Detailed validation dataset results

This document provides details on the framework's performance in predicting for the substructure probabilities and the ranking of candidate molecular structures for each molecule in our validation set, as well as the experimental ^{1}H and ^{13}C NMR spectra used as input. The data is ordered by the number of possible constitutional isomers generated by OMG using the molecular formula (SI section 3.5), starting with the largest. For each molecule, the SMILES string and molecular formula corresponding to the true molecular structure are listed first.

"Index of correct structure" denotes the rank of the correct structure as predicted for by our framework, with an index of "0" meaning that the correct structure was ranked as the most likely structure by our framework, "1" meaning the correct structure was the second ranked structure, and so on. An index of "-1" indicates that the correct structure was not generated as part of the ranked list of structures predicted for by our molecular graph generation algorithm. This index is reported alongside the total number of possible constitutional isomers for this molecular formula as generated by OMG.

"True structure loss" is the binary cross-entropy (BCE) loss between the predicted substructure probabilities and the correct structure substructure labels (SI section 3.5). A lower loss indicates better agreement between the ML-predicted substructure probabilities and the true substructure label, with 0 being perfect agreement.

The true structure is shown next along with the experimental ^{13}C and ^{1}H NMR spectra. The solvent in which the NMR spectra was collected in is noted in parentheses when available.

The 10 structures with the lowest BCE loss generated by our framework, sorted from lowest (most likely) to highest, are shown next. For each of the top 10 predicted molecular structures, the BCE loss between its ML-predicted substructure probabilities and the true structure's substructure label is displayed below an image of the predicted molecule's 2D structure.

For each molecule, additional details for the substructure predictions are shown on the following page. First, the top 10 highest probability substructures predicted for by our ML model are shown as SMARTS strings alongside their respective predicted probabilities. Next, the 10 highest probability true positive substructures ("best positives") are shown. These are the substructures present in the true structure that the model predicted to be present with a high probability. Substructures listed under "best negatives", "worst negatives", and "worst positives" correspond to the lowest probability true negatives, highest probability false positives, and lowest probability false negatives, respectively.

In [136…

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Example 0 true smiles: N=C(N)NCCCC(=O)O formula: C5H11N3O2
Index of correct structure: 8 of 677501
True structure loss: 0.030339
True structure:
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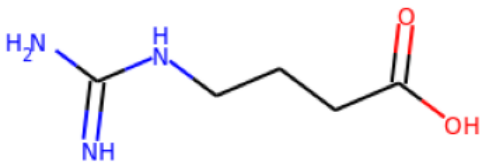
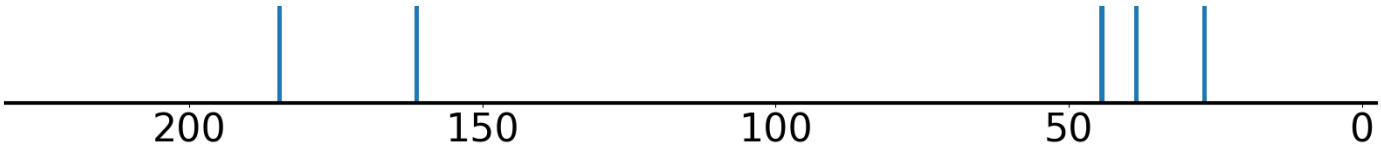
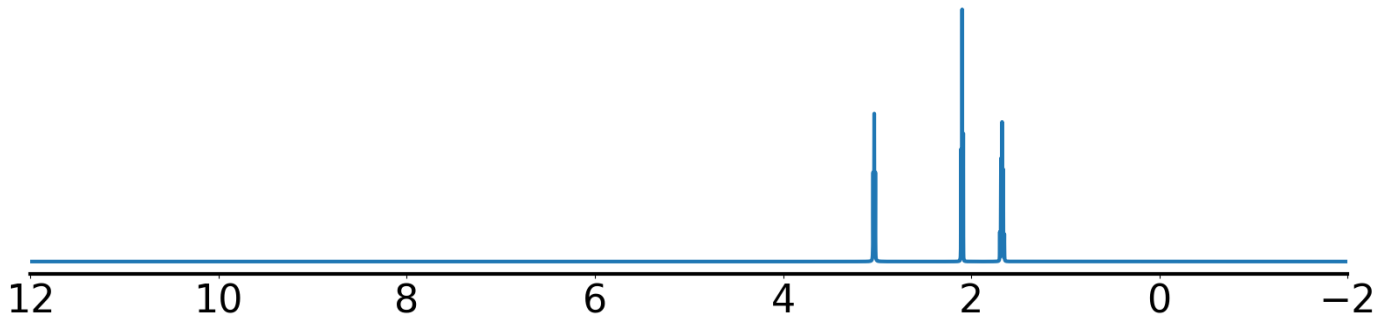


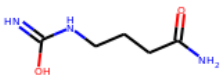
Experimental 13C NMR (solvent: D2O)



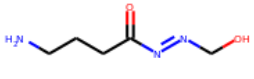
Experimental 1H NMR (solvent: D2O)



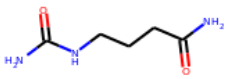
Top predicted structures (loss):



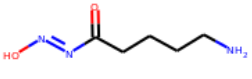
0.021364



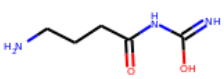
0.024313



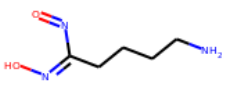
0.02474



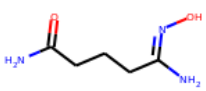
0.025733



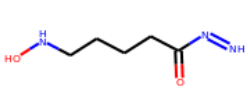
0.028428



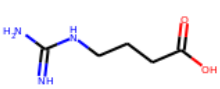
0.029822



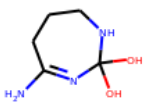
0.030128



0.030274



0.030339



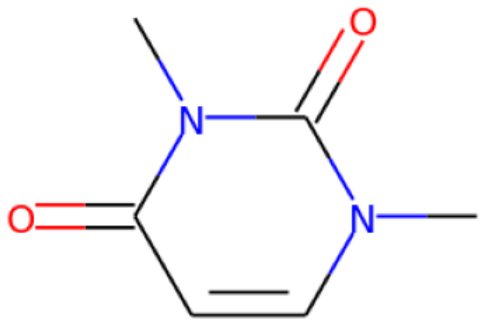
0.030498

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9972	[#7X3][#6H2]	0.9146
[#7X3H2]	0.9838	[OX2H1]	0.8938
[CX3](=[OX1])C	0.9587	[CX4H2][CX4H2]	0.8604
[#7][#6H2][#6H2]	0.9538	[CX4H2]CC=O	0.841
[#7][#6H2]	0.9306	[CX4H2]([CX4H2])[CX3H0]	0.7779

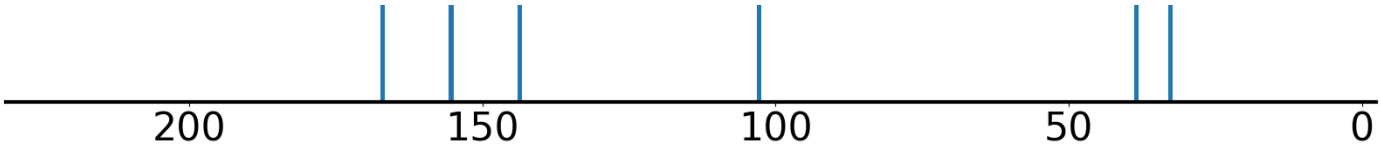
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9972	C=CC=CC#C	0.0
[#7X3H2]	0.9838	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9587	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7][#6H2][#6H2]	0.9538	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#7][#6H2]	0.9306	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3][#6H2]	0.9146	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[OX2H1]	0.8938	CC#CCC=C	0.0
[CX4H2][CX4H2]	0.8604	CC=CCC#C	0.0
[CX4H2]CC=O	0.841	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2]([CX4H2])[CX3H0]	0.7779	C=CCCC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([NX3H2])[CX4H2]	0.5724	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.0418
[#7H2][#6H2]	0.5509	[#7][#6]([#7])=[#7]	0.0897
[#7][#6][#6][#6X3]	0.3595	[#8][#6][#6H2]	0.1089
[#7][#6][#6][#6][#7]	0.2792	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.134
[#6H1][#6H2]	0.272	[#8]=[#6][#8]	0.2531
[#7][#6][#6][#6][#6][#7]	0.2362	[CX3](=[OX1])O	0.2953
[#8]=[#6H0][#6H1]	0.1883	OCC[CH2]	0.3515
[#6H1]	0.1817	[#7H2][#6H0]	0.5193
[#7X3H0]	0.1753	[#7X3H1]	0.5285
[#7][#6][#6X3]	0.1204	[CX4H2]([NX3H1])[CX4H2]	0.5364

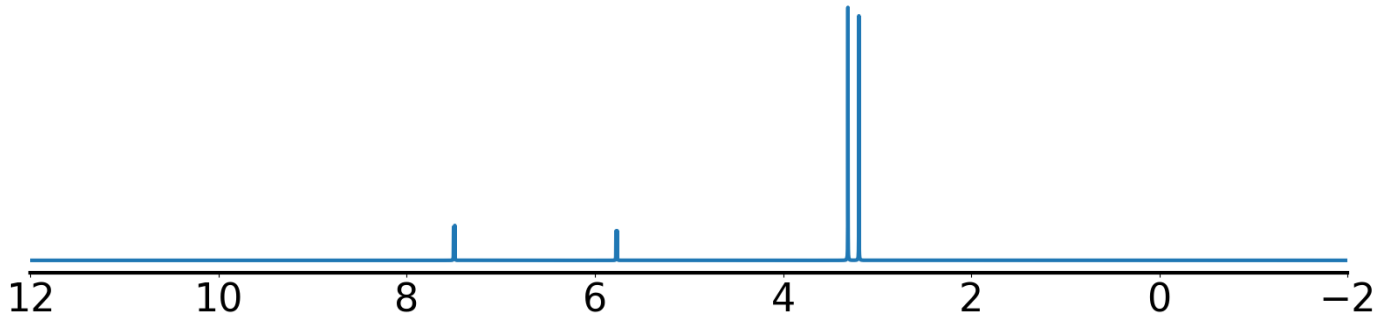
Example 1 true smiles: Cn1ccc(=O)n(C)c1=O formula: C6H8N2O2
Index of correct structure: 0 of 623393
True structure loss: 0.031526
True structure:



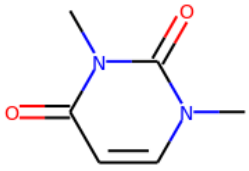
Experimental 13C NMR (solvent: CDCl3)



Experimental 1H NMR (solvent: D2O)

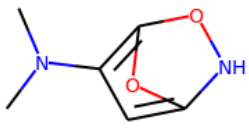


Top predicted structures (loss):



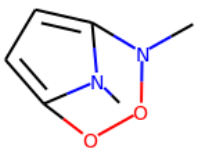
0.031526

0.03894

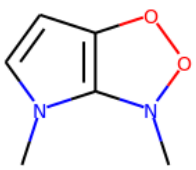


0.041776

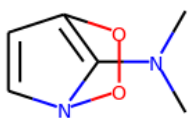
0.042338



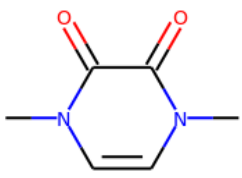
0.044092



0.0446

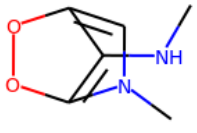


0.045601



0.047015

0.047597



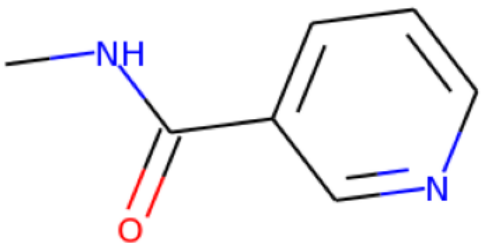
0.047685

Top predicted substructures	prob		
[#7X3][#6H3]	0.9986	[#6H3][#7][#6X3]	0.8865
[#6H1]	0.988	[#6X3][#7][#6X3]	0.8583
[#6H3][#7]	0.969	[#7][#6][#6X3]	0.8576
[CX4H3]	0.9559	[#7][#6][#6][#6X3]	0.8361
[#6X3][#6X3]	0.9119	[#7X3H0]	0.766

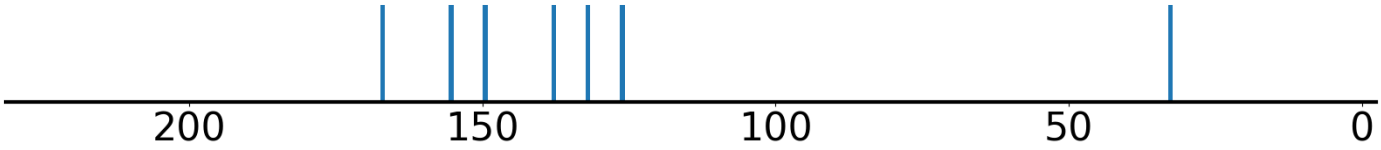
best positives	prob	best negatives	prob
[#7X3][#6H3]	0.9986	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H1]	0.988	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6H3][#7]	0.969	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[CX4H3]	0.9559	CCC#CC#C	0.0
[#6X3][#6X3]	0.9119	[#6H3][#6H2][#6H1r4]	0.0
[#6H3][#7][#6X3]	0.8865	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#7][#6X3]	0.8583	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#7][#6][#6X3]	0.8576	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.8361	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7X3H0]	0.766	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H3][NX3H0]	0.5633	[cX3H1]([nX3H0])[cX3H1]	0.1523
[CX3](=[OX1])C	0.53	[#7][#6H0][#7]	0.2196
[#8][#6][#6][#6X3]	0.4202	[#7][#6][#7]	0.2353
[#8][#6H0][#6H1]	0.4173	[#7][#6][#6][#6][#7]	0.2377
[CX4H2]([#6])[#6]	0.3802	[OX1H0]=[cX3H0][cX3H1]	0.2437
[#6X3][#6H2][#6X3]	0.367	[#8]=[#6][#6H1][#6H1]	0.259
[#8][#6][#6H2]	0.3665	[#8]=[#6H0][#6H1]	0.3397
[#7X3H1]	0.3581	[#6H1][#6H1]	0.3729
[OX2H1]	0.3365	O=[cX3]	0.4465
[#6H1][#6H2]	0.3315	[#7][#6X3H0][#6X3H1]	0.4526

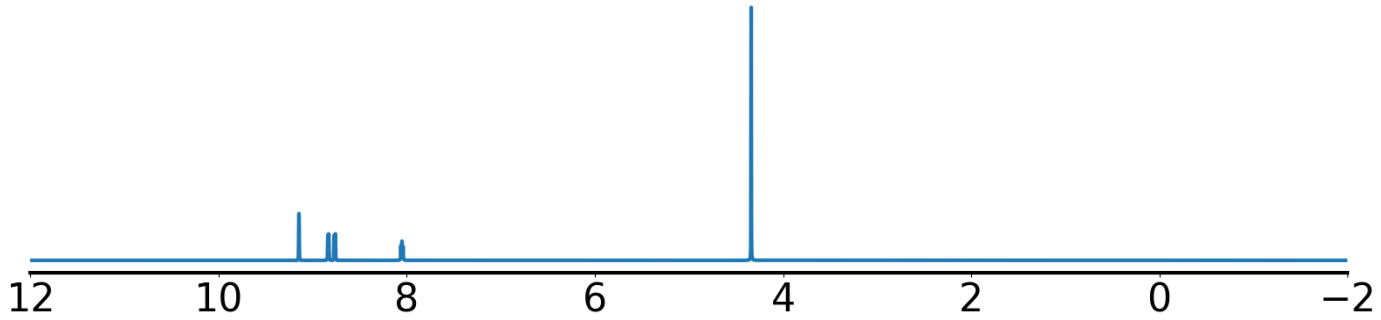
Example 2 true smiles: CNC(=O)c1cccnc1 formula: C7H8N2O
Index of correct structure: -1 of 376372
True structure loss: 0.02822
True structure:



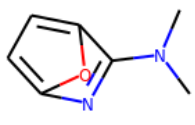
Experimental 13C NMR (solvent: CDCl3)



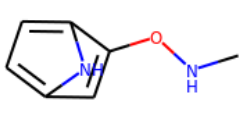
Experimental 1H NMR (solvent: D2O)



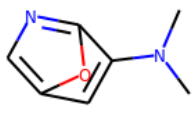
Top predicted structures (loss):



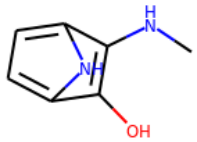
0.038564



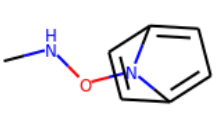
0.039903



0.040848



0.041371



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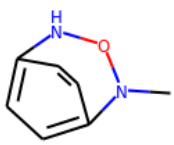

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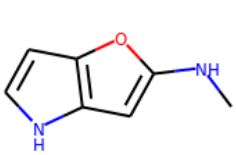
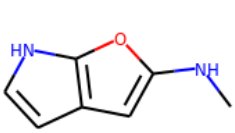
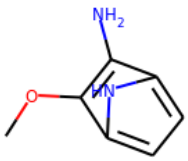


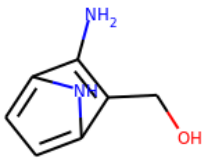
0.044615



0.04582



0.046694



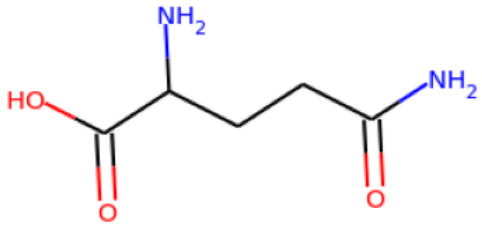
0.046896

Top predicted substructures	prob		
[#6X3][#6X3]	0.9993	[#6X3][#6X3][#6X3][#6X3]	0.8868
[#6H1]	0.9993	[cH]	0.8516
[#6X3H1][#6X3H0]	0.9883	[#6X3][#7][#6X3]	0.8217
[#7][#6][#6X3]	0.9696	[#7][#6X3H0][#6X3H1]	0.6519
[#7][#6][#6][#6X3]	0.894	[cH][cH]	0.6439

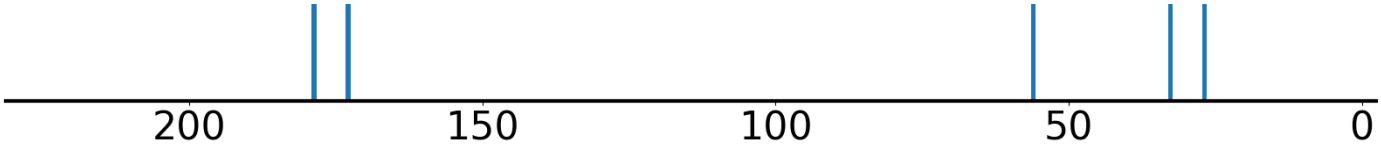
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9993	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H1]	0.9993	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3H1][#6X3H0]	0.9883	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#7][#6][#6X3]	0.9696	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.894	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.8868	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.8516	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3][#7][#6X3]	0.8217	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[cH][cH]	0.6439	[#6]1[#8][#6][#6]1=[#8]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.6405	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#7][#6X3H0][#6X3H1]	0.6519	[CX4H3][NX3H1]	0.1382
[#7][#6H0][#6H1]	0.5931	[#6H1][#7][#6H1]	0.1653
[#8][#6][#6][#6X3]	0.5206	[#7X3H1]	0.208
[OX2H1]	0.4645	O=[#6][#6][#6X3]	0.2701
[#8][#6H0][#6H1]	0.3266	[#6H3][#7]	0.2975
[#7X3H2]	0.3261	[cX3H1]([cX3H1])[cX3H1]	0.316
[#6X3][#6][#6][#6H3]	0.244	[cX3H1]([nX2H0])[cX3H1]	0.3174
[#7H2][#6H0]	0.2241	[#7][#6][#6][#6][#7]	0.3245
[#7][#6][#7]	0.2103	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3677
[cH]cO	0.207	[CX4H3]	0.4011

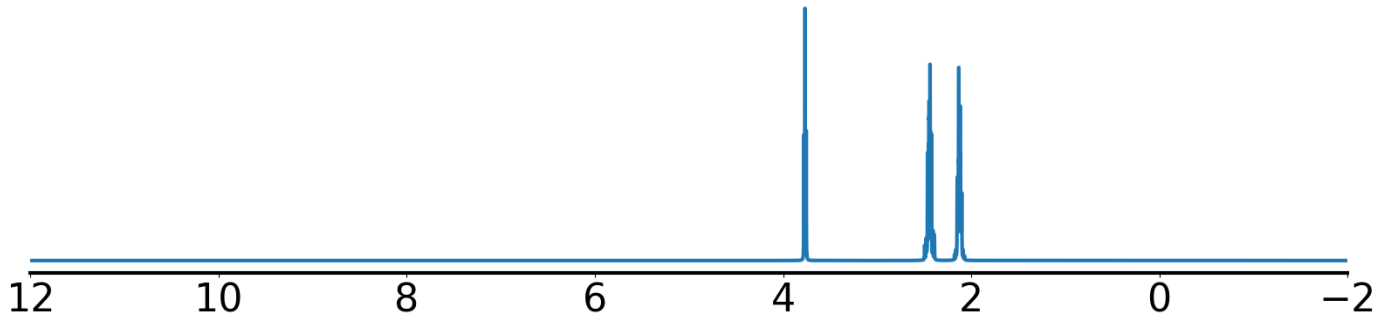
Example 3 true smiles: NC(=O)CCC(N)C(=O)O formula: C5H10N2O3
Index of correct structure: 3 of 371534
True structure loss: 0.024882
True structure:



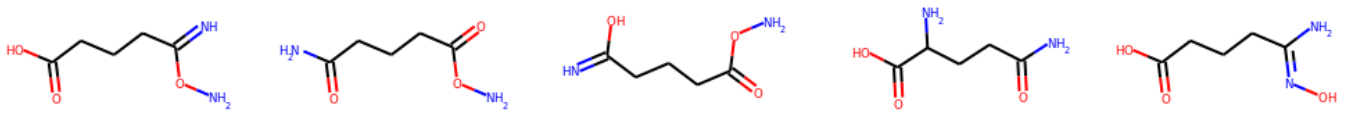
Experimental 13C NMR (solvent: D2O)



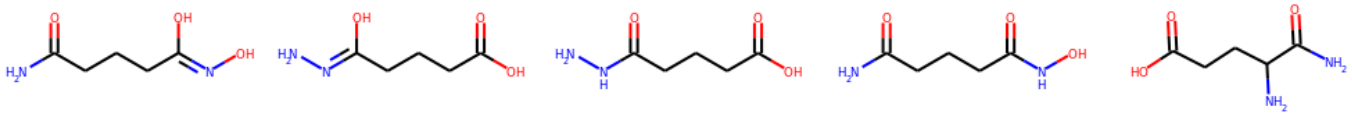
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.020751 0.022857 0.023199 0.024882 0.025053



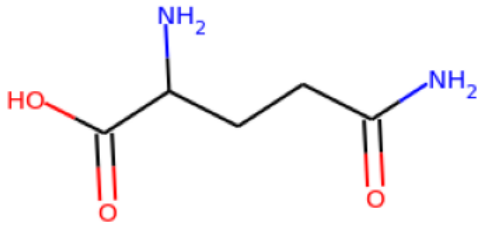
0.025267 0.02767 0.028047 0.028804 0.029394

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	O=[CX3H0][CX4H2][CX4H2]	0.9637
[CX3](=[OX1])C	0.9966	[CX3](=[OX1])O	0.9542
[#7X3H2]	0.9756	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.8848
[#8]=[#6][#8]	0.9745	[CX4H2][CX4H2]	0.882
[CX4H2]([CX4H2])[CX3H0]	0.9706	[CX4H2]CC=O	0.8812

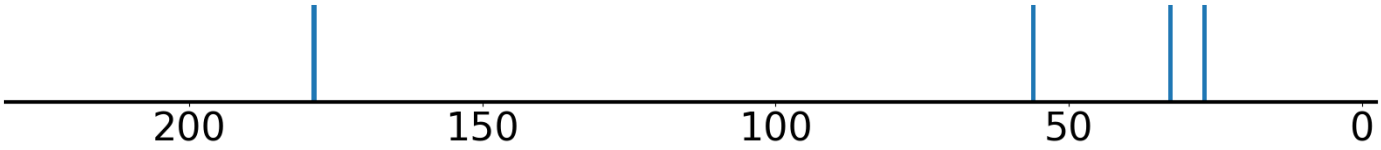
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9966	[CX2H0](#[CX2H0])[CX4H0]	0.0
[#7X3H2]	0.9756	CC=CCC#C	0.0
[#8]=[#6][#8]	0.9745	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2]([CX4H2])[CX3H0]	0.9706	CC#CCC#C	0.0
O=[CX3H0][CX4H2][CX4H2]	0.9637	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])O	0.9542	C=CC=CC#C	0.0
[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.8848	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2][CX4H2]	0.882	[CX2H0](#[CX2H1])[CX4H1]	0.0
[CX4H2]CC=O	0.8812	CC#CCC=C	0.0

worst negatives	prob	worst positives	prob
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.7335	[#7][#6][#6][#6][#6][#7]	0.06
[#8][#6][#6H2]	0.5612	[#8][#6H0][#6H1]	0.0741
[CX4H2]([CX4H2])[CX4H2]	0.3529	O=[CX3][CX4H]	0.2028
[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.3079	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2269
[#7X3H1]	0.3015	[#6H1][#6H2][#6][#6][#7]	0.2545
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2988	[#6H1]	0.2758
[OX2H0][CX3H0][CX4H2]	0.1659	[#6H1][#6H2]	0.3254
[#7][#6H2][#6H2]	0.1615	[CX4H2]([CX4H2])[CX4H1]	0.3759
[#6]=[#7H]	0.1517	[#8]=[#6H0][#6H1]	0.3908
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.118	[#7H2][#6H0]	0.59

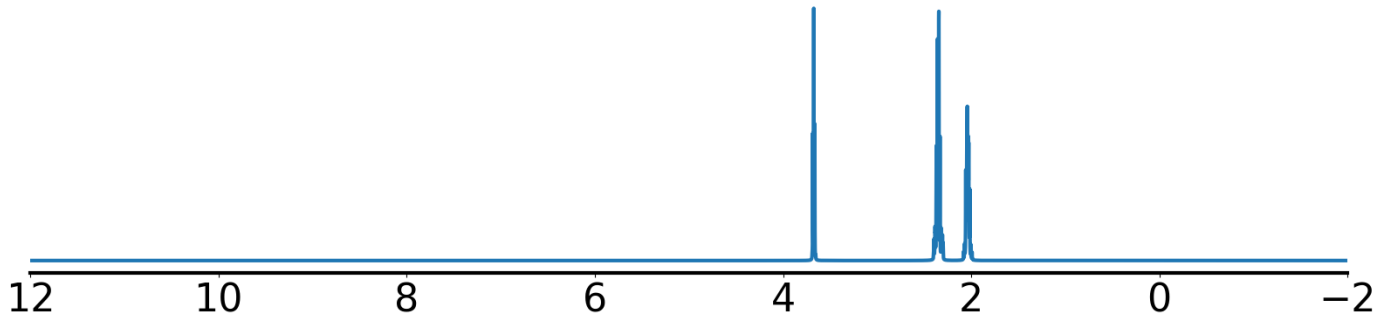
Example 4 true smiles: NC(=O)CCC(N)C(=O)O formula: C5H10N2O3
Index of correct structure: -1 of 371534
True structure loss: 0.020849
True structure:



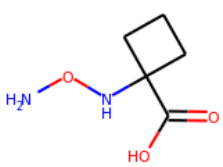
Experimental 13C NMR (solvent: N/A)



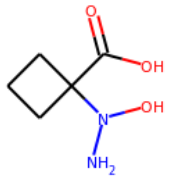
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



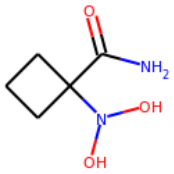
0.040077



0.044054

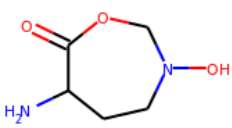
0.045911

0.046316

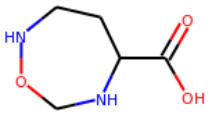


0.046643

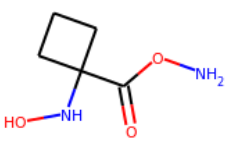
0.047568



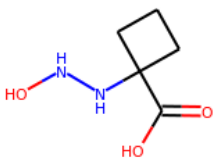
0.047568



0.048043



0.048543



0.048938

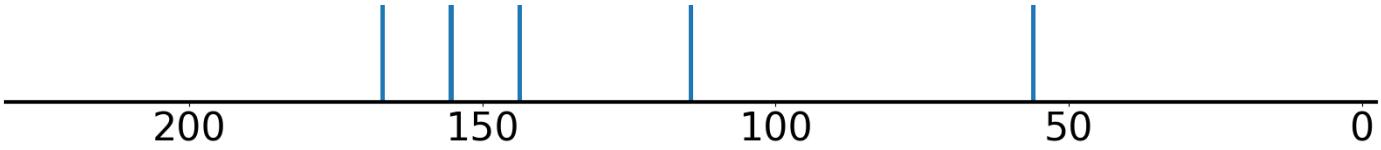
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9992	[#7X3H2]	0.8733
[CX3](=[OX1])C	0.9823	[#8]=[#6][#8]	0.8292
[OX2H1]	0.9796	[#7][#6][#6X3]	0.8207
[CX4H2][CX4H2]	0.8941	[CX4H2]CC=O	0.8164
[#7H2][#6H1]	0.8829	OCC[CH2]	0.7604

best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9992	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9823	CC=CCC#C	0.0
[OX2H1]	0.9796	CCC=CC#C	0.0
[CX4H2][CX4H2]	0.8941	C=CC=CC#C	0.0
[#7H2][#6H1]	0.8829	CC=CC#CC	0.0
[#7X3H2]	0.8733	CC#CCC=C	0.0
[#8]=[#6][#8]	0.8292	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#7][#6][#6X3]	0.8207	C=CCCC#C	0.0
[CX4H2]CC=O	0.8164	CCC#CC=C	0.0
OCC[CH2]	0.7604	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

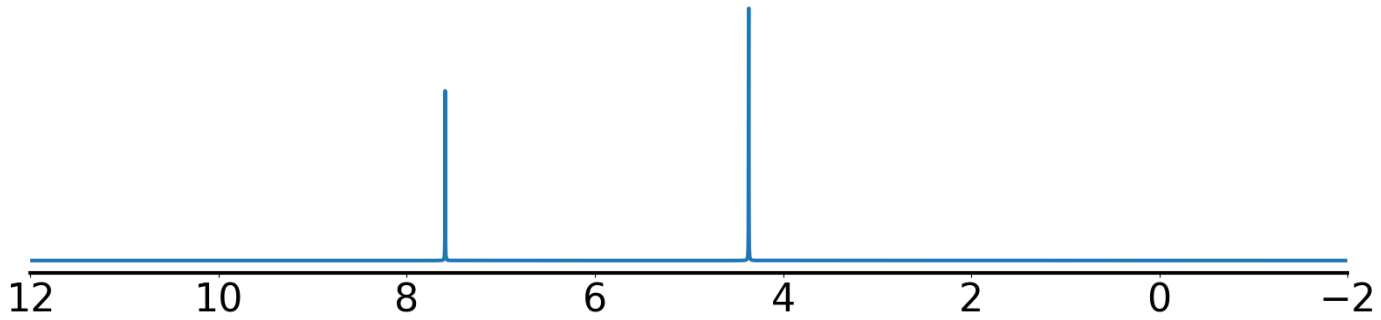
worst negatives	prob	worst positives	prob
[#7X3H1]	0.4857	[#7H2][#6H0]	0.1693
[#7][#6][#6][#7]	0.3365	[#8][#6H0][#6H1]	0.2032
[#7X3H0]	0.3296	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2892
[#8][#6][#6H2]	0.2799	[#7][#6][#6][#6][#6][#7]	0.4205
[#6H1][#6H1]	0.2698	[CX3](=O)[OX2H1]	0.451
[#7][#6][#6][#6][#7]	0.258	[#8]=[#6H0][#6H1]	0.5107
[OH][CX4H]	0.2145	O=[CX3][CX4H]	0.5163
[CX4H1]([OX2H1])([CX4H1])[CX4H1]	0.1968	[CX4H2][CX3]=O	0.5288
[CX4H2]([CX4H2])[CX4H2]	0.1663	[#6H1]	0.6315
[#7][#6H2]	0.1604	[CX4H2]([CX4H2])[CX4H1]	0.6329

Example 5 true smiles: O=c1[nH]cc(CO)c(=O)[nH]1 formula: C5H6N2O3
Index of correct structure: -1 of 354279
True structure loss: 0.035503
True structure:

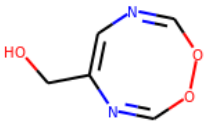
Experimental 13C NMR (solvent: DMSO-d6)



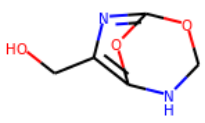
Experimental 1H NMR (solvent: D2O)



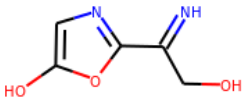
Top predicted structures (loss):



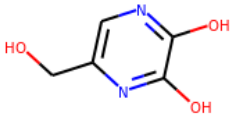
0.038209



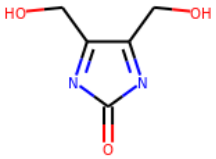
0.039649



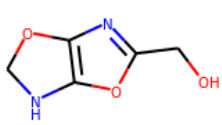
0.039969



0.040077

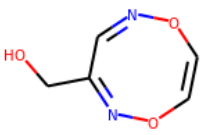


0.041477

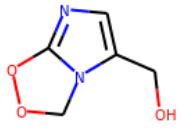


0.042268

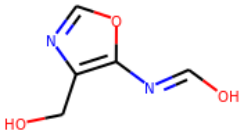
0.042466



0.043108



0.044141



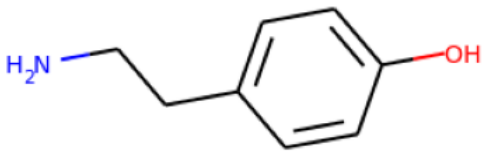
0.044431

Top predicted substructures	prob		
[#6H1]	0.9707	[CX4H2]([#6])[O]	0.82
[#6X3][#6X3]	0.9662	[OX2H1]	0.8045
[#7][#6][#6X3]	0.8608	[cH]	0.7152
[OX2H1][CX4H2][#6X3H0]	0.8345	[#6X3][#6H2][#8]	0.6931
[#6X3H1][#6X3H0]	0.8231	[#8][#6][#6][#6X3]	0.6841

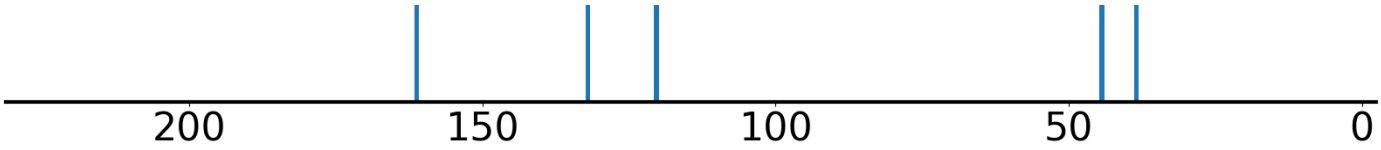
best positives	prob	best negatives	prob
[#6H1]	0.9707	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#6X3][#6X3]	0.9662	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.8608	[CX4H0]1[CX4H2][CX4H2][CX4H1]1	0.0
[OX2H1][CX4H2][#6X3H0]	0.8345	CCC#CC#C	0.0
[#6X3H1][#6X3H0]	0.8231	CC#CCC#C	0.0
[CX4H2]([#6])[O]	0.82	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[OX2H1]	0.8045	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[cH]	0.7152	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3][#6H2][#8]	0.6931	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#8][#6][#6][#6X3]	0.6841	[CX4H2]([CX4H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX3](=[OX1])O	0.6236	[#7][#6H0][#7]	0.0932
[#8]=[#6][#8]	0.61	[cX3H1]([nX3H1])[cX3H0]	0.1081
[#8][#6H0][#6H1]	0.3938	[cX3H0]([cX3H1])([cX3H0])[CX4H2]	0.1192
[#8][#6][#6]=[#6X3]	0.3719	[#7][#6][#6][#6][#7]	0.1998
[CX3](=[OX1])C	0.3667	[#7H][#6X3H1]	0.201
[#7X3H2]	0.3287	[#7][#6][#7]	0.2328
[#6H1r5][#7]	0.2875	O=[cX3]	0.2369
[#7]=[#6][#6X3]	0.2841	[#6X3][#7X3][#6X3]	0.286
[#7][#6X3H0][#6X3H1]	0.2766	O=[#6][#6][#6X3]	0.3261
[#6X3H1]=[#6X3H0]	0.2739	[#7X3H1]	0.4011

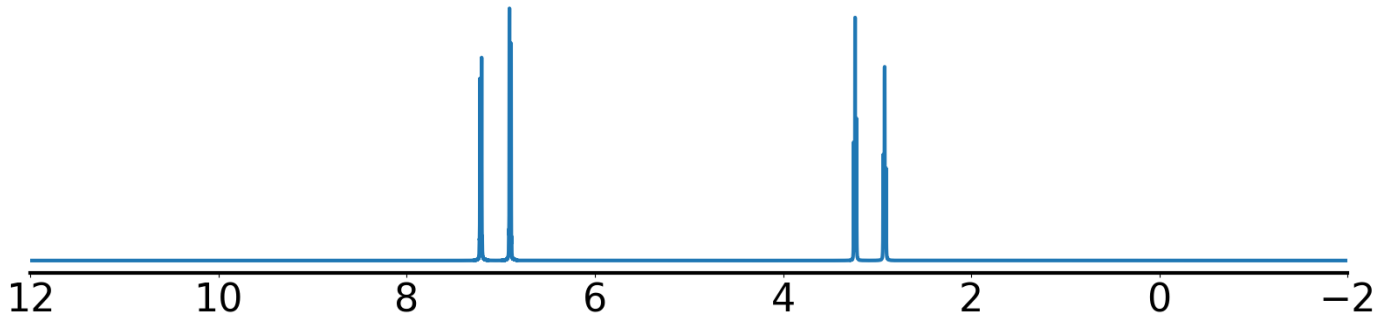
Example 6 true smiles: NCCc1ccc(O)cc1 formula: C8H11NO
Index of correct structure: 0 of 193269
True structure loss: 0.024764
True structure:



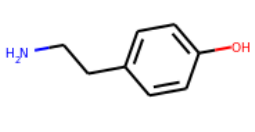
Experimental 13C NMR (solvent: CD3OD)



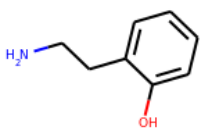
Experimental 1H NMR (solvent: D2O)



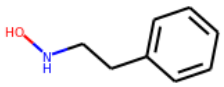
Top predicted structures (loss):



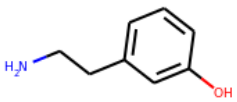
0.024764



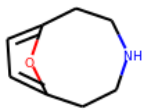
0.026646



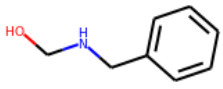
0.029193



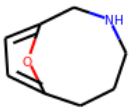
0.030488



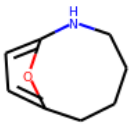
0.035378



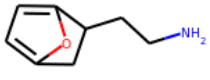
0.039365



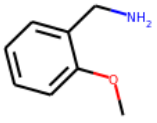
0.041407



0.042634



0.043999



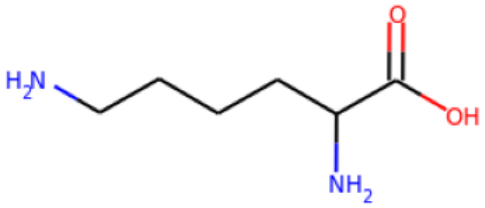
0.046839

Top predicted substructures	prob		
[#6H1]	0.9993	[CX4H2]([CX4H2])[cX3H0]	0.9351
[CX4H2]([#6])[#6]	0.9958	[#7][#6][#6X3]	0.8705
[cH][cH]	0.9816	[#6H1][#6H1]	0.8443
[#6X3][#6X3][#6X3][#6X3]	0.9614	[CX4H2]([NX3H2])[CX4H2]	0.8428
[#6X3][#6X3]	0.9439	[cH]	0.8401

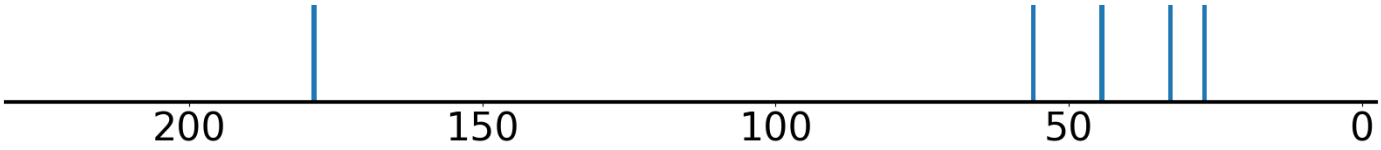
best positives	prob	best negatives	prob
[#6H1]	0.9993	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[CX4H2]([#6])[#6]	0.9958	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9816	[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9614	[OX2H0]1[CX4H0][CX4H1]1	0.0
[#6X3][#6X3]	0.9439	CC#CCC#C	0.0
[CX4H2]([CX4H2])[cX3H0]	0.9351	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[#6H1][#6H1]	0.8443	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[CX4H2]([NX3H2])[CX4H2]	0.8428	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[cH]	0.8401	[OX2H0][CX4H2][CX3H0][CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8379	[CX3H2]=[CX3H1][CX4H0][OX2H1]	0.0

worst negatives	prob	worst positives	prob
[#7][#6][#6X3]	0.8705	[cX3H0][cX3H1][cX3H1][cX3H0]	0.1148
[#6H1][#6H2]	0.6122	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.141
[cX3H1]([cX3H1])[cX3H1]	0.5428	[cH]cO	0.2988
[CX4H2][CX3H]	0.4241	[OX2H1]	0.3204
[#6X3][#7][#6X3]	0.3728	[CX4H2][CX4H2]	0.3796
[#6]1[#6][#6][#6][#6][#7]1	0.2982	[OX2H][cX3]:[c]	0.3968
[#7X3H1]	0.2617	[#6]1[#6][#6][#6][#6][#6]1	0.427
[#7][#6H0][#6H1]	0.2514	[#8][#6H0][#6H1]	0.4371
[#6H2][#7][#6X3]	0.2111	[#8][#6][#6][#6X3]	0.4734
[cX3H0]([cX3H1])([cX3H0])[CX4H2]	0.1989	[#7][#6H2][#6H2]	0.5587

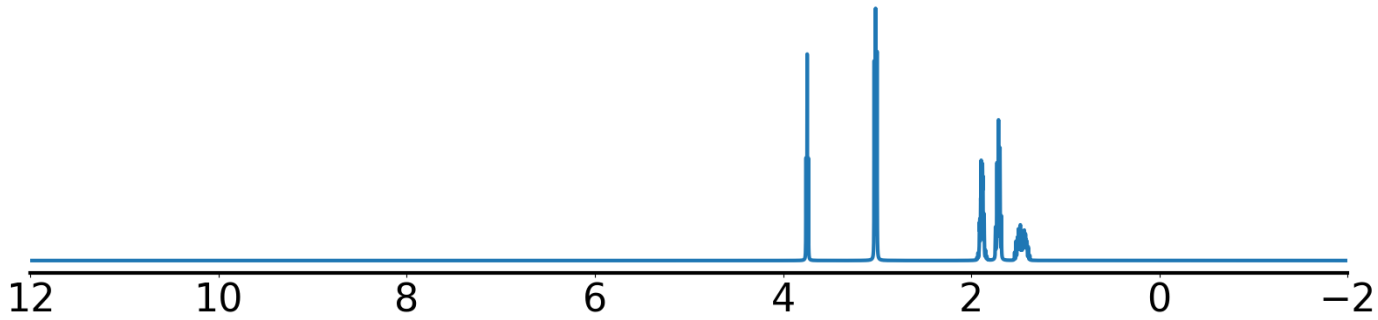
Example 7 true smiles: NCCCCC(N)C(=O)O formula: C6H14N2O2
Index of correct structure: 0 of 143634
True structure loss: 0.021445
True structure:



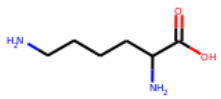
Experimental 13C NMR (solvent: D2O)



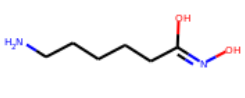
Experimental 1H NMR (solvent: D2O)



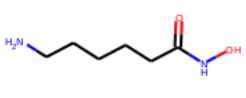
Top predicted structures (loss):



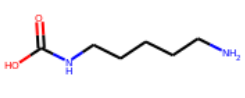
0.021445



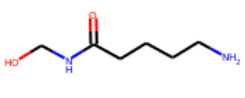
0.032197



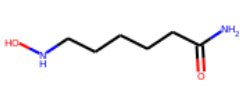
0.033694



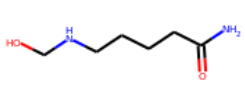
0.034373



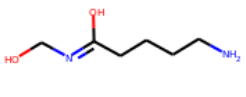
0.034638



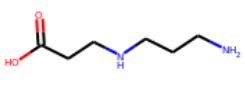
0.034681



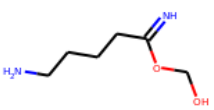
0.036561



0.03884



0.040982



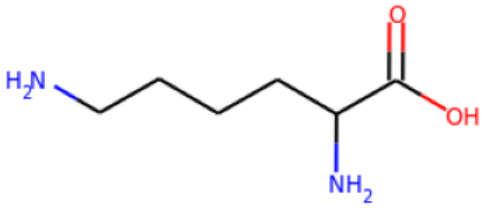
0.041044

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H2]([CX4H2])[CX4H2]	0.9238
[#7X3H2]	0.9909	OCC[CH2]	0.9076
[OX2H1]	0.9893	[CX4H2]CC=O	0.8824
[CX4H2][CX4H2]	0.968	[CX4H2]([CX4H2])[CX4H1]	0.8577
[CX3](=[OX1])C	0.9354	[#7][#6H2][#6H2]	0.8489

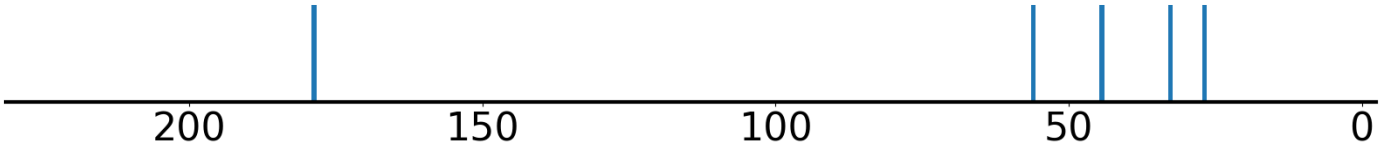
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3H2]	0.9909	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX2H1]	0.9893	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H2][CX4H2]	0.968	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX3](=[OX1])C	0.9354	CCC=CC#C	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9238	CCC#CC#C	0.0
OCC[CH2]	0.9076	C=CCCC#C	0.0
[CX4H2]CC=O	0.8824	CC#CCC=C	0.0
[CX4H2]([CX4H2])[CX4H1]	0.8577	CC=CC#CC	0.0
[#7][#6H2][#6H2]	0.8489	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.569	CCCCCC	0.069
[#7H2][#6H0]	0.5649	[#8][#6H0][#6H1]	0.1173
[CX4H2][CX3]=O	0.5159	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2924
O=[CX3H0][CX4H2][CX4H2]	0.451	[#6H1][#6H2]	0.4028
[CX4H2]([OX2H1])[CX4H2]	0.3368	[#6H1]	0.4525
[#7X3H1]	0.275	[CX3](=[OX1])O	0.479
[#7][#6][#6][#6][#6][#7]	0.2494	[#7][#6][#6X3]	0.4943
[CX4H2]([NX3H1])[CX4H2]	0.2047	[#8]=[#6][#8]	0.57
[#6H1][#6H2][#6][#6][#7]	0.1833	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.6514
[#7][#6][#6][#7]	0.143	[#8]=[#6H0][#6H1]	0.6631

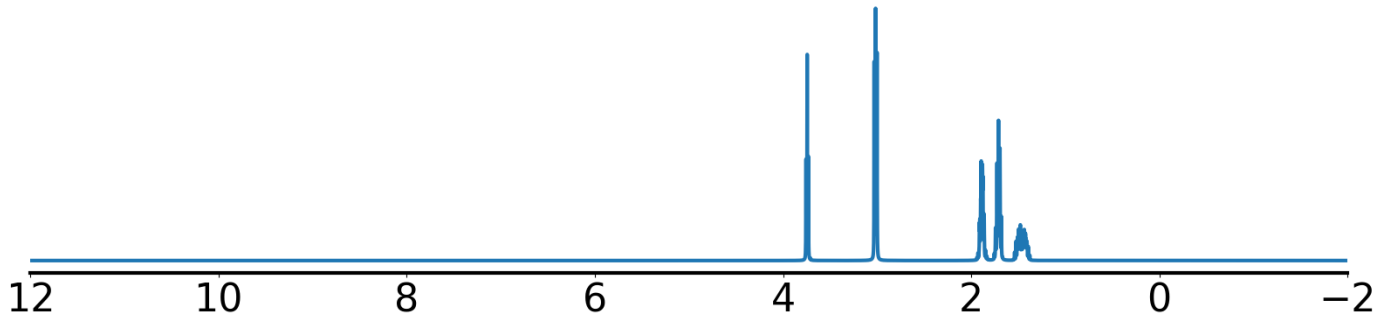
Example 8 true smiles: NCCCCC(N)C(=O)O formula: C6H14N2O2
Index of correct structure: 0 of 143634
True structure loss: 0.021405
True structure:



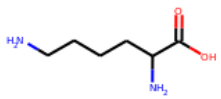
Experimental 13C NMR (solvent: D2O)



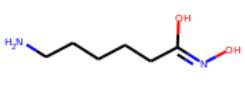
Experimental 1H NMR (solvent: D2O)



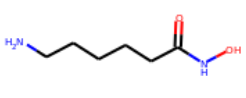
Top predicted structures (loss):



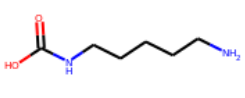
0.021405



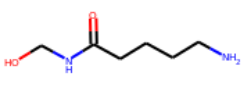
0.03232



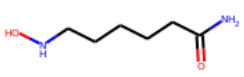
0.033761



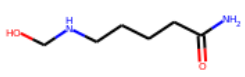
0.034453



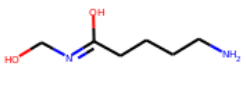
0.034698



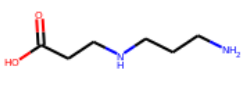
0.03472



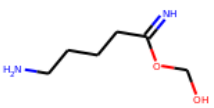
0.036615



0.038955



0.041103



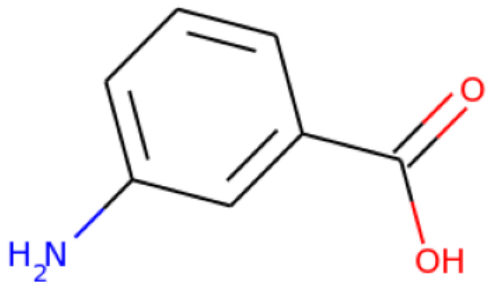
0.04116

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H2]([CX4H2])[CX4H2]	0.9238
[#7X3H2]	0.9903	OCC[CH2]	0.9076
[OX2H1]	0.9892	[CX4H2]CC=O	0.8846
[CX4H2][CX4H2]	0.9679	[CX4H2]([CX4H2])[CX4H1]	0.8567
[CX3](=[OX1])C	0.9363	[#7][#6H2][#6H2]	0.8521

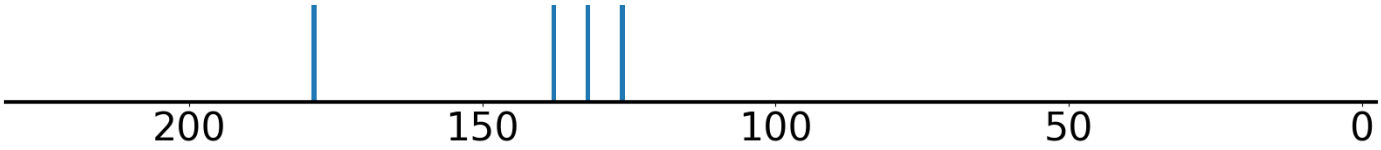
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3H2]	0.9903	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX2H1]	0.9892	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H2][CX4H2]	0.9679	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX3](=[OX1])C	0.9363	CCC=CC#C	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9238	CCC#CC#C	0.0
OCC[CH2]	0.9076	C=CCCC#C	0.0
[CX4H2]CC=O	0.8846	CC=CC#CC	0.0
[CX4H2]([CX4H2])[CX4H1]	0.8567	CC#CCC=C	0.0
[#7][#6H2][#6H2]	0.8521	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.5669	CCCCCC	0.0696
[#7H2][#6H0]	0.5601	[#8][#6H0][#6H1]	0.1181
[CX4H2][CX3]=O	0.5139	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2946
O=[CX3H0][CX4H2][CX4H2]	0.4554	[#6H1][#6H2]	0.4037
[CX4H2]([OX2H1])[CX4H2]	0.3334	[#6H1]	0.4478
[#7X3H1]	0.2746	[CX3](=[OX1])O	0.4781
[#7][#6][#6][#6][#6][#7]	0.2487	[#7][#6][#6X3]	0.4964
[CX4H2]([NX3H1])[CX4H2]	0.2068	[#8]=[#6][#8]	0.5679
[#6H1][#6H2][#6][#6][#7]	0.1832	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.6545
[#7][#6][#6][#7]	0.1446	[#8]=[#6H0][#6H1]	0.6676

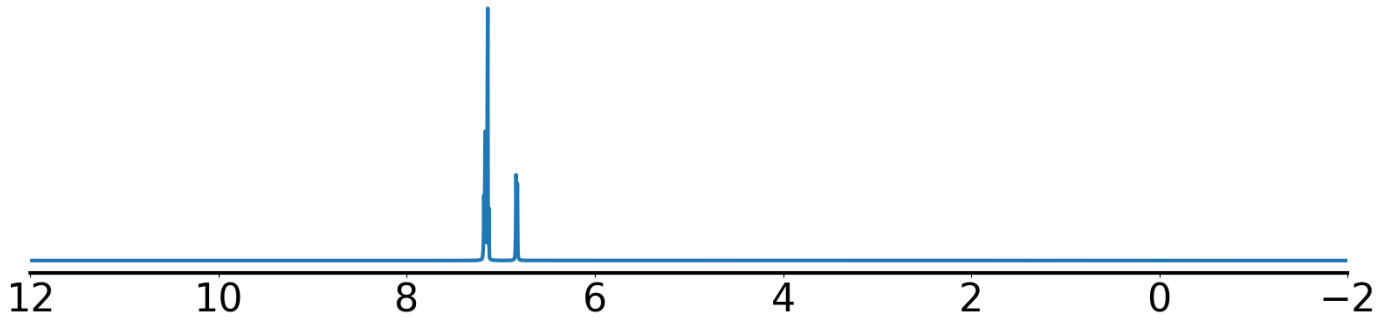
Example 9 true smiles: Nc1cccc(C(=O)O)c1 formula: C7H7NO2
Index of correct structure: 4 of 141060
True structure loss: 0.027383
True structure:



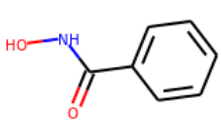
Experimental 13C NMR (solvent: D2O)



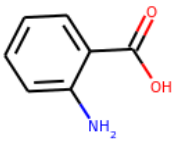
Experimental 1H NMR (solvent: D2O)



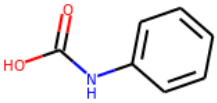
Top predicted structures (loss):



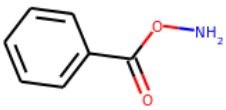
0.020355



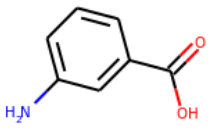
0.023262



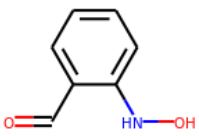
0.023546



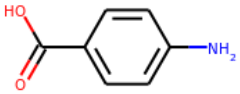
0.027078



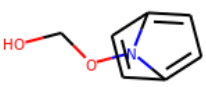
0.027383



0.028523

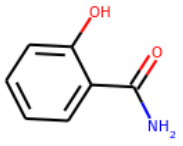


0.029103



0.029256

0.029341



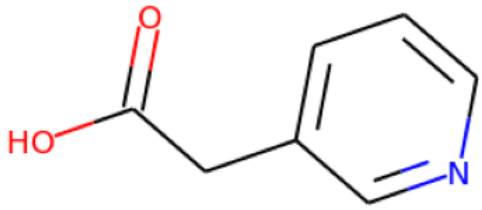
0.02951

Top predicted substructures	prob		
[#6X3][#6X3]	0.9953	[#6X3][#6X3][#6X3][#6X3]	0.8839
[#6H1]	0.9934	O=[#6][#6][#6X3]	0.8684
[cH][cH]	0.9704	[#6H1][#6H1]	0.8621
[#7][#6][#6X3]	0.9217	[cX3H1]([cX3H1])[cX3H0]	0.8292
[#6X3H1][#6X3H0]	0.9036	[cX3H1]([cX3H1])[cX3H1]	0.784

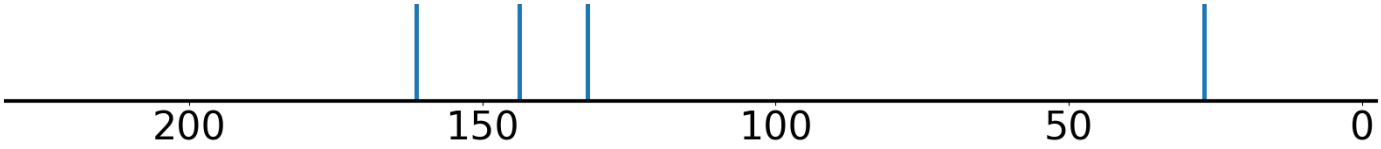
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9953	[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H1]	0.0
[#6H1]	0.9934	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9704	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#7][#6][#6X3]	0.9217	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3H1][#6X3H0]	0.9036	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.8839	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
O=[#6][#6][#6X3]	0.8684	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[#6H1][#6H1]	0.8621	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8292	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.784	[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7][#6X3]	0.6616	[cX3H1]([cX3H0])[cX3H0]	0.0297
[CX3](=[OX1])C	0.5236	[#7H2][#6H0]	0.1932
[#8]=[#6H0][#6H1]	0.5104	[#7X3H2]	0.2562
[#6X3][#7X3][#6X3]	0.4153	[CX3](=[OX1])O	0.2603
O=[#6][#6]=[#6X3]	0.3436	[#8][#6][#6][#6X3]	0.2658
[#8]=[#6][#6H1][#6H1]	0.3163	[#8]=[#6][#8]	0.3523
[OX1H0]=[cX3H0][cX3H1]	0.2981	[CX3](=O)[OX2H1]	0.3685
[#8]=[#6][#6H1]=[#6H1]	0.251	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3873
O=[cX3]	0.229	[#6]1[#6][#6][#6][#6][#6]1	0.4473
[#6H1r5][#7]	0.2272	[#7][#6X3H0][#6X3H1]	0.5636

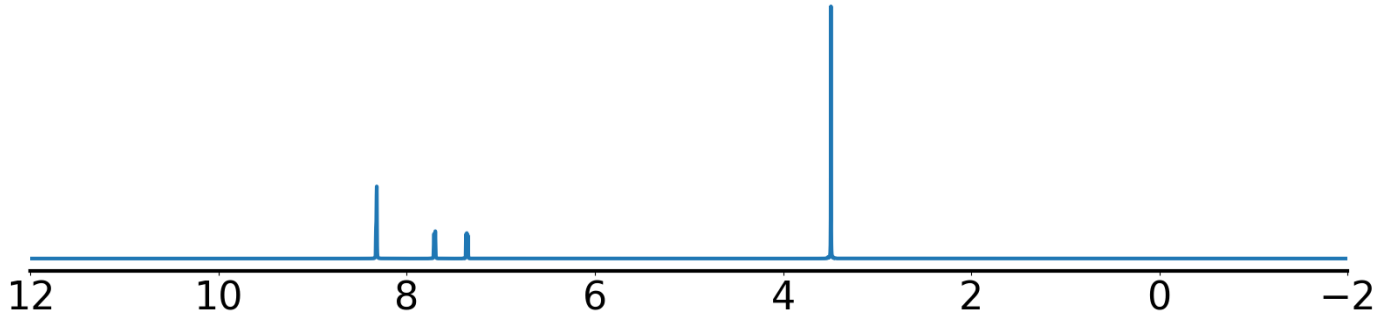
Example 10 true smiles: O=C(O)Cc1cccnc1 formula: C7H7NO2
Index of correct structure: -1 of 141060
True structure loss: 0.050539
True structure:



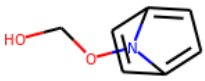
Experimental 13C NMR (solvent: DMSO-d6)



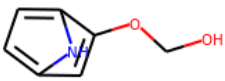
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



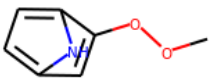
0.035522



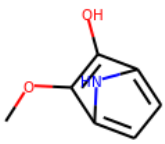
0.037206

0.038745

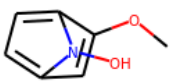
0.039656



0.040429

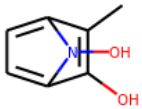


0.040517

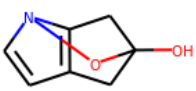


0.040547

0.042879



0.043882



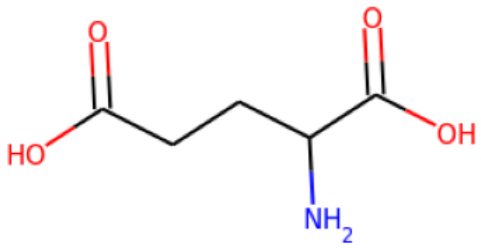
0.046072

Top predicted substructures	prob		
[#6X3][#6X3]	0.9987	[#7][#6][#6X3]	0.9655
[cH]	0.9935	[#6X3][#6X3][#6X3][#6X3]	0.9642
[#6H1]	0.9921	[#7][#6][#6][#6X3]	0.9103
[#6X3H1][#6X3H0]	0.9772	[cX3H1]([cX3H1])[cX3H0]	0.8783
[cH][cH]	0.9702	[#8][#6][#6][#6X3]	0.8771

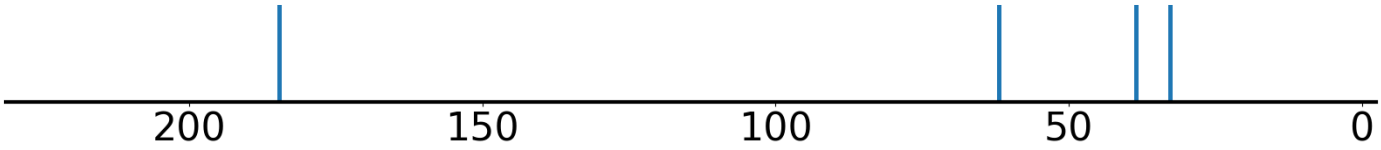
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9987	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9935	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H1]	0.9921	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3H1][#6X3H0]	0.9772	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9702	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.9655	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9642	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6][#6][#6X3]	0.9103	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8783	[OX2H1][CX4H0][CX4H2][CX4H0]	0.0
[#8][#6][#6][#6X3]	0.8771	[CX3H0](=[OX1H0])([CX4H1])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.5451	[CX4H2][CX3]=O	0.0029
[#7][#6H0][#6H1]	0.4829	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.0065
[#6X3][#6][#6][#6H3]	0.4767	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.012
[CX4H3]	0.4473	[#8X1]=[#6X3][#6H2][#6H0]	0.0414
[#7][#6X3H0][#6X3H1]	0.4087	[CX3](=[OX1])C	0.0485
[#6H3][#6][#6X3]	0.3535	[CX3](=[OX1])O	0.1004
[cH]cO	0.3506	[CX3](=O)[OX2H1]	0.1019
[CX4H3][cX3H0]	0.3258	[#8][#6][#6H2]	0.1745
[#6]1[#6][#6][#6][#6][#6]1	0.3213	[#6H1][#7][#6H1]	0.2382
o[cH]	0.3205	[#6X3][#6H2][#6X3]	0.2408

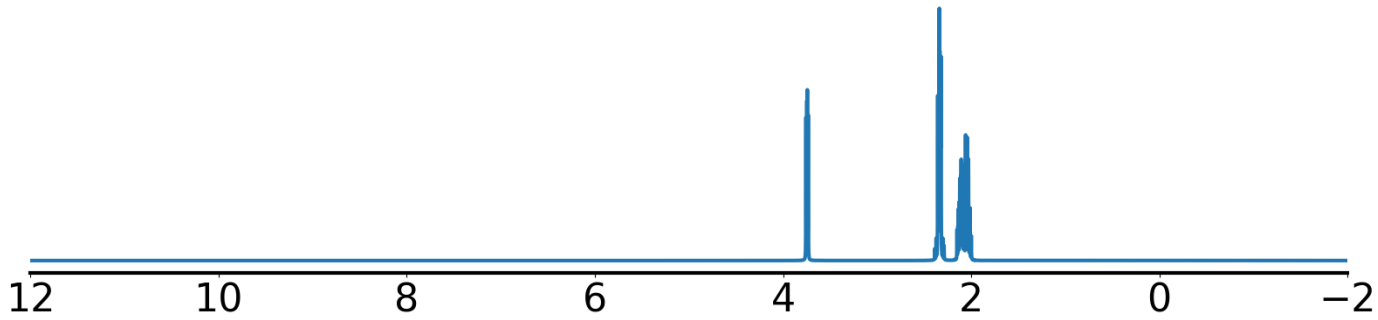
Example 11 true smiles: NC(CCC(=O)O)C(=O)O formula: C5H9NO4
Index of correct structure: 0 of 92537
True structure loss: 0.028545
True structure:



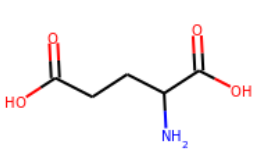
Experimental 13C NMR (solvent: D2O)



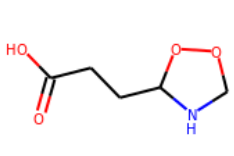
Experimental 1H NMR (solvent: D2O)



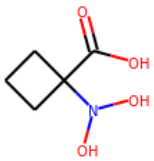
Top predicted structures (loss):



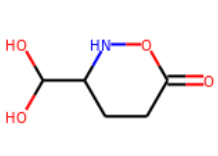
0.028545



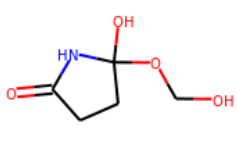
0.037194



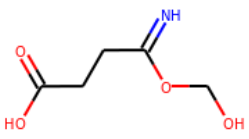
0.039214



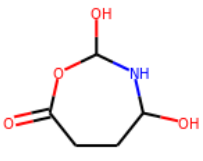
0.042218



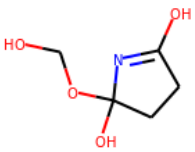
0.042586



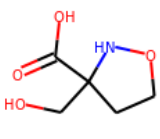
0.042857



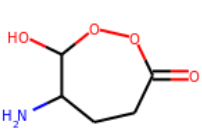
0.043528



0.043671



0.044099



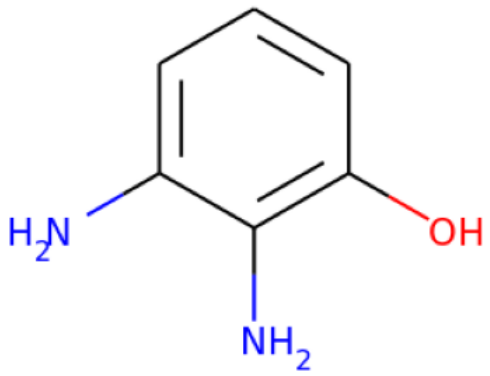
0.044258

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9996	[CX3](=[OX1])O	0.8933
[OX2H1]	0.9984	[CX3](=O)[OX2H1]	0.8039
[CX3](=[OX1])C	0.9976	O=[CX3H0][CX4H2][CX4H2]	0.7848
[#8]=[#6][#8]	0.9298	[#6H1]	0.7701
OCC[CH2]	0.905	[#8][#6][#6H2]	0.7503

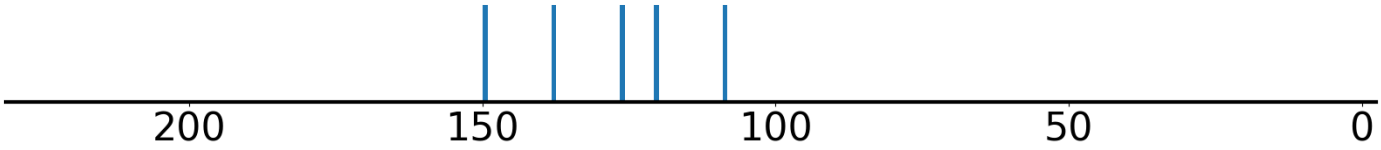
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9996	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9984	CC=CCC#C	0.0
[CX3](=[OX1])C	0.9976	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[#8]=[#6][#8]	0.9298	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
OCC[CH2]	0.905	CCC=CC#C	0.0
[CX3](=[OX1])O	0.8933	CC=CC#CC	0.0
[CX3](=O)[OX2H1]	0.8039	[CX3H1](=[CX3H1])[CX2H0]	0.0
O=[CX3H0][CX4H2][CX4H2]	0.7848	CC#CCC=C	0.0
[#6H1]	0.7701	C=CC=CC#C	0.0
[#8][#6][#6H2]	0.7503	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6][#6][#6]=[#8]	0.5993	[#7H2][#6X4H1][#6X3]	0.0157
[#8][#6][#6][#6][#6][#8]	0.3958	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.0617
[#6H1][#6H1]	0.3574	[#7X3H2]	0.2904
[CX4H]O	0.3514	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.3337
[#7X3H1]	0.3479	[#8]=[#6H0][#6H1]	0.3363
[CX4H2]([OX2H1])[CX4H2]	0.3249	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.3559
[#8][#6][#6][#6X3]	0.2829	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.4671
[OH][CX4H]	0.2425	[#7H2][#6H1]	0.4793
[#7][#6H1][#6H2r5]	0.232	O=[CX3][CX4H]	0.5061
[CH2X4](O)[CX4H2]	0.2256	[CX4H2]([CX4H2])[CX4H1]	0.5111

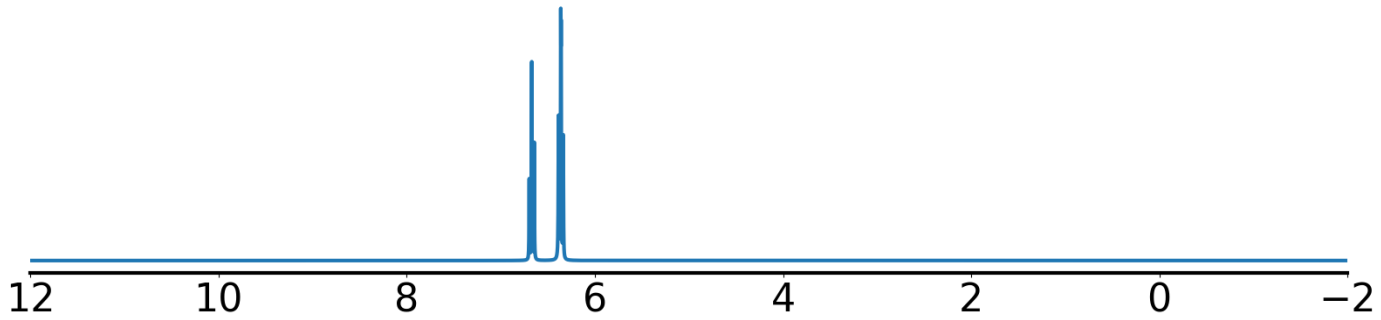
Example 12 true smiles: Nc1cccc(O)c1N formula: C6H8N2O
Index of correct structure: 3 of 75211
True structure loss: 0.022729
True structure:



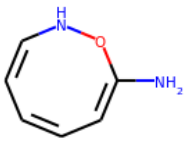
Experimental 13C NMR (solvent: DMSO)



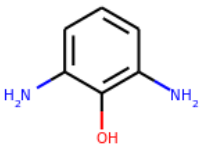
Experimental 1H NMR (solvent: CDCl3)



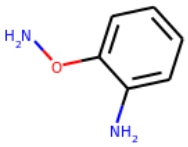
Top predicted structures (loss):



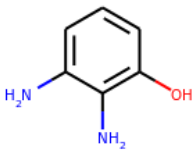
0.021308



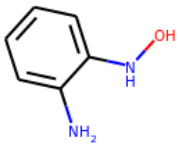
0.02231



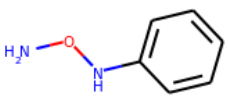
0.022402



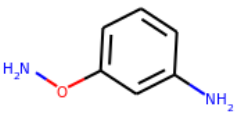
0.022729



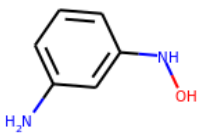
0.022749



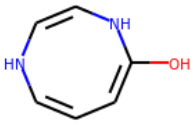
0.023122



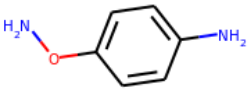
0.024044



0.02418



0.025169



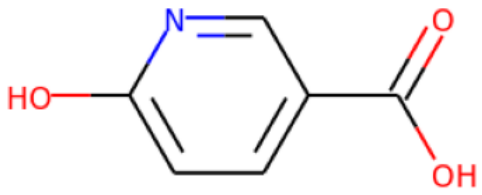
0.025648

Top predicted substructures	prob		
[#6H1]	0.9989	[cH]	0.9648
[#6X3][#6X3]	0.9954	[#7][#6][#6][#6X3]	0.9045
[#6X3H1][#6X3H0]	0.9932	[cH][cH]	0.9043
[#6X3][#6X3][#6X3][#6X3]	0.9837	[#7][#6X3H0][#6X3H1]	0.8842
[#7][#6][#6X3]	0.9791	[#6H1][#6H1]	0.8818

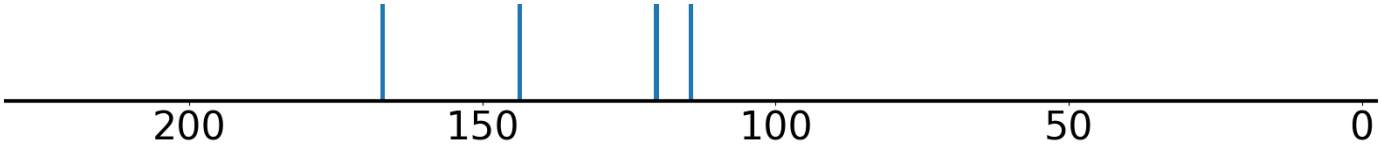
best positives	prob	best negatives	prob
[#6H1]	0.9989	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3]	0.9954	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9932	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9837	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#7][#6][#6X3]	0.9791	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[cH]	0.9648	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.9045	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[cH][cH]	0.9043	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[#7][#6X3H0][#6X3H1]	0.8842	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#6H1][#6H1]	0.8818	[OX2H0]1[CX4H2][CX4H1]1[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7][#6X3]	0.7913	[#6]1[#6][#6][#6][#6][#6]1	0.1071
[#6X3][#7X3][#6X3]	0.7362	[#7][#6][#6][#7]	0.1733
[#6]1[#6][#6][#6][#7]1	0.6031	[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.3688
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5985	[#8][#6H0][#6H1]	0.4102
[#7X3H1]	0.5688	[#8][#6][#6][#6X3]	0.4976
[#7H][#6X3H1]	0.5175	[OX2H][cX3]:[c]	0.6236
[#6H1r5][#7]	0.4436	[cH]cO	0.6685
[CH2X3](=C)	0.3305	[cX3H1]([cX3H1])[cX3H1]	0.7057
[cX3H1]([nX3H1])[cX3H1]	0.3278	[#7H2][#6H0]	0.7382
[#6X3H2]	0.3046	[OX2H1]	0.7828

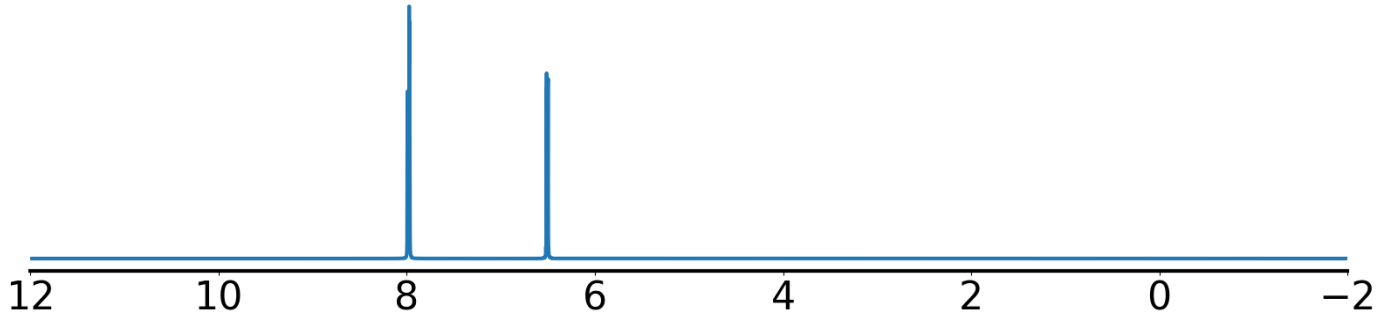
Example 13 true smiles: O=C(O)c1ccc(O)nc1 formula: C6H5NO3
Index of correct structure: -1 of 67881
True structure loss: 0.023869
True structure:



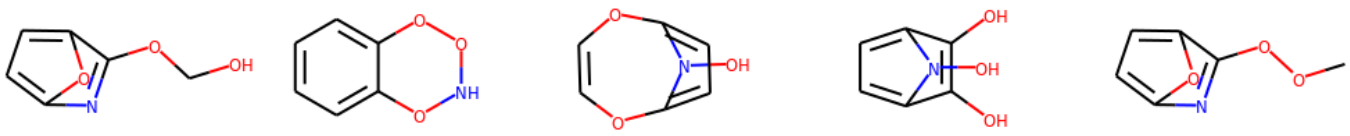
Experimental 13C NMR (solvent: DMSO-d6)



Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.022012 0.028095 0.033325 0.034622 0.034832

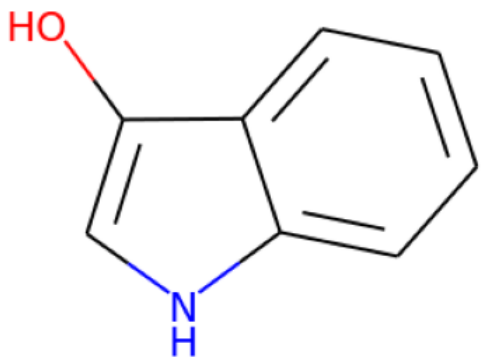
0.035773 0.035795 0.03586 0.036143 0.036339

Top predicted substructures	prob		
[#6H1]	0.9991	[#6X3H1][#6X3H0]	0.9599
[#6X3][#6X3]	0.9979	[cX3H1]([cX3H1])[cX3H0]	0.9263
[cH][cH]	0.9821	[#8][#6][#6][#6X3]	0.8933
[cH]	0.9786	[#6H1][#6H1]	0.8554
[#6X3][#6X3][#6X3][#6X3]	0.9604	[#8]=[#6][#8]	0.7644

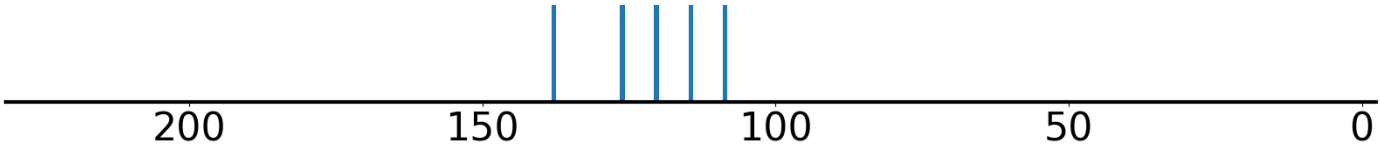
best positives	prob	best negatives	prob
[#6H1]	0.9991	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9979	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[cH][cH]	0.9821	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH]	0.9786	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9604	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9599	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9263	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#8][#6][#6][#6X3]	0.8933	[#6H3][#7][#6X4H1][#6H3]	0.0
[#6H1][#6H1]	0.8554	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#8]=[#6][#8]	0.7644	[CX3H0](=[CX3H2])([CX4H2])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.5307	[cX3H1]([nX2H0])[cX3H0]	0.0381
O=[cX3]	0.4282	[#6]1[#6][#6][#6][#6][#7]1	0.1533
[#8]=[#6][#6H1][#6H1]	0.4053	[cX3H0][cX3H1][cX3H1][cX3H0]	0.2571
[#8]=[#6H0][#6H1]	0.3276	[CX3](=O)[OX2H1]	0.3034
[OX1H0]=[cX3H0][cX3H1]	0.3043	[#7][#6H0][#6H1]	0.361
[#8][#6H1][#6H1]	0.2957	[#7][#6X3H0][#6X3H1]	0.3825
[#8][#6][#6][#8]	0.2587	[OX2H][cX3]:[c]	0.4119
[#8][#6][#6][#6][#6][#8]	0.2504	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.4151
[cX3H1]([oX2H0])[cX3H1]	0.2409	[#6X3][#7][#6X3]	0.4175
o[cH]	0.2264	[cH]cO	0.4361

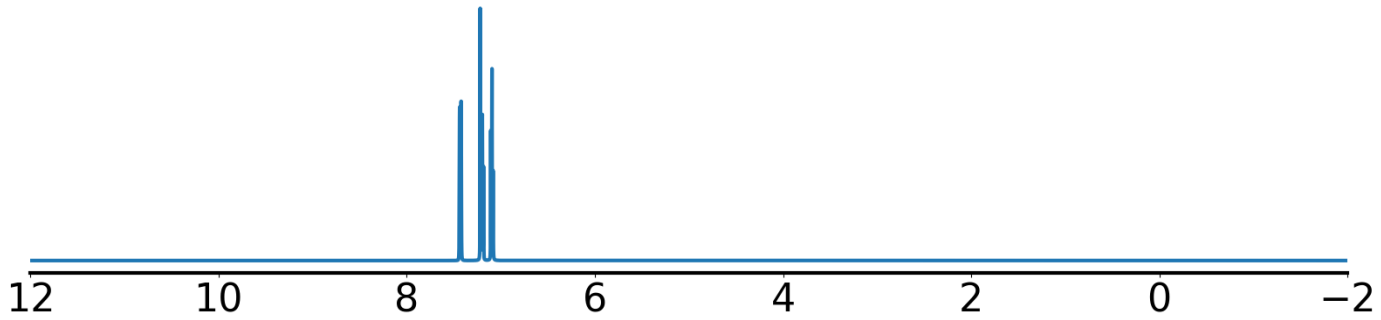
Example 14 true smiles: Oc1c[nH]c2ccccc12 formula: C8H7NO
Index of correct structure: 3 of 59121
True structure loss: 0.016676
True structure:



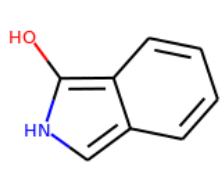
Experimental 13C NMR (solvent: DMSO-d6)



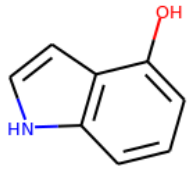
Experimental 1H NMR (solvent: D2O)



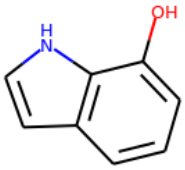
Top predicted structures (loss):



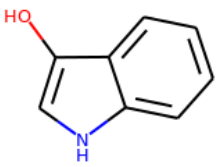
0.014749



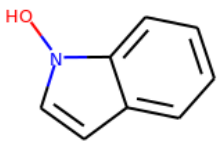
0.015962



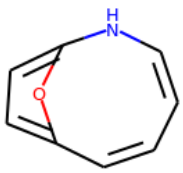
0.016278



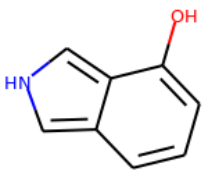
0.016676



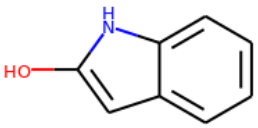
0.018786



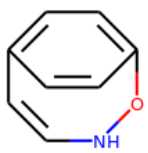
0.01948



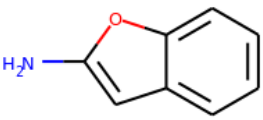
0.020223



0.020537



0.022308



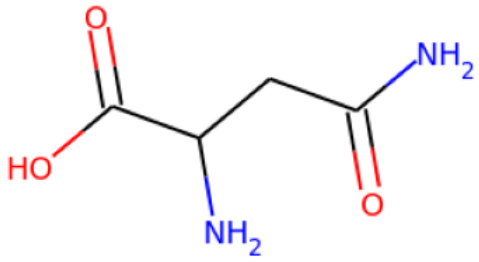
0.023469

Top predicted substructures	prob		
[#6H1]	0.9997	[#6X3H1][#6X3H0]	0.9876
[#6X3][#6X3][#6X3][#6X3]	0.9992	[cX3H1]([cX3H1])[cX3H0]	0.9814
[#6X3][#6X3]	0.9981	[#6H1][#6H1]	0.9794
[cH][cH]	0.9978	[#6]1[#6][#6][#6][#6][#6]1	0.9362
[cH]	0.9976	[cX3H1]([cX3H1])[cX3H1]	0.9113

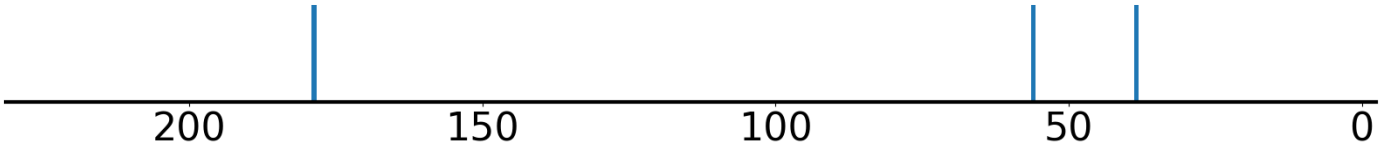
best positives	prob	best negatives	prob
[#6H1]	0.9997	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9992	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3]	0.9981	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9978	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cH]	0.9976	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3H1][#6X3H0]	0.9876	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9814	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[#6H1][#6H1]	0.9794	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.9362	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9113	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6089	[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.1816
[cX3H1]([nX3H1])[cX3H1]	0.425	[OX2H][cX3]:[c]	0.2116
[#7]#[#6][#6][#6X3]	0.222	[cX3H1]([nX3H1])[cX3H0]	0.2718
[#8][#6H1][#6H1]	0.1837	[cH]cO	0.307
[#6]#[#7]	0.1277	[#7X3H1]	0.3084
o[cH]	0.1139	[OX2H1]	0.4599
[#7X3H0]	0.1139	[#7H][#6X3H1]	0.526
[#7]#[#6][#6X3]	0.1137	[#8][#6H0][#6H1]	0.5433
[#6X3H1][#7X3H0]	0.1058	[#6H1r5][#7]	0.567
[cX3H1]([nX3H0])[cX3H1]	0.1032	[#7][#6X3H0][#6X3H1]	0.5792

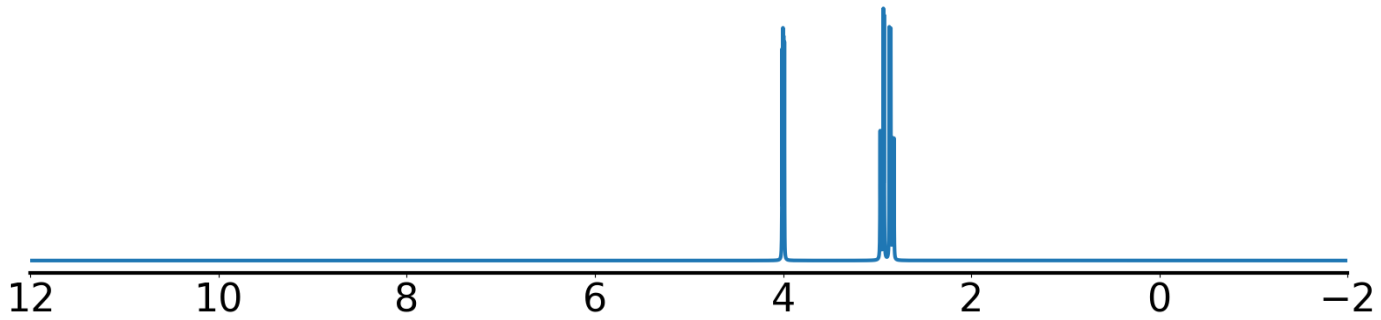
Example 15 true smiles: NC(=O)CC(N)C(=O)O formula: C4H8N2O3
Index of correct structure: 0 of 58024
True structure loss: 0.033268
True structure:



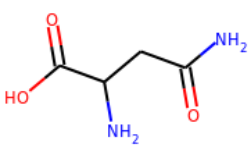
Experimental 13C NMR (solvent: D2O)



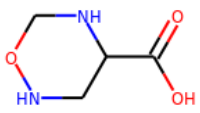
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.033268

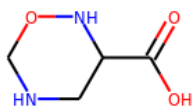


0.035903

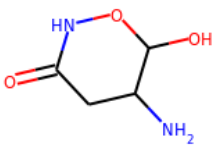
0.037272

0.03757

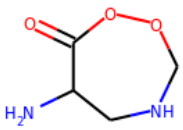
0.037613



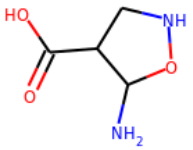
0.03893



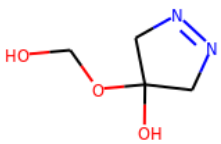
0.041735



0.042075



0.042357



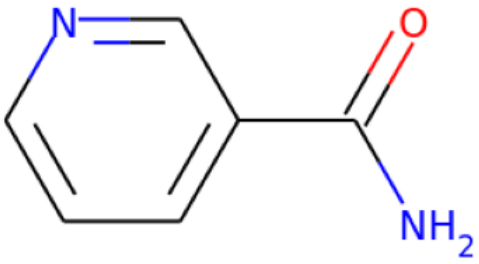
0.042735

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9811	[#8]=[#6H0][#6H1]	0.7567
[OX2H1]	0.9512	O=[CX3][CX4H]	0.7458
[#7X3H2]	0.8666	[CX3](=[OX1])O	0.726
[#8]=[#6][#8]	0.848	[#6H1][#6H2]	0.7157
[#6H1]	0.794	[#7H2][#6H1]	0.6811

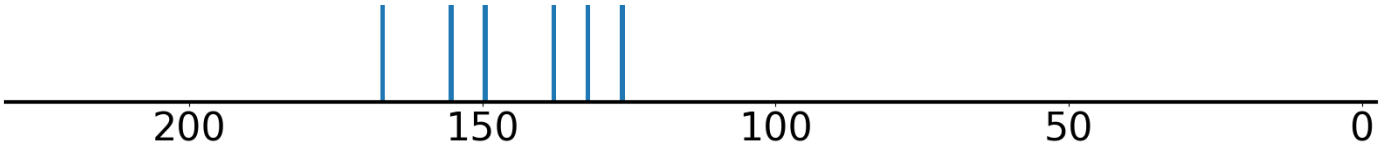
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9811	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9512	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#7X3H2]	0.8666	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#8]=[#6][#8]	0.848	CC=CCC#C	0.0
[#6H1]	0.794	CC#CCC=C	0.0
[#8]=[#6H0][#6H1]	0.7567	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
O=[CX3][CX4H]	0.7458	C=CC=CC#C	0.0
[CX3](=[OX1])O	0.726	[CX3H0](=[CX3H0])([CX4H3])[CX3H1]	0.0
[#6H1][#6H2]	0.7157	C=CCCC#C	0.0
[#7H2][#6H1]	0.6811	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0

worst negatives	prob	worst positives	prob
[#7][#6H2]	0.58	[#8]=[#6][#6][#6][#6]=[#8]	0.0702
[#6H1][#6H1]	0.5766	[#7H2][#6H0]	0.1389
[#7X3][#6H2]	0.5574	[#8][#6H0][#6H1]	0.2347
[#7X3H1]	0.5368	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.305
[#8][#6][#6][#6X3]	0.4624	[CX4H2]([CX4H1])[CX3H0]	0.3183
[#8][#6H1][#6H1]	0.4136	[#8]=[#6][#6H2][#6H1]	0.3464
[CX4H]O	0.4038	O=[CX3H0][CX4H2][CX4H1]	0.3882
[#8]=[#6][#6H1][#6H1]	0.2947	[#8][#6][#6][#6][#6]=[#8]	0.3999
[#7H1][#6X4H1][#6X3]	0.2866	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5026
[CX4H2]([NX3H1])[CX4H1]	0.2677	[CX4H2]([#6])[#6]	0.5386

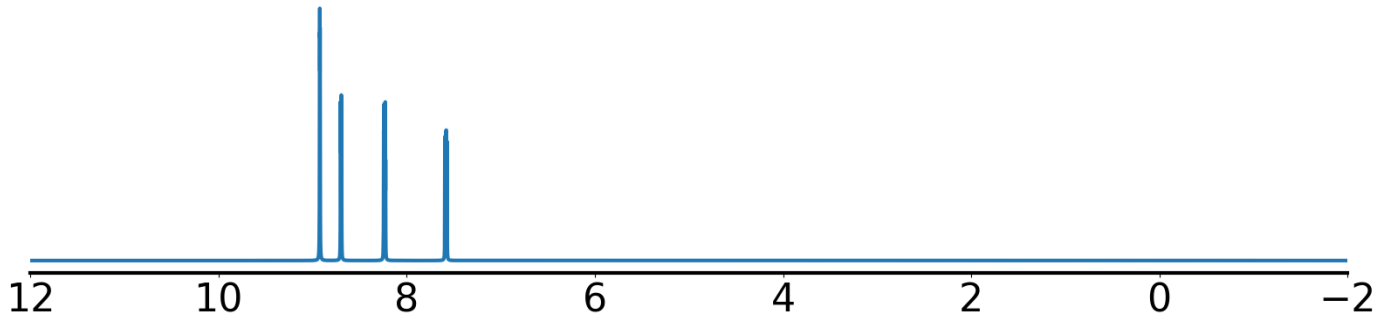
Example 16 true smiles: NC(=O)c1cccnc1 formula: C6H6N2O
Index of correct structure: -1 of 31495
True structure loss: 0.014517
True structure:



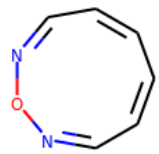
Experimental 13C NMR (solvent: DMSO)



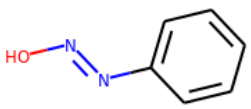
Experimental 1H NMR (solvent: d2o)



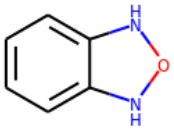
Top predicted structures (loss):



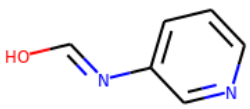
0.019746



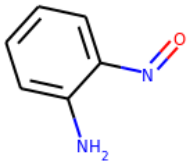
0.023498



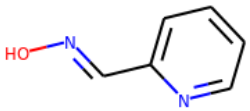
0.025849



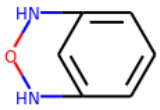
0.027113



0.027799

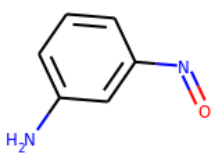


0.028293

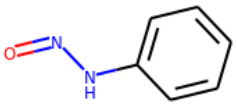


0.028402

0.030001



0.030352



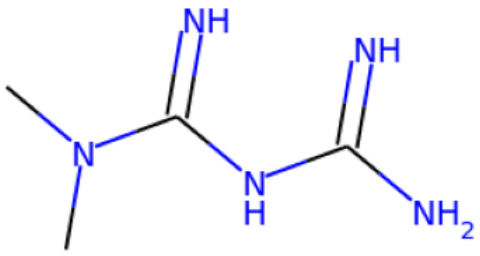
0.030973

Top predicted substructures	prob		
[#6H1]	1.0	[cH][cH]	0.9122
[#6X3][#6X3]	0.9989	[#6X3][#6X3][#6X3][#6X3]	0.9103
[#7][#6][#6][#6X3]	0.9754	[#7][#6][#6X3]	0.8758
[cH]	0.9649	[#6H1][#7][#6H1]	0.8639
[#6X3H1][#6X3H0]	0.9639	[#6H1][#6H1]	0.847

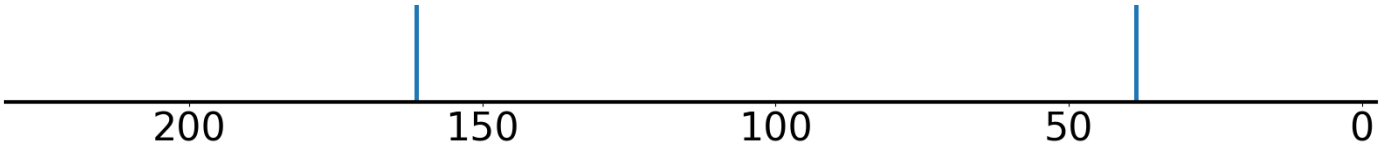
best positives	prob	best negatives	prob
[#6H1]	1.0	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9989	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.9754	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cH]	0.9649	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3H1][#6X3H0]	0.9639	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
[cH][cH]	0.9122	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9103	[OX2H0]1[CX4H2][CX4H1]1[CX4H2]	0.0
[#7][#6][#6X3]	0.8758	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6H1][#7][#6H1]	0.8639	[#6H3][#6H2][#6H1r4]	0.0
[#6H1][#6H1]	0.847	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0

worst negatives	prob	worst positives	prob
[#7][#6H0][#6H1]	0.5251	[#7X3H2]	0.1455
[#7][#6X3H0][#6X3H1]	0.4934	[#7H2][#6H0]	0.1551
[cH]cO	0.2763	[#7][#6][#6][#6][#7]	0.3388
[#8][#6][#6][#6X3]	0.2686	O=[#6][#6][#6X3]	0.4086
[#7H][#6X3H1]	0.1733	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6152
[#7X3H1]	0.1682	[cX3H1]([nX2H0])[cX3H0]	0.6357
[OX2H1]	0.1197	[cX3H1]([cX3H1])[cX3H0]	0.6695
[#7]=[#6][#6X3]	0.1191	[#6]1[#6][#6][#6][#6][#7]1	0.72
[#7][#7]	0.1179	[cX3H1]([cX3H1])[cX3H1]	0.791
[#7][#6][#7]	0.109	[cX3H1]([nX2H0])[cX3H1]	0.8094

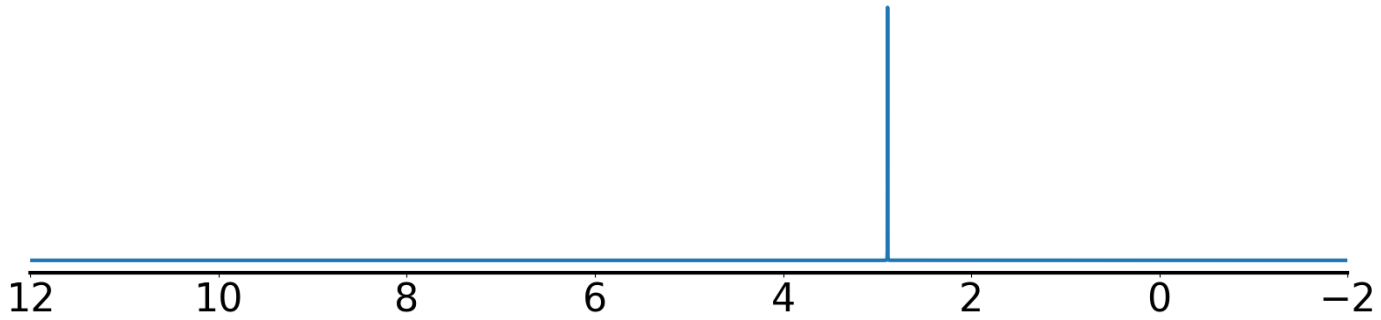
Example 17 true smiles: CN(C)C(=N)NC(=N)N formula: C4H11N5
Index of correct structure: 3 of 30817
True structure loss: 0.01683
True structure:



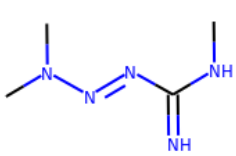
Experimental 13C NMR (solvent: D2O)



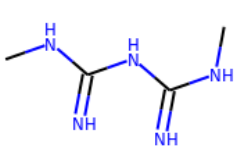
Experimental 1H NMR (solvent: d2o)



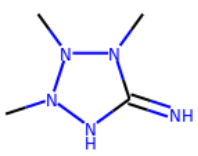
Top predicted structures (loss):



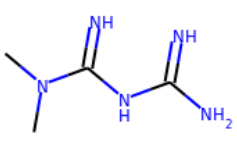
0.015959



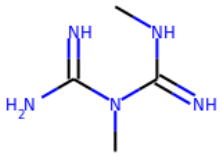
0.016287



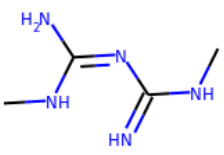
0.016689



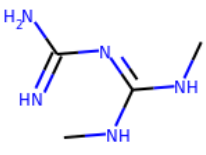
0.01683



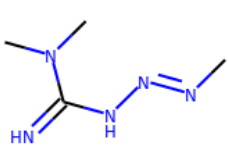
0.016899



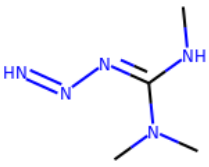
0.017047



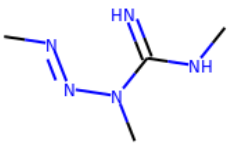
0.017159



0.017536



0.018149



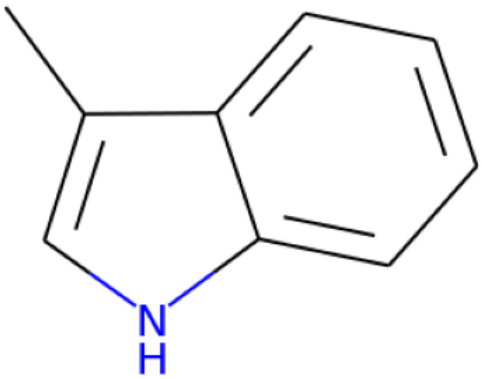
0.018632

Top predicted substructures	prob		
[CX4H3]	0.9746	[#7][#6][#7]	0.9401
[#7][#6]([#7])=[#7]	0.9737	[#7][#6]=[#7]	0.9356
[#6H3][#7]	0.9719	[#7X3][#6H3]	0.8762
[#7][#6H0]=[#7]	0.946	[NH1][#6]=[#7]	0.8544
[#7][#6H0][#7]	0.944	[NH1][#6][#7]	0.7823

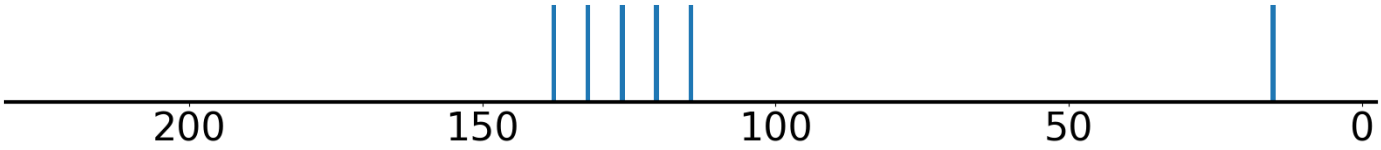
best positives	prob	best negatives	prob
[CX4H3]	0.9746	[#8][#6H1]=[#6H1][#6H3]	0.0
[#7][#6]([#7])=[#7]	0.9737	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H3][#7]	0.9719	[#6X3H2]=[#6][#6H2][#8H]	0.0
[#7][#6H0]=[#7]	0.946	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#7][#6H0][#7]	0.944	[OX2H0]1[CX4H2][CX4H1][CX3H0]=[CX3H1]1	0.0
[#7][#6][#7]	0.9401	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[#7][#6]=[#7]	0.9356	[#8]1[#6][#6]=[#6][#6]=[#6]1	0.0
[#7X3][#6H3]	0.8762	C=CCCC#C	0.0
[NH1][#6]=[#7]	0.8544	C=CC=CC#C	0.0
[NH1][#6][#7]	0.7823	[CX3H0](=[CX3H2])([OX2H0])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[CX4H3][NX3H1]	0.4833	[#6X3][#7][#6X3]	0.1032
[#7][#7]	0.471	[#6X3][#7X3][#6X3]	0.1357
[#7][#6][#6X3]	0.3816	[#7H2][#6H0]	0.2716
[#6]1[#6][#7][#6][#7]1	0.28	[CX4H3][NX3H0]	0.3068
[#7][#6H0][#6H1]	0.2613	[#7X3H0]	0.5055
[#7][#6][#6][#7]	0.2198	[#6]=[#7H]	0.6239
[#7][#7H1]	0.2163	[#7H1][#6H0][#7X3][#6H3]	0.6275
[#7][#6][#6][#6X3]	0.1824	[#7H1]=[#6H0][#7X3][#6H3]	0.6521
[#6H1]	0.18	[NH1]=[#6][#7]	0.7112
[#7X3][#6H2]	0.1377	[#6H3][#7][#6X3]	0.7473

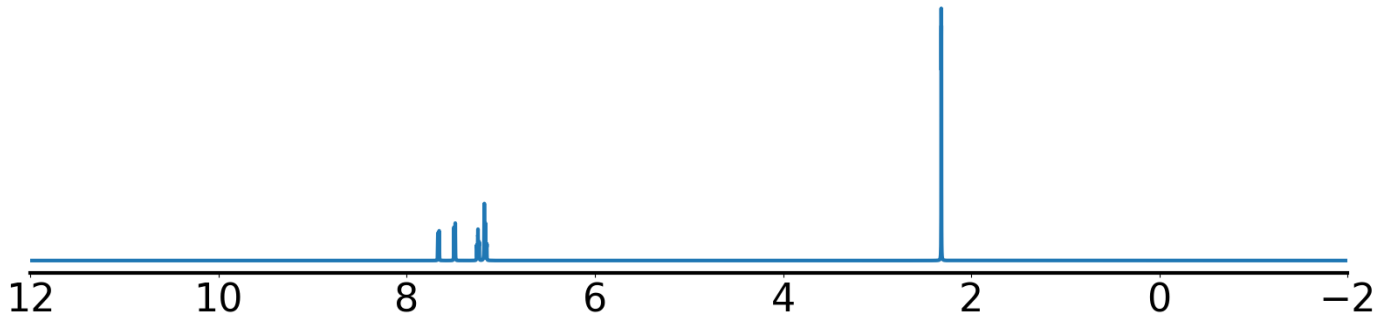
Example 18 true smiles: Cc1c[nH]c2ccccc12 formula: C9H9N
Index of correct structure: 0 of 29511
True structure loss: 0.013431
True structure:



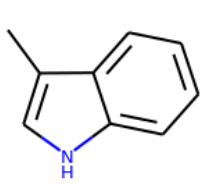
Experimental 13C NMR (solvent: CDCl3)



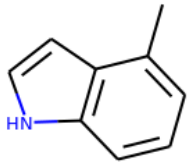
Experimental 1H NMR (solvent: d2o)



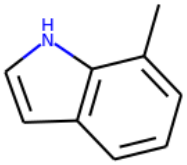
Top predicted structures (loss):



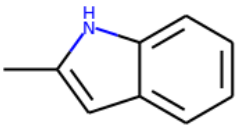
0.013431



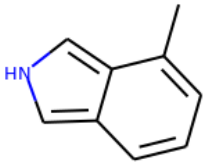
0.014915



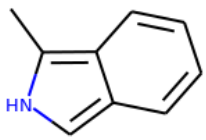
0.015945



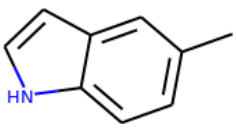
0.016185



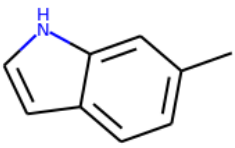
0.018507



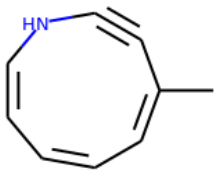
0.019129



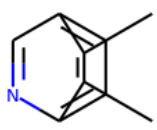
0.020373



0.020373



0.021081



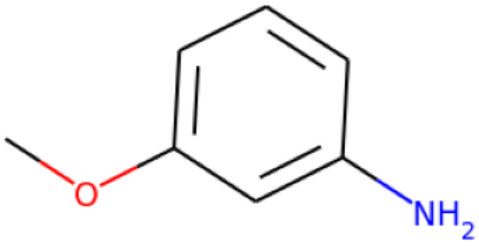
0.022922

Top predicted substructures	prob		
[#6H1]	0.9998	[cH]	0.9964
[#6X3][#6X3][#6X3][#6X3]	0.9998	[#6X3H1][#6X3H0]	0.9958
[#6X3][#6X3]	0.9997	[#6H3][#6H0]	0.9949
[#6H3][#6][#6]	0.9996	[cH][cH]	0.993
[CX4H3]	0.9995	[#6X3][#6][#6][#6H3]	0.9926

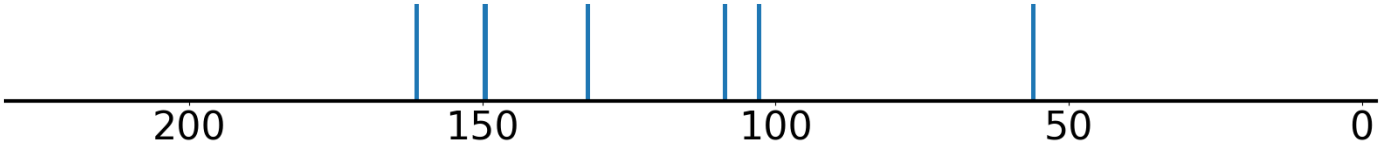
best positives	prob	best negatives	prob
[#6H1]	0.9998	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9998	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3]	0.9997	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6H3][#6][#6]	0.9996	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[CX4H3]	0.9995	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9964	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6X3H1][#6X3H0]	0.9958	[OX2H1][CX4H0][CX4H1]([CX4H2])[CX4H1]	0.0
[#6H3][#6H0]	0.9949	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[cH][cH]	0.993	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6X3][#6][#6][#6H3]	0.9926	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6176	[#7X3H1]	0.1356
[#6]1[#6][#6][#6][#6][#7]1	0.4272	[#7H][#6X3H1]	0.1907
[cX3H1]([nX3H0])[cX3H1]	0.2115	[#6H1r5][#7]	0.3164
[cX3H1]([cX3H0])[cX3H0]	0.1724	[cX3H1]([nX3H1])[cX3H0]	0.3305
[cX3H0][cX3H1][cX3H1][cX3H0]	0.1673	[#6X3][#7X3][#6X3]	0.5106
[#7][#[#6][#6][#6X3]	0.1381	[#6H3][#6H0][#6H1][#7]	0.5436
[cX3H1]([nX3H1])[cX3H1]	0.1244	[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.6386
[#7][#[#6][#6X3]	0.1079	[#7][#6H0][#6H1]	0.6627
[#6X3H1][#7X3H0]	0.0927	[#7][#6X3H0][#6X3H1]	0.6877
o[cH]	0.0587	[#6]1[#6][#6][#6][#7]1	0.6971

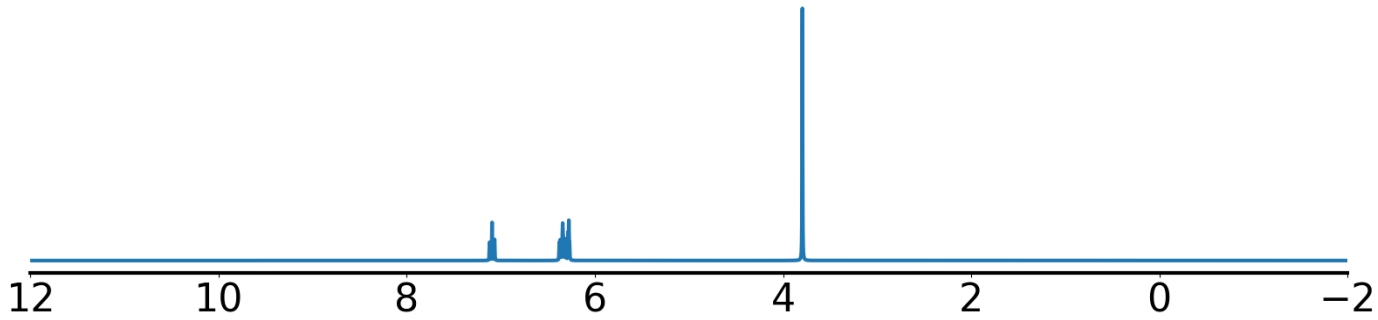
Example 19 true smiles: COc1cccc(N)c1 formula: C7H9NO
Index of correct structure: 1 of 29421
True structure loss: 0.022269
True structure:



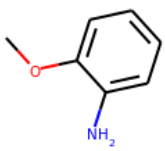
Experimental 13C NMR (solvent: CDCl3)



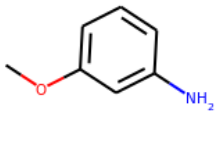
Experimental 1H NMR (solvent: CDCl3)



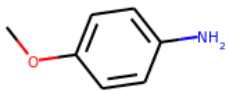
Top predicted structures (loss):



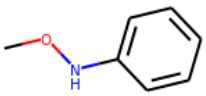
0.020336



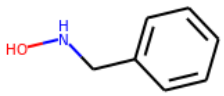
0.022269



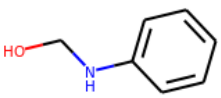
0.026384



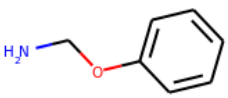
0.029129



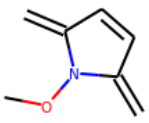
0.032354



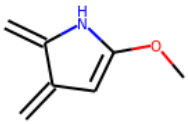
0.032459



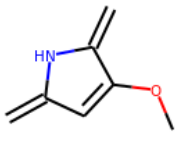
0.036699



0.0424



0.042488



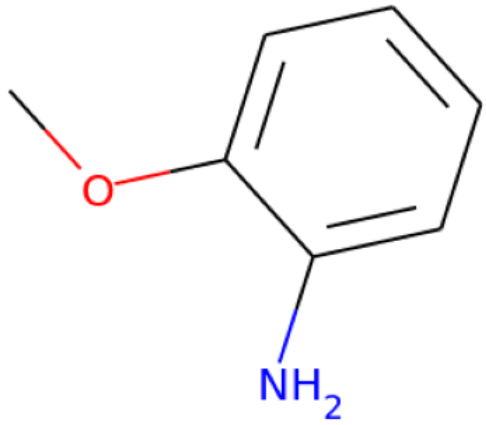
0.04278

Top predicted substructures	prob		
[#6H1]	0.9992	[cH][cH]	0.9391
[#6X3][#6X3]	0.9868	[CX4H3][OX2H0]	0.9129
[CX4H3]	0.9649	[cX3H1]([cX3H1])[cX3H0]	0.9118
[#6X3H1][#6X3H0]	0.9553	[cH]	0.9067
[#7][#6][#6X3]	0.95	[#6H1][#6H1]	0.8959

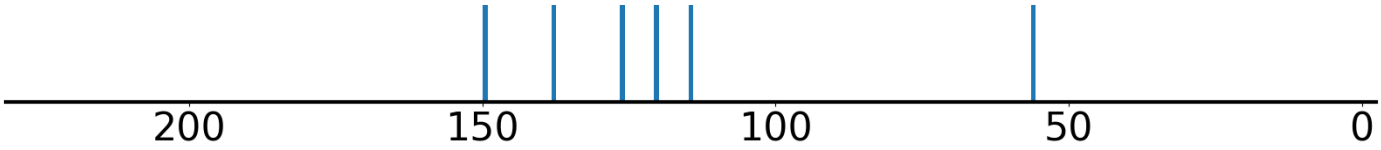
best positives	prob	best negatives	prob
[#6H1]	0.9992	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9868	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[CX4H3]	0.9649	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9553	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.95	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9391	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[CX4H3][OX2H0]	0.9129	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9118	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[cH]	0.9067	CCC#CC#C	0.0
[#6H1][#6H1]	0.8959	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0

worst negatives	prob	worst positives	prob
[CHX3](=C)C	0.5402	[#6]1[#6][#6][#6][#6][#6]1	0.0966
[#6X3][#7][#6X3]	0.4149	[#7H2][#6H0]	0.1806
[#7X3H1]	0.4128	[cX3H1]([cX3H0])[cX3H0]	0.2022
[#7X3][#6H2]	0.3836	[#7X3H2]	0.2045
[#6X3][#7X3][#6X3]	0.3677	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3828
[CHX3]=[CHX3]	0.3589	[#8][#6][#6][#6X3]	0.4801
[#6]1[#6][#6][#6][#7]1	0.3152	[cH]cO	0.4876
[#6X3][#6H2][#7]	0.2789	[#7][#6H0][#6H1]	0.599
[CX3H1](=[CX3H1])[CX3H0]	0.2697	[#7][#6X3H0][#6X3H1]	0.6884
[#6X3H2]	0.2192	[cX3H1]([cX3H1])[cX3H1]	0.7187

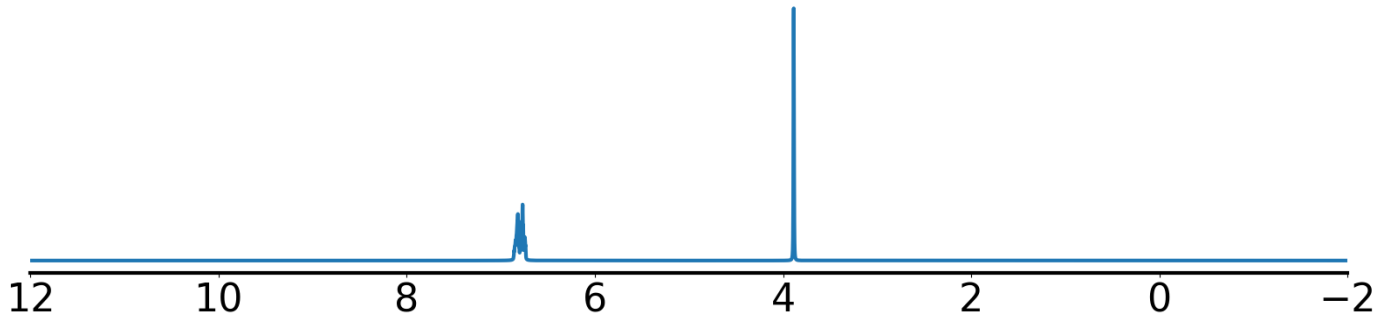
Example 20 true smiles: COc1ccccc1N formula: C7H9NO
Index of correct structure: 0 of 29421
True structure loss: 0.017036
True structure:



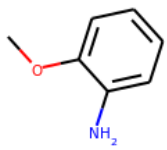
Experimental 13C NMR (solvent: CDCl3)



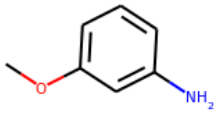
Experimental 1H NMR (solvent: CDCl3)



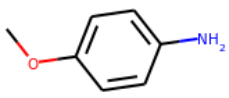
Top predicted structures (loss):



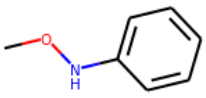
0.017036



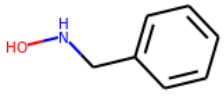
0.02047



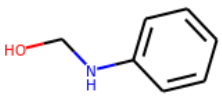
0.022668



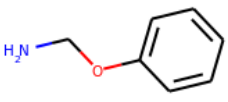
0.022859



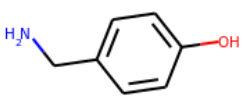
0.024341



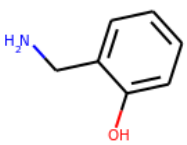
0.027768



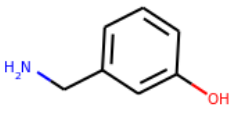
0.027878



0.032987



0.034698



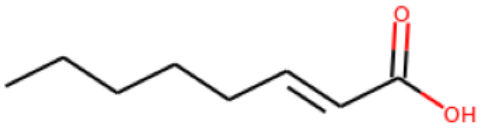
0.035239

Top predicted substructures	prob		
[#6H1]	0.9979	[#6X3H1][#6X3H0]	0.9036
[#6X3][#6X3]	0.9911	[cH][cH]	0.8995
[cH]	0.9658	[#6H1][#6H1]	0.8945
[#7][#6][#6X3]	0.9588	[cX3H1]([cX3H1])[cX3H0]	0.8733
[#6X3][#6X3][#6X3][#6X3]	0.9265	[#7][#6][#6][#6X3]	0.8635

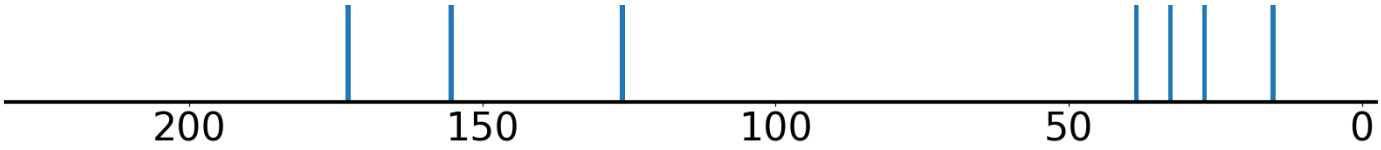
best positives	prob	best negatives	prob
[#6H1]	0.9979	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3][#6X3]	0.9911	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.9658	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#7][#6][#6X3]	0.9588	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9265	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9036	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[cH][cH]	0.8995	[#6]1[#8][#6][#6]1=[#8]	0.0
[#6H1][#6H1]	0.8945	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8733	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#7][#6][#6][#6X3]	0.8635	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0

worst negatives	prob	worst positives	prob
[#7X3][#6H2]	0.3931	[#7H2][#6H0]	0.183
[CHX3](=C)C	0.3794	[#7X3H2]	0.3159
[#6X3][#7][#6X3]	0.3564	[#7][#6H0][#6H1]	0.3398
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.341	[#7][#6X3H0][#6X3H1]	0.4599
[#6]1[#6][#6][#6][#7]1	0.3371	[#6]1[#6][#6][#6][#6][#6]1	0.5398
[#7X3H1]	0.3174	[CX4H3]	0.6248
[#6]1[#6][#6][#6][#6][#7]1	0.2989	[cH]cO	0.6338
[#7][#6H2]	0.2977	[#8][#6][#6][#6X3]	0.7336
[#7H][#6X3H1]	0.2636	[cX3H1]([cX3H1])[cX3H1]	0.7413
[#6H1r5][#7]	0.2606	[#8][#6H0][#6H1]	0.7598

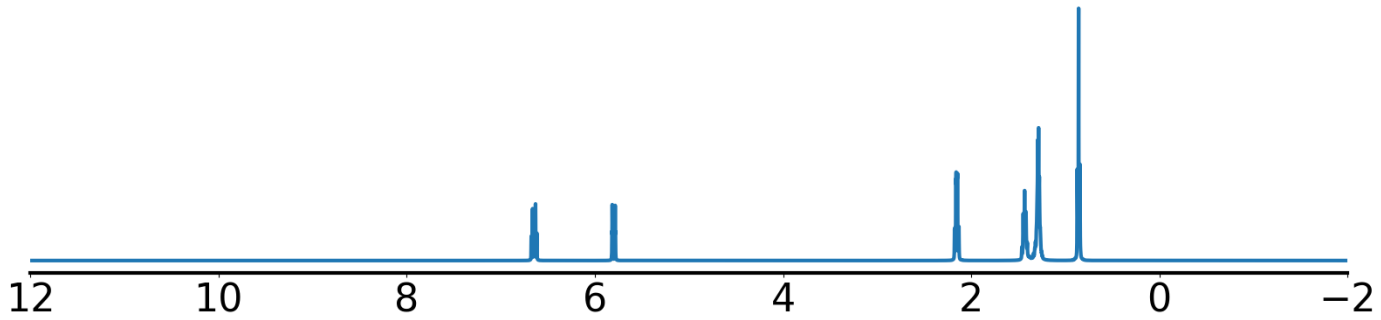
Example 21 true smiles: CCCCCC=CC(=O)O formula: C8H14O2
Index of correct structure: 0 of 28834
True structure loss: 0.008703
True structure:



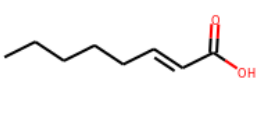
Experimental 13C NMR (solvent: CDCl3)



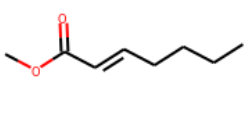
Experimental 1H NMR (solvent: D2O)



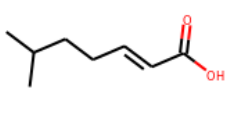
Top predicted structures (loss):



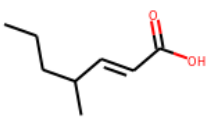
0.008703



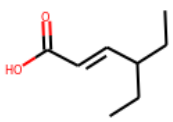
0.039766



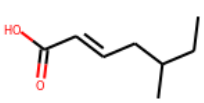
0.048218



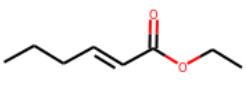
0.051362



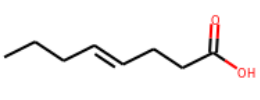
0.055961



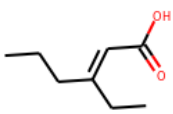
0.056054



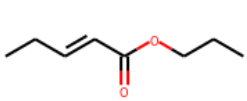
0.058186



0.06541



0.070585



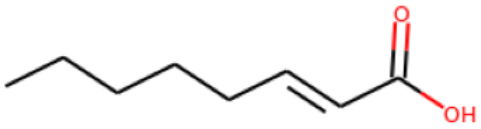
0.074826

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H3][#6]	0.9991
[CX4H3]	0.9998	O=[#6][#6]=[#6X3]	0.9989
[CX4H3][CX4H2]	0.9997	[CHX3](=C)C	0.9975
[#6H3][#6][#6]	0.9995	[#8]=[#6][#8]	0.9975
[#6H1]	0.9994	[CX3](=[OX1])O	0.996

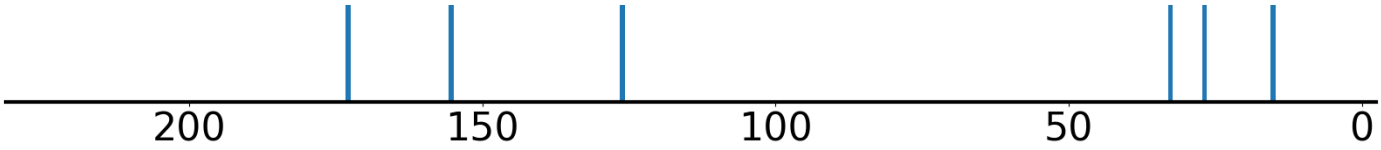
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	0.9998	[CX2H0](#[CX2H1])[CX4H1]	0.0
[CX4H3][CX4H2]	0.9997	CC#CCC#C	0.0
[#6H3][#6][#6]	0.9995	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H1]	0.9994	[#6X2][#6H1][#6X2]	0.0
[CX4H3][#6]	0.9991	[CX2H0](#[CX2H0])[CX2H0]	0.0
O=[#6][#6]=[#6X3]	0.9989	[CX2H0](#[CX2H0])[CX4H0]	0.0
[CHX3](=C)C	0.9975	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#8]=[#6][#8]	0.9975	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.996	[#7][#6H1][#6X2]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6][#6][#6H3]	0.5747	CCCCCC	0.5444
[#8][#6][#6H2]	0.3697	[CX4H2][CX4H2][CX4H2][CX4H2]	0.5653
[CX4H2]CC=O	0.3541	[CX4H2][CX3H]	0.6269
[CX4H2]([CX4H2])[CX3H0]	0.33	[#8][#6H0][#6H1]	0.6786
OCC[CH2]	0.2329	[#8][#6][#6]=[#6X3]	0.7211
[CX4H2][CX3]=O	0.1889	[CX4H2]([CX4H2])[CX4H2]	0.7384
[#6H3][#6][#6X3]	0.1584	[CX4H2]([CX4H2])[CX3H1]	0.8075
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.1566	CCCCC=C	0.8152
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.0917	[#8]=[#6H0][#6H1]	0.8167
[CX4H3][CX4H1]	0.0723	[#6H1][#6H2]	0.823

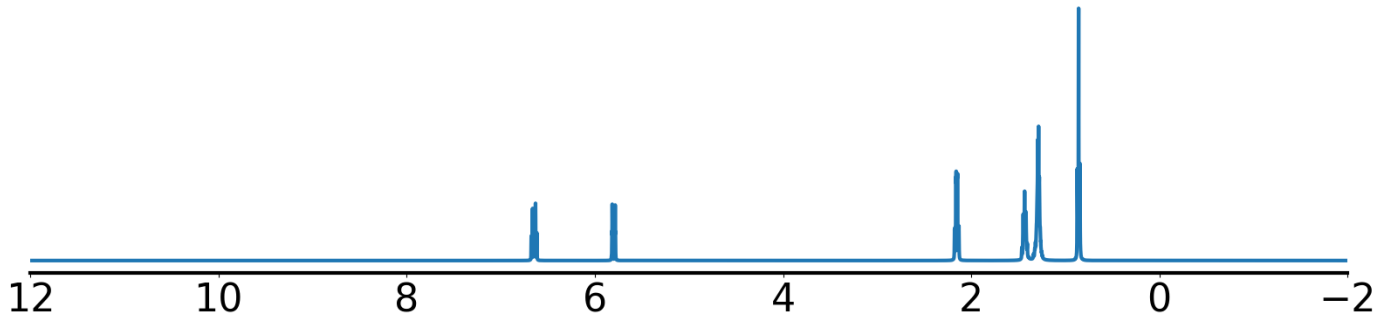
Example 22 true smiles: CCCCCC=CC(=O)O formula: C8H14O2
Index of correct structure: 0 of 28834
True structure loss: 0.008863
True structure:



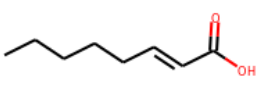
Experimental 13C NMR (solvent: CDCl3)



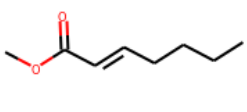
Experimental 1H NMR (solvent: d2o)



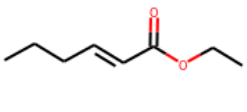
Top predicted structures (loss):



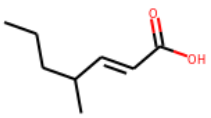
0.008863



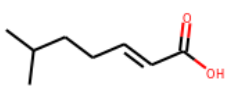
0.035556



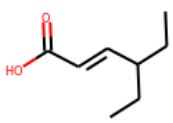
0.048876



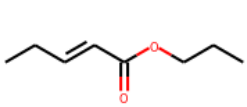
0.053914



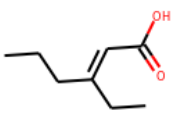
0.055939



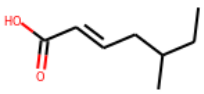
0.056741



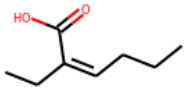
0.063285



0.066027



0.067133



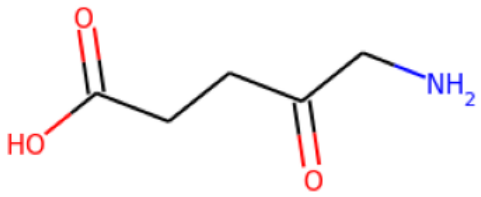
0.078098

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[#6H1]	0.9993
[CX4H3][CX4H2]	0.9999	O=[#6][#6]=[#6X3]	0.9991
[CX4H3]	0.9999	[CHX3](=C)C	0.9983
[CX4H3][#6]	0.9995	[#8]=[#6][#6H1]=[#6H1]	0.9977
[#6H3][#6][#6]	0.9995	[#6X3][#6X3]	0.9963

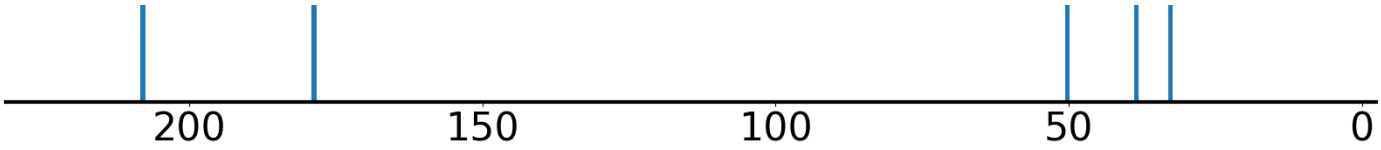
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[#6X2][#6H1][#6X2]	0.0
[CX4H3][CX4H2]	0.9999	CC#CCC#C	0.0
[CX4H3]	0.9999	[#7][#6H1][#6X2]	0.0
[CX4H3][#6]	0.9995	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6H3][#6][#6]	0.9995	[CX2H0](#[CX2H1])[CX4H1]	0.0
[#6H1]	0.9993	[CX2H0](#[CX2H1])[cX3H0]	0.0
O=[#6][#6]=[#6X3]	0.9991	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CHX3](=C)C	0.9983	[CX2H0](#[CX2H0])[CX4H0]	0.0
[#8]=[#6][#6H1]=[#6H1]	0.9977	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#6X3][#6X3]	0.9963	[#6H2][#6]#[#6X2]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6][#6][#6H3]	0.5245	CCCCCC	0.2862
[#8][#6][#6H2]	0.2748	[CX4H2][CX4H2][CX4H2][CX4H2]	0.5175
[CX4H2]CC=O	0.2187	[CX4H2][CX3H]	0.544
OCC[CH2]	0.2143	CCCCC=C	0.5958
[#6H3][#6][#6X3]	0.2035	[CX4H2]([CX4H2])[CX4H2]	0.6958
[CX4H2]([CX4H2])[CX3H0]	0.1177	[#6H1][#6H2]	0.746
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.1001	[CX4H2]([CX4H2])[CX3H1]	0.7582
[CX3H0](=[OX1H0])([OX2H0])[CX3H1]	0.0912	[#8][#6H0][#6H1]	0.7866
[#6H1][#6H1]	0.0748	[#8][#6][#6]=[#6X3]	0.8162
[CX4H3][CX4H1]	0.0585	[CHX3]=[CHX3]	0.8426

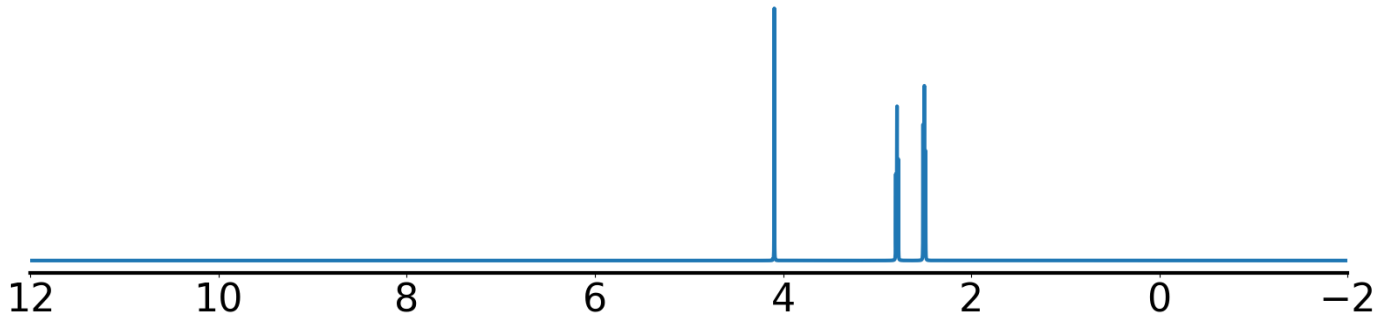
Example 23 true smiles: NCC(=O)CCC(=O)O formula: C5H9NO3
Index of correct structure: 0 of 27953
True structure loss: 0.019908
True structure:



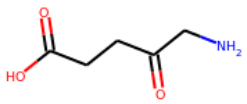
Experimental 13C NMR (solvent: D2O)



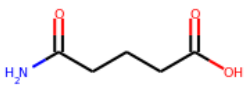
Experimental 1H NMR (solvent: D2O)



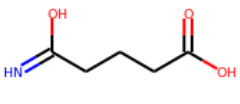
Top predicted structures (loss):



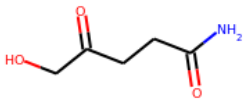
0.019908



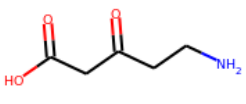
0.034361



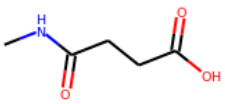
0.040346



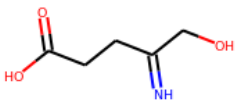
0.041791



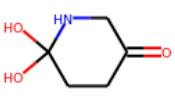
0.043131



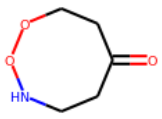
0.044076



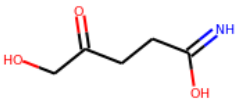
0.045778



0.048403



0.048685



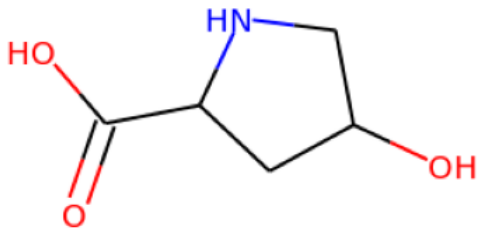
0.049151

Top predicted substructures	prob		
[CX3](=[OX1])C	1.0	[CX4H2][CX3]=O	0.988
[CX4H2]([#6])[#6]	0.9997	[OX2H1]	0.9756
[CX4H2]([CX4H2])[CX3H0]	0.9985	[#7X3][#6H2]	0.9679
O=[CX3H0][CX4H2][CX4H2]	0.9963	[CX4H2]CC=O	0.9206
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9962	[#7][#6H2]	0.9169

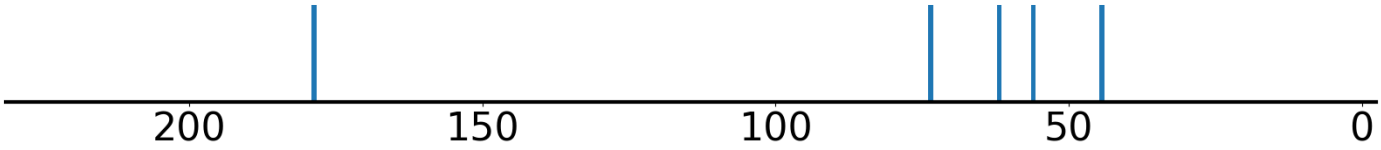
best positives	prob	best negatives	prob
[CX3](=[OX1])C	1.0	CC=CCC#C	0.0
[CX4H2]([#6])[#6]	0.9997	CC=CC#CC	0.0
[CX4H2]([CX4H2])[CX3H0]	0.9985	C=CC=CC#C	0.0
O=[CX3H0][CX4H2][CX4H2]	0.9963	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9962	[#6X2][#6H1][#6X2]	0.0
[CX4H2][CX3]=O	0.988	C=CCCC#C	0.0
[OX2H1]	0.9756	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7X3][#6H2]	0.9679	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]CC=O	0.9206	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#7][#6H2]	0.9169	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[#7][#6H2][#6H2]	0.6196	[CX4H2]([NX3H2])[CX3H0]	0.0503
[#7X3H1]	0.4542	[#7H2][#6H2]	0.1256
[CX4H2]([NX3H1])[CX4H2]	0.3455	[#8][#6][#6H2]	0.359
[#7][#6][#6][#6X3]	0.3301	[#6X3][#6H2][#7]	0.3748
[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.2928	[#8][#6][#6][#6][#6]=[#8]	0.4503
[OX2H1][CX4H2][#6X3H0]	0.2697	[#8]=[#6][#6][#6][#6]=[#8]	0.6313
[#7H2][#6H0]	0.2321	[#7][#6][#6X3]	0.6397
[#8]=[#6][#6H2][#8]	0.2189	[#7X3H2]	0.7007
[CX4H2]([#6])[O]	0.211	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.7035
[#6H2][#7][#6X3]	0.1922	[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.7186

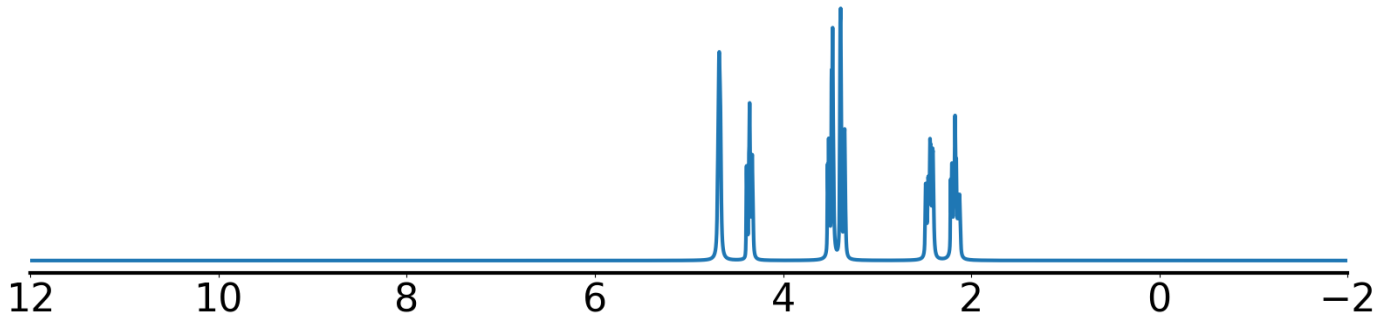
Example 24 true smiles: O=C(O)C1CC(O)CN1 formula: C5H9NO3
Index of correct structure: 0 of 27953
True structure loss: 0.032393
True structure:



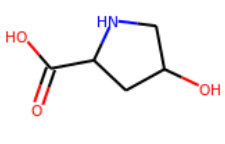
Experimental 13C NMR (solvent: D2O)



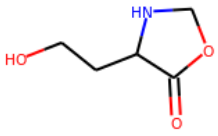
Experimental 1H NMR (solvent: D2O)



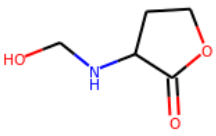
Top predicted structures (loss):



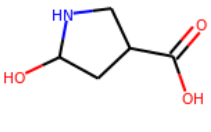
0.032393



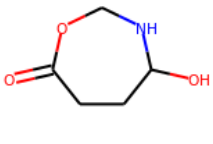
0.035936



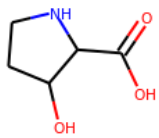
0.041696



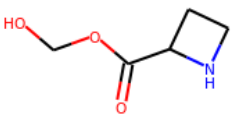
0.042455



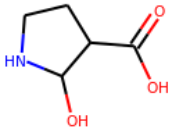
0.043932



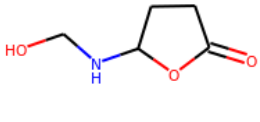
0.048112



0.048123



0.04834



0.048575

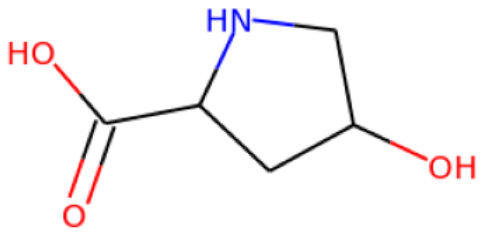
0.050339

Top predicted substructures	prob		
[#6H1]	0.9989	[#6H1][#6H2]	0.9335
[CX4H2]([#6])[#6]	0.9987	[OX2H1]	0.922
[CX3](=[OX1])C	0.9942	[#8]=[#6H0][#6H1]	0.8957
[#8]=[#6][#8]	0.9446	OCC[CH2]	0.8849
[#7X3][#6H2]	0.9414	[CX3](=[OX1])O	0.8714

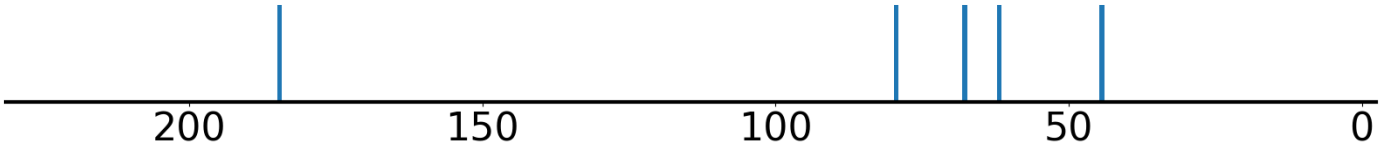
best positives	prob	best negatives	prob
[#6H1]	0.9989	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[#6]	0.9987	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[CX3](=[OX1])C	0.9942	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#8]=[#6][#8]	0.9446	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[#7X3][#6H2]	0.9414	C=CC=CC#C	0.0
[#6H1][#6H2]	0.9335	[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	0.0
[OX2H1]	0.922	[#6H3][#6H1][#6H1]=[#7]	0.0
[#8]=[#6H0][#6H1]	0.8957	[CX3H0](=[CX3H0])([CX4H3])[CX4H2]	0.0
OCC[CH2]	0.8849	[CX2H0](#[CX2H0])[CX3H0]	0.0
[CX3](=[OX1])O	0.8714	[#6X3][#6]#[#6][#6H3]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6][#6X3]	0.5012	[CX4H2]([NX3H1])[CX4H1]	0.164
[CX4H2]([CX4H2])[CX4H1]	0.4633	[#6H1]([#6H2])[#6H2]	0.2168
[CX4H2]([#6])[O]	0.4506	[#7][#6H2][#6H1]	0.2253
[CX4H2][CX4H2]	0.4158	[CX3](=O)[OX2H1]	0.2954
[#7X3H2]	0.4148	[CX4H2]([CH])[CH]	0.3104
[CX4H2][CX3]=O	0.3846	[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.3143
[#8][#6H1][#6H1]	0.3578	[#6H1][#6H2][#6][#6][#7]	0.3234
[#7H2][#6H1]	0.3093	[#8][#6][#6][#6][#6][#8]	0.3521
[#7][#6][#6][#6X3]	0.2444	[#6]1[#6][#6][#6][#7]1	0.3717
[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.2364	[#7X3H1]	0.3754

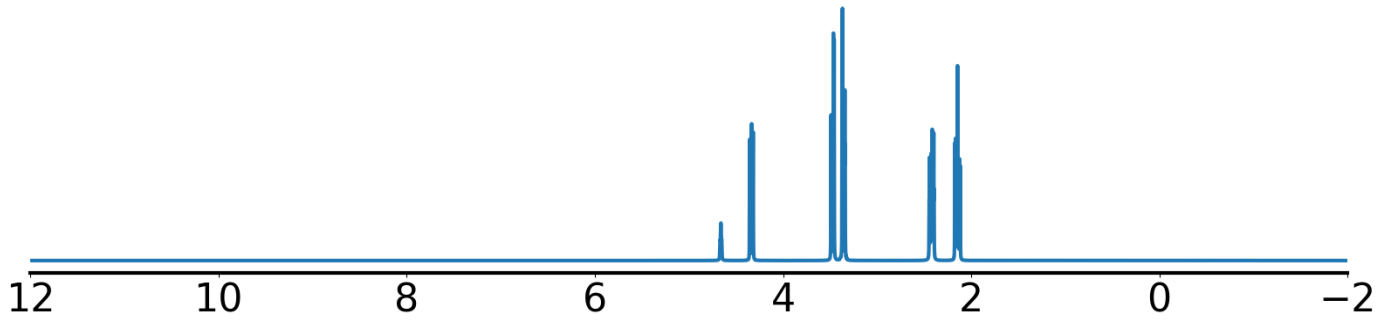
Example 25 true smiles: O=C(O)C1CC(O)CN1 formula: C5H9NO3
Index of correct structure: 0 of 27953
True structure loss: 0.032454
True structure:



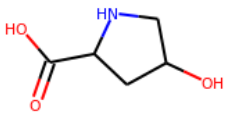
Experimental 13C NMR (solvent: D2O)



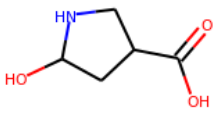
Experimental 1H NMR (solvent: D2O)



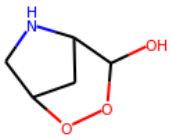
Top predicted structures (loss):



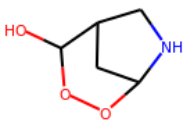
0.032454



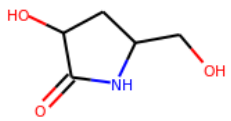
0.039223



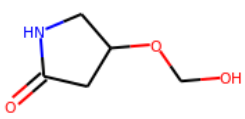
0.042535



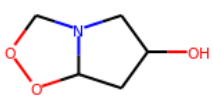
0.047224



0.052116



0.053022



0.053465

0.053893

0.05523

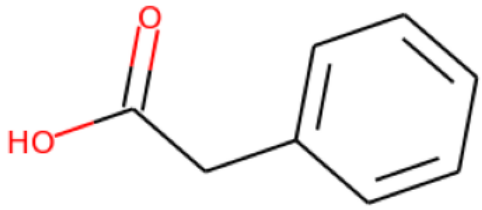
0.056236

Top predicted substructures	prob		
[#6H1]	0.9954	[CX4H]O	0.9004
[CX3](=[OX1])C	0.9942	O[CX4H][CX4H2]	0.8361
[CX4H2]([#6])[#6]	0.9744	[#8][#6][#6H2]	0.8266
[OX2H1]	0.9694	OCC[CH2]	0.7816
[#6H1][#6H2]	0.96	[#8]=[#6][#8]	0.7606

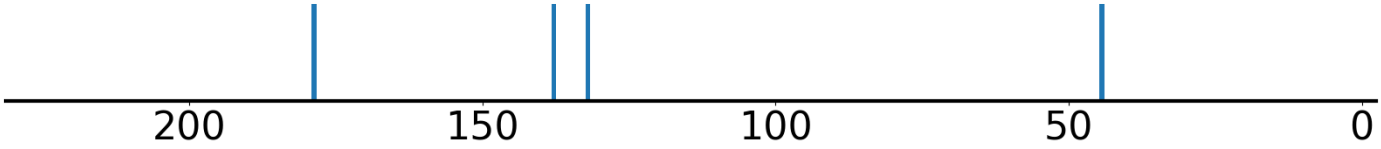
best positives	prob	best negatives	prob
[#6H1]	0.9954	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[CX3](=[OX1])C	0.9942	[CX3H0](=[CX3H1])([CX4H3])[CX3H1]	0.0
[CX4H2]([#6])[#6]	0.9744	CC=CC#CC	0.0
[OX2H1]	0.9694	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H1][#6H2]	0.96	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[CX4H]O	0.9004	CCC=CC#C	0.0
O[CX4H][CX4H2]	0.8361	[CX3H0](=[CX3H0])([CX4H3])[CX4H2]	0.0
[#8][#6][#6H2]	0.8266	[CX3H1](=[CX3H1])[CX2H0]	0.0
OCC[CH2]	0.7816	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#8]=[#6][#8]	0.7606	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H1][#6H1]	0.4266	[CX3](=O)[OX2H1]	0.14
[#8][#6][#6]=[#8]	0.4079	[#7H1][#6X4H1][#6X3]	0.2058
[#8][#6][#6][#6X3]	0.3946	[CX4H2]([NX3H1])[CX4H1]	0.2465
[#6H1][#6H1]	0.3882	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2565
[#7X3H2]	0.3711	[#8][#6][#6][#6][#6][#8]	0.2721
[CX4H2][CX3]=O	0.3122	[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.3053
[CX4H2]([#6])[O]	0.3048	[CX4H1]([NX3H1])([CX4H2])[CX3H0]	0.3349
[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.2694	[#6H1r5][#7]	0.3536
[#7][#6][#6][#6X3]	0.2688	[#8][#6H0][#6H1]	0.3608
O[CX4H]([CX4H2])[CX4H1]	0.2429	[CX3](=[OX1])O	0.4072

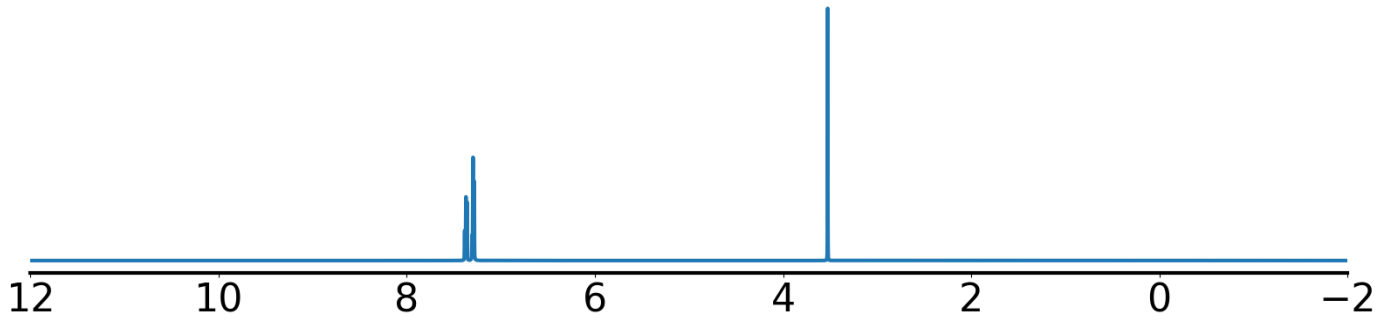
Example 26 true smiles: O=C(O)Cc1ccccc1 formula: C8H8O2
Index of correct structure: 0 of 26562
True structure loss: 0.023907
True structure:



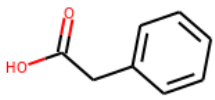
Experimental 13C NMR (solvent: CDCl3)



Experimental 1H NMR (solvent: d2o)

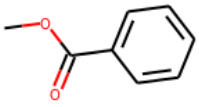


Top predicted structures (loss):

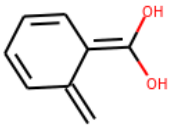


0.023907

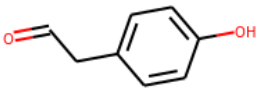
0.042161



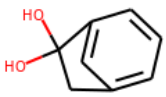
0.046921



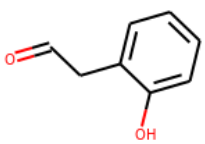
0.054306



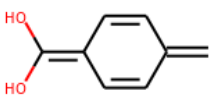
0.054605



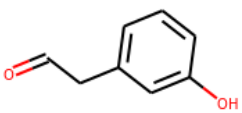
0.055526



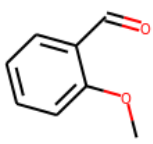
0.058364



0.058816



0.059834



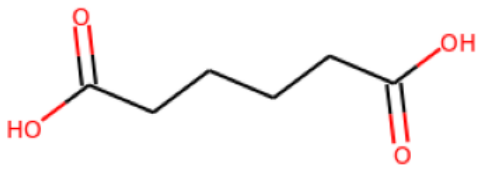
0.060167

Top predicted substructures	prob		
[#6H1]	0.9973	[CX3](=[OX1])C	0.9338
[#6X3][#6H2][#6X3]	0.9812	[#6X3H1][#6X3H0]	0.8959
[#6X3][#6X3]	0.977	[#8X1]=[#6X3][#6H2][#6H0]	0.8538
O=[#6][#6][#6X3]	0.9614	[#6X3][#6X3][#6X3][#6X3]	0.7715
[CX4H2]([#6])[#6]	0.9439	[#8]=[#6][#8]	0.757

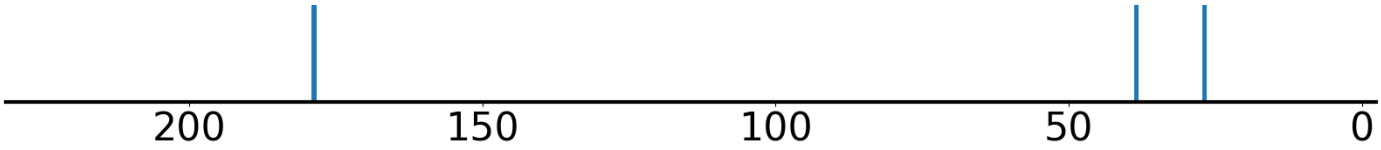
best positives	prob	best negatives	prob
[#6H1]	0.9973	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.0
[#6X3][#6H2][#6X3]	0.9812	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.977	[#6H3][#6H1][#7][#7]	0.0
O=[#6][#6][#6X3]	0.9614	[CX4H1]([OX2H1])([CX4H3])[CX4H0]	0.0
[CX4H2]([#6])[#6]	0.9439	[#8][#6H2][#6H2][#6X2]	0.0
[CX3](=[OX1])C	0.9338	[CX4H1]([NX3H2])([CX4H2])[CX4H0]	0.0
[#6X3H1][#6X3H0]	0.8959	[CX4H2]([NX2H0])[CX4H1]	0.0
[#8X1]=[#6X3][#6H2][#6H0]	0.8538	[CX4H1]([NX3H0])([CX4H3])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.7715	[CX4H2]([NX3H1])[CX4H3]	0.0
[#8]=[#6][#8]	0.757	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[CHX3](=C)C	0.3903	[#6]1[#6][#6][#6][#6][#6]1	0.1447
[CHX3]=[CHX3]	0.3433	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.1576
[#6X3][#6X3]=[#6X3][#6X3]	0.3093	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1624
[#8]=[#6H0][#6H1]	0.2914	[cX3H1]([cX3H1])[cX3H1]	0.1718
O=[#6][#6]=[#6X3]	0.2842	[OX2H1]	0.315
[OX1H0]=[CX3H0][CX4H2][CX3H0]	0.2613	[#8][#6][#6H2]	0.3455
[CX4H2]([CX3H0])[CX3H0]	0.2419	[CX3](=O)[OX2H1]	0.4395
[CX3H1](=[CX3H1])[CX3H0]	0.2409	[cH][cH]	0.4548
[#6H1][#6H2]	0.2295	[cX3H1]([cX3H1])[cX3H0]	0.5049
[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.2126	[#6H1][#6H1]	0.6281

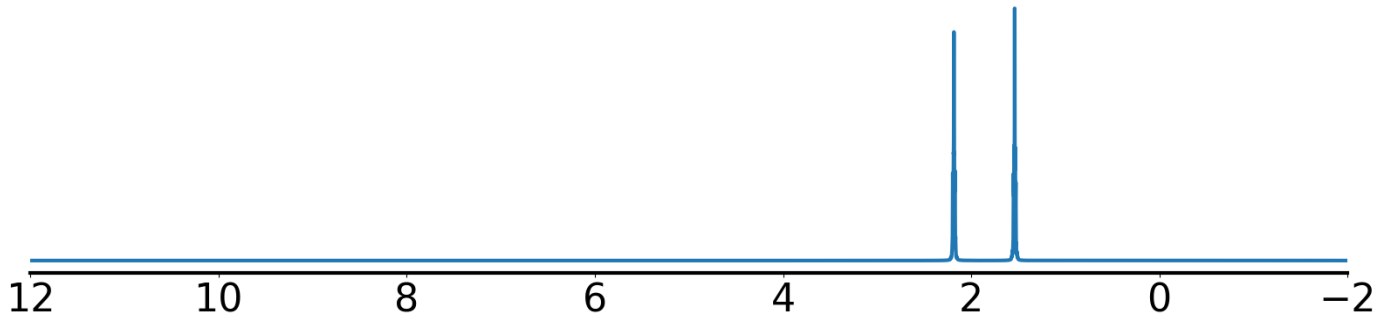
Example 27 true smiles: O=C(O)CCCCC(=O)O formula: C6H10O4
Index of correct structure: 0 of 19323
True structure loss: 0.011026
True structure:



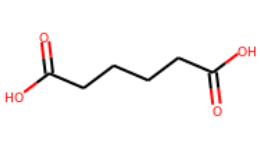
Experimental 13C NMR (solvent: DMSO)



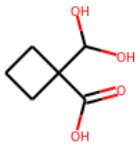
Experimental 1H NMR (solvent: d2o)



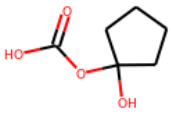
Top predicted structures (loss):



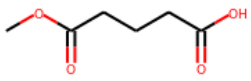
0.011026



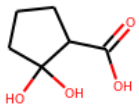
0.035414



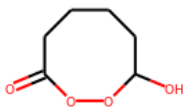
0.039191



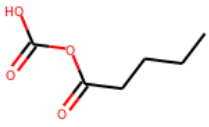
0.040383



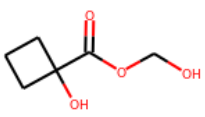
0.050711



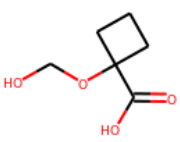
0.053052



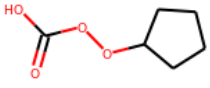
0.05349



0.054585



0.054696



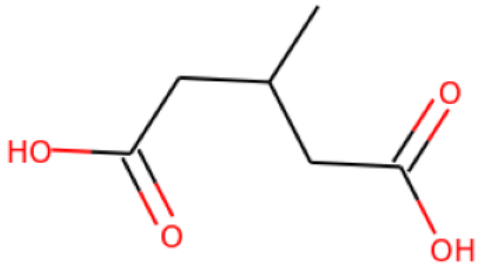
0.058132

Top predicted substructures	prob		
[#8]=[#6][#8]	0.9997	[OX2H1]	0.9961
[CX3](=[OX1])O	0.9995	OCC[CH2]	0.9672
[CX3](=[OX1])C	0.9994	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.9449
[CX3](=O)[OX2H1]	0.9982	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.8528
[CX4H2]([#6])[#6]	0.9972	O=[CX3H0][CX4H2][CX4H2]	0.7998

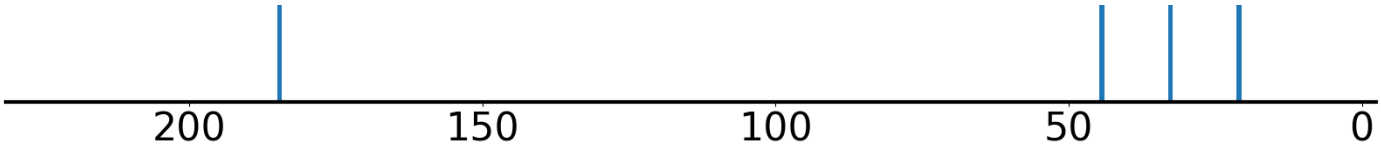
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9997	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])O	0.9995	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9994	[#7][#6]=[#6][#6]#[#7]	0.0
[CX3](=O)[OX2H1]	0.9982	C=CC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9972	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX2H1]	0.9961	CC#CCC=C	0.0
OCC[CH2]	0.9672	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.9449	CC=CCC#C	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.8528	[#7][#6]=[#6][#6][#6]=[#7]	0.0
O=[CX3H0][CX4H2][CX4H2]	0.7998	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.5891	CCCCCC	0.3714
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5782	[CX4H2][CX4H2][CX4H2][CX4H2]	0.4663
[#8][#6H0][#6H1]	0.5444	[CX4H2]([CX4H2])[CX3H0]	0.5775
[#6H1][#6H2]	0.3208	[CX4H2]([CX4H2])[CX4H2]	0.6523
[#8][#6][#6][#6][#6][#8]	0.1871	[#8][#6][#6H2]	0.7061
[#8]=[#6H0][#6H1]	0.1718	[CX4H2]CC=O	0.7156
O=[CX3][CX4H]	0.1504	[CX4H2][CX4H2]	0.7204
[#8]=[#6][#6H2][#6H1]	0.1349	[CX4H2][CX3]=O	0.775
[#8][#6][#6][#8]	0.1309	O=[CX3H0][CX4H2][CX4H2]	0.7998
O=[CX3H0][CX4H2][CX4H1]	0.1186	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.8528

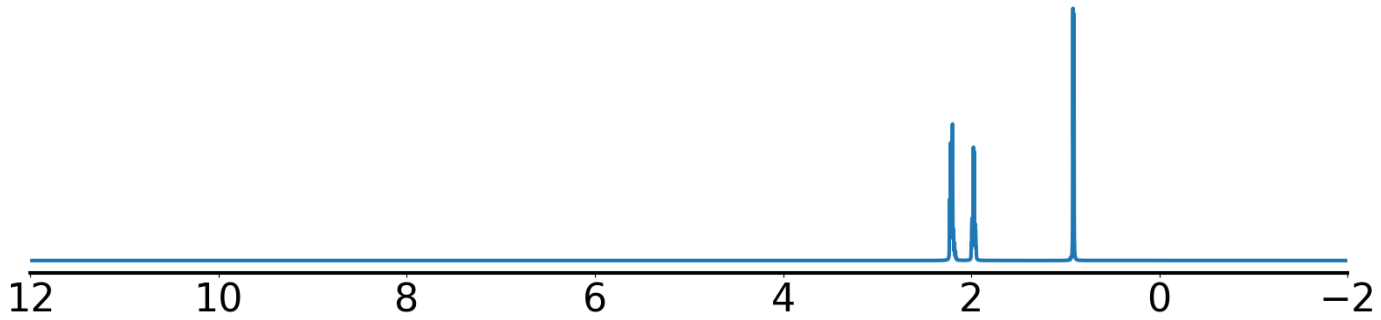
Example 28 true smiles: CC(CC(=O)O)CC(=O)O formula: C6H10O4
Index of correct structure: 0 of 19323
True structure loss: 0.027036
True structure:



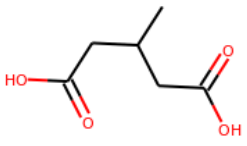
Experimental 13C NMR (solvent: CDCl3)



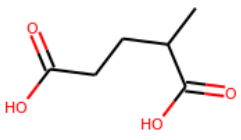
Experimental 1H NMR (solvent: D2O)



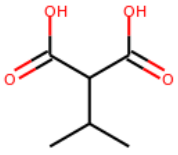
Top predicted structures (loss):



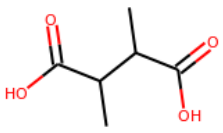
0.027036



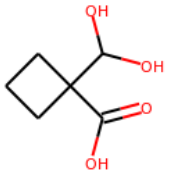
0.05023



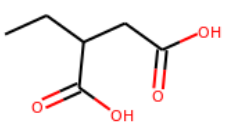
0.050384



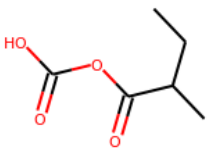
0.053722



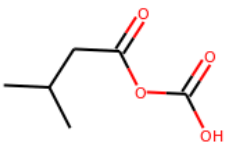
0.058615



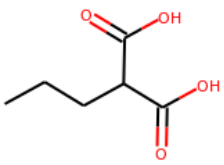
0.060752



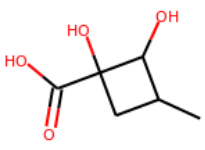
0.062412



0.064204



0.066972



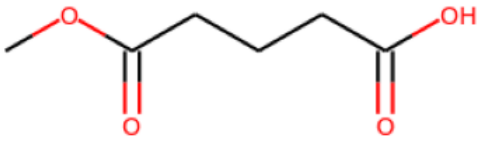
0.06846

Top predicted substructures	prob		
[OX2H1]	0.9997	[#6H3][#6][#6]	0.9977
[#8]=[#6][#8]	0.9996	[#6H1]	0.9973
[CX3](=[OX1])C	0.9993	[CX4H2]([#6])[#6]	0.9785
[CX3](=O)[OX2H1]	0.9991	[CX4H3]	0.9692
[CX3](=[OX1])O	0.9989	[#8][#6H0][#6H1]	0.8976

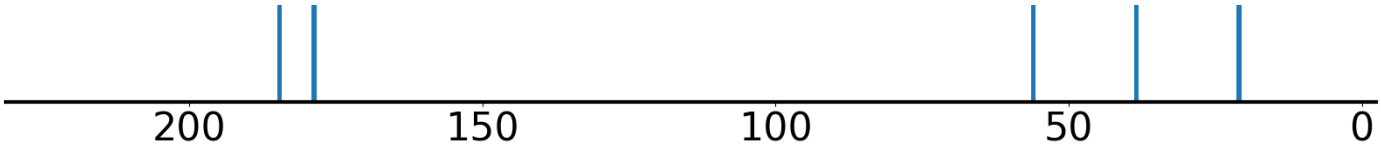
best positives	prob	best negatives	prob
[OX2H1]	0.9997	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8]=[#6][#8]	0.9996	CCC=CC#C	0.0
[CX3](=[OX1])C	0.9993	CC#CCC=C	0.0
[CX3](=O)[OX2H1]	0.9991	CC=CC#CC	0.0
[CX3](=[OX1])O	0.9989	[CX2H0](#[CX2H1])[CX3H1]	0.0
[#6H3][#6][#6]	0.9977	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#6H1]	0.9973	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H2]([#6])[#6]	0.9785	C=CC=CC#C	0.0
[CX4H3]	0.9692	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][#6]	0.8892	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.8976	[#6H1]([#6H2])[#6H2]	0.0805
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.8575	[CX4H2]([CX4H1])[CX3H0]	0.1352
OCC[CH2]	0.7204	[#8]=[#6][#6H2][#6H1]	0.2174
[#6H1][#6H1]	0.5838	[CX4H1]([CX4H3])([CX4H2])[CX4H2]	0.2215
[CX4H2]CC=O	0.5367	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2762
O=[CX3][CX4H]	0.5217	O=[CX3H0][CX4H2][CX4H1]	0.3053
[CH3]CC[OH]	0.4633	[CX4H2][CX3]=O	0.4156
[#8]=[#6H0][#6H1]	0.4464	[#8][#6][#6H2]	0.4676
[#8]=[#6][#6H1][#6H1]	0.2848	[CHX4]([CH3X4])[CH2X4]	0.6297
[#8][#6][#6][#6][#6]=[#8]	0.2233	[#6X3][#6][#6][#6H3]	0.7351

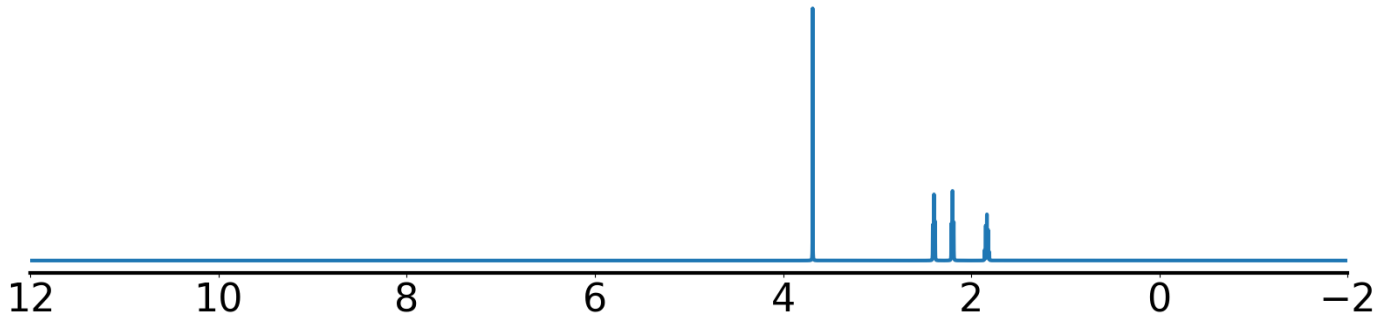
Example 29 true smiles: COC(=O)CCCC(=O)O formula: C6H10O4
Index of correct structure: 0 of 19323
True structure loss: 0.011848
True structure:



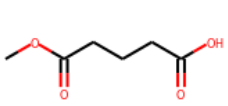
Experimental 13C NMR (solvent: CDCl3)



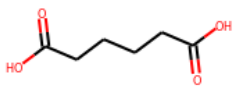
Experimental 1H NMR (solvent: d2o)



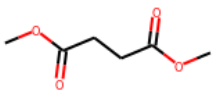
Top predicted structures (loss):



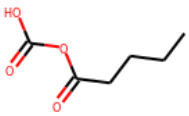
0.011848



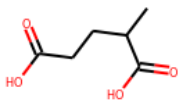
0.029618



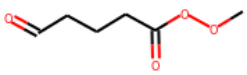
0.031528



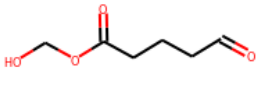
0.034056



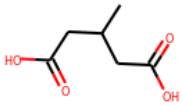
0.048556



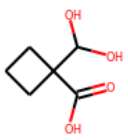
0.049282



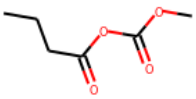
0.050412



0.050809



0.055695



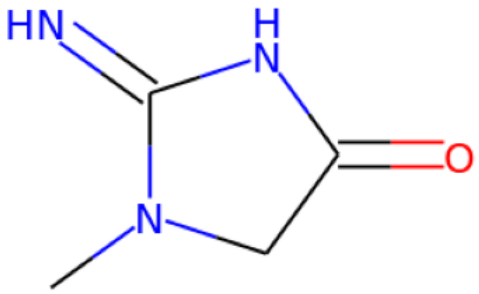
0.055804

Top predicted substructures	prob		
[CX3](=[OX1])C	1.0	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9786
[#8]=[#6][#8]	0.9999	[OX2H1]	0.9713
[CX3](=[OX1])O	0.9998	[CX4H3]	0.9612
[CX4H2]([#6])[#6]	0.9994	[CX3](=O)[OX2H1]	0.9606
OCC[CH2]	0.9793	[CX4H2]CC=O	0.9045

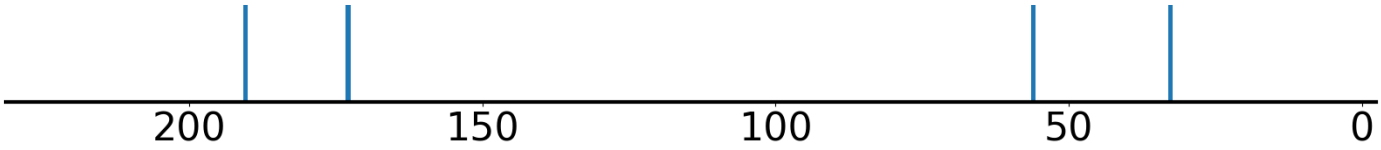
best positives	prob	best negatives	prob
[CX3](=[OX1])C	1.0	CCC#CC#C	0.0
[#8]=[#6][#8]	0.9999	C=CC=CC#C	0.0
[CX3](=[OX1])O	0.9998	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9994	[CX2H0](#[CX2H1])[cX3H0]	0.0
OCC[CH2]	0.9793	[#6X2][#6H1][#6X2]	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9786	CC#CCC#C	0.0
[OX2H1]	0.9713	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3]	0.9612	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=O)[OX2H1]	0.9606	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2]CC=O	0.9045	CC=CC#CC	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.7252	[OX2H0][CX3H0][CX4H2]	0.4948
[#8]=[#6H0][#6H1]	0.6052	[CX4H2]([CX4H2])[CX4H2]	0.577
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.4646	[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.5975
[#6H1]	0.375	[#8][#6][#6H2]	0.6469
[#8][#6][#6][#6][#6]=[#8]	0.3241	[CX4H2]([CX4H2])[CX3H0]	0.696
[#6H1][#6H2]	0.231	[CX4H2][CX4H2]	0.7094
O=[CX3][CX4H]	0.2265	[CX4H3][OX2H0]	0.8011
O=[CX3H0][CX4H2][CX4H1]	0.217	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.8159
[CX4H3][#6]	0.2016	O=[CX3H0][CX4H2][CX4H2]	0.8435
[#8][#6][#6][#6X3]	0.1879	[CX4H2][CX3]=O	0.8545

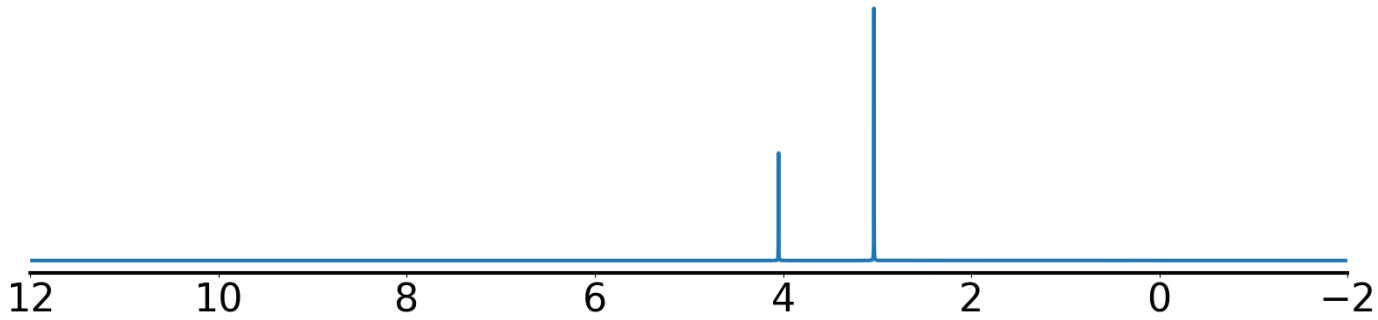
Example 30 true smiles: CN1CC(=O)NC1=N formula: C4H7N3O
Index of correct structure: 0 of 16898
True structure loss: 0.02136
True structure:



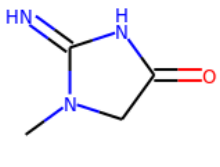
Experimental 13C NMR (solvent: DMSO)



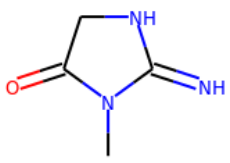
Experimental 1H NMR (solvent: D2O)



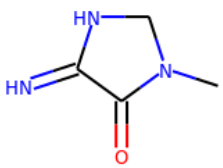
Top predicted structures (loss):



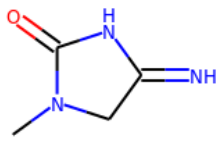
0.02136



0.028479

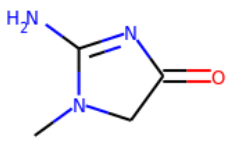


0.030813

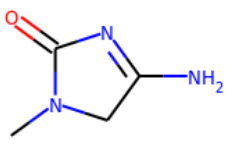


0.031246

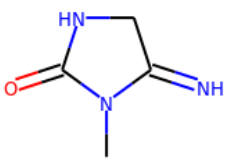
0.032402



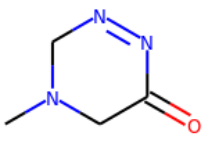
0.032854



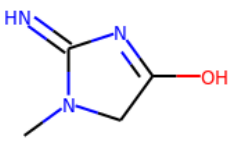
0.035052



0.035694



0.036352



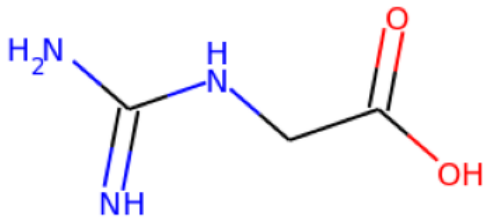
0.036589

Top predicted substructures	prob		
[#7][#6H0]=[#7]	0.9591	[#7X3][#6H3]	0.9161
[#7][#6][#6X3]	0.9489	[#6]=[#7H]	0.9137
[CX4H3]	0.9448	[#6X3][#6H2][#7]	0.8906
[#6H3][#7]	0.9423	[CX4H2]([NX3H0])[CX3H0]	0.879
[#7][#6]=[#7]	0.935	[#7X3][#6H2]	0.8653

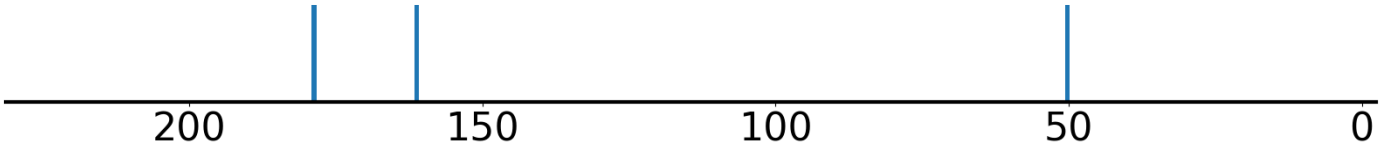
best positives	prob	best negatives	prob
[#7][#6H0]=[#7]	0.9591	[#8]1[#6][#6]=[#6][#6]=[#6]1	0.0
[#7][#6][#6X3]	0.9489	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H3]	0.9448	[OX2H0][CX3H1]=[#6X3H0][#8X2H0]	0.0
[#6H3][#7]	0.9423	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[#7][#6]=[#7]	0.935	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#7X3][#6H3]	0.9161	[CX3H2]=[CX3H1][CX4H1]([CX4H1])[OX2H0]	0.0
[#6]=[#7H]	0.9137	[CX3H2]=[CX3H1][CX4H0][OX2H1]	0.0
[#6X3][#6H2][#7]	0.8906	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[CX4H2]([NX3H0])[CX3H0]	0.879	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7X3][#6H2]	0.8653	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#7][#6][#6][#6X3]	0.3453	[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.1109
[#6H1]	0.2854	[#6X3][#7][#6X3]	0.116
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.2757	[#6]1[#6][#7][#6][#7]1	0.2475
[#7H2][#6H0]	0.2753	[#6X3][#7X3][#6X3]	0.2662
[#7X3H2]	0.2702	[#7][#6][#6][#7]	0.473
[#6X3][#6X3]	0.2385	[NH1][#6][#7]	0.5192
[#7][#6H0][#6H1]	0.2225	[CX4H2][CX3]=O	0.5537
[#7][#6][#6][#6][#7]	0.1786	[#7X3H1]	0.5837
O=[#6][#6][#6X3]	0.1695	[#6H3][#7][#6H2]	0.6003
[CX4H2]([#6])[#6]	0.1665	[CX4H3][NX3H0]	0.656

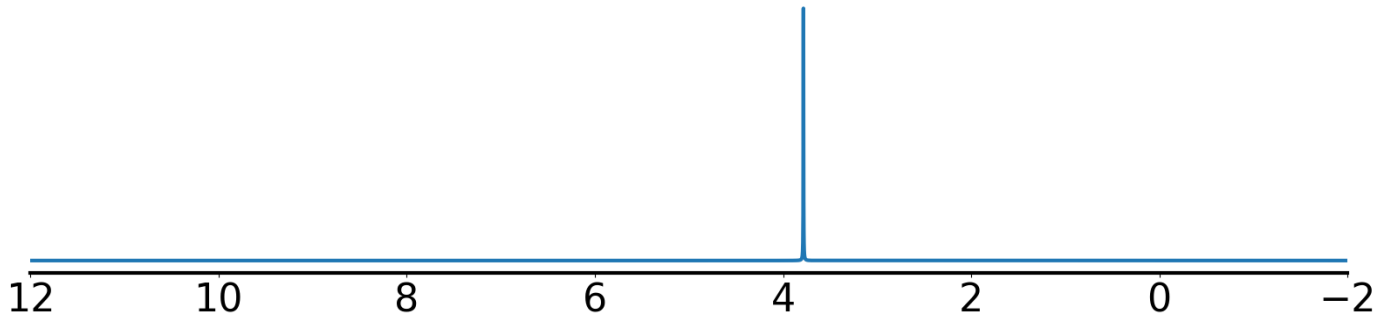
Example 31 true smiles: N=C(N)NCC(=O)O formula: C3H7N3O2
Index of correct structure: 6 of 15726
True structure loss: 0.026552
True structure:



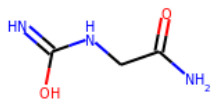
Experimental 13C NMR (solvent: D2O)



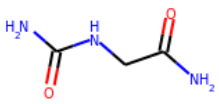
Experimental 1H NMR (solvent: D2O)



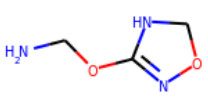
Top predicted structures (loss):



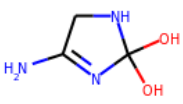
0.020384



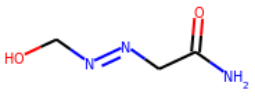
0.021752



0.026122

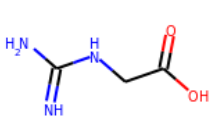


0.026445

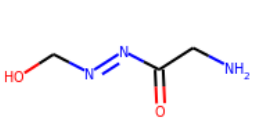


0.026499

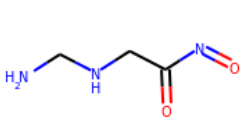
0.026551



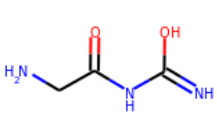
0.026552



0.027227



0.027468



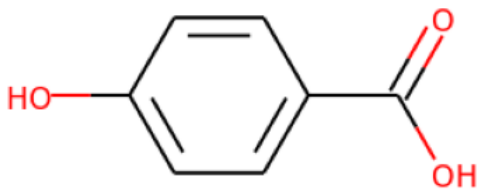
0.027487

Top predicted substructures	prob		
[#7][#6H2]	0.9313	[#7][#6H0][#7]	0.742
[#7X3H2]	0.9283	[#7][#6H0]=[#7]	0.7324
[#7X3][#6H2]	0.856	[#7][#6][#6X3]	0.7294
[CX3](=[OX1])C	0.8397	[#7][#6]=[#7]	0.6917
[#6X3][#6H2][#7]	0.82	[CX4H2]([NX3H1])[CX3H0]	0.6779

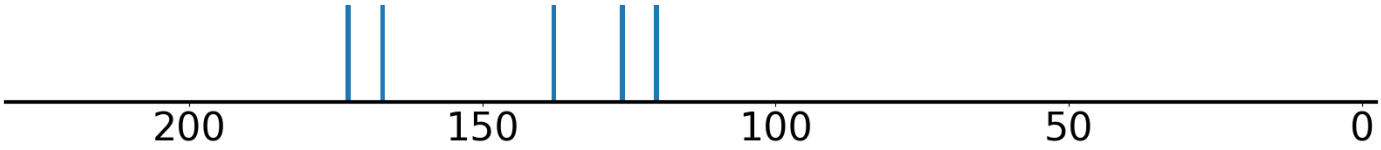
best positives	prob	best negatives	prob
[#7][#6H2]	0.9313	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7X3H2]	0.9283	C=CCCC#C	0.0
[#7X3][#6H2]	0.856	CC=CCC#C	0.0
[CX3](=[OX1])C	0.8397	CCC=CC#C	0.0
[#6X3][#6H2][#7]	0.82	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7][#6H0][#7]	0.742	[CX2H0](#[CX2H1])[CX4H1]	0.0
[#7][#6H0]=[#7]	0.7324	[#6X2][#6H1][#6X2]	0.0
[#7][#6][#6X3]	0.7294	CC#CCC#C	0.0
[#7][#6]=[#7]	0.6917	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2]([NX3H1])[CX3H0]	0.6779	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0

worst negatives	prob	worst positives	prob
[#7][#6][#6][#7]	0.4249	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1549
[#7H2][#6H2]	0.4205	[CX3](=O)[OX2H1]	0.1707
[CX4H3]	0.375	[OX2H1]	0.2216
[#6X3][#7X3][#6X3]	0.3605	[#7][#6]([#7])=[#7]	0.2506
[#6X3][#7][#6X3]	0.2295	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.3006
[CX4H3][OX2H0]	0.2196	[#8][#6][#6H2]	0.3498
[#7X3H0]	0.2149	[CX3](=[OX1])O	0.3662
O=[#6][#6][#6X3]	0.2102	[NH1][#6][#7]	0.37
[CX4H3][NX3H0]	0.1828	[#7][#6][#7]	0.4565
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.1801	[#8]=[#6][#8]	0.4577

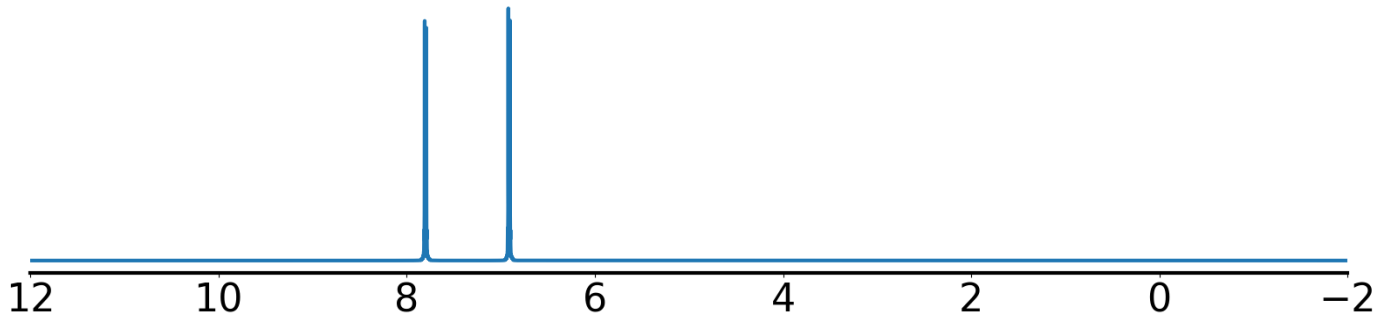
Example 32 true smiles: O=C(O)c1ccc(O)cc1 formula: C7H6O3
Index of correct structure: 0 of 15458
True structure loss: 0.015458
True structure:



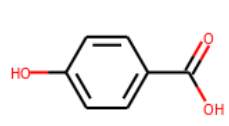
Experimental 13C NMR (solvent: D2O)



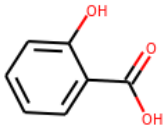
Experimental 1H NMR (solvent: D2O)



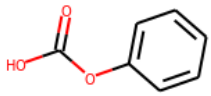
Top predicted structures (loss):



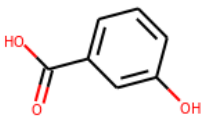
0.015458



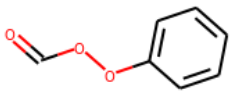
0.016028



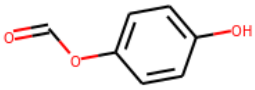
0.016751



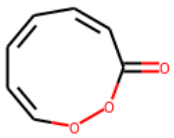
0.023018



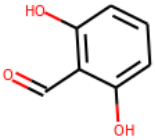
0.027588



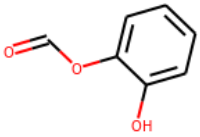
0.029742



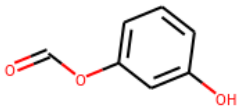
0.029754



0.030721



0.031412



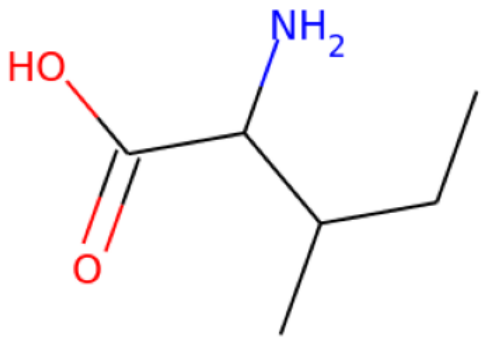
0.031722

Top predicted substructures	prob		
[#6X3][#6X3]	0.9996	[CX3](=[OX1])O	0.9809
[#6H1]	0.9994	[#6X3][#6X3][#6X3][#6X3]	0.9746
[#8]=[#6][#8]	0.995	O=[#6][#6][#6X3]	0.9355
[cH][cH]	0.9895	[cX3H1]([cX3H1])[cX3H0]	0.9325
[#6X3H1][#6X3H0]	0.9843	[cH]	0.8623

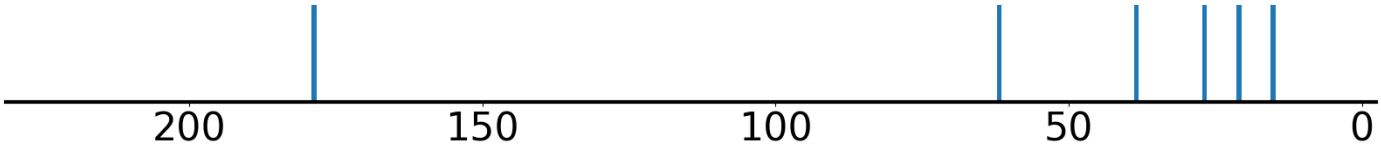
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9996	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6H1]	0.9994	[#6H3][#7][#6X4H1][#6H3]	0.0
[#8]=[#6][#8]	0.995	[#6H3][#6H0][#7][#6H3]	0.0
[cH][cH]	0.9895	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9843	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[CX3](=[OX1])O	0.9809	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9746	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
O=[#6][#6][#6X3]	0.9355	[CX4H2]([NX3H0])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9325	[CX4H1]([NX3H2])([CX4H2])[CX4H0]	0.0
[cH]	0.8623	[#8][#6H1][#6H2][#6H1]=[#8]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.7692	[#6]1[#6][#6][#6][#6][#6]1	0.4336
[CX3](=[OX1])C	0.5981	[OX2H][cX3]:[c]	0.4412
[#8]=[#6H0][#6H1]	0.5847	[cX3H0][cX3H1][cX3H1][cX3H0]	0.5008
[OX1H0]=[cX3H0][cX3H1]	0.5116	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5032
O=[cX3]	0.4958	[cH]cO	0.5104
[#8][#6][#6]=[#6X3]	0.3654	[CX3](=O)[OX2H1]	0.7037
[#8]=[#6][#6H1][#6H1]	0.295	[OX2H1]	0.7737
[#8]=[#6][#6H1]=[#6H1]	0.2343	[#6H1][#6H1]	0.7992
[#8][#6H1][#6H1]	0.1717	[#8][#6][#6][#6X3]	0.8104
[#8][#6][#6]=[#6][#6]=[#8]	0.164	[#8][#6H0][#6H1]	0.8359

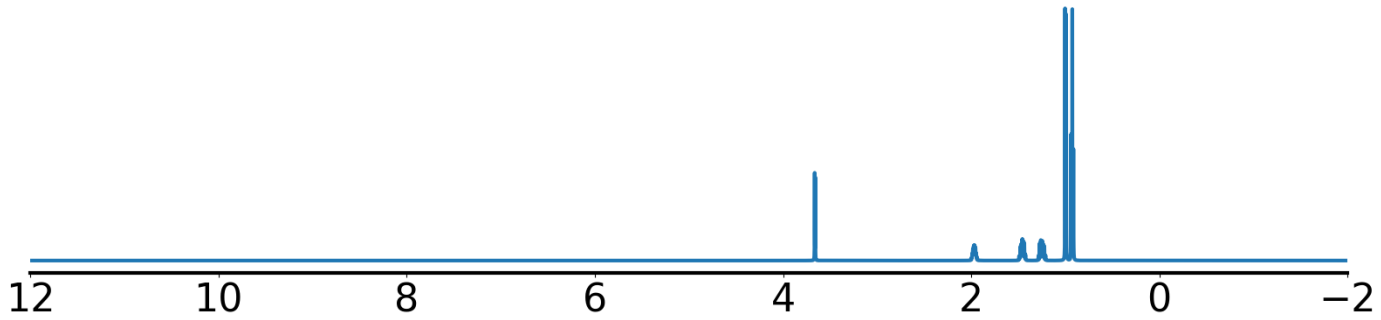
Example 33 true smiles: CCC(C)C(N)C(=O)O formula: C6H13NO2
Index of correct structure: 0 of 14628
True structure loss: 0.020782
True structure:



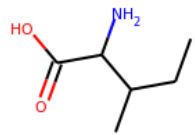
Experimental 13C NMR (solvent: D2O)



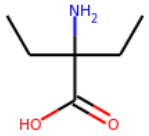
Experimental 1H NMR (solvent: #N/A)



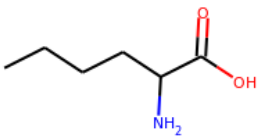
Top predicted structures (loss):



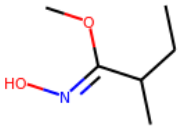
0.020782



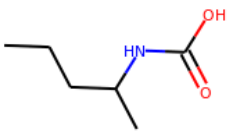
0.032973



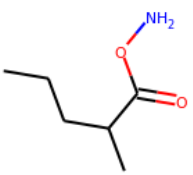
0.035784



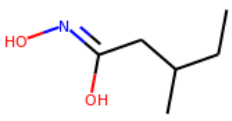
0.038178



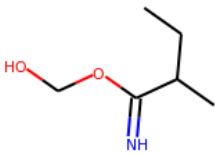
0.040487



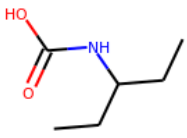
0.04087



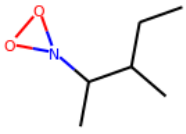
0.041271



0.041349



0.041494



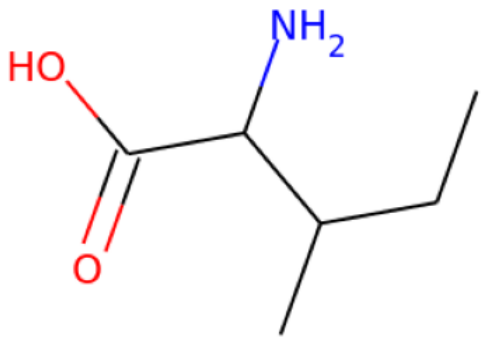
0.042415

Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][CX4H2]	0.9696
[#6H3][#6][#6]	0.9993	[OX2H1]	0.951
[CX4H3][#6]	0.9978	[#6H1]	0.9104
[CX4H2]([#6])[#6]	0.9951	[#6H1][#6H2]	0.8587
[CX3](=[OX1])C	0.9701	[CX4H3][CX4H1]	0.8132

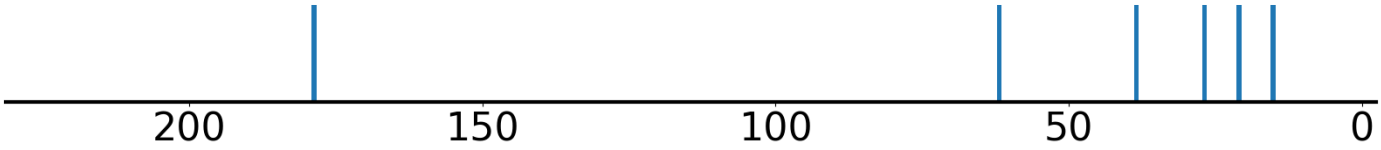
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9993	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9978	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	0.9951	C=CCCC#C	0.0
[CX3](=[OX1])C	0.9701	CC=CC#CC	0.0
[CX4H3][CX4H2]	0.9696	CCC=CC#C	0.0
[OX2H1]	0.951	CC#CCC=C	0.0
[#6H1]	0.9104	CC#CCC#C	0.0
[#6H1][#6H2]	0.8587	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][CX4H1]	0.8132	[CX2H0](#[CX2H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
OCC[CH2]	0.6286	[#6H1][#6H1]	0.1391
[CX4H2]CC=O	0.5128	[CX4H1]([CX4H3])([CX4H2])[CX4H1]	0.2299
[#7H2][#6H0]	0.3307	[#7H2][#6X4H1][#6X3]	0.2724
[CX4H2]([CX4H3])[CX4H2]	0.3005	[#6H3][#6H1][#6H1][#7]	0.28
[CX4H2][CX3]=O	0.2648	[#8][#6H0][#6H1]	0.3544
[#7][#6H0][#6H1]	0.2337	[#7H2][#6H1]	0.4785
[#6H3][#6][#6X3]	0.2278	[#6H3][#6][#6][#6H3]	0.5045
[CX4H2]([CX4H2])[CX4H1]	0.2163	[#8]=[#6][#6H1][#6H1]	0.5385
[#7X3H1]	0.2044	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5623
[CX4H2][CX4H2]	0.1429	[CX4H2]([CX4H3])[CX4H1]	0.568

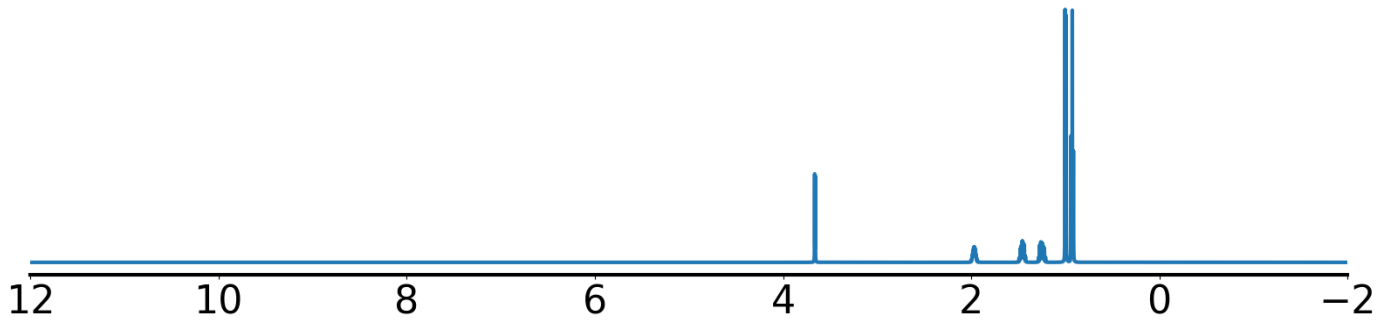
Example 34 true smiles: CCC(C)C(N)C(=O)O formula: C6H13NO2
Index of correct structure: 0 of 14628
True structure loss: 0.020715
True structure:



Experimental 13C NMR (solvent: D2O)

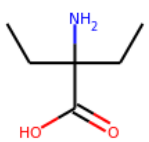


Experimental 1H NMR (solvent: d2o)

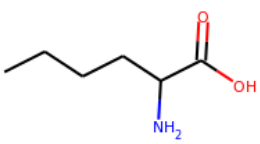


Top predicted structures (loss):

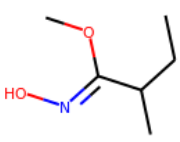
0.020715



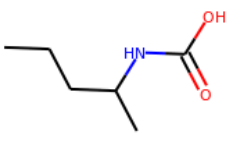
0.03305



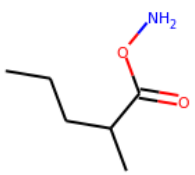
0.035674



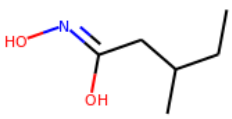
0.038283



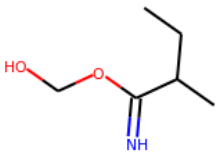
0.040448



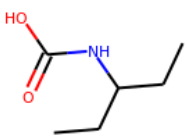
0.040841



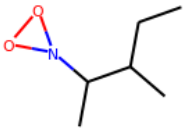
0.041151



0.04141



0.041454



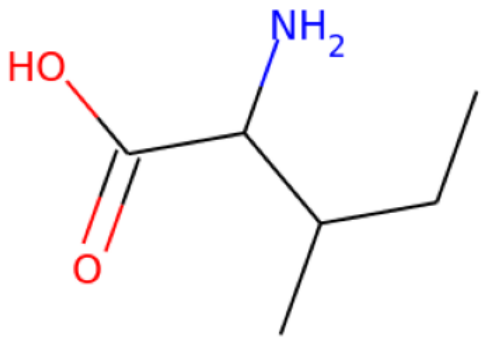
0.042373

Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][CX4H2]	0.9698
[#6H3][#6][#6]	0.9993	[OX2H1]	0.951
[CX4H3][#6]	0.9978	[#6H1]	0.912
[CX4H2]([#6])[#6]	0.9952	[#6H1][#6H2]	0.8584
[CX3](=[OX1])C	0.9698	[CX4H3][CX4H1]	0.8102

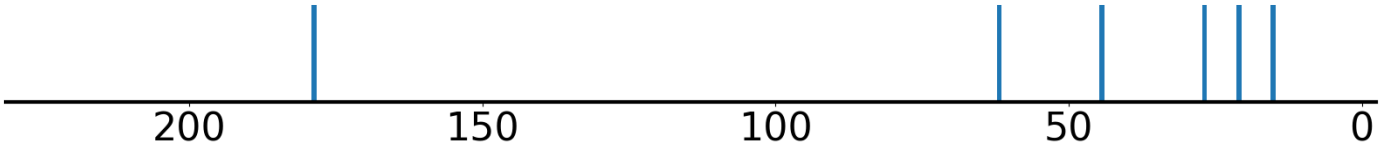
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9993	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9978	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	0.9952	C=CCCC#C	0.0
[CX3](=[OX1])C	0.9698	CC=CC#CC	0.0
[CX4H3][CX4H2]	0.9698	CCC=CC#C	0.0
[OX2H1]	0.951	CC#CCC=C	0.0
[#6H1]	0.912	CC#CCC#C	0.0
[#6H1][#6H2]	0.8584	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][CX4H1]	0.8102	[CX2H0](#[CX2H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
OCC[CH2]	0.6303	[#6H1][#6H1]	0.1428
[CX4H2]CC=O	0.5085	[CX4H1]([CX4H3])([CX4H2])[CX4H1]	0.2332
[#7H2][#6H0]	0.3281	[#6H3][#6H1][#6H1][#7]	0.2782
[CX4H2]([CX4H3])[CX4H2]	0.2986	[#7H2][#6X4H1][#6X3]	0.2805
[CX4H2][CX3]=O	0.2681	[#8][#6H0][#6H1]	0.3512
[#7][#6H0][#6H1]	0.2309	[#7H2][#6H1]	0.488
[#6H3][#6][#6X3]	0.2298	[#6H3][#6][#6][#6H3]	0.5034
[CX4H2]([CX4H2])[CX4H1]	0.2201	[#8]=[#6][#6H1][#6H1]	0.542
[#7X3H1]	0.206	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5655
[CX4H2][CX4H2]	0.1459	[CX4H2]([CX4H3])[CX4H1]	0.5706

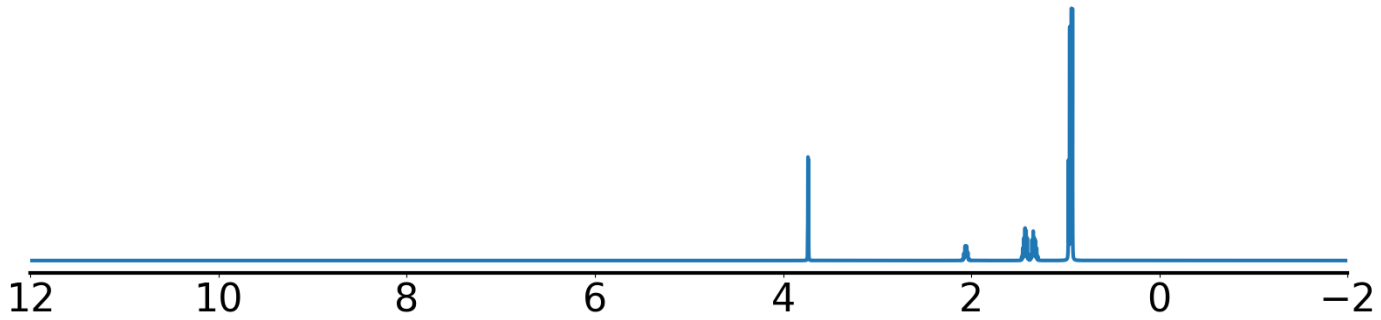
Example 35 true smiles: CCC(C)C(N)C(=O)O formula: C6H13NO2
Index of correct structure: 0 of 14628
True structure loss: 0.021957
True structure:



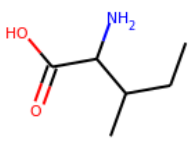
Experimental 13C NMR (solvent: D2O)



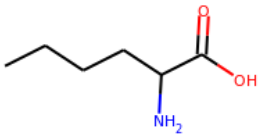
Experimental 1H NMR (solvent: D2O)



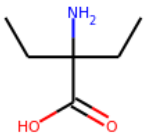
Top predicted structures (loss):



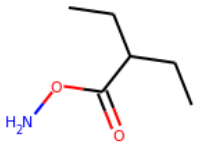
0.021957



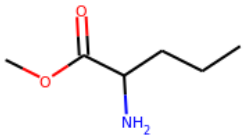
0.032026



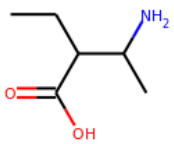
0.033232



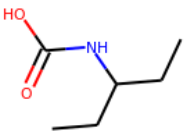
0.037734



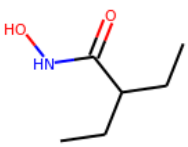
0.039877



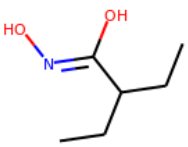
0.043138



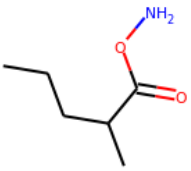
0.044492



0.044893



0.047251



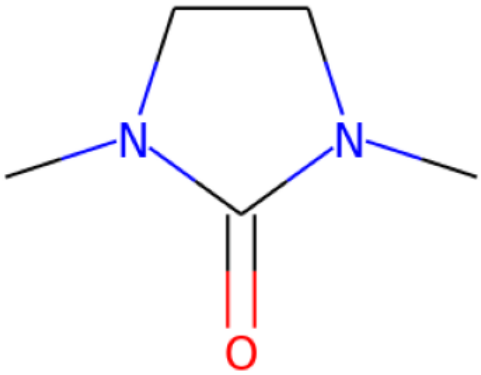
0.047937

Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H2]([#6])[#6]	0.9859
[#6H3][#6][#6]	0.9996	O=[CX3][CX4H]	0.9175
[CX4H3][#6]	0.9987	[#7X3H2]	0.8853
[CX4H3][CX4H2]	0.9974	[OX2H1]	0.8583
[CX3](=[OX1])C	0.9872	[#8]=[#6][#8]	0.8435

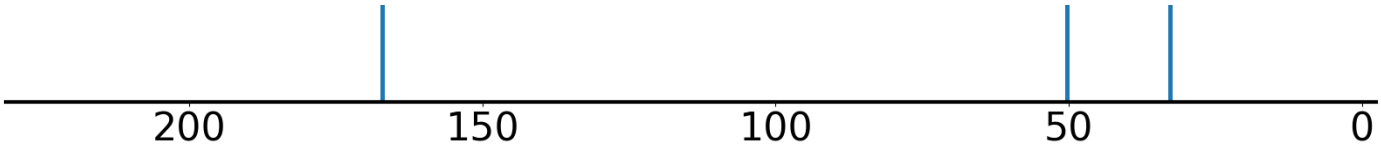
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9996	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][#6]	0.9987	C=CC=CC#C	0.0
[CX4H3][CX4H2]	0.9974	CC=CC#CC	0.0
[CX3](=[OX1])C	0.9872	C=CCCC#C	0.0
[CX4H2]([#6])[#6]	0.9859	CCC=CC#C	0.0
O=[CX3][CX4H]	0.9175	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7X3H2]	0.8853	CC#CCC=C	0.0
[OX2H1]	0.8583	[CX2H0](#[CX2H1])[CX3H1]	0.0
[#8]=[#6][#8]	0.8435	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[CX4H2]CC=O	0.611	[#6H1][#6H1]	0.093
OCC[CH2]	0.5543	[CX4H1]([CX4H3])([CX4H2])[CX4H1]	0.1567
[CX4H2]([CX4H3])[CX4H2]	0.5193	[#6H3][#6][#6][#6H3]	0.2537
[#7H2][#6H0]	0.3486	[#6H3][#6H1][#6H1][#7]	0.369
[#7][#6H0][#6H1]	0.2973	[CX4H3][CX4H1]	0.3748
[CX4H2][CX3]=O	0.2736	[#8][#6H0][#6H1]	0.4466
[CX4H2][CX4H2]	0.263	[#7H2][#6H1]	0.4537
[#7X3H1]	0.2456	[CHX4]([CH3X4])[CH2X4]	0.5275
[#8][#6][#6H2]	0.2017	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6592
[#8][#6][#6][#6X3]	0.1416	[#7H2][#6X4H1][#6X3]	0.6768

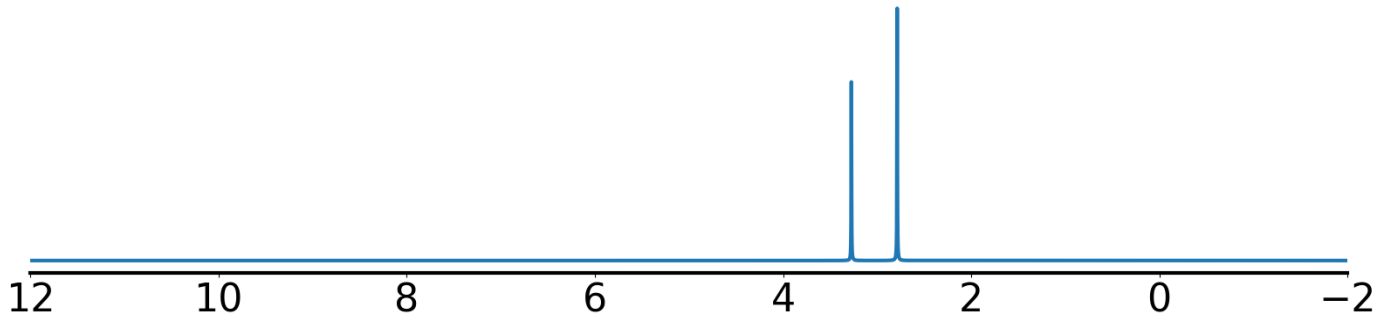
Example 36 true smiles: CN1CCN(C)C1=O formula: C5H10N2O
Index of correct structure: 0 of 14072
True structure loss: 0.02034
True structure:



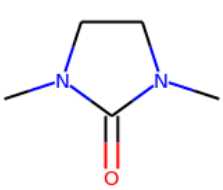
Experimental 13C NMR (solvent: CDCl3)



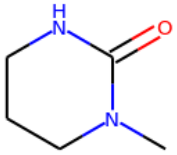
Experimental 1H NMR (solvent: CDCl3)



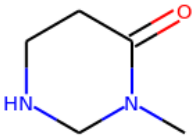
Top predicted structures (loss):



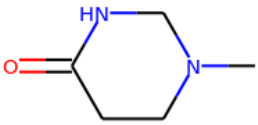
0.02034



0.024699

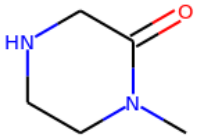


0.027254

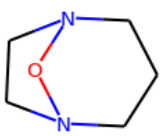


0.027517

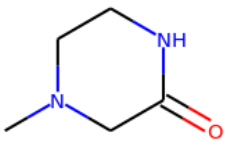
0.029084



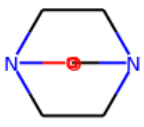
0.029595



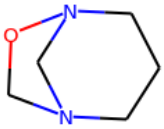
0.031556



0.031675



0.032324



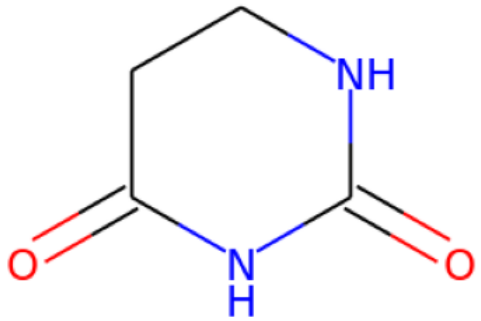
0.032494

Top predicted substructures	prob		
[#7X3][#6H2]	0.968	[CX4H2][CX4H2]	0.818
[#7][#6H2]	0.9601	[#6H2][#7][#6X3]	0.7848
[#7][#6H2][#6H2]	0.9204	[#6H3][#7][#6X3]	0.7758
[#7X3][#6H3]	0.8688	[CX4H2]([NX3H0])[CX4H2]	0.7597
[#6H3][#7]	0.8488	[#7X3H0]	0.7487

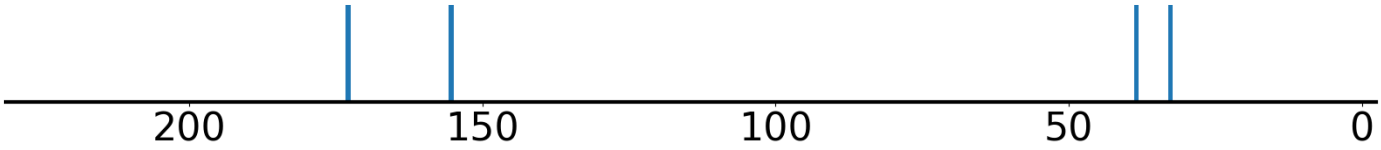
best positives	prob	best negatives	prob
[#7X3][#6H2]	0.968	C=CC=CC#C	0.0
[#7][#6H2]	0.9601	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7][#6H2][#6H2]	0.9204	[CX2H1]#[CX2H0][CX4H1][OX2H1]	0.0
[#7X3][#6H3]	0.8688	C=CCCC#C	0.0
[#6H3][#7]	0.8488	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2][CX4H2]	0.818	CC=CC#CC	0.0
[#6H2][#7][#6X3]	0.7848	CCC=CC#C	0.0
[#6H3][#7][#6X3]	0.7758	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H2]([NX3H0])[CX4H2]	0.7597	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#7X3H0]	0.7487	[CX4H2]([CX4H3])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7X3H1]	0.6854	[#6]1[#6][#7][#6][#7]1	0.2071
[CX4H2]([CX4H2])[CX3H0]	0.5299	[#7][#6H0][#7]	0.4379
[CX4H2][CX3]=O	0.5005	[#7][#6][#7]	0.4784
[CX4H2]([#6])[#6]	0.4992	[#7][#6][#6][#7]	0.5494
[CX4H2]([NX3H1])[CX4H2]	0.467	[#6H3][#7][#6H2]	0.6348
[CX3](=[OX1])C	0.4186	[CX4H3]	0.6473
[#7][#6][#6][#6X3]	0.4131	[#7][#6H2][#6H2][#7]	0.6488
[#6H2][#7][#6H2]	0.35	[#6H3][#7X3H0][#6X4H2][#6X4H2]	0.6674
[#7][#6][#6][#6][#7]	0.3382	[CX4H3][NX3H0]	0.741
[NH1][#6][#7]	0.3333	[#7X3H0]	0.7487

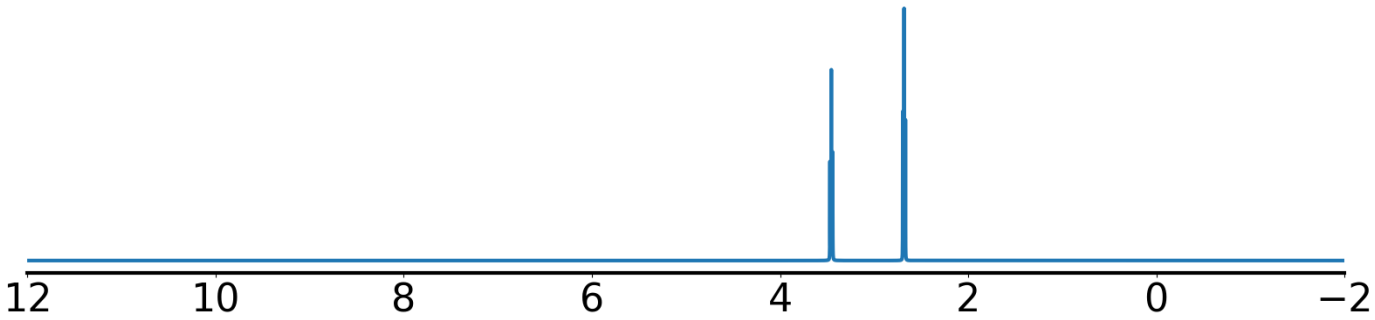
Example 37 true smiles: O=C1CCNC(=O)N1 formula: C4H6N2O2
Index of correct structure: 0 of 12102
True structure loss: 0.026577
True structure:



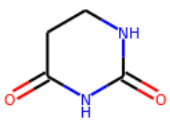
Experimental 13C NMR (solvent: DMSO)



Experimental 1H NMR (solvent: D2O)

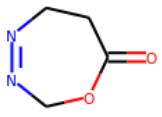


Top predicted structures (loss):



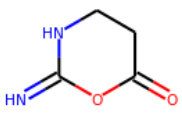
0.026577

0.036055

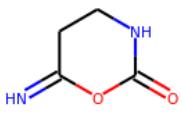


0.036253

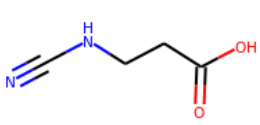
0.036614



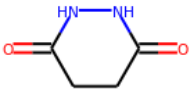
0.037828



0.03805



0.039202



0.039352

0.040693

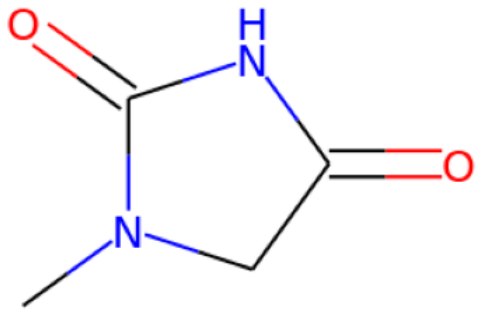
0.043407

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9954	[#7][#6H2]	0.8652
[CX4H2]([CX4H2])[CX3H0]	0.922	[CX4H2][CX3]=O	0.8137
[CX3](=[OX1])C	0.8961	[CX4H2]CC=O	0.7189
[CX4H2][CX4H2]	0.8837	[#6X3][#7X3][#6X3]	0.652
O=[CX3H0][CX4H2][CX4H2]	0.8827	[#8]=[#6][#8]	0.6518

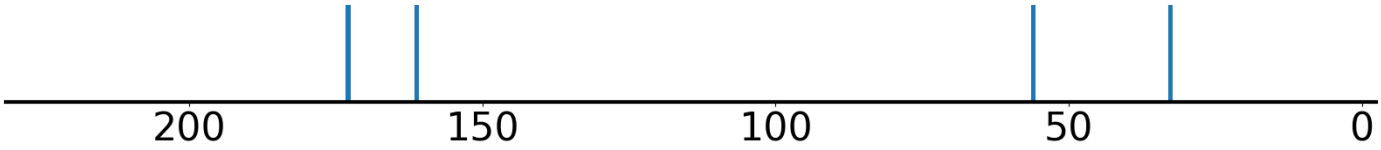
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9954	C=CC=CC#C	0.0
[CX4H2]([CX4H2])[CX3H0]	0.922	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[CX3](=[OX1])C	0.8961	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX3H1]	0.0
[CX4H2][CX4H2]	0.8837	CC=CC#CC	0.0
O=[CX3H0][CX4H2][CX4H2]	0.8827	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[#7][#6H2]	0.8652	C=CCCC#C	0.0
[CX4H2][CX3]=O	0.8137	CC=CCC#C	0.0
[CX4H2]CC=O	0.7189	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6X3][#7X3][#6X3]	0.652	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7][#6H2][#6H2]	0.6169	[CX3H1](=[CX3H2])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#8]	0.6518	[#7][#6][#6][#6][#7]	0.1724
[CX3](=[OX1])O	0.6105	[CX4H2]([NX3H1])[CX4H2]	0.1782
[#8][#6][#6H2]	0.6076	[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.2742
[#7X3H0]	0.515	[NH1][#6][#7]	0.3606
[#7][#6][#6X3]	0.5004	[#7][#6][#6][#6X3]	0.394
OCC[CH2]	0.4191	[#7X3H1]	0.4338
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.3048	[#7][#6][#7]	0.4994
[OX2H1]	0.3046	[#6X3][#7][#6X3]	0.5718
[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.2809	[#7][#6H0][#7]	0.5769
[#6H3][#7]	0.2805	[#7X3][#6H2]	0.5941

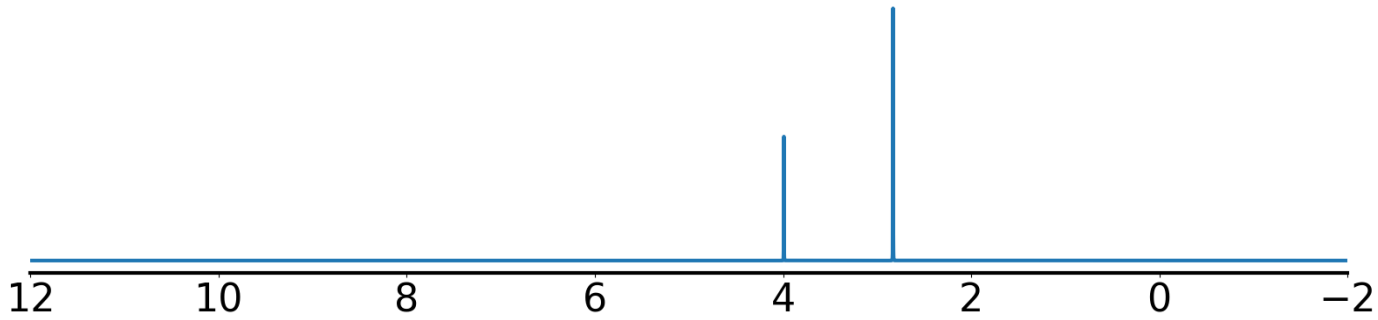
Example 38 true smiles: CN1CC(=O)NC1=O formula: C4H6N2O2
Index of correct structure: 0 of 12102
True structure loss: 0.027381
True structure:



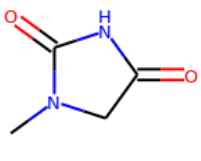
Experimental 13C NMR (solvent: DMSO-d6)



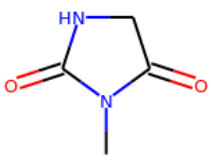
Experimental 1H NMR (solvent: D2O)



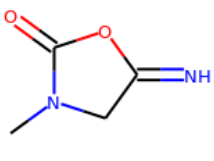
Top predicted structures (loss):



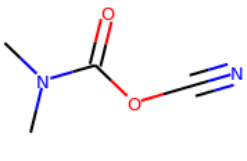
0.027381



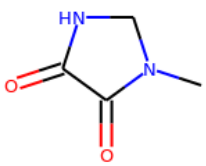
0.031975



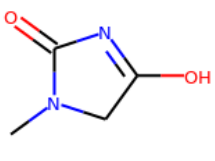
0.035806



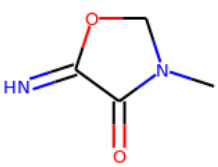
0.036366



0.037764

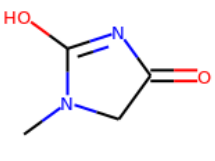


0.038849

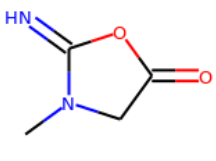


0.039835

0.041758



0.04187



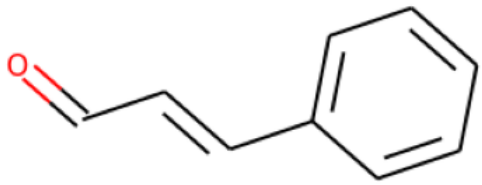
0.041875

Top predicted substructures	prob		
[#7X3][#6H3]	0.985	[CX3](=[OX1])C	0.781
[CX4H3]	0.9838	[#8]=[#6][#8]	0.7127
[#6H3][#7]	0.9497	[CX4H2]([NX3H0])[CX3H0]	0.6611
[#6H3][#7][#6X3]	0.8954	[#7][#6H0][#7]	0.6152
[#7][#6][#6X3]	0.8333	[#7][#6][#7]	0.6151

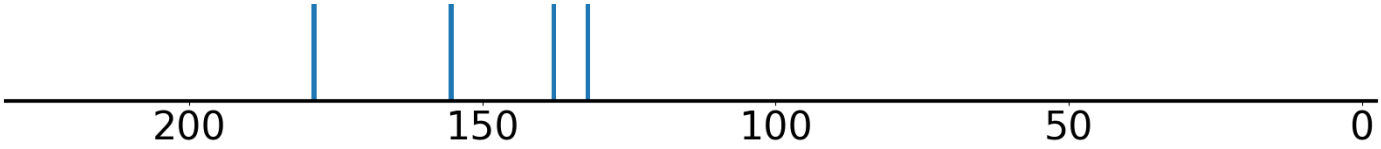
best positives	prob	best negatives	prob
[#7X3][#6H3]	0.985	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H3]	0.9838	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H3][#7]	0.9497	CC=CC#CC	0.0
[#6H3][#7][#6X3]	0.8954	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#7][#6][#6X3]	0.8333	[CX4H2]([CX4H3])[CX2H0]	0.0
[CX3](=[OX1])C	0.781	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX4H2]([NX3H0])[CX3H0]	0.6611	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[#7][#6H0][#7]	0.6152	CCC#CC=C	0.0
[#7][#6][#7]	0.6151	C=CCCC#C	0.0
[#6X3][#6H2][#7]	0.5738	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#8]	0.7127	[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.2485
O=[#6][#6][#6X3]	0.489	[#6H3][#7][#6H2]	0.3652
[CX3](=[OX1])O	0.462	[#7H1][#6H0][#7X3][#6H3]	0.3771
[#6H1]	0.3336	[#6H2][#7][#6X3]	0.3873
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.3033	[#6X3][#7][#6X3]	0.4383
[CX4H3][NX3H1]	0.3005	[#7][#6H2]	0.4448
[#6X3][#6X3]	0.2966	[NH1][#6][#7]	0.4489
[#7][#6][#6][#6X3]	0.2926	[#6X3][#7X3][#6X3]	0.4554
[#7][#6H0][#6H1]	0.2765	[CX4H3][NX3H0]	0.4566
[#8][#6][#6][#6X3]	0.2634	[CX4H2][CX3]=O	0.458

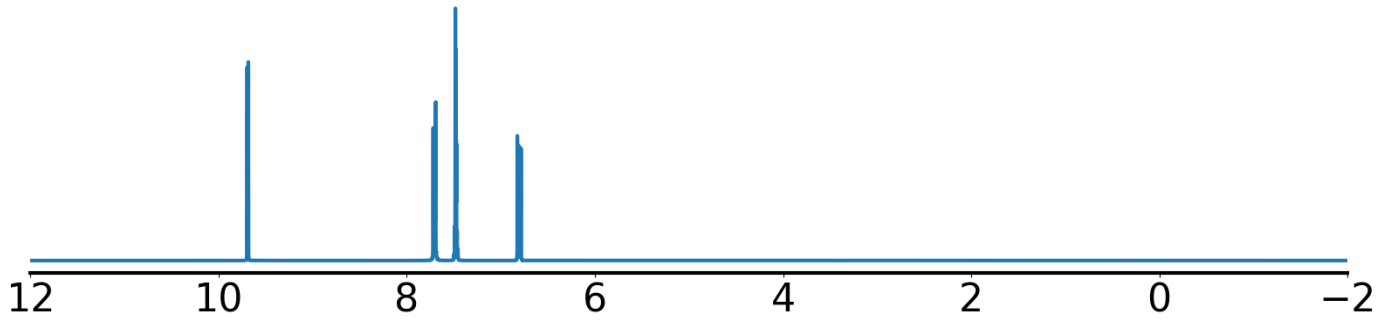
Example 39 true smiles: O=CC=Cc1ccccc1 formula: C9H8O
Index of correct structure: 1 of 10441
True structure loss: 0.026198
True structure:



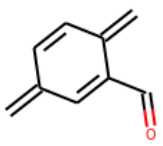
Experimental 13C NMR (solvent: CDCl3)



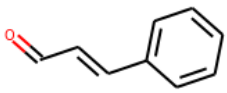
Experimental 1H NMR (solvent: MeOD)



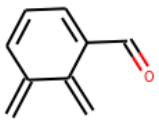
Top predicted structures (loss):



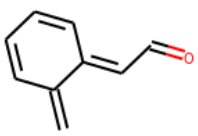
0.023761



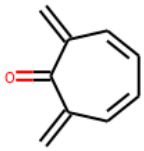
0.026198



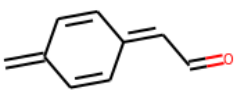
0.027599



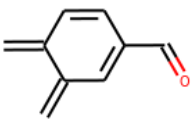
0.034457



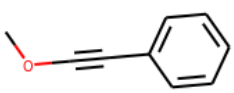
0.034579



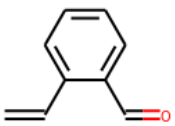
0.034709



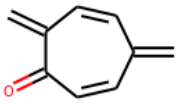
0.035367



0.041816



0.046832



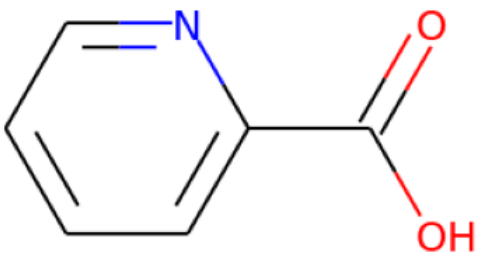
0.047059

Top predicted substructures	prob		
[#6H1]	0.9998	[#6H1][#6H1]	0.973
[#6X3][#6X3]	0.9996	[cH]	0.9162
[#6X3][#6X3][#6X3][#6X3]	0.9882	[cX3H1]([cX3H1])[cX3H0]	0.8928
[cH][cH]	0.9804	[CX3H1](=O)[#6]	0.8851
[#6X3H1][#6X3H0]	0.9793	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.8614

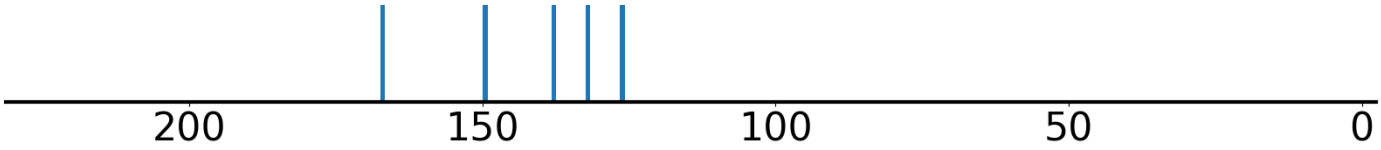
best positives	prob	best negatives	prob
[#6H1]	0.9998	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9996	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9882	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH][cH]	0.9804	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9793	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H1][#6H1]	0.973	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.9162	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8928	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[CX3H1](=O)[#6]	0.8851	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.8614	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6][#6X3]	0.4865	[#8]=[#6][#6H1]=[#6H1]	0.1025
[#8]=[#6H][#6X3][#6X3H]	0.2813	[CHX3](=C)C	0.1122
[#8]=[#6H0][#6H1]	0.1435	O=[#6][#6]=[#6X3]	0.1177
[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.1225	[CX3H1](=[CX3H1])[CX3H1]	0.1526
[#6X3]=[#6X3][#6X3]=[#6X3]	0.1159	[CX3H1](=[CX3H1])[cX3H0]	0.1569
[#8][#6H0][#6H1]	0.099	[#6X3][#6X3][#6X3]=[#6X3]	0.1891
[cX3H0][cX3H1][cX3H1][cX3H0]	0.0927	[#6X3H1]=[#6X3H1][#6X3H0][#6X3H1]	0.2076
[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.0819	[#8]=[#6H1][#6H1]	0.2111
[#8][#6][#6][#6X3]	0.08	[#8]=[#6H][#6X3]=[#6X3H]	0.2295
[cX3H0]([cX3H1])([cX3H0])[CX4H2]	0.0574	[CX3H1](=[OX1H0])[CX3H1]	0.266

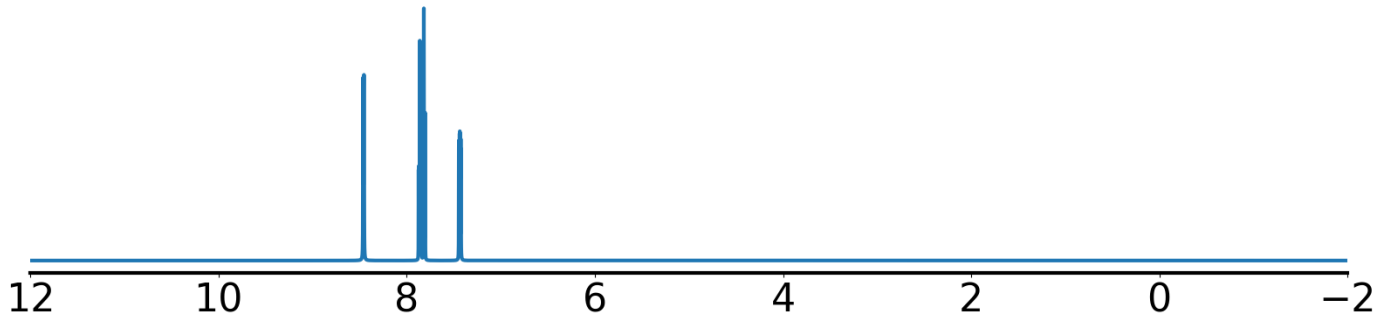
Example 40 true smiles: O=C(O)c1ccccn1 formula: C6H5NO2
Index of correct structure: 0 of 10337
True structure loss: 0.012249
True structure:



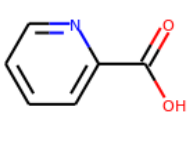
Experimental 13C NMR (solvent: DMSO)



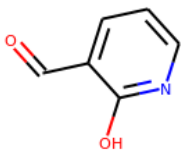
Experimental 1H NMR (solvent: D2O)



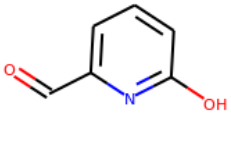
Top predicted structures (loss):



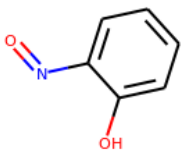
0.012249



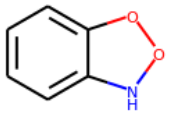
0.021685



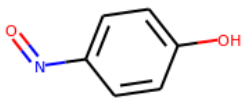
0.022058



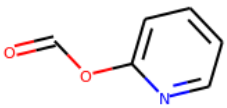
0.023854



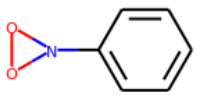
0.023959



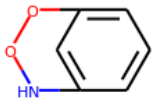
0.025189



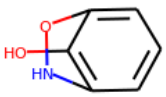
0.02572



0.026606



0.027178



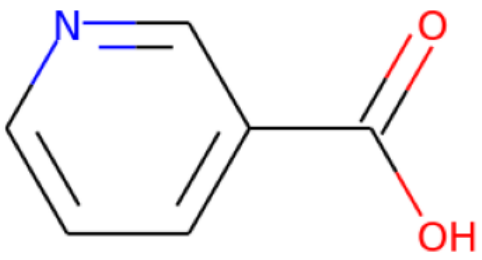
0.027365

Top predicted substructures	prob		
[#6H1]	0.9999	[#6X3H1][#6X3H0]	0.9854
[#6X3][#6X3]	0.9999	[cX3H1]([cX3H1])[cX3H0]	0.9823
[#6X3][#6X3][#6X3][#6X3]	0.9979	[#7][#6][#6X3]	0.9737
[cH][cH]	0.9959	[cX3H1]([cX3H1])[cX3H1]	0.9459
[cH]	0.9906	[#7][#6][#6][#6X3]	0.936

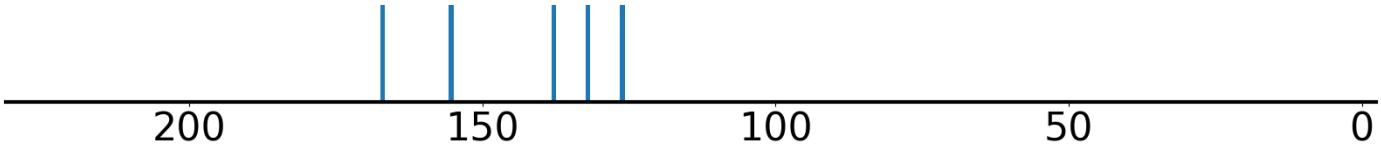
best positives	prob	best negatives	prob
[#6H1]	0.9999	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#6X3][#6X3]	0.9999	[#6H3][#7][#6X4H1][#6H3]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9979	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[cH][cH]	0.9959	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
[cH]	0.9906	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[#6X3H1][#6X3H0]	0.9854	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9823	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6][#6X3]	0.9737	[CX4H1r6][CX4H2r6][CX4H2r6][OX2H0r6]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9459	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.936	[CX3H0](=[CX3H2])([CX4H2])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6739	[CX3](=O)[OX2H1]	0.3303
[#8][#6H0][#6H1]	0.6009	[CX3](=[OX1])O	0.4173
[#8]=[#6H0][#6H1]	0.4033	[#7][#6H0][#6H1]	0.6587
[cH]cO	0.362	[#7][#6X3H0][#6X3H1]	0.6808
[OX2H][cX3]:[c]	0.2602	[#8]=[#6][#8]	0.7033
[#6]1[#6][#6][#6][#6][#6]1	0.2469	[OX2H1]	0.7728
[#8][#6H][#6X3][#6X3H]	0.2368	[#6X3][#7][#6X3]	0.792
o[cH]	0.2277	[#8][#6][#6][#6X3]	0.8158
[#8][#6H1][#6H1]	0.2194	[#6]1[#6][#6][#6][#6][#7]1	0.816
[OX1H0]=[cX3H0][cX3H1]	0.1811	[cX3H1]([nX2H0])[cX3H1]	0.834

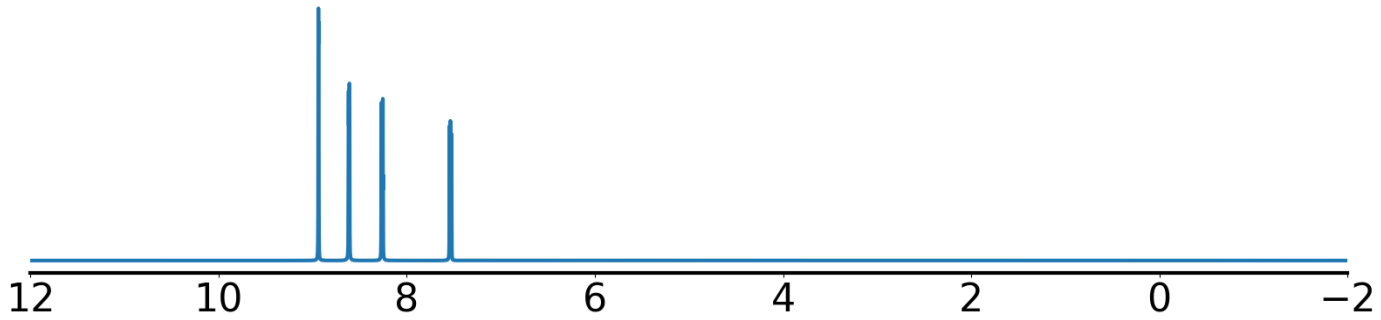
Example 41 true smiles: O=C(O)c1cccnc1 formula: C6H5NO2
Index of correct structure: -1 of 10337
True structure loss: 0.013704
True structure:



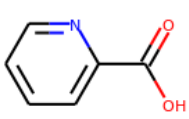
Experimental 13C NMR (solvent: DMSO-d6)



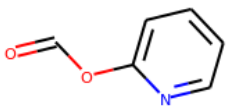
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):

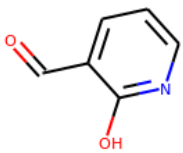


0.019113

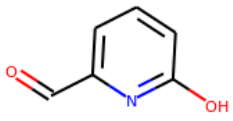


0.022086

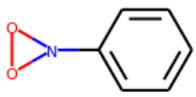
0.026728



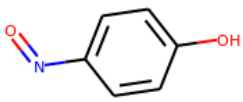
0.026819



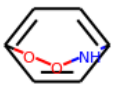
0.028933



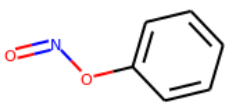
0.02929



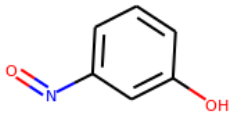
0.029411



0.030296



0.030497



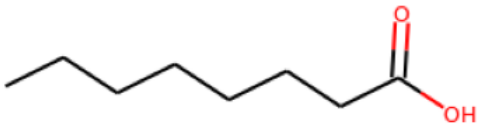
0.031821

Top predicted substructures	prob		
[#6H1]	1.0	[#6X3H1][#6X3H0]	0.9764
[#6X3][#6X3]	0.9997	[#6X3][#6X3][#6X3][#6X3]	0.9601
[#7][#6][#6][#6X3]	0.9848	[cH][cH]	0.9597
[#7][#6][#6X3]	0.9844	[#6H1][#7][#6H1]	0.8798
[cH]	0.9829	[cX3H1]([nX2H0])[cX3H0]	0.8575

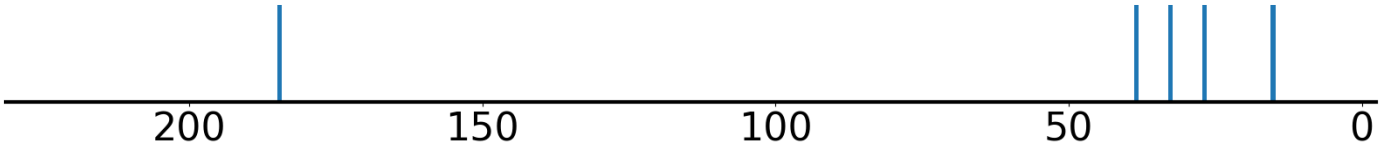
best positives	prob	best negatives	prob
[#6H1]	1.0	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9997	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.9848	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6X3]	0.9844	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[cH]	0.9829	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9764	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9601	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cH][cH]	0.9597	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H1][#7][#6H1]	0.8798	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[cX3H1]([nX2H0])[cX3H0]	0.8575	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[cH]cO	0.4969	[CX3](=O)[OX2H1]	0.0398
[#7][#6H0][#6H1]	0.429	[OX2H1]	0.4263
[#8][#6H0][#6H1]	0.4127	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6266
[#7][#6X3H0][#6X3H1]	0.357	[#6]1[#6][#6][#6][#6][#7]1	0.6847
[#6]1[#6][#6][#6][#6][#6]1	0.3183	[cX3H1]([nX2H0])[cX3H1]	0.6865
[OX2H][cX3]:[c]	0.2553	O=[#6][#6][#6X3]	0.6931
O=[cX3]	0.168	[#8]=[#6][#8]	0.7289
[#7H][#6X3H1]	0.1393	[#6H1][#6H1]	0.7302
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.1244	[CX3](=[OX1])O	0.7675
o[cH]	0.1183	[cX3H1]([cX3H1])[cX3H1]	0.7856

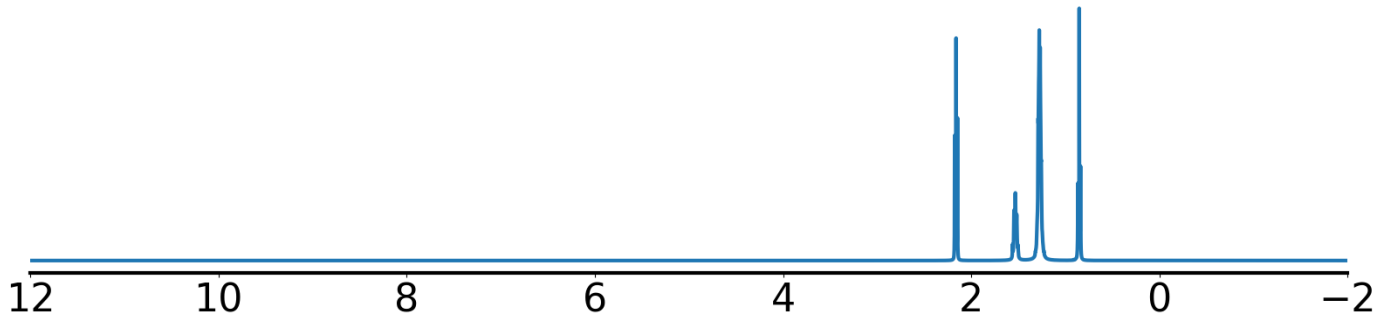
Example 42 true smiles: CCCCCCCC(=O)O formula: C8H16O2
Index of correct structure: 0 of 9984
True structure loss: 0.006326
True structure:



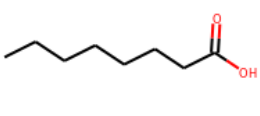
Experimental 13C NMR (solvent: CDCl3)



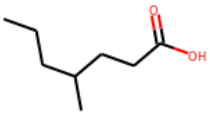
Experimental 1H NMR (solvent: D2O)



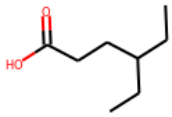
Top predicted structures (loss):



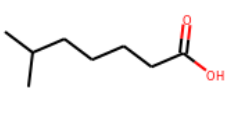
0.006326



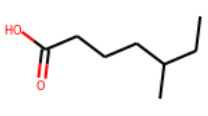
0.024303



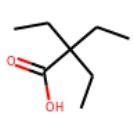
0.027016



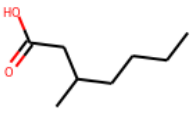
0.028162



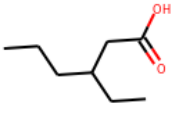
0.030015



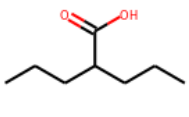
0.036825



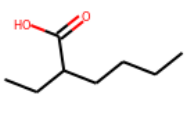
0.044071



0.044708



0.045575



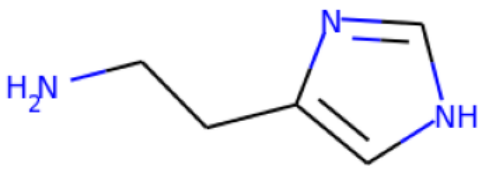
0.049083

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9999	[CX4H3]	0.9986
[#6H3][#6][#6]	0.9999	[CX3](=O)[OX2H1]	0.9972
[CX4H3][#6]	0.9996	[CX3](=[OX1])O	0.9763
[CX4H3][CX4H2]	0.999	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9679
[CX3](=[OX1])C	0.9987	[OX2H1]	0.9673

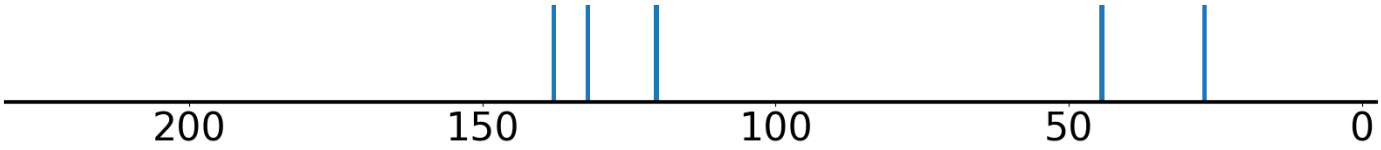
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H3][#6][#6]	0.9999	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][#6]	0.9996	[#6X2][#6H1][#6X2]	0.0
[CX4H3][CX4H2]	0.999	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9987	CC#CCC#C	0.0
[CX4H3]	0.9986	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=O)[OX2H1]	0.9972	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])O	0.9763	CCC#CC#C	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.9679	CC=CC#CC	0.0
[OX2H1]	0.9673	C=CC=CC#C	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H2]	0.4448	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.6574
[#6H1]	0.3232	[#8][#6][#6H2]	0.6788
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2239	O=[CX3H0][CX4H2][CX4H2]	0.7064
[CHX4]([CH3X4])[CH2X4]	0.1533	[CX4H2][CX3]=O	0.7251
[CX4H3][CX4H1]	0.1484	[CX4H2]CC=O	0.7729
[CX4H2]([CX4H2])[CX4H1]	0.1437	CCCCCC	0.8335
[#6H3][#6H0]	0.1234	OCC[CH2]	0.838
[#6H1]([#6H2])[#6H2]	0.1131	[CX4H2]([CX4H2])[CX3H0]	0.8454
[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.1007	[CX4H2]([CX4H3])[CX4H2]	0.8628
[#6X3][#6][#6][#6H3]	0.096	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.8756

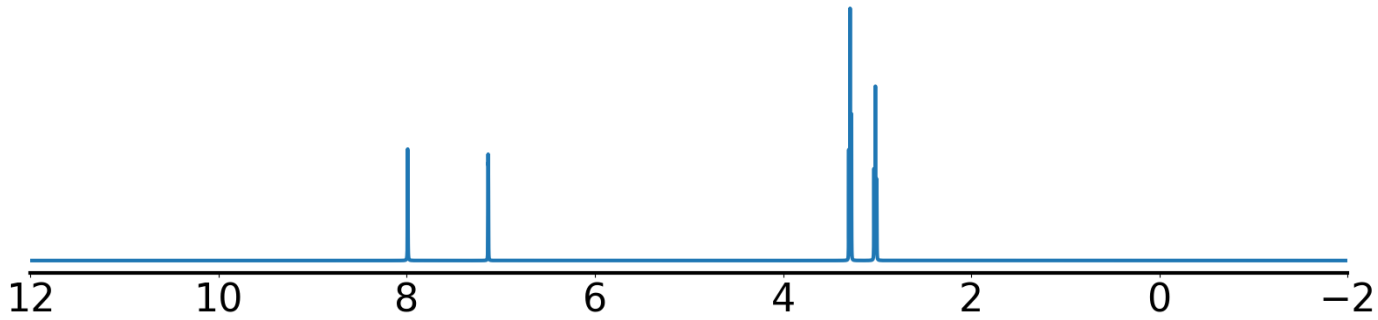
Example 43 true smiles: NCCc1c[nH]cn1 formula: C5H9N3
Index of correct structure: 1 of 8824
True structure loss: 0.022963
True structure:



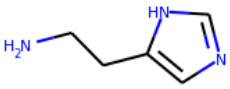
Experimental 13C NMR (solvent: D2O)



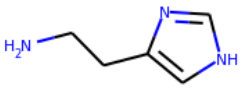
Experimental 1H NMR (solvent: D2O)



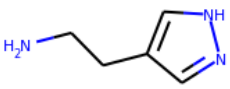
Top predicted structures (loss):



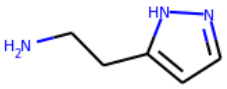
0.021891



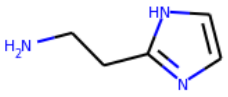
0.022963



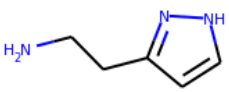
0.024396



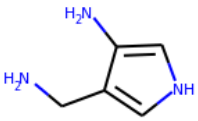
0.032793



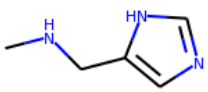
0.033342



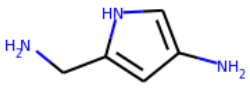
0.035301



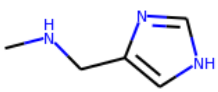
0.052169



0.052178



0.052482



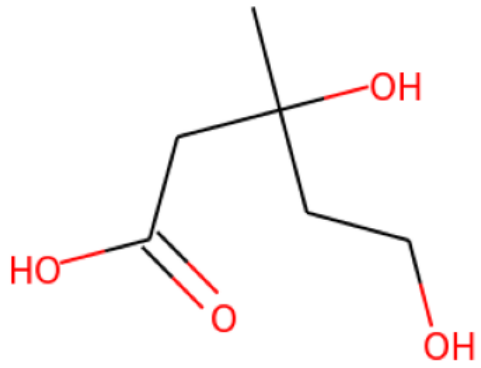
0.05325

Top predicted substructures	prob		
[#6H1]	0.9983	[#6X3][#6X3]	0.9092
[CX4H2]([#6])[#6]	0.9917	[#7X3][#6H2]	0.878
[cH]	0.9369	[#7][#6][#6][#6X3]	0.8601
[#7X3H2]	0.9196	[#7][#6][#6X3]	0.829
[#7][#6H2][#6H2]	0.9176	[#7][#6H2]	0.8177

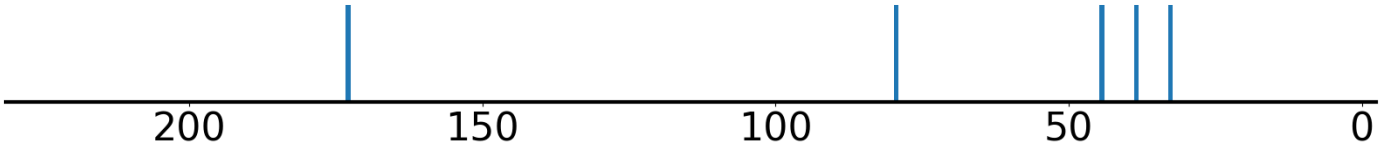
best positives	prob	best negatives	prob
[#6H1]	0.9983	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[CX4H2]([#6])[#6]	0.9917	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9369	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#7X3H2]	0.9196	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7][#6H2][#6H2]	0.9176	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3]	0.9092	[#6]1[#8][#6][#6]1=[#8]	0.0
[#7X3][#6H2]	0.878	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#7][#6][#6][#6X3]	0.8601	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[#7][#6][#6X3]	0.829	[CX3H0](=[OX1H0])([CX4H1])[CX4H0]	0.0
[#7][#6H2]	0.8177	[#8][#6H1][#6H2][#6H1]=[#8]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([nX2H0])[cX3H0]	0.5003	[#7][#6][#6][#6][#6][#7]	0.2249
[#7][#7]	0.4353	[cX3H1]([nX3H1])[cX3H0]	0.2641
[#7X3H0]	0.3889	[#7][#6X3H0][#6X3H1]	0.2764
[#6X3H1][#7X3H0]	0.2955	[#7][#6H0][#6H1]	0.3113
[cH][cH]	0.2886	[#6X3][#7X3][#6X3]	0.3797
[CX4H2][CX3H]	0.2386	[#6X3][#7][#6X3]	0.4547
[#6H2][#7][#6X3]	0.2327	[#7H][#6X3H1]	0.4658
[CX4H3]	0.2311	[#6]1[#6][#7][#6][#7]1	0.4963
[CX4H2]([NX3H1])[CX4H2]	0.2053	[#6H1][#7][#6H1]	0.5013
[#7][#7H1]	0.1818	[#7][#6][#6][#7]	0.5562

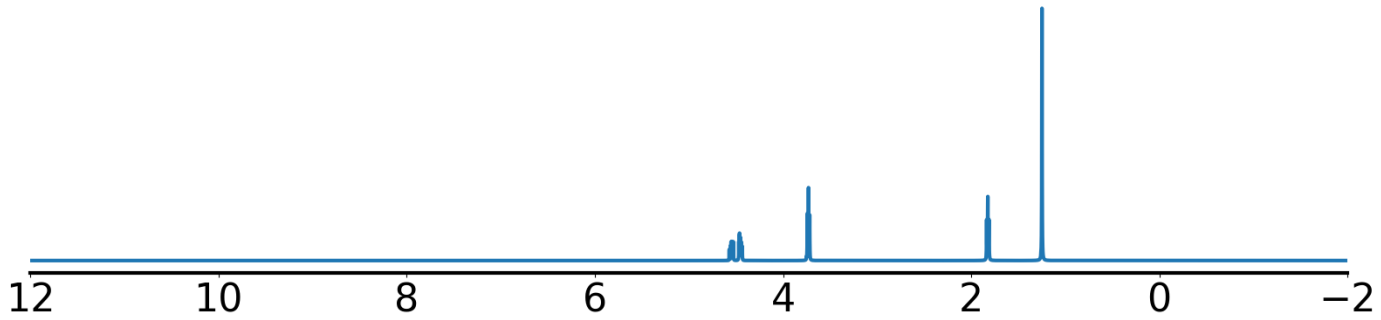
Example 44 true smiles: CC(O)(CCO)CC(=O)O formula: C6H12O4
Index of correct structure: 6 of 8605
True structure loss: 0.047542
True structure:



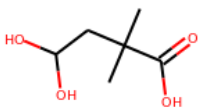
Experimental 13C NMR (solvent: CDCl3)

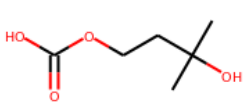


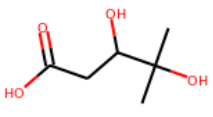
Experimental 1H NMR (solvent: D2O)

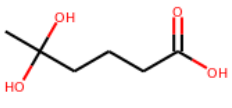


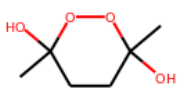
Top predicted structures (loss):

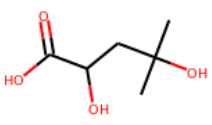

0.038973

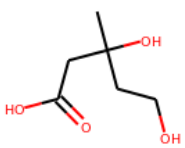

0.044147

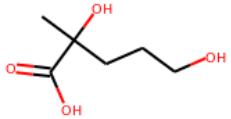

0.044396

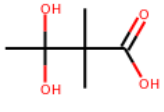

0.046009

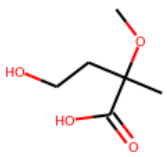

0.046128


0.046747


0.047542


0.048719


0.049301

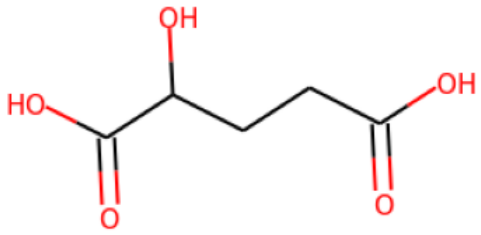

0.049788

Top predicted substructures	prob		
[#8]=[#6][#8]	0.9998	[CX4H3][CX4H0]	0.9767
[#6H3][#6][#6]	0.9996	[CX4H3]	0.9765
[OX2H1]	0.9994	[#8][#6][#6H2]	0.9746
[CX3](=[OX1])O	0.9981	[#6H3][#6H0]	0.9675
OCC[CH2]	0.9786	[CX4H3][#6]	0.9652

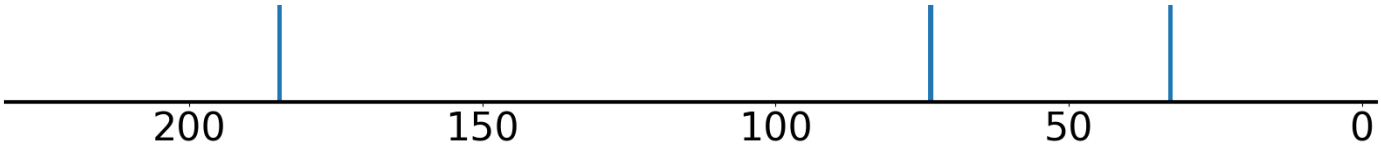
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9998	CCC#CC#C	0.0
[#6H3][#6][#6]	0.9996	CC=CC#CC	0.0
[OX2H1]	0.9994	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])O	0.9981	CCC#CC=C	0.0
OCC[CH2]	0.9786	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][CX4H0]	0.9767	[#7][#6]=[#6][#6]#[#7]	0.0
[CX4H3]	0.9765	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#8][#6][#6H2]	0.9746	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6H3][#6H0]	0.9675	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H3][#6]	0.9652	[CX2H0](#[CX2H1])[cX3H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H2]	0.8107	[OX2H1][CX4H0][CX4H2][CX3H0]	0.0341
[OH][CX4H]	0.8098	[CH2X4](O)[CX4H2]	0.0486
[#6H1]	0.71	[OX1H0]=[CX3H0][CX4H2][CX4H0]	0.0732
[#8][#6][#6][#6][#6][#8]	0.6329	[CX4H2]([OX2H1])[CX4H2]	0.0746
[#6X4H2][#6H1][#8H]	0.6155	[#8X1]=[#6X3][#6H2][#6H0]	0.0878
[CH3]CC[OH]	0.55	[#6X3][#6][#6][#6H3]	0.1341
[#8][#6H0][#6H1]	0.5262	[CX4H2]([CX4H0])[CX3H0]	0.1563
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5178	[#6H3][#6H0]([#6H2])[#6H2]	0.1825
[#8H][#6X4H1][#6X3H0]	0.4365	[#8][#6][#6][#6X3]	0.1873
O[CX4H][CX4H2]	0.4348	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2188

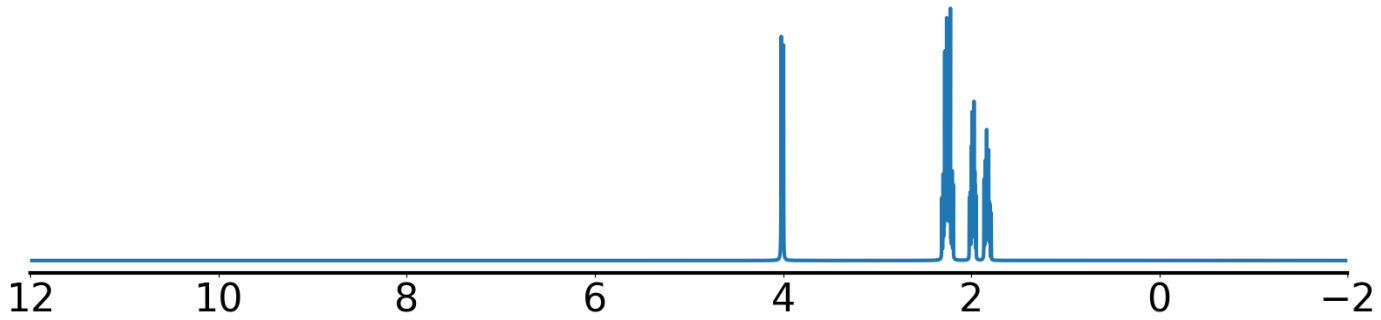
Example 45 true smiles: O=C(O)CCC(O)C(=O)O formula: C5H8O5
Index of correct structure: 1 of 8115
True structure loss: 0.028053
True structure:



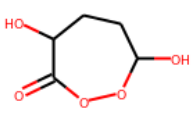
Experimental 13C NMR (solvent: D2O)



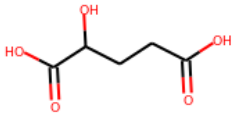
Experimental 1H NMR (solvent: D2O)



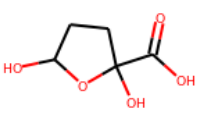
Top predicted structures (loss):



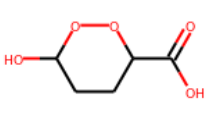
0.024143



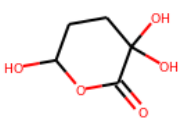
0.028053



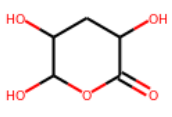
0.033235



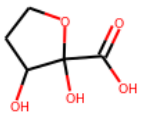
0.034373



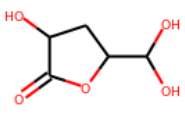
0.037587



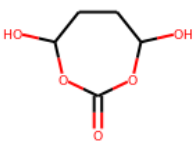
0.037689



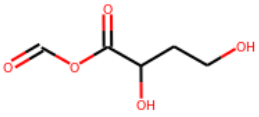
0.039094



0.040344



0.043423



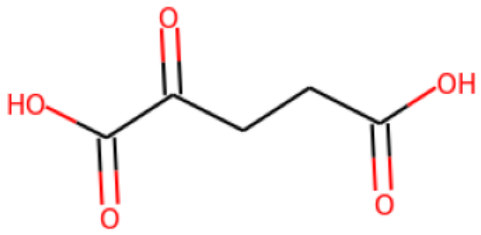
0.046571

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9993	[CX3](=[OX1])O	0.9786
[CX3](=[OX1])C	0.9979	[#8][#6][#6H2]	0.9463
[OX2H1]	0.9968	[#6H1]	0.9449
OCC[CH2]	0.9962	[#8][#6][#6]=[#8]	0.9435
[#8]=[#6][#8]	0.9805	[#6H1][#6H2]	0.9345

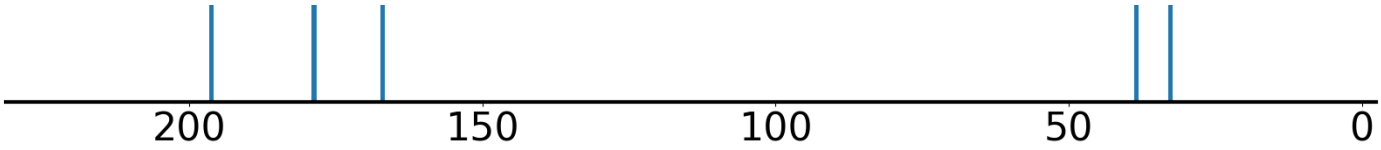
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9993	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9979	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[OX2H1]	0.9968	[#6X3H2]=[#6][#6H2][#8H]	0.0
OCC[CH2]	0.9962	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[#8]=[#6][#8]	0.9805	CC#CCC=C	0.0
[CX3](=[OX1])O	0.9786	CC=CCC#C	0.0
[#8][#6][#6H2]	0.9463	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[#6H1]	0.9449	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#8][#6][#6]=[#8]	0.9435	C=CC=CC#C	0.0
[#6H1][#6H2]	0.9345	[#6H3][#6H1][#6H1]=[#7]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H1]	0.4845	O=[CX3H0][CX4H2][CX4H2]	0.0235
[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.4505	[CX4H2]([CX4H2])[CX3H0]	0.0243
[#8][#6][#6][#6X3]	0.2572	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.0271
O[CX4H]([CX4H2])[CX4H1]	0.2434	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.0532
[#6H1]([#6H2])[#6H2]	0.2176	[CX4H2][CX3]=O	0.1769
[#8][#6H1][#6H1]	0.2031	[#8][#6][#6][#6][#6]=[#8]	0.3892
[#8]=[#6][#6H1][#6H1]	0.1938	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5714
CCCCCC	0.1754	[#8][#6][#6][#6][#6][#8]	0.6148
[OX2H1][CX4H1][CX4H1][OX2H1]	0.1595	[#8H][#6X4H1][#6X3H0]	0.7179
[CX4H2]([OX2H0])[CX4H2]	0.1491	[CX3](=O)[OX2H1]	0.718

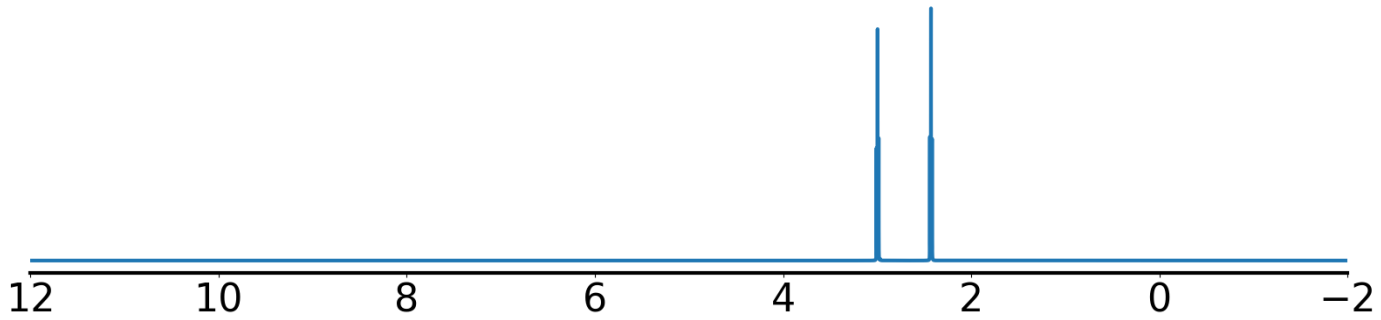
Example 46 true smiles: O=C(O)CCC(=O)C(=O)O formula: C5H6O5
Index of correct structure: 0 of 7597
True structure loss: 0.008162
True structure:



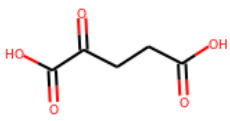
Experimental 13C NMR (solvent: DMSO)



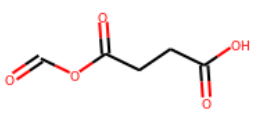
Experimental 1H NMR (solvent: d2o)



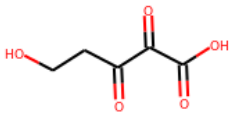
Top predicted structures (loss):



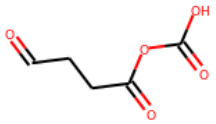
0.008162



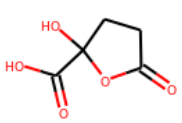
0.042883



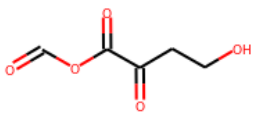
0.049861



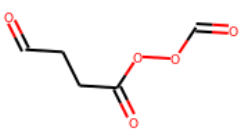
0.049914



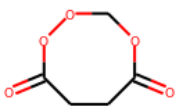
0.06086



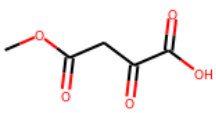
0.062934



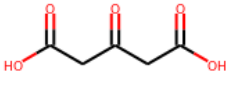
0.064672



0.066055



0.068078



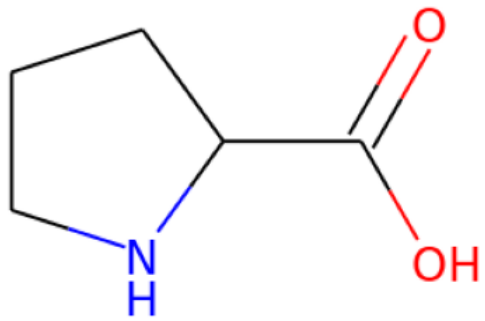
0.069021

Top predicted substructures	prob		
[CX3](=[OX1])C	1.0	O=[CX3H0][CX4H2][CX4H2]	0.9903
[CX4H2]([#6])[#6]	0.9999	[CX4H2][CX3]=O	0.9811
[CX3](=[OX1])O	0.9997	OCC[CH2]	0.9543
[#8]=[#6][#8]	0.9986	[CX4H2]CC=O	0.9518
[CX4H2]([CX4H2])[CX3H0]	0.9938	[#8]=[#6][#6]=[#8]	0.9427

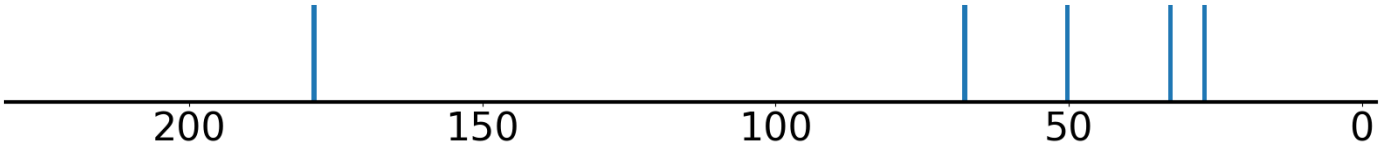
best positives	prob	best negatives	prob
[CX3](=[OX1])C	1.0	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2]([#6])[#6]	0.9999	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[CX3](=[OX1])O	0.9997	[#6X2][#6H1][#6X2]	0.0
[#8]=[#6][#8]	0.9986	C=CC=CC#C	0.0
[CX4H2]([CX4H2])[CX3H0]	0.9938	CCC#CC#C	0.0
O=[CX3H0][CX4H2][CX4H2]	0.9903	CC#CCC#C	0.0
[CX4H2][CX3]=O	0.9811	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
OCC[CH2]	0.9543	[OX2H0][CX4H2][CX2H0]#[CX2H1]	0.0
[CX4H2]CC=O	0.9518	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#8]=[#6][#6]=[#8]	0.9427	CCC=CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H3][CX3H0]	0.3481	[#8][#6][#6][#6][#6]=[#8]	0.514
[CX4H3]	0.3122	[#8][#6][#6]=[#8]	0.5427
[OX2H0][CX3H0][CX4H2]	0.2447	[#8]=[#6][#6][#6][#6]=[#8]	0.7041
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.1992	[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.7116
[#8][#6][#6][#6X3]	0.1964	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.7351
[OX1H0]=[CX3H0][CX4H3]	0.1642	[#8][#6][#6H2]	0.805
O=[#6][#6][#6X3]	0.1515	[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.8141
[#6H3][#6][#6]	0.1462	[CX3](=O)[OX2H1]	0.8203
[CX4H3][CX3]	0.1116	O=CC=O	0.8269
[#6X3][#6][#6][#6H3]	0.1064	[OX2H1]	0.8935

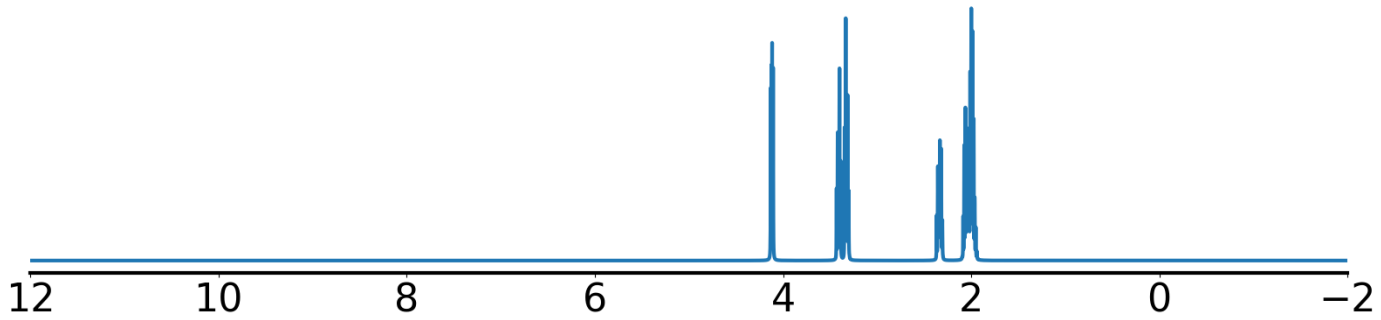
Example 47 true smiles: O=C(O)C1CCCN1 formula: C5H9NO2
Index of correct structure: 0 of 6935
True structure loss: 0.024354
True structure:



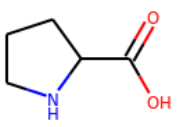
Experimental 13C NMR (solvent: D2O)



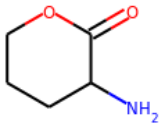
Experimental 1H NMR (solvent: d2o)



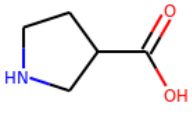
Top predicted structures (loss):



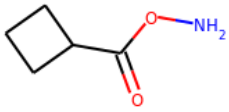
0.024354



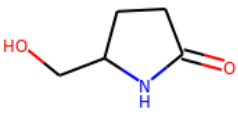
0.040611



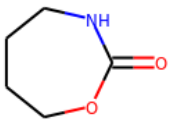
0.045086



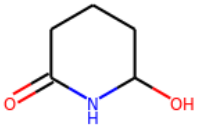
0.049682



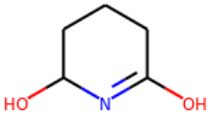
0.051446



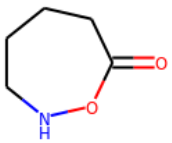
0.052438



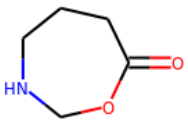
0.053394



0.054517



0.05542



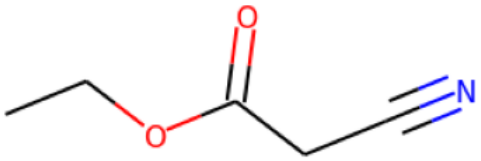
0.055889

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9998	[CX4H2]CC=O	0.9264
[CX4H2][CX4H2]	0.9861	[#6H1][#6H2]	0.8996
[CX3](=[OX1])C	0.9834	[#7X3][#6H2]	0.89
[CX4H2]([CX4H2])[CX4H1]	0.972	[#6H1]	0.8844
OCC[CH2]	0.9593	O=[CX3][CX4H]	0.8749

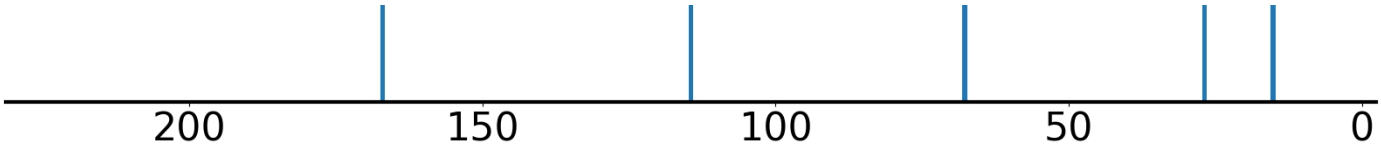
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9998	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2][CX4H2]	0.9861	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX3](=[OX1])C	0.9834	CC=CCC#C	0.0
[CX4H2]([CX4H2])[CX4H1]	0.972	[#6X3][#6]#[#6][#6H3]	0.0
OCC[CH2]	0.9593	CC=CC#CC	0.0
[CX4H2]CC=O	0.9264	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#6H1][#6H2]	0.8996	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[#7X3][#6H2]	0.89	C=CC=CC#C	0.0
[#6H1]	0.8844	[CX2H0](#[CX2H0])[CX4H0]	0.0
O=[CX3][CX4H]	0.8749	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([#6])[O]	0.5716	[#6H1r5][#7]	0.2458
[CH2X4](O)[CX4H2]	0.4952	[CX3](=O)[OX2H1]	0.3091
[#8][#6][#6H2]	0.4821	[#6]1[#6][#6][#6][#7]1	0.3217
[#7X3H2]	0.4455	[#7H1][#6X4H1][#6X3]	0.393
O=[CX3H0][CX4H2][CX4H2]	0.3793	[CX4H2]([CX4H2])[CX4H2]	0.4148
[CX4H2][CX3]=O	0.3654	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.4385
[CX4H2]([OX2H0])[CX4H2]	0.3401	[#7][#6H1][#6H2r5]	0.4651
[#7H2][#6H1]	0.2664	[#7X3H1]	0.4668
[#7][#6H0][#6H1]	0.2564	[#8][#6H0][#6H1]	0.5972
[#7H2][#6X4H1][#6X3]	0.2398	[#6H1][#6H2][#6][#6][#7]	0.6125

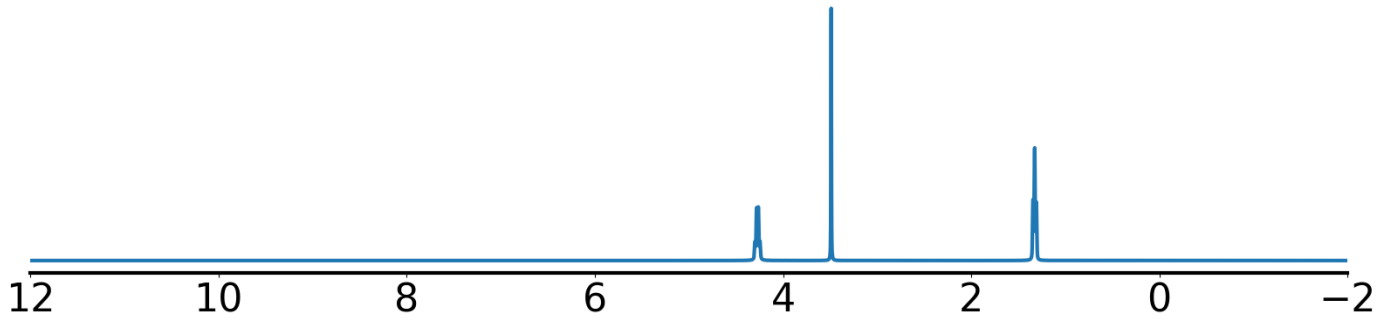
Example 48 true smiles: CCOC(=O)CC#N formula: C5H7NO2
Index of correct structure: 0 of 6308
True structure loss: 0.028354
True structure:



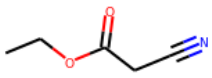
Experimental 13C NMR (solvent: CDCl3)



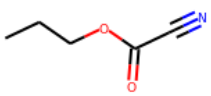
Experimental 1H NMR (solvent: CDCl3)



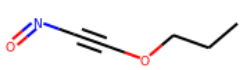
Top predicted structures (loss):



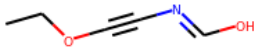
0.028354



0.042572

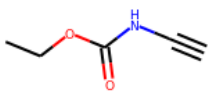


0.046532

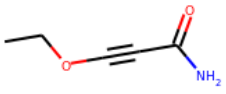


0.048316

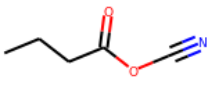
0.050451



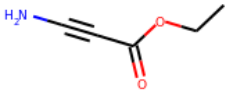
0.053284



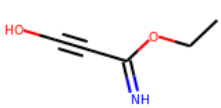
0.055955



0.055974



0.056476



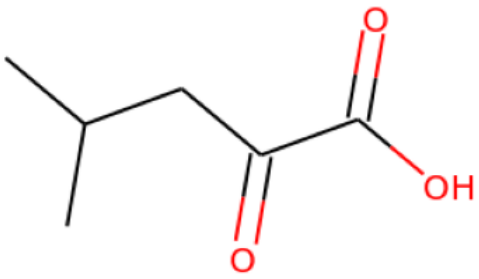
0.058853

Top predicted substructures	prob		
[CX4H3]	0.9878	[CX4H2]([CX3H0])[CX2H0]	0.7995
[CX4H3][#6]	0.8479	[#8][#6][#6H2]	0.7796
[#6]#[#7]	0.8474	[#8]=[#6][#6H2][#6X2]	0.7432
[CX2H0][CX4H2][#6X3H0]	0.8455	[#6H1]	0.6899
[CX4H3][CX4H2]	0.8052	[CX4H2]([#6])[#6]	0.6827

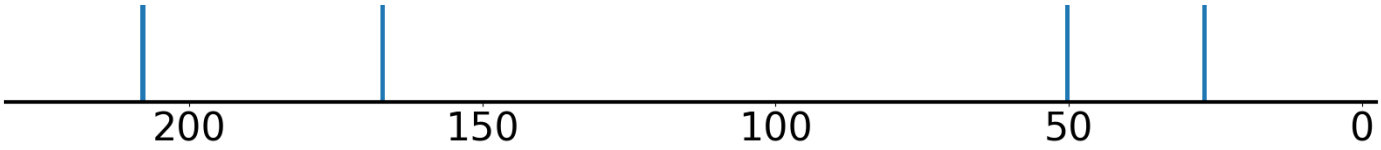
best positives	prob	best negatives	prob
[CX4H3]	0.9878	[CX3H1](=[CX3H2])[CX3H1]	0.0
[CX4H3][#6]	0.8479	[CX3H1](=[CX3H2])[CX4H2]	0.0
[#6]#[#7]	0.8474	[CX4H3][CX3H0][CX4H2][CX3H1]	0.0
[CX2H0][CX4H2][#6X3H0]	0.8455	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
[CX4H3][CX4H2]	0.8052	C=CC=CC#C	0.0
[CX4H2]([CX3H0])[CX2H0]	0.7995	[CX3H1](=[CX3H2])[cX3H0]	0.0
[#8][#6][#6H2]	0.7796	C=CC=CC=C	0.0
[#8]=[#6][#6H2][#6X2]	0.7432	[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	0.0
[CX4H2]([#6])[#6]	0.6827	[OX1H0]=[CX3H1][CX3H0]=[CX3H2]	0.0
[CX4H2]([OX2H0])[CX4H3]	0.6696	[CX3H1](=[CX3H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.6899	[CX4H2][CX3]=O	0.0745
[#8][#6][#6][#6X3]	0.4729	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.1265
[#6H1][#6H1]	0.373	[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.1695
[CX4H]O	0.2989	[CX4H2]([#6])[O]	0.3515
[#8][#6][#6][#8]	0.2475	[OX2H0][CX3H0][CX4H2]	0.3763
[CX4H2]([OX2H0])[CX4H2]	0.2435	[CX3](=[OX1])O	0.3783
O=[CX3][CX4H]	0.2361	[#8X1]=[#6X3][#6H2][#6H0]	0.3915
C1CC1	0.2336	[CX4H3][CX4]O	0.4134
[#8][#6H0][#6H1]	0.214	[#6H2][#6X2]	0.4931
OCC[CH2]	0.2077	[#8]=[#6][#8]	0.4994

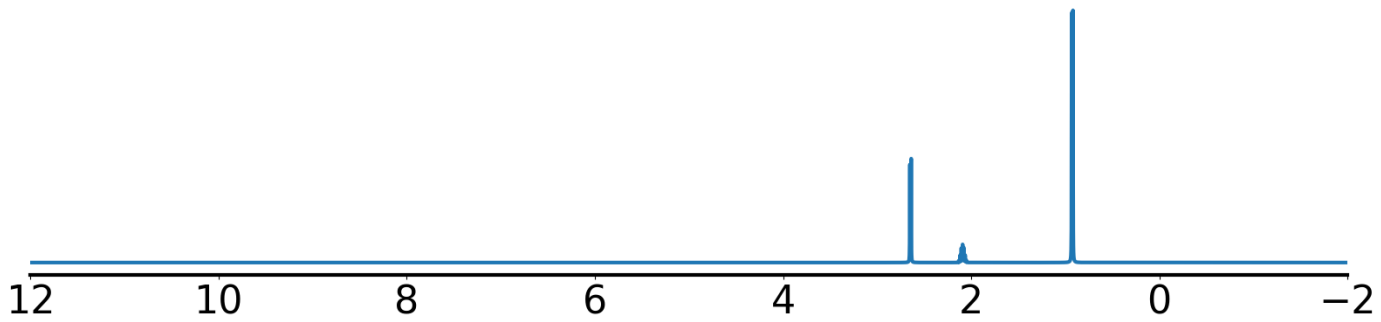
Example 49 true smiles: CC(C)CC(=O)C(=O)O formula: C6H10O3
Index of correct structure: 0 of 6069
True structure loss: 0.016838
True structure:



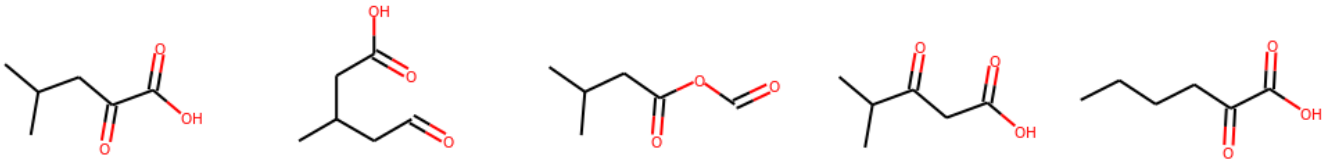
Experimental 13C NMR (solvent: DMSO)



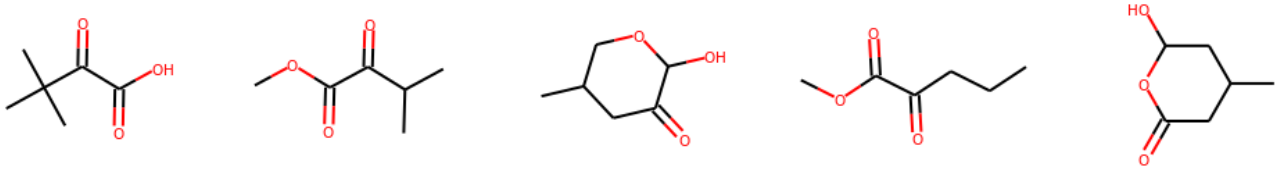
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.016838 0.054685 0.055422 0.064634 0.073687



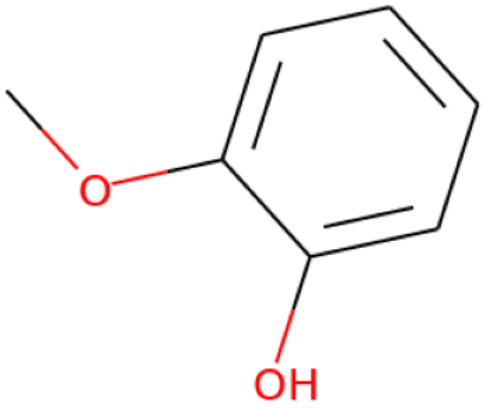
0.077413 0.078502 0.082401 0.082986 0.083879

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9999	O=[CX3H0][CX4H2][CX4H1]	0.9608
[CX4H3]	0.999	[CX4H2]([#6])[#6]	0.9539
[#6H3][#6][#6]	0.9953	[CX3](=[OX1])O	0.9525
[CX4H3][#6]	0.9894	[CX4H2][CX3]=O	0.95
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9842	[#6H1]	0.9455

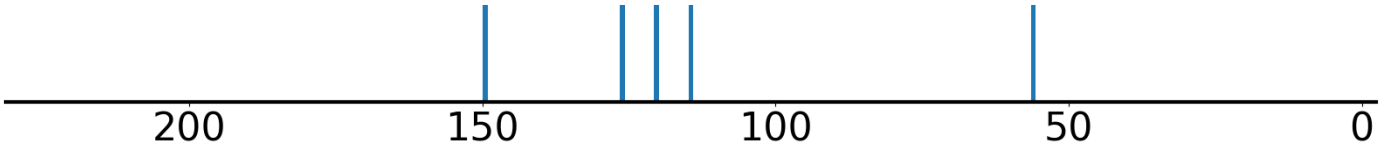
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9999	C=CC=CC#C	0.0
[CX4H3]	0.999	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6H3][#6][#6]	0.9953	CCC#CC#C	0.0
[CX4H3][#6]	0.9894	[CX2H0](#[CX2H1])[CX4H0]	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9842	CC=CC#CC	0.0
O=[CX3H0][CX4H2][CX4H1]	0.9608	CCC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9539	[CX4H3][CX2H0]	0.0
[CX3](=[OX1])O	0.9525	C=CCCC#C	0.0
[CX4H2][CX3]=O	0.95	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H1]	0.9455	[CX2H0](#[CX2H1])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.7481	OCC[CH2]	0.1562
O[CX4H][CX4H2]	0.4988	[#8][#6][#6]=[#8]	0.3936
[#8][#6][#6][#6X3]	0.3854	[CX4H2]CC=O	0.397
[#6H2][#8][#6H1]	0.3465	[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.5962
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.3268	[#6X3][#6X3]	0.6026
[CX4H2](O)[CHX4]	0.3212	[#8]=[#6][#6]=[#8]	0.7001
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2723	[CHX4]([CH3X4])[CH2X4]	0.7511
[#8]=[#6][#6][#6][#6]=[#8]	0.2611	[#8]=[#6][#6H2][#6H1]	0.7651
[CX4H]O	0.2494	[CX3](=O)[OX2H1]	0.7694
[CX4H2]([#6])[O]	0.2027	[CX4H3][CX4H1]	0.7729

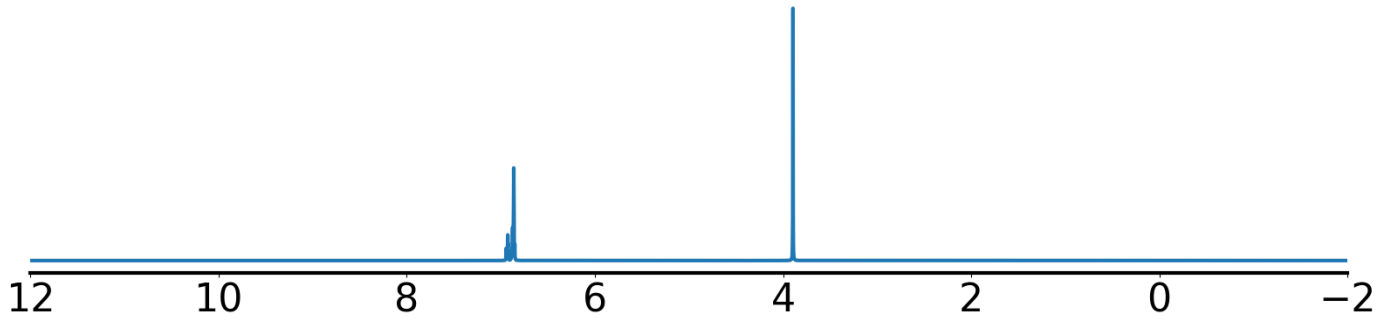
Example 50 true smiles: COc1ccccc1O formula: C7H8O2
Index of correct structure: 1 of 5977
True structure loss: 0.008976
True structure:



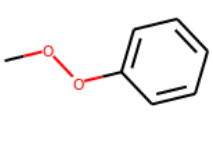
Experimental 13C NMR (solvent: CDCl3)



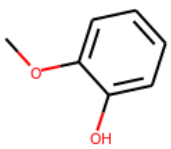
Experimental 1H NMR (solvent: CDCL3)



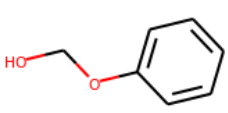
Top predicted structures (loss):



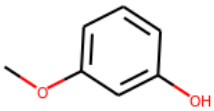
0.006759



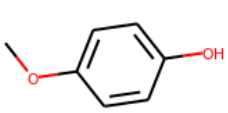
0.008976



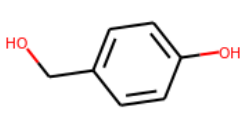
0.011707



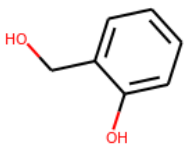
0.011993



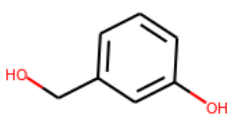
0.013973



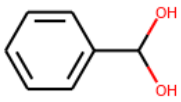
0.032486



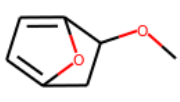
0.032625



0.035157



0.040894



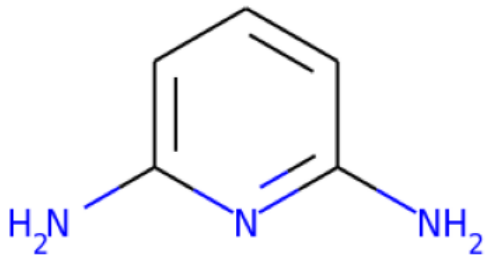
0.049135

Top predicted substructures	prob		
[#6X3][#6X3][#6X3][#6X3]	0.9979	[#6X3H1][#6X3H0]	0.9792
[#6H1]	0.9976	[cH][cH]	0.9617
[#6X3][#6X3]	0.9973	[cX3H1]([cX3H1])[cX3H0]	0.9536
[cH]	0.9864	[#6H1][#6H1]	0.9455
[#8][#6][#6][#6X3]	0.9828	[#8][#6H0][#6H1]	0.8961

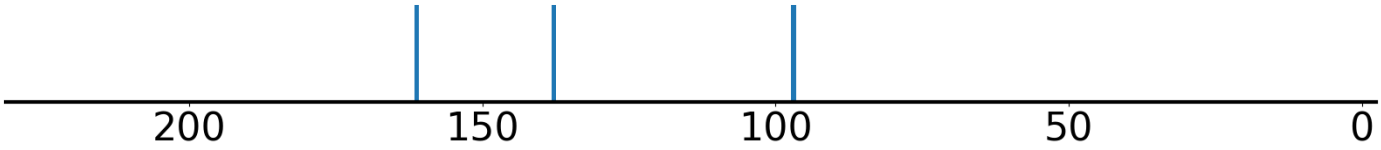
best positives	prob	best negatives	prob
[#6X3][#6X3][#6X3][#6X3]	0.9979	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H1]	0.9976	[#6H3][#6H1][#7][#7]	0.0
[#6X3][#6X3]	0.9973	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[cH]	0.9864	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.0
[#8][#6][#6][#6X3]	0.9828	[CX4H2]([NX3H0])[CX4H3]	0.0
[#6X3H1][#6X3H0]	0.9792	[CX4H1]([NX3H2])([CX4H2])[CX4H0]	0.0
[cH][cH]	0.9617	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9536	[#6H3][#6H1][#6H1]=[#7]	0.0
[#6H1][#6H1]	0.9455	[CX4H1]([NX3H0])([CX4H3])[CX4H2]	0.0
[#8][#6H0][#6H1]	0.8961	[CX4H1]([NX3H1])([CX4H2])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.4438	[OX2H1]	0.3102
[#8][#6H1][#6H1]	0.223	[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.3169
[#8][#6H][#6X3][#6X3H]	0.1817	[OX2H][cX3]:[c]	0.3804
[cX3H1]([cX3H0])[cX3H0]	0.1601	[#8][#6][#6][#8]	0.4274
[#8][#6][#6H2]	0.1257	[#6]1[#6][#6][#6][#6][#6]1	0.5898
[cX3H0][cX3H1][cX3H0][OX2H1]	0.1126	[cX3H1]([cX3H1])[cX3H1]	0.7576
o[cH]	0.1048	[CX4H3]	0.8693
[#8][#6][#6][#6][#6][#8]	0.0975	[CX4H3][OX2H0]	0.885
[cX3H1]([oX2H0])[cX3H1]	0.097	[cH]cO	0.8922
[cX3H0][cX3H1][cX3H1][cX3H0]	0.0953	[#8][#6H0][#6H1]	0.8961

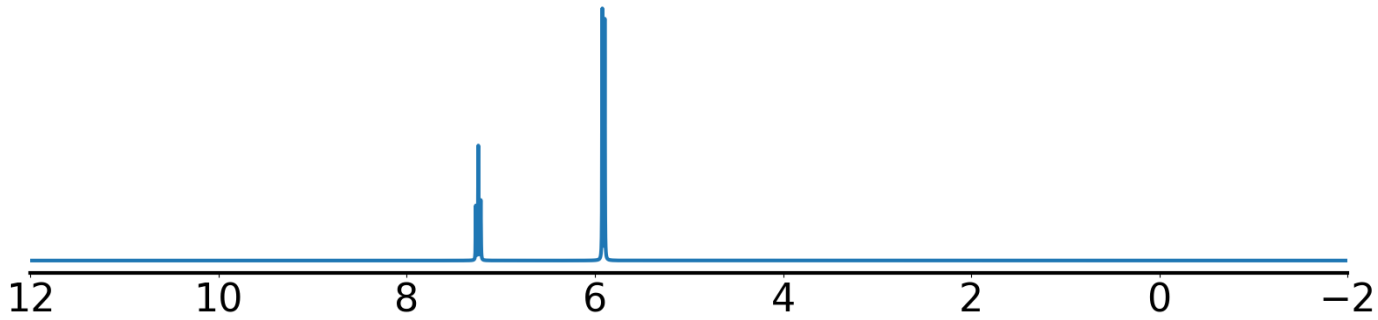
Example 51 true smiles: Nc1cccc(N)n1 formula: C5H7N3
Index of correct structure: 0 of 5951
True structure loss: 0.015978
True structure:



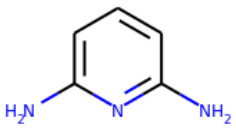
Experimental 13C NMR (solvent: Benzene-d6)



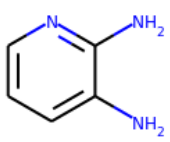
Experimental 1H NMR (solvent: CDCl3)



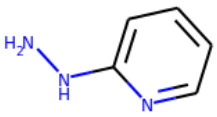
Top predicted structures (loss):



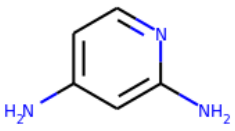
0.015978



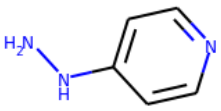
0.021855



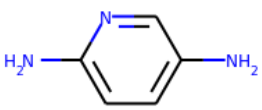
0.023035



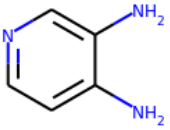
0.023718



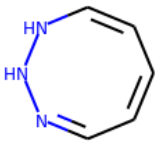
0.025275



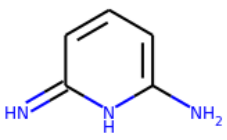
0.028579



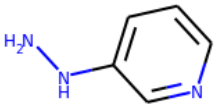
0.029698



0.031166



0.031357



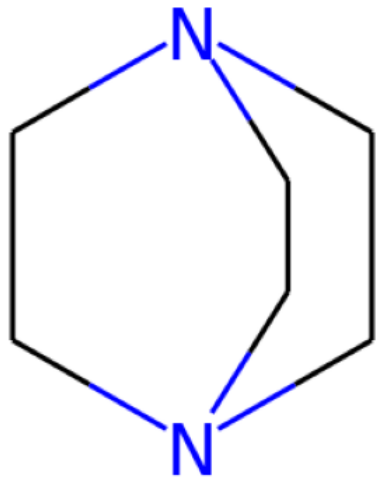
0.031773

Top predicted substructures	prob		
[#6H1]	0.9965	[#7][#6][#6X3]	0.9124
[#6X3][#6X3]	0.9714	[cX3H1]([cX3H1])[cX3H0]	0.8833
[cH][cH]	0.9446	[cH]	0.8383
[#7X3H2]	0.9273	[#7][#6][#6][#6X3]	0.8363
[#6X3H1][#6X3H0]	0.9227	[#7][#6H0][#6H1]	0.8301

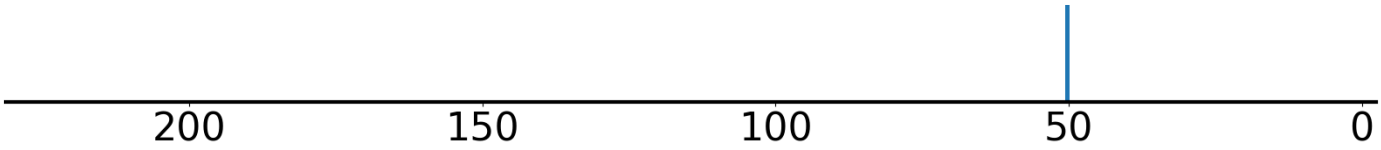
best positives	prob	best negatives	prob
[#6H1]	0.9965	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[#6X3][#6X3]	0.9714	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cH][cH]	0.9446	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#7X3H2]	0.9273	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9227	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#7][#6][#6X3]	0.9124	[#8][#6H2][#6H2][#6X2]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8833	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[cH]	0.8383	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.8363	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6H0][#6H1]	0.8301	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#7X3H1]	0.5125	[#6]1[#6][#6][#6][#6][#7]1	0.1723
[#7][#7]	0.4241	[#7][#6H0][#7]	0.5165
[#7][#6][#6][#6][#7]	0.3785	[#7H2][#6H0]	0.5818
[#7H][#6X3H1]	0.3693	[#6X3][#7][#6X3]	0.6083
[#6X3][#7X3][#6X3]	0.3563	[#7][#6X3H0][#6X3H1]	0.6478
[cX3H1]([nX3H1])[cX3H1]	0.3339	[#7][#6][#7]	0.6642
[#6H1][#7][#6H1]	0.2824	[#6X3][#6X3][#6X3][#6X3]	0.7195
[NH1]=[#6][#7]	0.2799	[cX3H1]([cX3H1])[cX3H1]	0.7327
[#6]=[#7H]	0.2438	[#6H1][#6H1]	0.8143
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.2195	[#7][#6H0][#6H1]	0.8301

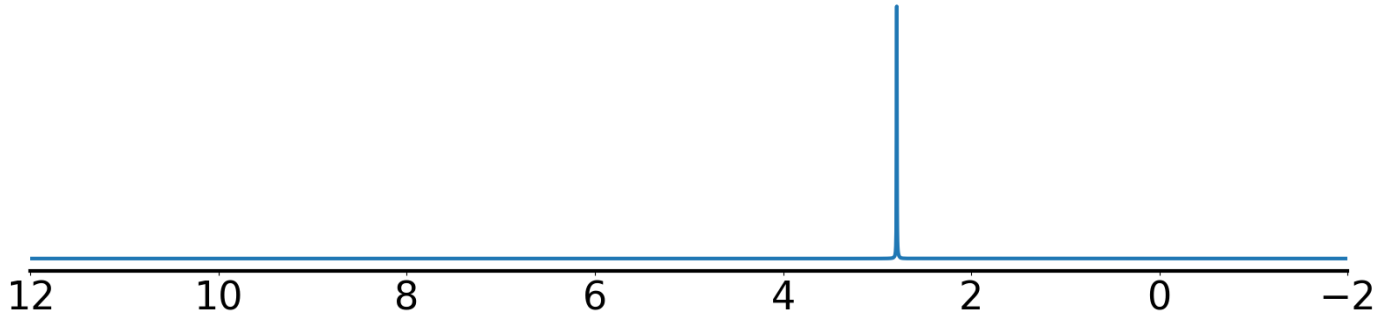
Example 52 true smiles: C1CN2CCN1CC2 formula: C6H12N2
Index of correct structure: 0 of 5002
True structure loss: 0.010484
True structure:



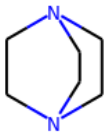
Experimental 13C NMR (solvent: CDCl3)



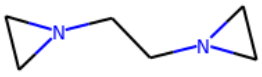
Experimental 1H NMR (solvent: CDCl3)



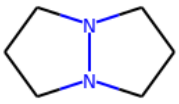
Top predicted structures (loss):



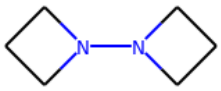
0.010484



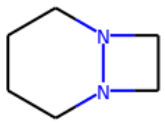
0.030006



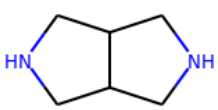
0.035419



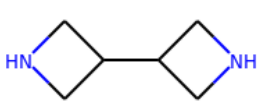
0.036905



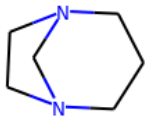
0.037147



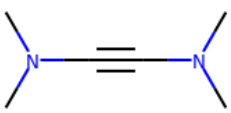
0.038104



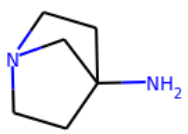
0.038266



0.038602



0.040673



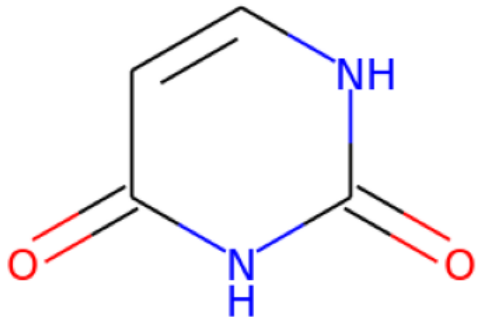
0.041273

Top predicted substructures	prob		
[#7X3][#6H2]	0.9364	[#7][#6H2][#6H2]	0.6456
[#7][#6H2][#6H2][#7]	0.9076	[#7][#6][#6][#7]	0.6298
[#6]1[#6][#7][#6][#6][#7]1	0.8213	[#7X3H0]	0.6207
[#6H2][#7][#6H2]	0.7831	[#7X3H1]	0.55
[#7][#6H2]	0.6834	[CX4H2][CX4H2]	0.4638

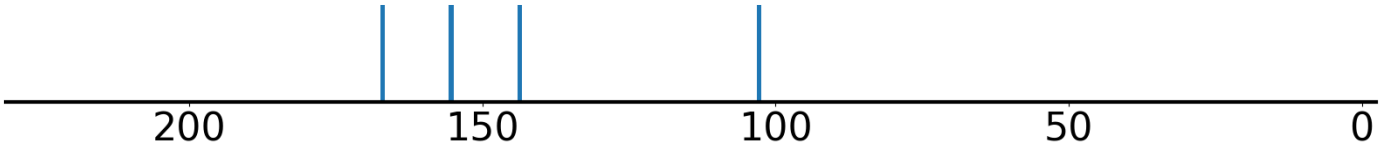
best positives	prob	best negatives	prob
[#7X3][#6H2]	0.9364	[OX2H0][CX3H1]=[#6X3H0][#8X2H0]	0.0
[#7][#6H2][#6H2][#7]	0.9076	[CX3H0](=[CX3H2])([OX2H0])[CX4H3]	0.0
[#6]1[#6][#7][#6][#6][#7]1	0.8213	[OX2H0][CX4H2][OX2H0][CX3H0]	0.0
[#6H2][#7][#6H2]	0.7831	[#6X3H1][#8][#6H2][#8]	0.0
[#7][#6H2]	0.6834	[OX2H0]1[CX4H2][CX4H1][CX3H0]=[CX3H1]1	0.0
[#7][#6H2][#6H2]	0.6456	[CX3H0](=[CX3H2])([OX2H0])[CX3H0]	0.0
[#7][#6][#6][#7]	0.6298	[#8]1[#6][#6]=[#6][#6]=[#6]1	0.0
[#7X3H0]	0.6207	[#8][#6X3]=[#6X3][#6X3][#6H3]	0.0
[CX4H2][CX4H2]	0.4638	[CX3H0](=[CX3H2])([OX2H0])[CX4H0]	0.0
[CX4H2]([NX3H0])[CX4H2]	0.3561	[#6H3][#6H1][#6H1]=[#7]	0.0

worst negatives	prob	worst positives	prob
[#7X3H1]	0.55	[CX4H2]([NX3H0])[CX4H2]	0.3561
[#6H3][#7]	0.3664	[CX4H2][CX4H2]	0.4638
[#7][#6][#6][#6][#7]	0.318	[#7X3H0]	0.6207
[#7X3H2]	0.2662	[#7][#6][#6][#7]	0.6298
[#6H1]([#6H2])[#6H2]	0.2369	[#7][#6H2][#6H2]	0.6456
[#6H1][#6H1]	0.2203	[#7][#6H2]	0.6834
[#6]1[#6][#6][#6][#7]1	0.2197	[#6H2][#7][#6H2]	0.7831
[CX4H2]([NX3H1])[CX4H2]	0.2188	[#6]1[#6][#7][#6][#6][#7]1	0.8213
[#6H1][#6H2]	0.2164	[#7][#6H2][#6H2][#7]	0.9076
[#6H1]	0.1993	[#7X3][#6H2]	0.9364

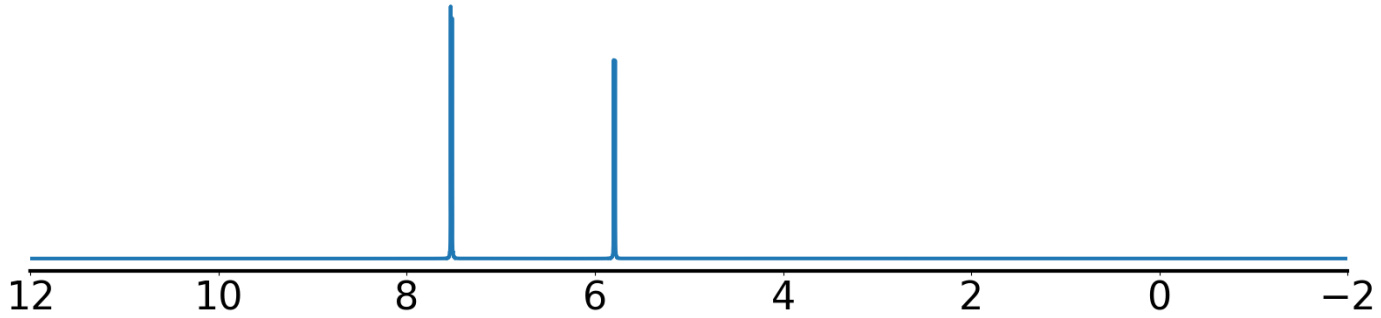
Example 53 true smiles: O=c1cc[nH]c(=O)[nH]1 formula: C4H4N2O2
Index of correct structure: 5 of 4792
True structure loss: 0.030097
True structure:



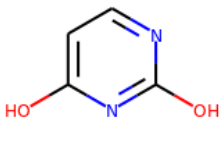
Experimental 13C NMR (solvent: DMSO)



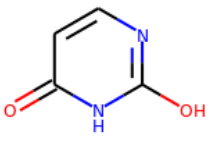
Experimental 1H NMR (solvent: D2O)



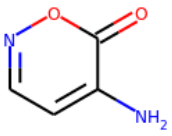
Top predicted structures (loss):



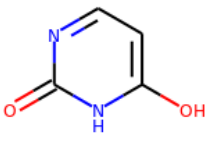
0.027947



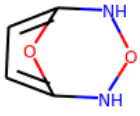
0.02828



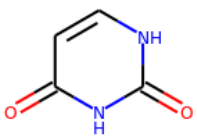
0.028299



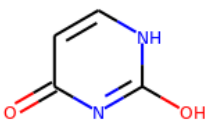
0.028616



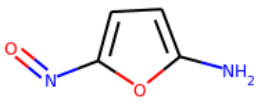
0.028707



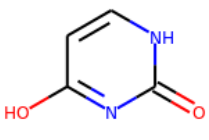
0.030097



0.030224



0.030357



0.03056

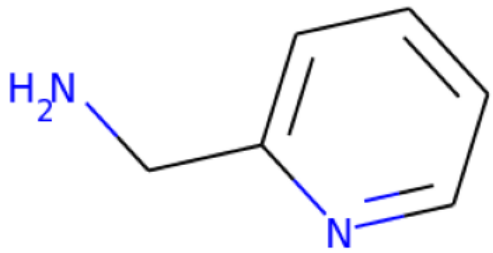
0.030795

Top predicted substructures	prob		
[#6H1]	0.9941	[cX3H1]([cX3H1])[cX3H0]	0.7864
[#6X3][#6X3]	0.9803	[#7][#6][#6][#6X3]	0.738
[#6X3H1][#6X3H0]	0.9093	[cH][cH]	0.7282
[cH]	0.8626	[#7][#6H0][#6H1]	0.6851
[#7][#6][#6X3]	0.8431	[#7][#6X3H0][#6X3H1]	0.6356

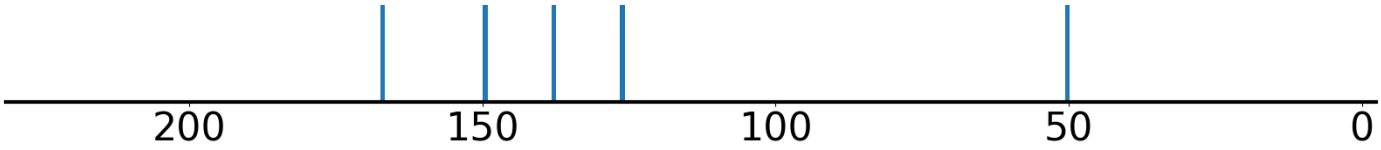
best positives	prob	best negatives	prob
[#6H1]	0.9941	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9803	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9093	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.8626	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#7][#6][#6X3]	0.8431	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.7864	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6][#6][#6X3]	0.738	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[cH][cH]	0.7282	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[#7][#6H0][#6H1]	0.6851	[CX4H2]([CX4H0])[CX2H0]	0.0
[#7][#6X3H0][#6X3H1]	0.6356	[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.4699	[cX3H1]([nX3H1])[cX3H1]	0.0997
[OX2H1]	0.4697	[#7H][#6X3H1]	0.1612
[#6X3][#6X3][#6X3][#6X3]	0.4444	[#8]=[#6][#6H1][#6H1]	0.2121
[#8]=[#6][#8]	0.4013	[#7][#6][#6][#6][#7]	0.2122
[#8][#6][#6][#6X3]	0.3816	[#7][#6H0][#7]	0.278
[#7X3H2]	0.3228	[#7X3H1]	0.4124
[OX2H][cX3]:[c]	0.3076	O=[#6][#6][#6X3]	0.4135
[cH]cO	0.2842	[OX1H0]=[cX3H0][cX3H1]	0.4206
[#7][#7]	0.2816	O=[cX3]	0.4341
[CX3](=[OX1])O	0.2715	[#7][#6][#7]	0.463

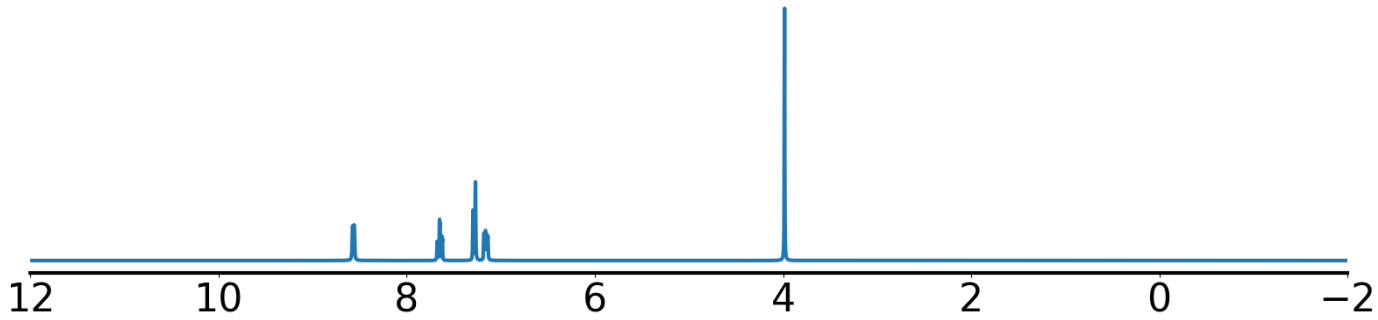
Example 54 true smiles: NCc1ccccn1 formula: C6H8N2
Index of correct structure: 0 of 4358
True structure loss: 0.012161
True structure:



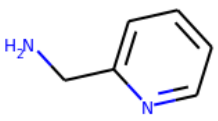
Experimental 13C NMR (solvent: CDCl3)



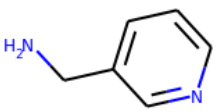
Experimental 1H NMR (solvent: CDCl3)



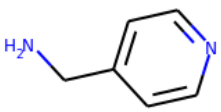
Top predicted structures (loss):



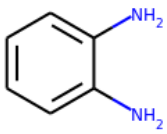
0.012161



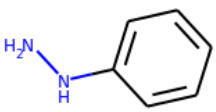
0.020249



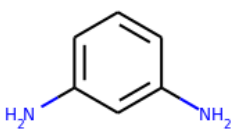
0.021371



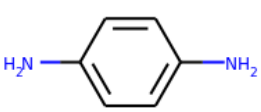
0.025413



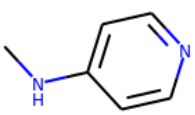
0.030034



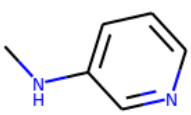
0.031805



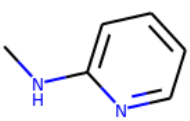
0.035658



0.035862



0.037262



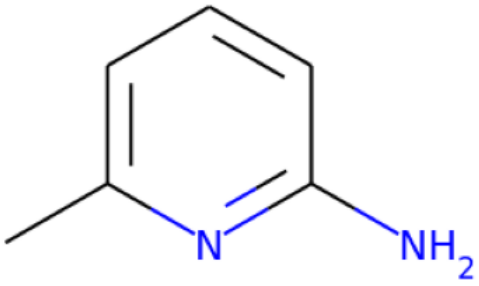
0.037527

Top predicted substructures	prob		
[#6H1]	0.9999	[cH]	0.9518
[#7][#6][#6X3]	0.9927	[#6H1][#6H1]	0.9483
[cH][cH]	0.9887	[cX3H1]([nX2H0])[cX3H1]	0.9449
[#6X3][#6X3]	0.9842	[#6X3][#6X3][#6X3][#6X3]	0.935
[cX3H1]([cX3H1])[cX3H1]	0.9703	[cX3H1]([cX3H1])[cX3H0]	0.9303

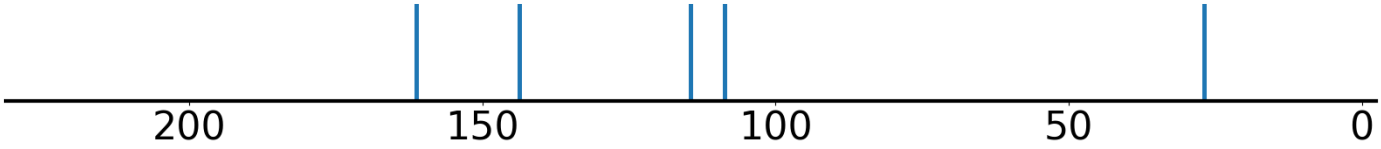
best positives	prob	best negatives	prob
[#6H1]	0.9999	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#7][#6][#6X3]	0.9927	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9887	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3]	0.9842	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9703	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9518	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6H1][#6H1]	0.9483	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[cX3H1]([nX2H0])[cX3H1]	0.9449	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.935	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9303	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.4853	[#7][#6][#6][#7]	0.2992
[CX4H3]	0.4706	[#7X3H2]	0.5031
[#7X3H1]	0.2605	[#6X3][#7][#6X3]	0.5142
[CHX3]=[CHX3]	0.2578	[#7H2][#6H2]	0.528
[#7][#6][#7]	0.244	[#7X3][#6H2]	0.6095
[#6H1][#7][#6H1]	0.2378	[#7][#6H2]	0.6933
[#6H3][#7]	0.1691	[#7][#6H0][#6H1]	0.7268
[CX4H2][CX3H]	0.1506	[#7][#6X3H0][#6X3H1]	0.7429
[#7][#6H0][#7]	0.1391	[#6X3][#6H2][#7]	0.8122
[#7H2][#6H0]	0.1267	[#6X3H1][#6X3H0]	0.8232

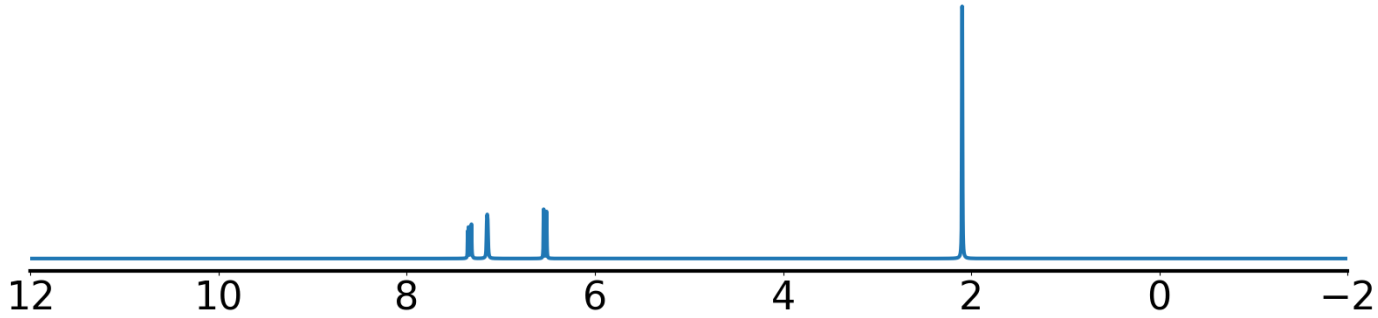
Example 55 true smiles: Cc1cccc(N)n1 formula: C6H8N2
Index of correct structure: 0 of 4358
True structure loss: 0.017386
True structure:



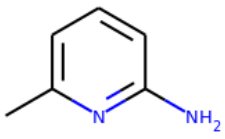
Experimental 13C NMR (solvent: CDCl3)



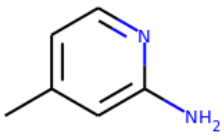
Experimental 1H NMR (solvent: CDCl3)



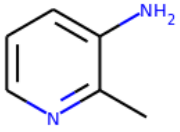
Top predicted structures (loss):



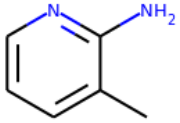
0.017386



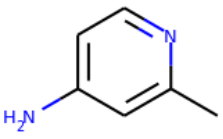
0.023935



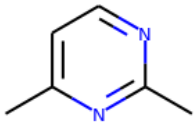
0.02415



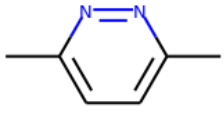
0.024627



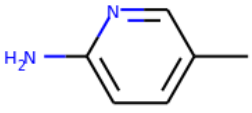
0.025266



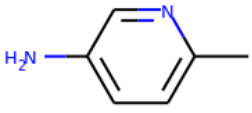
0.025368



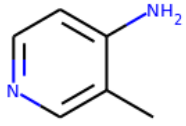
0.027708



0.03032



0.032023



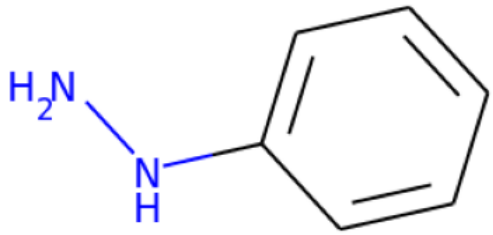
0.035372

Top predicted substructures	prob		
[#6H1]	0.9981	[cX3H1]([cX3H1])[cX3H0]	0.977
[cH][cH]	0.9943	[#7][#6][#6X3]	0.9361
[CX4H3]	0.9924	[#6X3][#6X3][#6X3][#6X3]	0.9352
[#6X3][#6X3]	0.9852	[#6H3][#6H0]	0.928
[cH]	0.9783	[#6X3H1][#6X3H0]	0.9121

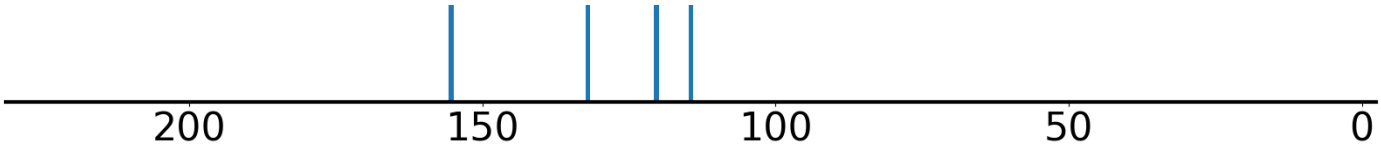
best positives	prob	best negatives	prob
[#6H1]	0.9981	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[cH][cH]	0.9943	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3]	0.9924	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3]	0.9852	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cH]	0.9783	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.977	[OX2H1][CX4H0][CX4H2][CX4H0]	0.0
[#7][#6][#6X3]	0.9361	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9352	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6H3][#6H0]	0.928	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9121	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7X3][#6X3]	0.6413	[#7H2][#6H0]	0.3514
[#7X3H1]	0.554	[#6]1[#6][#6][#6][#6][#7]1	0.422
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5275	[#7][#6H0][#7]	0.4561
[#7H][#6X3H1]	0.277	[#6H3][#6H0][#7H0][#6H0]	0.4617
[CX4H3][CX3]	0.2544	[#7][#6][#7]	0.5142
[#6]1[#6][#6][#6][#7]1	0.2539	[#7X3H2]	0.5202
[#7][#7]	0.2366	[#6X3][#6][#6][#6H3]	0.5282
[#7X3H0]	0.1952	[#6H3][#6][#6X3]	0.5868
[#6]=[#7H]	0.1843	[#7][#6][#6H3]	0.6043
[CX4H3][CX3H0]	0.1842	[#7][#6X3H0][#6X3H1]	0.734

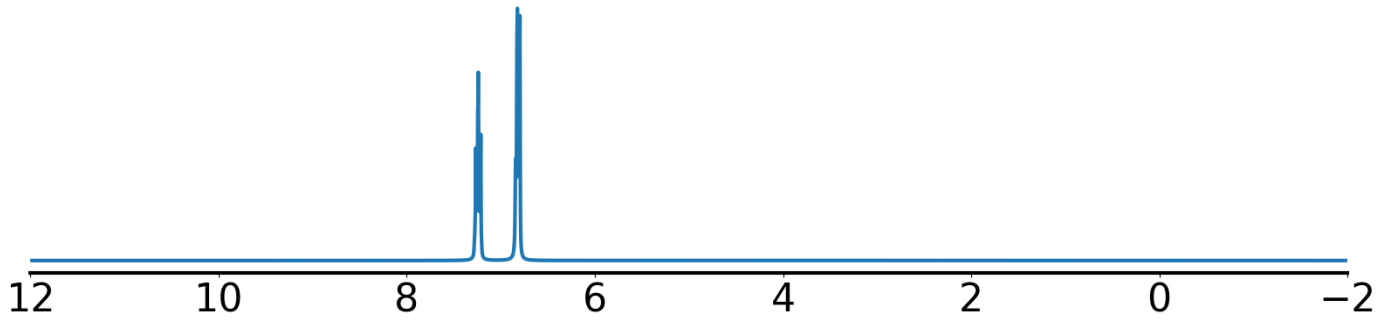
Example 56 true smiles: NNc1ccccc1 formula: C6H8N2
Index of correct structure: 1 of 4358
True structure loss: 0.019757
True structure:



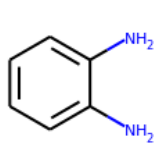
Experimental 13C NMR (solvent: CDCl3)



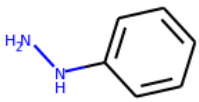
Experimental 1H NMR (solvent: CDCl3)



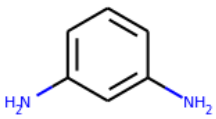
Top predicted structures (loss):



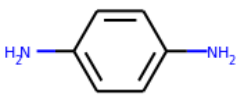
0.018309



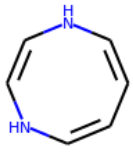
0.019757



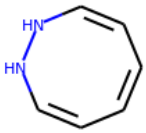
0.021042



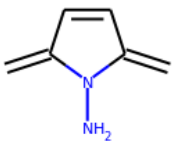
0.024399



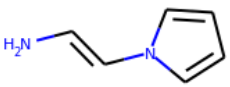
0.032753



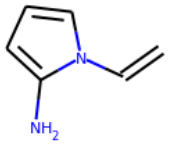
0.035244



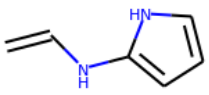
0.043157



0.04647



0.050038



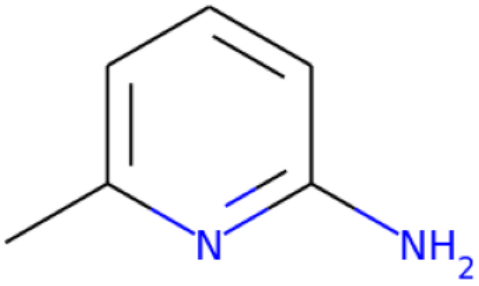
0.051222

Top predicted substructures	prob		
[cH][cH]	0.9995	[cX3H1]([cX3H1])[cX3H0]	0.9884
[#6H1]	0.9994	[cH]	0.9875
[#6X3][#6X3]	0.9954	[cX3H1]([cX3H1])[cX3H1]	0.9844
[#6X3][#6X3][#6X3][#6X3]	0.9949	[#7][#6][#6][#6X3]	0.9666
[#7][#6][#6X3]	0.9921	[#6X3H1][#6X3H0]	0.9489

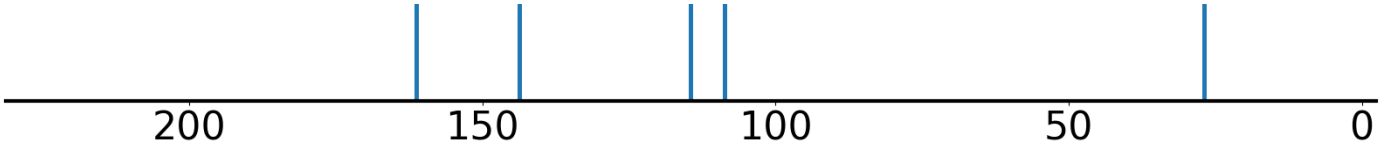
best positives	prob	best negatives	prob
[cH][cH]	0.9995	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H1]	0.9994	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3]	0.9954	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9949	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#7][#6][#6X3]	0.9921	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9884	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9875	[OX2H0]1[CX4H2][CX4H2][CX4H0]1	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9844	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.9666	[OX2H1][CX4H0][CX4H1]([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9489	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7][#6X3]	0.8957	[#7][#7H1]	0.0997
[#6X3][#7X3][#6X3]	0.8123	[#7][#7]	0.1497
[#6]1[#6][#6][#6][#6][#7]1	0.6365	[#7X3H1]	0.549
[#7H2][#6H0]	0.5821	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7398
[#7][#6H0][#7]	0.5793	[#7][#6X3H0][#6X3H1]	0.7727
[#7H][#6X3H1]	0.5137	[#7][#6H0][#6H1]	0.7849
[#7][#6][#7]	0.4792	[#6]1[#6][#6][#6][#6][#6]1	0.8317
[#6]1[#6][#6][#6][#7]1	0.4378	[#7X3H2]	0.8412
[#7X3H0]	0.3779	[#6H1][#6H1]	0.9061
[cX3H1]([nX3H1])[cX3H1]	0.3363	[#6X3H1][#6X3H0]	0.9489

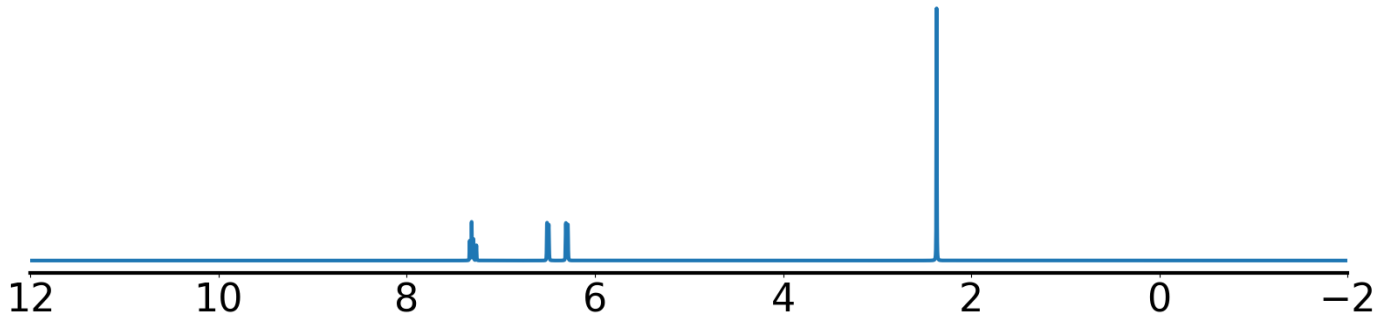
Example 57 true smiles: Cc1cccc(N)n1 formula: C6H8N2
Index of correct structure: 0 of 4358
True structure loss: 0.016728
True structure:



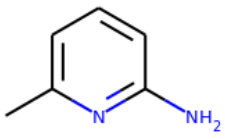
Experimental 13C NMR (solvent: CDCl3)



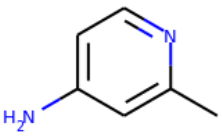
Experimental 1H NMR (solvent: CDCl3)



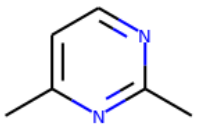
Top predicted structures (loss):



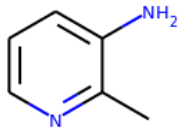
0.016728



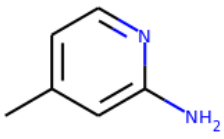
0.022537



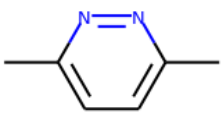
0.023097



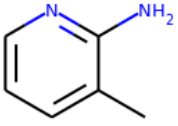
0.023302



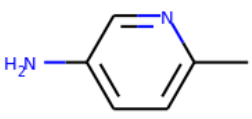
0.024167



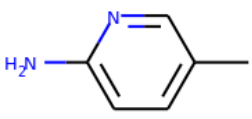
0.025751



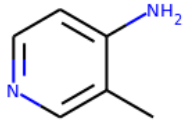
0.029256



0.030268



0.030902



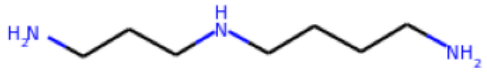
0.037129

Top predicted substructures	prob		
[#6H1]	0.9989	[cH]	0.9807
[cH][cH]	0.9967	[#7][#6][#6X3]	0.9724
[CX4H3]	0.995	[#6X3H1][#6X3H0]	0.968
[#6X3][#6X3]	0.9881	[#6X3][#6X3][#6X3][#6X3]	0.9596
[cX3H1]([cX3H1])[cX3H0]	0.9852	[#6H3][#6H0]	0.9539

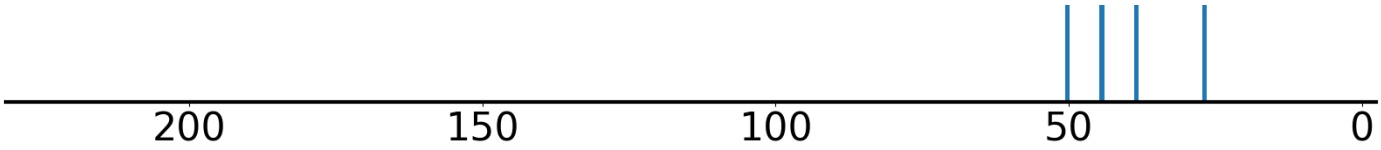
best positives	prob	best negatives	prob
[#6H1]	0.9989	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9967	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[CX4H3]	0.995	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6X3][#6X3]	0.9881	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9852	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cH]	0.9807	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.9724	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.968	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9596	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6H3][#6H0]	0.9539	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7X3][#6X3]	0.7699	[#7H2][#6H0]	0.2438
[#7X3H1]	0.629	[#7X3H2]	0.2453
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5472	[#7][#6][#7]	0.379
[#7H][#6X3H1]	0.2591	[#7][#6H0][#7]	0.4221
[cX3H1]([cX3H0])[cX3H0]	0.2153	[#6]1[#6][#6][#6][#6][#7]1	0.6541
[#6H3][#7]	0.2029	[#6H3][#6H0][#7H0][#6H0]	0.6721
[#7X3H0]	0.2019	[#6H3][#6][#6X3]	0.7687
[#7][#6][#6][#6][#7]	0.1944	[#6X3][#6][#6][#6H3]	0.7763
[cX3H1]([nX2H0])[cX3H1]	0.1778	[cX3H1]([cX3H1])[cX3H1]	0.8309
[cX3H1]([nX3H1])[cX3H1]	0.1711	[#7][#6X3H0][#6X3H1]	0.8473

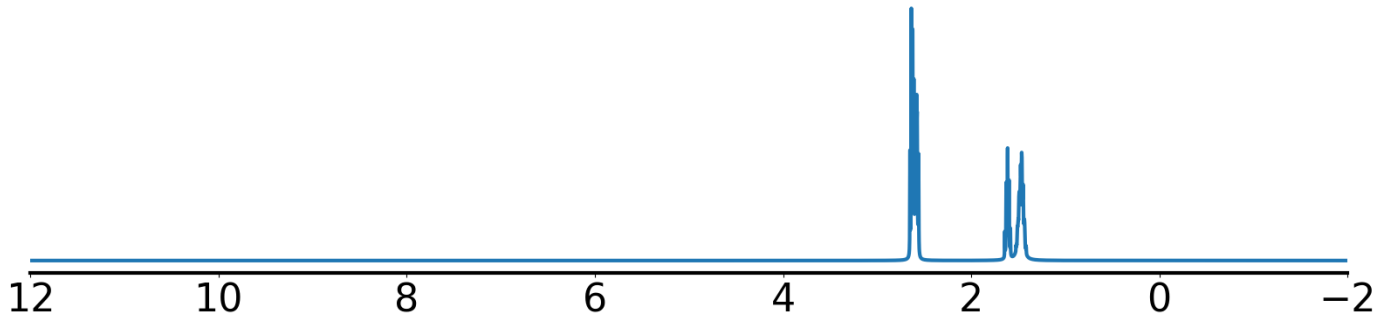
Example 58 true smiles: NCCCCNCCCN formula: C7H19N3
Index of correct structure: 0 of 4058
True structure loss: 0.010241
True structure:



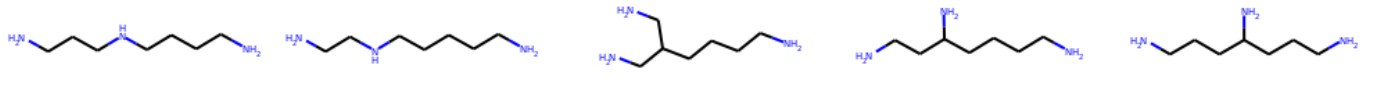
Experimental 13C NMR (solvent: D2O)



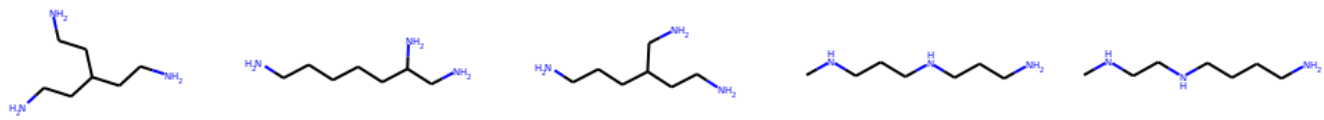
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.010241 0.016137 0.020638 0.022335 0.023653



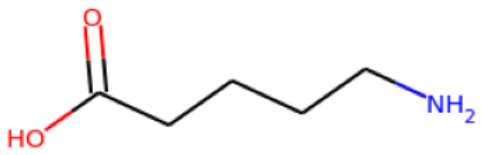
0.023821 0.025178 0.028091 0.031008 0.03336

Top predicted substructures	prob		
[#7X3H2]	1.0	[#7][#6H2][#6H2]	0.9648
[CX4H2]([#6])[#6]	0.9995	[CX4H2]([NX3H2])[CX4H2]	0.9246
[#7X3][#6H2]	0.9936	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9006
[#7][#6H2]	0.9891	[CX4H2][CX4H2]	0.8929
[#7H2][#6H2]	0.9855	[CX4H2]([CX4H2])[CX4H2]	0.8557

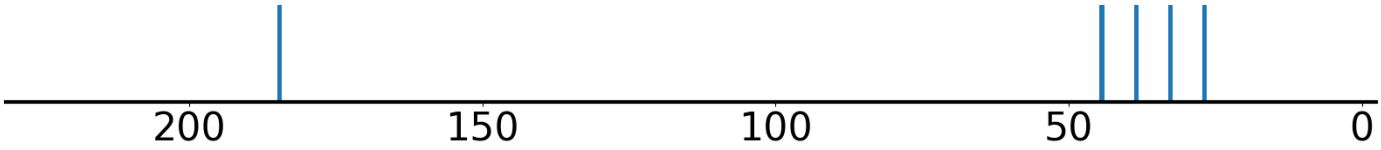
best positives	prob	best negatives	prob
[#7X3H2]	1.0	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9995	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3][#6H2]	0.9936	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7][#6H2]	0.9891	C=CC=CC#C	0.0
[#7H2][#6H2]	0.9855	[#6X2][#6H1][#6X2]	0.0
[#7][#6H2][#6H2]	0.9648	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2]([NX3H2])[CX4H2]	0.9246	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.9006	CC#CCC=C	0.0
[CX4H2][CX4H2]	0.8929	C=CCCC#C	0.0
[CX4H2]([CX4H2])[CX4H2]	0.8557	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7H2][#6H1]	0.5241	[#6H2][#7][#6H2]	0.0919
[#6H1][#6H2]	0.4136	[#7X3H1]	0.2527
[#6H1]	0.3811	[CX4H2]([NX3H1])[CX4H2]	0.5462
[CX4H2]([NX3H2])[CX4H1]	0.2582	[#7][#6][#6][#6][#6][#7]	0.6442
[#7][#6][#6][#7]	0.2526	[#7][#6][#6][#6][#7]	0.7666
[#6H1][#6H2][#6][#6][#7]	0.1983	[CX4H2]([CX4H2])[CX4H2]	0.8557
CCCCCC	0.1571	[CX4H2][CX4H2]	0.8929
[CX4H2]([CX4H2])[CX4H1]	0.1543	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9006
[#6H1]([#6H2])[#6H2]	0.1199	[CX4H2]([NX3H2])[CX4H2]	0.9246
[CX4H3][#6]	0.1152	[#7][#6H2][#6H2]	0.9648

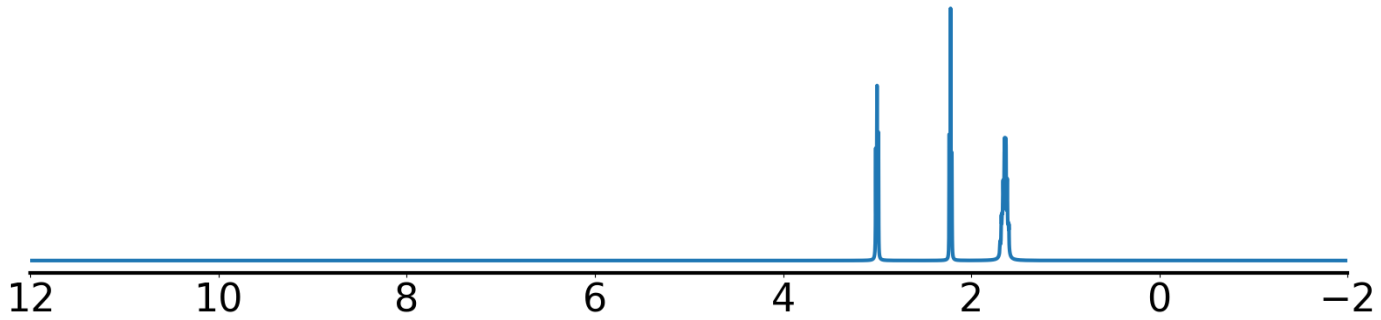
Example 59 true smiles: NCCCCC(=O)O formula: C5H11NO2
Index of correct structure: 0 of 3703
True structure loss: 0.006702
True structure:



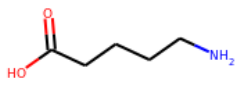
Experimental 13C NMR (solvent: D2O)



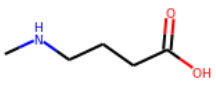
Experimental 1H NMR (solvent: D2O)



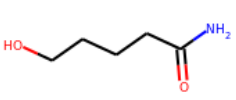
Top predicted structures (loss):



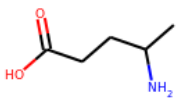
0.006702



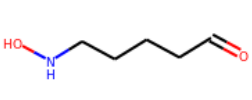
0.042572



0.05026

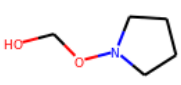


0.060383

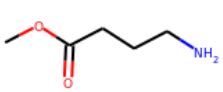


0.062468

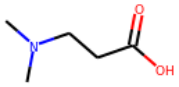
0.064524



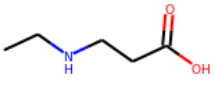
0.065611



0.066211



0.068058



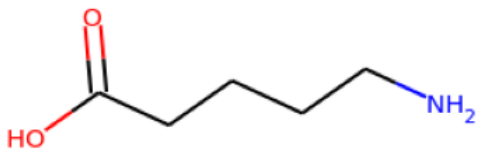
0.069829

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9999	[CX4H2]([CX4H2])[CX4H2]	0.9688
[OX2H1]	0.9971	[#7][#6H2][#6H2]	0.9436
[CX3](=[OX1])C	0.9947	[#7][#6H2]	0.9371
[CX4H2][CX4H2]	0.9898	[#7X3][#6H2]	0.9334
[CX3](=O)[OX2H1]	0.9785	OCC[CH2]	0.9257

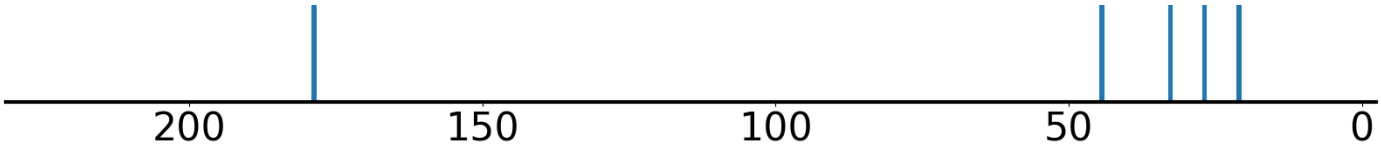
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9971	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9947	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2][CX4H2]	0.9898	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=O)[OX2H1]	0.9785	CCC#CC#C	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9688	CCC=CC#C	0.0
[#7][#6H2][#6H2]	0.9436	CC=CC#CC	0.0
[#7][#6H2]	0.9371	[#6X2][#6H1][#6X2]	0.0
[#7X3][#6H2]	0.9334	CC=CCC#C	0.0
OCC[CH2]	0.9257	[CX2H0](#[CX2H1])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#7H2][#6H0]	0.2692	[#8][#6][#6H2]	0.5826
[#6H1][#6H2]	0.2619	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.5931
[#6H1]	0.2432	[#8]=[#6][#8]	0.7553
[#7X3H1]	0.2313	[CX4H2][CX4H2][CX4H2][CX4H2]	0.8275
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.1962	[#7H2][#6H2]	0.854
[CX4H2]([CX4H2])[CX4H1]	0.1888	[#7X3H2]	0.8691
[#8]=[#6H0][#6H1]	0.1744	[CX3](=[OX1])O	0.8712
[#8][#6H0][#6H1]	0.1424	[CX4H2][CX3]=O	0.8768
CCCCCC	0.0969	[CX4H2]([CX4H2])[CX3H0]	0.8926
[#6H2][#7][#6X3]	0.0887	[CX4H2]([NX3H2])[CX4H2]	0.9041

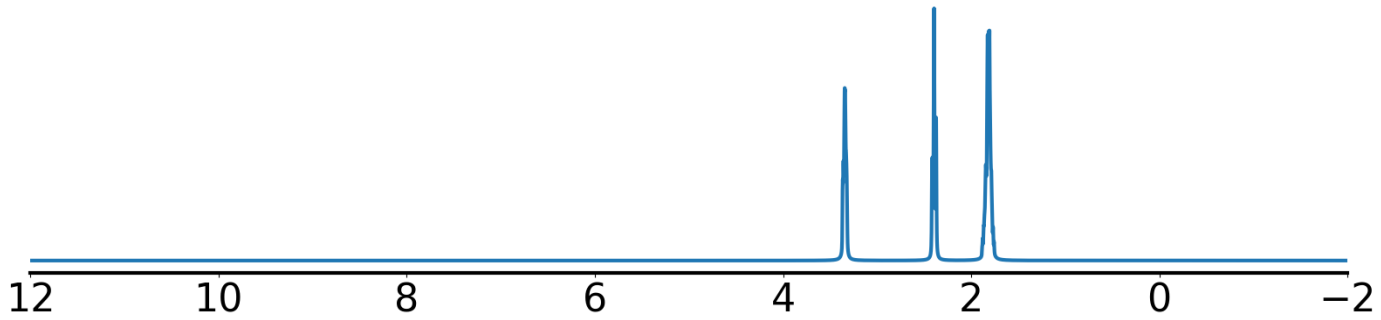
Example 60 true smiles: NCCCCC(=O)O formula: C5H11NO2
Index of correct structure: 0 of 3703
True structure loss: 0.013067
True structure:



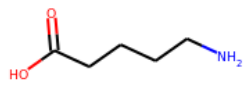
Experimental 13C NMR (solvent: D2O)



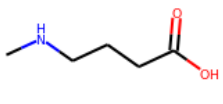
Experimental 1H NMR (solvent: CDCl3)



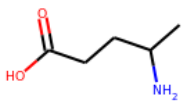
Top predicted structures (loss):



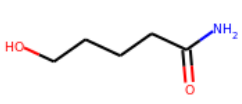
0.013067



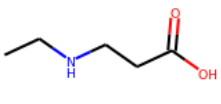
0.044319



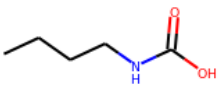
0.044563



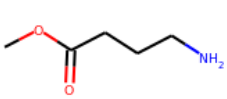
0.053856



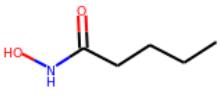
0.055854



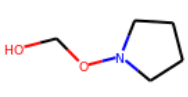
0.05827



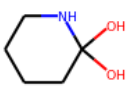
0.060447



0.060671



0.062129



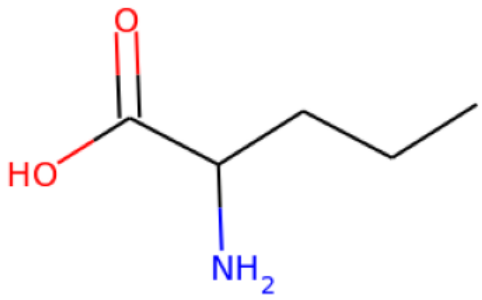
0.063969

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9997	[CX3](=[OX1])O	0.9267
[OX2H1]	0.9955	[CX4H2]CC=O	0.9198
[CX3](=[OX1])C	0.9939	[#7X3][#6H2]	0.9149
[CX3](=O)[OX2H1]	0.9903	[CX4H2][CX4H2]	0.9055
[#7X3H2]	0.9354	[#8]=[#6][#8]	0.8731

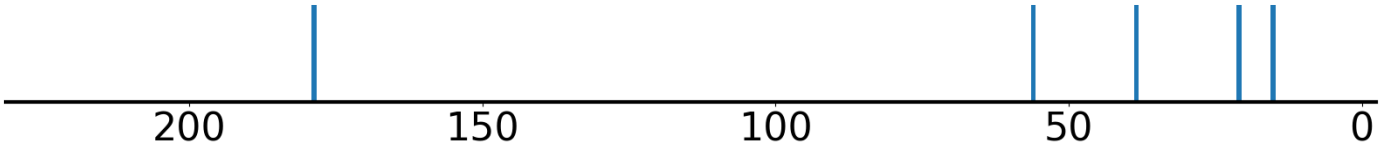
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9997	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9955	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])C	0.9939	CCC=CC#C	0.0
[CX3](=O)[OX2H1]	0.9903	C=CC=CC#C	0.0
[#7X3H2]	0.9354	CC#CCC=C	0.0
[CX3](=[OX1])O	0.9267	CC=CC#CC	0.0
[CX4H2]CC=O	0.9198	CCC#CC#C	0.0
[#7X3][#6H2]	0.9149	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H2][CX4H2]	0.9055	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#8]=[#6][#8]	0.8731	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6386	[#8][#6][#6H2]	0.2864
[#6H1][#6H2]	0.5189	[CX4H2]([NX3H2])[CX4H2]	0.4032
[CX4H2]([CX4H2])[CX4H1]	0.4361	[CX4H2][CX4H2][CX4H2][CX4H2]	0.5129
[#8]=[#6H0][#6H1]	0.327	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.5794
[#6H1]	0.2799	[CX4H2][CX3]=O	0.7031
[CX4H2]([NX3H1])[CX4H2]	0.277	[CX4H2]([CX4H2])[CX3H0]	0.7047
[#7X3H1]	0.263	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.7413
O=[CX3][CX4H]	0.2276	[#7H2][#6H2]	0.7751
[CX4H3][#6]	0.2261	[#7][#6H2]	0.8079
[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.1673	O=[CX3H0][CX4H2][CX4H2]	0.8115

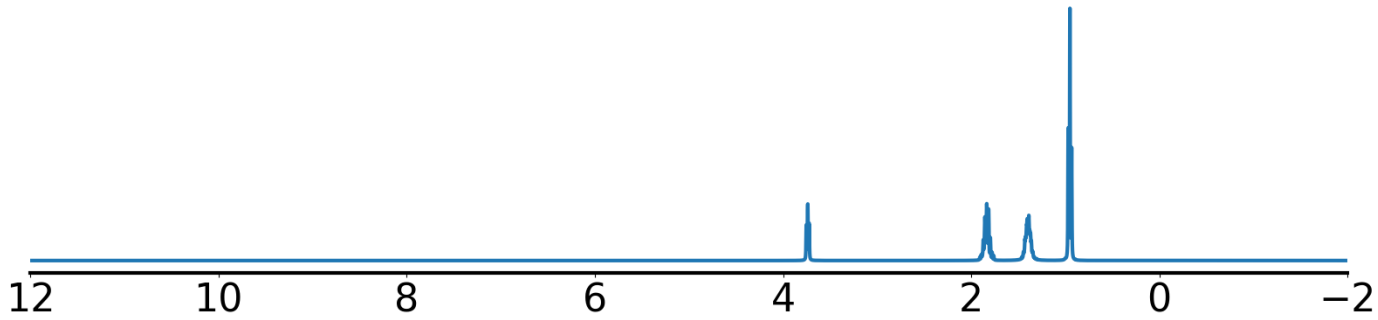
Example 61 true smiles: CCCC(N)C(=O)O formula: C5H11NO2
Index of correct structure: 0 of 3703
True structure loss: 0.01618
True structure:



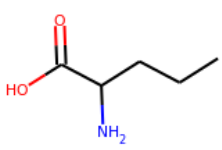
Experimental 13C NMR (solvent: D2O)



Experimental 1H NMR (solvent: D2O)

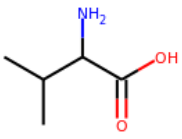


Top predicted structures (loss):



0.01618

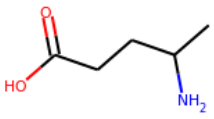
0.040724



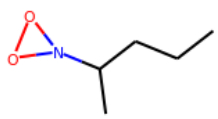
0.043792

0.047883

0.052978

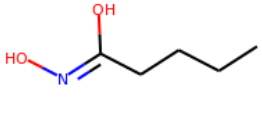


0.054491

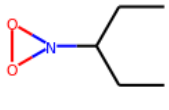


0.055547

0.056181



0.057161



0.058635

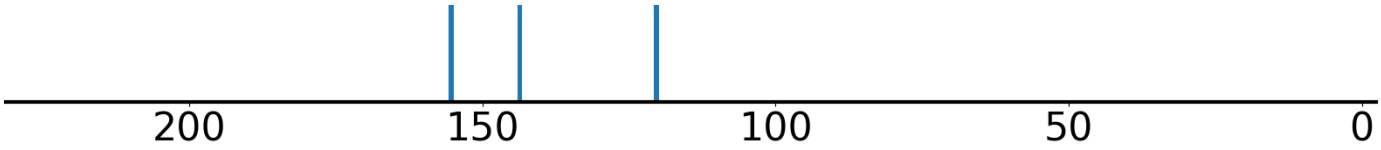
Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][CX4H2]	0.9839
[#6H3][#6][#6]	0.9994	[OX2H1]	0.9725
[CX4H2]([#6])[#6]	0.9958	[#6H1]	0.9698
[CX4H3][#6]	0.9953	[#7X3H2]	0.9613
[CX3](=[OX1])C	0.9874	O=[CX3][CX4H]	0.953

best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9994	CCC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9958	C=CC=CC#C	0.0
[CX4H3][#6]	0.9953	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX3](=[OX1])C	0.9874	CC#CCC=C	0.0
[CX4H3][CX4H2]	0.9839	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX2H1]	0.9725	CC=CC#CC	0.0
[#6H1]	0.9698	CCC#CC#C	0.0
[#7X3H2]	0.9613	CC=CCC#C	0.0
O=[CX3][CX4H]	0.953	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

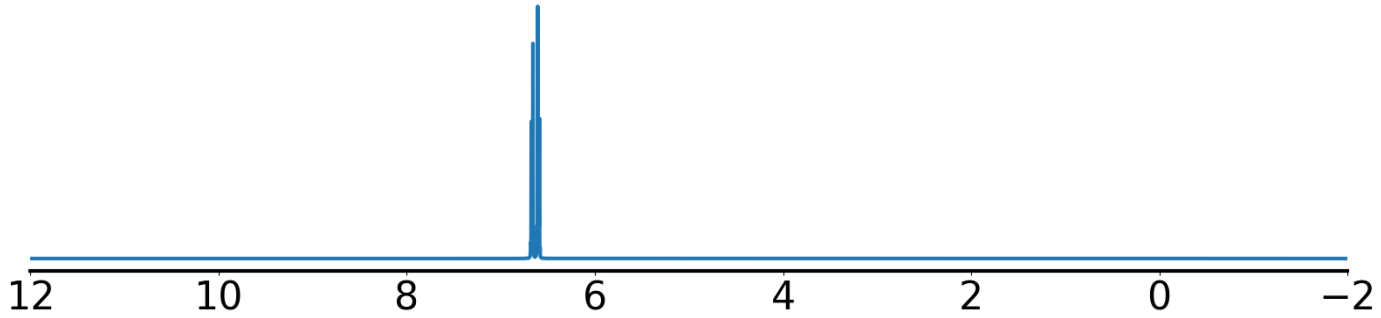
worst negatives	prob	worst positives	prob
[#6X3][#6][#6][#6H3]	0.7254	[CX4H2][CX4H2]	0.3276
[#8]=[#6][#6H1][#6H1]	0.6122	[CX4H2]([CX4H2])[CX4H1]	0.361
[#7H2][#6H0]	0.55	[#8][#6H0][#6H1]	0.4191
[#7][#6H0][#6H1]	0.4041	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.4832
[CX4H2]([CX4H3])[CX4H1]	0.3409	OCC[CH2]	0.4987
[CHX4]([CH3X4])[CH2X4]	0.3215	[#7][#6][#6X3]	0.555
[#6H3][#6H1][#6H1][#7]	0.3063	[#7H2][#6H1]	0.7282
[OH][CX4H]	0.2758	[CX4H2]CC=O	0.7748
[#6H1][#6H1]	0.2632	[#6H1][#6H2]	0.7758
[CX4H3][CX4H1]	0.2398	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.8049

Example 62 true smiles: Nc1ccc(O)cc1 formula: C6H7NO
Index of correct structure: 0 of 3639
True structure loss: 0.014456
True structure:

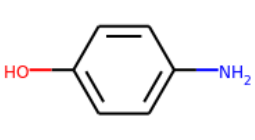
Experimental 13C NMR (solvent: CDCl3)



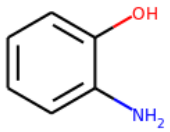
Experimental 1H NMR (solvent: CDCl3)



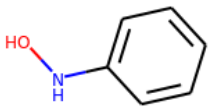
Top predicted structures (loss):



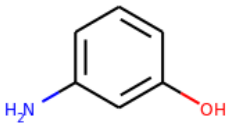
0.014456



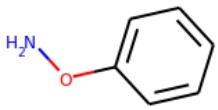
0.01564



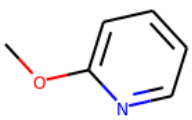
0.017236



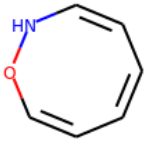
0.018273



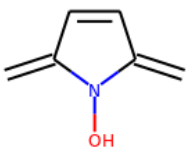
0.019053



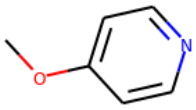
0.033679



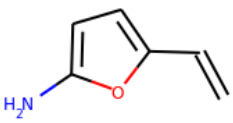
0.038067



0.038271



0.038935



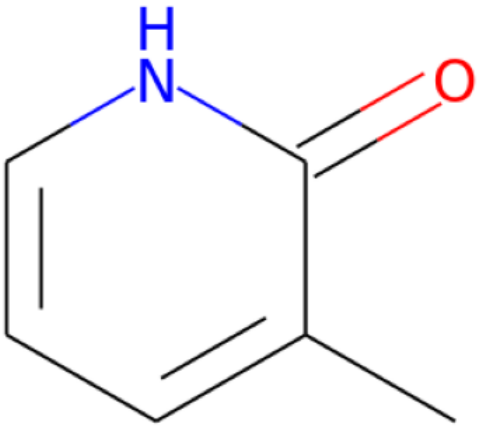
0.039351

Top predicted substructures	prob		
[#6H1]	0.9951	[cH][cH]	0.9133
[#6X3][#6X3]	0.9937	[#7][#6][#6X3]	0.8843
[#6X3][#6X3][#6X3][#6X3]	0.9583	[#7][#6][#6][#6X3]	0.8665
[#6X3H1][#6X3H0]	0.9366	[cX3H1]([cX3H1])[cX3H0]	0.8445
[cH]	0.9182	[#6H1][#6H1]	0.8359

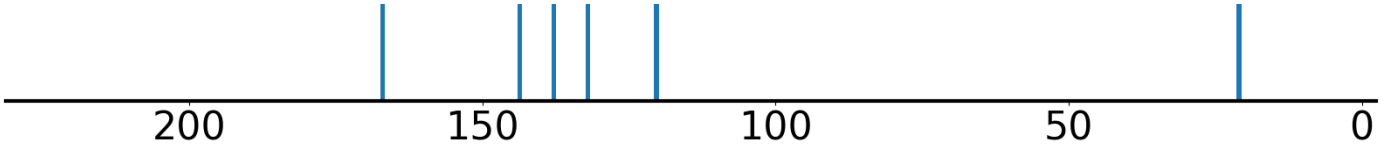
best positives	prob	best negatives	prob
[#6H1]	0.9951	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3]	0.9937	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9583	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9366	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[cH]	0.9182	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cH][cH]	0.9133	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#7][#6][#6X3]	0.8843	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.8665	[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8445	[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.0
[#6H1][#6H1]	0.8359	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.7017	[cX3H0][cX3H1][cX3H1][cX3H0]	0.4082
[#6X3][#7][#6X3]	0.4324	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5256
[#6]1[#6][#6][#6][#6][#7]1	0.3094	[OX2H1]	0.55
[#7X3H1]	0.2147	[cH]cO	0.5598
[#6]1[#6][#6][#6][#7]1	0.1769	[#7][#6X3H0][#6X3H1]	0.5652
[#7H][#6X3H1]	0.1769	[#8][#6][#6][#6X3]	0.5818
[#6X3][#6X3][#6X3]=[#6X3]	0.1658	[#7][#6H0][#6H1]	0.5827
[cX3H1]([nX3H1])[cX3H1]	0.1526	[#8][#6H0][#6H1]	0.595
[#6X3][#7X3][#6X3]	0.1443	[OX2H][cX3]:[c]	0.6068
[CHX3](=C)C	0.1398	[#7H2][#6H0]	0.6205

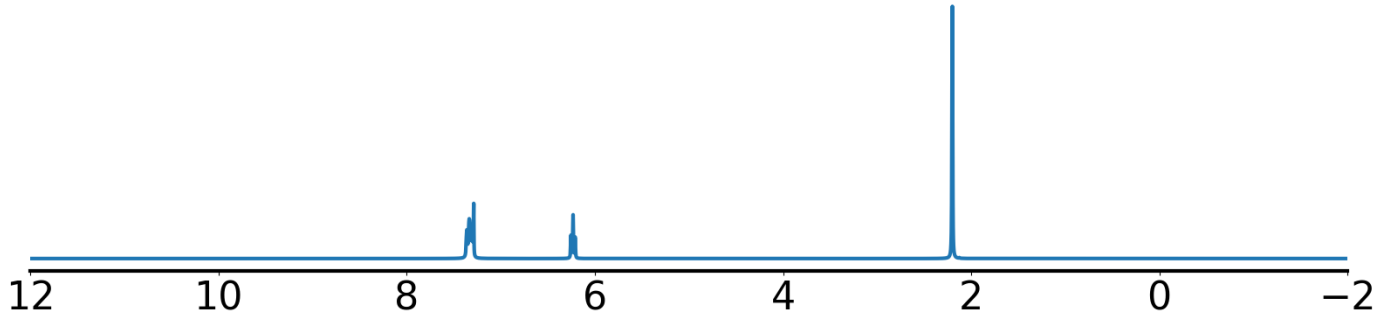
Example 63 true smiles: Cc1ccc[nH]c1=O formula: C6H7NO
Index of correct structure: 2 of 3639
True structure loss: 0.026615
True structure:



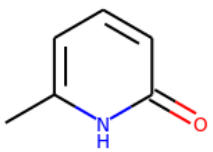
Experimental 13C NMR (solvent: CDCl3)



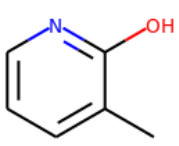
Experimental 1H NMR (solvent: CDCl3)



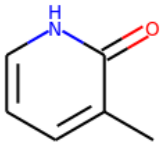
Top predicted structures (loss):



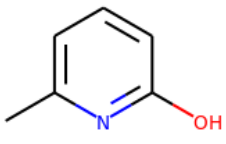
0.021851



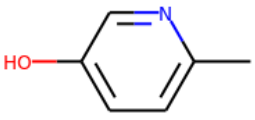
0.025291



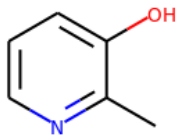
0.026615



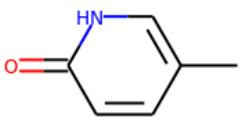
0.028358



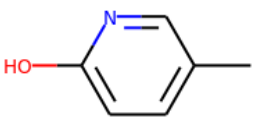
0.03163



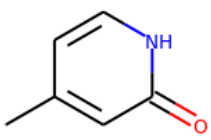
0.03252



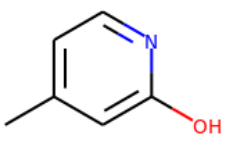
0.033951



0.034559



0.038276



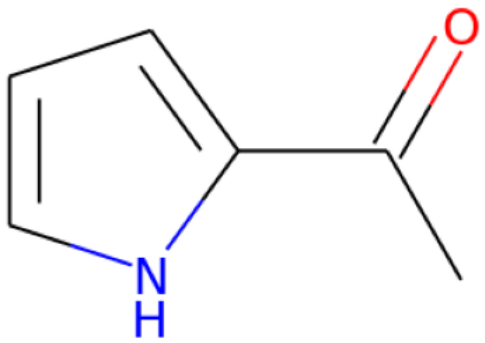
0.040865

Top predicted substructures	prob		
[#6X3][#6X3]	0.9994	[#6H3][#6][#6]	0.969
[#6H1]	0.9987	[#6X3H1][#6X3H0]	0.9507
[CX4H3][#6]	0.9981	[#7][#6][#6X3]	0.9422
[CX4H3]	0.9971	[cH][cH]	0.9314
[#6H3][#6H0]	0.9876	[#6X3][#6X3][#6X3][#6X3]	0.9178

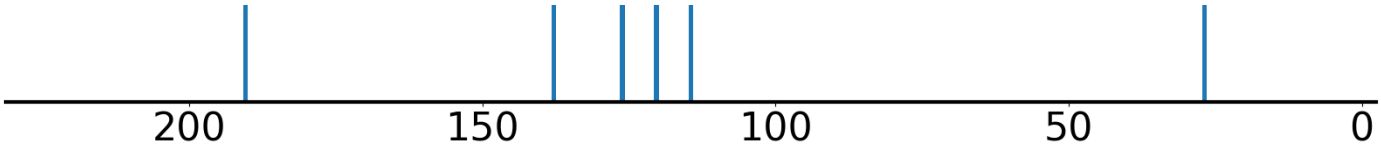
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9994	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H1]	0.9987	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX4H3][#6]	0.9981	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[CX4H3]	0.9971	[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H1]	0.0
[#6H3][#6H0]	0.9876	[CX4H0]([OX2H0])([CX4H2])([CX4H1])[CX4H1]	0.0
[#6H3][#6][#6]	0.969	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9507	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#7][#6][#6X3]	0.9422	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9314	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9178	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#7][#6X3H0][#6X3H1]	0.6262	[cX3H1]([nX3H1])[cX3H1]	0.0321
[#8]=[#6H0][#6H1]	0.591	[#7H][#6X3H1]	0.0995
[#7][#6H0][#6H1]	0.5833	[#7X3H1]	0.2203
[OX2H1]	0.4969	[#6X3][#7X3][#6X3]	0.2368
[#7][#6][#6H3]	0.3692	[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.2751
[OX1H0]=[cX3H0][cX3H1]	0.3616	[cX3H1]([cX3H1])[cX3H1]	0.5041
[CHX3](=C)C	0.3216	O=[cX3]	0.5396
[#7X3H2]	0.2955	O=[#6][#6][#6X3]	0.5542
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.283	[#6X3][#6][#6][#6H3]	0.5731
[#6H3][#6]=[#6X3]	0.2397	[#6]1[#6][#6][#6][#6][#7]1	0.62

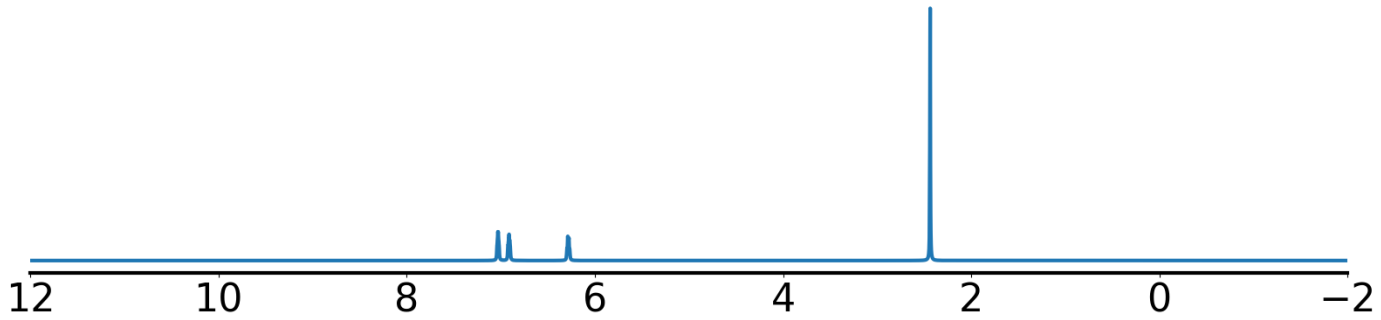
Example 64 true smiles: CC(=O)c1ccc[nH]1 formula: C6H7NO
Index of correct structure: 0 of 3639
True structure loss: 0.022279
True structure:



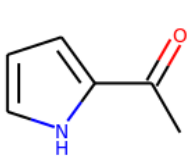
Experimental 13C NMR (solvent: CDCl3)



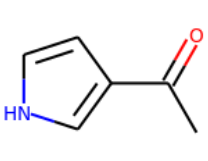
Experimental 1H NMR (solvent: CDCl3)



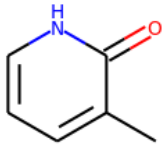
Top predicted structures (loss):



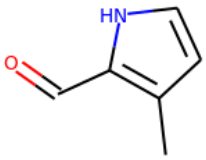
0.022279



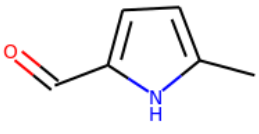
0.029047



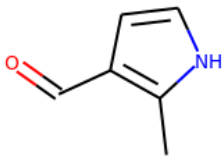
0.038817



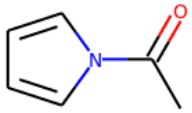
0.042603



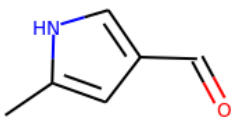
0.043372



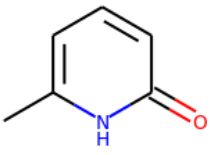
0.043547



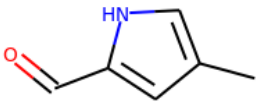
0.045681



0.048993



0.049163



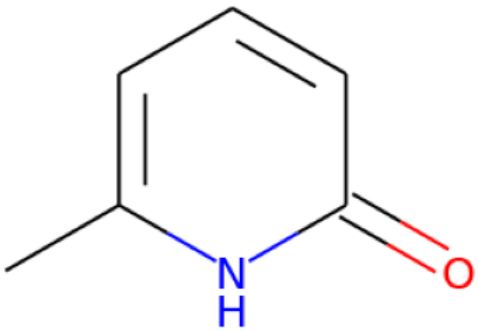
0.050744

Top predicted substructures	prob		
[#6H1]	0.9964	[OX1H0]=[CX3H0][CX4H3]	0.9259
[#6X3][#6X3]	0.9911	[#6H3][#6H0]	0.9225
[CX4H3]	0.9884	[#6H1][#6H1]	0.8845
[#6H3][#6][#6]	0.9632	[CX4H3][CX3]	0.8653
[CX4H3][#6]	0.9604	[cH][cH]	0.8462

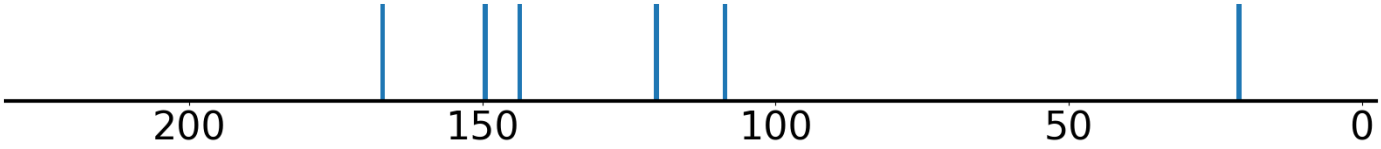
best positives	prob	best negatives	prob
[#6H1]	0.9964	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9911	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[CX4H3]	0.9884	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#6H3][#6][#6]	0.9632	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX4H3][#6]	0.9604	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9259	[CX4H0]([OX2H0])([CX4H2])([CX4H1])[CX4H1]	0.0
[#6H3][#6H0]	0.9225	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6H1][#6H1]	0.8845	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[CX4H3][CX3]	0.8653	[OX2H1][CX4H1][CX4H1]([CX4H2])[CX4H2]	0.0
[cH][cH]	0.8462	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6]=[#6X3]	0.5372	[#7][#6H0][#6H1]	0.2855
[CHX3](=C)C	0.3737	[#7][#6X3H0][#6X3H1]	0.2927
[CX4H2]([#6])[#6]	0.2578	[#6H1r5][#7]	0.3125
[#7X3H2]	0.2476	[cX3H1]([nX3H1])[cX3H1]	0.329
[#7H2][#6H0]	0.2456	[#6]1[#6][#6][#6][#7]1	0.3496
[#6]#[#7]	0.2436	[#7X3H1]	0.4309
[#6H1][#6H2]	0.2259	[#6X3][#6][#6][#6H3]	0.4659
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.2223	[#7H][#6X3H1]	0.4737
[CX4H2][CX4H2]	0.2172	[cX3H1]([cX3H1])[cX3H1]	0.4826
[CX4H3][cX3H0]	0.1866	[#7][#6][#6][#6X3]	0.4884

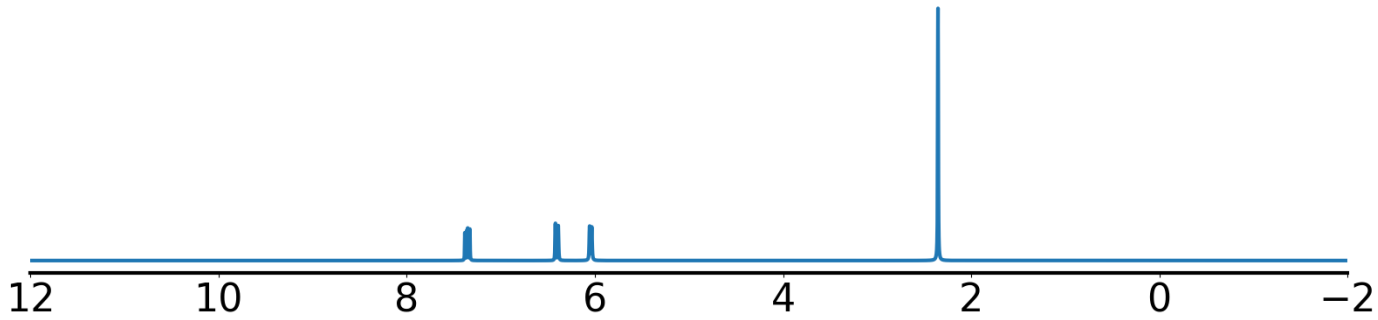
Example 65 true smiles: Cc1cccc(=O)[nH]1 formula: C6H7NO
Index of correct structure: 0 of 3639
True structure loss: 0.018889
True structure:



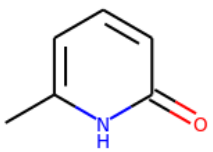
Experimental 13C NMR (solvent: CDCl3)



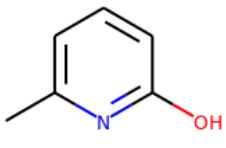
Experimental 1H NMR (solvent: CDCl3)



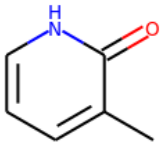
Top predicted structures (loss):



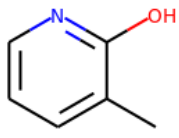
0.018889



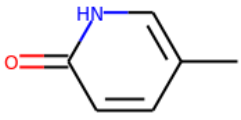
0.025633



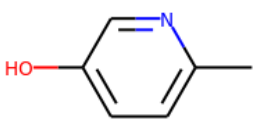
0.029254



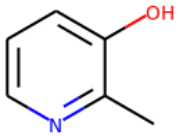
0.029349



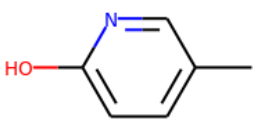
0.029649



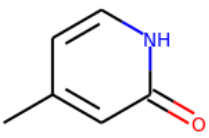
0.029797



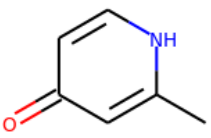
0.031335



0.032642



0.033015



0.034282

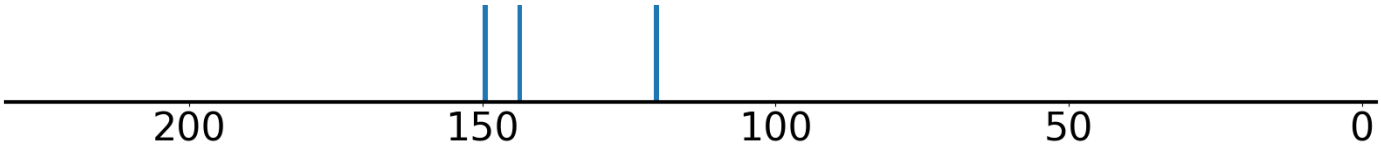
Top predicted substructures	prob		
[#6H1]	0.9989	[cX3H1]([cX3H1])[cX3H0]	0.9802
[#6X3][#6X3]	0.9986	[CX4H3]	0.9788
[cH][cH]	0.9943	[#6X3][#6X3][#6X3][#6X3]	0.9711
[CX4H3][#6]	0.9881	[cH]	0.9365
[#6X3H1][#6X3H0]	0.9857	[#7][#6][#6X3]	0.9303

best positives	prob	best negatives	prob
[#6H1]	0.9989	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9986	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[cH][cH]	0.9943	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX4H3][#6]	0.9881	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3H1][#6X3H0]	0.9857	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9802	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[CX4H3]	0.9788	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9711	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cH]	0.9365	[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.9303	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0

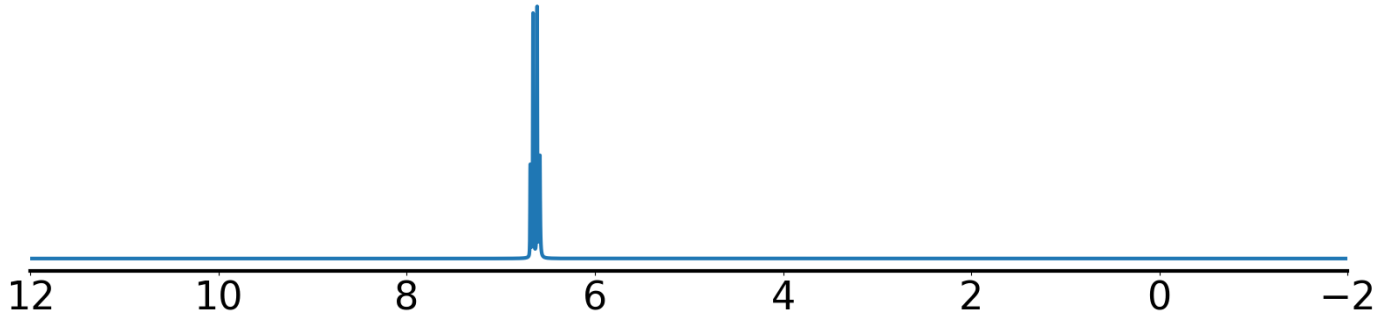
worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.6411	[#7X3H1]	0.261
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5062	[#6X3][#7X3][#6X3]	0.2929
[#8][#6][#6][#6X3]	0.3913	[#8]=[#6][#6H1][#6H1]	0.3071
[cX3H1]([cX3H0])[cX3H0]	0.2753	[#7][#6][#6H3]	0.4016
[cX3H1]([oX2H0])[cX3H1]	0.2596	O=[cX3]	0.4845
[cX3H0][cX3H1][cX3H1][cX3H0]	0.2345	[#6]1[#6][#6][#6][#6][#7]1	0.5562
[#8][#6H1][#6H1]	0.2197	[#8]=[#6H0][#6H1]	0.6413
[#6H3][#6H0][#7H0][#6H0]	0.1723	[OX1H0]=[cX3H0][cX3H1]	0.6471
[cX3H1]([nX2H0])[cX3H1]	0.1685	O=[#6][#6][#6X3]	0.6626
[#7H2][#6H0]	0.1585	[cX3H1]([cX3H1])[cX3H1]	0.7113

Example 66 true smiles: Nc1ccc(O)cc1 formula: C6H7NO
Index of correct structure: 0 of 3639
True structure loss: 0.015917
True structure:

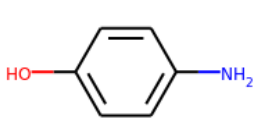
Experimental 13C NMR (solvent: DMSO)



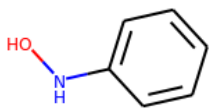
Experimental 1H NMR (solvent: CDCl3)



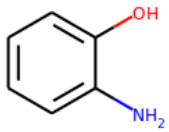
Top predicted structures (loss):



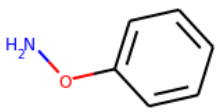
0.015917



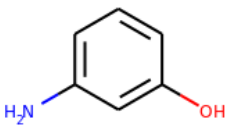
0.016321



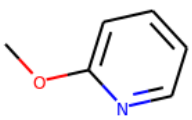
0.016459



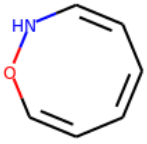
0.017054



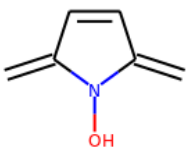
0.018874



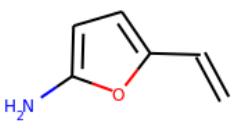
0.036082



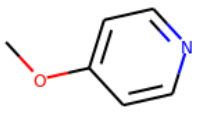
0.036564



0.038092



0.038165



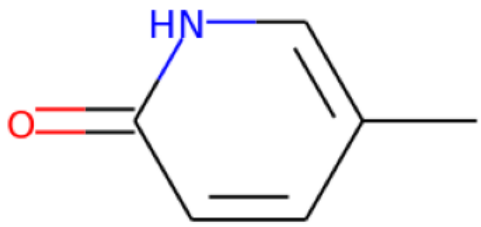
0.040932

Top predicted substructures	prob		
[#6H1]	0.994	[cH]	0.8872
[#6X3][#6X3]	0.9916	[cX3H1]([cX3H1])[cX3H0]	0.8649
[#6X3][#6X3][#6X3][#6X3]	0.9268	[#6H1][#6H1]	0.8164
[#6X3H1][#6X3H0]	0.9192	[#7][#6][#6X3]	0.7911
[cH][cH]	0.8966	[#7][#6][#6][#6X3]	0.7567

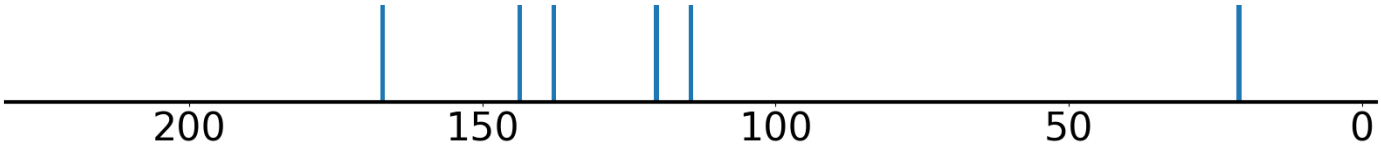
best positives	prob	best negatives	prob
[#6H1]	0.994	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9916	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9268	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9192	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH][cH]	0.8966	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.8872	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8649	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#6H1][#6H1]	0.8164	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.7911	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[#7][#6][#6][#6X3]	0.7567	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.7149	[cX3H0][cX3H1][cX3H1][cX3H0]	0.2257
[#6X3][#7][#6X3]	0.3167	[#8][#6H0][#6H1]	0.4292
[#7X3H1]	0.1862	[#7H2][#6H0]	0.4944
[#6]1[#6][#6][#6][#7]1	0.1815	[OX2H][cX3]:[c]	0.5058
[cX3H1]([nX3H1])[cX3H1]	0.1616	[#7][#6H0][#6H1]	0.5097
[CX3H1](=[CX3H1])[CX3H0]	0.1569	[#7][#6X3H0][#6X3H1]	0.5117
[#7H][#6X3H1]	0.1421	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.538
[CHX3]=[CHX3]	0.1406	[#8][#6][#6][#6X3]	0.5505
[#6X3][#6X3][#6X3]=[#6X3]	0.1382	[#6]1[#6][#6][#6][#6][#6]1	0.5859
[CHX3](=C)C	0.1368	[cH]cO	0.6107

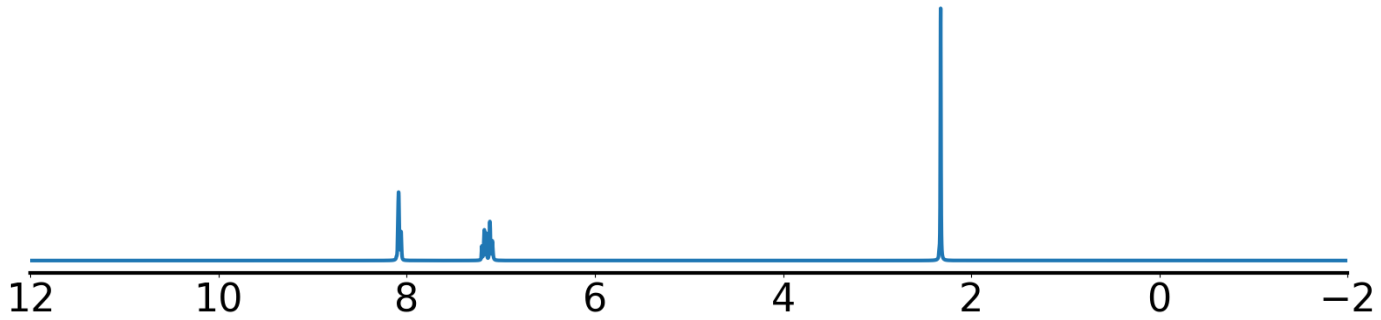
Example 67 true smiles: Cc1ccc(=O)[nH]c1 formula: C6H7NO
Index of correct structure: 7 of 3639
True structure loss: 0.025019
True structure:



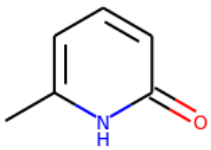
Experimental 13C NMR (solvent: DMSO)



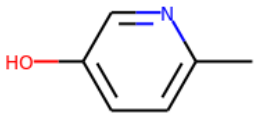
Experimental 1H NMR (solvent: CDCl3)



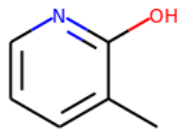
Top predicted structures (loss):



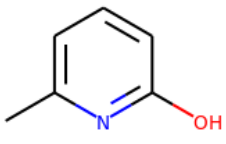
0.0201



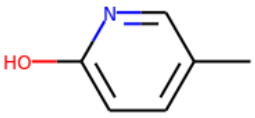
0.02148



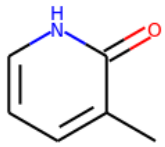
0.022151



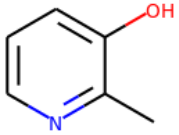
0.022284



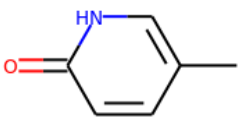
0.022527



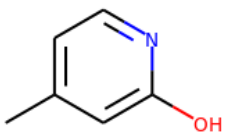
0.024836



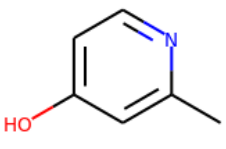
0.024973



0.025019



0.028234



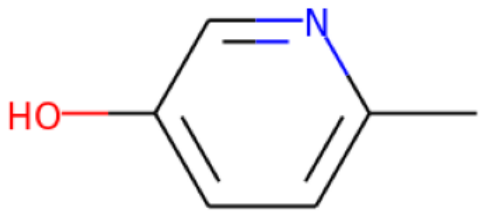
0.028482

Top predicted substructures	prob		
[#6X3][#6X3]	0.9991	[cX3H1]([cX3H1])[cX3H0]	0.9874
[#6H1]	0.9987	[#6H3][#6H0]	0.9847
[cH][cH]	0.9977	[CX4H3]	0.9825
[CX4H3][#6]	0.9958	[cH]	0.981
[#6X3][#6X3][#6X3][#6X3]	0.9926	[#6X3][#6][#6][#6H3]	0.9765

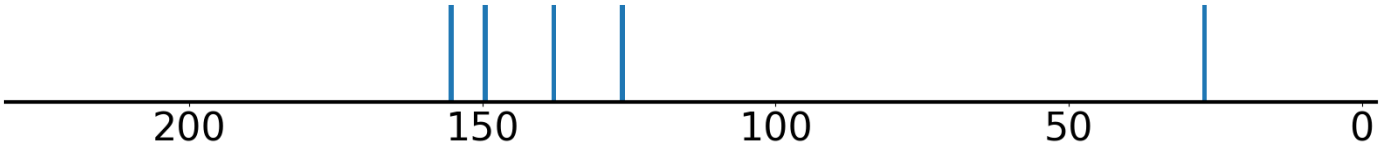
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9991	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H1]	0.9987	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cH][cH]	0.9977	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3][#6]	0.9958	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9926	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9874	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6H3][#6H0]	0.9847	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[CX4H3]	0.9825	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.981	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#6X3][#6][#6][#6H3]	0.9765	[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.6229	[cX3H1]([nX3H1])[cX3H0]	0.0509
[#8][#6][#6][#6X3]	0.5198	[#7H][#6X3H1]	0.1924
[#6]1[#6][#6][#6][#6][#6]1	0.4919	[#6H3][#6H0][#6H1][#7]	0.2246
[#7][#6][#6H3]	0.441	[#7X3H1]	0.2317
[#8][#6H0][#6H1]	0.4295	[#8]=[#6][#6H1][#6H1]	0.244
[cX3H1]([nX2H0])[cX3H1]	0.3516	[#8]=[#6H0][#6H1]	0.2469
[OX2H][cX3]:[c]	0.3225	[OX1H0]=[cX3H0][cX3H1]	0.349
[cX3H1]([cX3H0])[cX3H0]	0.2778	[#6X3][#7X3][#6X3]	0.3921
[OX2H1]	0.2355	O=[cX3]	0.5208
[#7H2][#6H0]	0.2172	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6062

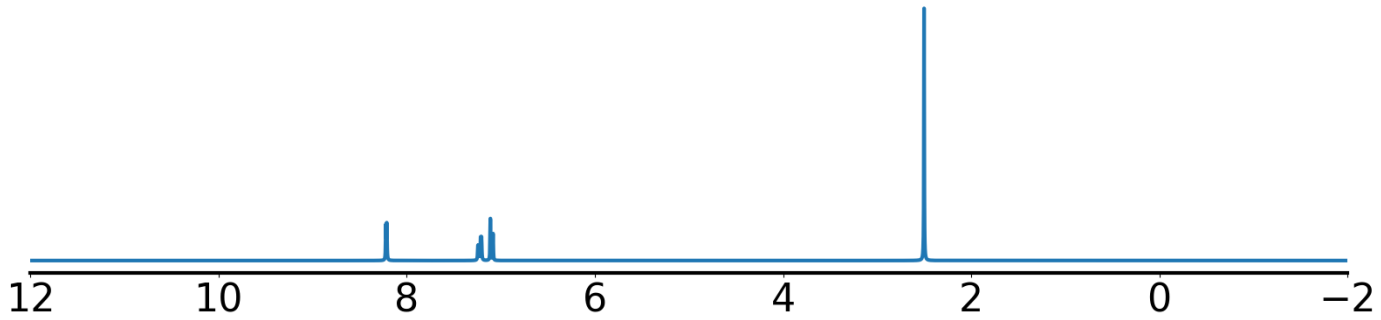
Example 68 true smiles: Cc1ccc(O)cn1 formula: C6H7NO
Index of correct structure: 0 of 3639
True structure loss: 0.014215
True structure:



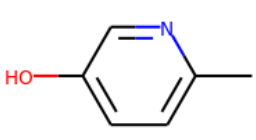
Experimental 13C NMR (solvent: DMSO)



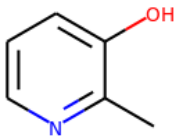
Experimental 1H NMR (solvent: CDCl3)



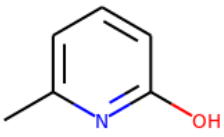
Top predicted structures (loss):



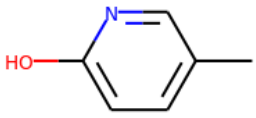
0.014215



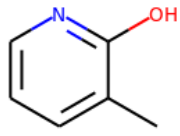
0.01648



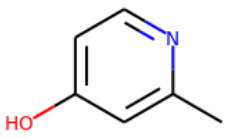
0.016908



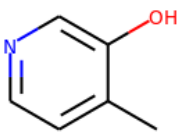
0.01717



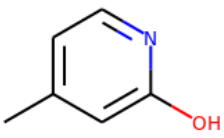
0.018078



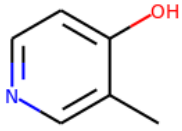
0.020607



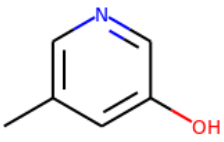
0.020746



0.021498



0.02281



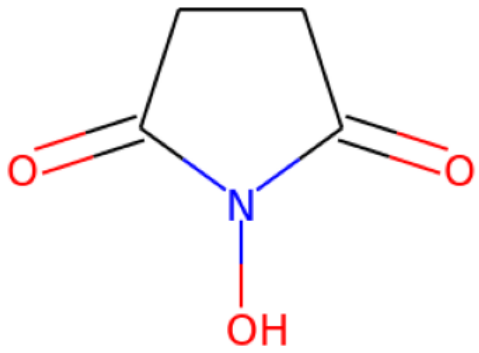
0.038462

Top predicted substructures	prob		
[#6H1]	0.9995	[cH]	0.9883
[#6X3][#6X3]	0.9992	[#6H3][#6][#6]	0.9882
[#6X3][#6X3][#6X3][#6X3]	0.9968	[#6X3H1][#6X3H0]	0.9762
[cH][cH]	0.9949	[#7][#6][#6][#6X3]	0.9745
[#7][#6][#6X3]	0.9946	[CX4H3][cX3H0]	0.9574

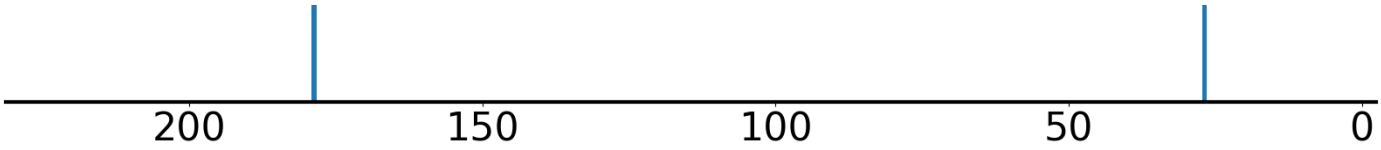
best positives	prob	best negatives	prob
[#6H1]	0.9995	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3]	0.9992	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9968	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[cH][cH]	0.9949	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#7][#6][#6X3]	0.9946	[#6]1[#8][#6][#6]1=[#8]	0.0
[cH]	0.9883	[CX3H0](=[OX1H0])([CX4H1])[CX4H0]	0.0
[#6H3][#6][#6]	0.9882	[CX3H2]=[CX3H1][CX4H0][OX2H1]	0.0
[#6X3H1][#6X3H0]	0.9762	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.9745	[OX2H1][CX4H0][CX4H2][CX4H0]	0.0
[CX4H3][cX3H0]	0.9574	[OX1H0]=[CX3H1][CX4H2][CX4H0]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([nX2H0])[cX3H1]	0.8243	[cX3H0][cX3H1][cX3H1][cX3H0]	0.308
[cX3H1]([cX3H1])[cX3H1]	0.6093	[OX2H][cX3]:[c]	0.4507
[#6]1[#6][#6][#6][#6][#6]1	0.4328	[#8][#6H0][#6H1]	0.5102
[#6H1][#7][#6H1]	0.2702	[cH]cO	0.6077
o[cH]	0.1784	[cX3H1]([nX2H0])[cX3H0]	0.6364
[CX4H2][CX4H2]	0.1745	[#7][#6H0][#6H1]	0.6517
[cX3H1]([cX3H0])[cX3H0]	0.1509	[#7][#6X3H0][#6X3H1]	0.6748
O=[cX3]	0.1503	[OX2H1]	0.6857
[#7H2][#6H0]	0.1391	[#7][#6][#6H3]	0.7011
[#6H3][#6H0][#6H1][#7]	0.1218	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7104

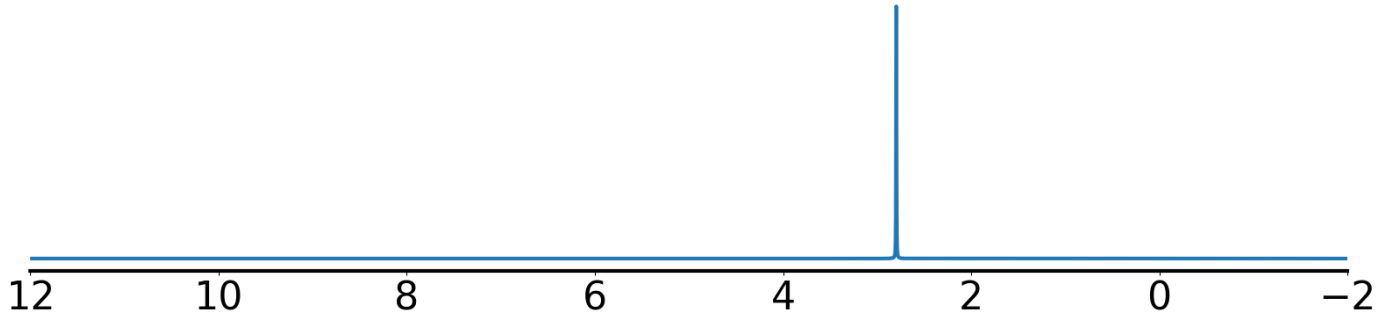
Example 69 true smiles: O=C1CCC(=O)N1O formula: C4H5NO3
Index of correct structure: 0 of 3337
True structure loss: 0.036294
True structure:



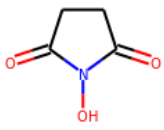
Experimental 13C NMR (solvent: DMSO-d6)



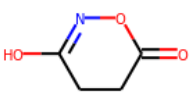
Experimental 1H NMR (solvent: D2O)



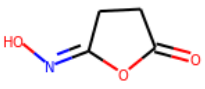
Top predicted structures (loss):



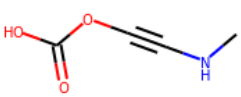
0.036294



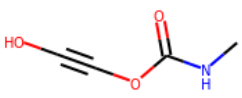
0.042469



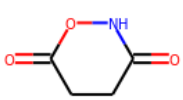
0.042616



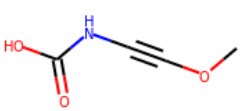
0.04262



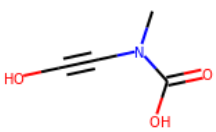
0.043709



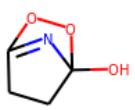
0.044092



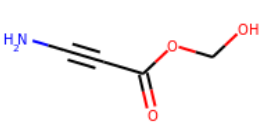
0.045782



0.047579



0.048092



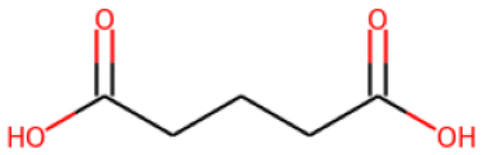
0.048961

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9693	[CX4H2]CC=O	0.5649
[#8]=[#6][#8]	0.9048	[#7X3H1]	0.5516
[OX2H1]	0.7909	O=[CX3][CX4H]	0.546
[CX3](=[OX1])O	0.765	[CX3](=O)[OX2H1]	0.5445
[#7][#6][#6X3]	0.7026	[CX4H2][CX3]=O	0.4891

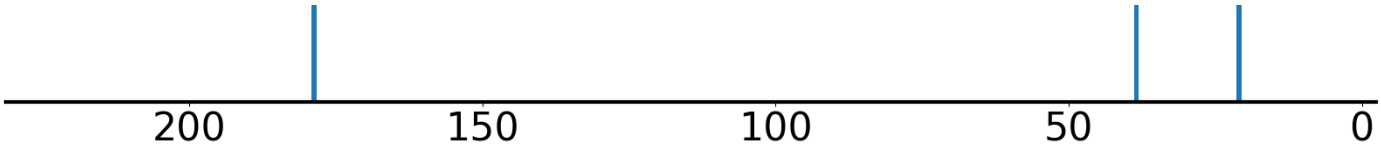
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9693	[CX3H0](=[CX3H2])([CX4H3])[CX4H1]	0.0
[OX2H1]	0.7909	[#6X3H2]=[#6][#6H2][#8H]	0.0
[CX4H2]CC=O	0.5649	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[CX4H2][CX3]=O	0.4891	CC=CC#CC	0.0
[CX4H2][CX4H2]	0.4783	[CX3H1](=[CX3H2])[CX4H0]	0.0
[#8]=[#6][#6][#6][#6]=[#8]	0.4352	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[#6]	0.4114	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.3634	[#8]1[#6][#6]=[#6][#6]=[#6]1	0.0
O=[CX3H0][CX4H2][CX4H2]	0.312	[#8][#6H2][#6H1]=[#6H0]	0.0
[CX4H2]([CX4H2])[CX3H0]	0.2522	[CX3H0](=[CX3H2])([CX4H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#8]	0.9048	[#6X3][#7X3][#6X3]	0.0468
[CX3](=[OX1])O	0.765	[#6]1[#6][#6][#6][#7]1	0.13
[#7][#6][#6X3]	0.7026	[CX3H0](=[OX1H0])([NX3H0])[CX4H2]	0.1403
[#7X3H1]	0.5516	[#6X3][#7][#6X3]	0.1464
O=[CX3][CX4H]	0.546	[#7X3H0]	0.2023
[CX3](=O)[OX2H1]	0.5445	[CX4H2]([CX4H2])[CX3H0]	0.2522
[#7][#6][#6][#6X3]	0.4025	O=[CX3H0][CX4H2][CX4H2]	0.312
[#8]=[#6H0][#6H1]	0.3922	[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.3634
[#6H1][#6H1]	0.3124	[CX4H2]([#6])[#6]	0.4114
[#6H3][#7][#6X3]	0.2966	[#8]=[#6][#6][#6][#6]=[#8]	0.4352

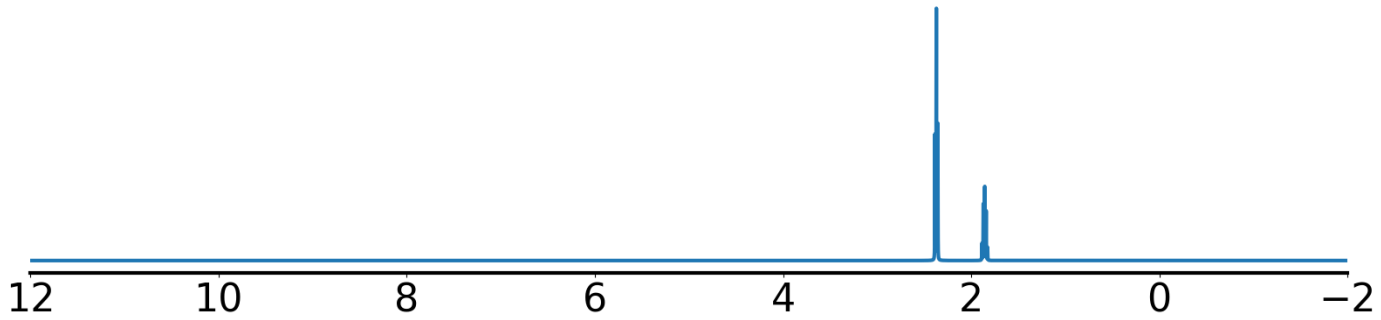
Example 70 true smiles: O=C(O)CCCC(=O)O formula: C5H8O4
Index of correct structure: 0 of 3240
True structure loss: 0.006856
True structure:



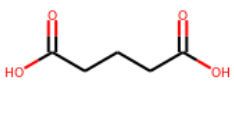
Experimental 13C NMR (solvent: D2O)

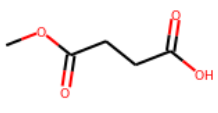


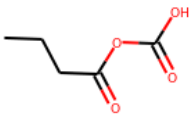
Experimental 1H NMR (solvent: D2O)

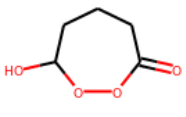


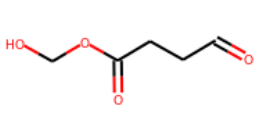
Top predicted structures (loss):

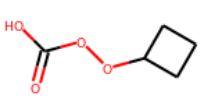

0.006856

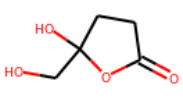

0.049658

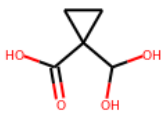

0.051419

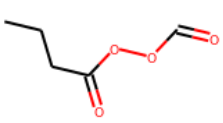

0.053181

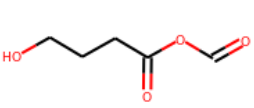

0.067022


0.069207


0.072057


0.073864


0.078546

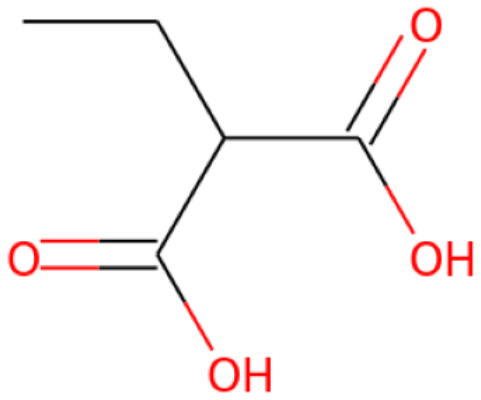

0.078714

Top predicted substructures	prob		
[#8]=[#6][#8]	0.9995	[CX3](=O)[OX2H1]	0.9928
[CX4H2]([#6])[#6]	0.9994	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.9675
[CX3](=[OX1])C	0.9993	OCC[CH2]	0.9647
[OX2H1]	0.999	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9249
[CX3](=[OX1])O	0.9987	O=[CX3H0][CX4H2][CX4H2]	0.9091

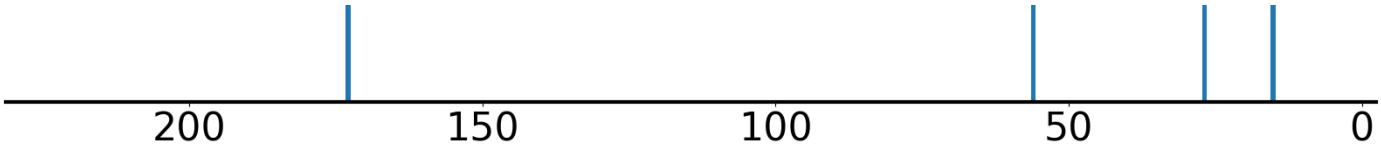
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9995	CCC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9994	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9993	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[OX2H1]	0.999	CC#CCC=C	0.0
[CX3](=[OX1])O	0.9987	CC=CC#CC	0.0
[CX3](=O)[OX2H1]	0.9928	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.9675	C=CC=CC#C	0.0
OCC[CH2]	0.9647	CC=CCC#C	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9249	[#7][#6]=[#6][#6]#[#7]	0.0
O=[CX3H0][CX4H2][CX4H2]	0.9091	[#6X3H2]=[#6][#6H2][#8H]	0.0

worst negatives	prob	worst positives	prob
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.4232	[CX4H2]([CX4H2])[CX4H2]	0.6467
[#8][#6H0][#6H1]	0.2917	[#8][#6][#6H2]	0.6586
[#8][#6][#6][#8]	0.2645	[CX4H2][CX4H2]	0.7593
[#6H1]	0.2518	[CX4H2]([CX4H2])[CX3H0]	0.7608
[#6H1][#6H2]	0.1751	[CX4H2]CC=O	0.8178
C1CCC1	0.1518	[CX4H2][CX3]=O	0.8831
[#6H1][#6H1]	0.1502	O=[CX3H0][CX4H2][CX4H2]	0.9091
CCCCCC	0.1427	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9249
[CX4H2]([CX4H2])[CX4H0]	0.1401	OCC[CH2]	0.9647
[#8][#6][#6][#6][#6]=[#8]	0.131	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.9675

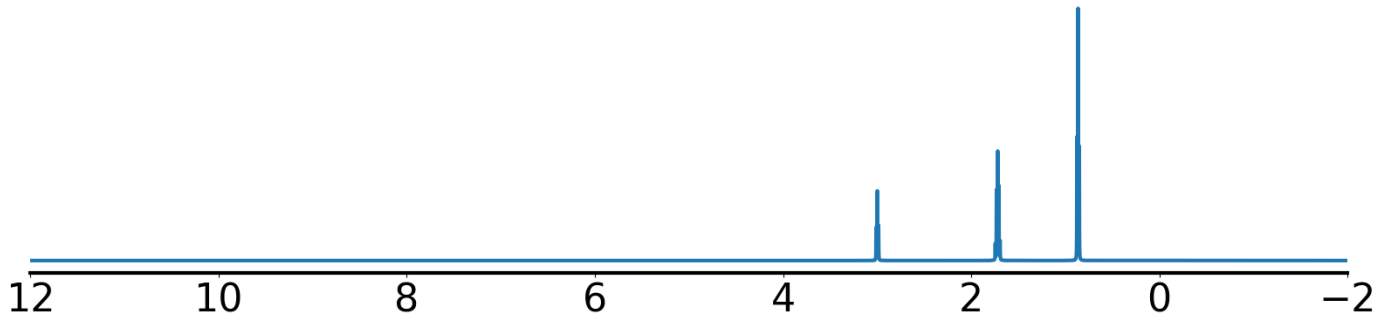
Example 71 true smiles: CCC(C(=O)O)C(=O)O formula: C5H8O4
Index of correct structure: 0 of 3240
True structure loss: 0.022372
True structure:



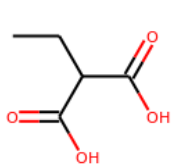
Experimental 13C NMR (solvent: CDCl3, DMSO-d6)



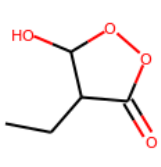
Experimental 1H NMR (solvent: D2O)



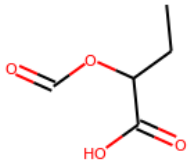
Top predicted structures (loss):



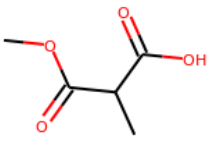
0.022372



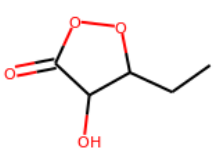
0.036184



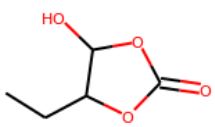
0.046682



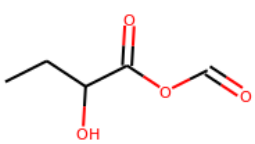
0.052213



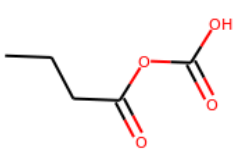
0.056183



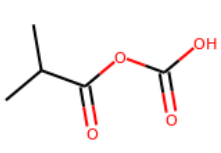
0.057518



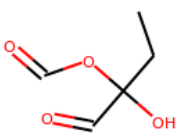
0.060492



0.061483



0.061659



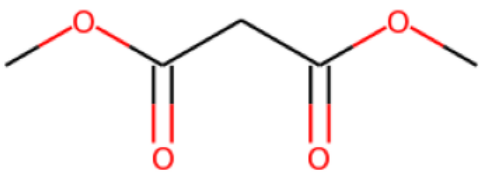
0.063964

Top predicted substructures	prob		
[#8]=[#6][#8]	0.9992	[CX4H2]([#6])[#6]	0.9796
[CX3](=[OX1])O	0.999	[OX2H1]	0.968
[CX3](=[OX1])C	0.9974	[CX4H3][CX4H2]	0.9487
[CX4H3]	0.9969	OCC[CH2]	0.9179
[#6H3][#6][#6]	0.991	[CX4H3][#6]	0.8938

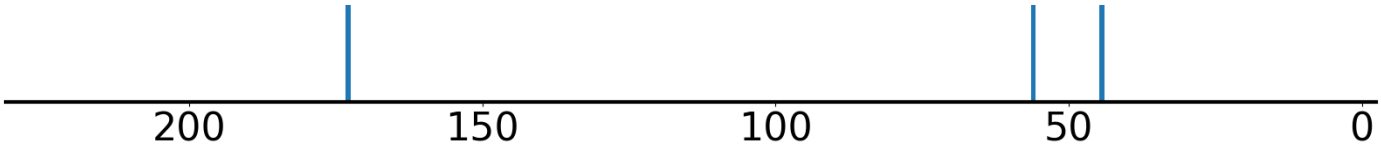
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9992	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])O	0.999	CCC=CC#C	0.0
[CX3](=[OX1])C	0.9974	CC=CC#CC	0.0
[CX4H3]	0.9969	[#6X3H2]=[#6][#6H2][#8H]	0.0
[#6H3][#6][#6]	0.991	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H2]([#6])[#6]	0.9796	[#7][#6][#6]=[#6][#6][#7]	0.0
[OX2H1]	0.968	CCC#CC=C	0.0
[CX4H3][CX4H2]	0.9487	CC=CCC#C	0.0
OCC[CH2]	0.9179	CC#CCC=C	0.0
[CX4H3][#6]	0.8938	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.6206	O=[#6][#6][#6X3]	0.0208
[#8][#6][#6]=[#8]	0.5807	[CX4H1]([CX4H2])([CX3H0])[CX3H0]	0.0307
[CX4H](O)CO	0.547	O=[#6][#6H][#6H0]	0.345
[#8][#6][#6][#8]	0.5149	[#6X3][#6][#6][#6H3]	0.4315
[#6H1][#6H1]	0.4777	[#8][#6][#6][#6X3]	0.4636
[CX4H]O	0.4307	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5555
[#6H2][#6H1r3]	0.217	[#6H1][#6H2]	0.6022
[#8][#6H1][#6H1]	0.2032	O=[CX3][CX4H]	0.6614
O[CX4H][CX4H2]	0.1817	[CX4H2]CC=O	0.6936
O[CX4H]([CX4H2])[CX4H1]	0.1784	[#8]=[#6H0][#6H1]	0.7015

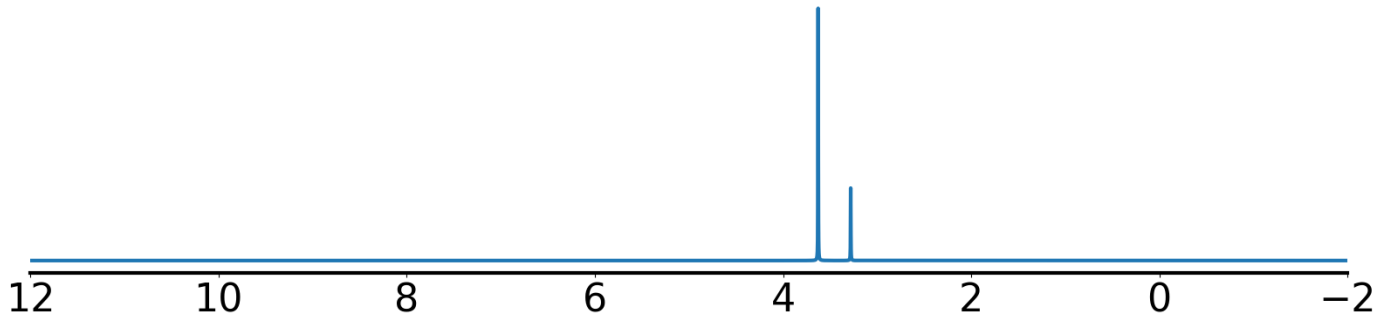
Example 72 true smiles: COC(=O)CC(=O)OC formula: C5H8O4
Index of correct structure: 0 of 3240
True structure loss: 0.014072
True structure:



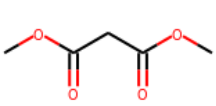
Experimental 13C NMR (solvent: CDCl3)



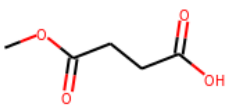
Experimental 1H NMR (solvent: CDCl3)



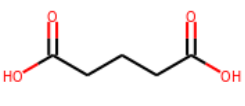
Top predicted structures (loss):



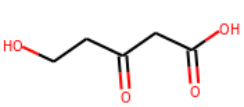
0.014072



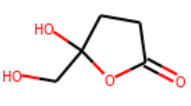
0.037693



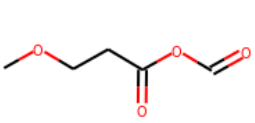
0.040552



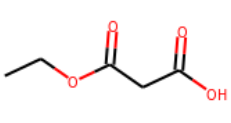
0.056913



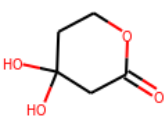
0.065685



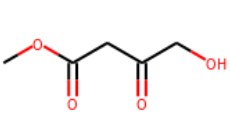
0.067063



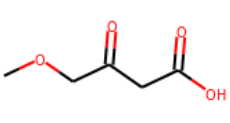
0.068575



0.069116



0.070151



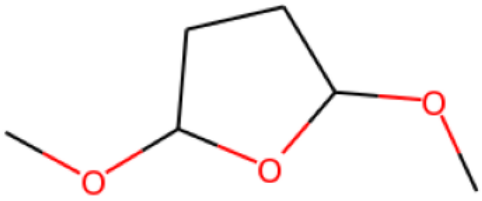
0.070197

Top predicted substructures	prob		
[#8]=[#6][#8]	0.9995	[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.9199
[CX3](=[OX1])O	0.9985	[CX4H3]	0.9055
[CX3](=[OX1])C	0.9961	[CX4H2][CX3]=O	0.8437
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9675	[CX4H2]([CX3H0])[CX3H0]	0.7876
[#8][#6][#6H2]	0.9433	[CX4H3][OX2H0]	0.785

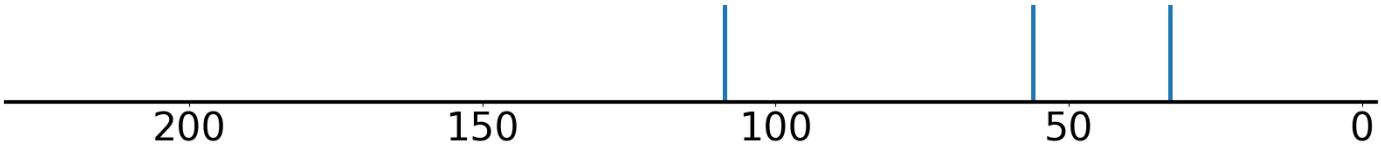
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9995	C=CC=CC#C	0.0
[CX3](=[OX1])O	0.9985	CC=CCC#C	0.0
[CX3](=[OX1])C	0.9961	CC=CC#CC	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9675	CC#CCC#C	0.0
[#8][#6][#6H2]	0.9433	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.9199	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3]	0.9055	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H2][CX3]=O	0.8437	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([CX3H0])[CX3H0]	0.7876	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H3][OX2H0]	0.785	[CX3H1](=[CX3H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX3](=O)[OX2H1]	0.5757	O=[#6][#6][#6X3]	0.2881
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.5191	[OX1H0]=[CX3H0][CX4H2][CX3H0]	0.6372
[OX2H1]	0.5179	[#6X3][#6H2][#6X3]	0.6722
OCC[CH2]	0.4732	[#8][#6][#6][#6X3]	0.6724
[CX4H2]CC=O	0.3523	[#8X1]=[#6X3][#6H2][#6H0]	0.6963
O=[CX3][CX4H]	0.2395	[CX4H2]([#6])[#6]	0.7071
[#8]=[#6H0][#6H1]	0.2368	[OX2H0][CX3H0][CX4H2]	0.7075
[#6H1][#6H2]	0.2221	[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.7429
[#8][#6][#6][#8]	0.208	[CX4H3][OX2H0]	0.785
[#6H1]	0.199	[CX4H2]([CX3H0])[CX3H0]	0.7876

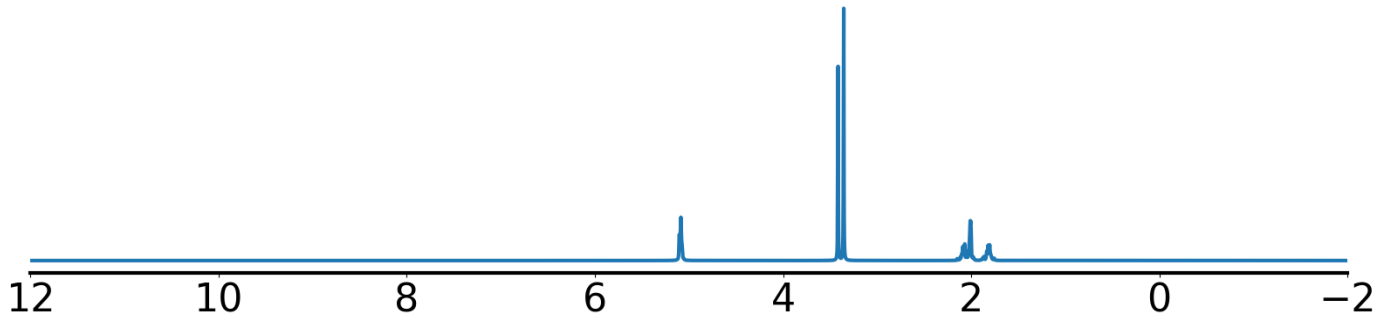
Example 73 true smiles: COC1CCC(OC)O1 formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.009313
True structure:



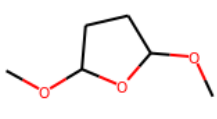
Experimental 13C NMR (solvent: CDCl3)



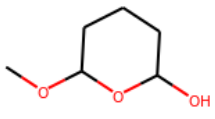
Experimental 1H NMR (solvent: CDCl3)



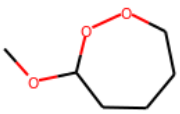
Top predicted structures (loss):



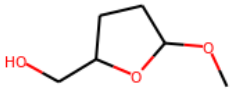
0.009313



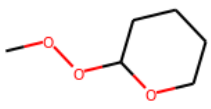
0.021802



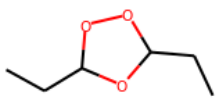
0.041438



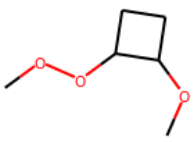
0.04503



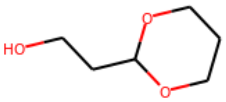
0.052808



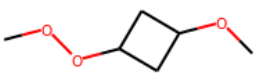
0.056076



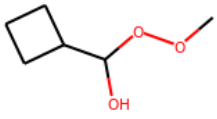
0.057516



0.058041



0.05979



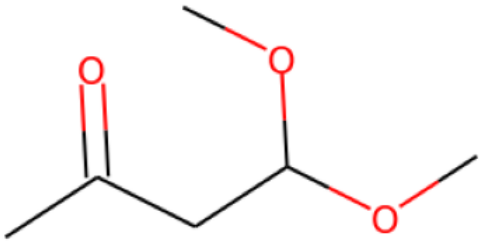
0.061794

Top predicted substructures	prob		
[OX2H0][CX4H1][OX2H0]	1.0	[CX4H1]([OX2H0])([OX2H0])[CX4H2]	0.9881
[CX4H3]	0.9973	OCC[CH2]	0.9771
[CX4H2]([#6])[#6]	0.9969	[#8][#6][#6H2]	0.9757
[CX4H]O	0.9959	[CX4H3][OX2H0]	0.9754
[#6H1]	0.9938	[#6H1][#6H2]	0.9412

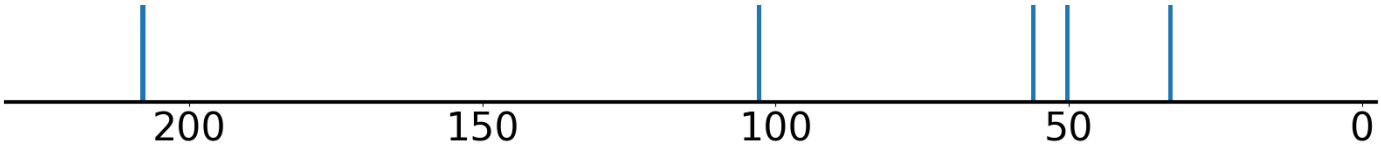
best positives	prob	best negatives	prob
[OX2H0][CX4H1][OX2H0]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	0.9973	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[#6]	0.9969	C=CC=CC#C	0.0
[CX4H]O	0.9959	CC=CCC#C	0.0
[#6H1]	0.9938	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
[CX4H1]([OX2H0])([OX2H0])[CX4H2]	0.9881	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
OCC[CH2]	0.9771	[#6H3][#6H1][#6H1]=[#7]	0.0
[#8][#6][#6H2]	0.9757	[#6H2]=[#6][#6X2]	0.0
[CX4H3][OX2H0]	0.9754	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H1][#6H2]	0.9412	[CX2H0](#[NX1H0])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H1][#6H1]	0.3907	C1OCCC1	0.3183
[CX4H2]([CH])[CH]	0.3743	[CX4H1][CX4H2][CX4H2][CX4H1]	0.3884
[#8][#6][#6][#8]	0.3585	[#6H1][#6H2][#6H2][#6H1]	0.5084
[#6H1][#6H1]	0.2965	[#8][#6][#6][#6][#6][#8]	0.5436
[CX4H2]([CX4H1])[CX4H1]	0.2902	[#6H][#8][#6H]	0.593
[CX4H](O)CO	0.2698	[OX2H0][CX4H1][CX4H2][CX4H2]	0.7509
[CX4H2]([CX4H2])[CX4H2]	0.1569	[CX4H2]([CX4H2])[CX4H1]	0.785
[#6H1]([#6H2])[#6H2]	0.1488	[CX4H2][CX4H2]	0.7876
[OX2H1]	0.1441	O[CX4H][CX4H2]	0.9053
[OH][CX4H]	0.1313	[#6H1][#6H2]	0.9412

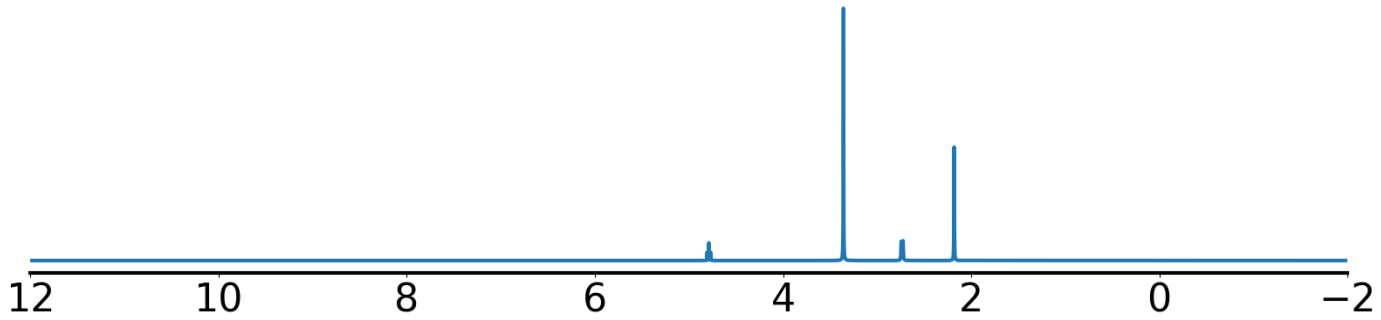
Example 74 true smiles: COC(CC(C)=O)OC formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.009806
True structure:



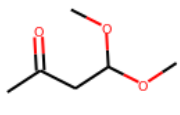
Experimental 13C NMR (solvent: CDCl3)



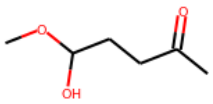
Experimental 1H NMR (solvent: CDCl3)



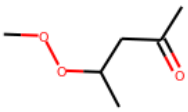
Top predicted structures (loss):



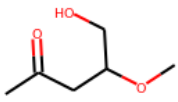
0.009806



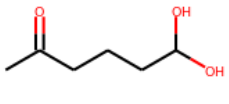
0.048452



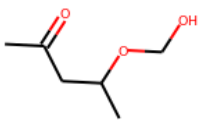
0.050987



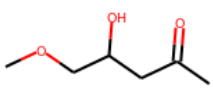
0.06019



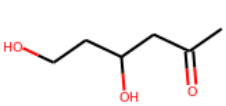
0.06186



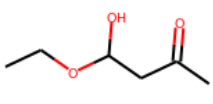
0.062557



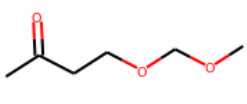
0.065114



0.068028



0.069773



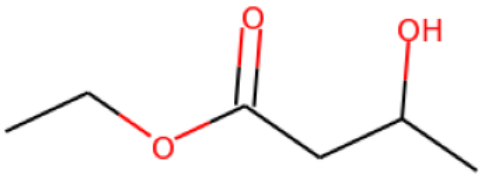
0.071497

Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][#6]	0.9871
[CX3](=[OX1])C	0.9997	[OX1H0]=[CX3H0][CX4H3]	0.9862
[CX4H3][CX3]	0.9993	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9781
[CX4H3][OX2H0]	0.9978	[#6H3][#6H0]	0.9743
[CX4H3][CX3H0]	0.9976	[CX4H2]([#6])[#6]	0.9631

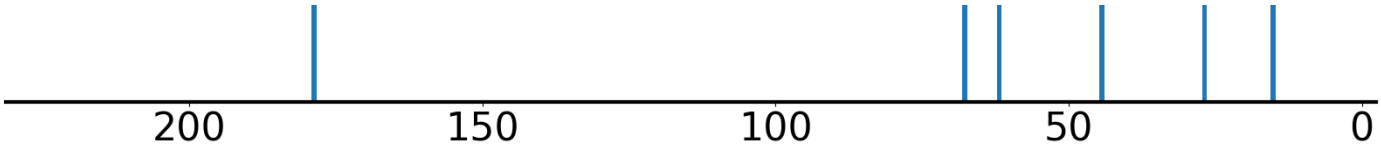
best positives	prob	best negatives	prob
[CX4H3]	1.0	CCC#CC#C	0.0
[CX3](=[OX1])C	0.9997	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][CX3]	0.9993	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][OX2H0]	0.9978	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX4H3][CX3H0]	0.9976	[#6X2][#6H1][#6X2]	0.0
[CX4H3][#6]	0.9871	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9862	C=CC=CC#C	0.0
[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9781	CC#CCC#C	0.0
[#6H3][#6H0]	0.9743	CC=CC#CC	0.0
[CX4H2]([#6])[#6]	0.9631	CC=CCC#C	0.0

worst negatives	prob	worst positives	prob
OCC[CH2]	0.5148	[#8][#6][#6][#6X3]	0.3459
[#8][#6][#6][#6][#6]=[#8]	0.3456	[CX4H2]([CX4H1])[CX3H0]	0.5104
[CX4H3][OX2H0][CX4H2]	0.2748	[#8]=[#6][#6H2][#6H1]	0.5135
[#6H2][#8][#6H1]	0.254	O=[CX3H0][CX4H2][CX4H1]	0.7588
[CX4H2]([#6])[O]	0.2386	[CX4H]O	0.7665
[CX3H1](=[OX1H0])[CX4H2]	0.2345	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.8124
[#6X3][#6][#6][#6H3]	0.2013	[#6H1]	0.8274
[CX4H2](O)[CHX4]	0.2009	[#6H1][#6H2]	0.846
[CX4H2]CC=O	0.1827	O[CX4H][CX4H2]	0.8753
[CX4H2][CX3H]	0.1803	[#6H3][#6X3H0][#6H2]	0.8755

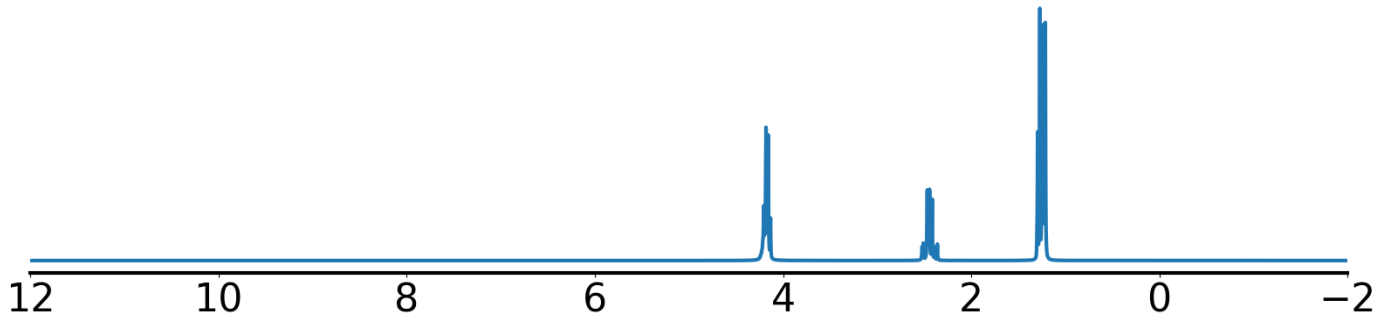
Example 75 true smiles: CCOC(=O)CC(C)O formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.031697
True structure:



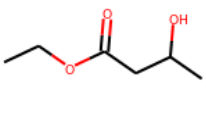
Experimental 13C NMR (solvent: CDCl3)



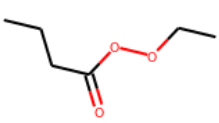
Experimental 1H NMR (solvent: CDCl3)



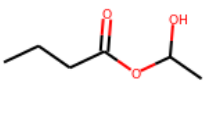
Top predicted structures (loss):



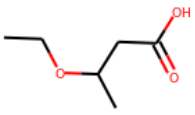
0.031697



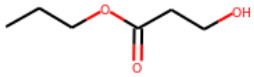
0.039367



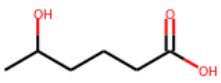
0.043515



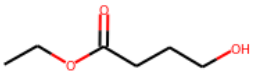
0.046002



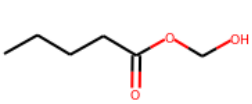
0.048921



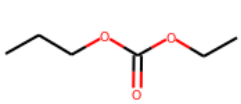
0.049044



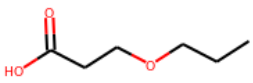
0.04967



0.050377



0.051692



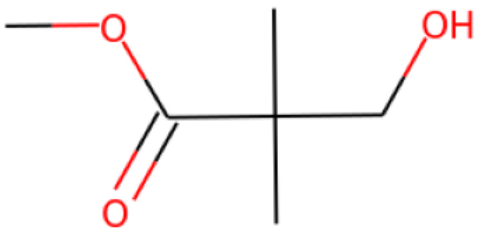
0.052115

Top predicted substructures	prob		
[CX4H3]	1.0	[#6H3][#6][#6]	0.9953
[CX3](=[OX1])C	0.9986	[CX4H3][CX4]O	0.9908
[#8]=[#6][#8]	0.9984	[OX2H1]	0.9903
[CX4H3][#6]	0.9979	[CX4H2]([#6])[O]	0.9799
[CX3](=[OX1])O	0.9971	[CX4H2]([#6])[#6]	0.9706

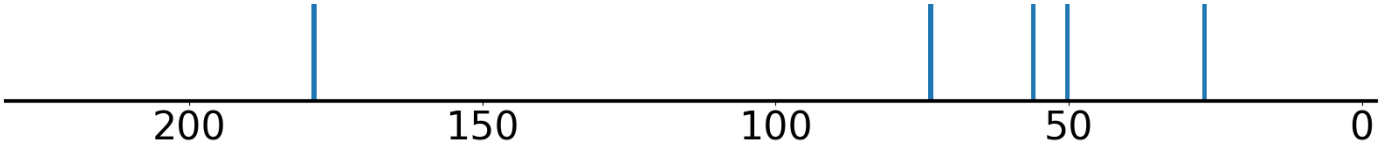
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9986	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8]=[#6][#8]	0.9984	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][#6]	0.9979	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX3](=[OX1])O	0.9971	[#6X2][#6H1][#6X2]	0.0
[#6H3][#6][#6]	0.9953	CC#CCC#C	0.0
[CX4H3][CX4]O	0.9908	CCC#CC#C	0.0
[OX2H1]	0.9903	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2]([#6])[O]	0.9799	[#7][#6H1][#6X2]	0.0
[CX4H2]([#6])[#6]	0.9706	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[CX3](=O)[OX2H1]	0.9255	O[CX4H][CX4H2]	0.1878
OCC[CH2]	0.7836	[#6X4H2][#6H1][#8H]	0.2528
[#8][#6H0][#6H1]	0.6518	[OH][CX4H]	0.2538
[CX4H2]CC=O	0.634	[CX4H]O	0.2555
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.5426	[#8]=[#6][#6H2][#6H1]	0.2812
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.38	O=[CX3H0][CX4H2][CX4H1]	0.3086
[#8][#6][#6][#6][#6][#8]	0.3667	[#6X3][#6][#6][#6H3]	0.3252
[#8][#6][#6][#6][#6]=[#8]	0.3665	[#8X2H0][#6X3H0][CX4H2][CX4H1]	0.3313
[#8H][#6H2][#6H1]	0.2805	[CHX4]([CH3X4])[CH2X4]	0.3742
[#8]=[#6H0][#6H1]	0.2401	[#6X4H3][#6][#8H]	0.4506

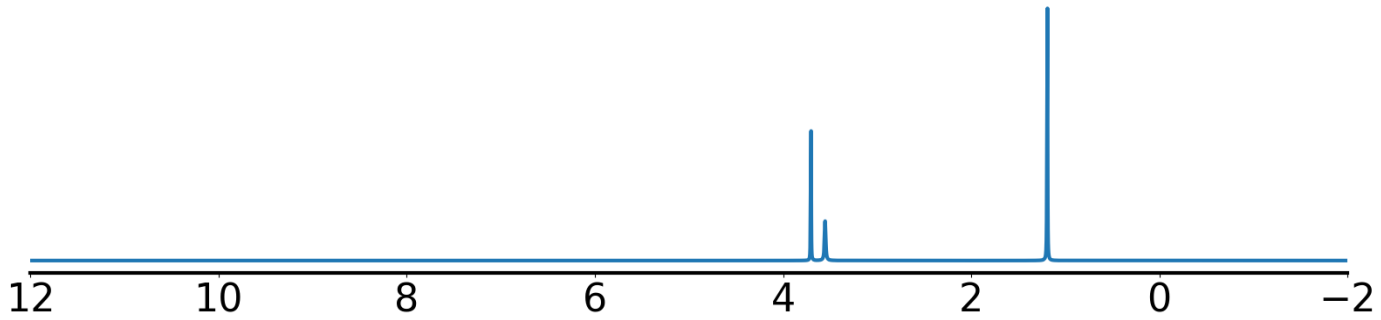
Example 76 true smiles: COC(=O)C(C)(C)CO formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.026019
True structure:



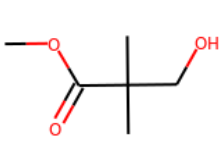
Experimental 13C NMR (solvent: CDCl3)



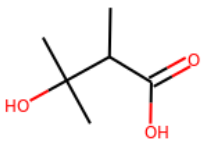
Experimental 1H NMR (solvent: CDCl3)



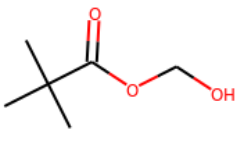
Top predicted structures (loss):



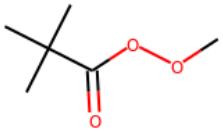
0.026019



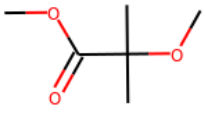
0.03807



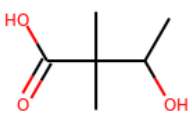
0.040402



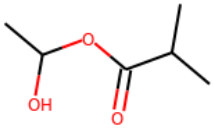
0.041319



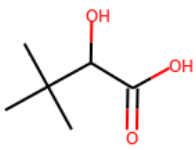
0.041943



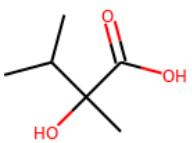
0.043469



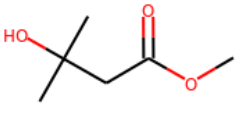
0.049183



0.049239



0.050928



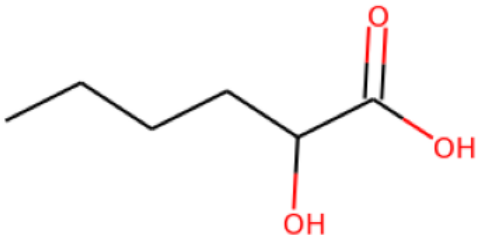
0.052917

Top predicted substructures	prob		
[CX4H3]	1.0	[CX3](=[OX1])O	0.9853
[#6H3][#6][#6]	1.0	[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.9576
[CX4H3][#6]	0.9996	[CX4H3][CX4H0][CX4H3]	0.9297
[#8]=[#6][#8]	0.9969	[#6H1]	0.9187
[CX3](=[OX1])C	0.9969	[OX2H1]	0.9066

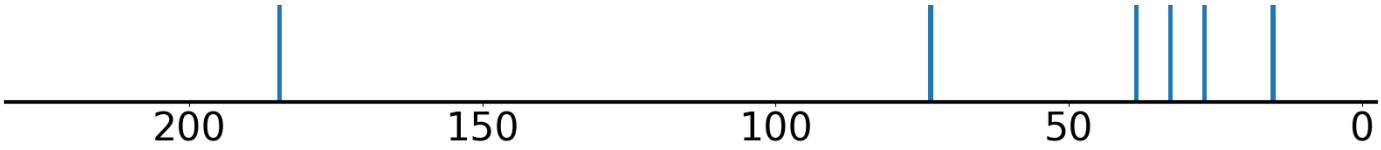
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[#6H3][#6][#6]	1.0	CCC#CC#C	0.0
[CX4H3][#6]	0.9996	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#8]=[#6][#8]	0.9969	CC=CC#CC	0.0
[CX3](=[OX1])C	0.9969	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.9853	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.9576	[#7][#6][#6][#6]#[#7]	0.0
[CX4H3][CX4H0][CX4H3]	0.9297	[#7][#6]=[#6][#6]#[#7]	0.0
[OX2H1]	0.9066	CC#CCC#C	0.0
[#6H3][#6H0]	0.9008	CC=CCC#C	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.9187	[CX4H2]([#6])[O]	0.2454
[CX3](=O)[OX2H1]	0.6856	[CX4H2]CC=O	0.3517
O=[CX3][CX4H]	0.6163	[#6H3][#6][#6X3]	0.3788
[CH3][#6][#8]	0.5652	OCC[CH2]	0.3985
[#8]=[#6H0][#6H1]	0.5512	[CX4H2]([OX2H1])[CX4H0]	0.408
[OH][CX4H]	0.5503	[CX3H0](=[OX1H0])([OX2H0])[CX4H0]	0.4116
[#8][#6H0][#6H1]	0.5489	[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.5749
[#6X4H3][#6][#8H]	0.52	[CH3]CC[OH]	0.6069
[CX4H3][CX4]O	0.4838	[CX4H3][CX4H0]	0.8012
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.4567	[CX4H3][OX2H0]	0.8014

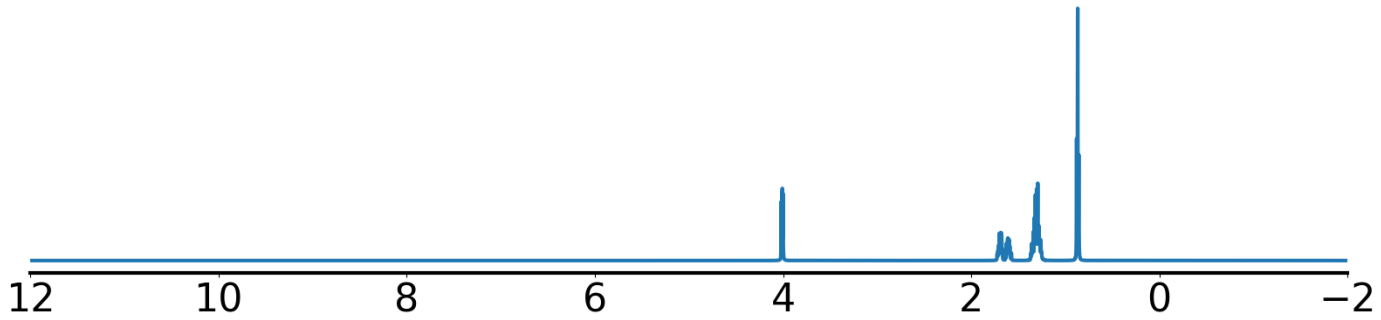
Example 77 true smiles: CCCCC(O)C(=O)O formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.014868
True structure:



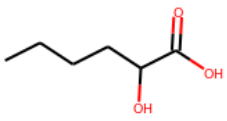
Experimental 13C NMR (solvent: CDCl3)



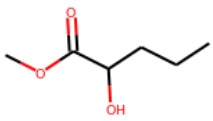
Experimental 1H NMR (solvent: D2O)



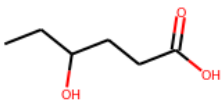
Top predicted structures (loss):



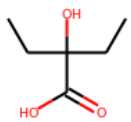
0.014868



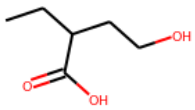
0.043137



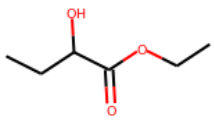
0.049736



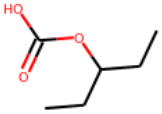
0.051526



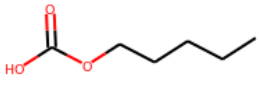
0.051833



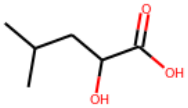
0.053758



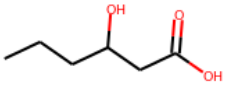
0.054139



0.054479



0.054607



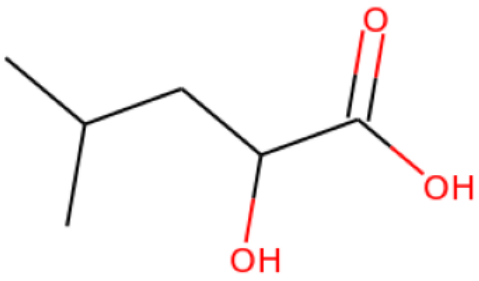
0.057478

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9999	[#8]=[#6][#8]	0.9969
[#6H3][#6][#6]	0.9999	[CX4H3][#6]	0.9969
[CX4H3]	0.9987	[CX4H3][CX4H2]	0.9953
[CX3](=[OX1])C	0.9984	OCC[CH2]	0.9889
[OX2H1]	0.9982	[CX3](=[OX1])O	0.9876

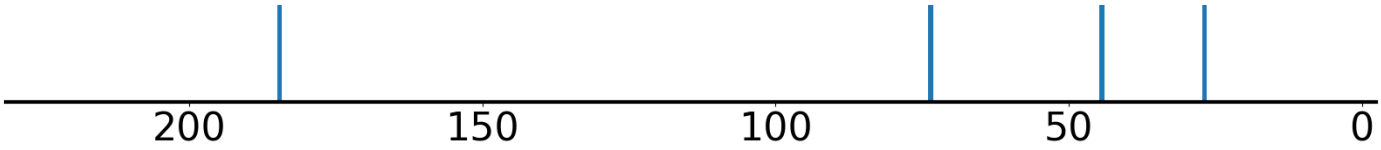
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9999	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9999	CCC=CC#C	0.0
[CX4H3]	0.9987	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9984	[CX2H0](#[CX2H1])[CX3H1]	0.0
[OX2H1]	0.9982	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8]=[#6][#8]	0.9969	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][#6]	0.9969	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][CX4H2]	0.9953	CC=CC#CC	0.0
OCC[CH2]	0.9889	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])O	0.9876	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H3])[CX4H1]	0.4451	[#8][#6][#6][#8]	0.2349
[CH3]CC[OH]	0.4013	[CX4H](O)CO	0.2531
[CX4H2]([#6])[O]	0.3404	CCCCCC	0.3469
[#6X3][#6][#6][#6H3]	0.2414	[CX4H]O	0.5352
[#8]=[#6][#6H1][#6H1]	0.2159	[#8][#6H0][#6H1]	0.5735
[#8][#6][#6][#6][#6][#8]	0.1468	[CX4H2]([CX4H2])[CX4H2]	0.5994
[#8][#6H1][#6H1]	0.1437	[#8]=[#6H0][#6H1]	0.6093
[#8][#6][#6][#6X3]	0.1303	[CX4H2]([CX4H2])[CX4H1]	0.6379
[CH2X4](O)[CX4H2]	0.1208	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6563
[#6H1]([#6H2])[#6H2]	0.1111	O=[CX3][CX4H]	0.6845

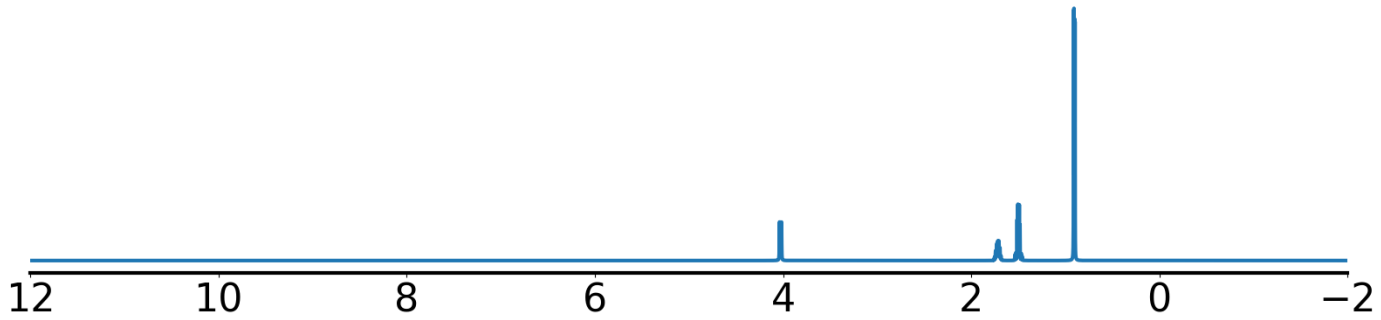
Example 78 true smiles: CC(C)CC(O)C(=O)O formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.01545
True structure:



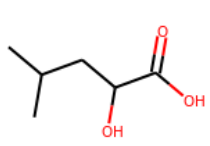
Experimental 13C NMR (solvent: CDCl3)



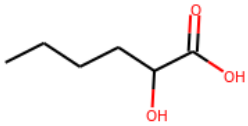
Experimental 1H NMR (solvent: D2O)



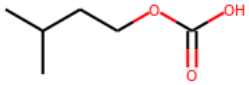
Top predicted structures (loss):



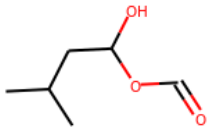
0.01545



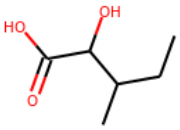
0.04494



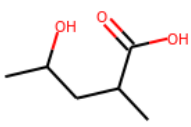
0.051578



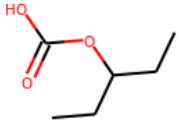
0.059144



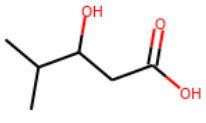
0.06263



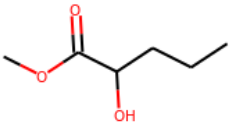
0.064006



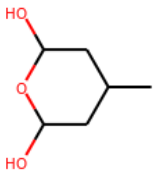
0.064863



0.066002



0.066504



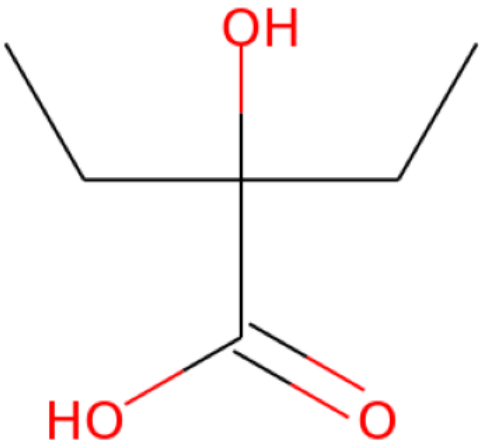
0.06662

Top predicted substructures	prob		
[#6H3][#6][#6]	1.0	[CX4H3][#6]	0.9942
[CX4H3]	0.9995	[CX3](=O)[OX2H1]	0.9895
[#6H1]	0.9985	[#8]=[#6][#8]	0.989
[OX2H1]	0.998	[CX4H2]([#6])[#6]	0.9887
[CX3](=[OX1])C	0.998	[CX3](=[OX1])O	0.9694

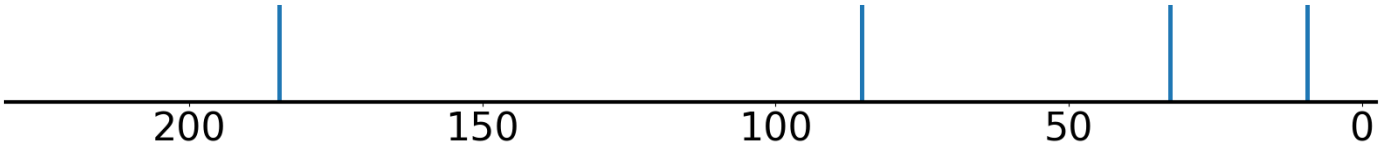
best positives	prob	best negatives	prob
[#6H3][#6][#6]	1.0	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3]	0.9995	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H1]	0.9985	C=CC=CC#C	0.0
[OX2H1]	0.998	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX3](=[OX1])C	0.998	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][#6]	0.9942	CC#CCC#C	0.0
[CX3](=O)[OX2H1]	0.9895	[#6X2][#6H1][#6X2]	0.0
[#8]=[#6][#8]	0.989	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9887	CC#CCC=C	0.0
[CX3](=[OX1])O	0.9694	[#7][#6]=[#6][#6]#[#7]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6][#6][#6H3]	0.4718	[#8][#6][#6][#8]	0.144
[CH3]CC[OH]	0.4167	[CX4H](O)CO	0.2109
[#8][#6][#6][#6X3]	0.3104	[CX4H2]([CH])[CH]	0.5079
[CX4H2][CX4H2]	0.2503	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.529
[CX4H2]([CX4H2])[CX4H1]	0.1786	[#8][#6H0][#6H1]	0.5358
[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.1505	[CX4H1]([OX2H1])([CX4H2])[CX3H0]	0.5521
[#8][#6H1][#6H1]	0.146	[CX4H2]([CX4H1])[CX4H1]	0.6033
[#6H1]([#6H2])[#6H2]	0.1447	O[CX4H][CX4H2]	0.7054
[#8]=[#6][#6H1][#6H1]	0.1338	[#8H][#6X4H1][#6X3H0]	0.7262
CCCCCC	0.1186	[CX4H]O	0.729

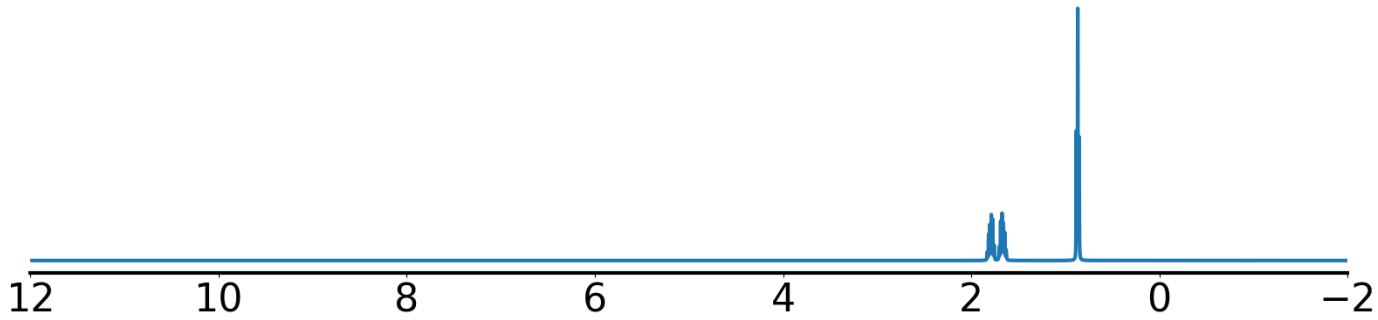
Example 79 true smiles: CCC(O)(CC)C(=O)O formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.008672
True structure:



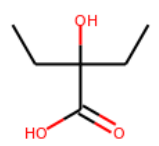
Experimental 13C NMR (solvent: D2O)



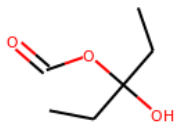
Experimental 1H NMR (solvent: D2O)



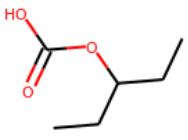
Top predicted structures (loss):



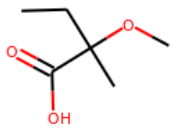
0.008672



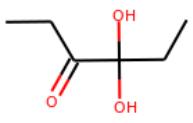
0.040807



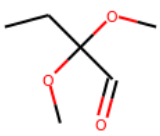
0.047832



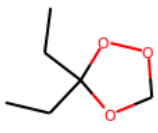
0.052271



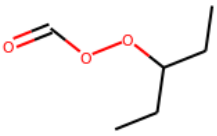
0.056101



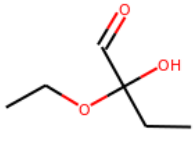
0.065144



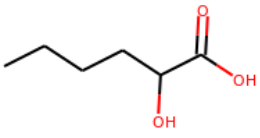
0.067416



0.068534



0.069311



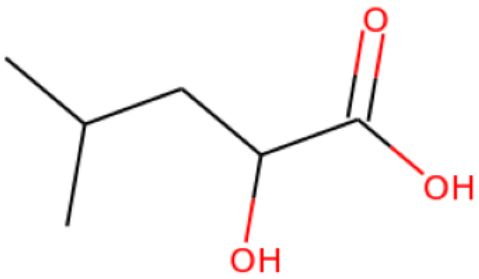
0.071234

Top predicted substructures	prob		
[#6H3][#6][#6]	1.0	[CX4H2]([#6])[#6]	0.9969
[CX4H3]	1.0	[OX2H1]	0.9963
[CX4H3][#6]	0.9998	[#8][#6][#6]=[#8]	0.9937
[CX4H3][CX4H2]	0.9986	[OX2H1][CX4H0][CX4H2][CX4H3]	0.984
[CX3](=[OX1])C	0.9982	[#8][#6][#6H2]	0.9778

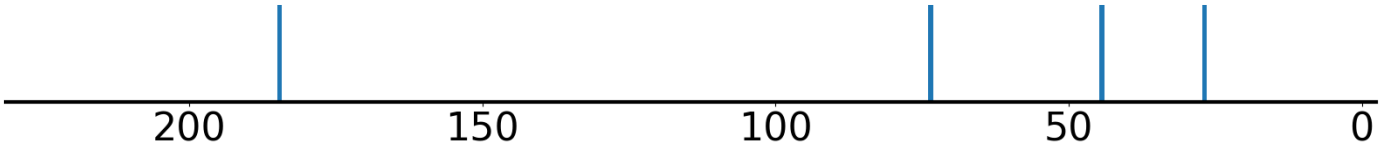
best positives	prob	best negatives	prob
[#6H3][#6][#6]	1.0	CC#CCC#C	0.0
[CX4H3]	1.0	CC=CC#CC	0.0
[CX4H3][#6]	0.9998	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H3][CX4H2]	0.9986	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])C	0.9982	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9969	[CX2H0](#[CX2H1])[CX2H0]	0.0
[OX2H1]	0.9963	CCC=CC#C	0.0
[#8][#6][#6]=[#8]	0.9937	[CX3H1](=[CX3H2])[CX2H0]	0.0
[OX2H1][CX4H0][CX4H2][CX4H3]	0.984	[#7][#6H1][#6X2]	0.0
[#8][#6][#6H2]	0.9778	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.581	OCC[CH2]	0.4724
[CX4H]O	0.425	[CX4H2]CC=O	0.6997
[CX4H2]([CX4H3])[CX4H1]	0.4098	[#8][#6][#6][#8]	0.7739
[#8]=[#6H0][#6H1]	0.3691	[CX3](=O)[OX2H1]	0.8499
O[CX4H][CX4H2]	0.3389	[CX4H2]([CX4H3])[CX4H0]	0.892
[#6H1]	0.3331	[CX3](=[OX1])O	0.9214
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.324	[#6X3][#6][#6][#6H3]	0.9237
O=[CX3][CX4H]	0.3215	[CH3]CC[OH]	0.9642
[CX4H](O)CO	0.3008	[#8]=[#6][#8]	0.9762
[#6H1][#6H2]	0.2877	[#8][#6][#6H2]	0.9778

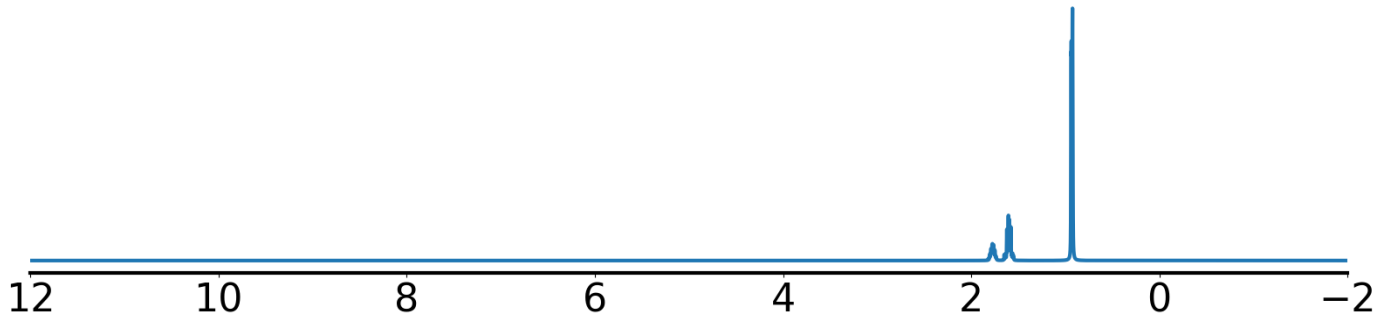
Example 80 true smiles: CC(C)CC(O)C(=O)O formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.020035
True structure:



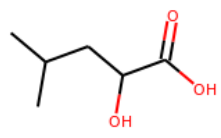
Experimental 13C NMR (solvent: CDCl3)



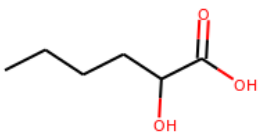
Experimental 1H NMR (solvent: D2O)



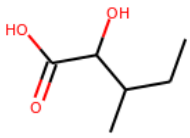
Top predicted structures (loss):



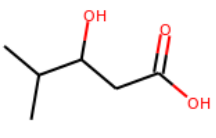
0.020035



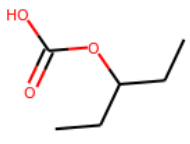
0.051365



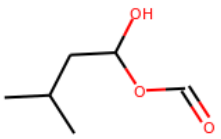
0.057001



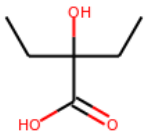
0.057718



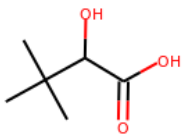
0.06121



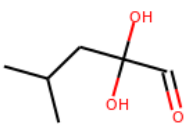
0.061549



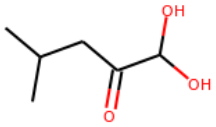
0.061987



0.063275



0.063397



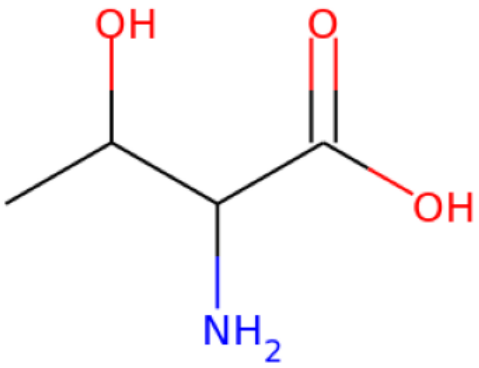
0.064033

Top predicted substructures	prob		
[#6H3][#6][#6]	1.0	[#6H1]	0.9954
[CX4H3]	1.0	[#8]=[#6][#8]	0.9947
[OX2H1]	0.9991	[CX4H3][#6]	0.9943
[CX3](=[OX1])C	0.9984	[CX3](=[OX1])O	0.9802
[CX3](=O)[OX2H1]	0.9977	[CHX4]([CH3X4])[CH3X4]	0.9068

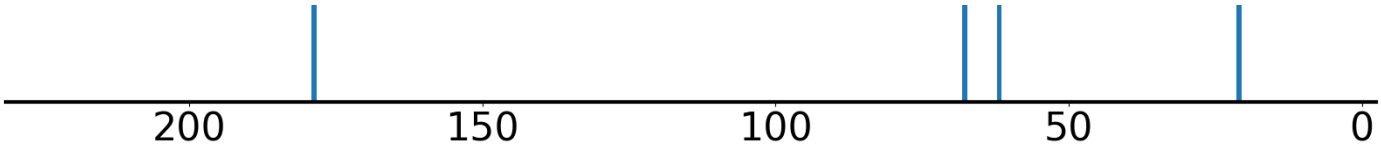
best positives	prob	best negatives	prob
[#6H3][#6][#6]	1.0	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9991	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9984	CC#CCC=C	0.0
[CX3](=O)[OX2H1]	0.9977	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H1]	0.9954	CC#CCC#C	0.0
[#8]=[#6][#8]	0.9947	C=CCCC#C	0.0
[CX4H3][#6]	0.9943	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])O	0.9802	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CHX4]([CH3X4])[CH3X4]	0.9068	CC=CC#CC	0.0

worst negatives	prob	worst positives	prob
[CH3]CC[OH]	0.6814	[#8][#6][#6][#8]	0.1115
[#6X3][#6][#6][#6H3]	0.6175	[CX4H](O)CO	0.2115
[#8]=[#6][#6H1][#6H1]	0.3635	[#8H][#6X4H1][#6X3H0]	0.3629
[#8][#6][#6][#6X3]	0.2167	[CX4H1]([OX2H1])([CX4H2])[CX3H0]	0.3949
[#8][#6H1][#6H1]	0.2121	O[CX4H][CX4H2]	0.415
CCCCCC	0.1994	[CX4H2]([CH])[CH]	0.507
[#6H1][#6H1]	0.1652	[CX4H2]([CX4H1])[CX4H1]	0.5643
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1641	OCC[CH2]	0.5726
[CX4H2][CX3]=O	0.1207	[#8][#6H0][#6H1]	0.5812
[CX4H2][CX4H2]	0.0943	[CX4H]O	0.5939

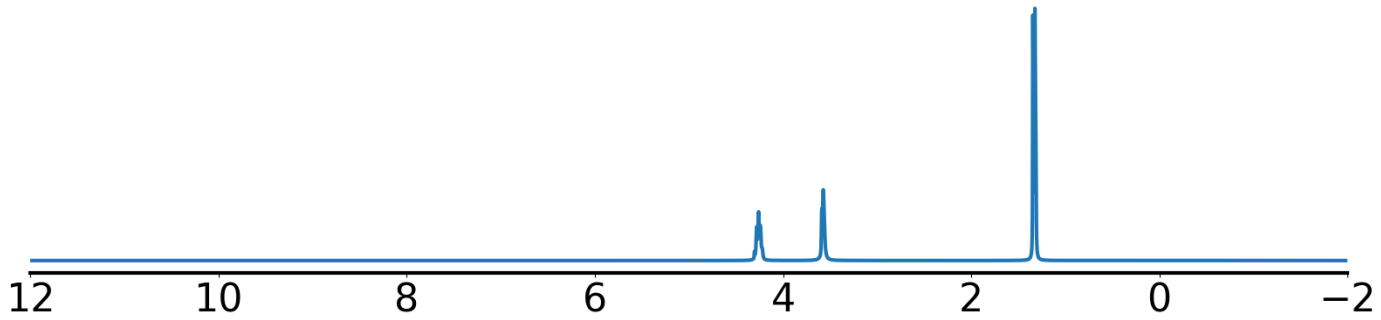
Example 81 true smiles: CC(O)C(N)C(=O)O formula: C4H9NO3
Index of correct structure: 0 of 2840
True structure loss: 0.019032
True structure:



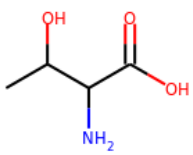
Experimental 13C NMR (solvent: D2O)



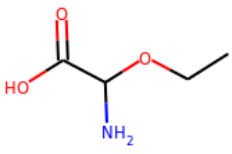
Experimental 1H NMR (solvent: D2O)



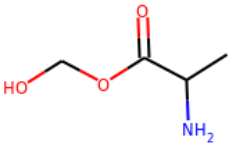
Top predicted structures (loss):



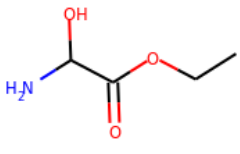
0.019032



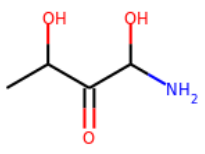
0.032936



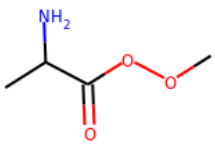
0.03333



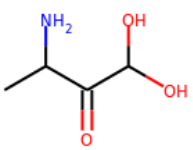
0.036132



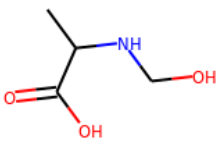
0.040698



0.04141

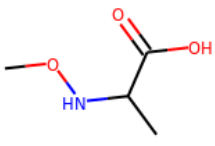


0.047184



0.048481

0.050476



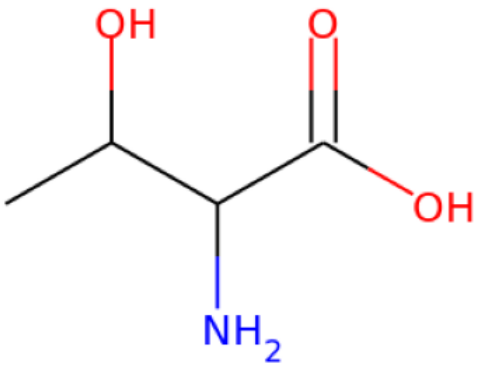
0.050609

Top predicted substructures	prob		
[CX4H3]	0.9999	[#6H3][#6][#6]	0.9789
[CX4H3][#6]	0.9918	[CX4H3][CX4]O	0.966
[CX3](=[OX1])C	0.9875	O=[CX3][CX4H]	0.9246
[#6H1]	0.9859	[#8]=[#6H0][#6H1]	0.9232
[OX2H1]	0.9848	[#8]=[#6][#8]	0.9216

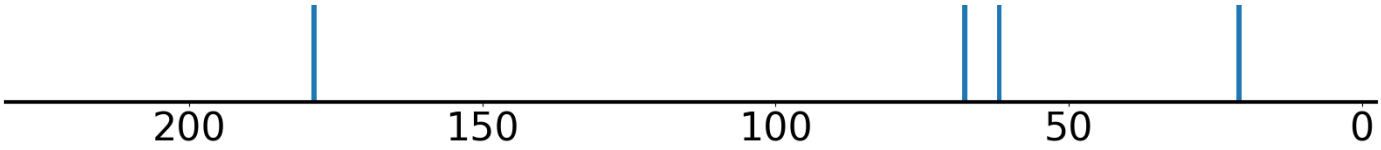
best positives	prob	best negatives	prob
[CX4H3]	0.9999	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H3][#6]	0.9918	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9875	CC=CCC#C	0.0
[#6H1]	0.9859	CC=CC#CC	0.0
[OX2H1]	0.9848	[#6X2][#6H1][#6X2]	0.0
[#6H3][#6][#6]	0.9789	C=CC=CC#C	0.0
[CX4H3][CX4]O	0.966	CC#CCC=C	0.0
O=[CX3][CX4H]	0.9246	C=CCCC#C	0.0
[#8]=[#6H0][#6H1]	0.9232	[#6H2][#6]#[#6X2]	0.0
[#8]=[#6][#8]	0.9216	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([#6])[O]	0.5983	[#6X3][#6][#6][#6H3]	0.2785
[#8][#6][#6]=[#8]	0.4209	[#6H3][#6H1][#6H1][#7]	0.2965
[#6H3][#6][#6X3]	0.3388	[#8][#6][#6][#6X3]	0.3994
[CX4H2]CC=O	0.3001	[#6X4H3][#6][#8H]	0.4933
[#7][#6H0][#6H1]	0.2864	[#6H1][#6H1]	0.5406
[CX4H2]([OX2H0])[CX4H3]	0.2696	[OH][CX4H]	0.5581
[CX4H2][CX4H2]	0.2452	[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.576
[#8][#6][#6][#8]	0.2327	[#8][#6H1][#6H1]	0.5925
[CH3]CC[OH]	0.2293	[CX4H3][CX4H1][OX2H1]	0.6009
[#7H2][#6H0]	0.2184	[#7H2][#6X4H1][#6X3]	0.609

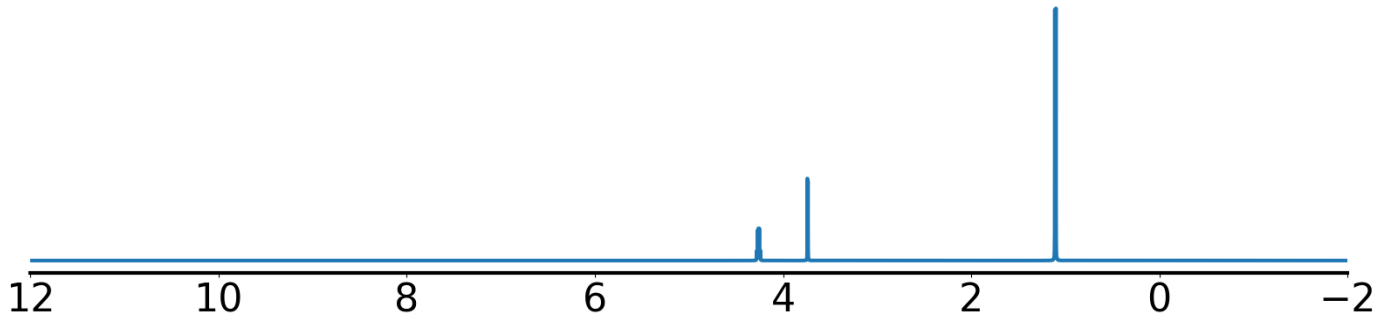
Example 82 true smiles: CC(O)C(N)C(=O)O formula: C4H9NO3
Index of correct structure: 1 of 2840
True structure loss: 0.031016
True structure:



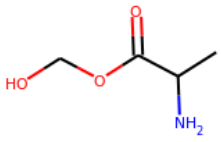
Experimental 13C NMR (solvent: D2O)



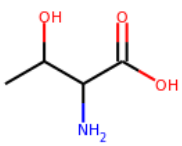
Experimental 1H NMR (solvent: D2O)



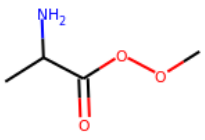
Top predicted structures (loss):



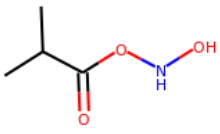
0.025



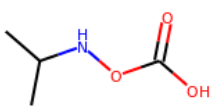
0.031016



0.031602

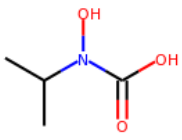


0.033318

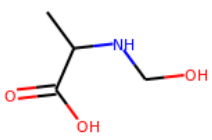


0.033689

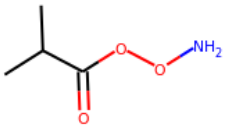
0.033888



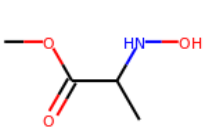
0.035416



0.035595



0.03611



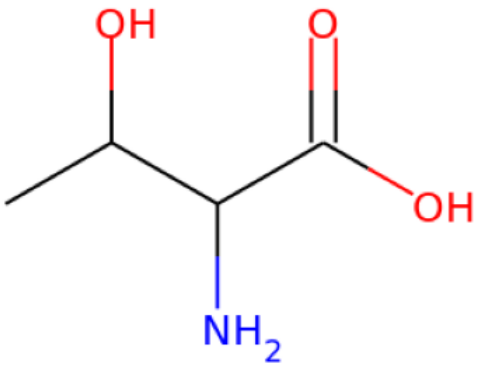
0.037933

Top predicted substructures	prob		
[CX4H3]	1.0	[#6H1]	0.9642
[CX4H3][#6]	0.9918	[#8]=[#6][#8]	0.9089
[OX2H1]	0.9871	O=[CX3][CX4H]	0.8589
[CX3](=[OX1])C	0.9834	[#8]=[#6H0][#6H1]	0.8369
[#6H3][#6][#6]	0.9697	[CX3](=[OX1])O	0.8324

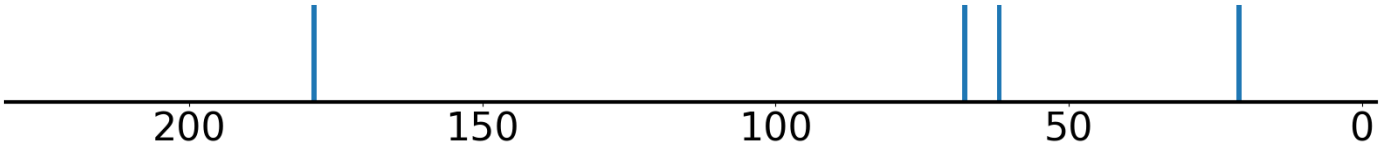
best positives	prob	best negatives	prob
[CX4H3]	1.0	CC=CC#CC	0.0
[CX4H3][#6]	0.9918	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9871	CC=CCC#C	0.0
[CX3](=[OX1])C	0.9834	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#6H3][#6][#6]	0.9697	C=CCCC#C	0.0
[#6H1]	0.9642	CCC#CC#C	0.0
[#8]=[#6][#8]	0.9089	[#6X2][#6H1][#6X2]	0.0
O=[CX3][CX4H]	0.8589	CCC#CC=C	0.0
[#8]=[#6H0][#6H1]	0.8369	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX3](=[OX1])O	0.8324	C=CC=CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([#6])[O]	0.5832	[#6H3][#6H1][#6H1][#7]	0.1181
[#8][#6][#6]=[#8]	0.4536	[#8]=[#6][#6H1][#6H1]	0.1507
[#7][#6][#6H3]	0.4487	[#8][#6H1][#6H1]	0.1525
[#8][#6][#6][#8]	0.3676	[#6H1][#6H1]	0.1635
[CH3]CC[OH]	0.3278	[#6X3][#6][#6][#6H3]	0.1894
[#6H3][#6][#6X3]	0.3236	[#8][#6][#6][#6X3]	0.2548
[#6H1][#6H2]	0.3038	[CH3][#6][#8]	0.342
[#8][#6][#6H2]	0.2832	[#7H2][#6H1]	0.3963
[#7][#6H0][#6H1]	0.2473	[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.4086
[#8H][#6H2][#6H1]	0.2472	[CX4H]O	0.4222

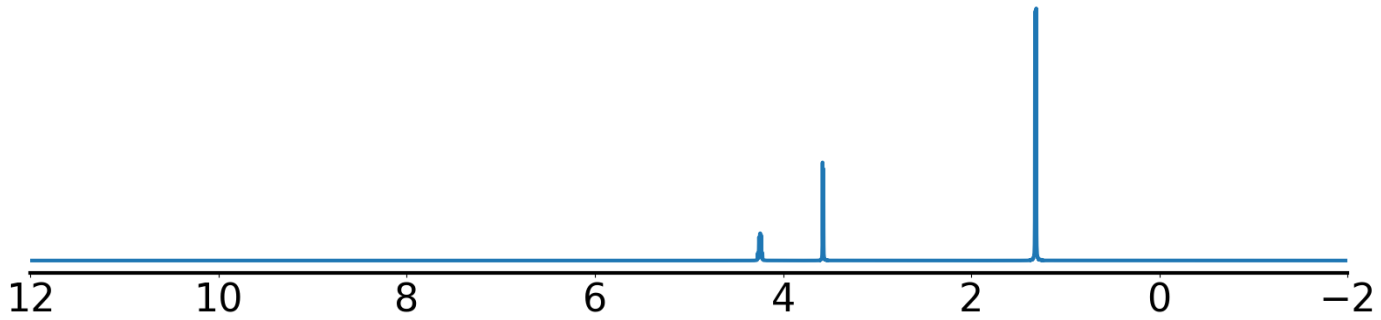
Example 83 true smiles: CC(O)C(N)C(=O)O formula: C4H9NO3
Index of correct structure: 0 of 2840
True structure loss: 0.019013
True structure:



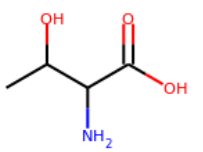
Experimental 13C NMR (solvent: D2O)



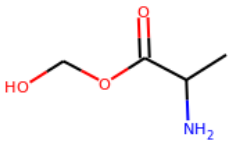
Experimental 1H NMR (solvent: D2O)



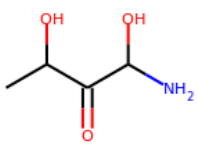
Top predicted structures (loss):



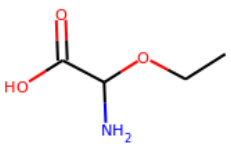
0.019013



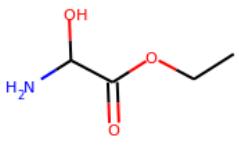
0.0327



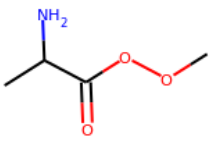
0.035489



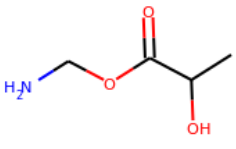
0.037584



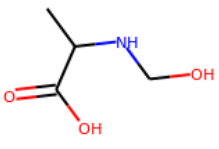
0.038551



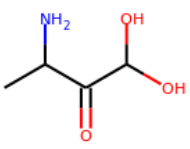
0.038865



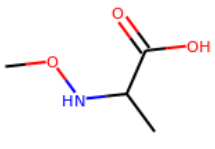
0.042675



0.043992



0.044356



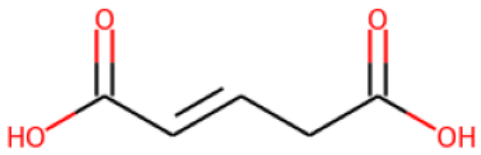
0.045511

Top predicted substructures	prob		
[CX4H3]	1.0	[CX3](=[OX1])C	0.9751
[CX4H3][#6]	0.9925	[#6H1]	0.9466
[OX2H1]	0.9821	O=[CX3][CX4H]	0.9127
[#6H3][#6][#6]	0.9819	[#8]=[#6H0][#6H1]	0.9064
[CX4H3][CX4]O	0.9773	[#8]=[#6][#8]	0.8861

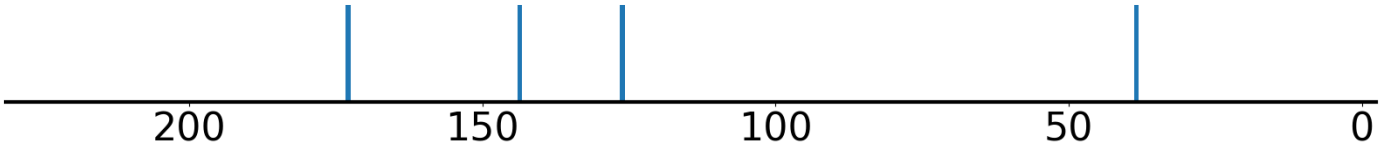
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9925	CC=CC#CC	0.0
[OX2H1]	0.9821	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#6H3][#6][#6]	0.9819	[#6X2][#6H1][#6X2]	0.0
[CX4H3][CX4]O	0.9773	CC=CCC#C	0.0
[CX3](=[OX1])C	0.9751	C=CCCC#C	0.0
[#6H1]	0.9466	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
O=[CX3][CX4H]	0.9127	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#8]=[#6H0][#6H1]	0.9064	CCC#CC=C	0.0
[#8]=[#6][#8]	0.8861	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6]=[#8]	0.5384	[#6X3][#6][#6][#6H3]	0.2192
[#6H3][#6][#6X3]	0.5148	[#8][#6][#6][#6X3]	0.2821
[CH3]CC[OH]	0.2652	[#8][#6H1][#6H1]	0.328
[#8][#6][#6][#8]	0.2423	[#6H3][#6H1][#6H1][#7]	0.3898
[CX4H2]([#6])[O]	0.2382	[#6H1][#6H1]	0.4927
[#7H2][#6H0]	0.2323	[#8]=[#6][#6H1][#6H1]	0.5244
[#7][#6H0][#6H1]	0.2256	[#7H2][#6X4H1][#6X3]	0.6013
[#8H][#6X4H1][#6X3H0]	0.2222	[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.6032
[#6H1r5][#7]	0.2187	[#7H2][#6H1]	0.6123
[CX4H](O)CO	0.211	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6604

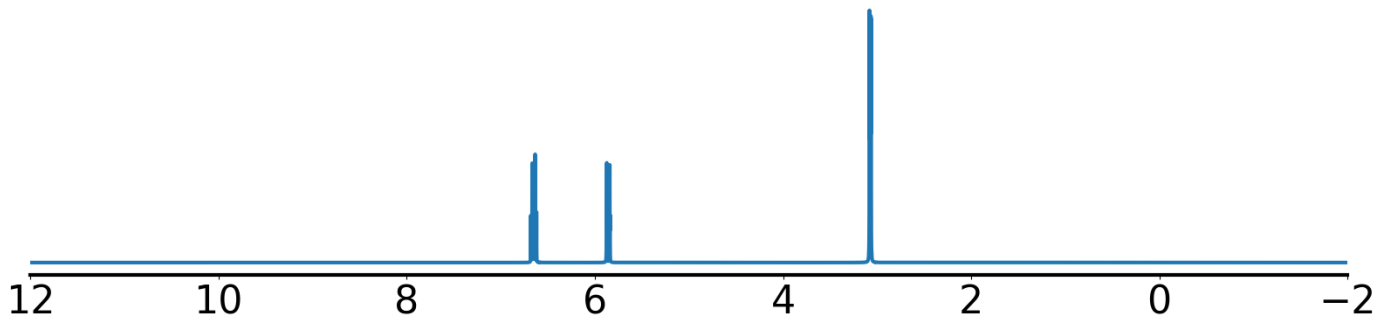
Example 84 true smiles: O=C(O)C=CCC(=O)O formula: C5H6O4
Index of correct structure: 0 of 2762
True structure loss: 0.016883
True structure:



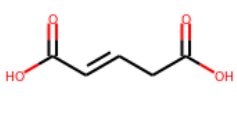
Experimental 13C NMR (solvent: CDCl3)



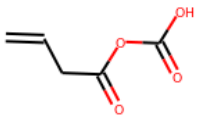
Experimental 1H NMR (solvent: D2O)



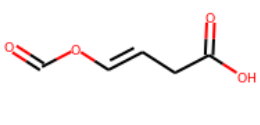
Top predicted structures (loss):



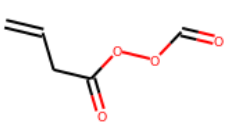
0.016883



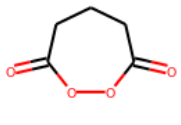
0.05633



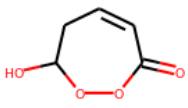
0.059739



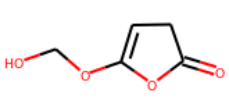
0.071016



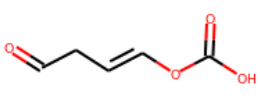
0.071765



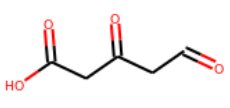
0.074151



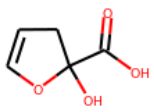
0.07869



0.081863



0.082281



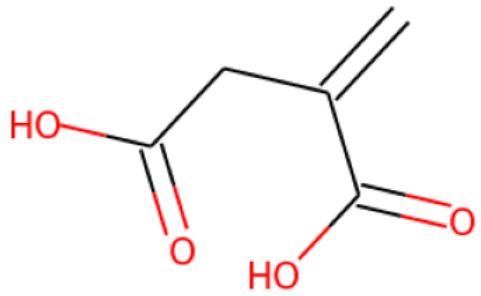
0.083658

Top predicted substructures	prob		
[#8]=[#6][#8]	0.9998	[CX3](=O)[OX2H1]	0.9559
[CX3](=[OX1])O	0.9992	[CHX3](=C)C	0.9552
[#6H1]	0.9781	[OX2H1]	0.9543
O=C[CH2][CX3H1]	0.9628	[OX1H0]=[CX3H0][CX4H2][CX3H1]	0.9305
[CX3](=[OX1])C	0.9561	[CX4H2]([#6])[#6]	0.928

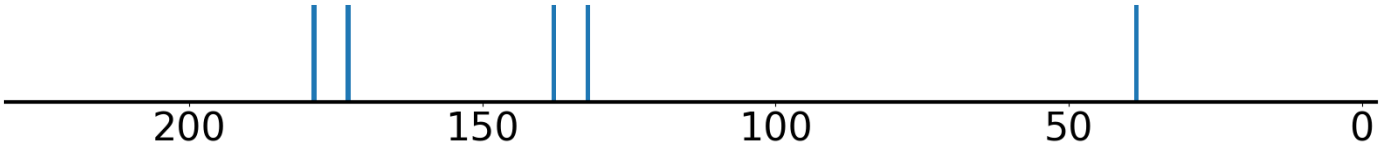
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9998	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.9992	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H1]	0.9781	C=CC=CC#C	0.0
O=C[CH2][CX3H1]	0.9628	CC#CCC#C	0.0
[CX3](=[OX1])C	0.9561	[#6X2][#6H1][#6X2]	0.0
[CX3](=O)[OX2H1]	0.9559	[CX2H0](#[CX2H1])[CX4H1]	0.0
[CHX3](=C)C	0.9552	[CX4H2]([CX4H3])[CX2H0]	0.0
[OX2H1]	0.9543	[OX2H0][CX4H2][CX2H0]#[CX2H1]	0.0
[OX1H0]=[CX3H0][CX4H2][CX3H1]	0.9305	[#7][#6H1][#6X2]	0.0
[CX4H2]([#6])[#6]	0.928	[CX2H0](#[CX2H0])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.6393	[CX3H1](=[CX3H1])[CX3H0]	0.2616
[CX4H2]CC=O	0.6297	[#8]=[#6H0][#6H1]	0.3787
OCC[CH2]	0.3754	[#8]=[#6][#6H2][#6H1]	0.4918
[OX2H0][CX3H0][CX4H2]	0.2364	[#8]=[#6][#6H1]=[#6H1]	0.5197
[#8][#6][#6][#8]	0.1611	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.5227
[CX4H2][CX4H2]	0.1489	O=C[CX3H]	0.6198
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.1372	O=[#6][#6][#6X3]	0.6245
[#8][#6][#6]=[#6][#6]=[#8]	0.1308	[#6X3H1][#6X3H0]	0.6268
[#6X3H2]	0.1296	[CX4H2][CX3H]	0.6295
[CX3H](O)	0.1002	[#8][#6H0][#6H1]	0.663

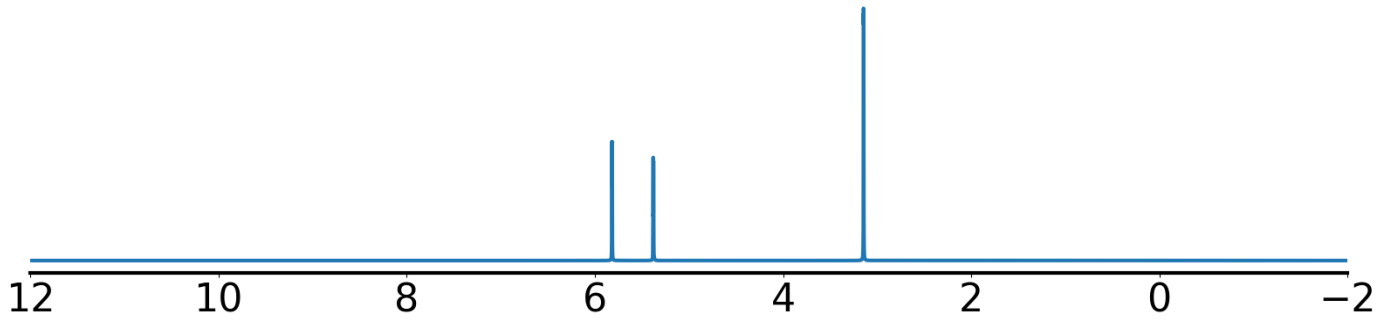
Example 85 true smiles: C=C(CC(=O)O)C(=O)O formula: C5H6O4
Index of correct structure: 0 of 2762
True structure loss: 0.01308
True structure:



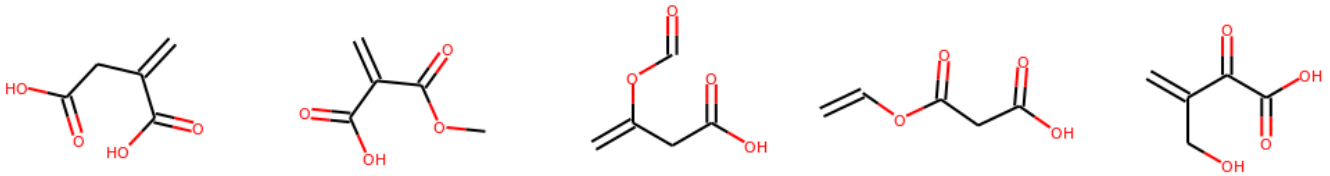
Experimental 13C NMR (solvent: D2O)

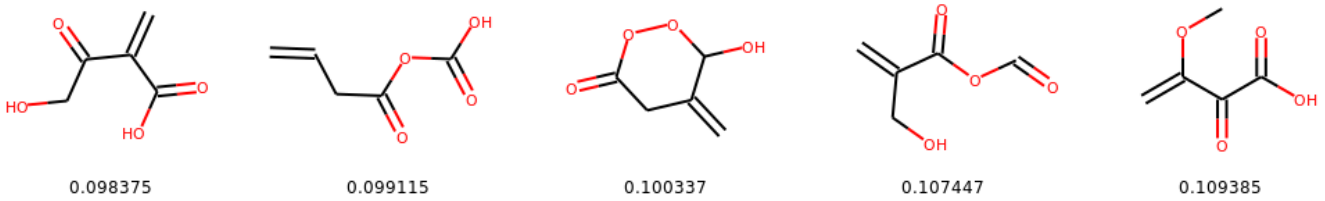


Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



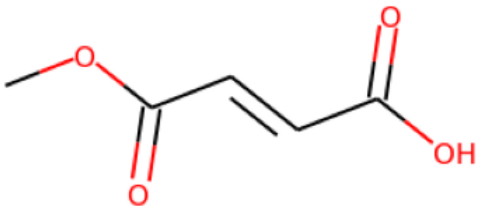


Top predicted substructures	prob		
[#8]=[#6][#8]	0.9999	[CX3H2]=[CX3H0]([#6])[#6]	0.9956
[CX3](=[OX1])O	0.9999	[CX4H2]([CX3H0])[CX3H0]	0.989
[#6X3H2]	0.9996	[CX4H2]([#6])[#6]	0.986
[CX3](=[OX1])C	0.9991	[CH2X3](=C)	0.9855
[CX3](=O)[OX2H1]	0.9978	[CX3H2]=[CX3H0][CX3H0]	0.9796

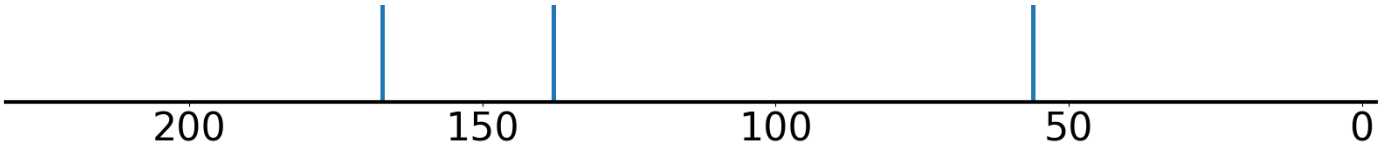
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9999	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])O	0.9999	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6X3H2]	0.9996	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[CX3](=[OX1])C	0.9991	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=O)[OX2H1]	0.9978	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[CX3H2]=[CX3H0]([#6])[#6]	0.9956	CCC#CC#C	0.0
[CX4H2]([CX3H0])[CX3H0]	0.989	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.986	[CX2H0](#[CX2H0])[CX4H0]	0.0
[CH2X3](=C)	0.9855	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[CX3H2]=[CX3H0][CX3H0]	0.9796	[OX2H1][CX4H1][CX4H1][CX2H0]	0.0

worst negatives	prob	worst positives	prob
[OX2H0][CX3H0][CX4H2]	0.4063	[#8][#6][#6][#6][#6][#8]	0.0349
[#6H1]	0.2111	[#8]=[#6][#6][#6][#6]=[#8]	0.1646
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.1825	[#8][#6][#6][#6][#6]=[#8]	0.4123
[#8][#6][#6]=[#6][#6]=[#8]	0.1558	[CX4H2]CC=O	0.5706
[#8][#6H0][#6H1]	0.1497	[CX3H0](=[CX3H2])([CX4H2])[CX3H0]	0.7751
[#6X3H1][#6X3H0]	0.1425	[#8][#6][#6]=[#6X3]	0.777
[CX4H2][CX3H]	0.1416	[#8][#6][#6][#6X3]	0.7802
[#8]=[#6][#6H2][#6H1]	0.1256	[#6H2][#6X3H0]=[#6H2]	0.8025
[#8][#6][#6]=[#8]	0.1026	[CX3H2]=[CX3H0]	0.8101
[CX4H3]	0.0873	OCC[CH2]	0.8142

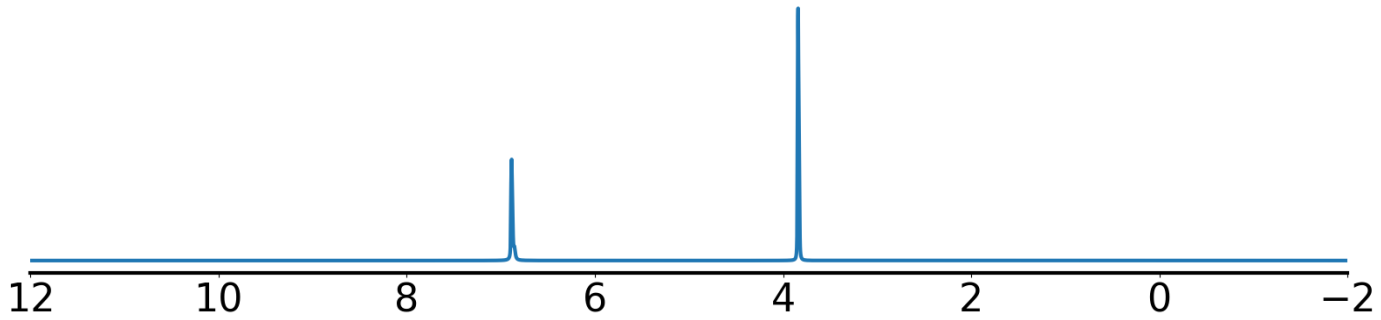
Example 86 true smiles: COC(=O)C=CC(=O)O formula: C5H6O4
Index of correct structure: 0 of 2762
True structure loss: 0.040183
True structure:



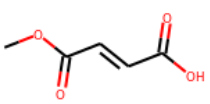
Experimental 13C NMR (solvent: CDCl3)



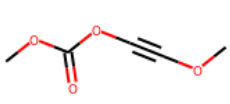
Experimental 1H NMR (solvent: D2O)



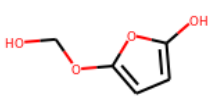
Top predicted structures (loss):



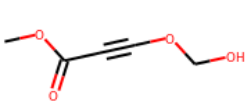
0.040183



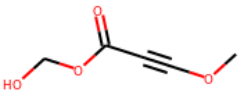
0.047029



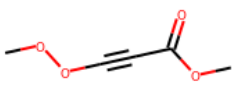
0.0508



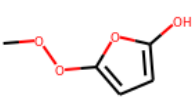
0.051253



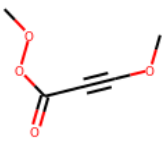
0.051843



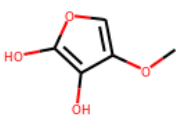
0.052214



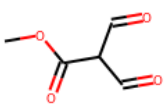
0.052267



0.052804



0.053883



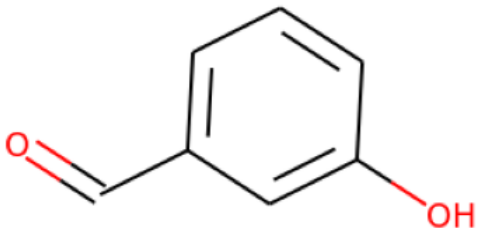
0.056626

Top predicted substructures	prob		
[#6H1]	0.9951	[CX3](=[OX1])C	0.7348
[#8]=[#6][#8]	0.9951	[#6H1][#6H1]	0.7214
[CX3](=[OX1])O	0.9796	[OX2H1]	0.715
[#6X3][#6X3]	0.8261	[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.6375
[#8][#6][#6][#6X3]	0.737	O=[#6][#6]=[#6X3]	0.6018

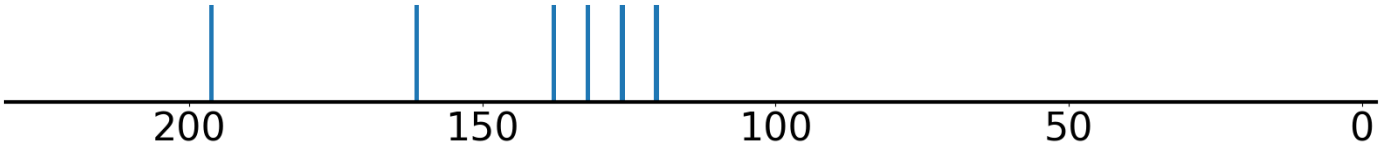
best positives	prob	best negatives	prob
[#6H1]	0.9951	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#8]=[#6][#8]	0.9951	[CX4H2]([CX4H3])[CX2H0]	0.0
[CX3](=[OX1])O	0.9796	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[#6X3][#6X3]	0.8261	[CX4H2]([NX3H0])[CX4H3]	0.0
[CX3](=[OX1])C	0.7348	CCC#CC#C	0.0
[OX2H1]	0.715	[CX2H0](#[CX2H1])[CX4H0]	0.0
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.6375	[#7][#6][#6][#6]#[#7]	0.0
O=[#6][#6]=[#6X3]	0.6018	[#6H3][#6H0][#7][#6H3]	0.0
[CHX3](=C)C	0.5702	CC#CCC#C	0.0
[#8][#6][#6]=[#6X3]	0.549	[#7X2]=[#6X3H1][#7X3H0][#6H3]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6][#6X3]	0.737	[#6X3][#6X3]=[#6X3][#6X3]	0.0222
[#6H1][#6H1]	0.7214	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.0512
[CX4H](O)([CH])[CH]	0.4793	[CX3H1](=[CX3H1])[CX3H0]	0.0923
[#8]=[#6][#6H1][#6H1]	0.3353	[#8][#6][#6]=[#6][#6]=[#8]	0.1654
[#8][#6][#6][#8]	0.3227	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.1749
[#8][#6H1][#6H1]	0.2854	[CX4H3]	0.1827
[cH]	0.2787	[#8]=[#6][#6]=[#6][#6]=[#8]	0.1836
O=[#6][#6][#6X3]	0.2746	[CX3H0](=[OX1H0])([OX2H0])[CX3H1]	0.2073
[#8][#6][#6]=[#8]	0.2572	[#8][#6][#6]=[#6][#6][#8]	0.2336
[CX4H](O)CO	0.2002	[#8]=[#6][#6H1]=[#6H1]	0.2805

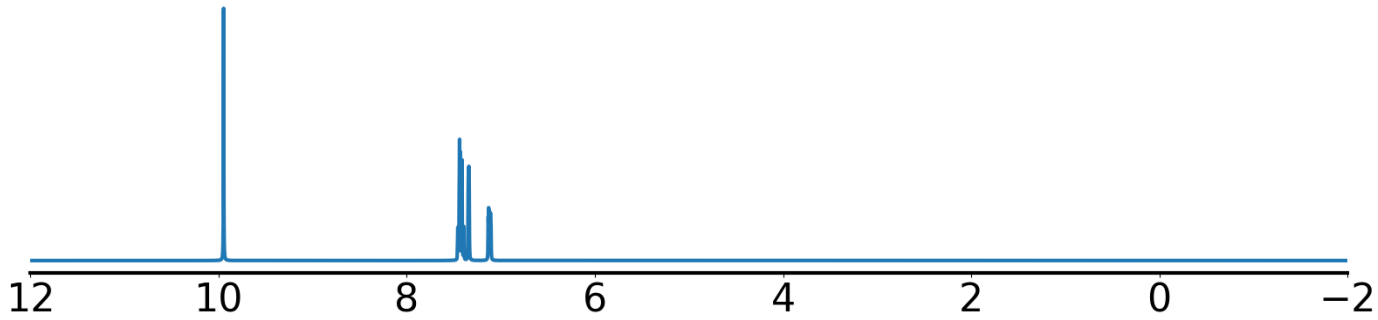
Example 87 true smiles: O=Cc1cccc(O)c1 formula: C7H6O2
Index of correct structure: 2 of 2390
True structure loss: 0.014748
True structure:



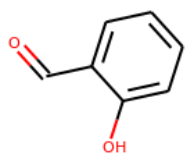
Experimental 13C NMR (solvent: CDCl3)



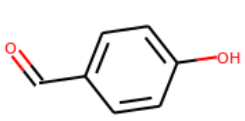
Experimental 1H NMR (solvent: CDCl3)



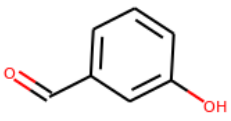
Top predicted structures (loss):



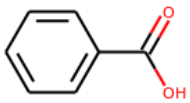
0.012713



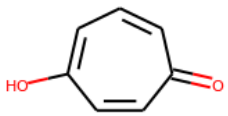
0.013394



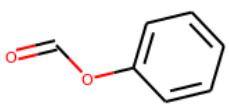
0.014748



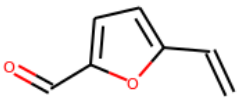
0.030149



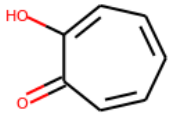
0.044794



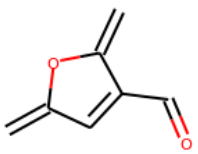
0.045856



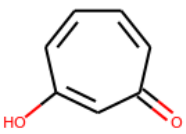
0.048388



0.049905



0.051083



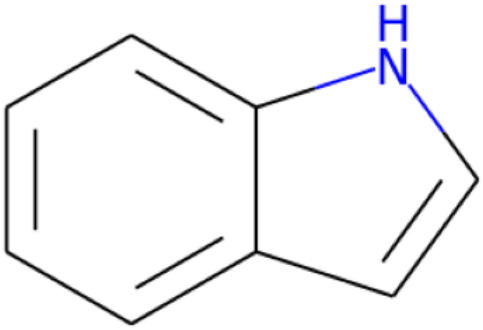
0.051486

Top predicted substructures	prob		
[#6X3][#6X3]	1.0	O=[#6][#6][#6X3]	0.9974
[#6H1]	0.9999	[cH][cH]	0.991
[CX3H1](=O)[#6]	0.9996	[cH]	0.9868
[#6X3][#6X3][#6X3][#6X3]	0.9994	[#6H1][#6H1]	0.9561
[#6X3H1][#6X3H0]	0.9985	[cX3H1]([cX3H1])[cX3H0]	0.9441

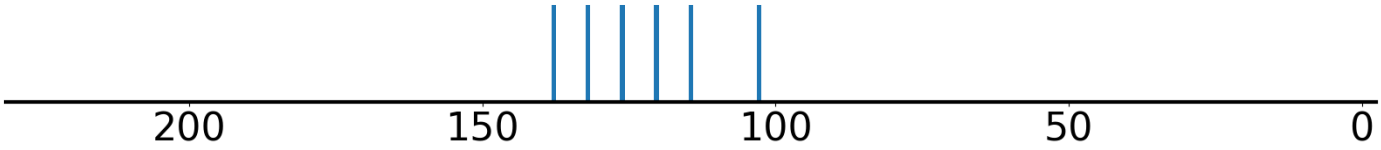
best positives	prob	best negatives	prob
[#6X3][#6X3]	1.0	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6H1]	0.9999	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[CX3H1](=O)[#6]	0.9996	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9994	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9985	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
O=[#6][#6][#6X3]	0.9974	[CX4H1]([NX3H0])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.991	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[cH]	0.9868	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6H1][#6H1]	0.9561	[CX4H1]([NX3H1])([CX4H2])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9441	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[CX3](=[OX1])C	0.5104	[cX3H1]([cX3H0])[cX3H0]	0.1209
[#8]=[#6][#6H1][#6H1]	0.3707	[cX3H0][cX3H1][cX3H0][OX2H1]	0.1317
[cX3H0][cX3H1][cX3H1][cX3H0]	0.2449	[cH]cO	0.2764
O=C[CX3H]	0.1634	[OX2H][cX3]:[c]	0.2978
[#8]=[#6H0][#6H1]	0.1448	[#8][#6][#6][#6][#6]=[#8]	0.3558
[#8]=[#6H][#6X3]=[#6X3H]	0.1373	[OX2H1]	0.5037
[#8][#6H][#6X3][#6X3H]	0.1056	[#8][#6H0][#6H1]	0.6102
[#8]=[#6H1][#6H1]	0.0906	[#8][#6][#6][#6X3]	0.6365
[OX1H0]=[cX3H0][cX3H1]	0.0877	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7175
[CX3H1](=[CX3H1])[CX3H1]	0.0872	[#6]1[#6][#6][#6][#6][#6]1	0.7588

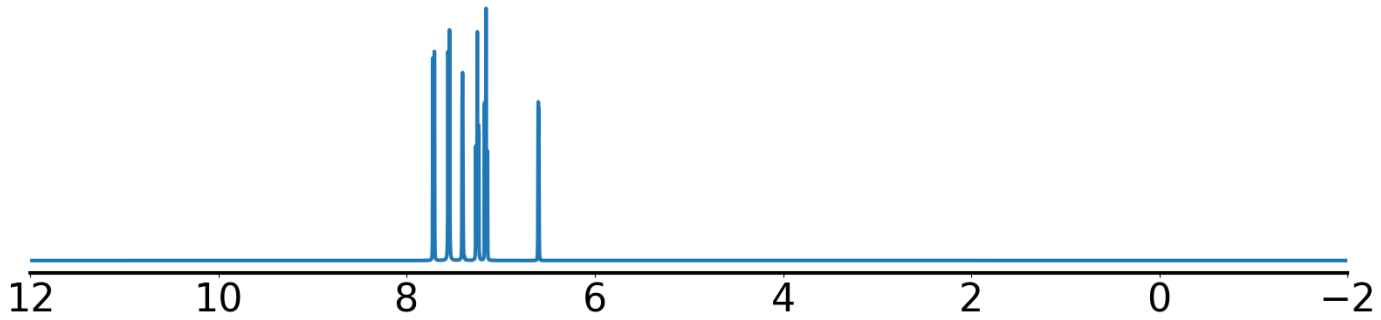
Example 88 true smiles: c1ccc2[nH]ccc2c1 formula: C8H7N
Index of correct structure: 0 of 2370
True structure loss: 0.008669
True structure:



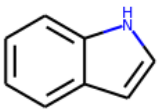
Experimental 13C NMR (solvent: CDCl3)



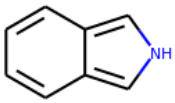
Experimental 1H NMR (solvent: D2O)



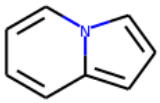
Top predicted structures (loss):



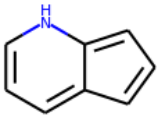
0.008669



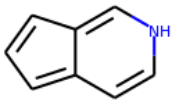
0.013965



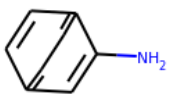
0.015204



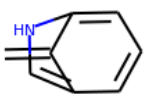
0.021481



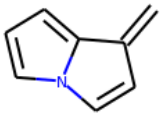
0.02677



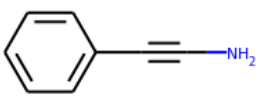
0.030027



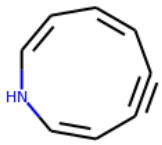
0.033928



0.034423



0.03612



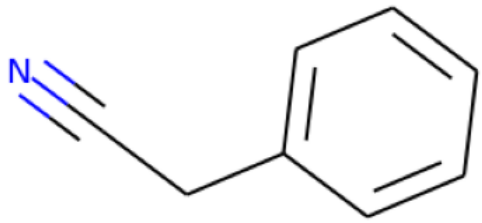
0.037248

Top predicted substructures	prob		
[#6H1]	1.0	[#6X3H1][#6X3H0]	0.997
[#6X3][#6X3][#6X3][#6X3]	0.9996	[cX3H1]([cX3H1])[cX3H0]	0.9959
[cH][cH]	0.9995	[#7][#6][#6][#6X3]	0.9855
[#6X3][#6X3]	0.9991	[#6H1][#6H1]	0.9757
[cH]	0.9982	[cX3H1]([cX3H1])[cX3H1]	0.9709

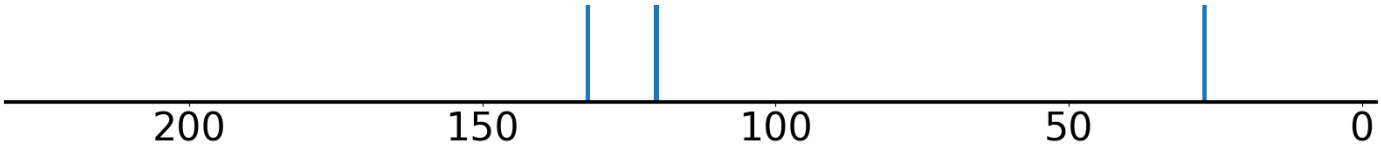
best positives	prob	best negatives	prob
[#6H1]	1.0	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9996	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cH][cH]	0.9995	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.9991	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH]	0.9982	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.997	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9959	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#7][#6][#6][#6X3]	0.9855	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6H1][#6H1]	0.9757	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9709	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6]1[#6][#6][#6][#6][#7]1	0.4302	[#7X3H1]	0.3501
[#6X3H1][#7X3H0]	0.3404	[#7H][#6X3H1]	0.4439
[#7X3H0]	0.2446	[cX3H1]([nX3H1])[cX3H1]	0.5017
[#6H1][#7][#6H1]	0.1904	[#6X3][#7X3][#6X3]	0.6953
[cX3H1]([nX3H1])[cX3H0]	0.1673	[#7][#6H0][#6H1]	0.7286
[#8][#6][#6][#6X3]	0.1434	[#6H1r5][#7]	0.729
[CX3H1](=[CX3H1])[cX3H0]	0.1274	[#7][#6X3H0][#6X3H1]	0.7353
[#7]#[#6][#6][#6X3]	0.1197	[#6]1[#6][#6][#6][#7]1	0.7535
[#7X3H2]	0.1181	[#6]1[#6][#6][#6][#6][#6]1	0.7983
[cX3H1]([nX3H0])[cX3H1]	0.0999	[#6X3][#7][#6X3]	0.8553

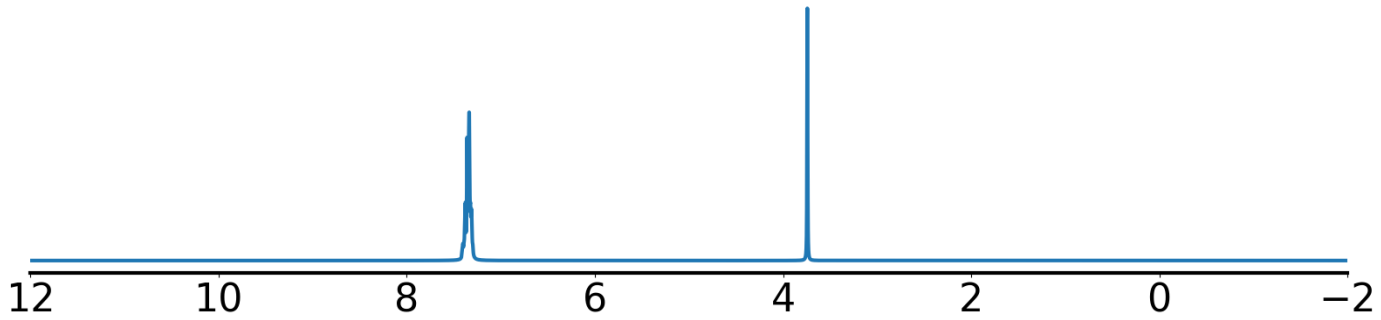
Example 89 true smiles: N#CCc1ccccc1 formula: C8H7N
Index of correct structure: 0 of 2370
True structure loss: 0.010376
True structure:



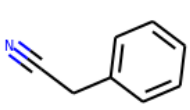
Experimental 13C NMR (solvent: CDCl3)



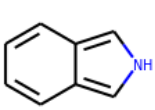
Experimental 1H NMR (solvent: CDCl3)



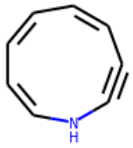
Top predicted structures (loss):



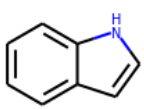
0.010376



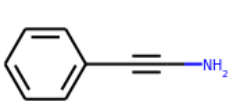
0.037804



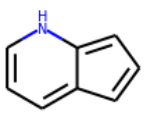
0.038478



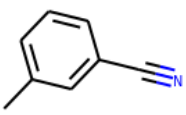
0.038617



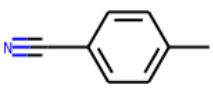
0.039793



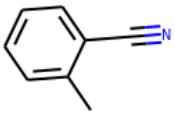
0.042286



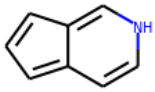
0.042591



0.04324



0.043593



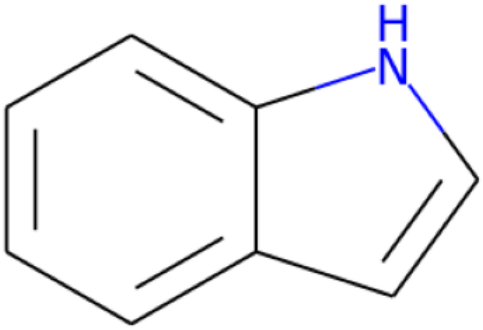
0.044861

Top predicted substructures	prob		
[#6H1]	0.9911	[#7]#[#6][#6][#6X3]	0.8348
[#6X3][#6X3]	0.974	[#6]#[#7]	0.8272
[cH]	0.9498	[#6X3][#6X3][#6X3][#6X3]	0.8072
[#6H1][#6H1]	0.8974	[cX3H1]([cX3H1])[cX3H0]	0.7411
[cH][cH]	0.8905	[#6X3H1][#6X3H0]	0.7025

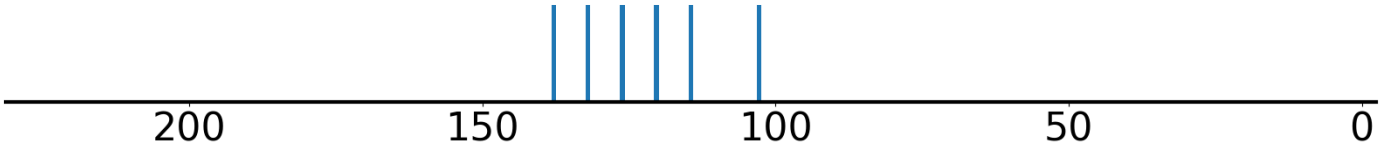
best positives	prob	best negatives	prob
[#6H1]	0.9911	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.974	[OX2H1][CX4H0][CX4H2][CX4H0]	0.0
[cH]	0.9498	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[#6H1][#6H1]	0.8974	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH][cH]	0.8905	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#7]#[#6][#6][#6X3]	0.8348	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#6]#[#7]	0.8272	[OX2H0r5][CX4H2][OX2H0r5]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.8072	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H0]	0.7411	[OX2H0][CX4H2][CX4H2][OX2H0]	0.0
[#6X3H1][#6X3H0]	0.7025	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7][#6X3]	0.3284	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.4732
[#7][#6][#6][#6X3]	0.2673	[CX2H0][CX4H2][#6X3H0]	0.5449
[CHX3]=[CHX3]	0.2171	[CX2H0](#[NX1H0])[CX4H2]	0.551
[#7][#6][#6X3]	0.2057	[CX4H2]([#6])[#6]	0.5849
[CX4H2][CX4H2]	0.1484	[#6]1[#6][#6][#6][#6][#6]1	0.5978
[#6X3][#7X3][#6X3]	0.1366	[cX3H1]([cX3H1])[cX3H1]	0.6208
[#6H3][#6][#6X3]	0.1208	[#6H2][#6X2]	0.6864
[#7][#6X3H0][#6X3H1]	0.1195	[#6X3H1][#6X3H0]	0.7025
[cX3H0]([cX3H1])([cX3H0])[CX4H2]	0.1184	[cX3H1]([cX3H1])[cX3H0]	0.7411
[CX4H2]([CX4H2])[cX3H0]	0.1108	[#6X3][#6X3][#6X3][#6X3]	0.8072

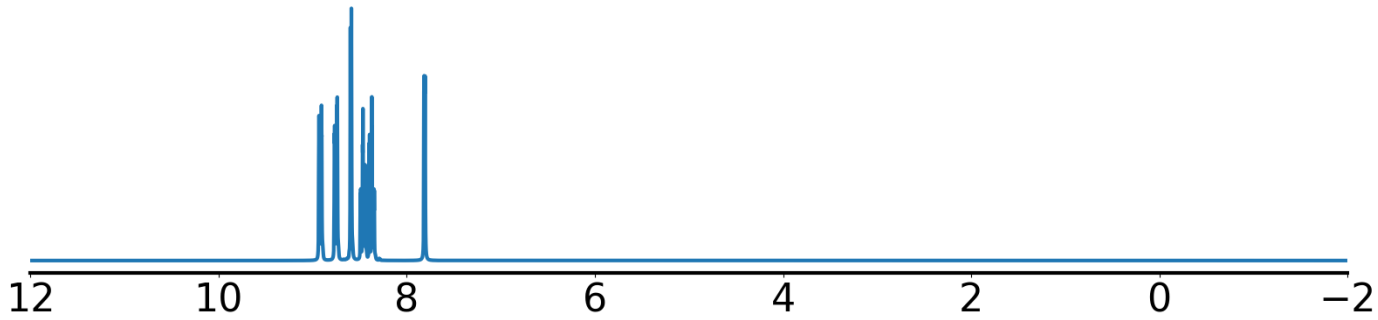
Example 90 true smiles: c1ccc2[nH]ccc2c1 formula: C8H7N
Index of correct structure: 0 of 2370
True structure loss: 0.015342
True structure:



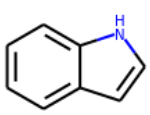
Experimental 13C NMR (solvent: CDCl3)



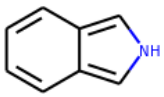
Experimental 1H NMR (solvent: D2O)



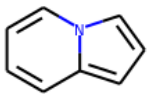
Top predicted structures (loss):



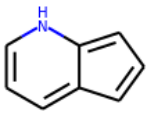
0.015342



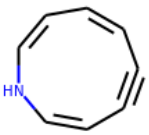
0.016765



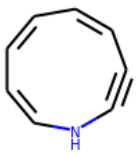
0.024085



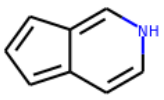
0.02584



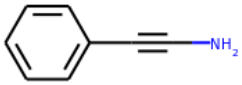
0.02696



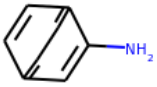
0.026964



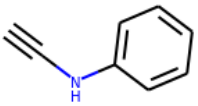
0.027941



0.03207



0.035016



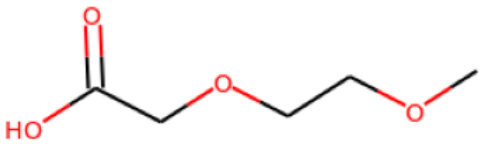
0.042892

Top predicted substructures	prob		
[#6H1]	1.0	[#6H1][#6H1]	0.9744
[cH][cH]	0.9982	[cX3H1]([cX3H1])[cX3H1]	0.9553
[#6X3][#6X3]	0.9977	[#7][#6][#6][#6X3]	0.9436
[#6X3][#6X3][#6X3][#6X3]	0.9976	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.935
[cH]	0.9952	[cX3H1]([cX3H1])[cX3H0]	0.9074

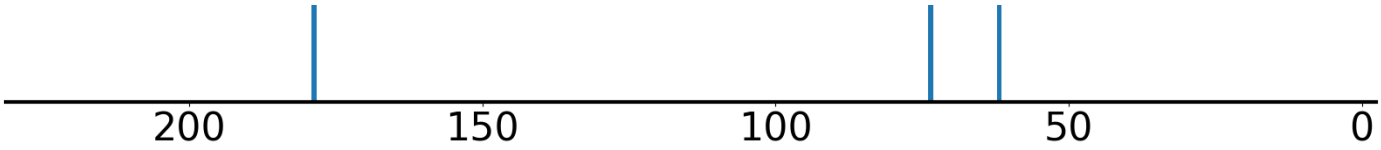
best positives	prob	best negatives	prob
[#6H1]	1.0	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cH][cH]	0.9982	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3]	0.9977	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9976	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.9952	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H1][#6H1]	0.9744	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9553	[OX2H0]1[CX4H2][CX4H2][CX4H0]1	0.0
[#7][#6][#6][#6X3]	0.9436	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.935	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9074	[OX2H1][CX4H0][CX4H1]([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6]1[#6][#6][#6][#6][#7]1	0.519	[#7X3H1]	0.1423
[#6H1][#7][#6H1]	0.3843	[#6]1[#6][#6][#6][#6][#6]1	0.265
[cX3H1]([nX2H0])[cX3H1]	0.3199	[#6X3][#7X3][#6X3]	0.2913
[#8][#6H0][#6H1]	0.1613	[#6]1[#6][#6][#6][#7]1	0.2929
[CHX3]=[CHX3]	0.1012	[#7H][#6X3H1]	0.2982
[cX3H1]([nX3H1])[cX3H0]	0.0932	[cX3H1]([nX3H1])[cX3H1]	0.3431
[#6X3]=[#6X3][#6X3]=[#6X3]	0.073	[#7][#6H0][#6H1]	0.3842
[cX3H1]([nX3H0])[cX3H1]	0.0708	[#7][#6X3H0][#6X3H1]	0.4345
[#7H2][#6H0]	0.0694	[#6H1r5][#7]	0.4396
[#8][#6][#6][#6X3]	0.0646	[#6X3][#7][#6X3]	0.7965

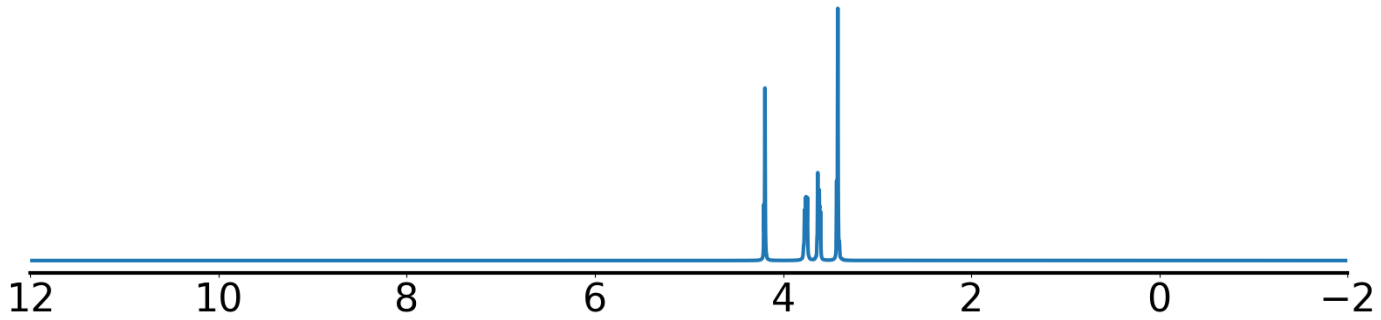
Example 91 true smiles: COCCOCC(=O)O formula: C5H10O4
Index of correct structure: 0 of 1865
True structure loss: 0.026528
True structure:



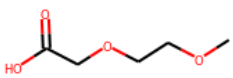
Experimental 13C NMR (solvent: CDCl3)



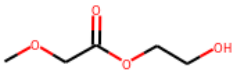
Experimental 1H NMR (solvent: CDCl3)



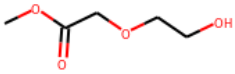
Top predicted structures (loss):



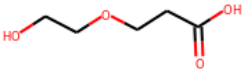
0.026528



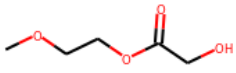
0.03734



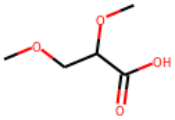
0.044413



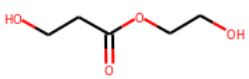
0.046428



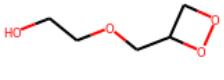
0.047324



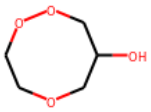
0.047717



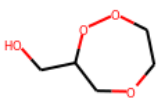
0.049079



0.050718



0.050792



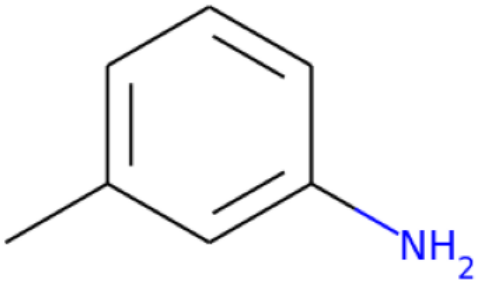
0.05223

Top predicted substructures	prob		
[CX4H2]([#6])[O]	0.9939	[OX2H1]	0.9492
[CX3](=[OX1])C	0.9898	[#8]=[#6][#8]	0.9316
[#8][#6][#6H2]	0.9656	[#8][#6][#6][#8]	0.8986
[#8][#6][#6H2][#8]	0.9514	[#8][#6][#6]=[#8]	0.825
[CX3](=[OX1])O	0.9505	[OX2H0][CX4H2][CX4H2][OX2H0]	0.8082

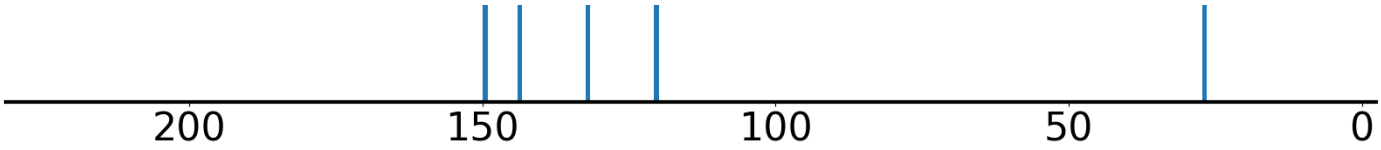
best positives	prob	best negatives	prob
[CX4H2]([#6])[O]	0.9939	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])C	0.9898	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6H2]	0.9656	[#7][#6][#6]#[#7]	0.0
[#8][#6][#6H2][#8]	0.9514	CC=CCC#C	0.0
[CX3](=[OX1])O	0.9505	C=CC=CC#C	0.0
[OX2H1]	0.9492	[CX2H0](#[CX2H0])[CX3H0]	0.0
[#8]=[#6][#8]	0.9316	[#7][#6H1][#6X2]	0.0
[#8][#6][#6][#8]	0.8986	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#8][#6][#6]=[#8]	0.825	[CX3H1](=[CX3H1])[CX2H0]	0.0
[OX2H0][CX4H2][CX4H2][OX2H0]	0.8082	[#6X3][#6]#[#6][#6H3]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.7644	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2785
[CX4H](O)CO	0.7529	[OX2H0][CX4H2][#6H0]	0.3665
OCC[CH2]	0.6905	[CX4H3][OX2H0][CX4H2]	0.3847
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6822	[CX4H2][OX2H0][CX4H2]	0.4226
[#6H1][#6H2]	0.5431	[CX4H3]	0.465
[CX4H2]CC=O	0.5052	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.4731
O[CX4H][CX4H2]	0.4774	[CX4H3][OX2H0]	0.5149
[CX4H2](O)[CHX4]	0.447	[CX4H2]([OX2H0])[CX4H2]	0.5459
[#8]=[#6H0][#6H1]	0.4139	[#8]=[#6][#6H2][#8]	0.5688
O=[CX3][CX4H]	0.3913	[CX4H2][CX3]=O	0.5734

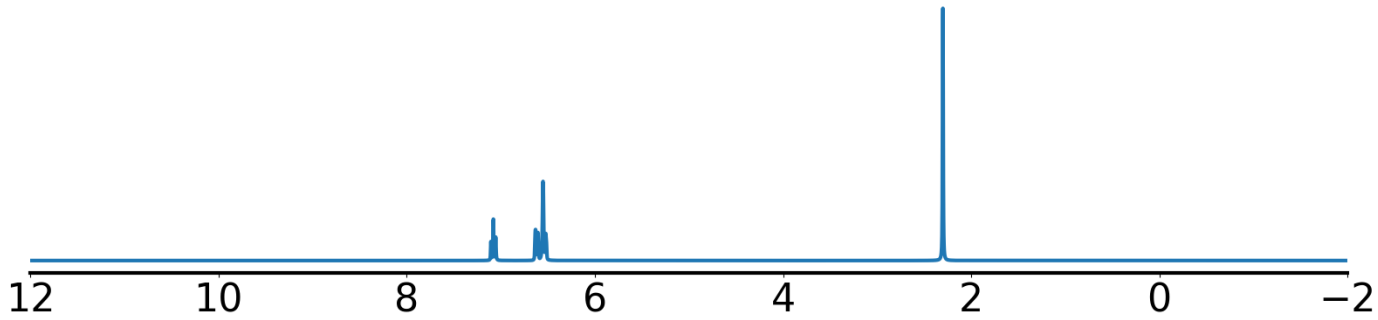
Example 92 true smiles: Cc1cccc(N)c1 formula: C7H9N
Index of correct structure: 0 of 1755
True structure loss: 0.01404
True structure:



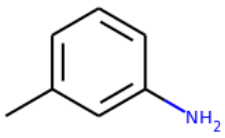
Experimental 13C NMR (solvent: CDCl3)



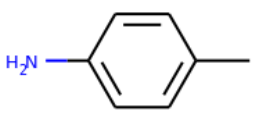
Experimental 1H NMR (solvent: CDCl3)



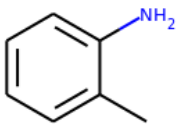
Top predicted structures (loss):



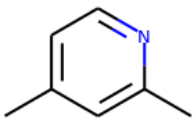
0.01404



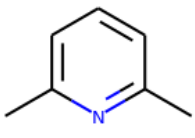
0.014554



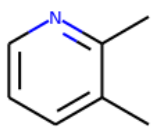
0.016638



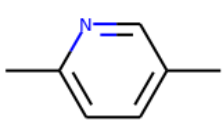
0.01955



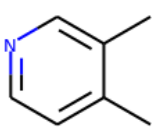
0.020187



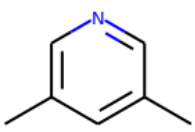
0.026088



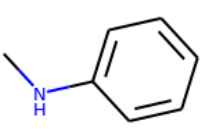
0.026829



0.038456



0.039593



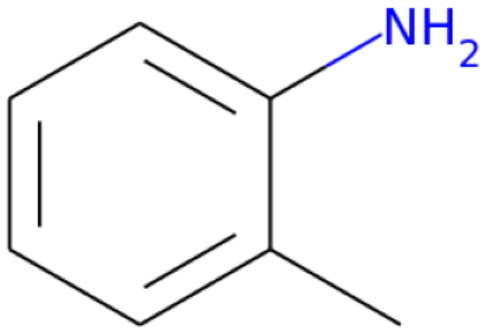
0.041978

Top predicted substructures	prob		
[#6H1]	0.9981	[#6H3][#6H0]	0.9376
[#6X3][#6X3]	0.9977	[cX3H1]([cX3H1])[cX3H0]	0.9155
[cH][cH]	0.9839	[#7][#6][#6X3]	0.9146
[#6X3][#6X3][#6X3][#6X3]	0.9803	[#6H1][#6H1]	0.9016
[#6X3H1][#6X3H0]	0.9448	[#7][#6][#6][#6X3]	0.8958

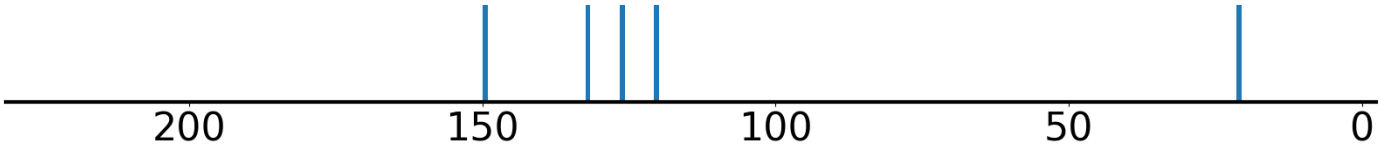
best positives	prob	best negatives	prob
[#6H1]	0.9981	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3]	0.9977	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9839	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9803	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9448	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[#6H3][#6H0]	0.9376	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9155	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#7][#6][#6X3]	0.9146	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6H1][#6H1]	0.9016	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#7][#6][#6][#6X3]	0.8958	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6]1[#6][#6][#6][#6][#7]1	0.403	[cX3H1]([cX3H0])[cX3H0]	0.133
[CHX3](=C)C	0.392	[#7H2][#6H0]	0.2834
[#6X3][#7][#6X3]	0.3811	[#7][#6H0][#6H1]	0.4359
[#7X3H1]	0.2731	[#7X3H2]	0.491
[CX4H2]([#6])[#6]	0.1712	[#7][#6X3H0][#6X3H1]	0.5626
[#7][#6][#6H3]	0.1604	[#6X3][#6][#6][#6H3]	0.6209
[cX3H0][cX3H1][cX3H1][cX3H0]	0.1428	[cX3H1]([cX3H1])[cX3H1]	0.6398
[#6X3]=[#6X3][#6X3]=[#6X3]	0.1392	[#6]1[#6][#6][#6][#6][#6]1	0.7191
[CHX3]=[CHX3]	0.1351	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.8029
[CX4H2][CX3H]	0.1084	[CX4H3][#6]	0.8394

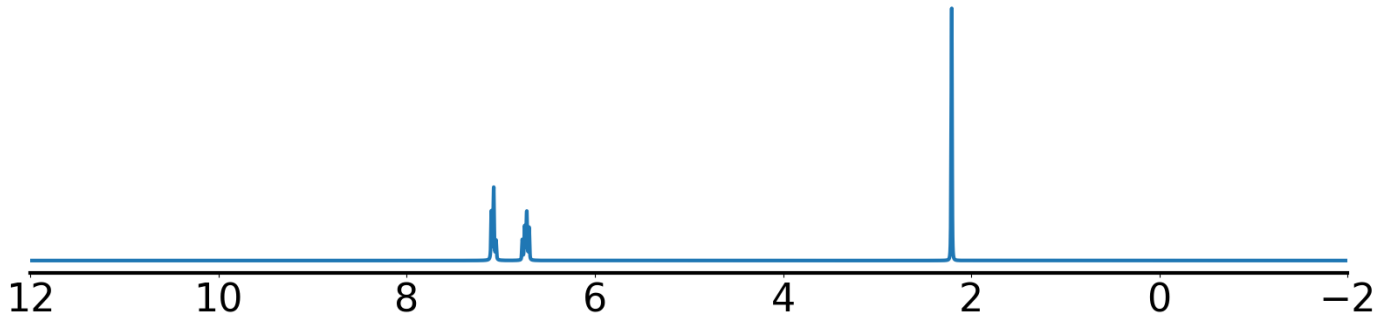
Example 93 true smiles: Cc1ccccc1N formula: C7H9N
Index of correct structure: 0 of 1755
True structure loss: 0.015657
True structure:



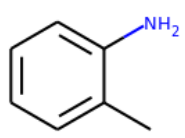
Experimental 13C NMR (solvent: CDCl3)



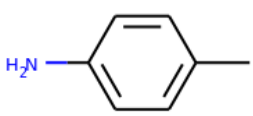
Experimental 1H NMR (solvent: CDCl3)



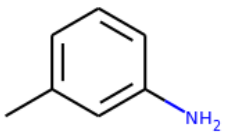
Top predicted structures (loss):



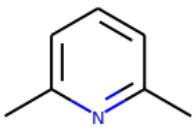
0.015657



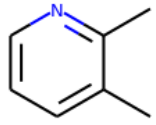
0.018607



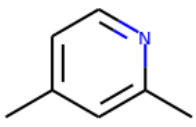
0.019227



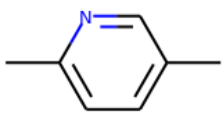
0.027272



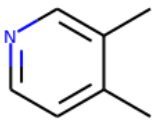
0.029253



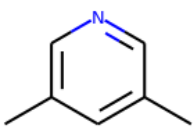
0.029578



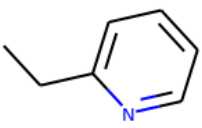
0.034941



0.039918



0.04112



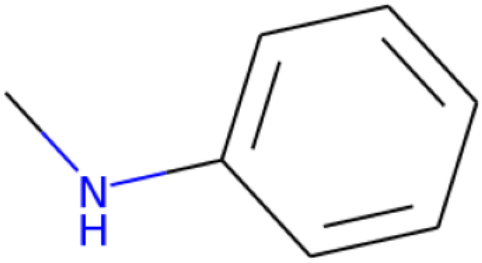
0.048189

Top predicted substructures	prob		
[#6X3][#6X3]	0.9979	[#6X3][#6X3][#6X3][#6X3]	0.9424
[#6H1]	0.9962	[#6H3][#6][#6]	0.9326
[CX4H3][#6]	0.9958	[#6H3][#6H0]	0.8925
[CX4H3]	0.9887	[#6X3H1][#6X3H0]	0.8825
[cH][cH]	0.9576	[#6]1[#6][#6][#6][#6][#6]1	0.8556

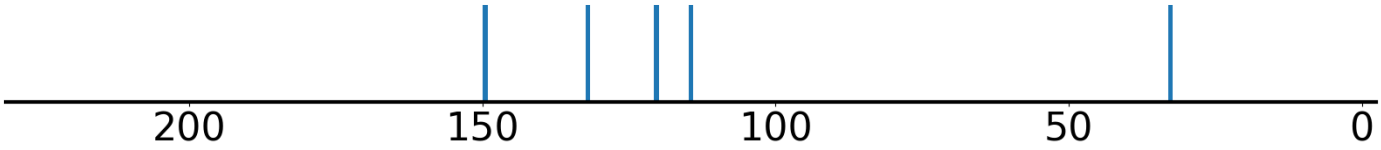
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9979	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H1]	0.9962	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3][#6]	0.9958	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3]	0.9887	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9576	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9424	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6H3][#6][#6]	0.9326	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6H3][#6H0]	0.8925	[#6]1[#8][#6][#6]1=[#8]	0.0
[#6X3H1][#6X3H0]	0.8825	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.8556	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3797	[#7H2][#6H0]	0.1473
[CHX3](=C)C	0.324	[#7][#6H0][#6H1]	0.3268
[#6X3][#7][#6X3]	0.322	[#7X3H2]	0.4268
[#6H3][#6]=[#6X3]	0.2535	[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.431
[CHX3]=[CHX3]	0.2174	[#7][#6X3H0][#6X3H1]	0.4638
[#7H][#6X3H1]	0.2059	[#6X3][#6][#6][#6H3]	0.5048
[#6X3][#6]=[#6][#6H3]	0.1997	[#7][#6][#6X3]	0.5873
[#6]1[#6][#6][#6][#6][#7]1	0.1941	[cX3H1]([cX3H1])[cX3H1]	0.5915
[CX4H2][CX3]=C	0.1888	[CX4H3][cX3H0]	0.6959
[#7X3H1]	0.1866	[#6H3][#6][#6X3]	0.744

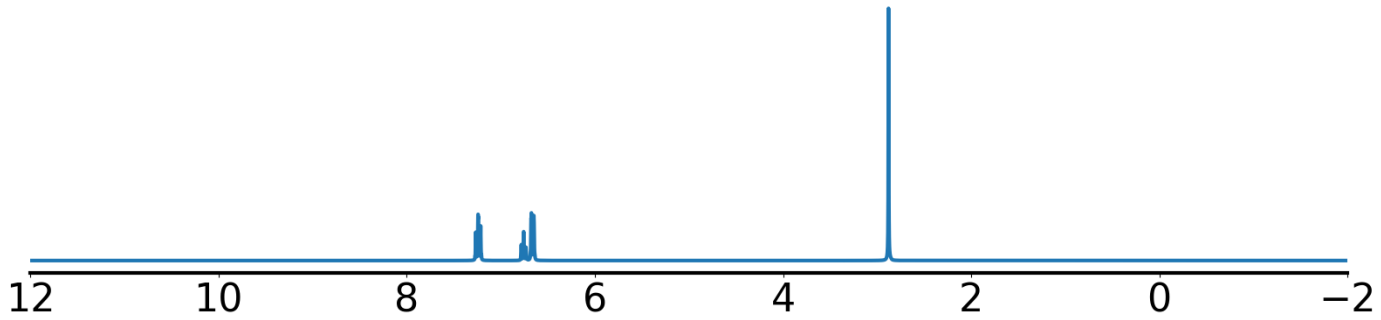
Example 94 true smiles: CNc1ccccc1 formula: C7H9N
Index of correct structure: 0 of 1755
True structure loss: 0.009893
True structure:



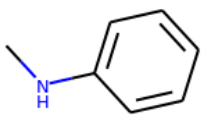
Experimental 13C NMR (solvent: CDCl3)



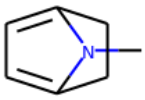
Experimental 1H NMR (solvent: CDCl3)



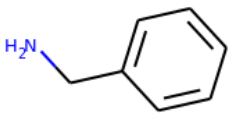
Top predicted structures (loss):



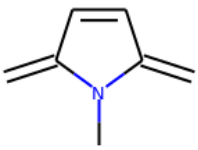
0.009893



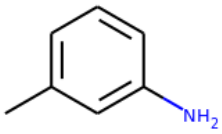
0.041262



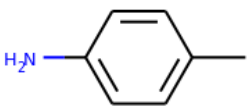
0.042546



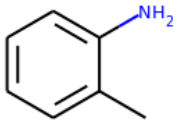
0.043419



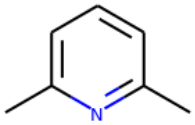
0.044812



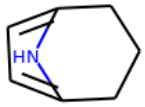
0.046776



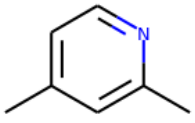
0.048976



0.054249



0.054935



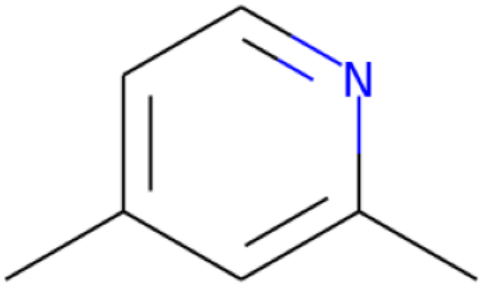
0.056296

Top predicted substructures	prob		
[#6H1]	0.9997	[cH]	0.9739
[#6X3][#6X3][#6X3][#6X3]	0.9949	[cX3H1]([cX3H1])[cX3H0]	0.9728
[#6X3][#6X3]	0.9933	[#7][#6][#6X3]	0.9542
[cH][cH]	0.9899	[cX3H1]([cX3H1])[cX3H1]	0.9153
[#6X3H1][#6X3H0]	0.9763	[#6H3][#7]	0.8853

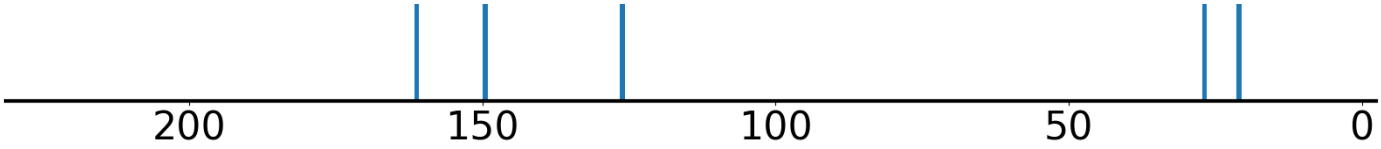
best positives	prob	best negatives	prob
[#6H1]	0.9997	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9949	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3]	0.9933	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9899	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9763	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9739	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9728	[#6]1[#8][#6][#6]1=[#8]	0.0
[#7][#6][#6X3]	0.9542	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9153	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#6H3][#7]	0.8853	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7][#6X3]	0.5759	[CX4H3][NX3H1]	0.4815
[#6]1[#6][#6][#6][#6][#7]1	0.474	[#7X3H1]	0.5255
[#6X3][#7X3][#6X3]	0.2969	[#7][#6X3H0][#6X3H1]	0.6407
[#6H1r5][#7]	0.2498	[#7][#6H0][#6H1]	0.715
[#7H][#6X3H1]	0.2331	[#6H3][#7][#6X3]	0.7178
[#6]1[#6][#6][#6][#7]1	0.1981	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7768
[#6X3][#6H2][#6X3]	0.1453	[CX4H3]	0.8312
[#7X3H2]	0.1385	[#6]1[#6][#6][#6][#6][#6]1	0.855
[CX4H2]([#6])[#6]	0.138	[#7][#6][#6][#6X3]	0.8725
[#6H3][#6][#6X3]	0.1187	[#6H1][#6H1]	0.878

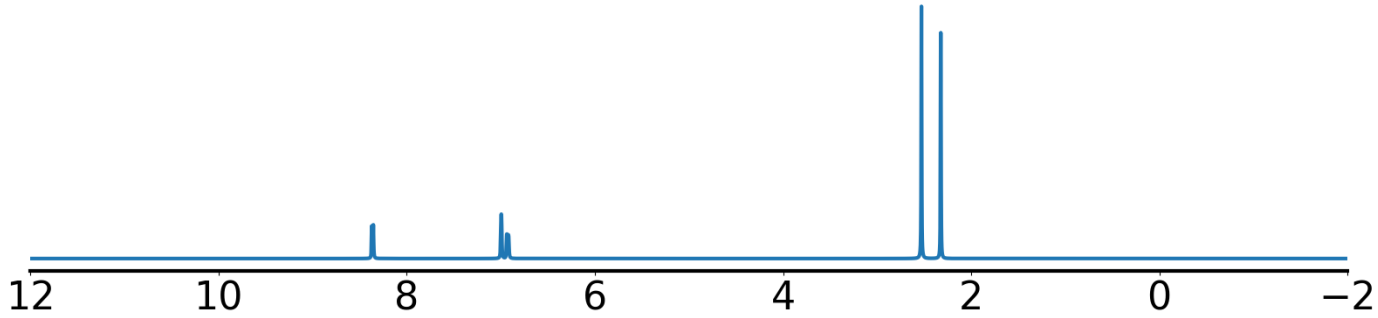
Example 95 true smiles: Cc1ccnc(C)c1 formula: C7H9N
Index of correct structure: 0 of 1755
True structure loss: 0.013298
True structure:



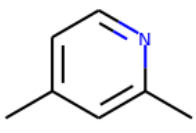
Experimental 13C NMR (solvent: CDCl3)



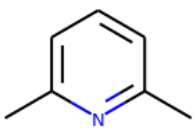
Experimental 1H NMR (solvent: CDCl3)



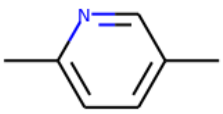
Top predicted structures (loss):



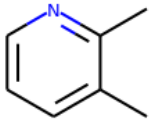
0.013298



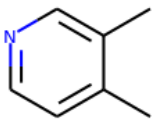
0.015574



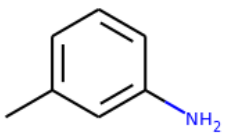
0.016487



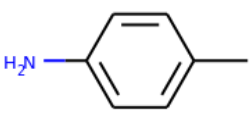
0.017267



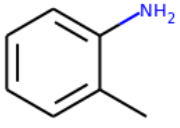
0.022711



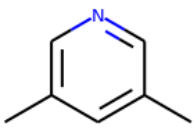
0.02455



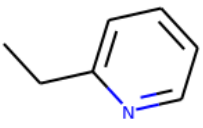
0.024582



0.024994



0.028351



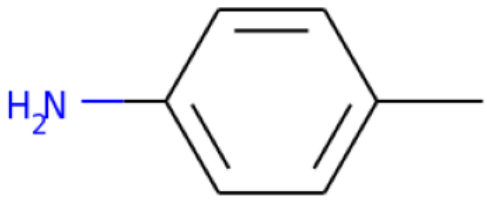
0.038191

Top predicted substructures	prob		
[#6X3][#6X3]	0.9933	[#6H3][#6H0]	0.9868
[#6H3][#6][#6]	0.9932	[cH][cH]	0.9862
[#6H1]	0.993	[CX4H3][cX3H0]	0.9798
[CX4H3]	0.9926	[CX4H3][#6]	0.9668
[#6X3][#6X3][#6X3][#6X3]	0.9925	[#6X3][#6][#6][#6H3]	0.9488

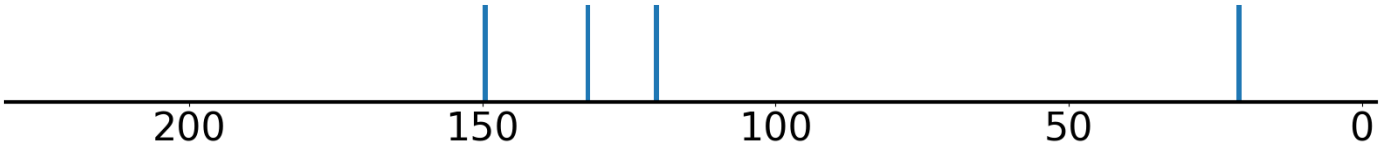
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9933	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H3][#6][#6]	0.9932	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H1]	0.993	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3]	0.9926	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9925	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#6H3][#6H0]	0.9868	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[cH][cH]	0.9862	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[CX4H3][cX3H0]	0.9798	[OX2H0]1[CX4H2][CX4H2][CX4H0]1	0.0
[CX4H3][#6]	0.9668	[#6]1[#8][#6][#6]1=[#8]	0.0
[#6X3][#6][#6][#6H3]	0.9488	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([#6])[#6]	0.6798	[cX3H1]([cX3H0])[cX3H0]	0.237
[CX4H2][CX4H2]	0.6223	[#7][#6H0][#6H1]	0.3474
[#6]1[#6][#6][#6][#6][#6]1	0.4063	[cX3H1]([nX2H0])[cX3H1]	0.5246
[cX3H1]([cX3H1])[cX3H1]	0.3669	[#7][#6X3H0][#6X3H1]	0.5552
[cX3H1]([nX2H0])[cX3H0]	0.2575	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5771
[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.2169	[#7][#6][#6H3]	0.5941
[#6H3][#6H0][#6H1][#7]	0.2112	[#6X3][#7][#6X3]	0.6808
[#6H1][#6H2]	0.1912	[#6]1[#6][#6][#6][#6][#7]1	0.6813
[cX3H0][cX3H1][cX3H1][cX3H0]	0.1486	[#7][#6][#6X3]	0.887
[CX4H2]([CX4H2])[CX3H1]	0.1246	[#6H1][#6H1]	0.8948

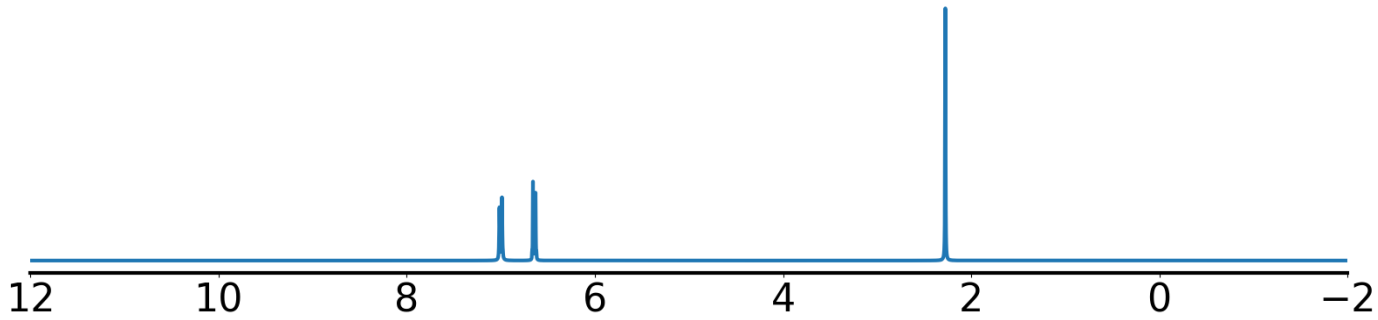
Example 96 true smiles: Cc1ccc(N)cc1 formula: C7H9N
Index of correct structure: 0 of 1755
True structure loss: 0.012272
True structure:



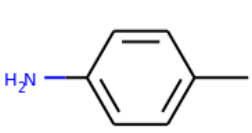
Experimental 13C NMR (solvent: CDCl3)



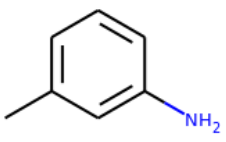
Experimental 1H NMR (solvent: CDCl3)



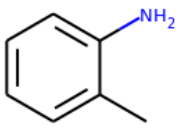
Top predicted structures (loss):



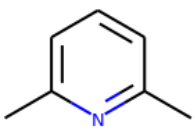
0.012272



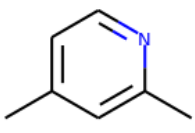
0.012897



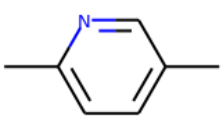
0.013551



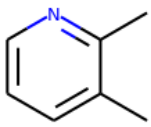
0.021013



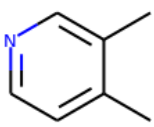
0.021516



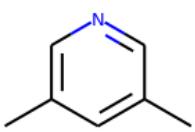
0.022322



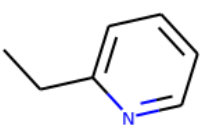
0.024314



0.031965



0.035487



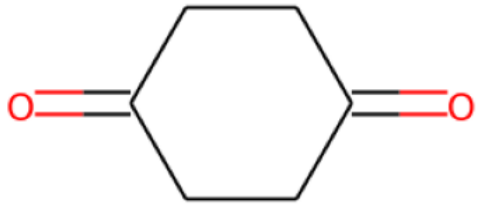
0.048218

Top predicted substructures	prob		
[#6X3][#6X3]	0.9963	[cH][cH]	0.9841
[#6H1]	0.9929	[#6H3][#6H0]	0.9714
[CX4H3][#6]	0.9899	[#6H3][#6][#6]	0.9517
[#6X3][#6X3][#6X3][#6X3]	0.9894	[#6X3H1][#6X3H0]	0.9512
[CX4H3]	0.9874	[cX3H1]([cX3H1])[cX3H0]	0.9414

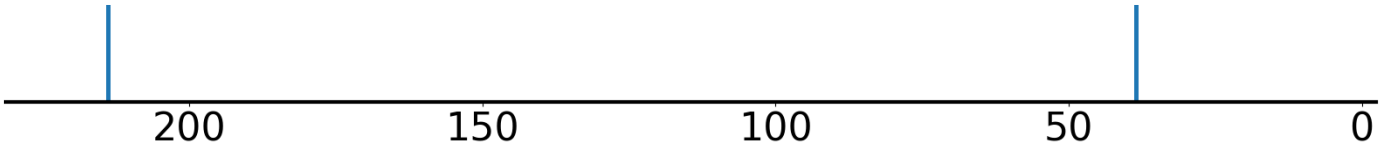
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9963	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H1]	0.9929	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3][#6]	0.9899	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9894	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[CX4H3]	0.9874	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[cH][cH]	0.9841	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#6H3][#6H0]	0.9714	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6H3][#6][#6]	0.9517	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9512	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9414	[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.7615	[#7H2][#6H0]	0.1784
[#6]1[#6][#6][#6][#6][#7]1	0.4605	[#7X3H2]	0.5267
[#6X3][#7][#6X3]	0.3779	[#7][#6H0][#6H1]	0.545
[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.2914	[cX3H0][cX3H1][cX3H1][cX3H0]	0.6044
[#7X3H1]	0.2149	[#7][#6X3H0][#6X3H1]	0.6059
[cX3H1]([cX3H0])[cX3H0]	0.2082	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7451
[#6]1[#6][#6][#6][#7]1	0.1856	[#6H1][#6H1]	0.8463
[#7H][#6X3H1]	0.1657	[CX4H3][cX3H0]	0.8543
[#6X3][#7X3][#6X3]	0.1316	[#6X3][#6][#6][#6H3]	0.8705
[#6H3][#6]=[#6X3]	0.125	[#6]1[#6][#6][#6][#6][#6]1	0.882

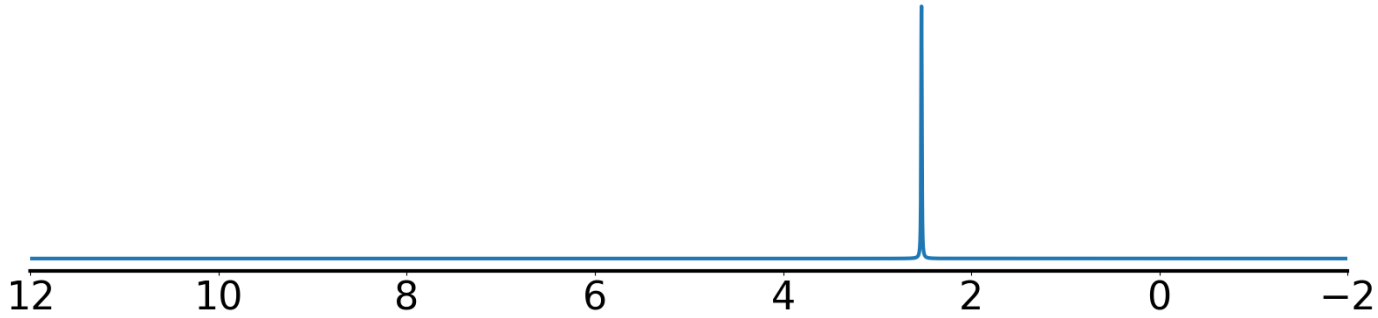
Example 97 true smiles: O=C1CCC(=O)CC1 formula: C6H8O2
Index of correct structure: 0 of 1578
True structure loss: 0.007099
True structure:



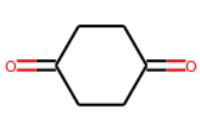
Experimental 13C NMR (solvent: CDCl3)



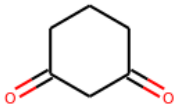
Experimental 1H NMR (solvent: CDCl3)



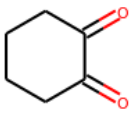
Top predicted structures (loss):



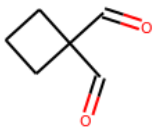
0.007099



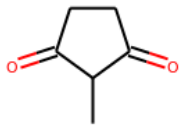
0.032071



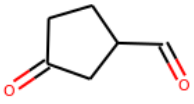
0.032482



0.069982

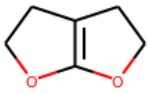


0.0849

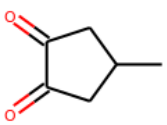


0.091144

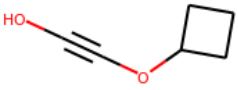
0.111186



0.119501



0.120469



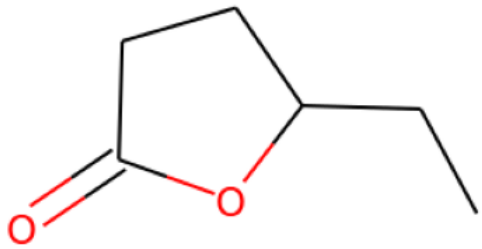
0.121847

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9991	O=[CX3H0][CX4H2][CX4H2]	0.8807
[CX4H2]([#6])[#6]	0.9903	[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.8596
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9902	[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.8429
[CX4H2][CX3]=O	0.9252	[CX4H2]CC=O	0.8414
[CX4H2]([CX4H2])[CX3H0]	0.9108	[#6H2][#6X3H0][#6H2]	0.789

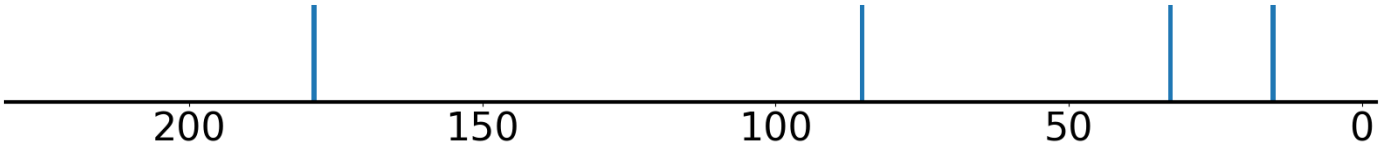
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9991	[CX3H1](=[CX3H2])[NX3H0]	0.0
[CX4H2]([#6])[#6]	0.9903	[#6H3][#6H1][#6H1]=[#7]	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9902	[CX3H0](=[CX3H2])([OX2H0])[CX4H3]	0.0
[CX4H2][CX3]=O	0.9252	C=CC=CC#C	0.0
[CX4H2]([CX4H2])[CX3H0]	0.9108	CC=CC#CC	0.0
O=[CX3H0][CX4H2][CX4H2]	0.8807	[#8][#6H1]=[#6H1][#6H3]	0.0
[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.8596	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.8429	[CX3H1](=[CX3H2])[OX2H0]	0.0
[CX4H2]CC=O	0.8414	[#6H3][#6H1][#7][#7]	0.0
[#6H2][#6X3H0][#6H2]	0.789	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#6H2][#6H1]	0.1947	[#8]=[#6][#6][#6][#6]=[#8]	0.5238
[#6]1[#6][#6][#6][#6]1	0.1936	[CX4H2][CX4H2]	0.5709
C1CCCC1	0.1675	[#6]1[#6][#6][#6][#6][#6]1	0.6172
[#6H1][#6H2]	0.1624	CCCCCC	0.6319
[#6H1][#6H1]	0.1547	[#6H2][#6X3H0][#6H2]	0.789
[CX3H0](=[OX1H0])([CX4H2])[CX3H0]	0.1515	[CX4H2]CC=O	0.8414
[#8][#6][#6][#6][#6]=[#8]	0.1312	[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.8429
OCC[CH2]	0.1253	[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.8596
[#6H1]	0.114	O=[CX3H0][CX4H2][CX4H2]	0.8807
O=CC=O	0.1094	[CX4H2]([CX4H2])[CX3H0]	0.9108

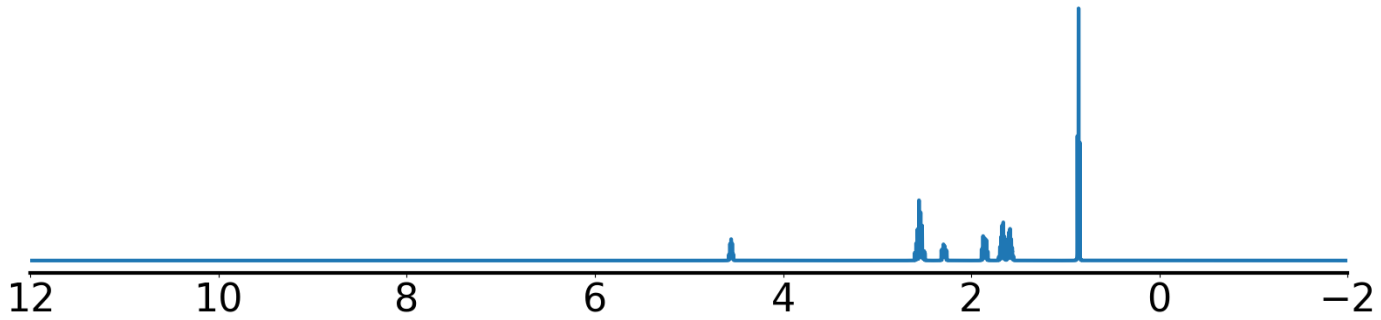
Example 98 true smiles: CCC1CCC(=O)O1 formula: C6H10O2
Index of correct structure: 0 of 1567
True structure loss: 0.013298
True structure:



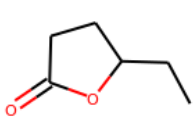
Experimental 13C NMR (solvent: CDCl3)



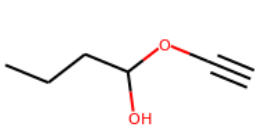
Experimental 1H NMR (solvent: D2O)



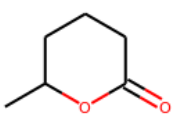
Top predicted structures (loss):



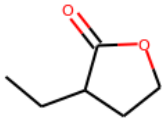
0.013298



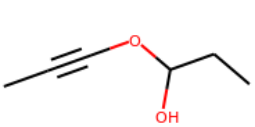
0.062732



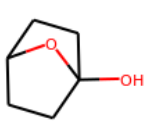
0.063131



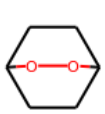
0.076545



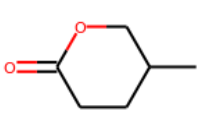
0.078268



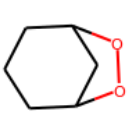
0.080148



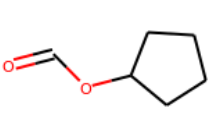
0.082432



0.085663



0.08738



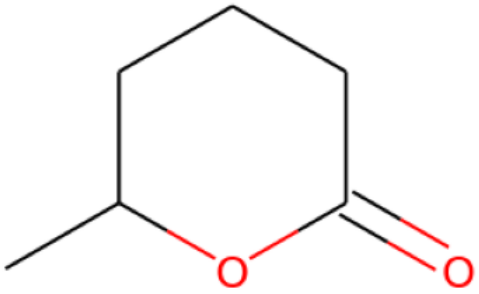
0.088436

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[#8][#6][#6H2]	0.9888
[CX4H3]	0.999	[#8]=[#6][#8]	0.9856
[#6H3][#6][#6]	0.9979	[CX3](=[OX1])O	0.9756
[CX4H3][CX4H2]	0.9963	[CX4H3][#6]	0.9684
[CX3](=[OX1])C	0.9955	OCC[CH2]	0.9411

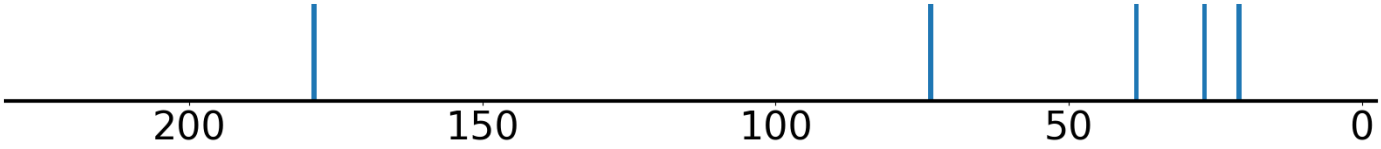
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H3]	0.999	[CX3H1](=[CX3H2])[NX3H0]	0.0
[#6H3][#6][#6]	0.9979	[#6H2]=[#7][#7]	0.0
[CX4H3][CX4H2]	0.9963	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9955	C=CC=CC=C	0.0
[#8][#6][#6H2]	0.9888	[CX3H0](=[NX2H1])([NX3H1])[CX4H1]	0.0
[#8]=[#6][#8]	0.9856	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX3](=[OX1])O	0.9756	[#6H2][#7]=[#6X3H1]	0.0
[CX4H3][#6]	0.9684	[CX4H2]([NX3H0])[CX3H1]	0.0
OCC[CH2]	0.9411	[CX3H1](=[CX3H2])[cX3H0]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6H0][#6H1]	0.3823	[#8][#6][#6][#6][#6]=[#8]	0.2797
[CX3](=O)[OX2H1]	0.3644	[#6H1]([#6H2])[#6H2]	0.3485
O=[CX3][CX4H]	0.3437	[CX4H2][CX3]=O	0.5141
[#8][#6H0][#6H1]	0.2691	CCCCCC	0.558
[CX4H2]([CX4H2])[CX4H2]	0.2266	[OX2H0][CX3H0][CX4H2]	0.5787
[OX2H1]	0.2063	[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.5794
[CX4H2]([CX4H3])[CX4H2]	0.1943	[CX4H2]([CX4H2])[CX3H0]	0.6016
[#8][#6][#6]=[#8]	0.1765	[OX2H0][CX4H1][CX4H2][CX4H2]	0.6804
[#6X3][#6][#6][#6H3]	0.1456	O=[CX3H0][CX4H2][CX4H2]	0.7081
[CX4H1]([OX2H1])([CX4H2])[CX3H0]	0.1372	C1OCCC1	0.737

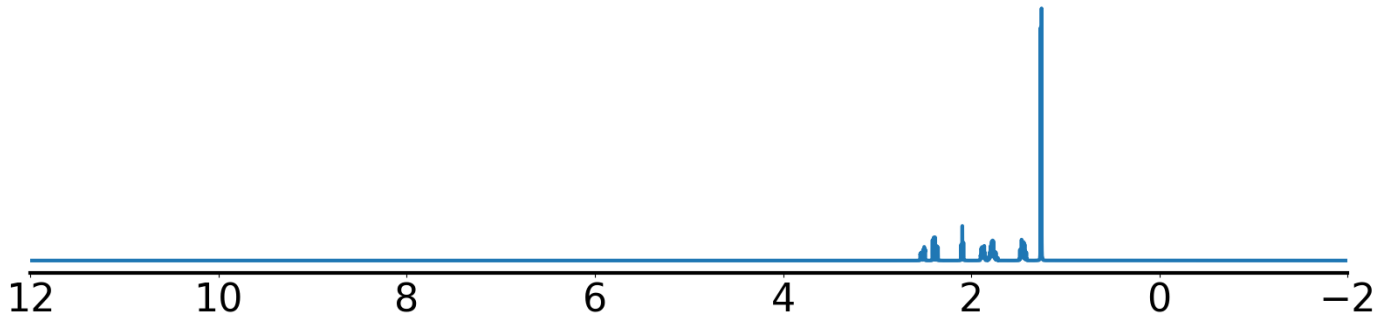
Example 99 true smiles: CC1CCCC(=O)O1 formula: C6H10O2
Index of correct structure: 0 of 1567
True structure loss: 0.012951
True structure:



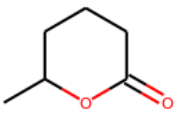
Experimental 13C NMR (solvent: CDCl3)



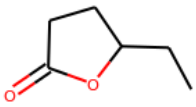
Experimental 1H NMR (solvent: D2O)



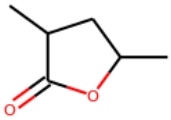
Top predicted structures (loss):



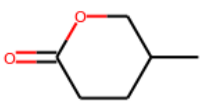
0.012951



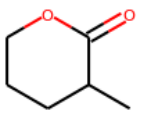
0.053548



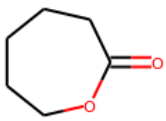
0.057716



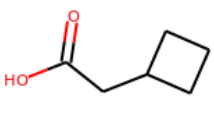
0.0581



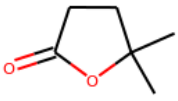
0.068806



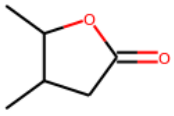
0.078512



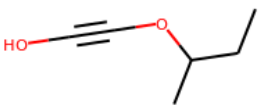
0.078936



0.079061



0.079458



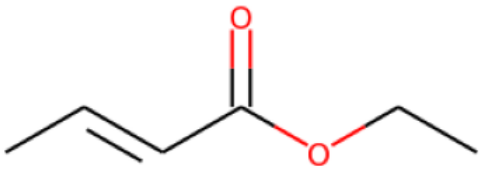
0.082227

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9999	[#8]=[#6][#8]	0.9887
[CX4H3]	0.9994	OCC[CH2]	0.978
[CX3](=[OX1])C	0.9969	[CX4H3][#6]	0.9714
[CX3](=[OX1])O	0.9945	[#6H1]	0.9636
[#6H3][#6][#6]	0.9938	[#8][#6][#6H2]	0.9499

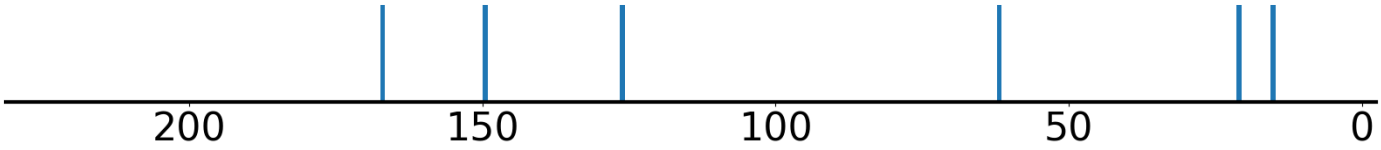
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9999	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H3]	0.9994	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9969	C=CC=CC#C	0.0
[CX3](=[OX1])O	0.9945	CC#CCC#C	0.0
[#6H3][#6][#6]	0.9938	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#8]=[#6][#8]	0.9887	[CX3H1](=[CX3H2])[NX3H0]	0.0
OCC[CH2]	0.978	CC#CCC=C	0.0
[CX4H3][#6]	0.9714	[#7][#6]=[#6][#6]#[#7]	0.0
[#6H1]	0.9636	[#6X3H2]=[#6][#6H2][#8H]	0.0
[#8][#6][#6H2]	0.9499	[#7][#6][#6]=[#6][#6][#7]	0.0

worst negatives	prob	worst positives	prob
[CX3](=O)[OX2H1]	0.5415	[#8]1[#6][#6][#6][#6][#6]1	0.3076
[#8][#6H0][#6H1]	0.4763	O[CX4H][CX4H2]	0.4531
O=[CX3][CX4H]	0.1904	[OX2H0][CX4H1][CX4H2][CX4H2]	0.4649
[OX2H1]	0.1717	[OX2H0][CX3H0][CX4H2]	0.5592
[#8]=[#6H0][#6H1]	0.15	[CX4H]O	0.5862
[CX4H2][CX4H2][CX4H2][CX4H2]	0.1423	[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.588
[CX3H0](=[OX1H0])([OX2H0])[CX4H1]	0.1377	[CX4H2]([CX4H2])[CX4H2]	0.6125
[#6X3][#6][#6][#6H3]	0.1335	CCCCCC	0.7465
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1298	[OX2H0][CX4H1][CX4H3]	0.7621
[#6H1]([#6H2])[#6H2]	0.1261	[CX4H2][CX3]=O	0.7856

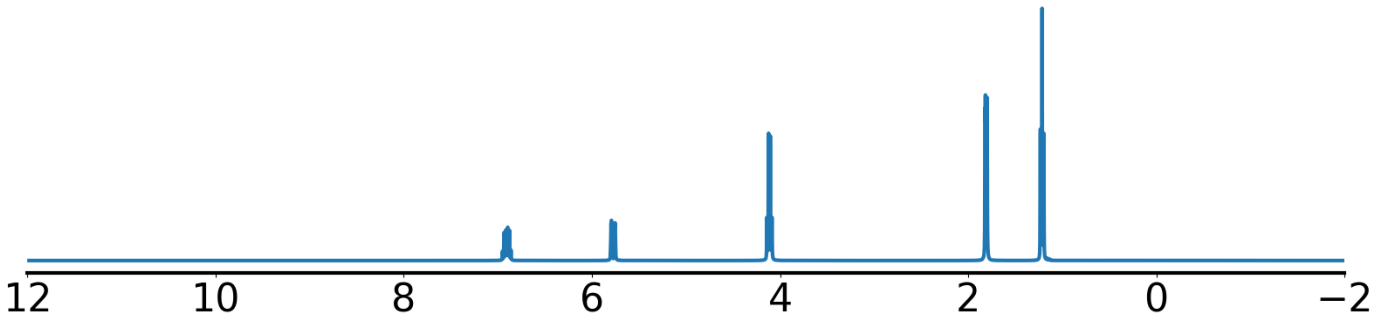
Example 100 true smiles: CC=CC(=O)OCC formula: C6H10O2
Index of correct structure: 0 of 1567
True structure loss: 0.013429
True structure:



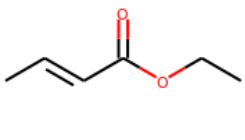
Experimental 13C NMR (solvent: CDCl3)



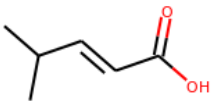
Experimental 1H NMR (solvent: CDCl3)



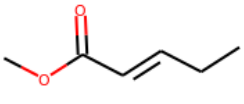
Top predicted structures (loss):



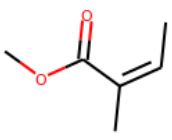
0.013429



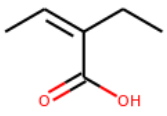
0.058213



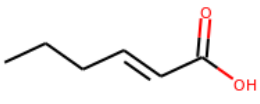
0.064394



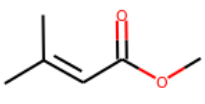
0.070942



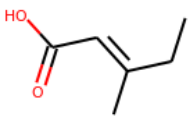
0.073778



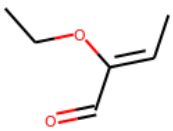
0.075099



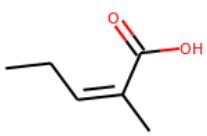
0.075477



0.080694



0.083619



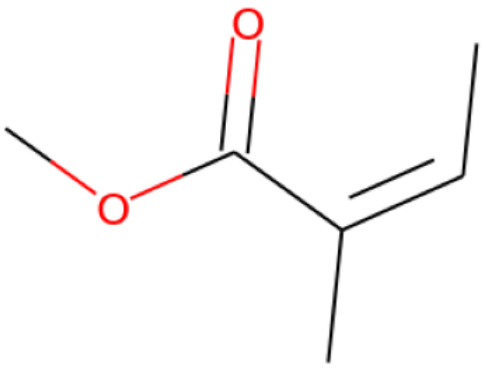
0.084162

Top predicted substructures	prob		
[CX4H3]	1.0	[#6X3][#6X3]	0.9906
[CX4H3][#6]	0.9998	[CX4H3][CX3]	0.9756
[#6H1]	0.9996	[CX4H3][CX4H2]	0.9689
[CHX3](=C)C	0.9961	[#8]=[#6][#8]	0.9596
O=[#6][#6]=[#6X3]	0.9909	[CX3](=[OX1])O	0.9418

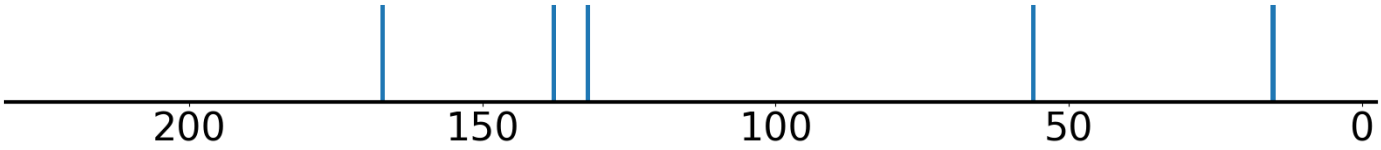
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][#6]	0.9998	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H1]	0.9996	[CX4H2]([CX4H0])[CX2H0]	0.0
[CHX3](=C)C	0.9961	CC#CCC#C	0.0
O=[#6][#6]=[#6X3]	0.9909	[#7][#6H1][#6X2]	0.0
[#6X3][#6X3]	0.9906	C=CC=CC#C	0.0
[CX4H3][CX3]	0.9756	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H3][CX4H2]	0.9689	[#6X2][#6H1][#6X2]	0.0
[#8]=[#6][#8]	0.9596	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.9418	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H3][#6][#6]	0.7024	[CX3H1](=[CX3H1])[CX4H3]	0.5893
[OX2H1]	0.5216	[CHX3]=[CHX3]	0.6116
[#6H3][#6][#6X3]	0.501	[#8]=[#6H0][#6H1]	0.6337
[CX3](=O)[OX2H1]	0.2613	[CH3][#6][#8]	0.6669
[#8H][#6H2][#6H1]	0.2237	[#8][#6X3][#6X3]=[#6X3][#6H3]	0.6737
[#6X3H1]=[#6X3H0]	0.2202	O=C[CX3H]	0.6854
[CX4H2][CX3]=C	0.2159	[CX3H0](=[OX1H0])([OX2H0])[CX3H1]	0.7018
[CX4H3][CX3H0]	0.1933	[CX3](=[OX1])C	0.7144
[#6H1][#6H1]	0.1752	[#8][#6H0][#6H1]	0.7589
[#6H1][#6H2]	0.1688	[#6X3][#6]=[#6][#6H3]	0.7708

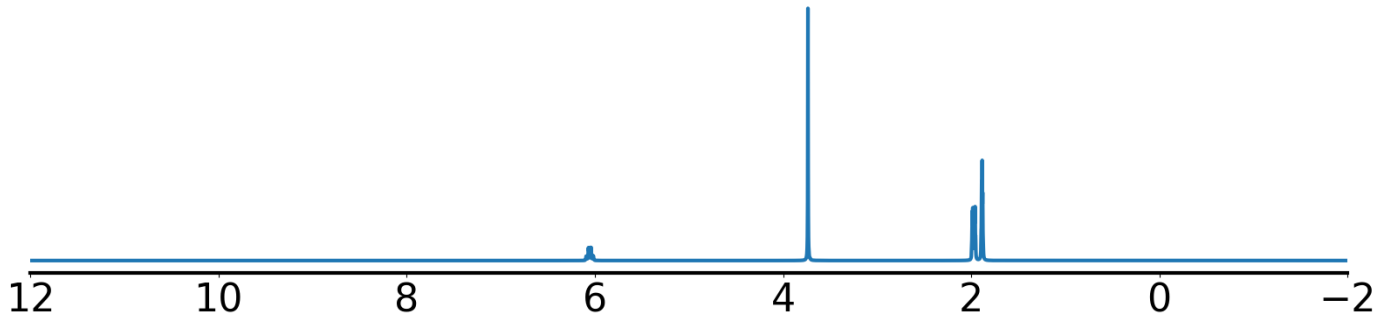
Example 101 true smiles: CC=C(C)C(=O)OC formula: C6H10O2
Index of correct structure: 0 of 1567
True structure loss: 0.016688
True structure:



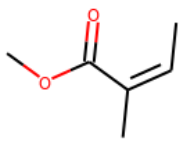
Experimental 13C NMR (solvent: CDCl3)



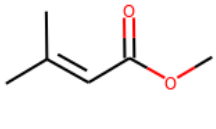
Experimental 1H NMR (solvent: CDCl3)



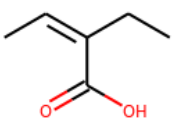
Top predicted structures (loss):



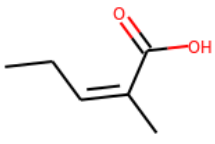
0.016688



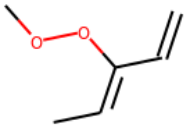
0.054286



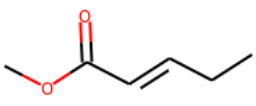
0.063237



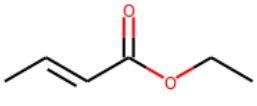
0.066651



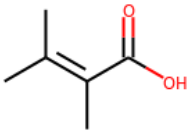
0.067998



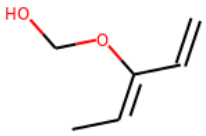
0.069045



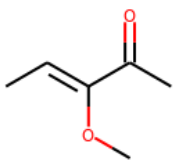
0.069707



0.072092



0.073025



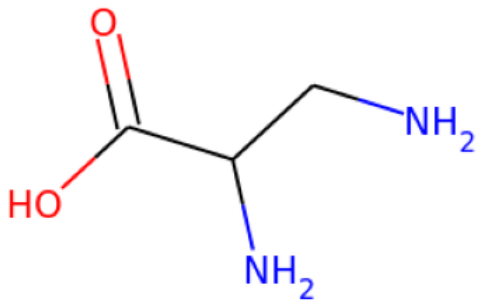
0.07791

Top predicted substructures	prob		
[CX4H3]	1.0	[#6X3][#6X3]	0.9818
[CX4H3][CX3]	0.9987	[CX4H3][OX2H0]	0.9761
[CHX3](=C)C	0.9959	[#8]=[#6][#8]	0.9703
[CX4H3][#6]	0.9953	[CX3](=[OX1])O	0.9578
[#6H1]	0.9883	[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.9462

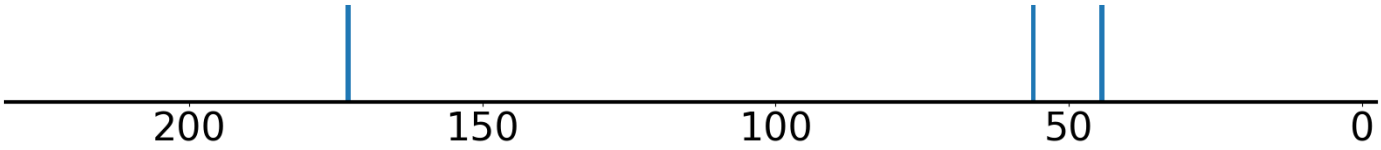
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][CX3]	0.9987	CCC#CC#C	0.0
[CHX3](=C)C	0.9959	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][#6]	0.9953	[#6X2][#6H1][#6X2]	0.0
[#6H1]	0.9883	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#6X3][#6X3]	0.9818	[#7][#6H1][#6X2]	0.0
[CX4H3][OX2H0]	0.9761	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[#8]=[#6][#8]	0.9703	CC#CCC#C	0.0
[CX3](=[OX1])O	0.9578	[CX2H1]#[CX2H0]	0.0
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.9462	[#7][#6][#6]#[#7]	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H0]	0.5715	[#6H3][#6][#6X3]	0.2463
[#8][#6H0][#6H1]	0.5222	[#6H3][#6H0]	0.2868
[CX3H1](=[CX3H1])[CX3H0]	0.3951	[#6H3][#6][#6]	0.363
[#6H1][#6H2]	0.3063	[CX4H3][CX3H0]	0.4756
[CHX3]=[CHX3]	0.3	[OX1H0]=[CX3H0][CX3H0][CX4H3]	0.4879
OCC[CH2]	0.2782	[CX4H3][CX3H0][CX3]=O	0.5088
[OX2H1]	0.2497	[#6H3][#6]=[#6][#6H3]	0.5642
[CX4H2]([#6])[#6]	0.2103	[CX3H0](=[OX1H0])([OX2H0])[CX3H0]	0.6444
[#6X3]=[#6X3][#6X3]=[#6X3]	0.1917	[#6X3H1]=[#6X3H0]	0.684
[#8]=[#6H0][#6H1]	0.169	[CX3H0](=[CX3H1])([CX4H3])[CX3H0]	0.7601

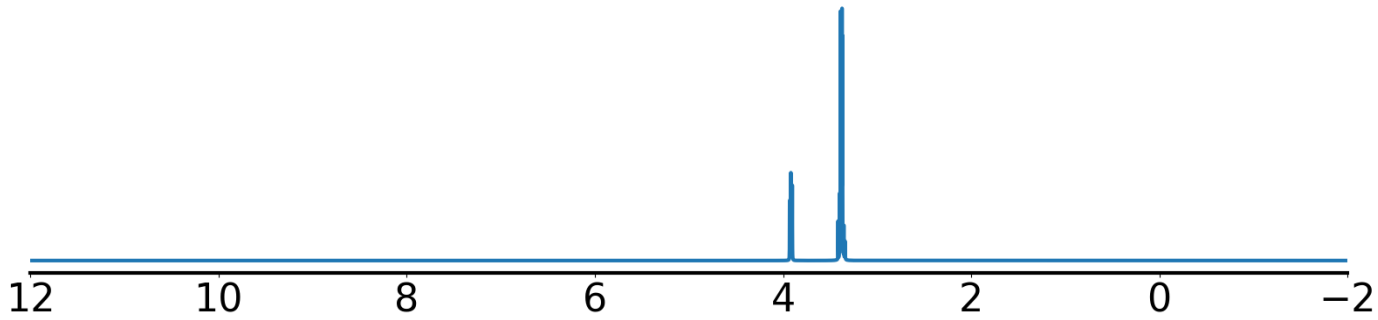
Example 102 true smiles: NCC(N)C(=O)O formula: C3H8N2O2
Index of correct structure: 3 of 1492
True structure loss: 0.033238
True structure:



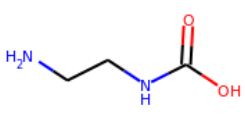
Experimental 13C NMR (solvent: D2O)



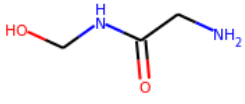
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):

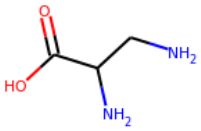


0.027831



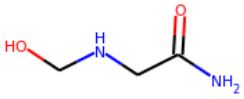
0.029552

0.032872



0.033238

0.033761

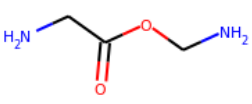


0.035094

0.035784

0.035784

0.035784



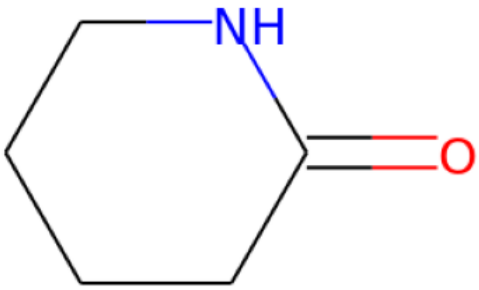
0.035919

Top predicted substructures	prob		
[#7X3][#6H2]	0.9757	[#6H2][#7][#6X3]	0.747
[#7][#6H2]	0.9703	[CX3](=[OX1])O	0.704
[CX3](=[OX1])C	0.9503	[#7][#6][#6X3]	0.6932
[#7X3H2]	0.8974	[OX2H1]	0.6901
[#8]=[#6][#8]	0.7911	[#7][#6H2][#6H2]	0.6776

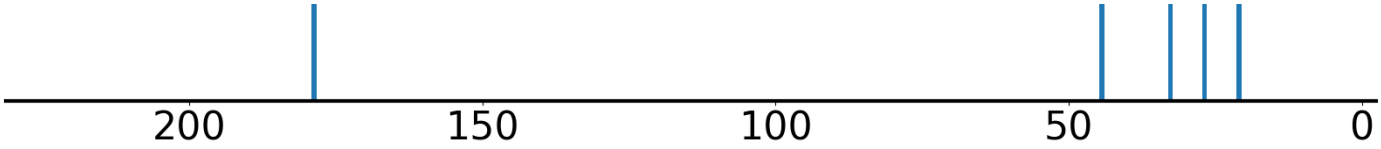
best positives	prob	best negatives	prob
[#7X3][#6H2]	0.9757	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7][#6H2]	0.9703	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9503	CC=CCC#C	0.0
[#7X3H2]	0.8974	C=CCCC#C	0.0
[#8]=[#6][#8]	0.7911	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])O	0.704	CC=CC#CC	0.0
[#7][#6][#6X3]	0.6932	CCC=CC#C	0.0
[OX2H1]	0.6901	[CX2H0](#[CX2H1])[CX4H1]	0.0
[#7H2][#6X4H1][#6X3]	0.6597	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.5951	[CX4H2]([CX4H3])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H2][#7][#6X3]	0.747	[#8][#6H0][#6H1]	0.0814
[#7][#6H2][#6H2]	0.6776	[CX4H2]([NX3H2])[CX4H1]	0.0905
[CX4H2][CX4H2]	0.5541	[#7][#6][#6][#6X3]	0.1933
[#7X3H1]	0.5117	OCC[CH2]	0.2037
[#7][#6H2][#6H2][#7]	0.3901	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.247
[CX4H2]([NX3H1])[CX4H2]	0.3779	[#7][#6H2][#6H1]	0.2681
[CX4H2][CX3]=O	0.3691	[#6H1][#6H2]	0.3226
[#8][#6][#6H2]	0.3554	[CX3](=O)[OX2H1]	0.3505
[#7][#6H0][#6H1]	0.2894	O=[CX3][CX4H]	0.373
[#7][#6][#7]	0.2414	[#6H1]	0.3959

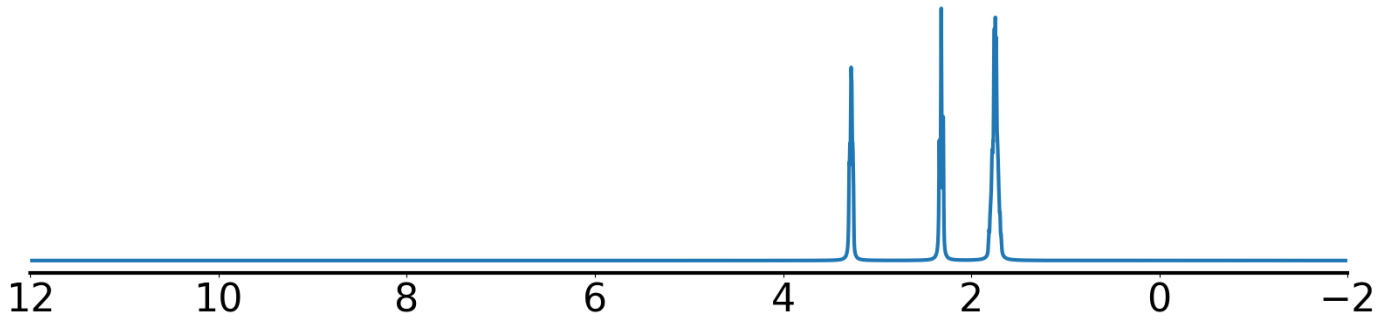
Example 103 true smiles: O=C1CCCCN1 formula: C5H9NO
Index of correct structure: 0 of 1318
True structure loss: 0.021931
True structure:



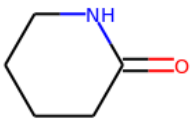
Experimental 13C NMR (solvent: CDCl3)



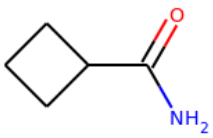
Experimental 1H NMR (solvent: CDCl3)



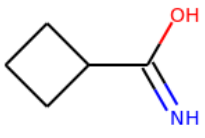
Top predicted structures (loss):



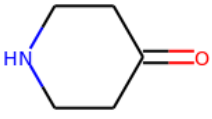
0.021931



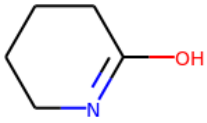
0.039314



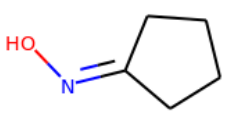
0.053053



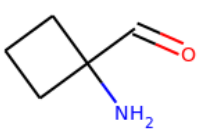
0.056398



0.057907

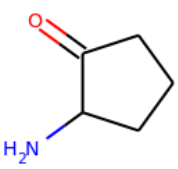


0.061226

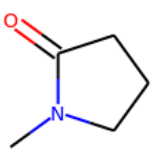


0.066954

0.067872



0.068434



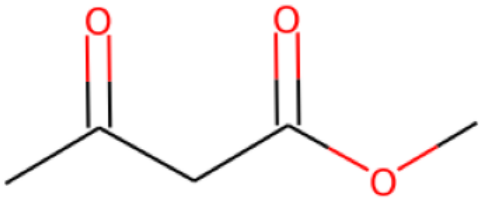
0.069597

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9997	[CX4H2]([CX4H2])[CX4H1]	0.8712
[CX3](=[OX1])C	0.9803	[#6H1][#6H2]	0.8172
[CX4H2][CX4H2]	0.9471	[#7][#6H2]	0.7855
[CX4H2]CC=O	0.9007	[#7X3][#6H2]	0.7626
[CX4H2]([CX4H2])[CX4H2]	0.8927	[#7][#6H2][#6H2]	0.7342

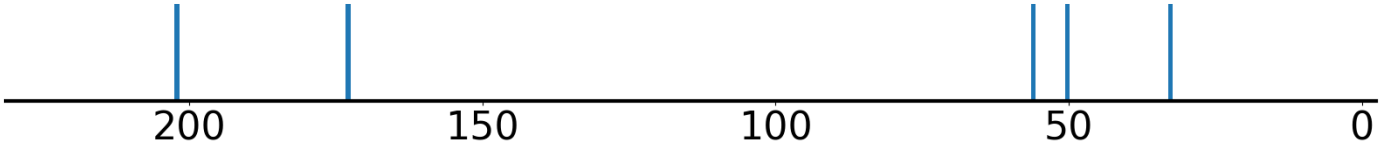
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9997	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9803	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2][CX4H2]	0.9471	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]CC=O	0.9007	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.8927	CC=CC#CC	0.0
[#7][#6H2]	0.7855	CC=CCC#C	0.0
[#7X3][#6H2]	0.7626	CC#CCC=C	0.0
[#7][#6H2][#6H2]	0.7342	[#6H2]=[#6][#6X2]	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.6299	[OX2H0]1[CX4H2][CX4H1][CX3H0]=[CX3H1]1	0.0
[CX4H2]([CX4H2])[CX3H0]	0.5912	[CX3H1](=[CX3H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H1]	0.8712	[#6]1[#6][#6][#6][#6][#7]1	0.2652
[#6H1][#6H2]	0.8172	[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.3322
[#8]=[#6H0][#6H1]	0.6528	[#7X3H1]	0.4776
O=[CX3][CX4H]	0.5727	[CX4H2]([NX3H1])[CX4H2]	0.5186
[#6H1]	0.5518	[#6H2][#7][#6X3]	0.5292
C1CCC1	0.4851	[CX4H2][CX3]=O	0.5444
[#7X3H2]	0.3897	O=[CX3H0][CX4H2][CX4H2]	0.5865
[#6]1[#6][#6][#6][#7]1	0.3607	[CX4H2]([CX4H2])[CX3H0]	0.5912
CCCCCC	0.3148	[CX4H2][CX4H2][CX4H2][CX4H2]	0.6299
[#6H1][#6H2][#6][#6][#7]	0.3014	[#7][#6H2][#6H2]	0.7342

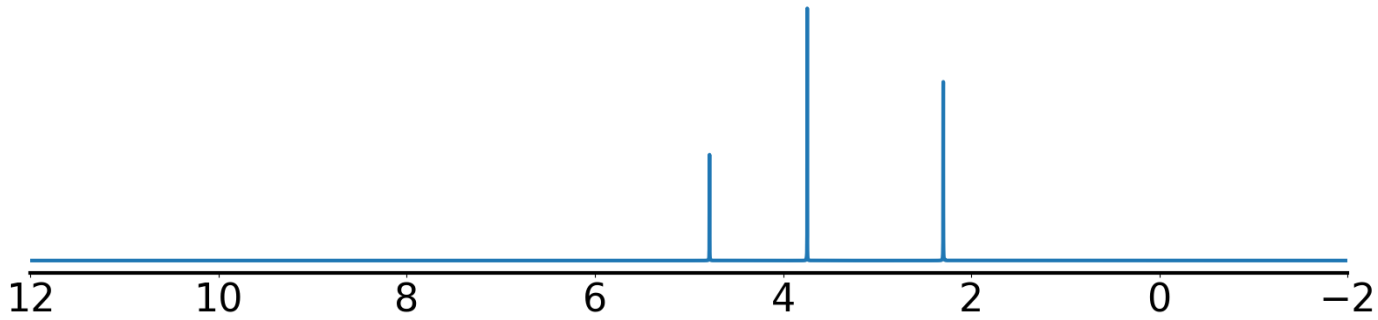
Example 104 true smiles: COC(=O)CC(C)=O formula: C5H8O3
Index of correct structure: 0 of 1131
True structure loss: 0.014216
True structure:



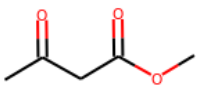
Experimental 13C NMR (solvent: CDCl3)



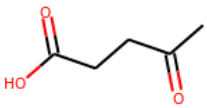
Experimental 1H NMR (solvent: d2o)



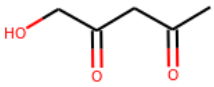
Top predicted structures (loss):



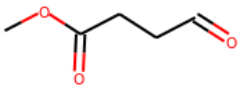
0.014216



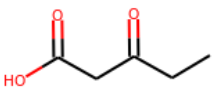
0.052128



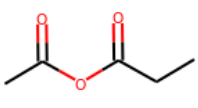
0.066422



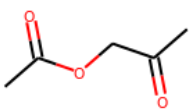
0.072955



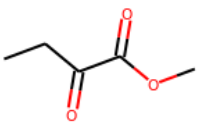
0.078236



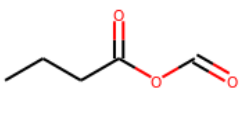
0.081265



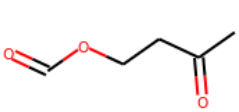
0.081615



0.085724



0.086552



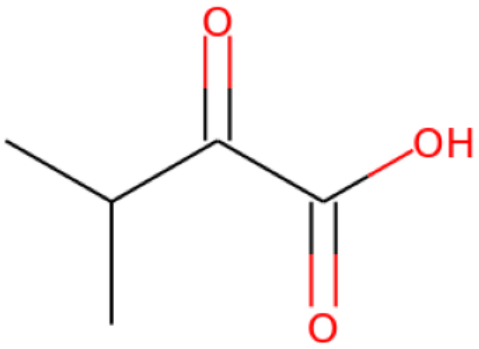
0.087887

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9999	[CX4H2][CX3]=O	0.979
[CX4H3]	0.996	[#6H3][#6H0]	0.9559
[#8]=[#6][#8]	0.9906	[CX4H3][CX3]	0.9502
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.988	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9338
[CX3](=[OX1])O	0.9844	[CX4H3][CX3H0]	0.9332

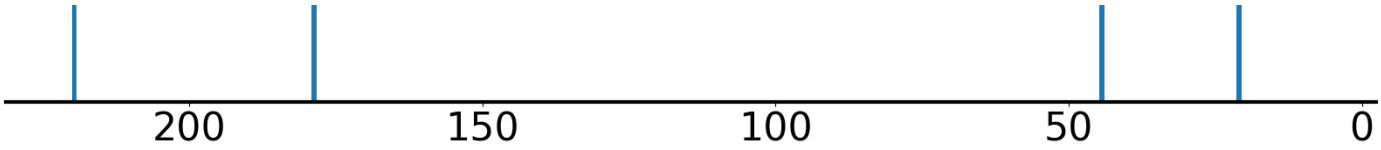
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9999	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3]	0.996	CCC#CC#C	0.0
[#8]=[#6][#8]	0.9906	C=CC=CC#C	0.0
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.988	CCC=CC#C	0.0
[CX3](=[OX1])O	0.9844	[#6X2][#6H1][#6X2]	0.0
[CX4H2][CX3]=O	0.979	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#6H3][#6H0]	0.9559	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[CX4H3][CX3]	0.9502	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9338	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX4H3][CX3H0]	0.9332	[#7][#6H1][#6X2]	0.0

worst negatives	prob	worst positives	prob
OCC[CH2]	0.3999	[#6X3][#6][#6][#6H3]	0.1515
[CX4H2]CC=O	0.3695	[CX4H2]([CX3H0])[CX3H0]	0.5671
[CX4H2]([#6])[O]	0.3341	[#8][#6][#6][#6X3]	0.572
[#6X3][#6X3]	0.2794	O=[#6][#6][#6X3]	0.619
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2406	[#6H3][#6X3H0][#6H2]	0.6379
[#8]=[#6][#6]=[#8]	0.1996	[#6H3][#6][#6]	0.6951
[#6X3][#6H2][#8]	0.199	[OX1H0]=[CX3H0][CX4H2][CX3H0]	0.6999
[CX3H1](=[OX1H0])[CX4H2]	0.1962	[#6X3][#6H2][#6X3]	0.7
[OX2H1][CX4H2][#6X3H0]	0.1949	[OX2H0][CX3H0][CX4H2]	0.7147
[#8]=[#6][#6][#6][#6]=[#8]	0.1804	[#8][#6][#6H2]	0.7324

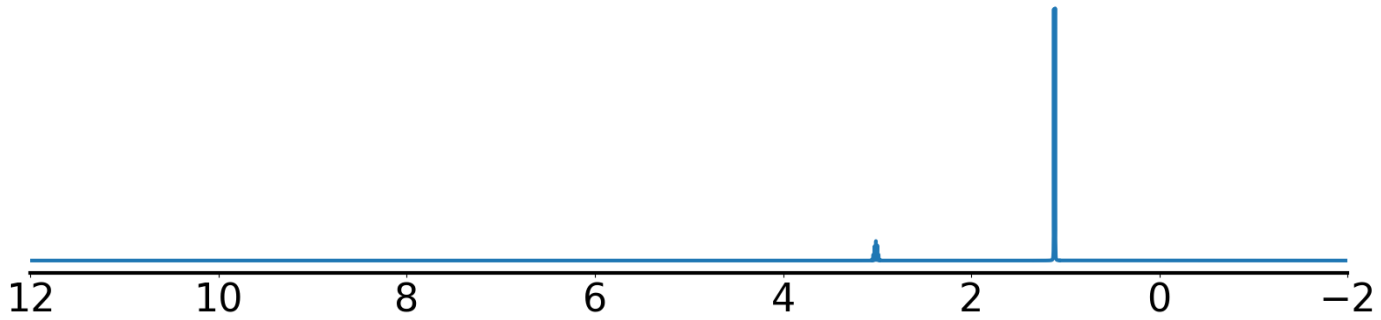
Example 105 true smiles: CC(C)C(=O)C(=O)O formula: C5H8O3
Index of correct structure: 0 of 1131
True structure loss: 0.01553
True structure:



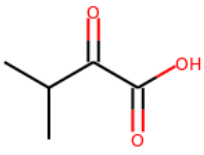
Experimental 13C NMR (solvent: D2O)



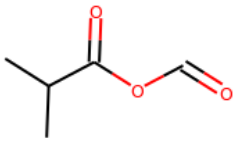
Experimental 1H NMR (solvent: D2O)



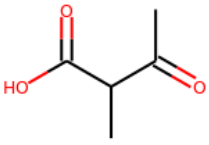
Top predicted structures (loss):



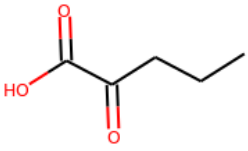
0.01553



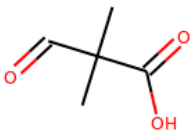
0.039704



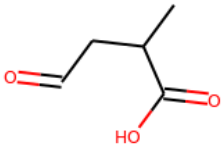
0.070354



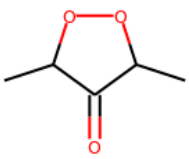
0.074231



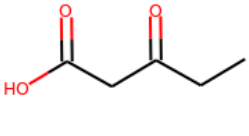
0.076095



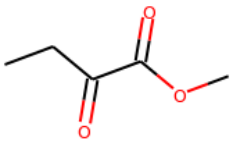
0.083627



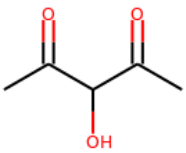
0.085353



0.08562



0.092913



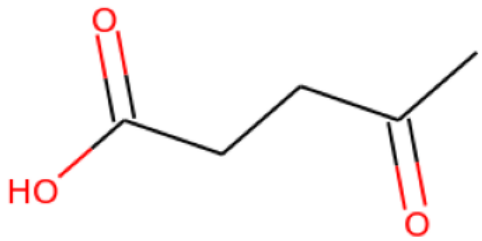
0.096611

Top predicted substructures	prob		
[CX3](=[OX1])C	1.0	[CX3](=[OX1])O	0.986
[CX4H3]	0.9994	[#8]=[#6][#8]	0.9764
[#6H3][#6][#6]	0.9971	[CX3](=O)[OX2H1]	0.9725
[CX4H3][#6]	0.9946	[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.9523
[OX2H1]	0.9936	[CHX4]([CH3X4])[CH3X4]	0.9512

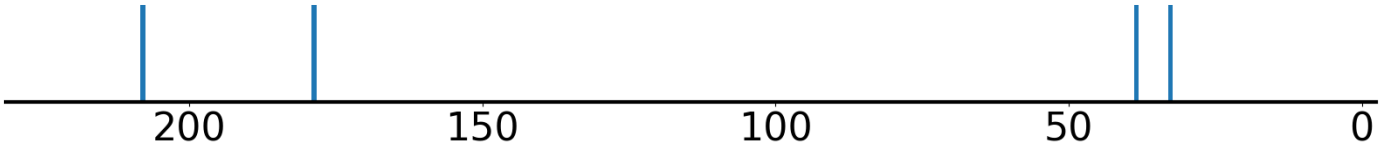
best positives	prob	best negatives	prob
[CX3](=[OX1])C	1.0	CC=CCC#C	0.0
[CX4H3]	0.9994	CCC=CC#C	0.0
[#6H3][#6][#6]	0.9971	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9946	CCC#CC#C	0.0
[OX2H1]	0.9936	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.986	[CX4H3][CX2H0]	0.0
[#8]=[#6][#8]	0.9764	CC=CC#CC	0.0
[CX3](=O)[OX2H1]	0.9725	[#6X2][#6H1][#6X2]	0.0
[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.9523	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CHX4]([CH3X4])[CH3X4]	0.9512	C=CC=CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX3]=O	0.6438	[#6X3][#6X3]	0.1274
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6319	[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.2547
[#8][#6H0][#6H1]	0.5364	[#8]=[#6][#6]=[#8]	0.4514
[CX4H2]CC=O	0.4105	[#8][#6][#6]=[#8]	0.5127
[CH3]CC[OH]	0.3886	[CX3H0](=[OX1H0])([CX4H1])[CX3H0]	0.5151
O=[#6][#6][#6X3]	0.3837	[#6X3][#6][#6][#6H3]	0.5841
[#8]=[#6][#6][#6][#6]=[#8]	0.3575	O=CC=O	0.596
[#8][#6][#6][#6X3]	0.2902	[#6H1]	0.8389
[CX4H2]([#6])[#6]	0.2431	[#8]=[#6H0][#6H1]	0.8818
CCCCCC	0.1383	O=[CX3][CX4H]	0.8887

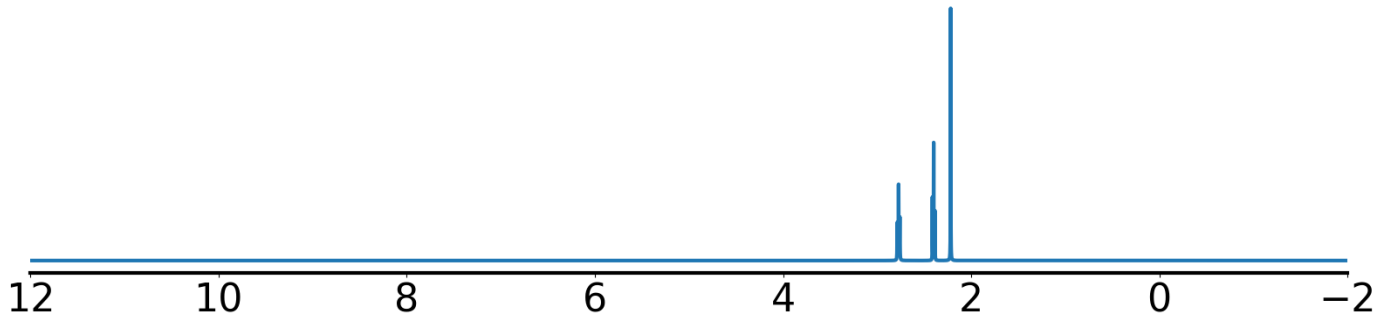
Example 106 true smiles: CC(=O)CCC(=O)O formula: C5H8O3
Index of correct structure: 0 of 1131
True structure loss: 0.004847
True structure:



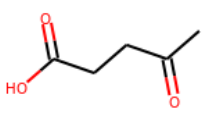
Experimental 13C NMR (solvent: CDCl3)



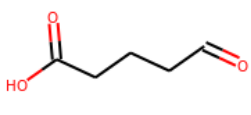
Experimental 1H NMR (solvent: D2O)



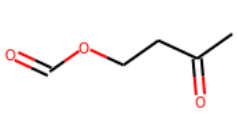
Top predicted structures (loss):



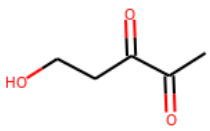
0.004847



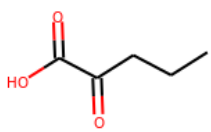
0.080461



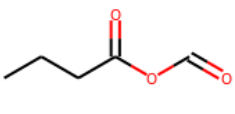
0.083891



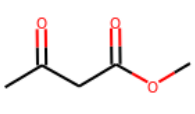
0.083916



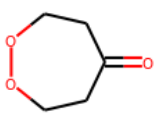
0.08424



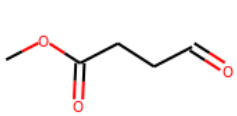
0.091077



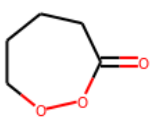
0.098337



0.105338



0.106729



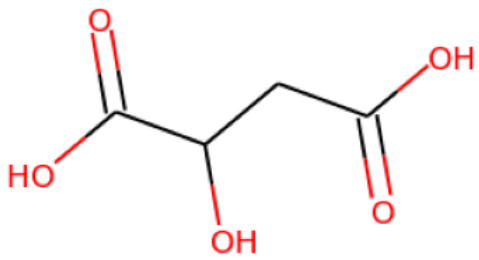
0.111187

Top predicted substructures	prob		
[CX3](=[OX1])C	1.0	[CX4H3][CX3H0]	0.9941
[CX4H2]([#6])[#6]	0.9995	O=[CX3H0][CX4H2][CX4H2]	0.993
[CX4H3][CX3]	0.9983	[CX4H2]([CX4H2])[CX3H0]	0.9922
[OX1H0]=[CX3H0][CX4H3]	0.997	[#8]=[#6][#8]	0.9914
[#6H3][#6H0]	0.995	[CX4H2][CX3]=O	0.9872

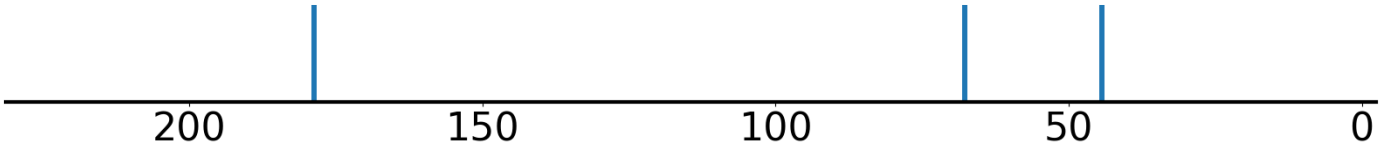
best positives	prob	best negatives	prob
[CX3](=[OX1])C	1.0	C=CC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9995	CCC#CC#C	0.0
[CX4H3][CX3]	0.9983	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX1H0]=[CX3H0][CX4H3]	0.997	[#6X2][#6H1][#6X2]	0.0
[#6H3][#6H0]	0.995	CCC=CC#C	0.0
[CX4H3][CX3H0]	0.9941	[CX2H0](#[CX2H1])[CX3H1]	0.0
O=[CX3H0][CX4H2][CX4H2]	0.993	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2]([CX4H2])[CX3H0]	0.9922	CC=CC#CC	0.0
[#8]=[#6][#8]	0.9914	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX4H2][CX3]=O	0.9872	CC=CCC#C	0.0

worst negatives	prob	worst positives	prob
CCCCCC	0.2577	[#8][#6][#6][#6][#6]=[#8]	0.5867
[CX4H2]([CX4H2])[CX4H2]	0.2181	[#8]=[#6][#6][#6][#6]=[#8]	0.6627
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.1606	OCC[CH2]	0.8379
[#8]=[#6H0][#6H1]	0.1477	[#6H3][#6X3H0][#6H2]	0.8718
O=CC=O	0.1172	[CX4H3][#6]	0.8852
[CX4H2][CX3H]	0.0851	[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.9004
[#6X3][#6X3]	0.0825	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9064
[#8]=[#6][#6H2][#6H1]	0.0791	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.909
[#8]=[#6][#6]=[#8]	0.0775	[CX4H2]CC=O	0.921
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.0613	[OX2H1]	0.9392

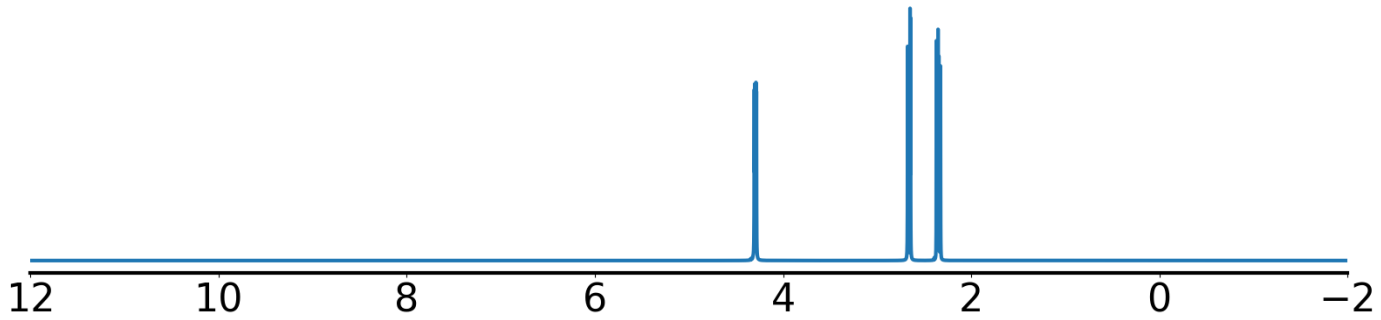
Example 107 true smiles: O=C(O)CC(O)C(=O)O formula: C4H6O5
Index of correct structure: 0 of 1119
True structure loss: 0.029603
True structure:



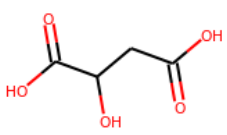
Experimental 13C NMR (solvent: D2O)



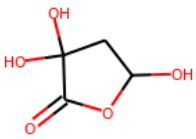
Experimental 1H NMR (solvent: d2o)



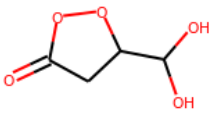
Top predicted structures (loss):



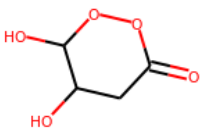
0.029603



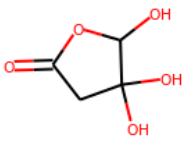
0.034938



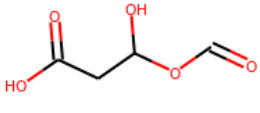
0.038943



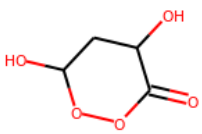
0.039548



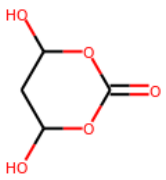
0.04211



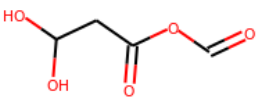
0.046565



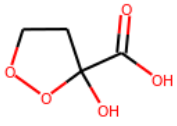
0.047419



0.04804



0.048508



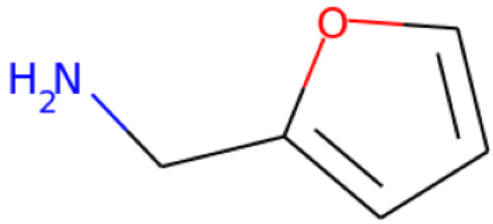
0.049697

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9995	[#8][#6][#6H2]	0.9694
[#8]=[#6][#8]	0.9988	OCC[CH2]	0.9374
[OX2H1]	0.9982	[#6H1]	0.8988
[CX3](=[OX1])O	0.9935	[#6H1][#6H2]	0.7982
[CX4H2]([#6])[#6]	0.9911	[CX4H2][CX3]=O	0.7758

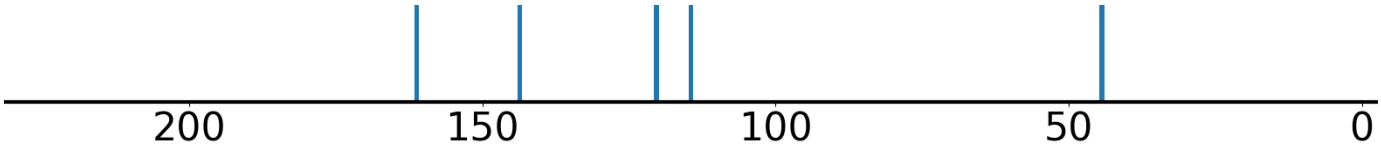
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9995	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[#8]=[#6][#8]	0.9988	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[OX2H1]	0.9982	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])O	0.9935	CC#CCC=C	0.0
[CX4H2]([#6])[#6]	0.9911	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[#8][#6][#6H2]	0.9694	[CX3H0](=[CX3H1])([CX4H3])[CX3H1]	0.0
OCC[CH2]	0.9374	CCC=CC#C	0.0
[#6H1]	0.8988	[#6H3][#6H1][#6H1]=[#7]	0.0
[#6H1][#6H2]	0.7982	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H2][CX3]=O	0.7758	[CX3H0](=[CX3H0])([CX4H3])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([#6])[O]	0.3773	[#8]=[#6][#6][#6][#6]=[#8]	0.0659
[#6H1][#6H1]	0.3479	[CX4H1]([OX2H1])([CX4H2])[CX3H0]	0.0977
[#6H1]([#6H2])[#6H2]	0.2463	[OX1H0]=[CX3H0][CX4H1]([OX2H1])[CX4H2]	0.1663
[CX4H2](O)[CHX4]	0.1937	O=[CX3][CX4H]	0.1757
[#8][#6H1][#6H1]	0.1826	[#8H][#6X4H1][#6X3H0]	0.2003
[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.1557	[#8]=[#6H0][#6H1]	0.2463
[#7][#6][#6X3]	0.1468	[#8][#6][#6]=[#8]	0.2987
[CX4H2]([CX4H1])[CX4H0]	0.1286	[CX4H2]CC=O	0.4384
[OX2H0][CX3H0][CX4H2]	0.1186	[OH][CX4H]	0.4442
C1OCCC1	0.1107	[#8]=[#6][#6H2][#6H1]	0.4543

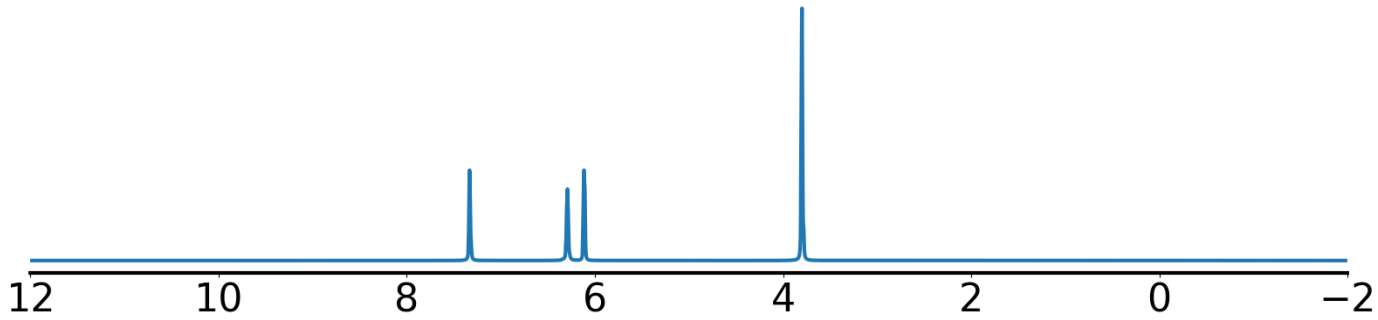
Example 108 true smiles: NCc1ccco1 formula: C5H7NO
Index of correct structure: 0 of 1024
True structure loss: 0.028721
True structure:



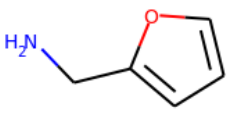
Experimental 13C NMR (solvent: CDCl3)



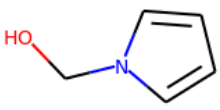
Experimental 1H NMR (solvent: CDCl3)



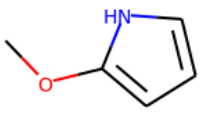
Top predicted structures (loss):



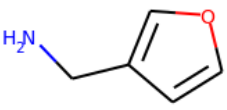
0.028721



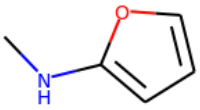
0.043498



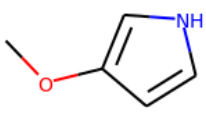
0.052437



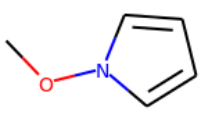
0.059929



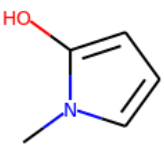
0.060608



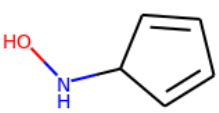
0.062206



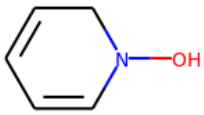
0.065483



0.066442



0.067302



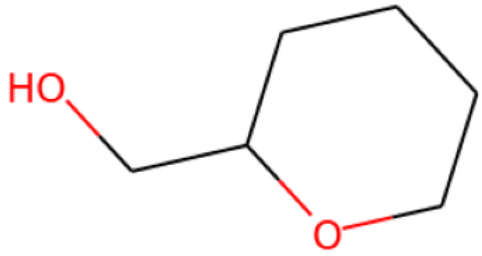
0.068634

Top predicted substructures	prob		
[#6H1]	0.9995	[cH]	0.8507
[#7][#6H2]	0.9652	[#6H1][#6H1]	0.8482
[#6X3][#6X3]	0.9642	[#7X3H2]	0.8372
[#7][#6][#6X3]	0.9179	[cH][cH]	0.8349
[#7X3][#6H2]	0.8774	[#6X3][#6H2][#7]	0.7894

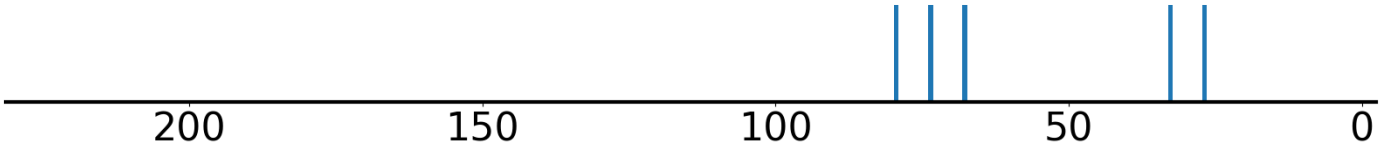
best positives	prob	best negatives	prob
[#6H1]	0.9995	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7][#6H2]	0.9652	[OX2H0][CX4H2][CX2H0]#[CX2H1]	0.0
[#6X3][#6X3]	0.9642	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7][#6][#6X3]	0.9179	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3][#6H2]	0.8774	[CX2H0](#[CX2H1])[CX4H1]	0.0
[cH]	0.8507	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H1][#6H1]	0.8482	CCC#CC#C	0.0
[#7X3H2]	0.8372	[CX2H0](#[CX2H1])[CX2H0]	0.0
[cH][cH]	0.8349	CC=CCC#C	0.0
[#6X3][#6H2][#7]	0.7894	[CX2H0](#[CX2H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[CHX3](=C)C	0.5954	[#8][#6H1][#6H1]	0.0087
[#6X3][#7][#6X3]	0.5573	[#8][#6H][#6X3][#6X3H]	0.0734
[#6H2][#7][#6X3]	0.4365	o[cH]	0.1203
[CHX3]=[CHX3]	0.4179	[cX3H1]([oX2H0])[cX3H1]	0.2167
[#6X3][#7X3][#6X3]	0.4093	[#8][#6H0][#6H1]	0.4846
[#7][#6H0][#6H1]	0.3005	[#6X3][#6X3][#6X3][#6X3]	0.4908
[#6H1][#6H2]	0.2936	[#8][#6][#6H2]	0.4909
[#7][#6X3H0][#6X3H1]	0.2918	[#7H2][#6H2]	0.4961
[#7][#6H2][#6H1]	0.2891	[#8][#6][#6][#6X3]	0.5389
[#7X3H1]	0.2768	[#7][#6][#6][#6X3]	0.5895

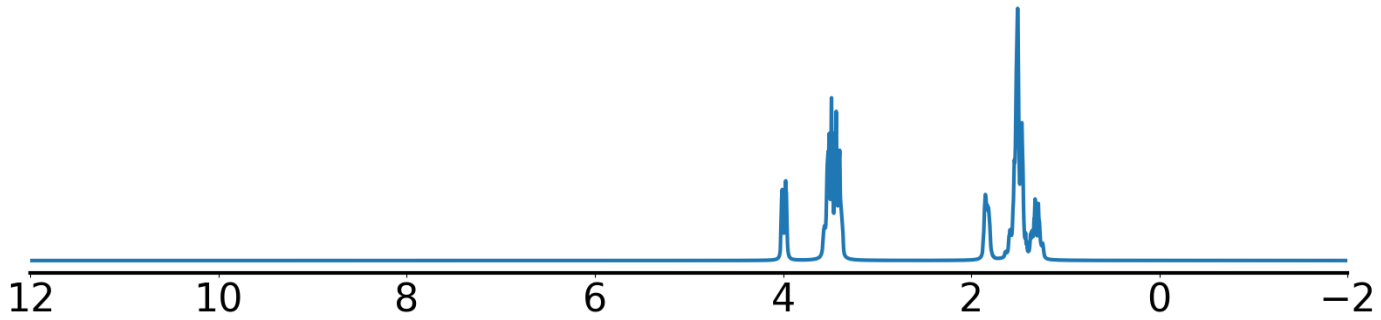
Example 109 true smiles: OCC1CCCCO1 formula: C6H12O2
Index of correct structure: 0 of 903
True structure loss: 0.016167
True structure:



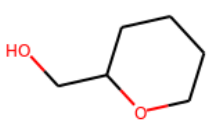
Experimental 13C NMR (solvent: CDCl3)



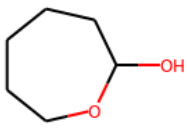
Experimental 1H NMR (solvent: CDCl3)



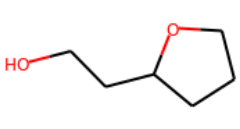
Top predicted structures (loss):



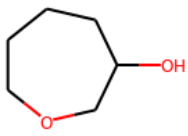
0.016167



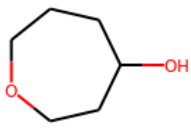
0.019617



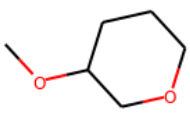
0.02226



0.032337

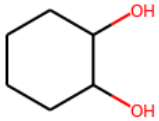


0.034418

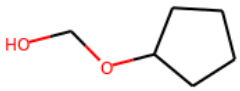


0.040589

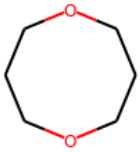
0.041438



0.041947



0.042096



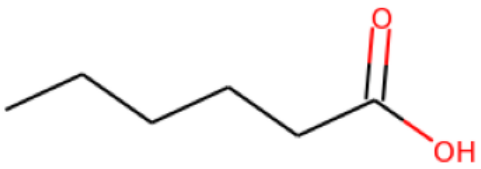
0.046171

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H2][CX4H2]	0.9866
OCC[CH2]	0.9997	[CX4H]O	0.9866
[#8][#6][#6H2]	0.999	[#6H1]	0.9857
[CX4H2]([CX4H2])[CX4H1]	0.997	O[CX4H][CX4H2]	0.9662
[CX4H2]([#6])[O]	0.9963	[#6H1][#6H2]	0.9605

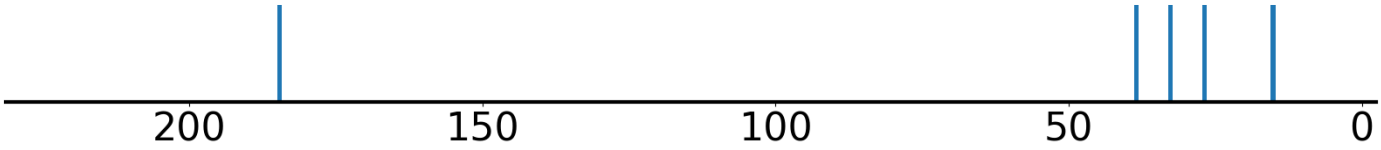
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
OCC[CH2]	0.9997	C=CC=CC#C	0.0
[#8][#6][#6H2]	0.999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([CX4H2])[CX4H1]	0.997	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2]([#6])[O]	0.9963	[CX2H0](#[CX2H0])[CX4H0]	0.0
[CX4H2][CX4H2]	0.9866	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H]O	0.9866	[CX3H1](=[CX3H2])[cX3H0]	0.0
[#6H1]	0.9857	[#6X3H1][#6X3H0][#6X4H1][#7]	0.0
O[CX4H][CX4H2]	0.9662	CC#CCC=C	0.0
[#6H1][#6H2]	0.9605	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.0

worst negatives	prob	worst positives	prob
[#6X4H2][#6H1][#8H]	0.5738	[CX4H2]([OX2H1])[CX4H1]	0.1718
[#8][#6][#6][#6][#6][#8]	0.5118	[CX4H2](O)[CHX4]	0.1948
[#8][#6H1][#6H1]	0.42	[#8H][#6H2][#6H1]	0.2252
O[CX4H]([CX4H2])[CX4H1]	0.4182	[#6H1]([#6H2])[#6H2]	0.2796
[OH][CX4H]	0.361	[#8][#6][#6H2][#8]	0.612
[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.2831	[#8]1[#6][#6][#6][#6][#6]1	0.6319
[#6H1][#6H1]	0.2603	[CX4H](O)CO	0.6398
[CX4H1][CX4H2][CX4H2][CX4H1]	0.1723	[CX4H1]([OX2H0])([CX4H2])[CX4H2]	0.6677
[CX4H2][OX2H0][CX4H2]	0.1527	CCCCCC	0.6845
[#6]1[#6][#6][#6][#6][#6]1	0.1491	[#6H2][#8][#6H1]	0.7462

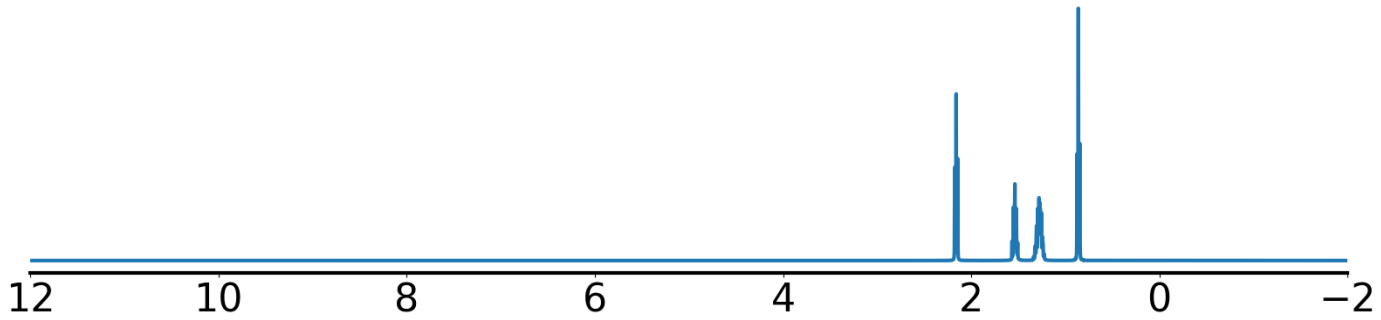
Example 110 true smiles: CCCCCC(=O)O formula: C6H12O2
Index of correct structure: 0 of 903
True structure loss: 0.004445
True structure:



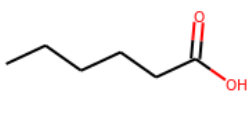
Experimental 13C NMR (solvent: CDCl3)



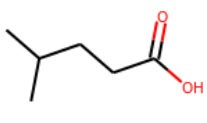
Experimental 1H NMR (solvent: D2O)



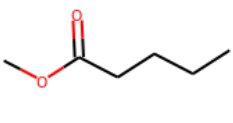
Top predicted structures (loss):



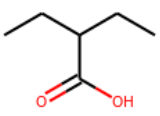
0.004445



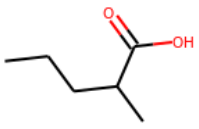
0.042294



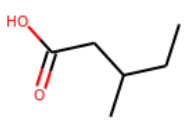
0.056974



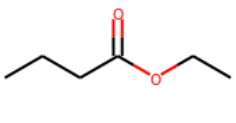
0.05836



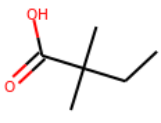
0.061383



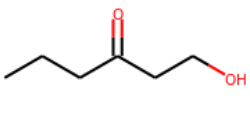
0.062021



0.0807



0.085363



0.092392

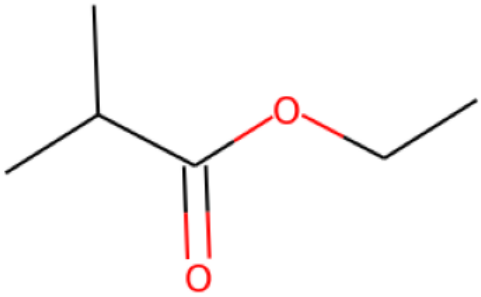
0.095194

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H3][#6]	0.9981
[#6H3][#6][#6]	0.9998	[CX4H3]	0.9971
[CX4H3][CX4H2]	0.9993	[#8]=[#6][#8]	0.9947
[CX3](=O)[OX2H1]	0.9991	[CX3](=[OX1])O	0.9835
[CX3](=[OX1])C	0.999	[OX2H1]	0.9755

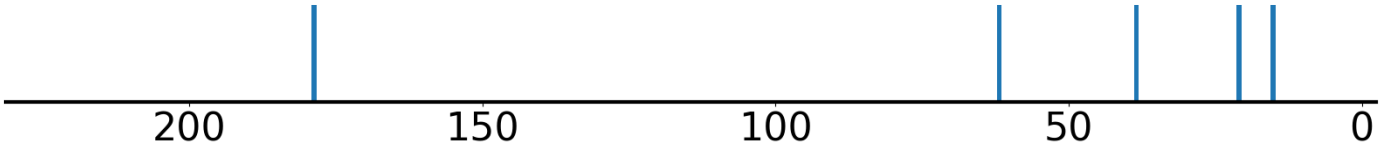
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H3][#6][#6]	0.9998	C=CC=CC#C	0.0
[CX4H3][CX4H2]	0.9993	CCC=CC#C	0.0
[CX3](=O)[OX2H1]	0.9991	CCC#CC#C	0.0
[CX3](=[OX1])C	0.999	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][#6]	0.9981	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3]	0.9971	CC=CC#CC	0.0
[#8]=[#6][#8]	0.9947	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])O	0.9835	CC#CCC#C	0.0
[OX2H1]	0.9755	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H2]	0.3048	CCCCCC	0.6494
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2195	[#8][#6][#6H2]	0.688
[#6H1]	0.1738	[CX4H2][CX3]=O	0.8214
[#6X3][#6][#6][#6H3]	0.1248	[CX4H2][CX4H2][CX4H2][CX4H2]	0.8511
[#8]=[#6H0][#6H1]	0.0998	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.8614
[CHX4]([CH3X4])[CH2X4]	0.0806	OCC[CH2]	0.8741
[CH3]CC[OH]	0.0799	O=[CX3H0][CX4H2][CX4H2]	0.8788
[#8][#6H0][#6H1]	0.071	[CX4H2]([CX4H2])[CX4H2]	0.8848
[#6H1]([#6H2])[#6H2]	0.071	[CX4H2]CC=O	0.8945
[#6H3][#6][#6X3]	0.0699	[CX4H2]([CX4H2])[CX3H0]	0.9015

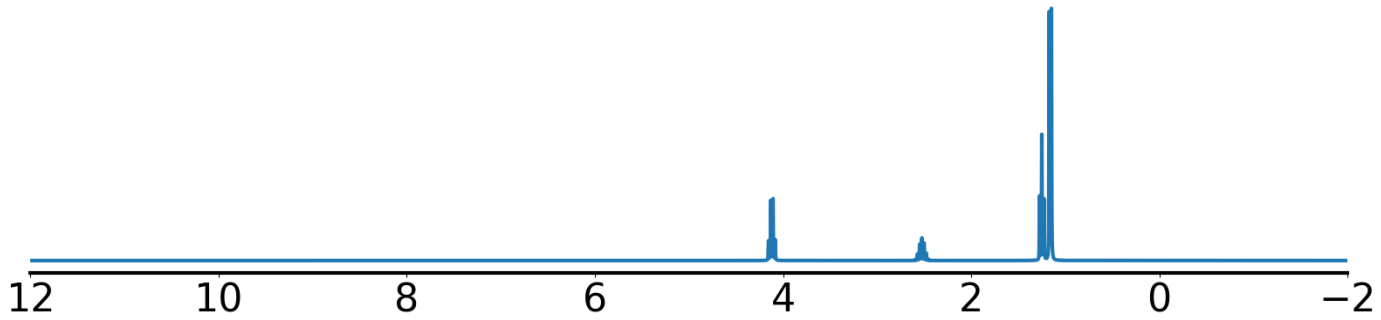
Example 111 true smiles: CCOC(=O)C(C)C formula: C6H12O2
Index of correct structure: 0 of 903
True structure loss: 0.022851
True structure:



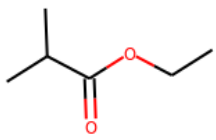
Experimental 13C NMR (solvent: CDCl3)



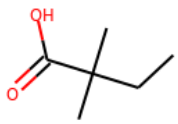
Experimental 1H NMR (solvent: CDCl3)



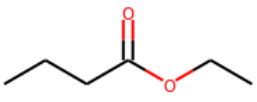
Top predicted structures (loss):



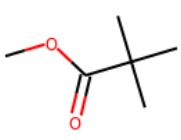
0.022851



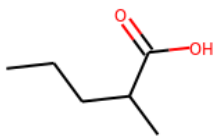
0.044646



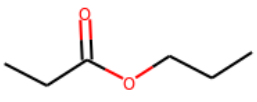
0.047757



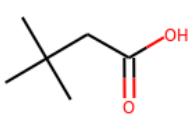
0.050781



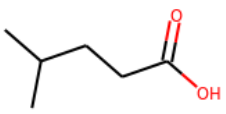
0.053552



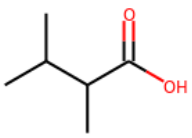
0.05806



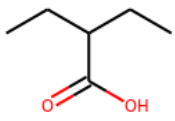
0.058515



0.058806



0.058854



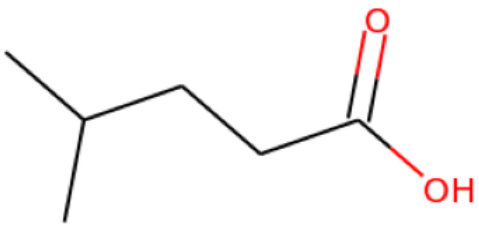
0.059992

Top predicted substructures	prob		
[CX4H3]	1.0	[CX3](=[OX1])O	0.9329
[#6H3][#6][#6]	0.9999	[CX4H2]([#6])[O]	0.9303
[CX4H3][#6]	0.999	[CX4H3][CX4H1]	0.8783
[CX3](=[OX1])C	0.9873	[#6H3][#6][#6X3]	0.8551
[#8]=[#6][#8]	0.9825	[CX4H3][CX4H2]	0.8471

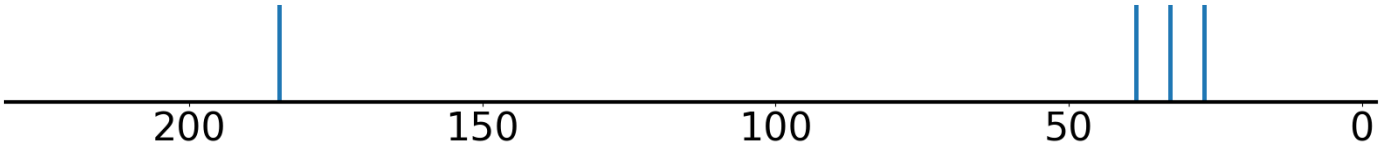
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][#6]	0.999	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9873	CC#CCC#C	0.0
[#8]=[#6][#8]	0.9825	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX3](=[OX1])O	0.9329	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2]([#6])[O]	0.9303	CCC=CC#C	0.0
[CX4H3][CX4H1]	0.8783	[#6X2][#6H1][#6X2]	0.0
[#6H3][#6][#6X3]	0.8551	CC=CC#CC	0.0
[CX4H3][CX4H2]	0.8471	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[OX2H1]	0.7563	[CX3H0](=[OX1H0])([OX2H0])[CX4H1]	0.1421
[#6H3][#6][#6][#6H3]	0.6401	[#8]=[#6H0][#6H1]	0.1627
[CX3](=O)[OX2H1]	0.614	[CHX4]([CH3X4])[CH3X4]	0.2393
[#6H3][#6H0]	0.5914	[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.3492
[CX4H3][CX4H0]	0.5165	O=[CX3][CX4H]	0.3638
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.4751	[CH3][#6][#8]	0.5874
[CX4H2][CX3]=O	0.3545	[#8][#6H0][#6H1]	0.6496
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.3298	[CX4H3][CX4]O	0.6655
[OX2H1][CX4H2][#6X3H0]	0.319	[#6H1]	0.7254
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2715	[CX4H2]([OX2H0])[CX4H3]	0.7587

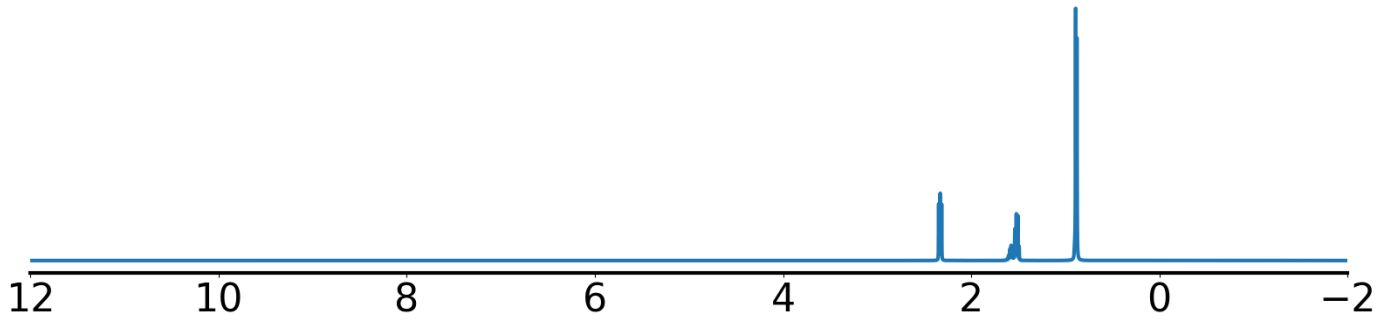
Example 112 true smiles: CC(C)CCC(=O)O formula: C6H12O2
Index of correct structure: 0 of 903
True structure loss: 0.006743
True structure:



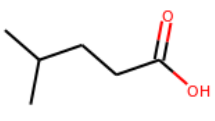
Experimental 13C NMR (solvent: CDCl3)



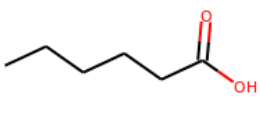
Experimental 1H NMR (solvent: cdcl3)



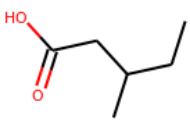
Top predicted structures (loss):



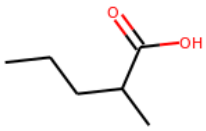
0.006743



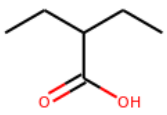
0.033622



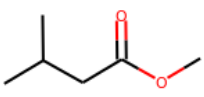
0.0486



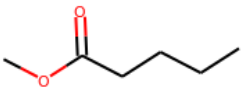
0.066608



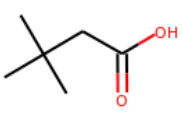
0.069353



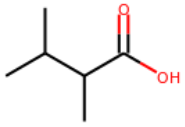
0.072996



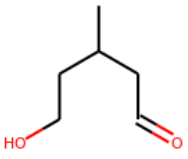
0.076831



0.087612



0.094259



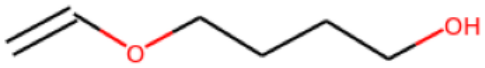
0.103345

Top predicted substructures	prob		
[#6H3][#6][#6]	1.0	[#8]=[#6][#8]	0.9914
[CX4H2]([#6])[#6]	0.9991	[CX4H3][#6]	0.9866
[CX3](=O)[OX2H1]	0.999	[CX3](=[OX1])O	0.985
[CX4H3]	0.9986	[OX2H1]	0.9754
[CX3](=[OX1])C	0.9974	[CHX4]([CH3X4])[CH3X4]	0.9549

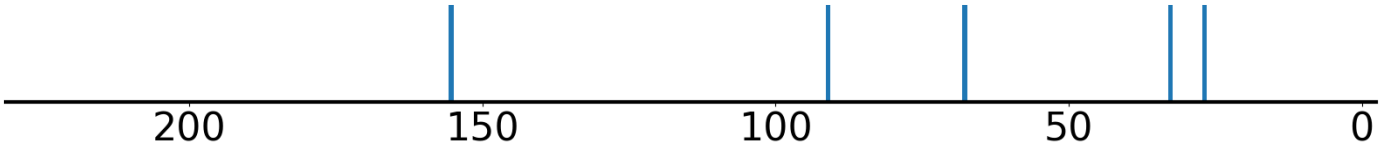
best positives	prob	best negatives	prob
[#6H3][#6][#6]	1.0	C=CC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9991	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=O)[OX2H1]	0.999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	0.9986	CCC=CC#C	0.0
[CX3](=[OX1])C	0.9974	CCC#CC#C	0.0
[#8]=[#6][#8]	0.9914	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][#6]	0.9866	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.985	CC=CCC#C	0.0
[OX2H1]	0.9754	[CX4H3][CX2H0]	0.0
[CHX4]([CH3X4])[CH3X4]	0.9549	CC#CCC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H2]	0.404	[CX4H2]([CX4H2])[CX4H1]	0.5845
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3546	[#8][#6][#6H2]	0.7081
[CX4H2][CX4H2][CX4H2][CX4H2]	0.2974	OCC[CH2]	0.7314
CCCCCC	0.277	[CX4H2][CX4H2]	0.7585
O=[CX3H0][CX4H2][CX4H1]	0.1705	[#6H1][#6H2]	0.7799
[#6X3][#6][#6][#6H3]	0.1614	[CX4H2]CC=O	0.8074
[#8]=[#6][#6H2][#6H1]	0.1584	[CX4H2][CX3]=O	0.8337
[CX4H2]([CX4H1])[CX3H0]	0.1343	[CHX4]([CH3X4])[CH2X4]	0.8768
[#8][#6H0][#6H1]	0.0971	[#6H1]	0.8814
[#8]=[#6H0][#6H1]	0.0934	[CX4H2]([CX4H2])[CX3H0]	0.8892

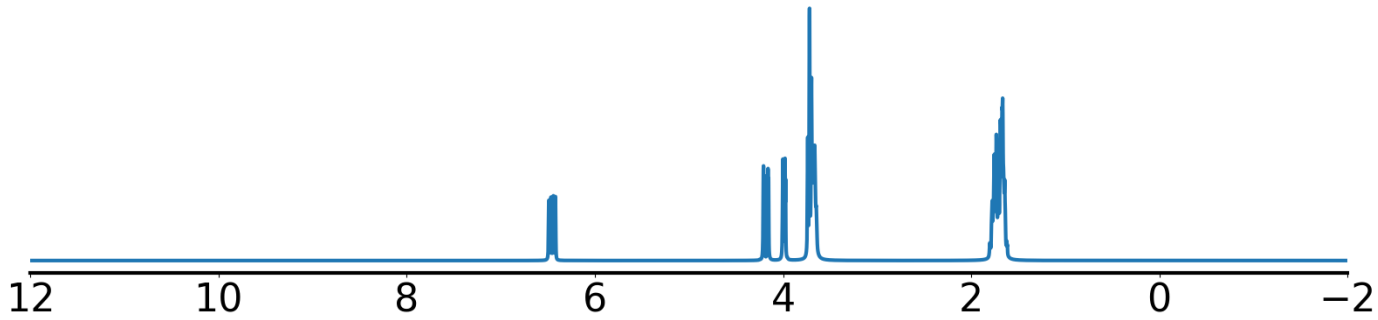
Example 113 true smiles: C=COCCCCO formula: C6H12O2
Index of correct structure: 0 of 903
True structure loss: 0.006823
True structure:



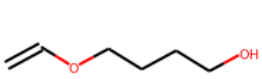
Experimental 13C NMR (solvent: CDCl3)



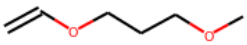
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



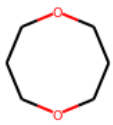
0.006823



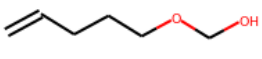
0.029637

0.046928

0.063585

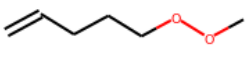


0.066065

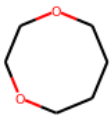


0.068251

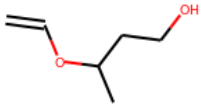
0.072528



0.076116



0.078152



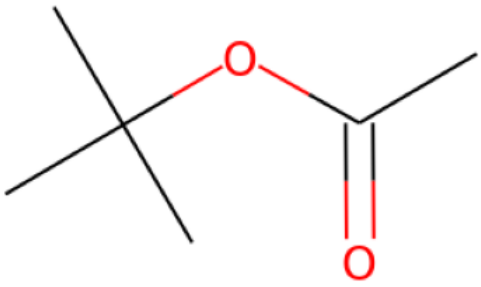
0.080675

Top predicted substructures	prob		
[CX3H1](=[CX3H2])[OX2H0]	0.9999	[CX4H2]([#6])[O]	0.9969
[#8][#6]=[#6H2]	0.9998	OCC[CH2]	0.9961
[#8][#6][#6H2]	0.9993	[#6X3H2]	0.9949
[CH2X3](=C)	0.9988	[CH2X4](O)[CX4H2][CX4H2]	0.9938
[CX4H2]([#6])[#6]	0.9983	[CX3H2]=[CX3H1]	0.9918

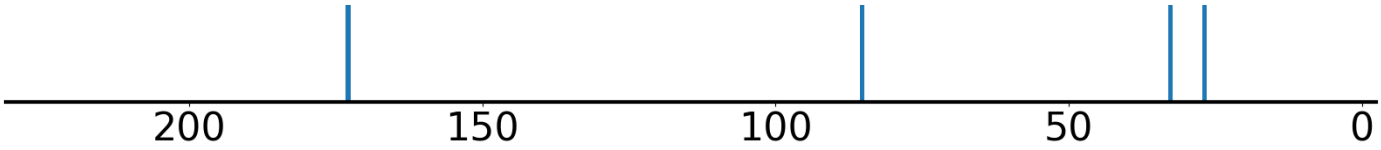
best positives	prob	best negatives	prob
[CX3H1](=[CX3H2])[OX2H0]	0.9999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8][#6]=[#6H2]	0.9998	[#6X2][#6H1][#6X2]	0.0
[#8][#6][#6H2]	0.9993	[#7][#6H1][#6X2]	0.0
[CH2X3](=C)	0.9988	[#7][#6][#6][#6]#[#7]	0.0
[CX4H2]([#6])[#6]	0.9983	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2]([#6])[O]	0.9969	C=CC=CC#C	0.0
OCC[CH2]	0.9961	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6X3H2]	0.9949	CC#CCC#C	0.0
[CH2X4](O)[CX4H2][CX4H2]	0.9938	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX3H2]=[CX3H1]	0.9918	[CX2H0](#[CX2H0])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H1]	0.4017	[#8][#6][#6][#6][#6][#8]	0.4203
[#6H1][#6H2]	0.3617	[CX4H2]([OX2H1])[CX4H2]	0.5112
[#8H][#6H2][#6H1]	0.3321	[#6H2][#8][#6H1]	0.6835
[#8][#6][#6][#8]	0.2209	[CX4H2]([OX2H0])[CX4H2]	0.7658
[CX4H2]([CX4H2])[CX3H1]	0.2048	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9231
O[CX4H][CX4H2]	0.2016	[CX3H]O[CX4H2]	0.9254
[CHX3](=C)C	0.1509	[OX2H1]	0.9329
[CX4H2][CX3H]	0.1259	[#6H1]	0.9364
[CX4H]O	0.1192	[CX3H](O)	0.9484
[#8][#6][#6H2][#8]	0.1084	[CH2X4](O)[CX4H2]	0.9484

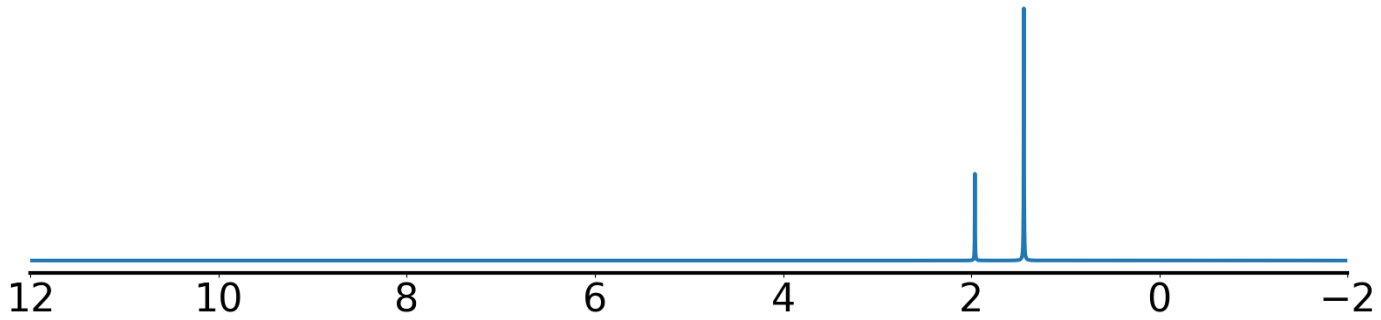
Example 114 true smiles: CC(=O)OC(C)(C)C formula: C6H12O2
Index of correct structure: 0 of 903
True structure loss: 0.007652
True structure:



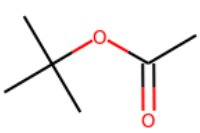
Experimental 13C NMR (solvent: CDCl3)



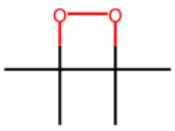
Experimental 1H NMR (solvent: CDCl3)



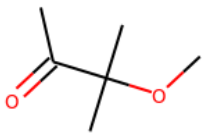
Top predicted structures (loss):



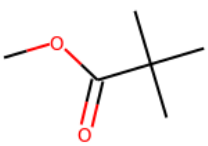
0.007652



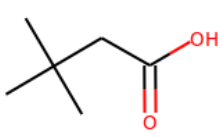
0.036201



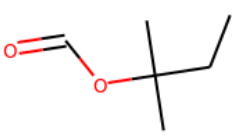
0.041301



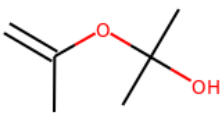
0.061614



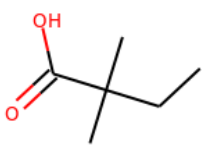
0.064295



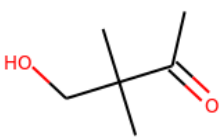
0.064928



0.07172



0.075579



0.076905

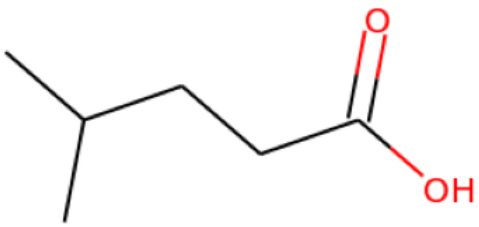
0.080629

Top predicted substructures	prob		
[#6H3][#6H0]	0.9996	[CX4H3][#6]	0.9958
[CX4H3]	0.9993	[CX4H3][CX4H0][CX4H3]	0.9946
[CX4H3][CX4H0]	0.9987	[CX4H3][CX3]	0.9811
[#6H3][#6][#6]	0.9972	[CX4H3][CX4H0]([CX4H3])[OX2H0]	0.9765
[CX4H3][CX4]O	0.9967	[#8]=[#6][#8]	0.9606

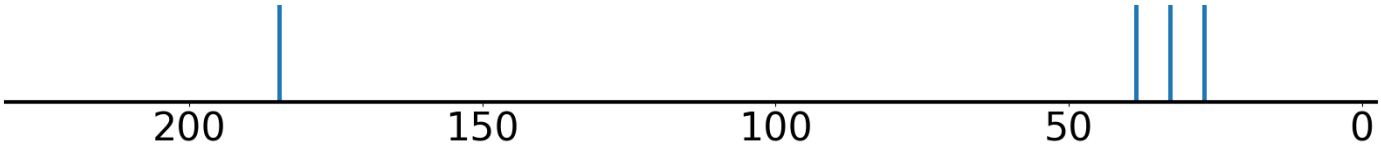
best positives	prob	best negatives	prob
[#6H3][#6H0]	0.9996	[#7][#6][#6][#6]#[#7]	0.0
[CX4H3]	0.9993	CCC#CC#C	0.0
[CX4H3][CX4H0]	0.9987	[#7][#6]=[#6][#6]#[#7]	0.0
[#6H3][#6][#6]	0.9972	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][CX4]O	0.9967	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX4H3][#6]	0.9958	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[CX4H3][CX4H0][CX4H3]	0.9946	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H3][CX3]	0.9811	[#7][#6H1][#6X2]	0.0
[CX4H3][CX4H0]([CX4H3])[OX2H0]	0.9765	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8]=[#6][#8]	0.9606	[#6X2][#6H1][#6X2]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.5603	[OX1H0]=[CX3H0][CX4H3]	0.7527
OCC[CH2]	0.5255	[CX4]([CX4H3])([CX4H3])[CX4H3]	0.8171
[OX2H1]	0.4812	[CX3H0](=[OX1H0])([OX2H0])[CX4H3]	0.877
[#6X4H3][#6][#8H]	0.2951	[OX2H0][CX3H0][CX4H3]	0.9063
[#8][#6][#6]=[#8]	0.2695	[CH3][#6][#8]	0.9194
[CX4H2]([#6])[#6]	0.2636	[CX3](=[OX1])C	0.9364
[CX4H2][CX4H2]	0.2233	[CX4H3][CX3H0]	0.9375
[CX3](=O)[OX2H1]	0.2005	[CX3](=[OX1])O	0.9389
[#8][#6][#6]=[#6X3]	0.1911	[#6H0]([#6H3])([#6H3])[#8]	0.9579
[#8][#6H0][#6H1]	0.176	[#8]=[#6][#8]	0.9606

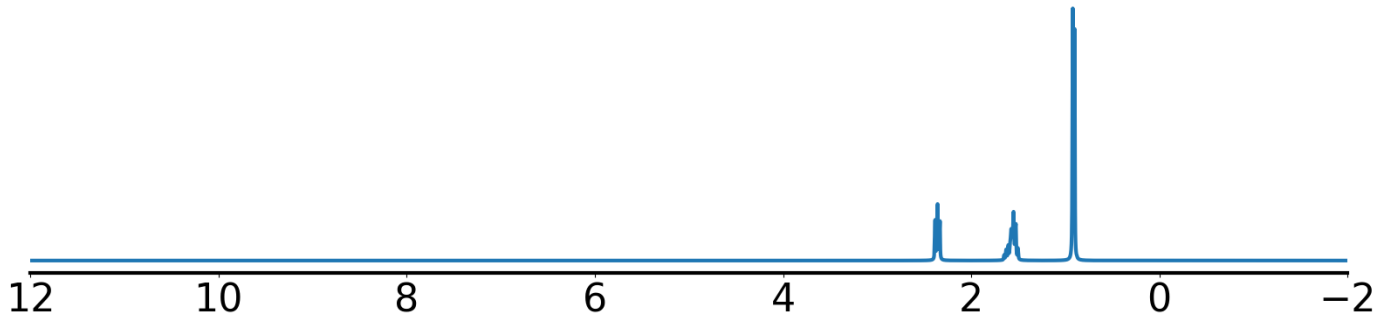
Example 115 true smiles: CC(C)CCC(=O)O formula: C6H12O2
Index of correct structure: 0 of 903
True structure loss: 0.007335
True structure:



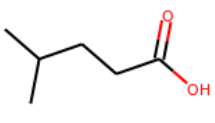
Experimental 13C NMR (solvent: CDCl3)



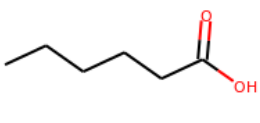
Experimental 1H NMR (solvent: CDCl3)



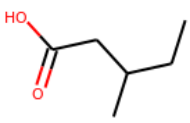
Top predicted structures (loss):



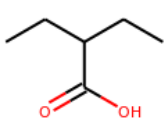
0.007335



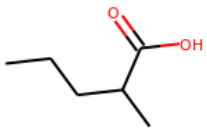
0.034777



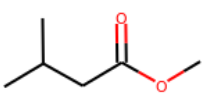
0.044111



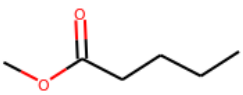
0.063887



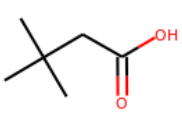
0.066391



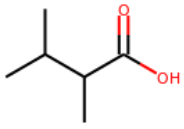
0.075492



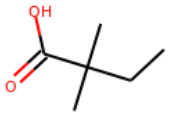
0.078784



0.081609



0.089869



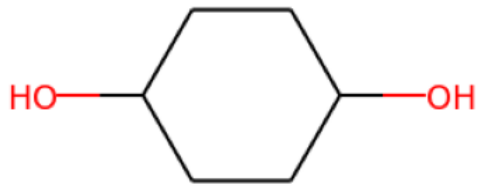
0.099078

Top predicted substructures	prob		
[#6H3][#6][#6]	1.0	[#8]=[#6][#8]	0.9945
[CX3](=O)[OX2H1]	0.9996	[CX4H3][#6]	0.9865
[CX4H3]	0.9992	[CX3](=[OX1])O	0.9862
[CX4H2]([#6])[#6]	0.9981	[OX2H1]	0.978
[CX3](=[OX1])C	0.9976	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9616

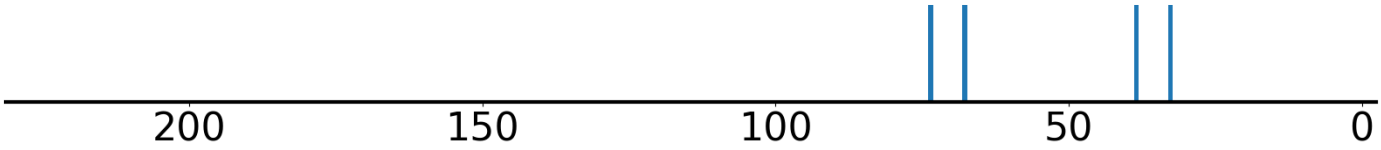
best positives	prob	best negatives	prob
[#6H3][#6][#6]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=O)[OX2H1]	0.9996	C=CC=CC#C	0.0
[CX4H3]	0.9992	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[#6]	0.9981	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX3](=[OX1])C	0.9976	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#8]=[#6][#8]	0.9945	CC=CCC#C	0.0
[CX4H3][#6]	0.9865	CCC#CC#C	0.0
[CX3](=[OX1])O	0.9862	CCC=CC#C	0.0
[OX2H1]	0.978	CC#CCC#C	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9616	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.4638	[CX4H2]([CX4H2])[CX4H1]	0.7047
CCCCCC	0.3535	[#8][#6][#6H2]	0.7051
[CX4H2]([CX4H2])[CX4H2]	0.2871	[#6H1][#6H2]	0.7086
[CX4H2][CX4H2][CX4H2][CX4H2]	0.2199	[CX4H2][CX4H2]	0.7485
[CX4H2]([CX4H1])[CX3H0]	0.2009	OCC[CH2]	0.7533
O=[CX3H0][CX4H2][CX4H1]	0.1997	[CX4H2][CX3]=O	0.7896
[#6X3][#6][#6][#6H3]	0.1769	[CHX4]([CH3X4])[CH2X4]	0.8125
[CX4H1]([CX4H3])([CX4H2])[CX4H2]	0.1685	[CX4H2]CC=O	0.8385
[#8]=[#6][#6H2][#6H1]	0.1656	[#6H1]	0.9088
[#8]=[#6H0][#6H1]	0.1466	[CX4H2]([CX4H2])[CX3H0]	0.9167

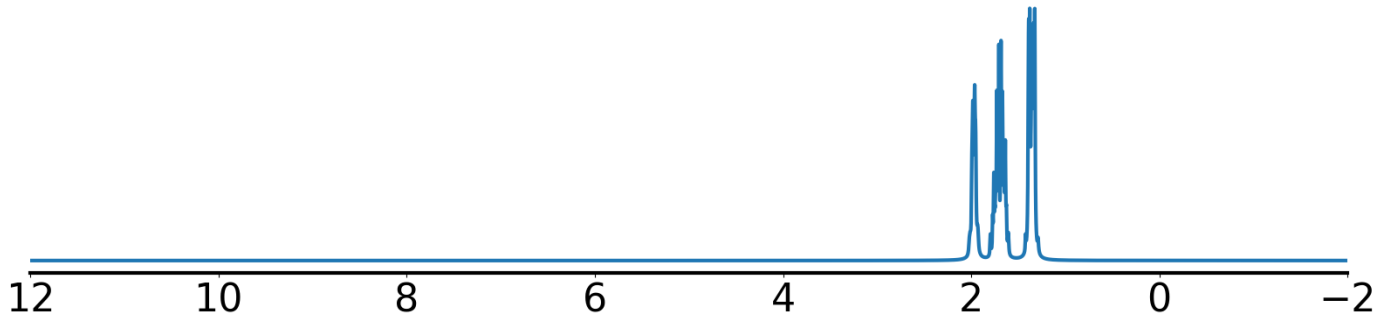
Example 116 true smiles: OC1CCC(O)CC1 formula: C6H12O2
Index of correct structure: 0 of 903
True structure loss: 0.012793
True structure:



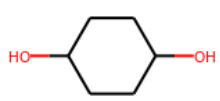
Experimental 13C NMR (solvent: DMSO)



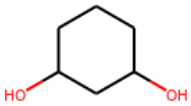
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):

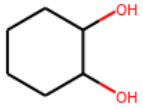


0.012793

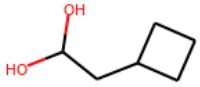


0.019807

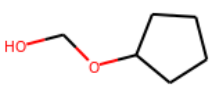
0.026045



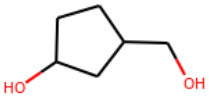
0.03449



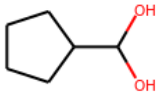
0.035419



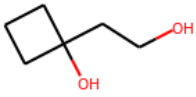
0.040487



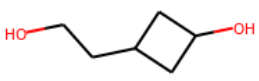
0.041637



0.041827



0.044251



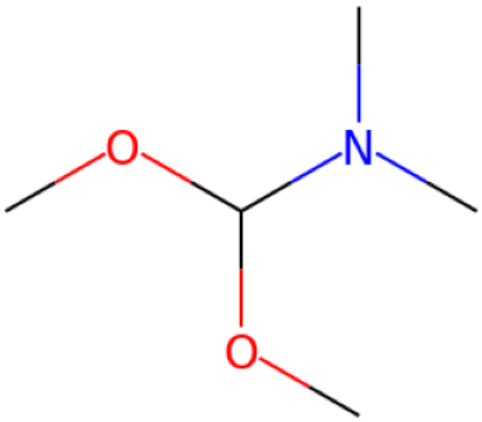
0.049836

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H2]([CX4H2])[CX4H1]	0.9566
OCC[CH2]	0.9986	[#6H1][#6H2]	0.8993
[OX2H1]	0.9933	CCCCCC	0.8891
[#8][#6][#6H2]	0.988	[#6H1]	0.853
[CX4H2][CX4H2]	0.9741	[#6X4H2][#6H1][#8H]	0.852

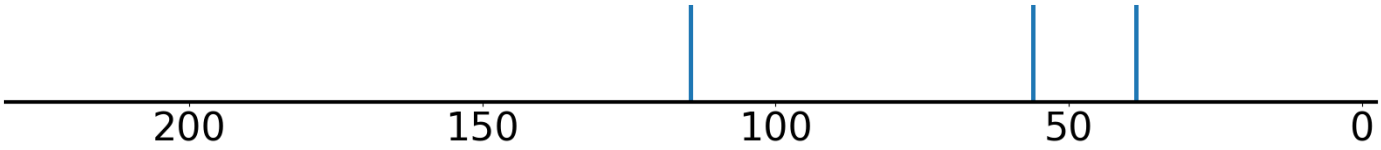
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
OCC[CH2]	0.9986	CC#CCC=C	0.0
[OX2H1]	0.9933	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6H2]	0.988	C=CC=CC#C	0.0
[CX4H2][CX4H2]	0.9741	[CX2H0](#[NX1H0])[CX3H1]	0.0
[CX4H2]([CX4H2])[CX4H1]	0.9566	[#6X2][#6H1][#6X2]	0.0
[#6H1][#6H2]	0.8993	[CX2H0](#[CX2H1])[cX3H0]	0.0
CCCCCC	0.8891	CC=CCC#C	0.0
[#6H1]	0.853	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#6X4H2][#6H1][#8H]	0.852	[CX2H0](#[CX2H0])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H2]	0.6622	[#6H1][#6H2][#6H2][#6H1]	0.2112
[#8][#6H0][#6H1]	0.411	[CX4H1][CX4H2][CX4H2][CX4H1]	0.478
[CX4H2]([CX4H2])[CX4H0]	0.3947	[OH][CX4H]	0.5191
[CX4H2][CX4H2][CX4H2][CX4H2]	0.3146	[#8][#6][#6][#6][#6][#8]	0.52
[CX4H1]([CX4H2])([CX4H2])[CX4H2]	0.2233	[CX4H]O	0.5359
[OX2H1][CX4H0][CX4H2][CX4H2]	0.2213	[#6H1]([#6H2])[#6H2]	0.6636
[#8][#6][#6][#8]	0.2099	[#6]1[#6][#6][#6][#6][#6]1	0.7286
[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.2015	O[CX4H][CX4H2]	0.7783
[CX4H3][CX4]O	0.1937	[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.7806
[CX4H2]([CX4H1])[CX4H1]	0.1927	[#6X4H2][#6H1][#8H]	0.852

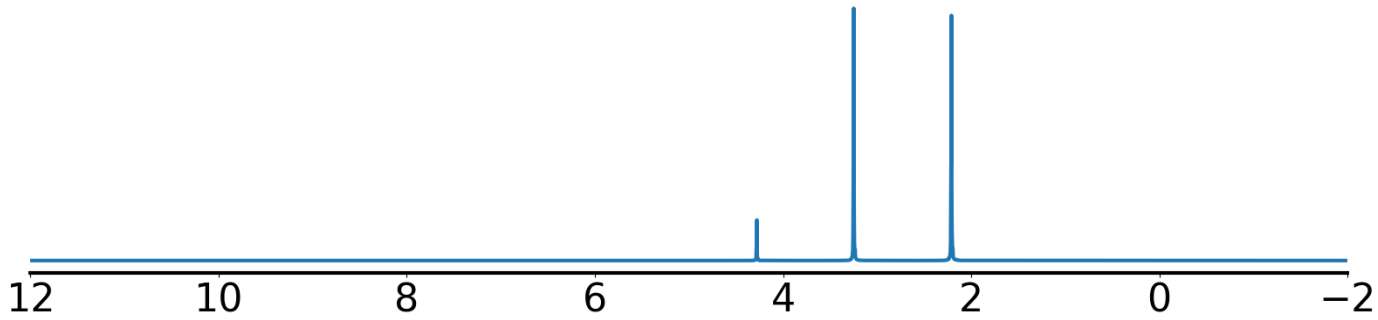
Example 117 true smiles: COC(OC)N(C)C formula: C5H13NO2
Index of correct structure: 0 of 900
True structure loss: 0.022358
True structure:



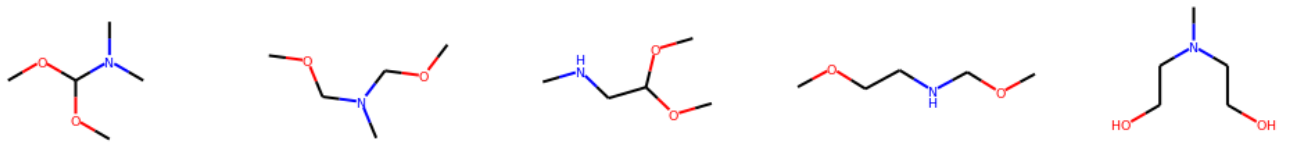
Experimental 13C NMR (solvent: CCl4)



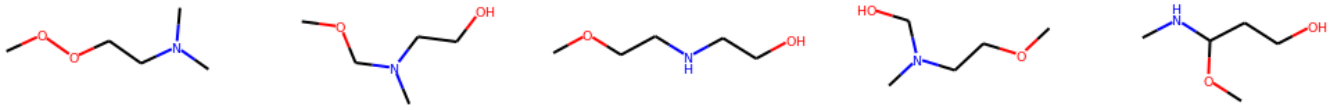
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.022358 0.022391 0.029448 0.034865 0.034961



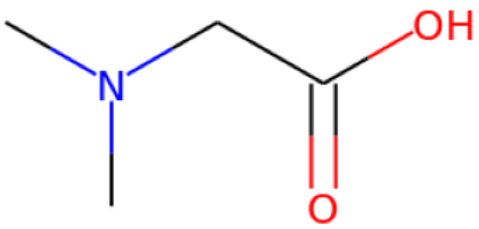
0.035292 0.036968 0.037916 0.040704 0.042838

Top predicted substructures	prob		
[CX4H3]	0.9868	[#7X3][#6H3]	0.7403
[#7X3][#6H2]	0.8904	[CX4H3][OX2H0]	0.6847
[#7][#6H2]	0.8376	[#6H3][#7]	0.6589
[#8][#6][#6H2]	0.8367	[CX4H2]([#6])[O]	0.5379
[OX2H0][CX4H1][OX2H0]	0.8311	[#6H3][#7][#6H2]	0.5316

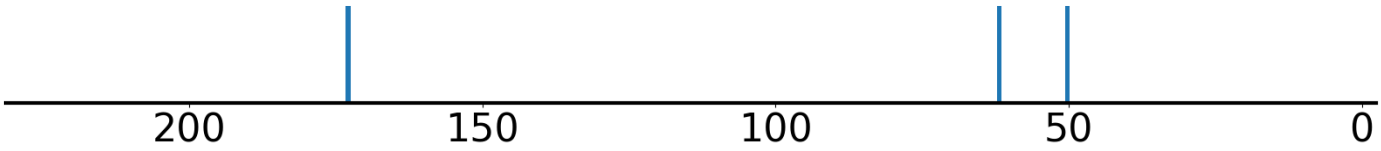
best positives	prob	best negatives	prob
[CX4H3]	0.9868	[#6X2][#6H1][#6X2]	0.0
[OX2H0][CX4H1][OX2H0]	0.8311	CCC=CC#C	0.0
[#7X3][#6H3]	0.7403	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
[CX4H3][OX2H0]	0.6847	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#7]	0.6589	CC=CCC#C	0.0
[CX4H]O	0.3619	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][NX3H0]	0.342	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H1]	0.0901	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#7X3H0]	0.0888	CC=CC#CC	0.0

worst negatives	prob	worst positives	prob
[#7X3][#6H2]	0.8904	[#7X3H0]	0.0888
[#7][#6H2]	0.8376	[#6H1]	0.0901
[#8][#6][#6H2]	0.8367	[CX4H3][NX3H0]	0.342
[CX4H2]([#6])[O]	0.5379	[CX4H]O	0.3619
[#6H3][#7][#6H2]	0.5316	[#6H3][#7]	0.6589
[CX4H2][CX4H2]	0.5118	[CX4H3][OX2H0]	0.6847
[OX2H1]	0.5003	[#7X3][#6H3]	0.7403
OCC[CH2]	0.4523	[OX2H0][CX4H1][OX2H0]	0.8311
[#7H2][#6H2]	0.3649	[CX4H3]	0.9868

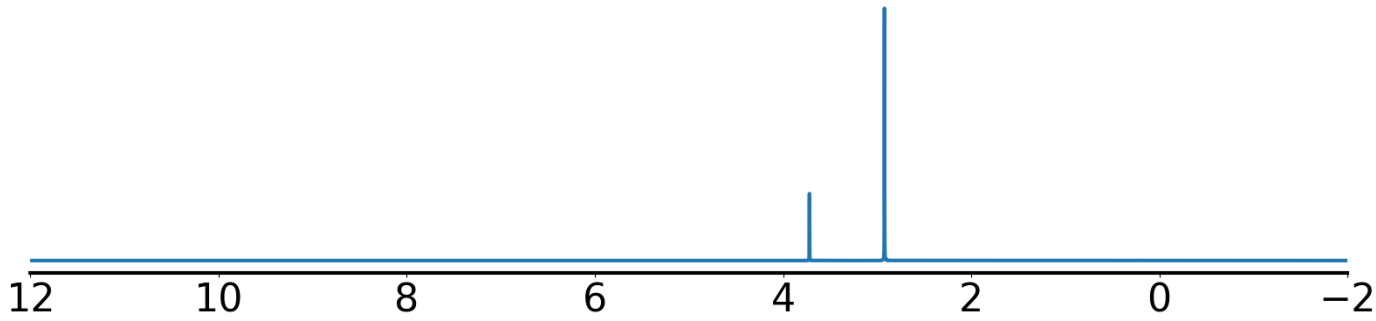
Example 118 true smiles: CN(C)CC(=O)O formula: C4H9NO2
Index of correct structure: 0 of 896
True structure loss: 0.018376
True structure:



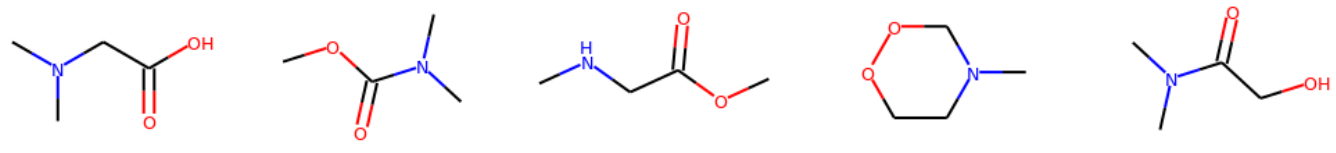
Experimental 13C NMR (solvent: D2O)



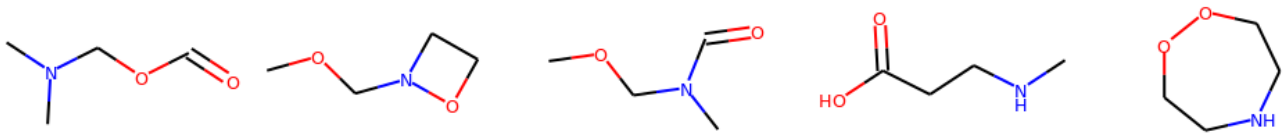
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.018376 0.024773 0.030801 0.040296 0.043706



0.046476 0.049585 0.051787 0.053629 0.054158

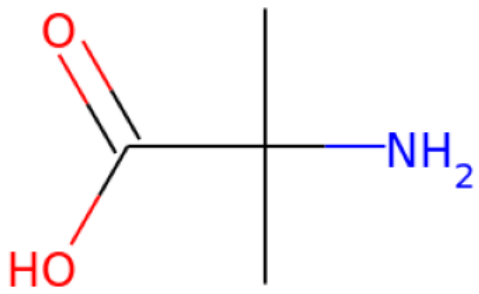
Top predicted substructures	prob		
[CX4H3]	0.9839	[CX4H3][NX3H0]	0.8289

[#7X3][#6H3]	0.9544	[#6H3][#7][#6H2]	0.8185
[CX3](=[OX1])C	0.9517	[CX3](=[OX1])O	0.7896
[#6H3][#7]	0.9203	[#7X3H0]	0.7793
[#8]=[#6][#8]	0.8577	[#7][#6H2]	0.7557

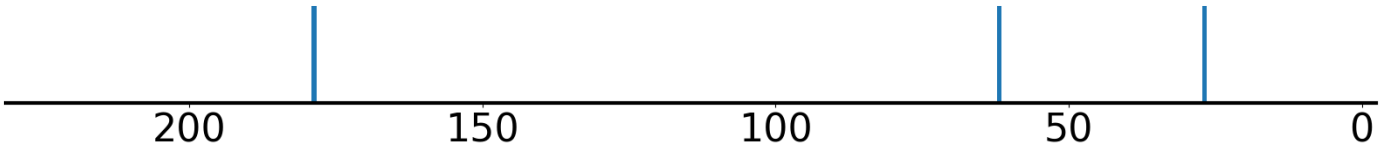
best positives	prob	best negatives	prob
[CX4H3]	0.9839	C=CCCC#C	0.0
[#7X3][#6H3]	0.9544	CCC#CC#C	0.0
[CX3](=[OX1])C	0.9517	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6H3][#7]	0.9203	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#8]=[#6][#8]	0.8577	CC=CC#CC	0.0
[CX4H3][NX3H0]	0.8289	[CX2H0](#[CX2H0])[CX3H1]	0.0
[#6H3][#7][#6H2]	0.8185	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[CX3](=[OX1])O	0.7896	[CX2H0](#[CX2H0])[CX4H1]	0.0
[#7X3H0]	0.7793	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#7][#6H2]	0.7557	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[CX4H3][OX2H0]	0.5766	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1351
[#6H3][#7][#6X3]	0.3678	[OX2H1]	0.2571
[#6H2][#7][#6X3]	0.3098	[CX3](=O)[OX2H1]	0.3188
[#8][#6][#6]=[#8]	0.2945	[#7][#6][#6X3]	0.4147
[#7X3H1]	0.2937	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.4513
[CX4H2]([#6])[O]	0.2519	[#6X3][#6H2][#7]	0.4727
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.2169	[CX4H2]([NX3H0])[CX3H0]	0.6611
[#8]=[#6H0][#6H1]	0.2107	[#8][#6][#6H2]	0.6755
[#8][#6][#6][#6X3]	0.2044	[#7X3][#6H2]	0.7197
[CH2X4](O)[CX4H2]	0.1983	[CX4H2][CX3]=O	0.7255

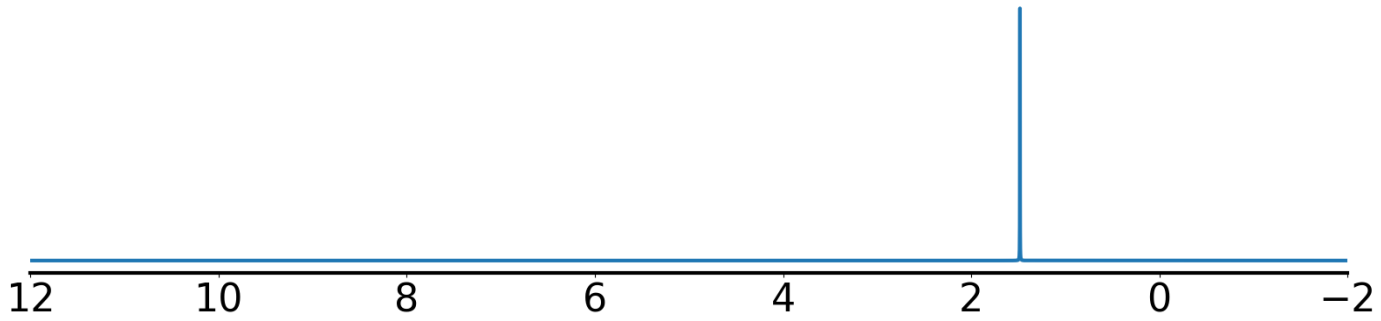
Example 119 true smiles: CC(C)(N)C(=O)O formula: C4H9NO2
Index of correct structure: 0 of 896
True structure loss: 0.010581
True structure:



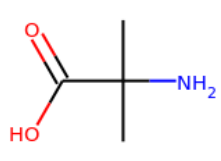
Experimental 13C NMR (solvent: D2O)



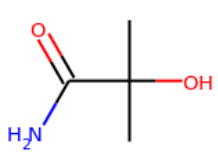
Experimental 1H NMR (solvent: D2O)



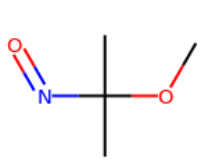
Top predicted structures (loss):



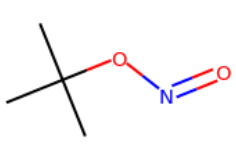
0.010581



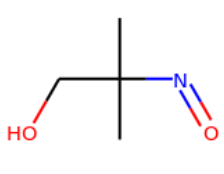
0.023607



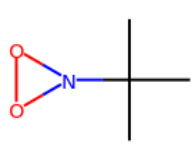
0.035324



0.036309

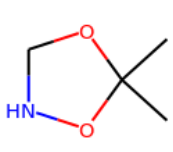


0.036552



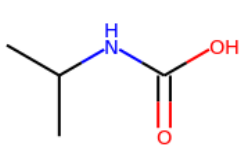
0.037491

0.03961



0.041186

0.045326



0.046072

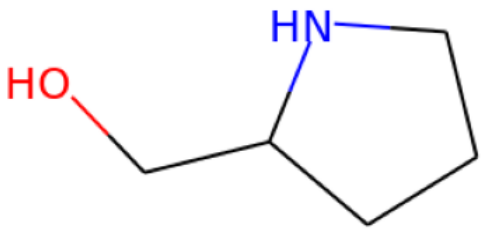
Top predicted substructures	prob		
[#6H3][#6][#6]	0.998	[CX4H3][#6]	0.9769

[CX4H3]	0.9966	[CX3](=[OX1])C	0.9693
[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.9952	[#6H3][#6H0]	0.9646
[CX4H3][CX4H0]	0.9883	[#7][#6][#6H3]	0.8187
[CX4H3][CX4H0][CX4H3]	0.9867	[OX2H1]	0.8171

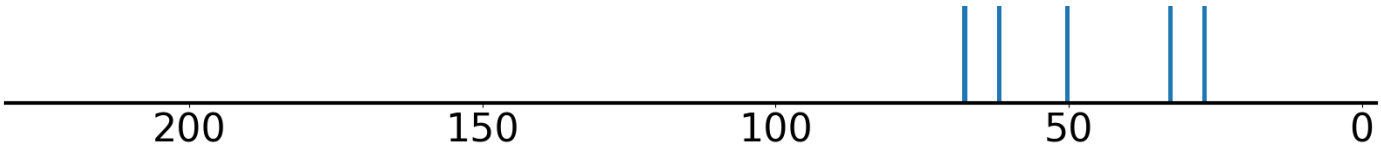
best positives	prob	best negatives	prob
[#6H3][#6][#6]	0.998	C=CCCC#C	0.0
[CX4H3]	0.9966	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.9952	CC=CCC#C	0.0
[CX4H3][CX4H0]	0.9883	CCC=CC#C	0.0
[CX4H3][CX4H0][CX4H3]	0.9867	CC=CC#CC	0.0
[CX4H3][#6]	0.9769	[#6H2]=[#6][#6X2]	0.0
[CX3](=[OX1])C	0.9693	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H3][#6H0]	0.9646	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#7][#6][#6H3]	0.8187	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[OX2H1]	0.8171	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H3][CX4]O	0.6106	[CH3]CC[OH]	0.1509
[#8][#6][#6]=[#8]	0.4852	[#7H2][#6H0]	0.569
[CH3][#6][#8]	0.2555	[CX3](=O)[OX2H1]	0.5965
[#7X3H1]	0.1904	[#7][#6][#6X3]	0.6135
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.154	[#6H3][#6][#6X3]	0.6418
[#6X4H3][#6][#8H]	0.1539	[CX3](=[OX1])O	0.7782
[CX3H0](=[OX1H0])([OX2H0])[CX4H0]	0.1486	[#8]=[#6][#8]	0.801
[#8][#6][#6][#6X3]	0.137	[#7X3H2]	0.8151
[#8]=[#6H0][#6H1]	0.1316	[OX2H1]	0.8171
[CX4H2]CC=O	0.1212	[#7][#6][#6H3]	0.8187

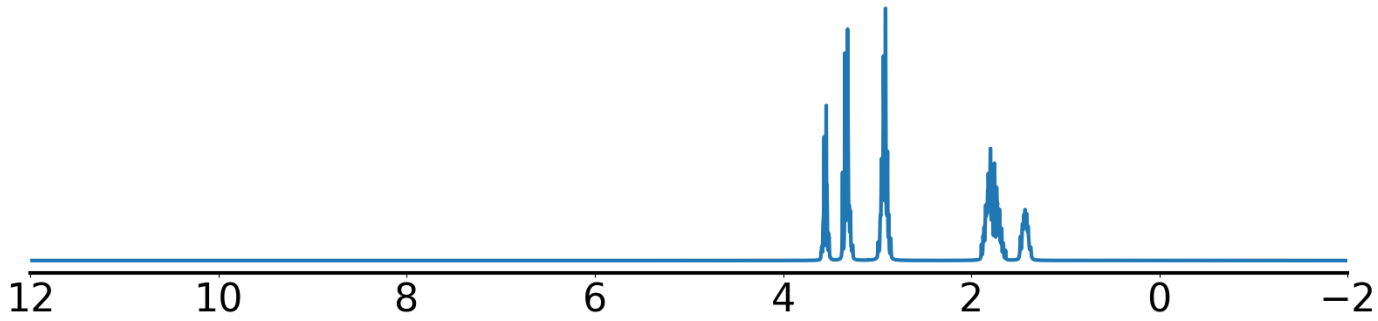
Example 120 true smiles: OCC1CCCN1 formula: C5H11NO
Index of correct structure: 0 of 864
True structure loss: 0.017582
True structure:



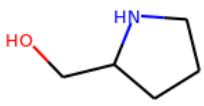
Experimental 13C NMR (solvent: CDCl3)



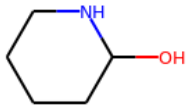
Experimental 1H NMR (solvent: CDCl3)



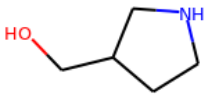
Top predicted structures (loss):



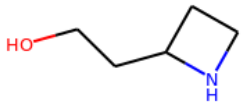
0.017582



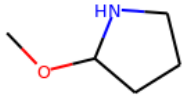
0.029427



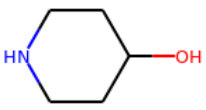
0.033329



0.033571

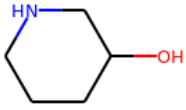


0.035319

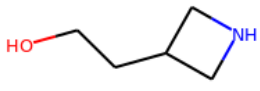


0.036991

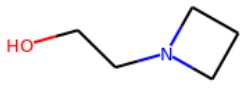
0.037958



0.03799



0.040106



0.041079

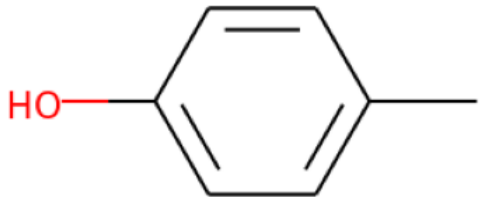
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9998	[#7][#6H2][#6H2]	0.9635

[#7X3][#6H2]	0.9973	[CX4H2][CX4H2]	0.9607
[CX4H2]([CX4H2])[CX4H1]	0.9937	[#6H1]	0.9599
[#7][#6H2]	0.9882	[#6H1][#6H2]	0.9563
OCC[CH2]	0.9659	[OX2H1]	0.9499

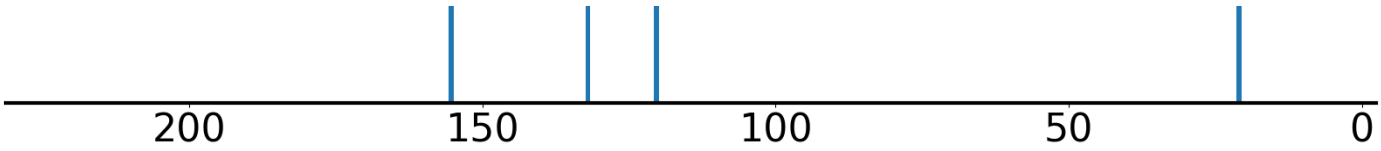
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9998	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7X3][#6H2]	0.9973	C=CC=CC#C	0.0
[CX4H2]([CX4H2])[CX4H1]	0.9937	C=CCCC#C	0.0
[#7][#6H2]	0.9882	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
OCC[CH2]	0.9659	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7][#6H2][#6H2]	0.9635	CC=CC#CC	0.0
[CX4H2][CX4H2]	0.9607	CC#CCC=C	0.0
[#6H1]	0.9599	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#6H1][#6H2]	0.9563	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[OX2H1]	0.9499	[CX3H1](=[CX3H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.7279	[CX4H2](O)[CHX4]	0.3232
[CH2X4](O)[CX4H2]	0.4326	[#6H1r5][#7]	0.3537
[#6H1][#6H1]	0.3638	[#7X3H1]	0.425
[#6]1[#6][#6][#6][#6][#7]1	0.351	[CX4H1]([NX3H1])([CX4H2])[CX4H2]	0.4256
CCCCCC	0.3119	[#6]1[#6][#6][#6][#7]1	0.4421
[#6H2][#7][#6H2]	0.2833	[#8H][#6H2][#6H1]	0.4455
O[CX4H][CX4H2]	0.2463	[#6H1]([#6H2])[#6H2]	0.4624
[CX4H2][CX4H2][CX4H2][CX4H2]	0.2156	[#6H1][#6H2][#6][#6][#7]	0.4735
[CH2X4](O)[CX4H2][CX4H2]	0.2076	[CX4H2]([OX2H1])[CX4H1]	0.5672
[CX4H2]([OX2H1])[CX4H2]	0.2025	[#7][#6H1][#6H2r5]	0.6475

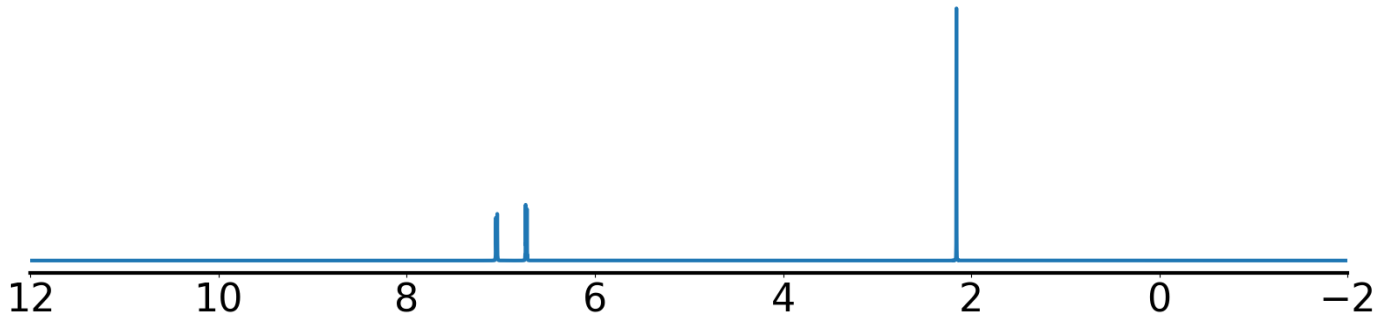
Example 121 true smiles: Cc1ccc(O)cc1 formula: C7H8O
Index of correct structure: 0 of 746
True structure loss: 0.009113
True structure:



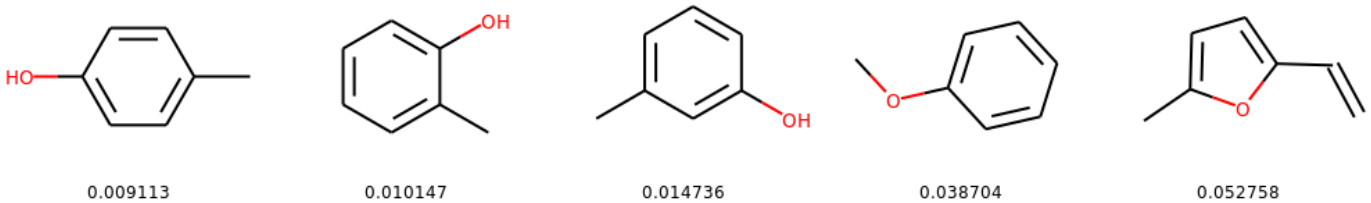
Experimental 13C NMR (solvent: CDCl3)



Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



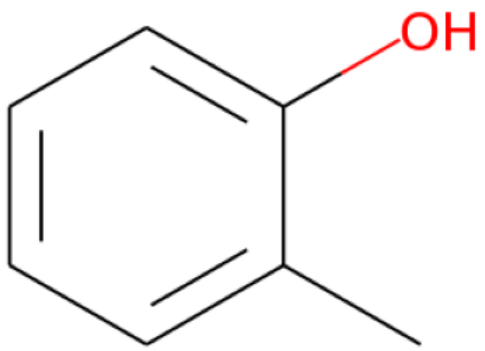
Top predicted substructures	prob		
[#6X3][#6X3]	0.9987	[#6H3][#6][#6]	0.9822

[#6X3][#6X3][#6X3][#6X3]	0.9973	[cH][cH]	0.9801
[#6H1]	0.9971	[#6X3H1][#6X3H0]	0.9753
[CX4H3][#6]	0.9935	[#6H3][#6H0]	0.9711
[CX4H3]	0.9914	[#6]1[#6][#6][#6][#6][#6]1	0.9661

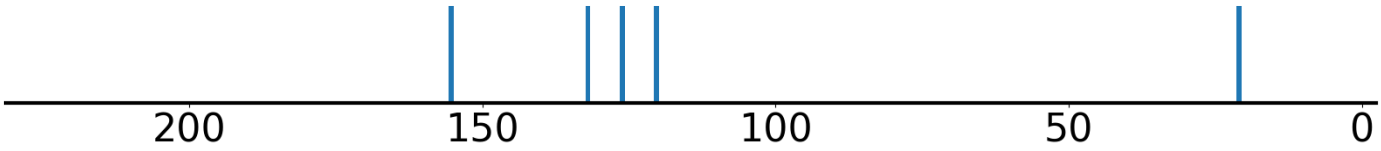
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9987	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9973	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H1]	0.9971	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[CX4H3][#6]	0.9935	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3]	0.9914	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H3][#6][#6]	0.9822	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9801	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6X3H1][#6X3H0]	0.9753	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[#6H3][#6H0]	0.9711	[#6H3][#6H1][#7][#7]	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.9661	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.7674	[OX2H1]	0.534
[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.5336	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5378
[cX3H1]([cX3H0])[cX3H0]	0.2326	[#8][#6][#6][#6X3]	0.6178
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.2013	[OX2H][cX3]:[c]	0.6537
[CH3][#6][#8]	0.1295	[#8][#6H0][#6H1]	0.6667
[#6X3][#6]=[#6][#6H3]	0.1127	[cX3H0][cX3H1][cX3H1][cX3H0]	0.6875
[#6H3][#6]=[#6X3]	0.1111	[cH]cO	0.7683
[cX3H0][cX3H1][cX3H0][OX2H1]	0.0968	[#6H1][#6H1]	0.8509
[CHX3]=[CHX3]	0.0938	[#6H3][#6][#6X3]	0.8858
[#8][#6X3][#6X3][#6X3][#6H3]	0.0863	[CX4H3][cX3H0]	0.8944

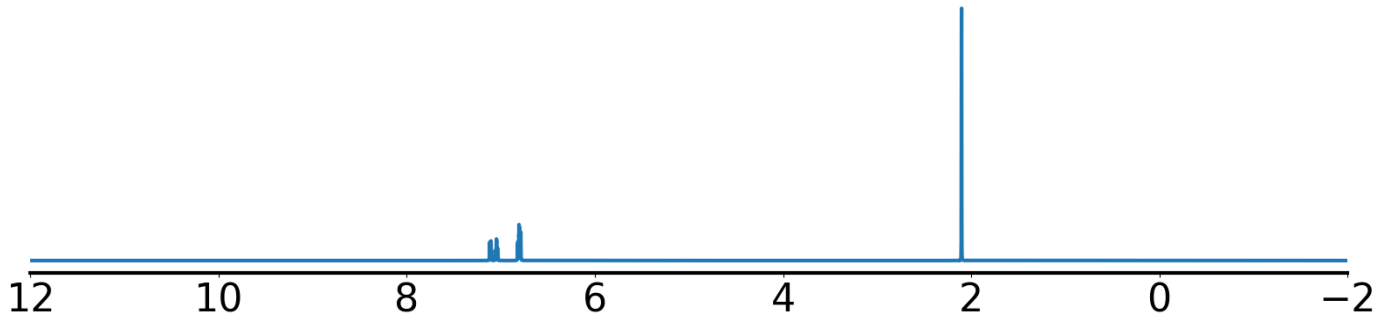
Example 122 true smiles: Cc1ccccc1O formula: C7H8O
Index of correct structure: 0 of 746
True structure loss: 0.007141
True structure:



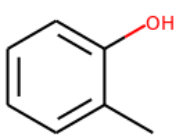
Experimental 13C NMR (solvent: CDCl3)



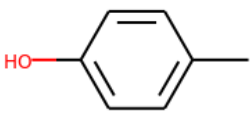
Experimental 1H NMR (solvent: D2O)



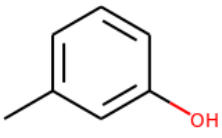
Top predicted structures (loss):



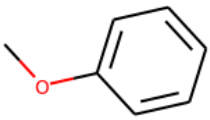
0.007141



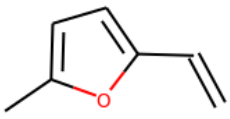
0.010702



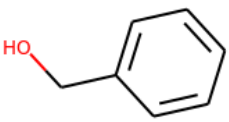
0.013357



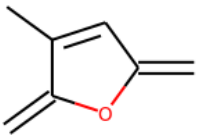
0.041378



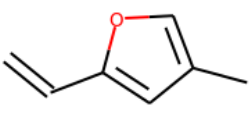
0.064152



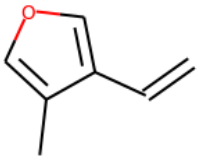
0.073154



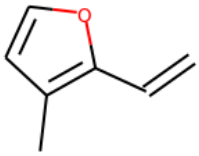
0.075647



0.07753



0.077702



0.078329

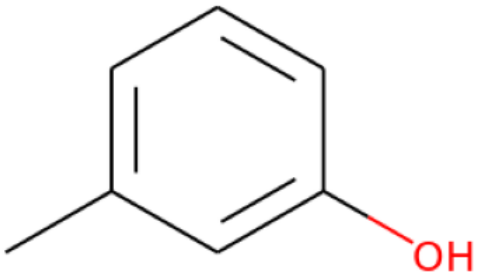
Top predicted substructures	prob		
[#6X3][#6X3]	0.9994	[#6H3][#6H0]	0.9938

[#6H1]	0.9985	[#6H3][#6][#6]	0.98
[#6X3][#6X3][#6X3][#6X3]	0.9983	[cH][cH]	0.9766
[CX4H3]	0.9977	[#6X3H1][#6X3H0]	0.9761
[CX4H3][#6]	0.9964	[#6X3][#6][#6][#6H3]	0.97

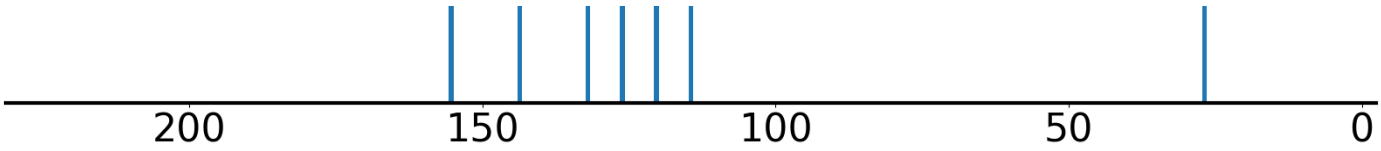
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9994	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H1]	0.9985	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9983	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[CX4H3]	0.9977	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[CX4H3][#6]	0.9964	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H3][#6H0]	0.9938	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6H3][#6][#6]	0.98	[CX4H1]([NX3H0])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9766	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[#6X3H1][#6X3H0]	0.9761	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6X3][#6][#6][#6H3]	0.97	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3628	[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.3608
[cX3H0][cX3H1][cX3H1][cX3H0]	0.3205	[#8][#6H0][#6H1]	0.643
[CHX3]=[CHX3]	0.1941	[#8][#6][#6][#6X3]	0.7155
[cX3H0][cX3H1][cX3H0][OX2H1]	0.19	[OX2H][cX3]:[c]	0.7402
[cX3H1]([cX3H0])[cX3H0]	0.1843	[OX2H1]	0.7458
[#8][#6X3][#6X3][#6X3][#6H3]	0.1509	[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.7845
[#6H3][#6]=[#6X3]	0.1331	[cX3H1]([cX3H1])[cX3H1]	0.7979
[#6X3][#6]=[#6][#6H3]	0.1009	[cH]cO	0.8557
o[cH]	0.092	[#6H3][#6][#6X3]	0.8741
[CH3][#6][#8]	0.0723	[#6H1][#6H1]	0.8827

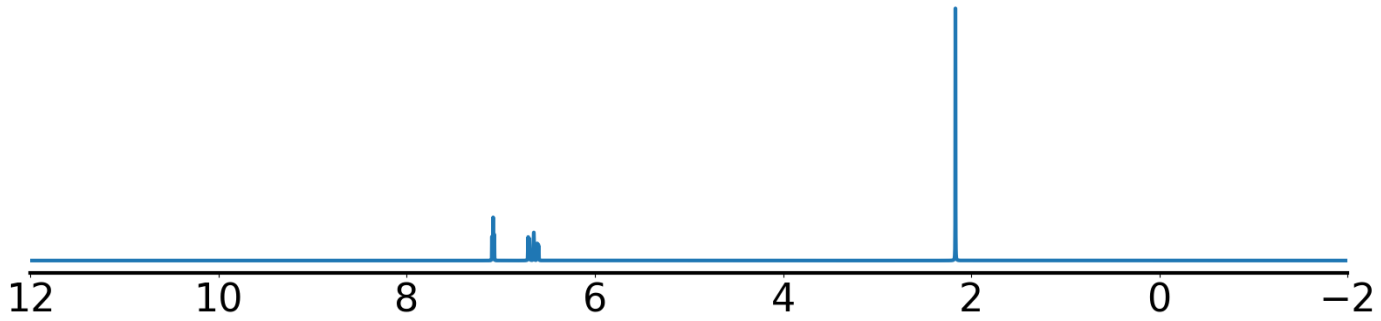
Example 123 true smiles: Cc1cccc(O)c1 formula: C7H8O
Index of correct structure: 0 of 746
True structure loss: 0.00733
True structure:



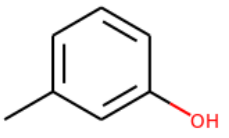
Experimental 13C NMR (solvent: CDCl3)



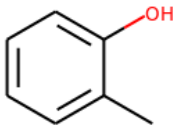
Experimental 1H NMR (solvent: D2O)



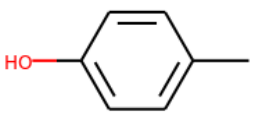
Top predicted structures (loss):



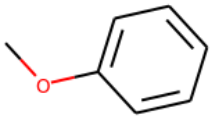
0.00733



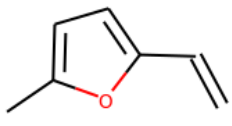
0.009841



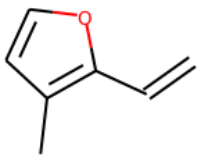
0.01076



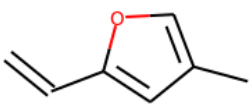
0.041811



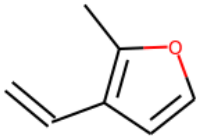
0.060376



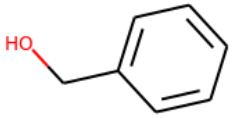
0.071828



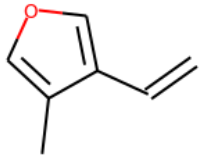
0.073556



0.076027



0.076688



0.076963

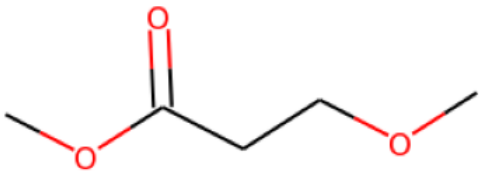
Top predicted substructures	prob		
[#6X3][#6X3][#6X3][#6X3]	0.9998	[#6X3H1][#6X3H0]	0.9959

[#6X3][#6X3]	0.9997	[#6H3][#6][#6]	0.9953
[CX4H3]	0.9993	[cH][cH]	0.9884
[#6H1]	0.9991	[CX4H3][#6]	0.9831
[#6H3][#6H0]	0.9972	[#6X3][#6][#6][#6H3]	0.9772

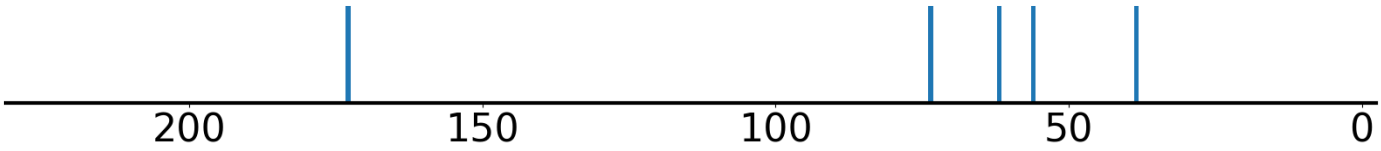
best positives	prob	best negatives	prob
[#6X3][#6X3][#6X3][#6X3]	0.9998	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#6X3][#6X3]	0.9997	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3]	0.9993	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[#6H1]	0.9991	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H3][#6H0]	0.9972	[CX4H1]([NX3H0])([CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9959	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6H3][#6][#6]	0.9953	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[cH][cH]	0.9884	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[CX4H3][#6]	0.9831	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6][#6][#6H3]	0.9772	[OX2H1][CX4H1][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.3974	[cX3H1]([cX3H0])[cX3H0]	0.4304
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.2473	[cX3H0][cX3H1][cX3H0][OX2H1]	0.5777
[cX3H0][cX3H1][cX3H1][cX3H0]	0.2423	[#8][#6X3][#6X3][#6X3][#6H3]	0.59
o[cH]	0.1662	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6168
[cX3H1]([oX2H0])[cX3H1]	0.1624	[OX2H1]	0.6697
[#8][#6H1][#6H1]	0.1325	[OX2H][cX3]:[c]	0.7578
[#8][#6H][#6X3][#6X3H]	0.0895	[cX3H1]([cX3H1])[cX3H1]	0.8513
[CH3][#6][#8]	0.0789	[cH]cO	0.8614
[CX3H](O)	0.0753	[#6]1[#6][#6][#6][#6][#6]1	0.8717
[CHX3]=[CHX3]	0.0711	[CX4H3][cX3H0]	0.8898

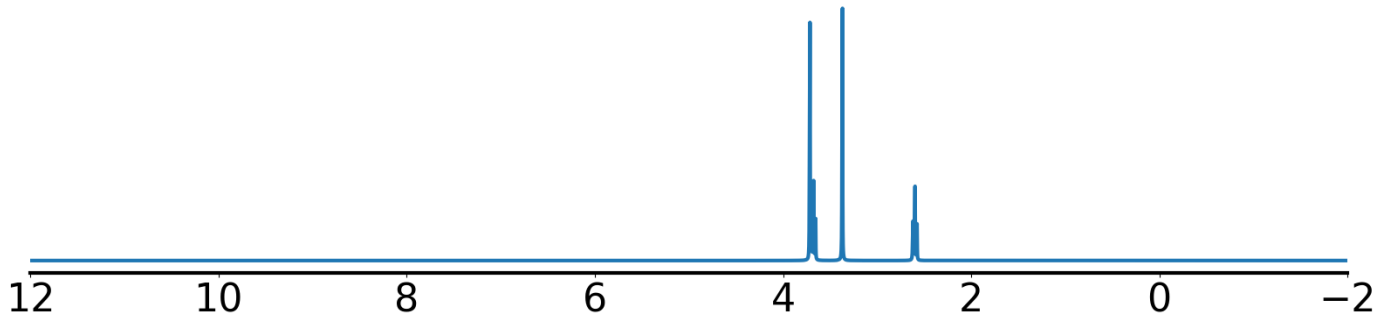
Example 124 true smiles: COCCC(=O)OC formula: C5H10O3
Index of correct structure: 0 of 739
True structure loss: 0.015744
True structure:



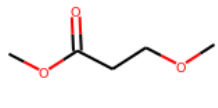
Experimental 13C NMR (solvent: CDCl3)



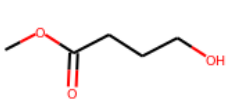
Experimental 1H NMR (solvent: CDCl3)



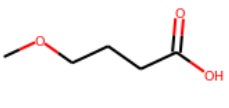
Top predicted structures (loss):



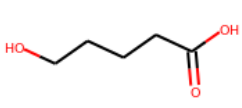
0.015744



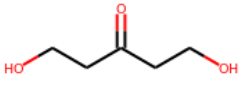
0.029944



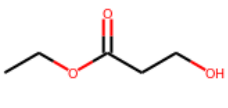
0.044809



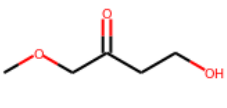
0.054369



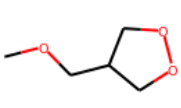
0.062483



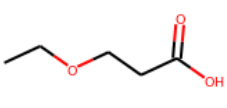
0.062567



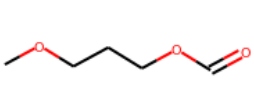
0.068845



0.069994



0.073498



0.073922

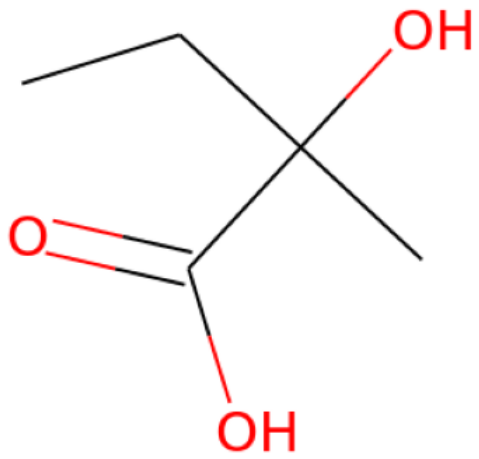
Top predicted substructures	prob		
[CX4H3]	0.9947	[CX4H2]([#6])[#6]	0.9747

[CX4H3][OX2H0]	0.9902	OCC[CH2]	0.968
[#8]=[#6][#8]	0.9882	[CX4H2]([#6])[O]	0.9516
[CX3](=[OX1])C	0.984	[CX3](=[OX1])O	0.9431
[#8][#6][#6H2]	0.9827	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9132

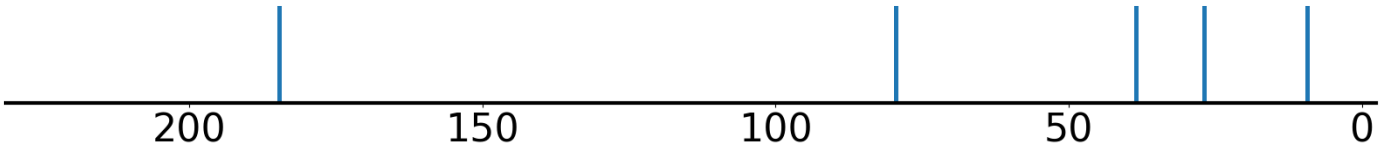
best positives	prob	best negatives	prob
[CX4H3]	0.9947	[#6X2][#6H1][#6X2]	0.0
[CX4H3][OX2H0]	0.9902	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#8]=[#6][#8]	0.9882	CCC#CC#C	0.0
[CX3](=[OX1])C	0.984	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8][#6][#6H2]	0.9827	CC=CC#CC	0.0
[CX4H2]([#6])[#6]	0.9747	CC#CCC#C	0.0
OCC[CH2]	0.968	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[CX4H2]([#6])[O]	0.9516	[#7][#6][#6]#[#7]	0.0
[CX3](=[OX1])O	0.9431	[CX3H1](=[CX3H2])[CX2H0]	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9132	CCC#CCC	0.0

worst negatives	prob	worst positives	prob
[OX2H1]	0.6442	[CX4H2]([OX2H0])[CX4H2]	0.4155
[#6H1]	0.5462	O=C[CH2][CH2]O	0.4215
[CX4H2]([CX4H1])[CX3H0]	0.4867	[CX4H2]CC=O	0.4565
O[CX4H][CX4H2]	0.4474	O=[CX3H0][CX4H2][CX4H2]	0.5104
[CX4H2]([OX2H1])[CX4H2]	0.4127	[CX4H2][CX4H2]	0.636
[#6H1][#6H2]	0.3868	[CH2X4](O)[CX4H2]	0.6647
O=[CX3H0][CX4H2][CX4H1]	0.3527	[#8][#6][#6][#6X3]	0.7787
[#8][#6][#6][#6][#6][#8]	0.3374	[CX4H2][CX3]=O	0.7963
[#6H1]([#6H2])[#6H2]	0.3015	[OX2H0][CX3H0][CX4H2]	0.8028
[#8X2H0][#6X3H0][CX4H2][CX4H1]	0.2812	[CX4H3][OX2H0][CX4H2]	0.8143

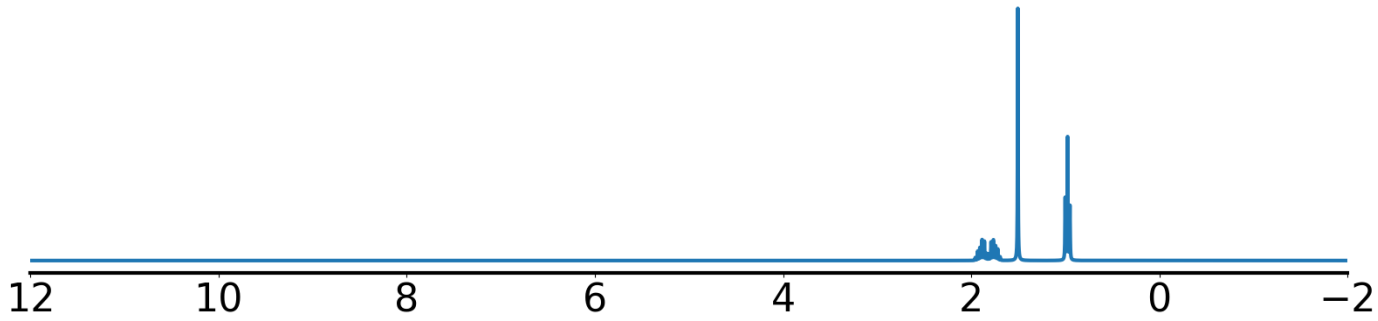
Example 125 true smiles: CCC(C)(O)C(=O)O formula: C5H10O3
Index of correct structure: 0 of 739
True structure loss: 0.009601
True structure:



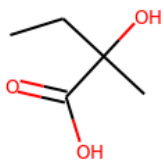
Experimental 13C NMR (solvent: CDCl3)



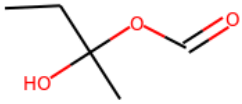
Experimental 1H NMR (solvent: CDCl3)



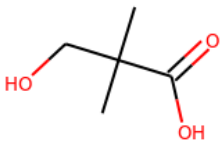
Top predicted structures (loss):



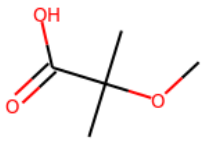
0.009601



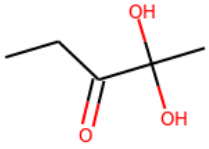
0.046423



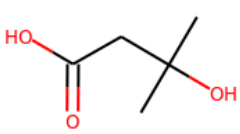
0.061202



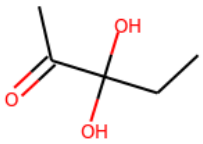
0.06516



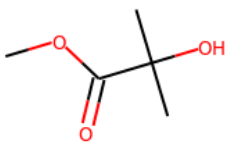
0.065722



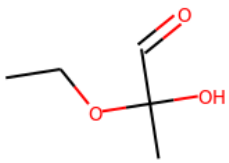
0.0741



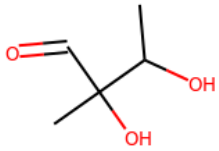
0.07679



0.07681



0.078138



0.078969

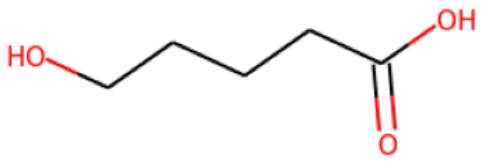
Top predicted substructures	prob		
[#6H3][#6][#6]	1.0	[#8]=[#6][#8]	0.9927

[CX4H3]	0.9999	[#6H3][#6H0]	0.9914
[CX4H3][#6]	0.9998	[CX4H2]([#6])[#6]	0.9913
[OX2H1]	0.9993	[CH3]CC[OH]	0.9907
[CX3](=[OX1])C	0.9988	[CX4H3][CX4H2]	0.9868

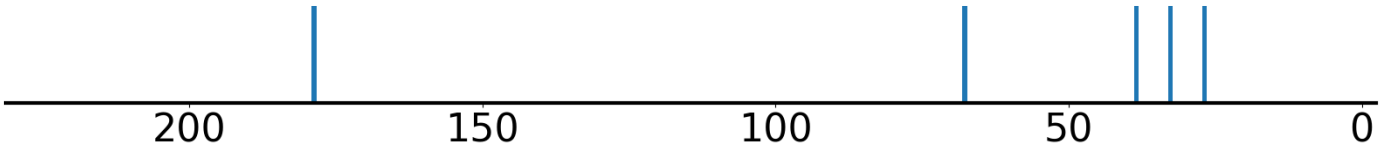
best positives	prob	best negatives	prob
[#6H3][#6][#6]	1.0	CC=CC#CC	0.0
[CX4H3]	0.9999	C=CC=CC#C	0.0
[CX4H3][#6]	0.9998	CCC=CC#C	0.0
[OX2H1]	0.9993	CC#CCC#C	0.0
[CX3](=[OX1])C	0.9988	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8]=[#6][#8]	0.9927	CCC#CC#C	0.0
[#6H3][#6H0]	0.9914	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9913	[#6X2][#6H1][#6X2]	0.0
[CH3]CC[OH]	0.9907	[#7][#6]=[#6][#6]#[#7]	0.0
[CX4H3][CX4H2]	0.9868	[CX2H0](#[CX2H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.6323	[#8][#6][#6][#8]	0.5714
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6148	[CX4H2]CC=O	0.6551
[#6H1]	0.3919	[#6H3][#6][#6][#6H3]	0.711
[#6H1][#6H2]	0.3251	[CX4H2]([CX4H3])[CX4H0]	0.722
[OH][CX4H]	0.3065	[#6H3][#6][#6X3]	0.76
[#8][#6][#6][#6X3]	0.3041	[#8][#6][#6]=[#8]	0.8058
[#8]=[#6H0][#6H1]	0.2186	[#6X3][#6][#6][#6H3]	0.8131
O=[#6][#6H][#6H0]	0.1529	[OX2H1][CX4H0][CX4H2][CX4H3]	0.8562
[#8H][#6X4H1][#6X3H0]	0.1368	[CH3][#6][#8]	0.8638
O[CX4H][CX4H2]	0.1345	[#8][#6][#6H2]	0.8913

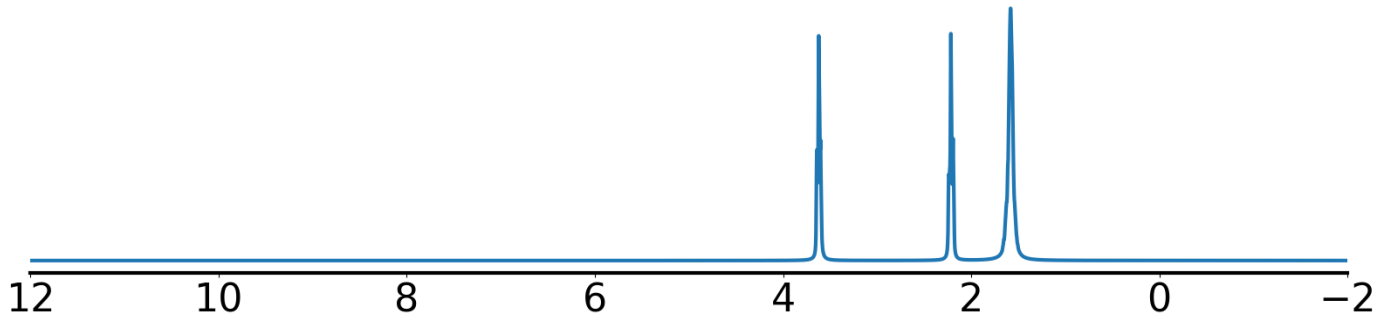
Example 126 true smiles: O=C(O)CCCCO formula: C5H10O3
Index of correct structure: 0 of 739
True structure loss: 0.007485
True structure:



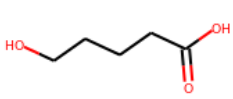
Experimental 13C NMR (solvent: CDCl3)



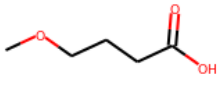
Experimental 1H NMR (solvent: D2O)



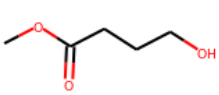
Top predicted structures (loss):



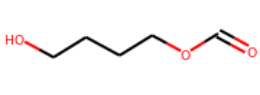
0.007485



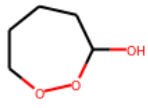
0.046104



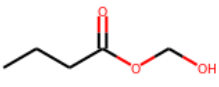
0.048947



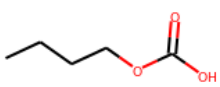
0.07109



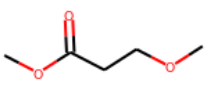
0.076818



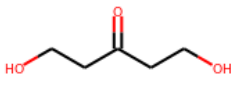
0.08025



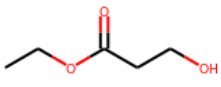
0.080297



0.082838



0.083664



0.083805

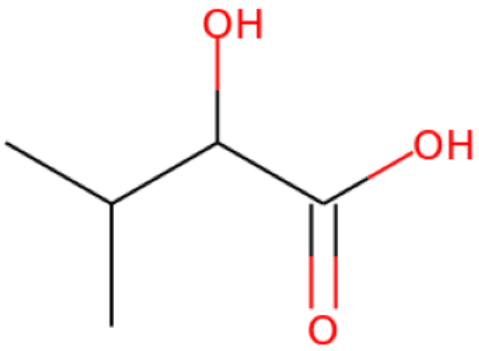
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX3](=[OX1])O	0.9973

[#8]=[#6][#8]	0.9993	[CX4H2][CX4H2]	0.9973
OCC[CH2]	0.9989	[#8][#6][#6H2]	0.997
[OX2H1]	0.9989	[CX4H2]([CX4H2])[CX4H2]	0.9894
[CX3](=[OX1])C	0.9976	O=[CX3H0][CX4H2][CX4H2]	0.9851

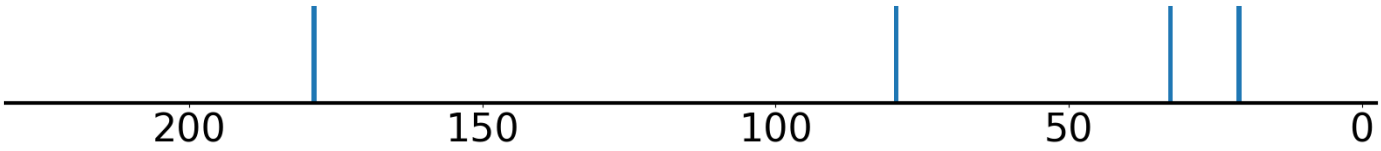
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#8]=[#6][#8]	0.9993	[CX2H0](#[CX2H1])[cX3H0]	0.0
OCC[CH2]	0.9989	CCC#CC#C	0.0
[OX2H1]	0.9989	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9976	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX3](=[OX1])O	0.9973	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2][CX4H2]	0.9973	CC=CC#CC	0.0
[#8][#6][#6H2]	0.997	CCC=CC#C	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9894	CC#CCC#C	0.0
O=[CX3H0][CX4H2][CX4H2]	0.9851	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H1]	0.8182	[CX4H2]([OX2H1])[CX4H2]	0.7688
[#6H1]	0.5007	[CH2X4](O)[CX4H2]	0.8153
[#6H1][#6H2]	0.4171	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.8454
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3302	[CX4H2]CC=O	0.8848
CCCCCC	0.3113	[CX4H2][CX3]=O	0.8888
[#8][#6][#6][#6][#6][#8]	0.2269	[CH2X4](O)[CX4H2][CX4H2]	0.9355
[#8H][#6H2][#6H1]	0.1407	[CX4H2]([CX4H2])[CX3H0]	0.9543
[OX2H0][CX3H0][CX4H2]	0.1292	[CX4H2]([#6])[O]	0.9638
[#8][#6][#6][#6][#6]=[#8]	0.126	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9759
[#8]=[#6H0][#6H1]	0.1064	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9799

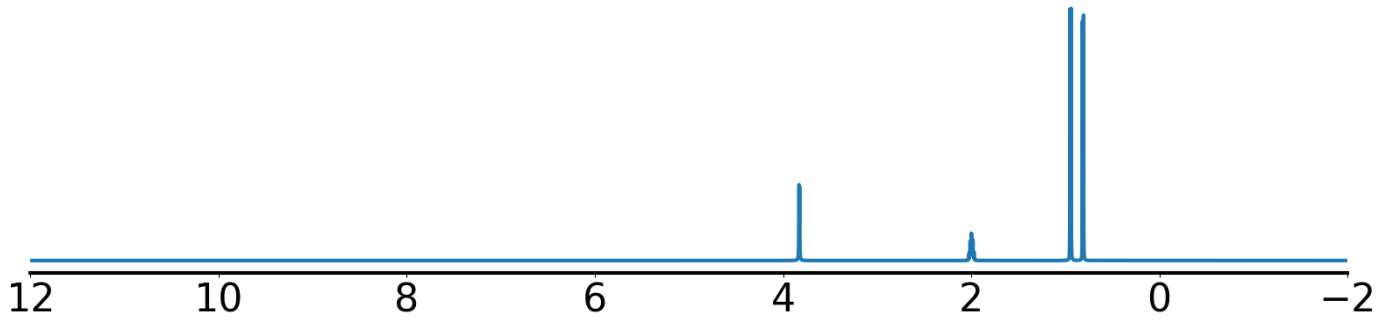
Example 127 true smiles: CC(C)C(O)C(=O)O formula: C5H10O3
Index of correct structure: 0 of 739
True structure loss: 0.011302
True structure:



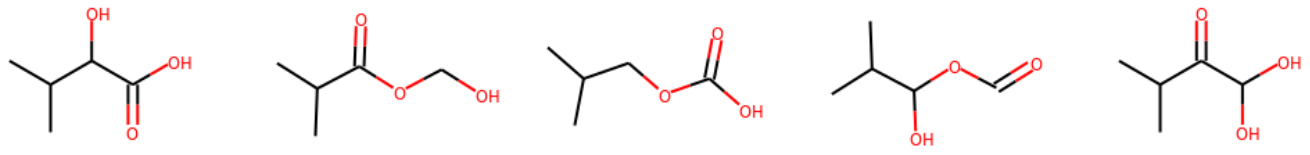
Experimental 13C NMR (solvent: DMSO)



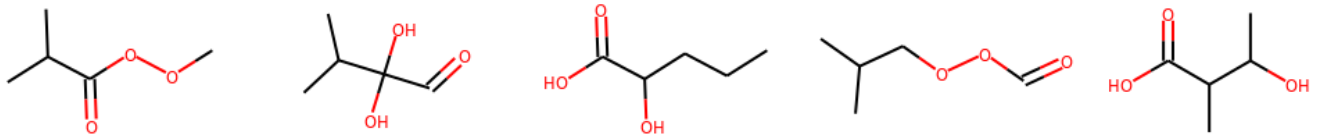
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.011302 0.050509 0.061464 0.062112 0.06217



0.063761 0.070679 0.072699 0.077151 0.079581

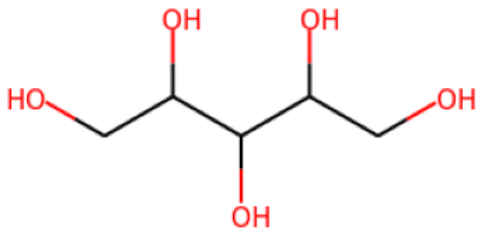
Top predicted substructures	prob		
[#6H3][#6][#6]	0.9999	[CX3](=[OX1])C	0.996

[CX4H3]	0.9998	[CX3](=[OX1])O	0.9949
[CX4H3][#6]	0.9997	[OX2H1]	0.9937
[#8]=[#6][#8]	0.9985	[CHX4]([CH3X4])[CH3X4]	0.9933
[#6H1]	0.9981	[CX3](=O)[OX2H1]	0.9722

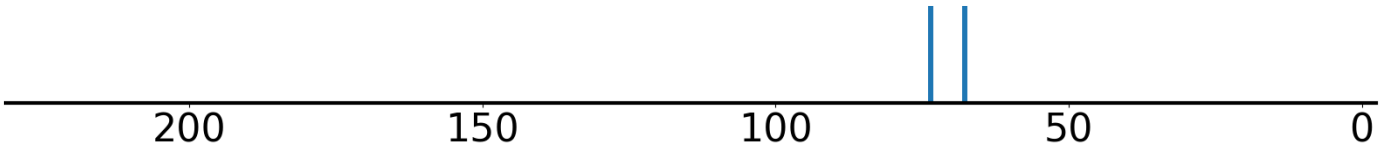
best positives	prob	best negatives	prob
[#6H3][#6][#6]	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3]	0.9998	CC#CCC#C	0.0
[CX4H3][#6]	0.9997	CCC#CC#C	0.0
[#8]=[#6][#8]	0.9985	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6H1]	0.9981	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX3](=[OX1])C	0.996	CCC=CC#C	0.0
[CX3](=[OX1])O	0.9949	CC=CC#CC	0.0
[OX2H1]	0.9937	[#6X2][#6H1][#6X2]	0.0
[CHX4]([CH3X4])[CH3X4]	0.9933	CCC#CC=C	0.0
[CX3](=O)[OX2H1]	0.9722	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H2]	0.5933	[#8][#6H1][#6H1]	0.3302
[CHX4]([CH3X4])[CH2X4]	0.2751	[#6H1][#6H1]	0.4853
[#8][#6][#6H2]	0.2661	[OH][CX4H]	0.5715
[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.254	[#8]=[#6][#6H1][#6H1]	0.6868
OCC[CH2]	0.2407	[CX4H]O	0.6907
[CX4H1]([OX2H1])([CX4H2])[CX3H0]	0.2365	[#8]=[#6H0][#6H1]	0.7058
[CX4H2]CC=O	0.2329	[#8][#6H0][#6H1]	0.7568
[#8][#6][#6][#6X3]	0.197	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.7572
[CX4H2][CX3]=O	0.1727	[CH3]CC[OH]	0.7739
[CH3][#6][#8]	0.1348	O=[CX3][CX4H]	0.776

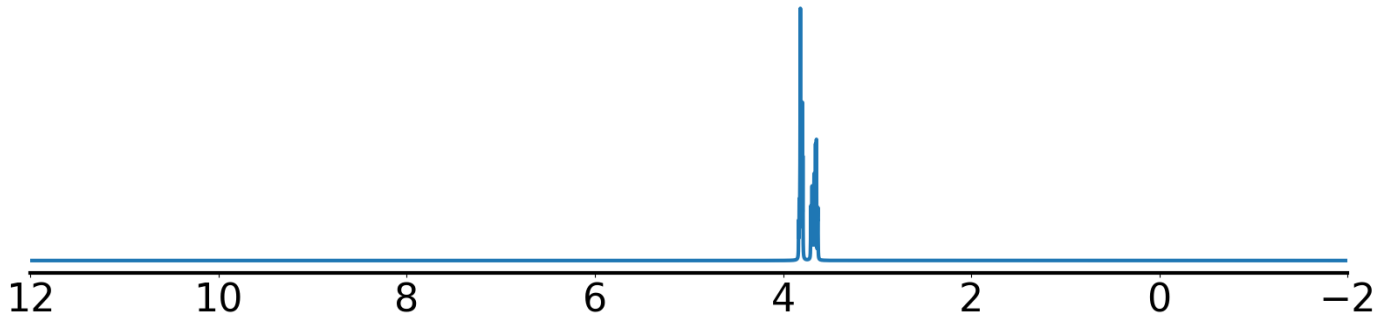
Example 128 true smiles: OCC(O)C(O)C(O)CO formula: C5H12O5
Index of correct structure: 0 of 734
True structure loss: 0.010997
True structure:



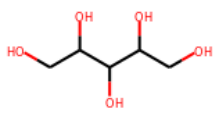
Experimental 13C NMR (solvent: D2O)



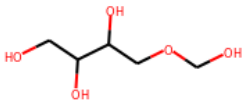
Experimental 1H NMR (solvent: D2O)



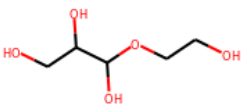
Top predicted structures (loss):



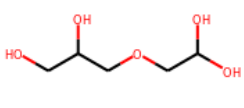
0.010997



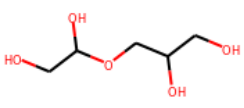
0.013642



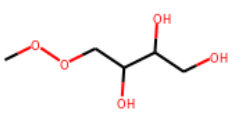
0.019935



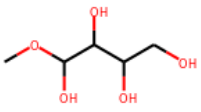
0.022565



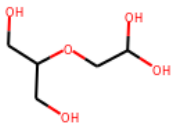
0.022975



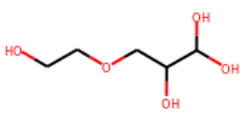
0.022978



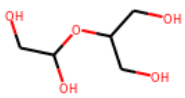
0.023036



0.024061



0.024443



0.025249

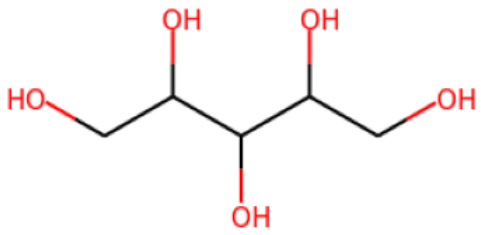
Top predicted substructures	prob		
[OX2H1]	0.9997	[CX4H2]([#6])[O]	0.9862

[#8][#6][#6][#8]	0.9966	[CX4H]O	0.9561
[#8][#6][#6H2][#8]	0.9958	OCC[CH2]	0.9414
[CX4H](O)CO	0.9954	[#6H1]	0.9312
[#8][#6][#6H2]	0.9884	O[CX4H][CX4H2]	0.9255

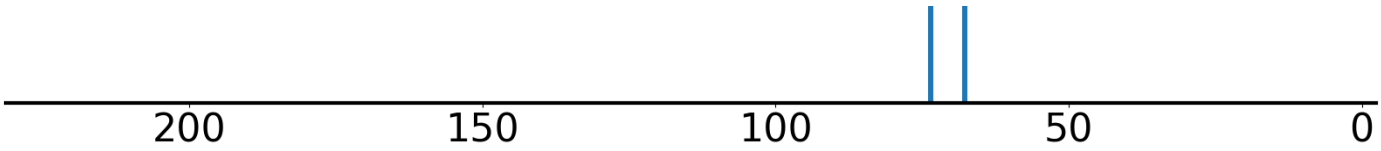
best positives	prob	best negatives	prob
[OX2H1]	0.9997	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6][#8]	0.9966	CC#CCC=C	0.0
[#8][#6][#6H2][#8]	0.9958	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H](O)CO	0.9954	CC=CC#CC	0.0
[#8][#6][#6H2]	0.9884	[CX3H0][CX4H2][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[O]	0.9862	CC=CCC#C	0.0
[CX4H]O	0.9561	[#7][#6][#6]#[#7]	0.0
OCC[CH2]	0.9414	C=CCCC#C	0.0
[#6H1]	0.9312	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
O[CX4H][CX4H2]	0.9255	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX4H2]	0.4875	[#6X4H1][#6X4H1][#6X4H1]	0.2404
[#6H2][#6H1][#6H1][#6H2]	0.3715	[CX4H](O)([CH])[CH]	0.2744
[CH2X4](O)[CX4H2]	0.3071	[CX4H1]([OX2H1])([CX4H1])[CX4H1]	0.4353
[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.2426	[#8][#6][#6][#6][#6][#8]	0.4735
[CX4H2]([OX2H0])[CX4H2]	0.2124	[#8][#6H1][#6H1]	0.4889
[#6H1]([#6H2])[#6H2]	0.159	[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.6617
[CX4H2]([OX2H0])[CX4H1]	0.1416	[#6H1][#6H1]	0.7223
[OX2H0][CX4H2][CX4H1][CX4H2]	0.0988	[CX4H2]([OX2H1])[CX4H1]	0.7763
O[CX4H2][CX4H2]O	0.0701	[OX2H1][CX4H1][CX4H1][OX2H1]	0.7805
[CX4H2][OX2H0][CX4H2]	0.07	O[CX4H]([CX4H2])[CX4H1]	0.7868

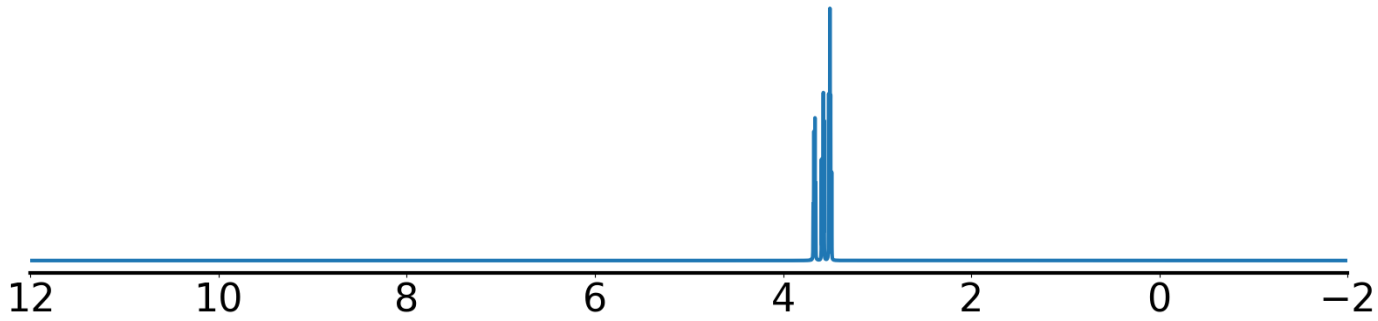
Example 129 true smiles: OCC(O)C(O)C(O)CO formula: C5H12O5
Index of correct structure: 0 of 734
True structure loss: 0.012278
True structure:



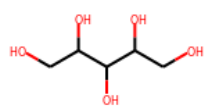
Experimental 13C NMR (solvent: D2O)



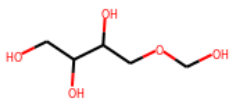
Experimental 1H NMR (solvent: D2O)



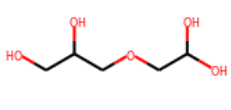
Top predicted structures (loss):



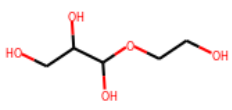
0.012278



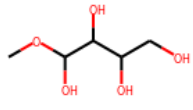
0.015361



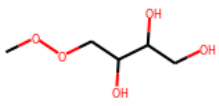
0.022517



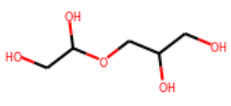
0.022808



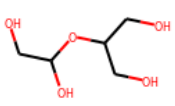
0.023509



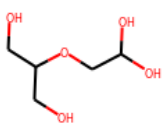
0.024467



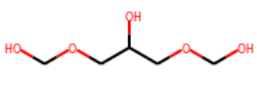
0.024473



0.025082



0.025642



0.026691

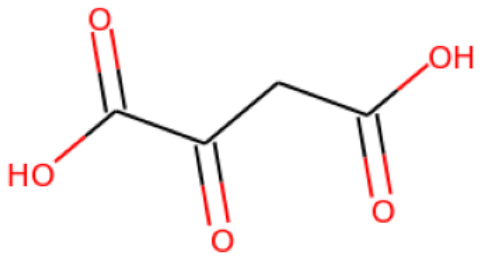
Top predicted substructures	prob		
[OX2H1]	0.9997	[#8][#6][#6H2]	0.9788

[#8][#6][#6][#8]	0.9952	[CX4H2](O)[CHX4]	0.8962
[#8][#6][#6H2][#8]	0.9941	[#8H][#6H2][#6H1]	0.894
[CX4H2]([#6])[O]	0.9927	[CX4H2]([OX2H1])[CX4H1]	0.8655
[CX4H](O)CO	0.9808	OCC[CH2]	0.8429

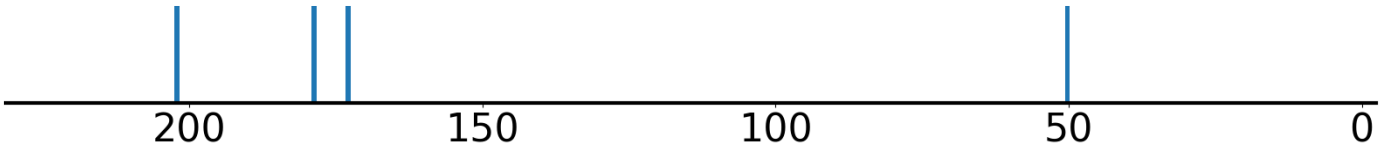
best positives	prob	best negatives	prob
[OX2H1]	0.9997	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6][#8]	0.9952	CC=CCC#C	0.0
[#8][#6][#6H2][#8]	0.9941	CC=CC#CC	0.0
[CX4H2]([#6])[O]	0.9927	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H](O)CO	0.9808	CCC#CC=C	0.0
[#8][#6][#6H2]	0.9788	[CX3H0][CX4H2][CX3H1]=[CX3H0]	0.0
[CX4H2](O)[CHX4]	0.8962	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
[#8H][#6H2][#6H1]	0.894	C=CCCC#C	0.0
[CX4H2]([OX2H1])[CX4H1]	0.8655	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
OCC[CH2]	0.8429	CC#CCC=C	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX4H2]	0.3729	[#6X4H1][#6X4H1][#6X4H1]	0.1873
[#6H2][#6H1][#6H1][#6H2]	0.3319	[CX4H](O)([CH])[CH]	0.3487
[CH2X4](O)[CX4H2]	0.2954	[#8][#6H1][#6H1]	0.4164
[#6H1]([#6H2])[#6H2]	0.2299	[CX4H1]([OX2H1])([CX4H1])[CX4H1]	0.4488
[CX4H2]([OX2H0])[CX4H2]	0.2114	[#8][#6][#6][#6][#6][#8]	0.5216
[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.1435	[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.5363
[CX4H2][OX2H0][CX4H2]	0.1157	[#6H1][#6H1]	0.5527
[#8][#6H2][#6H0][#6H2][#8]	0.103	[#6X4H2][#6H1][#8H]	0.6557
O[CX4H2][CX4H2]O	0.0868	O[CX4H]([CX4H2])[CX4H1]	0.6767
[CX4H2]([OX2H0])[CX4H1]	0.0748	[OX2H1][CX4H1][CX4H1][OX2H1]	0.7484

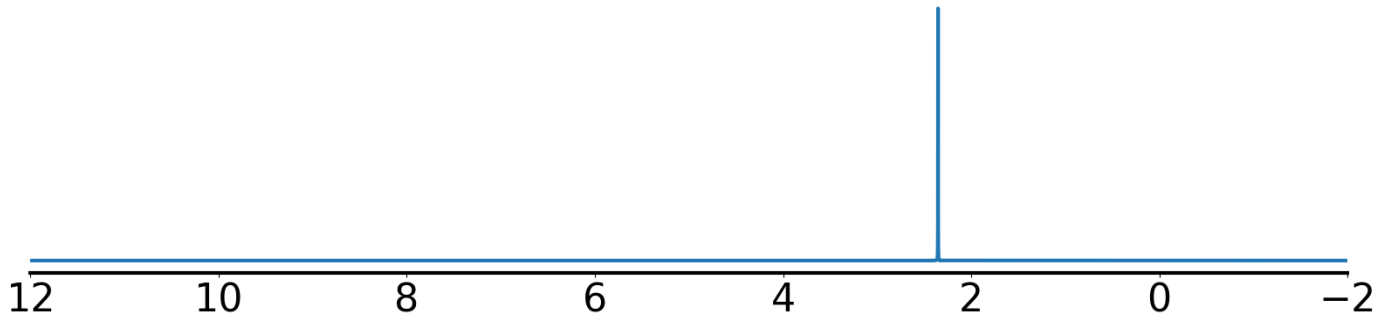
Example 130 true smiles: O=C(O)CC(=O)C(=O)O formula: C4H4O5
Index of correct structure: 0 of 729
True structure loss: 0.025576
True structure:



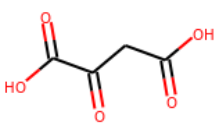
Experimental 13C NMR (solvent: D2O)



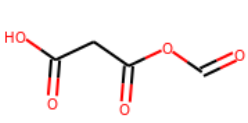
Experimental 1H NMR (solvent: D2O)



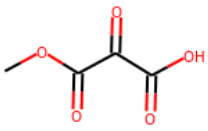
Top predicted structures (loss):



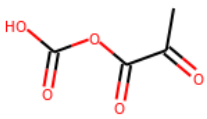
0.025576



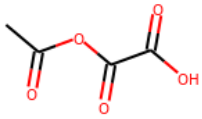
0.04397



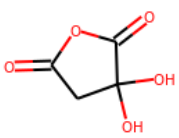
0.05027



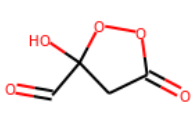
0.052274



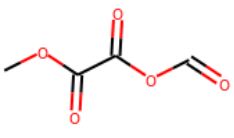
0.062491



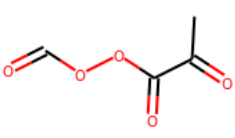
0.065158



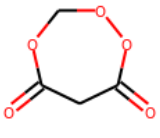
0.065795



0.069105



0.070087



0.070771

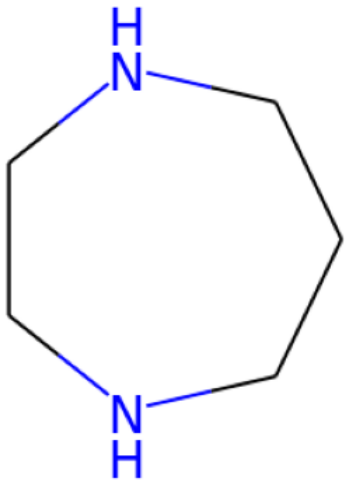
Top predicted substructures	prob		
[CX3](=[OX1])C	0.9999	[OX2H1]	0.8852

[CX3](=[OX1])O	0.999	[#6X3][#6X3]	0.8842
[#8]=[#6][#8]	0.9974	[#8]=[#6][#6]=[#8]	0.8829
[CX4H3]	0.9562	O=CC=O	0.8771
[#8X1]=[#6X3][#6H2][#6H0]	0.9017	[CX4H2][CX3]=O	0.8736

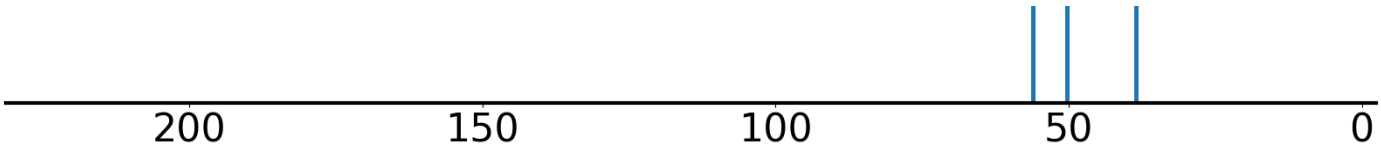
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9999	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX3](=[OX1])O	0.999	CC#CCC=C	0.0
[#8]=[#6][#8]	0.9974	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#8X1]=[#6X3][#6H2][#6H0]	0.9017	CC#CCC#C	0.0
[OX2H1]	0.8852	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6X3][#6X3]	0.8842	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#8]=[#6][#6]=[#8]	0.8829	CCC#CC#C	0.0
O=CC=O	0.8771	CC=CC#CC	0.0
[CX4H2][CX3]=O	0.8736	[CX4H1]([CX4H1])([CX4H1])[CX4H0]	0.0
O=[#6][#6][#6X3]	0.8399	[#6X2][#6H1][#6X2]	0.0

worst negatives	prob	worst positives	prob
[CX4H3]	0.9562	[#8][#6][#6][#6][#6][#8]	0.0311
[#6H3][#6H0]	0.7074	OCC[CH2]	0.2489
[#6H3][#6][#6]	0.5015	[CX4H2]CC=O	0.3009
[#6X3][#6][#6][#6H3]	0.4794	[#8][#6][#6][#6][#6]=[#8]	0.3196
[CX4H3][#6]	0.3592	[#8][#6][#6]=[#8]	0.3571
[OX2H0][CX3H0][CX4H2]	0.3371	[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.5088
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.321	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.575
[CX4H3][CX3]	0.3208	[CX3H0](=[OX1H0])([CX4H2])[CX3H0]	0.5817
[#8][#6H0][#6H1]	0.223	[CX4H2]([#6])[#6]	0.7039
[OX1H0]=[CX3H0][CX4H3]	0.1903	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.7233

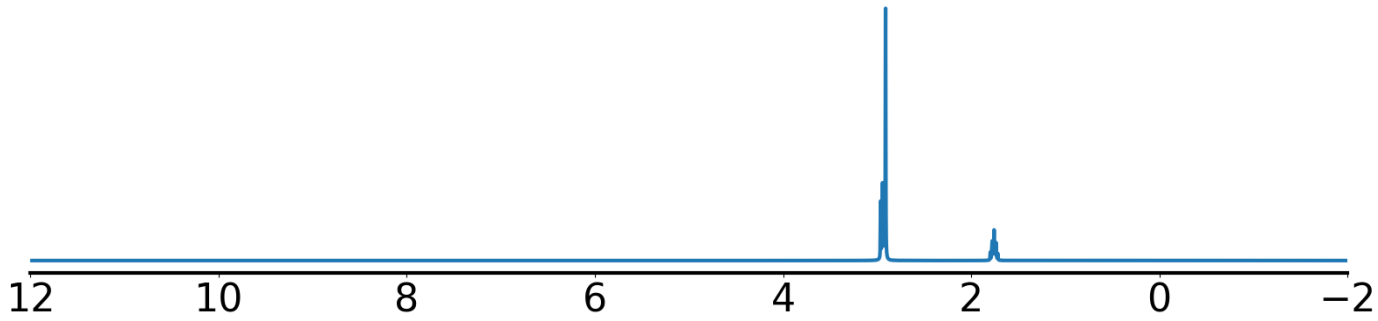
Example 131 true smiles: C1CNCCNC1 formula: C5H12N2
Index of correct structure: 0 of 619
True structure loss: 0.012311
True structure:



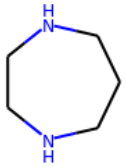
Experimental 13C NMR (solvent: CDCl3)



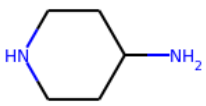
Experimental 1H NMR (solvent: CDCl3)



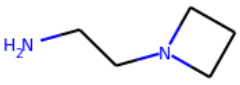
Top predicted structures (loss):



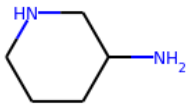
0.012311



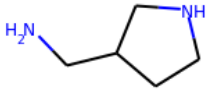
0.023138



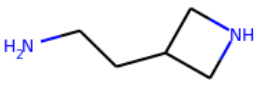
0.023454



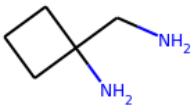
0.027873



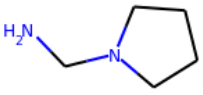
0.028366



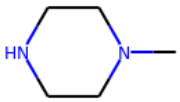
0.030343



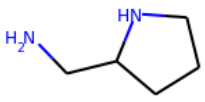
0.033374



0.033552



0.034828



0.035725

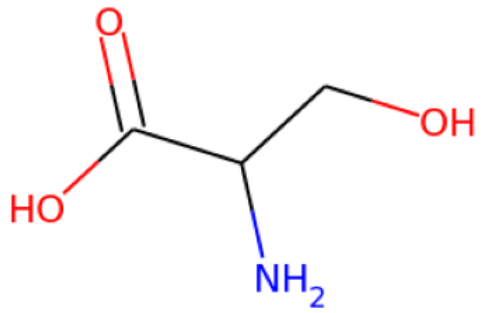
Top predicted substructures	prob		
[#7X3][#6H2]	0.9729	[CX4H2][CX4H2]	0.8451

[CX4H2]([#6])[#6]	0.9663	[#6H2][#7][#6H2]	0.7754
[#7][#6H2]	0.9604	[CX4H2]([NX3H1])[CX4H2]	0.7481
[#7][#6H2][#6H2]	0.9363	[#7X3H1]	0.7274
[#7][#6H2][#6H2][#7]	0.8547	[#7X3H2]	0.6358

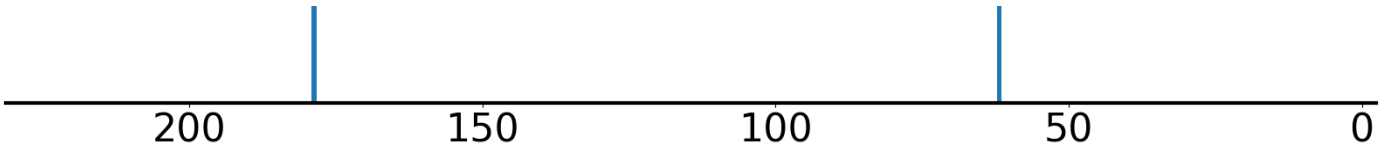
best positives	prob	best negatives	prob
[#7X3][#6H2]	0.9729	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9663	[CX3H0](=[CX3H2])([OX2H0])[CX3H0]	0.0
[#7][#6H2]	0.9604	[OX2H0][CX3H1]=[#6X3H0][#8X2H0]	0.0
[#7][#6H2][#6H2]	0.9363	[CX3H2]=[#6X3H0][#6X3H0][#8X2H0]	0.0
[#7][#6H2][#6H2][#7]	0.8547	C=CC=CC#C	0.0
[CX4H2][CX4H2]	0.8451	C=CCCC#C	0.0
[#6H2][#7][#6H2]	0.7754	[#8]1[#6][#6]=[#6][#6]=[#6]1	0.0
[CX4H2]([NX3H1])[CX4H2]	0.7481	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[#7X3H1]	0.7274	CC=CC#CC	0.0
[#7][#6][#6][#7]	0.6099	[CX4H1]([OX2H0])([CX3H1])[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[#7X3H2]	0.6358	[CX4H2]([CX4H2])[CX4H2]	0.3753
[#6H1]([#6H2])[#6H2]	0.4555	[#7][#6][#6][#6][#7]	0.5167
[#6H1][#6H2]	0.399	[#7][#6][#6][#7]	0.6099
[CX4H2]([NX3H1])[CX4H1]	0.39	[#7X3H1]	0.7274
[#7][#6][#6][#6][#6][#7]	0.3829	[CX4H2]([NX3H1])[CX4H2]	0.7481
[#6H1]	0.3811	[#6H2][#7][#6H2]	0.7754
[#7H2][#6H2]	0.3281	[CX4H2][CX4H2]	0.8451
[CX4H3]	0.2858	[#7][#6H2][#6H2][#7]	0.8547
[CX4H2]([CX4H2])[CX4H1]	0.2241	[#7][#6H2][#6H2]	0.9363
[#7H2][#6H1]	0.2211	[#7][#6H2]	0.9604

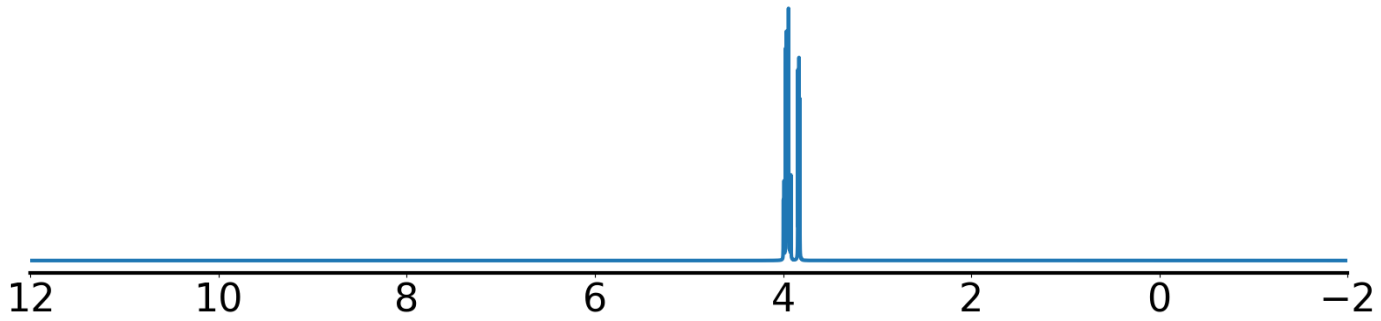
Example 132 true smiles: NC(CO)C(=O)O formula: C3H7NO3
Index of correct structure: 0 of 576
True structure loss: 0.021597
True structure:



Experimental 13C NMR (solvent: D2O)

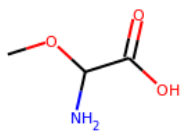


Experimental 1H NMR (solvent: D2O)

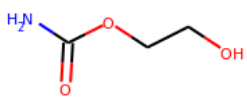


Top predicted structures (loss):

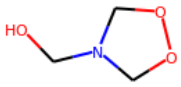
0.021597



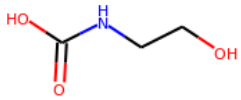
0.036092



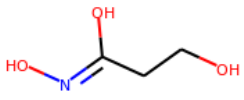
0.041058



0.04681

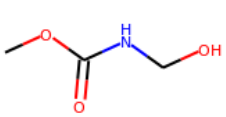


0.049029

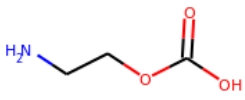


0.049246

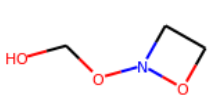
0.05125



0.051951



0.053941



0.054471

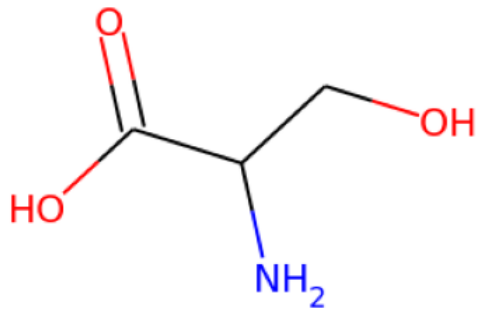
Top predicted substructures	prob		
[CX3](=[OX1])C	0.9709	[CX3](=[OX1])O	0.824

[OX2H1]	0.9666	[#8]=[#6H0][#6H1]	0.8081
[#8]=[#6][#8]	0.8923	O=[CX3][CX4H]	0.7797
[CX4H2]([#6])[O]	0.864	[#7X3H2]	0.7683
[CX3](=O)[OX2H1]	0.8283	[CX4H2]CC=O	0.7541

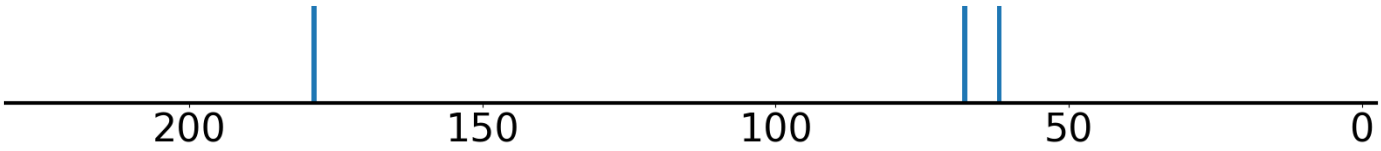
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9709	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9666	CC=CCC#C	0.0
[#8]=[#6][#8]	0.8923	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H2]([#6])[O]	0.864	CC=CC#CC	0.0
[CX3](=O)[OX2H1]	0.8283	[CX4H2]([CX4H3])[CX2H0]	0.0
[CX3](=[OX1])O	0.824	[#6H2][#6]#[#6X2]	0.0
[#8]=[#6H0][#6H1]	0.8081	[#6X3][#6]#[#6][#6H3]	0.0
O=[CX3][CX4H]	0.7797	[#6X2][#6H1][#6X2]	0.0
[#7X3H2]	0.7683	[CX2H0](#[CX2H0])[CX4H0]	0.0
[CX4H2]CC=O	0.7541	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.5467	[#8][#6H0][#6H1]	0.1484
[#7H2][#6H0]	0.3305	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.2368
[CX4H2]([OX2H1])[CX4H2]	0.3033	OCC[CH2]	0.2631
[#8][#6][#6][#8]	0.2452	[#6H1][#6H2]	0.3436
[CH2X4](O)[CX4H2]	0.2288	[CX4H2](O)[CHX4]	0.3481
[#7][#6H0][#6H1]	0.2254	[#8][#6H2][#6H][#6X3]	0.4181
[#7X3H1]	0.2071	[#8][#6][#6][#6X3]	0.419
[CX4H2][CX3]=O	0.2015	[CX4H2]([OX2H1])[CX4H1]	0.4192
[CX4H2][CX4H2]	0.1807	[#7][#6][#6X3]	0.5001
[#8]=[#6][#6H1][#6H1]	0.1802	[#7H2][#6H1]	0.5054

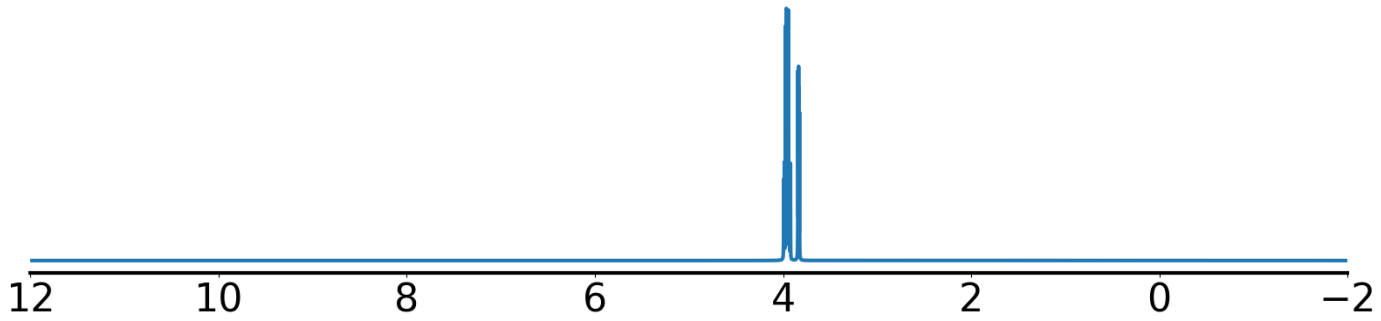
Example 133 true smiles: NC(CO)C(=O)O formula: C3H7NO3
Index of correct structure: 0 of 576
True structure loss: 0.023511
True structure:



Experimental 13C NMR (solvent: D2O)

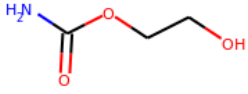


Experimental 1H NMR (solvent: d2o)

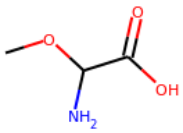


Top predicted structures (loss):

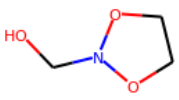
0.023511



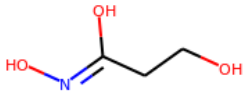
0.034598



0.04088



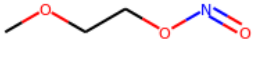
0.048102



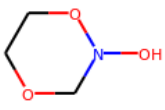
0.048228

0.048606

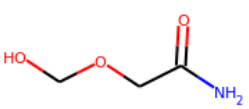
0.050717



0.052142



0.05223



0.05311

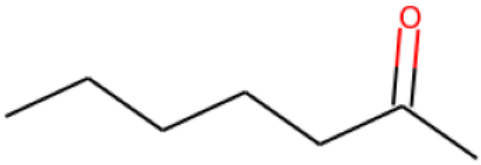
Top predicted substructures	prob		
[CX4H2]([#6])[O]	0.9831	[#7X3H2]	0.7948

[OX2H1]	0.9727	[#8]=[#6H0][#6H1]	0.7874
[CX3](=[OX1])C	0.9698	O=[CX3][CX4H]	0.7708
[#8]=[#6][#8]	0.8216	[#8][#6H2][#6H1][#6H0]	0.7487
[CX4H2]CC=O	0.7985	[#8H][#6H2][#6H1]	0.7033

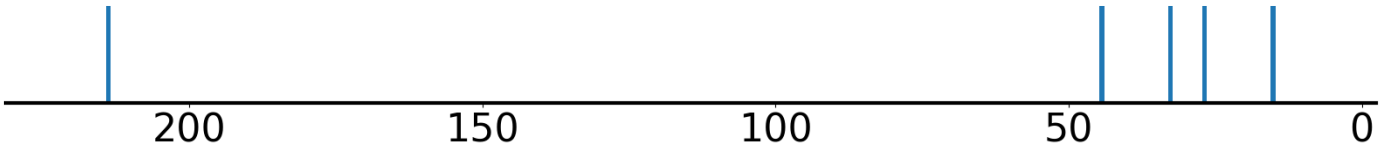
best positives	prob	best negatives	prob
[CX4H2]([#6])[O]	0.9831	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9727	CC=CCC#C	0.0
[CX3](=[OX1])C	0.9698	CC=CC#CC	0.0
[#8]=[#6][#8]	0.8216	[CX4H2]([CX4H3])[CX2H0]	0.0
[CX4H2]CC=O	0.7985	[#6X2][#6H1][#6X2]	0.0
[#7X3H2]	0.7948	[#6X3][#6]#[#6][#6H3]	0.0
[#8]=[#6H0][#6H1]	0.7874	[#6H2][#6]#[#6X2]	0.0
O=[CX3][CX4H]	0.7708	[CX4H2]([CX4H0])[CX2H0]	0.0
[#8][#6H2][#6H1][#6H0]	0.7487	CCC#CC=C	0.0
[#8H][#6H2][#6H1]	0.7033	[CX2H0](#[CX2H1])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.6953	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.1569
[#7H2][#6H0]	0.4281	[#8][#6H0][#6H1]	0.2227
[#8][#6][#6][#8]	0.4152	[#6H1][#6H2]	0.407
[CX4H2][CX4H2]	0.4071	[#7H2][#6H1]	0.4298
O[CX4H2][CX4H2]O	0.4031	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.436
[CH2X4](O)[CX4H2]	0.3962	[#8][#6][#6][#6X3]	0.4564
[#8][#6][#6H2][#8]	0.3961	OCC[CH2]	0.4856
[CX4H2]([OX2H0])[CX4H2]	0.3322	[CX4H2](O)[CHX4]	0.4961
[#8][#6][#6]=[#8]	0.2676	[#7][#6][#6X3]	0.5293
[OX2H0][CX4H2][CX4H2][OX2H0]	0.2431	[#7H2][#6X4H1][#6X3]	0.5381

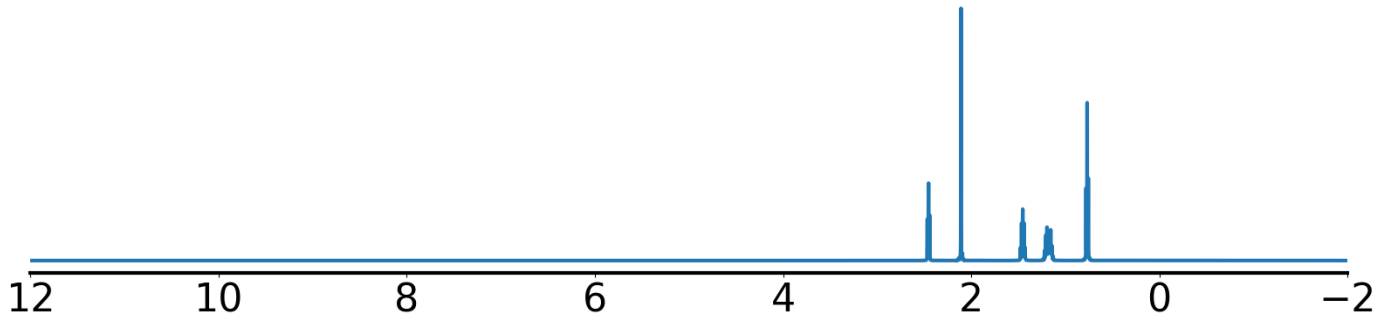
Example 134 true smiles: CCCCCC(C)=O formula: C7H14O
Index of correct structure: 0 of 556
True structure loss: 0.006778
True structure:



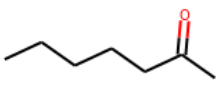
Experimental 13C NMR (solvent: CDCl3)



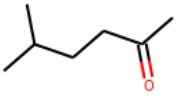
Experimental 1H NMR (solvent: D2O)



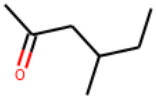
Top predicted structures (loss):



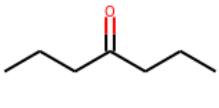
0.006778



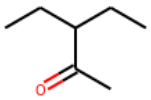
0.034776



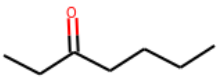
0.035885



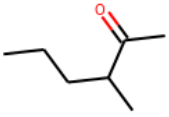
0.049086



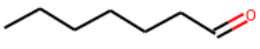
0.054234



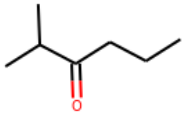
0.060119



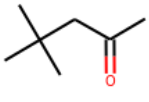
0.061917



0.067532



0.072748



0.079484

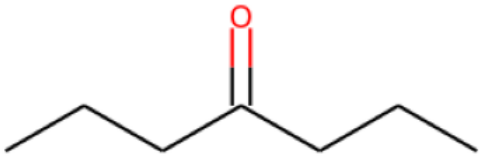
Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][CX4H2]	0.9995

[CX4H2]([#6])[#6]	0.9999	[CX4H3][CX3H0]	0.9992
[#6H3][#6][#6]	0.9999	[CX4H3][CX3]	0.9989
[CX3](=[OX1])C	0.9997	[OX1H0]=[CX3H0][CX4H3]	0.9987
[CX4H3][#6]	0.9996	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9769

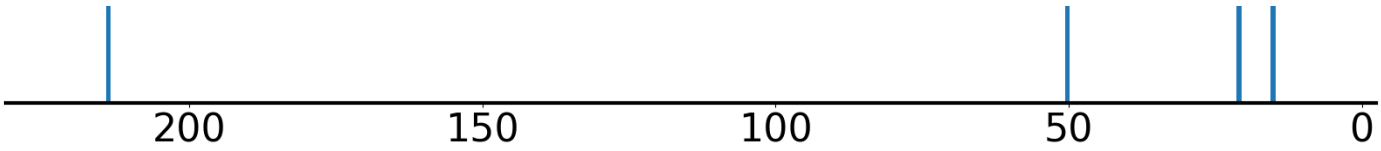
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	0.9999	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9999	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9997	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][#6]	0.9996	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CX4H3][CX4H2]	0.9995	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][CX3H0]	0.9992	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
[CX4H3][CX3]	0.9989	[#6X2][#6H1][#6X2]	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9987	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9769	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.4646	[CX4H2][CX4H2][CX4H2][CX4H2]	0.4765
[#6H1][#6H2]	0.4448	[CX4H2]([CX4H2])[CX4H2]	0.6509
[CX4H2]([CX4H1])[CX3H0]	0.3074	[CX4H2][CX4H2]	0.7293
[CX4H2]([CX4H3])[CX4H1]	0.2626	[CX4H2]([CX4H2])[CX3H0]	0.7635
[#6X3][#6][#6][#6H3]	0.2416	O=[CX3H0][CX4H2][CX4H2]	0.807
[#6H1]([#6H2])[#6H2]	0.2262	[CX4H2]CC=O	0.8609
O=[CX3H0][CX4H2][CX4H1]	0.1597	[CX4H2]([CX4H3])[CX4H2]	0.8841
[#6H3][#6][#6][#6H3]	0.1377	CCCCCC	0.9076
[#8]=[#6][#6H2][#6H1]	0.1072	[#6H3][#6X3H0][#6H2]	0.9153
[#6H3][#6][#6X3]	0.1032	[CX4H2][CX3]=O	0.9182

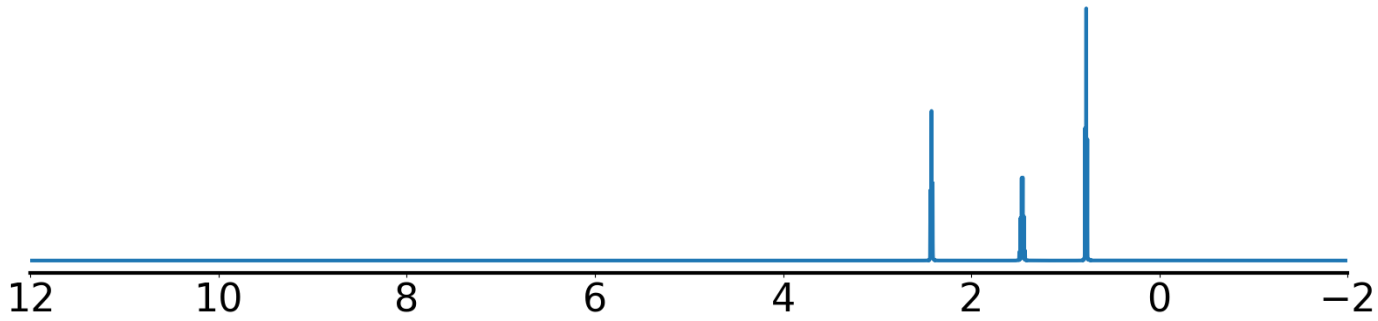
Example 135 true smiles: CCCC(=O)CCC formula: C7H14O
Index of correct structure: 0 of 556
True structure loss: 0.008486
True structure:



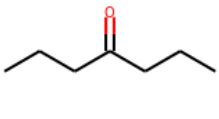
Experimental 13C NMR (solvent: CDCl3)



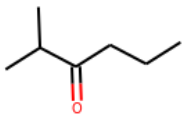
Experimental 1H NMR (solvent: D2O)



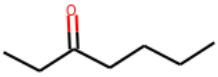
Top predicted structures (loss):



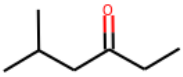
0.008486



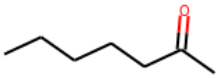
0.023597



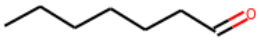
0.026207



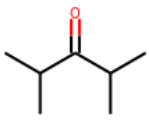
0.041165



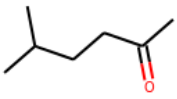
0.044167



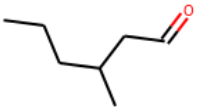
0.049743



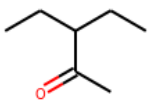
0.054679



0.05568



0.057693



0.058936

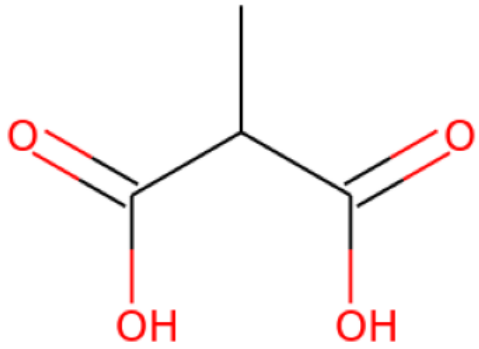
Top predicted substructures	prob		
[CX4H3][#6]	0.9999	[CX4H3][CX4H2]	0.9976

[CX4H3]	0.9998	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9847
[CX3](=[OX1])C	0.9997	[CX4H2]([CX4H3])[CX4H2]	0.9812
[CX4H2]([#6])[#6]	0.9994	[CX4H2][CX3]=O	0.8176
[#6H3][#6][#6]	0.9984	[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.816

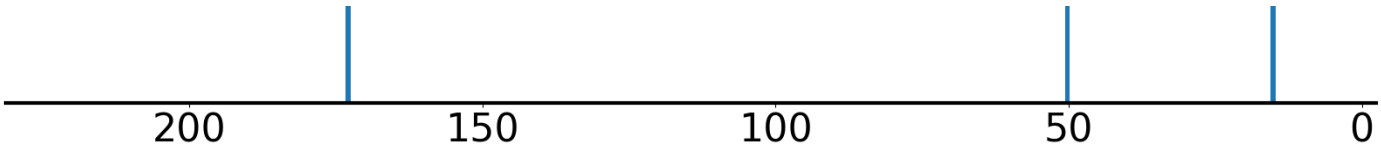
best positives	prob	best negatives	prob
[CX4H3][#6]	0.9999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	0.9998	CCC#CC#C	0.0
[CX3](=[OX1])C	0.9997	C=CC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9994	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9984	[CX2H0](#[NX1H0])[CX3H1]	0.0
[CX4H3][CX4H2]	0.9976	[#6X2][#6H1][#6X2]	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9847	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([CX4H3])[CX4H2]	0.9812	[CX2H1]#[CX2H0][CX4H1][OX2H1]	0.0
[CX4H2][CX3]=O	0.8176	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.816	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.4277	CCCCCC	0.5148
[CX4H3][CX4H1]	0.3791	[CX4H2]CC=O	0.6151
[#8]=[#6][#6H2][#6H1]	0.3503	O=[CX3H0][CX4H2][CX4H2]	0.6251
[#8]=[#6H0][#6H1]	0.2882	[CX4H2]([CX4H2])[CX3H0]	0.6543
[#6H1][#6H2]	0.2499	[#6H2][#6X3H0][#6H2]	0.6727
[#6H1]([#6H2])[#6H2]	0.2318	[CX4H2][CX4H2]	0.749
[#6H3][#6][#6X3]	0.2245	[#6X3][#6][#6][#6H3]	0.7993
[CX3H1](=[OX1H0])[CX4H2]	0.1605	[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.816
O=[CX3][CX4H]	0.1579	[CX4H2][CX3]=O	0.8176
[CHX4]([CH3X4])[CH3X4]	0.1528	[CX4H2]([CX4H3])[CX4H2]	0.9812

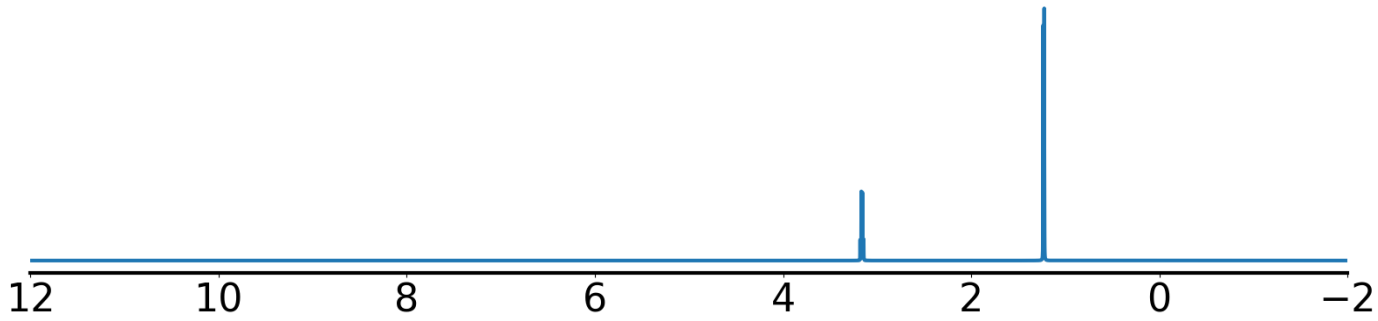
Example 136 true smiles: CC(C(=O)O)C(=O)O formula: C4H6O4
Index of correct structure: 0 of 502
True structure loss: 0.015123
True structure:



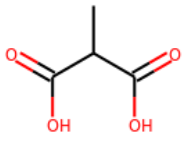
Experimental 13C NMR (solvent: DMSO)



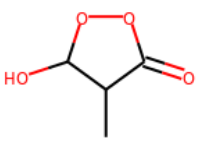
Experimental 1H NMR (solvent: D2O)



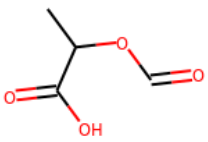
Top predicted structures (loss):



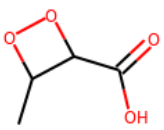
0.015123



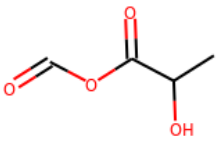
0.036391



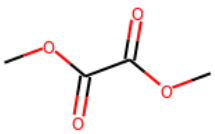
0.059477



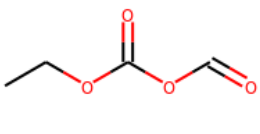
0.062217



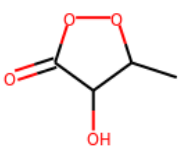
0.064527



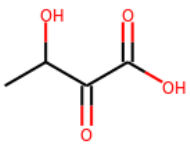
0.067327



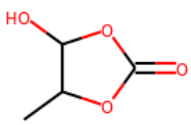
0.067581



0.068625



0.069131



0.070913

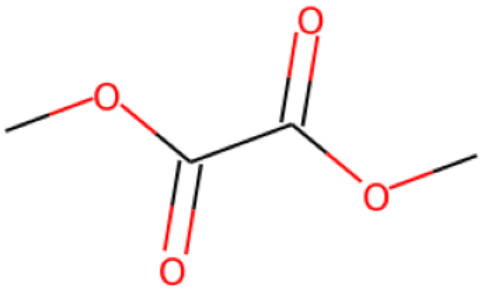
Top predicted substructures	prob		
[CX4H3]	0.9995	[#6H1]	0.9596

[#8]=[#6][#8]	0.9982	[OX2H1]	0.9491
[CX3](=[OX1])O	0.9972	[CX3](=O)[OX2H1]	0.8703
[CX3](=[OX1])C	0.9945	[CX4H3][#6]	0.8499
[#6H3][#6][#6]	0.9752	[#8][#6H0][#6H1]	0.8234

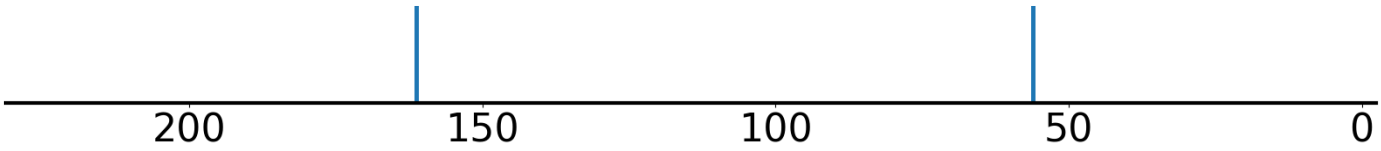
best positives	prob	best negatives	prob
[CX4H3]	0.9995	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8]=[#6][#8]	0.9982	C=CC=CC#C	0.0
[CX3](=[OX1])O	0.9972	CC=CCC#C	0.0
[CX3](=[OX1])C	0.9945	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9752	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
[#6H1]	0.9596	CC#CCC=C	0.0
[OX2H1]	0.9491	CCC=CC#C	0.0
[CX3](=O)[OX2H1]	0.8703	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H3][#6]	0.8499	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[#8][#6H0][#6H1]	0.8234	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H1]	0.5942	O=[#6][#6][#6X3]	0.1034
[#6X3][#6][#6][#6H3]	0.5008	[CH3]CC[OH]	0.3081
[#8][#6H1][#6H1]	0.3213	O=[#6][#6H][#6H0]	0.3483
[CX4H]O	0.2991	[#8][#6][#6][#6X3]	0.3989
[CX4H](O)CO	0.2863	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5252
[#8][#6][#6][#8]	0.2159	[#6H3][#6][#6X3]	0.5336
[#8]=[#6][#6H1][#6H1]	0.2106	[CX4H3][CX4H1]	0.7748
[CH3][#6][#8]	0.1993	[#8]=[#6H0][#6H1]	0.7992
[#8][#6][#6H2]	0.1807	O=[CX3][CX4H]	0.8184
[#8][#6H1][#6H1][#6H3]	0.1615	[#8][#6H0][#6H1]	0.8234

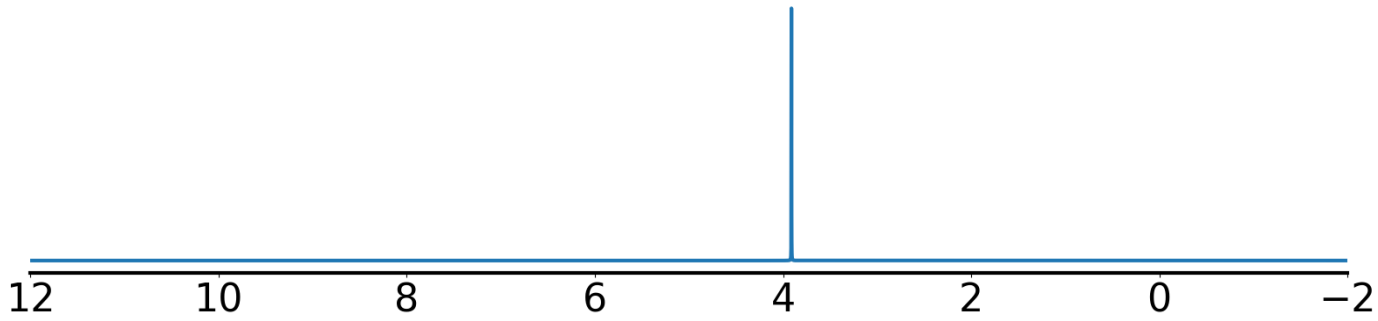
Example 137 true smiles: COC(=O)C(=O)OC formula: C4H6O4
Index of correct structure: 0 of 502
True structure loss: 0.02006
True structure:



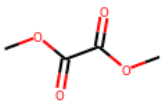
Experimental 13C NMR (solvent: CDCl3)



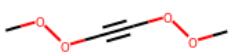
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):

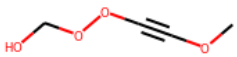


0.02006

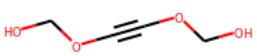


0.027254

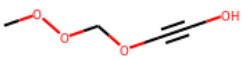
0.027367



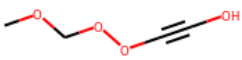
0.027367



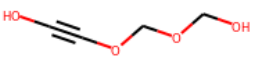
0.03017



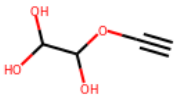
0.053531



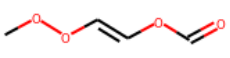
0.059798



0.064389



0.067154



0.067883

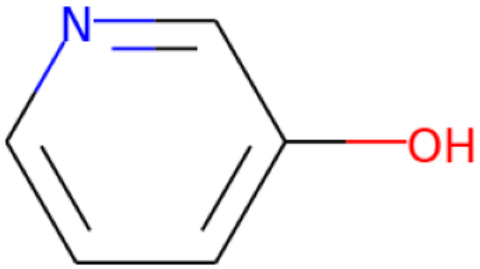
Top predicted substructures	prob		
[#8]=[#6][#8]	0.966	[CX4H3]	0.617

[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.9409	[OX2H1]	0.4729
[CX4H3][OX2H0]	0.9008	[#6X3][#6X3]	0.3049
[CX3](=[OX1])O	0.8793	[#8][#6][#6H2]	0.2585
[#8][#6][#6][#8]	0.6565	[#8][#6][#6][#6X3]	0.2551

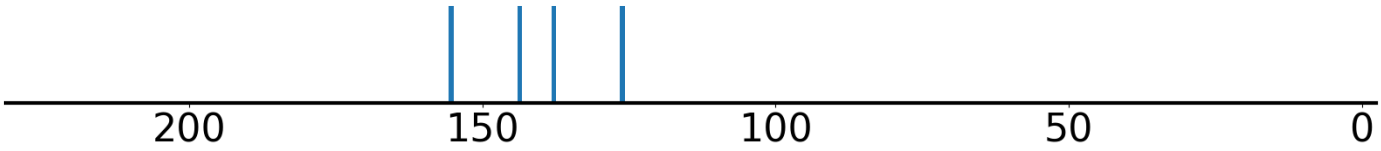
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.966	C=CC=CC#C	0.0
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.9409	CC=CCC#C	0.0
[CX4H3][OX2H0]	0.9008	CCC#CC#C	0.0
[CX3](=[OX1])O	0.8793	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6][#8]	0.6565	CC=CC#CC	0.0
[CX4H3]	0.617	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.3049	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[CX3H0](=[OX1H0])([OX2H0])[CX3H0]	0.2151	[CX4H3][CX3H0][CX4H2][CX3H1]	0.0
[CX3](=[OX1])C	0.1869	[CX3H0](=[CX3H2])([CX4H3])[CX4H1]	0.0
O=CC=O	0.0622	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0

worst negatives	prob	worst positives	prob
[OX2H1]	0.4729	[#8]=[#6][#6]=[#8]	0.0289
[#8][#6][#6H2]	0.2585	[#8][#6][#6]=[#8]	0.0408
[#8][#6][#6][#6X3]	0.2551	O=CC=O	0.0622
[#6H1]	0.2511	[CX3](=[OX1])C	0.1869
[CX3](=O)[OX2H1]	0.1924	[CX3H0](=[OX1H0])([OX2H0])[CX3H0]	0.2151
[#8][#6H0][#6H1]	0.1581	[#6X3][#6X3]	0.3049
[#6H1][#6H1]	0.1112	[CX4H3]	0.617
[#6H3][#8][#6H0][#8]	0.0907	[#8][#6][#6][#8]	0.6565
[#8][#6H1][#6H1]	0.0815	[CX3](=[OX1])O	0.8793
[CX4H](O)CO	0.0758	[CX4H3][OX2H0]	0.9008

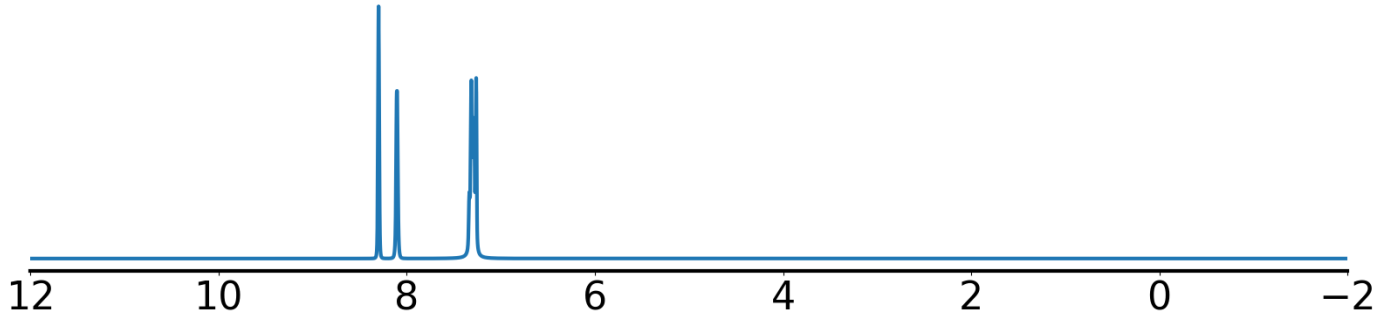
Example 138 true smiles: Oc1cccnc1 formula: C5H5NO
Index of correct structure: 0 of 371
True structure loss: 0.01149
True structure:



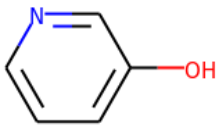
Experimental 13C NMR (solvent: CDCl3)



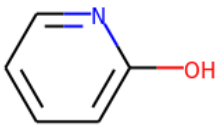
Experimental 1H NMR (solvent: CDCl3)



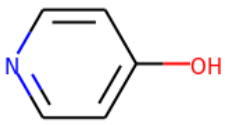
Top predicted structures (loss):



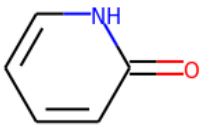
0.01149



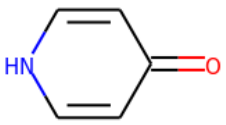
0.012264



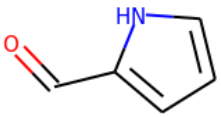
0.016269



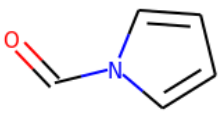
0.038359



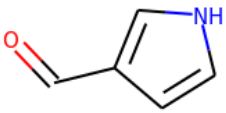
0.042365



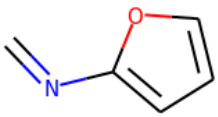
0.051



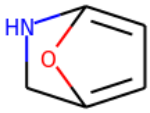
0.055451



0.05981



0.060799



0.07308

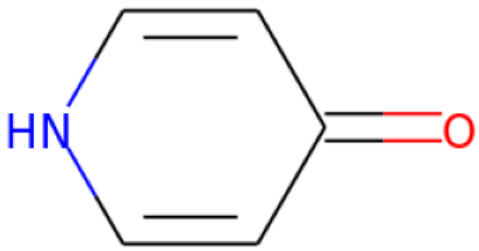
Top predicted substructures	prob		
[#6H1]	0.9999	[#7][#6][#6X3]	0.9911

[#6X3][#6X3]	0.9996	[cX3H1]([cX3H1])[cX3H1]	0.9846
[#6X3][#6X3][#6X3][#6X3]	0.9984	[#7][#6][#6][#6X3]	0.9807
[cH][cH]	0.9967	[#6]1[#6][#6][#6][#6][#7]1	0.9789
[cH]	0.9946	[#6X3H1][#6X3H0]	0.9628

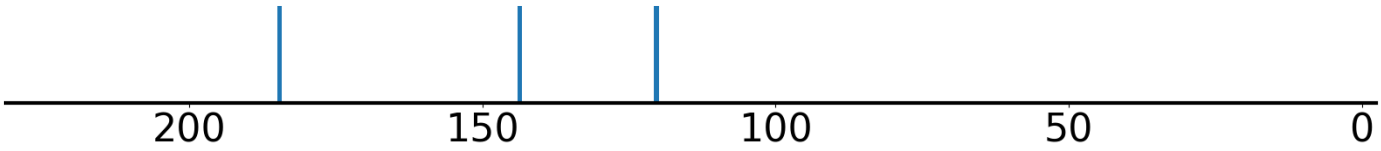
best positives	prob	best negatives	prob
[#6H1]	0.9999	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9996	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9984	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9967	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[cH]	0.9946	[OX2H0]1[CX4H2][CX4H2][CX4H0]1	0.0
[#7][#6][#6X3]	0.9911	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9846	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[#7][#6][#6][#6X3]	0.9807	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[#6]1[#6][#6][#6][#6][#7]1	0.9789	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9628	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#7][#6H0][#6H1]	0.7332	[OX2H][cX3]:[c]	0.347
[#7][#6X3H0][#6X3H1]	0.7118	[cH]cO	0.3983
[#6]1[#6][#6][#6][#6][#6]1	0.3251	[#8][#6H0][#6H1]	0.517
[#7X3H2]	0.3039	[cX3H1]([nX2H0])[cX3H0]	0.6028
O=[#6][#6][#6X3]	0.2547	[#6H1][#7][#6H1]	0.743
[#7H2][#6H0]	0.2275	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7644
[#6X3][#7X3][#6X3]	0.1575	[OX2H1]	0.7846
[#7H][#6X3H1]	0.1489	[#8][#6][#6][#6X3]	0.8555
o[cH]	0.1355	[#6X3][#7][#6X3]	0.9162
[#7X3H1]	0.1295	[#6H1][#6H1]	0.9212

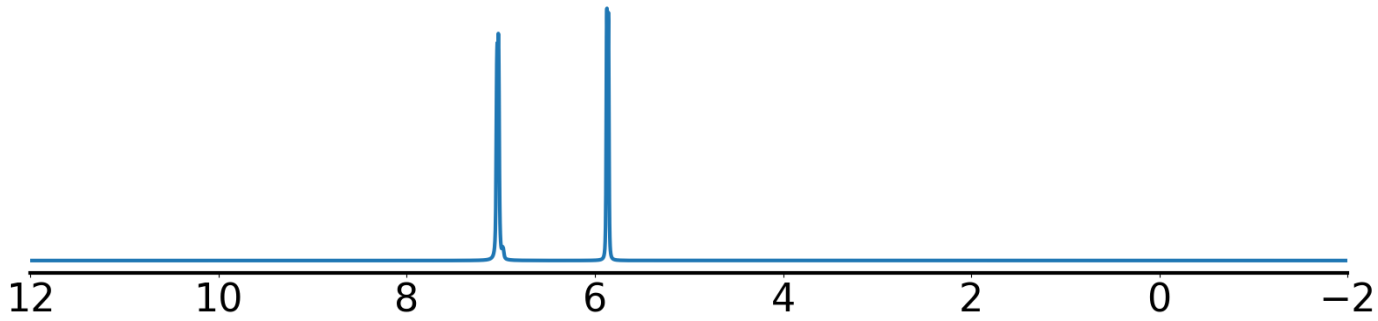
Example 139 true smiles: O=c1cc[nH]cc1 formula: C5H5NO
Index of correct structure: 1 of 371
True structure loss: 0.04109
True structure:



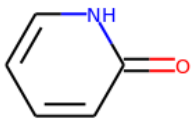
Experimental 13C NMR (solvent: D2O)



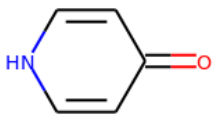
Experimental 1H NMR (solvent: CDCl3)



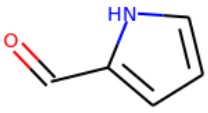
Top predicted structures (loss):



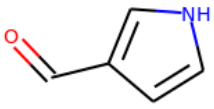
0.03829



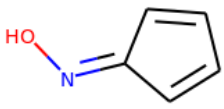
0.04109



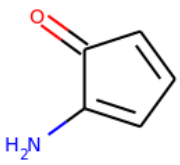
0.046299



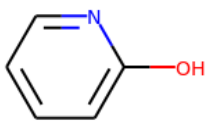
0.05235



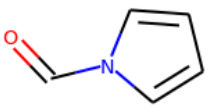
0.056054



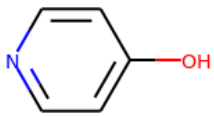
0.056478



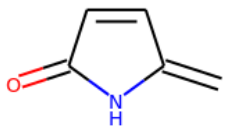
0.057749



0.058017



0.060548



0.060651

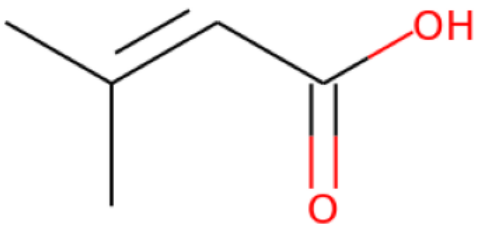
Top predicted substructures	prob		
[#6H1]	0.9992	[#8]=[#6H0][#6H1]	0.7819

[#6X3][#6X3]	0.9849	[CX3](=[OX1])C	0.7285
[#6X3H1][#6X3H0]	0.8087	O=[#6][#6][#6X3]	0.6833
[CHX3](=C)C	0.8007	O=[#6][#6]=[#6X3]	0.6584
[#6H1][#6H1]	0.7824	[#7][#6][#6][#6X3]	0.6362

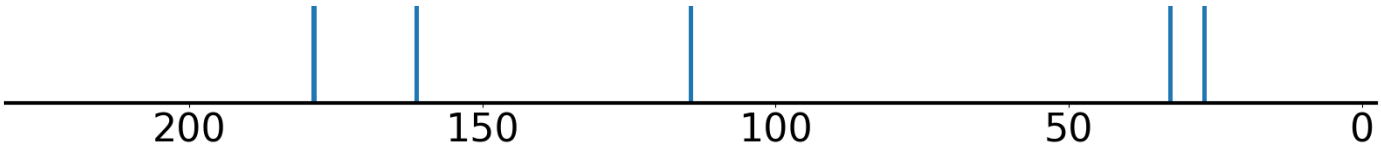
best positives	prob	best negatives	prob
[#6H1]	0.9992	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9849	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3H1][#6X3H0]	0.8087	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6H1][#6H1]	0.7824	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#8]=[#6H0][#6H1]	0.7819	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
O=[#6][#6][#6X3]	0.6833	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[#7][#6][#6][#6X3]	0.6362	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.606	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.549	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.4907	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[CHX3](=C)C	0.8007	O=[cX3]	0.0846
[CX3](=[OX1])C	0.7285	[#6]1[#6][#6][#6][#6][#7]1	0.104
O=[#6][#6]=[#6X3]	0.6584	[cX3H1]([nX3H1])[cX3H1]	0.1165
[#8]=[#6][#6H1]=[#6H1]	0.5599	[#6H1][#7][#6H1]	0.1263
[#7X3H2]	0.5528	[#7H][#6X3H1]	0.1638
[CHX3]=[CHX3]	0.5333	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.1797
O=C[CX3H]	0.5135	[cX3H1]([cX3H1])[cX3H0]	0.2238
[CX3H1](=[CX3H1])[CX3H0]	0.4813	[#7X3H1]	0.2569
[cX3H1]([cX3H1])[cX3H1]	0.4549	[cH]	0.2571
[#7][#6H0][#6H1]	0.4496	[#6X3][#7X3][#6X3]	0.2596

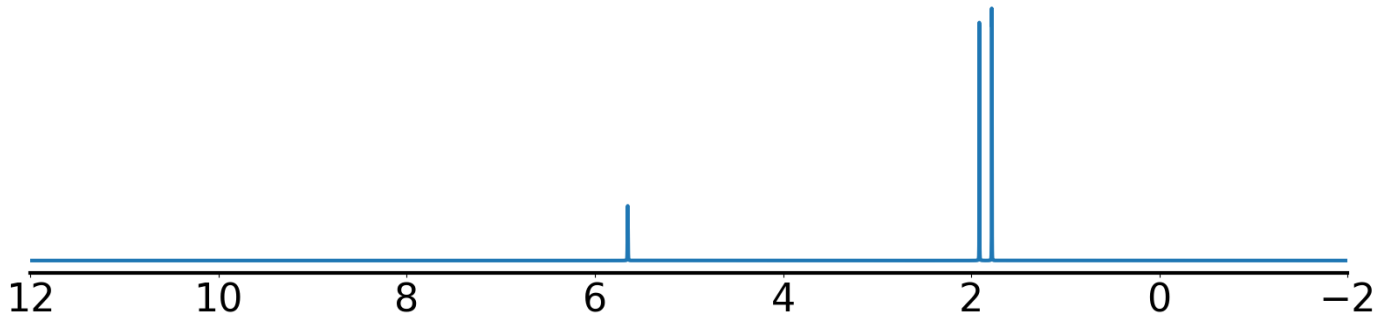
Example 140 true smiles: CC(C)=CC(=O)O formula: C5H8O2
Index of correct structure: 0 of 329
True structure loss: 0.015726
True structure:



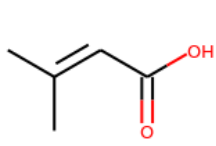
Experimental 13C NMR (solvent: CDCl3)



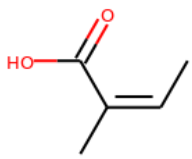
Experimental 1H NMR (solvent: D2O)



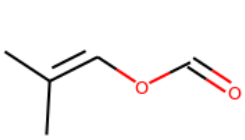
Top predicted structures (loss):



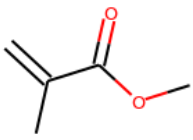
0.015726



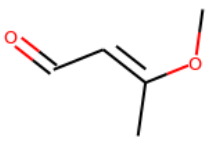
0.050235



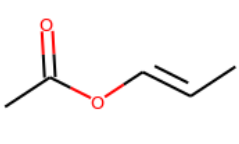
0.063737



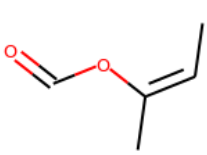
0.092419



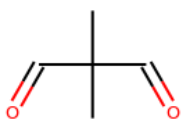
0.095791



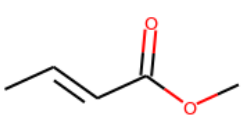
0.097581



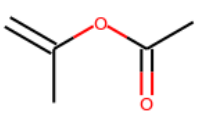
0.097622



0.099035



0.099102



0.108788

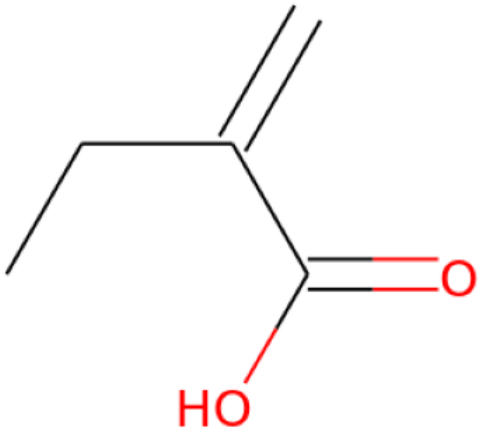
Top predicted substructures	prob		
[CX4H3]	0.9998	[#6H3][#6][#6]	0.9876

[#6H3][#6H0]	0.9993	[#8]=[#6][#8]	0.9839
[CX3](=[OX1])C	0.9958	[CX4H3][#6]	0.9644
[CX4H3][CX3]	0.9956	[#6X3][#6X3]	0.9566
[CX4H3][CX3H0]	0.994	[CX3](=[OX1])O	0.9282

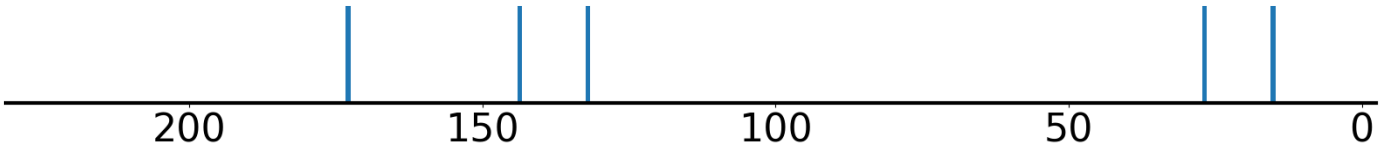
best positives	prob	best negatives	prob
[CX4H3]	0.9998	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[#6H3][#6H0]	0.9993	CCC#CC#C	0.0
[CX3](=[OX1])C	0.9958	[OX2H1][CX4H1][CX4H1][CX2H0]	0.0
[CX4H3][CX3]	0.9956	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX4H3][CX3H0]	0.994	[CX4H1]([CX4H2])([CX4H2])[CX2H0]	0.0
[#6H3][#6][#6]	0.9876	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#8]=[#6][#8]	0.9839	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[CX4H3][#6]	0.9644	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9566	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.9282	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6H3][#6][#6X3]	0.5667	[CHX3](=C)C	0.3164
[OX1H0]=[CX3H0][CX3H0][CX4H3]	0.4721	[#6H1]	0.4055
[CH3][#6][#8]	0.3466	[#8][#6][#6]=[#6X3]	0.425
[CX4H3][CX3H0][CX3]=O	0.3132	[#8]=[#6H0][#6H1]	0.4813
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2913	[#6X3][#6]=[#6][#6H3]	0.5015
O=[#6][#6][#6X3]	0.2827	[#8][#6X3][#6X3]=[#6X3][#6H3]	0.5736
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2557	[#6X3H1][#6X3H0]	0.5766
[CX4H2][CX3]=O	0.1673	[OX2H1]	0.5973
[OX1H0]=[CX3H0][CX4H3]	0.1398	[#8][#6H0][#6H1]	0.648
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.1133	O=C[CX3H]	0.6494

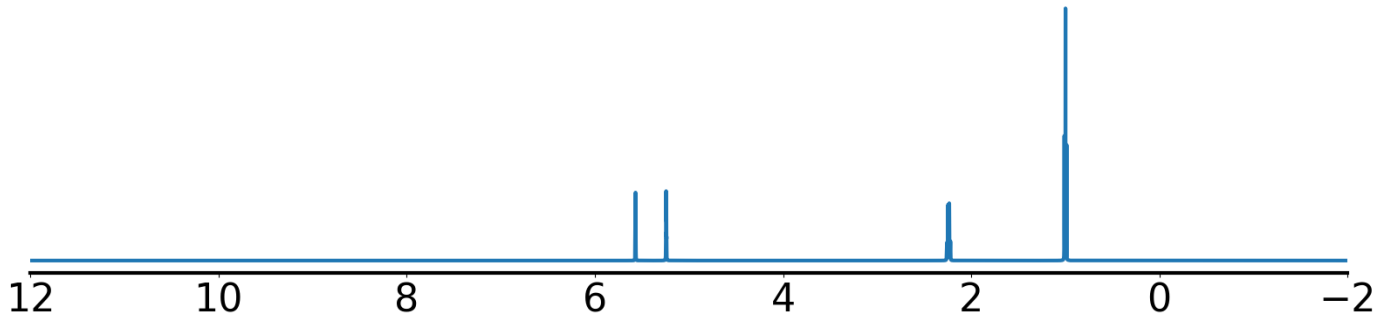
Example 141 true smiles: C=C(CC)C(=O)O formula: C5H8O2
Index of correct structure: 0 of 329
True structure loss: 0.012184
True structure:



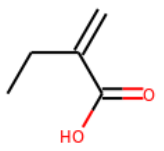
Experimental 13C NMR (solvent: CDCl3)



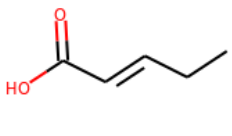
Experimental 1H NMR (solvent: D2O)



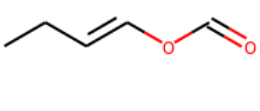
Top predicted structures (loss):



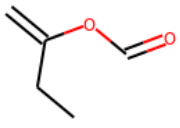
0.012184



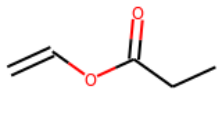
0.054155



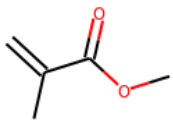
0.090765



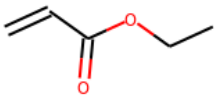
0.092741



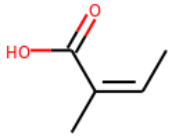
0.103478



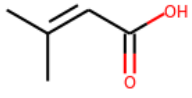
0.106921



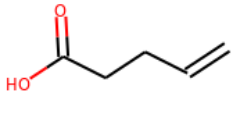
0.107536



0.113536



0.113587



0.118296

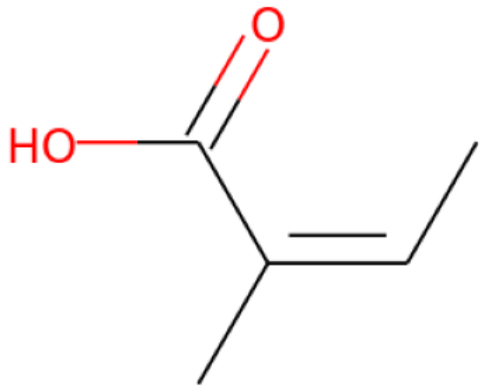
Top predicted substructures	prob		
[CX4H3][#6]	0.9998	[#8]=[#6][#8]	0.9953

[CX4H3]	0.9996	[CX3](=[OX1])O	0.9943
[CX4H2]([#6])[#6]	0.9992	[CX3](=[OX1])C	0.9912
[CX4H3][CX4H2]	0.9988	[CX4H2][CX3]=C	0.9701
[#6H3][#6][#6]	0.9954	[CX3](=O)[OX2H1]	0.967

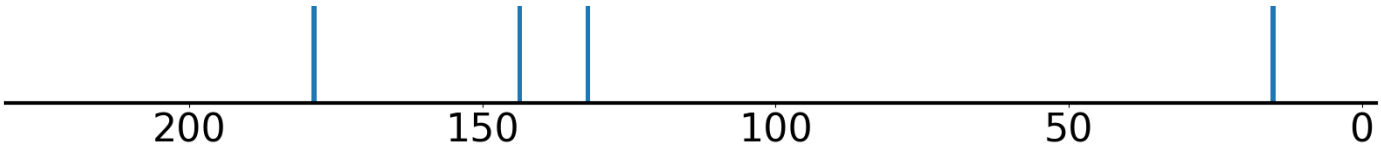
best positives	prob	best negatives	prob
[CX4H3][#6]	0.9998	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3]	0.9996	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H2]([#6])[#6]	0.9992	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][CX4H2]	0.9988	CCC#CC#C	0.0
[#6H3][#6][#6]	0.9954	[#6H2][#6]#[#6X2]	0.0
[#8]=[#6][#8]	0.9953	[CX2H0](#[CX2H1])[CX4H1]	0.0
[CX3](=[OX1])O	0.9943	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])C	0.9912	[CX2H0](#[CX2H0])[CX4H1]	0.0
[CX4H2][CX3]=C	0.9701	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX3](=O)[OX2H1]	0.967	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.6156	[#6X3][#6][#6][#6H3]	0.2924
[CHX3](=C)C	0.405	[CX4H2]CC=O	0.4542
O=[#6][#6][#6X3]	0.257	[CX3H0](=[CX3H2])([CX4H2])[CX3H0]	0.4638
[#8]=[#6H0][#6H1]	0.2322	OCC[CH2]	0.6192
[#6X3H1]=[#6X3H0]	0.2003	[#6H2][#6X3H0]=[#6H2]	0.628
[#6X3H1][#6X3H0]	0.1959	[#6X3H2]	0.724
[#6H1][#6H2]	0.1929	[CX3H2]=[CX3H0]	0.7368
[CHX3]=[CHX3]	0.1691	[CX3H2]=[CX3H0]([#6])[#6]	0.7982
[CX4H2][CX3H]	0.1475	[CX3H2]=[CX3H0][CX3H0]	0.802
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.1475	[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.8201

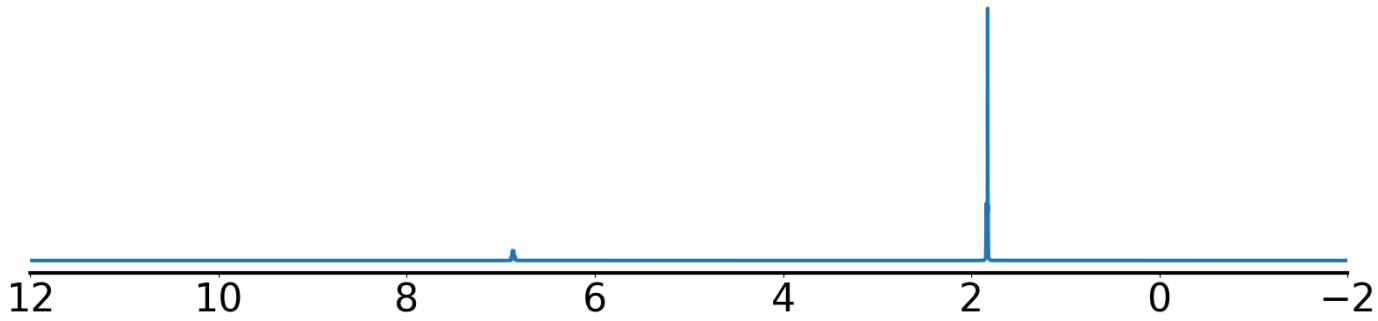
Example 142 true smiles: CC=C(C)C(=O)O formula: C5H8O2
Index of correct structure: 0 of 329
True structure loss: 0.010051
True structure:



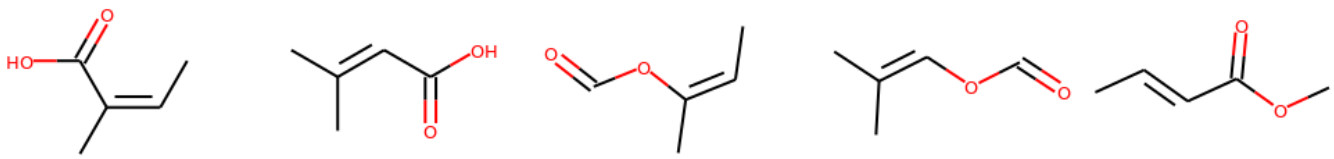
Experimental 13C NMR (solvent: CDCl3)



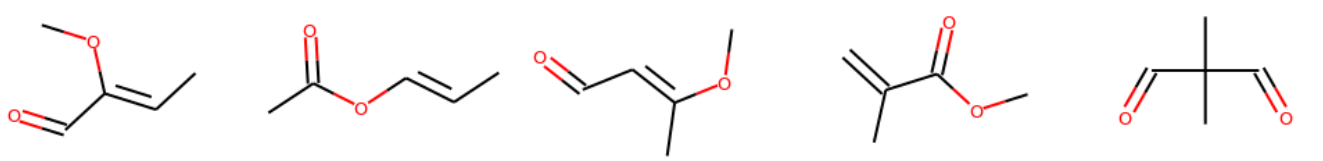
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.010051 0.060697 0.084163 0.090202 0.093542



0.093661 0.101289 0.110199 0.11225 0.112899

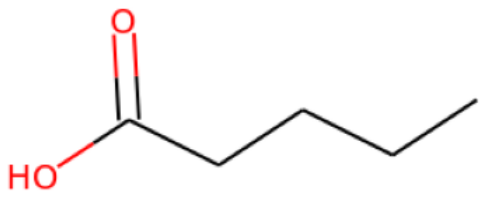
Top predicted substructures	prob		
[CX4H3]	1.0	[#6X3][#6X3]	0.9855

[CX4H3][CX3]	0.9994	[#8]=[#6][#8]	0.9811
[CX4H3][#6]	0.9993	[#6H3][#6]=[#6][#6H3]	0.9632
[CX3](=[OX1])C	0.9878	[#6H3][#6]=[#6X3]	0.9621
[#6H3][#6H0]	0.9868	[CX3](=O)[OX2H1]	0.9621

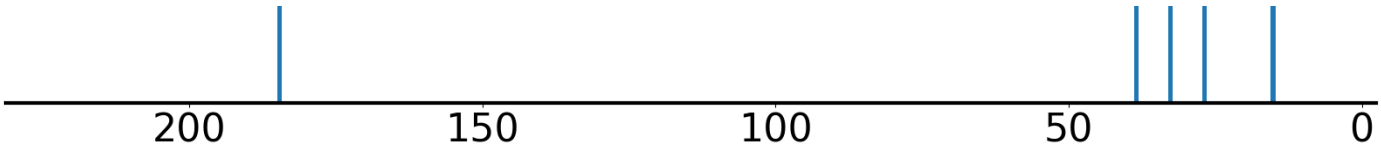
best positives	prob	best negatives	prob
[CX4H3]	1.0	[#6X2][#6H1][#6X2]	0.0
[CX4H3][CX3]	0.9994	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][#6]	0.9993	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX3](=[OX1])C	0.9878	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#6H3][#6H0]	0.9868	[CX2H0](#[CX2H1])[CX4H1]	0.0
[#6X3][#6X3]	0.9855	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#8]=[#6][#8]	0.9811	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H3][#6]=[#6][#6H3]	0.9632	[CX4H1]([CX4H1])([CX4H1])[CX4H0]	0.0
[#6H3][#6]=[#6X3]	0.9621	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX3](=O)[OX2H1]	0.9621	[CX4H2]([CX4H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6][#6X3]	0.4539	[CHX3](=C)C	0.3154
[#6X3H1][#6X3H0]	0.2332	[CH3]CC[OH]	0.4226
[#8][#6][#6][#6X3]	0.211	[#6H1]	0.4959
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1473	[#8][#6][#6]=[#6X3]	0.5751
[#8][#6H0][#6H1]	0.1394	[#6X3H1]=[#6X3H0]	0.6785
[#6X3][#6][#6][#6H3]	0.1384	[#6X3][#6]=[#6][#6H3]	0.6814
[#8][#6][#6]=[#8]	0.0977	[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.7244
[#8][#6][#6]=[#6][#6]=[#8]	0.0905	[#8][#6X3][#6X3]=[#6X3][#6H3]	0.7712
[CX4H2]CC=O	0.0869	[CX4H3][CX3H1]	0.7722
[#8]=[#6H0][#6H1]	0.0788	[CX3H0](=[CX3H1])([CX4H3])[CX3H0]	0.8203

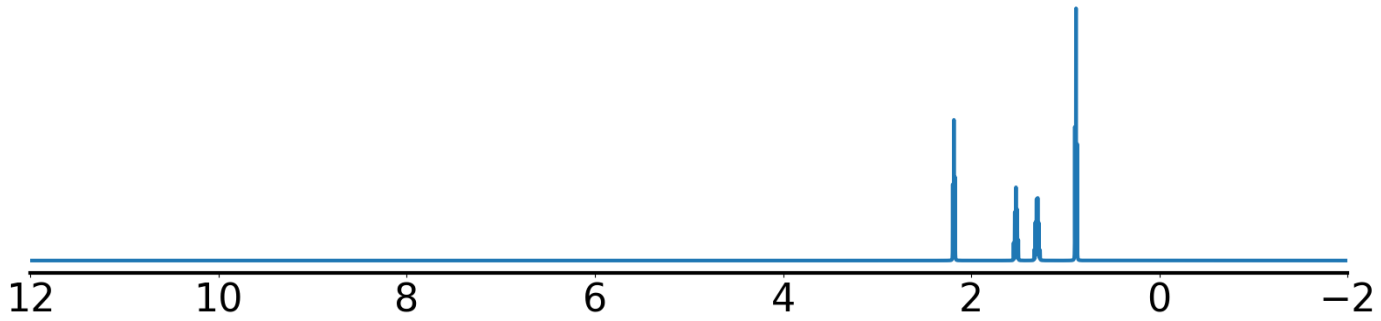
Example 143 true smiles: CCCCC(=O)O formula: C5H10O2
Index of correct structure: 0 of 303
True structure loss: 0.005996
True structure:



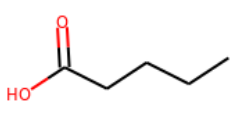
Experimental 13C NMR (solvent: CDCl3)



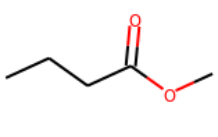
Experimental 1H NMR (solvent: D2O)



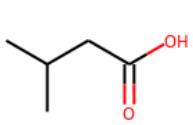
Top predicted structures (loss):



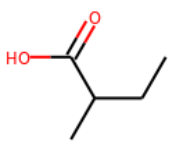
0.005996



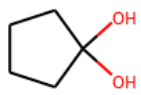
0.056613



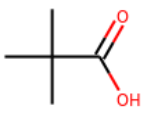
0.065769



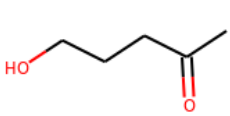
0.070666



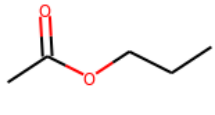
0.097018



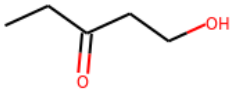
0.10027



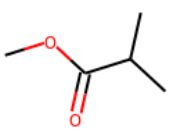
0.104816



0.106557



0.108538



0.111279

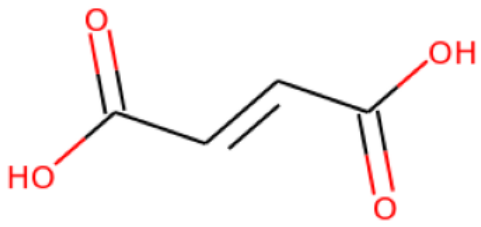
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9999	[CX4H3][#6]	0.9967

[#6H3][#6][#6]	0.9994	[#8]=[#6][#8]	0.9963
[CX3](=[OX1])C	0.999	[CX4H3]	0.9944
[CX3](=O)[OX2H1]	0.9988	[CX3](=[OX1])O	0.9863
[CX4H3][CX4H2]	0.9983	[OX2H1]	0.9793

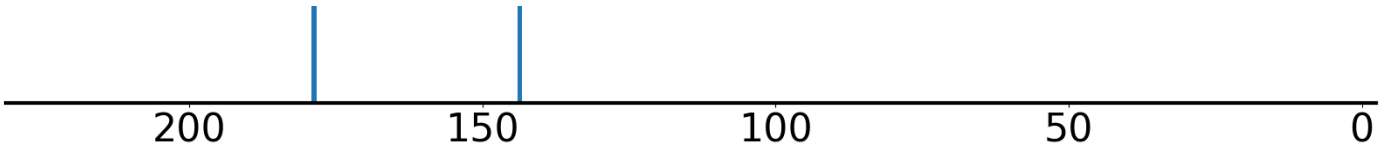
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9999	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9994	CCC=CC#C	0.0
[CX3](=[OX1])C	0.999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=O)[OX2H1]	0.9988	CCC#CC#C	0.0
[CX4H3][CX4H2]	0.9983	CC=CC#CC	0.0
[CX4H3][#6]	0.9967	CC=CCC#C	0.0
[#8]=[#6][#8]	0.9963	[CX2H0](#[CX2H1])[CX4H1]	0.0
[CX4H3]	0.9944	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CX3](=[OX1])O	0.9863	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9793	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX4H2][CX4H2][CX4H2]	0.6204	[#8][#6][#6H2]	0.6338
CCCCCC	0.4429	[CX4H2][CX3]=O	0.7568
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2647	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.8257
[#6H1][#6H2]	0.2375	[CX4H2]([CX4H2])[CX4H2]	0.8315
[#6H1]	0.236	OCC[CH2]	0.8508
[#8]=[#6H0][#6H1]	0.1819	O=[CX3H0][CX4H2][CX4H2]	0.8863
[#6X3][#6][#6][#6H3]	0.1805	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.9073
[CH3]CC[OH]	0.1211	[CX4H2]CC=O	0.9144
[#8][#6H0][#6H1]	0.0927	[CX4H2]([CX4H2])[CX3H0]	0.9252
[#6H3][#6][#6X3]	0.0594	[CX4H2]([CX4H3])[CX4H2]	0.9437

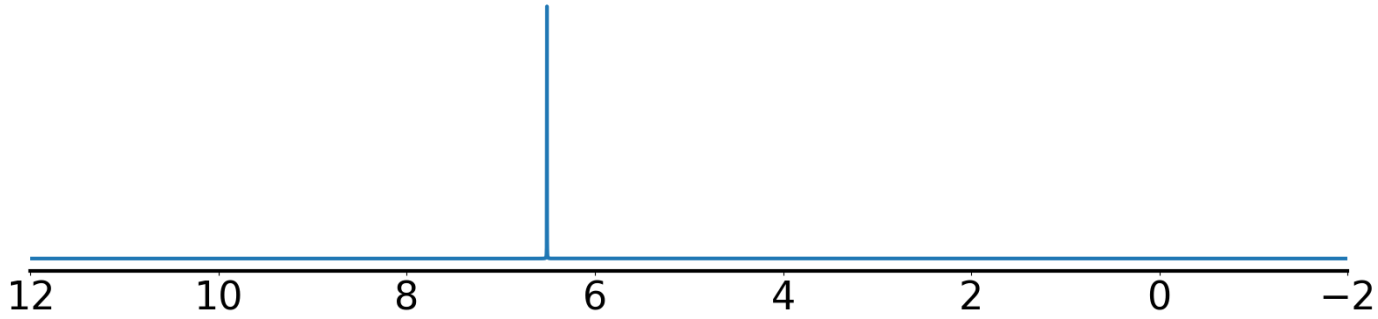
Example 144 true smiles: O=C(O)C=CC(=O)O formula: C4H4O4
Index of correct structure: 0 of 301
True structure loss: 0.035775
True structure:



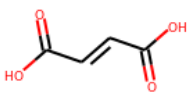
Experimental 13C NMR (solvent: D2O)



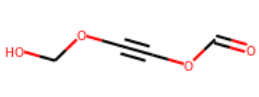
Experimental 1H NMR (solvent: D2O)



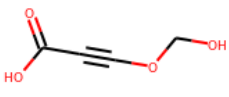
Top predicted structures (loss):



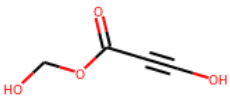
0.035775



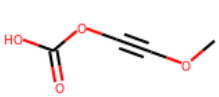
0.036655



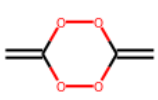
0.039464



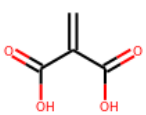
0.041437



0.041872

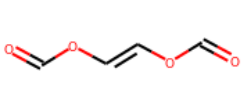


0.044606

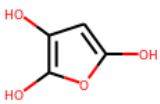


0.0447

0.047843



0.047968



0.049387

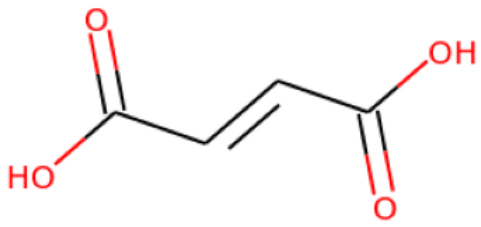
Top predicted substructures	prob		
[#8]=[#6][#8]	0.9905	[#6X3][#6X3]	0.8107

[CX3](=[OX1])O	0.9796	[OX2H1]	0.8064
[CX3](=[OX1])C	0.9322	O=[#6][#6][#6X3]	0.7505
[#6H1]	0.8799	[#8][#6H0][#6H1]	0.5214
[CX3](=O)[OX2H1]	0.8686	[#6X3H1][#6X3H0]	0.5068

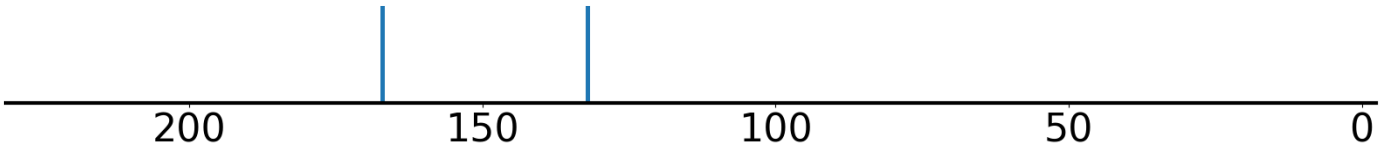
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9905	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX3](=[OX1])O	0.9796	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX3](=[OX1])C	0.9322	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6H1]	0.8799	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[CX3](=O)[OX2H1]	0.8686	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#6X3][#6X3]	0.8107	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[OX2H1]	0.8064	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#8][#6H0][#6H1]	0.5214	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6X3H1][#6X3H0]	0.5068	[CX4H1]([CX4H2])([CX4H2])[CX2H0]	0.0
O=[#6][#6]=[#6X3]	0.3217	[OX2H0]1[CX4H1][CX4H2][CX4H1][CX4H2]1	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6][#6X3]	0.7505	[#6X3][#6X3]=[#6X3][#6X3]	0.0732
[#8][#6][#6]=[#8]	0.4565	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.0765
[#8][#6][#6][#6X3]	0.4461	[CX3H1](=[CX3H1])[CX3H0]	0.087
[#8][#6][#6][#8]	0.3344	[#8][#6][#6]=[#6][#6][#8]	0.1074
[CX3H](O)	0.2135	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.1336
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.1982	[CHX3]=[CHX3]	0.1751
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1759	[#8]=[#6][#6H1]=[#6H1]	0.1897
O=CC=O	0.1679	[CHX3](=C)C	0.1901
[#8]=[#6][#6]=[#8]	0.1621	O=C[CX3H]	0.2013
[cH]	0.1419	[#8][#6][#6]=[#6][#6]=[#8]	0.2066

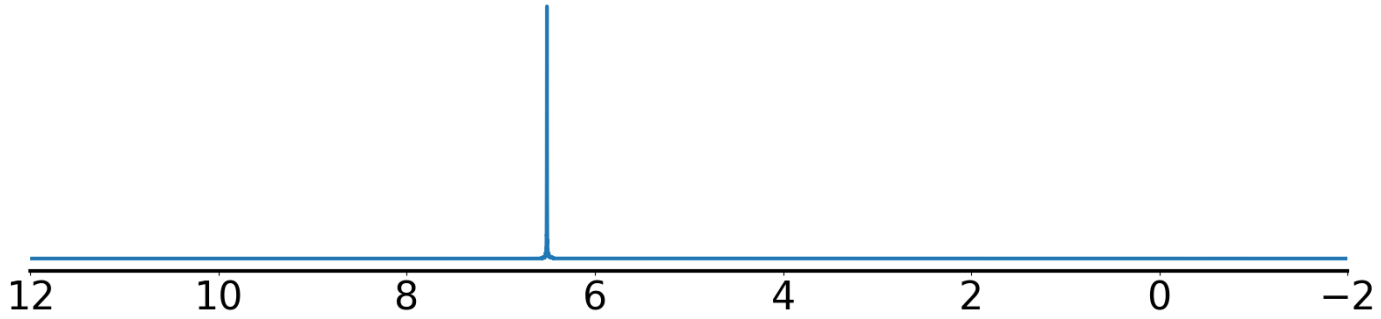
Example 145 true smiles: O=C(O)C=CC(=O)O formula: C4H4O4
Index of correct structure: 4 of 301
True structure loss: 0.039178
True structure:



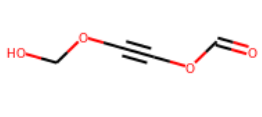
Experimental 13C NMR (solvent: DMSO)



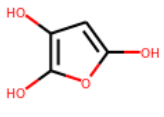
Experimental 1H NMR (solvent: D2O)



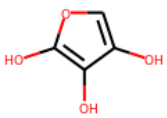
Top predicted structures (loss):



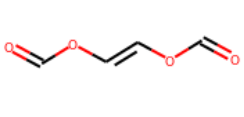
0.032792



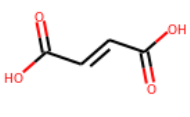
0.033734



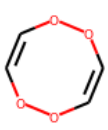
0.037724



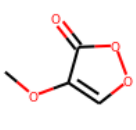
0.039167



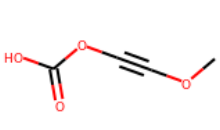
0.039178



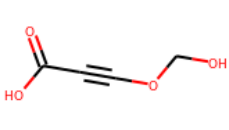
0.040963



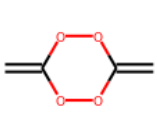
0.041943



0.042753



0.044155



0.044979

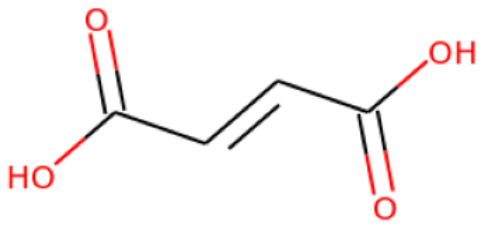
Top predicted substructures	prob		
[#8]=[#6][#8]	0.9843	[CX3](=O)[OX2H1]	0.7435

[#6H1]	0.9612	[#6X3H1][#6X3H0]	0.707
[CX3](=[OX1])O	0.9554	[#8][#6H0][#6H1]	0.6181
[#6X3][#6X3]	0.9177	O=[#6][#6][#6X3]	0.5864
[OX2H1]	0.7641	[CX3](=[OX1])C	0.5682

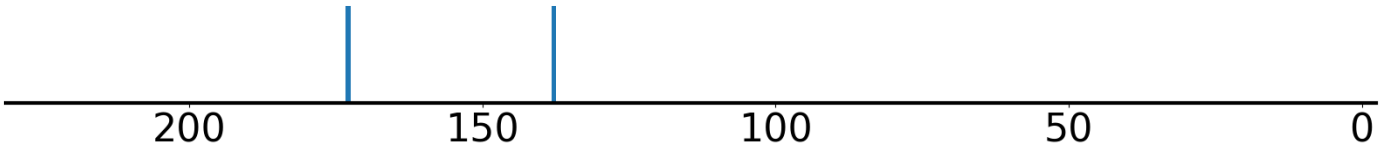
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9843	CCC#CC#C	0.0
[#6H1]	0.9612	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX3](=[OX1])O	0.9554	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6X3][#6X3]	0.9177	[CX2H0](#[CX2H0])[CX2H0]	0.0
[OX2H1]	0.7641	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[CX3](=O)[OX2H1]	0.7435	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.707	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#8][#6H0][#6H1]	0.6181	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[CX3](=[OX1])C	0.5682	[CX4H2]([CX4H1])[CX2H0]	0.0
O=[#6][#6]=[#6X3]	0.4426	[CX2H0](#[CX2H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6][#6X3]	0.5864	[#6X3][#6X3]=[#6X3][#6X3]	0.0226
[#8][#6][#6][#8]	0.4692	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.0487
[cH]	0.4523	[CHX3](=C)C	0.076
[OX2H][cX3]:[c]	0.3834	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.0949
[#8][#6][#6][#6X3]	0.3786	[CX3H1](=[CX3H1])[CX3H0]	0.097
[cH]cO	0.3112	[#8][#6][#6]=[#6][#6]=[#8]	0.1391
O=[cX3]	0.3085	[#8][#6][#6]=[#6X3]	0.1487
[#6X3][#6X3][#6X3][#6X3]	0.2756	[#8]=[#6][#6H1]=[#6H1]	0.1814
[CX3H](O)	0.2747	[#8]=[#6][#6]=[#6][#6]=[#8]	0.1879
[#8][#6][#6]=[#8]	0.2615	O=C[CX3H]	0.2223

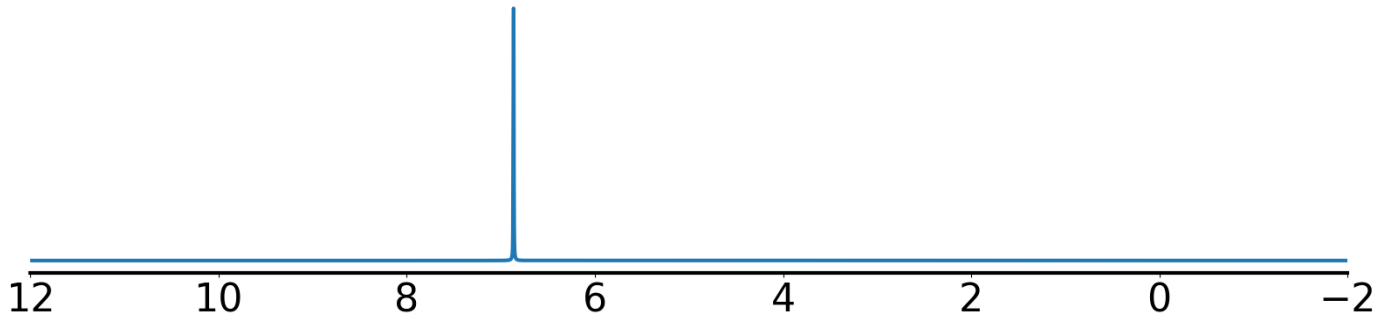
Example 146 true smiles: O=C(O)C=CC(=O)O formula: C4H4O4
Index of correct structure: 0 of 301
True structure loss: 0.026882
True structure:



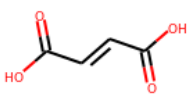
Experimental 13C NMR (solvent: CD3OD)



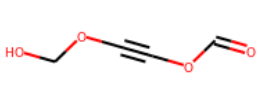
Experimental 1H NMR (solvent: D2O)



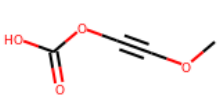
Top predicted structures (loss):



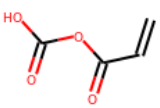
0.026882



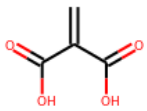
0.042347



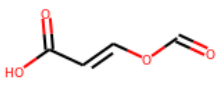
0.046889



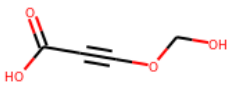
0.047066



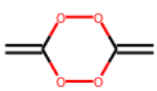
0.047417



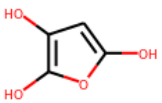
0.048399



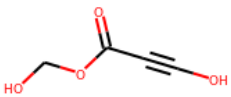
0.048745



0.049289



0.049371



0.050939

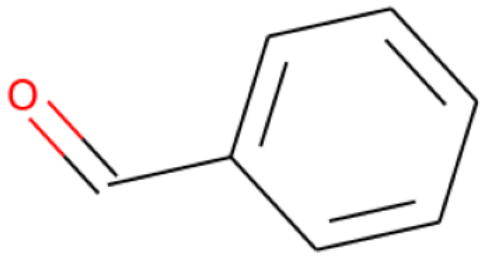
Top predicted substructures	prob		
[#8]=[#6][#8]	0.9941	[CX3](=O)[OX2H1]	0.8909

[CX3](=[OX1])O	0.9839	[CX3](=[OX1])C	0.8059
[#6X3][#6X3]	0.9369	O=[#6][#6]=[#6X3]	0.7132
[#6H1]	0.9104	[#6X3H1][#6X3H0]	0.7068
[OX2H1]	0.8964	O=[#6][#6][#6X3]	0.6379

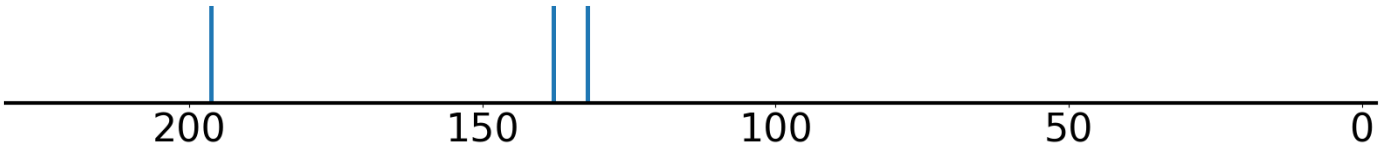
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9941	CCC#CC#C	0.0
[CX3](=[OX1])O	0.9839	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.9369	[#7][#6H1][#6X2]	0.0
[#6H1]	0.9104	[CX4H2]([CX4H3])[CX2H0]	0.0
[OX2H1]	0.8964	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[CX3](=O)[OX2H1]	0.8909	[CX4H2]([NX3H0])[CX4H3]	0.0
[CX3](=[OX1])C	0.8059	CC#CCC#C	0.0
O=[#6][#6]=[#6X3]	0.7132	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[#6X3H1][#6X3H0]	0.7068	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#8][#6][#6]=[#6X3]	0.5765	[CX2H0](#[CX2H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6][#6X3]	0.6379	[#8][#6][#6]=[#6][#6][#8]	0.1644
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.6203	[CX3H1](=[CX3H1])[CX3H0]	0.179
[#8][#6][#6][#6X3]	0.3569	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.184
[cH]	0.304	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.2162
[#8][#6][#6][#8]	0.2699	[CHX3]=[CHX3]	0.2722
[#8][#6][#6]=[#8]	0.26	[#8]=[#6][#6H1]=[#6H1]	0.2795
[#6X3H1]=[#6X3H0]	0.2421	[#8]=[#6H0][#6H1]	0.281
[cX3H1]([cX3H1])[cX3H0]	0.1815	[#6X3][#6X3]=[#6X3][#6X3]	0.2926
[cH]cO	0.1789	[CHX3](=C)C	0.3094
[#6X3][#6X3][#6X3][#6X3]	0.1728	O=C[CX3H]	0.3492

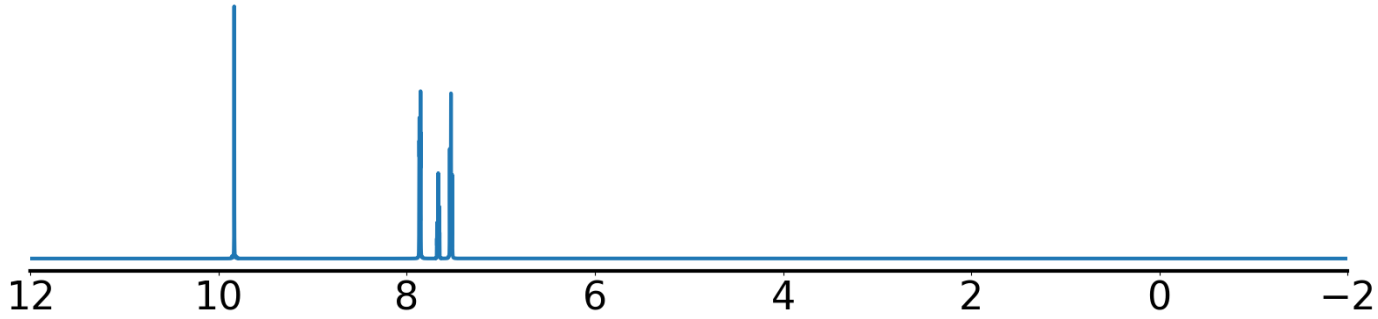
Example 147 true smiles: O=Cc1ccccc1 formula: C7H6O
Index of correct structure: 0 of 261
True structure loss: 0.010196
True structure:



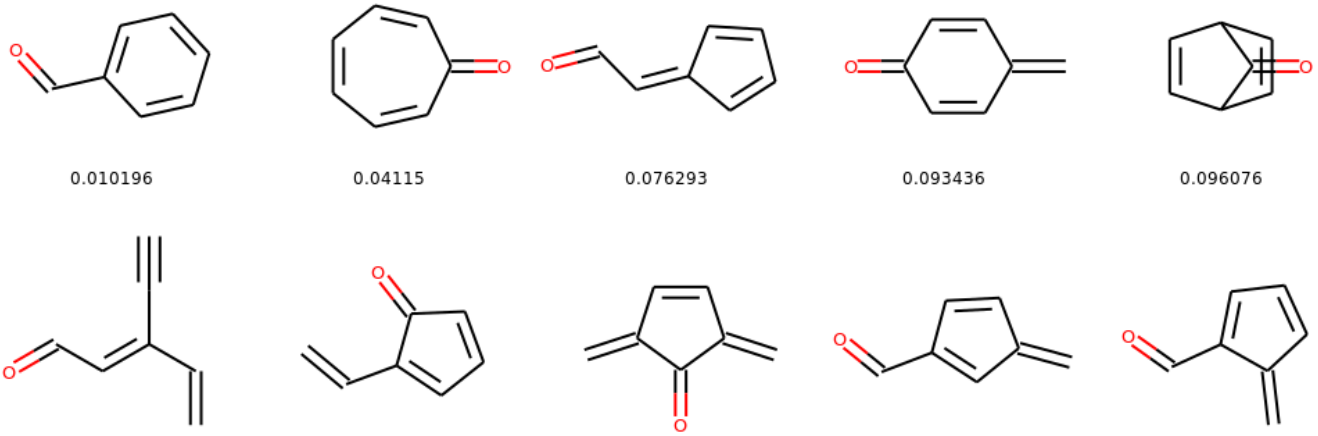
Experimental 13C NMR (solvent: CDCl3)



Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



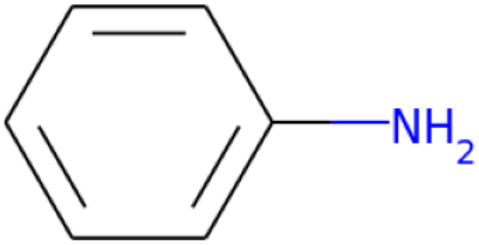
Top predicted substructures	prob		
[#6H1]	0.9998	[#6X3][#6X3][#6X3][#6X3]	0.9415

[#6X3][#6X3]	0.9992	[cH][cH]	0.8501
[CX3H1](=O)[#6]	0.9967	O=[#6][#6][#6X3]	0.8302
[#6X3H1][#6X3H0]	0.9905	[cX3H1]([cX3H1])[cX3H1]	0.827
[#6H1][#6H1]	0.9548	[CX3](=[OX1])C	0.8128

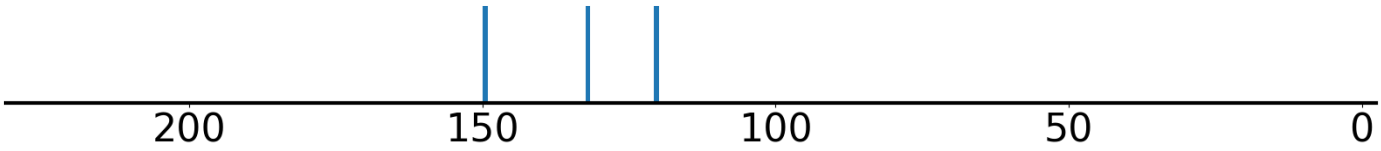
best positives	prob	best negatives	prob
[#6H1]	0.9998	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3]	0.9992	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX3H1](=O)[#6]	0.9967	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9905	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6H1][#6H1]	0.9548	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9415	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.8501	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
O=[#6][#6][#6X3]	0.8302	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.827	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.8049	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX3](=[OX1])C	0.8128	[#6]1[#6][#6][#6][#6][#6]1	0.5652
O=C[CX3H]	0.4753	[#8]=[#6H][#6X3][#6X3H]	0.6042
[#6X3][#6X3]=[#6X3][#6X3]	0.3759	[cX3H1]([cX3H1])[cX3H0]	0.6778
[CHX3]=[CHX3]	0.3655	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.8039
[#6X3H1]=[#6X3H1][#6X3H0][#6X3H1]	0.2878	[cH]	0.8049
[#8]=[#6H][#6X3]=[#6X3H]	0.2832	[cX3H1]([cX3H1])[cX3H1]	0.827
O=[#6][#6]=[#6X3]	0.2744	O=[#6][#6][#6X3]	0.8302
[#6X3][#6X3][#6X3]=[#6X3]	0.2684	[cH][cH]	0.8501
[#8]=[#6][#6]=[#6][#6]=[#8]	0.2366	[#6X3][#6X3][#6X3][#6X3]	0.9415
[#8]=[#6H0][#6H1]	0.2219	[#6H1][#6H1]	0.9548

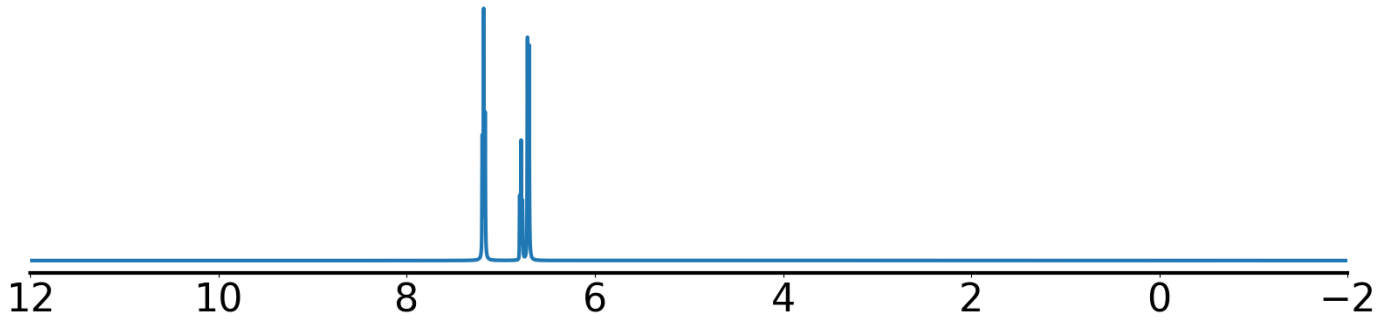
Example 148 true smiles: Nc1ccccc1 formula: C6H7N
Index of correct structure: 0 of 245
True structure loss: 0.008435
True structure:



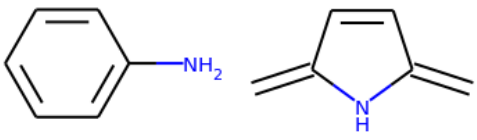
Experimental 13C NMR (solvent: CDCl3)



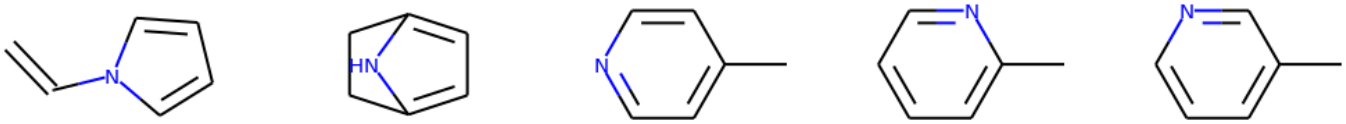
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.008435 0.038484 0.049658 0.054101 0.056782



0.057884 0.063464 0.08006 0.086147 0.090158

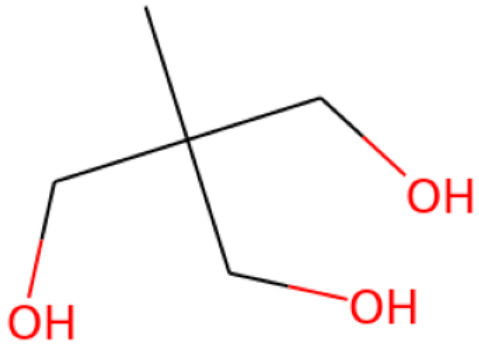
Top predicted substructures	prob		
[#6H1]	0.9989	[cH]	0.9652

[#6X3][#6X3]	0.9979	[#7][#6][#6X3]	0.9612
[cH][cH]	0.9964	[cX3H1]([cX3H1])[cX3H0]	0.955
[#6X3][#6X3][#6X3][#6X3]	0.9879	[#6]1[#6][#6][#6][#6][#6]1	0.9426
[cX3H1]([cX3H1])[cX3H1]	0.9798	[#6H1][#6H1]	0.9209

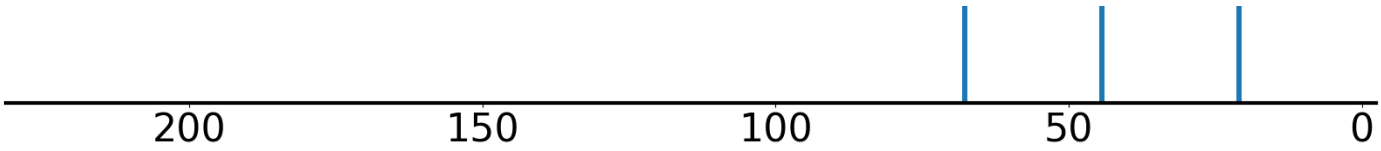
best positives	prob	best negatives	prob
[#6H1]	0.9989	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9979	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH][cH]	0.9964	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9879	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9798	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[cH]	0.9652	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6X3]	0.9612	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.955	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.9426	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H1][#6H1]	0.9209	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7][#6X3]	0.4874	[#7H2][#6H0]	0.4249
[#6]1[#6][#6][#6][#6][#7]1	0.4765	[#7][#6H0][#6H1]	0.5986
[#7X3H1]	0.3176	[#7][#6X3H0][#6X3H1]	0.66
[#7H][#6X3H1]	0.2547	[#7X3H2]	0.6981
[#6]1[#6][#6][#6][#7]1	0.2382	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.753
[#6H1][#7][#6H1]	0.2292	[#7][#6][#6][#6X3]	0.9116
[cH]cO	0.2147	[#6X3H1][#6X3H0]	0.9163
[cX3H1]([nX3H1])[cX3H1]	0.2034	[#6H1][#6H1]	0.9209
[#6X3][#7X3][#6X3]	0.18	[#6]1[#6][#6][#6][#6][#6]1	0.9426
[cX3H0][cX3H1][cX3H1][cX3H0]	0.1547	[cX3H1]([cX3H1])[cX3H0]	0.955

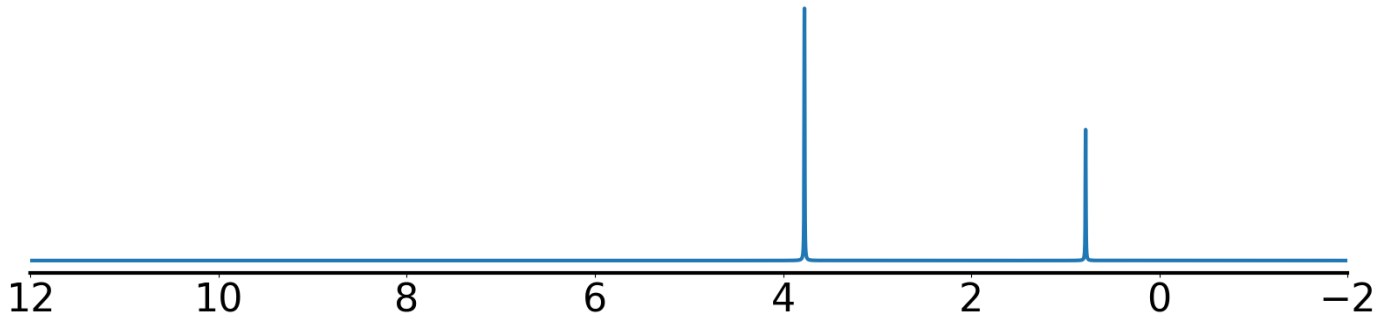
Example 149 true smiles: CC(CO)(CO)CO formula: C5H12O3
Index of correct structure: 0 of 238
True structure loss: 0.024948
True structure:



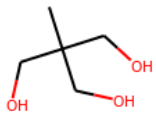
Experimental 13C NMR (solvent: D2O)



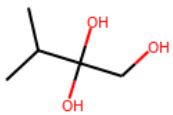
Experimental 1H NMR (solvent: CDCl3)



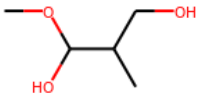
Top predicted structures (loss):



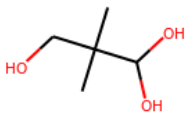
0.024948



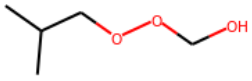
0.029405



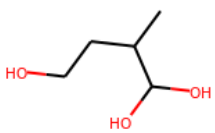
0.033083



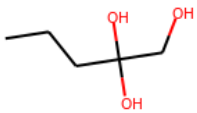
0.034161



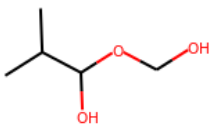
0.034384



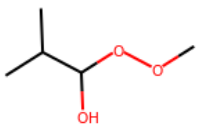
0.039017



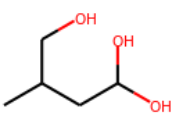
0.039642



0.040188



0.040273



0.041288

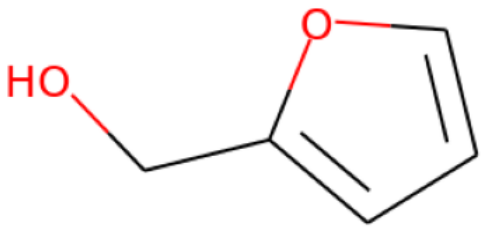
Top predicted substructures	prob		
[OX2H1]	0.9999	[OH][CX4H]	0.8238

[#6H3][#6][#6]	0.9948	[CH3]CC[OH]	0.7833
[CX4H3][#6]	0.9799	OCC[CH2]	0.7512
[CX4H3]	0.9762	[#6H1]	0.7329
[CX4H2]([#6])[O]	0.9332	[#8][#6][#6H2]	0.7134

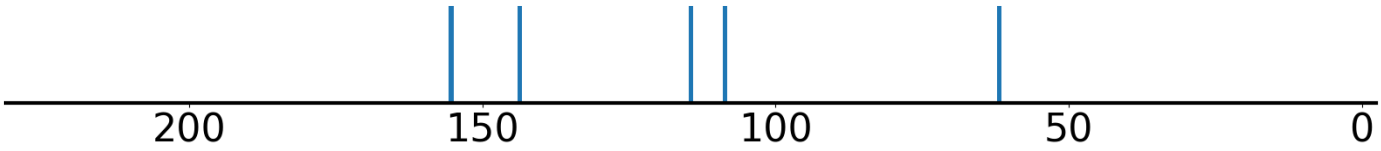
best positives	prob	best negatives	prob
[OX2H1]	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9948	C=CCCC#C	0.0
[CX4H3][#6]	0.9799	C=CC=CC#C	0.0
[CX4H3]	0.9762	CCC=CC#C	0.0
[CX4H2]([#6])[O]	0.9332	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CH3]CC[OH]	0.7833	CC#CCC=C	0.0
OCC[CH2]	0.7512	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2]([OX2H1])[CX4H0]	0.683	CC=CCC#C	0.0
[#8][#6H2][#6H0][#6H2][#8]	0.4732	CC=CC#CC	0.0
[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX4H2]	0.2748	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[OH][CX4H]	0.8238	[#6H3][#6H0]([#6H2])[#6H2]	0.1137
[#6H1]	0.7329	[#6H3][#6H0]	0.1245
[#8][#6][#6H2]	0.7134	[CX4H3][CX4H0]	0.1733
[CX4H3][CX4H1]	0.6912	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX4H2]	0.2748
[#8][#6][#6][#8]	0.4994	[#8][#6H2][#6H0][#6H2][#8]	0.4732
[#8H][#6H2][#6H1]	0.4967	[CX4H2]([OX2H1])[CX4H0]	0.683
C1CC1	0.4629	OCC[CH2]	0.7512
[#6H1][#6H2]	0.4514	[CH3]CC[OH]	0.7833
[CX4H2]([OX2H1])[CX4H1]	0.4394	[CX4H2]([#6])[O]	0.9332
[CX4H2](O)[CHX4]	0.4109	[CX4H3]	0.9762

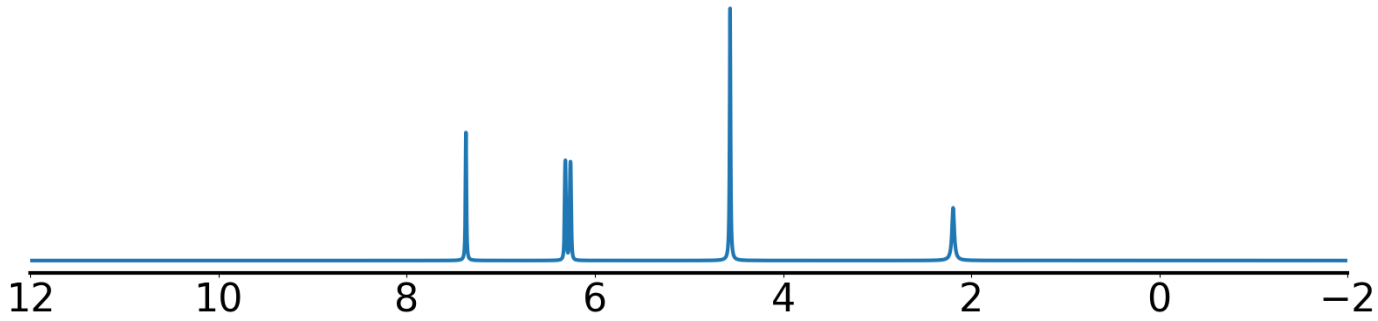
Example 150 true smiles: OCc1ccco1 formula: C5H6O2
Index of correct structure: 0 of 226
True structure loss: 0.023588
True structure:



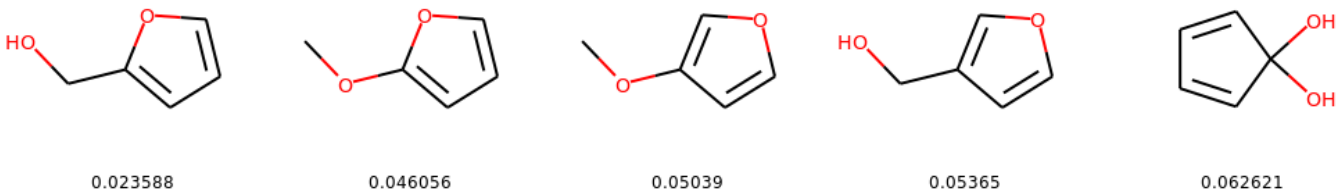
Experimental 13C NMR (solvent: CDCl3)



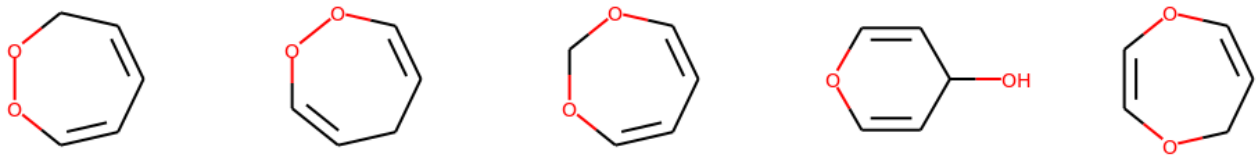
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.023588 0.046056 0.05039 0.05365 0.062621



0.069503 0.073489 0.082126 0.09083 0.091386

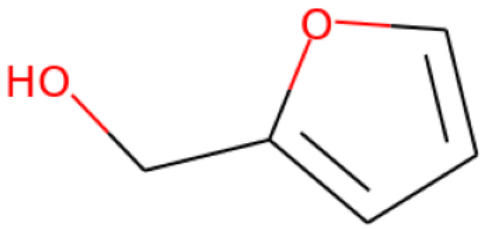
Top predicted substructures	prob		
[#6H1]	0.9999	[#6X3H1][#6X3H0]	0.8704

[#6X3][#6X3]	0.9911	[CX4H2]([#6])[O]	0.8523
[#6H1][#6H1]	0.9161	[#6X3][#6H2][#8]	0.8345
[#8][#6][#6][#6X3]	0.9149	[cH][cH]	0.8209
[OX2H1]	0.9142	[cX3H1]([cX3H1])[cX3H1]	0.7764

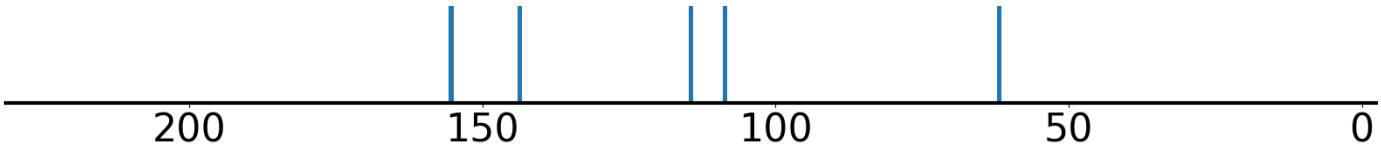
best positives	prob	best negatives	prob
[#6H1]	0.9999	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6X3][#6X3]	0.9911	[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	0.0
[#6H1][#6H1]	0.9161	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#8][#6][#6][#6X3]	0.9149	[CX4H2]([NX3H1])[CX2H0]	0.0
[OX2H1]	0.9142	[CX4H2]([NX3H0])[CX4H3]	0.0
[#6X3H1][#6X3H0]	0.8704	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[CX4H2]([#6])[O]	0.8523	CC#CCC#C	0.0
[#6X3][#6H2][#8]	0.8345	[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.0
[cH][cH]	0.8209	[CX4H2]([CX4H3])[CX2H0]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.7764	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[CHX3](=C)C	0.7159	[CX4H2]([OX2H1])[cX3H0]	0.0949
[CHX3]=[CHX3]	0.438	[#8][#6][#6H2][#8]	0.1477
[#6H1][#6H2]	0.4271	[OX2H1][CX4H2][#6X3H0]	0.1822
[#8][#6][#6]=[#6X3]	0.3879	o[cH]	0.3261
[CX4H2][CX3]=C	0.3824	[#8][#6][#6][#8]	0.3543
[CX3H1](=[CX3H1])[OX2H0]	0.3152	[#8][#6H][#6X3][#6X3H]	0.4084
[CX3H](O)	0.292	[OX2H1][CX4H2][#6X3H0][#8X2H0]	0.4557
[O][CX3H1]=[CX3H1]	0.2425	[#8][#6H0][#6H1]	0.4871
[CX4H]O	0.2304	[#8][#6][#6H2]	0.5545
[CX4H2][CX3H]	0.2241	[#6X3][#6X3][#6X3][#6X3]	0.5709

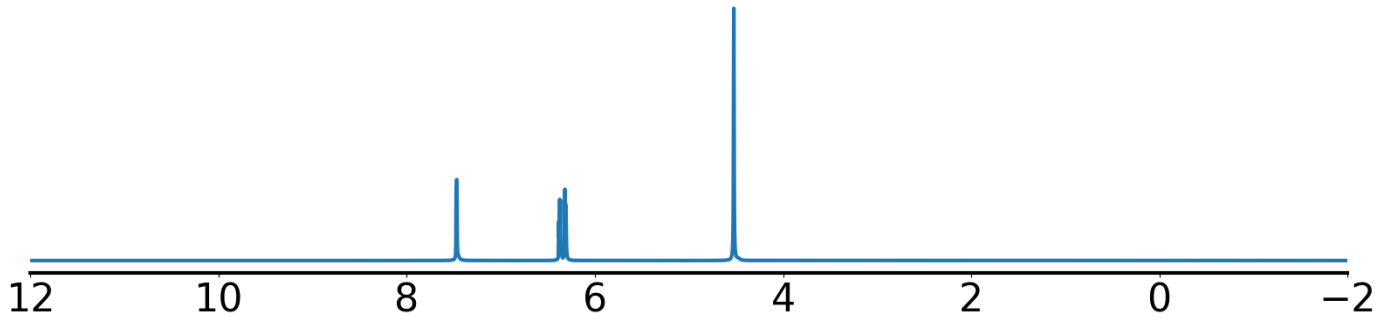
Example 151 true smiles: OCc1ccco1 formula: C5H6O2
Index of correct structure: 0 of 226
True structure loss: 0.017968
True structure:



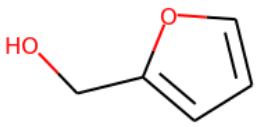
Experimental 13C NMR (solvent: CDCl3)



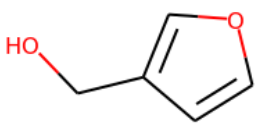
Experimental 1H NMR (solvent: CD3OD)



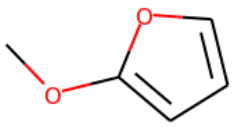
Top predicted structures (loss):



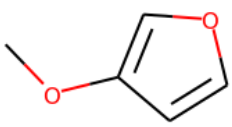
0.017968



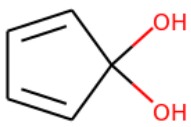
0.049957



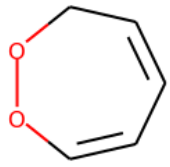
0.054671



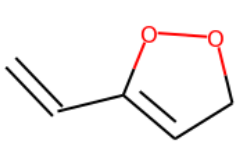
0.060977



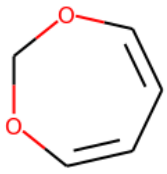
0.077338



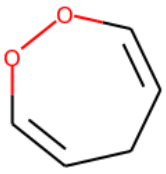
0.081317



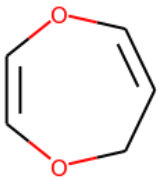
0.094199



0.101299



0.102284



0.102669

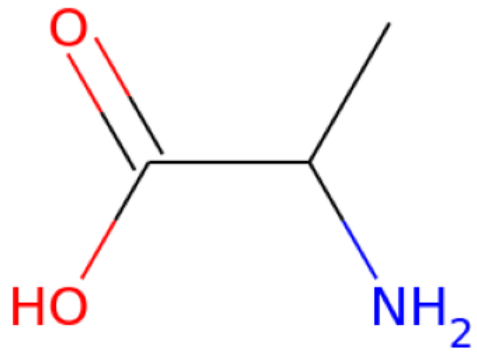
Top predicted substructures	prob		
[#6H1]	0.9995	[#6X3][#6H2][#8]	0.9504

[CX4H2]([#6])[O]	0.9965	[#6X3H1][#6X3H0]	0.9473
[#6X3][#6X3]	0.9931	[#8][#6][#6][#6X3]	0.9254
[OX2H1][CX4H2][#6X3H0]	0.9632	[cH][cH]	0.9207
[OX2H1]	0.9605	[#6X3][#6X3][#6X3][#6X3]	0.8966

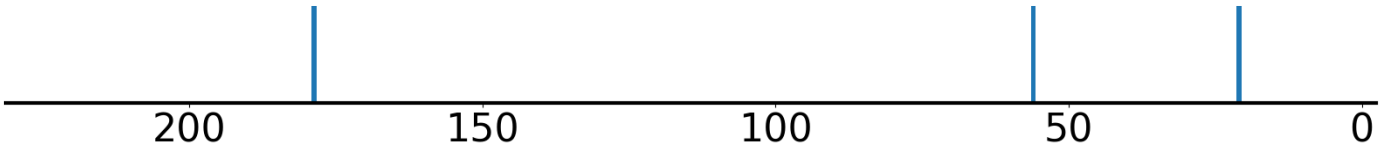
best positives	prob	best negatives	prob
[#6H1]	0.9995	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2]([#6])[O]	0.9965	[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	0.0
[#6X3][#6X3]	0.9931	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[OX2H1][CX4H2][#6X3H0]	0.9632	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[OX2H1]	0.9605	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6H2][#8]	0.9504	CCC#CC#C	0.0
[#6X3H1][#6X3H0]	0.9473	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#8][#6][#6][#6X3]	0.9254	[CX4H2]([CX4H3])[CX2H0]	0.0
[cH][cH]	0.9207	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.8966	[CX4H1]([NX3H0])([CX4H3])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6]=[#6X3]	0.6777	[#8][#6H][#6X3][#6X3H]	0.2424
[#8H][#6H2][#6H1]	0.524	[#8][#6][#6H2]	0.2536
[CHX3](=C)C	0.4629	[#8][#6H1][#6H1]	0.321
[CX4H2][CX3]=C	0.3372	o[cH]	0.3668
O[CX4H2][CX3H1]	0.3193	[#8][#6][#6][#8]	0.3999
[#6H1][#6H2]	0.2514	[#8][#6H0][#6H1]	0.4312
[CHX3]=[CHX3]	0.2479	[#8][#6][#6H2][#8]	0.4949
[CX4H2][CX3H]	0.2123	[cX3H1]([oX2H0])[cX3H1]	0.6041
[#6X3H1]=[#6X3H0]	0.2021	[CX4H2]([OX2H1])[cX3H0]	0.7003
[CX3H1](=[CX3H1])[OX2H0]	0.1898	[cX3H1]([cX3H1])[cX3H1]	0.7882

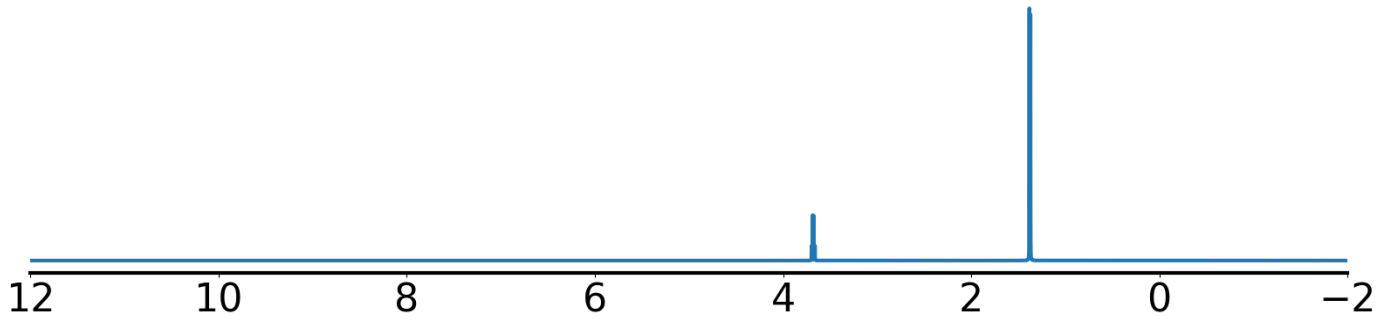
Example 152 true smiles: CC(N)C(=O)O formula: C3H7NO2
Index of correct structure: 0 of 207
True structure loss: 0.011071
True structure:



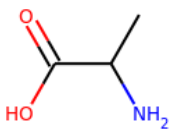
Experimental 13C NMR (solvent: D2O)



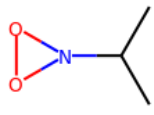
Experimental 1H NMR (solvent: D2O)



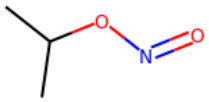
Top predicted structures (loss):



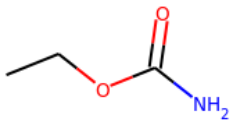
0.011071



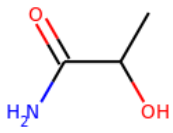
0.036461



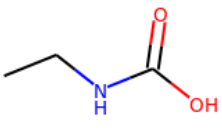
0.052779



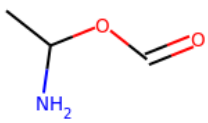
0.054028



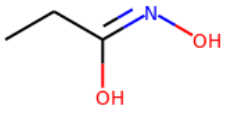
0.056523



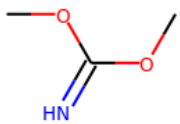
0.057483



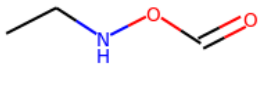
0.057575



0.061684



0.064723



0.067168

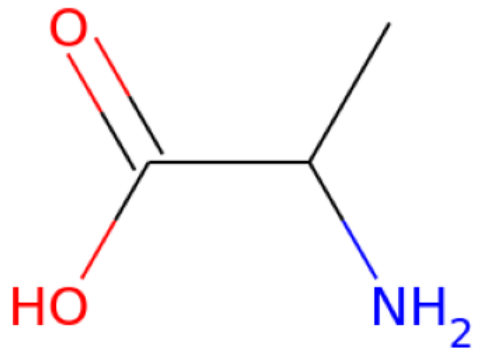
Top predicted substructures	prob		
[CX4H3]	0.9996	[CX4H3][CX4H1]	0.9063

[CX4H3][#6]	0.9967	O=[CX3][CX4H]	0.8844
[#6H3][#6][#6]	0.9886	[#7][#6][#6H3]	0.8753
[CX3](=[OX1])C	0.9771	[CX3](=[OX1])O	0.8642
[#8]=[#6][#8]	0.9273	[#7][#6][#6X3]	0.8558

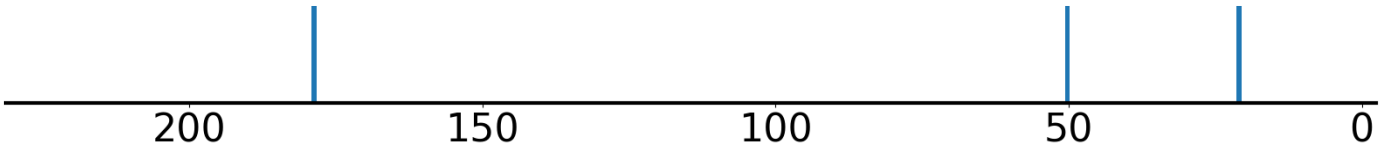
best positives	prob	best negatives	prob
[CX4H3]	0.9996	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H3][#6]	0.9967	C=CCCC#C	0.0
[#6H3][#6][#6]	0.9886	CC=CC#CC	0.0
[CX3](=[OX1])C	0.9771	C=CC=CC#C	0.0
[#8]=[#6][#8]	0.9273	CC=CCC#C	0.0
[CX4H3][CX4H1]	0.9063	[CX2H0](#[CX2H1])[cX3H0]	0.0
O=[CX3][CX4H]	0.8844	CCC#CC#C	0.0
[#7][#6][#6H3]	0.8753	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])O	0.8642	CC#CCC=C	0.0
[#7][#6][#6X3]	0.8558	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[#7H2][#6H0]	0.3668	[CH3]CC[OH]	0.1118
[#7][#6H0][#6H1]	0.2932	[#8][#6H0][#6H1]	0.4938
[#7X3H1]	0.2653	[#7H2][#6H1]	0.5558
[CX4H3][CX4]O	0.2616	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6897
[CX4H]O	0.2026	[OX2H1]	0.7058
[CH3][#6][#8]	0.1987	[#7X3H2]	0.7436
[#8][#6][#6][#6X3]	0.1209	[#6H1]	0.7454
[CX4H2][CX3]=O	0.11	[#6H3][#6][#6X3]	0.7826
[#6X3][#6][#6][#6H3]	0.1009	[#7H2][#6X4H1][#6X3]	0.8132
[OH][CX4H]	0.0873	[CX3](=O)[OX2H1]	0.8154

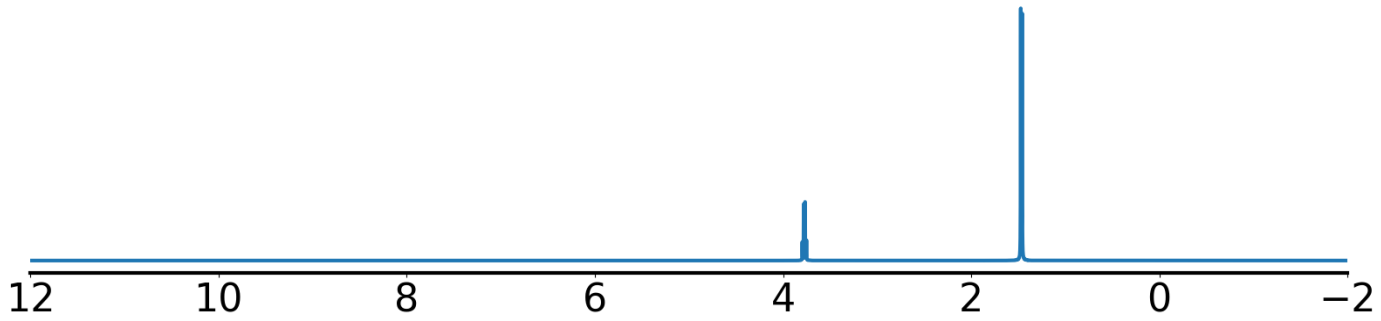
Example 153 true smiles: CC(N)C(=O)O formula: C3H7NO2
Index of correct structure: 0 of 207
True structure loss: 0.011341
True structure:



Experimental 13C NMR (solvent: D2O)

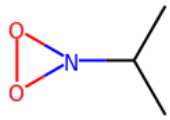


Experimental 1H NMR (solvent: D2O)

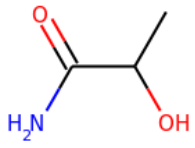


Top predicted structures (loss):

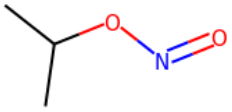
0.011341



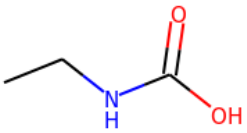
0.04266



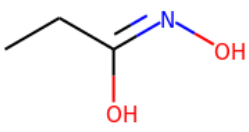
0.05316



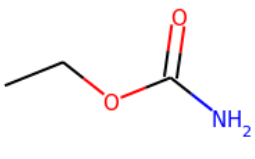
0.059448



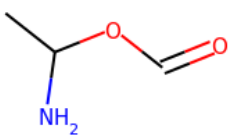
0.060436



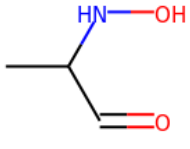
0.061857



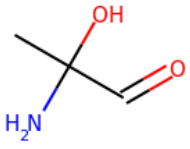
0.062952



0.065264



0.067683



0.070196

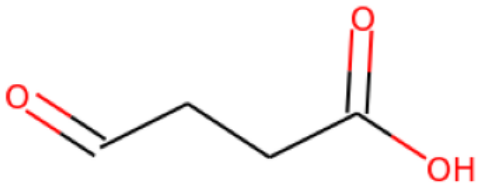
Top predicted substructures	prob		
[CX4H3]	0.9993	[#8]=[#6H0][#6H1]	0.9175

[CX4H3][#6]	0.9934	[#7X3H2]	0.9148
[#6H3][#6][#6]	0.9923	[#8]=[#6][#8]	0.9043
[CX3](=[OX1])C	0.985	[CX4H3][CX4H1]	0.89
O=[CX3][CX4H]	0.9442	[OX2H1]	0.8655

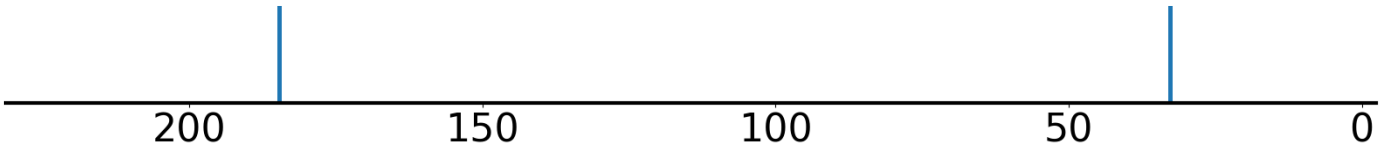
best positives	prob	best negatives	prob
[CX4H3]	0.9993	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9934	CC=CCC#C	0.0
[#6H3][#6][#6]	0.9923	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.985	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
O=[CX3][CX4H]	0.9442	CC=CC#CC	0.0
[#8]=[#6H0][#6H1]	0.9175	C=CCCC#C	0.0
[#7X3H2]	0.9148	CCC#CC#C	0.0
[#8]=[#6][#8]	0.9043	CCC#CC=C	0.0
[CX4H3][CX4H1]	0.89	[CX2H0](#[CX2H1])[CX4H2]	0.0
[OX2H1]	0.8655	[CX3H1](=[CX3H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7][#6H0][#6H1]	0.4468	[CH3]CC[OH]	0.153
[#8]=[#6][#6H1][#6H1]	0.3211	[#8][#6H0][#6H1]	0.5033
[#7H2][#6H0]	0.2911	[#7H2][#6X4H1][#6X3]	0.7191
[#7X3H1]	0.2705	[#7][#6][#6H3]	0.735
[CX4H]O	0.2573	[#7][#6][#6X3]	0.7472
[CX4H3][CX4]O	0.2464	[#7H2][#6H1]	0.7725
[#8][#6][#6][#6X3]	0.1986	[#6H3][#6][#6X3]	0.7916
[OH][CX4H]	0.1881	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.8314
[#6X4H3][#6][#8H]	0.1558	[#6H1]	0.8339
[CX4H2]CC=O	0.137	[CX3](=[OX1])O	0.8379

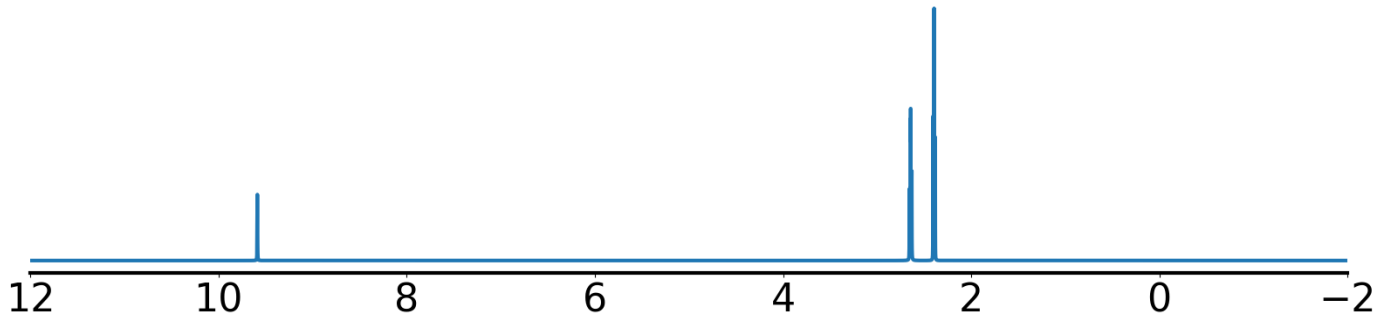
Example 154 true smiles: O=CCCC(=O)O formula: C4H6O3
Index of correct structure: 0 of 195
True structure loss: 0.029319
True structure:



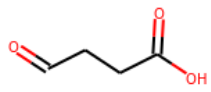
Experimental 13C NMR (solvent: D2O)



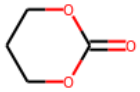
Experimental 1H NMR (solvent: D2O)



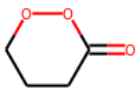
Top predicted structures (loss):



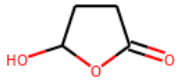
0.029319



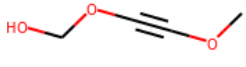
0.065265



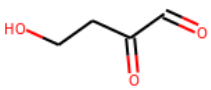
0.066793



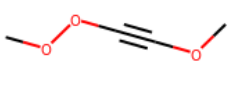
0.068062



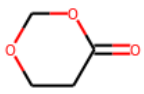
0.072635



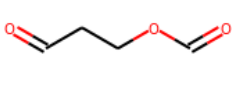
0.073666



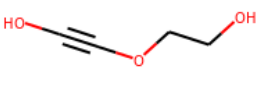
0.074645



0.089031



0.090288



0.097527

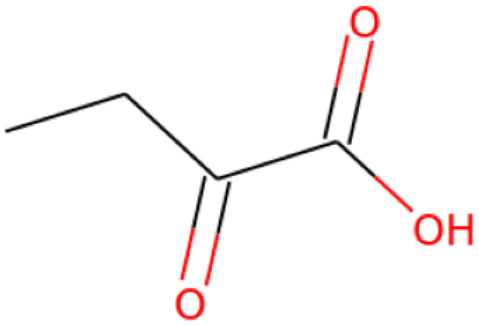
Top predicted substructures	prob		
[CX3](=[OX1])C	0.9962	[#6H1]	0.873

[CX3H1](=O)[#6]	0.9911	[OX2H1]	0.8726
[CX4H2]([#6])[#6]	0.9787	[CX4H2]CC=O	0.8403
[#8]=[#6][#8]	0.927	[CX4H2][CX4H2]	0.8351
[CX3](=[OX1])O	0.8876	OCC[CH2]	0.8214

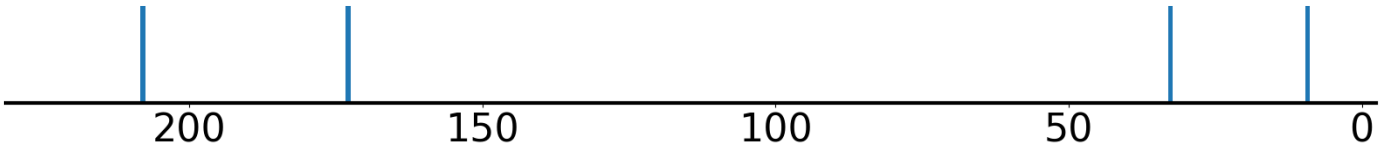
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9962	C=CC=CC#C	0.0
[CX3H1](=O)[#6]	0.9911	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[#6]	0.9787	CC=CC#CC	0.0
[#8]=[#6][#8]	0.927	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX3](=[OX1])O	0.8876	CCC#CC#C	0.0
[#6H1]	0.873	CCC=CC#C	0.0
[OX2H1]	0.8726	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2]CC=O	0.8403	[#6H2]=[#6][#6X2]	0.0
[CX4H2][CX4H2]	0.8351	[CX2H0](#[CX2H1])[cX3H0]	0.0
OCC[CH2]	0.8214	CC=CCC#C	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H0]	0.3981	[CX4H2][CX3H]	0.0117
O=CC=O	0.3297	[CX3H1](=[OX1H0])[CX4H2]	0.0423
[#8][#6H0][#6H1]	0.3077	[OX1H0]=[CX3H1][CX4H2][CX4H2]	0.0469
[#8][#6][#6]=[#8]	0.2754	[CX4H2]([CX4H2])[CX3H1]	0.0842
[CX4H2]([CX4H2])[CX4H2]	0.2414	[#8]=[#6][#6][#6][#6]=[#8]	0.1413
[#8]=[#6H0][#6H1]	0.189	[#8][#6][#6][#6][#6]=[#8]	0.1799
[OX2H0][CX3H0][CX4H2]	0.1776	[#6H1][#6H2]	0.1972
[#6X3][#6X3]	0.1597	[CX4H2][CX3]=O	0.3995
[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.1444	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.4094
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.1335	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.4332

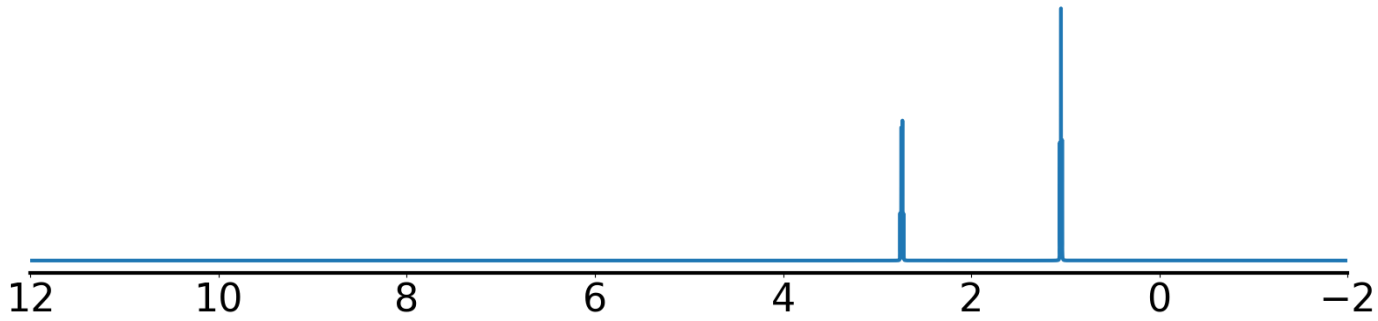
Example 155 true smiles: CCC(=O)C(=O)O formula: C4H6O3
Index of correct structure: 0 of 195
True structure loss: 0.008142
True structure:



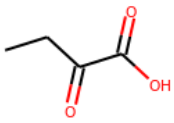
Experimental 13C NMR (solvent: DMSO)



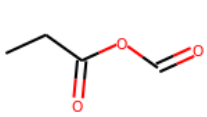
Experimental 1H NMR (solvent: D2O)



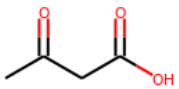
Top predicted structures (loss):



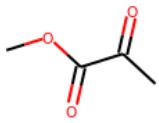
0.008142



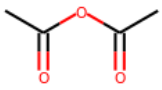
0.051879



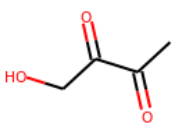
0.089521



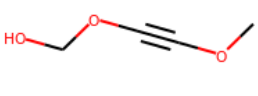
0.10688



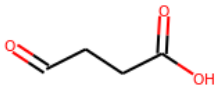
0.112216



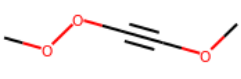
0.112651



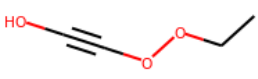
0.121922



0.122697



0.124217



0.130724

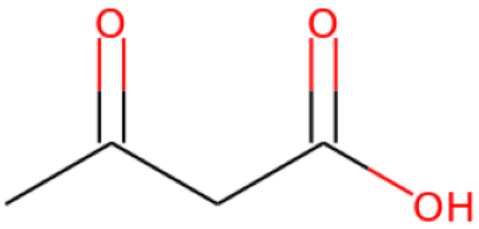
Top predicted substructures	prob		
[CX3](=[OX1])C	0.9999	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9965

[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9994	[CX4H3][#6]	0.9962
[CX4H2]([#6])[#6]	0.999	[#6H3][#6][#6]	0.995
[CX4H2]([CX4H3])[CX3H0]	0.997	[CX4H3][CX4H2]	0.9906
[CX4H3]	0.9966	[#8]=[#6][#8]	0.9831

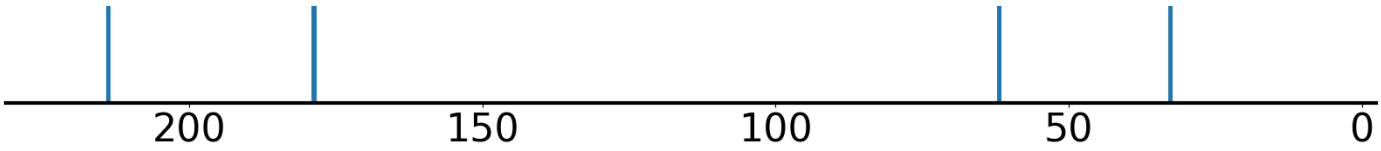
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9999	[CX2H0](#[CX2H1])[CX2H0]	0.0
[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9994	CCC#CC#C	0.0
[CX4H2]([#6])[#6]	0.999	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H2]([CX4H3])[CX3H0]	0.997	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3]	0.9966	CCC=CC#C	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9965	C=CCCC#C	0.0
[CX4H3][#6]	0.9962	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#6H3][#6][#6]	0.995	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][CX4H2]	0.9906	[CX2H0](#[CX2H1])[CX3H1]	0.0
[#8]=[#6][#8]	0.9831	C=CC=CC#C	0.0

worst negatives	prob	worst positives	prob
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.469	OCC[CH2]	0.5116
[#8][#6][#6H2]	0.3429	[CX4H2]CC=O	0.5538
[#8]=[#6][#6][#6][#6]=[#8]	0.2988	[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.5577
O=[#6][#6][#6X3]	0.277	[#6X3][#6X3]	0.6624
[OX2H0][CX3H0][CX4H2]	0.2184	[#6X3][#6][#6][#6H3]	0.6751
[#8X1]=[#6X3][#6H2][#6H0]	0.1557	[CX3](=O)[OX2H1]	0.6898
[#8][#6][#6][#6X3]	0.1495	[#8][#6][#6]=[#8]	0.7467
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1464	O=CC=O	0.8112
[#6X3][#6H2][#6X3]	0.0971	[#8]=[#6][#6]=[#8]	0.8589
CCCCCC	0.0713	[OX2H1]	0.8999

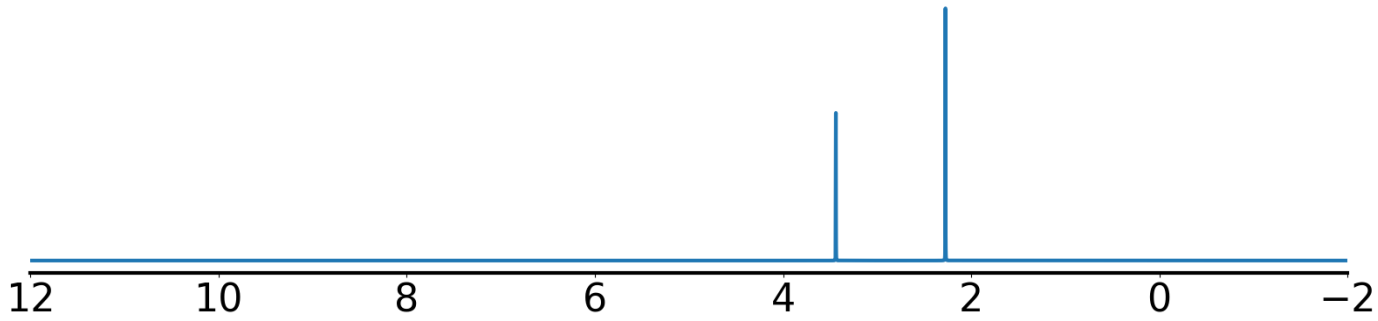
Example 156 true smiles: CC(=O)CC(=O)O formula: C4H6O3
Index of correct structure: 0 of 195
True structure loss: 0.015394
True structure:



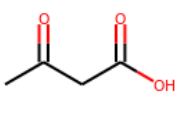
Experimental 13C NMR (solvent: D2O)



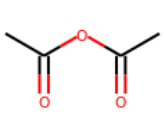
Experimental 1H NMR (solvent: D2O)



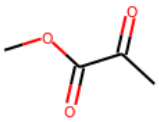
Top predicted structures (loss):



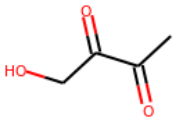
0.015394



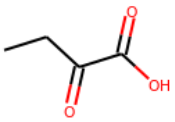
0.050129



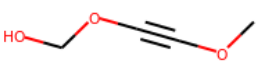
0.063121



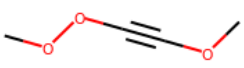
0.079611



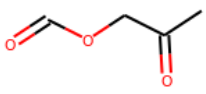
0.08312



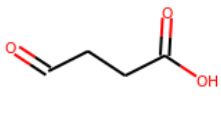
0.087835



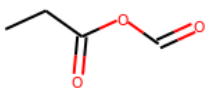
0.088136



0.094407



0.097968



0.106133

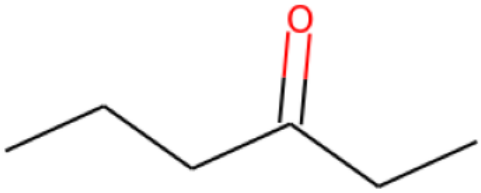
Top predicted substructures	prob		
[CX3](=[OX1])C	1.0	[OX1H0]=[CX3H0][CX4H3]	0.9704

[CX4H3]	0.997	[#6H3][#6H0]	0.9487
[CX4H3][CX3]	0.9862	[CX4H2][CX3]=O	0.9306
[CX4H3][CX3H0]	0.978	[#6H3][#6][#6]	0.8891
[CX4H2]([CX3H0])[CX3H0]	0.9753	[CX3](=[OX1])O	0.8459

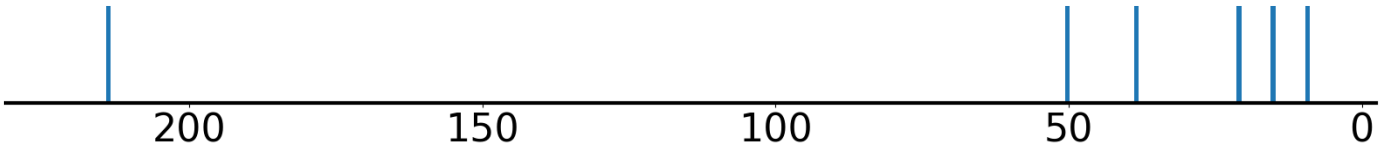
best positives	prob	best negatives	prob
[CX3](=[OX1])C	1.0	CC=CC#CC	0.0
[CX4H3]	0.997	[#6X2][#6H1][#6X2]	0.0
[CX4H3][CX3]	0.9862	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H3][CX3H0]	0.978	CC=CCC#C	0.0
[CX4H2]([CX3H0])[CX3H0]	0.9753	CCC#CC=C	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9704	C=CC=CC#C	0.0
[#6H3][#6H0]	0.9487	CCC=CC#C	0.0
[CX4H2][CX3]=O	0.9306	[#6H2]=[#6][#6X2]	0.0
[#6H3][#6][#6]	0.8891	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[CX3](=[OX1])O	0.8459	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H3][OX2H0]	0.4627	[#6X3][#6][#6][#6H3]	0.2811
[#8]=[#6][#6][#6][#6]=[#8]	0.4536	[#8][#6][#6][#6X3]	0.468
[CX4H2]CC=O	0.3838	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.4844
[#8][#6][#6][#6][#6]=[#8]	0.3529	[#6H3][#6X3H0][#6H2]	0.5088
O=CC=O	0.2683	[CX4H2]([#6])[#6]	0.5449
[#8][#6][#6]=[#8]	0.2257	[#8][#6][#6H2]	0.5671
[#6H3][#6][#6X3]	0.2101	[OX2H1]	0.5715
[#8]=[#6][#6]=[#8]	0.2052	O=[#6][#6][#6X3]	0.5936
[#8]=[#6H0][#6H1]	0.1744	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.6666
OCC[CH2]	0.1712	[CX3](=O)[OX2H1]	0.687

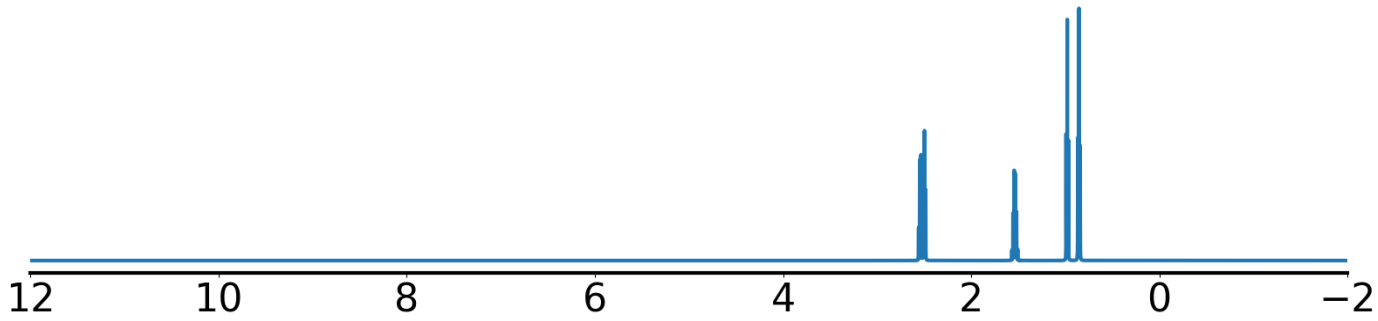
Example 157 true smiles: CCCC(=O)CC formula: C6H12O
Index of correct structure: 0 of 193
True structure loss: 0.004278
True structure:



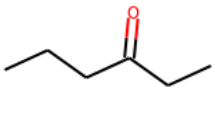
Experimental 13C NMR (solvent: CDCl3)



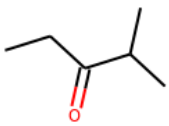
Experimental 1H NMR (solvent: D2O)



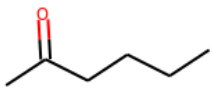
Top predicted structures (loss):



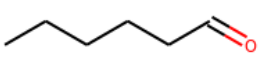
0.004278



0.043035

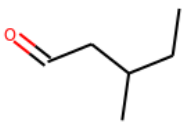


0.063048

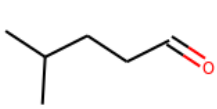


0.068929

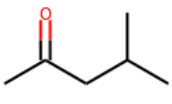
0.08883



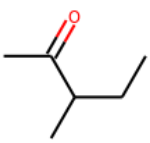
0.097767



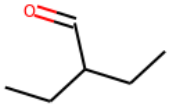
0.103281



0.110448



0.113741



0.117429

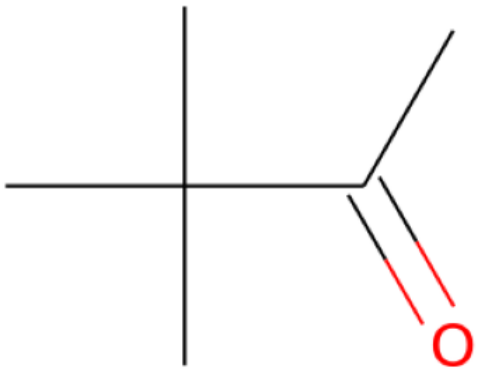
Top predicted substructures	prob		
[CX4H3][CX4H2]	1.0	[CX4H3][#6]	0.9997

[CX4H3]	1.0	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9996
[CX4H2]([#6])[#6]	1.0	[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9835
[CX3](=[OX1])C	0.9999	[CX4H2][CX3]=O	0.9814
[#6H3][#6][#6]	0.9999	[CX4H2]([CX4H3])[CX4H2]	0.9508

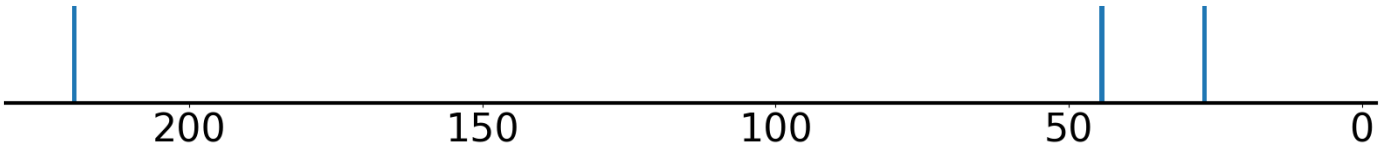
best positives	prob	best negatives	prob
[CX4H3][CX4H2]	1.0	C=CC=CC#C	0.0
[CX4H3]	1.0	C=CCCC#C	0.0
[CX4H2]([#6])[#6]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])C	0.9999	[CX2H0](#[CX2H1])[CX3H1]	0.0
[#6H3][#6][#6]	0.9999	CCC=CC#C	0.0
[CX4H3][#6]	0.9997	[CX2H0](#[CX2H0])[CX2H0]	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9996	[CX2H0](#[CX2H1])[CX2H0]	0.0
[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9835	CCC#CC=C	0.0
[CX4H2][CX3]=O	0.9814	CC=CC#CC	0.0
[CX4H2]([CX4H3])[CX4H2]	0.9508	[OX2H1][CX4H1][CX4H1][CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#6H2][#6H1]	0.1648	O=[CX3H0][CX4H2][CX4H2]	0.6941
[#8]=[#6H0][#6H1]	0.1392	[#6H3][#6][#6X3]	0.7058
[#6H3][#6][#6][#6H3]	0.1214	[CX4H2]CC=O	0.7405
[CX4H3][CX4H1]	0.1185	[#6X3][#6][#6][#6H3]	0.7461
[CX3H0](=[OX1H0])([CX4H2])[CX4H1]	0.1178	CCCCCC	0.8021
[#6H1]	0.1142	[#6H2][#6X3H0][#6H2]	0.8155
[#6H1][#6H2]	0.1054	[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.8414
O=[CX3][CX4H]	0.0938	[CX4H2][CX4H2]	0.8504
[CX4H2]([CX4H2])[CX4H1]	0.0815	[CX4H2]([CX4H2])[CX3H0]	0.8792
O=[CX3H0][CX4H2][CX4H1]	0.0606	[CX4H2]([CX4H3])[CX3H0]	0.9226

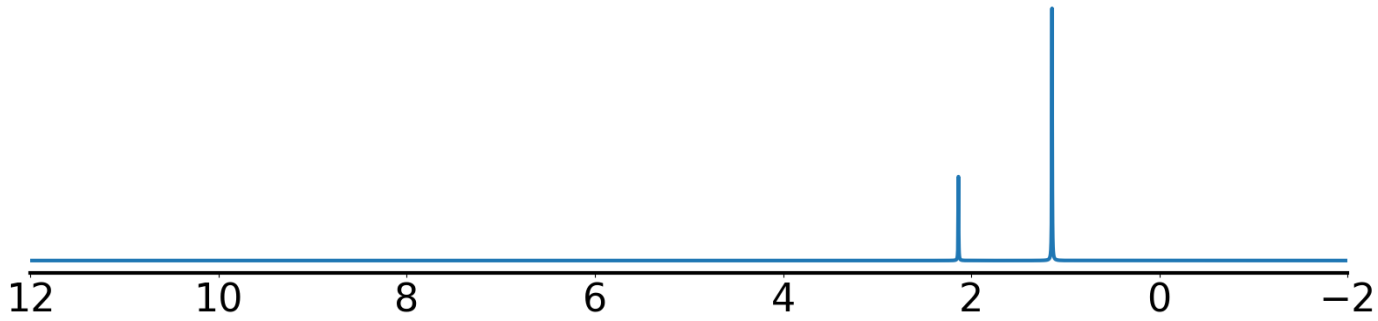
Example 158 true smiles: CC(=O)C(C)(C)C formula: C6H12O
Index of correct structure: 0 of 193
True structure loss: 0.007709
True structure:



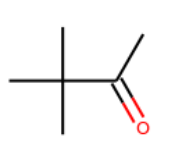
Experimental 13C NMR (solvent: CDCl3)

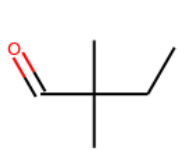


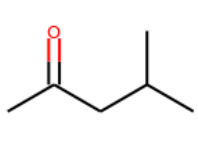
Experimental 1H NMR (solvent: CDCl3)

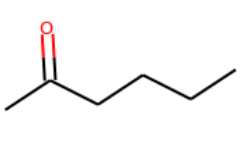


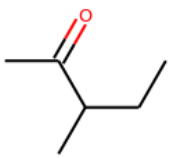
Top predicted structures (loss):

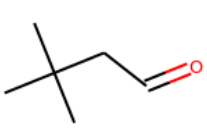

0.007709

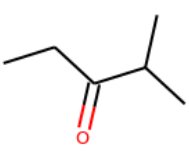

0.056767


0.065416

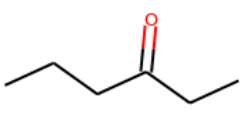

0.07255

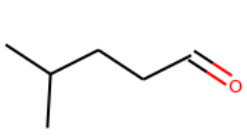

0.074018


0.074218


0.074584


0.089033


0.099302


0.103097

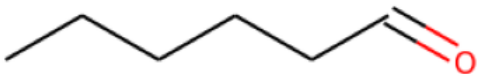
Top predicted substructures	prob		
[#6H3][#6][#6]	0.9999	[CX4H3][CX4H0][CX4H3]	0.9969

[CX3](=[OX1])C	0.9995	[CX4H3][CX4H0]	0.9915
[CX4H3]	0.9993	[CX4H3][CX3]	0.9662
[CX4H3][#6]	0.9987	[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.9079
[#6H3][#6H0]	0.9984	[CX4H3][CX3H0]	0.8839

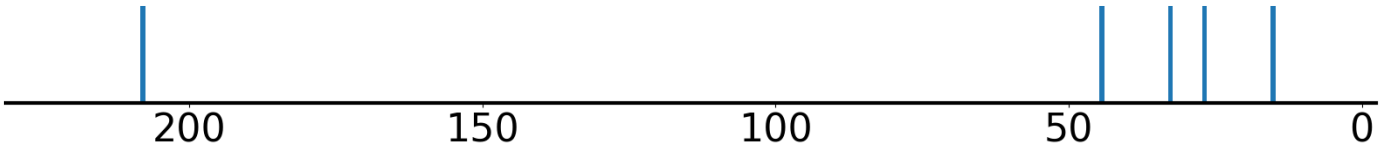
best positives	prob	best negatives	prob
[#6H3][#6][#6]	0.9999	CCC#CC#C	0.0
[CX3](=[OX1])C	0.9995	C=CC=CC#C	0.0
[CX4H3]	0.9993	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][#6]	0.9987	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H3][#6H0]	0.9984	CC=CCC#C	0.0
[CX4H3][CX4H0][CX4H3]	0.9969	[#7][#6]=[#6][#6]#[#7]	0.0
[CX4H3][CX4H0]	0.9915	CC=CC#CC	0.0
[CX4H3][CX3]	0.9662	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.9079	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][CX3H0]	0.8839	[CX2H0](#[CX2H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.5581	[#6H3][#6][#6][#6H3]	0.3797
[CX4H2][CX3]=O	0.5449	[#6H3][#6][#6X3]	0.7535
[#6X3][#6][#6][#6H3]	0.4247	[OX1H0]=[CX3H0][CX4H3]	0.8426
[CX4H3][CX4H1]	0.3629	[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.8432
[#8]=[#6H0][#6H1]	0.2848	[CX4]([CX4H3])([CX4H3])[CX4H3]	0.8489
[CX4H2]CC=O	0.2573	[CX4H3][CX3H0]	0.8839
[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.2202	[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.9079
O=[CX3][CX4H]	0.1856	[CX4H3][CX3]	0.9662
O=[#6][#6H][#6H0]	0.1538	[CX4H3][CX4H0]	0.9915
[CHX4]([CH3X4])[CH3X4]	0.1528	[CX4H3][CX4H0][CX4H3]	0.9969

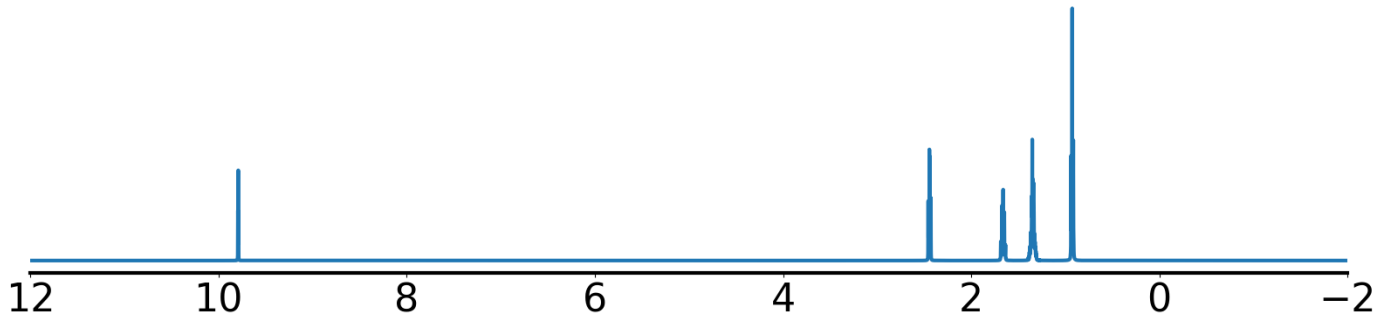
Example 159 true smiles: CCCCCC=O formula: C6H12O
Index of correct structure: 0 of 193
True structure loss: 0.006741
True structure:



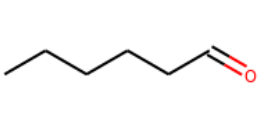
Experimental 13C NMR (solvent: CDCl3)



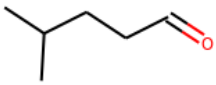
Experimental 1H NMR (solvent: CDCl3)



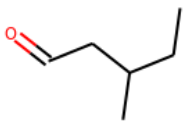
Top predicted structures (loss):



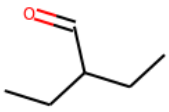
0.006741



0.040046

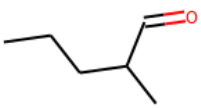


0.05417

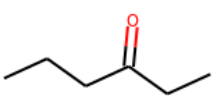


0.055096

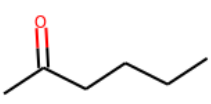
0.059002



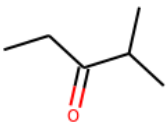
0.064702



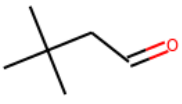
0.074501



0.093925



0.09467



0.107658

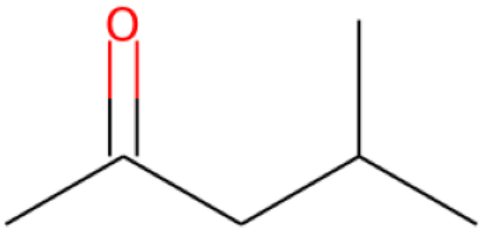
Top predicted substructures	prob		
[CX3H1](=O)[#6]	1.0	[CX4H3]	0.9973

[CX4H2]([#6])[#6]	0.9999	[#6H3][#6][#6]	0.9969
[CX3](=[OX1])C	0.9998	[#6H1]	0.995
[CX4H3][CX4H2]	0.9992	[CX4H2]CC=O	0.9574
[CX4H3][#6]	0.9979	[CX4H2]([CX4H2])[CX4H2]	0.9134

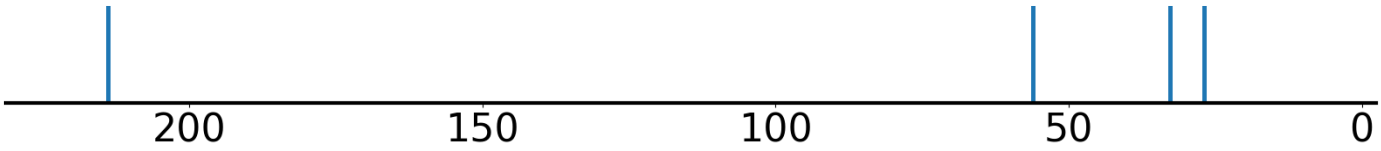
best positives	prob	best negatives	prob
[CX3H1](=O)[#6]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	0.9999	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9998	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][CX4H2]	0.9992	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9979	C=CC=CC#C	0.0
[CX4H3]	0.9973	[OX2H1][CX4H1][CX4H1][CX2H0]	0.0
[#6H3][#6][#6]	0.9969	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[#6H1]	0.995	CC#CCC#C	0.0
[CX4H2]CC=O	0.9574	CCC=CC#C	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9134	[#6X2][#6H1][#6X2]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6][#6][#6H3]	0.2147	[CX4H2][CX3H]	0.3727
[CX4H2]([CX4H3])[CX4H1]	0.1231	[CX4H2]([CX4H2])[CX3H1]	0.4797
[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.1108	[CX4H2][CX3]=O	0.5063
[CX3H1](=[OX1H0])[CX4H0]	0.1074	[#6H1][#6H2]	0.6097
[#6H1][#6H1]	0.107	CCCCCC	0.6468
[CX4H2]([CX4H2])[CX4H1]	0.1042	[OX1H0]=[CX3H1][CX4H2][CX4H2]	0.6508
[#6H1]([#6H2])[#6H2]	0.0985	[CX4H2][CX4H2][CX4H2][CX4H2]	0.7191
[CX4H3][CX4H1]	0.0728	[CX3H1](=[OX1H0])[CX4H2]	0.7238
[#6H3][#6][#6X3]	0.0519	[CX4H2][CX4H2]	0.8842
[CX4H2]([CX4H2])[CX3H0]	0.0481	[CX4H2]([CX4H3])[CX4H2]	0.8852

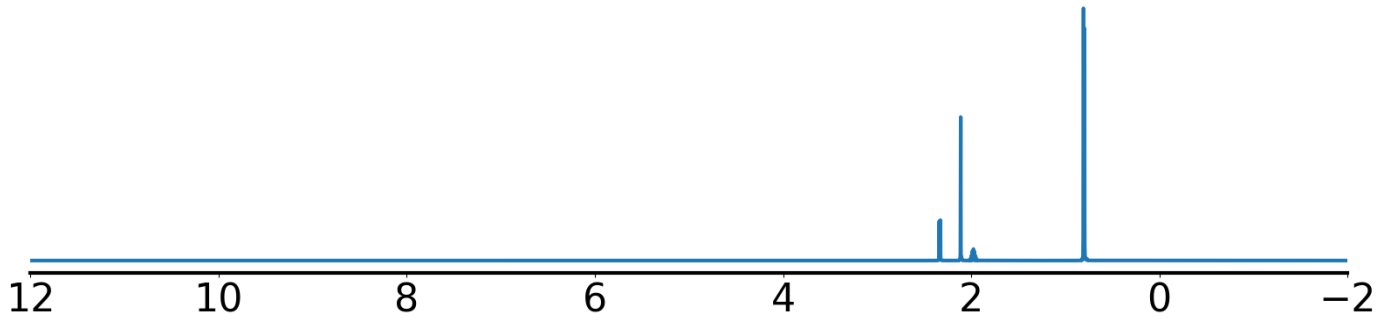
Example 160 true smiles: CC(=O)CC(C)C formula: C6H12O
Index of correct structure: 0 of 193
True structure loss: 0.009541
True structure:



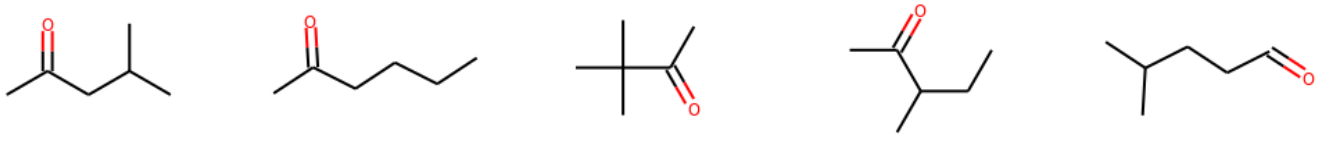
Experimental 13C NMR (solvent: CDCl3)



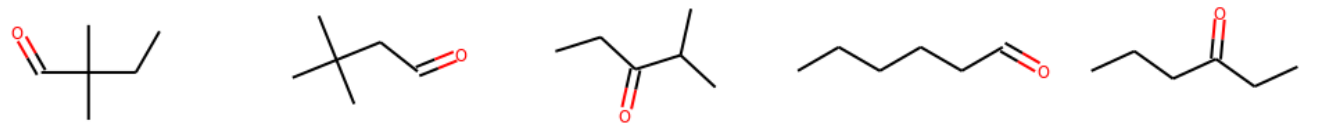
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.009541 0.043412 0.047147 0.070068 0.076053



0.083305 0.09189 0.09201 0.096687 0.099413

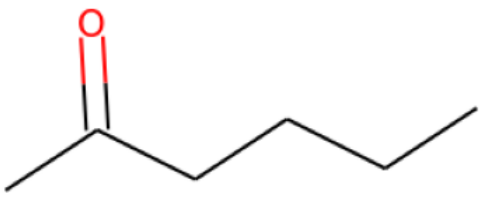
Top predicted substructures	prob		
[#6H3][#6][#6]	1.0	[OX1H0]=[CX3H0][CX4H3]	0.9982

[CX4H3]	1.0	[CX4H3][CX3]	0.9981
[CX3](=[OX1])C	0.9996	[#6H3][#6H0]	0.9626
[CX4H3][#6]	0.9993	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9611
[CX4H3][CX3H0]	0.9983	[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.9469

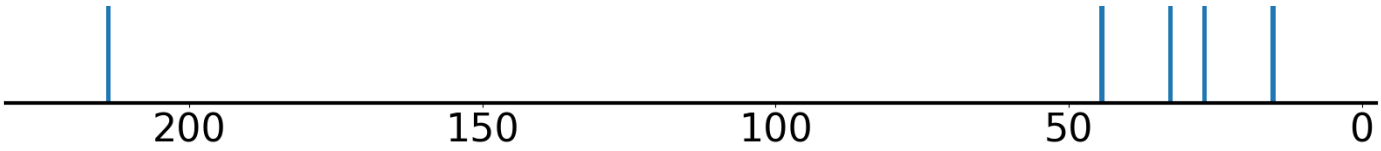
best positives	prob	best negatives	prob
[#6H3][#6][#6]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	1.0	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9996	CCC=CC#C	0.0
[CX4H3][#6]	0.9993	CC=CC#CC	0.0
[CX4H3][CX3H0]	0.9983	[CX2H0](#[CX2H0])[CX2H0]	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9982	CCC#CC#C	0.0
[CX4H3][CX3]	0.9981	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#6H3][#6H0]	0.9626	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9611	CCC#CC=C	0.0
[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.9469	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]CC=O	0.5612	[#6H1][#6H2]	0.4289
CCCCCC	0.2617	[CX4H2]([CX4H1])[CX3H0]	0.4298
[#6H3][#6H0]([#6H2])[#6H2]	0.2057	[#8]=[#6][#6H2][#6H1]	0.4642
[#8X1]=[#6X3][#6H2][#6H0]	0.1921	O=[CX3H0][CX4H2][CX4H1]	0.4758
[#6H3][#6][#6X3]	0.1103	[CHX4]([CH3X4])[CH2X4]	0.5663
[CX4H2][CX4H2]	0.1	[CX4H3][CX4H1]	0.5814
[OX1H0]=[CX3H0][CX4H2][CX4H0]	0.0946	[#6H1]	0.588
[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.0846	[CHX4]([CH3X4])[CH3X4]	0.7787
[CX4H3][CX4H0]	0.0749	[#6X3][#6][#6][#6H3]	0.7862
O=[CX3H0][CX4H2][CX4H2]	0.0741	[CX4H2][CX3]=O	0.8085

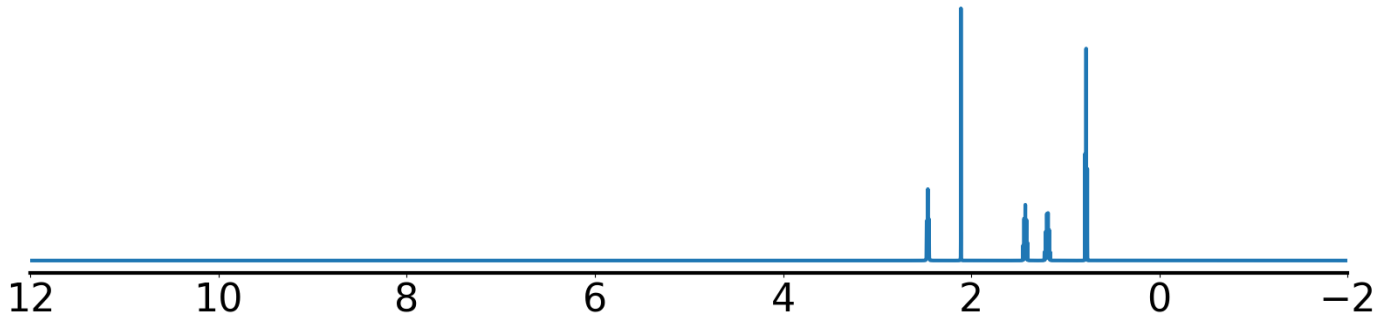
Example 161 true smiles: CCCCC(C)=O formula: C6H12O
Index of correct structure: 0 of 193
True structure loss: 0.003486
True structure:



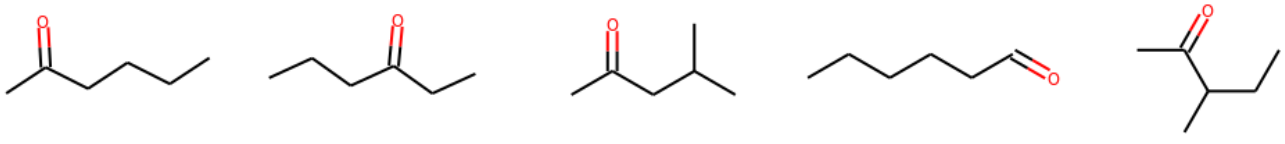
Experimental 13C NMR (solvent: CDCl3)



Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.003486 0.054926 0.057944 0.070309 0.078111

0.092744 0.097976 0.099465 0.109902 0.118524

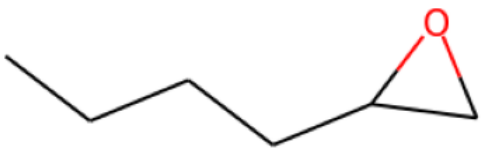
Top predicted substructures	prob		
[CX4H3]	0.9998	[CX4H3][CX4H2]	0.9985

[CX3](=[OX1])C	0.9998	[CX4H3][CX3H0]	0.9979
[#6H3][#6][#6]	0.9996	[CX4H3][CX3]	0.997
[CX4H2]([#6])[#6]	0.9995	[OX1H0]=[CX3H0][CX4H3]	0.9953
[CX4H3][#6]	0.9993	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9871

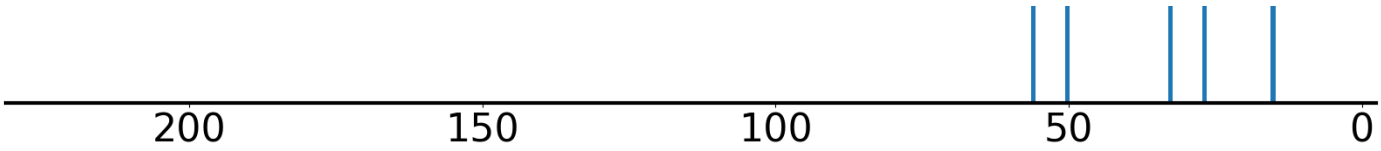
best positives	prob	best negatives	prob
[CX4H3]	0.9998	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])C	0.9998	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9996	CCC#CC#C	0.0
[CX4H2]([#6])[#6]	0.9995	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][#6]	0.9993	CCC=CC#C	0.0
[CX4H3][CX4H2]	0.9985	CC=CC#CC	0.0
[CX4H3][CX3H0]	0.9979	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CX4H3][CX3]	0.997	CC=CCC#C	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9953	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9871	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6][#6][#6H3]	0.2448	[CX4H2]([CX4H2])[CX4H2]	0.752
[CX4H2][CX4H2][CX4H2][CX4H2]	0.2329	CCCCCC	0.7559
[#6H1][#6H2]	0.1865	[CX4H2][CX4H2]	0.7812
[#6H3][#6][#6X3]	0.1378	[CX4H2]CC=O	0.9099
[#6H1]	0.1272	[CX4H2][CX3]=O	0.9109
[#6H3][#6][#6][#6H3]	0.1162	[#6H3][#6X3H0][#6H2]	0.9166
[#6H2][#6X3H0][#6H2]	0.0517	[CX4H2]([CX4H2])[CX3H0]	0.9228
[OX1H0]=[CX3H1][CX4H2][CX4H2]	0.0493	[#6H3][#6H0]	0.9492
[#8]=[#6H0][#6H1]	0.0469	[CX4H2]([CX4H3])[CX4H2]	0.9667
[CX4H3][CX4H1]	0.0448	O=[CX3H0][CX4H2][CX4H2]	0.9765

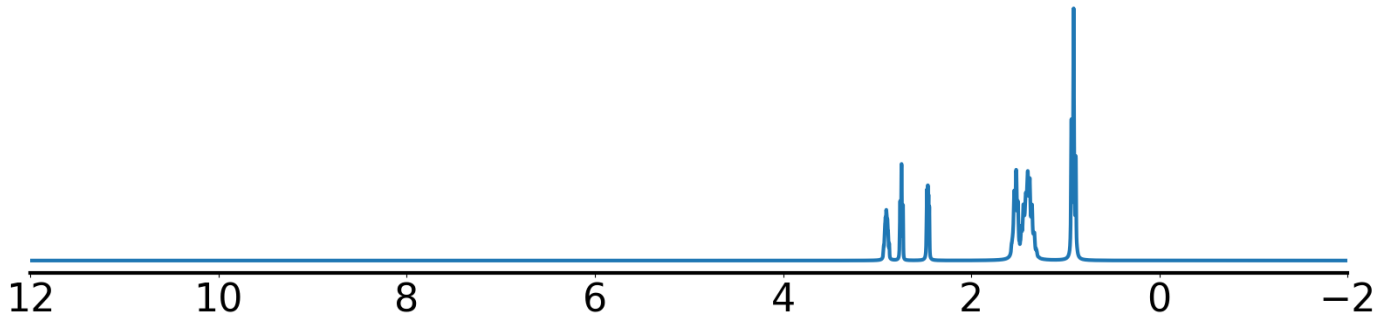
Example 162 true smiles: CCCCC1CO1 formula: C6H12O
Index of correct structure: 0 of 193
True structure loss: 0.010964
True structure:



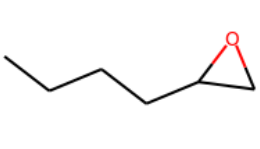
Experimental 13C NMR (solvent: CDCl3)



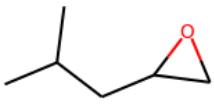
Experimental 1H NMR (solvent: CDCl3)



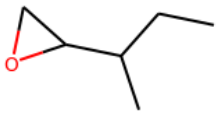
Top predicted structures (loss):



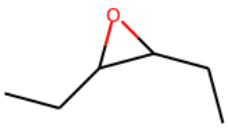
0.010964



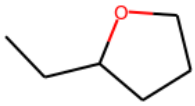
0.039952



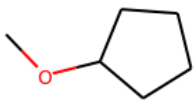
0.047401



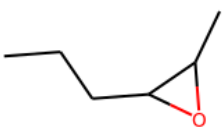
0.054853



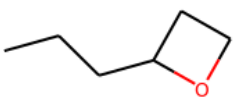
0.079513



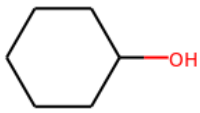
0.081922



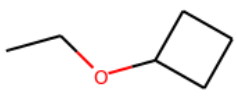
0.088865



0.092896



0.094128



0.094401

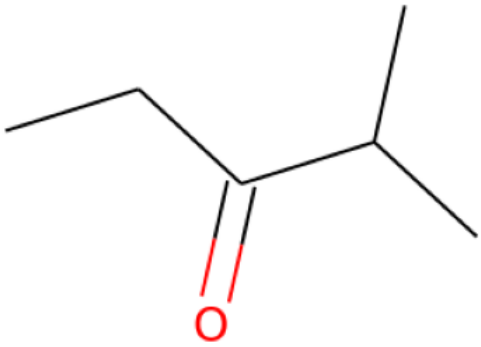
Top predicted substructures	prob		
[CX4H3]	0.9999	[CX4H3][#6]	0.9924

[#6H3][#6][#6]	0.9994	[#6H1]	0.9904
[CX4H2]([#6])[#6]	0.9993	[#6H2][#6H1r3]	0.9852
[CX4H3][CX4H2]	0.9983	[CX4H]O	0.985
[OX2H0]1[CX4H2][CX4H1]1	0.9978	C1OC1	0.9811

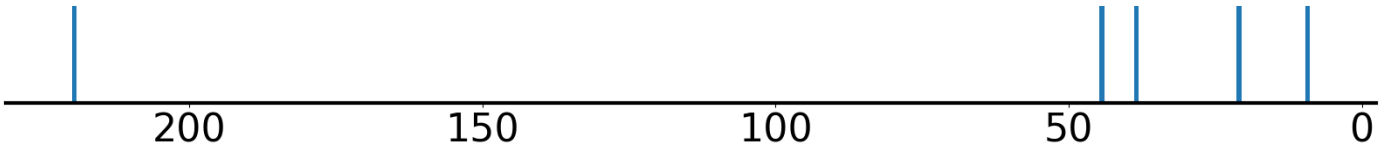
best positives	prob	best negatives	prob
[CX4H3]	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9994	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	0.9993	C=CC=CC#C	0.0
[CX4H3][CX4H2]	0.9983	C=CCCC#C	0.0
[OX2H0]1[CX4H2][CX4H1]1	0.9978	CC=CCC#C	0.0
[CX4H3][#6]	0.9924	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#6H1]	0.9904	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6H2][#6H1r3]	0.9852	[CX4H3][nX3H0]	0.0
[CX4H]O	0.985	[#7][#6]=[#6][#6]#[#7]	0.0
C1OC1	0.9811	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H3])[CX4H1]	0.7099	[OX2H0][CX4H1][CX4H2][CX4H2]	0.4635
[#8][#6H1][#6H1]	0.4617	CCCCCC	0.5569
[#6H1][#6H1]	0.4114	[#6H1]([#6H2])[#6H2]	0.5649
[CX4H2][CX4H2][CX4H2][CX4H2]	0.3018	[CX4H2]([CX4H2])[CX4H2]	0.607
O[CX4H]([CX4H2])[CX4H1]	0.3017	[CX4H2]([CX4H2])[CX4H1]	0.6125
[#6H2][#6H1][#6H1][#6H2]	0.2298	[CX4H2]([CX4H3])[CX4H2]	0.639
[OX2H1]	0.2169	[OX2H0][CX4H2][CX4H1][CX4H2]	0.7261
[#6X4H1][#6X4H1][#6X4H1]	0.1329	[CX4H2]([OX2H0])[CX4H1]	0.7728
[CX4H1]([OX2H0])([CX4H2])[CX4H1]	0.1243	[CX4H2](O)[CHX4]	0.7802
[CX4H2]([CH])[CH]	0.1047	[CX4H2][CX4H2]	0.7905

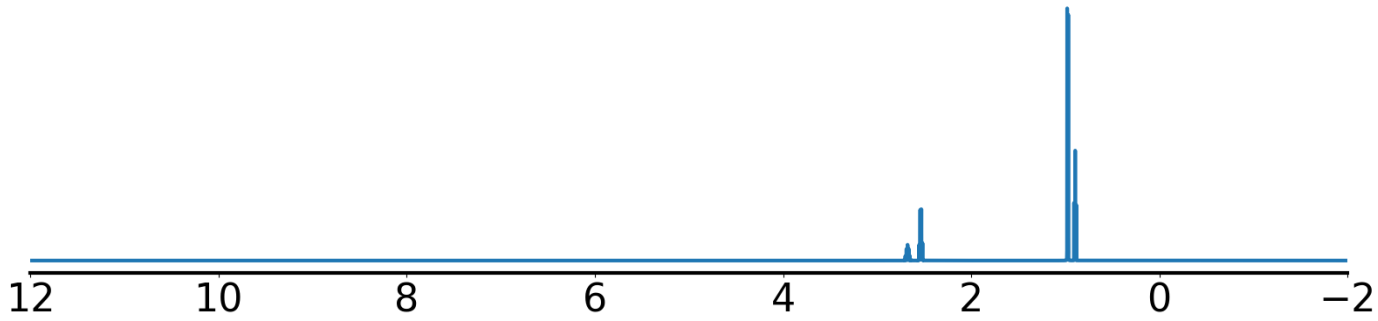
Example 163 true smiles: CCC(=O)C(C)C formula: C6H12O
Index of correct structure: 0 of 193
True structure loss: 0.011109
True structure:



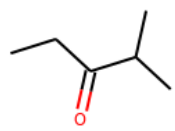
Experimental 13C NMR (solvent: CDCl3)



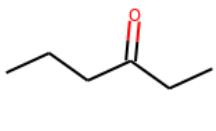
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):

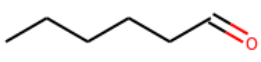


0.011109

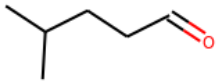


0.021622

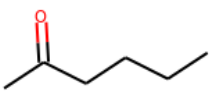
0.064929



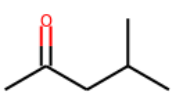
0.078475



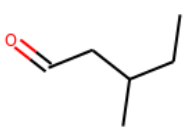
0.079066



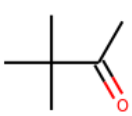
0.082231



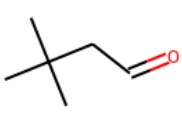
0.090535



0.094392



0.098022



0.105171

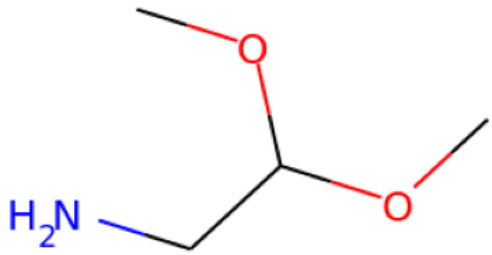
Top predicted substructures	prob		
[CX4H3]	1.0	[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9893

[CX3](=[OX1])C	0.9998	[CX4H3][CX4H2]	0.976
[#6H3][#6][#6]	0.9998	[CX4H2][CX3]=O	0.9728
[CX4H3][#6]	0.9996	[CX4H2]([CX4H3])[CX3H0]	0.9701
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9937	[CX4H2]([#6])[#6]	0.9469

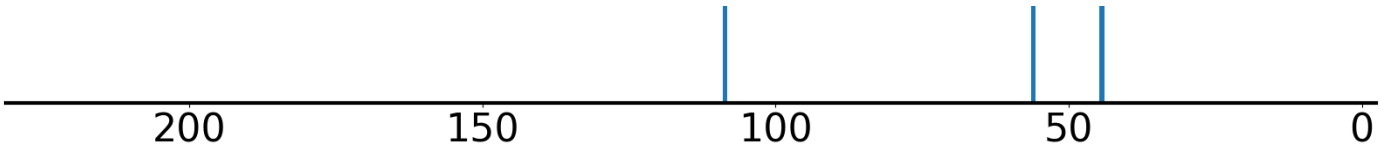
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CCCC#C	0.0
[CX3](=[OX1])C	0.9998	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H3][#6][#6]	0.9998	C=CC=CC#C	0.0
[CX4H3][#6]	0.9996	[CX2H0](#[CX2H0])[CX2H0]	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9937	[CX2H0](#[CX2H1])[CX3H1]	0.0
[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9893	CCC#CC=C	0.0
[CX4H3][CX4H2]	0.976	CC=CCC#C	0.0
[CX4H2][CX3]=O	0.9728	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H2]([CX4H3])[CX3H0]	0.9701	CCC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9469	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]CC=O	0.6438	[#6H1]	0.3709
O=[CX3H0][CX4H2][CX4H2]	0.592	[#8]=[#6H0][#6H1]	0.3781
CCCCCC	0.5814	O=[CX3][CX4H]	0.3997
[#6X3][#6][#6][#6H3]	0.544	[CX4H3][CX4H1]	0.7065
[CX4H2]([CX4H2])[CX3H0]	0.4469	[CX3H0](=[OX1H0])([CX4H2])[CX4H1]	0.8291
[CX4H2][CX4H2]	0.3034	[CHX4]([CH3X4])[CH3X4]	0.8738
[CHX4]([CH3X4])[CH2X4]	0.2059	[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.8744
[#6H2][#6X3H0][#6H2]	0.1574	[#6H3][#6][#6X3]	0.9389
[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.1299	[CX4H2]([#6])[#6]	0.9469
[#6H3][#6][#6][#6H3]	0.128	[CX4H2]([CX4H3])[CX3H0]	0.9701

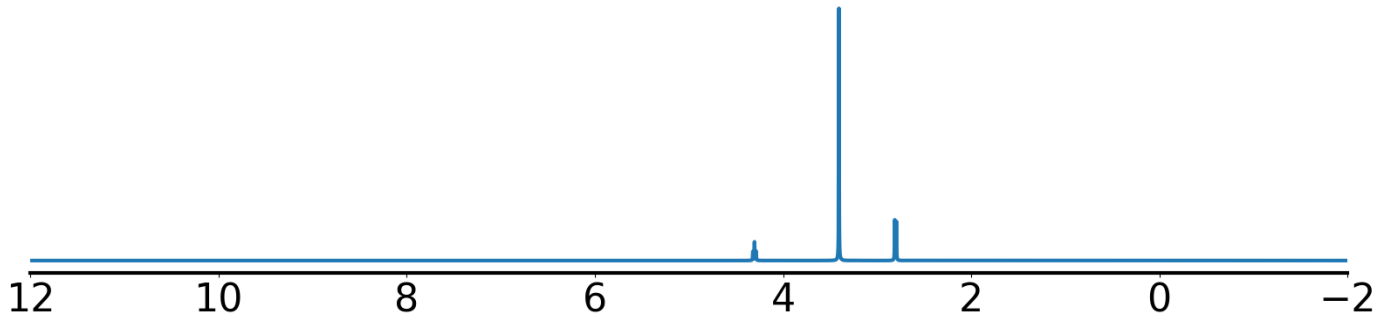
Example 164 true smiles: COC(CN)OC formula: C4H11NO2
Index of correct structure: 0 of 181
True structure loss: 0.005701
True structure:



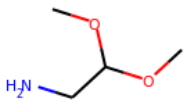
Experimental 13C NMR (solvent: CDCl3)



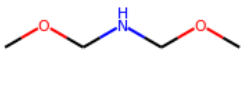
Experimental 1H NMR (solvent: CDCl3)



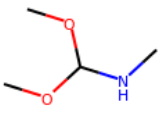
Top predicted structures (loss):



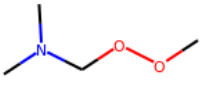
0.005701



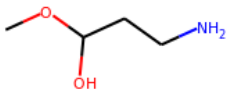
0.041941



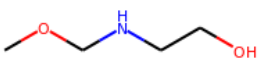
0.050458



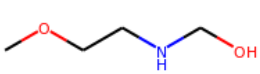
0.057218



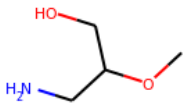
0.058905



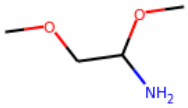
0.062322



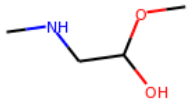
0.06277



0.063101



0.064976



0.065357

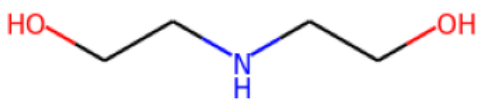
Top predicted substructures	prob		
[OX2H0][CX4H1][OX2H0]	0.9996	[CX4H3]	0.9748

[#7H2][#6H2]	0.9969	[#7X3H2]	0.9738
[#7][#6H2]	0.9935	[CX4H3][OX2H0]	0.9611
[#7X3][#6H2]	0.9909	[#7][#6H2][#6H1]	0.8323
[CX4H1]([OX2H0])([OX2H0])[CX4H2]	0.9851	[#8][#6][#6H2]	0.8168

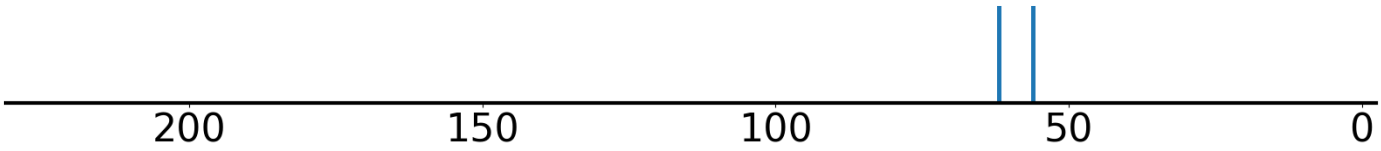
best positives	prob	best negatives	prob
[OX2H0][CX4H1][OX2H0]	0.9996	[#6X2][#6H1][#6X2]	0.0
[#7H2][#6H2]	0.9969	CC=CCC#C	0.0
[#7][#6H2]	0.9935	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3][#6H2]	0.9909	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
[CX4H1]([OX2H0])([OX2H0])[CX4H2]	0.9851	CCC#CC#C	0.0
[CX4H3]	0.9748	C=CC=CC#C	0.0
[#7X3H2]	0.9738	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H3][OX2H0]	0.9611	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7][#6H2][#6H1]	0.8323	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#8][#6][#6H2]	0.8168	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
OCC[CH2]	0.3533	[#6H1][#6H2]	0.581
[CX4H2]([NX3H2])[CX4H2]	0.3351	[#6H1]	0.6654
[CX4H2][CX4H2]	0.1797	[CX4H2]([NX3H2])[CX4H1]	0.7087
[#6H2][#7][#6H2]	0.1736	O[CX4H][CX4H2]	0.7146
[CX4H2]([#6])[O]	0.1499	[CX4H]O	0.775
[#7X3H1]	0.1424	[#8][#6][#6H2]	0.8168
[#6H2][#8][#6H1]	0.1335	[#7][#6H2][#6H1]	0.8323
[#7][#6H2][#6H2]	0.1166	[CX4H3][OX2H0]	0.9611
[CX4H3][OX2H0][CX4H2]	0.0628	[#7X3H2]	0.9738
[CX4H2](O)[CHX4]	0.0599	[CX4H3]	0.9748

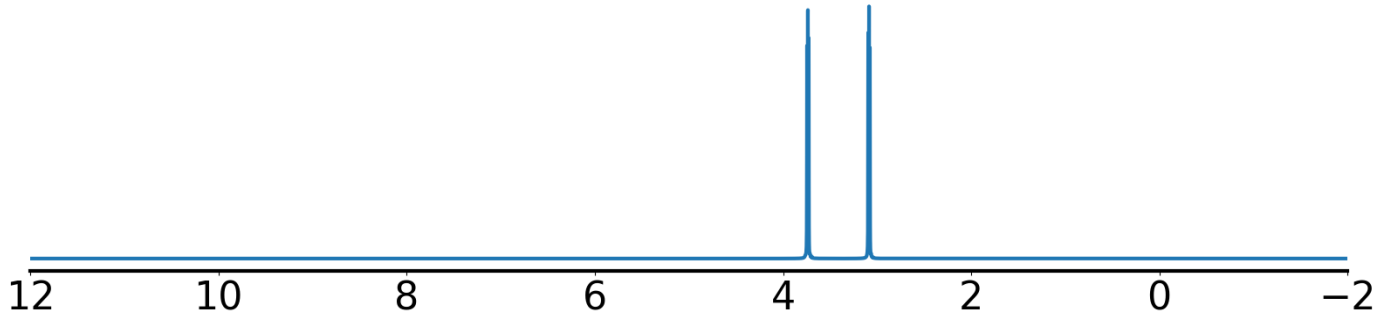
Example 165 true smiles: OCCNCCO formula: C4H11NO2
Index of correct structure: 0 of 181
True structure loss: 0.008394
True structure:



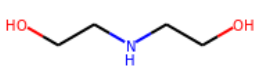
Experimental 13C NMR (solvent: CDCl3)



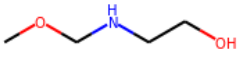
Experimental 1H NMR (solvent: D2O)



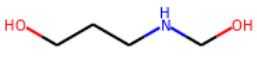
Top predicted structures (loss):



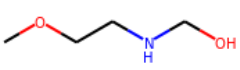
0.008394



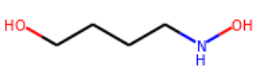
0.019748



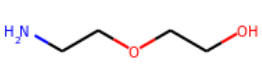
0.020764



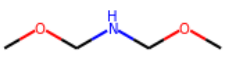
0.025876



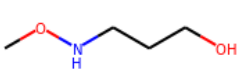
0.027609



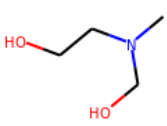
0.030531



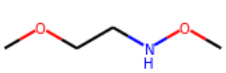
0.034585



0.037962



0.040601



0.041126

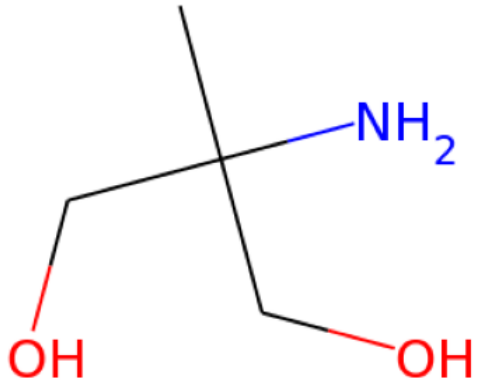
Top predicted substructures	prob		
[#7][#6H2]	0.9767	[CX4H2]([OX2H1])[CX4H2]	0.8669

[OX2H1]	0.9684	[#7][#6H2][#6H2]	0.8593
[#8][#6][#6H2]	0.9306	[CH2X4](O)[CX4H2]	0.7909
[CX4H2]([#6])[O]	0.9222	[CX4H2][CX4H2]	0.7214
[#7X3][#6H2]	0.9003	[#6H2][#7][#6H2]	0.6729

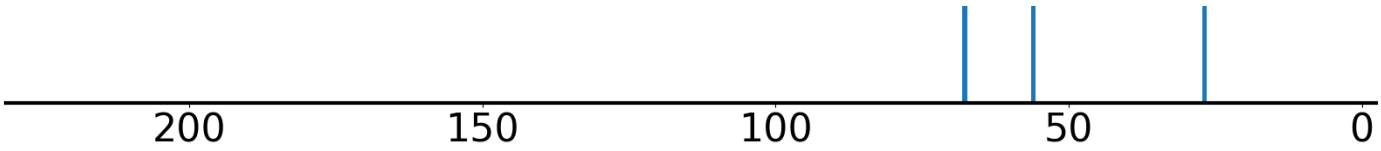
best positives	prob	best negatives	prob
[#7][#6H2]	0.9767	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX2H1]	0.9684	CCC=CC#C	0.0
[#8][#6][#6H2]	0.9306	CC=CC#CC	0.0
[CX4H2]([#6])[O]	0.9222	C=CC=CC#C	0.0
[#7X3][#6H2]	0.9003	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2]([OX2H1])[CX4H2]	0.8669	CCC#CC=C	0.0
[#7][#6H2][#6H2]	0.8593	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CH2X4](O)[CX4H2]	0.7909	C=CCCC#C	0.0
[CX4H2][CX4H2]	0.7214	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#6H2][#7][#6H2]	0.6729	[#6X2][#6H1][#6X2]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.3835	[#7X3H1]	0.247
OCC[CH2]	0.3122	[CX4H2]([NX3H1])[CX4H2]	0.4356
[#7X3H2]	0.2735	[#6H2][#7][#6H2]	0.6729
[CX4H2]([NX3H0])[CX4H2]	0.2625	[CX4H2][CX4H2]	0.7214
[#7X3H0]	0.2549	[CH2X4](O)[CX4H2]	0.7909
[#7][#6H2][#6H1]	0.1802	[#7][#6H2][#6H2]	0.8593
[#6H1][#6H2]	0.1761	[CX4H2]([OX2H1])[CX4H2]	0.8669
[CX4H2]([OX2H1])[CX4H1]	0.1491	[#7X3][#6H2]	0.9003
[#8][#6H1][#6H1]	0.131	[CX4H2]([#6])[O]	0.9222
[#7H2][#6H1]	0.107	[#8][#6][#6H2]	0.9306

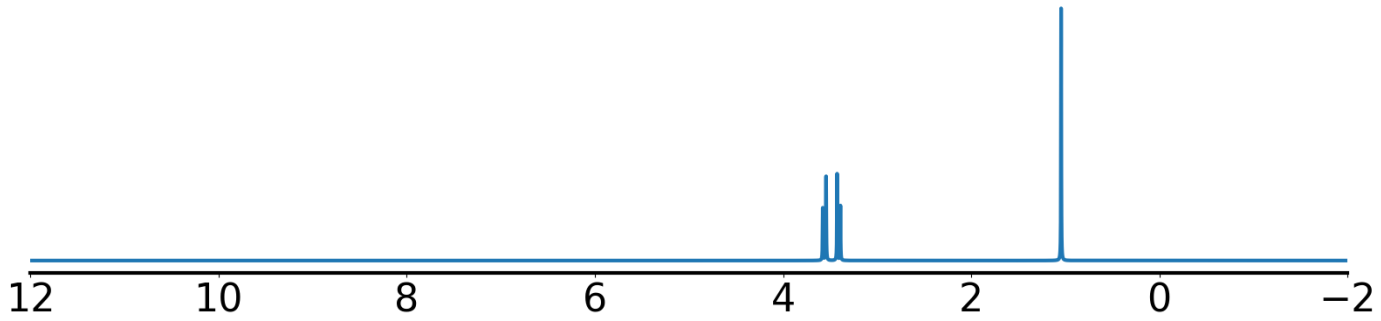
Example 166 true smiles: CC(N)(CO)CO formula: C4H11NO2
Index of correct structure: 0 of 181
True structure loss: 0.016605
True structure:



Experimental 13C NMR (solvent: DMSO-d6)

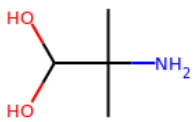


Experimental 1H NMR (solvent: CDCl3)



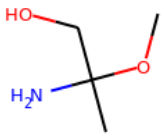
Top predicted structures (loss):

0.016605

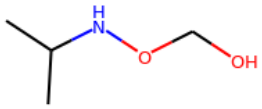


0.019313

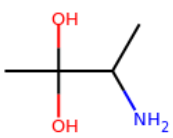
0.028744



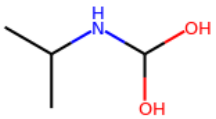
0.029283



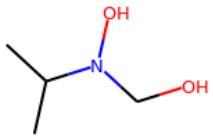
0.035906



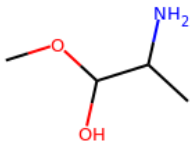
0.039362



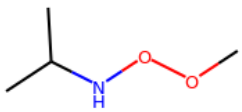
0.040474



0.042909



0.043992



0.044442

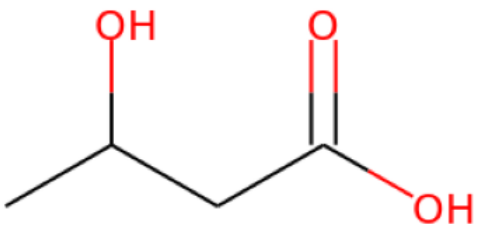
Top predicted substructures	prob		
[#6H3][#6][#6]	0.9992	[CX4H3][#6]	0.9544

[OX2H1]	0.9986	[#7X3H2]	0.9377
[CX4H3]	0.998	[CX4H2]([OX2H1])[CX4H0]	0.9033
[#6H3][#6H0]	0.9711	[CH3]CC[OH]	0.8724
[CX4H3][CX4H0]	0.9568	[#6H1]	0.7673

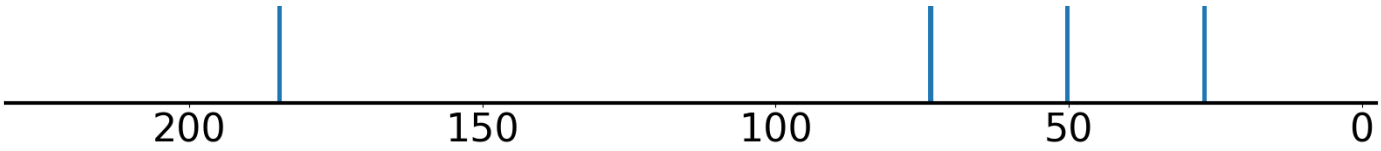
best positives	prob	best negatives	prob
[#6H3][#6][#6]	0.9992	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9986	C=CCCC#C	0.0
[CX4H3]	0.998	CCC=CC#C	0.0
[#6H3][#6H0]	0.9711	CC=CC#CC	0.0
[CX4H3][CX4H0]	0.9568	C=CC=CC#C	0.0
[CX4H3][#6]	0.9544	CCC#CC=C	0.0
[#7X3H2]	0.9377	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2]([OX2H1])[CX4H0]	0.9033	CC=CCC#C	0.0
[CH3]CC[OH]	0.8724	CC#CCC=C	0.0
[#7][#6][#6H3]	0.6764	[CX2H0](#[CX2H1])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.7673	[#8][#6H2][#6H0][#6H2][#8]	0.2105
[OH][CX4H]	0.7577	[#6H3][#6H0]([#6H2])[#6H2]	0.3025
[#7H2][#6H1]	0.554	[#7H2][#6H0]	0.3644
[CX4H2]([OX2H1])[CX4H1]	0.4928	OCC[CH2]	0.5283
[CX4H]O	0.4697	[CX4H2]([#6])[O]	0.5446
[#8H][#6H2][#6H1]	0.3081	[#7][#6][#6H3]	0.6764
[#6H1][#6H2]	0.2533	[CH3]CC[OH]	0.8724
[#7X3H1]	0.252	[CX4H2]([OX2H1])[CX4H0]	0.9033
[#7X3][#6H2]	0.2324	[#7X3H2]	0.9377
[#8][#6][#6][#8]	0.2322	[CX4H3][#6]	0.9544

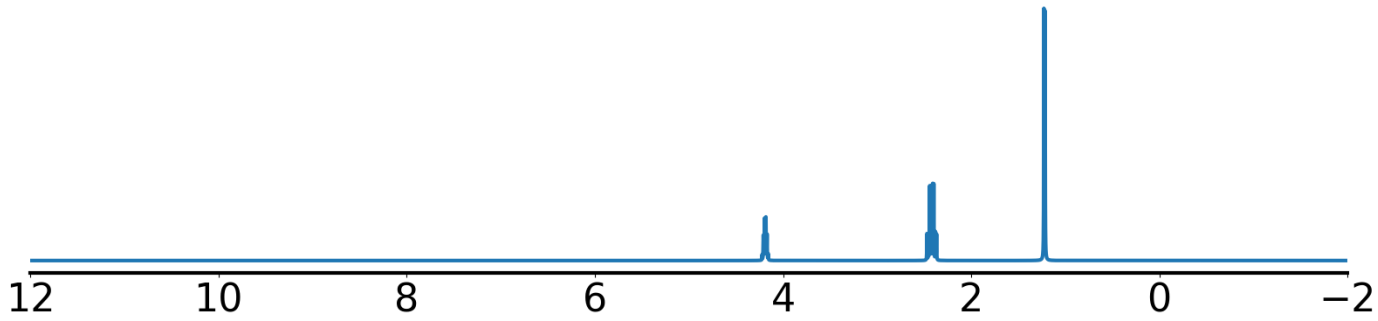
Example 167 true smiles: CC(O)CC(=O)O formula: C4H8O3
Index of correct structure: 0 of 172
True structure loss: 0.019179
True structure:



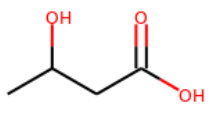
Experimental 13C NMR (solvent: CDCl3)



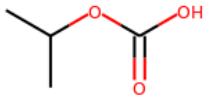
Experimental 1H NMR (solvent: D2O)



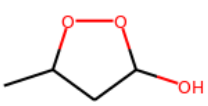
Top predicted structures (loss):



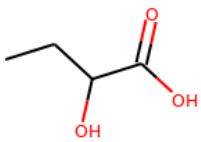
0.019179



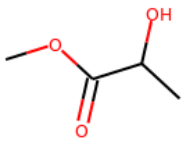
0.060651



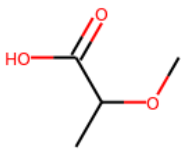
0.061101



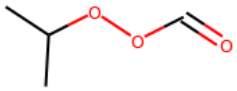
0.065334



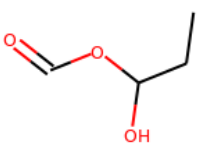
0.068097



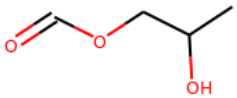
0.075476



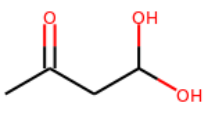
0.084514



0.086433



0.087185



0.093735

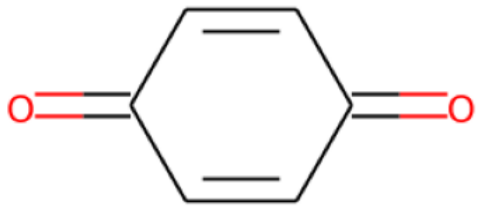
Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][#6]	0.995

[#6H3][#6][#6]	0.9996	[#6H1]	0.9888
[CX3](=[OX1])C	0.9988	[#8]=[#6][#8]	0.9872
[OX2H1]	0.9985	[CX4H]O	0.9811
[CX4H2]([#6])[#6]	0.9971	[CX3](=[OX1])O	0.9754

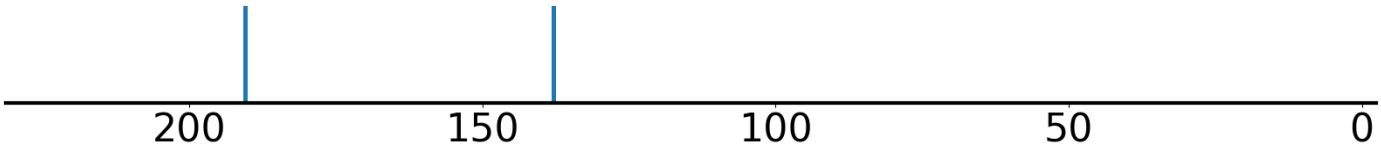
best positives	prob	best negatives	prob
[CX4H3]	1.0	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9996	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9988	CC=CCC#C	0.0
[OX2H1]	0.9985	CCC#CC#C	0.0
[CX4H2]([#6])[#6]	0.9971	[#6X2][#6H1][#6X2]	0.0
[CX4H3][#6]	0.995	CCC=CC#C	0.0
[#6H1]	0.9888	C=CC=CC#C	0.0
[#8]=[#6][#8]	0.9872	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H]O	0.9811	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.9754	CC#CCC#C	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.6222	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2133
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5987	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2865
[CX4H2]CC=O	0.5706	[#8]=[#6][#6H2][#6H1]	0.4054
[#8]=[#6H0][#6H1]	0.5622	[#6X3][#6][#6][#6H3]	0.5263
OCC[CH2]	0.465	[CX4H2][CX3]=O	0.5303
O=[CX3][CX4H]	0.4505	O=[CX3H0][CX4H2][CX4H1]	0.5886
[#8][#6H1][#6H1]	0.4225	[CHX4]([CH3X4])[CH2X4]	0.6628
[#8][#6][#6][#6][#6]=[#8]	0.3818	[CX4H1]([OX2H1])([CX4H3])[CX4H2]	0.6678
[CH3]CC[OH]	0.3735	[CX4H2]([CX4H1])[CX3H0]	0.6758
[CX4H2]([CH])[CH]	0.315	[#8][#6][#6][#6X3]	0.7748

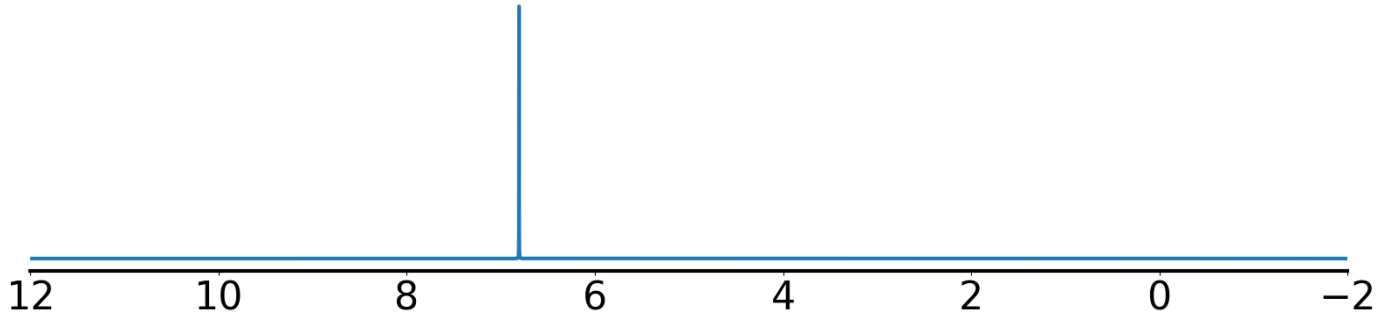
Example 168 true smiles: O=C1C=CC(=O)C=C1 formula: C6H4O2
Index of correct structure: 0 of 160
True structure loss: 0.018842
True structure:



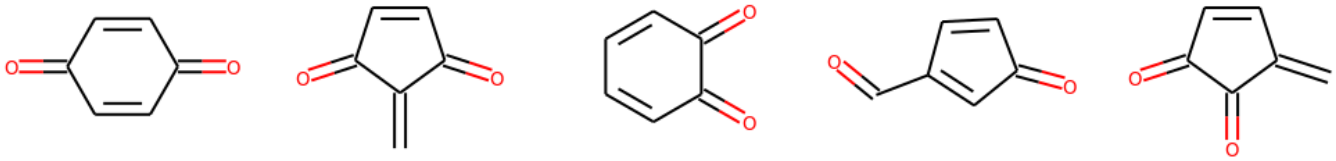
Experimental 13C NMR (solvent: CDCl3)



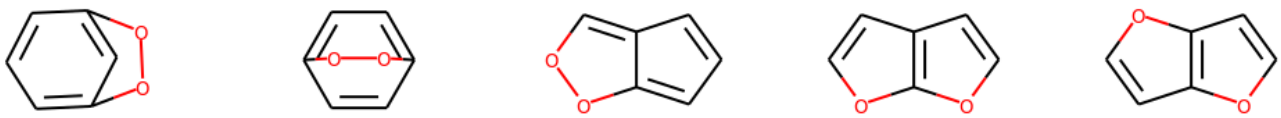
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.018842 0.03608 0.048474 0.056781 0.058536



0.061837 0.065505 0.066052 0.069136 0.069346

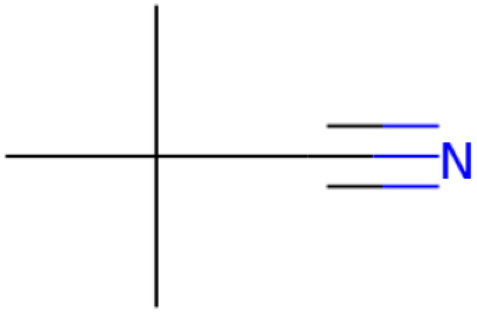
Top predicted substructures	prob		
[#6X3][#6X3]	0.9888	[#6X3][#6X3][#6X3]=[#6X3]	0.8337

O=[#6][#6]=[#6X3]	0.9266	[#6X3H1][#6X3H0]	0.8331
[CX3](=[OX1])C	0.9264	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.8195
[#8]=[#6][#6]=[#6][#6]=[#8]	0.8614	[#6H1]	0.8038
O=C[CX3H]	0.8553	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.774

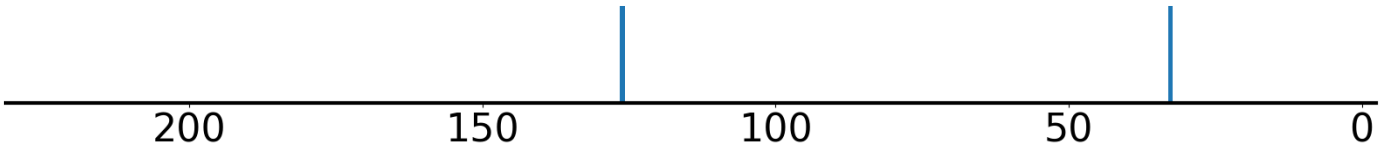
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9888	[#6H3][#7][#6X4H1][#6H3]	0.0
O=[#6][#6]=[#6X3]	0.9266	[CX4H2]([NX3H1])[CX4H3]	0.0
[CX3](=[OX1])C	0.9264	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#8]=[#6][#6]=[#6][#6]=[#8]	0.8614	[CX4H1]([NX3H0])([CX4H3])[CX4H1]	0.0
O=C[CX3H]	0.8553	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.0
[#6X3][#6X3][#6X3]=[#6X3]	0.8337	[CX4H1]([NX3H1])([CX4H3])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.8331	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.8195	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H1]	0.8038	[#6H3][#6H1][#6H1]=[#7]	0.0
[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.774	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6][#6X3]	0.7434	[#6X3H1]=[#6X3H1][#6X3H0][#6X3H1]	0.0869
[#6X3][#6X3][#6X3][#6X3]	0.6991	CCC=CCC	0.5204
O=CC=O	0.38	[CHX3]=[CHX3]	0.5284
[#8]=[#6][#6]=[#8]	0.3372	CC=CCC=C	0.5605
[cH]	0.3148	[CHX3](=C)C	0.5863
[#6]1[#6][#6][#6][#6][#6]1	0.2821	[#6]1[#6]=[#6][#6][#6]=[#6]1	0.6332
[#8]=[#6][#6][#6][#6]=[#8]	0.2751	[CX3H1](=[CX3H1])[CX3H0]	0.6345
[CX3H2]=[CX3H0][CX3H0]	0.2598	[#8]=[#6H0][#6H1]	0.6419
[#8][#6][#6][#6X3]	0.2581	[#8]=[#6][#6H1]=[#6H1]	0.7204
[#6H1][#6H1]	0.2391	[#6X3][#6X3]=[#6X3][#6X3]	0.7419

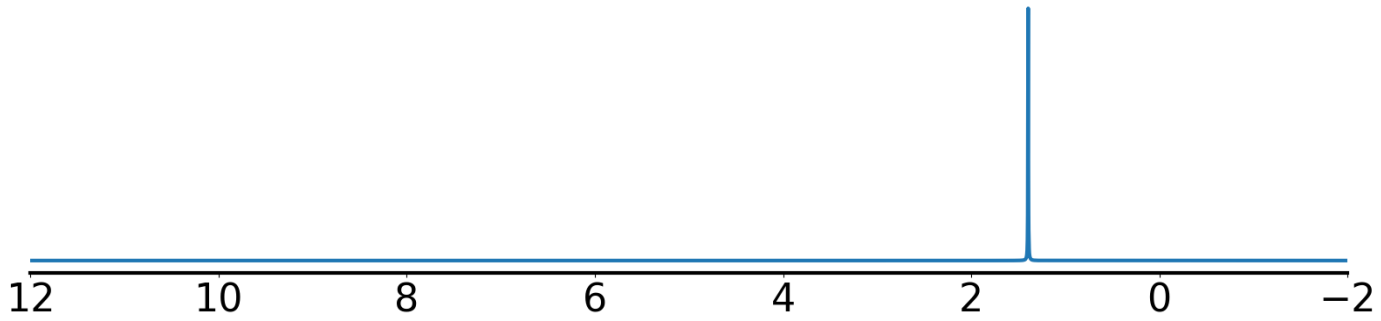
Example 169 true smiles: CC(C)(C)C#N formula: C5H9N
Index of correct structure: 0 of 125
True structure loss: 0.006086
True structure:



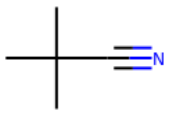
Experimental 13C NMR (solvent: CDCl3)



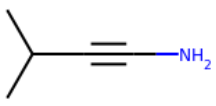
Experimental 1H NMR (solvent: CDCl3)



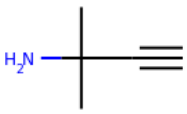
Top predicted structures (loss):



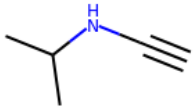
0.006086



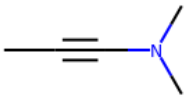
0.05987



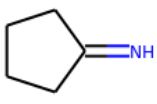
0.060118



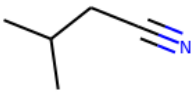
0.062975



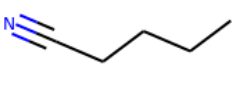
0.070877



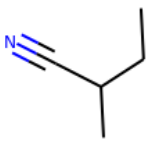
0.074554



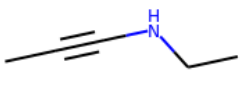
0.07724



0.079697



0.084828



0.085141

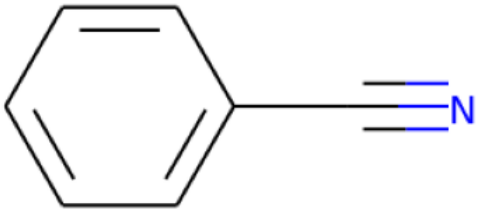
Top predicted substructures	prob		
[CX4H3][CX4H0][CX4H3]	0.9822	[CX4]([CX4H3])([CX4H3])[CX4H3]	0.8008

[CX2H0](#[NX1H0])[CX4H0]	0.9328	[CX4H3]	0.788
[CX4H3][#6]	0.8335	[#6]#[#7]	0.7521
[CX4H3][CX4H0]	0.8198	[#6H3][#6H0]	0.741
[#6H3][#6][#6]	0.8108	[#6H1]	0.3413

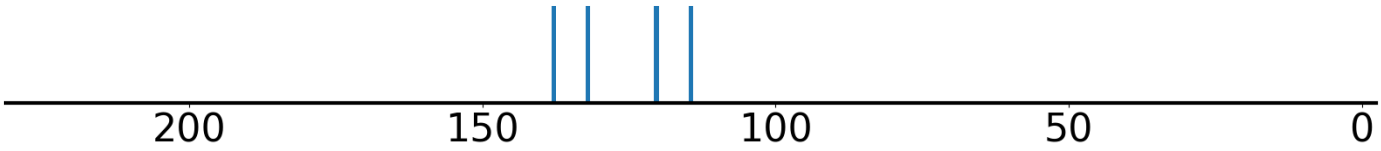
best positives	prob	best negatives	prob
[CX4H3][CX4H0][CX4H3]	0.9822	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX2H0](#[NX1H0])[CX4H0]	0.9328	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3][#6]	0.8335	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3][CX4H0]	0.8198	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H3][#6][#6]	0.8108	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[CX4]([CX4H3])([CX4H3])[CX4H3]	0.8008	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[CX4H3]	0.788	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6]#[#7]	0.7521	[CX3H0](=[CX3H2])([OX2H0])[CX3H0]	0.0
[#6H3][#6H0]	0.741	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.3413	[#6H3][#6H0]	0.741
[#7X3H1]	0.2462	[#6]#[#7]	0.7521
[#7X3H2]	0.2325	[CX4H3]	0.788
[CX4H2][CX4H2]	0.2317	[CX4]([CX4H3])([CX4H3])[CX4H3]	0.8008
[CHX3]=[CHX3]	0.1879	[#6H3][#6][#6]	0.8108
[#7H2][#6H0]	0.1472	[CX4H3][CX4H0]	0.8198
[#7][#6H0][#6H1]	0.1214	[CX4H3][#6]	0.8335
[#6H2][#7][#6H2]	0.1136	[CX2H0](#[NX1H0])[CX4H0]	0.9328
[#7][#6H2]	0.1089	[CX4H3][CX4H0][CX4H3]	0.9822

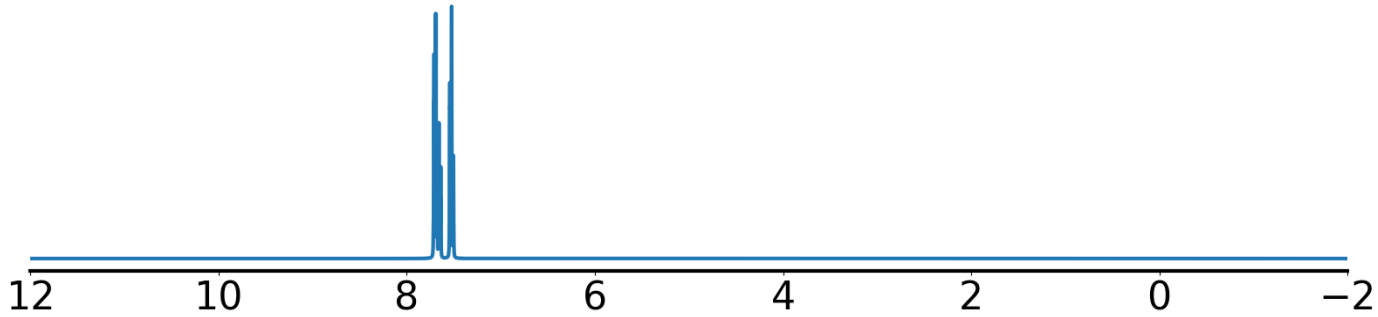
Example 170 true smiles: N#Cc1ccccc1 formula: C7H5N
Index of correct structure: 0 of 121
True structure loss: 0.012092
True structure:



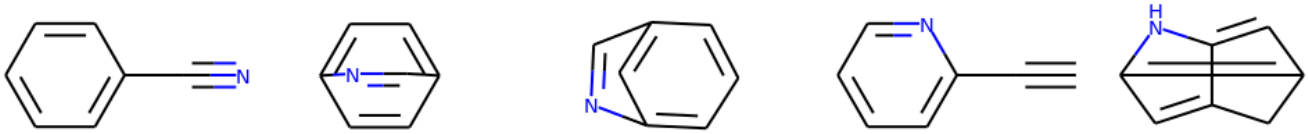
Experimental 13C NMR (solvent: CDCl3)



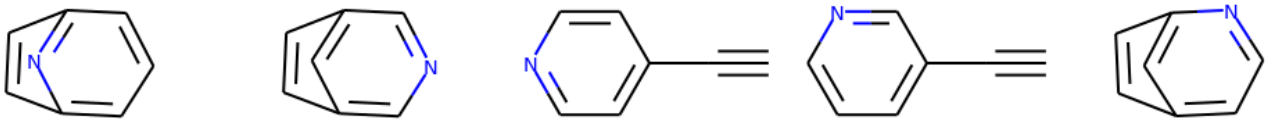
Experimental 1H NMR (solvent: CD3OD)



Top predicted structures (loss):



0.012092 0.018296 0.051488 0.060653 0.061253



0.061892 0.064748 0.066741 0.068065 0.075339

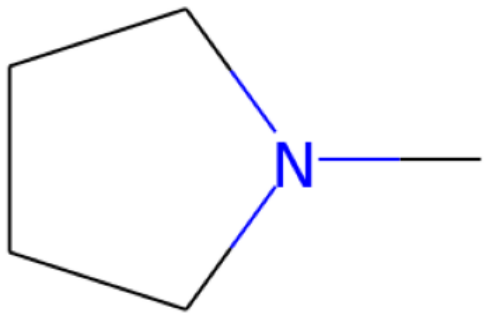
Top predicted substructures	prob		
[#6H1]	0.9992	[#6X3H1][#6X3H0]	0.9834
[#6X3][#6X3]	0.9988	[cX3H1]([cX3H1])[cX3H0]	0.9803
[#6X3][#6X3][#6X3][#6X3]	0.9985	[#6H1][#6H1]	0.9606

[cH][cH]	0.9924	[#6]1[#6][#6][#6][#6][#6]1	0.9276
[cH]	0.9912	[cX3H1]([cX3H1])[cX3H1]	0.8954

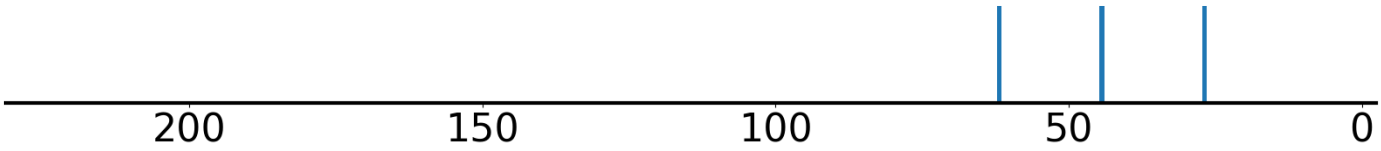
best positives	prob	best negatives	prob
[#6H1]	0.9992	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3]	0.9988	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9985	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[cH][cH]	0.9924	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9912	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3H1][#6X3H0]	0.9834	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9803	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[#6H1][#6H1]	0.9606	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.9276	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.8954	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#7][#6][#6X3]	0.7941	[#7]#[#6][#6X3]	0.5001
[#7][#6][#6][#6X3]	0.7814	[#6]#[#7]	0.5505
[#7][#6X3H0][#6X3H1]	0.5595	[#7]#[#6][#6][#6X3]	0.556
[#7][#6H0][#6H1]	0.5407	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7164
[#6]1[#6][#6][#6][#6][#7]1	0.4889	[cX3H1]([cX3H1])[cX3H1]	0.8954
[#6X3][#7][#6X3]	0.4874	[#6]1[#6][#6][#6][#6][#6]1	0.9276
[#6]1[#6][#6][#6][#7]1	0.3077	[#6H1][#6H1]	0.9606
[#7H][#6X3H1]	0.2102	[cX3H1]([cX3H1])[cX3H0]	0.9803
[cX3H1]([nX3H1])[cX3H1]	0.1785	[#6X3H1][#6X3H0]	0.9834
[#6X3][#7X3][#6X3]	0.1699	[cH]	0.9912

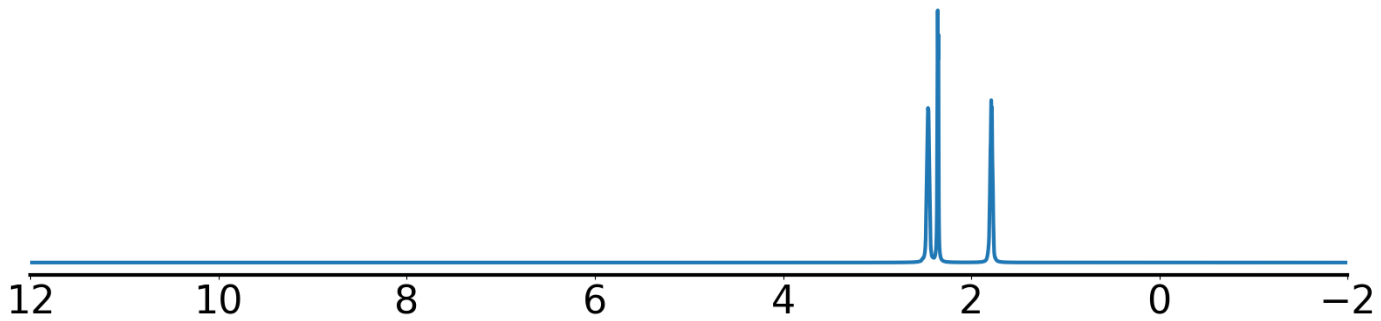
Example 171 true smiles: CN1CCCC1 formula: C5H11N
Index of correct structure: 0 of 100
True structure loss: 0.014178
True structure:



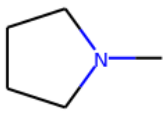
Experimental 13C NMR (solvent: CDCl3)



Experimental 1H NMR (solvent: CDCl3)

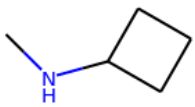


Top predicted structures (loss):

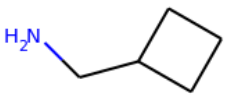


0.014178

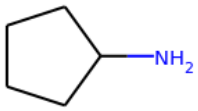
0.027459



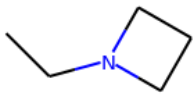
0.04011



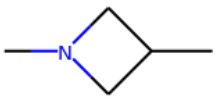
0.045611



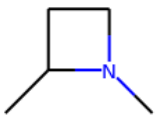
0.048858



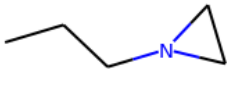
0.052041



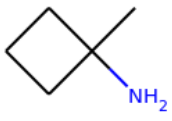
0.060631



0.065502



0.066835



0.069255

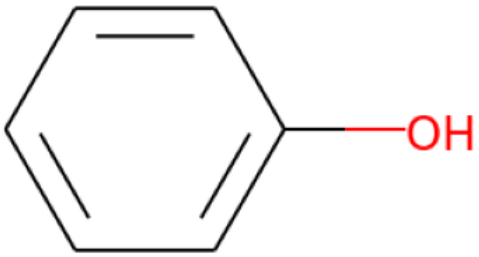
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9994	[CX4H3][NX3H0]	0.7773
[#7X3H0]	0.8612	[#6H3][#7]	0.7577
[CX4H2]([NX3H0])[CX4H2]	0.8396	[#7][#6H2][#6H2]	0.752

[CX4H2][CX4H2]	0.8359	[#6H3][#7X3H0][#6X4H2][#6X4H2]	0.7393
[#7X3][#6H3]	0.8244	[CX4H2]([CX4H2])[CX4H2]	0.727

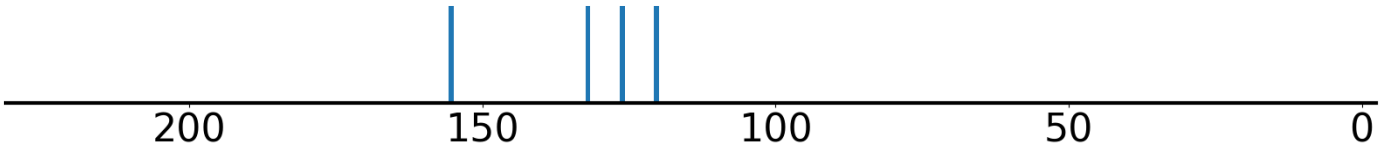
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9994	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3H0]	0.8612	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([NX3H0])[CX4H2]	0.8396	[cX3H0][cX3H1][cX3H0][OX2H1]	0.0
[CX4H2][CX4H2]	0.8359	C=CC=CC#C	0.0
[#7X3][#6H3]	0.8244	[OX2H0][CX3H1]=[#6X3H0][#8X2H0]	0.0
[CX4H3][NX3H0]	0.7773	[CX4H1]([OX2H0])([CX4H3])[CX3H0]	0.0
[#6H3][#7]	0.7577	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7][#6H2][#6H2]	0.752	[OX2H0r5][CX4H2][OX2H0r5]	0.0
[#6H3][#7X3H0][#6X4H2][#6X4H2]	0.7393	[CX3H0](=[CX3H2])([CX4H1])[CX3H1]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.727	[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H2]	0.5697	[#6]1[#6][#6][#6][#7]1	0.1489
[#7X3H2]	0.3576	[CX4H3]	0.2449
C1CCC1	0.2572	[#6H2][#7][#6H2]	0.2926
[#6H1]	0.2456	[#6H3][#7][#6H2]	0.4922
[#7X3H1]	0.2283	[#7X3][#6H2]	0.5065
[#6H1]([#6H2])[#6H2]	0.173	[CX4H2][CX4H2][CX4H2][CX4H2]	0.6648
CCCCCC	0.1713	[#7][#6H2]	0.7116
[#7][#6H1][#6H2r5]	0.1611	[CX4H2]([CX4H2])[CX4H2]	0.727
[CX4H2]([NX3H2])[CX4H2]	0.1259	[#6H3][#7X3H0][#6X4H2][#6X4H2]	0.7393
[CX4H2]([CX4H2])[CX4H1]	0.1252	[#7][#6H2][#6H2]	0.752

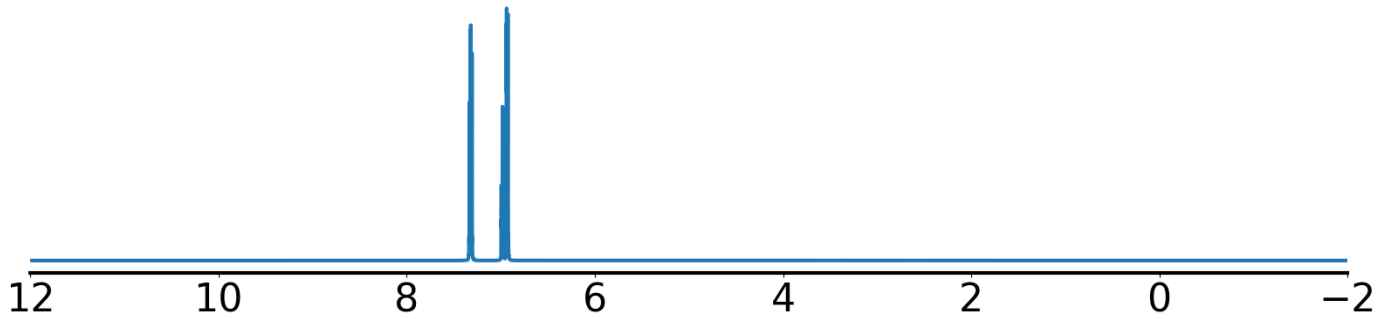
Example 172 true smiles: Oc1ccccc1 formula: C6H6O
Index of correct structure: 0 of 98
True structure loss: 0.005278
True structure:



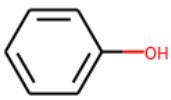
Experimental 13C NMR (solvent: CDCl3)



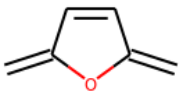
Experimental 1H NMR (solvent: D2O)



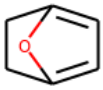
Top predicted structures (loss):



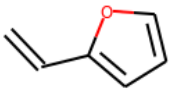
0.005278



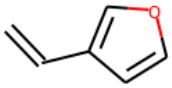
0.046617



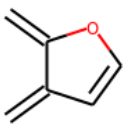
0.057299



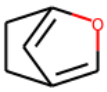
0.06161



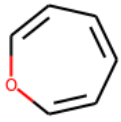
0.08174



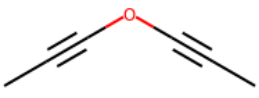
0.083112



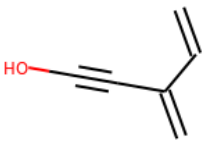
0.104978



0.13359



0.148344



0.166134

Top predicted substructures	prob		
[#6X3][#6X3]	0.9998	[cX3H1]([cX3H1])[cX3H0]	0.9851
[#6X3][#6X3][#6X3][#6X3]	0.9997	[#6X3H1][#6X3H0]	0.9816
[cH][cH]	0.9991	[#6]1[#6][#6][#6][#6][#6]1	0.9808

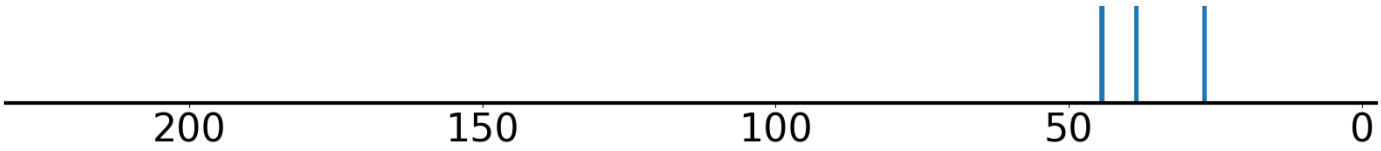
[#6H1]	0.9981	[cX3H1]([cX3H1])[cX3H1]	0.9659
[cH]	0.9853	[#6H1][#6H1]	0.9543

best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9998	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9997	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH][cH]	0.9991	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6H1]	0.9981	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.9853	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9851	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3H1][#6X3H0]	0.9816	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.9808	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9659	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6H1][#6H1]	0.9543	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0

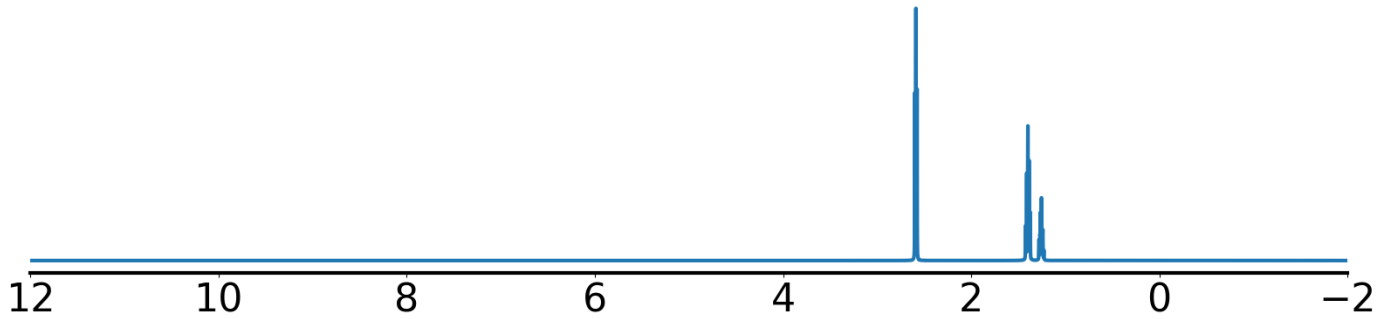
worst negatives	prob	worst positives	prob
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.3679	[OX2H1]	0.6808
[#7][#6][#6][#6X3]	0.2303	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7855
[cX3H0][cX3H1][cX3H1][cX3H0]	0.2131	[#8][#6][#6][#6X3]	0.8662
[cX3H1]([oX2H0])[cX3H1]	0.2107	[OX2H][cX3]:[c]	0.8725
[#8][#6H1][#6H1]	0.1858	[cH]cO	0.9132
[cX3H0][cX3H1][cX3H0][OX2H1]	0.1813	[#8][#6H0][#6H1]	0.9141
[#8][#6H][#6X3][#6X3H]	0.1665	[#6H1][#6H1]	0.9543
[#6X3][#7][#6X3]	0.1618	[cX3H1]([cX3H1])[cX3H1]	0.9659
[#6]1[#6][#6][#6][#6][#7]1	0.1551	[#6]1[#6][#6][#6][#6][#6]1	0.9808
[#7][#6][#6X3]	0.1461	[#6X3H1][#6X3H0]	0.9816

Example 173 true smiles: NCCCCCN formula: C5H14N2
Index of correct structure: 0 of 97
True structure loss: 0.005111
True structure:

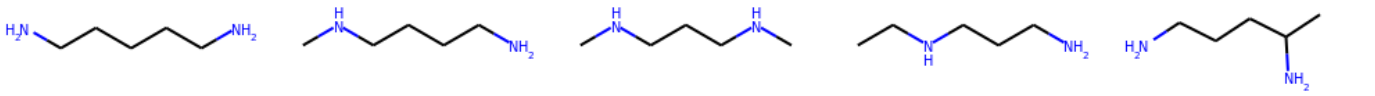
Experimental 13C NMR (solvent: CDCl3)



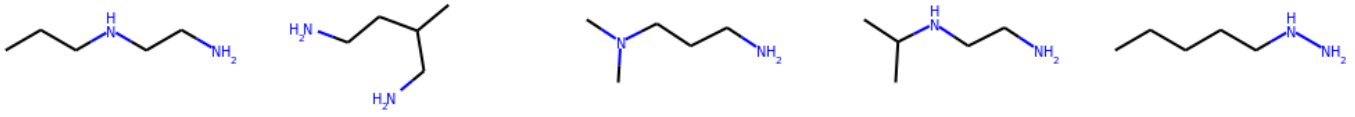
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.005111 0.023611 0.038452 0.042226 0.042658



0.045164 0.04917 0.05025 0.052515 0.059539

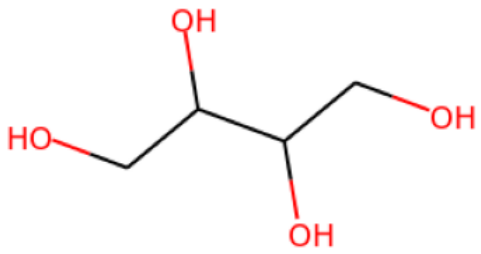
Top predicted substructures	prob		
[#7X3H2]	0.9977	[#7][#6H2][#6H2]	0.9659
[CX4H2]([#6])[#6]	0.9976	[#7H2][#6H2]	0.9278
[#7X3][#6H2]	0.997	[CX4H2][CX4H2]	0.9225

[#7][#6H2]	0.9815	[CX4H2]([NX3H2])[CX4H2]	0.9058
[CX4H2][CX4H2][CX4H2][CX4H2]	0.9811	[CX4H2]([CX4H2])[CX4H2]	0.9005

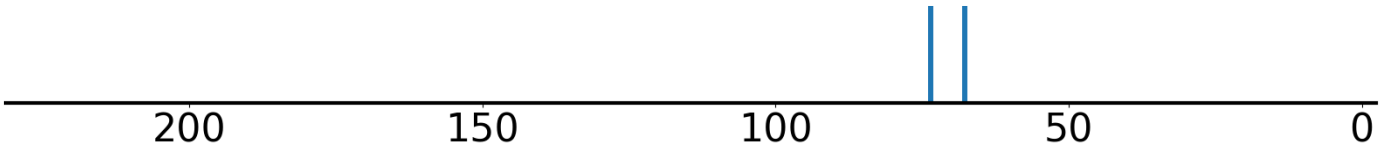
best positives	prob	best negatives	prob
[#7X3H2]	0.9977	C=CC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9976	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3][#6H2]	0.997	CC=CCC#C	0.0
[#7][#6H2]	0.9815	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.9811	[#6X2][#6H1][#6X2]	0.0
[#7][#6H2][#6H2]	0.9659	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#7H2][#6H2]	0.9278	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2][CX4H2]	0.9225	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([NX3H2])[CX4H2]	0.9058	CC=CC#CC	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9005	[CX2H0](#[CX2H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#7][#6][#6][#6][#7]	0.4748	[CX4H2]([CX4H2])[CX4H2]	0.9005
[#6H1]	0.3656	[CX4H2]([NX3H2])[CX4H2]	0.9058
[#7][#6][#6][#6][#6][#7]	0.3279	[CX4H2][CX4H2]	0.9225
[#7X3H1]	0.3252	[#7H2][#6H2]	0.9278
[#6H1][#6H2]	0.3106	[#7][#6H2][#6H2]	0.9659
[CX4H2]([NX3H1])[CX4H2]	0.2858	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9811
[CX4H3][NX3H1]	0.1631	[#7][#6H2]	0.9815
[CX4H3][#6]	0.1178	[#7X3][#6H2]	0.997
[#7][#6H2][#6H1]	0.1173	[CX4H2]([#6])[#6]	0.9976
[CX4H2]([CX4H2])[CX4H1]	0.1161	[#7X3H2]	0.9977

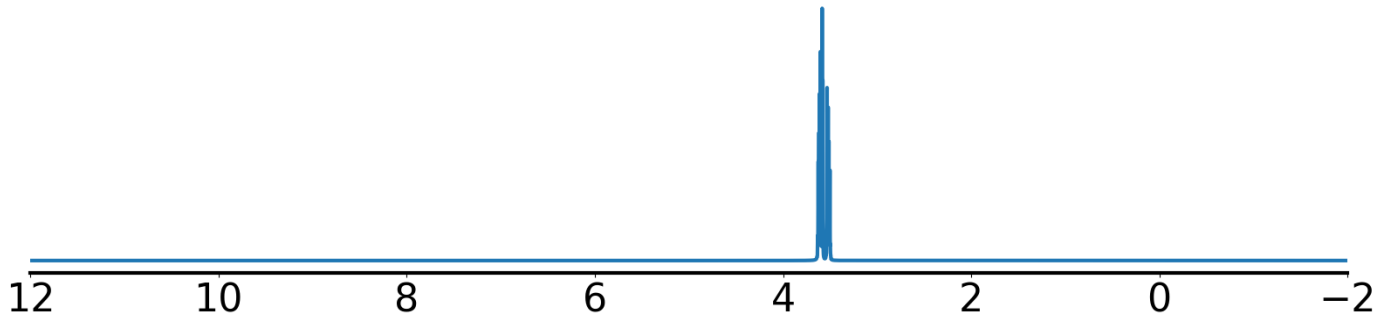
Example 174 true smiles: OCC(O)C(O)CO formula: C4H10O4
Index of correct structure: 0 of 92
True structure loss: 0.016919
True structure:



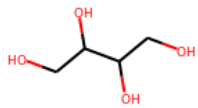
Experimental 13C NMR (solvent: D2O)



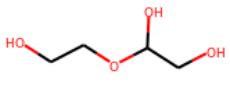
Experimental 1H NMR (solvent: D2O)



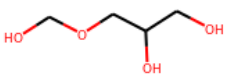
Top predicted structures (loss):



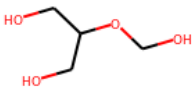
0.016919



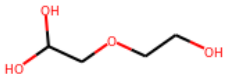
0.020653



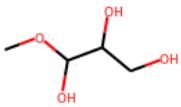
0.02189



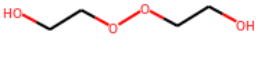
0.022483



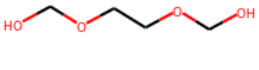
0.023681



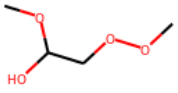
0.024666



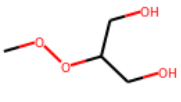
0.0254



0.026699



0.028374



0.029403

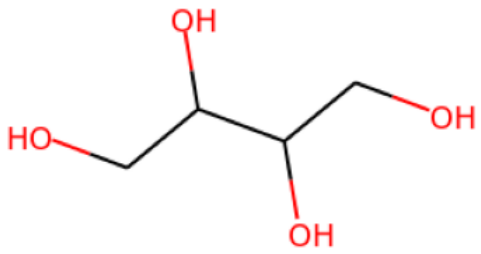
Top predicted substructures	prob		
[CX4H2]([#6])[O]	0.9975	[CX4H](O)CO	0.8638
[OX2H1]	0.9968	[CX4H2]([OX2H1])[CX4H1]	0.8315
[#8][#6][#6H2][#8]	0.9865	OCC[CH2]	0.8025

[#8][#6][#6][#8]	0.9858	[CX4H2](O)[CHX4]	0.7424
[#8][#6][#6H2]	0.9771	[#8H][#6H2][#6H1]	0.6962

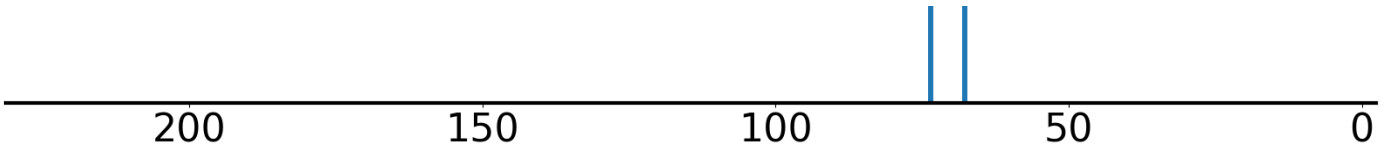
best positives	prob	best negatives	prob
[CX4H2]([#6])[O]	0.9975	CC=CCC#C	0.0
[OX2H1]	0.9968	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6H2][#8]	0.9865	CCC#CC=C	0.0
[#8][#6][#6][#8]	0.9858	CC=CC#CC	0.0
[#8][#6][#6H2]	0.9771	C=CCCC#C	0.0
[CX4H](O)CO	0.8638	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H2]([OX2H1])[CX4H1]	0.8315	[CX3H0][CX4H2][CX3H1]=[CX3H0]	0.0
OCC[CH2]	0.8025	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H2](O)[CHX4]	0.7424	CC#CCC=C	0.0
[#8H][#6H2][#6H1]	0.6962	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX4H2]	0.4858	[#6H2][#6H1][#6H1][#6H2]	0.1591
[CH2X4](O)[CX4H2]	0.4395	[#8][#6][#6][#6][#6][#8]	0.2583
[CX4H2]([OX2H0])[CX4H2]	0.371	[#8][#6H1][#6H1]	0.2611
O[CX4H2][CX4H2]O	0.2279	[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.2855
[CX4H2][OX2H0][CX4H2]	0.2006	[#6H1][#6H1]	0.3125
[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.1785	O[CX4H]([CX4H2])[CX4H1]	0.3703
[#6H1]([#6H2])[#6H2]	0.1477	O[CX4H][CX4H2]	0.5707
[OX2H0][CX4H2][CX4H2][OX2H0]	0.1118	[#6X4H2][#6H1][#8H]	0.5736
[CX4H1]([OX2H1])([CX4H1])[CX4H1]	0.1081	[#6H1][#6H2]	0.5941
[CX4H2]([OX2H1])[CX4H2]	0.0987	[OX2H1][CX4H1][CX4H1][OX2H1]	0.5981

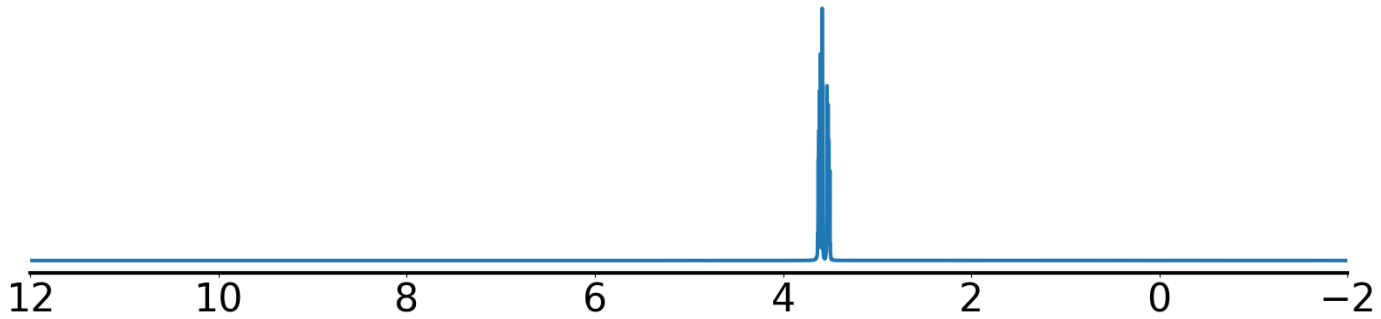
Example 175 true smiles: OCC(O)C(O)CO formula: C4H10O4
Index of correct structure: 0 of 92
True structure loss: 0.016768
True structure:



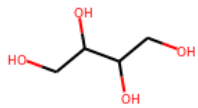
Experimental 13C NMR (solvent: CD3OD)



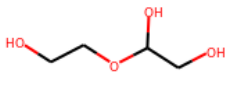
Experimental 1H NMR (solvent: D2O)



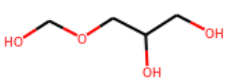
Top predicted structures (loss):



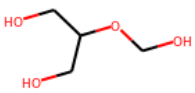
0.016768



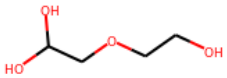
0.02061



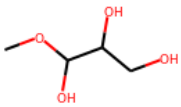
0.021821



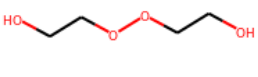
0.022514



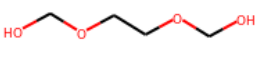
0.023665



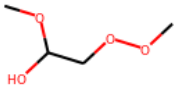
0.024513



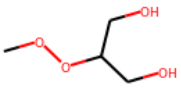
0.02567



0.026953



0.028259



0.029418

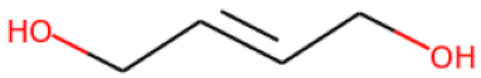
Top predicted substructures	prob		
[CX4H2]([#6])[O]	0.9976	[CX4H](O)CO	0.8726
[OX2H1]	0.997	[CX4H2]([OX2H1])[CX4H1]	0.8343
[#8][#6][#6H2][#8]	0.9868	OCC[CH2]	0.8025

[#8][#6][#6][#8]	0.986	[CX4H2](O)[CHX4]	0.743
[#8][#6][#6H2]	0.9768	[#8H][#6H2][#6H1]	0.6936

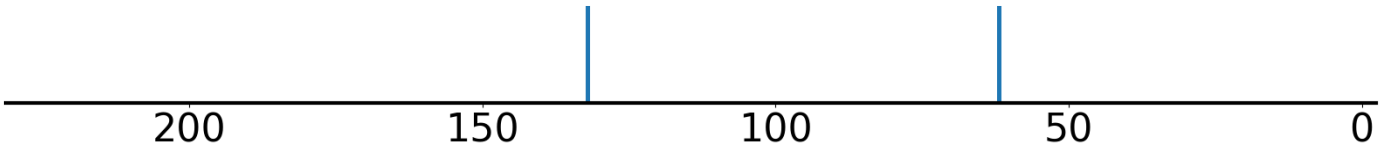
best positives	prob	best negatives	prob
[CX4H2]([#6])[O]	0.9976	CC=CCC#C	0.0
[OX2H1]	0.997	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6H2][#8]	0.9868	CCC#CC=C	0.0
[#8][#6][#6][#8]	0.986	CC=CC#CC	0.0
[#8][#6][#6H2]	0.9768	C=CCCC#C	0.0
[CX4H](O)CO	0.8726	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H2]([OX2H1])[CX4H1]	0.8343	[CX3H0][CX4H2][CX3H1]=[CX3H0]	0.0
OCC[CH2]	0.8025	CC#CCC=C	0.0
[CX4H2](O)[CHX4]	0.743	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#8H][#6H2][#6H1]	0.6936	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX4H2]	0.4851	[#6H2][#6H1][#6H1][#6H2]	0.1637
[CH2X4](O)[CX4H2]	0.4406	[#8][#6][#6][#6][#6][#8]	0.2587
[CX4H2]([OX2H0])[CX4H2]	0.3707	[#8][#6H1][#6H1]	0.2632
O[CX4H2][CX4H2]O	0.2245	[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.2898
[CX4H2][OX2H0][CX4H2]	0.1964	[#6H1][#6H1]	0.3079
[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.1786	O[CX4H]([CX4H2])[CX4H1]	0.379
[#6H1]([#6H2])[#6H2]	0.1469	O[CX4H][CX4H2]	0.5761
[OX2H0][CX4H2][CX4H2][OX2H0]	0.1147	[#6X4H2][#6H1][#8H]	0.5827
[CX4H1]([OX2H1])([CX4H1])[CX4H1]	0.1096	[#6H1][#6H2]	0.5944
[#6X4H1][#6X4H1][#6X4H1]	0.1004	[OX2H1][CX4H1][CX4H1][OX2H1]	0.6005

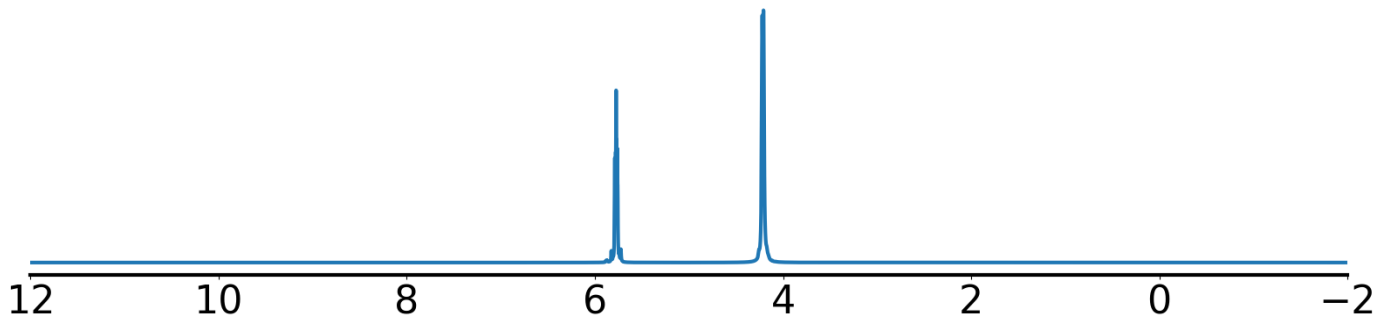
Example 176 true smiles: OCC=CCO formula: C4H8O2
Index of correct structure: 0 of 72
True structure loss: 0.00449
True structure:



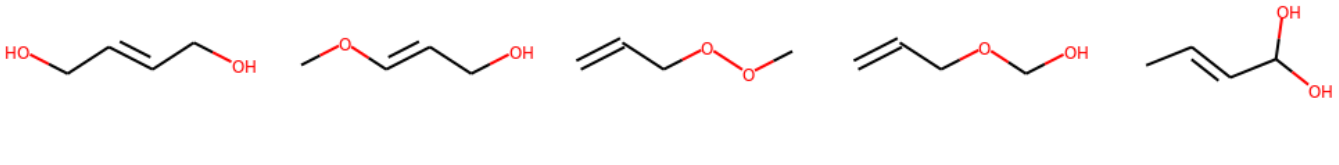
Experimental 13C NMR (solvent: DMSO-d6)



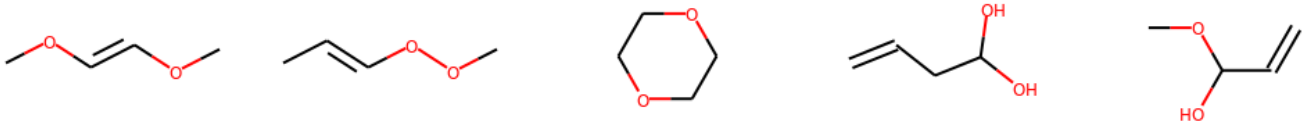
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.00449 0.065389 0.104814 0.10675 0.125735



0.131649 0.143793 0.146275 0.148439 0.148442

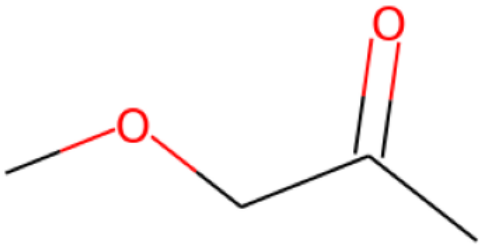
Top predicted substructures	prob		
[CHX3](=C)C	0.9998	[CX3H1](=[CX3H1])[CX4H2]	0.9912
[#6H1]	0.9996	[CX4H2]([#6])[O]	0.9907
[#8][#6H2][#6H]=[#6X3]	0.9992	O[CX4H2][CX3H1]	0.9892

[CX4H2][CX3]=C	0.998	[#8][#6][#6]=[#6X3]	0.9767
[#8H][#6H2][#6H1]	0.9952	[#6X3][#6H2][#8]	0.9551

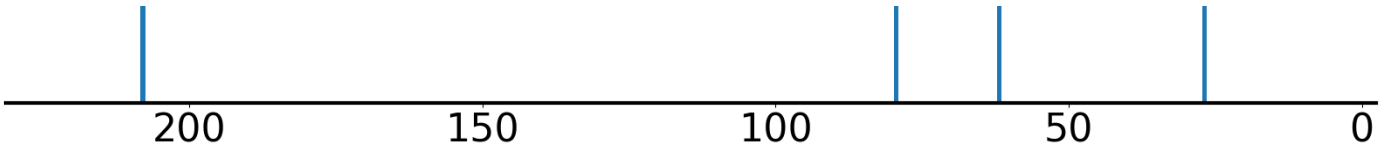
best positives	prob	best negatives	prob
[CHX3](=C)C	0.9998	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H1]	0.9996	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#8][#6H2][#6H]=[#6X3]	0.9992	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2][CX3]=C	0.998	C=CC=CC#C	0.0
[#8H][#6H2][#6H1]	0.9952	[#6X2][#6H1][#6X2]	0.0
[CX3H1](=[CX3H1])[CX4H2]	0.9912	CC#CCC#C	0.0
[CX4H2]([#6])[O]	0.9907	[CX2H0](#[CX2H1])[CX4H1]	0.0
O[CX4H2][CX3H1]	0.9892	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#8][#6][#6]=[#6X3]	0.9767	[CX4H2]([CX4H0])[CX2H0]	0.0
[#6X3][#6H2][#8]	0.9551	[CX2H0](#[CX2H1])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H1]	0.3787	[#8][#6][#6]=[#6][#6][#8]	0.499
[OH][CX4H]	0.2697	[CX4H2][CX3H]	0.6949
[CX3H][CX4H]	0.1495	[#6H1][#6H2]	0.8259
[#8][#6H1][#6H1]	0.1355	[CHX3]=[CHX3]	0.8984
[#8][#6][#6][#6X3]	0.1217	[CX4H2]([OX2H1])[CX3H1]	0.9102
[CX4H3][OX2H0]	0.1053	[OX2H1]	0.9327
[CX3H1](=[CX3H1])[CX4H1]	0.1026	[#8][#6H2][#6X3H]=[#6X3H]	0.9339
[CX3H1](=[CX3H1])[CX3H1]	0.0938	[#6H2][#6H1]=[#6H1][#6H2]	0.9548
[#6X3][#6X3]	0.0783	[#6X3][#6H2][#8]	0.9551
[CX4H3]	0.0777	[#8][#6][#6]=[#6X3]	0.9767

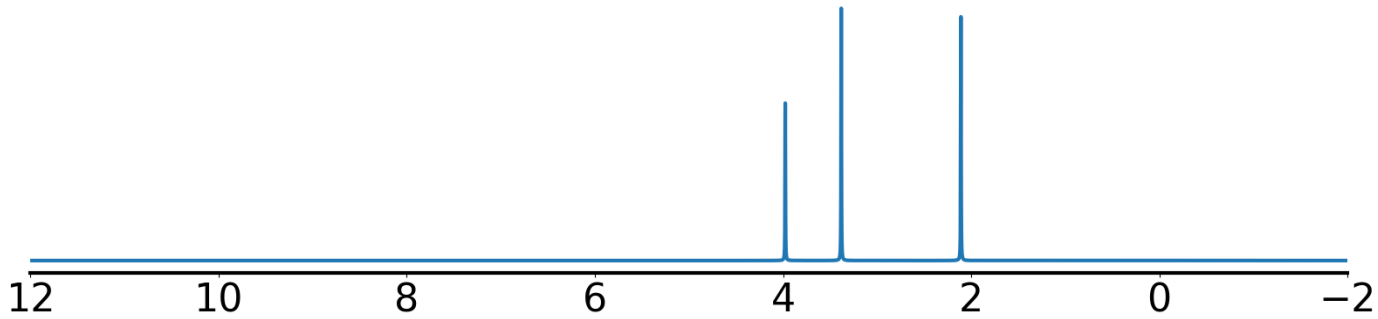
Example 177 true smiles: COCC(C)=O formula: C4H8O2
Index of correct structure: 0 of 72
True structure loss: 0.006544
True structure:



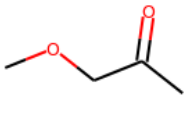
Experimental 13C NMR (solvent: CDCl3)



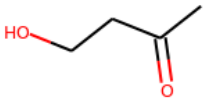
Experimental 1H NMR (solvent: CDCl3)



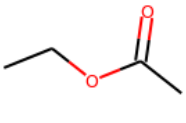
Top predicted structures (loss):



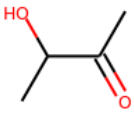
0.006544



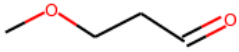
0.060101



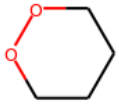
0.114435



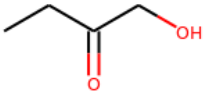
0.115004



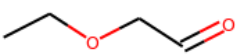
0.130328



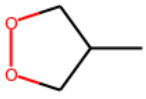
0.131932



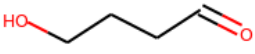
0.134524



0.138948



0.140668



0.141956

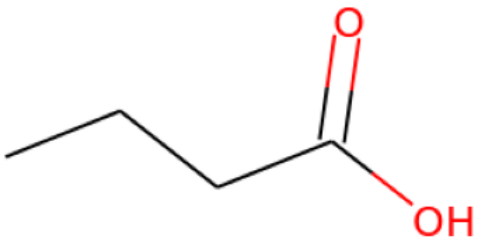
Top predicted substructures	prob		
[CX4H3][CX3]	1.0	[#6H3][#6][#6]	0.9977
[CX4H3][CX3H0]	0.9999	[#6H3][#6H0]	0.9962
[CX4H3]	0.9998	[CX4H3][#6]	0.9908

[CX3](=[OX1])C	0.9995	[OX2H0][CX4H2][CX3H0][CX4H3]	0.9906
[OX1H0]=[CX3H0][CX4H3]	0.9994	[CX4H2]([OX2H0])[CX3H0]	0.9724

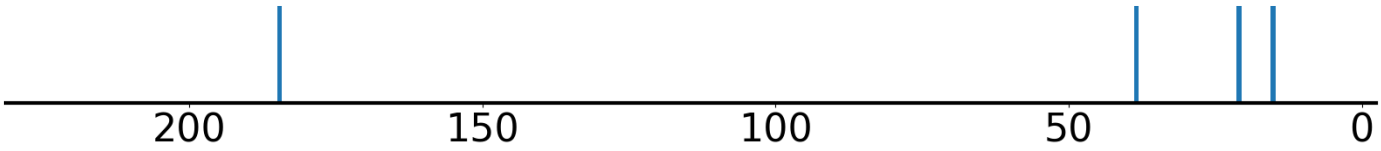
best positives	prob	best negatives	prob
[CX4H3][CX3]	1.0	CCC#CC#C	0.0
[CX4H3][CX3H0]	0.9999	C=CC=CC#C	0.0
[CX4H3]	0.9998	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX3](=[OX1])C	0.9995	CC=CC#CC	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9994	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H3][#6][#6]	0.9977	[#6X2][#6H1][#6X2]	0.0
[#6H3][#6H0]	0.9962	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][#6]	0.9908	[CX2H0](#[NX1H0])[CX3H1]	0.0
[OX2H0][CX4H2][CX3H0][CX4H3]	0.9906	[#7][#6][#6]#[#7]	0.0
[CX4H2]([OX2H0])[CX3H0]	0.9724	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
OCC[CH2]	0.3472	[#8][#6][#6]=[#8]	0.7237
[#8][#6][#6H2]	0.318	[#8]=[#6][#6H2][#8]	0.7293
[#8]=[#6H0][#6H1]	0.2955	[CX4H2][CX3]=O	0.7488
[CX4H2]CC=O	0.293	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.7952
[#6H1]	0.2557	[#6X3][#6H2][#8]	0.833
[#8][#6][#6][#6X3]	0.2477	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9026
[#6H1][#6H2]	0.2464	[#6H3][#6X3H0][#6H2]	0.906
[OX2H1]	0.1511	[CX4H3][OX2H0]	0.9204
[CX4H2][CX4H2]	0.1506	[CX4H2]([#6])[O]	0.928
[CX4H2]([OX2H0])[CX4H2]	0.1477	[CX4H3][OX2H0][CX4H2]	0.9368

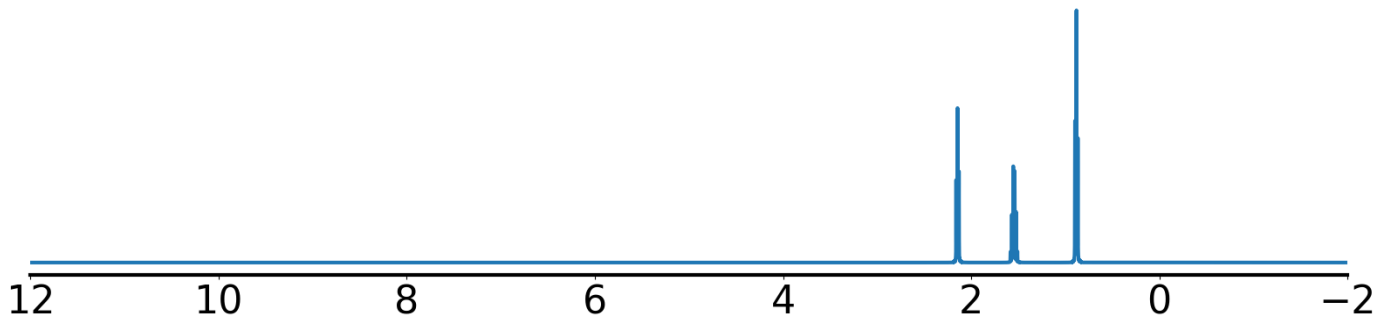
Example 178 true smiles: CCCC(=O)O formula: C4H8O2
Index of correct structure: 0 of 72
True structure loss: 0.00878
True structure:



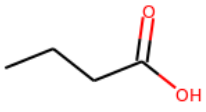
Experimental 13C NMR (solvent: CDCl3)



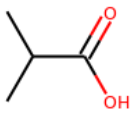
Experimental 1H NMR (solvent: D2O)



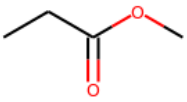
Top predicted structures (loss):



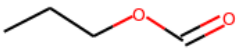
0.00878



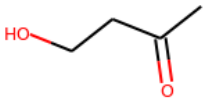
0.056313



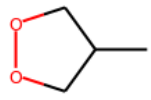
0.092859



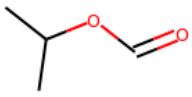
0.100006



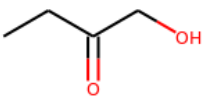
0.111503



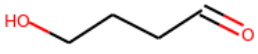
0.116315



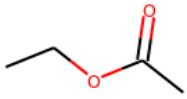
0.120523



0.126294



0.127472



0.128485

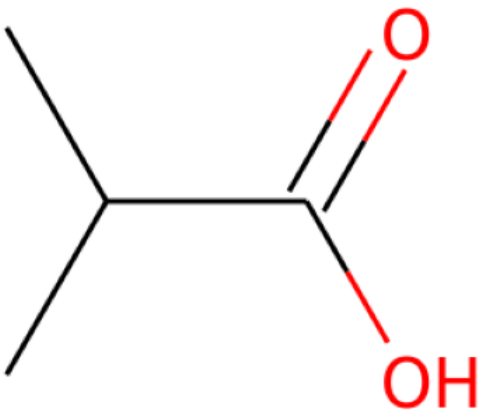
Top predicted substructures	prob		
[CX3](=[OX1])C	0.999	[CX4H3][CX4H2]	0.9942
[CX4H2]([#6])[#6]	0.9989	[#8]=[#6][#8]	0.9941
[#6H3][#6][#6]	0.9989	[CX3](=O)[OX2H1]	0.9921

[CX4H3][#6]	0.9977	[OX2H1]	0.987
[CX4H3]	0.9972	[CX3](=[OX1])O	0.9727

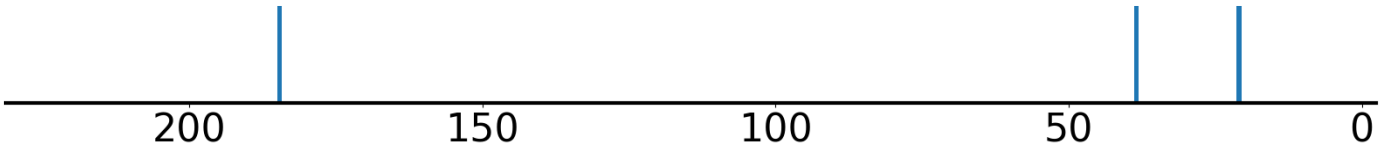
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.999	CCC=CC#C	0.0
[CX4H2]([#6])[#6]	0.9989	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9989	CCC#CC#C	0.0
[CX4H3][#6]	0.9977	CC=CC#CC	0.0
[CX4H3]	0.9972	CC=CCC#C	0.0
[CX4H3][CX4H2]	0.9942	C=CCCC#C	0.0
[#8]=[#6][#8]	0.9941	C=CC=CC#C	0.0
[CX3](=O)[OX2H1]	0.9921	[CX2H0](#[CX2H1])[CX3H1]	0.0
[OX2H1]	0.987	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX3](=[OX1])O	0.9727	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5366	[#8][#6][#6H2]	0.4587
[#8]=[#6H0][#6H1]	0.3821	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.5066
[#8][#6H0][#6H1]	0.3477	O=[CX3H0][CX4H2][CX4H2]	0.5954
O=[CX3][CX4H]	0.2241	[CX4H2][CX3]=O	0.6263
[CX4H3][CX4H1]	0.1645	OCC[CH2]	0.6402
[#6H1]	0.1644	[#6X3][#6][#6][#6H3]	0.7231
[#6H1][#6H2]	0.1625	[CX4H2]CC=O	0.7422
[#8]=[#6][#6]=[#8]	0.1511	[CX4H2]([CX4H2])[CX3H0]	0.7681
[#8][#6][#6]=[#8]	0.1134	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.8081
[CH3]CC[OH]	0.1129	[CX4H2][CX4H2]	0.8794

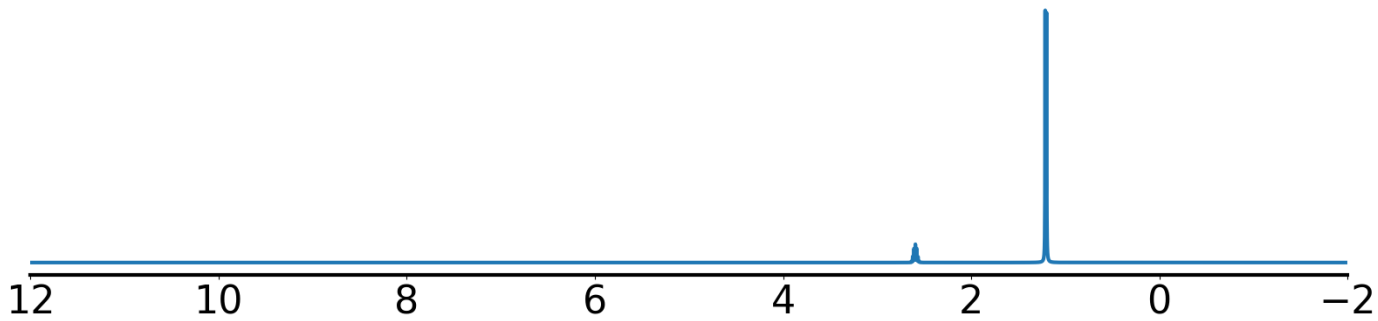
Example 179 true smiles: CC(C)C(=O)O formula: C4H8O2
Index of correct structure: 0 of 72
True structure loss: 0.005506
True structure:



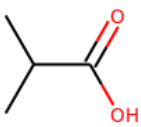
Experimental 13C NMR (solvent: CDCl3)



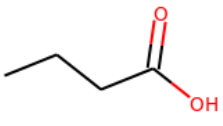
Experimental 1H NMR (solvent: CDCl3)



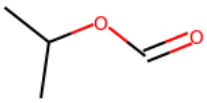
Top predicted structures (loss):



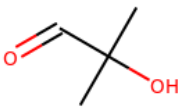
0.005506



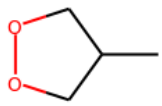
0.077914



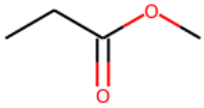
0.084234



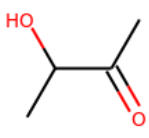
0.101948



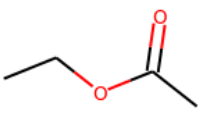
0.107408



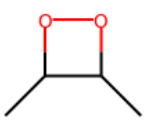
0.113703



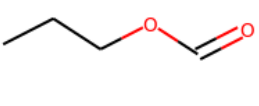
0.124453



0.127398



0.129836



0.132785

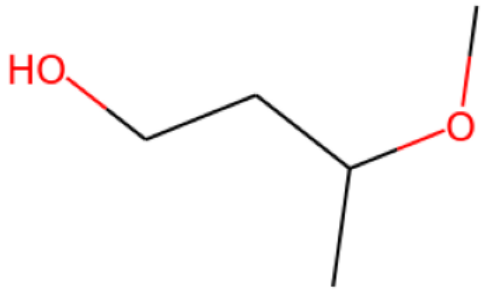
Top predicted substructures	prob		
[CX4H3]	1.0	[#8]=[#6][#8]	0.9846
[#6H3][#6][#6]	0.9999	[CX4H3][CX4H1]	0.9659
[CX4H3][#6]	0.9998	[CX3](=[OX1])O	0.9634

[CX3](=[OX1])C	0.9977	O=[CX3][CX4H]	0.9352
[CX3](=O)[OX2H1]	0.9969	[OX2H1]	0.9339

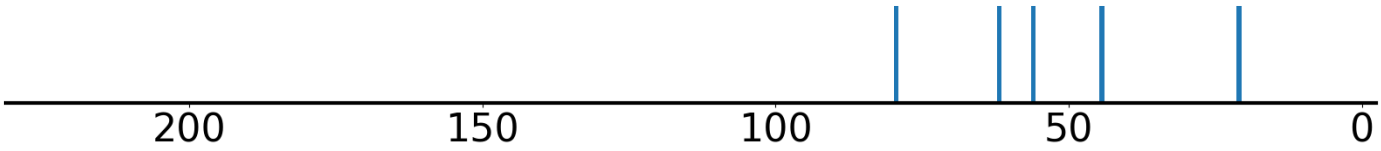
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9999	C=CC=CC#C	0.0
[CX4H3][#6]	0.9998	CCC#CC#C	0.0
[CX3](=[OX1])C	0.9977	CC=CC#CC	0.0
[CX3](=O)[OX2H1]	0.9969	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8]=[#6][#8]	0.9846	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H3][CX4H1]	0.9659	CCC=CC#C	0.0
[CX3](=[OX1])O	0.9634	[CX4H3][CX2H0]	0.0
O=[CX3][CX4H]	0.9352	[#6H2]=[#6][#6X2]	0.0
[OX2H1]	0.9339	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#6H1][#6H1]	0.4888	[CH3]CC[OH]	0.5814
[#6X3][#6][#6][#6H3]	0.2938	[CHX4]([CH3X4])[CH3X4]	0.7996
[#6H1][#6H1]	0.286	[#8][#6H0][#6H1]	0.8055
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2048	[#6H3][#6][#6X3]	0.8144
[CX4H2]CC=O	0.1892	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.864
[#6H3][#6][#6][#6H3]	0.1777	[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.8774
[CHX4]([CH3X4])[CH2X4]	0.168	[#8]=[#6H0][#6H1]	0.9054
[CX4H2][CX3]=O	0.0983	[#6H1]	0.9079
[CX4H2]([CH])[CH]	0.0814	[OX2H1]	0.9339
[#6H1][#6H2]	0.0726	O=[CX3][CX4H]	0.9352

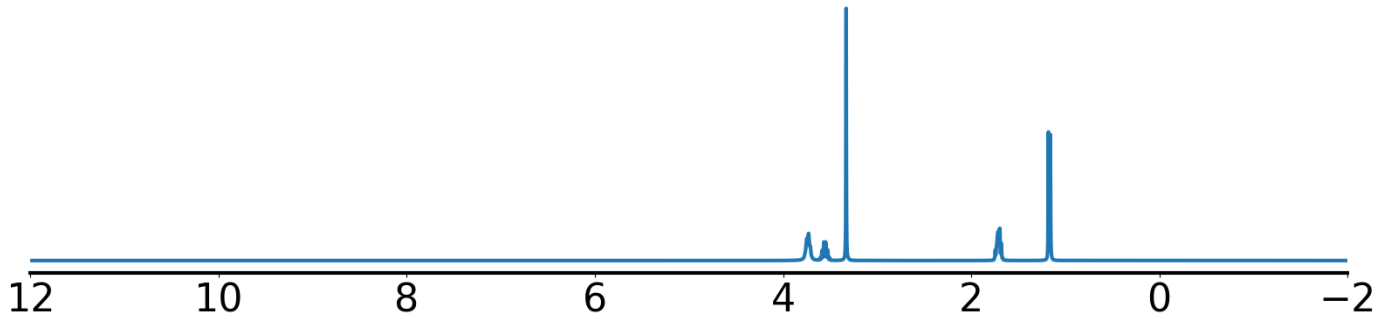
Example 180 true smiles: COC(C)CCO formula: C5H12O2
Index of correct structure: 0 of 69
True structure loss: 0.013422
True structure:



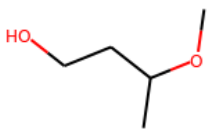
Experimental 13C NMR (solvent: CDCl3)



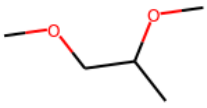
Experimental 1H NMR (solvent: CDCl3)



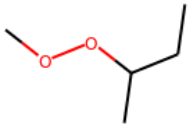
Top predicted structures (loss):



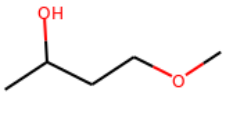
0.013422



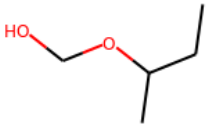
0.031664



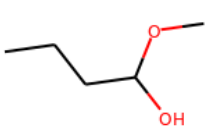
0.032577



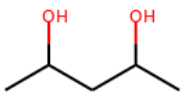
0.035588



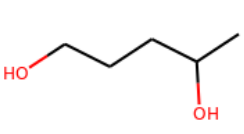
0.040513



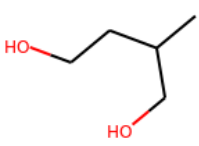
0.041928



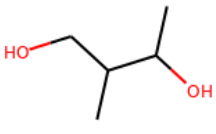
0.042913



0.043718



0.044175



0.044311

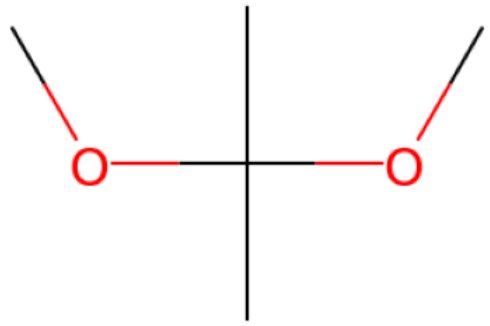
Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][CX4H1]	0.9701
[CX4H3][#6]	0.9974	[CX4H3][CX4]O	0.9668
[#6H3][#6][#6]	0.9944	[#6H1][#6H2]	0.9402

[CX4H3][OX2H0]	0.9924	[CX4H]O	0.9263
[#6H1]	0.9916	[CX4H2]([#6])[O]	0.8977

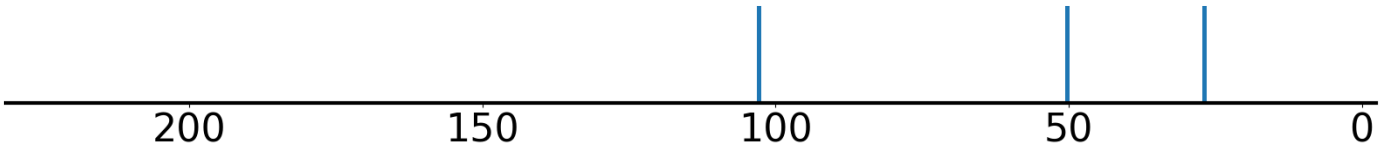
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][#6]	0.9974	CCC=CC#C	0.0
[#6H3][#6][#6]	0.9944	CC=CC#CC	0.0
[CX4H3][OX2H0]	0.9924	[#7][#6]=[#6][#6]#[#7]	0.0
[#6H1]	0.9916	C=CC=CC#C	0.0
[CX4H3][CX4H1]	0.9701	CC=CCC#C	0.0
[CX4H3][CX4]O	0.9668	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#6H1][#6H2]	0.9402	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H]O	0.9263	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[O]	0.8977	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[#8][#6H1][#6H1]	0.54	[OX2H0][CX4H1][CX4H2][CX4H2]	0.3091
[#6H1][#6H1]	0.429	[CH2X4](O)[CX4H2]	0.4421
[CX4H3][OX2H0][CX4H2]	0.3905	O[CX4H][CX4H2]	0.5162
[OH][CX4H]	0.292	[CX4H2]([OX2H1])[CX4H2]	0.5304
[CX4H2]([CX4H1])[CX4H1]	0.2727	[CX4H2][CX4H2]	0.5396
[#8][#6][#6][#6][#6][#8]	0.2527	[CHX4]([CH3X4])[CH2X4]	0.5901
[CX4H2](O)[CHX4]	0.2359	[CX4H2]([CX4H2])[CX4H1]	0.6575
O[CX4H]([CX4H2])[CX4H1]	0.1783	[CX4H2]([#6])[#6]	0.6716
[CX4H2]([CH])[CH]	0.1768	[CX4H1]([OX2H0])([CX4H3])[CX4H2]	0.761
[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.1731	[OX2H0][CX4H1][CX4H3]	0.8019

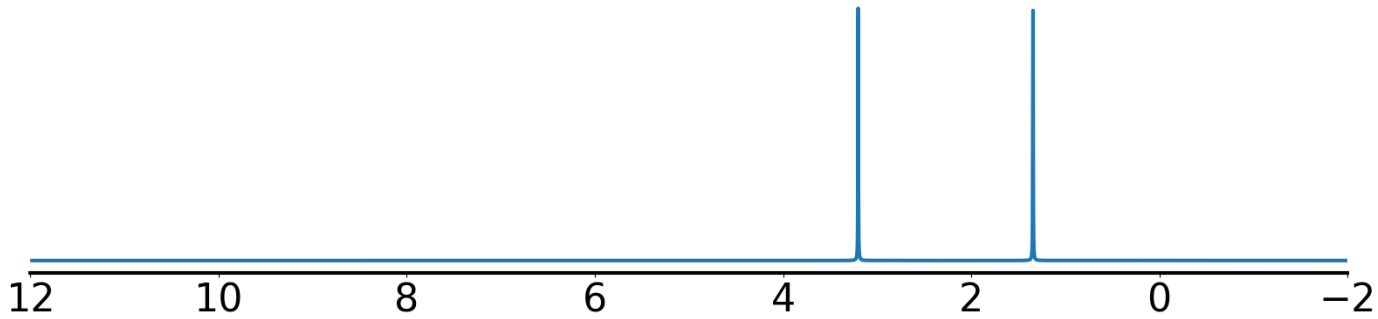
Example 181 true smiles: COC(C)(C)OC formula: C5H12O2
Index of correct structure: 0 of 69
True structure loss: 0.004759
True structure:



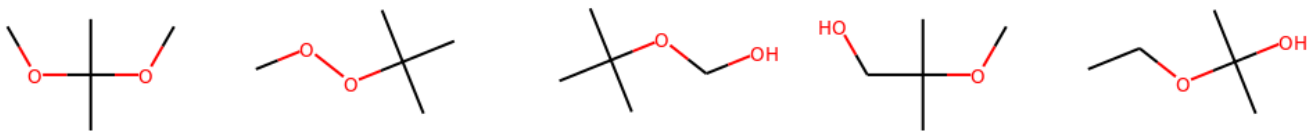
Experimental 13C NMR (solvent: CDCl3)



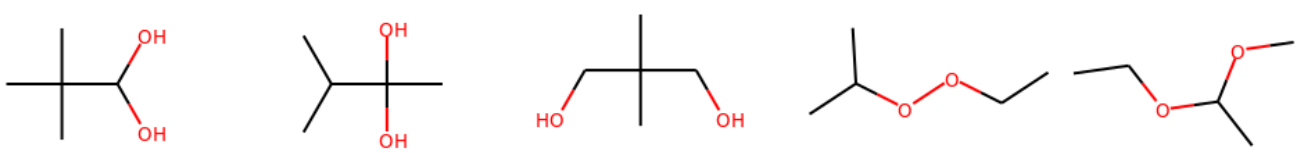
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.004759 0.014062 0.022775 0.045376 0.045577



0.04945 0.053543 0.062637 0.064374 0.066537

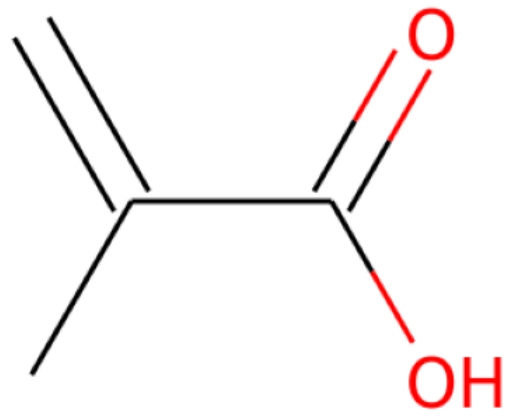
Top predicted substructures	prob		
[CX4H3]	0.9999	[#6H3][#6][#6]	0.9887
[CX4H3][#6]	0.9997	[#6H3][#8][#6H0][#8]	0.9717
[CX4H3][CX4]O	0.9995	[CH3][#6][#8]	0.9704

[CX4H3][CX4H0]	0.9935	[#6H3][#6H0]	0.9627
[CX4H3][OX2H0]	0.9935	[#6H0]([#6H3])([#6H3])[#8]	0.9389

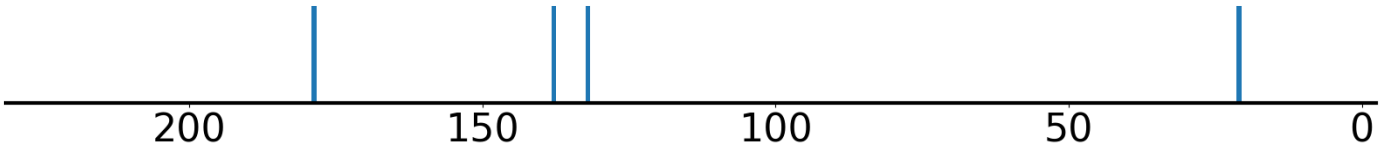
best positives	prob	best negatives	prob
[CX4H3]	0.9999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][#6]	0.9997	CCC#CC#C	0.0
[CX4H3][CX4]O	0.9995	C=CC=CC#C	0.0
[CX4H3][CX4H0]	0.9935	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][OX2H0]	0.9935	[#7][#6]=[#6][#6]#[#7]	0.0
[#6H3][#6][#6]	0.9887	CC#CCC#C	0.0
[#6H3][#8][#6H0][#8]	0.9717	[#6X2][#6H1][#6X2]	0.0
[CH3][#6][#8]	0.9704	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6H3][#6H0]	0.9627	CC=CCC#C	0.0
[#6H0]([#6H3])([#6H3])[#8]	0.9389	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.5702	[CX4H3][CX4H0]([CX4H3])[OX2H0]	0.9098
[CX4H]O	0.5465	[CX4H3][CX4H0][CX4H3]	0.9222
[#8][#6][#6H2]	0.4975	[#6H0]([#6H3])([#6H3])[#8]	0.9389
[#8][#6H0][#6H1]	0.2987	[#6H3][#6H0]	0.9627
[CX4H3][CX4H1]	0.2463	[CH3][#6][#8]	0.9704
[OX2H0][CX4H1][OX2H0]	0.1506	[#6H3][#8][#6H0][#8]	0.9717
OCC[CH2]	0.1153	[#6H3][#6][#6]	0.9887
[#8][#6H1][#6H1]	0.1044	[CX4H3][OX2H0]	0.9935
[#8][#6][#6][#8]	0.0941	[CX4H3][CX4H0]	0.9935
[#6H3][#6H0]([#6H2])[#6H2]	0.0532	[CX4H3][CX4]O	0.9995

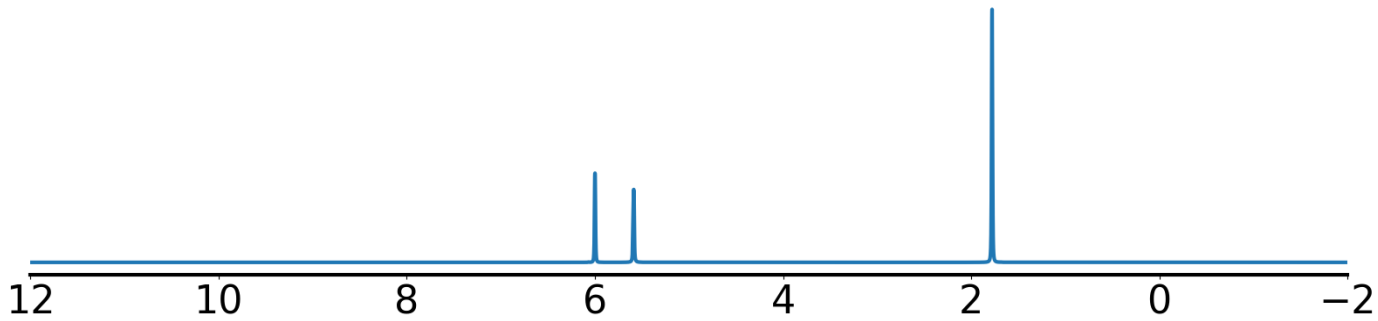
Example 182 true smiles: C=C(C)C(=O)O formula: C4H6O2
Index of correct structure: 0 of 68
True structure loss: 0.034097
True structure:



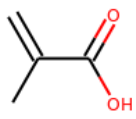
Experimental 13C NMR (solvent: CDCl3)



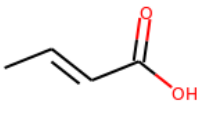
Experimental 1H NMR (solvent: D2O)



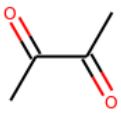
Top predicted structures (loss):



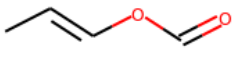
0.034097



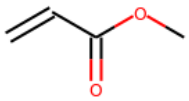
0.037208



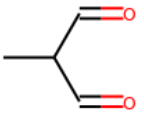
0.084706



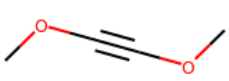
0.089645



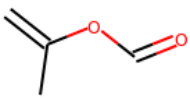
0.095468



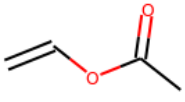
0.113819



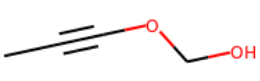
0.123603



0.127293



0.134404



0.141415

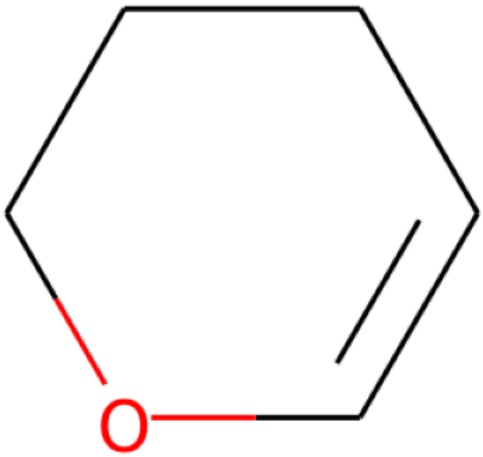
Top predicted substructures	prob		
[CX4H3]	0.9997	[#6H3][#6]=[#6X3]	0.9926
[CX4H3][#6]	0.9997	[#6H1]	0.9866
[CX4H3][CX3]	0.9997	[OX2H1]	0.9865

[CX3](=O)[OX2H1]	0.9976	[#8]=[#6][#8]	0.9827
[CX3](=[OX1])C	0.9935	[CX3](=[OX1])O	0.9798

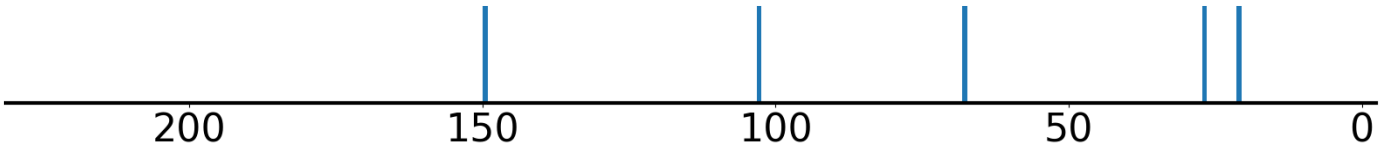
best positives	prob	best negatives	prob
[CX4H3]	0.9997	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][#6]	0.9997	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H3][CX3]	0.9997	[#6H2][#6]#[#6X2]	0.0
[CX3](=O)[OX2H1]	0.9976	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9935	[CX2H0](#[CX2H1])[CX4H1]	0.0
[#6H3][#6]=[#6X3]	0.9926	CCC#CC#C	0.0
[OX2H1]	0.9865	[#6X2][#6H1][#6X2]	0.0
[#8]=[#6][#8]	0.9827	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])O	0.9798	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6X3][#6X3]	0.9742	[CX2H0](#[CX2H1])[cX3H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.9866	[CX3H2]=[CX3H0]	0.2111
[CHX3](=C)C	0.9658	[CH2X3](=C)	0.3434
O=[#6][#6][#6X3]	0.7783	[CH3]CC[OH]	0.3681
[CX3H1](=[CX3H1])[CX4H3]	0.563	[#6X3H2]	0.3915
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5421	[CX3H2]=[CX3H0][CX3]=O	0.4052
[#6X3][#6]=[#6][#6H3]	0.5275	[CX4H3][CX3H0]	0.4053
[#8]=[#6H0][#6H1]	0.4829	[CX3H2]=[CX3H0]([#6])[#6]	0.4073
[#8][#6H0][#6H1]	0.4816	[#6H3][#6H0]	0.4215
[#6X3H1][#6X3H0]	0.4309	[CX3H0](=[CX3H2])([CX4H3])[CX3H0]	0.4381
[CHX3]=[CHX3]	0.3962	[CX4H3][CX3H0]=[CX3H2]	0.4399

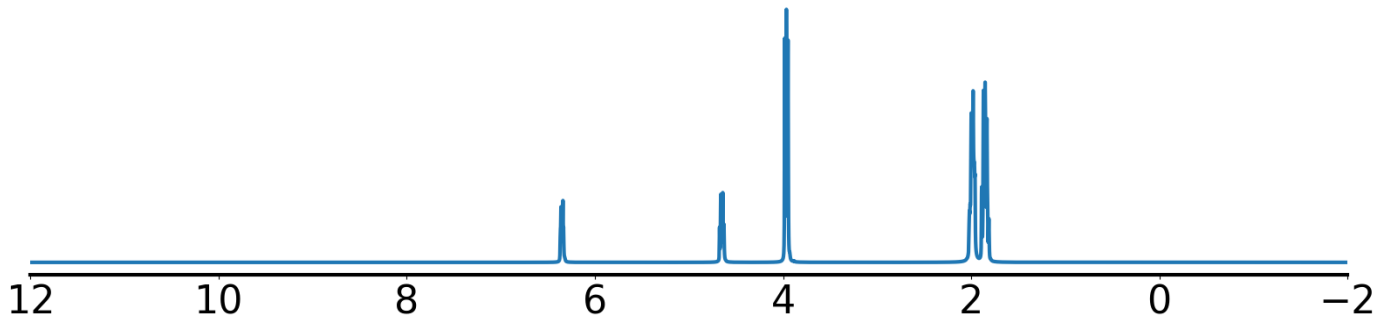
Example 183 true smiles: C1=COCCC1 formula: C5H8O
Index of correct structure: 0 of 66
True structure loss: 0.00998
True structure:



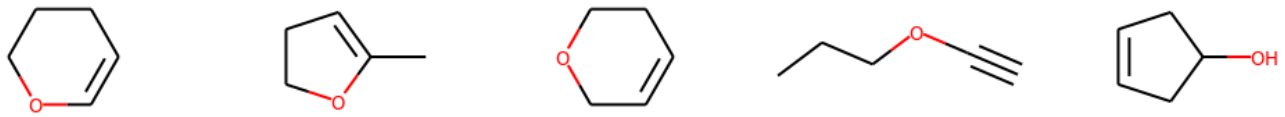
Experimental 13C NMR (solvent: CDCl3)



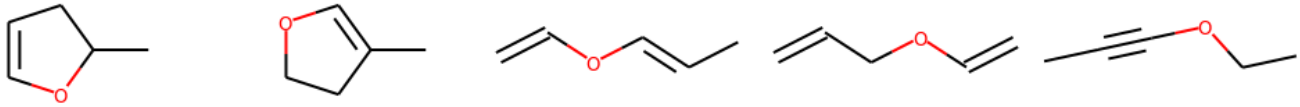
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.00998 0.077758 0.08154 0.103122 0.1057



0.116916 0.118393 0.120263 0.123239 0.127778

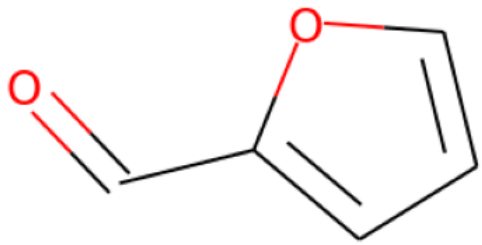
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9973	[CH2X4](O)[CX4H2][CX4H2]	0.9545
[CHX3](=C)C	0.9936	[O][CX3H1]=[CX3H1]	0.9385
[CX4H2]([#6])[O]	0.9934	[OX2H0][CX4H2][CX4H2][CX4H2]	0.9379

[#6H1]	0.9896	[CX4H2][CX3]=C	0.9142
[#8]1[#6][#6][#6][#6]=[#6]1	0.9723	[CX4H2][CX4H2]	0.9131

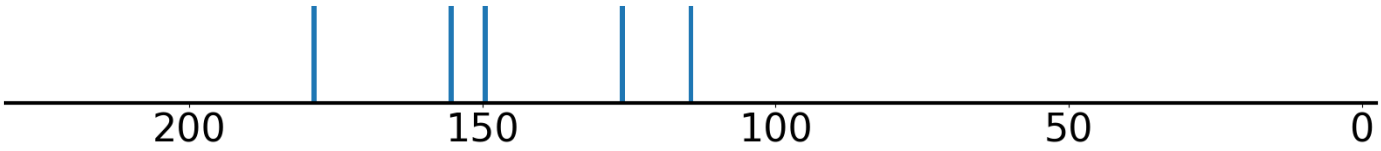
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9973	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CHX3](=C)C	0.9936	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H2]([#6])[O]	0.9934	[CX3H1](=[CX3H2])[cX3H0]	0.0
[#6H1]	0.9896	CC#CCC#C	0.0
[#8]1[#6][#6][#6][#6]=[#6]1	0.9723	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CH2X4](O)[CX4H2][CX4H2]	0.9545	[#7][#6][#6]#[#7]	0.0
[O][CX3H1]=[CX3H1]	0.9385	[#6X2][#6H1][#6X2]	0.0
[OX2H0][CX4H2][CX4H2][CX4H2]	0.9379	[CX4H2]([CX4H0])[CX2H0]	0.0
[CX4H2][CX3]=C	0.9142	[#7][#6]=[#6][#6]#[#7]	0.0
[CX4H2][CX4H2]	0.9131	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H3]	0.5509	[CX4H2]([CX4H2])[CX3H1]	0.6603
[CX4H3][#6]	0.5227	[CHX3]=[CHX3]	0.6832
[CX4H3][CX3]	0.3269	[CX4H2]([OX2H0])[CX4H2]	0.745
[#6H3][#6]=[#6X3]	0.2898	OCC[CH2]	0.7567
[CH3][#6][#8]	0.2083	[CX4H2][CX3H]	0.7916
[#8][#6][#6]=[#6X3]	0.1956	[CH2X4](O)[CX4H2]	0.795
C1OCCC1	0.1729	[CX3H1](=[CX3H1])[CX4H2]	0.7967
[#6X3][#6H2][#8]	0.1534	[#6H2][#8][#6H1]	0.7991
[CX4H3][CX3H0]	0.1265	[CX3H]O[CX4H2]	0.8047
CCCCC=C	0.1231	[CX4H2]([CX4H2])[CX4H2]	0.8114

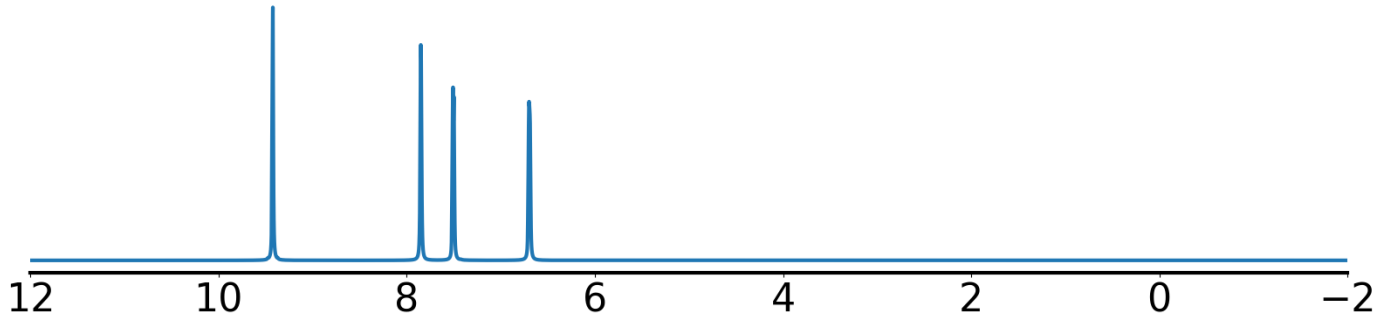
Example 184 true smiles: O=Cc1ccco1 formula: C5H4O2
Index of correct structure: 0 of 65
True structure loss: 0.026066
True structure:



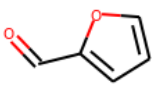
Experimental 13C NMR (solvent: CDCl3)



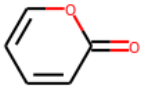
Experimental 1H NMR (solvent: D2O)



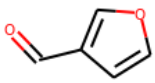
Top predicted structures (loss):



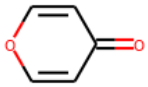
0.026066



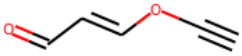
0.042903



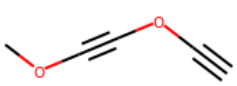
0.043117



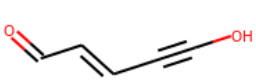
0.054581



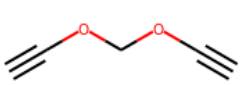
0.087684



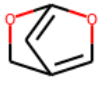
0.095056



0.100161



0.110948



0.110953

0.11748

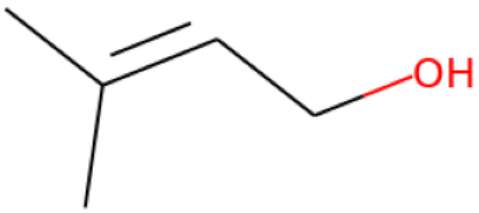
Top predicted substructures	prob		
[#6H1]	1.0	[cX3H1]([cX3H1])[cX3H1]	0.8774
[#6X3][#6X3]	0.9998	[#6X3H1][#6X3H0]	0.848
[CX3H1](=O)[#6]	0.9664	[#8]=[#6][#8]	0.7761

[cH][cH]	0.9129	[cH]	0.773
[#6H1][#6H1]	0.9086	[cX3H1]([cX3H1])[cX3H0]	0.7308

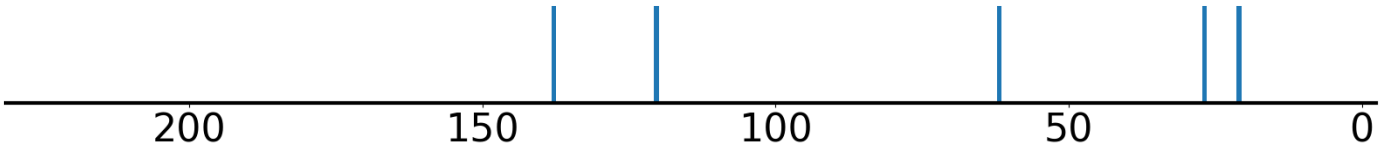
best positives	prob	best negatives	prob
[#6H1]	1.0	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9998	[#6H3][#6H2][#6H1r4]	0.0
[CX3H1](=O)[#6]	0.9664	[CX2H0](#[CX2H1])[CX4H0]	0.0
[cH][cH]	0.9129	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[#6H1][#6H1]	0.9086	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.8774	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.848	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[cH]	0.773	[#6H3][#6H0][#7][#6H3]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.7308	[CX4H1]([NX3H0])([CX4H3])[CX4H1]	0.0
[#8][#6][#6][#6X3]	0.665	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#8]	0.7761	[#8][#6][#6]=[#8]	0.0584
O=[#6][#6]=[#6X3]	0.5884	[cX3H1]([oX2H0])[cX3H1]	0.1085
[CX3](=[OX1])C	0.5206	[#8][#6H][#6X3][#6X3H]	0.179
[CHX3](=C)C	0.4888	o[cH]	0.2269
[CX3](=[OX1])O	0.4678	[#8][#6H1][#6H1]	0.3274
[CX3](=O)[OX2H1]	0.4635	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3378
[#8]=[#6H][#6X3]=[#6X3H]	0.3871	O=[#6][#6][#6X3]	0.3909
[CHX3]=[CHX3]	0.3216	[#8]=[#6H][#6X3][#6X3H]	0.4438
[#8]=[#6H1][#6H1]	0.3098	[#8][#6H0][#6H1]	0.596
O=C[CX3H]	0.285	[#6X3][#6X3][#6X3][#6X3]	0.6117

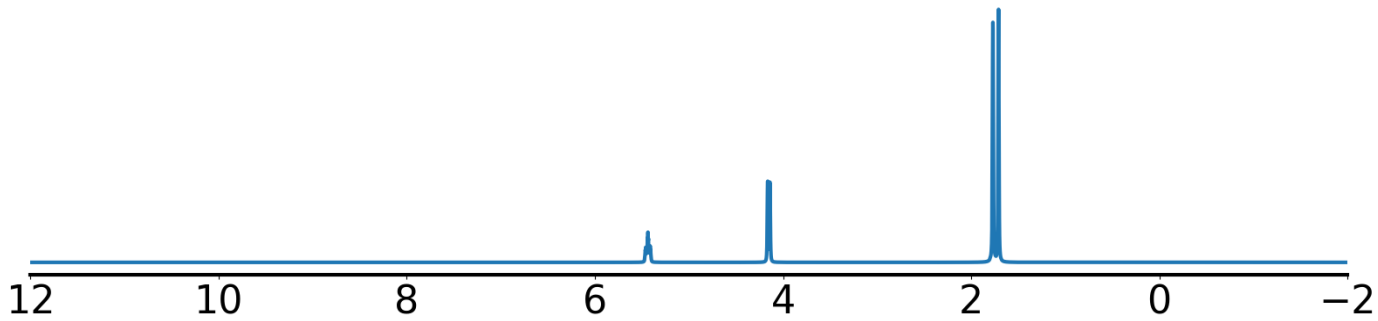
Example 185 true smiles: CC(C)=CCO formula: C5H10O
Index of correct structure: 0 of 65
True structure loss: 0.007174
True structure:



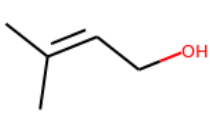
Experimental 13C NMR (solvent: CDCl3)



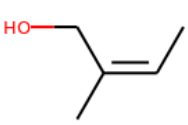
Experimental 1H NMR (solvent: CDCl3)



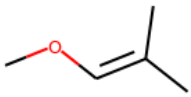
Top predicted structures (loss):



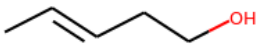
0.007174



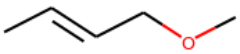
0.050776



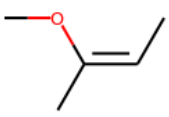
0.075936



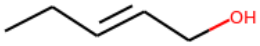
0.091646



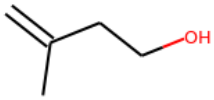
0.092371



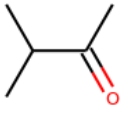
0.096789



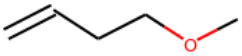
0.113027



0.117666



0.133113



0.138189

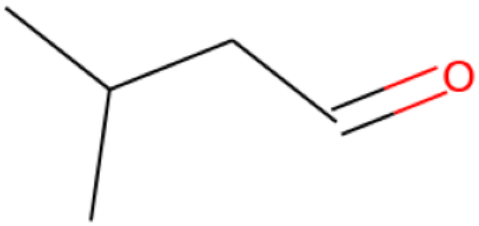
Top predicted substructures	prob		
[CX4H3]	1.0	[#6H3][#6][#6]	0.9927
[CX4H3][CX3]	1.0	[#8][#6H2][#6H1]=[#6H0]	0.9879
[#6H3][#6H0]	0.998	[CHX3](=C)C	0.9836

[CX4H3][CX3H0]	0.9978	[CX4H2]([#6])[O]	0.9772
[CX4H3][#6]	0.9962	[#6H1]	0.9699

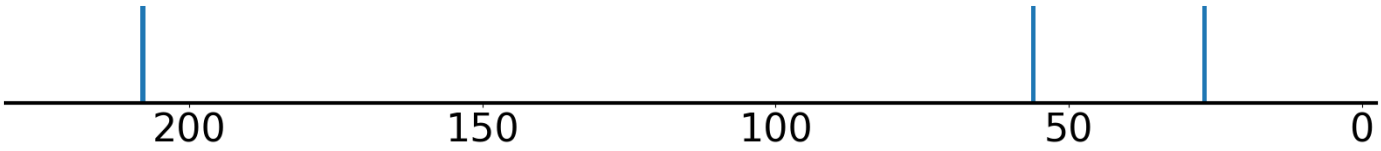
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][CX3]	1.0	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#6H3][#6H0]	0.998	CCC#CC#C	0.0
[CX4H3][CX3H0]	0.9978	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9962	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9927	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#8][#6H2][#6H1]=[#6H0]	0.9879	[#6X2][#6H1][#6X2]	0.0
[CHX3](=C)C	0.9836	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2]([#6])[O]	0.9772	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
[#6H1]	0.9699	[CX3H1](=[OX1H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[OX2H1][CX4H2][#6X3H0]	0.2203	[CX4H2][CX3H]	0.3513
[CX4H2][CX4H2]	0.2134	[#6H1][#6H2]	0.5218
[#6H3][#6]=[#6][#6H3]	0.1816	[CX4H2]([OX2H1])[CX3H1]	0.6781
[OH][CX4H]	0.1804	[CX4H3][CX3H0][CX4H3]	0.7829
[#8][#6][#6][#6X3]	0.1365	O[CX4H2][CX3H1]	0.7858
[#6H1][#6H1]	0.1291	[#6X3][#6H2][#8]	0.8034
[CX4H3][CX3H1]	0.1207	[CX3H0](=[CX3H1])([CX4H3])[CX4H3]	0.8119
[#6H3][#6X3H0][#6H2]	0.1066	[CX4H2][CX3]=C	0.8354
[CX3H1](=[CX3H1])[CX4H3]	0.1033	[#8][#6H2][#6H]=[#6X3]	0.8539
[CH2X4](O)[CX4H2]	0.0977	[#8H][#6H2][#6H1]	0.8616

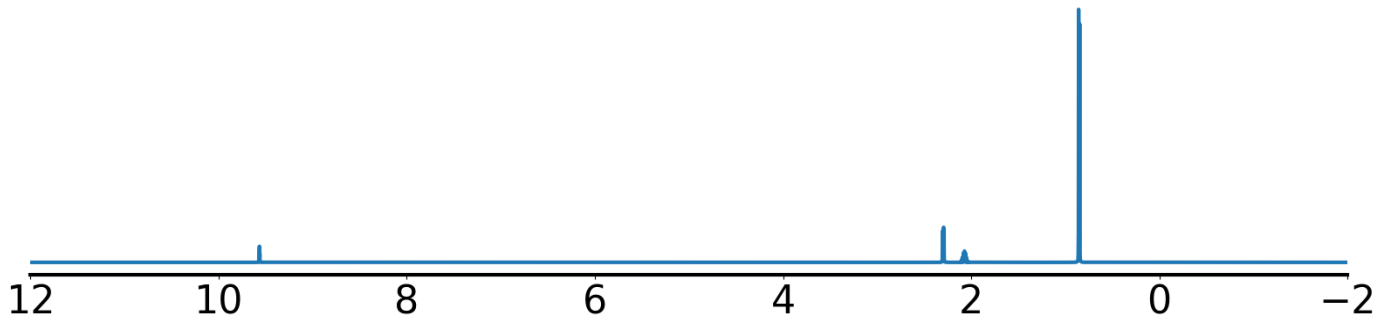
Example 186 true smiles: CC(C)CC=O formula: C5H10O
Index of correct structure: 0 of 65
True structure loss: 0.01415
True structure:



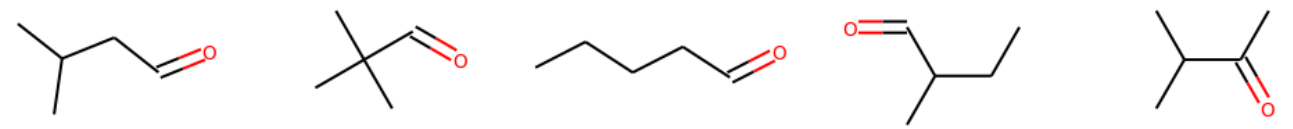
Experimental 13C NMR (solvent: CDCl3)



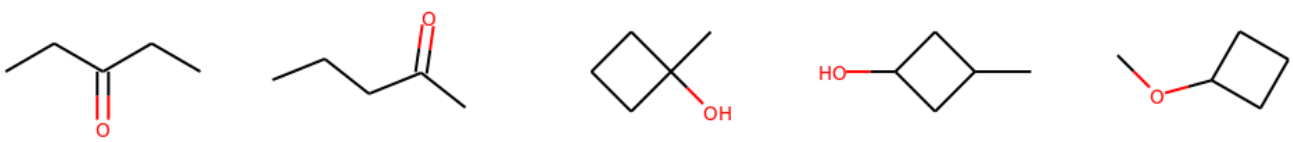
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.01415 0.030954 0.048717 0.067829 0.071756



0.081982 0.100525 0.156875 0.172101 0.176257

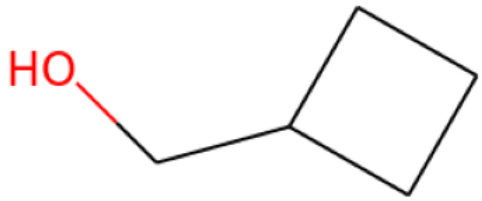
Top predicted substructures	prob		
[CX4H3]	0.9998	[#6H1]	0.9919
[CX3H1](=O)[#6]	0.9997	[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.9165
[CX3](=[OX1])C	0.9995	[#6X3][#6][#6][#6H3]	0.9031

[#6H3][#6][#6]	0.9994	[CHX4]([CH3X4])[CH3X4]	0.8389
[CX4H3][#6]	0.9985	[#6H1][#6H2]	0.6827

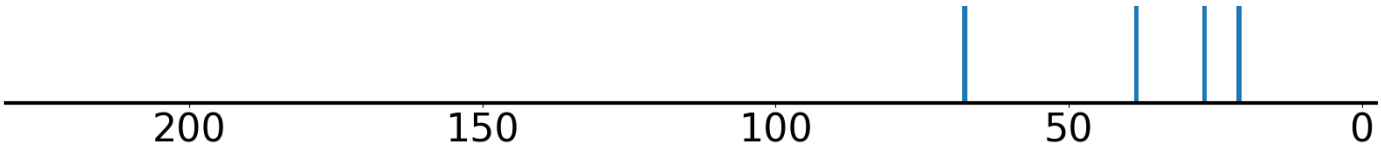
best positives	prob	best negatives	prob
[CX4H3]	0.9998	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3H1](=O)[#6]	0.9997	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9995	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H3][#6][#6]	0.9994	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9985	CCC#CC#C	0.0
[#6H1]	0.9919	CCC=CC#C	0.0
[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.9165	C=CCCC#C	0.0
[#6X3][#6][#6][#6H3]	0.9031	CCC#CC=C	0.0
[CHX4]([CH3X4])[CH3X4]	0.8389	CC=CC#CC	0.0
[#6H1][#6H2]	0.6827	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]CC=O	0.3359	[CX4H2]([CH])[CH]	0.1769
[#6H3][#6H0]	0.2868	[OX1H0]=[CX3H1][CX4H2][CX4H1]	0.2552
O=[CX3][CX4H]	0.2263	[CX3H1](=[OX1H0])[CX4H2]	0.2966
[CX4H3][CX4H0][CX4H3]	0.1848	[CX4H2][CX3H]	0.297
[#8]=[#6H1][#6H1]	0.1038	[#8]=[#6][#6H2][#6H1]	0.353
[CX4H2]([CX4H1])[CX3H0]	0.0991	[CX4H2]([CX4H1])[CX3H1]	0.4448
[#6X3H1][#6H1][#6H2]	0.0932	[CHX4]([CH3X4])[CH2X4]	0.4657
O=[CX3H0][CX4H2][CX4H1]	0.07	[CX4H2][CX3]=O	0.4971
[CX3H][CX4H]	0.0659	[CX4H2]([#6])[#6]	0.5473
[#6H1][#6H1]	0.0595	[CX4H3][CX4H1]	0.556

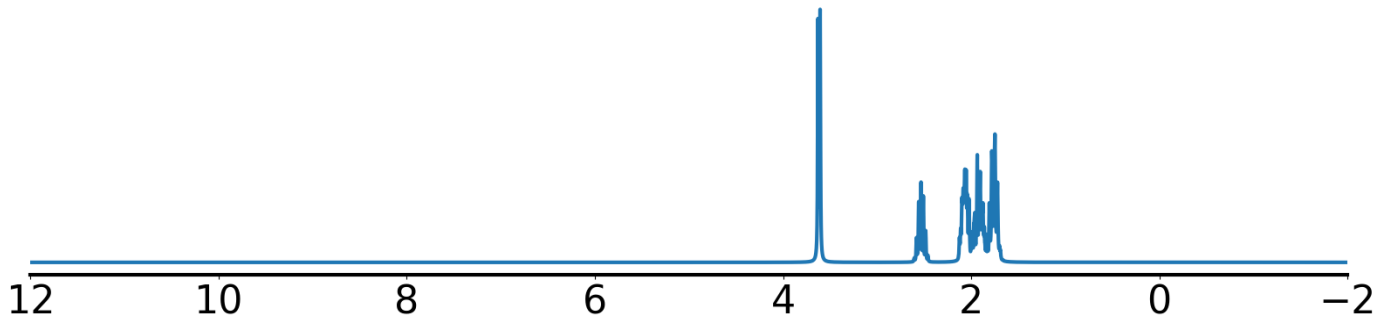
Example 187 true smiles: OCC1CCC1 formula: C5H10O
Index of correct structure: 0 of 65
True structure loss: 0.010513
True structure:



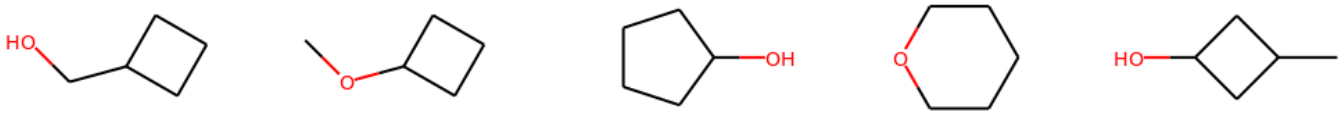
Experimental 13C NMR (solvent: CDCl3)



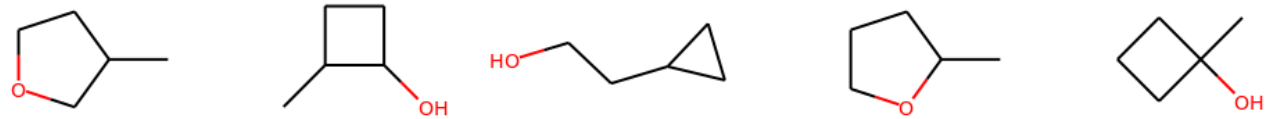
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.010513 0.045102 0.046123 0.055905 0.084224



0.08514 0.089069 0.092136 0.105299 0.108361

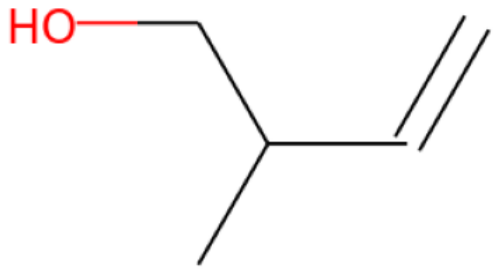
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H1]1[CX4H2][CX4H2][CX4H2]1	0.8752
[CX4H2]([#6])[O]	0.9711	[#6H1][#6H2]	0.8618
[OX2H1]	0.9696	[CX4H2][CX4H2]	0.8589

OCC[CH2]	0.9691	C1CCC1	0.8499
[CX4H2]([CX4H2])[CX4H1]	0.9639	[CX4H2]([OX2H1])[CX4H1]	0.8369

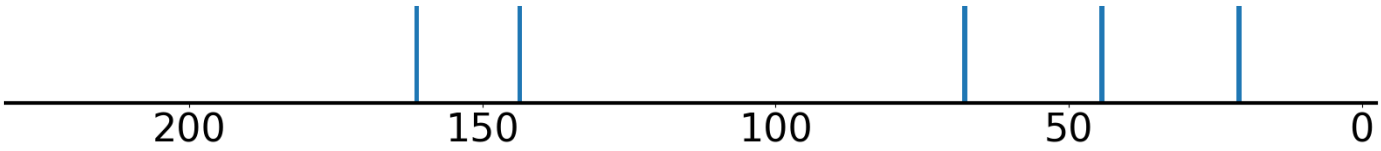
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	C=CC=CC#C	0.0
[CX4H2]([#6])[O]	0.9711	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[OX2H1]	0.9696	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
OCC[CH2]	0.9691	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([CX4H2])[CX4H1]	0.9639	CC#CCC=C	0.0
[CX4H1]1[CX4H2][CX4H2][CX4H2]1	0.8752	[CX3H0](=[CX3H2])([CX4H1])[CX3H1]	0.0
[#6H1][#6H2]	0.8618	[CX3H1](=[CX3H2])[cX3H0]	0.0
[CX4H2][CX4H2]	0.8589	[CX2H0](#[CX2H1])[cX3H0]	0.0
C1CCC1	0.8499	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2]([OX2H1])[CX4H1]	0.8369	[CX2H0](#[CX2H1])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
CCCCCC	0.6896	[CX4H2](O)[CHX4]	0.4939
[#8][#6][#6H2]	0.5911	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.6199
[#6H2][#6H1][#6H1][#6H2]	0.3961	[CX4H1]([CX4H2])([CX4H2])[CX4H2]	0.63
[#6H1][#6H1]	0.2758	[#6H1]([#6H2])[#6H2]	0.6596
[CH2X4](O)[CX4H2]	0.1841	[#8H][#6H2][#6H1]	0.6865
[CX4H3][#6]	0.1803	[#6H1]	0.7794
[CX4H]O	0.1787	[CX4H2]([CX4H2])[CX4H2]	0.8243
O[CX4H][CX4H2]	0.1749	[CX4H2]([OX2H1])[CX4H1]	0.8369
[CX4H1][CX4H2][CX4H2][CX4H1]	0.1528	C1CCC1	0.8499
[CX4H2][CX4H2][CX4H2][CX4H2]	0.1248	[CX4H2][CX4H2]	0.8589

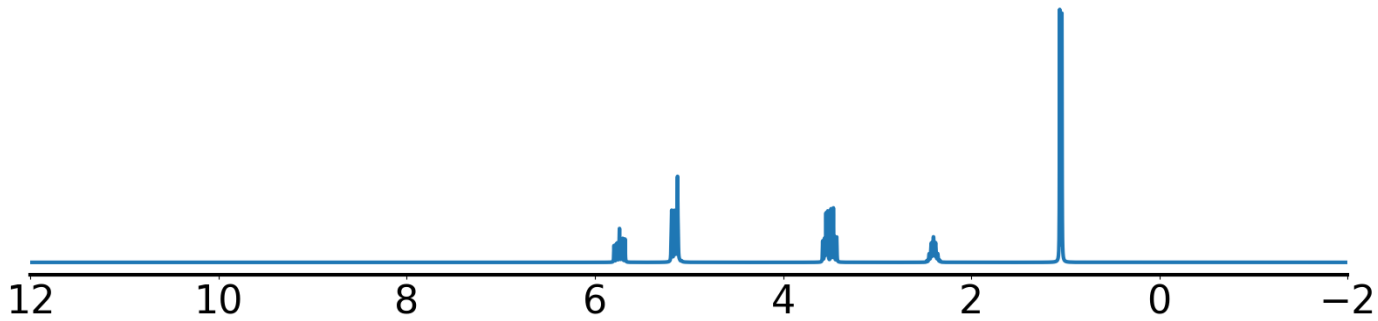
Example 188 true smiles: C=CC(C)CO formula: C5H10O
Index of correct structure: 0 of 65
True structure loss: 0.008143
True structure:



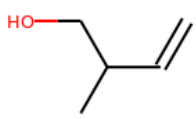
Experimental 13C NMR (solvent: CDCl3)



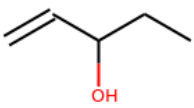
Experimental 1H NMR (solvent: CDCl3)



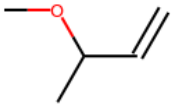
Top predicted structures (loss):



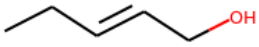
0.008143



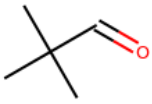
0.108944



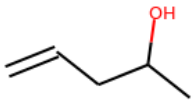
0.117814



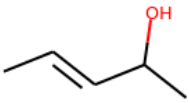
0.117941



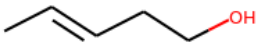
0.120557



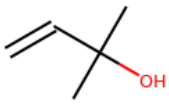
0.129866



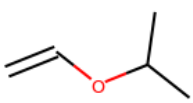
0.131551



0.134556



0.134644



0.134959

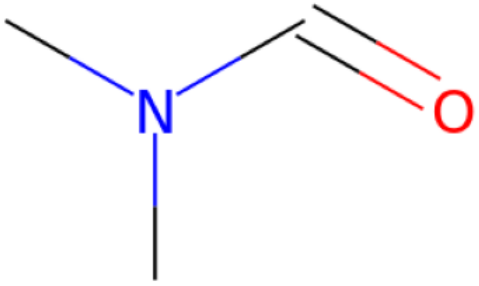
Top predicted substructures	prob		
[CX4H3][#6]	1.0	[#6X3]=[#6][#6][#6H3]	0.9972
[CX4H3]	1.0	[OX2H1]	0.9912
[#6H1]	0.9999	[#8H][#6H2][#6H1]	0.981

[#6H3][#6][#6]	0.9998	[CH3]CC[OH]	0.9591
[CHX3](=C)C	0.9994	[CX3H][CX4H]	0.9588

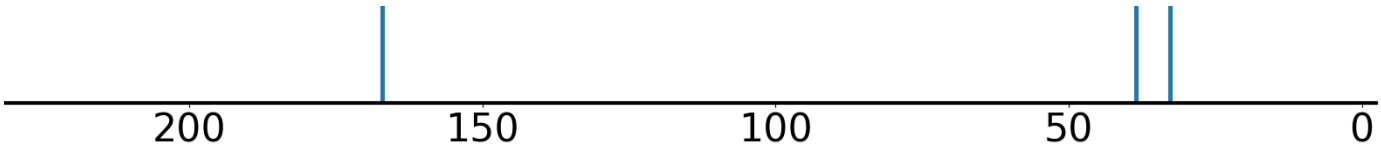
best positives	prob	best negatives	prob
[CX4H3][#6]	1.0	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H3]	1.0	[#6X2][#6H1][#6X2]	0.0
[#6H1]	0.9999	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H3][#6][#6]	0.9998	C=CC=CC#C	0.0
[CHX3](=C)C	0.9994	CCC#CCC	0.0
[#6X3]=[#6][#6][#6H3]	0.9972	CCC#CC#C	0.0
[OX2H1]	0.9912	[CX4H3][CX2H0]	0.0
[#8H][#6H2][#6H1]	0.981	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CH3]CC[OH]	0.9591	CC#CCC#C	0.0
[CX3H][CX4H]	0.9588	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#8]	0.3084	[CX4H2](O)[CHX4]	0.5132
[CHX3]=[CHX3]	0.2143	[CHX4]([CH3X4])[CH2X4]	0.6089
[CX3H1](=[CX3H1])[CX4H1]	0.1968	[#6H1][#6H2]	0.6395
[#6H3][#6H0]	0.1871	[#6H1][#6H1]	0.6582
[#8][#6][#6]=[#6X3]	0.149	[#8][#6][#6][#6X3]	0.6987
[#6H3][#6][#6][#6H3]	0.1465	[#6H2][#6H1][#6H1]=[#6H2]	0.7282
[#6H3][#6]=[#6X3]	0.1391	[#6X3H1][#6H1][#6H2]	0.7728
[#8][#6H0][#6H1]	0.1364	[#8][#6H2][#6H][#6X3]	0.857
[#6X3][#6][#6][#6H3]	0.1224	[CX3H2]=[CX3H1]	0.8646
[#8][#6H2][#6H1][#6H0]	0.1183	[CX4H2]([OX2H1])[CX4H1]	0.906

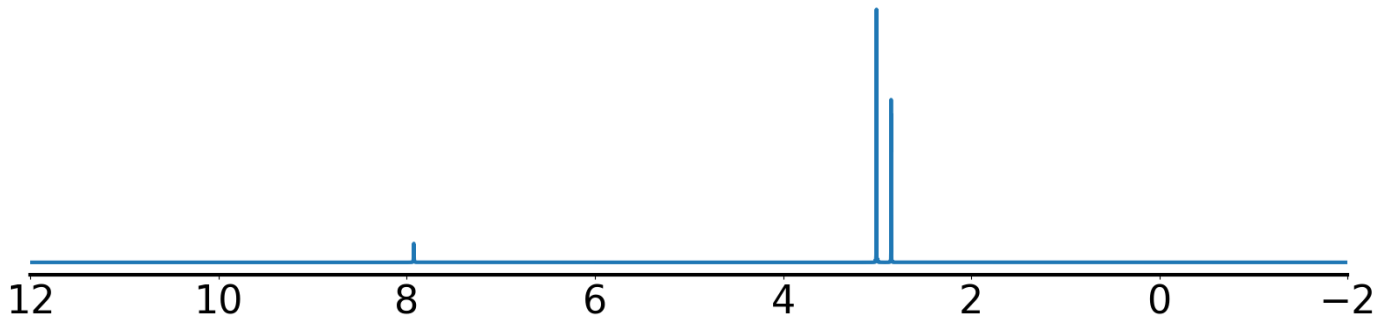
Example 189 true smiles: CN(C)C=O formula: C3H7NO
Index of correct structure: 0 of 59
True structure loss: 0.008732
True structure:



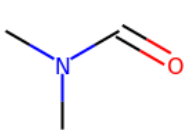
Experimental 13C NMR (solvent: CDCl3)



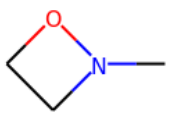
Experimental 1H NMR (solvent: D2O)



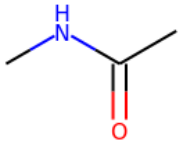
Top predicted structures (loss):



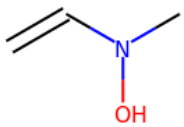
0.008732



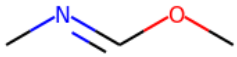
0.061035



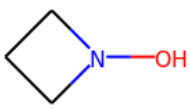
0.062484



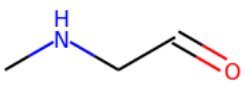
0.070628



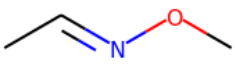
0.074575



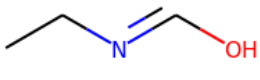
0.075067



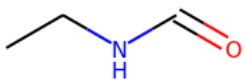
0.084416



0.084549



0.084706



0.085229

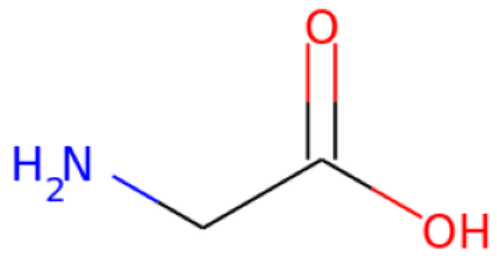
Top predicted substructures	prob		
[#7X3][#6H3]	0.9998	[#7X3H0]	0.7694
[#6H3][#7]	0.9995	[#8]=[#6H1][#7]	0.7625
[CX4H3]	0.9971	[#6H1]	0.7588

[#6H3][#7][#6X3]	0.9385	[CX3H1](=[OX1H0])[NX3H0]	0.707
[CX4H3][NX3H0]	0.8575	[#6X3H1][#7X3H0]	0.6201

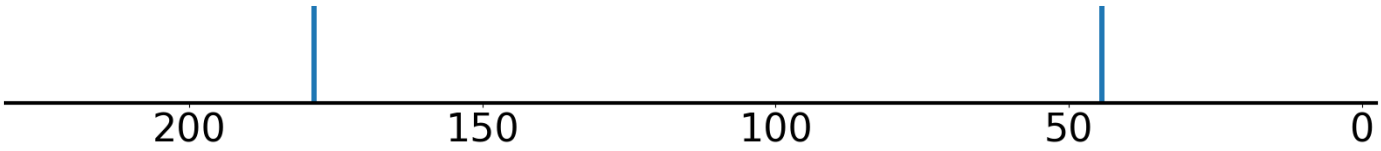
best positives	prob	best negatives	prob
[#7X3][#6H3]	0.9998	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6H3][#7]	0.9995	CCC#CC#C	0.0
[CX4H3]	0.9971	C=CCCC#C	0.0
[#6H3][#7][#6X3]	0.9385	C=CC=CC#C	0.0
[CX4H3][NX3H0]	0.8575	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3H0]	0.7694	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
[#8]=[#6H1][#7]	0.7625	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6H1]	0.7588	CCC#CC=C	0.0
[CX3H1](=[OX1H0])[NX3H0]	0.707	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3H1][#7X3H0]	0.6201	CCC=CC#C	0.0

worst negatives	prob	worst positives	prob
[CX3](=[OX1])C	0.4001	[#6X3H1][#7X3H0]	0.6201
[OX2H1]	0.3915	[CX3H1](=[OX1H0])[NX3H0]	0.707
[#7X3H1]	0.3817	[#6H1]	0.7588
[CX4H3][NX3H1]	0.3371	[#8]=[#6H1][#7]	0.7625
[CX3](=[OX1])O	0.3302	[#7X3H0]	0.7694
[#8]=[#6][#8]	0.2687	[CX4H3][NX3H0]	0.8575
[#7][#6H0][#7]	0.2298	[#6H3][#7][#6X3]	0.9385
[#7][#6]=[#7]	0.192	[CX4H3]	0.9971
[CX4H2][CX3]=O	0.1911	[#6H3][#7]	0.9995
[#6H3][#7][#6H2]	0.1903	[#7X3][#6H3]	0.9998

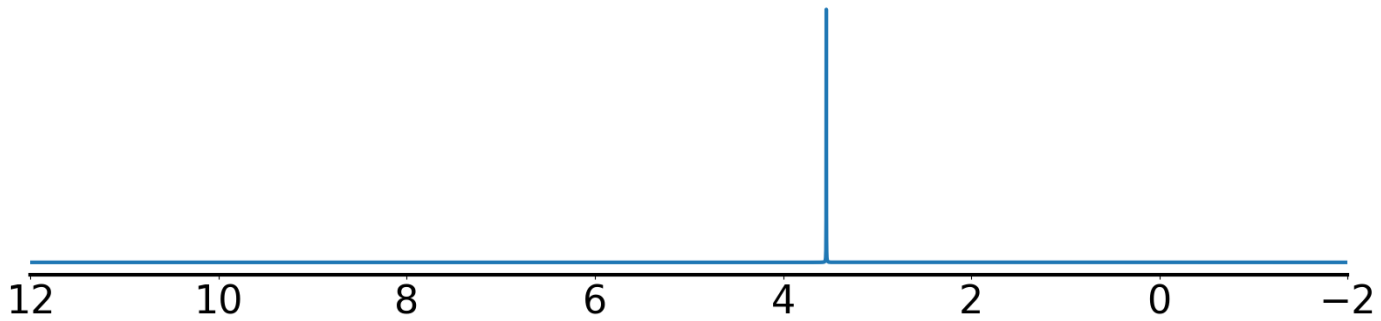
Example 190 true smiles: NCC(=O)O formula: C2H5NO2
Index of correct structure: 0 of 47
True structure loss: 0.010644
True structure:



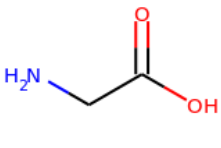
Experimental 13C NMR (solvent: D2O)



Experimental 1H NMR (solvent: D2O)

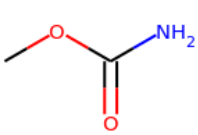


Top predicted structures (loss):

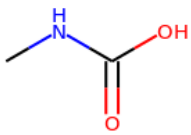


0.010644

0.036594



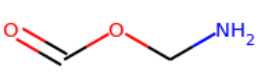
0.045586



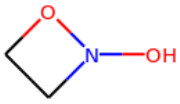
0.046442

0.060313

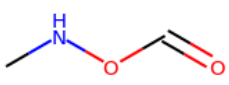
0.060766



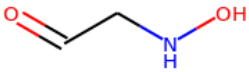
0.061471



0.062799



0.062933



0.062987

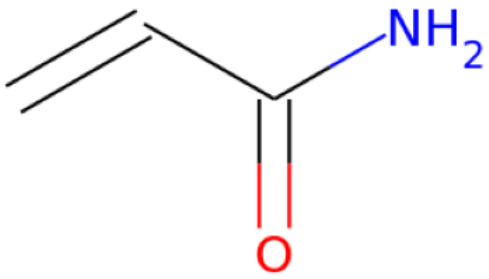
Top predicted substructures	prob		
[CX3](=[OX1])C	0.9844	[CX4H2][CX3]=O	0.8644
[#7X3][#6H2]	0.9755	[CX3](=[OX1])O	0.8606
[#8]=[#6][#8]	0.9195	[CX3](=O)[OX2H1]	0.8547

[#7][#6H2]	0.9154	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.8147
[#7H2][#6H2]	0.8698	[#7][#6][#6X3]	0.8007

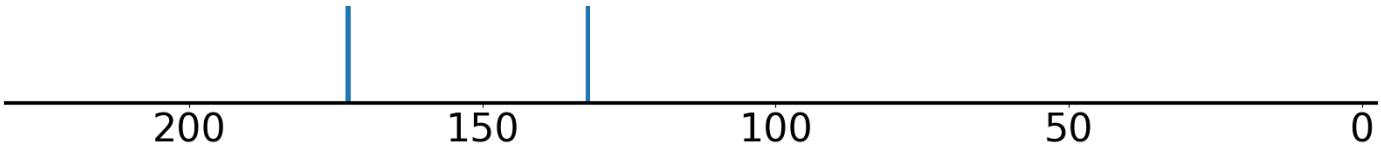
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9844	C=CC=CC#C	0.0
[#7X3][#6H2]	0.9755	CC=CCC#C	0.0
[#8]=[#6][#8]	0.9195	CCC#CC#C	0.0
[#7][#6H2]	0.9154	C=CCCC#C	0.0
[#7H2][#6H2]	0.8698	[#6H2]=[#6][#6X2]	0.0
[CX4H2][CX3]=O	0.8644	CC=CC#CC	0.0
[CX3](=[OX1])O	0.8606	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=O)[OX2H1]	0.8547	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.8147	CCC#CC=C	0.0
[#7][#6][#6X3]	0.8007	[CX2H0](#[CX2H0])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#7X3H1]	0.3652	[#8][#6][#6H2]	0.5088
[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.28	[CX4H2]([NX3H2])[CX3H0]	0.6126
[CX4H2]CC=O	0.262	[#7X3H2]	0.6902
[#6H2][#7][#6X3]	0.2507	[OX2H1]	0.7346
O=[#6][#6][#6X3]	0.2388	[#6X3][#6H2][#7]	0.7404
[CX4H3][NX3H0]	0.2271	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.7839
[#7X3H0]	0.2161	[#7][#6][#6X3]	0.8007
[CX4H2][CX4H2]	0.2102	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.8147
[OX1H0]=[CX3H0][CX4H2][CX3H0]	0.2003	[CX3](=O)[OX2H1]	0.8547
[#8X1]=[#6X3][#6H2][#6H0]	0.1971	[CX3](=[OX1])O	0.8606

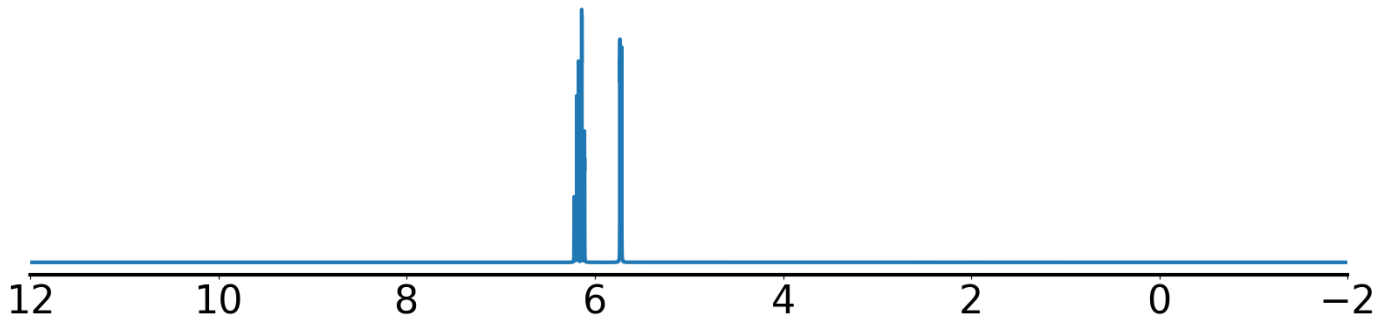
Example 191 true smiles: C=CC(N)=O formula: C3H5NO
Index of correct structure: 0 of 46
True structure loss: 0.014223
True structure:



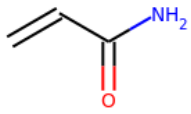
Experimental 13C NMR (solvent: D2O)



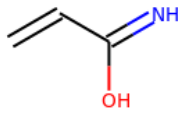
Experimental 1H NMR (solvent: D2O)



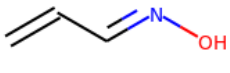
Top predicted structures (loss):



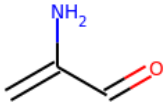
0.014223



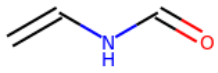
0.046104



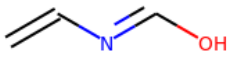
0.05967



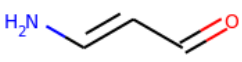
0.060387



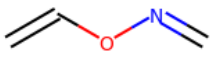
0.081697



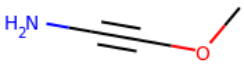
0.083348



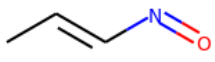
0.084012



0.084349



0.089945



0.095113

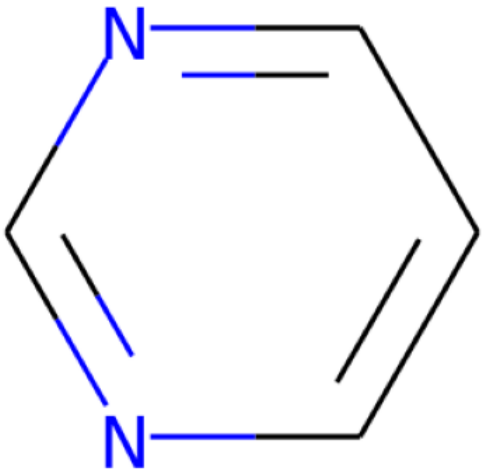
Top predicted substructures	prob		
[#6X3][#6X3]	0.9808	[#6X3H2]	0.9226
[CHX3](=C)C	0.9559	[#6X3H1][#6X3H0]	0.896
[OX1H0]=[CX3H0][CX3H1]=[CX3H2]	0.9431	[CH2X3](=C)	0.8817

[#7X3H2]	0.9299	O=[#6][#6]=[#6X3]	0.807
[#6H1]	0.9268	[#7H2][#6H0]	0.7796

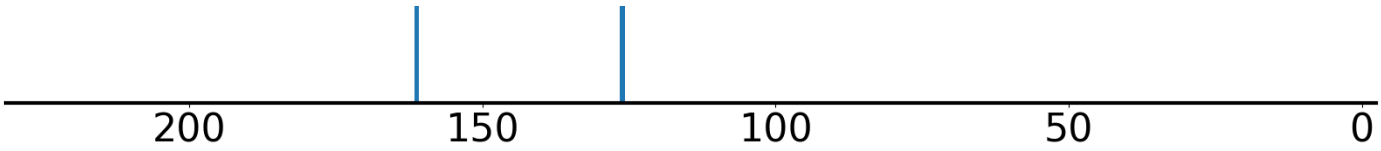
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9808	CCC#CC#C	0.0
[CHX3](=C)C	0.9559	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[OX1H0]=[CX3H0][CX3H1]=[CX3H2]	0.9431	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7X3H2]	0.9299	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H1]	0.9268	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3H2]	0.9226	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#6X3H1][#6X3H0]	0.896	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CH2X3](=C)	0.8817	[#6H2][#6]#[#6X2]	0.0
O=[#6][#6]=[#6X3]	0.807	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#7H2][#6H0]	0.7796	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[OX2H1]	0.5556	[#7][#6X3H0][#6X3H1]	0.5274
[CHX3]=[CHX3]	0.4558	[CX3H1](=[CX3H2])[CX3H0]	0.6151
[CX3](=O)[OX2H1]	0.4407	[CX3H2]=[CX3H1]	0.6272
[#8][#6H0][#6H1]	0.4225	[#8]=[#6H0][#6H1]	0.7066
[#8][#6][#6]=[#6X3]	0.4083	[#7][#6H0][#6H1]	0.7112
[CX3](=[OX1])O	0.3966	[#7][#6][#6]=[#6X3]	0.7204
[#8]=[#6][#8]	0.3516	[#7][#6][#6X3]	0.7261
[CX3H1](=[CX3H1])[CX3H0]	0.3497	[CX3](=[OX1])C	0.7582
O=[#6][#6][#6X3]	0.3404	O=C[CX3H]	0.7693
[#7][#6][#6][#6X3]	0.3309	[#7H2][#6H0]	0.7796

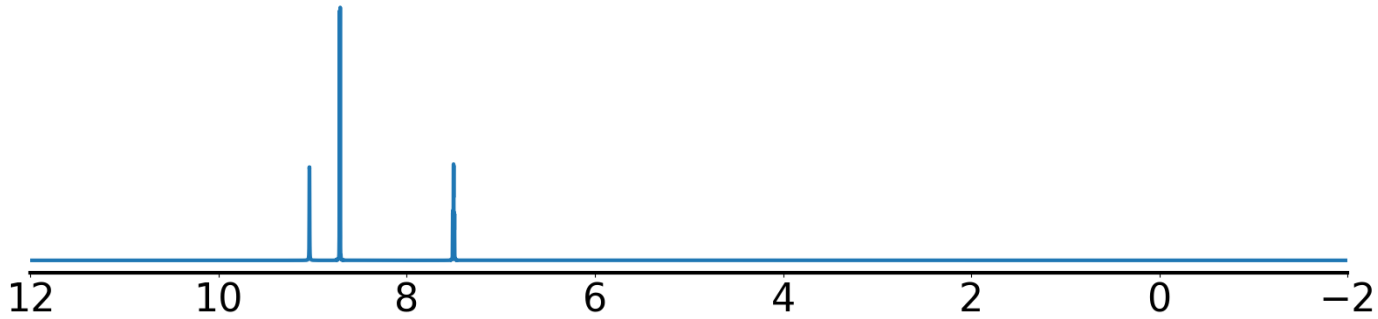
Example 192 true smiles: c1cncnc1 formula: C4H4N2
Index of correct structure: 0 of 46
True structure loss: 0.017585
True structure:



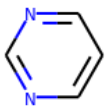
Experimental 13C NMR (solvent: CDCl3)



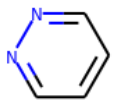
Experimental 1H NMR (solvent: D2O)



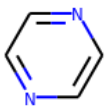
Top predicted structures (loss):



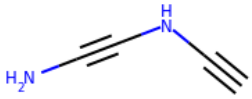
0.017585



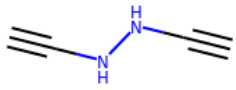
0.018729



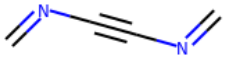
0.023258



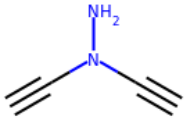
0.059451



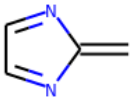
0.061355



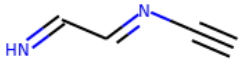
0.061403



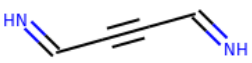
0.061855



0.067281



0.072427



0.073715

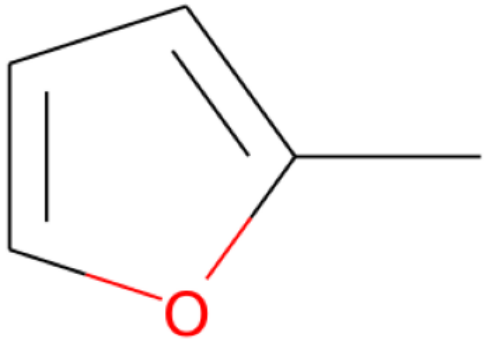
Top predicted substructures	prob		
[#6H1]	0.9993	[#7][#6][#6][#6X3]	0.8105
[#6X3][#6X3]	0.977	[#6H1][#6H1]	0.7943
[cH]	0.9504	[#6H1][#7][#6H1]	0.7546

[cH][cH]	0.9432	[#6X3][#6X3][#6X3][#6X3]	0.7448
[#7][#6][#6X3]	0.8217	[#6X3H1][#6X3H0]	0.6703

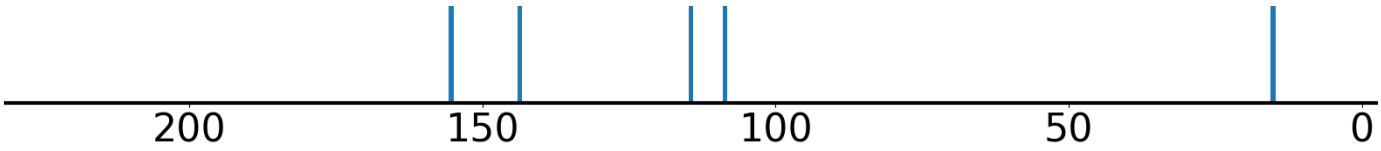
best positives	prob	best negatives	prob
[#6H1]	0.9993	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.977	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[cH]	0.9504	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH][cH]	0.9432	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6][#6X3]	0.8217	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.8105	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H1][#6H1]	0.7943	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H1][#7][#6H1]	0.7546	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
[cX3H1]([nX2H0])[cX3H1]	0.6421	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.6359	[OX2H0][CX4H1]([CX4H1])[CX4H1][CX4H3]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6X3][#6X3][#6X3]	0.7448	[#7][#6][#6][#6][#7]	0.2938
[#6X3H1][#6X3H0]	0.6703	[#7][#6H1][#7]	0.339
[cX3H1]([cX3H1])[cX3H0]	0.5854	[#7][#6][#7]	0.4802
[#7][#6X3H0][#6X3H1]	0.5144	[#6X3][#7][#6X3]	0.6103
[cX3H1]([nX2H0])[cX3H0]	0.418	[cX3H1]([cX3H1])[cX3H1]	0.6359
[#7][#6H0][#6H1]	0.3842	[cX3H1]([nX2H0])[cX3H1]	0.6421
[#7][#7]	0.3635	[#6H1][#7][#6H1]	0.7546
[#6X3][#7X3][#6X3]	0.3396	[#6H1][#6H1]	0.7943
[#6]1[#6][#6][#6][#6][#7]1	0.3349	[#7][#6][#6][#6X3]	0.8105
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3137	[#7][#6][#6X3]	0.8217

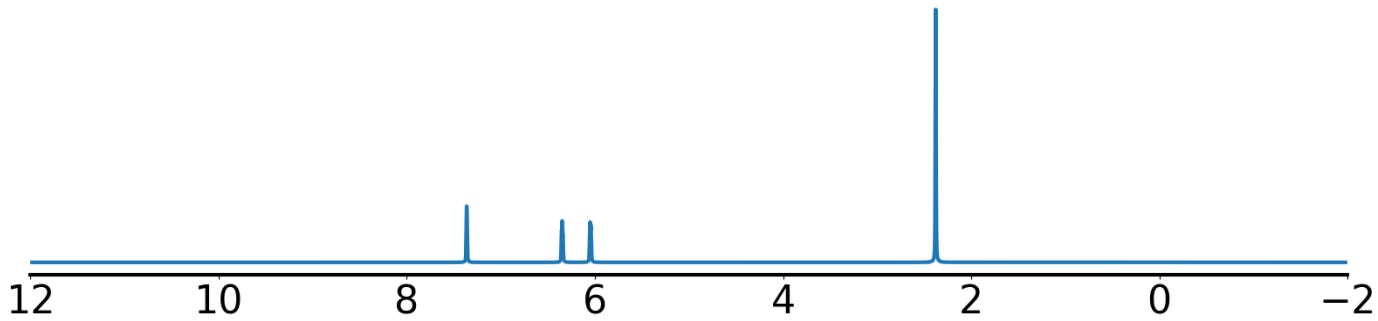
Example 193 true smiles: Cc1ccco1 formula: C5H6O
Index of correct structure: 0 of 45
True structure loss: 0.009801
True structure:



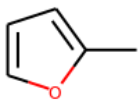
Experimental 13C NMR (solvent: CDCl3)



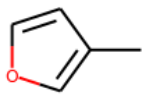
Experimental 1H NMR (solvent: CDCl3)



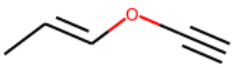
Top predicted structures (loss):



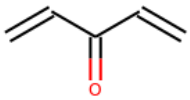
0.009801



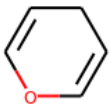
0.036472



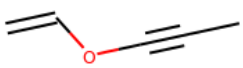
0.141783



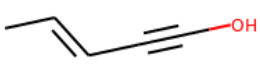
0.158804



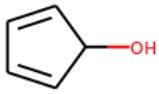
0.162743



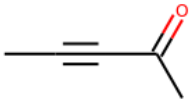
0.16676



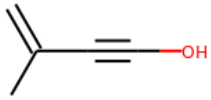
0.167792



0.176873



0.178773



0.183347

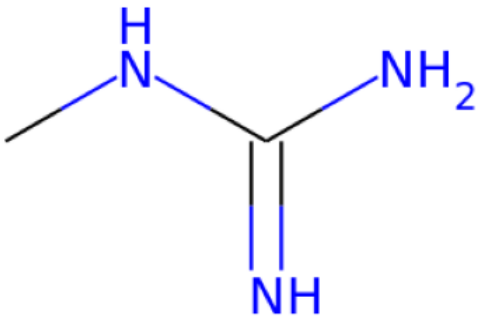
Top predicted substructures	prob		
[#6H1]	0.9995	[CX4H3][#6]	0.9925
[cH][cH]	0.999	[cH]	0.991
[#6X3][#6X3][#6X3][#6X3]	0.9983	[cX3H1]([cX3H1])[cX3H0]	0.986

[#6X3][#6X3]	0.998	[#6X3H1][#6X3H0]	0.9853
[CX4H3]	0.996	[#6H3][#6][#6]	0.9634

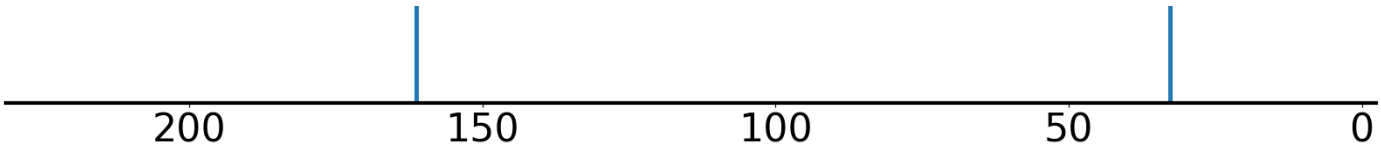
best positives	prob	best negatives	prob
[#6H1]	0.9995	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[cH][cH]	0.999	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9983	CCC#CC#C	0.0
[#6X3][#6X3]	0.998	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3]	0.996	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[CX4H3][#6]	0.9925	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[cH]	0.991	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.986	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9853	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6H3][#6][#6]	0.9634	[#6X2][#6H1][#6X2]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H0])[cX3H0]	0.3007	[#8][#6H][#6X3][#6X3H]	0.2426
[CX4H2]([#6])[#6]	0.2846	o[cH]	0.3342
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.2358	[#8][#6H1][#6H1]	0.4695
[cH]cO	0.2092	[CH3][#6][#8]	0.5045
[OX2H1]	0.2016	[cX3H1]([oX2H0])[cX3H1]	0.6672
[OX2H][cX3]:[c]	0.1938	[cX3H1]([cX3H1])[cX3H1]	0.7585
[cX3H0][cX3H1][cX3H1][cX3H0]	0.1833	[#8][#6H0][#6H1]	0.7773
[#8][#6][#6H2]	0.1577	[#6H3][#6H0]	0.844
[CX4H2][CX4H2]	0.1193	[CX4H3][cX3H0][oX2H0]	0.8865
[#7][#6][#6][#6X3]	0.0804	[#6H1][#6H1]	0.9041

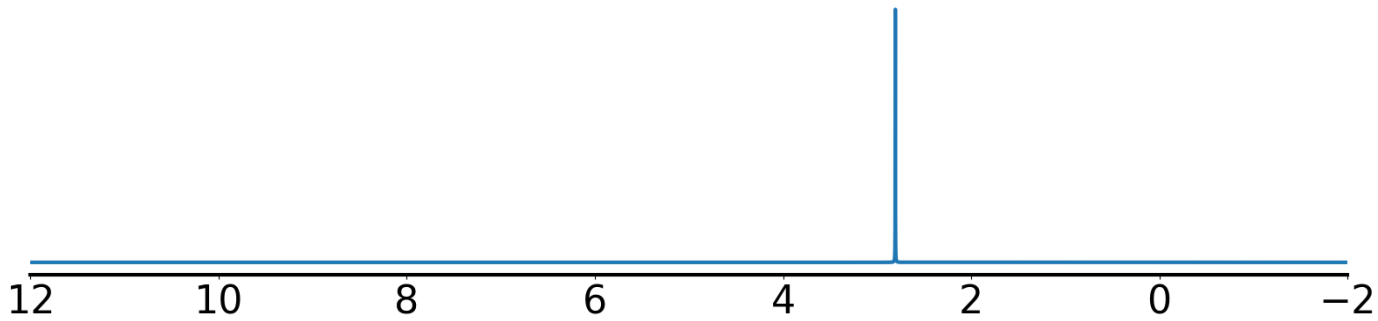
Example 194 true smiles: CNC(=N)N formula: C2H7N3
Index of correct structure: 0 of 39
True structure loss: 0.012255
True structure:



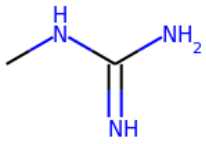
Experimental 13C NMR (solvent: D2O)



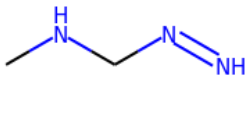
Experimental 1H NMR (solvent: D2O)



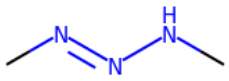
Top predicted structures (loss):



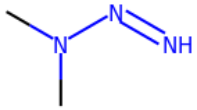
0.012255



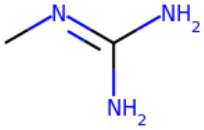
0.034622



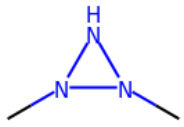
0.03556



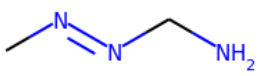
0.035682



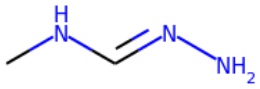
0.040991



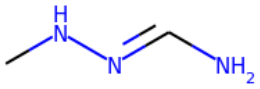
0.041908



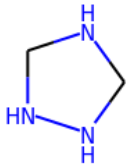
0.046539



0.050554



0.055232



0.058862

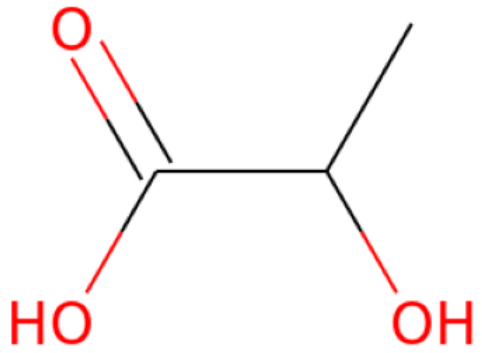
Top predicted substructures	prob		
[#7X3][#6H3]	0.9971	[#6H3][#7][#6X3]	0.9427
[#6H3][#7]	0.9757	[#7][#6][#7]	0.8712
[CX4H3]	0.9644	[#7X3H1]	0.7627

[#7][#6H0][#7]	0.9543	[#7][#6]([#7])=[#7]	0.7359
[NH1][#6][#7]	0.9455	[CX4H3][NX3H1]	0.7287

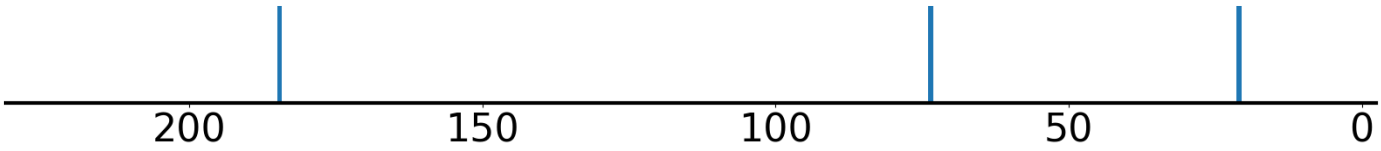
best positives	prob	best negatives	prob
[#7X3][#6H3]	0.9971	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6H3][#7]	0.9757	CCC#CC#C	0.0
[CX4H3]	0.9644	C=CCCC#C	0.0
[#7][#6H0][#7]	0.9543	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[NH1][#6][#7]	0.9455	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6H3][#7][#6X3]	0.9427	C=CC=CC#C	0.0
[#7][#6][#7]	0.8712	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#7X3H1]	0.7627	CC=CCC#C	0.0
[#7][#6]([#7])=[#7]	0.7359	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX4H3][NX3H1]	0.7287	CCC=CC#C	0.0

worst negatives	prob	worst positives	prob
[#7H1][#6H0][#7X3][#6H3]	0.5542	[#7H2][#6H0]	0.2385
[#7][#6H0][#6H1]	0.2709	[#6]=[#7H]	0.4274
[#7][#6][#6][#7]	0.27	[#7X3H2]	0.4319
[#7X3H0]	0.2491	[NH1]=[#6][#7]	0.5231
[#7][#7]	0.1917	[#7][#6]=[#7]	0.5239
[#6X3][#7X3][#6X3]	0.1657	[#7H1]=[#6H0][#7X3][#6H3]	0.5455
[#6H1]	0.1581	[NH1][#6]=[#7]	0.5767
[#7][#6][#6X3]	0.1494	[#7][#6H0]=[#7]	0.6009
[#7][#6X3H0][#6X3H1]	0.1283	[CX4H3][NX3H1]	0.7287
[cH]	0.1279	[#7][#6]([#7])=[#7]	0.7359

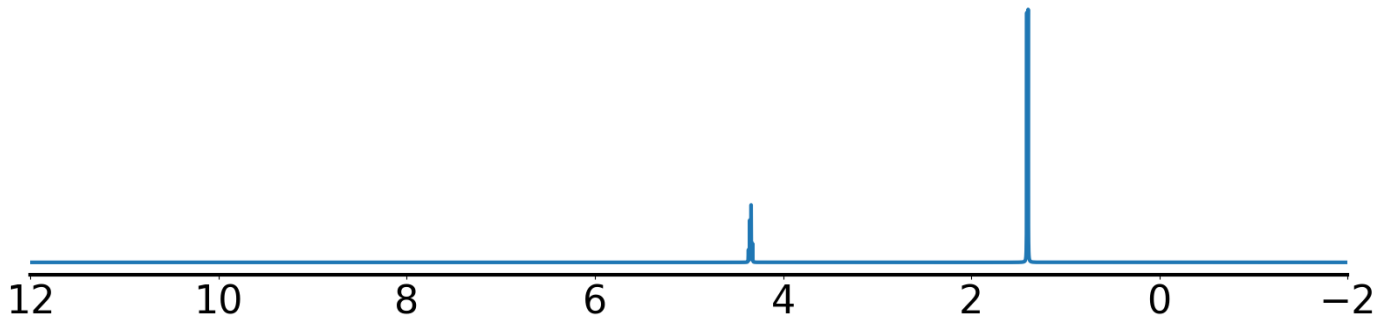
Example 195 true smiles: CC(O)C(=O)O formula: C3H6O3
Index of correct structure: 0 of 38
True structure loss: 0.008204
True structure:



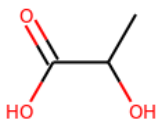
Experimental 13C NMR (solvent: D2O)



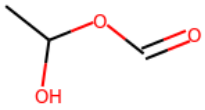
Experimental 1H NMR (solvent: D2O)



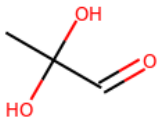
Top predicted structures (loss):



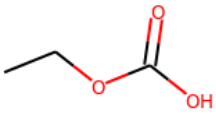
0.008204



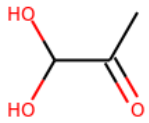
0.056712



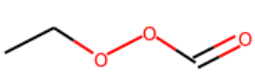
0.062729



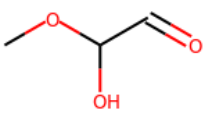
0.065243



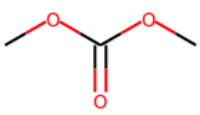
0.077549



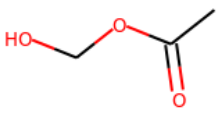
0.079312



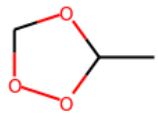
0.100439



0.102971



0.10319



0.111373

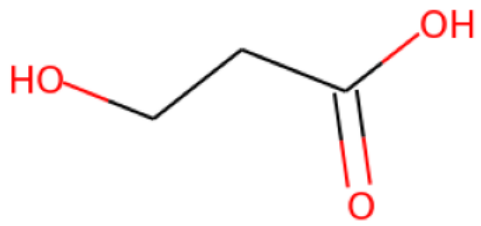
Top predicted substructures	prob		
[CX4H3]	0.9999	[CX4H]O	0.9812
[#6H3][#6][#6]	0.9973	[OX2H1]	0.9767
[CX4H3][#6]	0.9967	[CH3][#6][#8]	0.9437

[CX4H3][CX4]O	0.9966	[#8][#6][#6]=[#8]	0.941
[CX3](=[OX1])C	0.9966	[CX3](=[OX1])O	0.9326

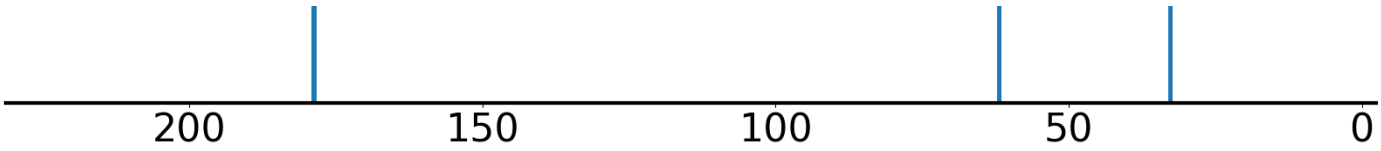
best positives	prob	best negatives	prob
[CX4H3]	0.9999	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9973	C=CCCC#C	0.0
[CX4H3][#6]	0.9967	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
[CX4H3][CX4]O	0.9966	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])C	0.9966	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H]O	0.9812	CC=CCC#C	0.0
[OX2H1]	0.9767	CCC#CC#C	0.0
[CH3][#6][#8]	0.9437	C=CC=CC#C	0.0
[#8][#6][#6]=[#8]	0.941	[CX4H2]([CX4H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.9326	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H1]	0.4131	[CH3]CC[OH]	0.5758
[#8][#6H1][#6H1]	0.3548	[CX3](=O)[OX2H1]	0.5904
[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.2444	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.6291
[#8]=[#6][#6H1][#6H1]	0.2316	[CX4H](O)CO	0.6409
[#6X3][#6][#6][#6H3]	0.18	[#8][#6H0][#6H1]	0.6977
[OX2H0][CX4H1][CX4H3]	0.1754	[#8H][#6X4H1][#6X3H0]	0.7316
[#8][#6][#6][#6X3]	0.1618	[#8][#6][#6][#8]	0.7592
[#6H1][#6H2]	0.075	[#6H3][#6][#6X3]	0.8117
[#8][#6H1][#6H1][#6H3]	0.0727	[OH][CX4H]	0.8204
[#6H3][#6][#6][#6H3]	0.0702	[CX4H1]([OX2H1])([CX4H3])[CX3H0]	0.8339

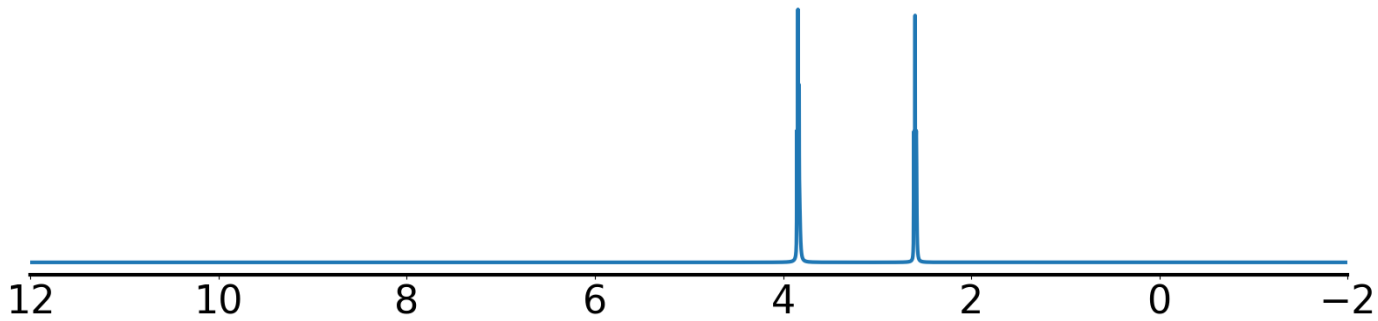
Example 196 true smiles: O=C(O)CCO formula: C3H6O3
Index of correct structure: 0 of 38
True structure loss: 0.007232
True structure:



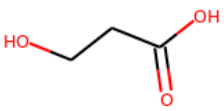
Experimental 13C NMR (solvent: D2O)



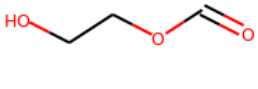
Experimental 1H NMR (solvent: D2O)



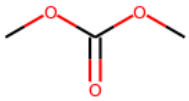
Top predicted structures (loss):



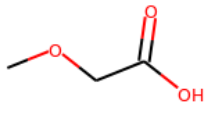
0.007232



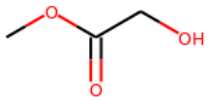
0.079487



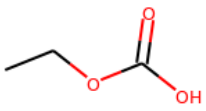
0.085344



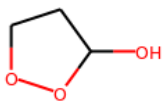
0.089833



0.092632

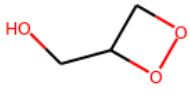


0.09286

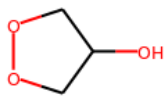


0.101687

0.111257



0.112307



0.112885

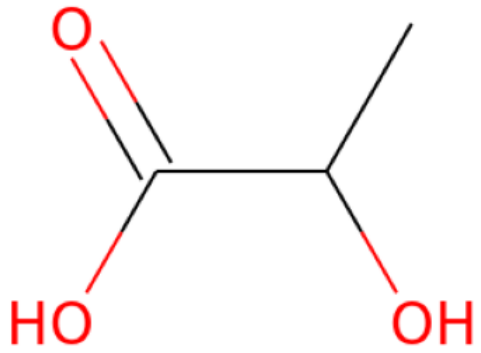
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9983	[CX4H2]([CX4H2])[CX3H0]	0.9746
[#8]=[#6][#8]	0.9953	[#8][#6][#6H2]	0.9727
[CX3](=[OX1])C	0.9952	[CX4H2]([#6])[O]	0.9628

[OX2H1]	0.9898	OCC[CH2]	0.9456
[CX3](=[OX1])O	0.9837	[CX4H2][CX4H2]	0.9252

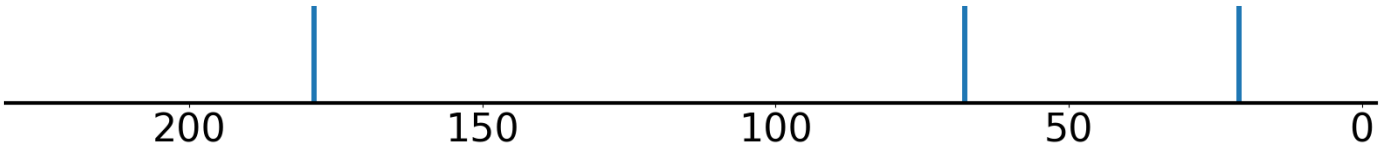
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9983	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8]=[#6][#8]	0.9953	CC=CCC#C	0.0
[CX3](=[OX1])C	0.9952	[#6X2][#6H1][#6X2]	0.0
[OX2H1]	0.9898	CC=CC#CC	0.0
[CX3](=[OX1])O	0.9837	C=CC=CC#C	0.0
[CX4H2]([CX4H2])[CX3H0]	0.9746	[#6X3][#6]#[#6][#6H3]	0.0
[#8][#6][#6H2]	0.9727	CCC#CC#C	0.0
[CX4H2]([#6])[O]	0.9628	[CX3H1](=[CX3H2])[CX2H0]	0.0
OCC[CH2]	0.9456	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H2][CX4H2]	0.9252	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6][#6][#6]=[#8]	0.3974	[#8][#6][#6][#6X3]	0.5021
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3022	O=C[CH2][CH2]O	0.555
[OX2H0][CX3H0][CX4H2]	0.2971	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.6778
[#8][#6][#6][#6][#6][#8]	0.271	[CX4H2][CX3]=O	0.7871
[CX4H2]([CX4H2])[CX4H2]	0.1846	[CX4H2]([OX2H1])[CX4H2]	0.8216
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.1766	[CX4H2]CC=O	0.8781
[#6H1][#6H2]	0.1619	O=[CX3H0][CX4H2][CX4H2]	0.9095
[#8]=[#6H0][#6H1]	0.1546	[CH2X4](O)[CX4H2]	0.9098
[CX4H2]([OX2H0])[CX4H2]	0.1542	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9172
[#7X3H2]	0.1086	[CX3](=O)[OX2H1]	0.9235

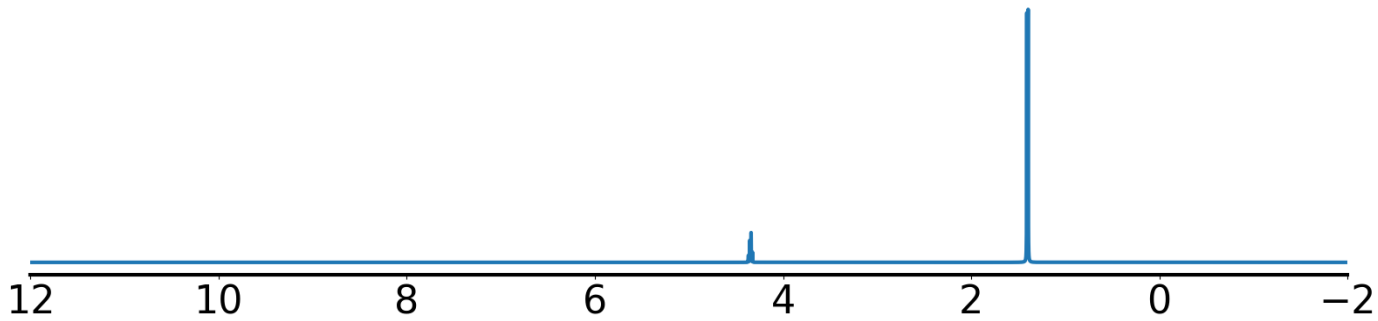
Example 197 true smiles: CC(O)C(=O)O formula: C3H6O3
Index of correct structure: 0 of 38
True structure loss: 0.010427
True structure:



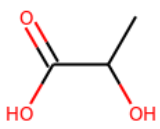
Experimental 13C NMR (solvent: DMSO)



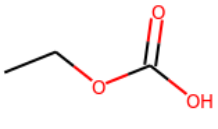
Experimental 1H NMR (solvent: D2O)



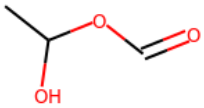
Top predicted structures (loss):



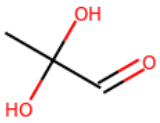
0.010427



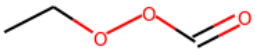
0.048633



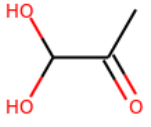
0.053373



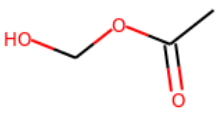
0.059115



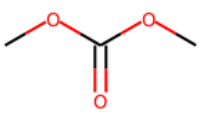
0.063273



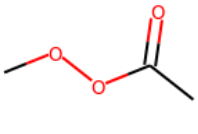
0.071394



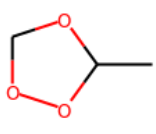
0.077329



0.085279



0.087326



0.108892

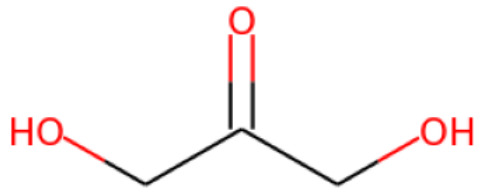
Top predicted substructures	prob		
[CX4H3]	0.9999	[CX3](=[OX1])O	0.9902
[#6H3][#6][#6]	0.9968	[#8]=[#6][#8]	0.9837
[CX3](=[OX1])C	0.9964	[OX2H1]	0.9517

[CX4H3][CX4]O	0.9954	[CH3][#6][#8]	0.9265
[CX4H3][#6]	0.993	[CX4H3][CX4H1][OX2H1]	0.9068

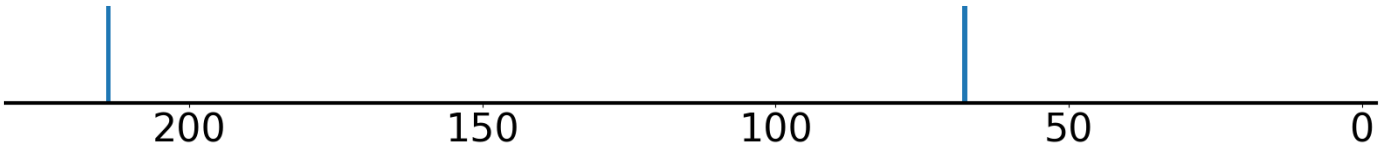
best positives	prob	best negatives	prob
[CX4H3]	0.9999	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9968	C=CCCC#C	0.0
[CX3](=[OX1])C	0.9964	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H3][CX4]O	0.9954	CCC#CC=C	0.0
[CX4H3][#6]	0.993	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])O	0.9902	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
[#8]=[#6][#8]	0.9837	[CX3H1](=[CX3H1])[CX2H0]	0.0
[OX2H1]	0.9517	C=CC=CC#C	0.0
[CH3][#6][#8]	0.9265	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][CX4H1][OX2H1]	0.9068	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([OX2H0])[CX4H3]	0.2077	[CH3]CC[OH]	0.3688
[#6H1][#6H1]	0.1839	[#8H][#6X4H1][#6X3H0]	0.3703
[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.1673	[CX4H](O)CO	0.3781
[#8][#6H1][#6H1]	0.1497	[#8][#6][#6][#8]	0.506
[#6X3][#6][#6][#6H3]	0.1369	[OH][CX4H]	0.6438
[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.1142	[#8][#6H0][#6H1]	0.6957
[CX3H0](=[OX1H0])([OX2H0])[CX4H1]	0.1111	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.7147
[CX4H2]CC=O	0.111	[CX4H1]([OX2H1])([CX4H3])[CX3H0]	0.7241
[#8][#6][#6][#6X3]	0.111	[#8][#6][#6]=[#8]	0.7607
[CX4H2][CX3]=O	0.1024	[#6H3][#6][#6X3]	0.7709

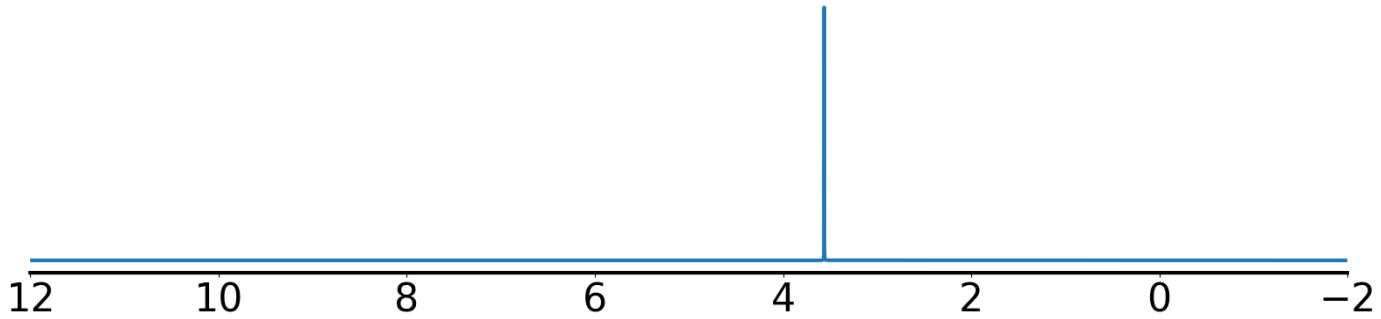
Example 198 true smiles: O=C(CO)CO formula: C3H6O3
Index of correct structure: 0 of 38
True structure loss: 0.013689
True structure:



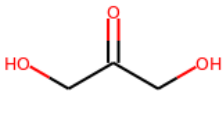
Experimental 13C NMR (solvent: N/A)



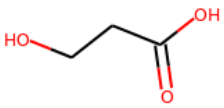
Experimental 1H NMR (solvent: D2O)



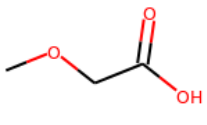
Top predicted structures (loss):



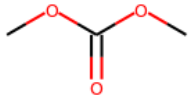
0.013689



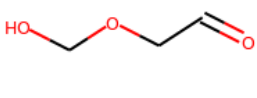
0.060303



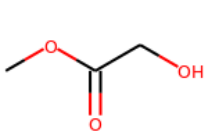
0.063898



0.065795

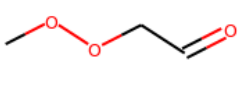


0.070775

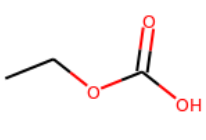


0.072064

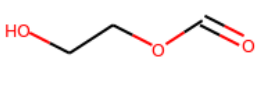
0.072961



0.073991



0.081297



0.091921

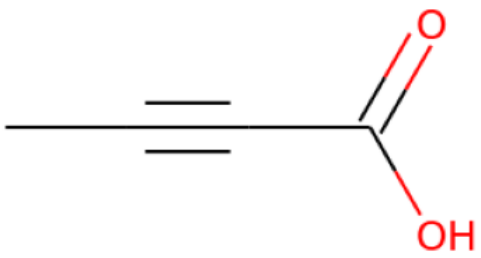
Top predicted substructures	prob		
[CX3](=[OX1])C	0.9996	[#8][#6][#6]=[#8]	0.7643
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9969	[#6H2][#6X3H0][#6H2]	0.7369
[OX2H1]	0.9841	OCC[CH2]	0.6381

[CX4H2][CX3]=O	0.8879	[CX4H2]([#6])[O]	0.5832
[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.8812	[CX4H2]([OX2H1])[CX3H0]	0.567

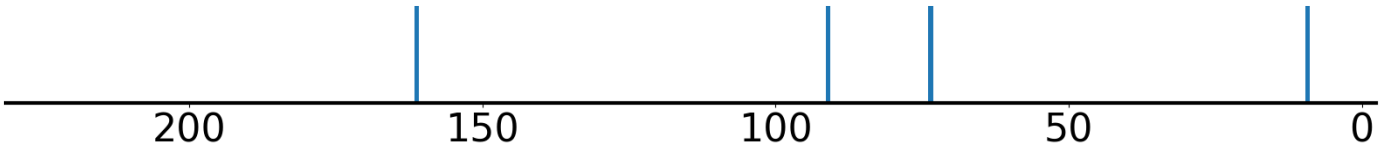
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9996	CC=CC#CC	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9969	C=CC=CC#C	0.0
[OX2H1]	0.9841	CC=CCC#C	0.0
[CX4H2][CX3]=O	0.8879	C=CCCC#C	0.0
[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.8812	[#6X2][#6H1][#6X2]	0.0
[#8][#6][#6]=[#8]	0.7643	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#6H2][#6X3H0][#6H2]	0.7369	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
OCC[CH2]	0.6381	CC#CCC=C	0.0
[CX4H2]([#6])[O]	0.5832	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H2]([OX2H1])[CX3H0]	0.567	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6H2]	0.5254	[#6X3][#6H2][#8]	0.2118
[#8][#6][#6][#6X3]	0.4512	[OX2H1][CX4H2][CX3H0][CX4H2]	0.43
[CX4H2]CC=O	0.4289	[OX2H1][CX4H2][#6X3H0]	0.4332
O=[#6][#6][#6X3]	0.2862	[#8]=[#6][#6H2][#8]	0.4421
[#8][#6][#6][#8]	0.2629	[#8][#6H2][#6H0][#6H2][#8]	0.5346
[#8][#6][#6H2][#8]	0.1799	[CX4H2]([OX2H1])[CX3H0]	0.567
[#6X3][#6H2][#6X3]	0.1772	[CX4H2]([#6])[O]	0.5832
[#8]=[#6H0][#6H1]	0.1447	OCC[CH2]	0.6381
[CX4H2]([OX2H1])[CX4H1]	0.1426	[#6H2][#6X3H0][#6H2]	0.7369
[CX4H3][OX2H0]	0.1343	[#8][#6][#6]=[#8]	0.7643

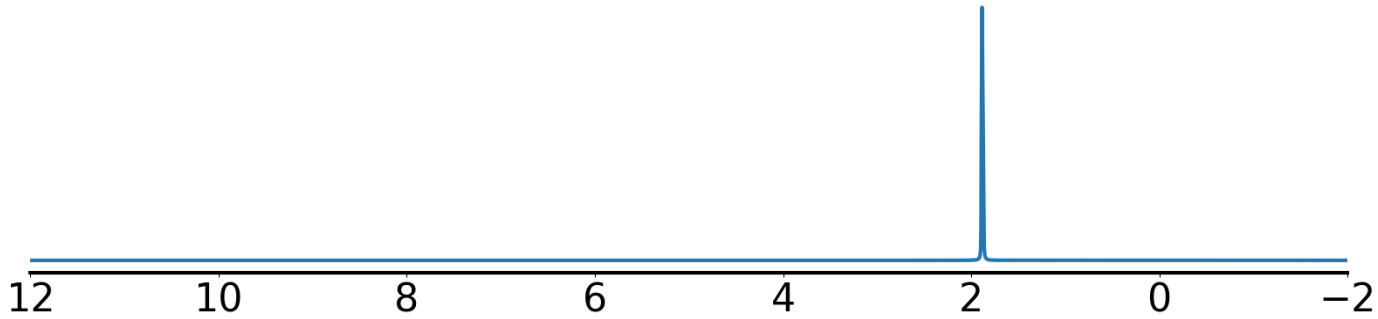
Example 199 true smiles: CC#CC(=O)O formula: C4H4O2
Index of correct structure: 0 of 32
True structure loss: 0.004418
True structure:



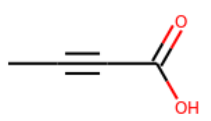
Experimental 13C NMR (solvent: CDCl3)



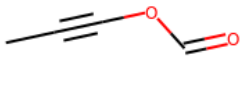
Experimental 1H NMR (solvent: D2O)



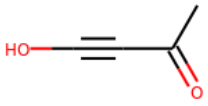
Top predicted structures (loss):



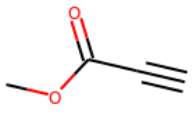
0.004418



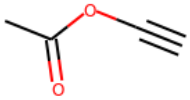
0.025247



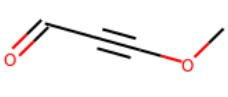
0.043696



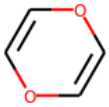
0.064242



0.072622



0.0809



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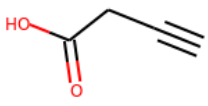
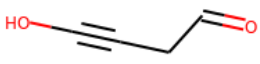
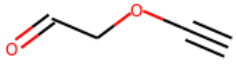


0.102659



0.107462



0.115173

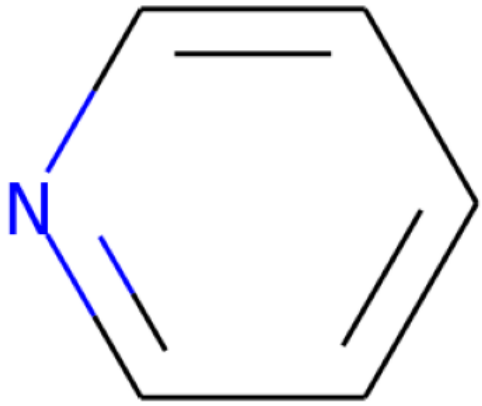
Top predicted substructures	prob		
[CX4H3][CX2H0]	0.9993	[#8]=[#6][#8]	0.9138
[$([CX2]#C)]	0.9983	[CX3](=[OX1])O	0.9026
[CX2H0](#[CX2H0])[CX3H0]	0.9928	[CX4H3]	0.8999

[#6X3][#6]#[#6][#6H3]	0.9864	[#6H3][#6H0]	0.7969
[CX4H3][#6]	0.9561	[CX3](=[OX1])C	0.7356

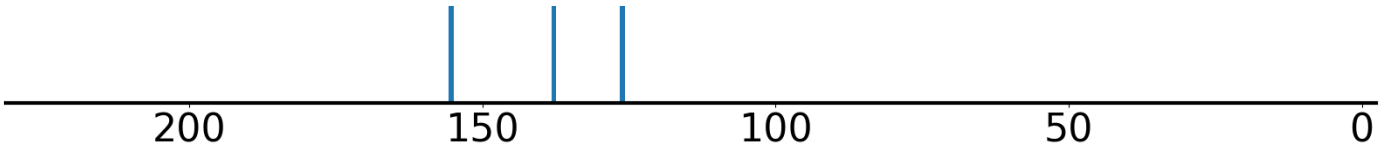
best positives	prob	best negatives	prob
[CX4H3][CX2H0]	0.9993	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[$([CX2]#C)]	0.9983	[CX3H1](=[CX3H2])[CX4H2]	0.0
[CX2H0](#[CX2H0])[CX3H0]	0.9928	[CX3H0](=[CX3H2])([CX4H2])[CX4H0]	0.0
[#6X3][#6]#[#6][#6H3]	0.9864	[CX3H1](=[CX3H2])[NX3H0]	0.0
[CX4H3][#6]	0.9561	[CX3H2]=[CX3H1][CX4H0][OX2H1]	0.0
[#8]=[#6][#8]	0.9138	[CX3H1](=[CX3H2])[CX4H0]	0.0
[CX3](=[OX1])O	0.9026	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[CX4H3]	0.8999	[CX3H1](=[CX3H2])[cX3H0]	0.0
[#6H3][#6H0]	0.7969	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
[CX3](=[OX1])C	0.7356	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6][#8]	0.2293	[OX2H1]	0.5969
[#6H1]	0.1463	[CX3](=O)[OX2H1]	0.7048
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.1024	[CX3](=[OX1])C	0.7356
[#8][#6][#6H2]	0.0799	[#6H3][#6H0]	0.7969
[#8][#6][#6]=[#8]	0.0743	[CX4H3]	0.8999
[CX4H2][CX3]=O	0.07	[CX3](=[OX1])O	0.9026
[CX3H](O)	0.0694	[#8]=[#6][#8]	0.9138
[#6H1][#6H2]	0.0676	[CX4H3][#6]	0.9561
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.0632	[#6X3][#6]#[#6][#6H3]	0.9864
[#8][#6][#6][#6X3]	0.0562	[CX2H0](#[CX2H0])[CX3H0]	0.9928

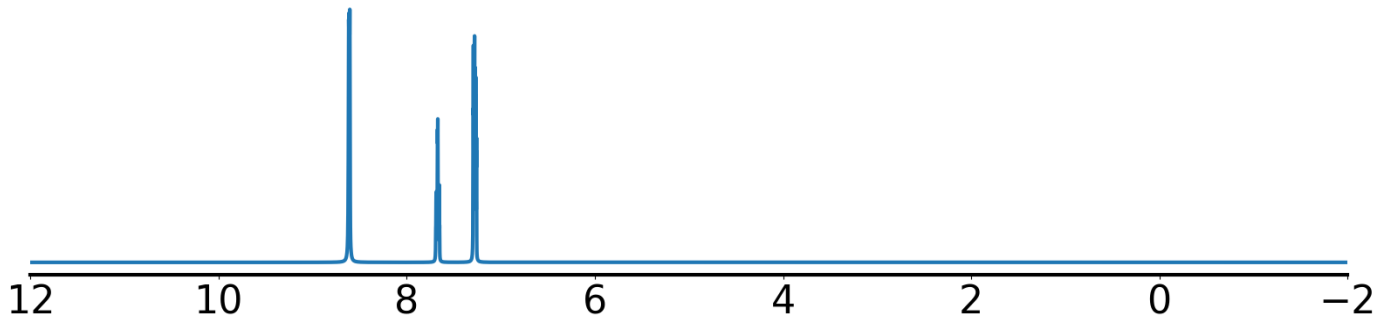
Example 200 true smiles: c1ccncc1 formula: C5H5N
Index of correct structure: 0 of 27
True structure loss: 0.016342
True structure:



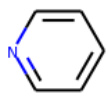
Experimental 13C NMR (solvent: CDCl3)



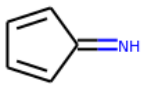
Experimental 1H NMR (solvent: CDCl3)



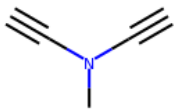
Top predicted structures (loss):



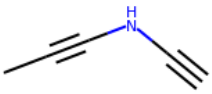
0.016342



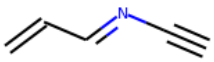
0.132606



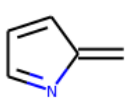
0.145075



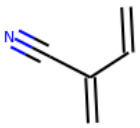
0.161712



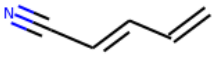
0.168013



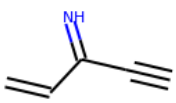
0.172207



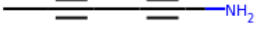
0.181046



0.18835



0.191809



0.196347

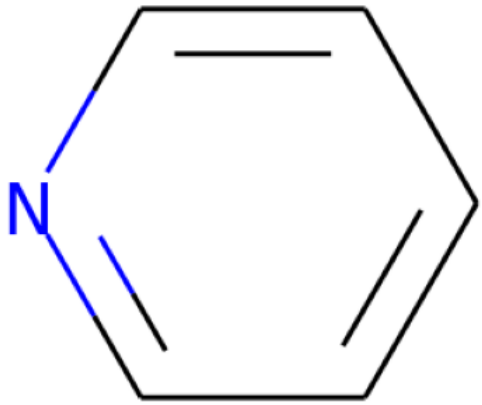
Top predicted substructures	prob		
[#6H1]	0.9998	[cX3H1]([cX3H1])[cX3H1]	0.9891
[cH][cH]	0.999	[#7][#6][#6][#6X3]	0.9837
[#6X3][#6X3]	0.9984	[cH]	0.9816

[#6X3][#6X3][#6X3][#6X3]	0.9969	[#6]1[#6][#6][#6][#6][#7]1	0.9665
[#7][#6][#6X3]	0.9914	[cX3H1]([cX3H1])[cX3H0]	0.9503

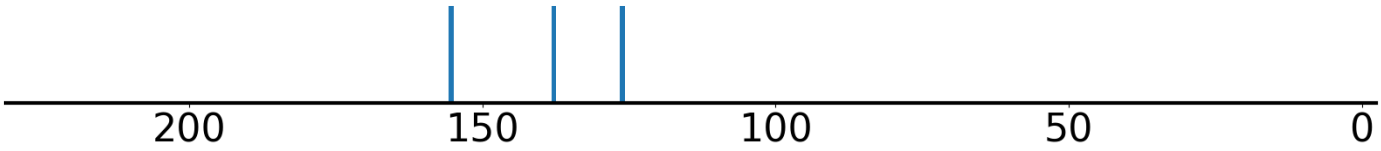
best positives	prob	best negatives	prob
[#6H1]	0.9998	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.999	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3]	0.9984	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9969	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6X3]	0.9914	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9891	[CX3H0](=[OX1H0])([CX4H1])[CX4H0]	0.0
[#7][#6][#6][#6X3]	0.9837	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[cH]	0.9816	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6]1[#6][#6][#6][#6][#7]1	0.9665	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[#6H1][#6H1]	0.9494	[OX2H1][CX4H0][CX4H1]([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H0]	0.9503	[#6H1][#7][#6H1]	0.5928
[#6X3H1][#6X3H0]	0.9077	[#6X3][#7][#6X3]	0.7718
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.8683	[cX3H1]([nX2H0])[cX3H1]	0.9044
[#6]1[#6][#6][#6][#6][#6]1	0.7428	[#6H1][#6H1]	0.9494
[#7][#6X3H0][#6X3H1]	0.6768	[#6]1[#6][#6][#6][#6][#7]1	0.9665
[#7][#6H0][#6H1]	0.6699	[cH]	0.9816
[#7X3H2]	0.4489	[#7][#6][#6][#6X3]	0.9837
[#7H2][#6H0]	0.2631	[cX3H1]([cX3H1])[cX3H1]	0.9891
[cX3H1]([nX2H0])[cX3H0]	0.2243	[#7][#6][#6X3]	0.9914
[cH]cO	0.1757	[#6X3][#6X3][#6X3][#6X3]	0.9969

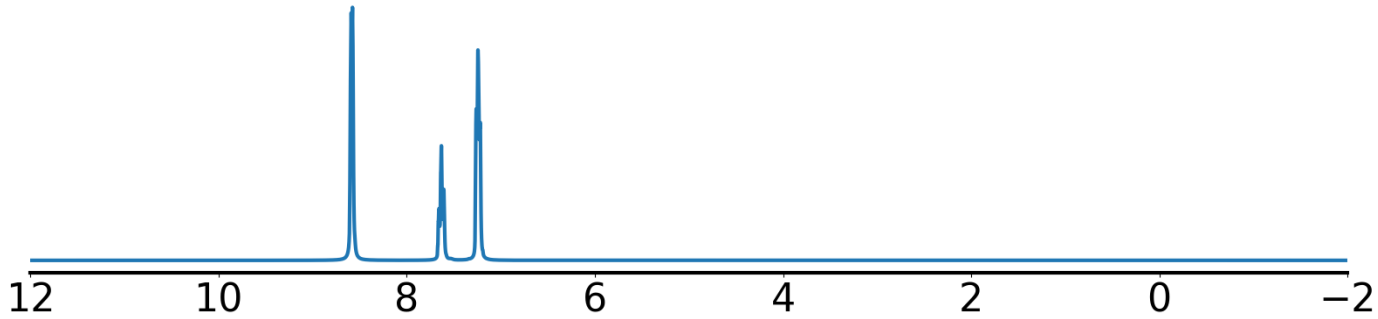
Example 201 true smiles: c1ccncc1 formula: C5H5N
Index of correct structure: 0 of 27
True structure loss: 0.015397
True structure:



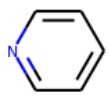
Experimental 13C NMR (solvent: CDCl3)



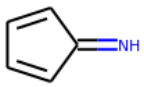
Experimental 1H NMR (solvent: CDCl3)



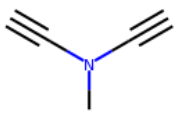
Top predicted structures (loss):



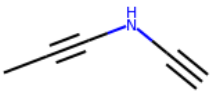
0.015397



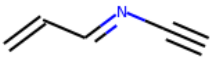
0.139172



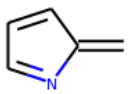
0.14969



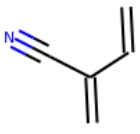
0.164619



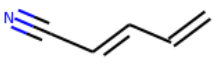
0.176428



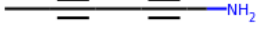
0.183814



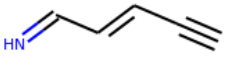
0.19823



0.199064



0.200105



0.205311

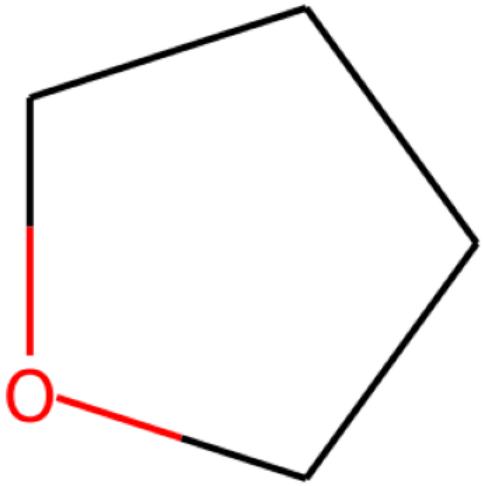
Top predicted substructures	prob		
[#6H1]	0.9999	[#7][#6][#6X3]	0.9872
[cH][cH]	0.9996	[cH]	0.9843
[#6X3][#6X3]	0.9984	[#6]1[#6][#6][#6][#6][#7]1	0.9775

[cX3H1]([cX3H1])[cX3H1]	0.9968	[#7][#6][#6][#6X3]	0.9751
[#6X3][#6X3][#6X3][#6X3]	0.9967	[#6H1][#6H1]	0.9512

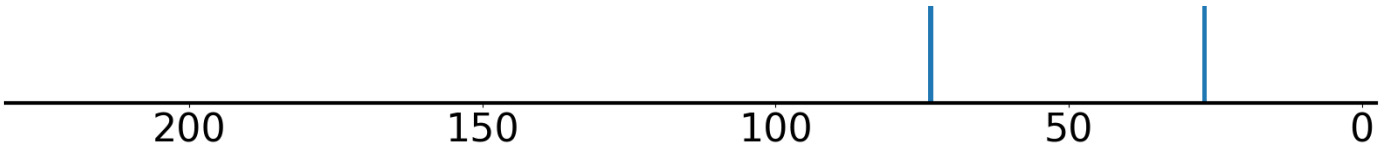
best positives	prob	best negatives	prob
[#6H1]	0.9999	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9996	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3]	0.9984	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9968	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9967	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#7][#6][#6X3]	0.9872	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[cH]	0.9843	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6]1[#6][#6][#6][#6][#7]1	0.9775	[CX3H0](=[OX1H0])([CX4H1])[CX4H0]	0.0
[#7][#6][#6][#6X3]	0.9751	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[#6H1][#6H1]	0.9512	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H0]	0.949	[#6H1][#7][#6H1]	0.4317
[#6]1[#6][#6][#6][#6][#6]1	0.9078	[#6X3][#7][#6X3]	0.6631
[#6X3H1][#6X3H0]	0.8516	[cX3H1]([nX2H0])[cX3H1]	0.8868
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7913	[#6H1][#6H1]	0.9512
[#7][#6H0][#6H1]	0.5639	[#7][#6][#6][#6X3]	0.9751
[#7][#6X3H0][#6X3H1]	0.5349	[#6]1[#6][#6][#6][#6][#7]1	0.9775
[#7X3H2]	0.3616	[cH]	0.9843
[#7H2][#6H0]	0.2407	[#7][#6][#6X3]	0.9872
[#8][#6][#6][#6X3]	0.1467	[#6X3][#6X3][#6X3][#6X3]	0.9967
[cH]cO	0.1409	[cX3H1]([cX3H1])[cX3H1]	0.9968

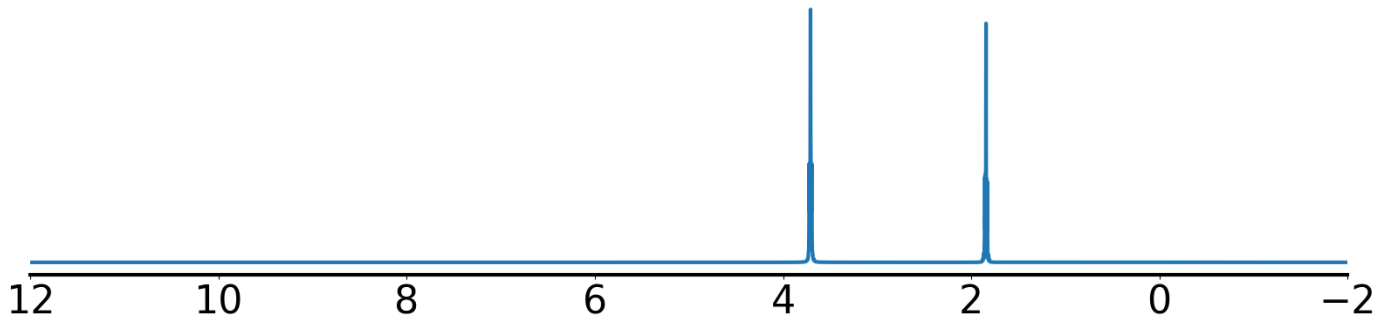
Example 202 true smiles: C1CCOC1 formula: C4H8O
Index of correct structure: 0 of 22
True structure loss: 0.006421
True structure:



Experimental 13C NMR (solvent: CDCl3)

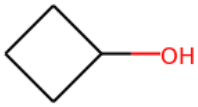


Experimental 1H NMR (solvent: D2O)

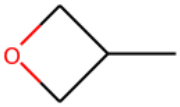


Top predicted structures (loss):

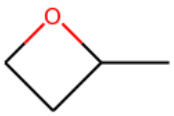
0.006421



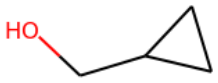
0.068256



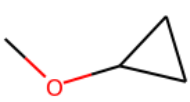
0.093125



0.121414



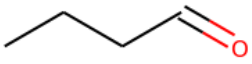
0.135288



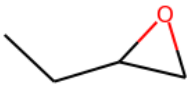
0.137885

0.150093

0.150942



0.153123



0.155557

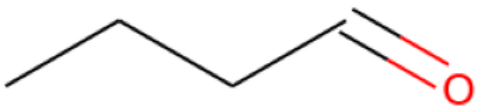
Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9896	[CX4H2][CX4H2]	0.8752
[#8][#6][#6H2]	0.9811	[CH2X4](O)[CX4H2][CX4H2]	0.8612
[CX4H2]([#6])[O]	0.9606	[CX4H2][CX4H2][CX4H2][CX4H2]	0.796

OCC[CH2]	0.9472	[CX4H2]([CX4H2])[CX4H2]	0.7903
[OX2H0][CX4H2][CX4H2][CX4H2]	0.9278	[CH2X4](O)[CX4H2]	0.741

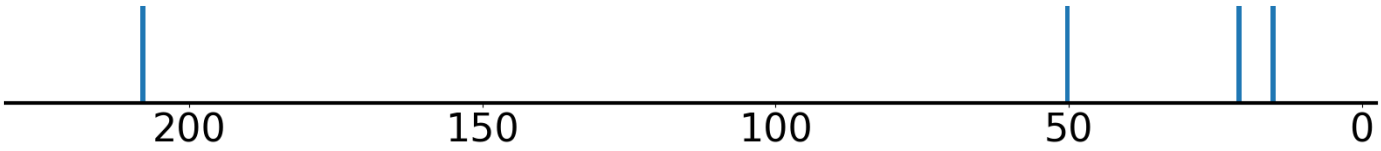
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9896	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#8][#6][#6H2]	0.9811	[#6H3][#6H1][#6H1]=[#7]	0.0
[CX4H2]([#6])[O]	0.9606	[CX2H0](#[CX2H1])[cX3H0]	0.0
OCC[CH2]	0.9472	[CX3H1](=[CX3H2])[cX3H0]	0.0
[OX2H0][CX4H2][CX4H2][CX4H2]	0.9278	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2][CX4H2]	0.8752	C=CC=CC#C	0.0
[CH2X4](O)[CX4H2][CX4H2]	0.8612	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.796	[CX3H0](=[CX3H2])([CX4H2])[CX4H1]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.7903	[CX3H0](=[CX3H2])([CX4H1])[CX3H1]	0.0
[CH2X4](O)[CX4H2]	0.741	[#7][#6]=[#6][#6]#[#7]	0.0

worst negatives	prob	worst positives	prob
[#8]1[#6][#6][#6][#6][#6]1	0.1766	C1OCCC1	0.295
[#8][#6][#6][#8]	0.1541	[CX4H2][OX2H0][CX4H2]	0.6094
[CX4H3][#6]	0.154	[CX4H2]([OX2H0])[CX4H2]	0.7178
[OX2H1]	0.1356	[CH2X4](O)[CX4H2]	0.741
[CH3][#6][#8]	0.1124	[CX4H2]([CX4H2])[CX4H2]	0.7903
[#6H1][#6H2]	0.111	[CX4H2][CX4H2][CX4H2][CX4H2]	0.796
[#8][#6][#6H2][#8]	0.1057	[CH2X4](O)[CX4H2][CX4H2]	0.8612
[#6H1]	0.1035	[CX4H2][CX4H2]	0.8752
CCCCCC	0.1033	[OX2H0][CX4H2][CX4H2][CX4H2]	0.9278
[OX2H0][CX4H1][CX4H3]	0.0868	OCC[CH2]	0.9472

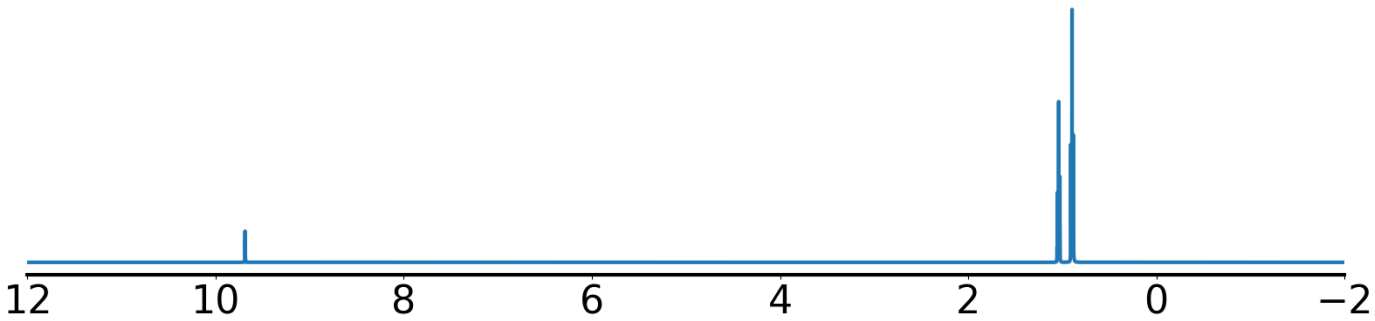
Example 203 true smiles: CCCC=O formula: C4H8O
Index of correct structure: 1 of 22
True structure loss: 0.030431
True structure:



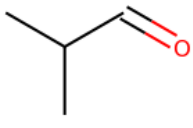
Experimental 13C NMR (solvent: CDCl3)



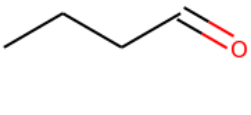
Experimental 1H NMR (solvent: D2O)



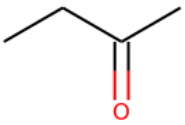
Top predicted structures (loss):



0.020199

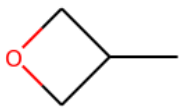


0.030431

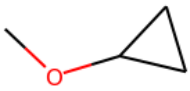


0.107416

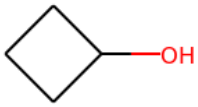
0.143962



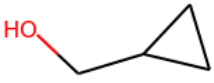
0.167981



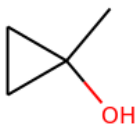
0.171477



0.174714



0.183314



0.188553

0.211463

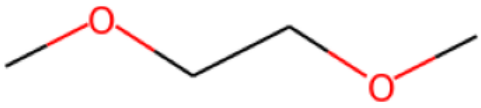
Top predicted substructures	prob		
[CX3H1](=O)[#6]	0.9997	[#6H3][#6][#6]	0.9862
[CX3](=[OX1])C	0.9994	[#6X3][#6][#6][#6H3]	0.7682
[CX4H3][#6]	0.9981	[CX4H3][CX4H1]	0.7426

[CX4H3]	0.9968	[CX4H2]([#6])[#6]	0.7244
[#6H1]	0.9951	[CX4H3][CX4H2]	0.6874

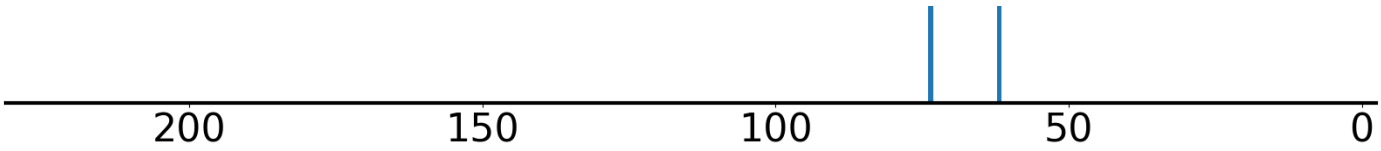
best positives	prob	best negatives	prob
[CX3H1](=O)[#6]	0.9997	C=CCCC#C	0.0
[CX3](=[OX1])C	0.9994	CCC=CC#C	0.0
[CX4H3][#6]	0.9981	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3]	0.9968	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#6H1]	0.9951	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9862	[CX2H0](#[CX2H1])[CX3H0]	0.0
[#6X3][#6][#6][#6H3]	0.7682	[CX3H2]=[CX3H0][OX2H0][CX4H2]	0.0
[CX4H2]([#6])[#6]	0.7244	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][CX4H2]	0.6874	CC=CCC#C	0.0
[CX4H2][CX4H2]	0.5008	[CX2H0](#[CX2H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H3][CX4H1]	0.7426	[CX4H2]([CX4H2])[CX3H1]	0.0019
O=[CX3][CX4H]	0.6661	[OX1H0]=[CX3H1][CX4H2][CX4H2]	0.0219
[#6H1][#6H1]	0.5494	[CX4H2][CX3H]	0.0652
[#8]=[#6H1][#6H1]	0.423	[CX4H2][CX3]=O	0.1516
[#6H3][#6][#6][#6H3]	0.382	[#6H1][#6H2]	0.174
[CX3H][CX4H]	0.3545	[CX3H1](=[OX1H0])[CX4H2]	0.2456
[CHX4]([CH3X4])[CH3X4]	0.3178	[CX4H2]CC=O	0.2582
[#6H3][#6][#6X3]	0.3024	[CX4H2]([CX4H3])[CX4H2]	0.4085
[CX3H1](=[OX1H0])[CX4H1]	0.1718	[CX4H2][CX4H2]	0.5008
[#8]=[#6][#6H1][#6H1]	0.1664	[CX4H3][CX4H2]	0.6874

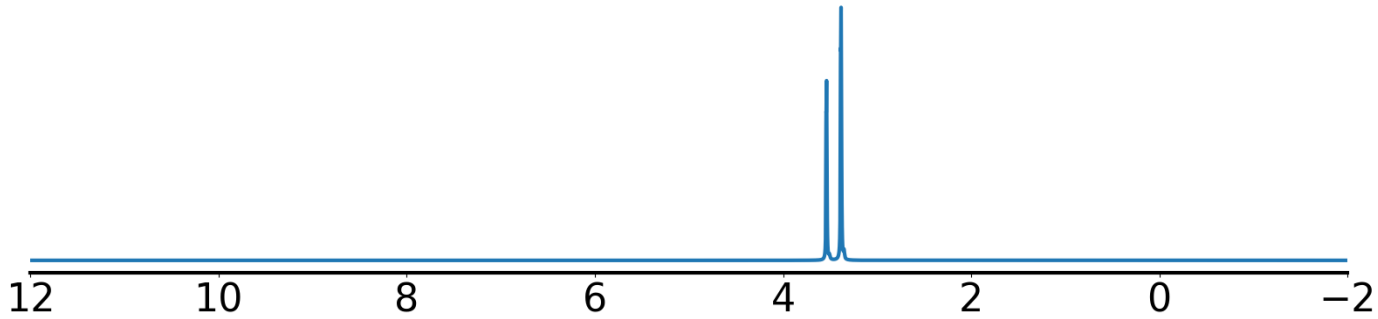
Example 204 true smiles: COCCOC formula: C4H10O2
Index of correct structure: 0 of 20
True structure loss: 0.006334
True structure:



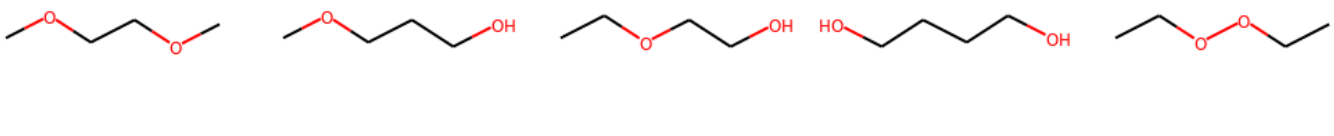
Experimental 13C NMR (solvent: CDCl3)



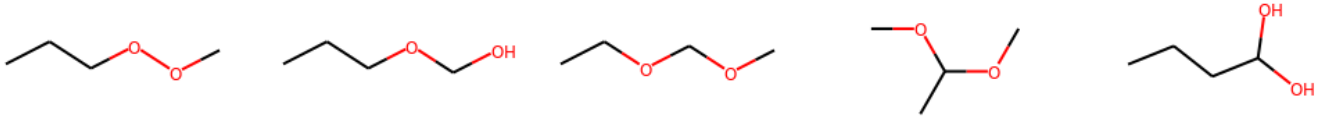
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.006334 0.034641 0.045662 0.046983 0.060173



0.060918 0.064007 0.083101 0.095612 0.097936

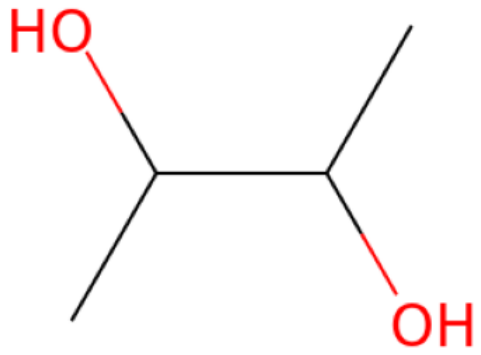
Top predicted substructures	prob		
[CX4H2]([#6])[O]	0.9976	[#8][#6][#6H2][#8]	0.8997
[#8][#6][#6H2]	0.9624	[OX2H0][CX4H2][CX4H2][OX2H0]	0.885
[CX4H2]([OX2H0])[CX4H2]	0.9415	[CX4H3]	0.8737

O[CX4H2][CX4H2]O	0.9395	[CX4H3][OX2H0]	0.8446
[CH2X4](O)[CX4H2]	0.9041	[CX4H2][CX4H2]	0.8434

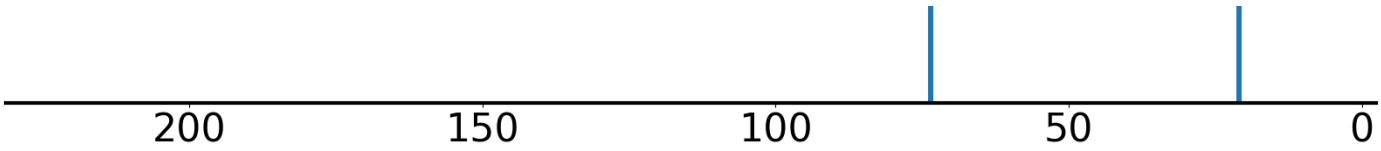
best positives	prob	best negatives	prob
[CX4H2]([#6])[O]	0.9976	[CX2H0](#[NX1H0])[CX3H1]	0.0
[#8][#6][#6H2]	0.9624	C=CC=CC#C	0.0
[CX4H2]([OX2H0])[CX4H2]	0.9415	[#6X2][#6H1][#6X2]	0.0
O[CX4H2][CX4H2]O	0.9395	[#7][#6]=[#6][#6]#[#7]	0.0
[CH2X4](O)[CX4H2]	0.9041	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6H2][#8]	0.8997	[CX3H0](=[OX1H0])([CX4H1])[CX4H0]	0.0
[OX2H0][CX4H2][CX4H2][OX2H0]	0.885	[CX4H2]([CX4H0])[CX2H0]	0.0
[CX4H3]	0.8737	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][OX2H0]	0.8446	[#7][#6][#6]#[#7]	0.0
[CX4H2][CX4H2]	0.8434	CCC=CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2][OX2H0][CX4H2]	0.5821	[CX4H3][OX2H0][CX4H2]	0.6928
OCC[CH2]	0.3817	[#8][#6][#6][#8]	0.6971
[CX4H2]([OX2H1])[CX4H2]	0.3618	[CX4H2][CX4H2]	0.8434
[CX4H2](O)[CHX4]	0.2719	[CX4H3][OX2H0]	0.8446
[#7X3][#6H2]	0.2673	[CX4H3]	0.8737
[CX4H]O	0.2498	[OX2H0][CX4H2][CX4H2][OX2H0]	0.885
[#6H1][#6H2]	0.2334	[#8][#6][#6H2][#8]	0.8997
[OX2H1]	0.1687	[CH2X4](O)[CX4H2]	0.9041
[#6H1]	0.1593	O[CX4H2][CX4H2]O	0.9395
O[CX4H][CX4H2]	0.0793	[CX4H2]([OX2H0])[CX4H2]	0.9415

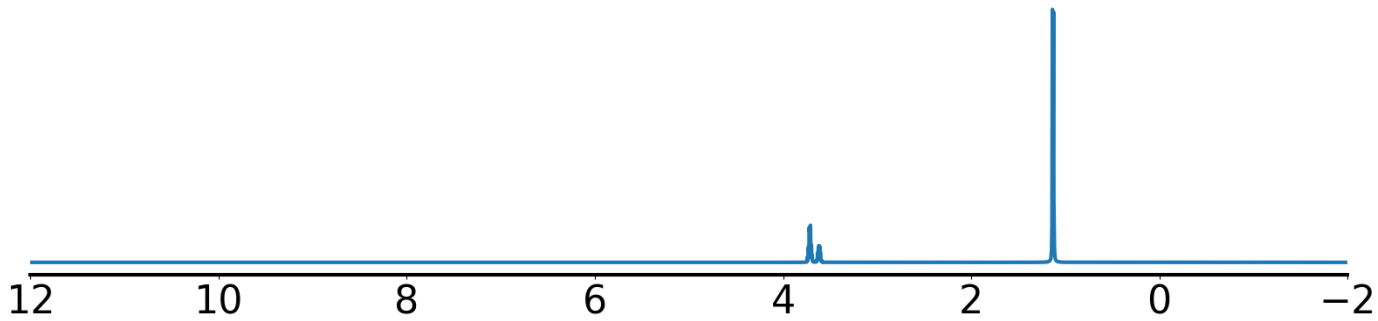
Example 205 true smiles: CC(O)C(C)O formula: C4H10O2
Index of correct structure: 0 of 20
True structure loss: 0.005398
True structure:



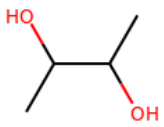
Experimental 13C NMR (solvent: CDCl3)



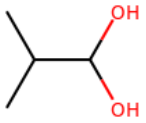
Experimental 1H NMR (solvent: D2O)



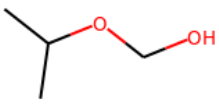
Top predicted structures (loss):



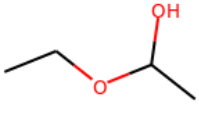
0.005398



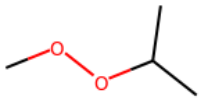
0.036003



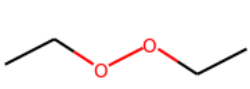
0.045253



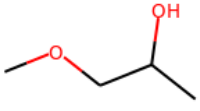
0.047717



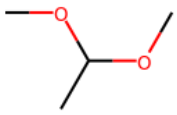
0.055175



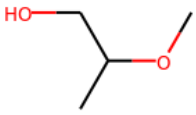
0.06866



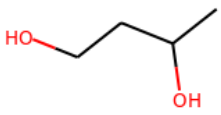
0.072792



0.074736



0.081616



0.082952

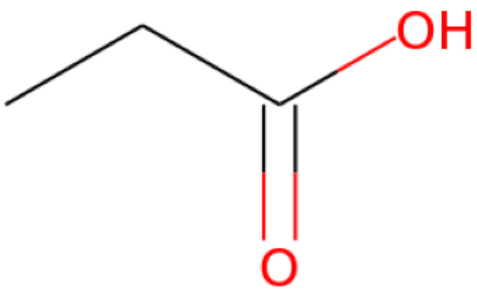
Top predicted substructures	prob		
[CX4H3]	0.9998	[OX2H1]	0.9901
[CX4H3][#6]	0.9996	[CX4H]O	0.9898
[CX4H3][CX4]O	0.9977	[CH3][#6][#8]	0.9815

[#6H3][#6][#6]	0.9962	[CX4H3][CX4H1][OX2H1]	0.9723
[#6H1]	0.9961	[#6X4H3][#6][#8H]	0.9686

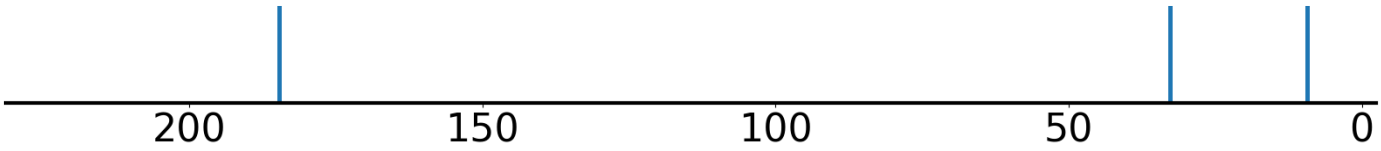
best positives	prob	best negatives	prob
[CX4H3]	0.9998	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9996	CCC=CC#C	0.0
[CX4H3][CX4]O	0.9977	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9962	CC=CCC#C	0.0
[#6H1]	0.9961	C=CCCC#C	0.0
[OX2H1]	0.9901	CC=CC#CC	0.0
[CX4H]O	0.9898	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CH3][#6][#8]	0.9815	CC#CCC=C	0.0
[CX4H3][CX4H1][OX2H1]	0.9723	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#6X4H3][#6][#8H]	0.9686	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H1]([OX2H1])([CX4H1])[CX4H1]	0.5259	[#6H3][#6][#6][#6H3]	0.5228
[CX4H](O)([CH])[CH]	0.4094	[OX2H1][CX4H1][CX4H1][OX2H1]	0.6797
[#6X4H1][#6X4H1][#6X4H1]	0.247	[#6H1][#6H1]	0.8192
[CHX4]([CH3X4])[CH3X4]	0.2416	[CX4H](O)CO	0.8483
[CX4H2](O)[CHX4]	0.1218	[#8][#6H1][#6H1][#6H3]	0.8717
[#8][#6][#6H2]	0.0845	[#8][#6][#6][#8]	0.8951
[CX4H1]([OX2H1])([CX4H2])[CX4H1]	0.0837	[CH3]CC[OH]	0.9001
O[CX4H2][CX4H2]O	0.0748	[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.9091
[#6X4H2][#6H1][#8H]	0.0573	[CX4H3][CX4H1]	0.9094
[OX2H0][CX4H1][CX4H3]	0.0567	[OH][CX4H]	0.9459

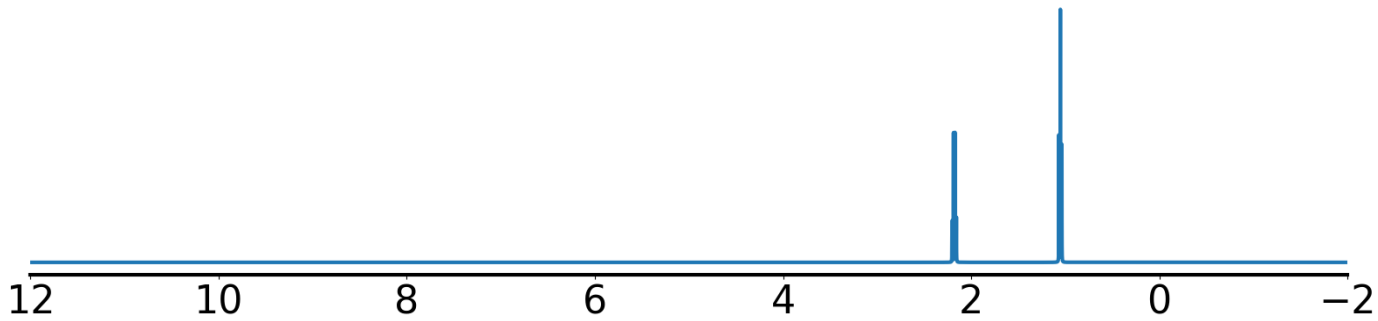
Example 206 true smiles: CCC(=O)O formula: C3H6O2
Index of correct structure: 0 of 18
True structure loss: 0.00581
True structure:



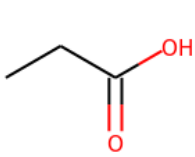
Experimental 13C NMR (solvent: CDCl3)



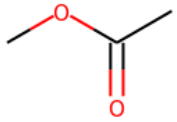
Experimental 1H NMR (solvent: D2O)



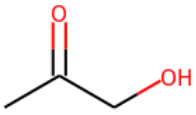
Top predicted structures (loss):



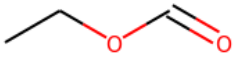
0.00581



0.093995

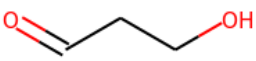


0.109935

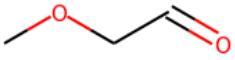


0.110616

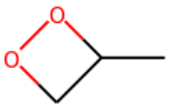
0.130769



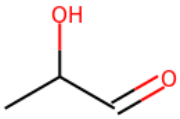
0.155919



0.162787



0.179026



0.201812

0.203705

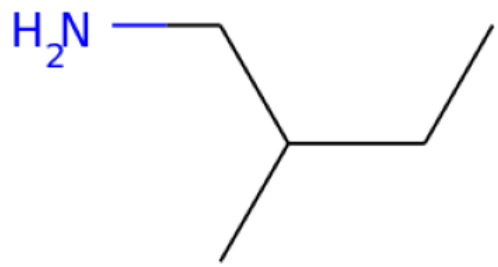
Top predicted substructures	prob		
[CX4H3]	0.9988	[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9943
[CX3](=[OX1])C	0.9986	[CX4H2]([#6])[#6]	0.9904
[CX4H3][#6]	0.9985	[#8]=[#6][#8]	0.972

[#6H3][#6][#6]	0.9979	[CX3](=O)[OX2H1]	0.9352
[CX4H3][CX4H2]	0.9958	[OX2H1]	0.9304

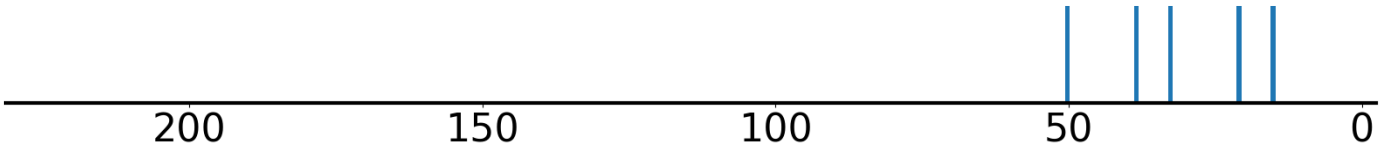
best positives	prob	best negatives	prob
[CX4H3]	0.9988	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9986	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H3][#6]	0.9985	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#6H3][#6][#6]	0.9979	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX4H3][CX4H2]	0.9958	C=CCCC#C	0.0
[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9943	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9904	[CX2H0](#[CX2H1])[CX3H1]	0.0
[#8]=[#6][#8]	0.972	CC=CC#CC	0.0
[CX3](=O)[OX2H1]	0.9352	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[OX2H1]	0.9304	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2]CC=O	0.2489	[CH3]CC[OH]	0.3225
[#6X3][#6][#6][#6H3]	0.193	[#8][#6][#6H2]	0.5833
[#6H3][#6H0]	0.1907	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.6094
OCC[CH2]	0.1886	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.7454
[#8][#6H0][#6H1]	0.1546	[CX4H2][CX3]=O	0.8182
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.0981	[#6H3][#6][#6X3]	0.8575
[#6H3][#6][#6][#6H3]	0.0943	[CX3](=[OX1])O	0.9017
[#8][#6][#6]=[#8]	0.0935	[CX4H2]([CX4H3])[CX3H0]	0.9274
[#8]=[#6][#6]=[#8]	0.0656	[OX2H1]	0.9304
[#8]=[#6H0][#6H1]	0.0571	[CX3](=O)[OX2H1]	0.9352

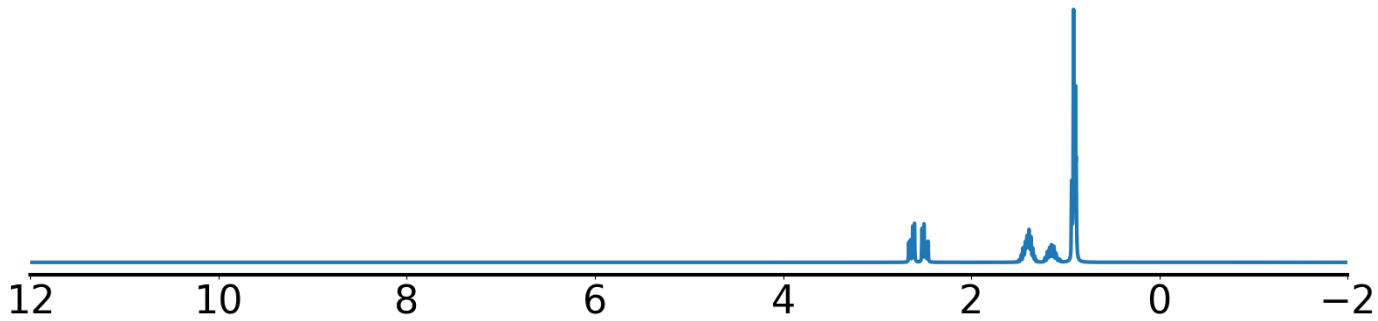
Example 207 true smiles: CCC(C)CN formula: C5H13N
Index of correct structure: 0 of 17
True structure loss: 0.013327
True structure:



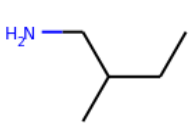
Experimental 13C NMR (solvent: CDCl3)



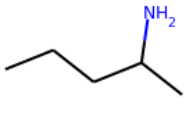
Experimental 1H NMR (solvent: CDCl3)



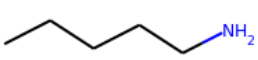
Top predicted structures (loss):



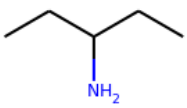
0.013327



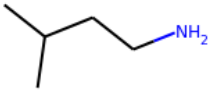
0.023625



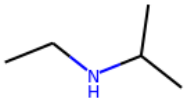
0.031055



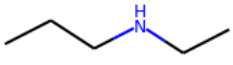
0.032795



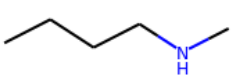
0.033844



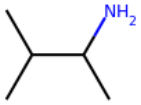
0.036681



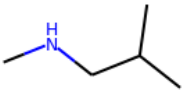
0.03987



0.045889



0.046605



0.055815

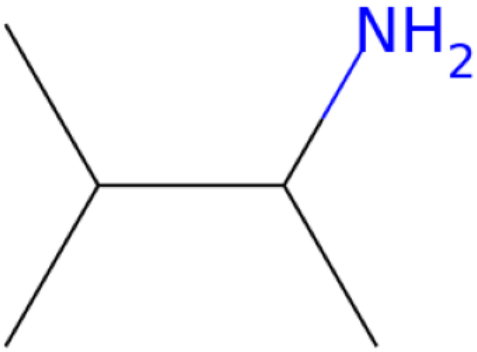
Top predicted substructures	prob		
[CX4H3]	1.0	[#7X3H2]	0.9619
[#6H3][#6][#6]	0.9999	[#6H1]	0.961
[CX4H3][#6]	0.9994	[#7][#6H2]	0.937

[CX4H3][CX4H2]	0.9907	[#7X3][#6H2]	0.9193
[CX4H2]([#6])[#6]	0.9789	[#6H1][#6H2]	0.8595

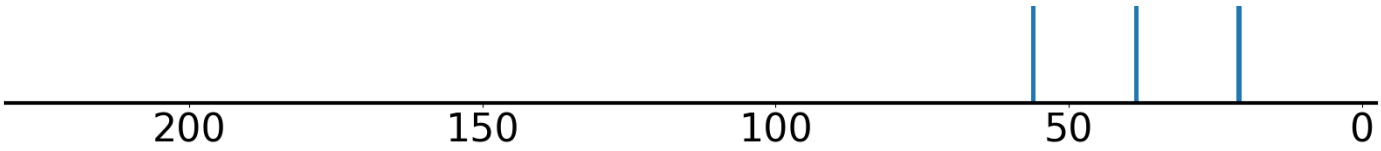
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9999	C=CCCC#C	0.0
[CX4H3][#6]	0.9994	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][CX4H2]	0.9907	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	0.9789	CCC=CC#C	0.0
[#7X3H2]	0.9619	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H1]	0.961	CC=CCC#C	0.0
[#7][#6H2]	0.937	CC=CC#CC	0.0
[#7X3][#6H2]	0.9193	CCC#CC=C	0.0
[#6H1][#6H2]	0.8595	CC#CCC=C	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX4H2]	0.5598	[#6H1]([#6H2])[#6H2]	0.3591
[CX4H2]([CX4H3])[CX4H2]	0.436	[CX4H1]([CX4H3])([CX4H2])[CX4H2]	0.389
[#6H1][#6H1]	0.4247	[#7][#6H2][#6H1]	0.4531
[#6H3][#6H1][#6H1][#7]	0.3729	[CX4H2]([CX4H3])[CX4H1]	0.4596
[CX4H2]([CX4H2])[CX4H1]	0.355	[#6H3][#6][#6][#6H3]	0.4993
[#7X3H1]	0.3259	[CX4H2]([NX3H2])[CX4H1]	0.5139
[#7H2][#6H1]	0.2999	[CHX4]([CH3X4])[CH2X4]	0.598
[CX4H2]([NX3H1])[CX4H2]	0.2291	[CX4H3][CX4H1]	0.79
[#7][#6H2][#6H2]	0.2033	[#7H2][#6H2]	0.841
[CX4H2]([CX4H2])[CX4H2]	0.2029	[#6H1][#6H2]	0.8595

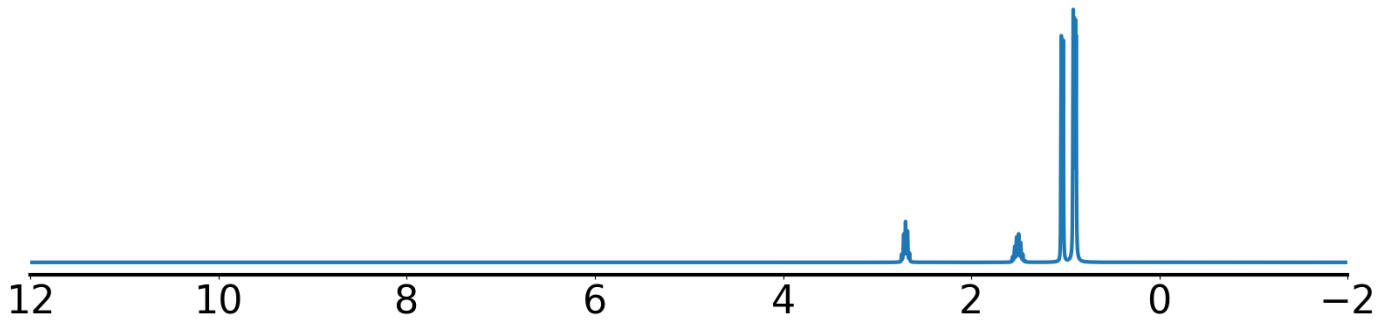
Example 208 true smiles: CC(C)C(C)N formula: C5H13N
Index of correct structure: 0 of 17
True structure loss: 0.009488
True structure:



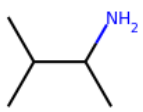
Experimental 13C NMR (solvent: CDCl3)



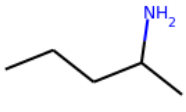
Experimental 1H NMR (solvent: CDCl3)



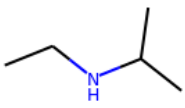
Top predicted structures (loss):



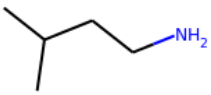
0.009488



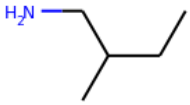
0.031909



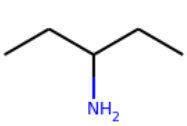
0.032797



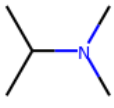
0.038971



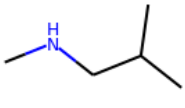
0.043152



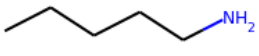
0.048335



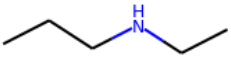
0.055476



0.060535



0.064514



0.066122

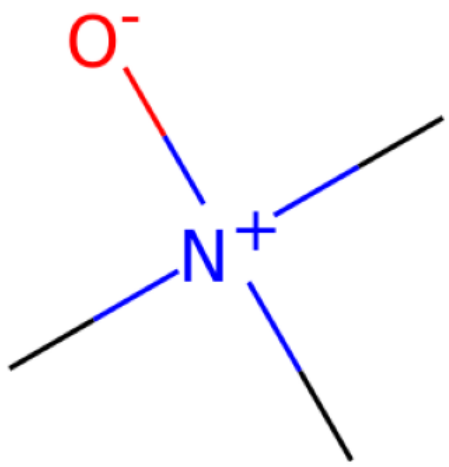
Top predicted substructures	prob		
[CX4H3]	1.0	[#7X3H2]	0.9732
[#6H3][#6][#6]	0.9999	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.9323
[CX4H3][#6]	0.9994	[CHX4]([CH3X4])[CH3X4]	0.8898

[#6H1]	0.9988	[#7H2][#6H1]	0.8561
[CX4H3][CX4H1]	0.9914	[CX4H1]([CX4H3])([CX4H3])[CX4H1]	0.6809

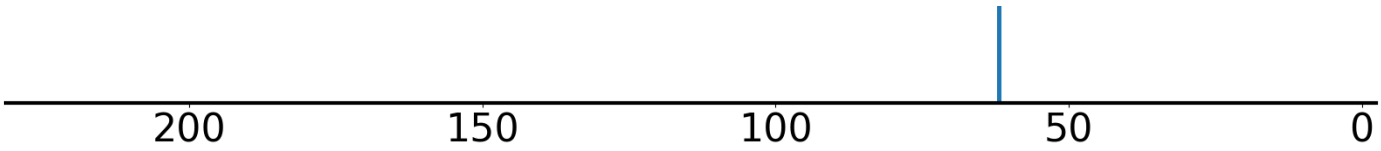
best positives	prob	best negatives	prob
[CX4H3]	1.0	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9999	CC=CCC#C	0.0
[CX4H3][#6]	0.9994	CCC=CC#C	0.0
[#6H1]	0.9988	C=CC=CC#C	0.0
[CX4H3][CX4H1]	0.9914	CC=CC#CC	0.0
[#7X3H2]	0.9732	C=CCCC#C	0.0
[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.9323	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CHX4]([CH3X4])[CH3X4]	0.8898	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7H2][#6H1]	0.8561	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H1]([CX4H3])([CX4H3])[CX4H1]	0.6809	[CX2H0](#[CX2H1])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[CHX4]([CH3X4])[CH2X4]	0.5107	[#7][#6][#6H3]	0.4809
[#7][#6H2]	0.5006	[#6H3][#6][#6][#6H3]	0.578
[#6H1][#6H2]	0.4811	[#6H1][#6H1]	0.6236
[CX4H1]([CX4H3])([CX4H2])[CX4H1]	0.3441	[#6H3][#6H1][#6H1][#7]	0.6475
[#7X3][#6H2]	0.3111	[CX4H1]([CX4H3])([CX4H3])[CX4H1]	0.6809
[#6X4H1][#6X4H1][#6X4H1]	0.294	[#7H2][#6H1]	0.8561
[#7X3H1]	0.2593	[CHX4]([CH3X4])[CH3X4]	0.8898
[#7H2][#6H2]	0.208	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.9323
[CX4H2]([#6])[#6]	0.1816	[#7X3H2]	0.9732
[#7][#6H2][#6H1]	0.1577	[CX4H3][CX4H1]	0.9914

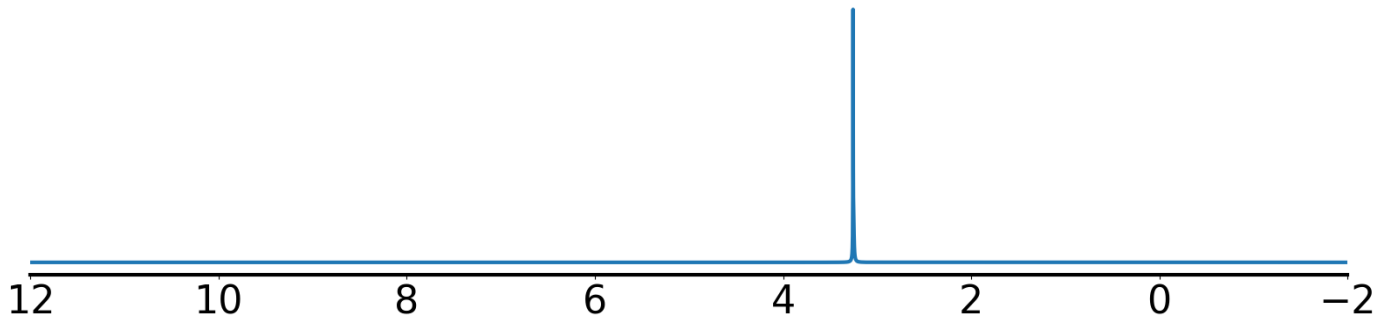
Example 209 true smiles: C[N+](C)(C)[O-] formula: C3H9NO
Index of correct structure: -1 of 17
True structure loss: 0.013455
True structure:



Experimental 13C NMR (solvent: D2O)

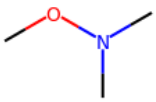


Experimental 1H NMR (solvent: D2O)



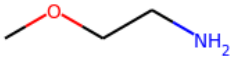
Top predicted structures (loss):

0.03226

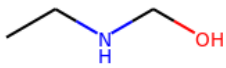


0.033582

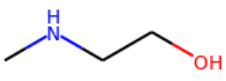
0.033637



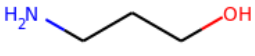
0.034276



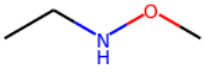
0.051929



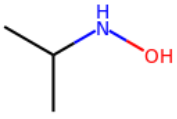
0.053221



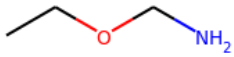
0.055904



0.057636



0.058774



0.06764

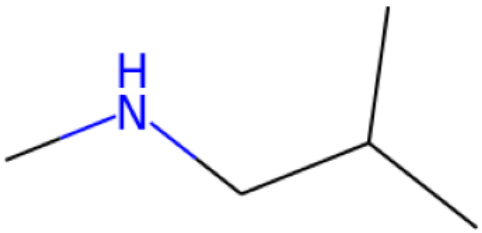
Top predicted substructures	prob		
[#7X3][#6H2]	0.9249	[#7X3H1]	0.3659
[CX4H3]	0.8394	[#7X3H2]	0.3623
[#7][#6H2]	0.6938	[#7][#6H2][#6H1]	0.2895

[CX4H3][OX2H0]	0.5514	[#8][#6][#6H2]	0.241
[#6H2][#7][#6H2]	0.5336	[OX2H1]	0.2003

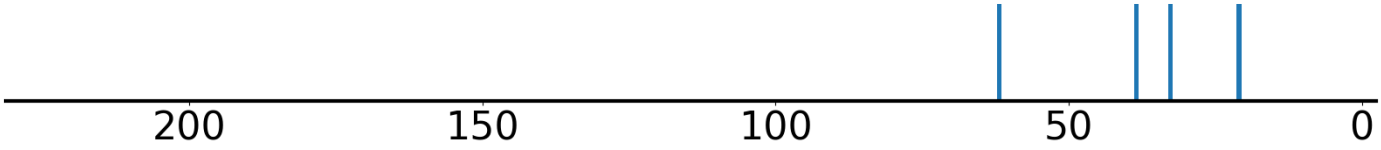
best positives	prob	best negatives	prob
[CX4H3]	0.8394	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H3][#7]	0.0278	C=CC=CC#C	0.0

worst negatives	prob	worst positives	prob
[#7X3][#6H2]	0.9249	[#6H3][#7]	0.0278
[#7][#6H2]	0.6938	[CX4H3]	0.8394

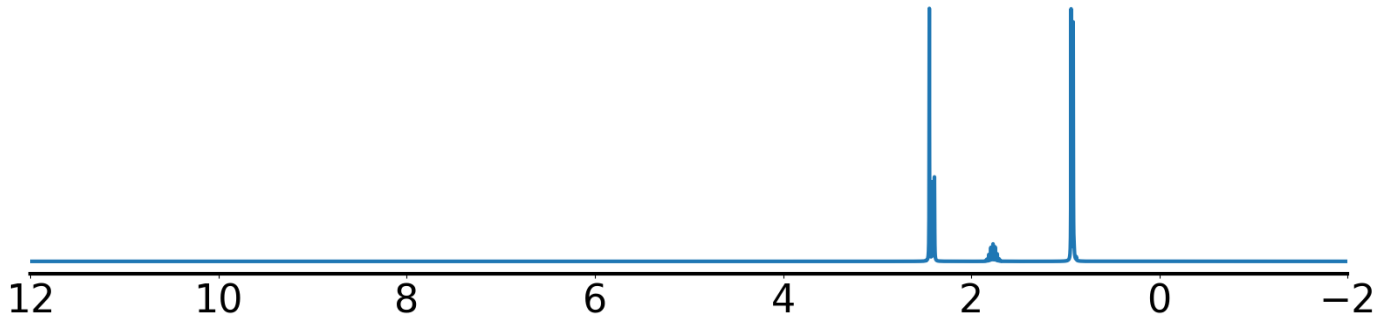
Example 210 true smiles: CNCC(C)C formula: C5H13N
Index of correct structure: 0 of 17
True structure loss: 0.01223
True structure:



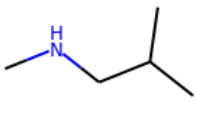
Experimental 13C NMR (solvent: CDCl3)



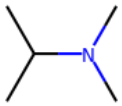
Experimental 1H NMR (solvent: CDCl3)



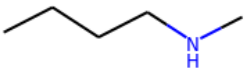
Top predicted structures (loss):



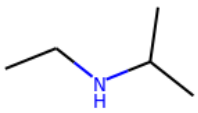
0.01223



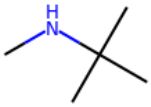
0.029804



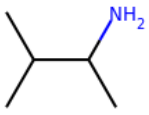
0.039926



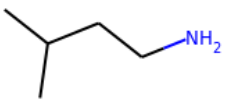
0.04073



0.04284



0.04435



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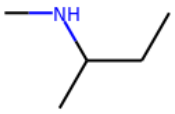
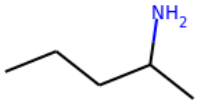


0.048238



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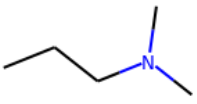


0.051006

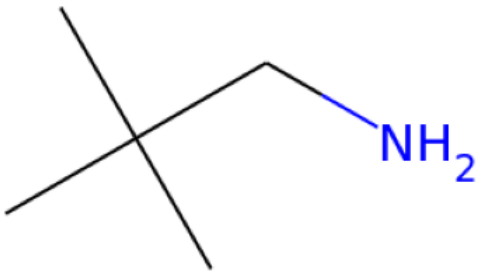
Top predicted substructures	prob		
[CX4H3]	1.0	[CHX4]([CH3X4])[CH3X4]	0.8869
[#6H3][#6][#6]	0.9997	[CX4H3][CX4H1]	0.867
[#7X3][#6H3]	0.9988	[CX4H3][NX3H1]	0.8502
[CX4H3][#6]	0.9955	[#6H1]	0.7825
[#6H3][#7]	0.9836	[#7X3][#6H2]	0.6849

best positives	prob	best negatives	prob

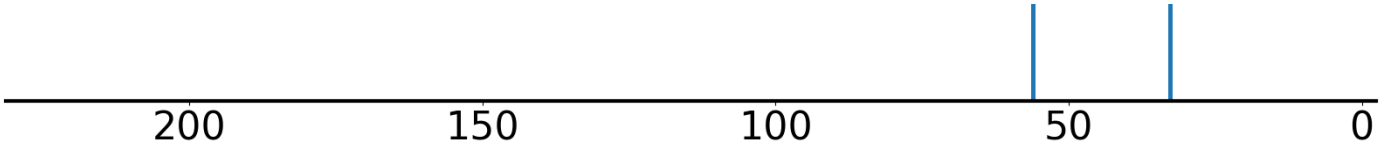
[CX4H3]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H3][#6][#6]	0.9997	C=CC=CC#C	0.0
[#7X3][#6H3]	0.9988	C=CCCC#C	0.0
[CX4H3][#6]	0.9955	CC=CC#CC	0.0
[#6H3][#7]	0.9836	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CHX4]([CH3X4])[CH3X4]	0.8869	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H3][CX4H1]	0.867	CCC=CC#C	0.0
[CX4H3][NX3H1]	0.8502	[#6X2][#6H1][#6X2]	0.0
[#6H1]	0.7825	CC=CCC#C	0.0
[#7X3][#6H2]	0.6849	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H3][#6H1][#6H1][#7]	0.4644	[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.133
[#7X3H2]	0.2384	[CX4H2]([NX3H1])[CX4H1]	0.3155
[CX4H1]([CX4H3])([CX4H3])[CX4H1]	0.2233	[#7][#6H2][#6H1]	0.3608
[CX4H2]([#6])[#6]	0.1995	[#6H1][#6H2]	0.5863
[#6H3][#6][#6][#6H3]	0.1972	[CHX4]([CH3X4])[CH2X4]	0.6006
[CX4H1]([CX4H3])([CX4H2])[CX4H2]	0.1588	[#6H3][#7][#6H2]	0.6081
[CX4H2][CX4H2]	0.1492	[#7][#6H2]	0.6609
[#6H1][#6H1]	0.1241	[#7X3H1]	0.6794
[#6H3][#6H0]	0.1006	[#7X3][#6H2]	0.6849
[#7H2][#6H1]	0.0946	[#6H1]	0.7825

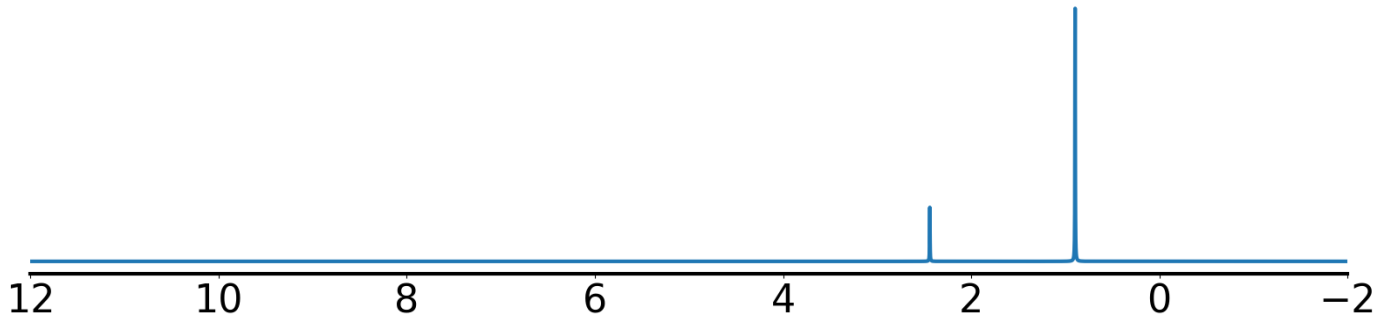
Example 211 true smiles: CC(C)(C)CN formula: C5H13N
Index of correct structure: 0 of 17
True structure loss: 0.011019
True structure:



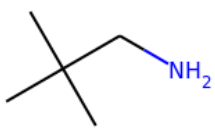
Experimental 13C NMR (solvent: CDCl3)



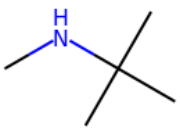
Experimental 1H NMR (solvent: CDCl3)



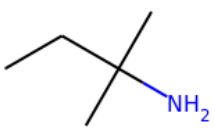
Top predicted structures (loss):



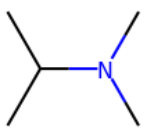
0.011019



0.02531



0.041095



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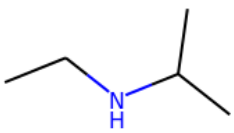
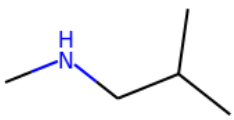
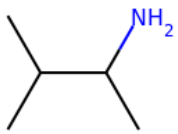


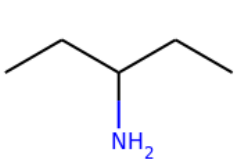
0.057282



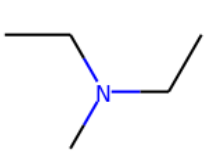
0.057635



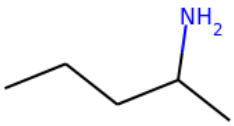
0.06509



0.065881



0.068679



0.071354

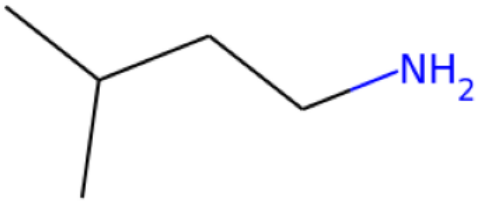
Top predicted substructures	prob		
[CX4H3]	0.9997	[CX4H3][CX4H0]	0.9741
[#6H3][#6][#6]	0.9991	[#6H3][#6H0]	0.9204
[CX4]([CX4H3])([CX4H3])[CX4H3]	0.9984	[#7X3H2]	0.6844
[CX4H3][CX4H0][CX4H3]	0.996	[#6H1]	0.5967
[CX4H3][#6]	0.9903	[#7X3][#6H2]	0.589

best positives	prob	best negatives	prob

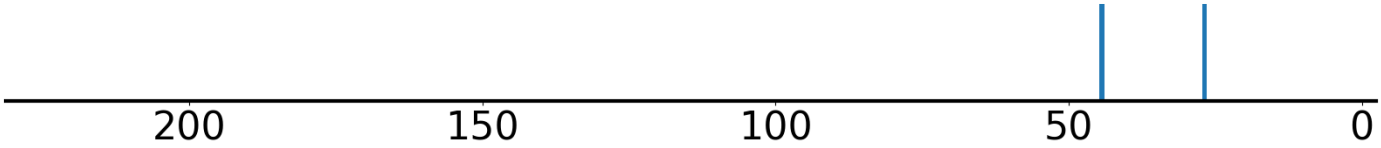
[CX4H3]	0.9997	CCC#CC#C	0.0
[#6H3][#6][#6]	0.9991	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4]([CX4H3])([CX4H3])[CX4H3]	0.9984	C=CCCC#C	0.0
[CX4H3][CX4H0][CX4H3]	0.996	CCC=CC#C	0.0
[CX4H3][#6]	0.9903	CC=CC#CC	0.0
[CX4H3][CX4H0]	0.9741	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#6H3][#6H0]	0.9204	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3H2]	0.6844	CC=CCC#C	0.0
[#7X3][#6H2]	0.589	C=CC=CC#C	0.0
[#7][#6H2]	0.5401	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.5967	[#7H2][#6H2]	0.1188
[#7X3H1]	0.4838	[CX4H2]([NX3H2])[CX4H0]	0.1987
[#7H2][#6H1]	0.3169	[#7][#6H2]	0.5401
[#6H3][#7]	0.2847	[#7X3][#6H2]	0.589
[#7][#6H2][#6H1]	0.2728	[#7X3H2]	0.6844
[#6H1][#6H2]	0.2358	[#6H3][#6H0]	0.9204
[#7X3][#6H3]	0.1789	[CX4H3][CX4H0]	0.9741
[#6H3][#6H0][#6H1][#7]	0.1607	[CX4H3][#6]	0.9903
[#6H2r3]	0.1085	[CX4H3][CX4H0][CX4H3]	0.996
[#6H2][#7][#6H2]	0.0996	[CX4]([CX4H3])([CX4H3])[CX4H3]	0.9984

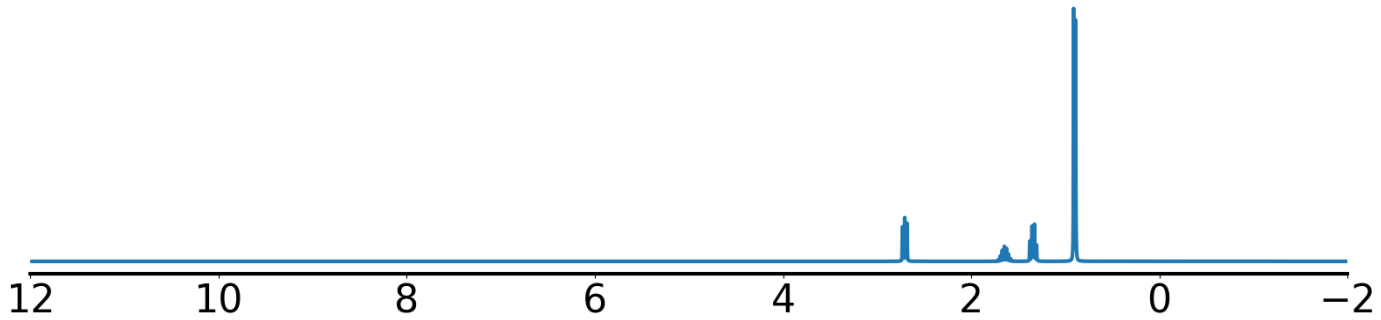
Example 212 true smiles: CC(C)CCN formula: C5H13N
Index of correct structure: 0 of 17
True structure loss: 0.014666
True structure:



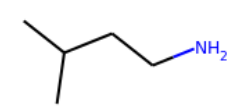
Experimental 13C NMR (solvent: CDCl3)



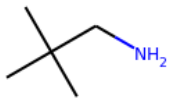
Experimental 1H NMR (solvent: CDCl3)



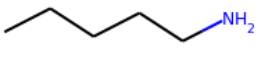
Top predicted structures (loss):



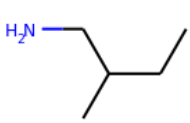
0.014666



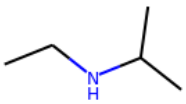
0.027713



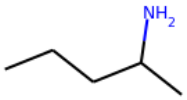
0.029321



0.032585



0.039837



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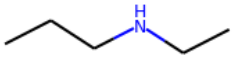
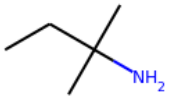
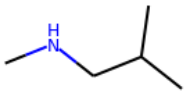


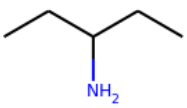
0.050835



0.052677



0.052687



0.056678

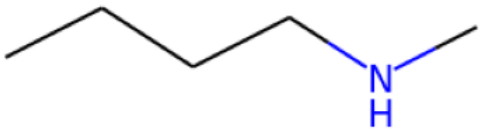
Top predicted substructures	prob		
[#6H3][#6][#6]	0.9996	[#7][#6H2]	0.9699
[CX4H3]	0.9978	[#7X3H2]	0.9186
[#7X3][#6H2]	0.9903	[CX4H2]([NX3H2])[CX4H2]	0.8439
[CX4H3][#6]	0.9893	[CX4H2]([#6])[#6]	0.8272
[#7H2][#6H2]	0.9732	[#7][#6H2][#6H2]	0.7821

best positives	prob	best negatives	prob

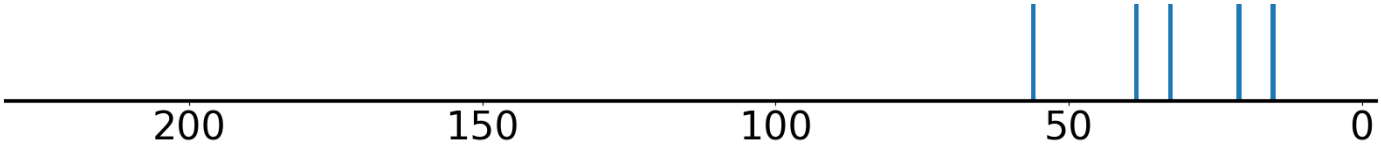
[#6H3][#6][#6]	0.9996	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	0.9978	C=CC=CC#C	0.0
[#7X3][#6H2]	0.9903	CC=CCC#C	0.0
[CX4H3][#6]	0.9893	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7H2][#6H2]	0.9732	CCC#CC#C	0.0
[#7][#6H2]	0.9699	C=CCCC#C	0.0
[#7X3H2]	0.9186	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2]([NX3H2])[CX4H2]	0.8439	CCC=CC#C	0.0
[CX4H2]([#6])[#6]	0.8272	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7][#6H2][#6H2]	0.7821	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7][#6H2][#6H1]	0.6092	[CX4H2]([CX4H2])[CX4H1]	0.0919
[#6H3][#6H0]	0.4801	[#7][#6H2][#6H2][#6H1]	0.2041
[#6H3][#6H0]([#6H2])[#6H2]	0.4039	[CX4H2][CX4H2]	0.4587
[CX4H3][CX4H0]	0.3601	[#6H1][#6H2]	0.541
[CX4H2]([NX3H2])[CX4H0]	0.3055	[#6H1]	0.59
[#6H1]([#6H2])[#6H2]	0.2877	[CX4H3][CX4H1]	0.6024
[CX4H2]([CX4H2])[CX4H2]	0.2648	[CHX4]([CH3X4])[CH2X4]	0.6604
[CX4H2]([NX3H2])[CX4H1]	0.2582	[CHX4]([CH3X4])[CH3X4]	0.7426
[#7X3H1]	0.1703	[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.7755
[#6H3][#6][#6][#6H3]	0.1669	[#7][#6H2][#6H2]	0.7821

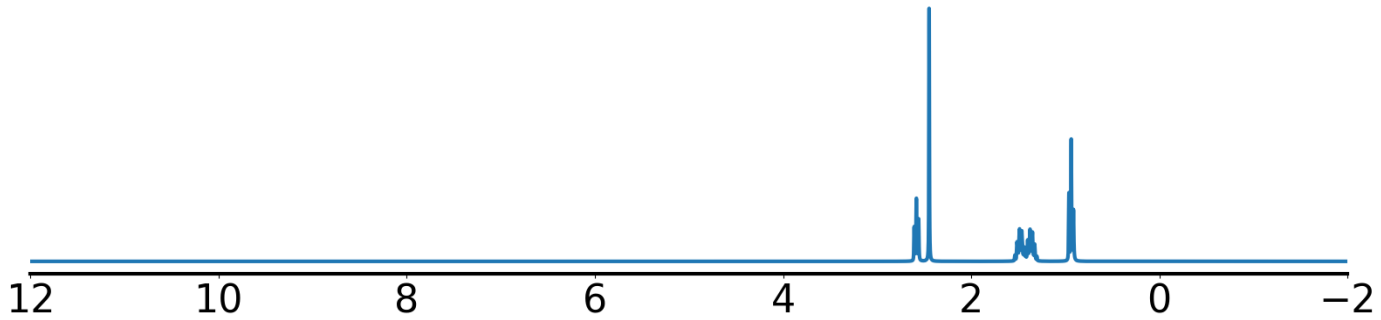
Example 213 true smiles: CCCCNC formula: C5H13N
Index of correct structure: 0 of 17
True structure loss: 0.016642
True structure:



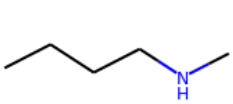
Experimental 13C NMR (solvent: CDCl3)



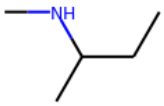
Experimental 1H NMR (solvent: CDCl3)



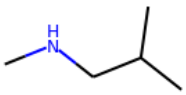
Top predicted structures (loss):



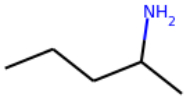
0.016642



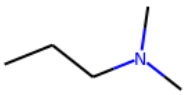
0.032647



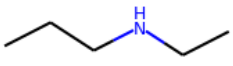
0.033403



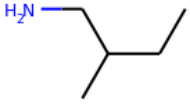
0.034261



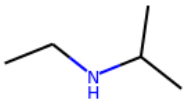
0.038543



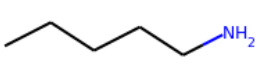
0.039711



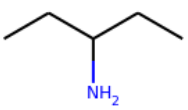
0.040719



0.042379



0.044044



0.044162

Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H2]([#6])[#6]	0.9874
[#6H3][#6][#6]	0.9994	[#6H3][#7]	0.9791
[CX4H3][#6]	0.9993	[CX4H3][NX3H1]	0.8863
[#7X3][#6H3]	0.9955	[#6H1]	0.8169
[CX4H3][CX4H2]	0.9908	[#7][#6H2]	0.796

best positives	prob	best negatives	prob

[CX4H3]	1.0	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9994	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][#6]	0.9993	CCC=CC#C	0.0
[#7X3][#6H3]	0.9955	C=CCCC#C	0.0
[CX4H3][CX4H2]	0.9908	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9874	CC=CC#CC	0.0
[#6H3][#7]	0.9791	CCC#CC#C	0.0
[CX4H3][NX3H1]	0.8863	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#7][#6H2]	0.796	[CX2H0](#[CX2H1])[CX3H1]	0.0
[#7X3H1]	0.7637	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.8169	[#7][#6H2][#6H2]	0.1223
[#6H1][#6H2]	0.6088	[CX4H2]([NX3H1])[CX4H2]	0.1841
[CX4H3][CX4H1]	0.5615	[CX4H2]([CX4H2])[CX4H2]	0.353
[CHX4]([CH3X4])[CH2X4]	0.5281	[CX4H2][CX4H2]	0.5532
[CX4H2]([NX3H1])[CX4H1]	0.4053	[#6H3][#7][#6H2]	0.6932
[CX4H2]([CX4H3])[CX4H1]	0.36	[#7X3][#6H2]	0.7106
[#6H3][#6H1][#6H1][#7]	0.3215	[CX4H2]([CX4H3])[CX4H2]	0.7297
[#7][#6H2][#6H1]	0.2725	[#7X3H1]	0.7637
CCCCCC	0.1812	[#7][#6H2]	0.796
[#7X3H2]	0.1655	[CX4H3][NX3H1]	0.8863
