Detailed test 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 test 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.

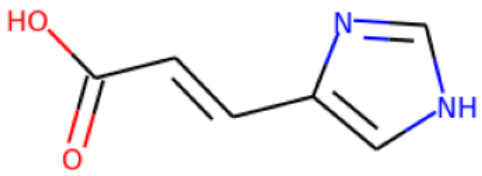
The true structure is shown next along with the experimental ^{13}C and ^{1}H NMR spectra. The solvent in which the NMR spectra was collected in is noted in parentheses when available.

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.

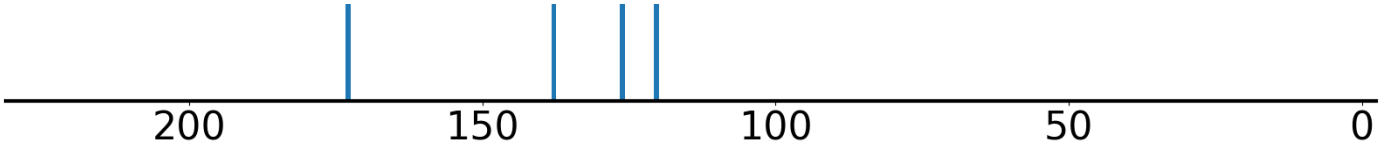
For each molecule, additional details for the substructure predictions are shown on the following page. First, the top 10 highest probability substructures predicted for by our ML model are shown as SMARTS strings alongside their respective predicted probabilities. Next, the 10 highest probability true 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 [129…

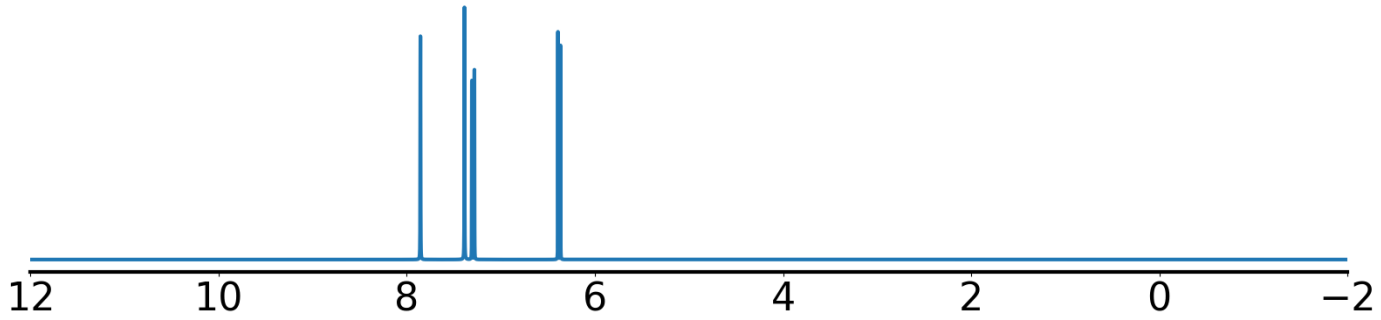
Example 0 true smiles: O=C(O)C=Cc1c[nH]cn1 formula: C6H6N2O2
Index of correct structure: -1 of 319796
True structure loss: 0.084946
True structure:



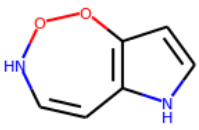
Experimental 13C NMR (solvent: DMSO)



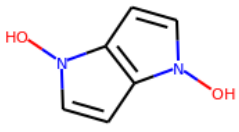
Experimental 1H NMR (solvent: D2O)



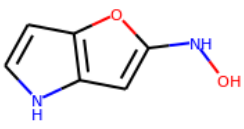
Top predicted structures (loss):



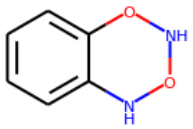
0.02923



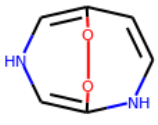
0.031375



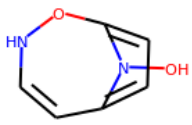
0.032855



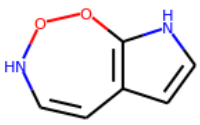
0.034147



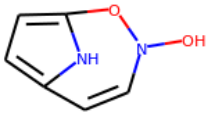
0.034643



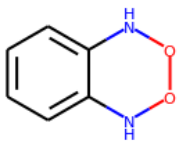
0.034753



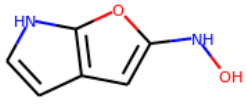
0.035312



0.035873



0.036152



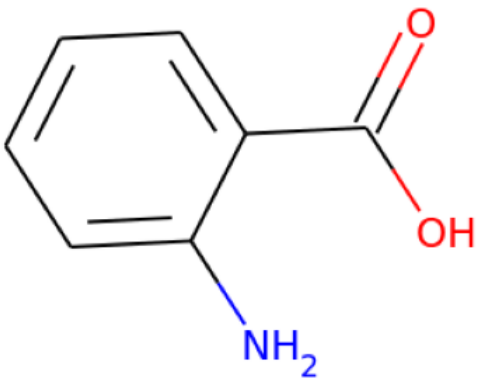
0.036976

Top predicted substructures	prob		
[#6H1]	0.9994	O=[#6][#6][#6X3]	0.8946
[#6X3][#6X3]	0.9945	[cH][cH]	0.7357
[#6X3H1][#6X3H0]	0.9782	[#7][#6X3H0][#6X3H1]	0.7178
[cH]	0.9777	[#6X3][#6X3][#6X3][#6X3]	0.7158
[#7][#6][#6X3]	0.9358	[#7][#6][#6][#6X3]	0.7103

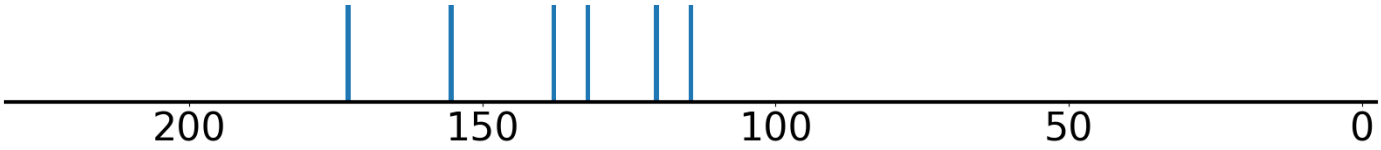
best positives	prob	best negatives	prob
[#6H1]	0.9994	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[#6X3][#6X3]	0.9945	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9782	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9777	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6X3]	0.9358	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[#7][#6X3H0][#6X3H1]	0.7178	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#7][#6][#6][#6X3]	0.7103	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX3H1]	0.0
[#6X3][#7][#6X3]	0.7075	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX3H1]	0.0
[#7][#6H0][#6H1]	0.6872	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[OX2H1]	0.5786	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6][#6X3]	0.8946	[#6X3][#6X3]=[#6X3][#6X3]	0.0091
[cH][cH]	0.7357	[#7][#6][#6]=[#6X3]	0.0166
[#6X3][#6X3][#6X3][#6X3]	0.7158	[CX3H1](=[CX3H1])[cX3H0]	0.0167
[#8][#6][#6][#6X3]	0.5835	[CX3H1](=[CX3H1])[CX3H0]	0.0196
[cX3H1]([cX3H1])[cX3H0]	0.5425	[#6X3H1]=[#6X3H1][#6X3H0][#6X3H1]	0.0201
[#6H1][#6H1]	0.5238	[#6X3][#6X3][#6X3]=[#6X3]	0.0234
[#7][#6][#6][#6][#7]	0.3947	[CHX3](=C)C	0.0257
[#7X3H0]	0.3928	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.0412
[#6X3H2]	0.3403	[CHX3]=[CHX3]	0.0521
[#7][#7]	0.2663	[#6]1[#6][#7][#6][#7]1	0.0653

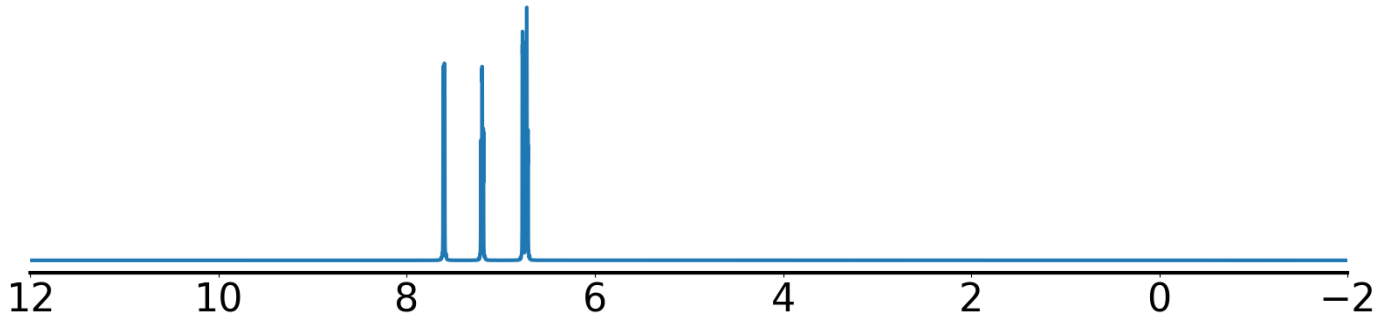
Example 1 true smiles: Nc1ccccc1C(=O)O formula: C7H7NO2
Index of correct structure: 0 of 141060
True structure loss: 0.020632
True structure:



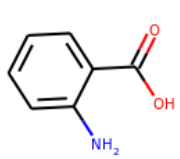
Experimental 13C NMR (solvent: DMSO-d6)



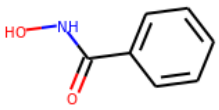
Experimental 1H NMR (solvent: MeOD)



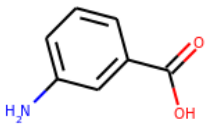
Top predicted structures (loss):



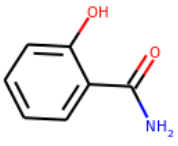
0.020632



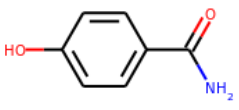
0.021651



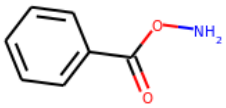
0.022241



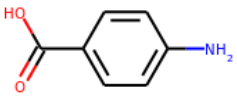
0.022304



0.023161

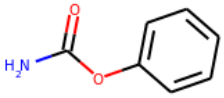


0.023205

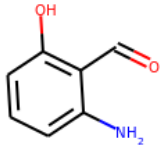


0.02394

0.024779



0.025236



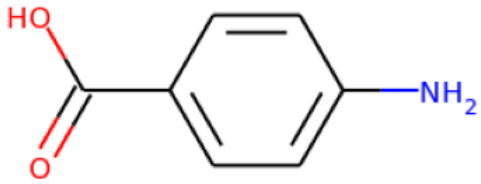
0.025271

Top predicted substructures	prob		
[#6H1]	0.9998	[cH]	0.9823
[#6X3][#6X3]	0.9996	[cX3H1]([cX3H1])[cX3H0]	0.9653
[cH][cH]	0.9919	[cX3H1]([cX3H1])[cX3H1]	0.9234
[#6X3H1][#6X3H0]	0.9886	O=[#6][#6][#6X3]	0.9193
[#6X3][#6X3][#6X3][#6X3]	0.984	[#6H1][#6H1]	0.9028

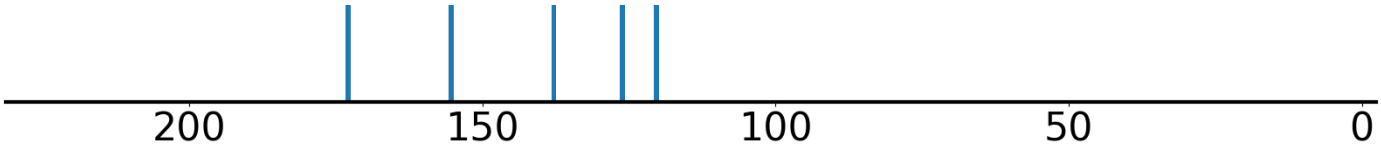
best positives	prob	best negatives	prob
[#6H1]	0.9998	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9996	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cH][cH]	0.9919	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#6X3H1][#6X3H0]	0.9886	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.984	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.9823	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9653	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9234	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
O=[#6][#6][#6X3]	0.9193	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#6H1][#6H1]	0.9028	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.7522	[CX3](=[OX1])O	0.2177
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.658	[CX3](=O)[OX2H1]	0.3572
[#6]1[#6][#6][#6][#6][#7]1	0.5493	[#7H2][#6H0]	0.3611
[#6X3][#7][#6X3]	0.5284	[#7X3H2]	0.4027
[cH]cO	0.4873	[#6]1[#6][#6][#6][#6][#6]1	0.4328
O=[cX3]	0.4022	[#8]=[#6][#8]	0.4892
[OX2H][cX3]:[c]	0.3668	[#7][#6][#6X3]	0.6413
[#8]=[#6H0][#6H1]	0.3135	[#7][#6X3H0][#6X3H1]	0.6701
[OX1H0]=[cX3H0][cX3H1]	0.3133	[#7][#6H0][#6H1]	0.7249
[#8]=[#6][#6H1][#6H1]	0.2988	[#7][#6][#6][#6X3]	0.7321

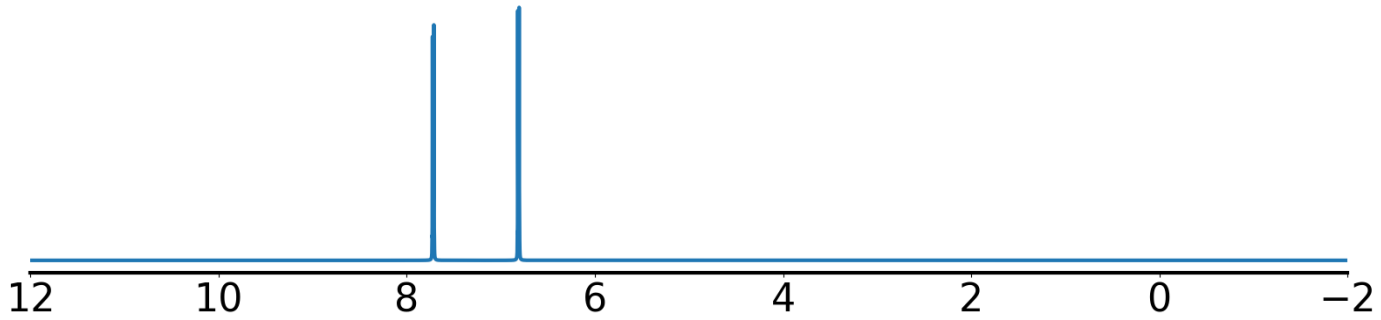
Example 2 true smiles: Nc1ccc(C(=O)O)cc1 formula: C7H7NO2
Index of correct structure: 5 of 141060
True structure loss: 0.024241
True structure:



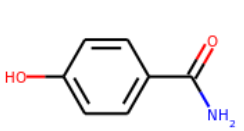
Experimental 13C NMR (solvent: D2O)



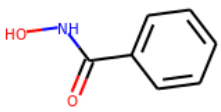
Experimental 1H NMR (solvent: d2o)



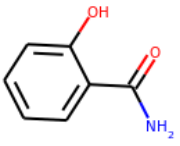
Top predicted structures (loss):



0.0215

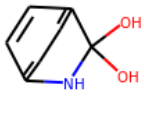


0.022439

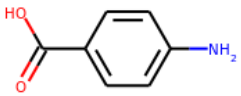


0.022546

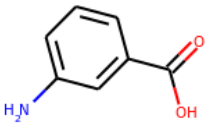
0.022904



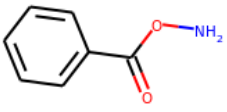
0.023697



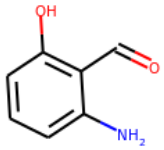
0.024241



0.024987



0.025089



0.025422

0.025852

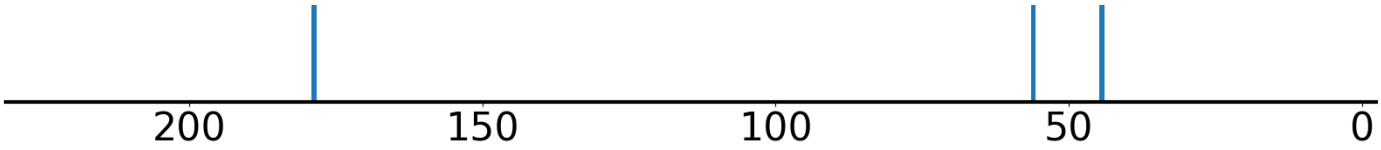
Top predicted substructures	prob		
[#6X3][#6X3]	0.9994	[cH]	0.9609
[#6H1]	0.9982	[cX3H1]([cX3H1])[cX3H0]	0.9395
[#6X3H1][#6X3H0]	0.9873	[#6H1][#6H1]	0.8885
[#6X3][#6X3][#6X3][#6X3]	0.9721	O=[#6][#6][#6X3]	0.8463
[cH][cH]	0.9673	[#7][#6][#6X3]	0.8193

best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9994	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H1]	0.9982	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#6X3H1][#6X3H0]	0.9873	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9721	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[cH][cH]	0.9673	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cH]	0.9609	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9395	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[#6H1][#6H1]	0.8885	[OX2H0][CX4H2][CX4H1]([CX4H2])[CX4H1]	0.0
O=[#6][#6][#6X3]	0.8463	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6][#6X3]	0.8193	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0

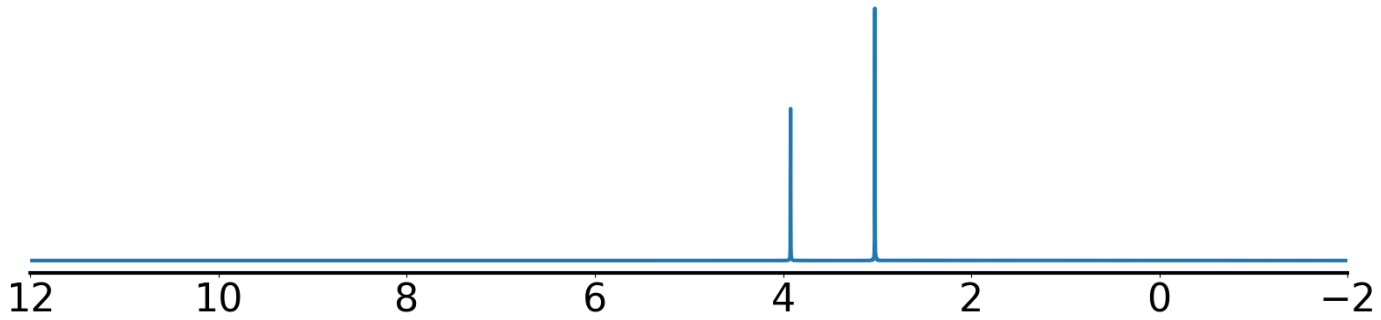
worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.7249	[CX3](=O)[OX2H1]	0.23
[#8][#6H0][#6H1]	0.6587	[CX3](=[OX1])O	0.2396
[cH]cO	0.6406	[#7X3H2]	0.2599
[#6]1[#6][#6][#6][#6][#7]1	0.6403	[cX3H0][cX3H1][cX3H1][cX3H0]	0.2996
[#6X3][#7][#6X3]	0.5149	[#6]1[#6][#6][#6][#6][#6]1	0.3605
[OX2H][cX3]:[c]	0.3907	[#7H2][#6H0]	0.395
O=[cX3]	0.3635	[#8]=[#6][#8]	0.4668
[cX3H1]([nX2H0])[cX3H1]	0.34	[#7][#6H0][#6H1]	0.5704
[#8]=[#6H0][#6H1]	0.3119	[#7][#6X3H0][#6X3H1]	0.594
[OX1H0]=[cX3H0][cX3H1]	0.2823	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6314

Example 3 true smiles: CN(CC(=O)O)C(=N)N formula: C4H9N3O2
Index of correct structure: -1 of 108327
True structure loss: 0.058628
True structure:

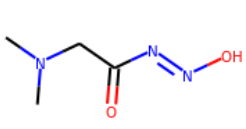
Experimental 13C NMR (solvent: D2O)



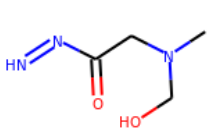
Experimental 1H NMR (solvent: D2O)



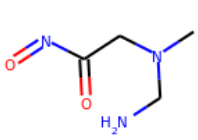
Top predicted structures (loss):



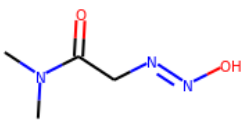
0.026265



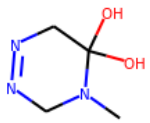
0.028464



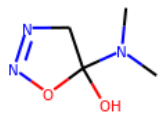
0.028839



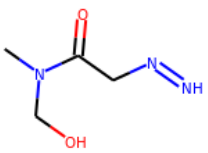
0.029077



0.029137



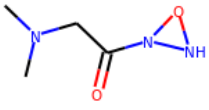
0.029213



0.029331

0.029553

0.030365



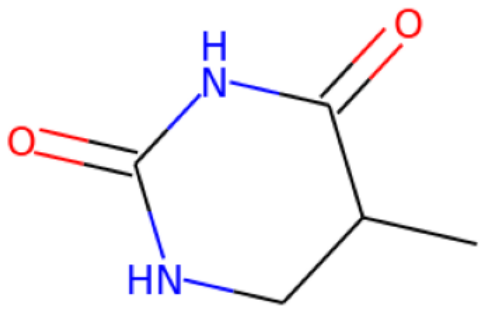
0.030413

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9128	[#7X3H2]	0.7896
[#7][#6][#6][#7]	0.8608	[#7X3][#6H3]	0.7794
[CX4H3]	0.838	[#7][#6][#6][#6][#7]	0.7379
[#7][#6][#6X3]	0.7978	[#6H3][#7]	0.674
[#7][#6H2]	0.7944	[#7X3][#6H2]	0.6623

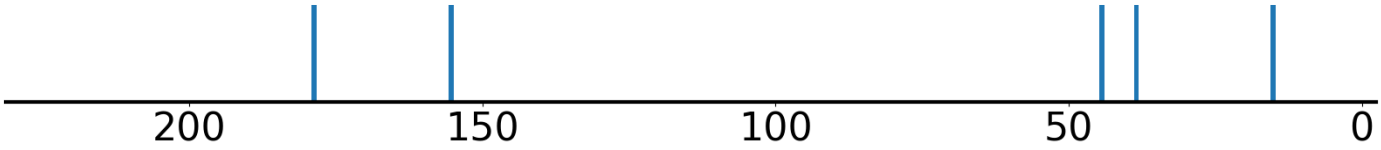
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9128	CC=CC#CC	0.0
[CX4H3]	0.838	C=CC=CC#C	0.0
[#7][#6][#6X3]	0.7978	CC=CCC#C	0.0
[#7][#6H2]	0.7944	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3H2]	0.7896	CCC=CC#C	0.0
[#7X3][#6H3]	0.7794	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#6H3][#7]	0.674	[CX3H0](=[CX3H1])([CX4H3])[CX3H1]	0.0
[#7X3][#6H2]	0.6623	CC#CCC=C	0.0
[CX4H3][NX3H0]	0.5483	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#6H3][#7][#6H2]	0.5226	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7][#6][#6][#7]	0.8608	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.015
[#7][#6][#6][#6][#7]	0.7379	[#7][#6]([#7])=[#7]	0.0251
[#7X3H1]	0.5663	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.0375
[#7H2][#6H1]	0.4283	[#7][#6]=[#7]	0.104
[#6H1]	0.3849	[#7H1]=[#6H0][#7X3][#6H3]	0.1049
[CX4H2]CC=O	0.3775	[#6]=[#7H]	0.1246
[#8]=[#6H0][#6H1]	0.3633	[CX4H2]([NX3H0])[CX3H0]	0.1364
O=[CX3][CX4H]	0.3399	[NH1]=[#6][#7]	0.1389
[#7][#6H0][#6H1]	0.3063	[#7][#6H0]=[#7]	0.1562
[#6]1[#6][#7][#6][#7]1	0.2866	[#8]=[#6][#8]	0.1903

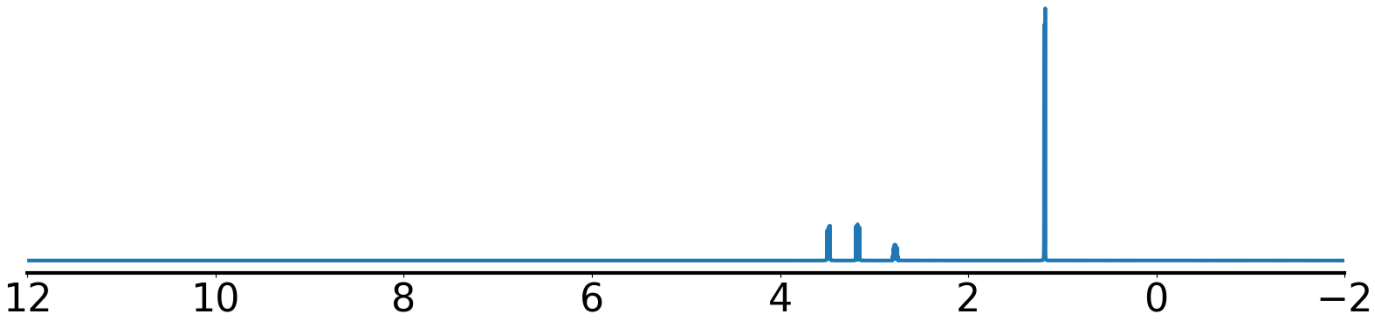
Example 4 true smiles: CC1CNC(=O)NC1=O formula: C5H8N2O2
Index of correct structure: 1 of 96528
True structure loss: 0.033156
True structure:



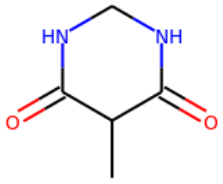
Experimental 13C NMR (solvent: DMSO)



Experimental 1H NMR (solvent: d2o)

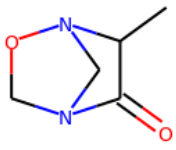


Top predicted structures (loss):

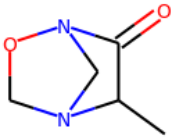


0.030971

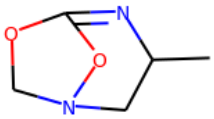
0.033156



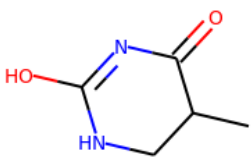
0.038271



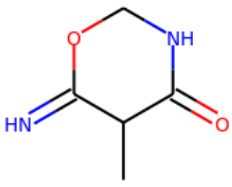
0.038271



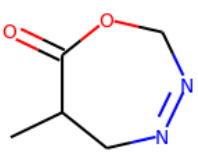
0.042304



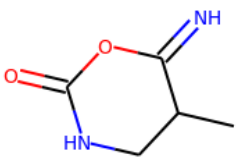
0.043594



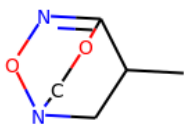
0.044369



0.046526



0.047441



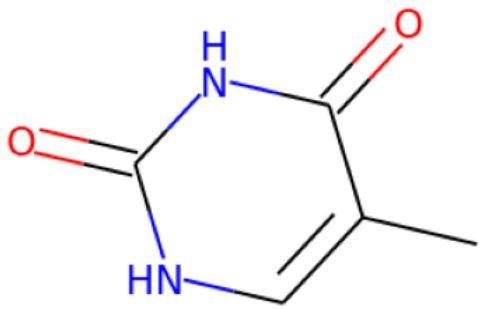
0.048062

Top predicted substructures	prob		
[CX4H3]	0.9992	[#6H3][#6][#6]	0.841
[CX4H3][#6]	0.9739	[#6H2][#7][#6X3]	0.8402
[CX3](=[OX1])C	0.9624	[#7][#6][#6][#6X3]	0.8164
[#7X3][#6H2]	0.9244	O=[CX3][CX4H]	0.787
[#7][#6H2]	0.9039	[#6H1]	0.7465

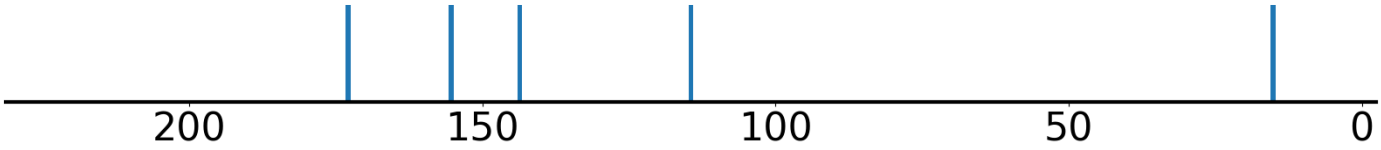
best positives	prob	best negatives	prob
[CX4H3]	0.9992	C=CC=CC#C	0.0
[CX4H3][#6]	0.9739	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9624	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7X3][#6H2]	0.9244	C=CCCC#C	0.0
[#7][#6H2]	0.9039	CC=CCC#C	0.0
[#6H3][#6][#6]	0.841	[#6]1[#6]=[#6][#6][#6]=[#6]1	0.0
[#6H2][#7][#6X3]	0.8402	CC=CC#CC	0.0
[#7][#6][#6][#6X3]	0.8164	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
O=[CX3][CX4H]	0.787	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#6H1]	0.7465	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0

worst negatives	prob	worst positives	prob
[#7][#6][#6X3]	0.5961	[CX4H2]([NX3H1])[CX4H1]	0.0431
[#7X3H0]	0.5931	[CX3H0](=[OX1H0])([NX3H1])[CX4H1]	0.0633
[CX3](=[OX1])O	0.4955	[NH1][#6][#7]	0.2195
[#8]=[#6][#8]	0.4362	[#7][#6H0][#7]	0.3114
O=[#6][#6][#6X3]	0.3658	[CX4H1]([CX4H3])([CX4H2])[CX3H0]	0.3541
[OX2H1]	0.3606	[OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]	0.3611
[CX4H2][CX3]=O	0.3383	[#7][#6][#6][#6][#7]	0.4043
[#7][#6][#6H3]	0.3324	[#7][#6][#7]	0.4481
[#6H3][#6H1r5]	0.3066	[#6H1][#6H2]	0.4902
[#8][#6H0][#6H1]	0.2849	[#7X3H1]	0.4976

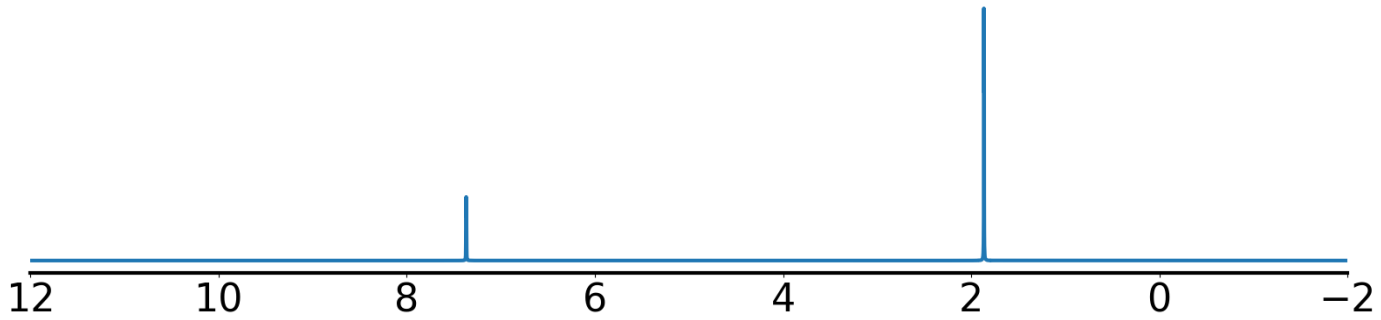
Example 5 true smiles: Cc1c[nH]c(=O)[nH]c1=O formula: C5H6N2O2
Index of correct structure: 3 of 62260
True structure loss: 0.033961
True structure:



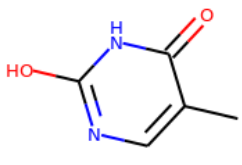
Experimental 13C NMR (solvent: D2O)



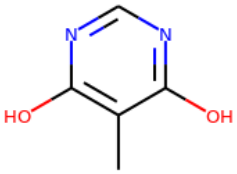
Experimental 1H NMR (solvent: D2O)



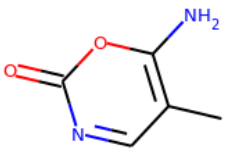
Top predicted structures (loss):



0.032831

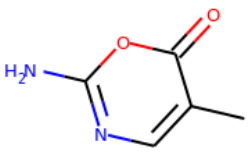


0.033598

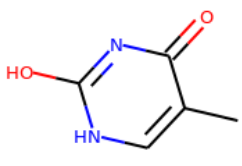


0.033841

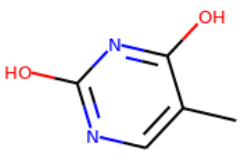
0.033961



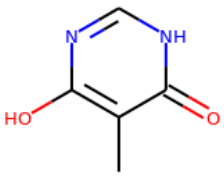
0.034243



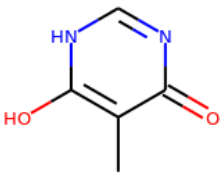
0.034362



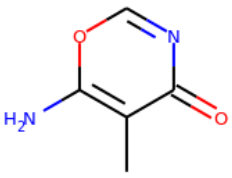
0.034596



0.035597



0.035597



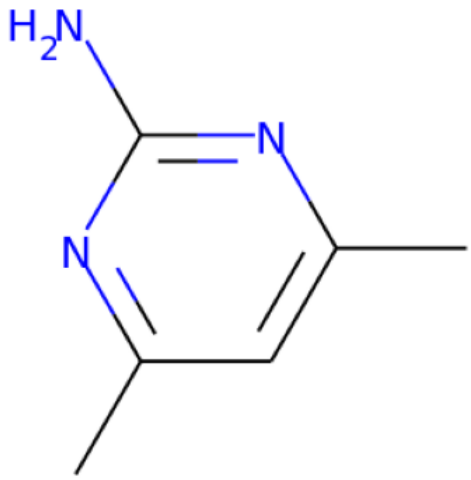
0.036021

Top predicted substructures	prob		
[CX4H3]	0.9999	[#6H3][#6][#6]	0.9771
[CX4H3][#6]	0.9993	[#6H3][#6][#6X3]	0.9423
[#6H3][#6H0]	0.9974	[#7][#6][#6X3]	0.9153
[#6X3][#6X3]	0.9956	[cH]	0.8754
[#6H1]	0.978	[CX4H3][cX3H0]	0.7591

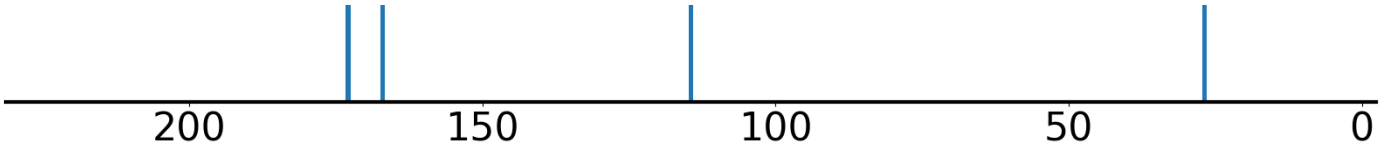
best positives	prob	best negatives	prob
[CX4H3]	0.9999	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[CX4H3][#6]	0.9993	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H3][#6H0]	0.9974	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6X3][#6X3]	0.9956	[CX4H1]1[CX4H2][CX4H1][CX4H2]1	0.0
[#6H1]	0.978	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6H3][#6][#6]	0.9771	[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	0.0
[#6H3][#6][#6X3]	0.9423	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6][#6X3]	0.9153	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[cH]	0.8754	[CX4H2]1[CX4H0][CX4H2][CX4H1]1	0.0
[CX4H3][cX3H0]	0.7591	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[CX3H0](=[CX3H1])([CX4H3])[CX3H0]	0.6398	[cX3H1]([nX3H1])[cX3H0]	0.0863
[CX4H3][CX3]	0.5363	[#7][#6H0][#7]	0.1327
[CX4H3][CX3H0]	0.5285	[#7H][#6X3H1]	0.174
[#8][#6][#6][#6X3]	0.5043	[#7][#6][#6][#6][#7]	0.21
[#7X3H2]	0.4588	[#6H3][#6H0][#6H1][#7]	0.2459
[#8]=[#6][#8]	0.4357	[#7][#6][#7]	0.3164
[OX1H0]=[CX3H0][CX3H0][CX4H3]	0.4099	[#7X3H1]	0.3202
[OX2H1]	0.4051	[#6X3][#7X3][#6X3]	0.3724
[#6H3][#6]=[#6X3]	0.364	[#6X3][#7][#6X3]	0.4391
[#7][#6H0][#6H1]	0.3537	O=[cX3]	0.4949

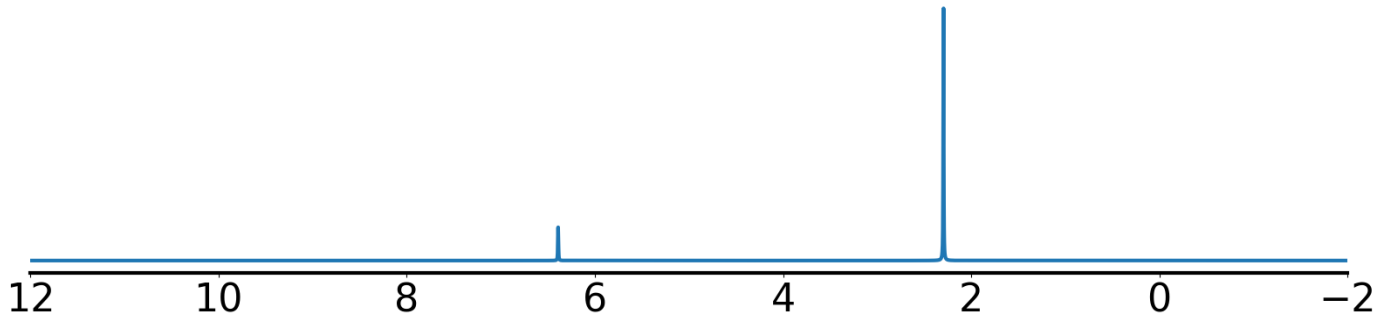
Example 6 true smiles: Cc1cc(C)nc(N)n1 formula: C6H9N3
Index of correct structure: 1 of 51623
True structure loss: 0.035975
True structure:



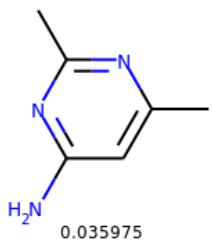
Experimental 13C NMR (solvent: CDCl3)

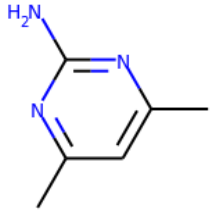


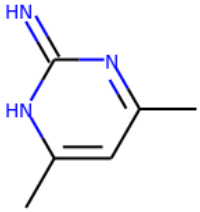
Experimental 1H NMR (solvent: CDCl3)

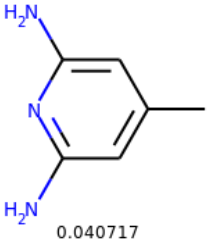


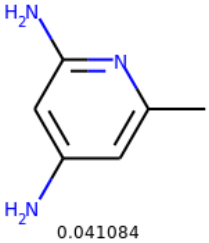
Top predicted structures (loss):

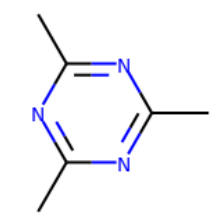

0.035975

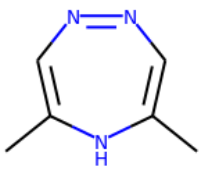

0.035975

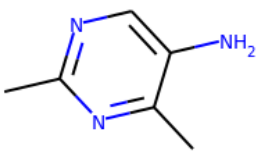

0.036304

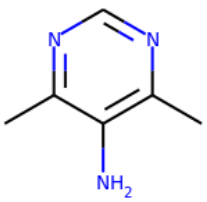

0.040717

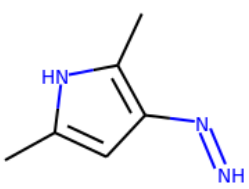

0.041084


0.04164


0.042354


0.043091


0.043377

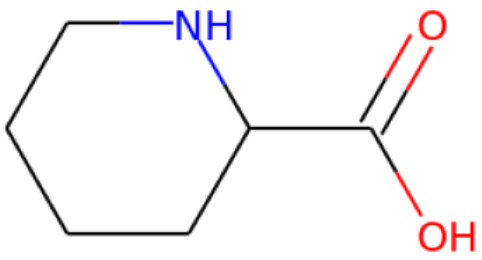

0.04373

Top predicted substructures	prob		
[#6H3][#6H0]	0.9833	[#7][#6][#6H3]	0.8367
[CX4H3]	0.9427	[#6X3H1][#6X3H0]	0.8047
[#7][#6][#6X3]	0.9397	[CX4H3][#6]	0.788
[#6X3][#6X3]	0.9394	[#7][#6H0]=[#7]	0.7858
[#6H1]	0.8559	[#6]=[#7H]	0.72

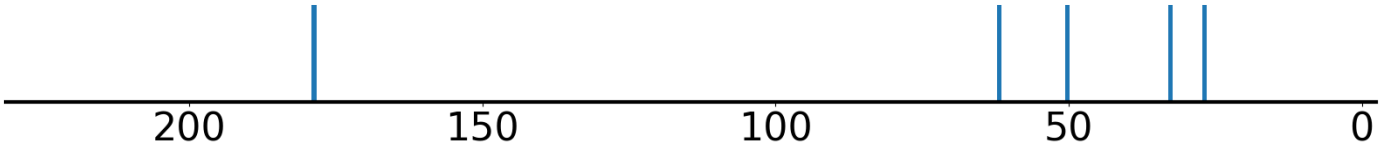
best positives	prob	best negatives	prob
[#6H3][#6H0]	0.9833	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3]	0.9427	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[#7][#6][#6X3]	0.9397	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3][#6X3]	0.9394	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6H1]	0.8559	[OX2H0r5][CX4H2][OX2H0r5]	0.0
[#7][#6][#6H3]	0.8367	[OX2H1][CX4H1][CX4H1]([CX4H2])[CX4H2]	0.0
[#6X3H1][#6X3H0]	0.8047	[OX2H0][CX3H1]=[#6X3H0][#8X2H0]	0.0
[CX4H3][#6]	0.788	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#7][#6X3H0][#6X3H1]	0.6724	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#7X3H2]	0.665	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7][#6H0]=[#7]	0.7858	[#6H3][#6][#6X3]	0.1936
[#6]=[#7H]	0.72	[cX3H1]([cX3H0])[cX3H0]	0.1954
[NH1]=[#6][#7]	0.6746	[#7][#6][#6][#6][#7]	0.254
[CX4H3][CX3H0]	0.6368	[#6X3][#6][#6][#6H3]	0.2772
[#7][#6]=[#7]	0.6093	[#6H3][#6H0][#7H0][#6H0]	0.2874
[#7X3H1]	0.5878	[CX4H3][cX3H0]	0.3318
[CHX3](=C)C	0.48	[#6X3][#7][#6X3]	0.3394
[#6X3H1]=[#6X3H0]	0.4224	[#7][#6][#7]	0.3575
[cH][cH]	0.3864	[#6H3][#6][#6]	0.3949
[#6X3][#7X3][#6X3]	0.3835	[#7][#6H0][#7]	0.3971

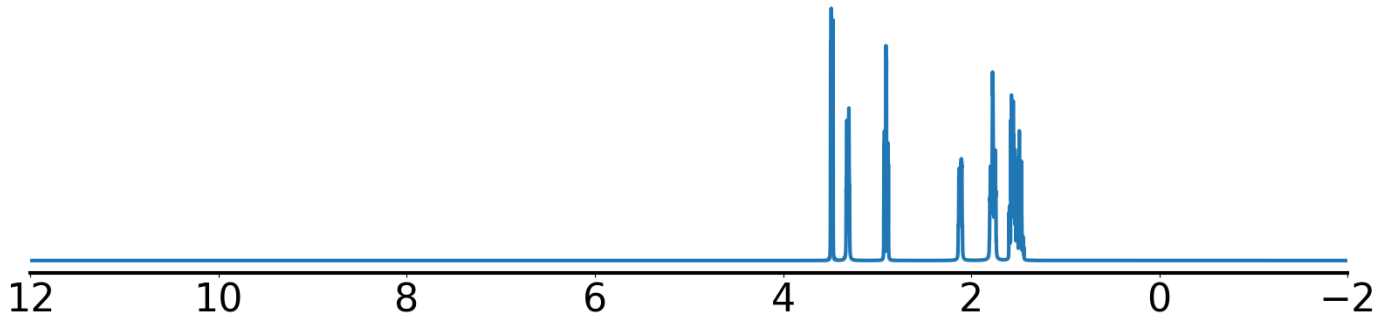
Example 7 true smiles: O=C(O)C1CCCCN1 formula: C6H11NO2
Index of correct structure: 0 of 35172
True structure loss: 0.028661
True structure:



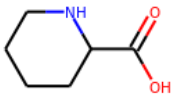
Experimental 13C NMR (solvent: D2O)



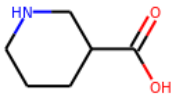
Experimental 1H NMR (solvent: D2O)



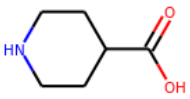
Top predicted structures (loss):



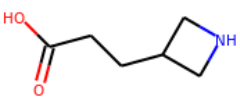
0.028661



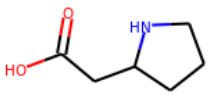
0.034049



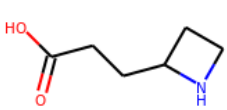
0.035513



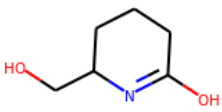
0.043542



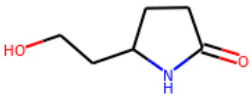
0.04653



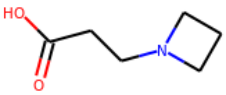
0.049435



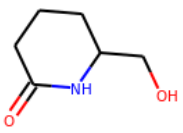
0.049899



0.050267



0.050356



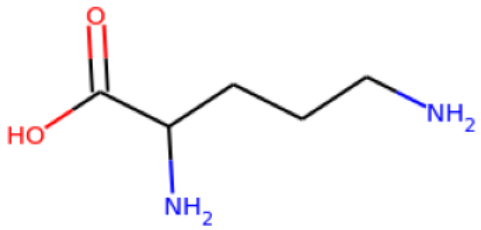
0.050651

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9998	OCC[CH2]	0.9393
[CX4H2]([CX4H2])[CX4H1]	0.9892	[#7][#6H2]	0.9392
[CX3](=[OX1])C	0.9835	[#6H1]	0.9286
[CX4H2][CX4H2]	0.9721	[OX2H1]	0.909
[#7X3][#6H2]	0.9464	[#6H1][#6H2]	0.8923

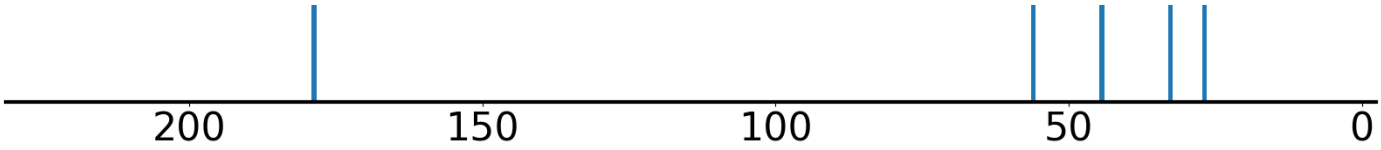
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9998	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([CX4H2])[CX4H1]	0.9892	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9835	CC#CCC=C	0.0
[CX4H2][CX4H2]	0.9721	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#7X3][#6H2]	0.9464	[CX4H2]([CX4H3])[CX2H0]	0.0
OCC[CH2]	0.9393	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7][#6H2]	0.9392	C=CCCC#C	0.0
[#6H1]	0.9286	CC=CCC#C	0.0
[OX2H1]	0.909	C=CC=CC#C	0.0
[#6H1][#6H2]	0.8923	[CX3H1](=[CX3H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7][#6H1][#6H2r5]	0.6369	[CX4H1]([NX3H1])([CX4H2])[CX3H0]	0.0878
[#8][#6][#6H2]	0.5651	[#7H1][#6X4H1][#6X3]	0.1329
[#6H1][#6H2][#6][#6][#7]	0.5252	[#7][#6][#6X3]	0.2719
[CX4H2][CX3]=O	0.5189	[#6]1[#6][#6][#6][#6][#7]1	0.3346
[#6]1[#6][#6][#6][#7]1	0.5154	[CX4H2][CX4H2][CX4H2][CX4H2]	0.3923
[#6H1]([#6H2])[#6H2]	0.4658	[#8][#6H0][#6H1]	0.4241
[#6H1r5][#7]	0.4086	CCCCCC	0.4379
[#7][#6H2][#6H1]	0.3915	[#7][#6H2][#6H2]	0.4389
O=[CX3H0][CX4H2][CX4H2]	0.364	[#7X3H1]	0.4434
[CX4H2]([CX4H2])[CX3H0]	0.3197	[CX3](=[OX1])O	0.5374

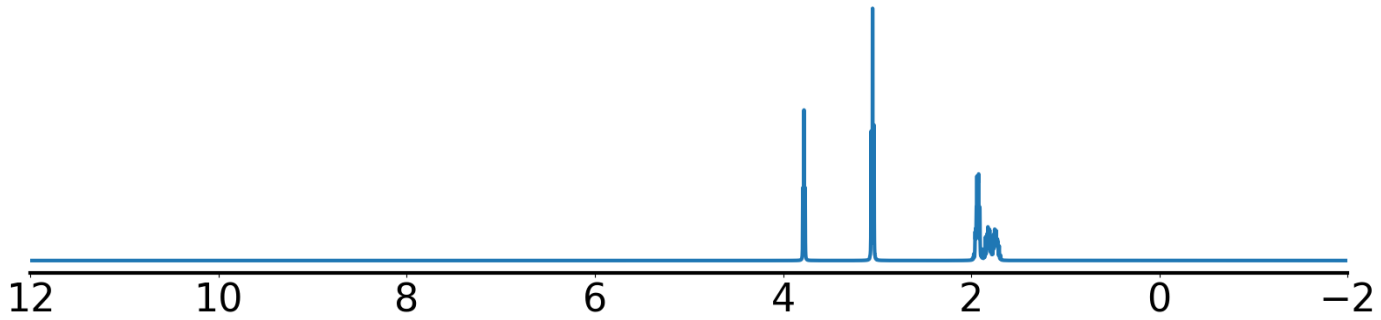
Example 8 true smiles: NCCCC(N)C(=O)O formula: C5H12N2O2
Index of correct structure: 0 of 32944
True structure loss: 0.02186
True structure:



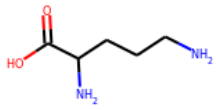
Experimental 13C NMR (solvent: D2O)



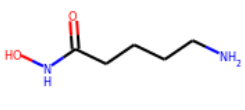
Experimental 1H NMR (solvent: D2O)



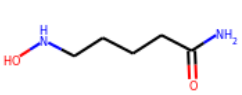
Top predicted structures (loss):



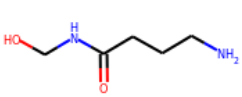
0.02186



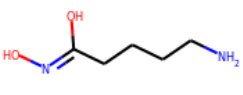
0.028496



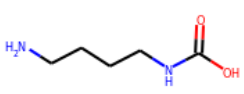
0.029016



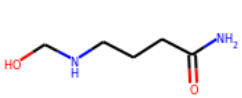
0.030358



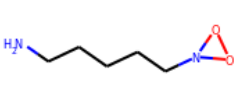
0.030825



0.031303

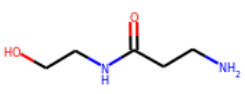


0.034377



0.03841

0.042354



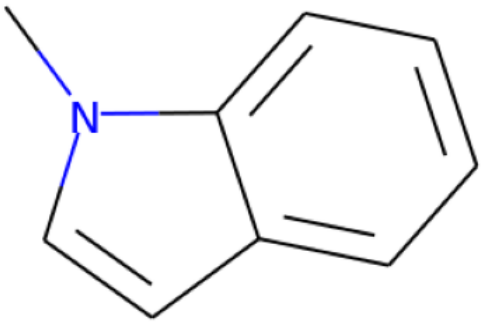
0.042625

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9999	[CX4H2][CX4H2]	0.9618
[#7X3H2]	0.9906	[#7][#6H2]	0.9149
[OX2H1]	0.9859	[CX4H2]CC=O	0.9079
[CX3](=[OX1])C	0.973	[CX4H2]([CX4H2])[CX4H2]	0.899
[#7][#6H2][#6H2]	0.9624	[#7X3][#6H2]	0.8755

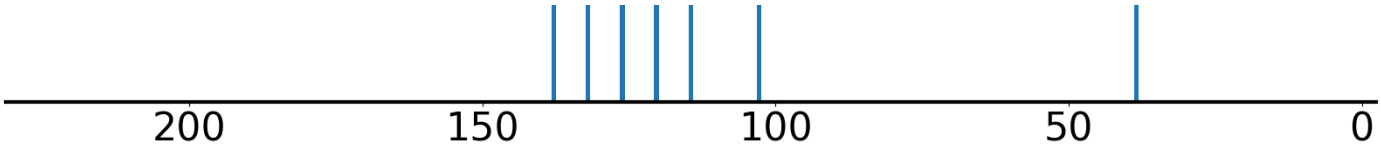
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3H2]	0.9906	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[OX2H1]	0.9859	CCC=CC#C	0.0
[CX3](=[OX1])C	0.973	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#7][#6H2][#6H2]	0.9624	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2][CX4H2]	0.9618	CC=CC#CC	0.0
[#7][#6H2]	0.9149	C=CCCC#C	0.0
[CX4H2]CC=O	0.9079	CCC#CC#C	0.0
[CX4H2]([CX4H2])[CX4H2]	0.899	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7X3][#6H2]	0.8755	CC=CCC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX3]=O	0.5232	[#8][#6H0][#6H1]	0.1534
O=[CX3H0][CX4H2][CX4H2]	0.4807	[#6H1][#6H2][#6][#6][#7]	0.2114
[CX4H2][CX4H2][CX4H2][CX4H2]	0.4418	[#6H1][#6H2]	0.2443
[#7X3H1]	0.4071	[#7][#6][#6][#6][#6][#7]	0.2867
[#8][#6][#6H2]	0.3773	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3746
[#7][#6][#6][#7]	0.3759	[#6H1]	0.3784
[CX4H2]([NX3H1])[CX4H2]	0.3642	[CX3](=[OX1])O	0.521
[#7H2][#6H0]	0.3526	[CX4H2]([CX4H2])[CX4H1]	0.6082
[#7][#6][#6][#6][#7]	0.2537	O=[CX3][CX4H]	0.6101
[#6H2][#7][#6X3]	0.2489	[#7H2][#6H1]	0.6526

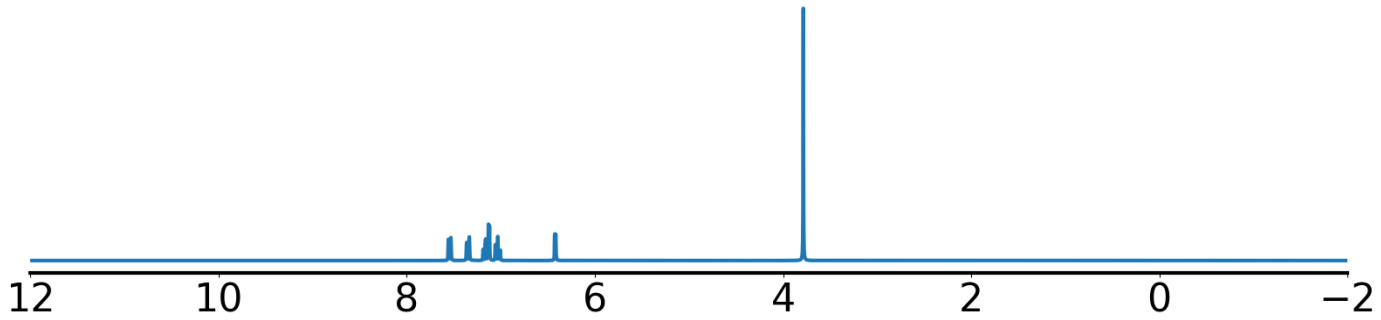
Example 9 true smiles: Cn1ccc2ccccc21 formula: C9H9N
Index of correct structure: 0 of 29511
True structure loss: 0.013237
True structure:



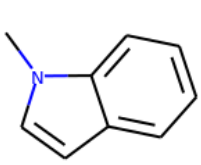
Experimental 13C NMR (solvent: CDCl3)



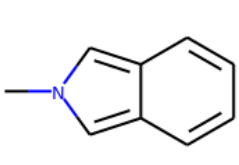
Experimental 1H NMR (solvent: CD3OD)



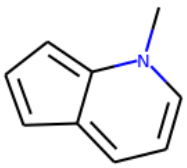
Top predicted structures (loss):



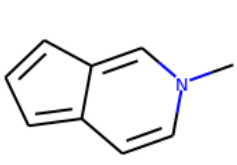
0.013237



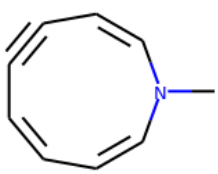
0.018262



0.026289

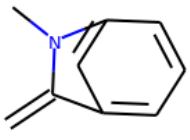


0.031304

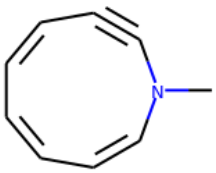


0.034869

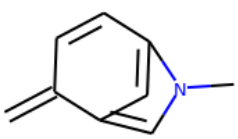
0.034901



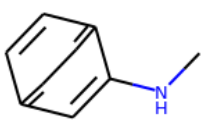
0.037159



0.039331



0.040262



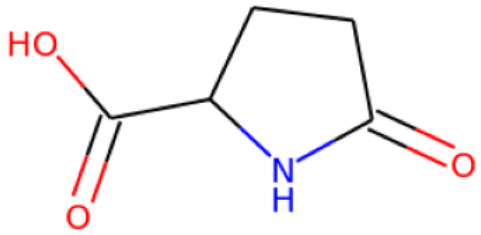
0.041778

Top predicted substructures	prob		
[#6H1]	0.9999	[cH][cH]	0.9938
[#6X3][#6X3][#6X3][#6X3]	0.9981	[#6X3H1][#6X3H0]	0.9883
[#7][#6][#6X3]	0.9977	[cX3H1]([cX3H1])[cX3H0]	0.9882
[#6X3][#6X3]	0.9952	[#7][#6][#6][#6X3]	0.9819
[cH]	0.9945	[#6H1][#6H1]	0.9583

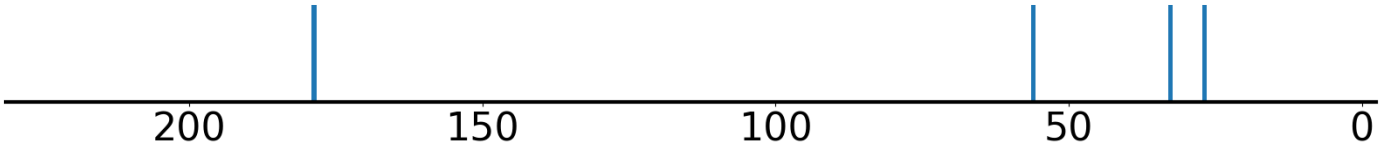
best positives	prob	best negatives	prob
[#6H1]	0.9999	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9981	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#7][#6][#6X3]	0.9977	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3]	0.9952	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9945	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9938	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#6X3H1][#6X3H0]	0.9883	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9882	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.9819	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[#6H1][#6H1]	0.9583	[OX2H1][CX4H0][CX4H1]([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6H2][#6X3]	0.7329	[#6]1[#6][#6][#6][#6][#6]1	0.2976
[#6H1][#7][#6H1]	0.5529	[cX3H1]([nX3H0])[cX3H1]	0.5026
[#7H][#6X3H1]	0.3855	[#7][#6X3H0][#6X3H1]	0.6196
[cX3H1]([nX3H1])[cX3H1]	0.3189	[CX4H3][nX3H0]	0.6924
[#7X3H1]	0.3102	[#6H3][#7]	0.7252
[#7][#6H2]	0.2576	[#6X3H1][#7X3H0]	0.7276
[#6]1[#6][#6][#6][#6][#7]1	0.2081	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.731
O=[#6][#6][#6X3]	0.1962	[CX4H3]	0.7366
[#6X3][#6H2][#7]	0.1776	[#7][#6H0][#6H1]	0.7521
[cX3H1]([nX3H1])[cX3H0]	0.1684	[#7X3][#6H3]	0.7782

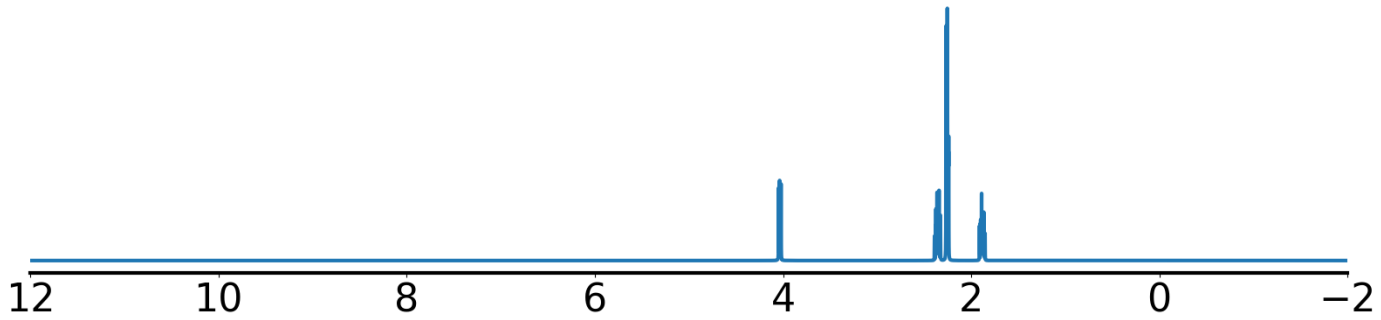
Example 10 true smiles: O=C1CCC(C(=O)O)N1 formula: C5H7NO3
Index of correct structure: 0 of 28551
True structure loss: 0.033519
True structure:



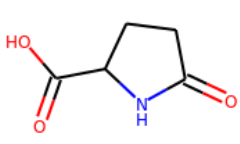
Experimental 13C NMR (solvent: DMSO)



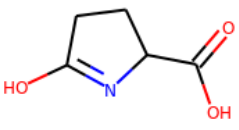
Experimental 1H NMR (solvent: D2O)



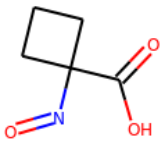
Top predicted structures (loss):



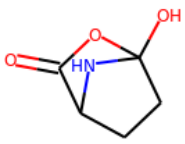
0.033519



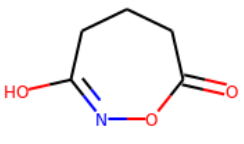
0.035021



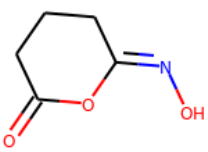
0.040787



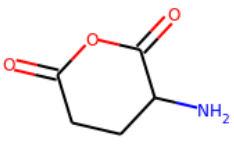
0.042966



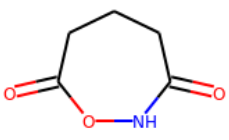
0.043186



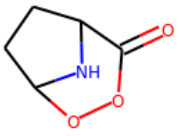
0.045337



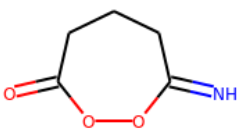
0.045787



0.048792



0.050969



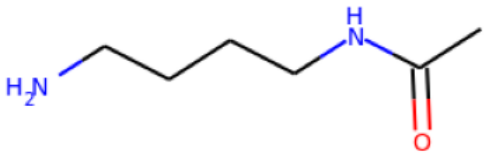
0.05319

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9949	[CX4H2]CC=O	0.8911
[CX4H2]([#6])[#6]	0.9872	OCC[CH2]	0.8885
[#8]=[#6][#8]	0.975	[#6H1]	0.8743
[CX3](=[OX1])O	0.9461	[#6H1][#6H2]	0.8295
[OX2H1]	0.8954	[#7][#6][#6X3]	0.7966

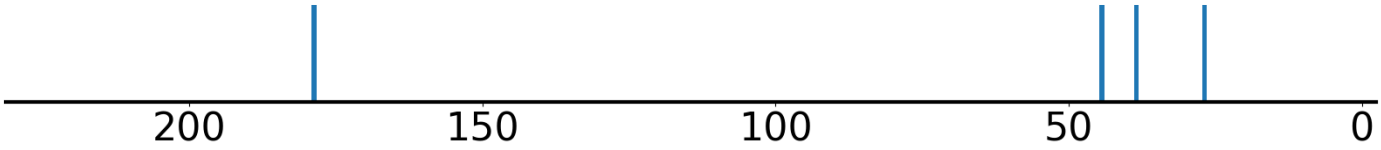
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9949	CC=CC#CC	0.0
[CX4H2]([#6])[#6]	0.9872	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[#8]=[#6][#8]	0.975	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[CX3](=[OX1])O	0.9461	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.8954	CCC=CC#C	0.0
[CX4H2]CC=O	0.8911	CCC#CC=C	0.0
OCC[CH2]	0.8885	[#6X3H2]=[#6][#6H2][#8H]	0.0
[#6H1]	0.8743	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[#6H1][#6H2]	0.8295	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#7][#6][#6X3]	0.7966	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H1]	0.7038	[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.0664
[#8][#6][#6][#6][#6]=[#8]	0.4216	[#6]1[#6][#6][#6][#7]1	0.1477
[CX4H](O)([CH])[CH]	0.4155	[CX4H1]([NX3H1])([CX4H2])[CX3H0]	0.1642
[#8][#6H1][#6H1]	0.4011	[#7H1][#6X4H1][#6X3]	0.1664
[CX4H]O	0.3761	[#6H1r5][#7]	0.252
[#8][#6][#6H2]	0.3638	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3141
[#7X3H0]	0.3569	[#7X3H1]	0.3602
[CX4H1]([OX2H1])([CX4H1])[CX4H1]	0.3542	[CX4H2][CX3]=O	0.4067
[OX2H1][CX4H1]1[CX4H1][CX4H1]1	0.3382	O=[CX3H0][CX4H2][CX4H2]	0.4439
[#6]1[#6][#6][#6][#6][#7]1	0.3115	[CX4H2]([CX4H2])[CX3H0]	0.4722

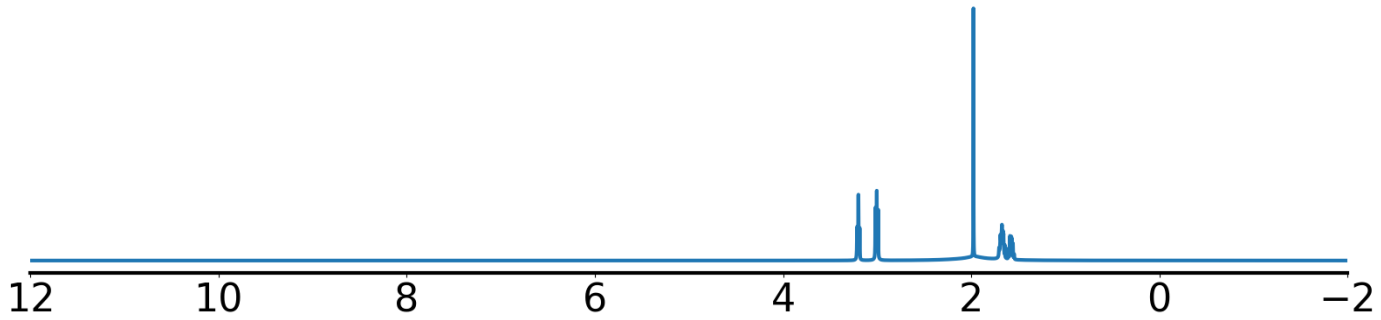
Example 11 true smiles: CC(=O)NCCCCN formula: C6H14N2O
Index of correct structure: 0 of 22876
True structure loss: 0.019508
True structure:



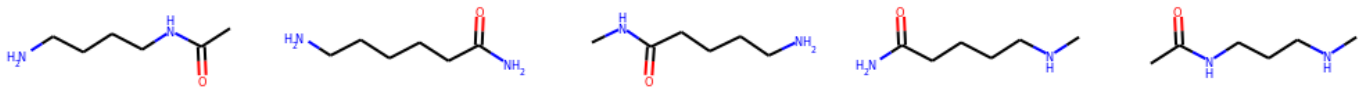
Experimental 13C NMR (solvent: D2O)



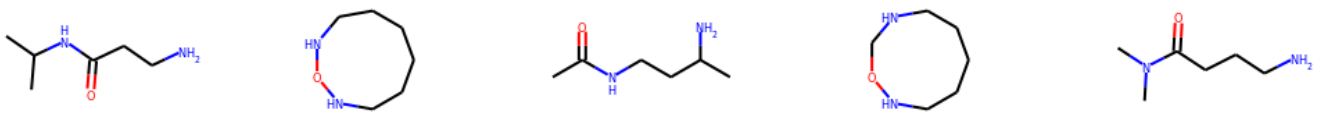
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.019508 0.026128 0.031322 0.033808 0.03422



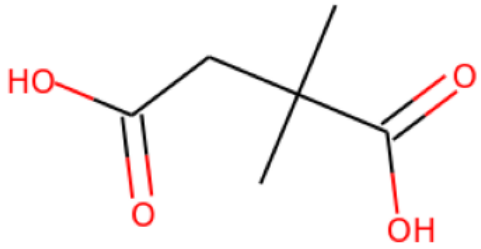
0.035583 0.035879 0.036409 0.036538 0.037347

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9965	[CX4H3]	0.9361
[#7X3][#6H2]	0.981	[CX4H2][CX4H2]	0.9265
[#7][#6H2][#6H2]	0.9598	[#7][#6H2]	0.9
[#7X3H2]	0.9584	[CX4H2]([NX3H2])[CX4H2]	0.883
[CX3](=[OX1])C	0.9396	[CX4H2]([CX4H2])[CX4H2]	0.8786

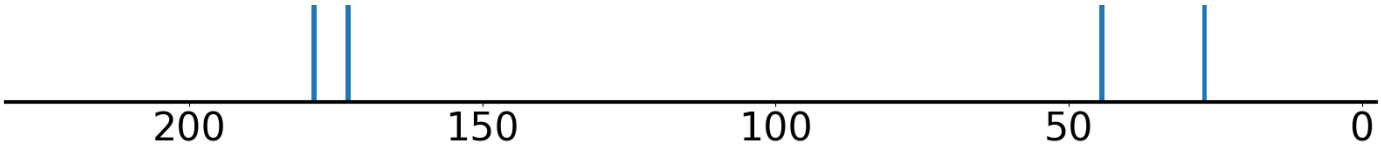
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9965	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3][#6H2]	0.981	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7][#6H2][#6H2]	0.9598	C=CC=CC#C	0.0
[#7X3H2]	0.9584	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9396	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3]	0.9361	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2][CX4H2]	0.9265	CC#CCC=C	0.0
[#7][#6H2]	0.9	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H2]([NX3H2])[CX4H2]	0.883	CC=CCC#C	0.0
[CX4H2]([CX4H2])[CX4H2]	0.8786	[#6X2][#6H1][#6X2]	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX3]=O	0.6277	[#7][#6][#6][#6][#6][#7]	0.2054
[CX4H2]CC=O	0.6044	[CX4H2][CX4H2][CX4H2][CX4H2]	0.2632
O=[CX3H0][CX4H2][CX4H2]	0.4071	[CX4H2]([NX3H1])[CX4H2]	0.3182
[#7H2][#6H0]	0.3995	[#6H3][#6H0]	0.4135
[CX4H2]([CX4H2])[CX4H1]	0.3928	[#7][#6][#6H3]	0.4473
[#6H1][#6H2]	0.3893	[OX1H0]=[CX3H0][CX4H3]	0.4637
[#6H3][#6][#6]	0.3394	[#7X3H1]	0.466
[#6H1]	0.3259	[#6H2][#7][#6X3]	0.5651
[CX4H2]([CX4H2])[CX3H0]	0.3133	[CX4H3][CX3]	0.6452
[#7][#6][#6][#6][#7]	0.3	[CX4H3][CX3H0]	0.6962

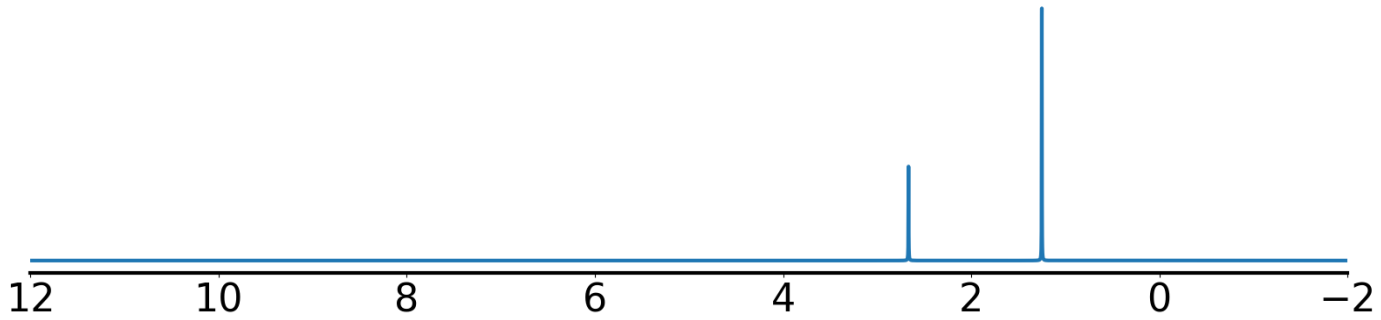
Example 12 true smiles: CC(C)(CC(=O)O)C(=O)O formula: C6H10O4
Index of correct structure: 0 of 19323
True structure loss: 0.018492
True structure:



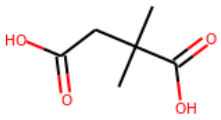
Experimental 13C NMR (solvent: DMSO)



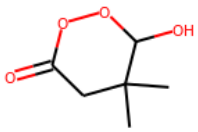
Experimental 1H NMR (solvent: D2O)



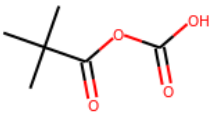
Top predicted structures (loss):



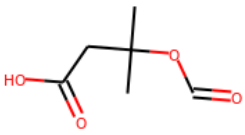
0.018492



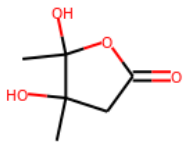
0.04651



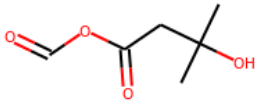
0.047561



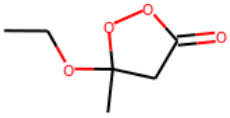
0.050277



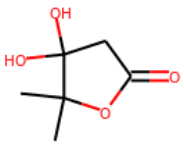
0.050498



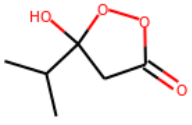
0.051003



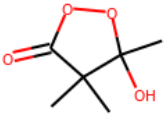
0.051862



0.052008



0.054245



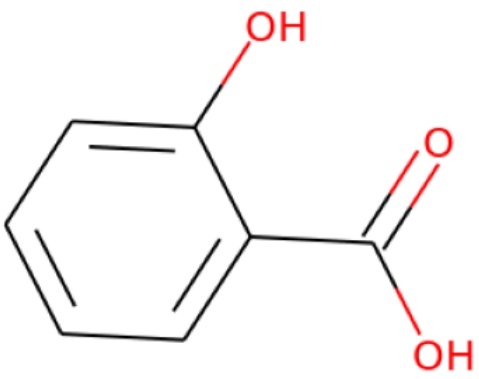
0.057978

Top predicted substructures	prob		
[#8]=[#6][#8]	1.0	[CX3](=O)[OX2H1]	0.9954
[CX3](=[OX1])O	1.0	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9932
[#6H3][#6][#6]	0.9998	[CX4H2]([#6])[#6]	0.9904
[CX3](=[OX1])C	0.9997	[CX4H3][CX4H0]	0.9884
[CX4H3]	0.9996	[#6H3][#6H0]	0.9853

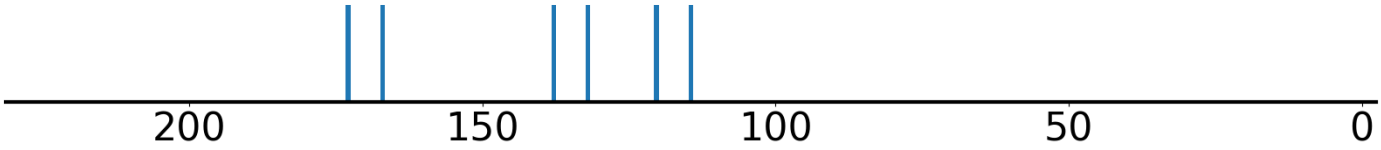
best positives	prob	best negatives	prob
[#8]=[#6][#8]	1.0	C=CC=CC#C	0.0
[CX3](=[OX1])O	1.0	[#6X2][#6H1][#6X2]	0.0
[#6H3][#6][#6]	0.9998	CC#CCC#C	0.0
[CX3](=[OX1])C	0.9997	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3]	0.9996	CCC#CC#C	0.0
[CX3](=O)[OX2H1]	0.9954	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9932	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2]([#6])[#6]	0.9904	CCC=CC#C	0.0
[CX4H3][CX4H0]	0.9884	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[#6H3][#6H0]	0.9853	CC=CCC#C	0.0

worst negatives	prob	worst positives	prob
[OX2H0][CX3H0][CX4H2]	0.6632	[#8][#6][#6][#6][#6][#8]	0.1451
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.5578	[#8][#6][#6][#6][#6]=[#8]	0.1897
[#8][#6][#6][#6X3]	0.4815	[CH3]CC[OH]	0.2266
[#8]=[#6][#6H2][#6H1]	0.2654	[CX4H2]CC=O	0.2849
[#6H1]	0.2399	[#8]=[#6][#6][#6][#6]=[#8]	0.3414
[#6X3][#6H2][#6X3]	0.2339	[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.3519
[CH3][#6][#8]	0.1937	[#6H3][#6][#6X3]	0.4082
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.1861	OCC[CH2]	0.514
[CX4H3][CX4]O	0.1801	[OX1H0]=[CX3H0][CX4H2][CX4H0]	0.6716
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.1433	[CX4H3][CX4H0][CX4H3]	0.7456

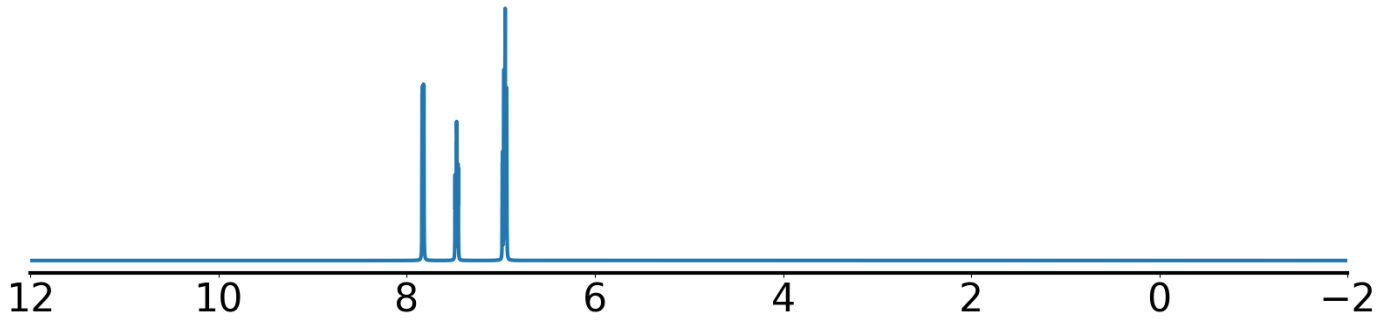
Example 13 true smiles: O=C(O)c1ccccc1O formula: C7H6O3
Index of correct structure: 0 of 15458
True structure loss: 0.016306
True structure:



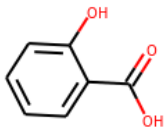
Experimental 13C NMR (solvent: N/A)



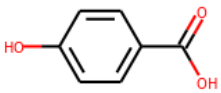
Experimental 1H NMR (solvent: D2O)



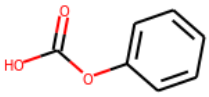
Top predicted structures (loss):



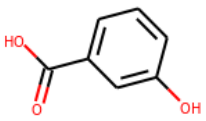
0.016306



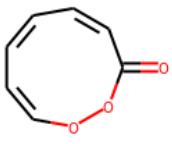
0.016401



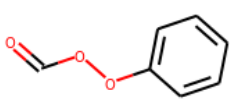
0.017178



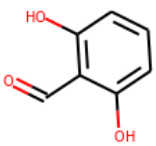
0.023257



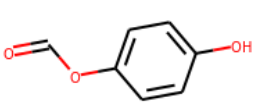
0.023758



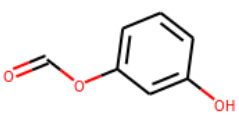
0.028966



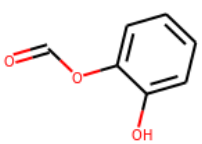
0.030215



0.03252



0.033484



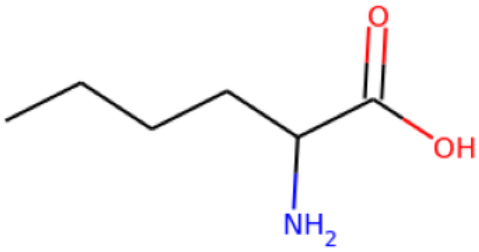
0.033797

Top predicted substructures	prob		
[#6H1]	0.9999	[#6X3H1][#6X3H0]	0.99
[#6X3][#6X3]	0.9998	[cX3H1]([cX3H1])[cX3H0]	0.9856
[cH][cH]	0.9968	O=[#6][#6][#6X3]	0.9786
[#6X3][#6X3][#6X3][#6X3]	0.9952	[CX3](=[OX1])O	0.9734
[#8]=[#6][#8]	0.9925	[cH]	0.9489

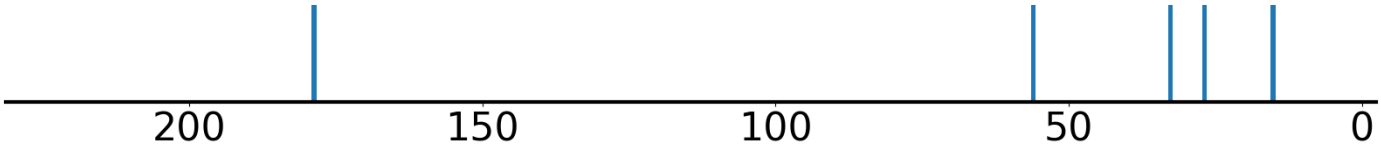
best positives	prob	best negatives	prob
[#6H1]	0.9999	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.9998	[#6H3][#7][#6X4H1][#6H3]	0.0
[cH][cH]	0.9968	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9952	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#8]=[#6][#8]	0.9925	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#6X3H1][#6X3H0]	0.99	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9856	[CX4H1]([NX3H2])([CX4H2])[CX4H0]	0.0
O=[#6][#6][#6X3]	0.9786	[CX4H0]([NX3H2])([CX4H2])([CX4H1])[CX4H1]	0.0
[CX3](=[OX1])O	0.9734	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[cH]	0.9489	[CX4H2]([NX3H0])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#6H1][#6H1]	0.6906	[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.1005
[OX1H0]=[cX3H0][cX3H1]	0.6486	[OX2H][cX3]:[c]	0.4525
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6475	[cH]cO	0.4689
[#8]=[#6H0][#6H1]	0.6392	[#6]1[#6][#6][#6][#6][#6]1	0.5237
O=[cX3]	0.6267	[CX3](=O)[OX2H1]	0.7912
[CX3](=[OX1])C	0.5293	[OX2H1]	0.8534
[#8][#6H1][#6H1]	0.4076	[#6H1][#6H1]	0.8561
[cX3H0][cX3H1][cX3H1][cX3H0]	0.3796	[#8][#6][#6][#6X3]	0.8807
[cX3H1]([oX2H0])[cX3H1]	0.1907	[#8][#6H0][#6H1]	0.8978
[#8][#6][#6][#6][#6]=[#8]	0.1862	[cX3H1]([cX3H1])[cX3H1]	0.9167

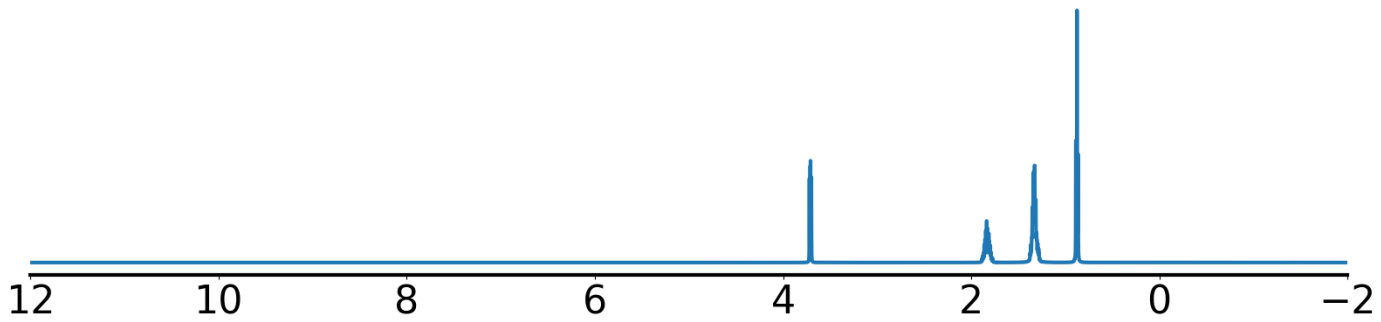
Example 14 true smiles: CCCCC(N)C(=O)O formula: C6H13NO2
Index of correct structure: 0 of 14628
True structure loss: 0.01752
True structure:



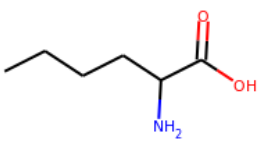
Experimental 13C NMR (solvent: D2O)



Experimental 1H NMR (solvent: D2O)

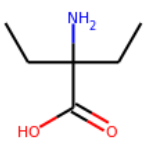


Top predicted structures (loss):

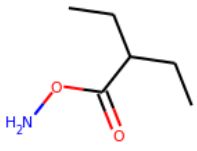


0.01752

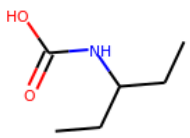
0.030179



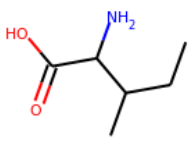
0.033519



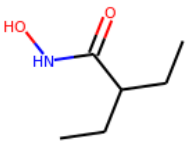
0.035605



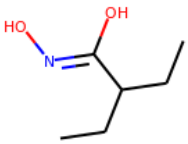
0.041748



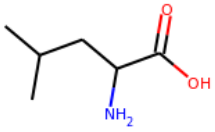
0.043004



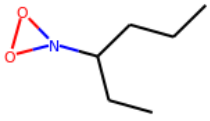
0.046331



0.050592



0.0525



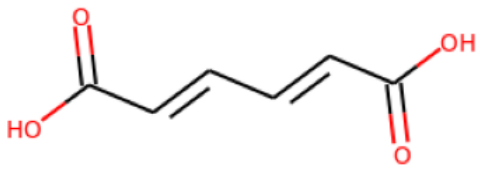
0.052515

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9999	[CX3](=[OX1])C	0.9855
[CX4H3]	0.9994	[#7X3H2]	0.9563
[CX4H3][CX4H2]	0.999	[#8]=[#6][#8]	0.9523
[#6H3][#6][#6]	0.9988	O=[CX3][CX4H]	0.9346
[CX4H3][#6]	0.9934	[OX2H1]	0.9136

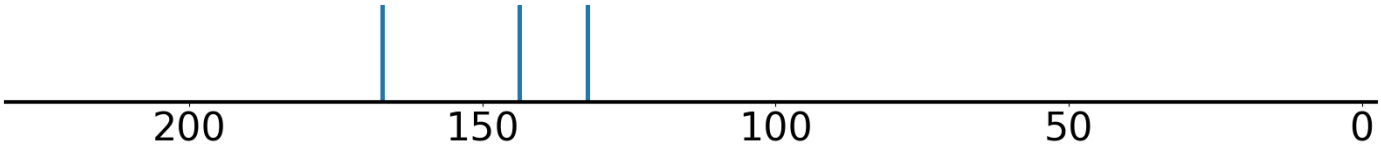
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	0.9994	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][CX4H2]	0.999	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9988	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][#6]	0.9934	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX3](=[OX1])C	0.9855	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7X3H2]	0.9563	CCC#CC#C	0.0
[#8]=[#6][#8]	0.9523	CC=CCC#C	0.0
O=[CX3][CX4H]	0.9346	CC#CCC=C	0.0
[OX2H1]	0.9136	[CX2H0](#[CX2H1])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H3])[CX4H1]	0.785	CCCCCC	0.1261
[#6X3][#6][#6][#6H3]	0.587	[#8][#6H0][#6H1]	0.2354
[#7H2][#6H0]	0.5192	[CX4H2]([CX4H2])[CX4H2]	0.2711
[#8]=[#6][#6H1][#6H1]	0.2955	[CX4H2][CX4H2]	0.3609
[#7][#6H0][#6H1]	0.2873	[CX4H2]([CX4H2])[CX4H1]	0.4169
[#8][#6][#6H2]	0.2732	[CX4H2]([CX4H3])[CX4H2]	0.513
[#6H3][#6H2][#6H1][#7]	0.1774	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.5782
[#7X3H1]	0.1619	[#7][#6][#6X3]	0.6265
[CX4H2][CX3]=O	0.1269	OCC[CH2]	0.7336
[OH][CX4H]	0.0816	[#7H2][#6H1]	0.777

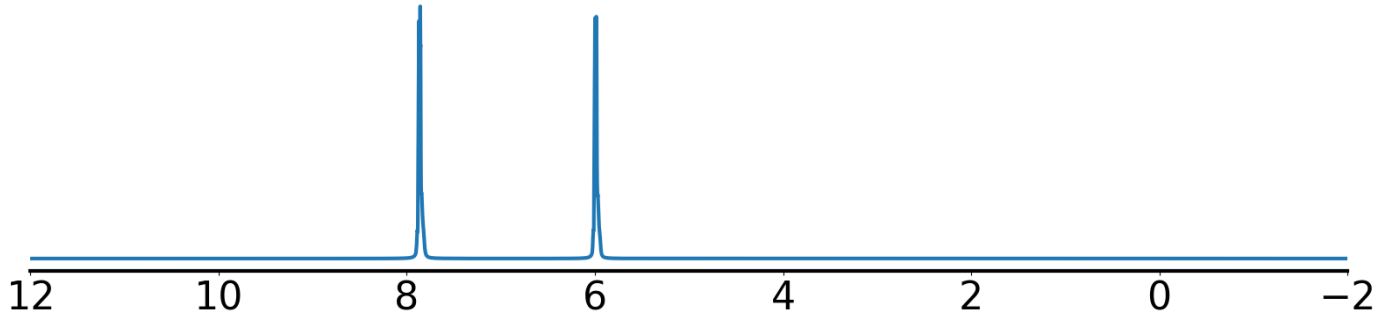
Example 15 true smiles: O=C(O)C=CC=CC(=O)O formula: C6H6O4
Index of correct structure: 0 of 14419
True structure loss: 0.027355
True structure:



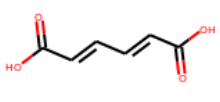
Experimental 13C NMR (solvent: DMSO)



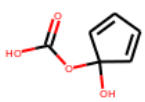
Experimental 1H NMR (solvent: #N/A)



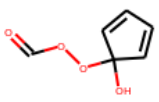
Top predicted structures (loss):



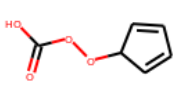
0.027355



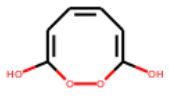
0.041066



0.047702

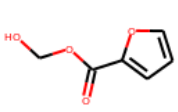


0.051506

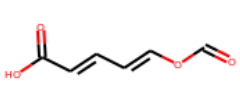


0.05409

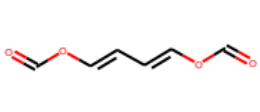
0.054502



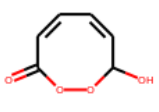
0.054963



0.055276



0.056261



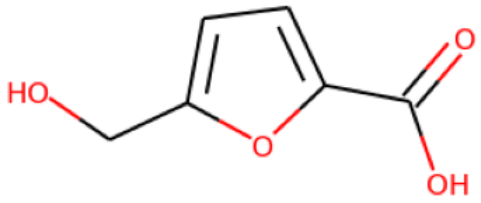
0.058764

Top predicted substructures	prob		
[#6H1]	0.9999	[OX2H1]	0.8686
[#6X3][#6X3]	0.9978	[CHX3]=[CHX3]	0.8266
[#8]=[#6][#8]	0.9977	[#6H1][#6H1]	0.818
[CX3](=[OX1])O	0.9953	O=[#6][#6]=[#6X3]	0.6731
[CHX3](=C)C	0.9616	[#6X3H1][#6X3H0]	0.673

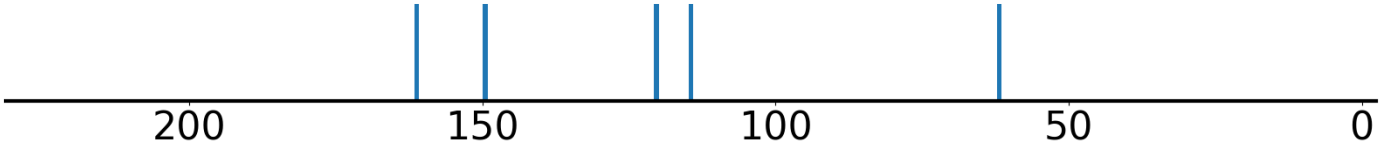
best positives	prob	best negatives	prob
[#6H1]	0.9999	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9978	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8]=[#6][#8]	0.9977	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX3](=[OX1])O	0.9953	[#7][#6][#6][#6]#[#7]	0.0
[CHX3](=C)C	0.9616	[#6H3][#6H0][#7][#6H3]	0.0
[OX2H1]	0.8686	[#6H3][#7][#6X4H1][#6H3]	0.0
[CHX3]=[CHX3]	0.8266	[#7][#6H1][#6X2]	0.0
[#6H1][#6H1]	0.818	[CX4H2]([NX3H0])[CX4H3]	0.0
O=[#6][#6]=[#6X3]	0.6731	[#7][#6][#6]#[#7]	0.0
[#6X3H1][#6X3H0]	0.673	[#6H3][#7][#7]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H1][#6H1]	0.3944	CC=CC=CC	0.0026
[#8][#6][#6][#8]	0.3279	[#6X3]=[#6X3][#6X3]=[#6X3]	0.0431
[#8][#6][#6]=[#6][#6][#8]	0.3082	[CX3H1](=[CX3H1])[CX3H1]	0.157
[CX3H][CX4H]	0.2747	[CX3H1](=[CX3H1])[CX3H0]	0.1874
[CX3H1](=[CX3H1])[CX4H1]	0.2425	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.2496
[CX4H](O)([CH])[CH]	0.2182	[#6X3][#6X3]=[#6X3][#6X3]	0.2813
[#8][#6][#6][#6X3]	0.2066	[#8]=[#6][#6H1]=[#6H1]	0.4025
[CX4H]O	0.1636	[#8]=[#6H0][#6H1]	0.4633
O=[#6][#6][#6X3]	0.149	[#8][#6H0][#6H1]	0.4713
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.1391	[CX3](=[OX1])C	0.5366

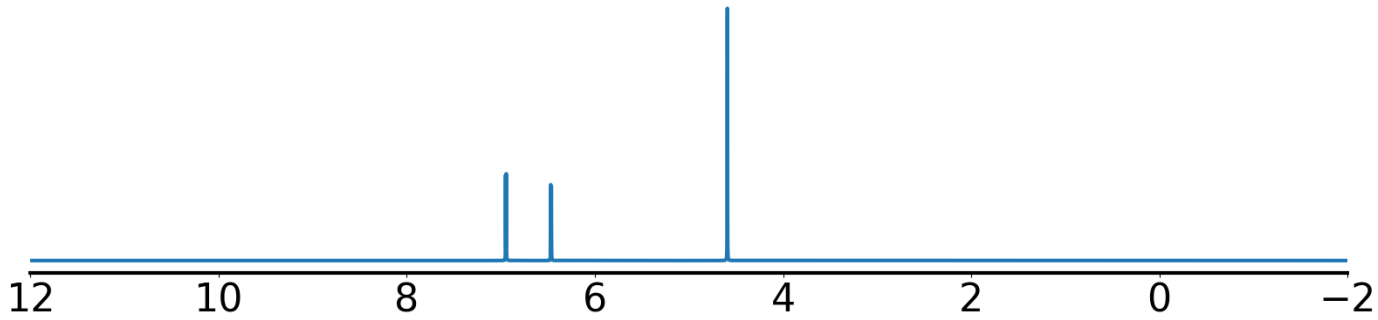
Example 16 true smiles: O=C(O)c1ccc(CO)o1 formula: C6H6O4
Index of correct structure: 5 of 14419
True structure loss: 0.027503
True structure:



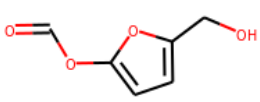
Experimental 13C NMR (solvent: Acetone-d6)



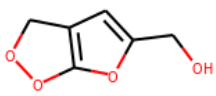
Experimental 1H NMR (solvent: D2O)



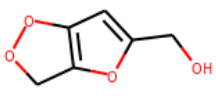
Top predicted structures (loss):



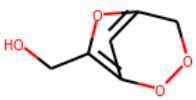
0.023982



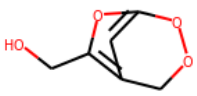
0.025608



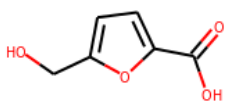
0.027161



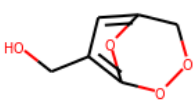
0.027161



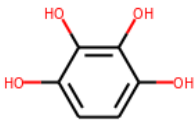
0.027475



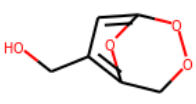
0.027503



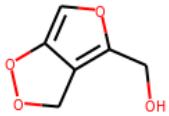
0.027658



0.029326



0.029526



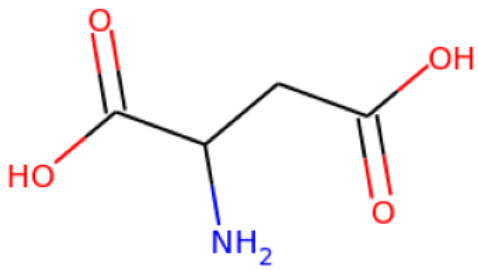
0.031459

Top predicted substructures	prob		
[#6X3][#6X3]	0.9984	[OX2H1][CX4H2][#6X3H0]	0.9807
[OX2H1]	0.9967	[#6X3H1][#6X3H0]	0.98
[#6X3][#6X3][#6X3][#6X3]	0.9962	[CX4H2]([#6])[O]	0.9639
[#6H1]	0.9955	[cH]	0.9406
[#8][#6][#6][#6X3]	0.9813	[CX4H2]([OX2H1])[cX3H0]	0.9278

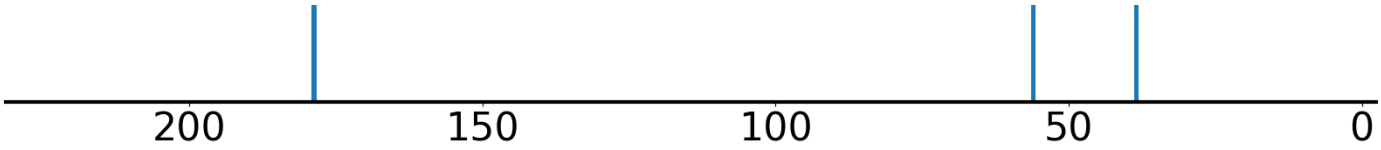
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9984	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[OX2H1]	0.9967	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9962	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6H1]	0.9955	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#8][#6][#6][#6X3]	0.9813	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[OX2H1][CX4H2][#6X3H0]	0.9807	[CX4H2]([NX3H1])[CX4H3]	0.0
[#6X3H1][#6X3H0]	0.98	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H2]([#6])[O]	0.9639	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[cH]	0.9406	[CX4H1]([NX3H0])([CX4H2])[CX3H1]	0.0
[CX4H2]([OX2H1])[cX3H0]	0.9278	[CX4H1]([NX3H2])([CX4H2])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[OX2H][cX3]:[c]	0.7758	[#8][#6][#6]=[#8]	0.0076
[#8][#6][#6][#6][#6][#8]	0.6978	[CX3](=O)[OX2H1]	0.0288
[cH]cO	0.6963	O=[#6][#6][#6X3]	0.0477
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.4846	[CX3](=[OX1])O	0.2277
[cX3H0]([cX3H1])([cX3H0])[CX4H2]	0.4254	[cX3H0][cX3H1][cX3H1][cX3H0]	0.3364
o[cH]	0.3731	[#8][#6][#6H2]	0.3535
[#8][#6H1][#6H1]	0.3526	[#8]=[#6][#8]	0.4866
[cX3H1]([oX2H0])[cX3H1]	0.3159	[#8][#6][#6H2][#8]	0.6704
[#8][#6][#6]=[#6X3]	0.233	[#6H1][#6H1]	0.6911
[#8][#6][#6]=[#6][#6][#8]	0.2187	[#8][#6H0][#6H1]	0.8119

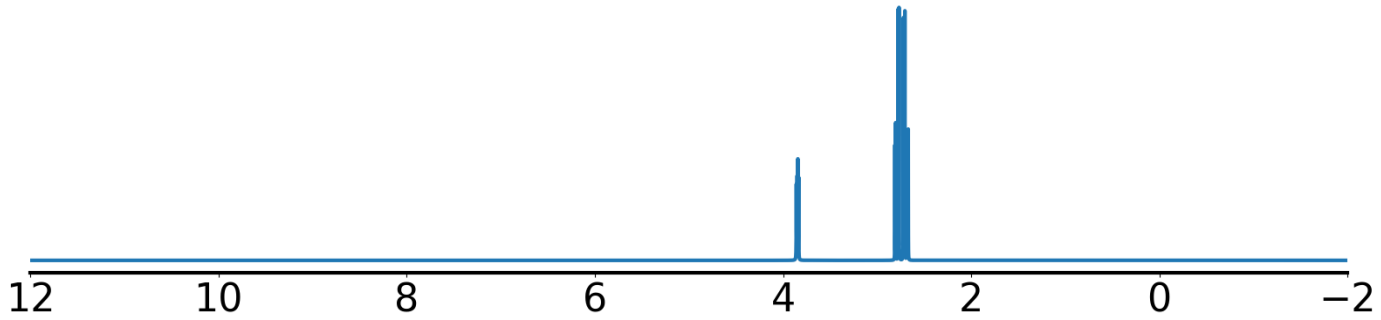
Example 17 true smiles: NC(CC(=O)O)C(=O)O formula: C4H7NO4
Index of correct structure: 0 of 13760
True structure loss: 0.037025
True structure:



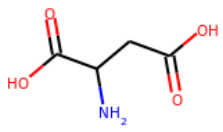
Experimental 13C NMR (solvent: D2O)



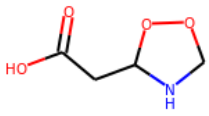
Experimental 1H NMR (solvent: D2O)



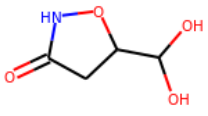
Top predicted structures (loss):



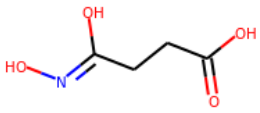
0.037025



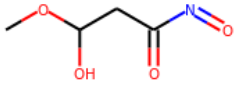
0.039541



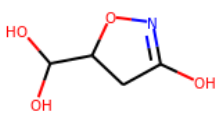
0.045378



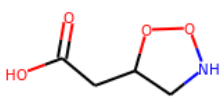
0.046676



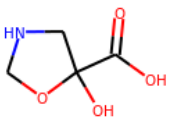
0.047823



0.048293

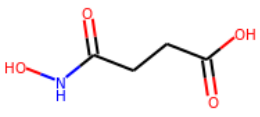


0.04834



0.050062

0.050409



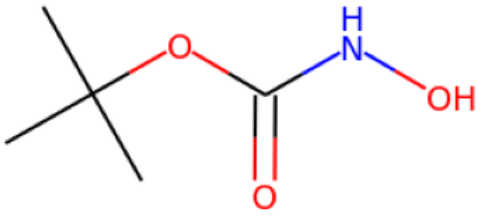
0.050734

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9946	[CX3](=O)[OX2H1]	0.8149
[OX2H1]	0.9837	[#6H1]	0.7734
[#8]=[#6][#8]	0.9751	[CX4H2][CX3]=O	0.7038
[CX3](=[OX1])O	0.9299	[#6H1][#6H1]	0.6788
OCC[CH2]	0.8344	[#8][#6][#6][#6X3]	0.674

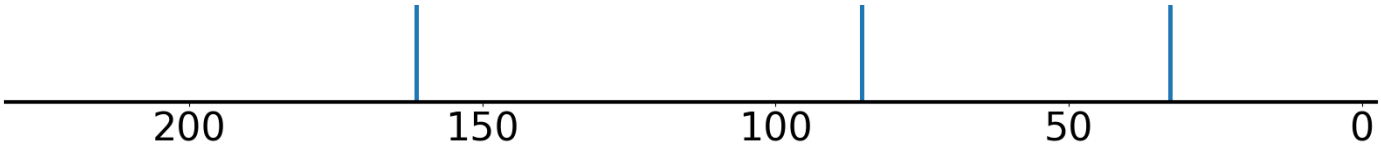
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9946	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9837	CC#CCC=C	0.0
[#8]=[#6][#8]	0.9751	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[CX3](=[OX1])O	0.9299	CC=CC#CC	0.0
OCC[CH2]	0.8344	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[CX3](=O)[OX2H1]	0.8149	CCC=CC#C	0.0
[#6H1]	0.7734	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[CX4H2][CX3]=O	0.7038	C=CCCC#C	0.0
[#8][#6][#6H2]	0.6337	CC=CCC#C	0.0
O=[CX3][CX4H]	0.6021	[CX3H1](=[CX3H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H1]	0.6788	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.0278
[#8][#6][#6][#6X3]	0.674	[#8]=[#6][#6][#6][#6]=[#8]	0.1507
[CX4H]O	0.5629	[#7H2][#6X4H1][#6X3]	0.2111
O[CX4H][CX4H2]	0.504	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2677
[#7X3H1]	0.5023	[#8]=[#6][#6H2][#6H1]	0.3254
[#8][#6H1][#6H1]	0.3657	[#8][#6H0][#6H1]	0.3468
[CX4H](O)CO	0.3344	[#8][#6][#6][#6][#6][#8]	0.3527
[#8]=[#6][#6H1][#6H1]	0.2981	[#7][#6][#6][#6X3]	0.4039
[#6H2][#6H1r3]	0.2649	O=[CX3H0][CX4H2][CX4H1]	0.4315
[CX4H2]([#6])[O]	0.2554	[CX4H2]([CX4H1])[CX3H0]	0.4445

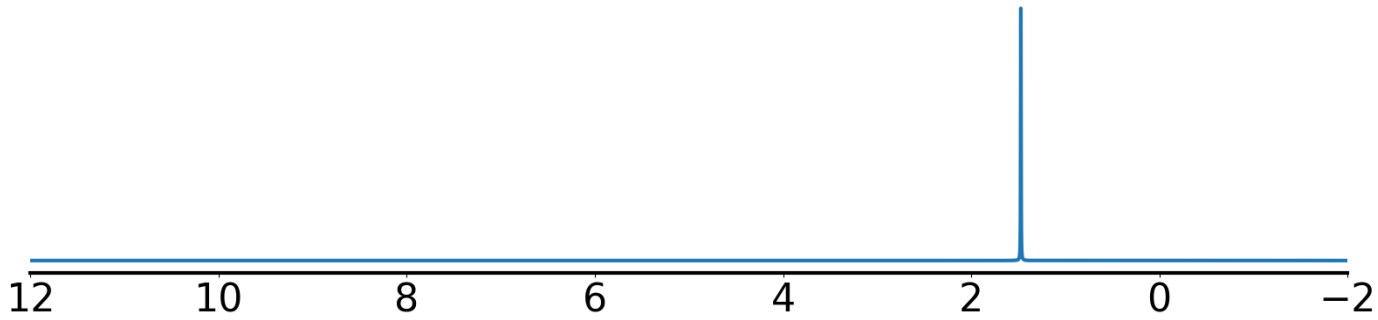
Example 18 true smiles: CC(C)(C)OC(=O)NO formula: C5H11NO3
Index of correct structure: 1 of 13267
True structure loss: 0.010181
True structure:



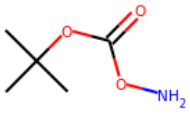
Experimental 13C NMR (solvent: CDCl3)



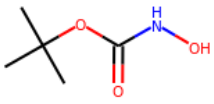
Experimental 1H NMR (solvent: D2O)



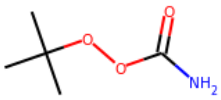
Top predicted structures (loss):



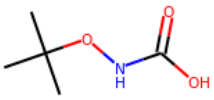
0.009659



0.010181



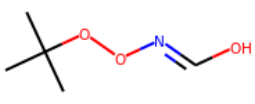
0.010868



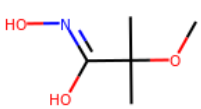
0.011906

0.017831

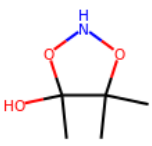
0.01825



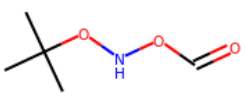
0.018278



0.019533



0.019639



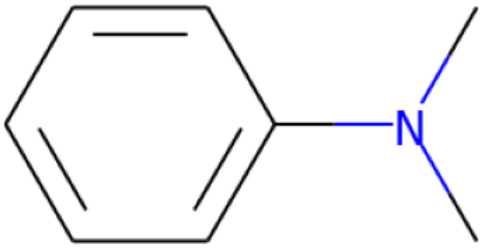
0.019836

Top predicted substructures	prob		
[CX4H3]	0.9976	[#6H3][#6H0]	0.9892
[#6H3][#6][#6]	0.9966	[CX4H3][#6]	0.9447
[CX4H3][CX4]O	0.9959	[#6H0]([#6H3])([#6H3])[#8]	0.9207
[CX4H3][CX4H0][CX4H3]	0.9957	[CX4H3][CX4H0]([CX4H3])[OX2H0]	0.9195
[CX4H3][CX4H0]	0.9949	[OX2H1]	0.8938

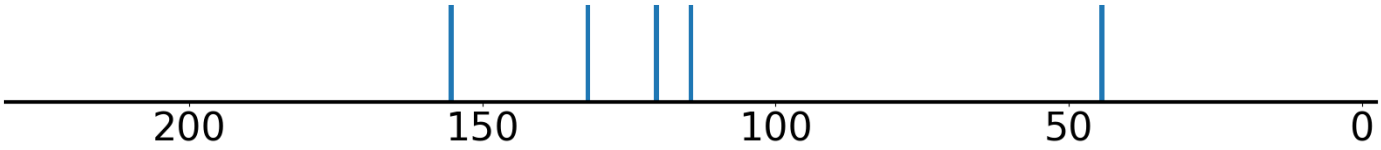
best positives	prob	best negatives	prob
[CX4H3]	0.9976	CCC#CC#C	0.0
[#6H3][#6][#6]	0.9966	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H3][CX4]O	0.9959	C=CC=CC#C	0.0
[CX4H3][CX4H0][CX4H3]	0.9957	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][CX4H0]	0.9949	CC=CC#CC	0.0
[#6H3][#6H0]	0.9892	[CX4H1]([CX4H2])([CX4H2])[CX2H0]	0.0
[CX4H3][#6]	0.9447	CC=CCC#C	0.0
[#6H0]([#6H3])([#6H3])[#8]	0.9207	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX4H3][CX4H0]([CX4H3])[OX2H0]	0.9195	[#6X2][#6H1][#6X2]	0.0
[OX2H1]	0.8938	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0

worst negatives	prob	worst positives	prob
[#6X4H3][#6][#8H]	0.4604	[#7X3H1]	0.0367
[#8][#6][#6][#8]	0.4109	[CX4]([CX4H3])([CX4H3])[CX4H3]	0.552
[#7X3H2]	0.3457	[CX3](=[OX1])O	0.6945
[#8][#6H0][#6H1]	0.2901	[#8]=[#6][#8]	0.7656
[OX2H1][CX4H0][CX4H3]	0.2894	[CH3][#6][#8]	0.8774
[#7H2][#6H0]	0.2393	[OX2H1]	0.8938
[#8][#6][#6H2]	0.2199	[CX4H3][CX4H0]([CX4H3])[OX2H0]	0.9195
[CX3](=O)[OX2H1]	0.161	[#6H0]([#6H3])([#6H3])[#8]	0.9207
[#6H1]	0.1518	[CX4H3][#6]	0.9447
[#6H3][#6][#6X3]	0.15	[#6H3][#6H0]	0.9892

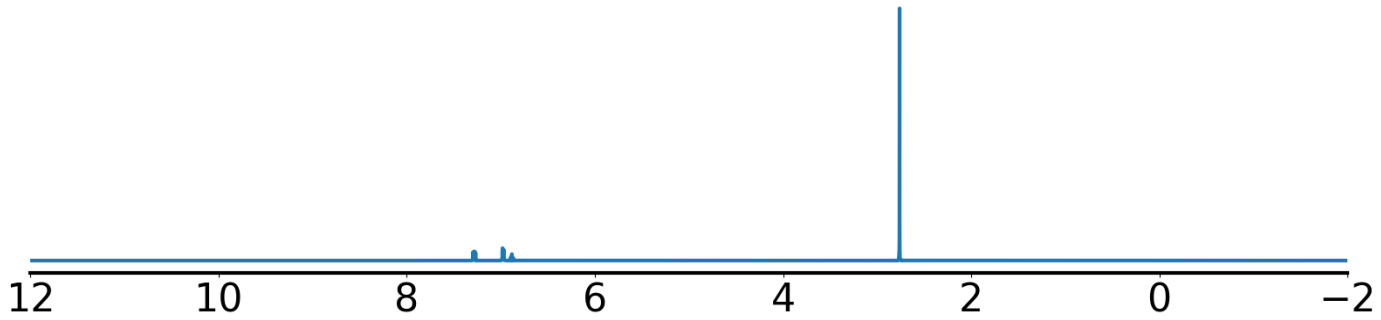
Example 19 true smiles: CN(C)c1ccccc1 formula: C8H11N
Index of correct structure: 0 of 10820
True structure loss: 0.018022
True structure:



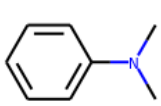
Experimental 13C NMR (solvent: CDCl3)



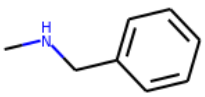
Experimental 1H NMR (solvent: D2O)



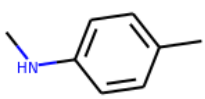
Top predicted structures (loss):



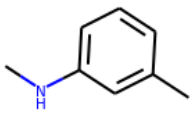
0.018022



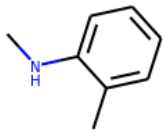
0.024033



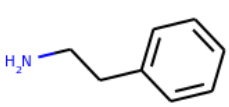
0.044352



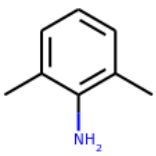
0.045717



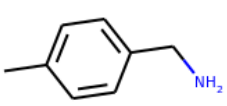
0.048424



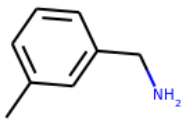
0.051874



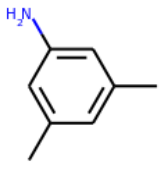
0.052251



0.052462



0.053827



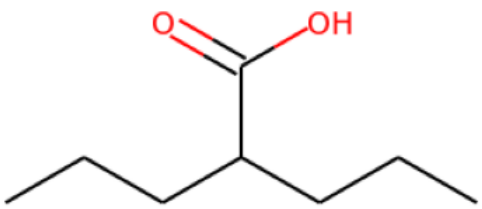
0.055472

Top predicted substructures	prob		
[#6H1]	0.9908	[#6H3][#7]	0.9085
[#6X3][#6X3]	0.9895	[#7][#6][#6][#6X3]	0.9024
[#6X3][#6X3][#6X3][#6X3]	0.9707	[cH]	0.8996
[#7X3][#6H3]	0.9186	[cH][cH]	0.8718
[#6X3H1][#6X3H0]	0.9179	[CX4H3]	0.861

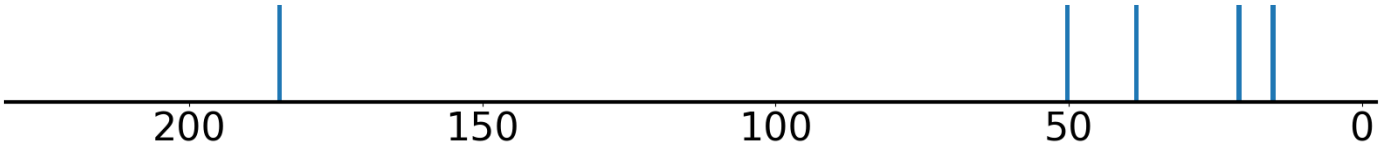
best positives	prob	best negatives	prob
[#6H1]	0.9908	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9895	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9707	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#7X3][#6H3]	0.9186	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9179	[#6]1[#8][#6][#6]1=[#8]	0.0
[#6H3][#7]	0.9085	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#7][#6][#6][#6X3]	0.9024	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[cH]	0.8996	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.8718	[CX4H1]([OX2H0])([CX4H3])[CX4H0]	0.0
[CX4H3]	0.861	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6H2][#6X3]	0.4836	[#7X3H0]	0.1399
[#7X3H1]	0.3138	[CX4H3][NX3H0]	0.203
[cX3H0][cX3H1][cX3H1][cX3H0]	0.3119	[#7][#6X3H0][#6X3H1]	0.2503
[#7X3][#6H2]	0.3078	[#7][#6H0][#6H1]	0.3137
[#6X3][#7][#6X3]	0.2768	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.4022
[#7X3H2]	0.2569	[#6H3][#7][#6X3]	0.6086
[#7H2][#6H2]	0.2227	[#6H1][#6H1]	0.6087
[CX4H2][CX3]=C	0.1977	[#6]1[#6][#6][#6][#6][#6]1	0.6263
[#6]1[#6][#6][#6][#7]1	0.1961	[cX3H1]([cX3H1])[cX3H1]	0.6802
[#6X3][#7X3][#6X3]	0.1922	[#7][#6][#6X3]	0.7452

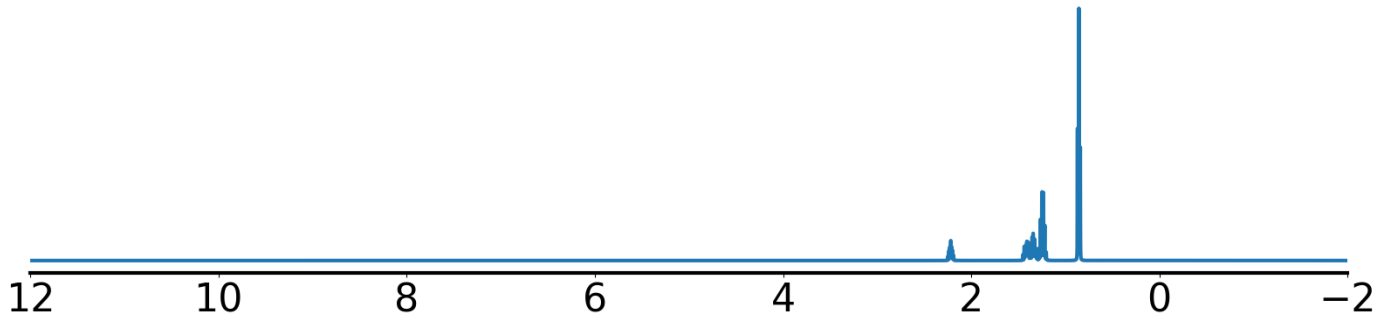
Example 20 true smiles: CCCC(CCC)C(=O)O formula: C8H16O2
Index of correct structure: 0 of 9984
True structure loss: 0.017342
True structure:



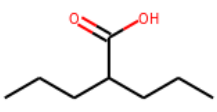
Experimental 13C NMR (solvent: CDCl3)



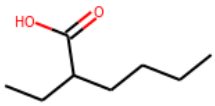
Experimental 1H NMR (solvent: D2O)



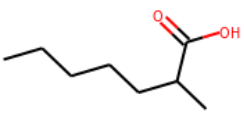
Top predicted structures (loss):



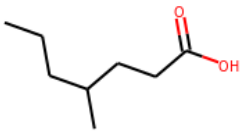
0.017342



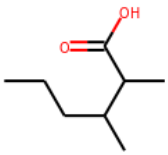
0.022903



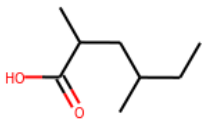
0.026993



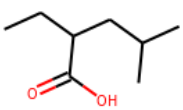
0.031791



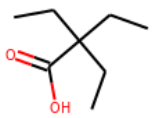
0.032951



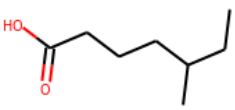
0.0331



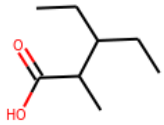
0.035662



0.037335



0.041204



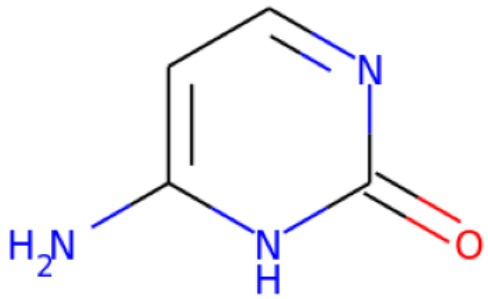
0.042131

Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][CX4H2]	0.9967
[#6H3][#6][#6]	1.0	[CX3](=O)[OX2H1]	0.9935
[CX4H3][#6]	0.9999	[CX3](=[OX1])O	0.9871
[CX4H2]([#6])[#6]	0.9993	[#8]=[#6][#8]	0.9806
[CX3](=[OX1])C	0.9992	[OX2H1]	0.9799

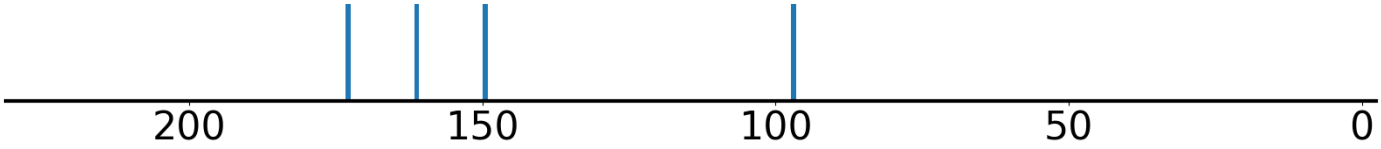
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[#6H3][#6][#6]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][#6]	0.9999	CC=CC#CC	0.0
[CX4H2]([#6])[#6]	0.9993	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9992	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H3][CX4H2]	0.9967	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX3](=O)[OX2H1]	0.9935	CC#CCC#C	0.0
[CX3](=[OX1])O	0.9871	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#8]=[#6][#8]	0.9806	CCC=CC#C	0.0
[OX2H1]	0.9799	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CHX4]([CH3X4])[CH2X4]	0.7421	[OX1H0]=[CX3H0][CX4H1]([CX4H2])[CX4H2]	0.0493
[CX4H3][CX4H1]	0.6922	[CX4H1]([CX4H2])([CX4H2])[CX3H0]	0.1727
[#6X3][#6][#6][#6H3]	0.6165	[#6H1]([#6H2])[#6H2]	0.3844
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.4988	CCCCCC	0.4191
[#6H3][#6][#6X3]	0.3757	[CX4H2]([CX4H2])[CX4H1]	0.6998
[CX4H2][CX3]=O	0.3629	[CX4H2]CC=O	0.7414
[#6H3][#6][#6][#6H3]	0.3247	[#6H1]	0.7691
[CX4H1]([CX4H3])([CX4H2])[CX3H0]	0.2418	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.7779
[#8][#6][#6H2]	0.155	[#6H1][#6H2]	0.8012
[#6H1][#6H1]	0.1488	[CX4H2][CX4H2]	0.8027

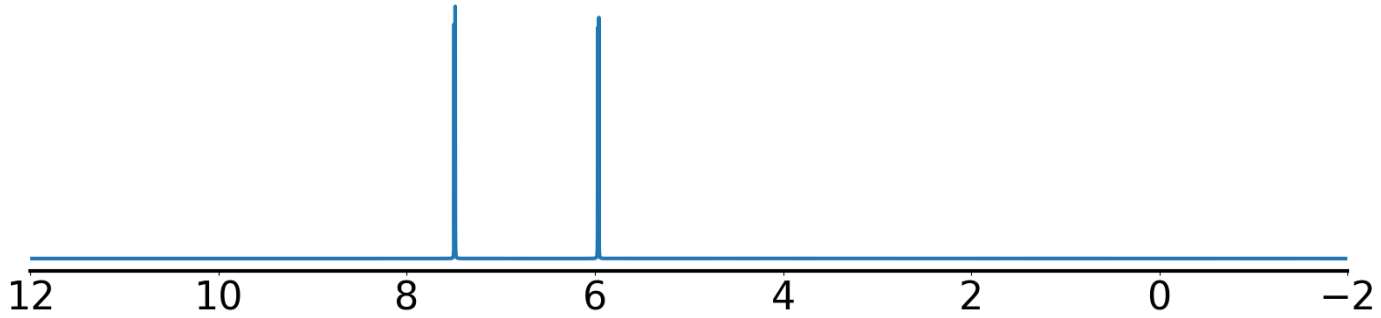
Example 21 true smiles: Nc1ccnc(=O)[nH]1 formula: C4H5N3O
Index of correct structure: 1 of 8616
True structure loss: 0.025688
True structure:



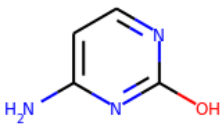
Experimental 13C NMR (solvent: D2O)



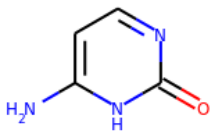
Experimental 1H NMR (solvent: d2o)



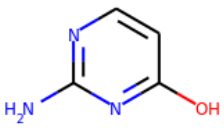
Top predicted structures (loss):



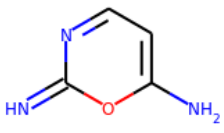
0.02392



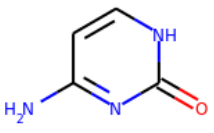
0.025688



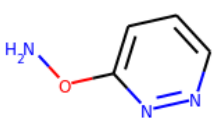
0.026505



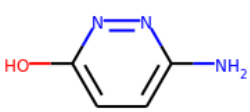
0.026884



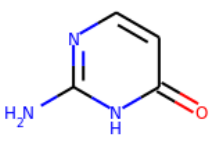
0.027135



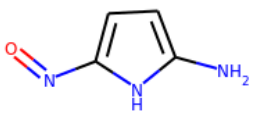
0.030327



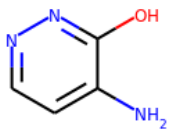
0.030571



0.030602



0.030929



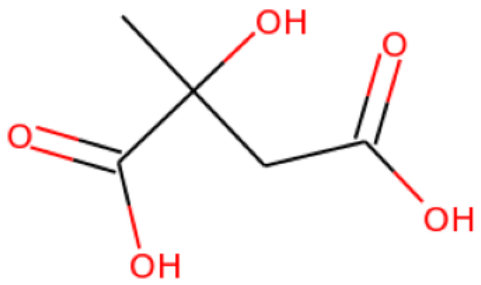
0.031199

Top predicted substructures	prob		
[#6H1]	0.9905	[cX3H1]([cX3H1])[cX3H0]	0.8583
[#6X3][#6X3]	0.9878	[cH][cH]	0.826
[#6X3H1][#6X3H0]	0.9355	[#7][#6H0][#6H1]	0.7848
[#7][#6][#6X3]	0.9096	[#7][#6][#6][#6X3]	0.7703
[#7X3H2]	0.8746	[cH]	0.7557

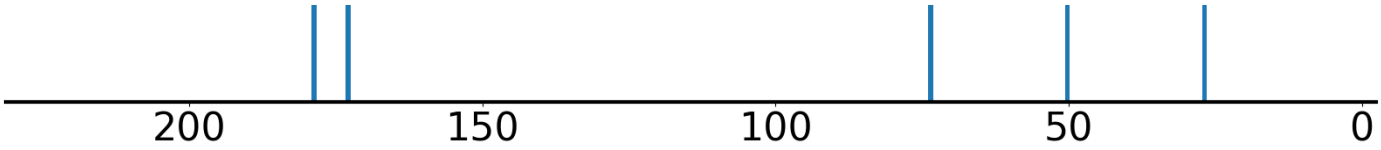
best positives	prob	best negatives	prob
[#6H1]	0.9905	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0
[#6X3][#6X3]	0.9878	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9355	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.9096	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[#7X3H2]	0.8746	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8583	[OX2H0]1[CX4H2][CX4H1]1[CX4H2]	0.0
[cH][cH]	0.826	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6H0][#6H1]	0.7848	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
[#7][#6][#6][#6X3]	0.7703	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[cH]	0.7557	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6X3][#6X3][#6X3]	0.5565	[cX3H1]([nX2H0])[cX3H1]	0.0774
[#8][#6H0][#6H1]	0.5207	O=[cX3]	0.1702
[#6]=[#7H]	0.4368	[#6X3][#7X3][#6X3]	0.2537
[#7][#6H0]=[#7]	0.3856	[#7X3H1]	0.4398
[NH1]=[#6][#7]	0.383	[#6X3][#7][#6X3]	0.4768
O=[#6][#6][#6X3]	0.3528	[#7][#6][#6][#6][#7]	0.504
[#8][#6][#6][#6X3]	0.3478	[#7][#6H0][#7]	0.5465
[OX1H0]=[cX3H0][cX3H1]	0.3236	[#7][#6][#7]	0.6236
[CX3H1](=[CX3H1])[CX3H0]	0.3167	[#7H2][#6H0]	0.6323
[CHX3](=C)C	0.3142	[#6H1][#6H1]	0.6424

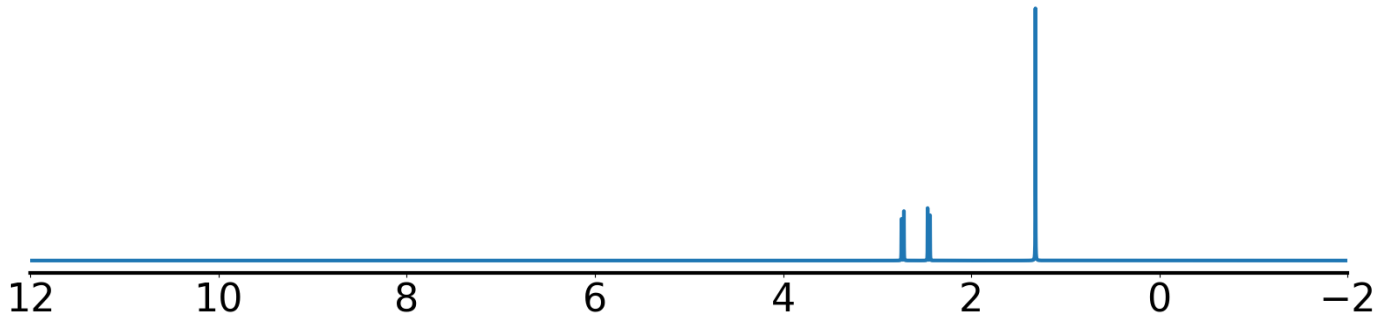
Example 22 true smiles: CC(O)(CC(=O)O)C(=O)O formula: C5H8O5
Index of correct structure: 1 of 8115
True structure loss: 0.022315
True structure:



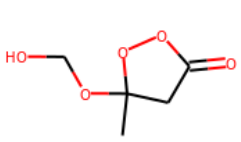
Experimental 13C NMR (solvent: DMSO)



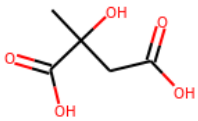
Experimental 1H NMR (solvent: D2O)



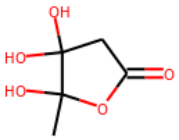
Top predicted structures (loss):



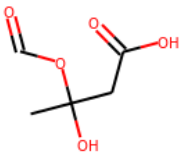
0.020519



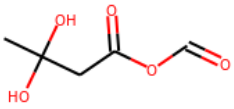
0.022315



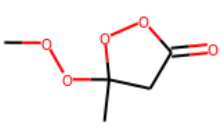
0.024159



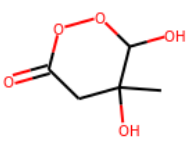
0.029605



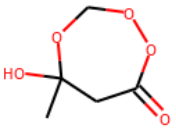
0.032483



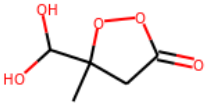
0.032936



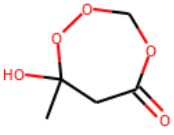
0.035614



0.039742



0.040299



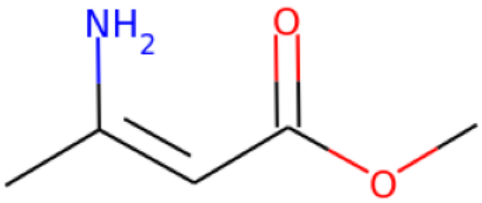
0.056143

Top predicted substructures	prob		
[#8]=[#6][#8]	1.0	[CX4H2]([#6])[#6]	0.9995
[CX3](=[OX1])O	1.0	[#8X1]=[#6X3][#6H2][#6H0]	0.9991
[#6H3][#6][#6]	0.9999	[#8][#6][#6H2]	0.9981
[CX4H3]	0.9999	[#6H3][#6H0]	0.9944
[CX3](=[OX1])C	0.9998	[OX2H1]	0.9929

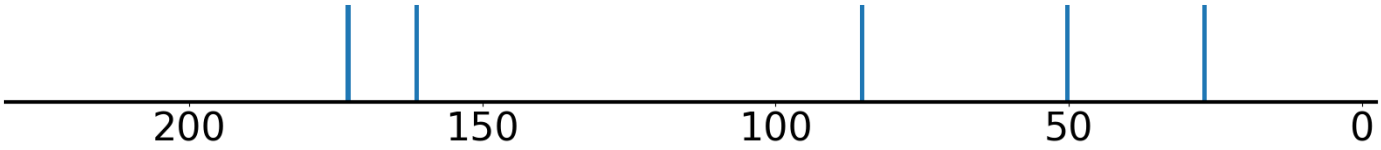
best positives	prob	best negatives	prob
[#8]=[#6][#8]	1.0	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])O	1.0	CC#CCC#C	0.0
[#6H3][#6][#6]	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3]	0.9999	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[CX3](=[OX1])C	0.9998	CC#CCC=C	0.0
[CX4H2]([#6])[#6]	0.9995	CCC#CC#C	0.0
[#8X1]=[#6X3][#6H2][#6H0]	0.9991	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#8][#6][#6H2]	0.9981	[#7][#6][#6]#[#7]	0.0
[#6H3][#6H0]	0.9944	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[OX2H1]	0.9929	C=CC=CC=C	0.0

worst negatives	prob	worst positives	prob
[OX2H0][CX3H0][CX4H2]	0.7164	[#8][#6][#6][#8]	0.147
[#6H3][#6H0]([#6H2])[#6H2]	0.4355	[#6H3][#6][#6X3]	0.1573
[CX4H2]([CX4H1])[CX3H0]	0.3879	[#8][#6][#6]=[#8]	0.1857
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.3158	[#8][#6][#6][#6][#6][#8]	0.2144
[#6H1]	0.2752	[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.2147
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2566	[#8]=[#6][#6][#6][#6]=[#8]	0.2256
[#8][#6H0][#6H1]	0.2381	[OX2H1][CX4H0][CX4H2][CX3H0]	0.3545
[CX4H2]([#6])[O]	0.1961	[CX4H2]CC=O	0.3627
[CX3H0](=[OX1H0])([OX2H0])[CX4H0]	0.1881	[CH3]CC[OH]	0.5273
[OX2H0][CX4H2][#6H0]	0.1277	[#8][#6][#6][#6][#6]=[#8]	0.5354

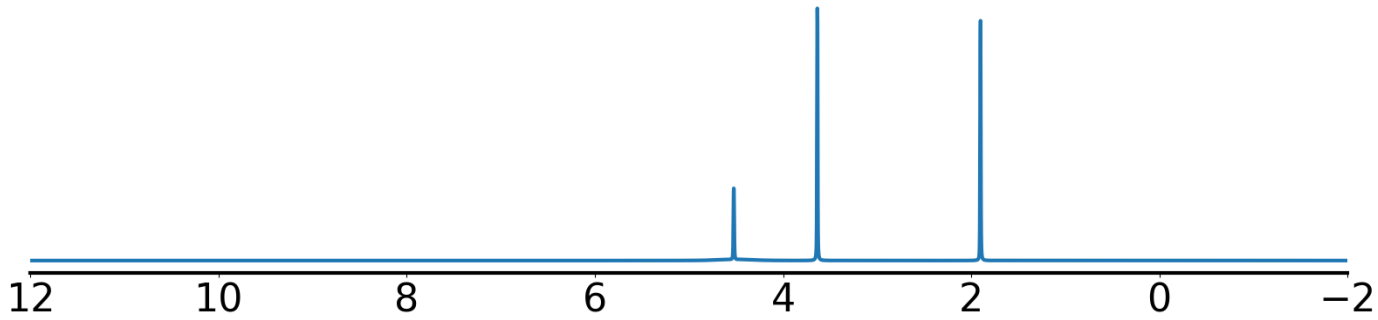
Example 23 true smiles: COC(=O)C=C(C)N formula: C5H9NO2
Index of correct structure: 32 of 6935
True structure loss: 0.068837
True structure:



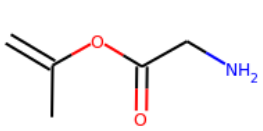
Experimental 13C NMR (solvent: CDCl3)



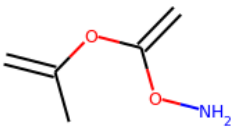
Experimental 1H NMR (solvent: CDCl3)



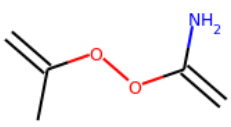
Top predicted structures (loss):



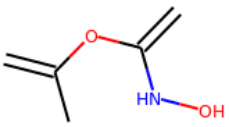
0.039482



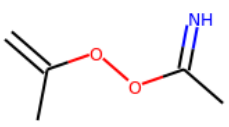
0.041694



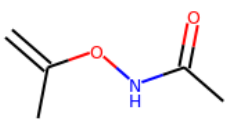
0.043046



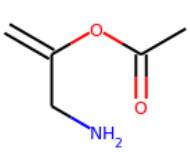
0.049456



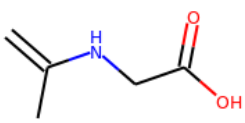
0.049768



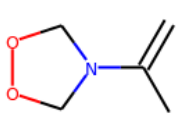
0.050278



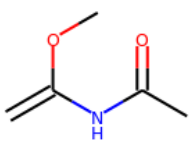
0.050999



0.051849



0.0528



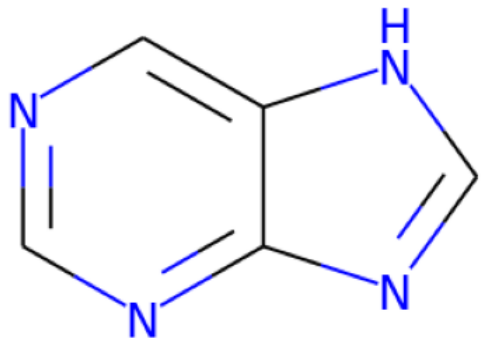
0.055925

Top predicted substructures	prob		
[CX4H3][CX3]	0.9979	[CX3](=[OX1])C	0.8923
[CX4H3]	0.9929	[CH2X3](=C)	0.8701
[CX4H3][CX3H0]	0.9525	[CX4H3][#6]	0.8517
[#6H3][#6H0]	0.9511	[#7X3H2]	0.8208
[CX3H2]=[CX3H0]	0.9031	[#8]=[#6][#8]	0.8111

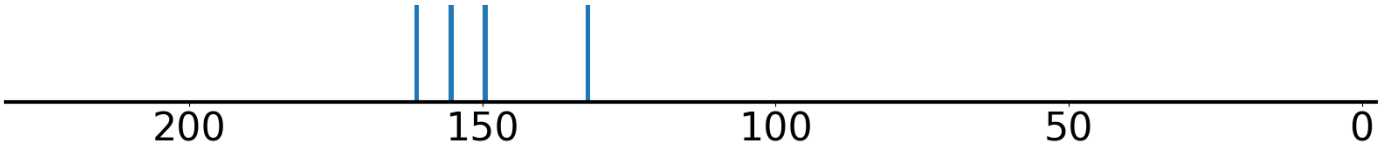
best positives	prob	best negatives	prob
[CX4H3][CX3]	0.9979	CCC#CC#C	0.0
[CX4H3]	0.9929	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][CX3H0]	0.9525	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6H3][#6H0]	0.9511	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[CX3](=[OX1])C	0.8923	[#6X2][#6H1][#6X2]	0.0
[CX4H3][#6]	0.8517	[CX4H2]([CX4H0])[CX2H0]	0.0
[#7X3H2]	0.8208	[CX4H1]([CX4H1])([CX4H1])[CX4H0]	0.0
[#8]=[#6][#8]	0.8111	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])O	0.7836	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#6H3][#6]=[#6X3]	0.7706	[CX2H0](#[CX2H1])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[CX3H2]=[CX3H0]	0.9031	[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.01
[CH2X3](=C)	0.8701	[#7][#6]=[#6X3]	0.0213
[#8][#6][#6H2]	0.8108	[#7][#6X3H0]=[#6X3H1]	0.0458
[CX4H3][CX3H0]=[CX3H2]	0.7892	[CX3H0](=[OX1H0])([OX2H0])[CX3H1]	0.0829
[#7X3][#6H2]	0.7751	[#6X3H1]=[#6X3H0]	0.0851
[#7][#6H2]	0.7264	[CX4H3][OX2H0]	0.1684
[#8][#6]=[#6H2]	0.6554	[#6H1]	0.1744
[#7][#6][#6X3]	0.6018	[#7][#6][#6H3]	0.2123
[#6X3H2]	0.5889	O=C[CX3H]	0.2371
[CX3H2]=CO	0.5568	[#8][#6][#6]=[#6X3]	0.253

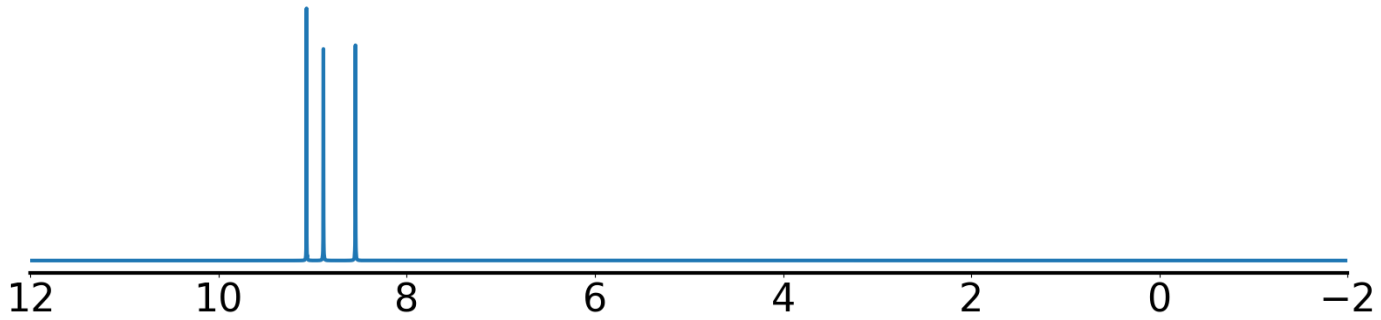
Example 24 true smiles: c1ncc2[nH]cnc2n1 formula: C5H4N4
Index of correct structure: 3 of 6256
True structure loss: 0.019535
True structure:



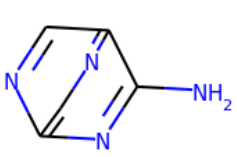
Experimental 13C NMR (solvent: D2O)



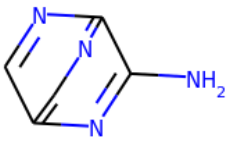
Experimental 1H NMR (solvent: D2O)



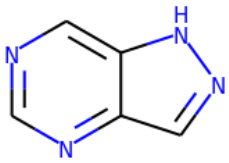
Top predicted structures (loss):



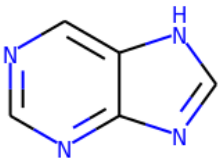
0.018063



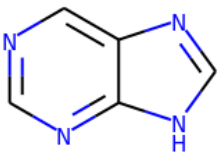
0.018063



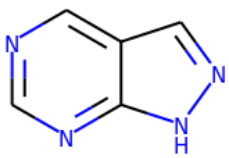
0.01853



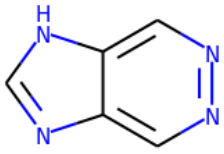
0.019535



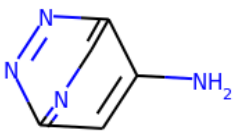
0.019535



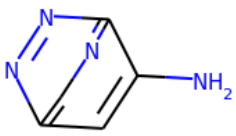
0.021099



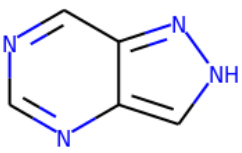
0.021188



0.022142



0.022142



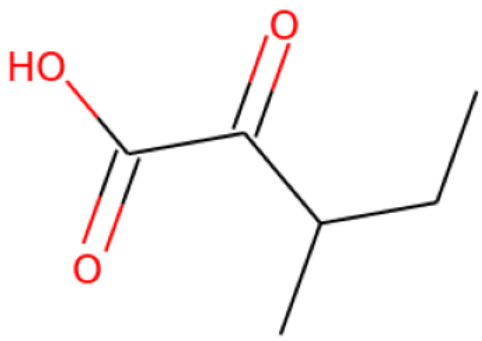
0.02358

Top predicted substructures	prob		
[#6H1]	0.9995	[#7][#6][#6][#6X3]	0.972
[#7][#6][#6X3]	0.9979	[cX3H1]([nX2H0])[cX3H0]	0.9328
[#6X3][#6X3]	0.9956	[#7][#6][#7]	0.9151
[cH]	0.9934	[#6X3][#7][#6X3]	0.9115
[#6X3H1][#6X3H0]	0.9906	[#7][#6][#6][#6][#7]	0.8856

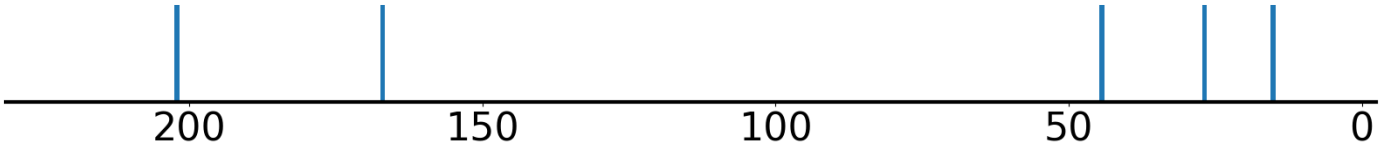
best positives	prob	best negatives	prob
[#6H1]	0.9995	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6][#6X3]	0.9979	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3]	0.9956	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[cH]	0.9934	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3H1][#6X3H0]	0.9906	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#7][#6][#6][#6X3]	0.972	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([nX2H0])[cX3H0]	0.9328	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[#7][#6][#7]	0.9151	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0
[#6X3][#7][#6X3]	0.9115	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6][#6][#7]	0.8856	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6X3][#6X3][#6X3]	0.699	[#6]1[#6][#7][#6][#7]1	0.0387
[cH][cH]	0.5086	[#7H][#6X3H1]	0.1374
[#7][#7]	0.4519	[#7X3H1]	0.2139
[cX3H1]([nX2H0])[cX3H1]	0.3823	[#6H1r5][#7]	0.2143
[#7][#6][#6][#6][#6][#7]	0.3706	[#6X3][#7X3][#6X3]	0.4718
[#7X3H2]	0.3652	[#7][#6][#6][#7]	0.5541
[cX3H1]([cX3H1])[cX3H0]	0.3639	[#7][#6H0][#7]	0.5701
[#7H2][#6H0]	0.3256	[#7][#6H0][#6H1]	0.7341
[#8][#6H0][#6H1]	0.2648	[#7][#6X3H0][#6X3H1]	0.7677
[#6H1][#6H1]	0.2312	[#6H1][#7][#6H1]	0.8053

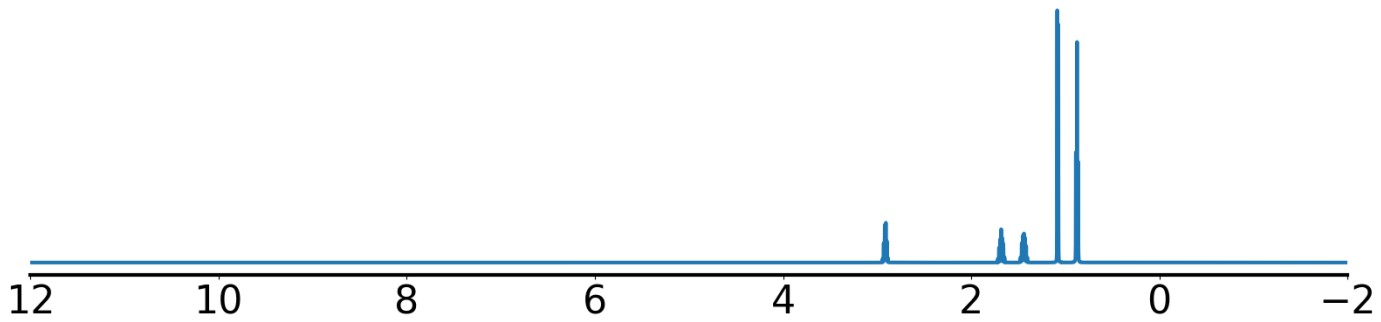
Example 25 true smiles: CCC(C)C(=O)C(=O)O formula: C6H10O3
Index of correct structure: 0 of 6069
True structure loss: 0.021241
True structure:



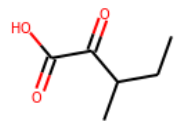
Experimental 13C NMR (solvent: CDCl3)



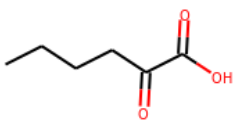
Experimental 1H NMR (solvent: D2O)



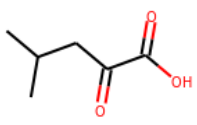
Top predicted structures (loss):



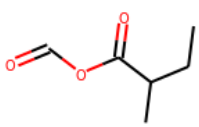
0.021241



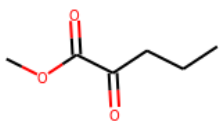
0.034124



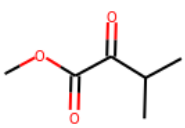
0.038773



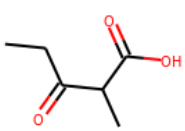
0.052157



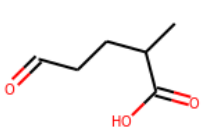
0.052959



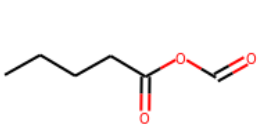
0.061265



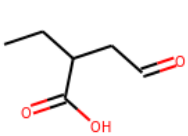
0.065131



0.066794



0.071492



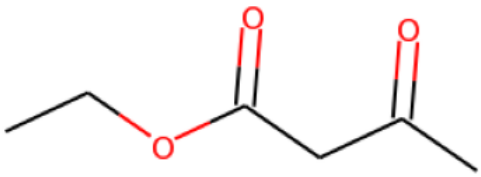
0.073254

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9999	[CX3](=[OX1])O	0.996
[CX4H3]	0.9993	[#8]=[#6][#6]=[#8]	0.9951
[#6H3][#6][#6]	0.9983	[CX4H3][#6]	0.9942
[CX4H2]([#6])[#6]	0.9974	O=CC=O	0.9839
[#8]=[#6][#8]	0.9961	[CX4H2]CC=O	0.9391

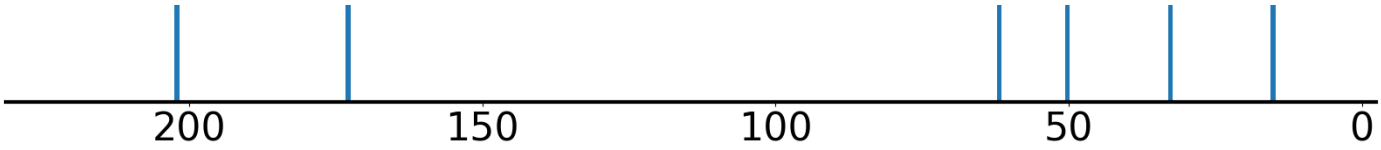
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3]	0.9993	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#6H3][#6][#6]	0.9983	CCC#CC#C	0.0
[CX4H2]([#6])[#6]	0.9974	CCC=CC#C	0.0
[#8]=[#6][#8]	0.9961	CC#CCC#C	0.0
[CX3](=[OX1])O	0.996	C=CCCC#C	0.0
[#8]=[#6][#6]=[#8]	0.9951	C=CC=CC#C	0.0
[CX4H3][#6]	0.9942	[#6H2][#6]#[#6X2]	0.0
O=CC=O	0.9839	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2]CC=O	0.9391	[CX2H0](#[CX2H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H3])[CX4H2]	0.7067	[#6H3][#6][#6][#6H3]	0.0972
[CX3H0](=[OX1H0])([CX4H2])[CX3H0]	0.5411	[CX4H1]([CX4H3])([CX4H2])[CX3H0]	0.1664
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.5047	[OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]	0.1812
[CX4H2][CX3]=O	0.4796	[#8][#6][#6]=[#8]	0.3767
[CX4H2][CX4H2]	0.4556	[CX4H3][CX4H1]	0.4931
[#8][#6][#6H2]	0.3548	[CX4H2]([CX4H3])[CX4H1]	0.5855
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3269	O=[CX3][CX4H]	0.5926
[#8][#6H0][#6H1]	0.256	[#8]=[#6H0][#6H1]	0.6546
OCC[CH2]	0.2413	[CHX4]([CH3X4])[CH2X4]	0.6852
CCCCCC	0.2125	[CX3H0](=[OX1H0])([CX4H1])[CX3H0]	0.708

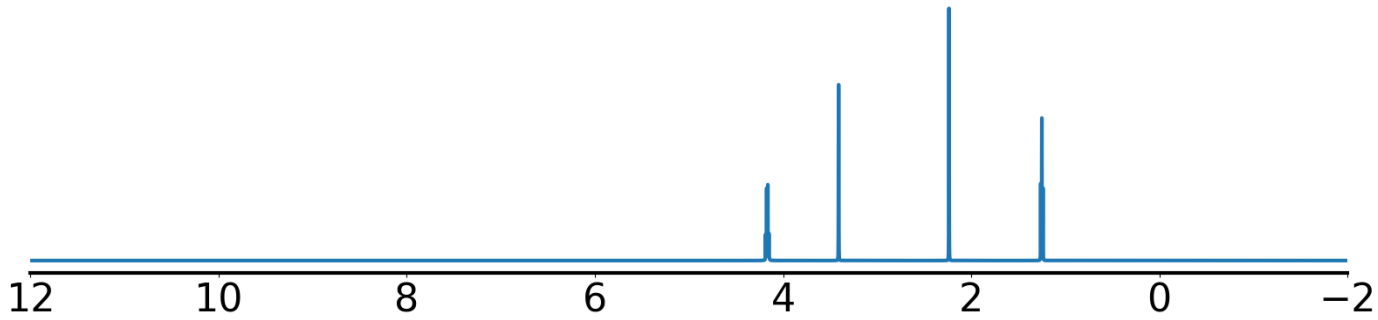
Example 26 true smiles: CCOC(=O)CC(C)=O formula: C6H10O3
Index of correct structure: 0 of 6069
True structure loss: 0.020259
True structure:



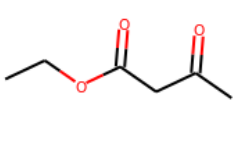
Experimental 13C NMR (solvent: CDCl3)



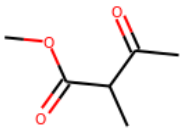
Experimental 1H NMR (solvent: CDCl3)



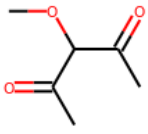
Top predicted structures (loss):



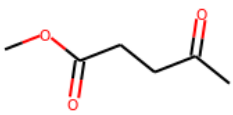
0.020259



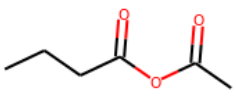
0.053425



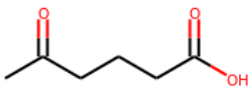
0.056301



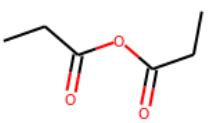
0.058655



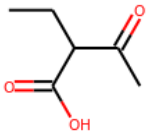
0.058773



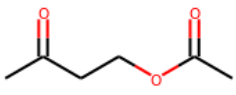
0.063125



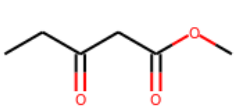
0.065091



0.066846



0.066941



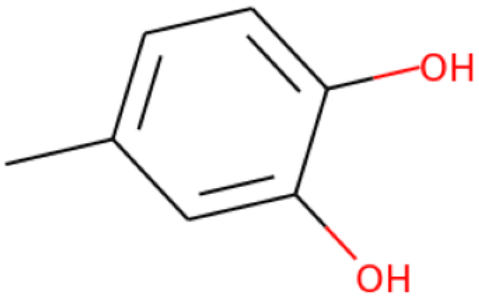
0.069215

Top predicted substructures	prob		
[CX4H3]	1.0	[OX1H0]=[CX3H0][CX4H3]	0.9894
[CX3](=[OX1])C	1.0	[#6H3][#6H0]	0.9881
[CX4H3][CX3H0]	0.9977	[CX3](=[OX1])O	0.9699
[CX4H3][#6]	0.9968	[#8]=[#6][#8]	0.9648
[CX4H3][CX3]	0.9959	[#6H3][#6][#6]	0.9262

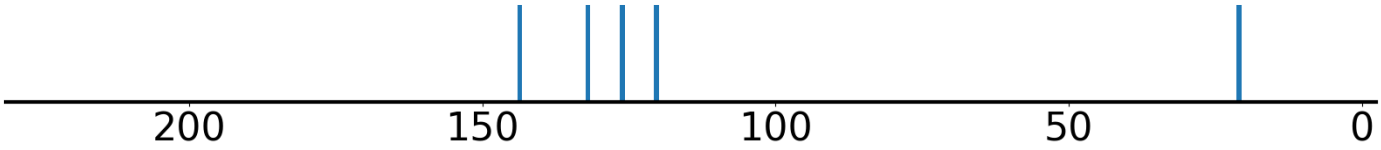
best positives	prob	best negatives	prob
[CX4H3]	1.0	CCC#CC#C	0.0
[CX3](=[OX1])C	1.0	[#6X2][#6H1][#6X2]	0.0
[CX4H3][CX3H0]	0.9977	CC=CC#CC	0.0
[CX4H3][#6]	0.9968	CCC=CC#C	0.0
[CX4H3][CX3]	0.9959	[CX3H1](=[CX3H2])[CX2H0]	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9894	[#7][#6]=[#6][#6]#[#7]	0.0
[#6H3][#6H0]	0.9881	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.9699	C=CC=CC#C	0.0
[#8]=[#6][#8]	0.9648	[CX2H0](#[CX2H1])[CX2H0]	0.0
[#6H3][#6][#6]	0.9262	[CX2H0](#[CX2H1])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[#6H3][#6][#6X3]	0.6399	[CX4H2]([#6])[O]	0.2969
[#6H1]	0.507	[OX2H0][CX3H0][CX4H2]	0.3147
[CX4H3][OX2H0]	0.4892	[#6H3][#6X3H0][#6H2]	0.3208
[#8]=[#6H0][#6H1]	0.3417	[CX4H3][CX4H2]	0.3337
[CX4H2]CC=O	0.3348	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.3771
[#8]=[#6][#6]=[#8]	0.2967	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.3901
[#8][#6][#6][#6][#6]=[#8]	0.2391	[CX4H3][CX4]O	0.488
[#8][#6H0][#6H1]	0.2331	[CH3][#6][#8]	0.523
[OX2H1]	0.2226	[#6X3][#6][#6][#6H3]	0.5452
[#6H1][#6H2]	0.2034	[CX4H2]([OX2H0])[CX4H3]	0.6337

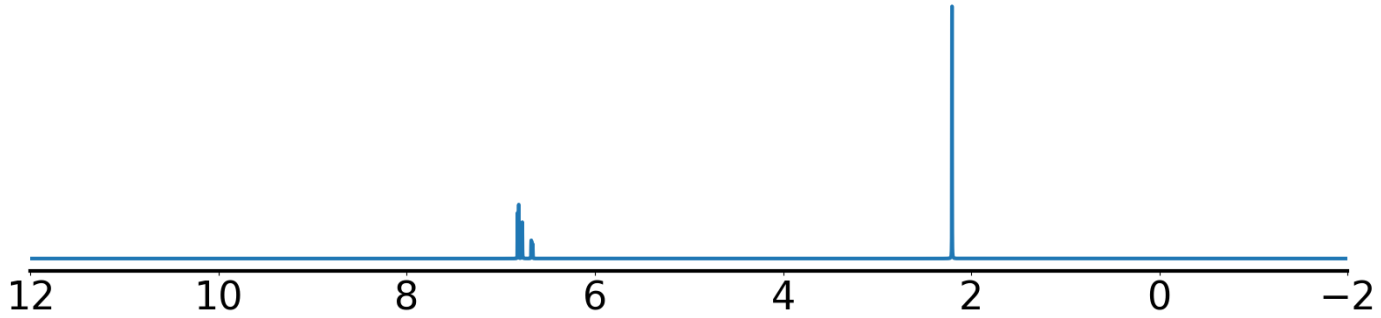
Example 27 true smiles: Cc1ccc(O)c(O)c1 formula: C7H8O2
Index of correct structure: 2 of 5977
True structure loss: 0.017126
True structure:



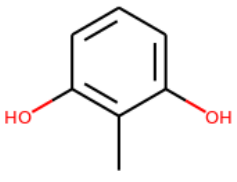
Experimental 13C NMR (solvent: CDCl3)



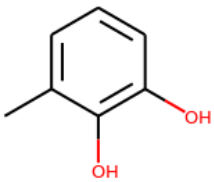
Experimental 1H NMR (solvent: D2O)



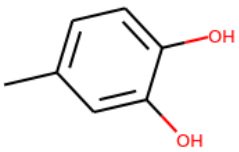
Top predicted structures (loss):



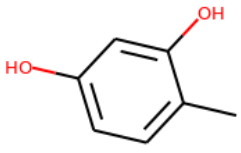
0.010273



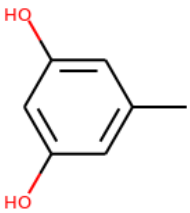
0.011851



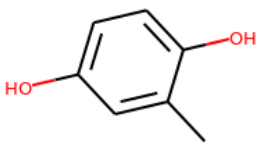
0.017126



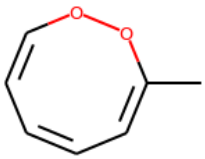
0.017484



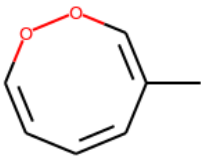
0.018236



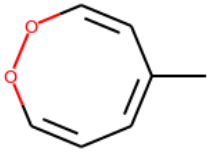
0.020811



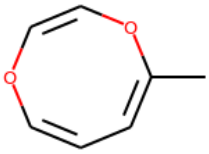
0.029144



0.032264



0.033178



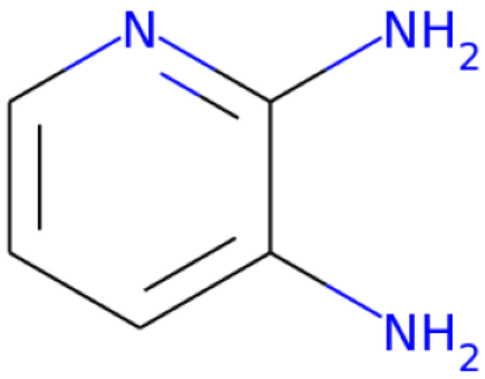
0.034198

Top predicted substructures	prob		
[#6X3][#6X3][#6X3][#6X3]	0.9969	[#6H3][#6H0]	0.9832
[#6X3][#6X3]	0.9952	[#6X3H1][#6X3H0]	0.9797
[#6H1]	0.9928	[#6H3][#6][#6]	0.9732
[CX4H3]	0.9919	[cH]	0.9326
[CX4H3][#6]	0.984	[#6X3][#6][#6][#6H3]	0.9161

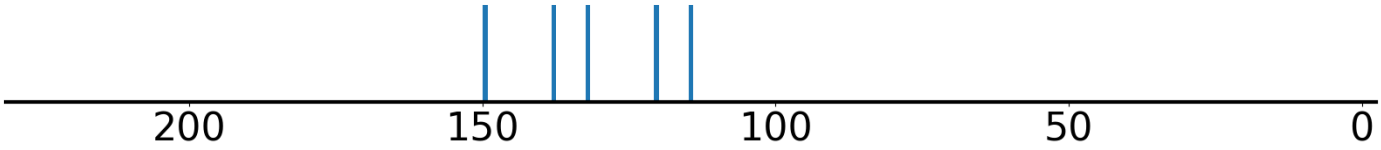
best positives	prob	best negatives	prob
[#6X3][#6X3][#6X3][#6X3]	0.9969	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#6X3][#6X3]	0.9952	[CX4H2]([NX2H0])[CX4H1]	0.0
[#6H1]	0.9928	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3]	0.9919	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[CX4H3][#6]	0.984	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6H3][#6H0]	0.9832	[#6H3][#6H1][#7][#7]	0.0
[#6X3H1][#6X3H0]	0.9797	[CX4H1]([NX3H0])([CX4H1])[CX4H1]	0.0
[#6H3][#6][#6]	0.9732	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[cH]	0.9326	[CX4H1]([NX3H0])([CX4H2])[CX4H1]	0.0
[#6X3][#6][#6][#6H3]	0.9161	[CX3H0](=[NX2H1])([NX3H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.3751	[cX3H0][cX3H1][cX3H0][OX2H1]	0.1083
[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.2836	[cX3H0][cX3H1][cX3H1][cX3H0]	0.1496
[CH3][#6][#8]	0.2673	[cX3H1]([cX3H0])[cX3H0]	0.1797
[CHX3]=[CHX3]	0.1661	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.2458
o[cH]	0.1549	[#8][#6X3][#6X3][#6X3][#6H3]	0.3621
[#8]=[#6][#8]	0.1518	[#8][#6][#6][#8]	0.4955
[CX3H](O)	0.131	[#6H1][#6H1]	0.558
[#6H3][#6]=[#6X3]	0.1016	[#8][#6H0][#6H1]	0.5874
[#6H][#8][#6H]	0.0997	[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.6927
[O][CX3H1]=[CX3H1]	0.0992	[#6]1[#6][#6][#6][#6][#6]1	0.7131

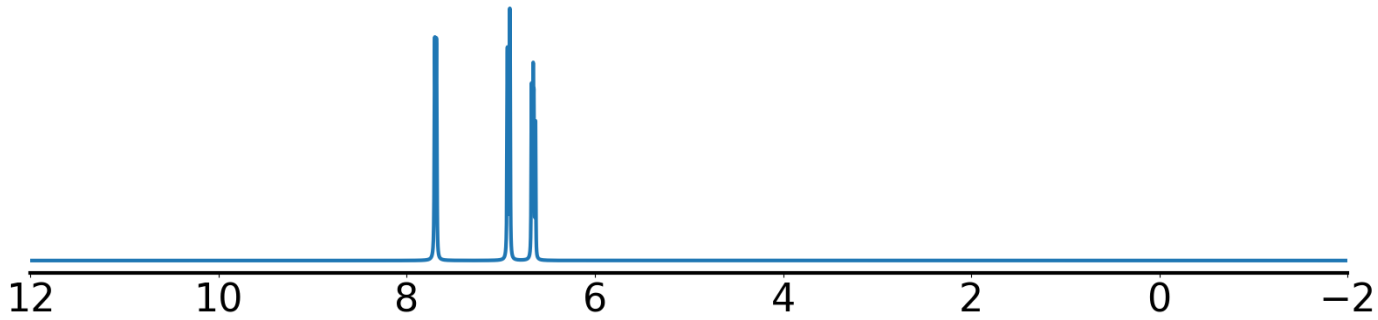
Example 28 true smiles: Nc1cccnc1N formula: C5H7N3
Index of correct structure: 1 of 5951
True structure loss: 0.017388
True structure:



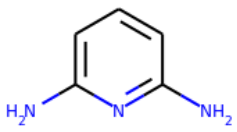
Experimental 13C NMR (solvent: DMSO)



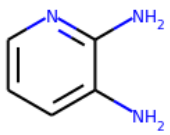
Experimental 1H NMR (solvent: CDCl3)



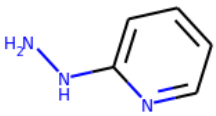
Top predicted structures (loss):



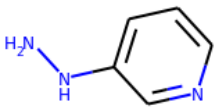
0.014871



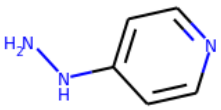
0.017388



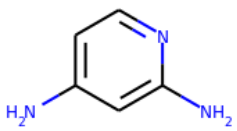
0.021729



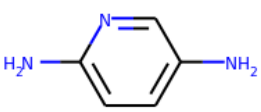
0.024243



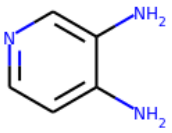
0.024512



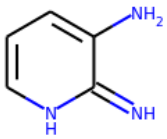
0.024764



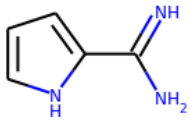
0.026398



0.027241



0.031042



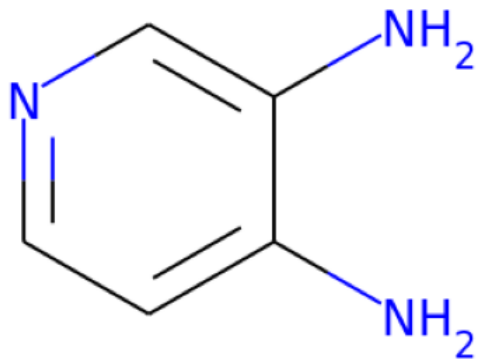
0.033035

Top predicted substructures	prob		
[#6H1]	0.9999	[#7][#6][#6X3]	0.9882
[cH][cH]	0.9993	[cX3H1]([cX3H1])[cX3H1]	0.9851
[#6X3][#6X3][#6X3][#6X3]	0.9974	[cH]	0.9827
[#6X3][#6X3]	0.9965	[#7][#6][#6][#6X3]	0.9598
[cX3H1]([cX3H1])[cX3H0]	0.9895	[#6X3H1][#6X3H0]	0.9563

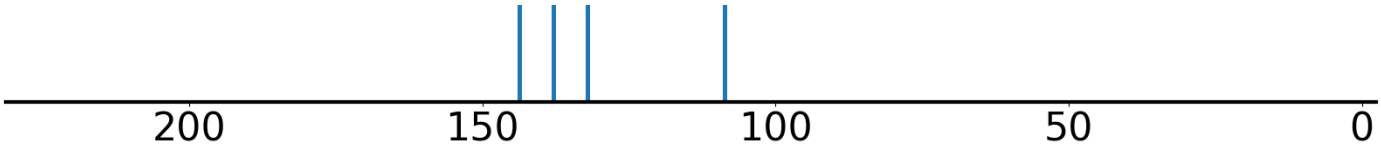
best positives	prob	best negatives	prob
[#6H1]	0.9999	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9993	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9974	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3][#6X3]	0.9965	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9895	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#7][#6][#6X3]	0.9882	[OX2H0][CX4H1][CX4H1]([CX4H1])[CX4H2]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9851	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
[cH]	0.9827	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#7][#6][#6][#6X3]	0.9598	[OX2H0]1[CX4H2][CX4H2][CX4H0]1	0.0
[#6X3H1][#6X3H0]	0.9563	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7X3][#6X3]	0.6904	[cX3H1]([nX2H0])[cX3H1]	0.2669
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6416	[#7][#6][#6][#7]	0.2723
[#7][#7]	0.4984	[#7][#6H0][#7]	0.35
[#7X3H1]	0.4727	[#7][#6][#6][#6][#6][#7]	0.3975
[#7H][#6X3H1]	0.4332	[#7][#6][#7]	0.5897
[#7]=[#6][#6][#6X3]	0.3247	[#6]1[#6][#6][#6][#6][#7]1	0.6015
[#6]1[#6][#6][#6][#6][#6]1	0.3178	[#7H2][#6H0]	0.7063
[#6]1[#6][#6][#6][#7]1	0.3151	[#7][#6H0][#6H1]	0.7875
[NH1]=[#6][#7]	0.2905	[#6X3][#7][#6X3]	0.8356
[#7][#6][#6][#6][#7]	0.2805	[#7][#6X3H0][#6X3H1]	0.8627

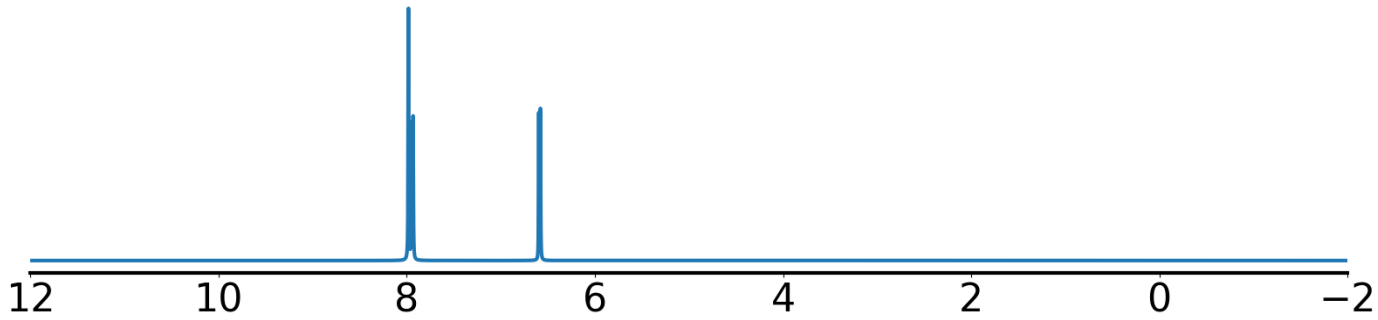
Example 29 true smiles: Nc1ccncc1N formula: C5H7N3
Index of correct structure: 5 of 5951
True structure loss: 0.025336
True structure:



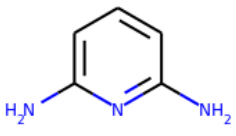
Experimental 13C NMR (solvent: DMSO)



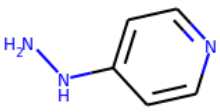
Experimental 1H NMR (solvent: CDCl3)



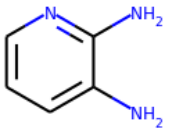
Top predicted structures (loss):



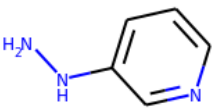
0.019781



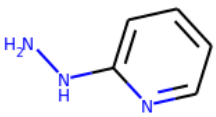
0.021108



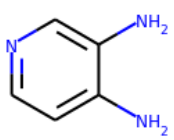
0.02353



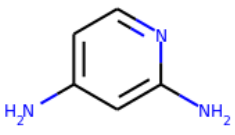
0.024253



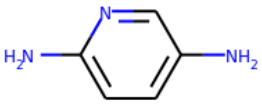
0.024296



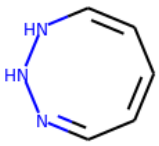
0.025336



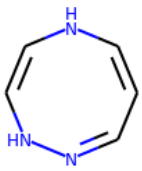
0.025991



0.02814



0.02965



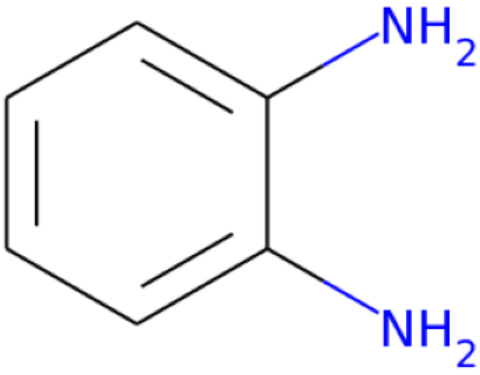
0.031571

Top predicted substructures	prob		
[#6H1]	0.9997	[#6X3H1][#6X3H0]	0.9422
[#6X3][#6X3]	0.9953	[cX3H1]([cX3H1])[cX3H0]	0.9216
[cH][cH]	0.9702	[#7][#6][#6][#6X3]	0.9143
[cH]	0.9672	[#6H1][#6H1]	0.8697
[#7][#6][#6X3]	0.9487	[#6X3][#7][#6X3]	0.7855

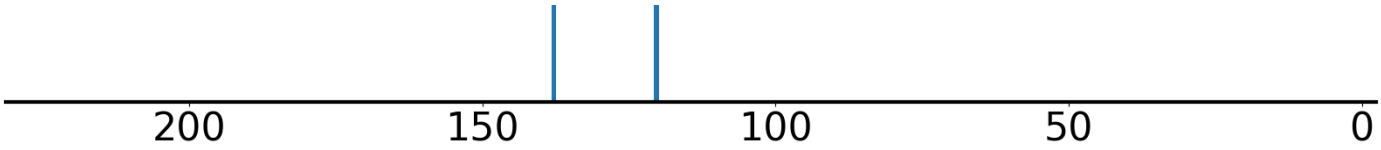
best positives	prob	best negatives	prob
[#6H1]	0.9997	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9953	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cH][cH]	0.9702	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
[cH]	0.9672	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6X3]	0.9487	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[#6X3H1][#6X3H0]	0.9422	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9216	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.9143	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H1][#6H1]	0.8697	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#6X3][#7][#6X3]	0.7855	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.7634	[#7][#6][#6][#6][#6][#7]	0.107
[#6X3][#7X3][#6X3]	0.5853	[cX3H1]([nX2H0])[cX3H0]	0.2153
[#7X3H1]	0.5513	[#7][#6][#6][#7]	0.2168
[#7][#7]	0.5195	[#7][#6][#6][#6][#7]	0.3733
[#7H][#6X3H1]	0.4874	[#6]1[#6][#6][#6][#6][#7]1	0.3814
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.4676	[#7H2][#6H0]	0.388
[NH1]=[#6][#7]	0.4448	[#6H1][#7][#6H1]	0.4014
[#6]=[#7H]	0.4223	[cX3H1]([nX2H0])[cX3H1]	0.455
[#7][#6][#7]	0.4072	[#7][#6H0][#6H1]	0.7144
[#7][#6]=[#7]	0.3363	[#7X3H2]	0.7193

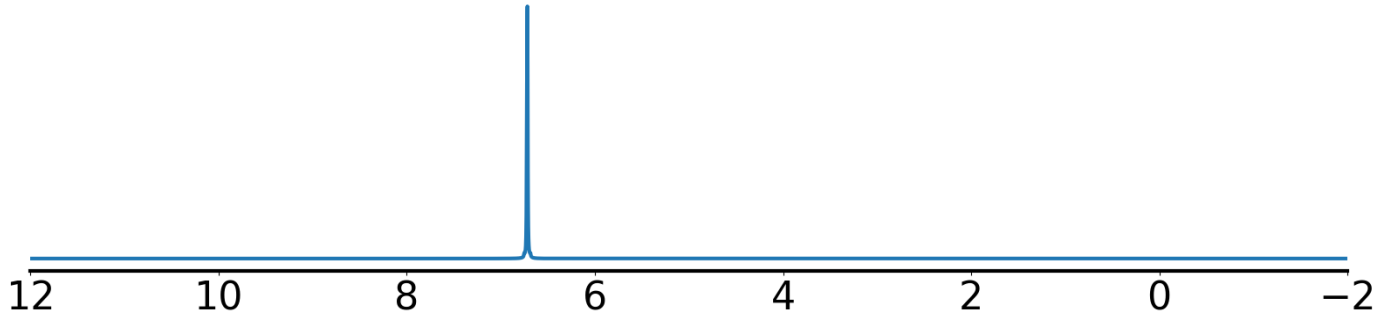
Example 30 true smiles: Nc1ccccc1N formula: C6H8N2
Index of correct structure: 0 of 4358
True structure loss: 0.01771
True structure:



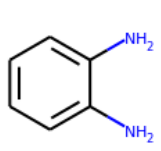
Experimental 13C NMR (solvent: CDCl3)



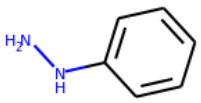
Experimental 1H NMR (solvent: CDCl3)



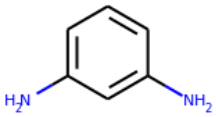
Top predicted structures (loss):



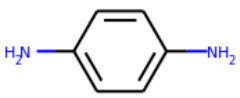
0.01771



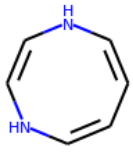
0.019543



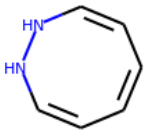
0.021588



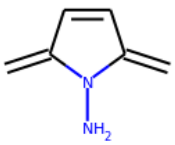
0.021869



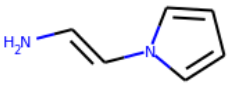
0.023951



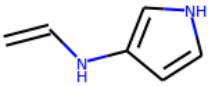
0.024944



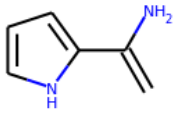
0.032202



0.036647



0.037697



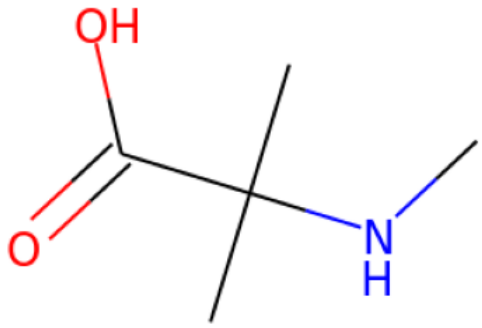
0.041615

Top predicted substructures	prob		
[#6H1]	0.981	[#7][#6][#6X3]	0.9058
[#6X3][#6X3]	0.9786	[#6X3H1][#6X3H0]	0.8657
[#6X3][#6X3][#6X3][#6X3]	0.9771	[#7][#6][#6][#6X3]	0.8447
[cH][cH]	0.9317	[#6H1][#6H1]	0.8107
[cH]	0.9289	[cX3H1]([cX3H1])[cX3H0]	0.7935

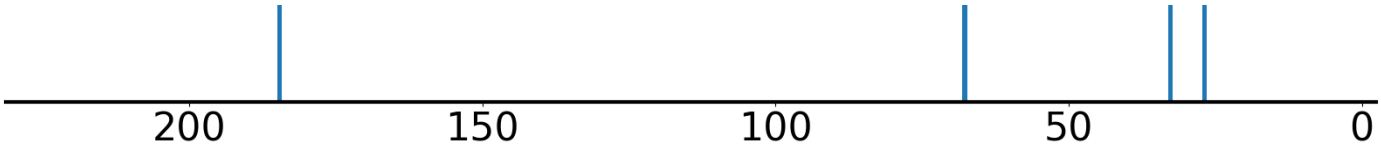
best positives	prob	best negatives	prob
[#6H1]	0.981	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9786	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9771	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH][cH]	0.9317	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cH]	0.9289	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[#7][#6][#6X3]	0.9058	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3H1][#6X3H0]	0.8657	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6][#6X3]	0.8447	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H1][#6H1]	0.8107	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.7935	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#7][#6H1]	0.6072	[#7][#6][#6][#7]	0.1767
[#6X3][#7][#6X3]	0.5978	[#6]1[#6][#6][#6][#6][#6]1	0.452
[#6X3][#7X3][#6X3]	0.5857	[#7H2][#6H0]	0.4854
[#6]1[#6][#6][#6][#7]1	0.5451	[#7][#6H0][#6H1]	0.5142
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5094	[#7][#6X3H0][#6X3H1]	0.5562
[#7H][#6X3H1]	0.5056	[#7X3H2]	0.7118
[#7X3H1]	0.5037	[cX3H1]([cX3H1])[cX3H1]	0.7809
[#6H1r5][#7]	0.4704	[cX3H1]([cX3H1])[cX3H0]	0.7935
[cX3H1]([nX3H1])[cX3H0]	0.3558	[#6H1][#6H1]	0.8107
[cX3H1]([nX3H1])[cX3H1]	0.2789	[#7][#6][#6][#6X3]	0.8447

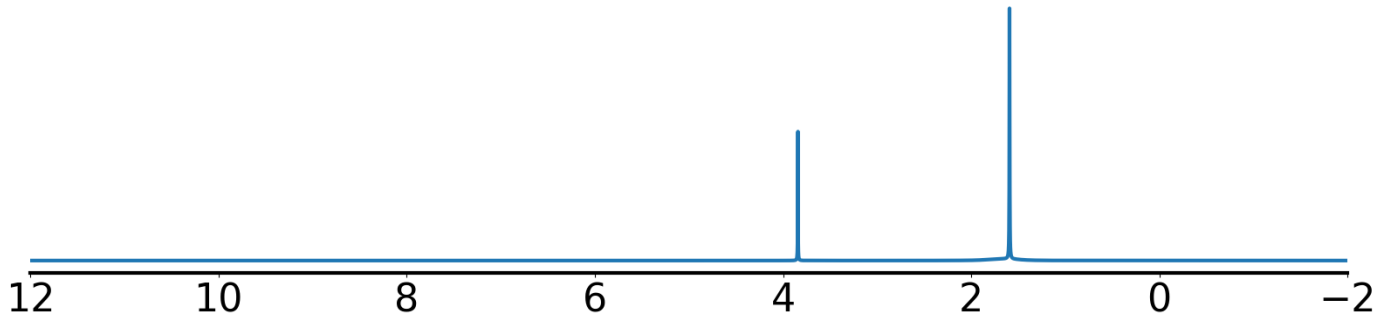
Example 31 true smiles: CNC(C)(C)C(=O)O formula: C5H11NO2
Index of correct structure: 15 of 3703
True structure loss: 0.046642
True structure:



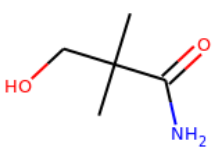
Experimental 13C NMR (solvent: D2O)



Experimental 1H NMR (solvent: D2O)



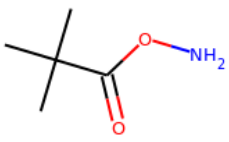
Top predicted structures (loss):



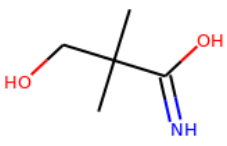
0.02522

0.027341

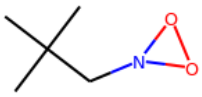
0.031369



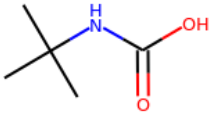
0.032131



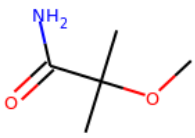
0.032692



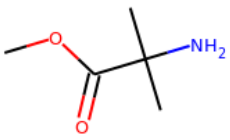
0.033951



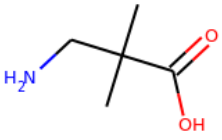
0.036758



0.03894



0.040791



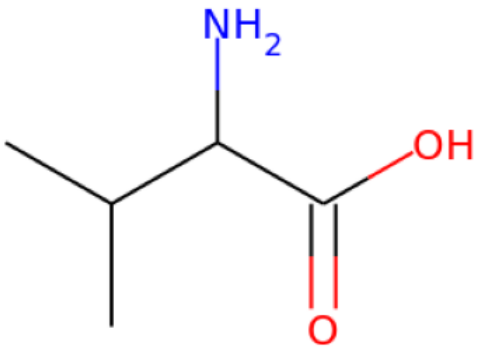
0.041005

Top predicted substructures	prob		
[CX4H3]	0.9759	[#6H3][#6H0]	0.8876
[CX4H3][#6]	0.9449	[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.7469
[CX3](=[OX1])C	0.9448	[#7X3H2]	0.7278
[OX2H1]	0.917	[CX4H2]([#6])[O]	0.7191
[#6H3][#6][#6]	0.9131	[#7X3][#6H2]	0.6466

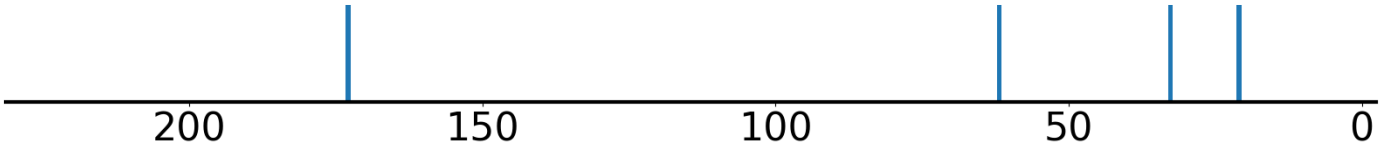
best positives	prob	best negatives	prob
[CX4H3]	0.9759	C=CCCC#C	0.0
[CX4H3][#6]	0.9449	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])C	0.9448	CCC#CC#C	0.0
[OX2H1]	0.917	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#6H3][#6][#6]	0.9131	C=CC=CC#C	0.0
[#6H3][#6H0]	0.8876	CCC=CC#C	0.0
[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.7469	CC#CCC#C	0.0
[CX4H3][CX4H0]	0.5924	[#6X2][#6H1][#6X2]	0.0
[#6H3][#6][#6X3]	0.4327	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8]=[#6][#8]	0.4136	[CX3H1](=[CX3H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7X3H2]	0.7278	[#6H3][#6H0][#7][#6H3]	0.0064
[CX4H2]([#6])[O]	0.7191	[#7X3][#6H3]	0.0114
[#7X3][#6H2]	0.6466	[#7][#6][#6H3]	0.0727
[CH2X4](O)[CX4H2][CX4H2]	0.558	[#6H3][#7]	0.087
[#7H2][#6H0]	0.4795	[CX4H3][NX3H1]	0.0945
OCC[CH2]	0.444	[CX3](=O)[OX2H1]	0.1341
[#7][#6H2]	0.4421	[#7X3H1]	0.152
[CX4H2][CX4H2]	0.428	[CH3]CC[OH]	0.161
[CX4H2]([OX2H1])[CX4H0]	0.3945	[#7][#6][#6X3]	0.1724
[#8][#6][#6]=[#8]	0.3779	[CX4H3][CX4H0][CX4H3]	0.2059

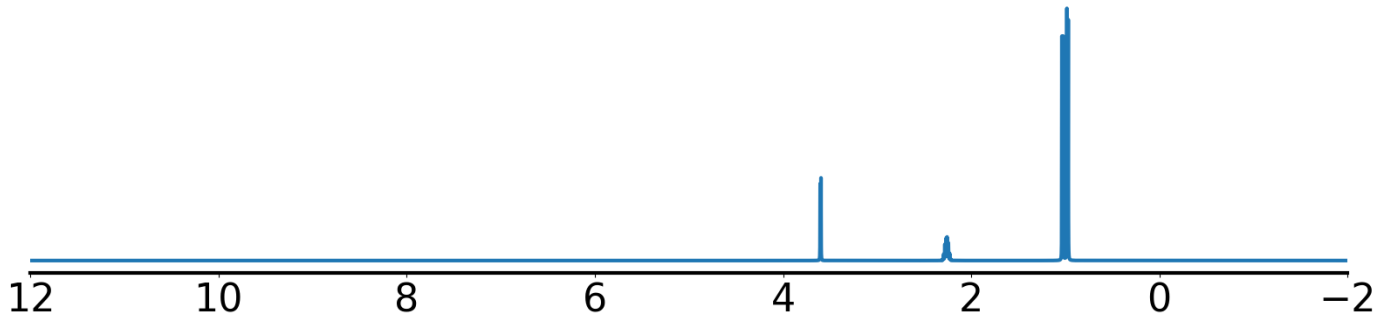
Example 32 true smiles: CC(C)C(N)C(=O)O formula: C5H11NO2
Index of correct structure: 4 of 3703
True structure loss: 0.029994
True structure:



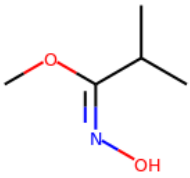
Experimental 13C NMR (solvent: D2O)



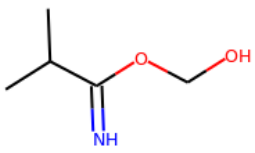
Experimental 1H NMR (solvent: D2O)



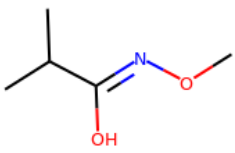
Top predicted structures (loss):



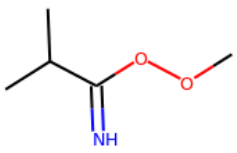
0.021598



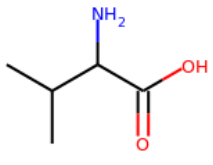
0.024027



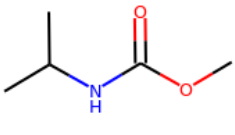
0.028045



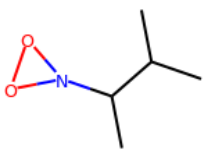
0.0287



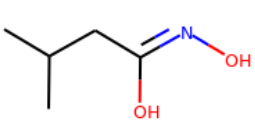
0.029994



0.030137

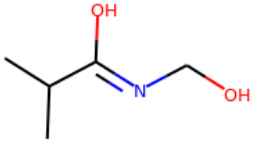


0.031042



0.033054

0.035145



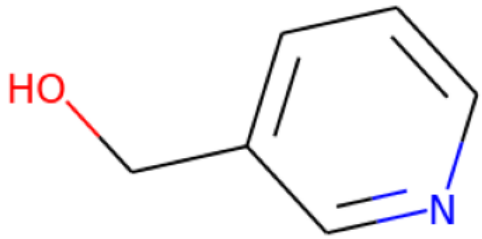
0.035147

Top predicted substructures	prob		
[CX4H3]	1.0	[#6H1]	0.9041
[#6H3][#6][#6]	0.9986	[CX4H3][CX4H1]	0.9018
[CX4H3][#6]	0.9905	[CX3](=[OX1])C	0.8841
[CHX4]([CH3X4])[CH3X4]	0.9588	[#8]=[#6][#8]	0.8539
[OX2H1]	0.9386	[CX3](=[OX1])O	0.7789

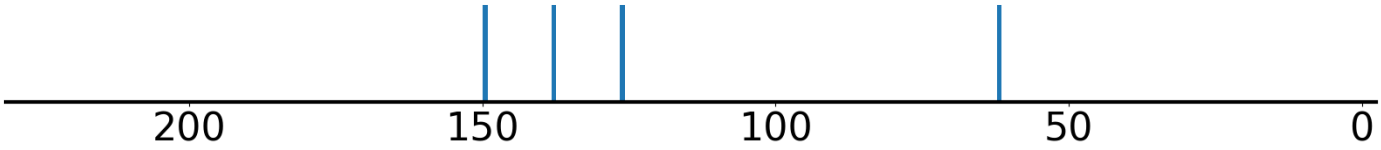
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9986	CC=CC#CC	0.0
[CX4H3][#6]	0.9905	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CHX4]([CH3X4])[CH3X4]	0.9588	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX2H1]	0.9386	CCC#CC#C	0.0
[#6H1]	0.9041	C=CCCC#C	0.0
[CX4H3][CX4H1]	0.9018	CCC=CC#C	0.0
[CX3](=[OX1])C	0.8841	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#8]=[#6][#8]	0.8539	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX3](=[OX1])O	0.7789	CC#CCC=C	0.0

worst negatives	prob	worst positives	prob
[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.7252	[#7H2][#6X4H1][#6X3]	0.0877
[#6H3][#6][#6X3]	0.5599	[CX4H1]([CX4H3])([CX4H3])[CX4H1]	0.0972
[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.3017	[#8]=[#6][#6H1][#6H1]	0.1208
[CX4H2]([#6])[O]	0.2911	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.1229
[#6H1][#6H2]	0.2774	O=[CX3][CX4H]	0.1951
[#7X3H1]	0.2222	[#8][#6H0][#6H1]	0.2224
[CX4H2][CX3]=O	0.2122	[#7][#6][#6X3]	0.255
[CHX4]([CH3X4])[CH2X4]	0.1853	[#6H3][#6H1][#6H1][#7]	0.3035
[#7H2][#6H0]	0.1523	[#7H2][#6H1]	0.3157
[#7]=[#6H0][#6H1]	0.1488	[#6X3][#6][#6][#6H3]	0.3222

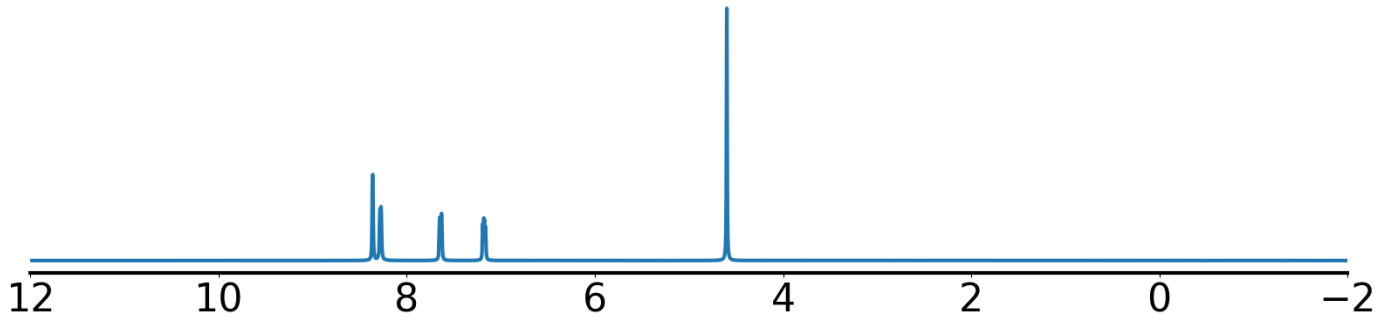
Example 33 true smiles: OCc1cccnc1 formula: C6H7NO
Index of correct structure: 0 of 3639
True structure loss: 0.012653
True structure:



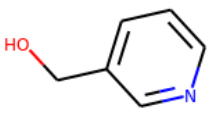
Experimental 13C NMR (solvent: CDCl3)



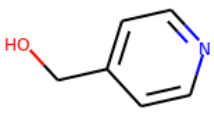
Experimental 1H NMR (solvent: CDCl3)



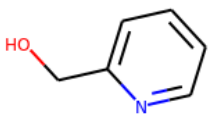
Top predicted structures (loss):



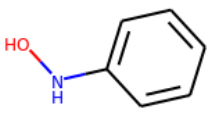
0.012653



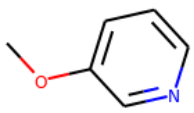
0.013761



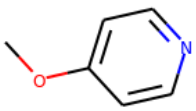
0.014018



0.02853

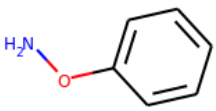


0.033872

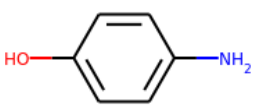


0.034979

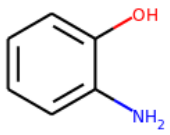
0.035236



0.036679



0.042206



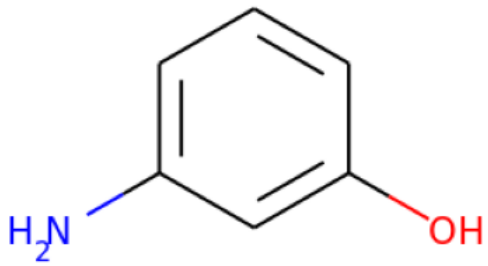
0.044977

Top predicted substructures	prob		
[#6H1]	0.9997	[#6X3][#6X3][#6X3][#6X3]	0.9476
[#6X3][#6X3]	0.9943	[cH]	0.9367
[CX4H2]([#6])[O]	0.993	[#6H1][#6H1]	0.9243
[cH][cH]	0.9846	[#6X3][#6H2][#8]	0.8929
[#7][#6][#6X3]	0.9809	[OX2H1]	0.8841

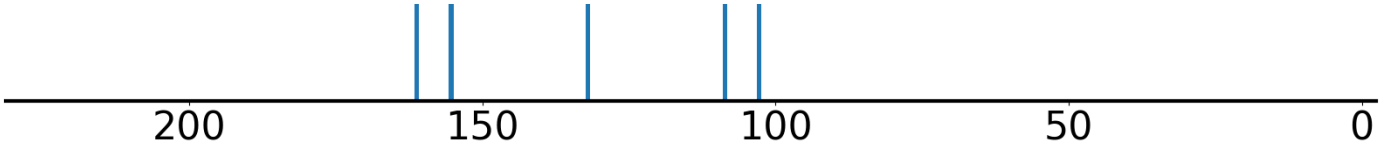
best positives	prob	best negatives	prob
[#6H1]	0.9997	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9943	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H2]([#6])[O]	0.993	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9846	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#7][#6][#6X3]	0.9809	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9476	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.9367	[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.0
[#6H1][#6H1]	0.9243	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6H2][#8]	0.8929	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[OX2H1]	0.8841	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[#6]1[#6][#6][#6][#6][#6]1	0.3921	[cX3H1]([nX2H0])[cX3H0]	0.3499
[#7][#6X3H0][#6X3H1]	0.3219	[#6H1][#7][#6H1]	0.4155
O[CX4H2][CX3H1]	0.2939	[#6]1[#6][#6][#6][#6][#7]1	0.4914
[#6H1r5][#7]	0.2464	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5667
[CHX3]=[CHX3]	0.2314	[#6X3][#7][#6X3]	0.6243
[#6H1][#6H2]	0.2237	[#8][#6][#6][#6X3]	0.6336
[#7][#6H0][#6H1]	0.2221	[OX2H1][CX4H2][#6X3H0]	0.7152
[#8][#6][#6]=[#6X3]	0.1747	[cX3H1]([nX2H0])[cX3H1]	0.7454
[#8][#6H0][#6H1]	0.1624	[CX4H2]([OX2H1])[cX3H0]	0.7696
[#7X3H2]	0.153	[#6X3H1][#6X3H0]	0.7854

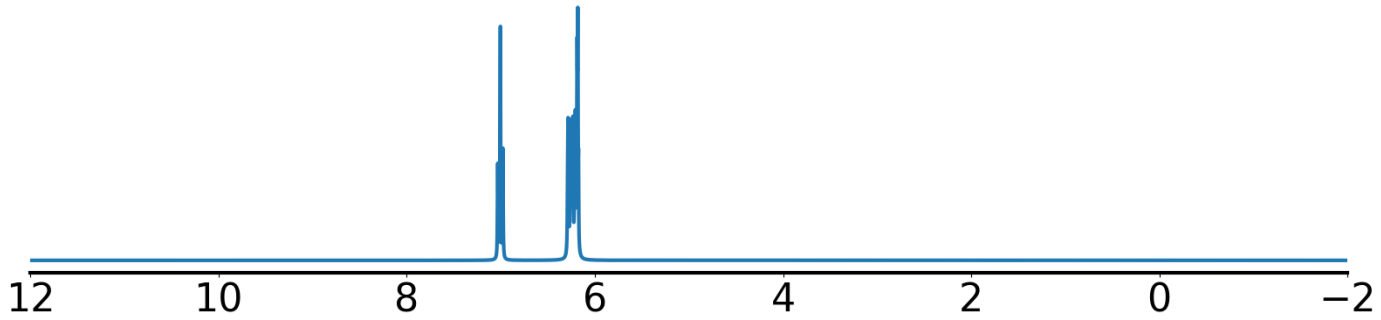
Example 34 true smiles: Nc1cccc(O)c1 formula: C6H7NO
Index of correct structure: 0 of 3639
True structure loss: 0.018182
True structure:



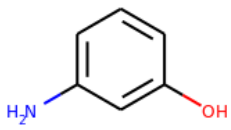
Experimental 13C NMR (solvent: DMSO)



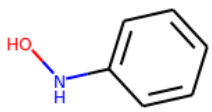
Experimental 1H NMR (solvent: CDCl3)



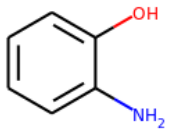
Top predicted structures (loss):



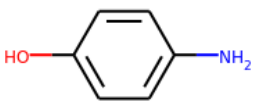
0.018182



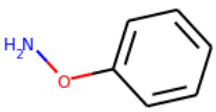
0.018349



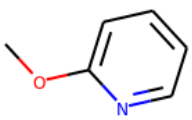
0.018708



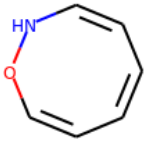
0.020537



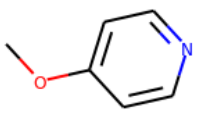
0.022258



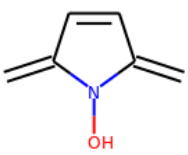
0.030054



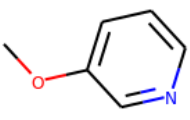
0.036553



0.039949



0.041059



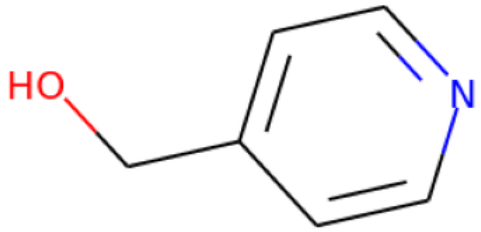
0.043486

Top predicted substructures	prob		
[#6H1]	0.9998	[cH]	0.9652
[#6X3][#6X3]	0.9981	[#7][#6][#6X3]	0.9646
[#6X3][#6X3][#6X3][#6X3]	0.9965	[cX3H1]([cX3H1])[cX3H0]	0.9628
[cH][cH]	0.9952	[#6H1][#6H1]	0.9453
[cX3H1]([cX3H1])[cX3H1]	0.9715	[#6X3H1][#6X3H0]	0.9376

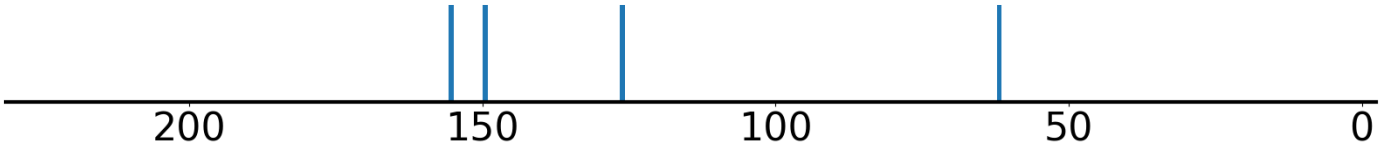
best positives	prob	best negatives	prob
[#6H1]	0.9998	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9981	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9965	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[cH][cH]	0.9952	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9715	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.9652	[CX4H0]([CX4H2])([CX4H2])([CX4H2])[CX4H1]	0.0
[#7][#6][#6X3]	0.9646	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9628	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6H1][#6H1]	0.9453	[OX2H0][CX4H2][CX2H0]#[CX2H1]	0.0
[#6X3H1][#6X3H0]	0.9376	[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#7][#6X3]	0.7759	[cX3H1]([cX3H0])[cX3H0]	0.1057
[#6X3][#7X3][#6X3]	0.6569	[cX3H0][cX3H1][cX3H0][OX2H1]	0.1613
[#6]1[#6][#6][#6][#7]1	0.3608	[#6]1[#6][#6][#6][#6][#6]1	0.2952
[#6]1[#6][#6][#6][#6][#7]1	0.3398	[#7H2][#6H0]	0.5162
[#7H][#6X3H1]	0.2825	[OX2H][cX3]:[c]	0.5249
[#7X3H1]	0.2585	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5666
[cX3H1]([nX3H1])[cX3H1]	0.1936	[#8][#6][#6][#6X3]	0.5754
[CX3H1](=[CX3H1])[CX3H1]	0.1823	[OX2H1]	0.6085
[#6H1r5][#7]	0.1756	[cH]cO	0.6246
[#8][#6H1][#6H1]	0.1646	[#7][#6H0][#6H1]	0.6887

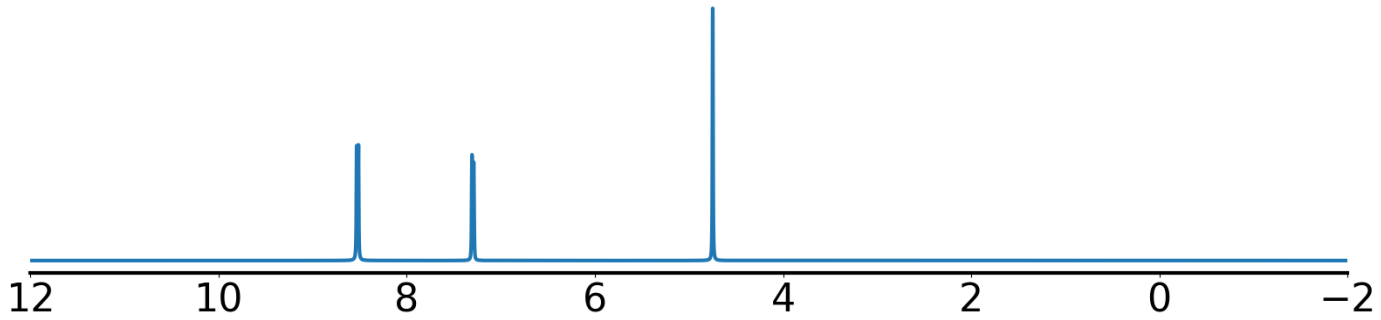
Example 35 true smiles: OCc1ccncc1 formula: C6H7NO
Index of correct structure: 1 of 3639
True structure loss: 0.019165
True structure:



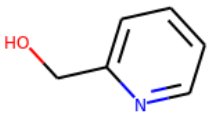
Experimental 13C NMR (solvent: DMSO)



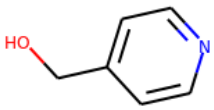
Experimental 1H NMR (solvent: CDCl3)



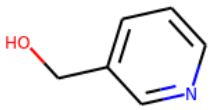
Top predicted structures (loss):



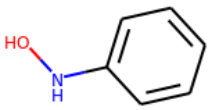
0.018144



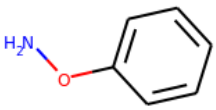
0.019165



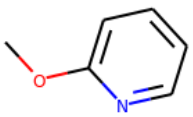
0.01946



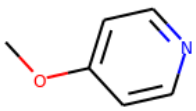
0.031282



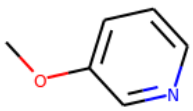
0.033728



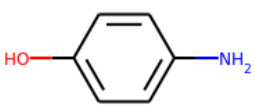
0.035811



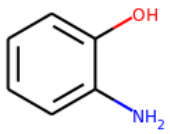
0.036833



0.037128



0.042436



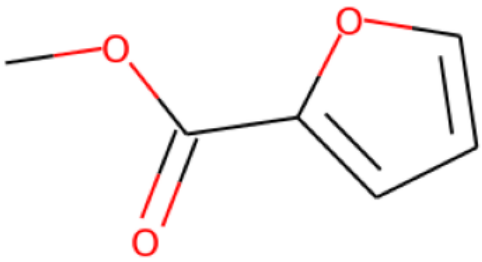
0.045147

Top predicted substructures	prob		
[#6H1]	0.9994	[#6X3][#6H2][#8]	0.8738
[#6X3][#6X3]	0.9906	[cH]	0.8691
[CX4H2]([#6])[O]	0.99	[#6H1][#6H1]	0.8305
[#7][#6][#6X3]	0.926	[#6X3H1][#6X3H0]	0.7402
[cH][cH]	0.8998	[cX3H1]([cX3H1])[cX3H1]	0.7399

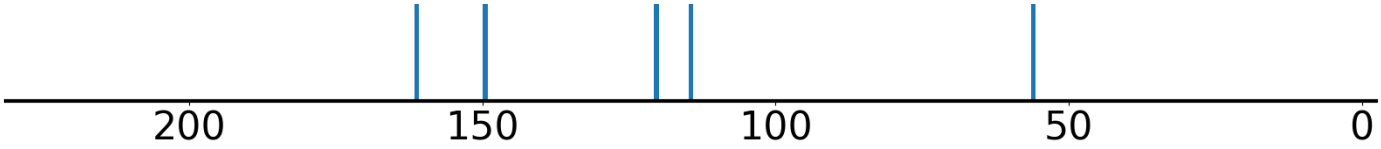
best positives	prob	best negatives	prob
[#6H1]	0.9994	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X3][#6X3]	0.9906	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[CX4H2]([#6])[O]	0.99	[CX4H0]1[CX4H2][CX4H2][CX4H1]1	0.0
[#7][#6][#6X3]	0.926	[CX3H0](=[OX1H0])([CX4H1])[CX4H0]	0.0
[cH][cH]	0.8998	[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.0
[#6X3][#6H2][#8]	0.8738	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[cH]	0.8691	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6H1][#6H1]	0.8305	[CX4H1]([CX4H3])([CX4H2])[CX4H0]	0.0
[#6X3H1][#6X3H0]	0.7402	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#8][#6][#6][#6X3]	0.7284	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H1])[cX3H1]	0.7399	[#6H1][#7][#6H1]	0.1156
O[CX4H2][CX3H1]	0.4765	[#6X3][#7][#6X3]	0.3768
[CX4H2]([OX2H0])[CX3H1]	0.3367	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3993
[#8][#6][#6]=[#6X3]	0.2925	[OX2H1][CX4H2][#6X3H0]	0.4618
[CX4H2][CX3H]	0.2904	[#6]1[#6][#6][#6][#6][#7]1	0.497
[#7][#6X3H0][#6X3H1]	0.2646	[#7][#6][#6][#6X3]	0.5777
[#8][#6H0][#6H1]	0.2407	[cX3H1]([cX3H1])[cX3H0]	0.644
[#6]1[#6][#6][#6][#6][#6]1	0.2294	[cX3H1]([nX2H0])[cX3H1]	0.6878
[#7]=[#6][#6]=[#6X3]	0.2232	[OX2H1]	0.6962
[#6H1r5][#7]	0.2144	[#6X3][#6X3][#6X3][#6X3]	0.7101

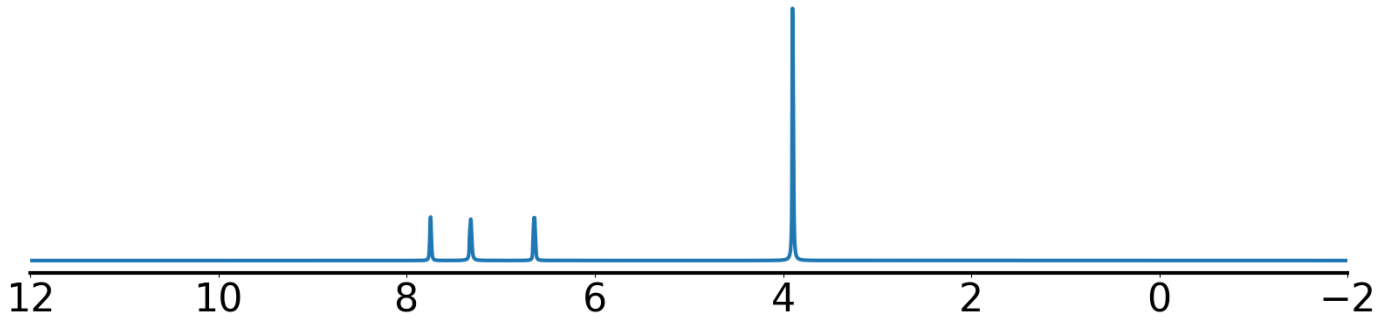
Example 36 true smiles: COC(=O)c1cccc1 formula: C6H6O3
Index of correct structure: 4 of 3580
True structure loss: 0.025458
True structure:



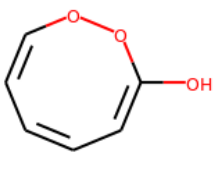
Experimental 13C NMR (solvent: Acetone-d6)



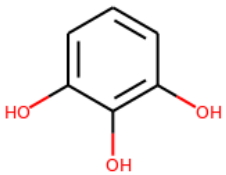
Experimental 1H NMR (solvent: D2O)



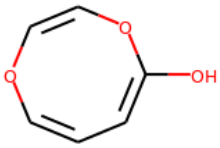
Top predicted structures (loss):



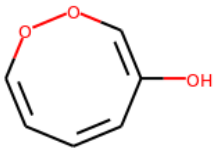
0.016006



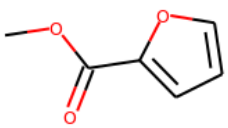
0.018703



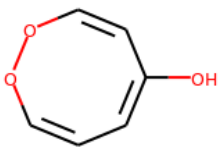
0.019293



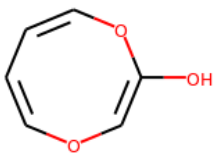
0.022271



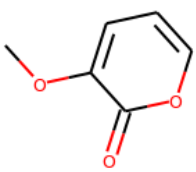
0.025458



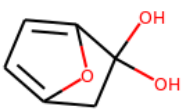
0.025614



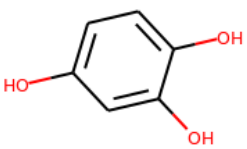
0.028323



0.02932



0.030657



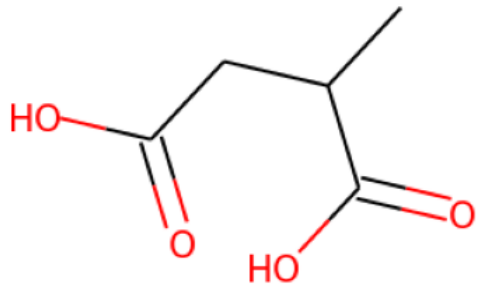
0.031311

Top predicted substructures	prob		
[#6H1]	0.9998	[cX3H1]([cX3H1])[cX3H0]	0.961
[#6X3][#6X3]	0.9977	[#6X3H1][#6X3H0]	0.9511
[cH][cH]	0.987	[#6X3][#6X3][#6X3][#6X3]	0.9499
[#8][#6][#6][#6X3]	0.9851	[#6H1][#6H1]	0.9261
[cH]	0.9843	[#8][#6H0][#6H1]	0.9149

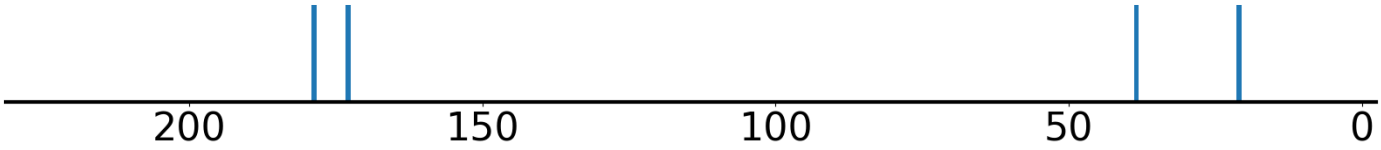
best positives	prob	best negatives	prob
[#6H1]	0.9998	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.9977	[CX4H1]([NX3H2])([CX4H2])[CX4H0]	0.0
[cH][cH]	0.987	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[#8][#6][#6][#6X3]	0.9851	[#6H3][#6H1][#7][#7]	0.0
[cH]	0.9843	[#6H3][#6H0][#7][#6H3]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.961	[CX3H0](=[NX2H0])([NX3H0])[CX4H2]	0.0
[#6X3H1][#6X3H0]	0.9511	[CX4H2]([NX3H0])[CX4H3]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9499	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.0
[#6H1][#6H1]	0.9261	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[#8][#6H0][#6H1]	0.9149	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[OX2H1]	0.8342	[#8][#6][#6]=[#8]	0.0291
[cH]cO	0.5813	[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.0871
[#8]=[#6][#6H1][#6H1]	0.4873	[CX4H3]	0.1211
[OX2H][cX3]:[c]	0.4661	o[cH]	0.2081
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.2416	O=[#6][#6][#6X3]	0.2261
[#8][#6][#6][#6][#6][#8]	0.2343	[#8][#6H][#6X3][#6X3H]	0.2646
[CX4H2]([#6])[O]	0.2048	[CX3](=[OX1])O	0.4402
[CHX3]=[CHX3]	0.1719	[CX4H3][OX2H0]	0.4662
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.1673	[cX3H1]([oX2H0])[cX3H1]	0.5109
O=[cX3]	0.1461	[#8][#6H1][#6H1]	0.5917

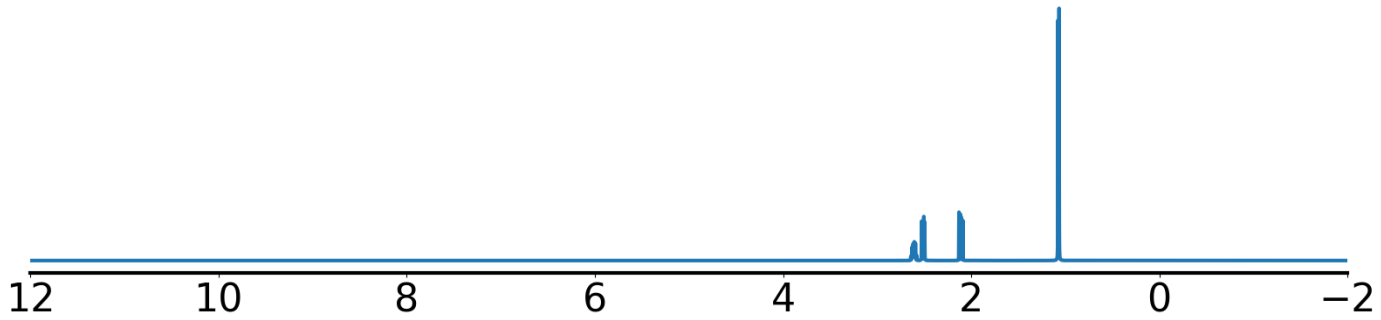
Example 37 true smiles: CC(CC(=O)O)C(=O)O formula: C5H8O4
Index of correct structure: 0 of 3240
True structure loss: 0.0312
True structure:



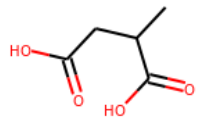
Experimental 13C NMR (solvent: DMSO)



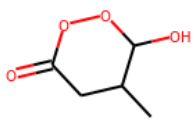
Experimental 1H NMR (solvent: D2O)



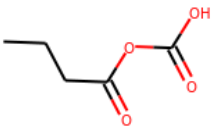
Top predicted structures (loss):



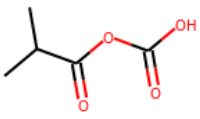
0.0312



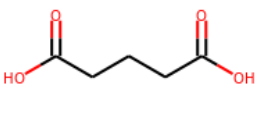
0.04632



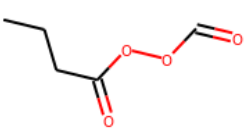
0.047054



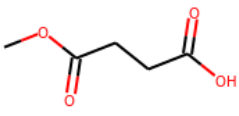
0.052269



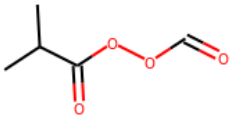
0.053122



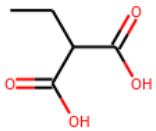
0.062345



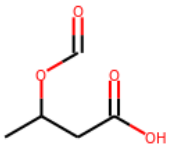
0.068231



0.069875



0.070738



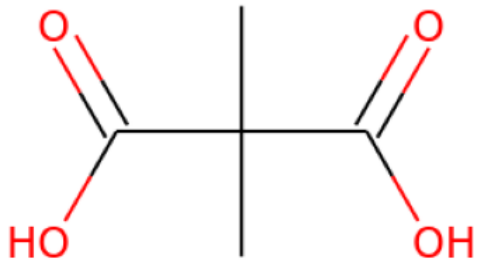
0.071324

Top predicted substructures	prob		
[#8]=[#6][#8]	1.0	[#6H3][#6][#6]	0.9963
[CX3](=[OX1])O	1.0	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9876
[CX4H3]	0.9998	[OX2H1]	0.9789
[CX3](=[OX1])C	0.9998	[CX3](=O)[OX2H1]	0.9563
[CX4H2]([#6])[#6]	0.9978	[CX4H2]([CX4H1])[CX3H0]	0.9495

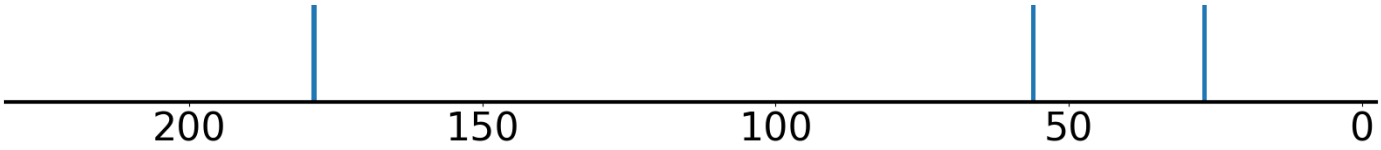
best positives	prob	best negatives	prob
[#8]=[#6][#8]	1.0	CC#CCC#C	0.0
[CX3](=[OX1])O	1.0	[#6X2][#6H1][#6X2]	0.0
[CX4H3]	0.9998	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9998	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2]([#6])[#6]	0.9978	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9963	CCC=CC#C	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9876	[CX2H0](#[CX2H0])[CX2H0]	0.0
[OX2H1]	0.9789	CCC#CCC	0.0
[CX3](=O)[OX2H1]	0.9563	CC#CCC=C	0.0
[CX4H2]([CX4H1])[CX3H0]	0.9495	[CX2H0](#[CX2H0])[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[OX2H0][CX3H0][CX4H2]	0.6583	[OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]	0.005
[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.434	[CX4H1]([CX4H3])([CX4H2])[CX3H0]	0.0416
[#8X2H0][#6X3H0][CX4H2][CX4H1]	0.3797	[#8][#6][#6][#6][#6][#8]	0.0517
[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.3061	[#8]=[#6][#6][#6][#6]=[#8]	0.1725
[CX3H0](=[OX1H0])([OX2H0])[CX4H3]	0.2867	O=[CX3][CX4H]	0.1926
O=[CX3H0][CX4H2][CX4H2]	0.2339	[#8]=[#6H0][#6H1]	0.2157
[#6H3][#6H1r5]	0.1782	[#6H3][#6][#6X3]	0.2451
[CX4H2]([CX4H2])[CX3H0]	0.1255	[#8][#6][#6][#6][#6]=[#8]	0.3035
[CH3][#6][#8]	0.1094	[CH3]CC[OH]	0.3227
[CHX4]([CH3X4])[CH3X4]	0.1019	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.503

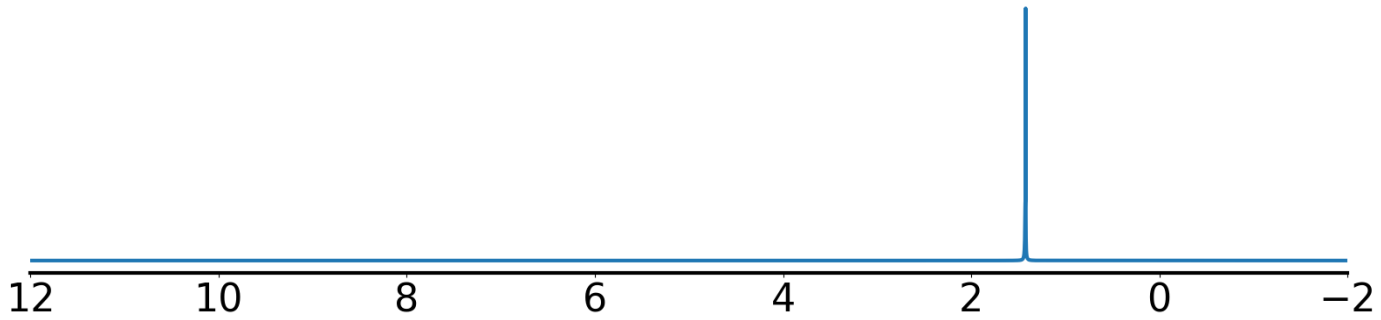
Example 38 true smiles: CC(C)(C(=O)O)C(=O)O formula: C5H8O4
Index of correct structure: 1 of 3240
True structure loss: 0.026307
True structure:



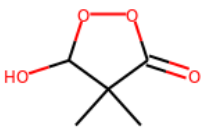
Experimental 13C NMR (solvent: D2O)



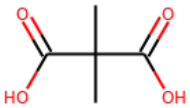
Experimental 1H NMR (solvent: D2O)



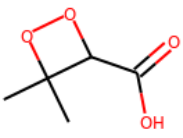
Top predicted structures (loss):



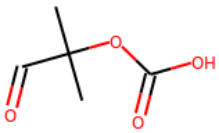
0.024814



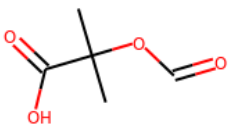
0.026307



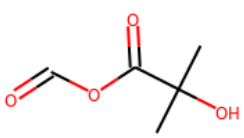
0.02928



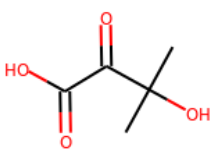
0.032178



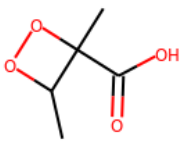
0.034096



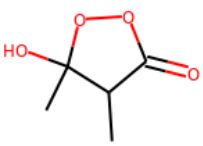
0.038497



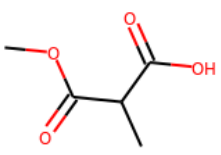
0.041365



0.043049



0.04502



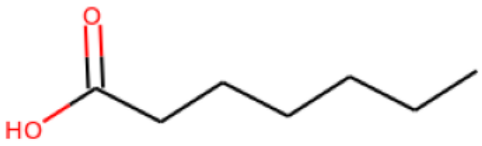
0.045022

Top predicted substructures	prob		
[CX3](=[OX1])C	0.999	[CX4H3][CX4H0]	0.9834
[#8]=[#6][#8]	0.9989	[#6H3][#6H0]	0.9703
[CX3](=[OX1])O	0.9981	[OX2H1]	0.9652
[CX4H3]	0.996	[CX3](=O)[OX2H1]	0.8972
[#6H3][#6][#6]	0.9929	[CX4H3][#6]	0.8477

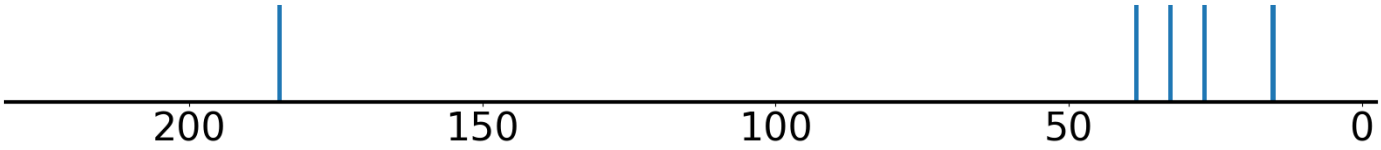
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8]=[#6][#8]	0.9989	C=CC=CC#C	0.0
[CX3](=[OX1])O	0.9981	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
[CX4H3]	0.996	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9929	CC=CCC#C	0.0
[CX4H3][CX4H0]	0.9834	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#6H3][#6H0]	0.9703	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[OX2H1]	0.9652	CCC#CC=C	0.0
[CX3](=O)[OX2H1]	0.8972	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H3][#6]	0.8477	[CX3H0](=[CX3H2])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H3][CX4]O	0.8176	[#8]=[#6][#6H0][#6]=[#8]	0.0034
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.7283	O=[#6][#6][#6X3]	0.0888
[CH3][#6][#8]	0.6137	[CH3]CC[OH]	0.3323
[#8][#6H0][#6H1]	0.5495	[#8][#6][#6][#6X3]	0.4338
[#6H1]	0.5052	[#6H3][#6][#6X3]	0.5108
[CX3H0](=[OX1H0])([OX2H0])[CX4H0]	0.4581	[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.7075
[#8][#6][#6]=[#8]	0.4316	[CX4H3][CX4H0][CX4H3]	0.7762
[CX4H2]CC=O	0.4033	[CX4H3][#6]	0.8477
[#8]=[#6H0][#6H1]	0.4007	[CX3](=O)[OX2H1]	0.8972
[#8][#6][#6][#8]	0.3391	[OX2H1]	0.9652

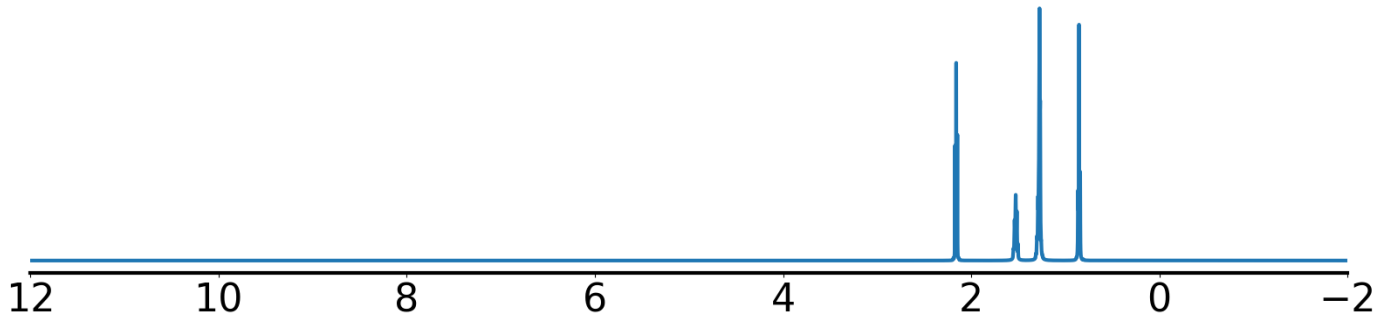
Example 39 true smiles: CCCCCCC(=O)O formula: C7H14O2
Index of correct structure: 0 of 3028
True structure loss: 0.008652
True structure:



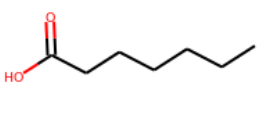
Experimental 13C NMR (solvent: CDCl3)



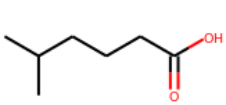
Experimental 1H NMR (solvent: d2o)



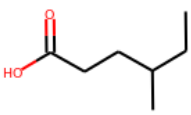
Top predicted structures (loss):



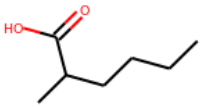
0.008652



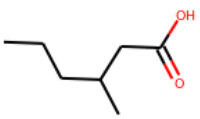
0.02813



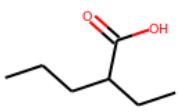
0.030004



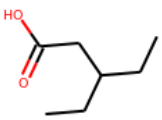
0.041653



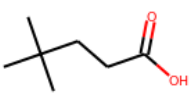
0.043735



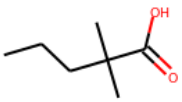
0.044891



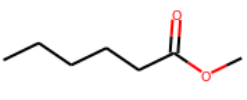
0.046682



0.052074



0.053962



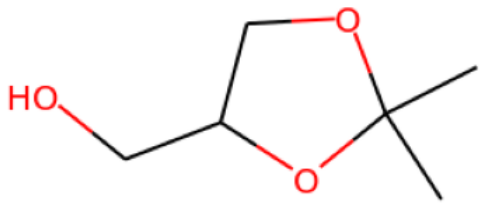
0.055838

Top predicted substructures	prob		
[#6H3][#6][#6]	0.9999	[CX3](=[OX1])C	0.9989
[CX4H2]([#6])[#6]	0.9995	[CX4H3][CX4H2]	0.9968
[CX4H3][#6]	0.9994	[#8]=[#6][#8]	0.9863
[CX4H3]	0.9992	[CX3](=[OX1])O	0.9851
[CX3](=O)[OX2H1]	0.999	[OX2H1]	0.9677

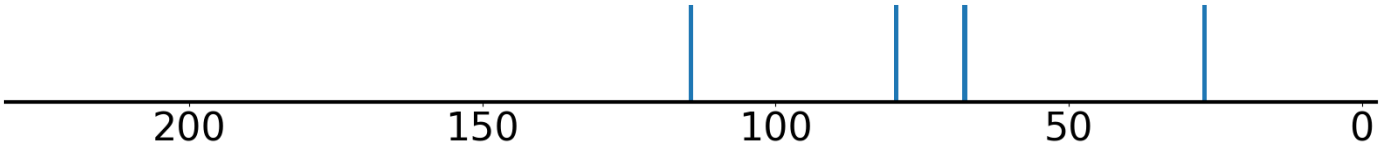
best positives	prob	best negatives	prob
[#6H3][#6][#6]	0.9999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	0.9995	CCC#CC#C	0.0
[CX4H3][#6]	0.9994	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3]	0.9992	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=O)[OX2H1]	0.999	CCC=CC#C	0.0
[CX3](=[OX1])C	0.9989	[#6X2][#6H1][#6X2]	0.0
[CX4H3][CX4H2]	0.9968	C=CC=CC#C	0.0
[#8]=[#6][#8]	0.9863	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])O	0.9851	CC=CC#CC	0.0
[OX2H1]	0.9677	CC#CCC#C	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.4501	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.5721
[#6H1][#6H2]	0.4491	[CX4H2][CX3]=O	0.6044
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3637	CCCCCC	0.6456
[CX4H3][CX4H1]	0.262	O=[CX3H0][CX4H2][CX4H2]	0.6516
[CHX4]([CH3X4])[CH2X4]	0.1828	[#8][#6][#6H2]	0.688
[#6H3][#6H0]	0.1589	[CX4H2]([CX4H2])[CX3H0]	0.7089
[CX4H2]([CX4H2])[CX4H1]	0.1484	[CX4H2]CC=O	0.7683
[#8]=[#6H0][#6H1]	0.1461	[CX4H2]([CX4H3])[CX4H2]	0.7715
[CX4H1]([CX4H3])([CX4H3])[CX4H2]	0.1437	OCC[CH2]	0.7969
[#6H3][#6][#6X3]	0.1392	[CX4H2]([CX4H2])[CX4H2]	0.817

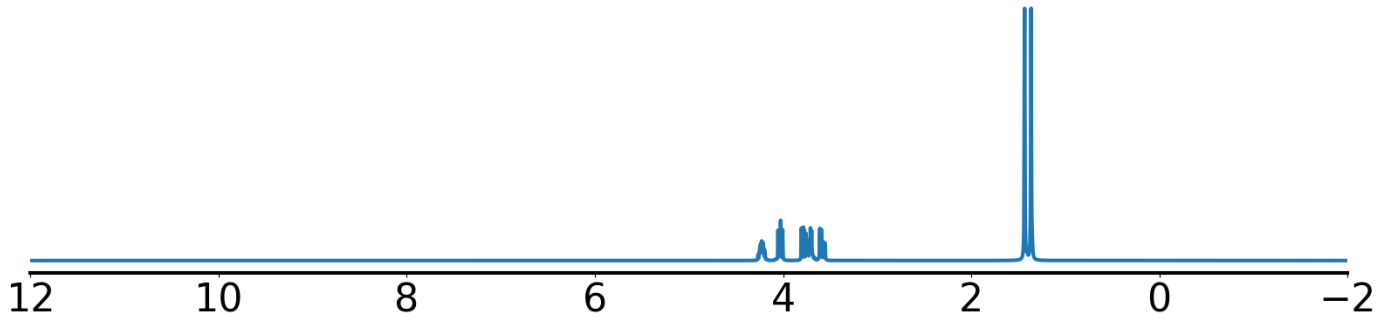
Example 40 true smiles: CC1(C)OCC(CO)O1 formula: C6H12O3
Index of correct structure: 0 of 3020
True structure loss: 0.035402
True structure:



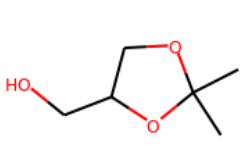
Experimental 13C NMR (solvent: CDCl3)



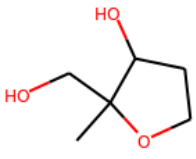
Experimental 1H NMR (solvent: CDCl3)



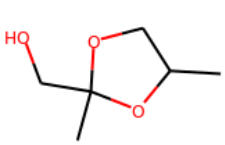
Top predicted structures (loss):



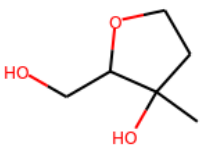
0.035402



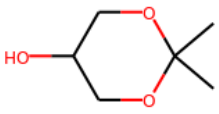
0.036146



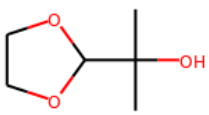
0.039829



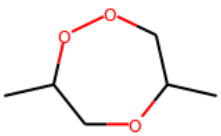
0.040292



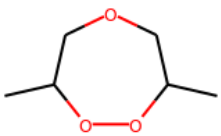
0.04119



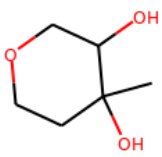
0.041192



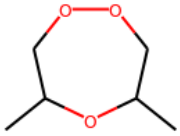
0.041906



0.042918



0.043665



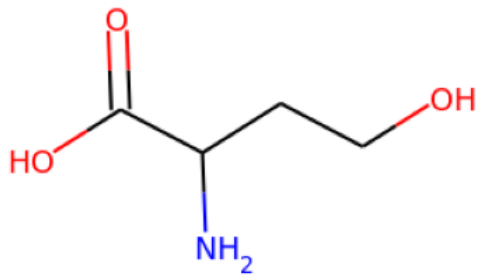
0.044431

Top predicted substructures	prob		
[CX4H2]([#6])[O]	0.9999	[#8][#6][#6H2][#8]	0.9943
[CX4H3]	0.9999	[#8][#6][#6][#8]	0.9897
[CX4H3][CX4]O	0.9997	[CX4H3][#6]	0.9875
[#6H3][#6][#6]	0.9988	OCC[CH2]	0.9845
[#8][#6][#6H2]	0.9947	[#6H1]	0.9823

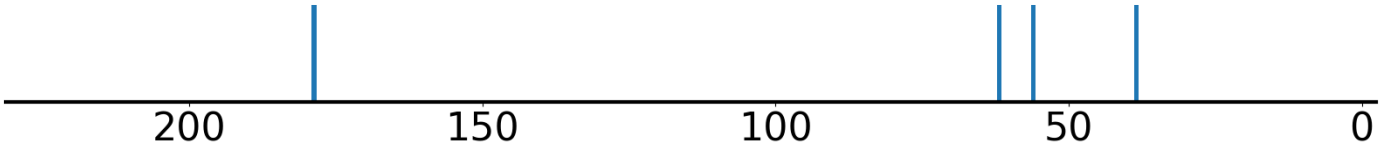
best positives	prob	best negatives	prob
[CX4H2]([#6])[O]	0.9999	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	0.9999	C=CC=CC#C	0.0
[CX4H3][CX4]O	0.9997	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[#6H3][#6][#6]	0.9988	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8][#6][#6H2]	0.9947	CC#CCC#C	0.0
[#8][#6][#6H2][#8]	0.9943	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.0
[#8][#6][#6][#8]	0.9897	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H3][#6]	0.9875	[CX2H0](#[CX2H0])[CX2H0]	0.0
OCC[CH2]	0.9845	[CX3H0](=[NX2H1])([NX3H1])[CX4H1]	0.0
[#6H1]	0.9823	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX4H2]	0.8369	[CX4H3][CX4H0][CX4H3]	0.0044
[CH2X4](O)[CX4H2]	0.6708	[CX4H3][CX4H0]([CX4H3])[OX2H0]	0.0161
[#8][#6H0][#6H1]	0.6319	[#6H0]([#6H3])([#6H3])[#8]	0.032
[#6X4H3][#6][#8H]	0.5238	[#6H1]([#6H2])[#6H2]	0.1036
[CX4H2]([OX2H0])[CX4H2]	0.5047	[OX2H0][CX4H2][CX4H1][CX4H2]	0.1992
[OH][CX4H]	0.4017	[CX4H1]([OX2H0])([CX4H2])[CX4H2]	0.2242
C1OCCC1	0.3782	[CX4H2]([OX2H1])[CX4H1]	0.3112
[#8][#6][#6][#6][#6][#8]	0.3387	[CX4H2]([OX2H0])[CX4H1]	0.4405
[OX2H0][CX4H2][#6H0]	0.3207	[#8H][#6H2][#6H1]	0.4854
[#6X4H2][#6H1][#8H]	0.3174	[#6]1[#8][#6][#8][#6]1	0.6221

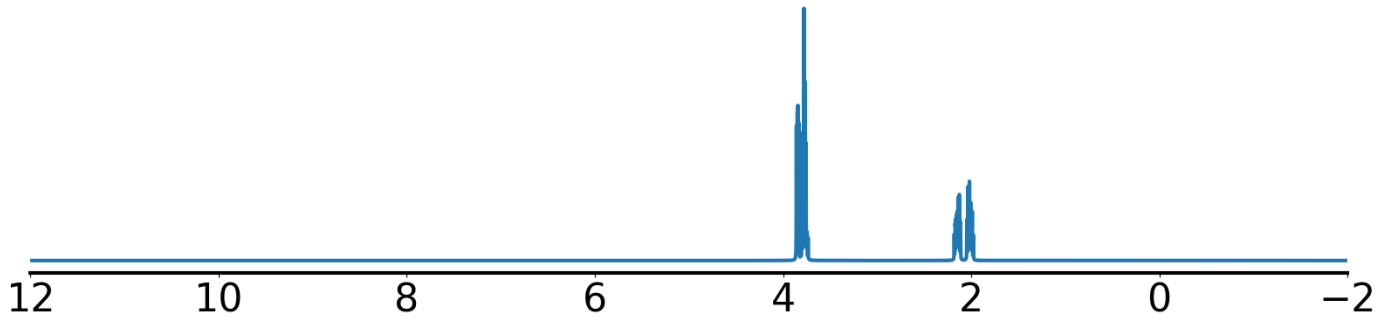
Example 41 true smiles: NC(CCO)C(=O)O formula: C4H9NO3
Index of correct structure: 0 of 2840
True structure loss: 0.01536
True structure:



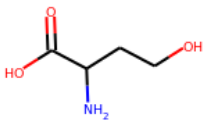
Experimental 13C NMR (solvent: D2O)



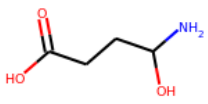
Experimental 1H NMR (solvent: D2O)



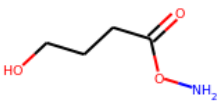
Top predicted structures (loss):



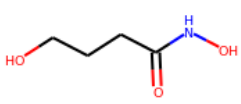
0.01536



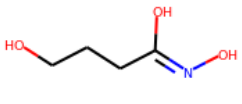
0.049893



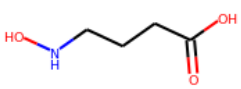
0.054603



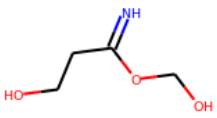
0.055064



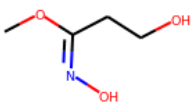
0.055355



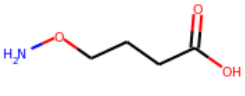
0.055844



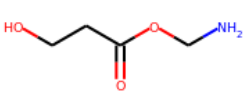
0.056444



0.056502



0.057623



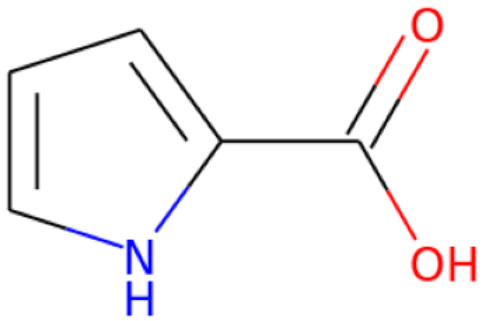
0.057921

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9949	[CX3](=O)[OX2H1]	0.9268
[CX4H2]([#6])[#6]	0.9946	[CX4H2]([OX2H1])[CX4H2]	0.9111
[OX2H1]	0.9909	[#8]=[#6H0][#6H1]	0.9006
[#8]=[#6][#8]	0.9735	[#7X3H2]	0.8953
[CX3](=[OX1])O	0.9401	[#8][#6][#6H2]	0.8872

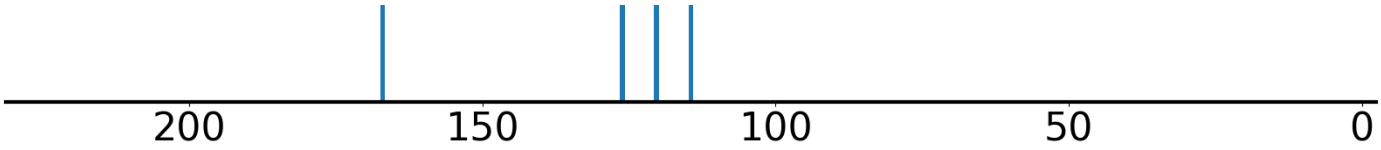
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9949	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[#6]	0.9946	CC=CCC#C	0.0
[OX2H1]	0.9909	[CX2H0](#[CX2H1])[CX4H2]	0.0
[#8]=[#6][#8]	0.9735	CC=CC#CC	0.0
[CX3](=[OX1])O	0.9401	CCC#CC#C	0.0
[CX3](=O)[OX2H1]	0.9268	CC#CCC=C	0.0
[CX4H2]([OX2H1])[CX4H2]	0.9111	[#6X2][#6H1][#6X2]	0.0
[#8]=[#6H0][#6H1]	0.9006	[CX2H0](#[CX2H1])[CX4H1]	0.0
[#7X3H2]	0.8953	[#6X3][#6]#[#6][#6H3]	0.0
[#8][#6][#6H2]	0.8872	[CX2H0](#[CX2H0])[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H1]([NX3H1])([CX4H2])[CX3H0]	0.4249	[#8][#6H0][#6H1]	0.1975
[CX4H2][CX3]=O	0.3888	[#8][#6][#6][#6][#6]=[#8]	0.2456
[#8][#6][#6][#6X3]	0.314	[#8][#6][#6][#6][#6][#8]	0.2613
[CX4H2]([CX4H2])[CX3H0]	0.2941	[#6H1][#6H2]	0.5729
[#7H2][#6H0]	0.2695	OCC[CH2]	0.6983
[#7X3H1]	0.2365	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.7064
O=[CX3H0][CX4H2][CX4H2]	0.2267	[#6H1]	0.761
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2218	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.7876
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.1981	[#7][#6][#6X3]	0.7902
[#7][#6H1][#6H2r5]	0.1873	O=[CX3][CX4H]	0.7941

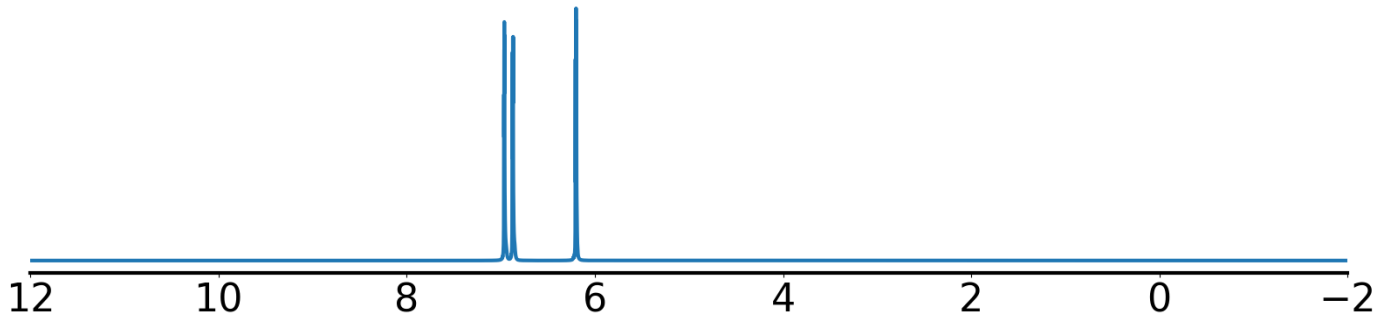
Example 42 true smiles: O=C(O)c1ccc[nH]1 formula: C5H5NO2
Index of correct structure: 1 of 2827
True structure loss: 0.023863
True structure:



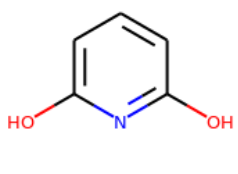
Experimental 13C NMR (solvent: CD3OD)



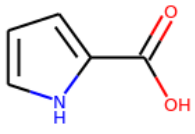
Experimental 1H NMR (solvent: MeOD)



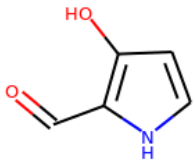
Top predicted structures (loss):



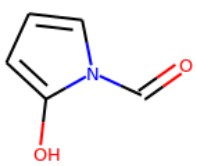
0.018317



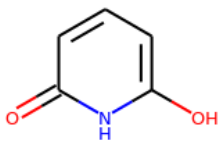
0.023863



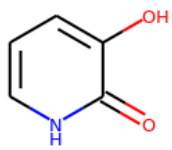
0.025028



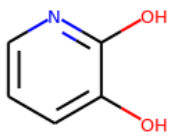
0.02595



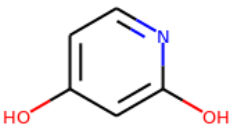
0.028001



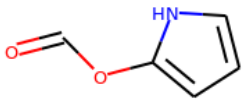
0.028305



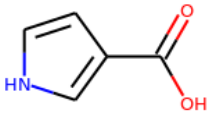
0.029159



0.029949



0.030875



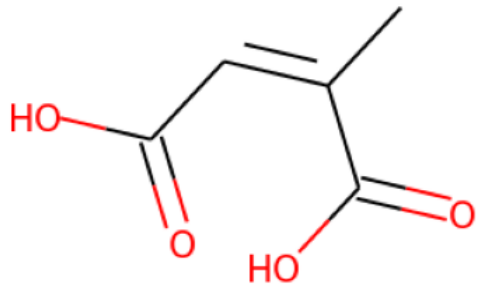
0.031187

Top predicted substructures	prob		
[#6H1]	0.9979	[cX3H1]([cX3H1])[cX3H0]	0.9565
[cH][cH]	0.9929	[#6X3H1][#6X3H0]	0.9508
[#6X3][#6X3]	0.9919	[#7][#6][#6X3]	0.9211
[#6X3][#6X3][#6X3][#6X3]	0.9906	[#6H1][#6H1]	0.9082
[cH]	0.9757	[#6X3][#7][#6X3]	0.8886

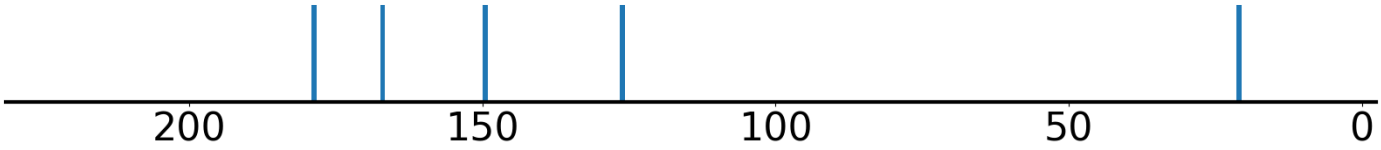
best positives	prob	best negatives	prob
[#6H1]	0.9979	[CX4H0]([CX4H3])([CX4H2])([CX4H2])[CX3H0]	0.0
[cH][cH]	0.9929	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9919	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9906	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH]	0.9757	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9565	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9508	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#7][#6][#6X3]	0.9211	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H2]	0.0
[#6H1][#6H1]	0.9082	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3][#7][#6X3]	0.8886	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.8139	[CX3](=[OX1])O	0.1568
[cH]cO	0.7154	O=[#6][#6][#6X3]	0.2142
[OX2H][cX3]:[c]	0.6126	[CX3](=O)[OX2H1]	0.2144
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.5717	[cX3H1]([nX3H1])[cX3H1]	0.274
[#6X3H1][#7X3H0]	0.3303	[#7X3H1]	0.3488
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.3166	[#8]=[#6][#8]	0.3893
[#6]1[#6][#6][#6][#6][#6]1	0.297	[#7H][#6X3H1]	0.458
[#7H2][#6H0]	0.276	[#6H1r5][#7]	0.5552
O=[cX3]	0.2728	[#7][#6H0][#6H1]	0.635
[#7X3H0]	0.2708	[#7][#6X3H0][#6X3H1]	0.6432

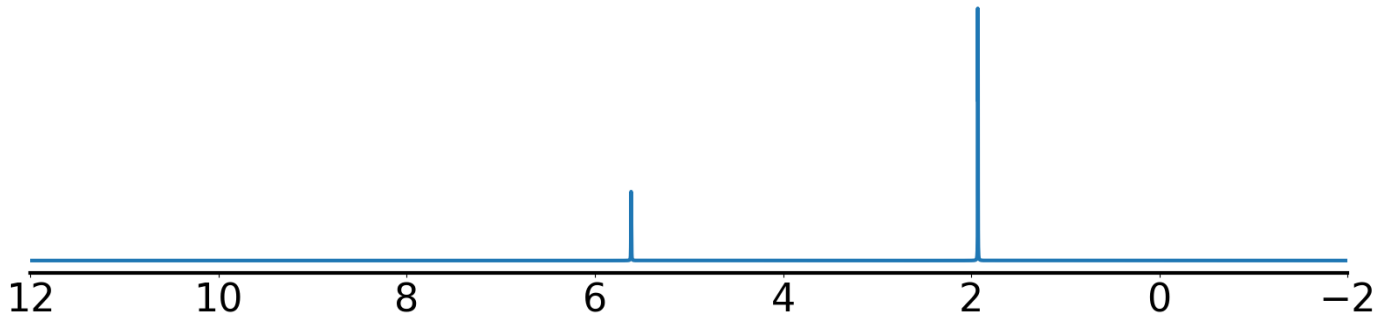
Example 43 true smiles: CC(=CC(=O)O)C(=O)O formula: C5H6O4
Index of correct structure: 1 of 2762
True structure loss: 0.04138
True structure:



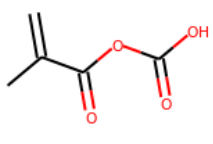
Experimental 13C NMR (solvent: N/A)



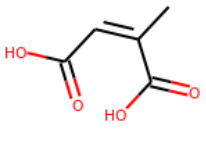
Experimental 1H NMR (solvent: D2O)



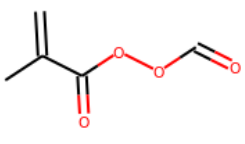
Top predicted structures (loss):



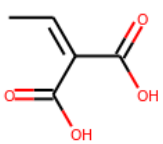
0.033174



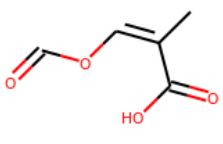
0.04138



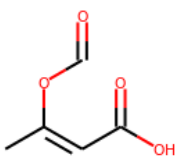
0.047924



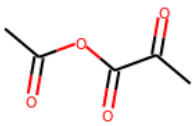
0.056259



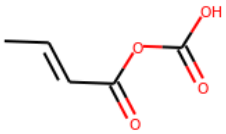
0.059278



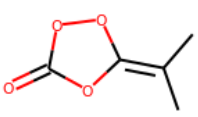
0.064331



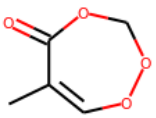
0.064575



0.068804



0.07264



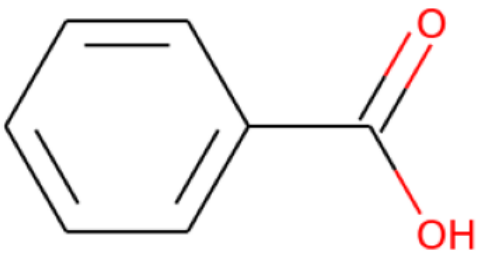
0.07275

Top predicted substructures	prob		
[CX4H3]	0.9998	[#6H3][#6H0]	0.9973
[#8]=[#6][#8]	0.9993	[CX3](=[OX1])C	0.9923
[CX3](=[OX1])O	0.999	[CX4H3][CX3]	0.9833
[CX4H3][#6]	0.9981	[CX4H3][CX3H0]	0.9736
[#6X3][#6X3]	0.9975	[CX3](=O)[OX2H1]	0.967

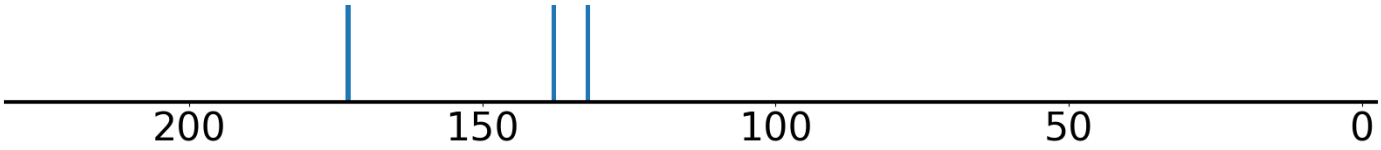
best positives	prob	best negatives	prob
[CX4H3]	0.9998	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#8]=[#6][#8]	0.9993	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX3](=[OX1])O	0.999	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[CX4H3][#6]	0.9981	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9975	[CX4H2]([CX4H0])[CX2H0]	0.0
[#6H3][#6H0]	0.9973	CCC#CC#C	0.0
[CX3](=[OX1])C	0.9923	[CX4H1]([CX4H2])([CX4H2])[CX2H0]	0.0
[CX4H3][CX3]	0.9833	[CX4H1]([CX4H1])([CX4H1])[CX2H0]	0.0
[CX4H3][CX3H0]	0.9736	CC#CCC#C	0.0
[CX3](=O)[OX2H1]	0.967	CCC=CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H3][CX3H0]=[CX3H2]	0.7484	[#6X3][#6X3]=[#6X3][#6X3]	0.0197
O=[#6][#6][#6X3]	0.7386	[CH3]CC[OH]	0.0361
[CX3H2]=[CX3H0][CX3H0]	0.653	[OX1H0]=[CX3H0][CX3H1]=[CX3H0]	0.0415
[#8][#6][#6]=[#8]	0.5941	[#8][#6][#6]=[#6][#6][#8]	0.0761
[#8]=[#6][#6]=[#8]	0.4737	[CHX3](=C)C	0.138
[CX3H0](=[CX3H2])([CX4H3])[CX3H0]	0.4466	[#8][#6][#6]=[#6][#6]=[#8]	0.2284
[CH2X3](=C)	0.4001	[#8]=[#6][#6]=[#6][#6]=[#8]	0.2333
O=CC=O	0.3651	[CX3H1](=[CX3H0])[CX3H0]	0.239
[#8][#6][#6][#6X3]	0.3648	[#6X3H1][#6X3H0]	0.3116
[CX3H2]=[CX3H0][CX3]=O	0.3647	[CX3H0](=[CX3H1])([CX4H3])[CX3H0]	0.3755

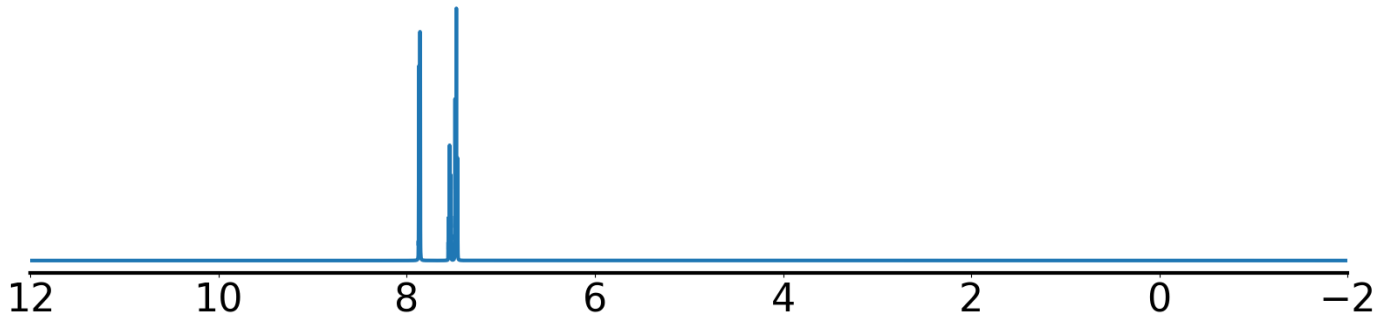
Example 44 true smiles: O=C(O)c1ccccc1 formula: C7H6O2
Index of correct structure: 0 of 2390
True structure loss: 0.013018
True structure:



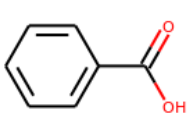
Experimental 13C NMR (solvent: CDCl3)



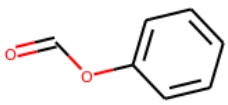
Experimental 1H NMR (solvent: d2o)



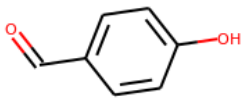
Top predicted structures (loss):



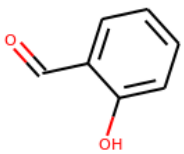
0.013018



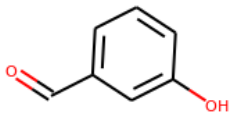
0.026863



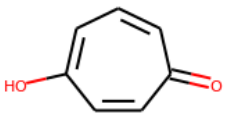
0.030436



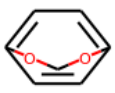
0.030571



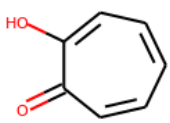
0.039667



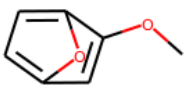
0.04025



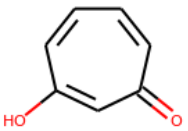
0.043328



0.044723



0.048973



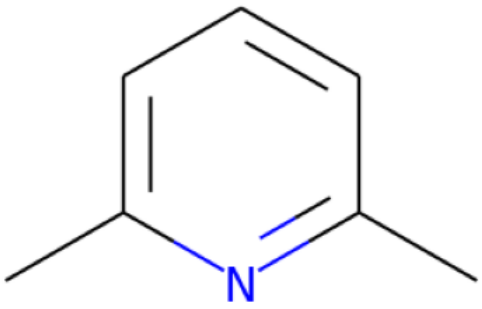
0.05015

Top predicted substructures	prob		
[#6X3][#6X3]	0.9993	[#8]=[#6][#8]	0.8863
[#6H1]	0.9989	[cH]	0.8725
[#6X3H1][#6X3H0]	0.9516	[cX3H1]([cX3H1])[cX3H0]	0.8503
[cH][cH]	0.9488	O=[#6][#6][#6X3]	0.8489
[#6X3][#6X3][#6X3][#6X3]	0.9487	[CX3](=[OX1])O	0.8424

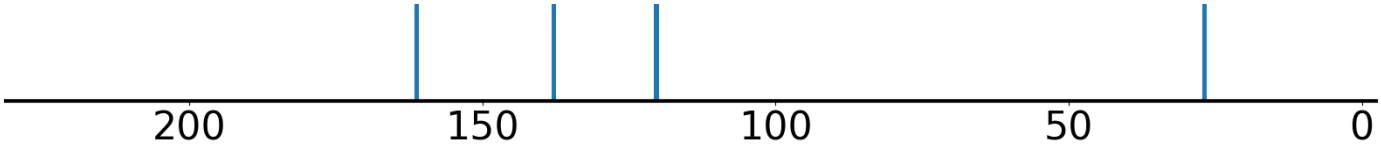
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9993	[#6H3][#7][#6X4H1][#6H3]	0.0
[#6H1]	0.9989	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9516	[#6H3][#6H0][#7][#6H3]	0.0
[cH][cH]	0.9488	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9487	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.0
[#8]=[#6][#8]	0.8863	[CX4H2]([NX3H1])[CX4H3]	0.0
[cH]	0.8725	[CX4H1]([NX3H0])([CX4H3])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.8503	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
O=[#6][#6][#6X3]	0.8489	[CX4H1]([NX3H1])([CX4H3])[CX4H1]	0.0
[CX3](=[OX1])O	0.8424	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[CX3](=[OX1])C	0.6131	[#6]1[#6][#6][#6][#6][#6]1	0.5472
[#8]=[#6H0][#6H1]	0.5705	[OX2H1]	0.5595
[#6X3][#6X3]=[#6X3][#6X3]	0.4553	[#8][#6][#6][#6X3]	0.5959
[#8][#6H0][#6H1]	0.3952	[CX3](=O)[OX2H1]	0.5966
[OX1H0]=[cX3H0][cX3H1]	0.2532	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6833
O=[cX3]	0.2422	[#6H1][#6H1]	0.8052
[#6H][#8][#6H]	0.24	[cX3H1]([cX3H1])[cX3H1]	0.8303
[cH]cO	0.2097	[CX3](=[OX1])O	0.8424
[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.1892	O=[#6][#6][#6X3]	0.8489
[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.1823	[cX3H1]([cX3H1])[cX3H0]	0.8503

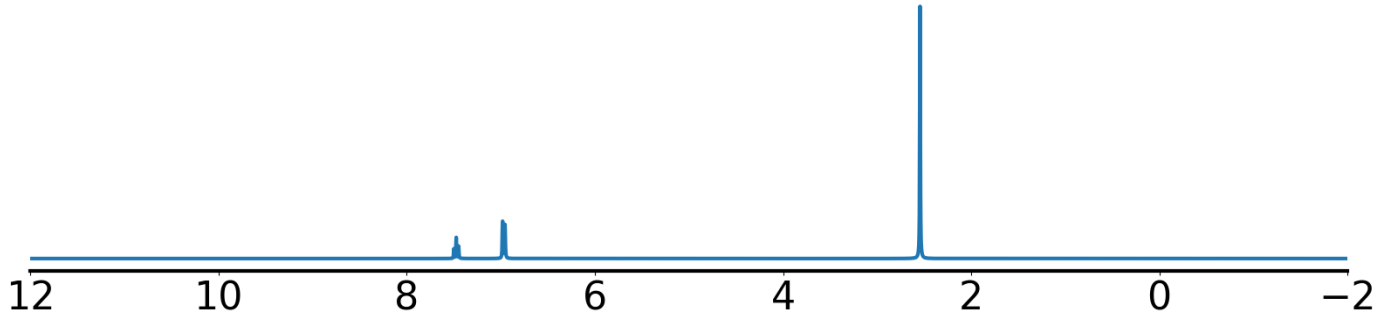
Example 45 true smiles: Cc1cccc(C)n1 formula: C7H9N
Index of correct structure: 1 of 1755
True structure loss: 0.017191
True structure:



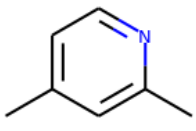
Experimental 13C NMR (solvent: CDCl3)



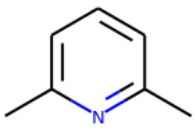
Experimental 1H NMR (solvent: CDCl3)



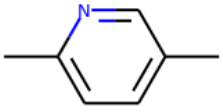
Top predicted structures (loss):



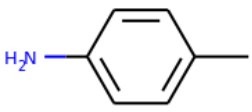
0.017047



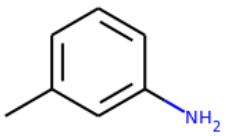
0.017191



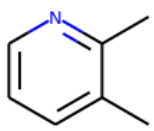
0.019012



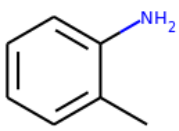
0.020059



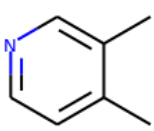
0.021291



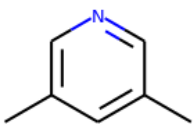
0.023169



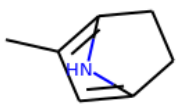
0.023339



0.030276



0.031111



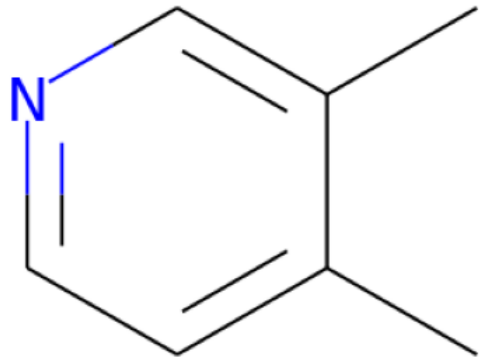
0.034149

Top predicted substructures	prob		
[#6X3][#6X3]	0.99	[cH][cH]	0.9405
[#6H1]	0.9892	[CX4H3][cX3H0]	0.9389
[#6H3][#6][#6]	0.9851	[cH]	0.9349
[#6X3][#6X3][#6X3][#6X3]	0.9797	[#7][#6][#6][#6X3]	0.9148
[#6X3H1][#6X3H0]	0.9457	[#7][#6][#6X3]	0.8934

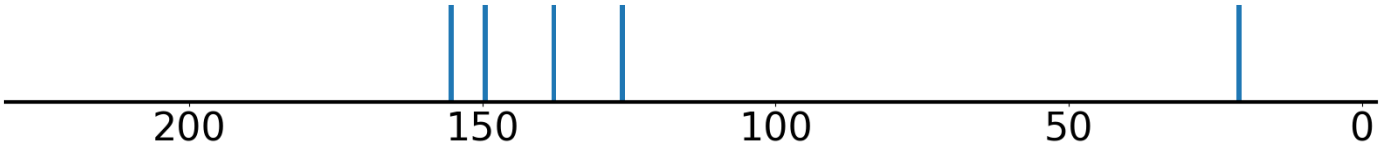
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.99	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[#6H1]	0.9892	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H3][#6][#6]	0.9851	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9797	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3H1][#6X3H0]	0.9457	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[cH][cH]	0.9405	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3][cX3H0]	0.9389	[OX2H1][CX4H0][CX4H2][CX4H0]	0.0
[cH]	0.9349	[#6]1[#8][#6][#6]1=[#8]	0.0
[#7][#6][#6][#6X3]	0.9148	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#7][#6][#6X3]	0.8934	[OX2H1][CX4H1][CX4H1]([CX4H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.726	[#6H3][#6H0][#7H0][#6H0]	0.1658
[CX4H2][CX4H2]	0.7115	[#7][#6][#6H3]	0.3638
[#6]1[#6][#6][#6][#6][#6]1	0.63	[#7][#6H0][#6H1]	0.4524
[cX3H0][cX3H1][cX3H1][cX3H0]	0.4074	[cX3H1]([cX3H1])[cX3H1]	0.4633
[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.3855	[#7][#6X3H0][#6X3H1]	0.555
[CX4H2]([#6])[#6]	0.3564	[#6X3][#7][#6X3]	0.6227
[cX3H1]([nX2H0])[cX3H1]	0.2327	[#6H3][#6H0]	0.7314
[CX4H2]([CX4H2])[cX3H0]	0.2276	[#6]1[#6][#6][#6][#6][#7]1	0.7467
[cX3H1]([cX3H0])[cX3H0]	0.1968	[#6H3][#6][#6X3]	0.802
[cX3H1]([nX2H0])[cX3H0]	0.1816	[#6X3][#6][#6][#6H3]	0.8164

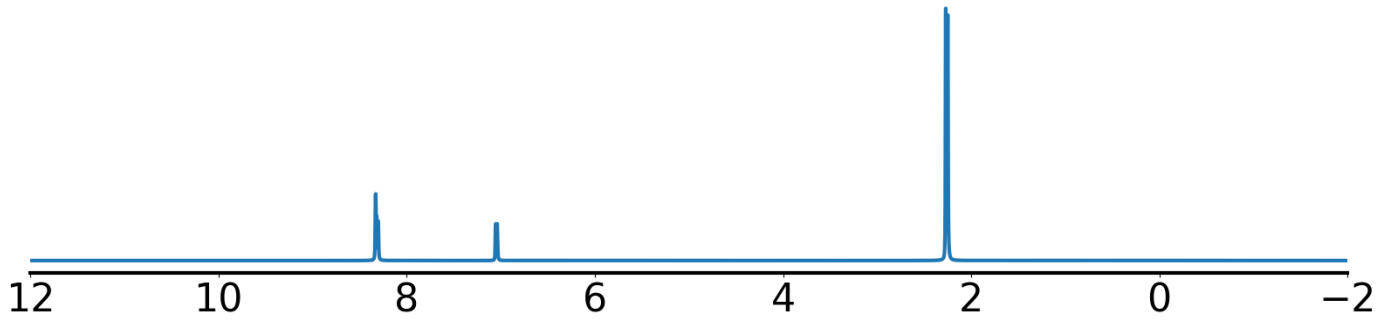
Example 46 true smiles: Cc1ccncc1C formula: C7H9N
Index of correct structure: 7 of 1755
True structure loss: 0.024065
True structure:



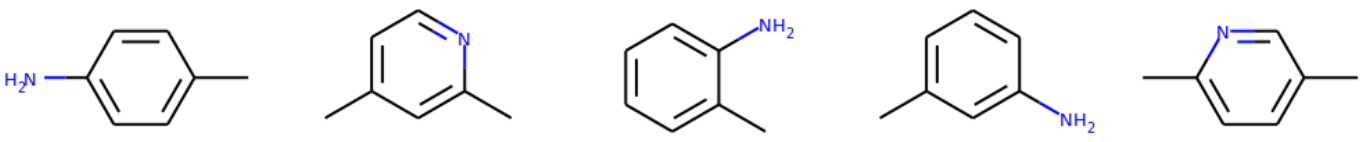
Experimental 13C NMR (solvent: CDCl3)



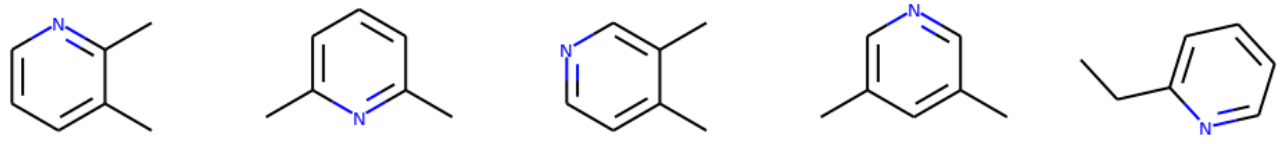
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.016077 0.016351 0.01637 0.017264 0.018944



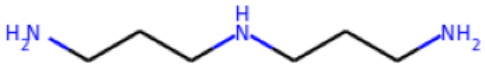
0.019078 0.019737 0.024065 0.029088 0.035916

Top predicted substructures	prob		
[#6X3][#6X3]	0.9986	[cH][cH]	0.9761
[#6H1]	0.9979	[#6X3H1][#6X3H0]	0.971
[#6X3][#6X3][#6X3][#6X3]	0.9952	[CX4H3][cX3H0]	0.971
[CX4H3][#6]	0.995	[CX4H3]	0.9617
[#6H3][#6][#6]	0.9947	[#6X3][#6][#6][#6H3]	0.9529

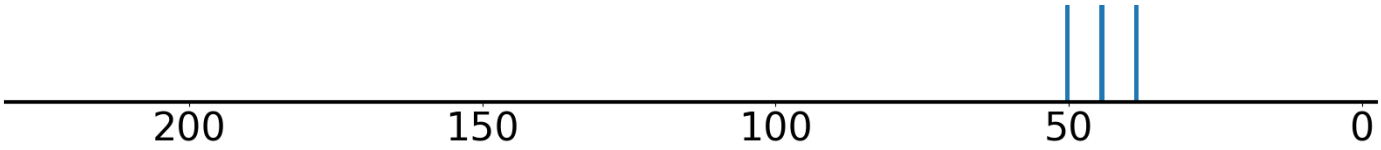
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9986	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H1]	0.9979	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9952	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3][#6]	0.995	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6H3][#6][#6]	0.9947	[#6]1[#8][#6][#6]1=[#8]	0.0
[cH][cH]	0.9761	[CX3H0](=[OX1H0])([OX2H0])[CX4H2]	0.0
[#6X3H1][#6X3H0]	0.971	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[CX4H3][cX3H0]	0.971	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[CX4H3]	0.9617	[OX2H0]1[CX4H0][CX4H1]1	0.0
[#6X3][#6][#6][#6H3]	0.9529	[OX2H0]1[CX4H2][CX4H1]1[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#6]1[#6][#6][#6][#6][#6]1	0.7845	[#6H3][#6][#6][#6H3]	0.0114
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6734	[#6H3][#6H0][#6H1][#7]	0.052
[cX3H1]([cX3H1])[cX3H1]	0.5304	[#6H1][#7][#6H1]	0.0541
[#7][#6X3H0][#6X3H1]	0.4605	[cX3H1]([nX2H0])[cX3H0]	0.3301
[#7X3H2]	0.3889	[cX3H0]([cX3H1])([cX3H0])[CX4H3]	0.4508
[CX4H2]([#6])[#6]	0.3765	[cX3H1]([nX2H0])[cX3H1]	0.5319
[cX3H0][cX3H1][cX3H1][cX3H0]	0.3731	[#6X3][#7][#6X3]	0.6087
[#7][#6H0][#6H1]	0.3277	[#6H3][#6H0]	0.8372
[#7H2][#6H0]	0.2506	[cX3H1]([cX3H1])[cX3H0]	0.867
[CX4H2][CX3H]	0.1766	[#6H1][#6H1]	0.8787

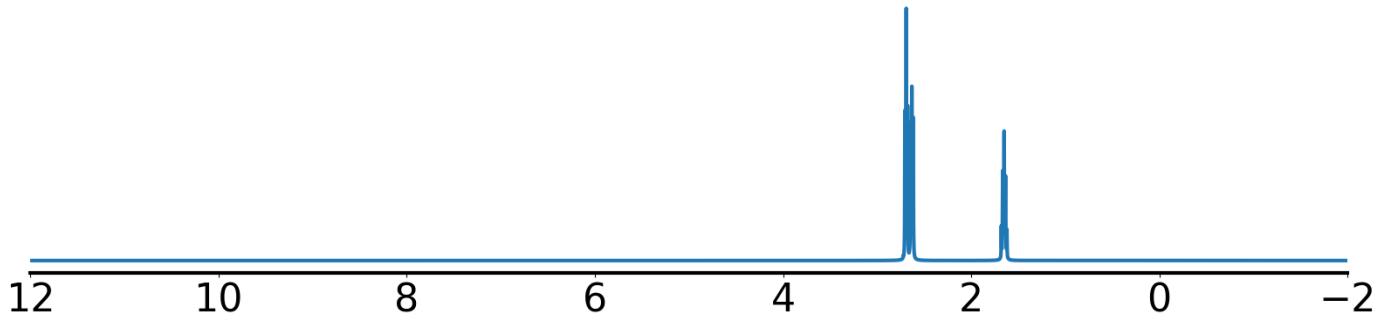
Example 47 true smiles: NCCCNCCCN formula: C6H17N3
Index of correct structure: 0 of 1323
True structure loss: 0.009571
True structure:



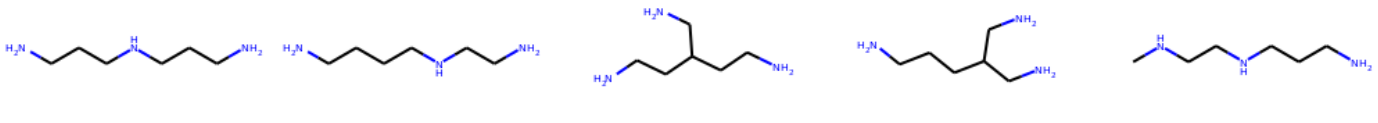
Experimental 13C NMR (solvent: CDCl3)



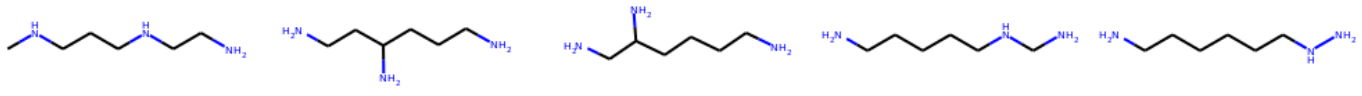
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.009571 0.010276 0.02442 0.024664 0.025912



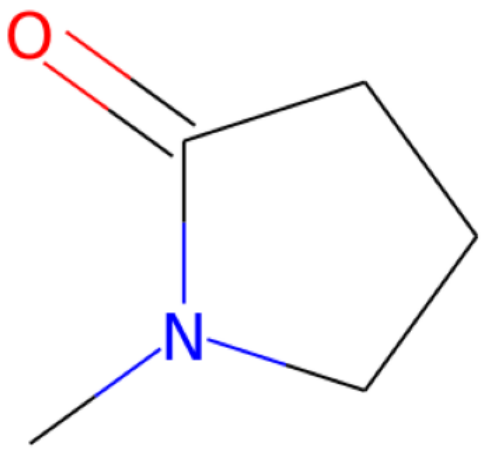
0.025912 0.030093 0.032774 0.034189 0.036315

Top predicted substructures	prob		
[#7X3H2]	0.9996	[#7][#6H2][#6H2]	0.9846
[#7X3][#6H2]	0.9987	[CX4H2]([NX3H2])[CX4H2]	0.9786
[#7][#6H2]	0.9971	[CX4H2][CX4H2]	0.905
[CX4H2]([#6])[#6]	0.9893	[CX4H2]([NX3H1])[CX4H2]	0.7325
[#7H2][#6H2]	0.9879	[#7][#6][#6][#6][#7]	0.7094

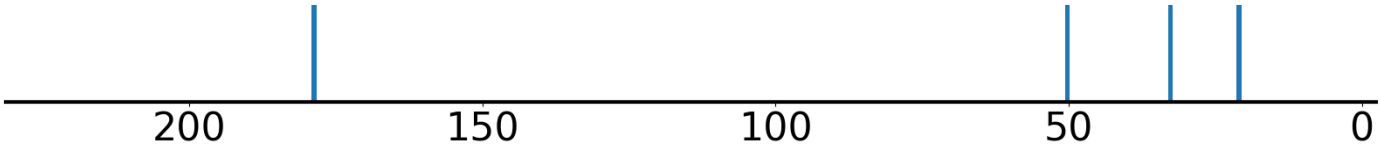
best positives	prob	best negatives	prob
[#7X3H2]	0.9996	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3][#6H2]	0.9987	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7][#6H2]	0.9971	[#6X2][#6H1][#6X2]	0.0
[CX4H2]([#6])[#6]	0.9893	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7H2][#6H2]	0.9879	C=CCCC#C	0.0
[#7][#6H2][#6H2]	0.9846	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([NX3H2])[CX4H2]	0.9786	C=CC=CC#C	0.0
[CX4H2][CX4H2]	0.905	CC=CC#CC	0.0
[CX4H2]([NX3H1])[CX4H2]	0.7325	[CX2H0](#[CX2H1])[CX3H0]	0.0
[#7][#6][#6][#6][#7]	0.7094	CC#CCC#C	0.0

worst negatives	prob	worst positives	prob
[#7][#6H2][#6H2][#7]	0.6931	[#6H2][#7][#6H2]	0.3072
[#7][#6][#6][#6][#6][#7]	0.616	[#7X3H1]	0.3477
[CX4H2][CX4H2][CX4H2][CX4H2]	0.4146	[CX4H2]([CX4H2])[CX4H2]	0.483
[#7][#6][#6][#7]	0.3264	[#7][#6][#6][#6][#7]	0.7094
[#6H1][#6H2]	0.2722	[CX4H2]([NX3H1])[CX4H2]	0.7325
[CX4H2]([NX3H2])[CX4H1]	0.2271	[CX4H2][CX4H2]	0.905
[#7][#6H2][#6H2][#6H1]	0.1618	[CX4H2]([NX3H2])[CX4H2]	0.9786
[#6H1]	0.1591	[#7][#6H2][#6H2]	0.9846
[CX4H1]([CX4H2])([CX4H2])[CX4H2]	0.1507	[#7H2][#6H2]	0.9879
[#6H1]([#6H2])[#6H2]	0.1469	[CX4H2]([#6])[#6]	0.9893

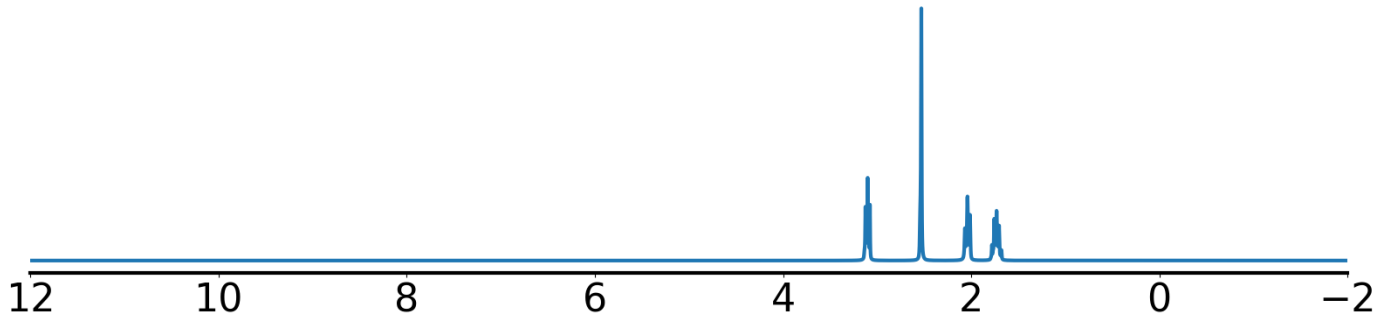
Example 48 true smiles: CN1CCCC1=O formula: C5H9NO
Index of correct structure: 2 of 1318
True structure loss: 0.045538
True structure:



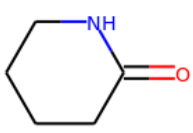
Experimental 13C NMR (solvent: CDCl3)



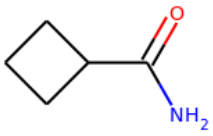
Experimental 1H NMR (solvent: CDCl3)



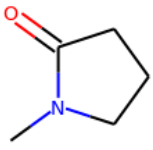
Top predicted structures (loss):



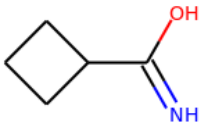
0.030037



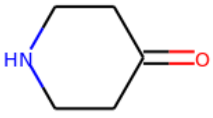
0.035512



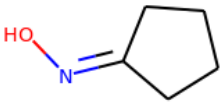
0.045538



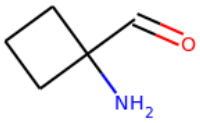
0.050304



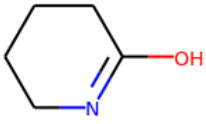
0.053616



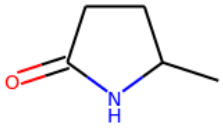
0.059961



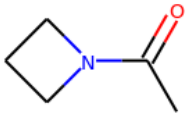
0.060548



0.061676



0.061735



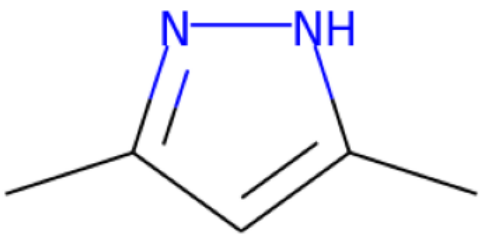
0.063207

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9949	[CX4H2]([CX4H2])[CX4H1]	0.8318
[CX3](=[OX1])C	0.9596	[CX4H2]([CX4H2])[CX4H2]	0.7864
[CX4H2][CX4H2]	0.9122	[#6H1][#6H2]	0.7342
[#7][#6H2]	0.8381	[#7X3][#6H2]	0.6885
[CX4H2]CC=O	0.8348	C1CCC1	0.6839

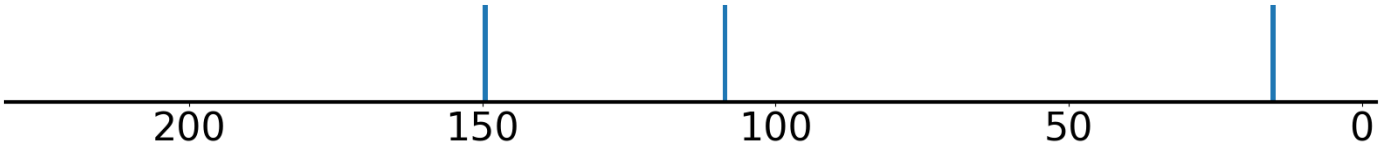
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9949	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9596	C=CC=CC#C	0.0
[CX4H2][CX4H2]	0.9122	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7][#6H2]	0.8381	CC=CC#CC	0.0
[CX4H2]CC=O	0.8348	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.7864	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#7X3][#6H2]	0.6885	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[#7][#6H2][#6H2]	0.6064	CCC#CC=C	0.0
[CX4H2][CX3]=O	0.4323	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([CX4H2])[CX3H0]	0.38	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H1]	0.8318	[#6H3][#7][#6X3]	0.036
[#6H1][#6H2]	0.7342	[CX3H0](=[OX1H0])([NX3H0])[CX4H2]	0.0564
C1CCC1	0.6839	[CX4H3][NX3H0]	0.0906
[#6H1]	0.6452	[#6H3][#7X3H0][#6X4H2][#6X4H2]	0.0997
[#8]=[#6H0][#6H1]	0.4937	[#6H3][#7]	0.1463
[#7X3H1]	0.4663	[#7X3H0]	0.1509
[#6H1]([#6H2])[#6H2]	0.4376	[CX4H2]([NX3H0])[CX4H2]	0.159
O=[CX3][CX4H]	0.4318	[#6H3][#7][#6H2]	0.1724
[CX4H1]1[CX4H2][CX4H2][CX4H2]1	0.3424	[#6H2][#7][#6X3]	0.2156
[#7][#6H0][#6H1]	0.3285	O=[CX3H0][CX4H2][CX4H2]	0.3021

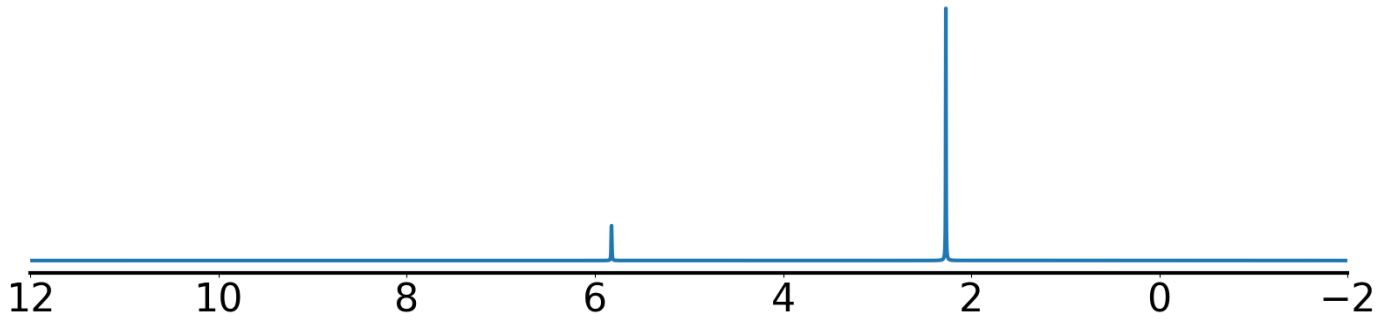
Example 49 true smiles: Cc1cc(C)[nH]n1 formula: C5H8N2
Index of correct structure: 4 of 1068
True structure loss: 0.027633
True structure:



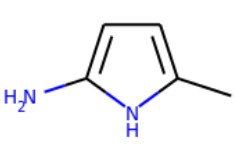
Experimental 13C NMR (solvent: CDCl3)



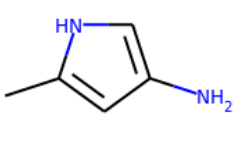
Experimental 1H NMR (solvent: CDCl3)



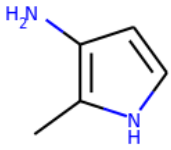
Top predicted structures (loss):



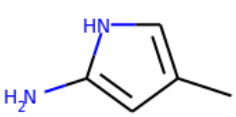
0.020162



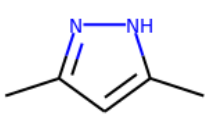
0.023502



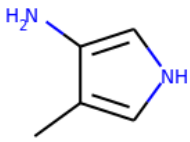
0.024498



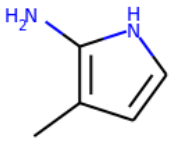
0.027619



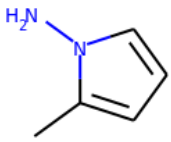
0.027633



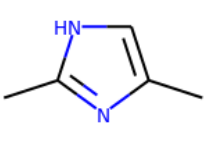
0.031007



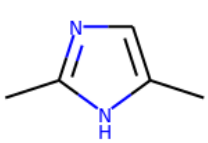
0.031025



0.032053



0.033125



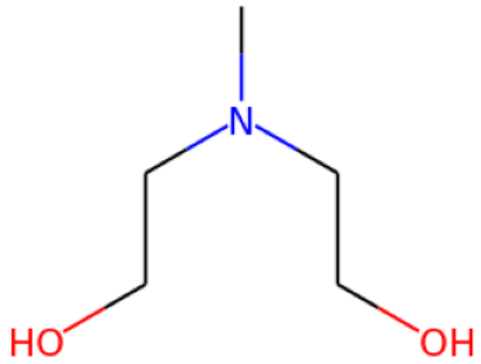
0.035215

Top predicted substructures	prob		
[CX4H3]	0.9981	[#6H3][#6][#6]	0.9385
[#6H3][#6H0]	0.991	[#6X3][#6][#6][#6H3]	0.915
[CX4H3][cX3H0]	0.9804	[#7][#6][#6][#6X3]	0.9105
[#6X3][#6X3]	0.969	[#7][#6][#6X3]	0.9095
[CX4H3][#6]	0.9594	[#7][#6][#6H3]	0.8995

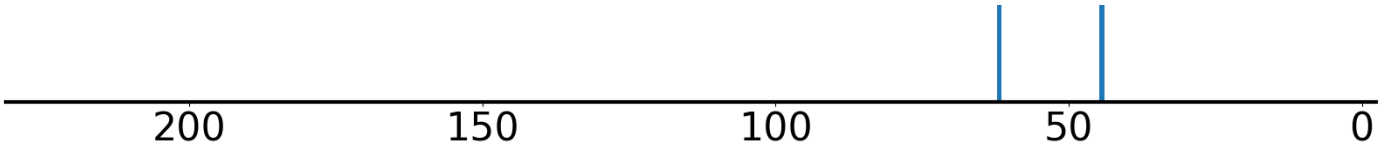
best positives	prob	best negatives	prob
[CX4H3]	0.9981	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H3][#6H0]	0.991	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3][cX3H0]	0.9804	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6X3][#6X3]	0.969	[OX2H1][CX4H2][CX4H1]([OX2H0])[CX4H1]	0.0
[CX4H3][#6]	0.9594	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6H3][#6][#6]	0.9385	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6][#6][#6H3]	0.915	[OX2H1][CX4H1][CX4H1]([CX4H2])[CX4H2]	0.0
[#7][#6][#6][#6X3]	0.9105	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[#7][#6][#6X3]	0.9095	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#7][#6][#6H3]	0.8995	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6X3][#6X3][#6X3][#6X3]	0.8876	[#7][#7H1]	0.0626
[#6X3][#7X3][#6X3]	0.8077	[cX3H1]([cX3H0])[cX3H0]	0.2896
[#6X3][#7][#6X3]	0.7695	[#7][#7]	0.3219
[#7X3H2]	0.6337	[#7][#6][#6][#6][#7]	0.3345
[cH][cH]	0.6071	[#7][#6H0][#6H1]	0.5491
[#7H2][#6H0]	0.5746	[#7X3H1]	0.5723
[cX3H1]([cX3H1])[cX3H0]	0.5189	[#7][#6X3H0][#6X3H1]	0.7222
[#7][#6][#7]	0.4856	[#6H1]	0.7804
[#7][#6H0][#7]	0.4636	[#6X3H1][#6X3H0]	0.8527
[#6H3][#6H0][#7H0][#6H0]	0.4243	[#6H3][#6][#6X3]	0.8563

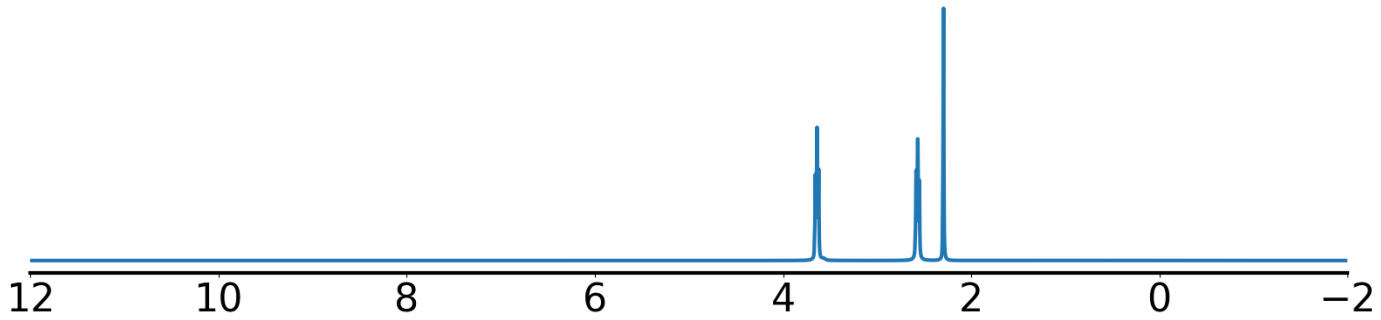
Example 50 true smiles: CN(CCO)CCO formula: C5H13NO2
Index of correct structure: 0 of 900
True structure loss: 0.022324
True structure:



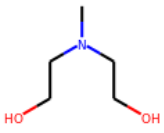
Experimental 13C NMR (solvent: CDCl3)



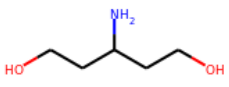
Experimental 1H NMR (solvent: CDCl3)



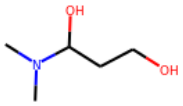
Top predicted structures (loss):



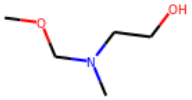
0.022324



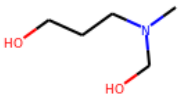
0.02863



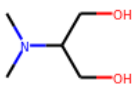
0.030825



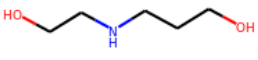
0.032305



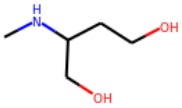
0.034111



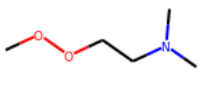
0.03543



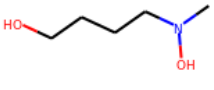
0.036206



0.036376



0.037714



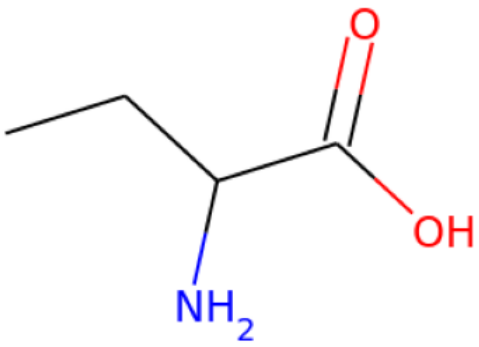
0.039016

Top predicted substructures	prob		
[OX2H1]	0.9936	[CX4H2][CX4H2]	0.7881
[CX4H2]([#6])[O]	0.9526	[CH2X4](O)[CX4H2]	0.7026
[#8][#6][#6H2]	0.946	[#7X3][#6H3]	0.6422
[CX4H2]([#6])[#6]	0.894	[CX4H3][NX3H0]	0.6388
[CX4H2]([OX2H1])[CX4H2]	0.8876	[#6H3][#7]	0.599

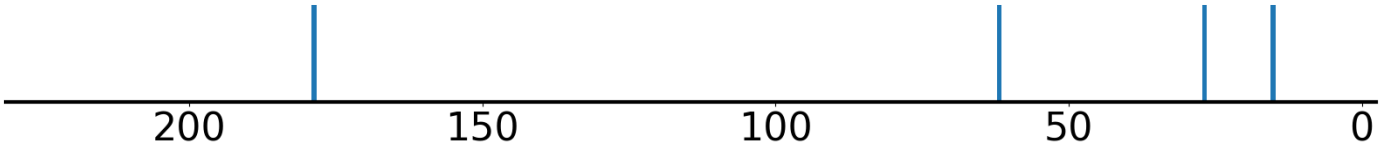
best positives	prob	best negatives	prob
[OX2H1]	0.9936	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[O]	0.9526	CC=CC#CC	0.0
[#8][#6][#6H2]	0.946	CCC=CC#C	0.0
[CX4H2]([OX2H1])[CX4H2]	0.8876	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2][CX4H2]	0.7881	CC=CCC#C	0.0
[CH2X4](O)[CX4H2]	0.7026	[CX2H0](#[CX2H0])[CX3H0]	0.0
[#7X3][#6H3]	0.6422	C=CC=CC#C	0.0
[CX4H3][NX3H0]	0.6388	CC#CCC=C	0.0
[#6H3][#7]	0.599	C=CCCC#C	0.0
[#7X3H0]	0.5847	[CX2H0](#[CX2H0])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([#6])[#6]	0.894	[#6H2][#7][#6H2]	0.0747
OCC[CH2]	0.4944	[#6H3][#7X3H0][#6X4H2][#6X4H2]	0.1001
[#7X3H2]	0.4723	[CX4H2]([NX3H0])[CX4H2]	0.198
[#6H1][#6H2]	0.4327	[#6H3][#7][#6H2]	0.2012
[#6H1]	0.4226	[CX4H3]	0.323
[CX4H2](O)[CHX4]	0.2109	[#7X3][#6H2]	0.4452
[#8H][#6H2][#6H1]	0.1621	[#7][#6H2][#6H2]	0.5133
[#7H2][#6H2]	0.1594	[#7][#6H2]	0.5271
[#6H1]([#6H2])[#6H2]	0.1485	[#7X3H0]	0.5847
[CX4H2]([NX3H2])[CX4H2]	0.1362	[#6H3][#7]	0.599

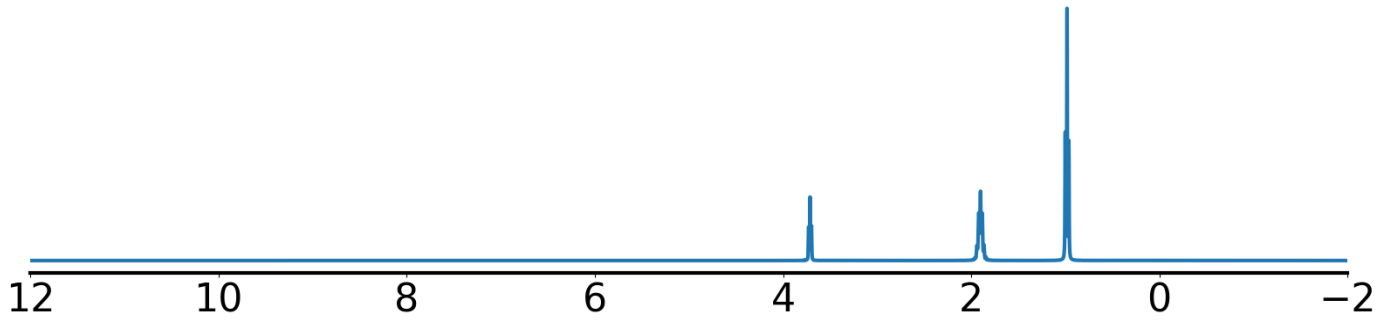
Example 51 true smiles: CCC(N)C(=O)O formula: C4H9NO2
Index of correct structure: 0 of 896
True structure loss: 0.017196
True structure:



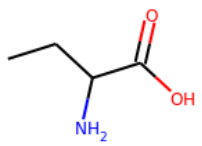
Experimental 13C NMR (solvent: D2O)



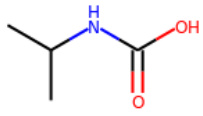
Experimental 1H NMR (solvent: D2O)



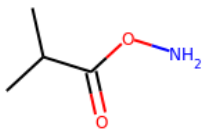
Top predicted structures (loss):



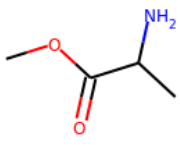
0.017196



0.04451

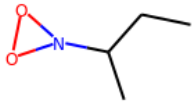


0.047569

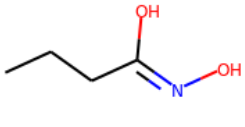


0.050225

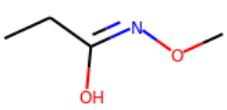
0.053337



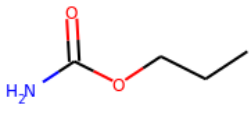
0.054463



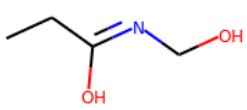
0.056389



0.056797



0.056952



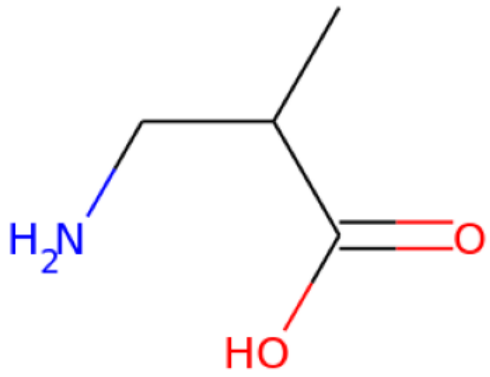
0.057627

Top predicted substructures	prob		
[CX4H3]	0.9998	[CX4H3][CX4H2]	0.9439
[#6H3][#6][#6]	0.9979	[#7X3H2]	0.9303
[CX4H3][#6]	0.9975	[CX3](=O)[OX2H1]	0.9061
[CX3](=[OX1])C	0.9834	[#8]=[#6H0][#6H1]	0.8742
[OX2H1]	0.9659	[CX4H2]([CX4H3])[CX4H1]	0.8656

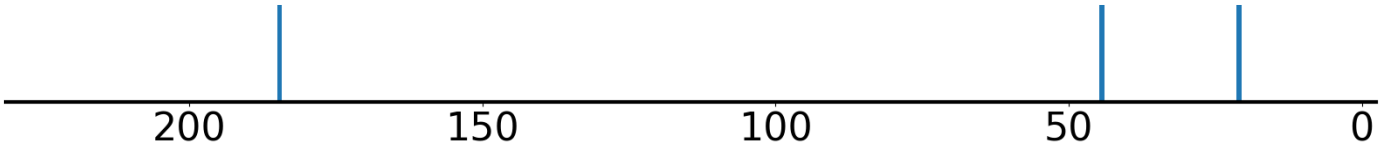
best positives	prob	best negatives	prob
[CX4H3]	0.9998	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6][#6]	0.9979	C=CC=CC#C	0.0
[CX4H3][#6]	0.9975	CC=CC#CC	0.0
[CX3](=[OX1])C	0.9834	CCC=CC#C	0.0
[OX2H1]	0.9659	C=CCCC#C	0.0
[CX4H3][CX4H2]	0.9439	CC#CCC=C	0.0
[#7X3H2]	0.9303	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX3](=O)[OX2H1]	0.9061	CCC#CC#C	0.0
[#8]=[#6H0][#6H1]	0.8742	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H2]([CX4H3])[CX4H1]	0.8656	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#6H1][#6H1]	0.4913	OCC[CH2]	0.0953
[#7H2][#6H0]	0.4635	[#6H3][#6H2][#6H1][#7]	0.3188
[#7][#6H0][#6H1]	0.3145	[CX4H1]([NX3H2])([CX4H2])[CX3H0]	0.3877
[#8][#6][#6H2]	0.3131	[#8][#6H0][#6H1]	0.4438
[#6H3][#6H1][#6H1][#7]	0.2994	[#7H2][#6H1]	0.4712
[#6H3][#6][#6X3]	0.2758	[CX4H2]([#6])[#6]	0.5339
[CH3]CC[OH]	0.2624	[#6H1][#6H2]	0.6182
[#7X3H1]	0.2603	[CX4H2]CC=O	0.6784
[OH][CX4H]	0.2305	[#7][#6][#6X3]	0.6901
[#6H1][#6H1]	0.1805	[#6X3][#6][#6][#6H3]	0.7073

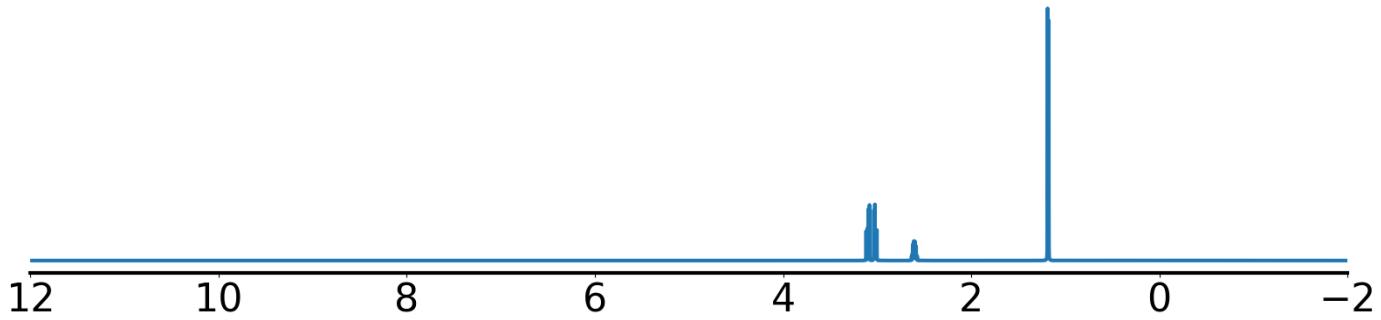
Example 52 true smiles: CC(CN)C(=O)O formula: C4H9NO2
Index of correct structure: 0 of 896
True structure loss: 0.016235
True structure:



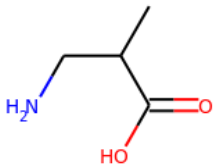
Experimental 13C NMR (solvent: D2O)



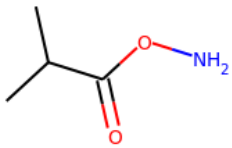
Experimental 1H NMR (solvent: D2O)



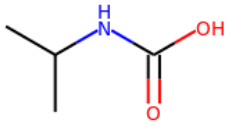
Top predicted structures (loss):



0.016235

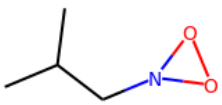


0.038758

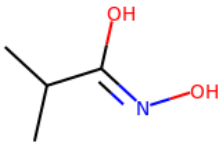


0.040326

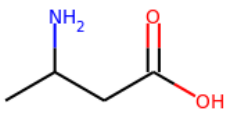
0.043098



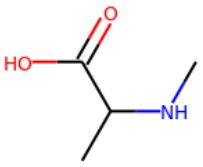
0.050884



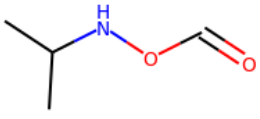
0.051074



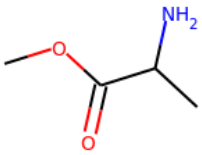
0.055718



0.058522



0.063079



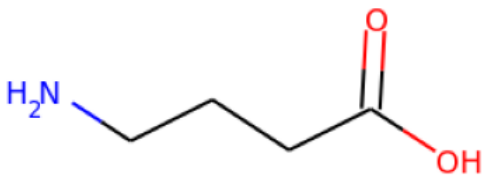
0.066704

Top predicted substructures	prob		
[CX4H3]	0.9997	[OX2H1]	0.9833
[CX4H3][#6]	0.9964	[#7X3][#6H2]	0.9574
[#6H3][#6][#6]	0.9962	[#6H1]	0.9544
[CX3](=[OX1])C	0.9937	[CX4H3][CX4H1]	0.9209
[CX3](=O)[OX2H1]	0.9937	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.9144

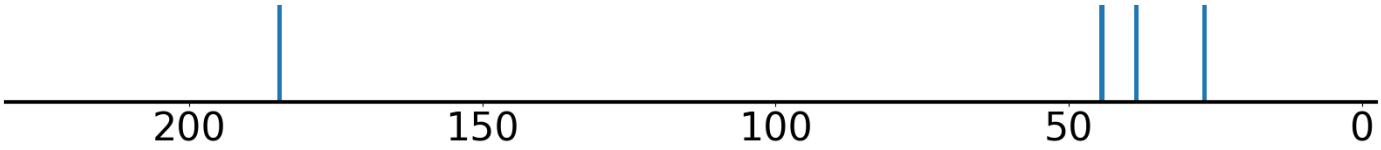
best positives	prob	best negatives	prob
[CX4H3]	0.9997	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9964	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9962	CC=CC#CC	0.0
[CX3](=[OX1])C	0.9937	CC=CCC#C	0.0
[CX3](=O)[OX2H1]	0.9937	CCC=CC#C	0.0
[OX2H1]	0.9833	CCC#CC#C	0.0
[#7X3][#6H2]	0.9574	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#6H1]	0.9544	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H3][CX4H1]	0.9209	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.9144	CC#CCC=C	0.0

worst negatives	prob	worst positives	prob
[#7][#6H0][#6H1]	0.4055	[OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]	0.2495
[CX4H1]([CX4H3])([CX4H3])[CX3H0]	0.3462	OCC[CH2]	0.341
[#7X3H1]	0.3242	[#7][#6][#6][#6X3]	0.3596
[#6X3][#6][#6][#6H3]	0.3115	[CH3]CC[OH]	0.3635
[#7H2][#6H0]	0.2364	[CX4H2]([NX3H2])[CX4H1]	0.4049
[CHX4]([CH3X4])[CH3X4]	0.2278	[CX4H1]([CX4H3])([CX4H2])[CX3H0]	0.4461
[#8]=[#6][#6H1][#6H1]	0.2174	[#6H1][#6H2]	0.5617
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.1888	[#7][#6H2][#6H1]	0.5643
[CX4H2][CX3]=O	0.1872	[#7][#6H2]	0.6809
[#7][#6][#6H3]	0.1307	[CX4H2]CC=O	0.6858

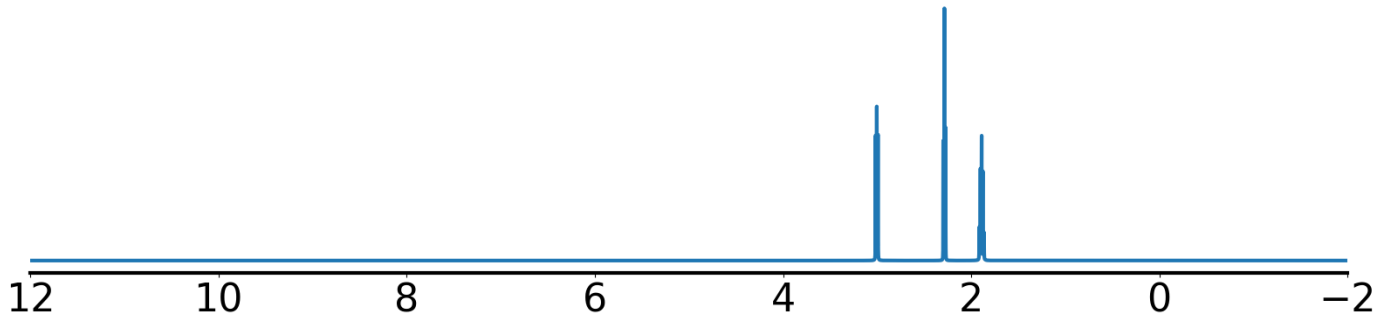
Example 53 true smiles: NCCCC(=O)O formula: C4H9NO2
Index of correct structure: 0 of 896
True structure loss: 0.009423
True structure:



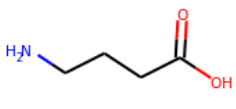
Experimental 13C NMR (solvent: D2O)



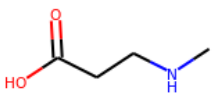
Experimental 1H NMR (solvent: D2O)



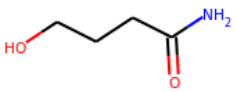
Top predicted structures (loss):



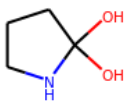
0.009423



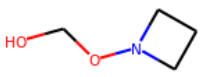
0.043282



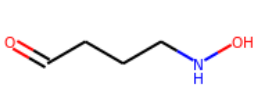
0.055838



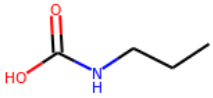
0.058892



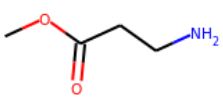
0.061202



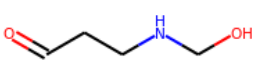
0.063165



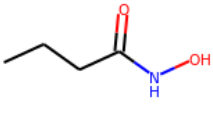
0.065322



0.066907



0.071745



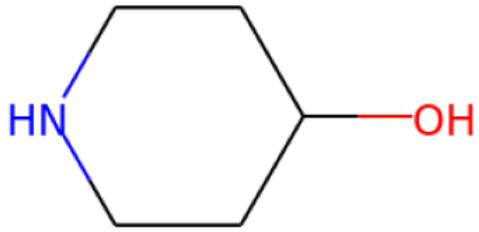
0.073503

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9973	[#7X3][#6H2]	0.9482
[CX4H2]([#6])[#6]	0.997	[CX4H2]CC=O	0.9318
[OX2H1]	0.9952	[CX4H2][CX4H2]	0.924
[CX3](=O)[OX2H1]	0.9919	[#7][#6H2][#6H2]	0.9218
[#7][#6H2]	0.965	O=[CX3H0][CX4H2][CX4H2]	0.8961

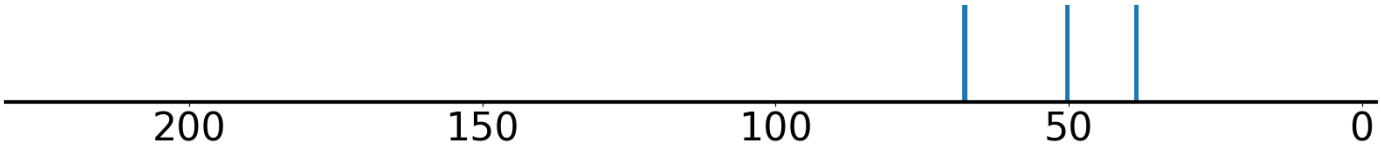
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9973	CCC=CC#C	0.0
[CX4H2]([#6])[#6]	0.997	[CX2H0](#[CX2H1])[cX3H0]	0.0
[OX2H1]	0.9952	CC=CC#CC	0.0
[CX3](=O)[OX2H1]	0.9919	C=CC=CC#C	0.0
[#7][#6H2]	0.965	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3][#6H2]	0.9482	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]CC=O	0.9318	CCC#CC#C	0.0
[CX4H2][CX4H2]	0.924	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7][#6H2][#6H2]	0.9218	CC=CCC#C	0.0
O=[CX3H0][CX4H2][CX4H2]	0.8961	[CX3H1](=[CX3H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#7X3H1]	0.2593	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2647
[#7H2][#6H0]	0.2362	[#8][#6][#6H2]	0.2824
[CX4H2][CX4H2][CX4H2][CX4H2]	0.2338	[CX4H2]([NX3H2])[CX4H2]	0.7698
[#6H2][#7][#6X3]	0.2223	OCC[CH2]	0.7986
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2156	[#7H2][#6H2]	0.8096
[#8]=[#6H0][#6H1]	0.2037	[#8]=[#6][#8]	0.8098
[#8][#6H0][#6H1]	0.156	[CX4H2][CX3]=O	0.8196
[#6H1][#6H2]	0.1536	[CX4H2]([CX4H2])[CX4H2]	0.8248
[#6H1]	0.143	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.839
[CX4H2]([NX3H1])[CX4H2]	0.1223	[CX4H2]([CX4H2])[CX3H0]	0.8477

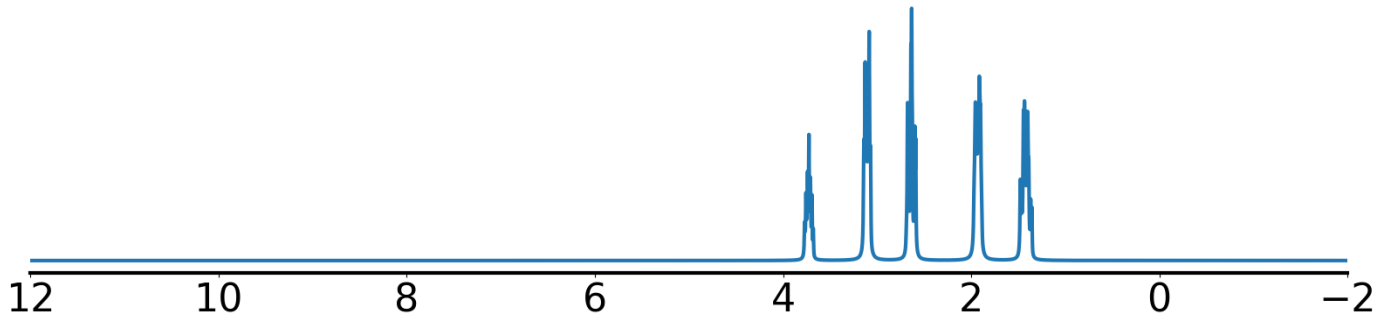
Example 54 true smiles: OC1CCNCC1 formula: C5H11NO
Index of correct structure: 0 of 864
True structure loss: 0.021376
True structure:



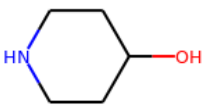
Experimental 13C NMR (solvent: CDCl3)



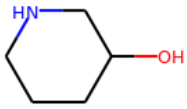
Experimental 1H NMR (solvent: CDCl3)



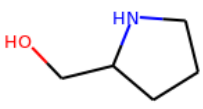
Top predicted structures (loss):



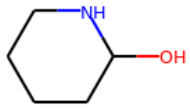
0.021376



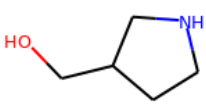
0.028397



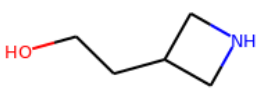
0.029413



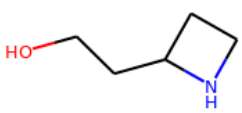
0.031179



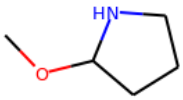
0.031396



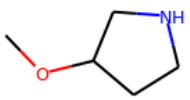
0.038322



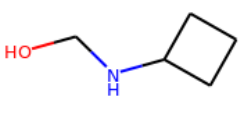
0.039979



0.044659



0.045066



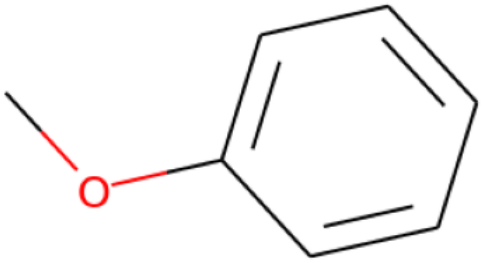
0.047455

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9987	[#6H1][#6H2]	0.9545
[#6H1]	0.9816	OCC[CH2]	0.9274
[#7][#6H2]	0.965	[OX2H1]	0.9168
[#7X3][#6H2]	0.9622	[CX4H2][CX4H2]	0.8776
[CX4H2]([CX4H2])[CX4H1]	0.9592	[#6H1]([#6H2])[#6H2]	0.8672

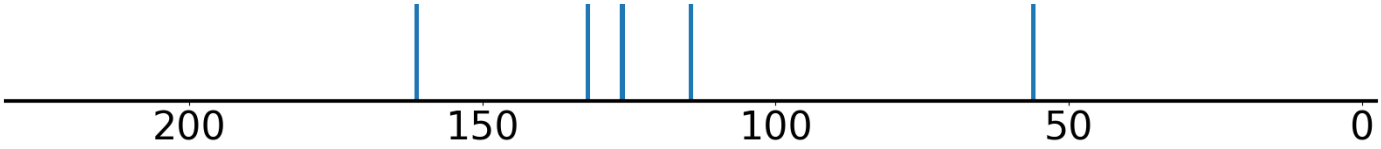
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9987	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H1]	0.9816	C=CC=CC#C	0.0
[#7][#6H2]	0.965	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3][#6H2]	0.9622	C=CCCC#C	0.0
[CX4H2]([CX4H2])[CX4H1]	0.9592	CC#CCC=C	0.0
[#6H1][#6H2]	0.9545	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
OCC[CH2]	0.9274	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[OX2H1]	0.9168	CCC#CC=C	0.0
[CX4H2][CX4H2]	0.8776	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[#6H1]([#6H2])[#6H2]	0.8672	CC=CC#CC	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H1])[CX4H1]	0.6905	[OH][CX4H]	0.251
[#7X3H2]	0.5904	[CX4H1]([OX2H1])([CX4H2])[CX4H2]	0.3287
[#6H1][#6H2][#6][#6][#7]	0.5554	[#7X3H1]	0.3429
[CX4H2]([CH])[CH]	0.5415	[#6X4H2][#6H1][#8H]	0.3631
[CX4H2](O)[CHX4]	0.4818	[#6H2][#7][#6H2]	0.4152
[CX4H2]([#6])[O]	0.4503	O[CX4H][CX4H2]	0.4281
[CH2X4](O)[CX4H2]	0.3133	[#6]1[#6][#6][#6][#6][#7]1	0.4324
CCCCCC	0.2891	[CX4H]O	0.5077
[CX4H2]([OX2H1])[CX4H1]	0.2804	[#7][#6H2][#6H2][#6H1]	0.6804
[#7][#6H1][#6H2r5]	0.279	[#8][#6][#6H2]	0.7243

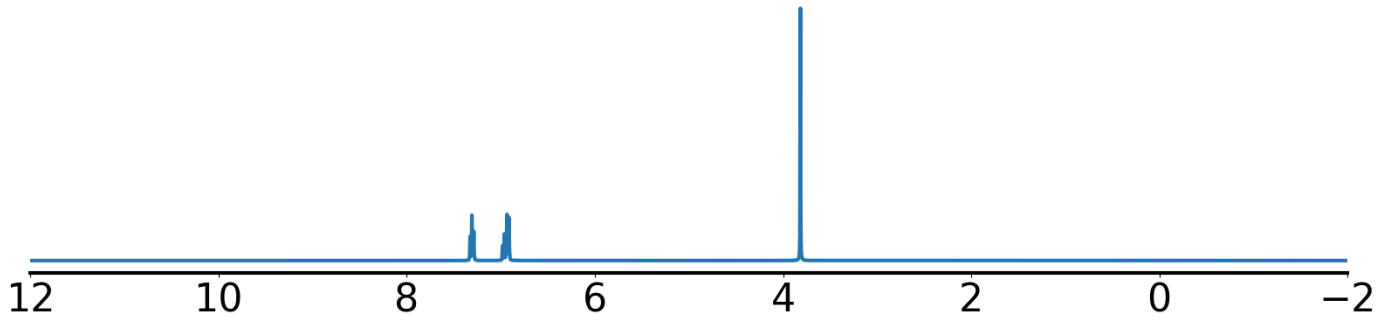
Example 55 true smiles: COc1ccccc1 formula: C7H8O
Index of correct structure: 0 of 746
True structure loss: 0.003697
True structure:



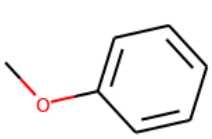
Experimental 13C NMR (solvent: CDCl3)



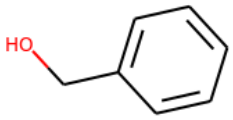
Experimental 1H NMR (solvent: CDCl3)



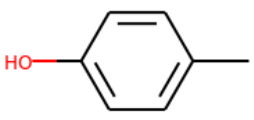
Top predicted structures (loss):



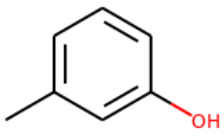
0.003696



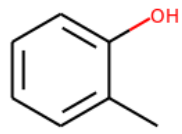
0.037556



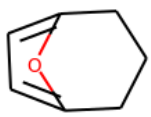
0.064552



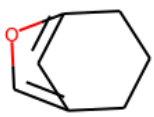
0.072269



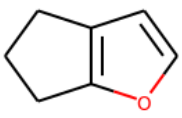
0.072973



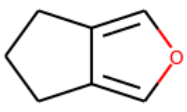
0.079819



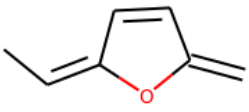
0.0904



0.097002



0.105886



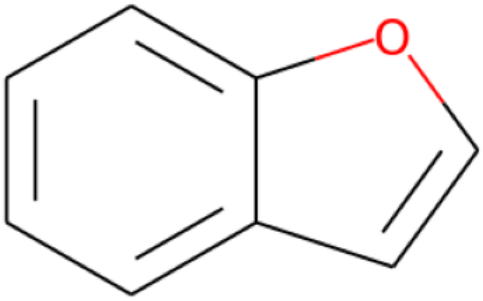
0.107218

Top predicted substructures	prob		
[#6H1]	0.9993	[#6X3H1][#6X3H0]	0.9821
[#6X3][#6X3]	0.9976	[cX3H1]([cX3H1])[cX3H0]	0.9807
[cH][cH]	0.997	[cX3H1]([cX3H1])[cX3H1]	0.9614
[#6X3][#6X3][#6X3][#6X3]	0.993	[#6H1][#6H1]	0.9596
[cH]	0.9897	[CX4H3][OX2H0]	0.957

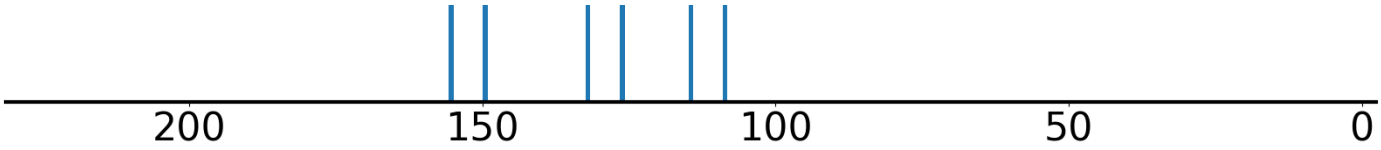
best positives	prob	best negatives	prob
[#6H1]	0.9993	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.9976	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[cH][cH]	0.997	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.993	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[cH]	0.9897	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#6X3H1][#6X3H0]	0.9821	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9807	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9614	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6H1][#6H1]	0.9596	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[CX4H3][OX2H0]	0.957	[CX4H1]([OX2H1])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[cX3H1]([cX3H0])[cX3H0]	0.1857	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.7749
[OX2H1]	0.1733	[cH]cO	0.8451
[CHX3]=[CHX3]	0.1605	[#8][#6][#6][#6X3]	0.8911
[OX2H][cX3]:[c]	0.1251	[#6]1[#6][#6][#6][#6][#6]1	0.9259
[#6X3][#6H2][#6X3]	0.1188	[CX4H3]	0.9492
[cX3H0][cX3H1][cX3H1][cX3H0]	0.1176	[#8][#6H0][#6H1]	0.9498
o[cH]	0.0994	[CX4H3][OX2H0]	0.957
[#7][#6][#6][#6X3]	0.0954	[#6H1][#6H1]	0.9596
[#8][#6H][#6X3][#6X3H]	0.0951	[cX3H1]([cX3H1])[cX3H1]	0.9614
[#6]1[#6][#6][#6][#6][#7]1	0.0944	[cX3H1]([cX3H1])[cX3H0]	0.9807

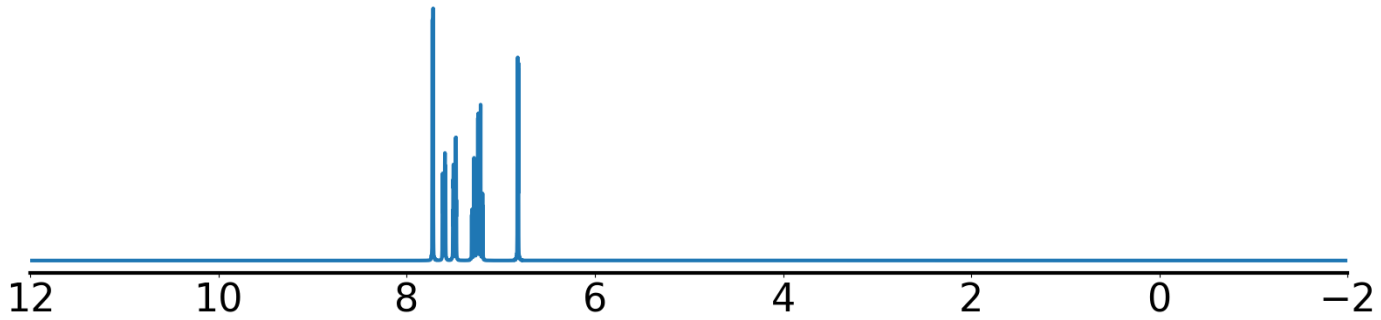
Example 56 true smiles: c1ccc2occc2c1 formula: C8H6O
Index of correct structure: 0 of 720
True structure loss: 0.009984
True structure:



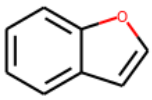
Experimental 13C NMR (solvent: CDCl3)



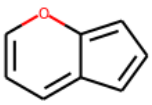
Experimental 1H NMR (solvent: CD3OD)



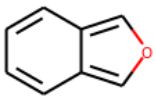
Top predicted structures (loss):



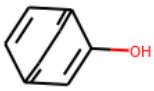
0.009984



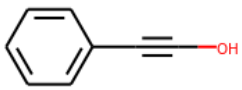
0.018026



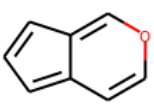
0.024484



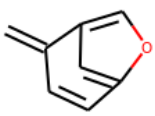
0.025727



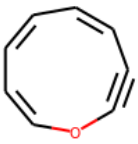
0.031534



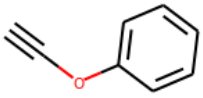
0.038981



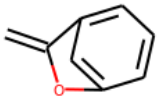
0.039189



0.039479



0.040704



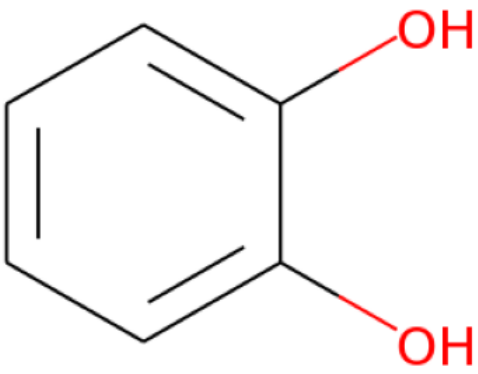
0.042596

Top predicted substructures	prob		
[#6H1]	1.0	[#6X3H1][#6X3H0]	0.9984
[#6X3][#6X3]	1.0	[cX3H1]([cX3H1])[cX3H0]	0.9965
[#6X3][#6X3][#6X3][#6X3]	0.9999	[#8][#6][#6][#6X3]	0.9941
[cH][cH]	0.9998	[#6]1[#6][#6][#6][#6][#6]1	0.9864
[cH]	0.9993	[#6H1][#6H1]	0.9846

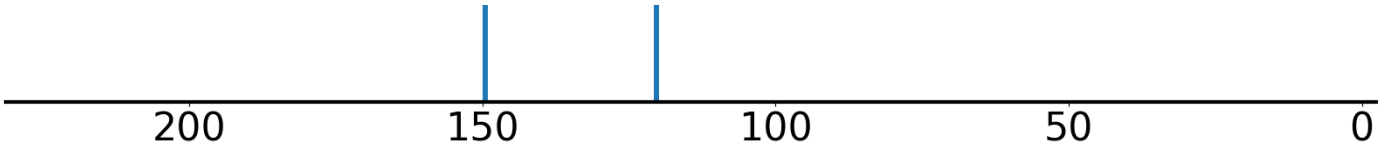
best positives	prob	best negatives	prob
[#6H1]	1.0	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	1.0	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9999	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[cH][cH]	0.9998	[#6H3][#6H0][#7][#6H3]	0.0
[cH]	0.9993	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6X3H1][#6X3H0]	0.9984	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H3]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9965	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX4H1]	0.0
[#8][#6][#6][#6X3]	0.9941	[CX3H0](=[NX2H0])([CX4H2])[CX4H1]	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.9864	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6H1][#6H1]	0.9846	[CX3H0](=[CX3H2])([CX4H3])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[cH]cO	0.4025	[#8X2H0][#6X3H1][#6X3H1][#6X3H0]	0.0043
[#8][#6H][#6X3][#6X3H]	0.3014	o[cH]	0.5279
[CX3H1](=[CX3H1])[cX3H0]	0.2094	[cX3H1]([oX2H0])[cX3H1]	0.8105
[OX2H][cX3]:[c]	0.1867	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.9165
[OX2H1]	0.1525	[#8][#6H1][#6H1]	0.9167
O=[#6][#6][#6X3]	0.1486	[#8][#6H0][#6H1]	0.9476
[#7][#6][#6][#6X3]	0.1267	[cX3H1]([cX3H1])[cX3H1]	0.9641
[cX3H1]([cX3H0])[cX3H0]	0.0995	[#6H1][#6H1]	0.9846
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.0879	[#6]1[#6][#6][#6][#6][#6]1	0.9864
[#7][#6X3H0][#6X3H1]	0.0867	[#8][#6][#6][#6X3]	0.9941

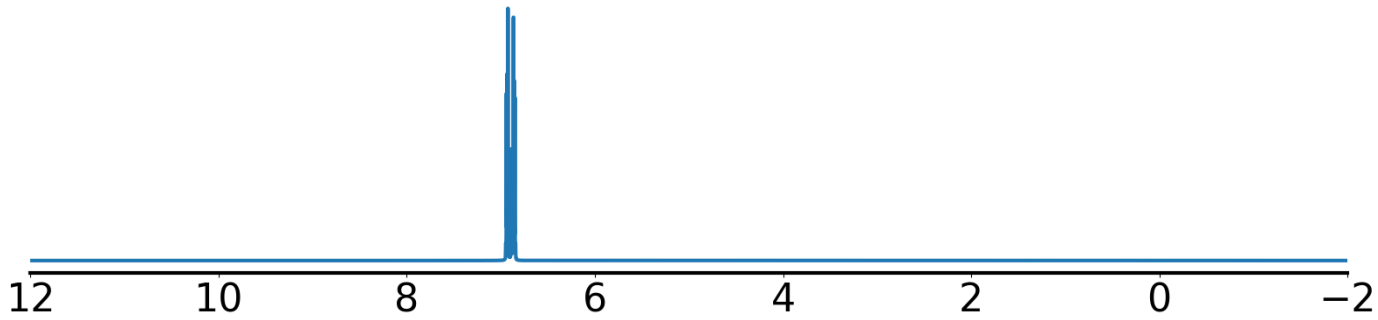
Example 57 true smiles: Oc1ccccc1O formula: C6H6O2
Index of correct structure: 0 of 711
True structure loss: 0.009254
True structure:



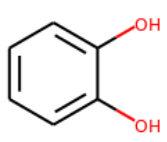
Experimental 13C NMR (solvent: CDCl3)



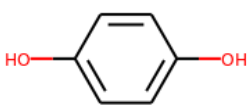
Experimental 1H NMR (solvent: D2O)



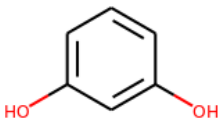
Top predicted structures (loss):



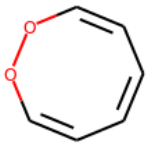
0.009254



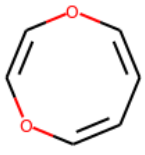
0.011482



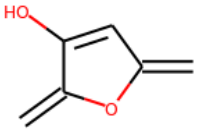
0.012204



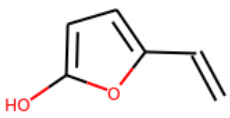
0.025279



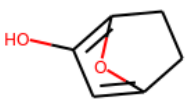
0.033056



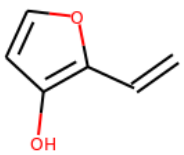
0.051641



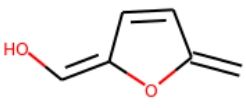
0.054744



0.063618



0.065229



0.065689

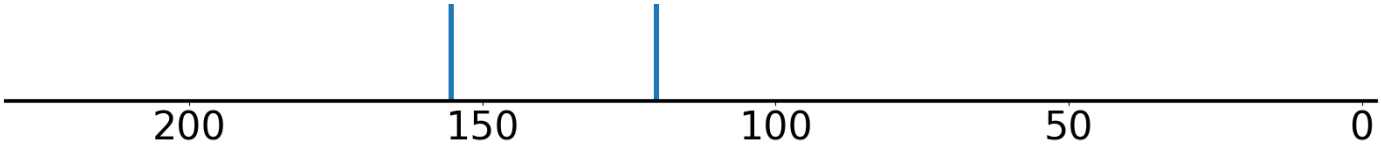
Top predicted substructures	prob		
[#6X3][#6X3][#6X3][#6X3]	0.9893	[cX3H1]([cX3H1])[cX3H0]	0.9235
[#6H1]	0.9874	[#6]1[#6][#6][#6][#6][#6]1	0.909
[#6X3][#6X3]	0.9862	[#6H1][#6H1]	0.8754
[cH][cH]	0.9844	[#6X3H1][#6X3H0]	0.8687
[cH]	0.9352	[#8][#6][#6][#6X3]	0.8469

best positives	prob	best negatives	prob
[#6X3][#6X3][#6X3][#6X3]	0.9893	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6H1]	0.9874	[CX4H2]([NX3H0])[CX4H3]	0.0
[#6X3][#6X3]	0.9862	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[cH][cH]	0.9844	[#6H3][#6H1][#7][#7]	0.0
[cH]	0.9352	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9235	[CX4H2]([NX2H0])[CX4H1]	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.909	[#6H3][#7][#6X4H1][#6H3]	0.0
[#6H1][#6H1]	0.8754	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.8687	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#8][#6][#6][#6X3]	0.8469	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0

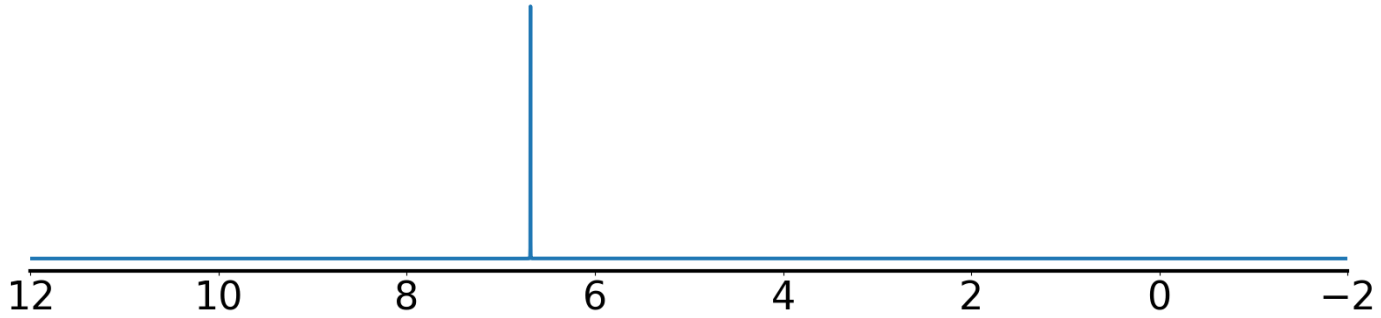
worst negatives	prob	worst positives	prob
[cX3H0][cX3H1][cX3H1][cX3H0]	0.4666	[#8][#6][#6][#8]	0.2663
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.4178	[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.2837
[#8]=[#6][#8]	0.279	[OX2H1]	0.5629
[cX3H1]([oX2H0])[cX3H1]	0.2249	[#8][#6H0][#6H1]	0.7258
[cX3H0][cX3H1][cX3H0][OX2H1]	0.1995	[cX3H1]([cX3H1])[cX3H1]	0.7509
[#8][#6H1][#6H1]	0.1495	[cH]cO	0.7681
[#8][#6H][#6X3][#6X3H]	0.1359	[OX2H][cX3]:[c]	0.7851
o[cH]	0.1142	[#8][#6][#6][#6X3]	0.8469
[CX3](=[OX1])O	0.1097	[#6X3H1][#6X3H0]	0.8687
[#8][#6][#6]=[#6][#6][#8]	0.0986	[#6H1][#6H1]	0.8754

Example 58 true smiles: Oc1ccc(O)cc1 formula: C6H6O2
Index of correct structure: 1 of 711
True structure loss: 0.016357
True structure:

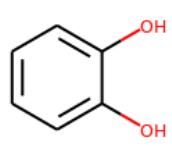
Experimental 13C NMR (solvent: DMSO)



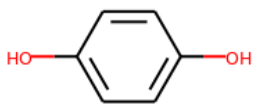
Experimental 1H NMR (solvent: D2O)



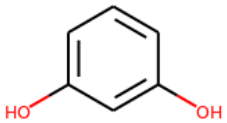
Top predicted structures (loss):



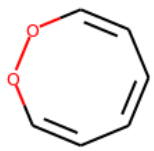
0.01542



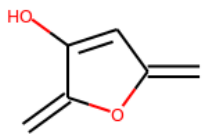
0.016357



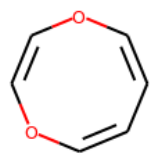
0.0206



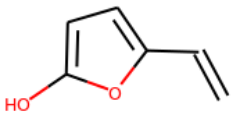
0.028024



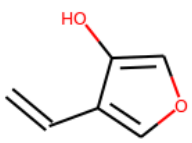
0.033216



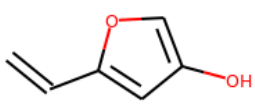
0.034636



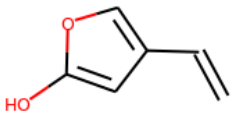
0.040065



0.0441



0.046645



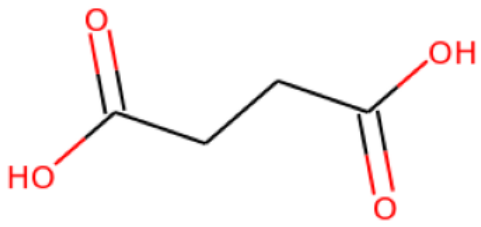
0.046909

Top predicted substructures	prob		
[#6X3][#6X3]	0.9921	[#8][#6][#6][#6X3]	0.8189
[#6H1]	0.9795	[OX2H][cX3]:[c]	0.684
[#6X3H1][#6X3H0]	0.9261	[#8][#6H0][#6H1]	0.6508
[cH]	0.9199	[#6]1[#6][#6][#6][#6][#6]1	0.6291
[#6X3][#6X3][#6X3][#6X3]	0.8914	[cH]cO	0.6013

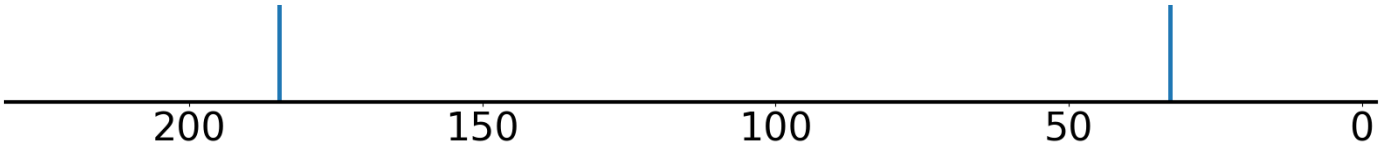
best positives	prob	best negatives	prob
[#6X3][#6X3]	0.9921	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H1]	0.9795	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3H1][#6X3H0]	0.9261	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[cH]	0.9199	[#6H3][#7][#6X4H1][#6H3]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.8914	[CX4H1]([NX3H2])([CX4H3])[CX4H1]	0.0
[#8][#6][#6][#6X3]	0.8189	[#6H3][#6H1][#6H1]=[#7]	0.0
[OX2H][cX3]:[c]	0.684	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[#8][#6H0][#6H1]	0.6508	[CX4H1]([NX3H0])([CX4H3])[CX4H1]	0.0
[#6]1[#6][#6][#6][#6][#6]1	0.6291	[CX4H1]([NX3H0])([CX4H2])[CX4H1]	0.0
[cH]cO	0.6013	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6][#8]	0.4815	[#8][#6][#6][#6][#6][#8]	0.058
[#8]=[#6][#8]	0.3829	[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.1692
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.3032	[cX3H1]([cX3H1])[cX3H0]	0.3135
o[cH]	0.1606	[#6H1][#6H1]	0.3433
[#6X3][#6X3][#6X3]=[#6X3]	0.1585	[OX2H1]	0.3669
[cX3H1]([cX3H0])[cX3H0]	0.1568	[cX3H0][cX3H1][cX3H1][cX3H0]	0.5317
[CHX3]=[CHX3]	0.1235	[cH][cH]	0.5336
[CX3](=[OX1])O	0.1145	[cH]cO	0.6013
O=[#6][#6][#6X3]	0.0989	[#6]1[#6][#6][#6][#6][#6]1	0.6291
[cX3H1]([oX2H0])[cX3H1]	0.0826	[#8][#6H0][#6H1]	0.6508

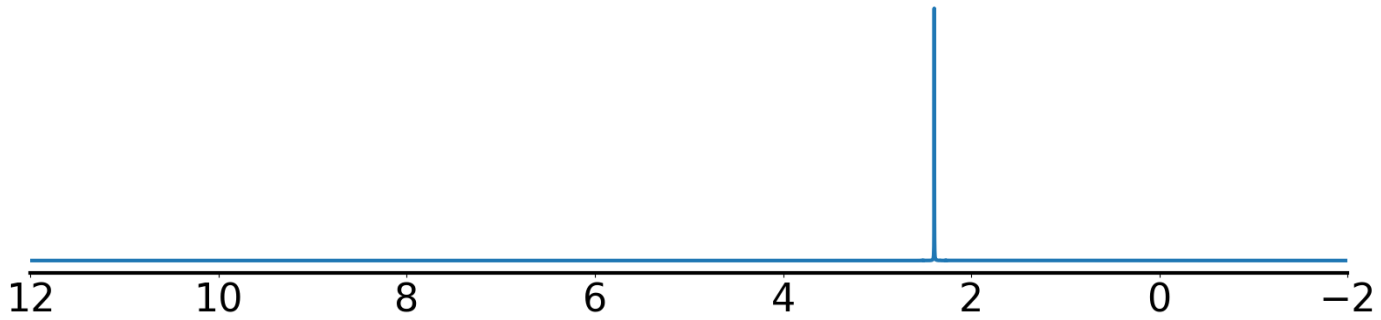
Example 59 true smiles: O=C(O)CCC(=O)O formula: C4H6O4
Index of correct structure: 0 of 502
True structure loss: 0.031774
True structure:



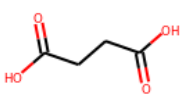
Experimental 13C NMR (solvent: D2O)



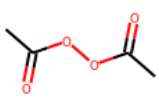
Experimental 1H NMR (solvent: D2O)



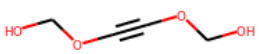
Top predicted structures (loss):



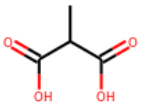
0.031774



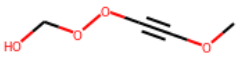
0.041147



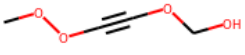
0.042675



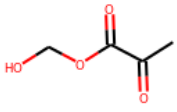
0.044818



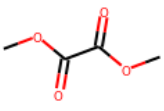
0.049815



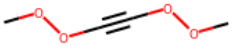
0.049815



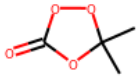
0.050201



0.050657



0.053666



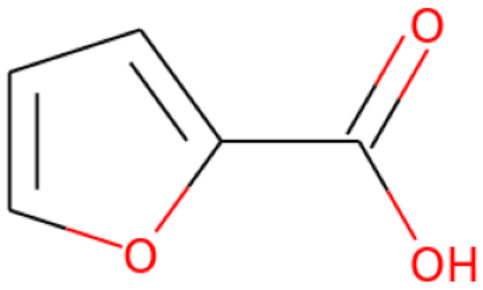
0.057383

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9966	[CX4H3]	0.6851
[#8]=[#6][#8]	0.9797	[#6H3][#6H0]	0.6646
[OX2H1]	0.9755	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.6119
[CX3](=O)[OX2H1]	0.9514	[OX1H0]=[CX3H0][CX4H3]	0.5685
[CX3](=[OX1])O	0.944	[#6H3][#6][#6]	0.4855

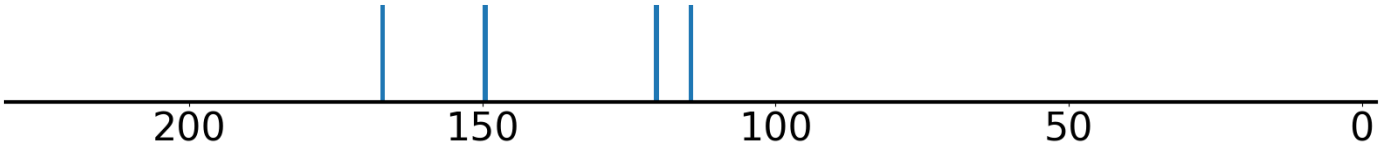
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9966	CC=CC#CC	0.0
[#8]=[#6][#8]	0.9797	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[OX2H1]	0.9755	CC=CCC#C	0.0
[CX3](=O)[OX2H1]	0.9514	C=CC=CC#C	0.0
[CX3](=[OX1])O	0.944	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.6119	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2]CC=O	0.4087	[#6H2]=[#6][#6X2]	0.0
[CX4H2][CX3]=O	0.371	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H2][CX4H2]	0.329	[CX3H0](=[CX3H2])([CX4H3])[CX4H1]	0.0
[#8]=[#6][#6][#6][#6]=[#8]	0.3273	[CX3H0](=[CX3H2])([CX4H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H3]	0.6851	[CX4H2]([#6])[#6]	0.0476
[#6H3][#6H0]	0.6646	[#8][#6][#6][#6][#6][#8]	0.0867
[OX1H0]=[CX3H0][CX4H3]	0.5685	[#8][#6][#6][#6][#6]=[#8]	0.1338
[#6H3][#6][#6]	0.4855	[#8][#6][#6H2]	0.175
[CX4H3][CX3H0]	0.401	[#6X3H0][CX4H2][CX4H2][#6X3H0]	0.186
O=CC=O	0.3188	[CX4H2]([CX4H2])[CX3H0]	0.1866
[#8]=[#6][#6]=[#8]	0.2301	O=[CX3H0][CX4H2][CX4H2]	0.2013
[#8][#6H0][#6H1]	0.2193	OCC[CH2]	0.2075
[#8][#6][#6]=[#8]	0.2155	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2393
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2037	[#8]=[#6][#6][#6][#6]=[#8]	0.3273

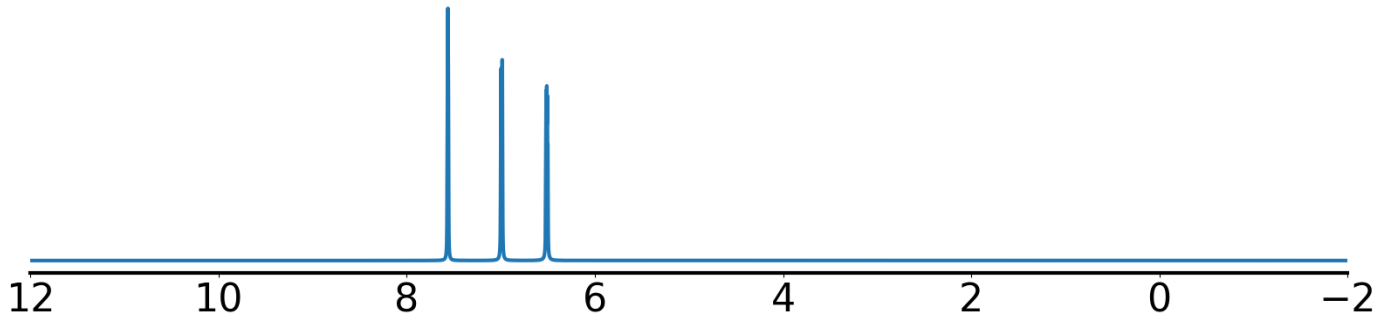
Example 60 true smiles: O=C(O)c1ccco1 formula: C5H4O3
Index of correct structure: 1 of 305
True structure loss: 0.019457
True structure:



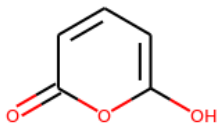
Experimental 13C NMR (solvent: CDCl3)



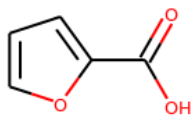
Experimental 1H NMR (solvent: D2O)



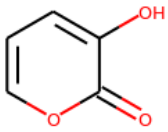
Top predicted structures (loss):



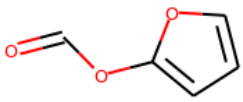
0.019025



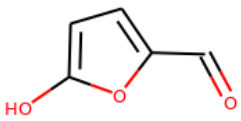
0.019457



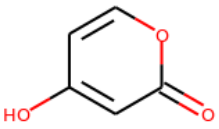
0.023511



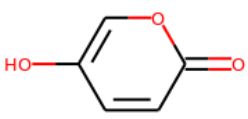
0.028772



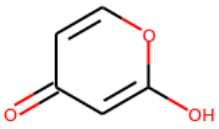
0.033818



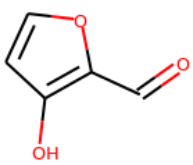
0.034053



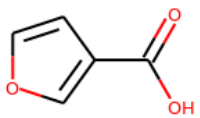
0.034793



0.037258



0.037339



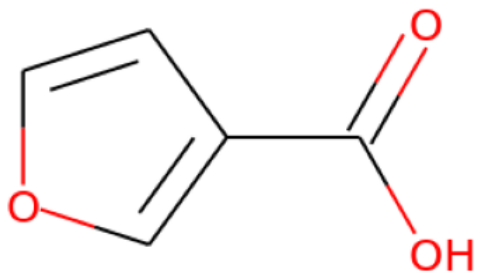
0.041355

Top predicted substructures	prob		
[#6H1]	0.9997	[cX3H1]([cX3H1])[cX3H0]	0.9818
[#6X3][#6X3]	0.9986	[cH]	0.9717
[cH][cH]	0.9973	[OX2H1]	0.9519
[#6X3][#6X3][#6X3][#6X3]	0.997	[#8][#6H0][#6H1]	0.9478
[#6X3H1][#6X3H0]	0.9819	[cX3H1]([cX3H1])[cX3H1]	0.9404

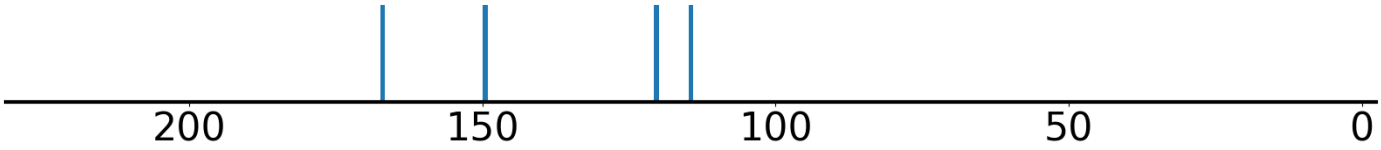
best positives	prob	best negatives	prob
[#6H1]	0.9997	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.9986	[#6H3][#6H0][#7][#6H3]	0.0
[cH][cH]	0.9973	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3][#6X3][#6X3]	0.997	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6X3H1][#6X3H0]	0.9819	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9818	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[cH]	0.9717	[CX4H2]([NX3H0])[CX4H3]	0.0
[OX2H1]	0.9519	[OX2H0]1[CX4H1][CX4H2][CX4H1][CX4H2]1	0.0
[#8][#6H0][#6H1]	0.9478	[CX4H1]([NX3H0])([CX4H2])[CX4H0]	0.0
[cX3H1]([cX3H1])[cX3H1]	0.9404	[CX4H1]([NX3H2])([CX4H2])[CX4H0]	0.0

worst negatives	prob	worst positives	prob
[OX2H][cX3]:[c]	0.7344	[#8][#6][#6]=[#8]	0.0671
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.6806	[#8][#6][#6][#8]	0.2244
[cH]cO	0.6606	[#8][#6H][#6X3][#6X3H]	0.2655
[#6]1[#6][#6][#6][#6][#6]1	0.5628	o[cH]	0.2833
O=[cX3]	0.4666	[cX3H1]([oX2H0])[cX3H1]	0.5095
[OX1H0]=[cX3H0][cX3H1]	0.4465	[#8][#6H1][#6H1]	0.6084
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.3877	[CX3](=O)[OX2H1]	0.6828
[#8]=[#6][#6H1][#6H1]	0.3289	[CX3](=[OX1])O	0.7246
[#8][#6][#6][#6][#6][#8]	0.3142	O=[#6][#6][#6X3]	0.7563
[cX3H0][cX3H1][cX3H1][cX3H0]	0.2662	[#6H1][#6H1]	0.9045

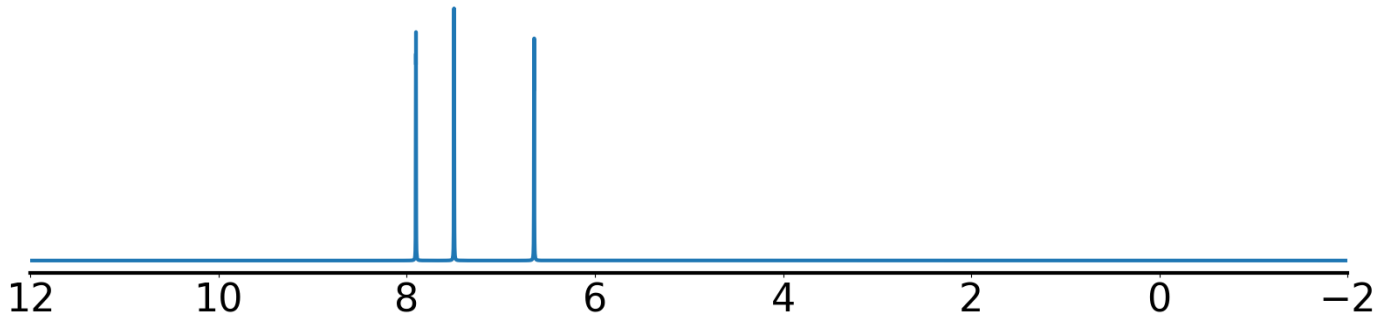
Example 61 true smiles: O=C(O)c1ccoc1 formula: C5H4O3
Index of correct structure: 0 of 305
True structure loss: 0.019856
True structure:



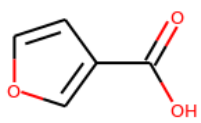
Experimental 13C NMR (solvent: DMSO)



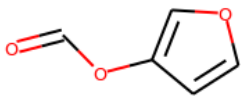
Experimental 1H NMR (solvent: D2O)



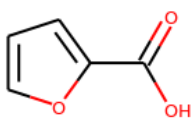
Top predicted structures (loss):



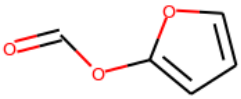
0.019856



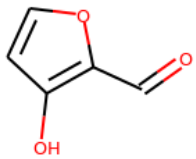
0.01998



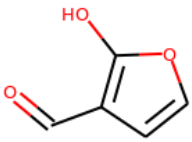
0.020896



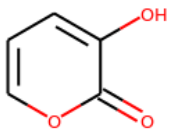
0.023368



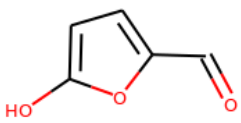
0.026213



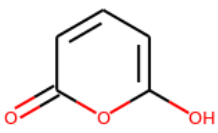
0.027661



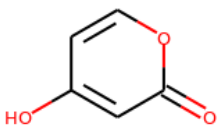
0.029271



0.029832



0.032661



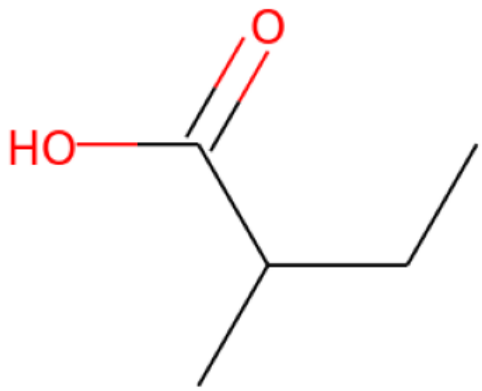
0.034723

Top predicted substructures	prob		
[#6H1]	0.9999	[#8][#6][#6][#6X3]	0.9565
[#6X3][#6X3]	0.9981	[cH]	0.9463
[#6X3][#6X3][#6X3][#6X3]	0.9921	[cX3H1]([cX3H1])[cX3H0]	0.9361
[#6X3H1][#6X3H0]	0.9864	[#6H1][#6H1]	0.8336
[cH][cH]	0.9838	[#6H][#8][#6H]	0.7888

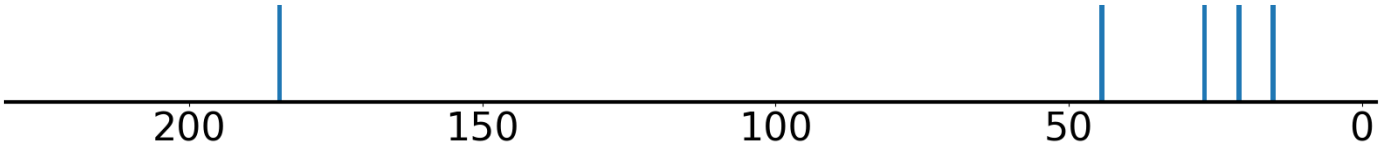
best positives	prob	best negatives	prob
[#6H1]	0.9999	[CX4H0]([NX3H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.9981	[CX4H1]([NX3H1])([CX4H3])[CX4H2]	0.0
[#6X3][#6X3][#6X3][#6X3]	0.9921	[#6H3][#6H0][#7][#6H3]	0.0
[#6X3H1][#6X3H0]	0.9864	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[cH][cH]	0.9838	[#6H3][#6H1][#7][#7]	0.0
[#8][#6][#6][#6X3]	0.9565	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[cH]	0.9463	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX4H1]	0.0
[cX3H1]([cX3H1])[cX3H0]	0.9361	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[#6H1][#6H1]	0.8336	[CX4H0]([CX4H2])([CX4H2])([CX4H1])[CX4H1]	0.0
[#6H][#8][#6H]	0.7888	[CX4H1]([NX3H0])([CX4H3])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[#8][#6H0][#6H1]	0.7747	[#8][#6][#6][#6][#6]=[#8]	0.1355
[#8][#6][#6][#8]	0.6262	[CX3](=O)[OX2H1]	0.2152
[OX2H][cX3]:[c]	0.5894	[#8X2H0][#6X3H1][#6X3H1][#6X3H0]	0.2304
[cH]cO	0.3322	o[cH]	0.3389
[CX3H1](=[OX1H0])[OX2H0]	0.2327	[cX3H1]([oX2H0])[cX3H0]	0.3688
[CX3](=[OX1])C	0.2234	[#8][#6][#6][#6][#6][#8]	0.3849
[cX3H1]([cX3H1])[cX3H1]	0.1932	[#8][#6H][#6X3][#6X3H]	0.4383
[cX3H0]([cX3H1])([cX3H0])[OX2H1]	0.1739	O=[#6][#6][#6X3]	0.565
[#8]=[#6H0][#6H1]	0.1672	[CX3](=[OX1])O	0.6526
[cX3H0][cX3H1][cX3H1][cX3H0]	0.1428	[#8][#6H1][#6H1]	0.6919

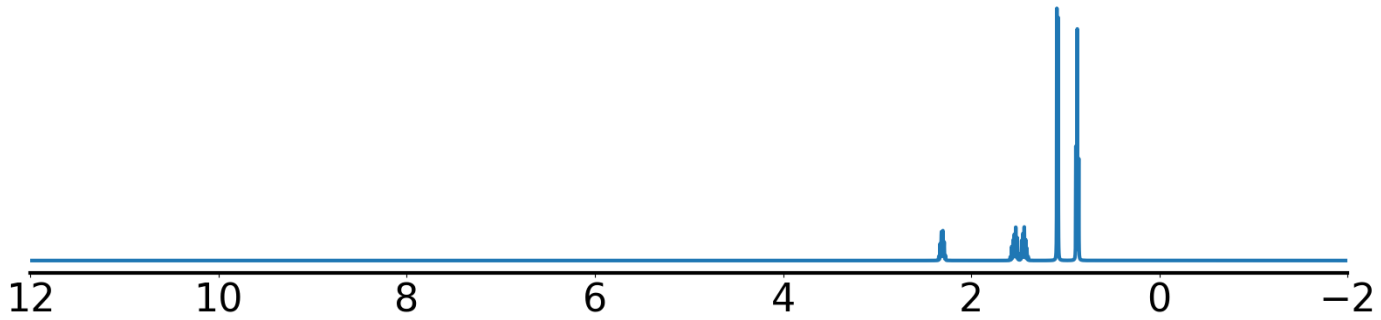
Example 62 true smiles: CCC(C)C(=O)O formula: C5H10O2
Index of correct structure: 0 of 303
True structure loss: 0.014043
True structure:



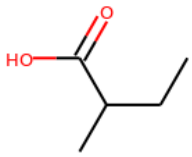
Experimental 13C NMR (solvent: CDCl3)



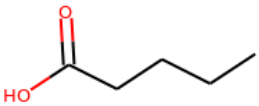
Experimental 1H NMR (solvent: D2O)



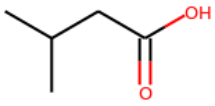
Top predicted structures (loss):



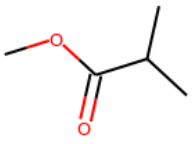
0.014043



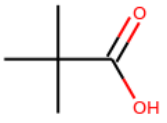
0.052993



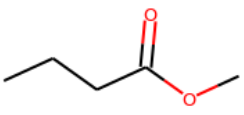
0.0563



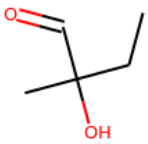
0.066355



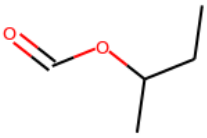
0.076886



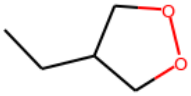
0.096807



0.112868



0.114389



0.114431

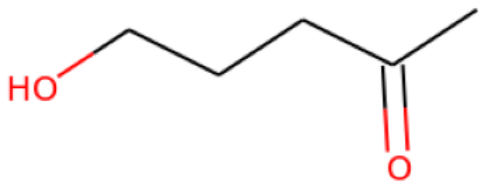
0.11941

Top predicted substructures	prob		
[#6H3][#6][#6]	0.9999	[#8]=[#6][#8]	0.9963
[CX4H3]	0.9999	[CX3](=[OX1])O	0.9936
[CX4H3][#6]	0.9997	[OX2H1]	0.9912
[CX3](=[OX1])C	0.9996	[CX4H3][CX4H2]	0.9858
[CX3](=O)[OX2H1]	0.9986	[CX4H2]([#6])[#6]	0.9838

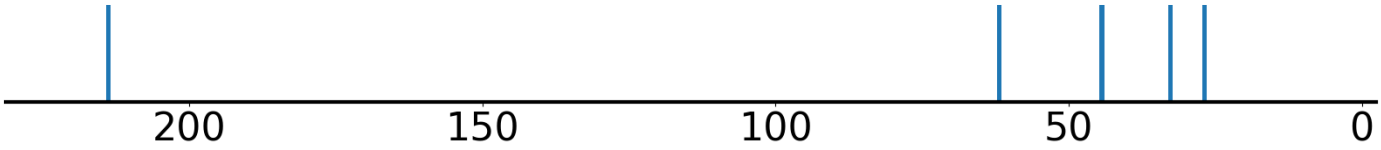
best positives	prob	best negatives	prob
[#6H3][#6][#6]	0.9999	CCC=CC#C	0.0
[CX4H3]	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9997	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9996	CC=CC#CC	0.0
[CX3](=O)[OX2H1]	0.9986	CCC#CC#C	0.0
[#8]=[#6][#8]	0.9963	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX3](=[OX1])O	0.9936	CCC#CC=C	0.0
[OX2H1]	0.9912	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H3][CX4H2]	0.9858	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9838	CC=CCC#C	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#6H1][#6H1]	0.5029	[OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]	0.057
[CX4H2]([CX4H3])[CX4H2]	0.4372	[CX4H1]([CX4H3])([CX4H2])[CX3H0]	0.1103
[CX4H1]([CX4H3])([CX4H2])[CX4H1]	0.2367	[CH3]CC[OH]	0.4417
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2289	OCC[CH2]	0.4992
[CX4H2][CX4H2]	0.1978	[#6H3][#6][#6][#6H3]	0.6141
[OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H3]	0.1775	[CX4H2]CC=O	0.7558
[CX4H2][CX3]=O	0.168	[#6H1][#6H2]	0.7588
CCCCCC	0.1628	[CX4H3][CX4H1]	0.7661
[#6H1][#6H1]	0.1216	[#6H3][#6][#6X3]	0.7788
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.1055	[CHX4]([CH3X4])[CH2X4]	0.7844

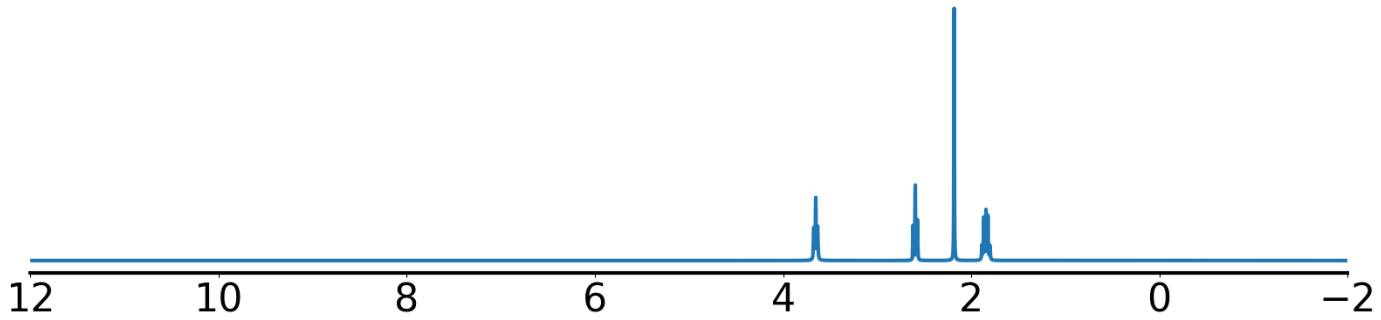
Example 63 true smiles: CC(=O)CCCO formula: C5H10O2
Index of correct structure: 0 of 303
True structure loss: 0.010088
True structure:



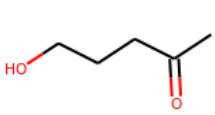
Experimental 13C NMR (solvent: CDCl3)



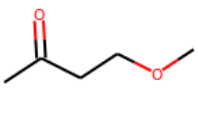
Experimental 1H NMR (solvent: CDCl3)



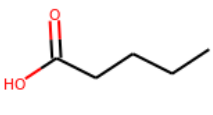
Top predicted structures (loss):



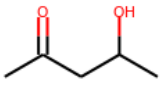
0.010088



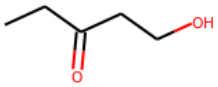
0.03921



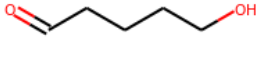
0.090852



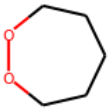
0.091266



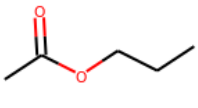
0.094873



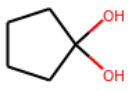
0.095749



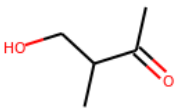
0.098055



0.104903



0.106108



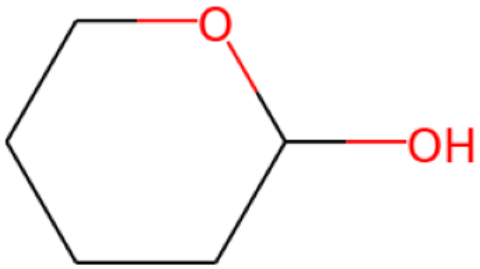
0.11082

Top predicted substructures	prob		
[CX4H3][CX3]	0.9998	[#6H3][#6][#6]	0.9918
[CX3](=[OX1])C	0.9998	[CX4H3]	0.9916
[CX4H3][CX3H0]	0.9996	[CX4H2][CX4H2]	0.9795
[CX4H2]([#6])[#6]	0.9993	[#6H3][#6H0]	0.9788
[OX1H0]=[CX3H0][CX4H3]	0.9963	[OX2H1]	0.9677

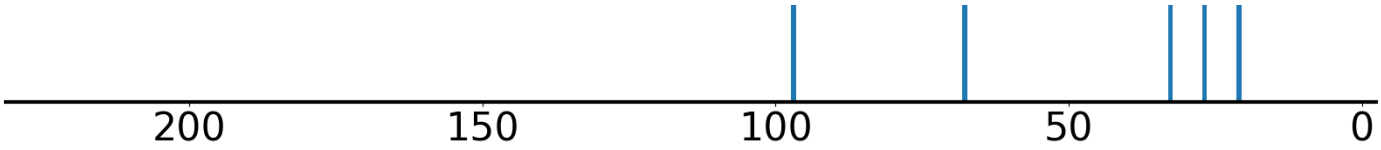
best positives	prob	best negatives	prob
[CX4H3][CX3]	0.9998	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])C	0.9998	CC=CC#CC	0.0
[CX4H3][CX3H0]	0.9996	CCC#CC#C	0.0
[CX4H2]([#6])[#6]	0.9993	CCC=CC#C	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9963	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9918	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CX4H3]	0.9916	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2][CX4H2]	0.9795	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6H0]	0.9788	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[OX2H1]	0.9677	[CX2H0](#[NX1H0])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H1]	0.5141	[CH2X4](O)[CX4H2][CX4H2]	0.1512
CCCCCC	0.4032	[CH2X4](O)[CX4H2]	0.6482
[#6H1][#6H2]	0.3595	[#8][#6][#6][#6][#6]=[#8]	0.6769
[#8][#6][#6][#6X3]	0.3522	[CX4H2]([CX4H2])[CX4H2]	0.8301
[#6H1]	0.2949	[CX4H2]([CX4H2])[CX3H0]	0.8455
[#8H][#6H2][#6H1]	0.2832	OCC[CH2]	0.8591
O=[CX3][CX4H]	0.2562	[CX4H2]([#6])[O]	0.8856
[CX3H0](=[OX1H0])([CX4H3])[CX4H1]	0.2165	[#6H3][#6X3H0][#6H2]	0.8945
[#6H1]([#6H2])[#6H2]	0.1998	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.8949
[#8]=[#6H0][#6H1]	0.1608	[CX4H3][#6]	0.9037

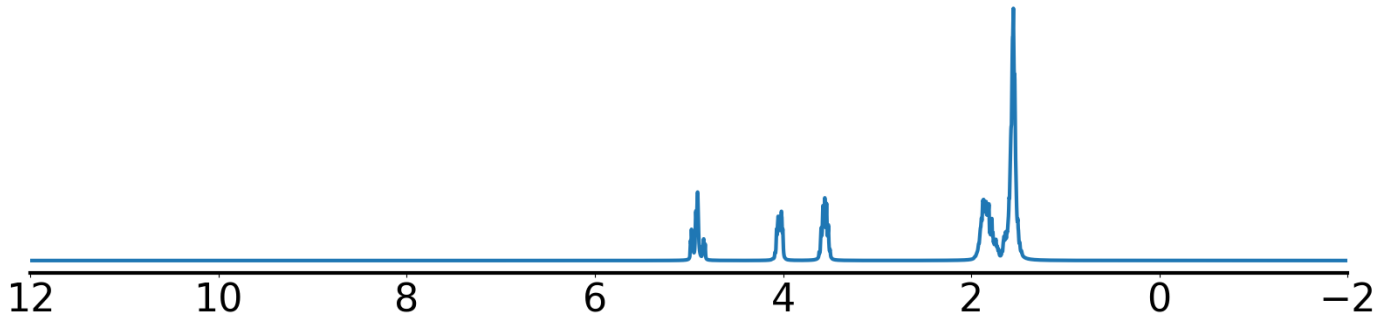
Example 64 true smiles: OC1CCCCO1 formula: C5H10O2
Index of correct structure: 0 of 303
True structure loss: 0.020487
True structure:



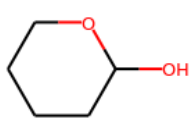
Experimental 13C NMR (solvent: CDCl3)



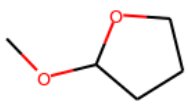
Experimental 1H NMR (solvent: CDCl3)



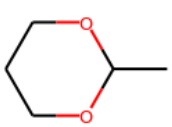
Top predicted structures (loss):



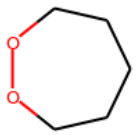
0.020487



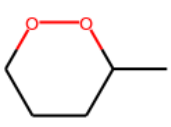
0.02636



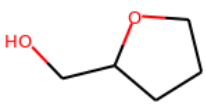
0.035684



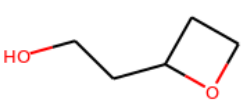
0.038011



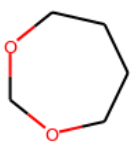
0.0395



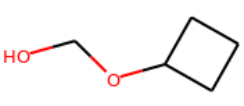
0.040049



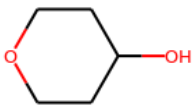
0.042894



0.043229



0.044938



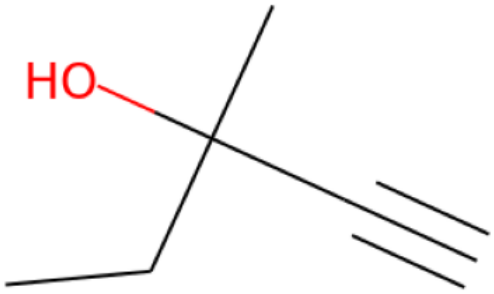
0.048109

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H2]([CX4H2])[CX4H1]	0.9946
OCC[CH2]	0.998	[CX4H]O	0.9825
[#6H1]	0.9974	[CX4H2][CX4H2]	0.9365
[#8][#6][#6H2]	0.9971	O[CX4H][CX4H2]	0.9079
[CX4H2]([#6])[O]	0.9956	[#6H1][#6H2]	0.9076

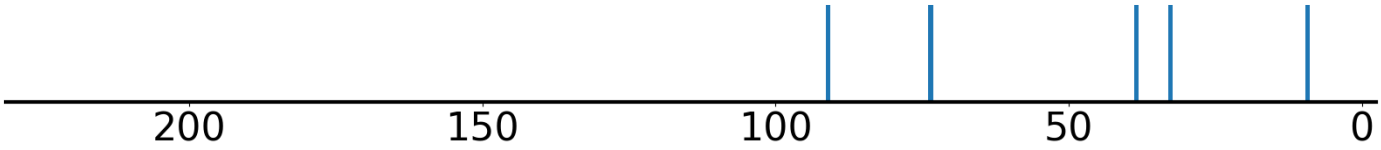
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	C=CC=CC#C	0.0
OCC[CH2]	0.998	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H1]	0.9974	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#8][#6][#6H2]	0.9971	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2]([#6])[O]	0.9956	[#6X2][#6H1][#6X2]	0.0
[CX4H2]([CX4H2])[CX4H1]	0.9946	[#7][#6]=[#6][#6]#[#7]	0.0
[CX4H]O	0.9825	CCC#CC#C	0.0
[CX4H2][CX4H2]	0.9365	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.0
O[CX4H][CX4H2]	0.9079	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#6H1][#6H2]	0.9076	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0

worst negatives	prob	worst positives	prob
[OX2H0][CX4H1][OX2H0]	0.6672	[#8]1[#6][#6][#6][#6][#6]1	0.048
[#8][#6H1][#6H1]	0.5624	[OH][CX4H]	0.1732
[#6H1][#6H1]	0.5456	[#6X4H2][#6H1][#8H]	0.2408
O[CX4H]([CX4H2])[CX4H1]	0.5033	[CX4H2][CX4H2][CX4H2][CX4H2]	0.3783
[#8][#6][#6][#6][#6][#8]	0.4638	[OX2H1]	0.5085
[CX4H](O)CO	0.4605	[OX2H0][CX4H1][CX4H2][CX4H2]	0.6416
[CX4H3]	0.4106	[CX4H2]([OX2H0])[CX4H2]	0.7132
[CX4H3][#6]	0.3516	[OX2H0][CX4H2][CX4H2][CX4H2]	0.7525
[CH3][#6][#8]	0.3455	[CX4H2]([CX4H2])[CX4H2]	0.8615
[#8][#6][#6][#8]	0.3393	[CH2X4](O)[CX4H2]	0.8654

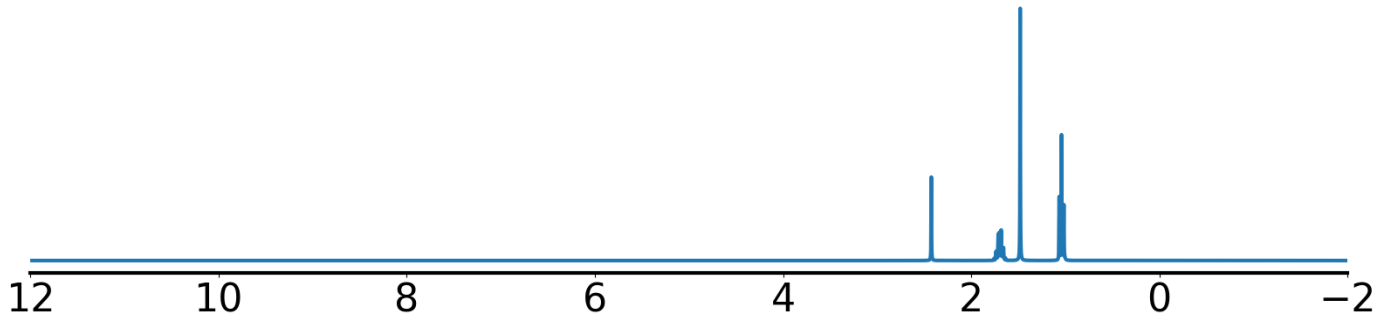
Example 65 true smiles: C#CC(C)(O)CC formula: C6H10O
Index of correct structure: 0 of 283
True structure loss: 0.017885
True structure:



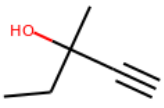
Experimental 13C NMR (solvent: CDCl3)



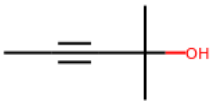
Experimental 1H NMR (solvent: CDCl3)



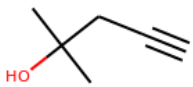
Top predicted structures (loss):



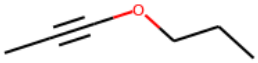
0.017885



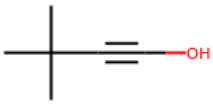
0.04282



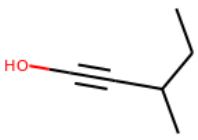
0.046047



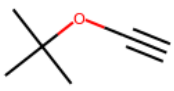
0.049568



0.053311



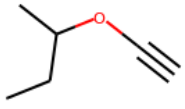
0.054724



0.05563

0.055832

0.055998



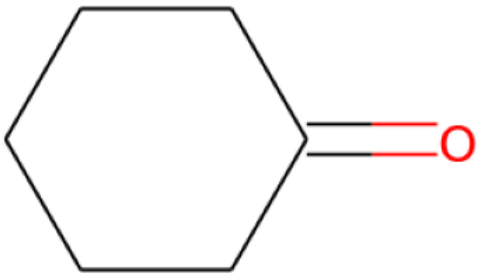
0.057715

Top predicted substructures	prob		
[#6H3][#6][#6]	0.9993	[#6H3][#6H0]	0.975
[CX4H3]	0.9951	[CX4H3][CX4H2]	0.9521
[CX4H2]([#6])[#6]	0.9948	[CX4H3][CX4]O	0.95
[CX4H3][CX4H0]	0.9851	[#8][#6][#6H2]	0.9194
[CX4H3][#6]	0.9802	[$([CX2]#C)]	0.8795

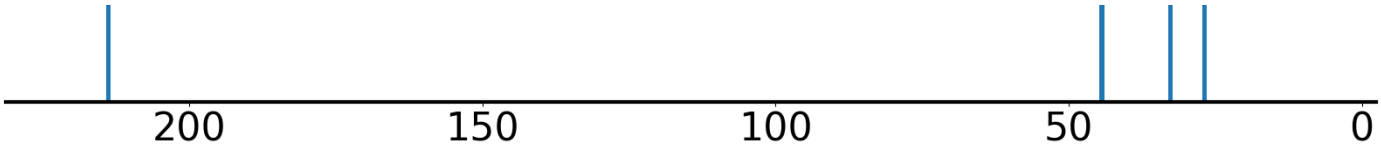
best positives	prob	best negatives	prob
[#6H3][#6][#6]	0.9993	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H3]	0.9951	[CX4H1]([NX3H2])([CX4H2])[CX3H1]	0.0
[CX4H2]([#6])[#6]	0.9948	[CX3H1](=[CX3H2])[NX3H0]	0.0
[CX4H3][CX4H0]	0.9851	[CX3H0](=[NX2H1])([NX3H1])[CX4H1]	0.0
[CX4H3][#6]	0.9802	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.0
[#6H3][#6H0]	0.975	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3][CX4H2]	0.9521	[CX4H2]([NX2H0])[CX4H1]	0.0
[CX4H3][CX4]O	0.95	[OX2H0]1[CX4H2][CX4H1][CX3H0]=[CX3H1]1	0.0
[#8][#6][#6H2]	0.9194	[CX3H0](=[CX3H2])([CX4H1])[CX3H1]	0.0
[$([CX2]#C)]	0.8795	[#7][#6]=[#6][#6]#[#7]	0.0

worst negatives	prob	worst positives	prob
OCC[CH2]	0.6462	[CX2H0](#[CX2H1])[CX4H0]	0.0328
[CX4H2][CX4H2]	0.3184	[#6H2][#6][#6X2]	0.3117
[#8][#6H0][#6H1]	0.3114	[#6H3][#6][#6][#6H3]	0.4323
[#6H1][#6H2]	0.3109	[CX2H1]#[CX2H0]	0.5117
[CX2H0](#[CX2H1])[CX4H1]	0.2883	[CX4H2]([CX4H3])[CX4H0]	0.5759
[#6H3][#6H0]([#6H2])[#6H2]	0.2628	[OX2H1][CX4H0][CX4H2][CX4H3]	0.6287
C1CC1	0.2592	[#6H1]	0.6414
CCCCCC	0.257	[CH3]CC[OH]	0.67
[CX4H2]([CX4H2])[CX4H0]	0.2373	[CH3][#6][#8]	0.755
CCCCC#C	0.2188	[#6X4H3][#6][#8H]	0.7729

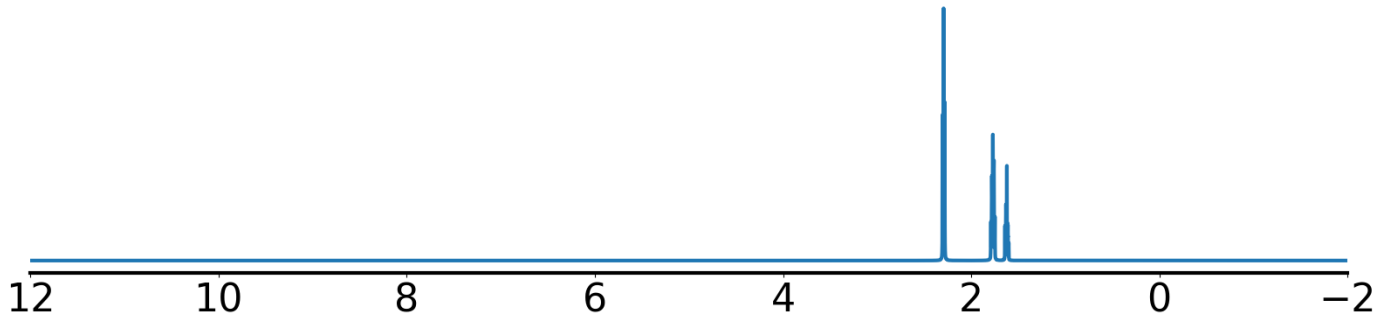
Example 66 true smiles: O=C1CCCCC1 formula: C6H10O
Index of correct structure: 0 of 283
True structure loss: 0.004536
True structure:



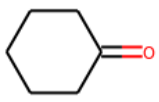
Experimental 13C NMR (solvent: CDCl3)



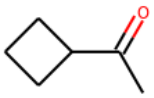
Experimental 1H NMR (solvent: D2O)



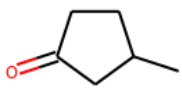
Top predicted structures (loss):



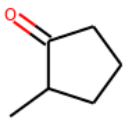
0.004536



0.077206

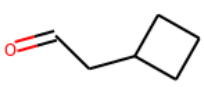


0.078029

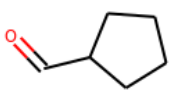


0.079376

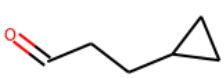
0.081844



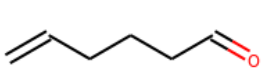
0.083365



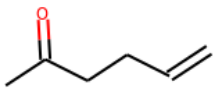
0.100834



0.132923



0.138809



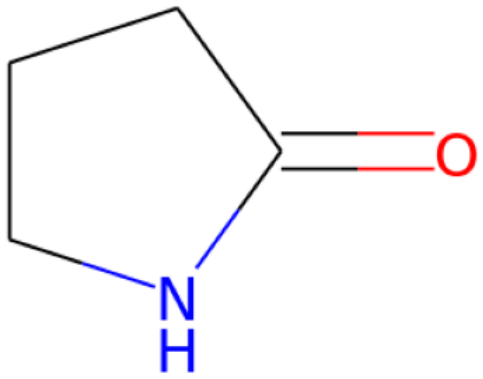
0.144015

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9998	[CX4H2][CX4H2]	0.9767
[CX3](=[OX1])C	0.9998	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9672
O=[CX3H0][CX4H2][CX4H2]	0.9891	[CX4H2]([CX4H2])[CX4H2]	0.9611
[CX4H2]([CX4H2])[CX3H0]	0.979	[CX4H2]CC=O	0.9474
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9772	CCCCCC	0.9209

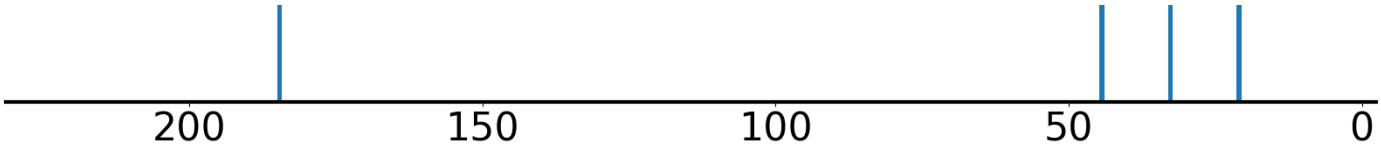
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9998	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])C	0.9998	C=CC=CC#C	0.0
O=[CX3H0][CX4H2][CX4H2]	0.9891	CC=CCC#C	0.0
[CX4H2]([CX4H2])[CX3H0]	0.979	[OX2H1][CX4H1][CX4H1][CX2H0]	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9772	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2][CX4H2]	0.9767	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.9672	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9611	CCC#CC#C	0.0
[CX4H2]CC=O	0.9474	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
CCCCCC	0.9209	C=CCCC#C	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H2]	0.2387	[#6]1[#6][#6][#6][#6][#6]1	0.5154
[#6H1]	0.187	[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.6664
[#6H3][#6H0]	0.1785	[#6H2][#6X3H0][#6H2]	0.7679
C1CCCC1	0.1673	[CX4H2][CX3]=O	0.9125
[CX4H3][CX3]	0.1437	CCCCCC	0.9209
[OX1H0]=[CX3H1][CX4H2][CX4H2]	0.1148	[CX4H2]CC=O	0.9474
[CX4H3][#6]	0.1057	[CX4H2]([CX4H2])[CX4H2]	0.9611
[CX4H2]([CX4H2])[CX4H1]	0.1041	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9672
[#8]=[#6H0][#6H1]	0.0888	[CX4H2][CX4H2]	0.9767
C1CCC1	0.0819	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.9772

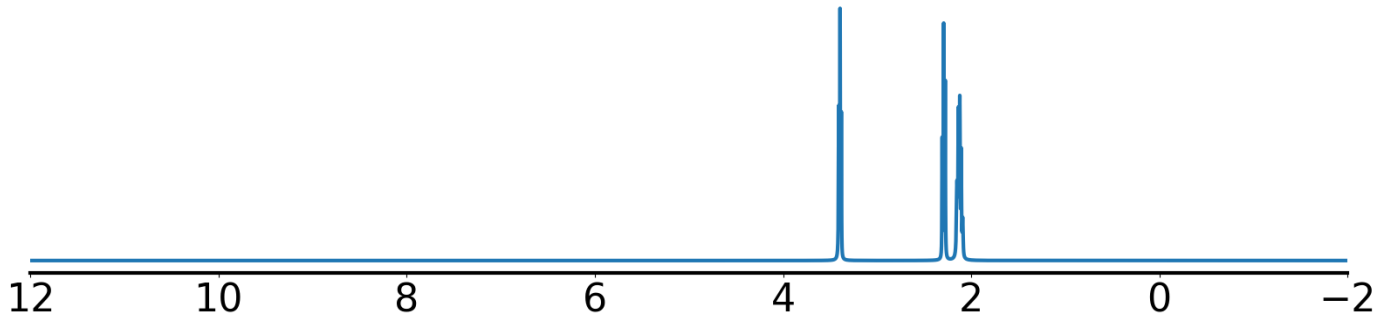
Example 67 true smiles: O=C1CCCN1 formula: C4H7NO
Index of correct structure: 0 of 253
True structure loss: 0.015705
True structure:



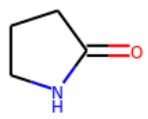
Experimental 13C NMR (solvent: CDCl3)



Experimental 1H NMR (solvent: CDCl3)



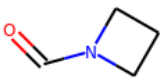
Top predicted structures (loss):



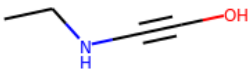
0.015705

0.047983

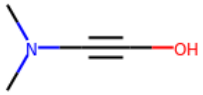
0.050845



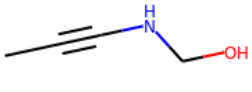
0.068081



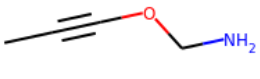
0.075688



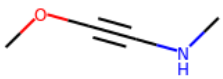
0.076671



0.08281



0.083603



0.083906

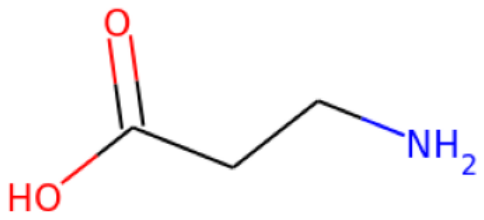
0.087963

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9984	[#7][#6H2][#6H2]	0.8243
[CX3](=[OX1])C	0.9682	[CX4H2]([CX4H2])[CX4H2]	0.7358
[#7X3][#6H2]	0.9589	[CX4H2]CC=O	0.7273
[#7][#6H2]	0.9225	[#6H2][#7][#6X3]	0.6801
[CX4H2][CX4H2]	0.8921	[CX4H2][CX3]=O	0.6556

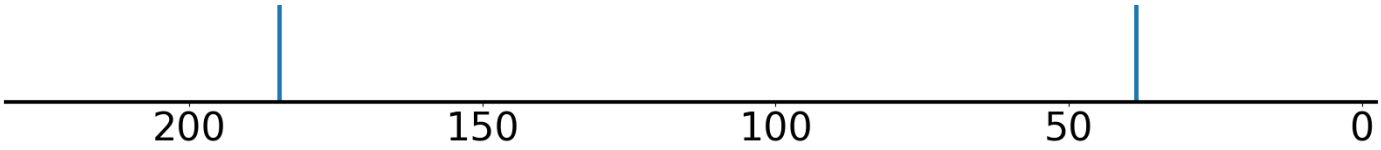
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9984	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9682	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3][#6H2]	0.9589	[OX2H0][CX3H1]=[#6X3H0][#8X2H0]	0.0
[#7][#6H2]	0.9225	CC=CC#CC	0.0
[CX4H2][CX4H2]	0.8921	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7][#6H2][#6H2]	0.8243	[OX2H0]1[CX4H2][CX4H1][CX3H0]=[CX3H1]1	0.0
[CX4H2]([CX4H2])[CX4H2]	0.7358	[#6H2]=[#6][#6X2]	0.0
[CX4H2]CC=O	0.7273	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#6H2][#7][#6X3]	0.6801	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2][CX3]=O	0.6556	[CX3H2]=[CX3H1][CX4H0][OX2H1]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H2]	0.4022	[CX3H0](=[OX1H0])([NX3H1])[CX4H2]	0.2453
[#7X3H2]	0.3854	[CX4H2]([NX3H1])[CX4H2]	0.4575
[#8]=[#6H0][#6H1]	0.3797	[#7X3H1]	0.4674
O=[CX3][CX4H]	0.326	[#6]1[#6][#6][#6][#7]1	0.4804
C1CCC1	0.3254	[CX4H2]([CX4H2])[CX3H0]	0.6058
[#6H1]	0.2596	O=[CX3H0][CX4H2][CX4H2]	0.6344
[CX4H2]([CX4H2])[CX4H1]	0.2446	[CX4H2][CX3]=O	0.6556
[#7][#6H0][#6H1]	0.2069	[#6H2][#7][#6X3]	0.6801
[#7][#6][#6X3]	0.2055	[CX4H2]CC=O	0.7273
[OX2H1]	0.2027	[CX4H2]([CX4H2])[CX4H2]	0.7358

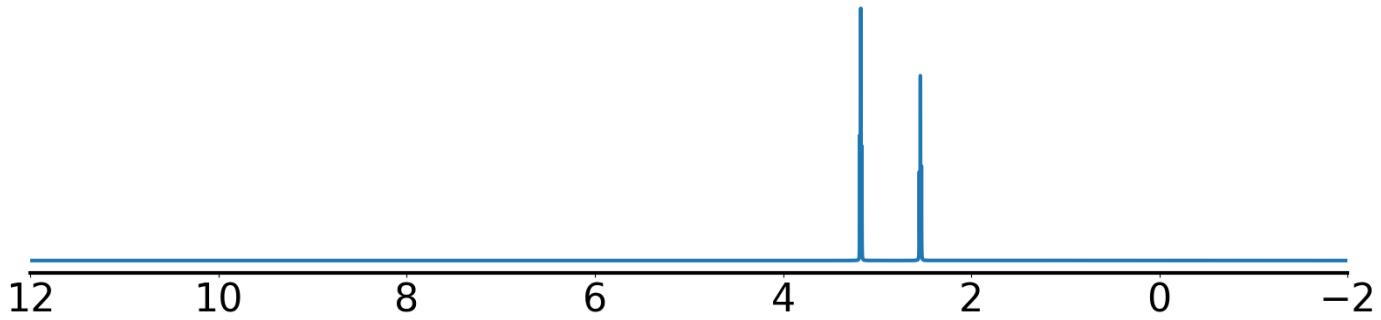
Example 68 true smiles: NCCC(=O)O formula: C3H7NO2
Index of correct structure: 0 of 207
True structure loss: 0.017592
True structure:



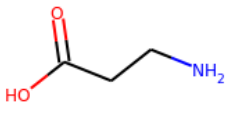
Experimental 13C NMR (solvent: D2O)



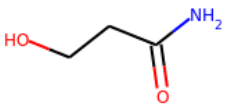
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):

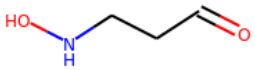


0.017592

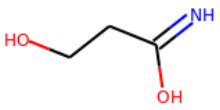


0.041783

0.051769



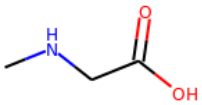
0.055945



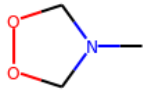
0.056672

0.061544

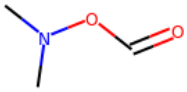
0.062582



0.064633



0.064962



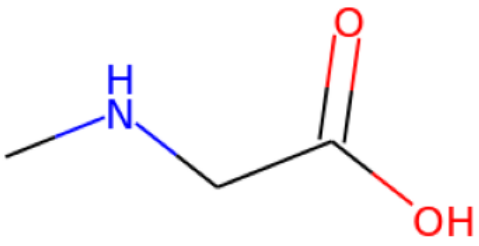
0.070064

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9913	[CX4H2]([CX4H2])[CX3H0]	0.8631
[OX2H1]	0.9717	[CX4H2]CC=O	0.857
[CX4H2]([#6])[#6]	0.9569	[#7X3H2]	0.8246
[CX3](=O)[OX2H1]	0.9489	[#7X3][#6H2]	0.7873
O=[CX3H0][CX4H2][CX4H2]	0.9143	[CX4H2][CX3]=O	0.7314

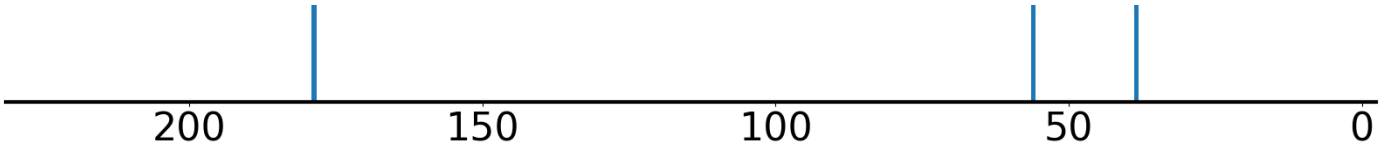
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9913	C=CC=CC#C	0.0
[OX2H1]	0.9717	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([#6])[#6]	0.9569	CC=CCC#C	0.0
[CX3](=O)[OX2H1]	0.9489	CC=CC#CC	0.0
O=[CX3H0][CX4H2][CX4H2]	0.9143	[CX2H0](#[CX2H1])[CX4H1]	0.0
[CX4H2]([CX4H2])[CX3H0]	0.8631	CCC#CC#C	0.0
[CX4H2]CC=O	0.857	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[#7X3H2]	0.8246	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#7X3][#6H2]	0.7873	[CX2H0](#[CX2H1])[CX4H0]	0.0
[CX4H2][CX3]=O	0.7314	[CX2H0](#[CX2H1])[cX3H0]	0.0

worst negatives	prob	worst positives	prob
[#7X3H1]	0.3625	[#7][#6][#6][#6X3]	0.1377
[#7H2][#6H0]	0.2898	[CX4H2]([NX3H2])[CX4H2]	0.1485
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.2645	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2032
[#6H2][#7][#6X3]	0.2431	[#8][#6][#6H2]	0.3472
[#8]=[#6H0][#6H1]	0.2181	OCC[CH2]	0.4213
[#6H1]	0.2085	[#7H2][#6H2]	0.4894
[#6H1][#6H2]	0.1645	[CX4H2][CX4H2]	0.5776
[#8][#6][#6][#6][#6]=[#8]	0.1068	[CX3](=[OX1])O	0.5795
[CX4H3][NX3H1]	0.0998	[#7][#6H2][#6H2]	0.5921
[CX4H2]([CX4H2])[CX4H2]	0.0978	[#8]=[#6][#8]	0.6398

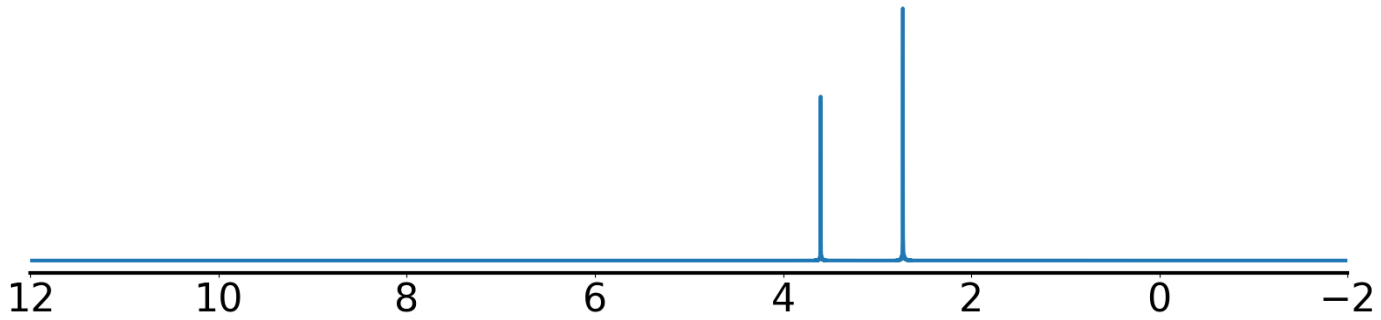
Example 69 true smiles: CNCC(=O)O formula: C3H7NO2
Index of correct structure: 0 of 207
True structure loss: 0.020239
True structure:



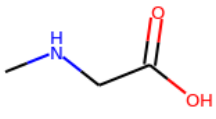
Experimental 13C NMR (solvent: D2O)



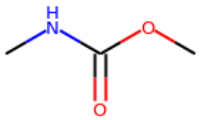
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):

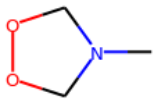


0.020239

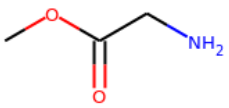


0.030472

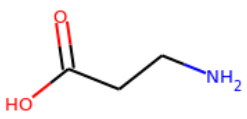
0.032011



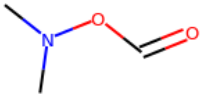
0.033912



0.03964

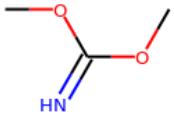


0.048822

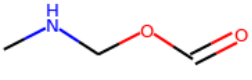


0.048851

0.05347



0.057421



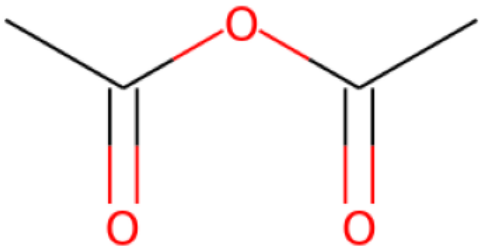
0.057782

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9853	[#6H3][#7][#6H2]	0.8383
[#7X3][#6H3]	0.976	[#7X3][#6H2]	0.8076
[CX4H3]	0.9718	[CX4H2][CX3]=O	0.807
[#8]=[#6][#8]	0.921	[CX3](=[OX1])O	0.787
[#6H3][#7]	0.8672	[#7][#6H2]	0.7753

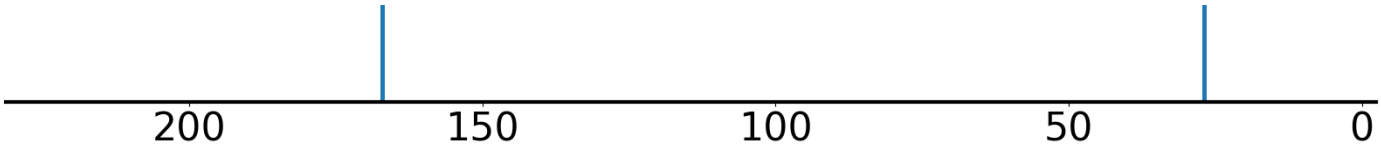
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9853	CCC#CC#C	0.0
[#7X3][#6H3]	0.976	C=CC=CC#C	0.0
[CX4H3]	0.9718	C=CCCC#C	0.0
[#8]=[#6][#8]	0.921	CC=CCC#C	0.0
[#6H3][#7]	0.8672	CC=CC#CC	0.0
[#6H3][#7][#6H2]	0.8383	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#7X3][#6H2]	0.8076	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H2][CX3]=O	0.807	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])O	0.787	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7][#6H2]	0.7753	[CX2H0](#[CX2H1])[CX4H1]	0.0

worst negatives	prob	worst positives	prob
[OX1H0]=[CX3H0][OX2H0][CX4H3]	0.614	[CX4H2]([NX3H1])[CX3H0]	0.0633
[#6H3][#7][#6X3]	0.5073	[#6X3][#6H2][#7]	0.4186
[CX4H2][CX4H2]	0.475	[OX2H1]	0.4278
[CX4H2]CC=O	0.4186	[CX4H3][NX3H1]	0.4652
[#7][#6H2][#6H2]	0.3836	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.577
O=[CX3H0][CX4H2][CX4H2]	0.3475	[#7X3H1]	0.5792
[CX4H3][NX3H0]	0.3352	[CX3](=O)[OX2H1]	0.6082
[CX4H3][OX2H0]	0.3241	[#7][#6][#6X3]	0.6231
[#7][#6][#6][#6X3]	0.3043	[#8][#6][#6H2]	0.6499
[CX3H0](=[OX1H0])([NX3H0])[CX4H2]	0.2809	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.7382

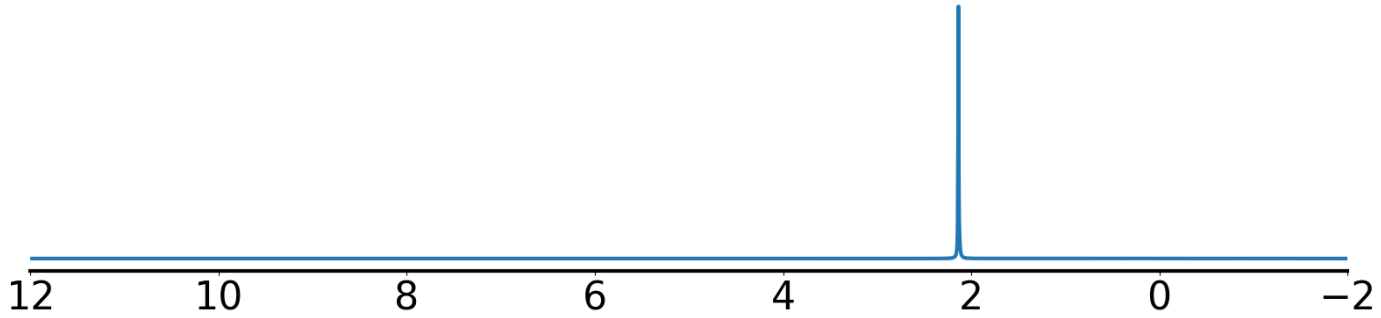
Example 70 true smiles: CC(=O)OC(C)=O formula: C4H6O3
Index of correct structure: 0 of 195
True structure loss: 0.029077
True structure:



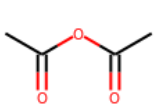
Experimental 13C NMR (solvent: CDCl3)



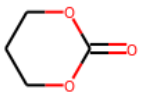
Experimental 1H NMR (solvent: CDCl3)



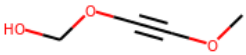
Top predicted structures (loss):



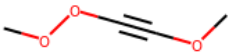
0.029077



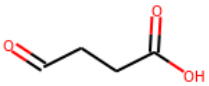
0.053927



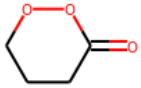
0.057677



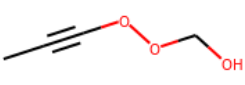
0.058027



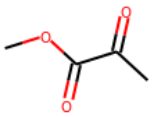
0.064953



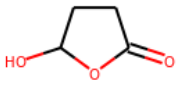
0.070062



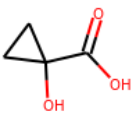
0.073171



0.075062



0.083163



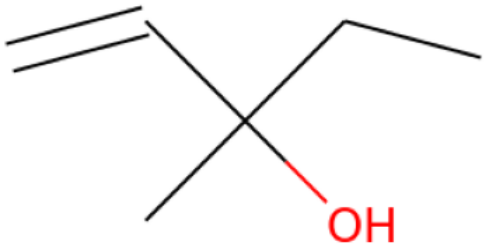
0.086985

Top predicted substructures	prob		
[#8]=[#6][#8]	0.9965	[CX3](=O)[OX2H1]	0.7998
[CX3](=[OX1])O	0.9938	[CX4H2]([#6])[#6]	0.7762
[CX3](=[OX1])C	0.87	[CX4H2]([CX4H2])[CX3H0]	0.6739
[#6H3][#6H0]	0.8477	[CX4H2]([CX4H2])[CX4H2]	0.6167
[CX4H2][CX4H2]	0.8324	[OX2H1]	0.5829

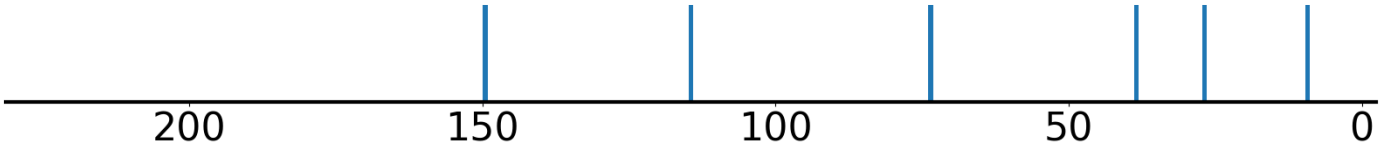
best positives	prob	best negatives	prob
[#8]=[#6][#8]	0.9965	C=CC=CC#C	0.0
[CX3](=[OX1])O	0.9938	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX3](=[OX1])C	0.87	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#6H3][#6H0]	0.8477	[#6H2]=[#6][#6X2]	0.0
[CX4H3][CX3H0]	0.5784	[#6X3H2]=[#6][#6H2][#8H]	0.0
[CX4H3]	0.5464	[CX3H1](=[CX3H2])[CX3H1]	0.0
[CX4H3][#6]	0.2541	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H3][CX3]	0.254	[OX2H0]1[CX4H2][CX4H1][CX3H0]=[CX3H1]1	0.0
[OX1H0]=[CX3H0][CX4H3]	0.1749	[CX2H0](#[CX2H1])[CX4H0]	0.0
[OX2H0][CX3H0][CX4H3]	0.1211	CC=CC#CC	0.0

worst negatives	prob	worst positives	prob
[CX4H2][CX4H2]	0.8324	[CX3H0](=[OX1H0])([OX2H0])[CX4H3]	0.0254
[CX3](=O)[OX2H1]	0.7998	[CH3][#6][#8]	0.0993
[CX4H2]([#6])[#6]	0.7762	[OX2H0][CX3H0][CX4H3]	0.1211
[CX4H2]([CX4H2])[CX3H0]	0.6739	[OX1H0]=[CX3H0][CX4H3]	0.1749
[CX4H2]([CX4H2])[CX4H2]	0.6167	[CX4H3][CX3]	0.254
[OX2H1]	0.5829	[CX4H3][#6]	0.2541
OCC[CH2]	0.5544	[CX4H3]	0.5464
O=[CX3H0][CX4H2][CX4H2]	0.4449	[CX4H3][CX3H0]	0.5784
[#8][#6][#6H2]	0.4103	[#6H3][#6H0]	0.8477
[CX4H2][CX3]=O	0.3091	[CX3](=[OX1])C	0.87

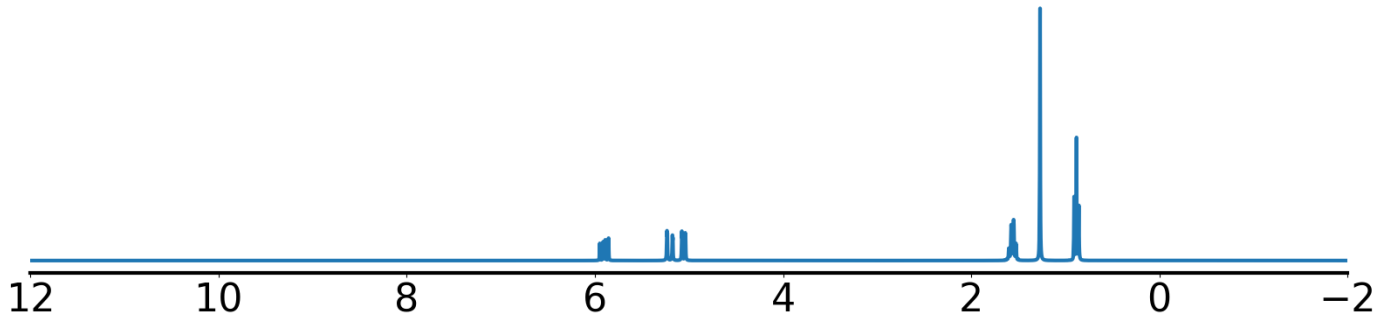
Example 71 true smiles: C=CC(C)(O)CC formula: C6H12O
Index of correct structure: 0 of 193
True structure loss: 0.007644
True structure:



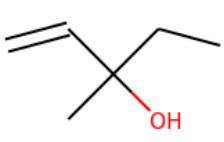
Experimental 13C NMR (solvent: CDCl3)



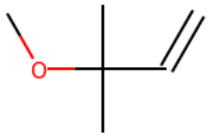
Experimental 1H NMR (solvent: CDCl3)



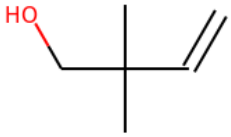
Top predicted structures (loss):



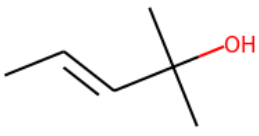
0.007644



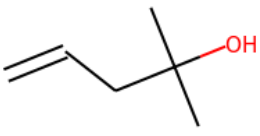
0.057481



0.058566

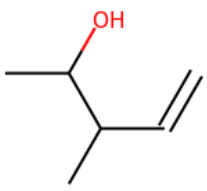


0.08332

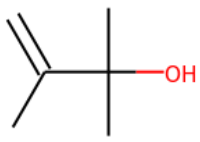


0.084626

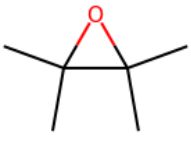
0.096872



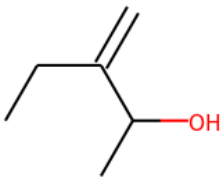
0.098502



0.100366



0.105097



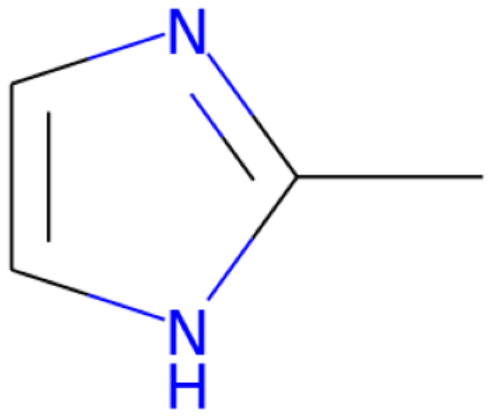
0.111478

Top predicted substructures	prob		
[#6H3][#6][#6]	1.0	[CX4H3][CX4]O	0.9977
[CX4H3]	1.0	[CX3H2]=[CX3H1]	0.9897
[CX4H3][#6]	0.9996	[#6H3][#6H0]	0.9841
[#6X3H2]	0.999	[CX4H3][CX4H0]	0.9834
[CX4H3][CX4H2]	0.9979	[OX2H1]	0.9819

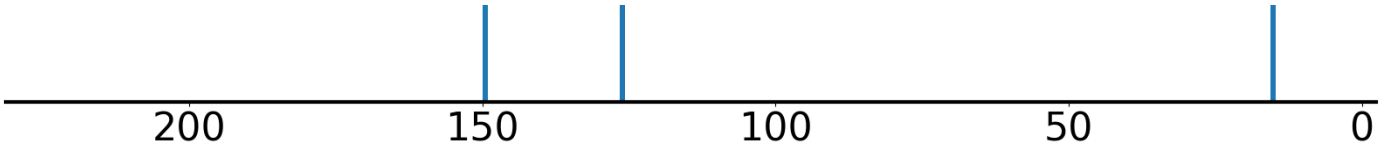
best positives	prob	best negatives	prob
[#6H3][#6][#6]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3]	1.0	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H3][#6]	0.9996	[#6X2][#6H1][#6X2]	0.0
[#6X3H2]	0.999	CCC#CC#C	0.0
[CX4H3][CX4H2]	0.9979	CC#CCC#C	0.0
[CX4H3][CX4]O	0.9977	C=CC=CC#C	0.0
[CX3H2]=[CX3H1]	0.9897	CC=CCC#C	0.0
[#6H3][#6H0]	0.9841	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[CX4H3][CX4H0]	0.9834	[CX2H0](#[CX2H1])[CX4H2]	0.0
[OX2H1]	0.9819	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[CHX4]([CH3X4])[CH2X4]	0.3003	[#8][#6][#6H2]	0.589
[#8][#6][#6][#6X3]	0.2464	[CH3]CC[OH]	0.5959
[O][CX3H1]=[CX3H1]	0.2399	[OX2H1][CX4H0][CX4H2][CX4H3]	0.6398
[CX3H](O)	0.2364	[CX4H2]([CX4H3])[CX4H0]	0.7549
[OH][CX4H]	0.2354	[CX3H2]=[CX3H1][CX4H0][OX2H1]	0.7929
CCCCC=C	0.2063	[CX4H2]([#6])[#6]	0.7934
[CX4H]O	0.1795	[#6H3][#6][#6][#6H3]	0.8481
[CX3H2]=[CX3H0]	0.1731	[CH3][#6][#8]	0.8698
[CX3H1](=[CX3H1])[OX2H0]	0.1603	[#6X3][#6][#6][#6H3]	0.8837
O[CX4H][CX4H2]	0.1583	[#8][#6H0][#6H1]	0.8858

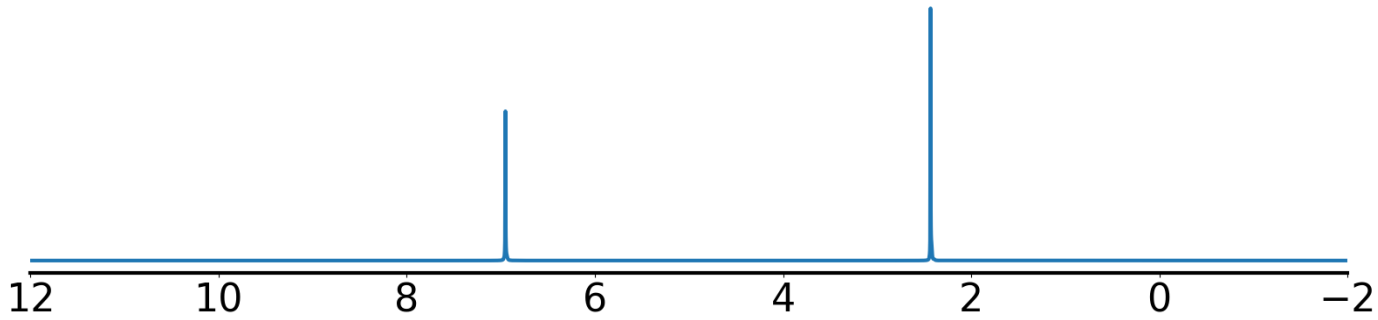
Example 72 true smiles: Cc1ncc[nH]1 formula: C4H6N2
Index of correct structure: 5 of 177
True structure loss: 0.034547
True structure:



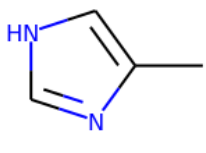
Experimental 13C NMR (solvent: CDCl3)



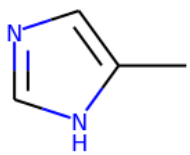
Experimental 1H NMR (solvent: CDCl3)



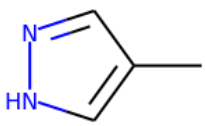
Top predicted structures (loss):



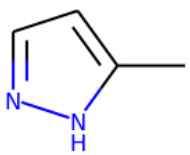
0.019913



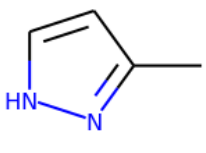
0.020212



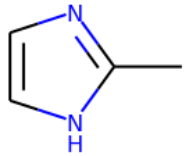
0.032869



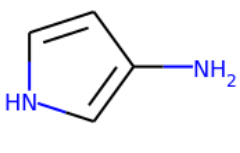
0.034049



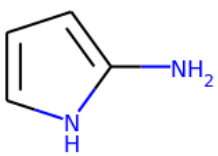
0.034259



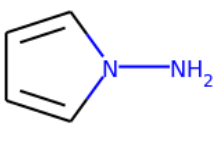
0.034547



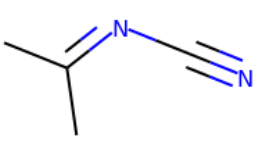
0.059508



0.061591



0.067517



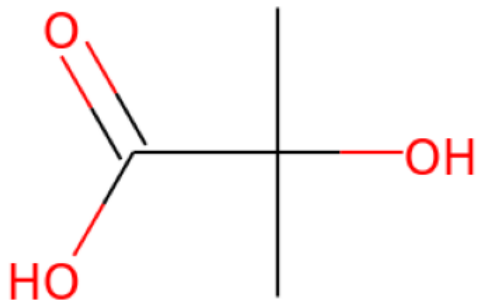
0.077065

Top predicted substructures	prob		
[CX4H3]	0.9951	[CX4H3][cX3H0]	0.9622
[#6X3][#6X3]	0.9889	[#6H3][#6][#6]	0.9597
[#6H3][#6H0]	0.9849	[cH]	0.9466
[CX4H3][#6]	0.9787	[#6H3][#6][#6X3]	0.9449
[#7][#6][#6X3]	0.9694	[#6H1]	0.9061

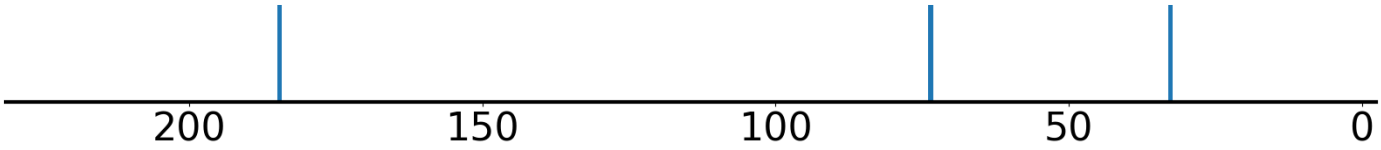
best positives	prob	best negatives	prob
[CX4H3]	0.9951	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9889	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H3][#6H0]	0.9849	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[CX4H3][#6]	0.9787	[OX2H0][CX4H2][CX4H2][CX4H1][OX2H0]	0.0
[#7][#6][#6X3]	0.9694	[OX2H1][CX4H1][CX4H1]([CX4H2])[CX4H2]	0.0
[CX4H3][cX3H0]	0.9622	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cH]	0.9466	[OX2H0][CX4H2][CX4H0][OX2H0]	0.0
[#6H1]	0.9061	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#7][#6X3]	0.8846	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
[#6]1[#6][#7][#6][#7]1	0.8077	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[#6H3][#6][#6]	0.9597	[cX3H1]([nX2H0])[cX3H1]	0.0539
[#6H3][#6][#6X3]	0.9449	[cX3H1]([nX3H1])[cX3H1]	0.0701
[#6X3H1][#6X3H0]	0.8633	[#6H1][#6H1]	0.2603
[#6H3][#6H0][#6H1][#7]	0.6748	[#7H][#6X3H1]	0.3819
[#7][#6H0][#6H1]	0.6646	[cH][cH]	0.4891
[#7][#6X3H0][#6X3H1]	0.6564	[#7X3H1]	0.5261
[#7][#6][#6][#6X3]	0.6393	[#7][#6H0][#7]	0.6467
[#6X3][#6][#6][#6H3]	0.6266	[#6H1r5][#7]	0.6611
[#7X3H2]	0.5322	[#7][#6][#6H3]	0.6726
[#7][#6H1][#7]	0.4653	[#7][#6][#6][#7]	0.7194

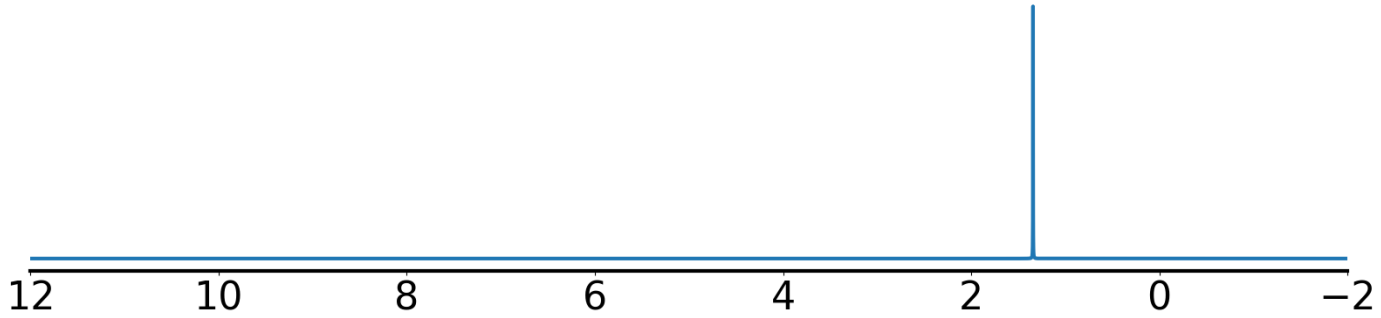
Example 73 true smiles: CC(C)(O)C(=O)O formula: C4H8O3
Index of correct structure: 0 of 172
True structure loss: 0.010936
True structure:



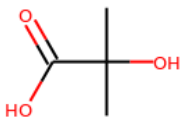
Experimental 13C NMR (solvent: CDCl3)



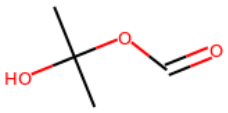
Experimental 1H NMR (solvent: d2o)



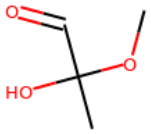
Top predicted structures (loss):



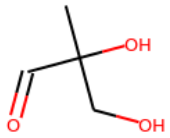
0.010936



0.035745

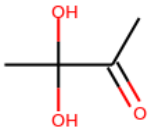


0.059714



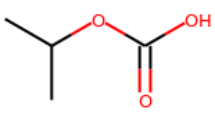
0.062249

0.062402

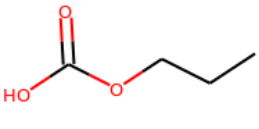


0.063627

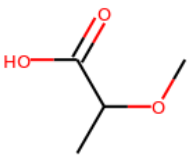
0.066481



0.06793



0.080043



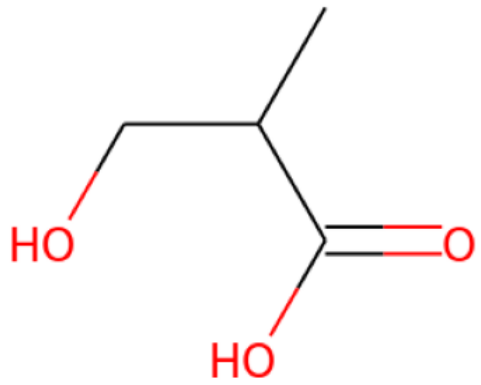
0.083611

Top predicted substructures	prob		
[CX4H3]	0.9964	[OX2H1]	0.9779
[#6H3][#6][#6]	0.9959	[#8]=[#6][#8]	0.9721
[CX3](=[OX1])C	0.9955	[CX3](=[OX1])O	0.9631
[CX4H3][CX4H0][CX4H3]	0.9947	[#6H3][#6H0]	0.9605
[CX4H3][CX4H0]	0.99	[CX4H3][CX4]O	0.9398

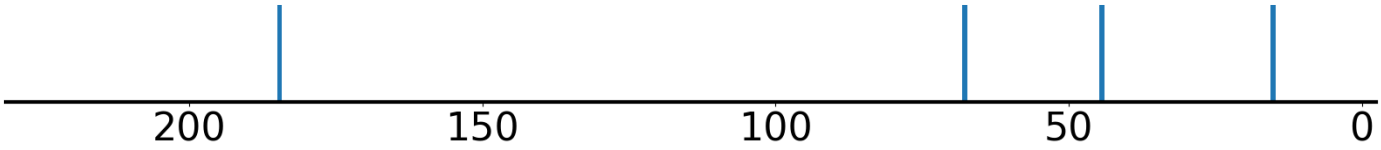
best positives	prob	best negatives	prob
[CX4H3]	0.9964	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9959	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9955	C=CCCC#C	0.0
[CX4H3][CX4H0][CX4H3]	0.9947	C=CC=CC#C	0.0
[CX4H3][CX4H0]	0.99	CCC=CC#C	0.0
[OX2H1]	0.9779	CC=CCC#C	0.0
[#8]=[#6][#8]	0.9721	[#6H2]=[#6][#6X2]	0.0
[CX3](=[OX1])O	0.9631	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#6H3][#6H0]	0.9605	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H3][CX4]O	0.9398	CCC#CC=C	0.0

worst negatives	prob	worst positives	prob
[CX4]([CX4H3])([CX4H3])[CX4H3]	0.6283	[#6H3][#6][#6X3]	0.4128
[CX4H2][CX3]=O	0.2579	[#8][#6][#6][#8]	0.4366
[#8]=[#6H0][#6H1]	0.2424	[OX1H0]=[CX3H0][CX4H0][CX4H3]	0.4372
[CX4H2]CC=O	0.1774	[CH3]CC[OH]	0.4975
[#8][#6][#6][#6X3]	0.1603	[OX2H1][CX4H0][CX4H3]	0.5635
OCC[CH2]	0.1602	[#8][#6][#6]=[#8]	0.6669
[#8][#6][#6H2]	0.1532	[#6X4H3][#6][#8H]	0.7006
[#8]=[#6][#6]=[#8]	0.1525	[CH3][#6][#8]	0.7295
O=[CX3][CX4H]	0.1477	[CX3](=O)[OX2H1]	0.8732
[CX3H0](=[OX1H0])([OX2H0])[CX4H0]	0.1473	[#6H0]([#6H3])([#6H3])[#8]	0.8876

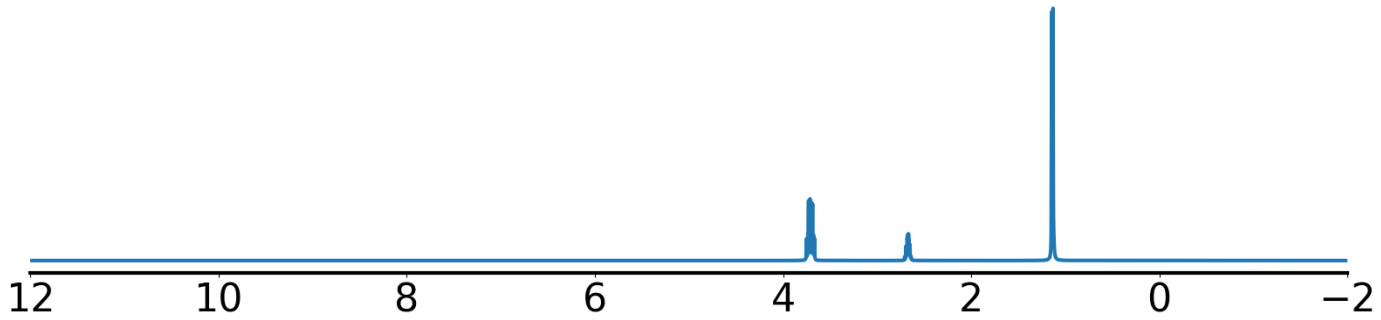
Example 74 true smiles: CC(CO)C(=O)O formula: C4H8O3
Index of correct structure: 0 of 172
True structure loss: 0.028466
True structure:



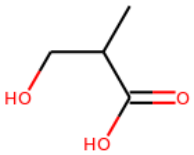
Experimental 13C NMR (solvent: CDCl3)



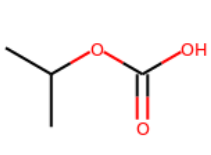
Experimental 1H NMR (solvent: D2O)



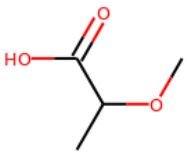
Top predicted structures (loss):



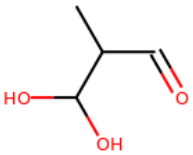
0.028466



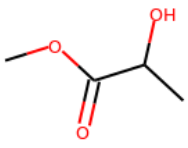
0.071441



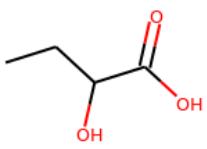
0.071878



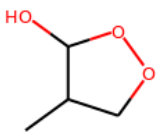
0.077025



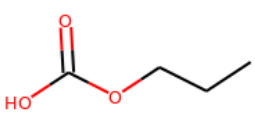
0.077177



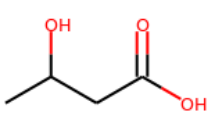
0.078321



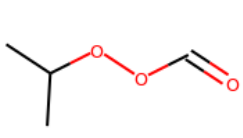
0.078839



0.078956



0.092249



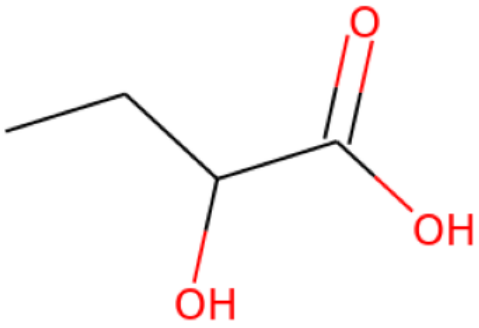
0.096201

Top predicted substructures	prob		
[CX4H3]	0.9999	[CX3](=[OX1])O	0.9869
[CX3](=[OX1])C	0.9988	[CX3](=O)[OX2H1]	0.9824
[OX2H1]	0.9988	[#6H1]	0.9807
[CX4H3][#6]	0.9963	O=[CX3][CX4H]	0.965
[#8]=[#6][#8]	0.9906	[#8]=[#6H0][#6H1]	0.9464

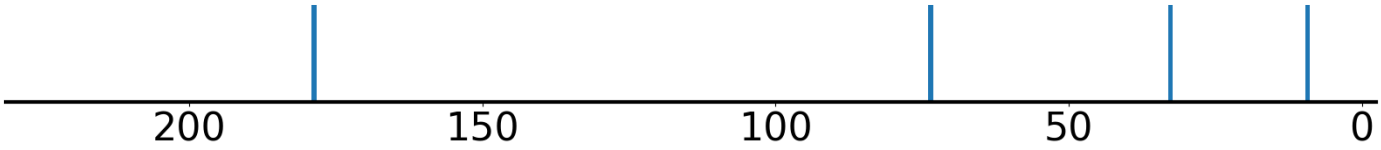
best positives	prob	best negatives	prob
[CX4H3]	0.9999	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.9988	CC=CC#CC	0.0
[OX2H1]	0.9988	CC=CCC#C	0.0
[CX4H3][#6]	0.9963	C=CC=CC#C	0.0
[#8]=[#6][#8]	0.9906	CCC=CC#C	0.0
[CX3](=[OX1])O	0.9869	CC#CCC=C	0.0
[CX3](=O)[OX2H1]	0.9824	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H1]	0.9807	[CX2H0](#[CX2H1])[cX3H0]	0.0
O=[CX3][CX4H]	0.965	CCC#CC#C	0.0
[#8]=[#6H0][#6H1]	0.9464	[CX2H0](#[CX2H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#6H1][#6H1]	0.8852	[OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]	0.0281
[#6H1][#6H1]	0.6724	OCC[CH2]	0.2063
[OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H3]	0.6681	[CX4H1]([CX4H3])([CX4H2])[CX3H0]	0.2209
[CX4H1]([CX4H3])([CX4H1])[CX3H0]	0.5862	[#8][#6H2][#6H][#6X3]	0.2225
[#8][#6H1][#6H1][#6H3]	0.374	[#8][#6H2][#6H1][#6H0]	0.2362
[OH][CX4H]	0.3591	[CHX4]([CH3X4])[CH2X4]	0.2928
[#8][#6][#6][#6][#6]=[#8]	0.3227	[CX4H2]CC=O	0.3623
[#8][#6H1][#6H1]	0.3136	[CX4H2](O)[CHX4]	0.3667
[#6X3][#6][#6][#6H3]	0.2885	[#8H][#6H2][#6H1]	0.4372
[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.2401	[#6H1][#6H2]	0.5085

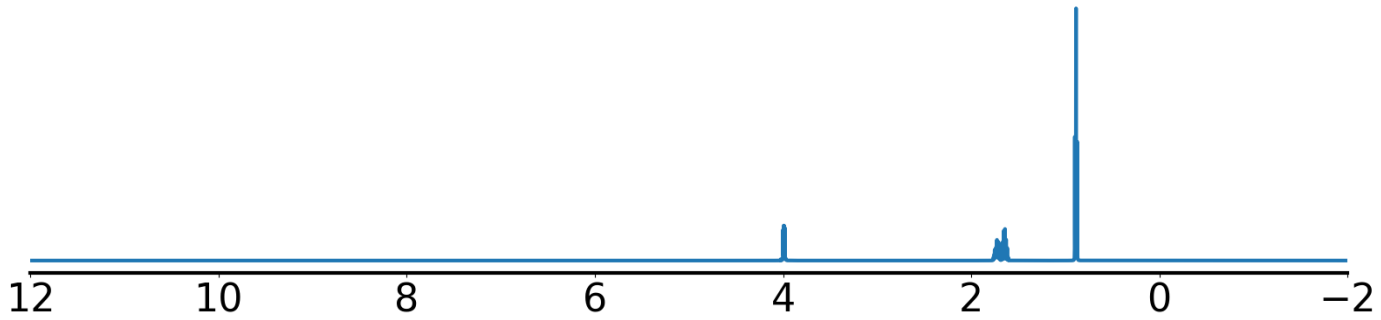
Example 75 true smiles: CCC(O)C(=O)O formula: C4H8O3
Index of correct structure: 0 of 172
True structure loss: 0.021028
True structure:



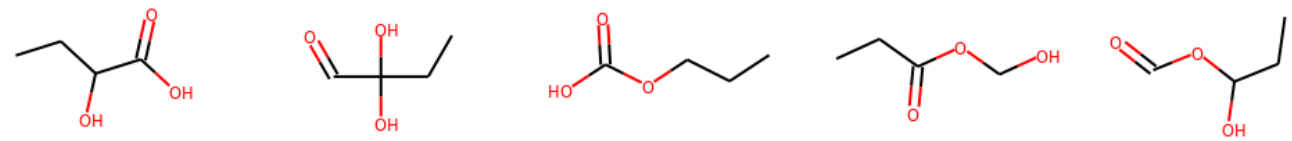
Experimental 13C NMR (solvent: CDCl3)



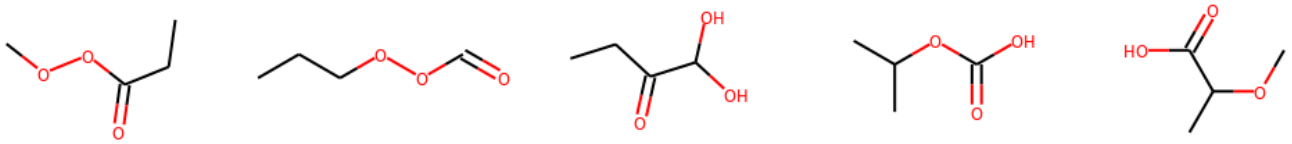
Experimental 1H NMR (solvent: d2o)



Top predicted structures (loss):



0.021028 0.049342 0.053294 0.058771 0.060748



0.071974 0.072581 0.075985 0.090438 0.091313

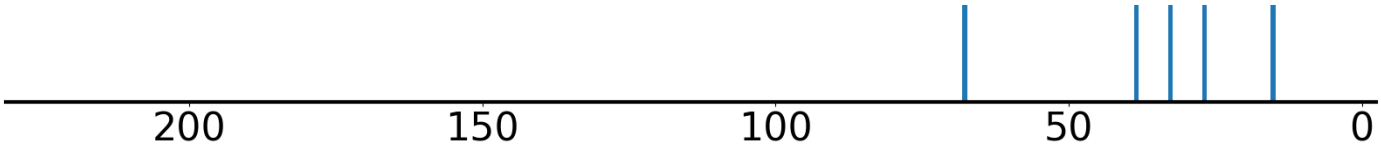
Top predicted substructures	prob		
[CX4H3]	0.9997	[CX4H2]([#6])[#6]	0.9969
[#6H3][#6][#6]	0.9988	[CX4H3][#6]	0.9959
[CX3](=[OX1])C	0.998	[CX3](=[OX1])O	0.9951
[#8]=[#6][#8]	0.9971	[OX2H1]	0.9902
[CX4H3][CX4H2]	0.9969	[#8][#6][#6H2]	0.9749

best positives	prob	best negatives	prob
[CX4H3]	0.9997	CC=CC#CC	0.0
[#6H3][#6][#6]	0.9988	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])C	0.998	[CX3H1](=[CX3H2])[CX2H0]	0.0
[#8]=[#6][#8]	0.9971	CCC#CC#C	0.0
[CX4H3][CX4H2]	0.9969	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9969	CCC#CC=C	0.0
[CX4H3][#6]	0.9959	[#6X2][#6H1][#6X2]	0.0
[CX3](=[OX1])O	0.9951	C=CC=CC#C	0.0
[OX2H1]	0.9902	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[#8][#6][#6H2]	0.9749	CC#CCC#C	0.0

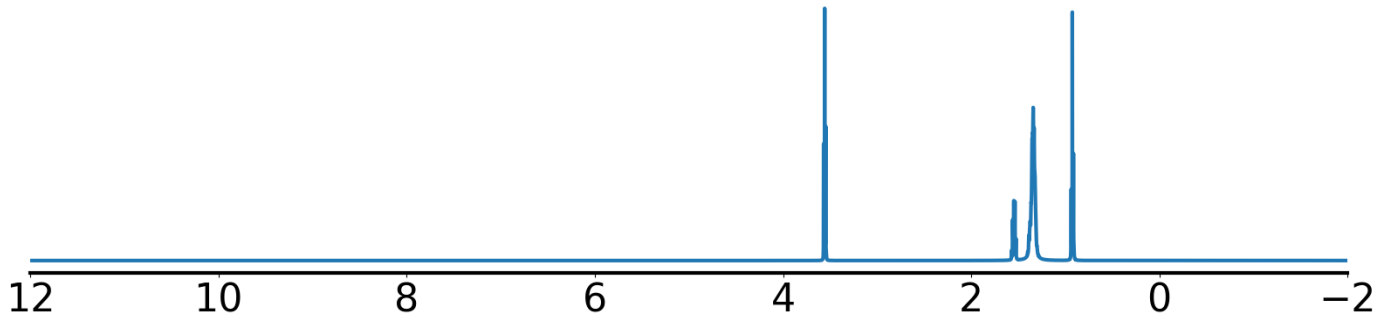
worst negatives	prob	worst positives	prob
[OX2H1][CX4H0][CX4H2][CX4H3]	0.8867	[CX4H2]([CX4H3])[CX4H1]	0.0687
[CX4H2]([CX4H3])[CX4H0]	0.6733	[#6H1][#6H2]	0.3109
[#8][#6][#6][#6X3]	0.3545	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.344
[CX4H2][CX3]=O	0.305	[#8][#6H0][#6H1]	0.451
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.2117	[#6X4H2][#6H1][#8H]	0.4582
[CX3H0](=[OX1H0])([OX2H0])[CX4H0]	0.1602	[CX4H](O)CO	0.4609
[#8][#6][#6H2][#8]	0.1396	[#8]=[#6H0][#6H1]	0.495
[CX4H2]([#6])[O]	0.1276	[OH][CX4H]	0.5045
[CX4H2]([CX4H3])[CX3H0]	0.1192	O[CX4H][CX4H2]	0.5068
[#6H3][#6][#6X3]	0.1018	O=[CX3][CX4H]	0.5208

Example 76 true smiles: CCCCCCCCO formula: C8H18O
Index of correct structure: 0 of 171
True structure loss: 0.008491
True structure:

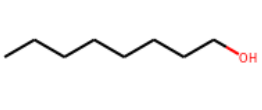
Experimental 13C NMR (solvent: CDCl3)



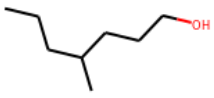
Experimental 1H NMR (solvent: MeOD)



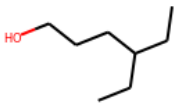
Top predicted structures (loss):



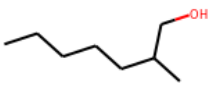
0.008491



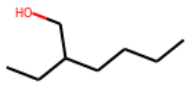
0.02378



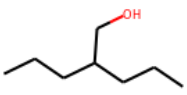
0.023828



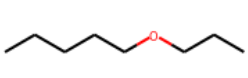
0.024177



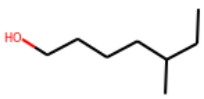
0.025258



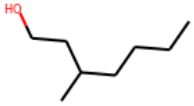
0.025781



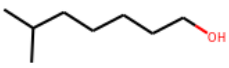
0.02613



0.02635



0.027431



0.027628

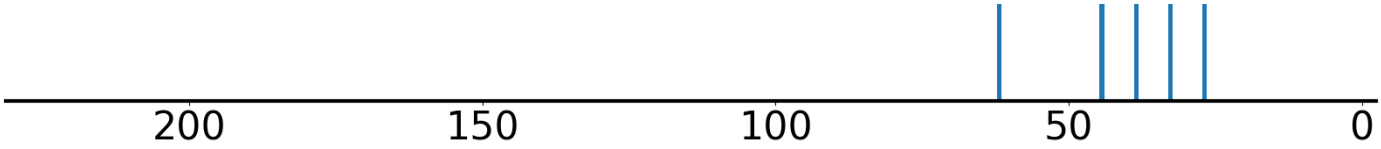
Top predicted substructures	prob		
[CX4H2]([#6])[O]	0.9997	[CX4H3][CX4H2]	0.9951
[CX4H2]([#6])[#6]	0.9994	[CX4H2][CX4H2][CX4H2][CX4H2]	0.9875
[CX4H3]	0.9992	[CX4H2]([CX4H2])[CX4H2]	0.9691
[CX4H3][#6]	0.9989	[CX4H2][CX4H2]	0.9627
[#6H3][#6][#6]	0.9989	OCC[CH2]	0.9258

best positives	prob	best negatives	prob
[CX4H2]([#6])[O]	0.9997	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	0.9994	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3]	0.9992	[#6X2][#6H1][#6X2]	0.0
[CX4H3][#6]	0.9989	C=CC=CC#C	0.0
[#6H3][#6][#6]	0.9989	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H3][CX4H2]	0.9951	C=CCCC#C	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.9875	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9691	[#7][#6]=[#6][#6]#[#7]	0.0
[CX4H2][CX4H2]	0.9627	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
OCC[CH2]	0.9258	[CX2H0](#[CX2H1])[CX4H2]	0.0

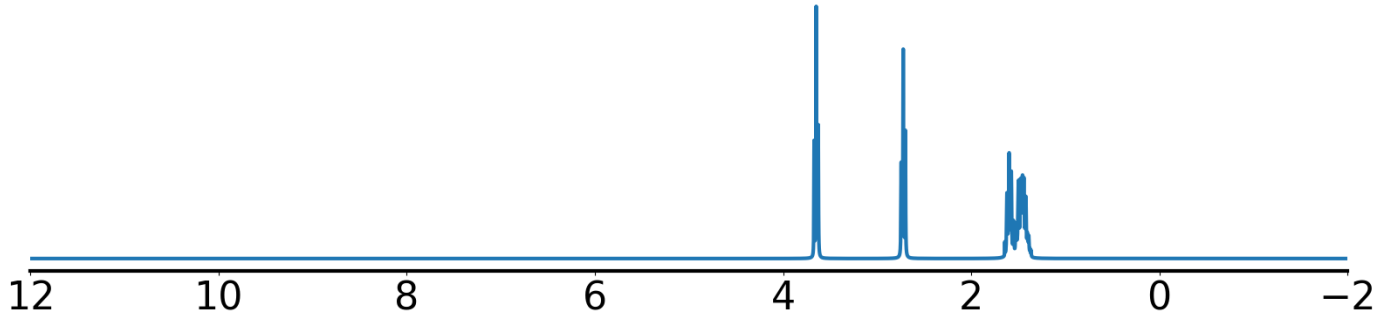
worst negatives	prob	worst positives	prob
[CX4H2]([OX2H1])[CX4H1]	0.7466	[CX4H2]([OX2H1])[CX4H2]	0.5119
[#6H1][#6H2]	0.5345	[#8][#6][#6H2]	0.5598
[#8H][#6H2][#6H1]	0.4214	[CH2X4](O)[CX4H2]	0.68
[#6H1]	0.4102	[CH2X4](O)[CX4H2][CX4H2]	0.7251
[OX2H1][CX4H2][CX4H1]([CX4H2])[CX4H2]	0.3709	CCCCCC	0.7923
[CX4H3][CX4H1]	0.2589	[CX4H2]([CX4H3])[CX4H2]	0.8484
[CX4H2](O)[CHX4]	0.2118	[OX2H1]	0.918
[CX4H1]([CX4H2])([CX4H2])[CX4H2]	0.1828	OCC[CH2]	0.9258
[#6H1]([#6H2])[#6H2]	0.1468	[CX4H2][CX4H2]	0.9627
[CHX4]([CH3X4])[CH2X4]	0.1073	[CX4H2]([CX4H2])[CX4H2]	0.9691

Example 77 true smiles: NCCCCCO formula: C5H13NO
Index of correct structure: 0 of 152
True structure loss: 0.008112
True structure:

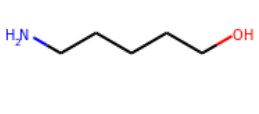
Experimental 13C NMR (solvent: CDCl3)



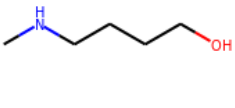
Experimental 1H NMR (solvent: CDCl3)



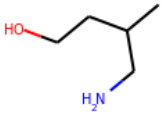
Top predicted structures (loss):



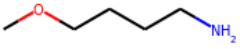
0.008112



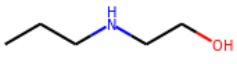
0.035379



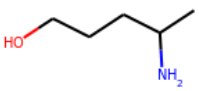
0.048434



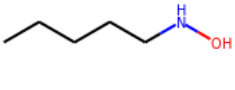
0.049003



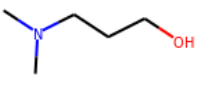
0.056304



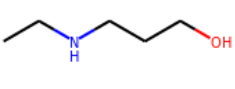
0.057765



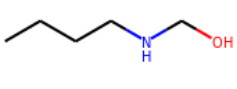
0.057902



0.062004



0.062756



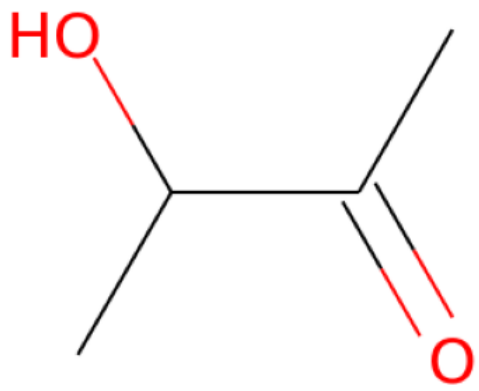
0.064579

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9998	[#7][#6H2]	0.978
[CX4H2][CX4H2]	0.9959	[CX4H2]([CX4H2])[CX4H2]	0.9756
[CX4H2]([OX2H1])[CX4H2]	0.9934	[#7H2][#6H2]	0.9756
[OX2H1]	0.9925	[#7X3][#6H2]	0.9543
[CX4H2]([#6])[O]	0.9841	[#7X3H2]	0.9275

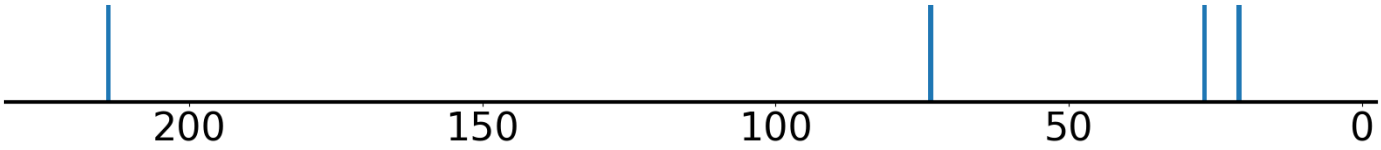
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9998	C=CC=CC#C	0.0
[CX4H2][CX4H2]	0.9959	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([OX2H1])[CX4H2]	0.9934	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[OX2H1]	0.9925	CCC=CC#C	0.0
[CX4H2]([#6])[O]	0.9841	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7][#6H2]	0.978	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.9756	C=CCCC#C	0.0
[#7H2][#6H2]	0.9756	[#6X2][#6H1][#6X2]	0.0
[#7X3][#6H2]	0.9543	[CX2H0](#[CX2H1])[CX4H1]	0.0
[#7X3H2]	0.9275	CCC#CC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H1]	0.7334	[CH2X4](O)[CX4H2][CX4H2]	0.3373
[#6H1]	0.3908	[#8][#6][#6H2]	0.6898
[#6H1][#6H2]	0.3426	OCC[CH2]	0.7685
[#6H1]([#6H2])[#6H2]	0.2877	[CH2X4](O)[CX4H2]	0.8428
[#7X3H1]	0.2846	[#7][#6H2][#6H2]	0.8809
[CX4H2]([NX3H1])[CX4H2]	0.2522	[CX4H2]([NX3H2])[CX4H2]	0.8812
CCCCCC	0.2318	[CX4H2][CX4H2][CX4H2][CX4H2]	0.923
[#8H][#6H2][#6H1]	0.2017	[#7X3H2]	0.9275
[CX4H2]([OX2H1])[CX4H1]	0.1515	[#7X3][#6H2]	0.9543
[CX4H2](O)[CHX4]	0.1313	[#7H2][#6H2]	0.9756

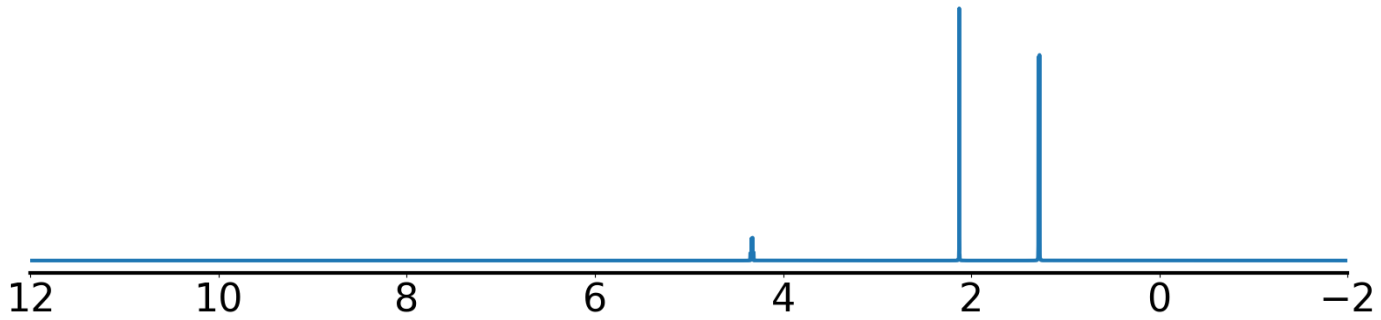
Example 78 true smiles: CC(=O)C(C)O formula: C4H8O2
Index of correct structure: 0 of 72
True structure loss: 0.008046
True structure:



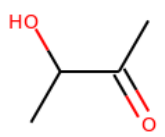
Experimental 13C NMR (solvent: CDCl3)



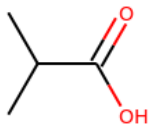
Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):

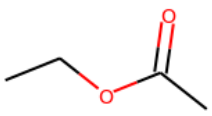


0.008046

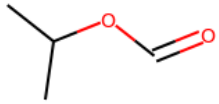


0.077084

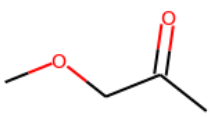
0.081874



0.083511

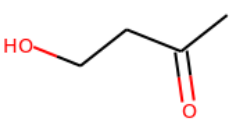


0.091763

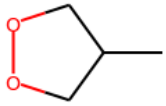


0.103167

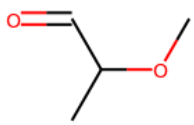
0.115577



0.127283



0.144516



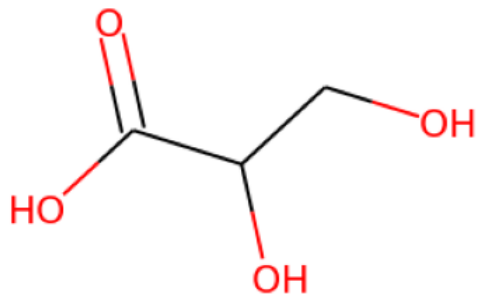
0.148293

Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H3][CX3]	0.9975
[CX3](=[OX1])C	0.9998	[CX4H3][CX3H0]	0.9972
[CX4H3][#6]	0.9995	[CX4H3][CX4]O	0.9872
[#6H3][#6][#6]	0.9993	[CX4H]O	0.9696
[OX1H0]=[CX3H0][CX4H3]	0.9985	[#6H3][#6H0]	0.963

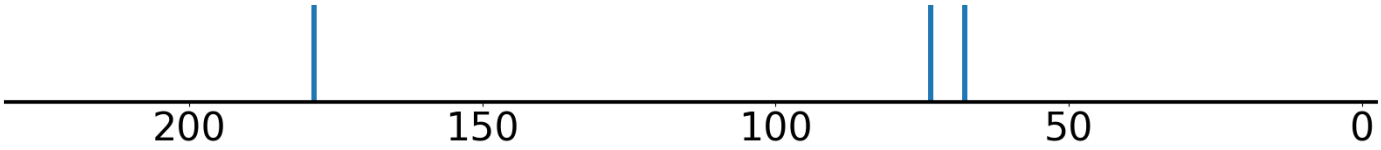
best positives	prob	best negatives	prob
[CX4H3]	1.0	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9998	C=CCCC#C	0.0
[CX4H3][#6]	0.9995	[#6H2]=[#6][#6X2]	0.0
[#6H3][#6][#6]	0.9993	CC=CC#CC	0.0
[OX1H0]=[CX3H0][CX4H3]	0.9985	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H3][CX3]	0.9975	CCC#CC=C	0.0
[CX4H3][CX3H0]	0.9972	[CX3H0](=[CX3H1])([CX4H2])[CX2H0]	0.0
[CX4H3][CX4]O	0.9872	[CX3H0](=[CX3H2])([CX4H2])[CX4H0]	0.0
[CX4H]O	0.9696	[CX2H0](#[CX2H0])[CX3H1]	0.0
[#6H3][#6H0]	0.963	[#6]1[#6]=[#6][#6][#6]=[#6]1	0.0

worst negatives	prob	worst positives	prob
[CX3H0](=[OX1H0])([CX4H3])[CX4H0]	0.2983	[CX3H0](=[OX1H0])([CX4H3])[CX4H1]	0.3801
[#6X3][#6][#6][#6H3]	0.2897	[#6H3][#6][#6][#6H3]	0.591
[#8][#6][#6][#6X3]	0.2299	[#8H][#6X4H1][#6X3H0]	0.6508
[CX4H2][CX3]=O	0.1798	[#8]=[#6H0][#6H1]	0.698
[CX4H1]([OX2H1])([CX4H3])[CX4H1]	0.1662	O=[CX3][CX4H]	0.7634
[CX4H2]CC=O	0.1548	[OH][CX4H]	0.7795
[OX1H0]=[CX3H0][CX3H0][CX4H3]	0.1474	[#6X4H3][#6][#8H]	0.7997
[CHX4]([CH3X4])[CH3X4]	0.1398	[#6H3][#6][#6X3]	0.8048
[#6H3][#6X3H0][#6H2]	0.084	[CH3]CC[OH]	0.808
[CX4H3][CX3H0][CX3]=O	0.0673	[CX4H1]([OX2H1])([CX4H3])[CX3H0]	0.8115

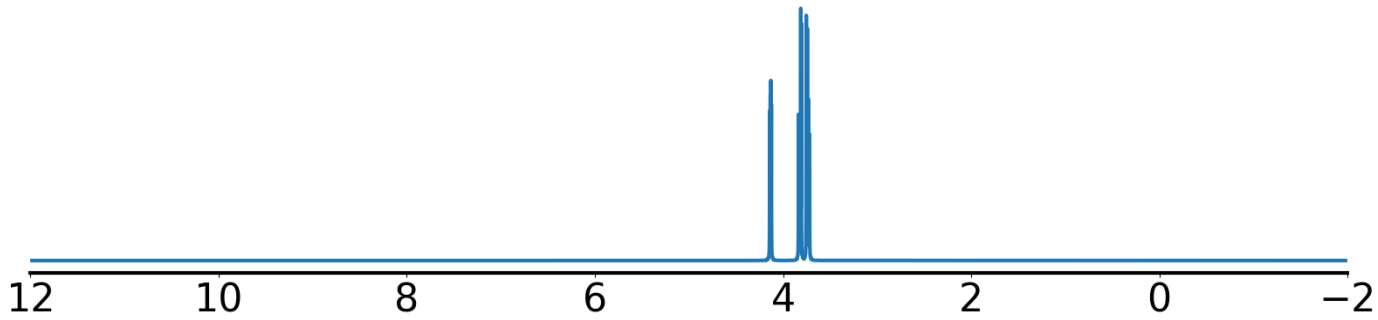
Example 79 true smiles: O=C(O)C(O)CO formula: C3H6O4
Index of correct structure: 0 of 71
True structure loss: 0.021543
True structure:



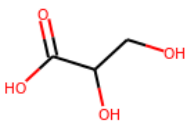
Experimental 13C NMR (solvent: D2O)



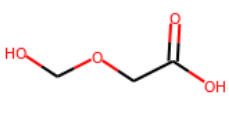
Experimental 1H NMR (solvent: D2O)



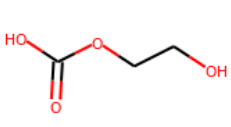
Top predicted structures (loss):



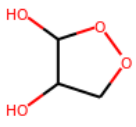
0.021543



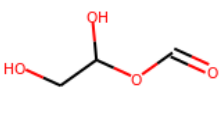
0.044352



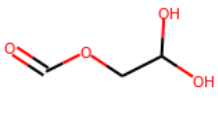
0.047151



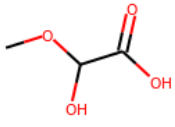
0.047896



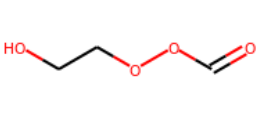
0.049885



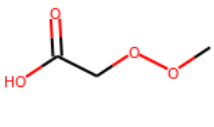
0.052381



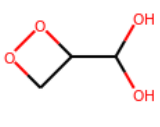
0.056455



0.057624



0.058404



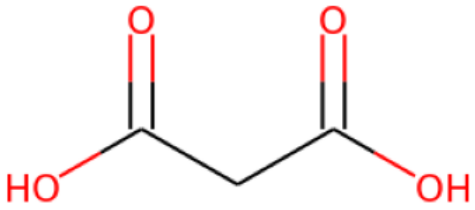
0.060583

Top predicted substructures	prob		
[CX4H2]([#6])[O]	0.9958	[CX3](=[OX1])O	0.9601
[OX2H1]	0.9803	[#8][#6][#6H2]	0.9595
[#8][#6][#6H2][#8]	0.9765	[CX4H](O)CO	0.9528
[#8][#6][#6][#8]	0.9709	[#8]=[#6][#8]	0.9428
[CX3](=[OX1])C	0.9707	[CX4H2](O)[CHX4]	0.8824

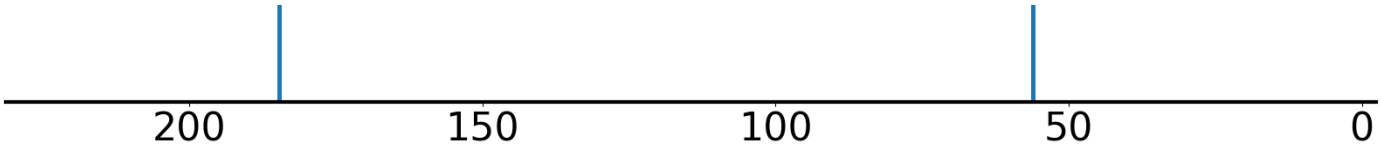
best positives	prob	best negatives	prob
[CX4H2]([#6])[O]	0.9958	[#6X2][#6H1][#6X2]	0.0
[OX2H1]	0.9803	CC=CCC#C	0.0
[#8][#6][#6H2][#8]	0.9765	CC#CCC=C	0.0
[#8][#6][#6][#8]	0.9709	[#7][#6][#6]#[#7]	0.0
[CX3](=[OX1])C	0.9707	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX3](=[OX1])O	0.9601	CCC#CC#C	0.0
[#8][#6][#6H2]	0.9595	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H](O)CO	0.9528	[CX2H0](#[CX2H0])[CX4H0]	0.0
[#8]=[#6][#8]	0.9428	[CX3H1](=[CX3H1])[CX2H0]	0.0
[CX4H2](O)[CHX4]	0.8824	[#6H2][#6]#[#6X2]	0.0

worst negatives	prob	worst positives	prob
[CX4H2][OX2H0][CX4H2]	0.4959	[#8][#6][#6][#6X3]	0.2983
[CX4H2][CX4H2]	0.4874	[#8][#6H0][#6H1]	0.3087
O[CX4H2][CX4H2]O	0.4826	[OX1H0]=[CX3H0][CX4H1]([OX2H1])[CX4H2]	0.3588
[OX2H0][CX4H2][CX4H2][OX2H0]	0.4747	[#8H][#6X4H1][#6X3H0]	0.4136
[CX4H2][CX3]=O	0.4013	[#8][#6H2][#6H][#6X3]	0.445
[CX4H2]([OX2H0])[CX3H0]	0.3274	[OH][CX4H]	0.4498
[CX4H2]([OX2H0])[CX4H2]	0.2791	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.4515
[#6X3][#6H2][#8]	0.2575	[#8][#6H2][#6H1][#6H0]	0.4696
[CX4H2]([OX2H0])[CX4H1]	0.2448	[#8]=[#6H0][#6H1]	0.5513
[#8][#6H1][#6H1]	0.2291	[#6X4H2][#6H1][#8H]	0.552

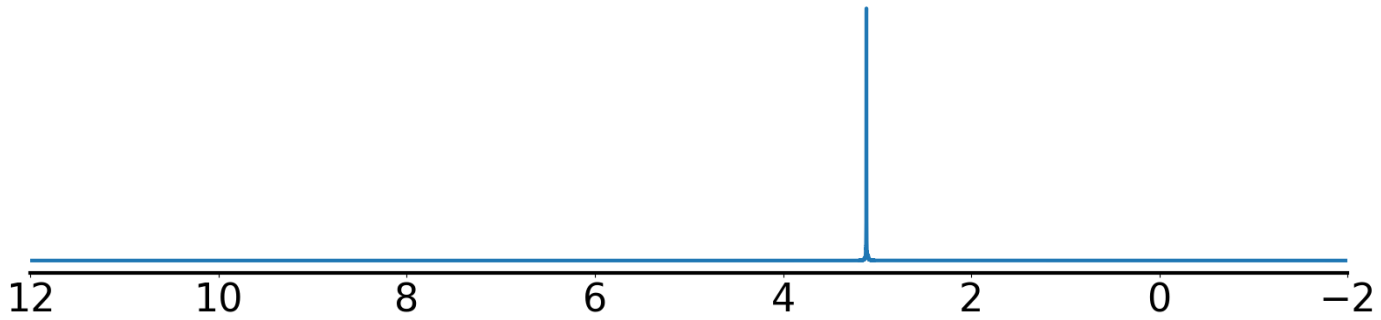
Example 80 true smiles: O=C(O)CC(=O)O formula: C3H4O4
Index of correct structure: 0 of 69
True structure loss: 0.035753
True structure:



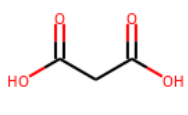
Experimental 13C NMR (solvent: D2O)



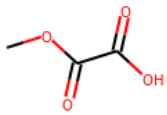
Experimental 1H NMR (solvent: D2O)



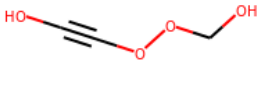
Top predicted structures (loss):



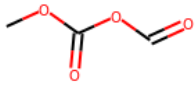
0.035753



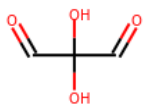
0.038212



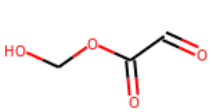
0.039043



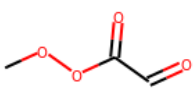
0.044505



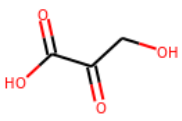
0.054523



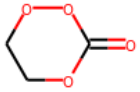
0.059851



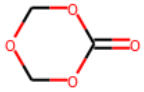
0.065053



0.068764



0.07055



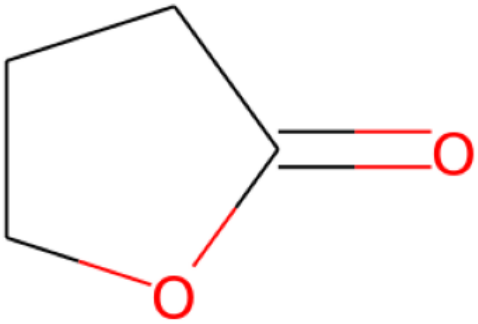
0.072

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9967	[#8][#6][#6][#6X3]	0.52
[#8]=[#6][#8]	0.9615	[#8][#6][#6H2]	0.4323
[OX2H1]	0.9267	[#8][#6][#6]=[#8]	0.4315
[CX3](=[OX1])O	0.847	[CX4H2][CX3]=O	0.4011
[CX3](=O)[OX2H1]	0.6954	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3988

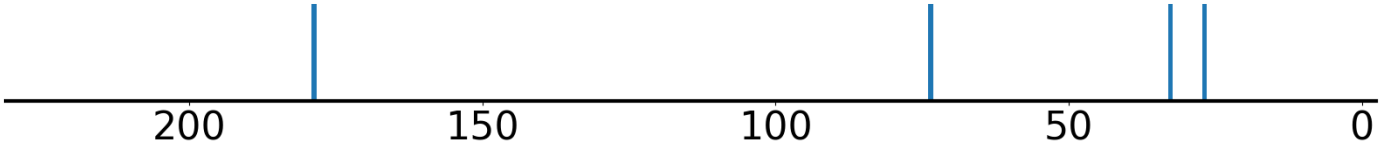
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9967	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#8]=[#6][#8]	0.9615	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.0
[OX2H1]	0.9267	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[CX3](=[OX1])O	0.847	C=CC=CC#C	0.0
[CX3](=O)[OX2H1]	0.6954	CCC=CC#C	0.0
[#8][#6][#6][#6X3]	0.52	CC=CCC#C	0.0
[#8][#6][#6H2]	0.4323	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[CX4H2][CX3]=O	0.4011	[CX3H0](=[CX3H2])([CX4H3])[CX4H1]	0.0
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.151	[CX3H0](=[CX3H2])([CX4H2])[CX4H2]	0.0
O=[#6][#6][#6X3]	0.1293	[#6X3H2]=[#6][#6H2][#8H]	0.0

worst negatives	prob	worst positives	prob
[#8][#6][#6]=[#8]	0.4315	[#6X3][#6H2][#6X3]	0.0077
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.3988	[OX1H0]=[CX3H0][CX4H2][CX3H0]	0.0242
[CX4H2]CC=O	0.3483	[CX4H2]([CX3H0])[CX3H0]	0.0312
O=[CX3][CX4H]	0.3318	[CX4H2]([#6])[#6]	0.0416
[#8][#6][#6][#8]	0.3293	[#8X1]=[#6X3][#6H2][#6H0]	0.1103
[CX4H3]	0.3247	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.1156
[#8]=[#6H0][#6H1]	0.2727	O=[#6][#6][#6X3]	0.1293
C1CC1O	0.2616	[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.151
[CX4H]O	0.2464	[CX4H2][CX3]=O	0.4011
[#6H1][#6H1]	0.2397	[#8][#6][#6H2]	0.4323

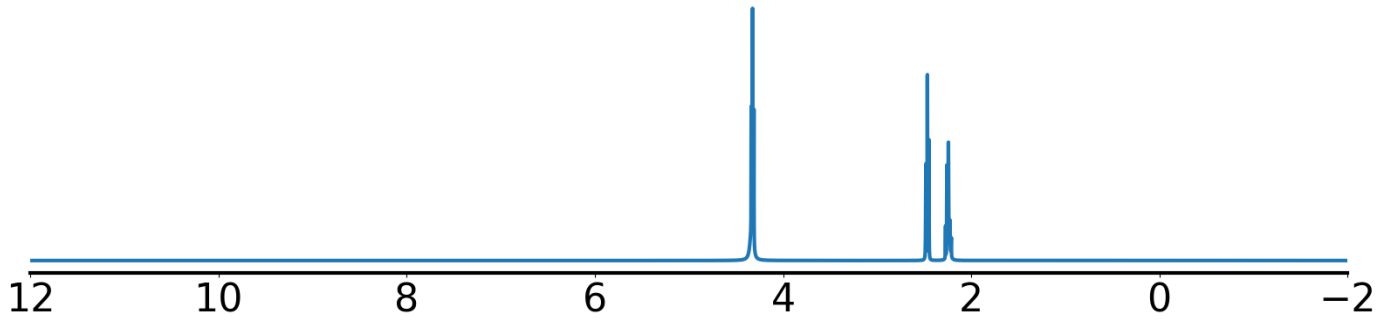
Example 81 true smiles: O=C1CCCO1 formula: C4H6O2
Index of correct structure: 0 of 68
True structure loss: 0.012881
True structure:



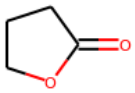
Experimental 13C NMR (solvent: CDCl3)



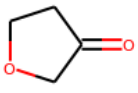
Experimental 1H NMR (solvent: CDCl3)



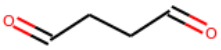
Top predicted structures (loss):



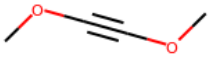
0.012881



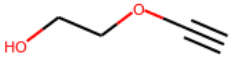
0.078109



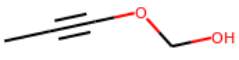
0.078619



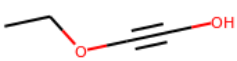
0.105713



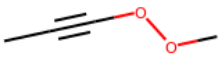
0.11641



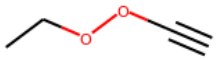
0.131362



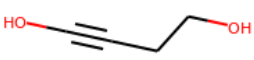
0.131877



0.138979



0.146089



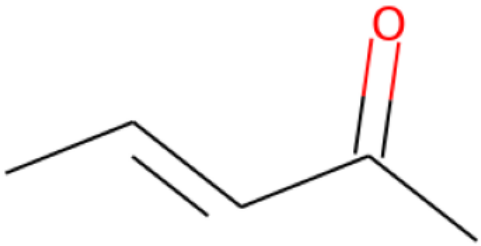
0.150866

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	O=[CX3H0][CX4H2][CX4H2]	0.9854
[CX3](=[OX1])C	0.9937	[CX4H2]([CX4H2])[CX3H0]	0.9817
[CX4H2][CX4H2]	0.9917	[CX3](=[OX1])O	0.9816
[#8]=[#6][#8]	0.9865	OCC[CH2]	0.9547
[#8][#6][#6H2]	0.9859	[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9465

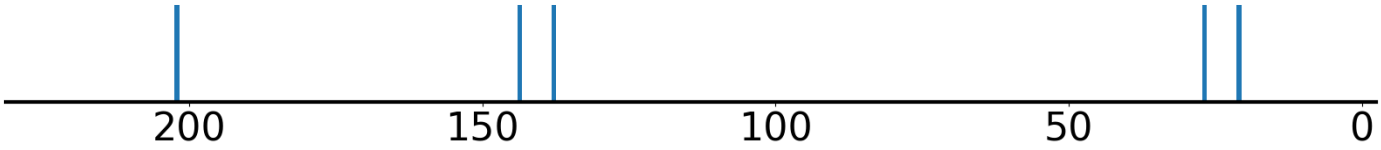
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	C=CC=CC#C	0.0
[CX3](=[OX1])C	0.9937	[#6H3][#6H1][#6H1]=[#7]	0.0
[CX4H2][CX4H2]	0.9917	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8]=[#6][#8]	0.9865	[CX4H1]([NX3H1])([CX4H1])[CX4H0]	0.0
[#8][#6][#6H2]	0.9859	[#7][#6]=[#6][#6][#6]=[#7]	0.0
O=[CX3H0][CX4H2][CX4H2]	0.9854	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2]([CX4H2])[CX3H0]	0.9817	[CX2H0](#[CX2H0])[CX4H0]	0.0
[CX3](=[OX1])O	0.9816	[CX3H1](=[CX3H2])[CX4H0]	0.0
OCC[CH2]	0.9547	[cX3H1]([nX2H0])[cX3H1]	0.0
[OX1H0]=[CX3H0]([#8])[CX4H2]	0.9465	[CX4H0]([CX4H3])([CX4H2])([CX4H1])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[#6H1][#6H2]	0.4527	[CH2X4](O)[CX4H2][CX4H2]	0.3247
[#6H1]	0.3246	[#8][#6][#6][#6][#6]=[#8]	0.3358
[#8][#6H0][#6H1]	0.2895	C1OCCC1	0.4169
[#8]1[#6][#6][#6][#6][#6]1	0.2852	[OX2H0][CX4H2][CX4H2][CX4H2]	0.4595
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2471	[CX4H2]([CX4H2])[CX4H2]	0.5617
[OX2H1]	0.2037	[CH2X4](O)[CX4H2]	0.5937
[CX4H2]([CX4H2])[CX4H1]	0.193	[CX4H2]([#6])[O]	0.6874
[CX4H]O	0.1919	[CX4H2]([OX2H0])[CX4H2]	0.6885
[#6X4H2][#6H1][#8H]	0.1893	[CX4H2][CX3]=O	0.8696
[CX4H2]([CX4H2])[CX3H1]	0.1827	[OX2H0][CX3H0][CX4H2]	0.8931

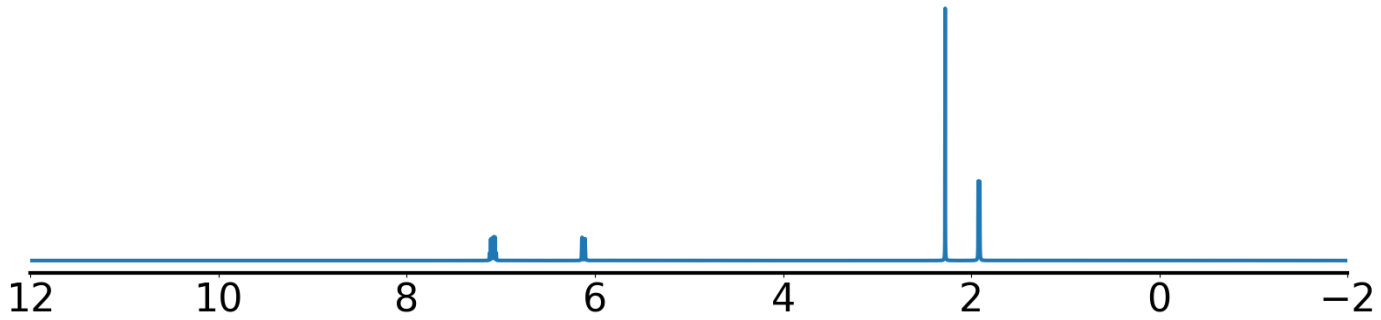
Example 82 true smiles: CC=CC(C)=O formula: C5H8O
Index of correct structure: 0 of 66
True structure loss: 0.009459
True structure:



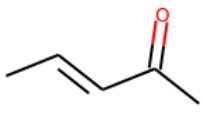
Experimental 13C NMR (solvent: CDCl3)



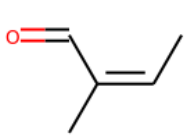
Experimental 1H NMR (solvent: D2O)



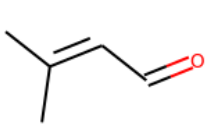
Top predicted structures (loss):



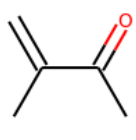
0.009459



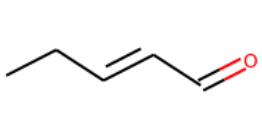
0.052656



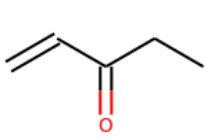
0.059911



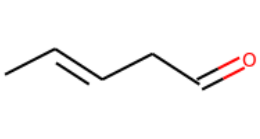
0.086267



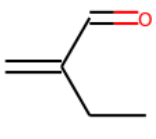
0.116485



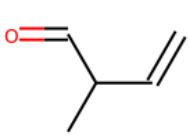
0.143647



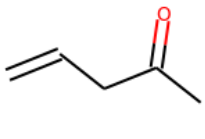
0.150581



0.185346



0.18705



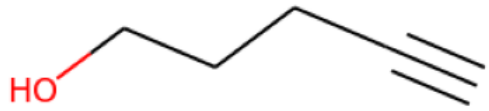
0.189319

Top predicted substructures	prob		
[CX4H3]	1.0	[#6X3][#6X3]	0.9976
[CX4H3][#6]	1.0	[#6H3][#6H0]	0.9971
[CX4H3][CX3]	1.0	[CX4H3][CX3H0]	0.9952
O=[#6][#6]=[#6X3]	0.9998	[#6H3][#6][#6]	0.9934
[CX3](=[OX1])C	0.9977	[#6H3][#6]=[#6X3]	0.992

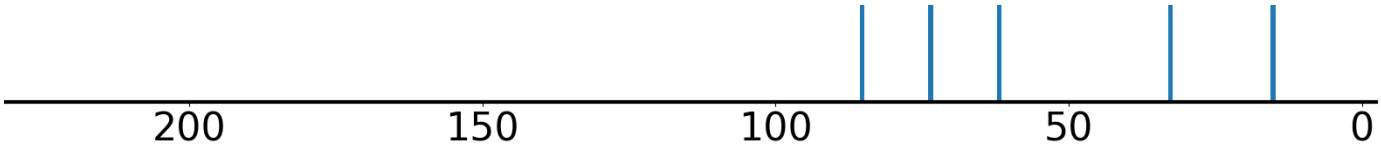
best positives	prob	best negatives	prob
[CX4H3]	1.0	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3][#6]	1.0	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[CX4H3][CX3]	1.0	[#6X2][#6H1][#6X2]	0.0
O=[#6][#6]=[#6X3]	0.9998	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX3](=[OX1])C	0.9977	[OX2H1][CX4H1][CX4H1][CX2H0]	0.0
[#6X3][#6X3]	0.9976	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H3][#6H0]	0.9971	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[CX4H3][CX3H0]	0.9952	CCC#CC#C	0.0
[#6H3][#6][#6]	0.9934	CCC=CC#C	0.0
[#6H3][#6]=[#6X3]	0.992	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[CX3H1](=[CX3H0])[CX4H3]	0.5167	[CX3H1](=[CX3H1])[CX4H3]	0.272
[CX4H3][CX3H0][CX3]=O	0.4214	[#8]=[#6H0][#6H1]	0.5397
[OX1H0]=[CX3H0][CX3H0][CX4H3]	0.3295	[CHX3]=[CHX3]	0.554
[#6X3H1]=[#6X3H0]	0.3267	[CX4H3][CX3H1]	0.7385
[CX3H0](=[CX3H1])([CX4H3])[CX3H0]	0.2832	[OX1H0]=[CX3H0][CX3H1]=[CX3H1]	0.7645
[CX3H0](=[OX1H0])([CX4H3])[CX3H0]	0.1733	[#6X3H1][#6X3H0]	0.7847
CCC=CCC	0.1469	[CX3H1](=[CX3H1])[CX3H0]	0.7862
[#6H1][#6H2]	0.14	[#6X3]=[#6][#6][#6H3]	0.801
[CX4H2]CC=O	0.1286	O=C[CX3H]	0.8111
[#6H3][#6]=[#6][#6H3]	0.1172	[#6X3][#6]=[#6][#6H3]	0.9067

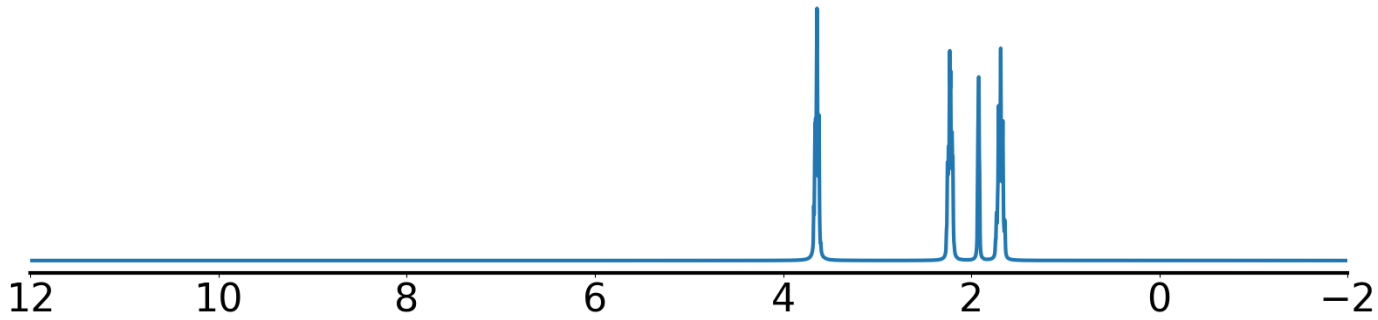
Example 83 true smiles: C#CCCCO formula: C5H8O
Index of correct structure: 0 of 66
True structure loss: 0.016951
True structure:



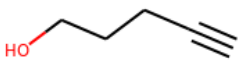
Experimental 13C NMR (solvent: CDCl3)



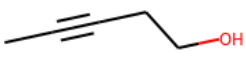
Experimental 1H NMR (solvent: CDCl3)



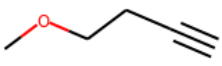
Top predicted structures (loss):



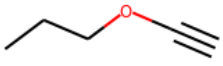
0.016951



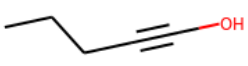
0.037868



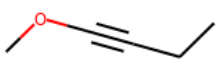
0.0395



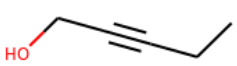
0.049389



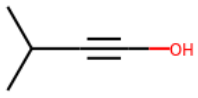
0.049925



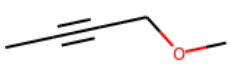
0.051962



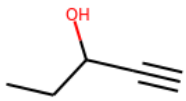
0.058943



0.075868



0.082002



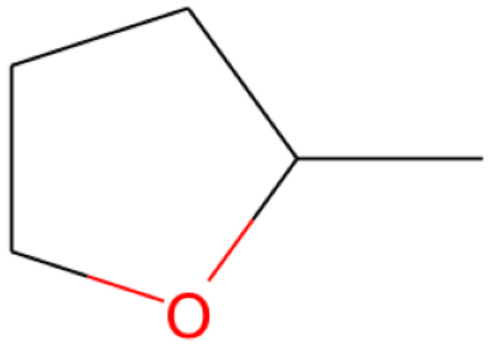
0.083761

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	1.0	[CX4H2][CX4H2]	0.8862
[$([CX2]#C)]	0.9873	[#6H1]	0.7888
[#8][#6][#6H2]	0.9817	[OX2H1]	0.7786
[#6H2][#6X2]	0.9468	[CX4H2]([CX4H2])[CX4H2]	0.7719
OCC[CH2]	0.9084	[CX4H2]([#6])[O]	0.7718

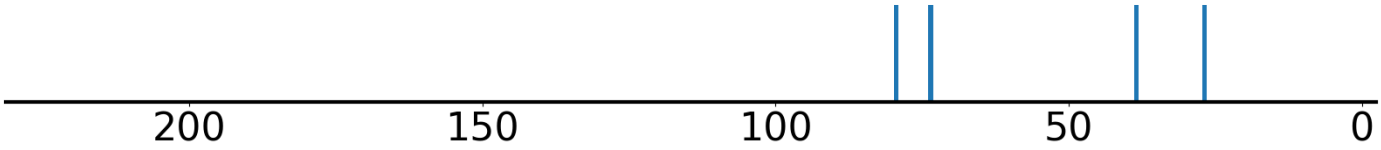
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	1.0	[CX3H1](=[CX3H2])[cX3H0]	0.0
[$([CX2]#C)]	0.9873	[#6H3][#6H1][#6H1]=[#7]	0.0
[#8][#6][#6H2]	0.9817	[#6X3H1]=[#6X3H1][#6X3H0]=[#6X3H1]	0.0
[#6H2][#6X2]	0.9468	[#7][#6]=[#6][#6][#6]=[#7]	0.0
OCC[CH2]	0.9084	[#6H3][#6X3][#6X3]=[#6X3H2]	0.0
[CX4H2][CX4H2]	0.8862	[CX4H3][nX3H0]	0.0
[#6H1]	0.7888	[#6X3H2]=[#6][#6H2][#8H]	0.0
[OX2H1]	0.7786	[CX3H2]=[CX3H0][CX4H2][CX3H1]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.7719	[CX4H1]([CX4H3])([CX3H1])[CX3H0]	0.0
[CX4H2]([#6])[O]	0.7718	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H1]	0.552	[CX2H1]#[CX2H0]	0.1858
[#6H1][#6H2]	0.4324	[CX2H0](#[CX2H1])[CX4H2]	0.2053
[CX2H0](#[CX2H0])[CX4H2]	0.4073	[#6H2][#6][#6X2]	0.4253
[CX4H2]([OX2H0])[CX4H2]	0.3957	[CH2X4](O)[CX4H2][CX4H2]	0.437
O[CX4H][CX4H2]	0.3157	[#6H2][#6]#[#6X2]	0.5926
[OX2H0][CX4H2][CX4H2][CX4H2]	0.2985	[CH2X4](O)[CX4H2]	0.6768
[OH][CX4H]	0.2508	[CX4H2]([OX2H1])[CX4H2]	0.7005
C1CCC1	0.24	[CX4H2]([CX4H2])[CX2H0]	0.7332
[CX4H]O	0.2393	[CX4H2]([#6])[O]	0.7718
O[CX4H]([CX4H2])[CX4H1]	0.1734	[CX4H2]([CX4H2])[CX4H2]	0.7719

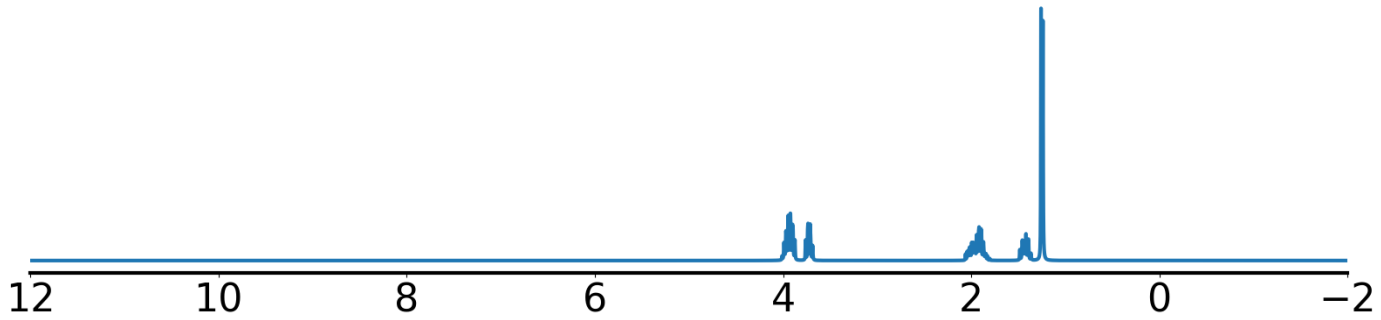
Example 84 true smiles: CC1CCCO1 formula: C5H10O
Index of correct structure: 0 of 65
True structure loss: 0.019401
True structure:



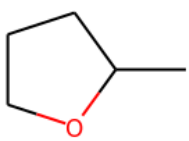
Experimental 13C NMR (solvent: CDCl3)



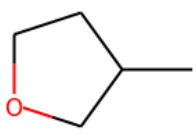
Experimental 1H NMR (solvent: CDCl3)



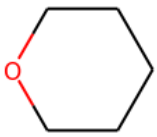
Top predicted structures (loss):



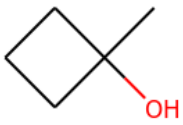
0.019401



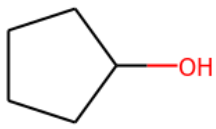
0.040693



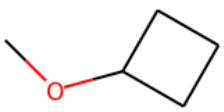
0.056381



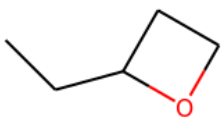
0.074822



0.074921

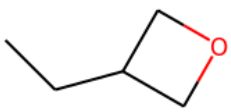


0.07954

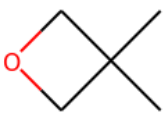


0.090534

0.092396



0.095725



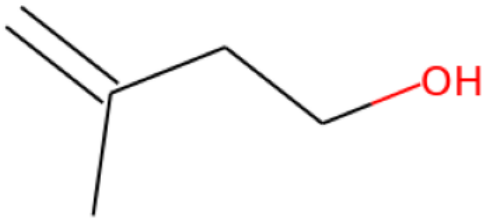
0.099106

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9999	[#8][#6][#6H2]	0.9866
[#6H3][#6][#6]	0.9983	[#6H1]	0.979
[CX4H3]	0.9975	[CX4H3][#6]	0.9772
[CX4H3][CX4]O	0.9971	[CX4H2]([#6])[O]	0.9586
OCC[CH2]	0.9906	[CX4H2][CX4H2]	0.906

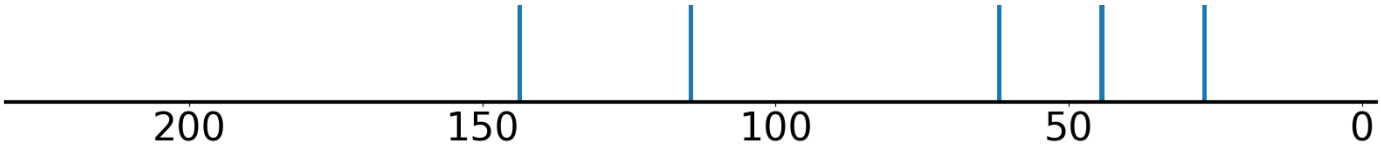
best positives	prob	best negatives	prob
[CX4H2]([#6])[#6]	0.9999	[#7][#6]=[#6][#6]#[#7]	0.0
[#6H3][#6][#6]	0.9983	C=CC=CC#C	0.0
[CX4H3]	0.9975	[#7][#6]=[#6][#6][#6]=[#7]	0.0
[CX4H3][CX4]O	0.9971	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
OCC[CH2]	0.9906	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#8][#6][#6H2]	0.9866	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[#6H1]	0.979	[CX4H2][#6X3H0][#6X3H1][#8X2H0]	0.0
[CX4H3][#6]	0.9772	[CX3H1](=[CX3H2])[cX3H0]	0.0
[CX4H2]([#6])[O]	0.9586	[CX3H0][CX3H1]=[CX3H1][CX3H0]	0.0
[CX4H2][CX4H2]	0.906	[CX4H2]([CX4H2])[cX3H0]	0.0

worst negatives	prob	worst positives	prob
CCCCCC	0.6438	[#6H3][#6H1r5]	0.1163
[#8]1[#6][#6][#6][#6][#6]1	0.618	[#6H2][#8][#6H1]	0.3522
[#6H1]([#6H2])[#6H2]	0.4381	[OX2H0][CX4H1][CX4H2][CX4H2]	0.4197
[CX4H2](O)[CHX4]	0.4361	[CHX4]([CH3X4])[CH2X4]	0.4844
[CX4H2]([OX2H0])[CX4H1]	0.4187	[CX4H2]([OX2H0])[CX4H2]	0.5425
[CX4H2]([CX4H2])[CX4H0]	0.2965	[CX4H1]([OX2H0])([CX4H3])[CX4H2]	0.5635
[OX2H0][CX4H2][CX4H1][CX4H2]	0.2461	[CH2X4](O)[CX4H2][CX4H2]	0.5916
[#6H3][#6H0]	0.2246	[CX4H2]([CX4H2])[CX4H2]	0.629
[CX4H2][OX2H0][CX4H2]	0.2071	[OX2H0][CX4H2][CX4H2][CX4H2]	0.6583
[OX2H0][CX4H2][#6H0]	0.183	O[CX4H][CX4H2]	0.6667

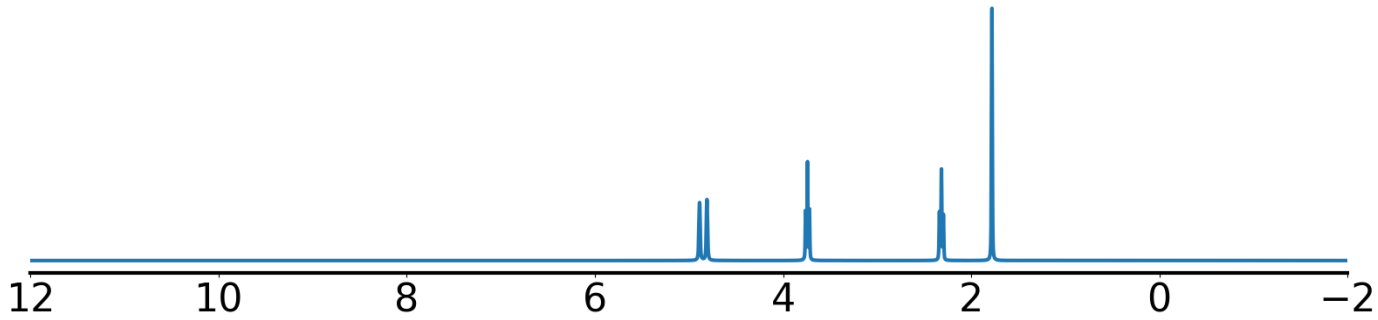
Example 85 true smiles: C=C(C)CCO formula: C5H10O
Index of correct structure: 0 of 65
True structure loss: 0.018763
True structure:



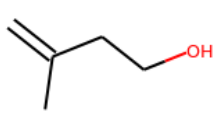
Experimental 13C NMR (solvent: CDCl3)



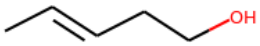
Experimental 1H NMR (solvent: CDCl3)



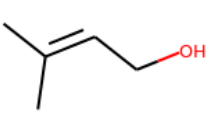
Top predicted structures (loss):



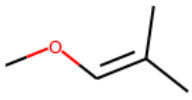
0.018763



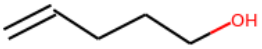
0.060426



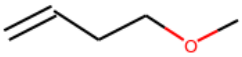
0.064155



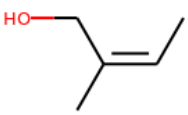
0.070333



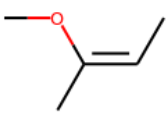
0.07931



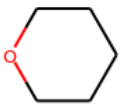
0.085347



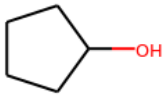
0.093263



0.094865



0.104729



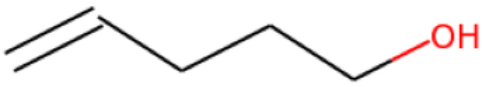
0.108799

Top predicted substructures	prob		
[CX4H3][CX3]	0.9994	[#6H3][#6][#6]	0.9862
[CX4H3][CX3H0]	0.9992	[#8][#6][#6H2]	0.9773
[CX4H3]	0.9979	[CX4H3][#6]	0.9488
[CX4H2]([#6])[#6]	0.9965	[CX4H2]([#6])[O]	0.9266
[#6H3][#6H0]	0.9882	[#6H3][#6]=[#6X3]	0.8826

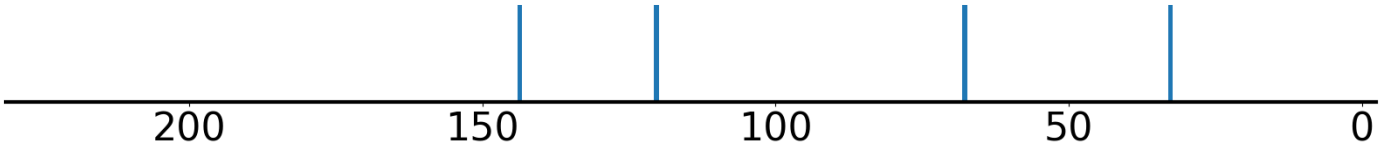
best positives	prob	best negatives	prob
[CX4H3][CX3]	0.9994	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][CX3H0]	0.9992	CCC#CC#C	0.0
[CX4H3]	0.9979	[#6X2][#6H1][#6X2]	0.0
[CX4H2]([#6])[#6]	0.9965	[CX2H0](#[CX2H0])[CX2H0]	0.0
[#6H3][#6H0]	0.9882	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
[#6H3][#6][#6]	0.9862	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#8][#6][#6H2]	0.9773	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H3][#6]	0.9488	[CX2H0](#[CX2H1])[CX4H1]	0.0
[CX4H2]([#6])[O]	0.9266	CC#CCC#C	0.0
[#6H3][#6]=[#6X3]	0.8826	C=CC=CC#C	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.8155	[CX3H2]=[CX3H0]	0.2335
[CX3H0](=[CX3H1])([CX4H3])[CX4H3]	0.5796	[CH2X3](=C)	0.2786
[#6H1][#6H2]	0.5512	[CX3H2]=[CX3H0]([#6])[#6]	0.3573
[CHX3](=C)C	0.4889	[#6H2][#6X3H0]=[#6H2]	0.3883
[#6X3H1]=[#6X3H0]	0.4438	[CX3H0](=[CX3H2])([CX4H3])[CX4H2]	0.4059
[CX3H1](=[CX3H0])[CX4H2]	0.2614	[#6H3][#6X3H0][#6H2]	0.4249
[CX4H2]([CX4H2])[CX3H1]	0.2405	[#6X3H2]	0.4339
[CX4H3][CX3H0][CX4H3]	0.2299	[CX4H2]([CX4H2])[CX3H0]	0.5982
[CX4H2][CX3H]	0.2041	[CX4H3][CX3H0]=[CX3H2]	0.6795
[#7X3H2]	0.1637	[#8][#6][#6][#6X3]	0.7215

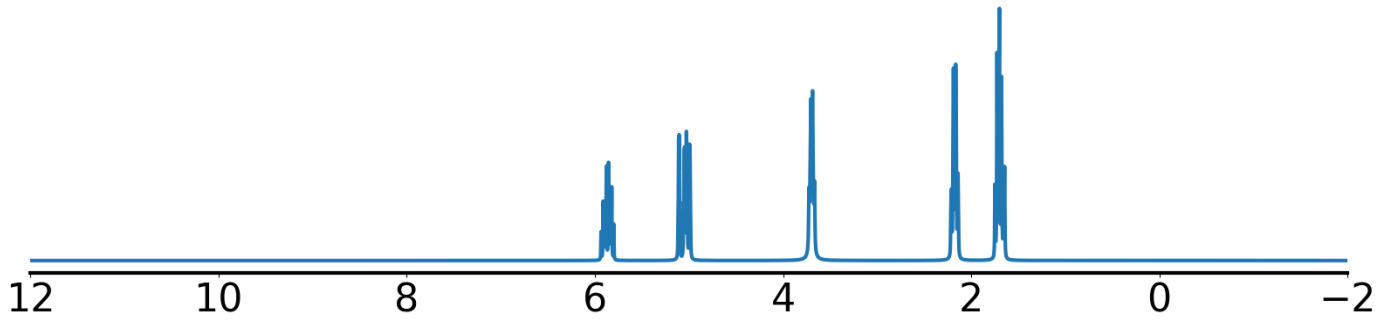
Example 86 true smiles: C=CCCCO formula: C5H10O
Index of correct structure: 0 of 65
True structure loss: 0.020514
True structure:



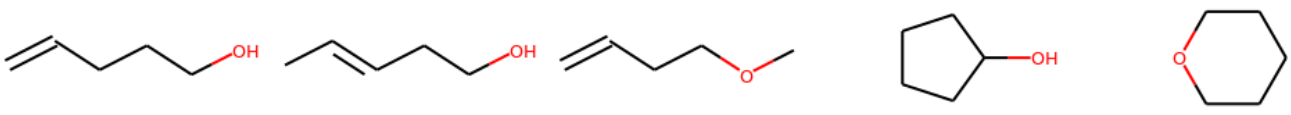
Experimental 13C NMR (solvent: CDCl3)



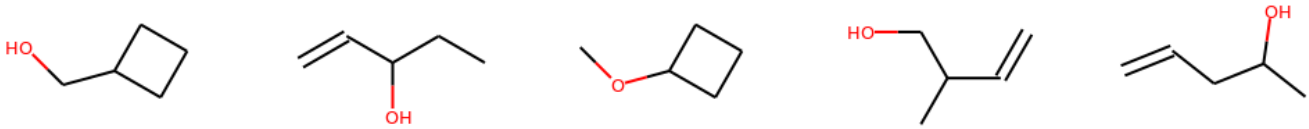
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.020514 0.051192 0.054973 0.066714 0.070372



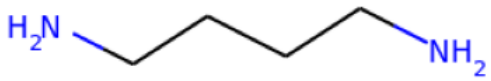
0.087205 0.094626 0.09868 0.108334 0.115583

Top predicted substructures	prob		
[CHX3](=C)C	1.0	[CX4H2][CX4H2]	0.9205
[CX4H2]([#6])[#6]	1.0	[CX4H2]([CX4H2])[CX4H2]	0.8843
[#6H1]	0.9999	[CX4H2]([#6])[O]	0.8636
[#8][#6][#6H2]	0.9914	[#6H1][#6H2]	0.852
[OX2H1]	0.9702	[CH2X4](O)[CX4H2]	0.8464

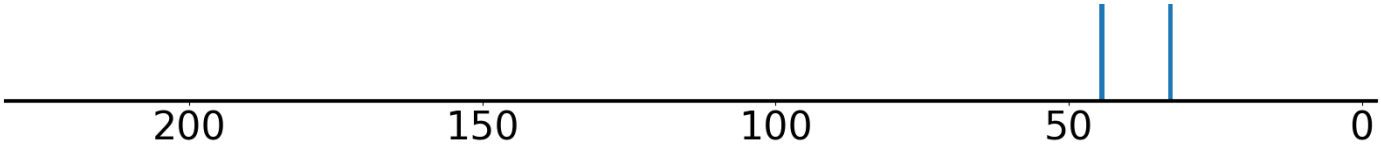
best positives	prob	best negatives	prob
[CHX3](=C)C	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([#6])[#6]	1.0	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#6H1]	0.9999	[#6X2][#6H1][#6X2]	0.0
[#8][#6][#6H2]	0.9914	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0
[OX2H1]	0.9702	[CX2H0](#[CX2H0])[CX2H0]	0.0
[CX4H2][CX4H2]	0.9205	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.8843	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([#6])[O]	0.8636	[CX2H0](#[CX2H0])[CX4H0]	0.0
[#6H1][#6H2]	0.852	CCC=CC#C	0.0
[CH2X4](O)[CX4H2]	0.8464	CC#CCC#C	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([CX4H2])[CX4H1]	0.642	[CX3H1](=[CX3H2])[CX4H2]	0.0799
[#6H2][#6H1][#6H1]=[#6H2]	0.6201	OCC[CH2]	0.544
[CX3H1](=[CX3H2])[CX4H1]	0.6049	[CX4H2][CX3H]	0.5633
[CX3H][CX4H]	0.5127	[CX4H2][CX3]=C	0.6176
O[CX4H][CX4H2]	0.5	[CX4H2]([CX4H2])[CX3H1]	0.6798
[#6H1][#6H1]	0.4361	[CX4H2]([OX2H1])[CX4H2]	0.6854
[#6H3][#6]=[#6X3]	0.4348	[CH2X3](=C)	0.7111
[#6X4H2][#6H1][#8H]	0.4044	[CX3H2]=[CX3H1]	0.8066
[#6X3H1][#6H1][#6H2]	0.3902	[CH2X4](O)[CX4H2][CX4H2]	0.8106
[OH][CX4H]	0.3704	[#6X3H2]	0.8268

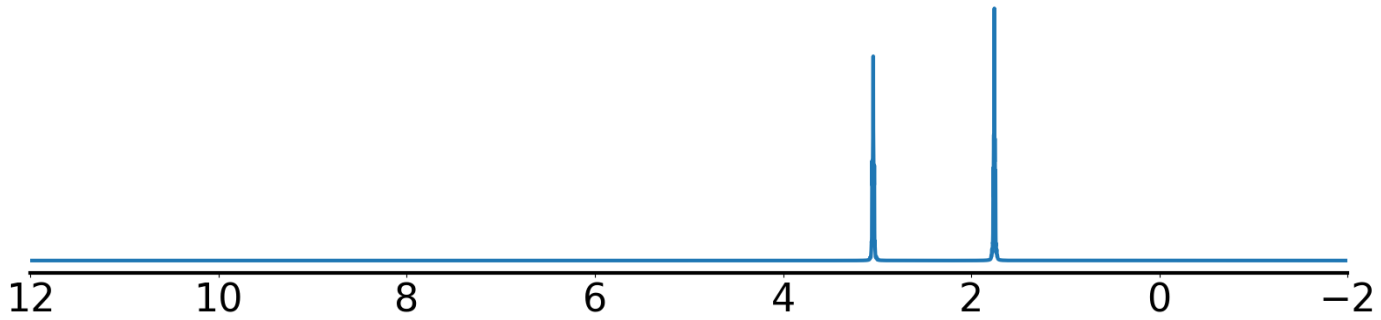
Example 87 true smiles: NCCCCN formula: C4H12N2
Index of correct structure: 0 of 38
True structure loss: 0.005709
True structure:



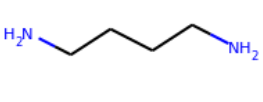
Experimental 13C NMR (solvent: DMSO-d6)



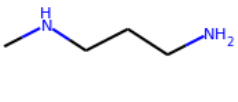
Experimental 1H NMR (solvent: d2o)



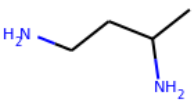
Top predicted structures (loss):



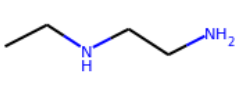
0.005709



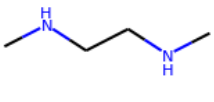
0.038795



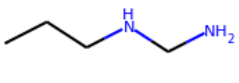
0.05247



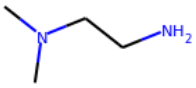
0.056211



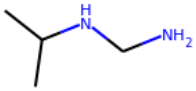
0.064029



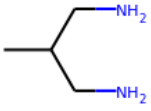
0.065404



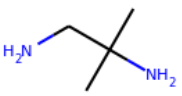
0.067194



0.074361



0.075511



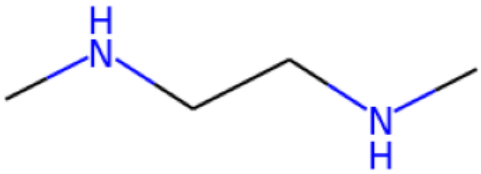
0.078909

Top predicted substructures	prob		
[#7X3H2]	0.9961	[#7][#6H2]	0.9615
[CX4H2]([#6])[#6]	0.9958	[#7X3][#6H2]	0.9447
[CX4H2]([NX3H2])[CX4H2]	0.9806	[CX4H2][CX4H2]	0.8832
[#7H2][#6H2]	0.9686	[CX4H2]([CX4H2])[CX4H2]	0.8122
[#7][#6H2][#6H2]	0.9668	[CX4H2][CX4H2][CX4H2][CX4H2]	0.6061

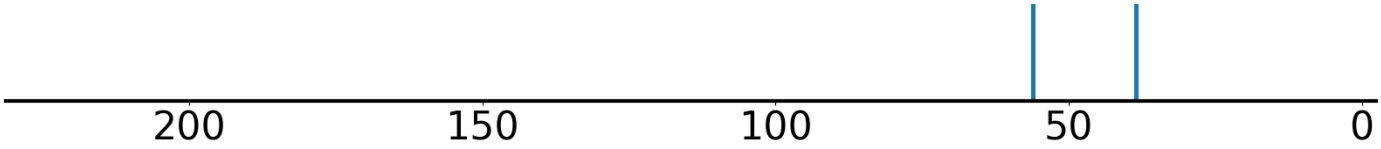
best positives	prob	best negatives	prob
[#7X3H2]	0.9961	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H2]([#6])[#6]	0.9958	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H2]([NX3H2])[CX4H2]	0.9806	C=CC=CC#C	0.0
[#7H2][#6H2]	0.9686	[CX2H0](#[CX2H1])[CX4H0]	0.0
[#7][#6H2][#6H2]	0.9668	CCC#CC#C	0.0
[#7][#6H2]	0.9615	[CX2H0](#[CX2H1])[CX3H1]	0.0
[#7X3][#6H2]	0.9447	C=CCCC#C	0.0
[CX4H2][CX4H2]	0.8832	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.8122	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.6061	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0

worst negatives	prob	worst positives	prob
[#7X3H1]	0.3223	[#7][#6][#6][#6][#6][#7]	0.2069
[#7][#6][#6][#6][#7]	0.2652	[CX4H2][CX4H2][CX4H2][CX4H2]	0.6061
[#6H1]	0.2029	[CX4H2]([CX4H2])[CX4H2]	0.8122
[CX4H2]([NX3H1])[CX4H2]	0.191	[CX4H2][CX4H2]	0.8832
[#6H2][#7][#6H2]	0.1893	[#7X3][#6H2]	0.9447
[#7][#6H2][#6H2][#6H1]	0.1671	[#7][#6H2]	0.9615
[#7H2][#6H1]	0.1173	[#7][#6H2][#6H2]	0.9668
[#6H1][#6H2]	0.1143	[#7H2][#6H2]	0.9686
[CX4H2]([CX4H2])[CX4H1]	0.0796	[CX4H2]([NX3H2])[CX4H2]	0.9806
[#7][#6H2][#6H2][#7]	0.0693	[CX4H2]([#6])[#6]	0.9958

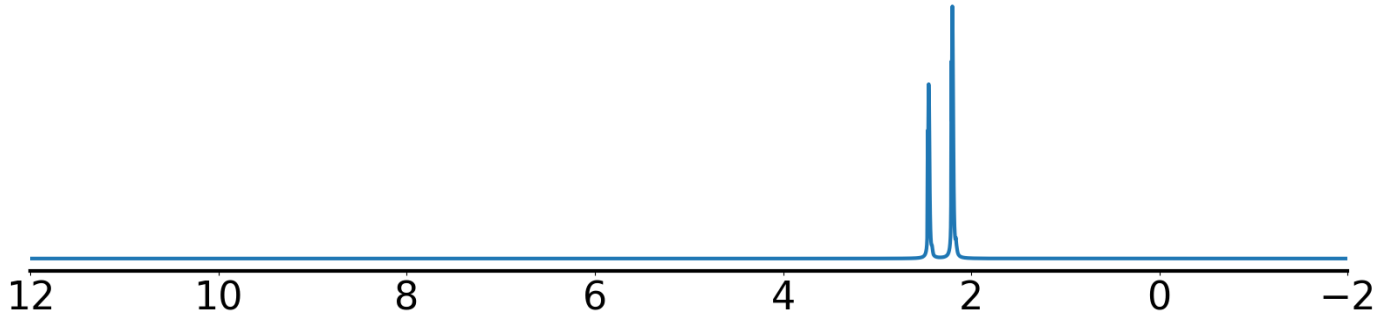
Example 88 true smiles: CNCCNC formula: C4H12N2
Index of correct structure: 2 of 38
True structure loss: 0.034946
True structure:



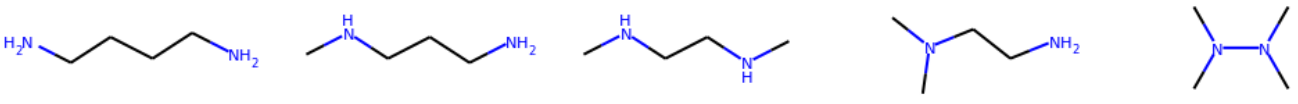
Experimental 13C NMR (solvent: CDCl3)



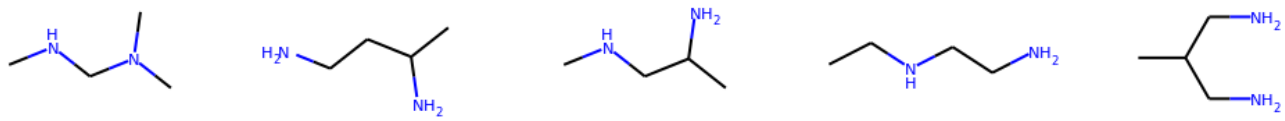
Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.026146 0.026977 0.034946 0.03562 0.047696



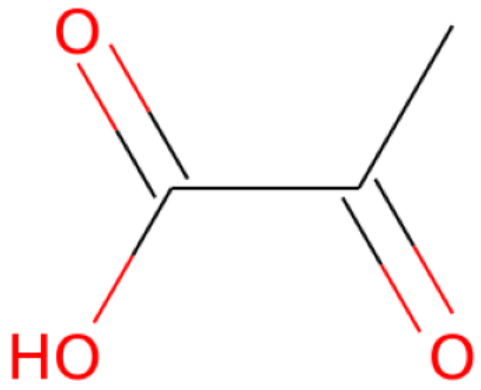
0.058505 0.06904 0.072935 0.075883 0.078749

Top predicted substructures	prob		
[CX4H2]([#6])[#6]	0.9963	[#6H1][#6H2]	0.5691
[#7X3H2]	0.9838	[#7][#6H2][#6H2]	0.5633
[#7][#6H2]	0.6338	[#7H2][#6H1]	0.5595
[#7X3][#6H3]	0.6169	[#6H1]	0.5207
[#6H3][#7]	0.5927	[CX4H2]([NX3H2])[CX4H2]	0.4082

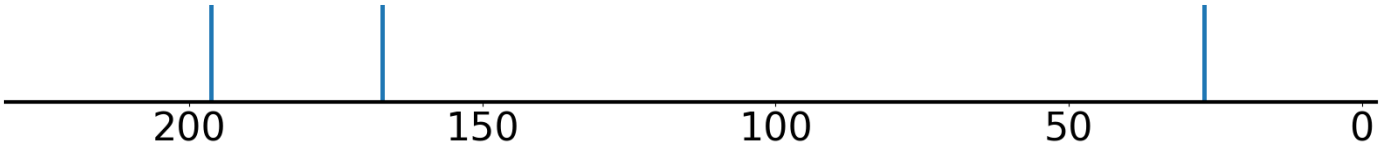
best positives	prob	best negatives	prob
[#7][#6H2]	0.6338	[CX2H0](#[CX2H1])[cX3H0]	0.0
[#7X3][#6H3]	0.6169	C=CC=CC#C	0.0
[#6H3][#7]	0.5927	CCC#CC#C	0.0
[#7][#6H2][#6H2]	0.5633	[#6X2][#6H1][#6X2]	0.0
[CX4H2][CX4H2]	0.3981	CC=CCC#C	0.0
[#7X3H1]	0.3914	[CX2H1]#[CX2H0][CX3H1]=[CX3H0]	0.0
[#7X3][#6H2]	0.3854	[CX3H0](=[CX3H1])([OX2H0])[CX2H0]	0.0
[CX4H3][NX3H1]	0.3205	CC=CC#CC	0.0
[#6H3][#7][#6H2]	0.2839	[CX2H0](#[CX2H1])[CX3H1]	0.0
[#7][#6][#6][#7]	0.2628	[OX1H0]=[CX3H0][CX2H0]#[CX2H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([#6])[#6]	0.9963	[CX4H2]([NX3H1])[CX4H2]	0.0396
[#7X3H2]	0.9838	[#7][#6H2][#6H2][#7]	0.0571
[#6H1][#6H2]	0.5691	[CX4H3]	0.1436
[#7H2][#6H1]	0.5595	[#7][#6][#6][#7]	0.2628
[#6H1]	0.5207	[#6H3][#7][#6H2]	0.2839
[CX4H2]([NX3H2])[CX4H2]	0.4082	[CX4H3][NX3H1]	0.3205
[#6H1]([#6H2])[#6H2]	0.3634	[#7X3][#6H2]	0.3854
[CX4H2]([CH])[CH]	0.2229	[#7X3H1]	0.3914
[#7X3H0]	0.2172	[CX4H2][CX4H2]	0.3981
[#7][#6][#6][#6][#6][#7]	0.208	[#7][#6H2][#6H2]	0.5633

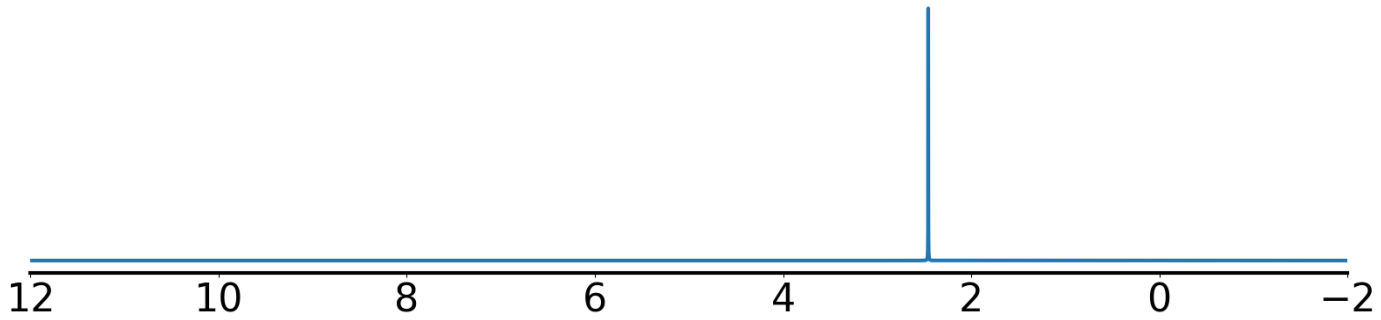
Example 89 true smiles: CC(=O)C(=O)O formula: C3H4O3
Index of correct structure: 0 of 31
True structure loss: 0.01426
True structure:



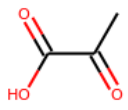
Experimental 13C NMR (solvent: CDCl3)



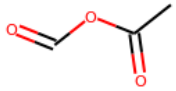
Experimental 1H NMR (solvent: D2O)



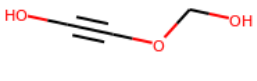
Top predicted structures (loss):



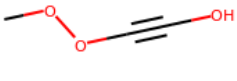
0.01426



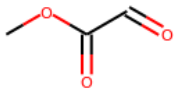
0.05062



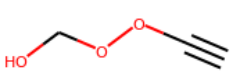
0.083965



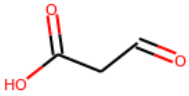
0.085776



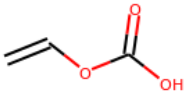
0.096801



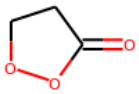
0.119405



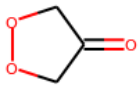
0.140115



0.140649



0.141668



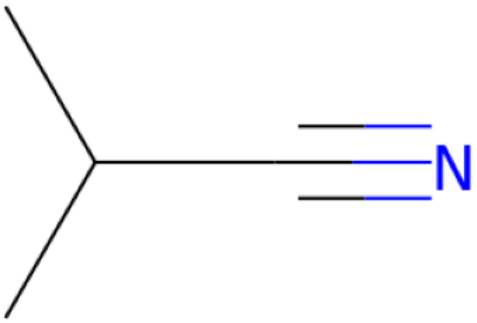
0.142443

Top predicted substructures	prob		
[CX3](=[OX1])C	0.9961	[CX4H3][#6]	0.9859
[CX4H3]	0.9941	[#6H3][#6H0]	0.9799
[CX4H3][CX3H0]	0.9918	[#6H3][#6][#6]	0.9725
[OX1H0]=[CX3H0][CX4H3]	0.991	[#6X3][#6X3]	0.9517
[CX4H3][CX3]	0.9888	[#8]=[#6][#8]	0.8887

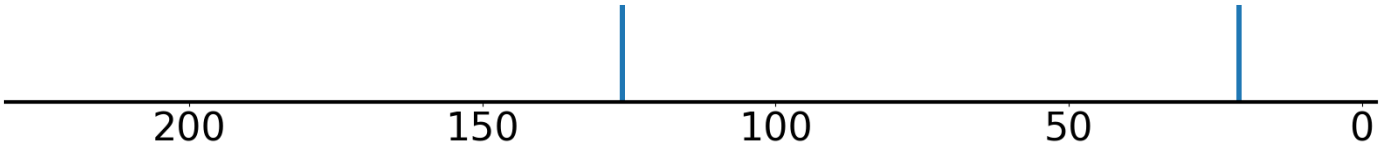
best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.9961	[OX2H0][CX4H2][CX4H1]([CX4H1])[CX4H1]	0.0
[CX4H3]	0.9941	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3][CX3H0]	0.9918	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[OX1H0]=[CX3H0][CX4H3]	0.991	CCC#CC#C	0.0
[CX4H3][CX3]	0.9888	[CX3H1](=[CX3H2])[CX2H0]	0.0
[CX4H3][#6]	0.9859	[CX4H3][CX2H0]	0.0
[#6H3][#6H0]	0.9799	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[#6H3][#6][#6]	0.9725	[CX4H0]([NX3H1])([CX4H2])([CX4H2])[CX4H1]	0.0
[#6X3][#6X3]	0.9517	CC=CC#CC	0.0
[#8]=[#6][#8]	0.8887	[CX2H0](#[CX2H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
O=[#6][#6][#6X3]	0.3758	[CH3]CC[OH]	0.0046
[CX4H2][CX3]=O	0.3067	[CX3H0](=[OX1H0])([OX2H1])[CX3H0]	0.5162
[#6X3][#6][#6][#6H3]	0.2158	[#8][#6][#6]=[#8]	0.5199
[CX4H2]CC=O	0.1623	[CX3H0](=[OX1H0])([CX4H3])[CX3H0]	0.5874
[#8]=[#6][#6][#6][#6]=[#8]	0.1588	[CX3](=O)[OX2H1]	0.6505
[#8]=[#6][#6]=[#6][#6]=[#8]	0.1415	[CX4H3][CX3H0][CX3]=O	0.684
[#8][#6][#6]=[#6][#6]=[#8]	0.1372	[OX1H0]=[CX3H0][CX3H0][CX4H3]	0.7392
[#8][#6][#6][#6X3]	0.1361	[OX2H1]	0.7812
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.1198	[CX3](=[OX1])O	0.7955
[#8]=[#6X3][#6X3][#6X3][#6H3]	0.1136	[#8]=[#6][#6]=[#8]	0.8025

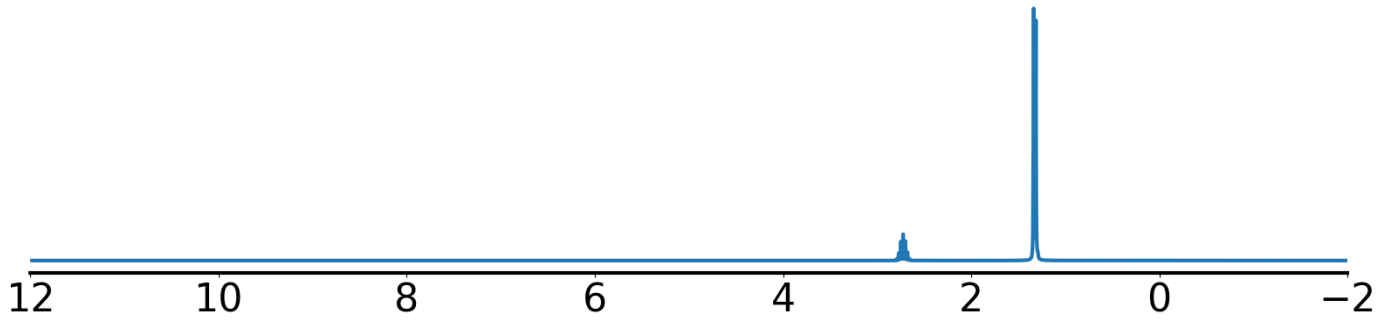
Example 90 true smiles: CC(C)C#N formula: C4H7N
Index of correct structure: 0 of 29
True structure loss: 0.016232
True structure:



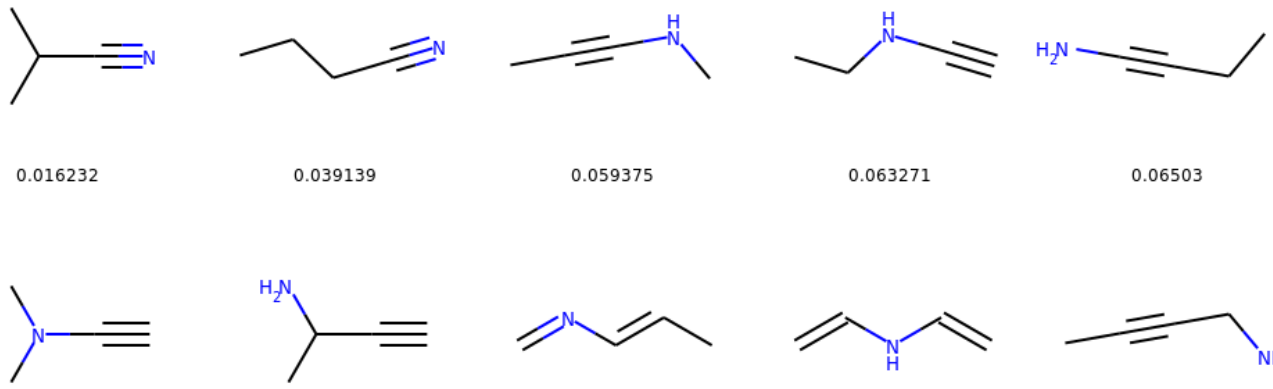
Experimental 13C NMR (solvent: CDCl3)



Experimental 1H NMR (solvent: CDCl3)



Top predicted structures (loss):



0.016232 0.039139 0.059375 0.063271 0.06503

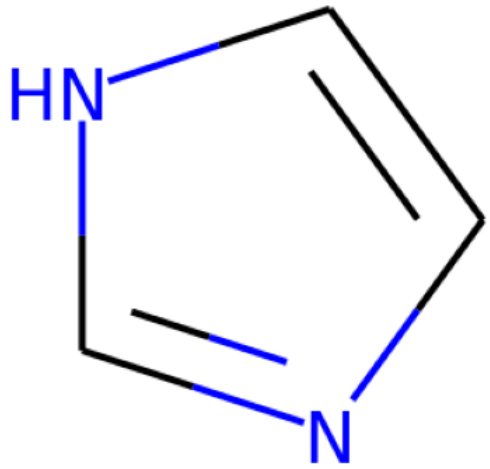
0.067799 0.070512 0.075706 0.076914 0.081474

Top predicted substructures	prob		
[#6H3][#6][#6]	0.9943	[CX4H3][CX4H1]	0.5524
[CX4H3]	0.9938	[CX4H2]([#6])[#6]	0.5225
[CX4H3][#6]	0.9934	[#6H3][#6H0]	0.3286
[#6]#[#7]	0.6312	[#7X3H1]	0.266
[#6H1]	0.6278	[#7X3H2]	0.2599

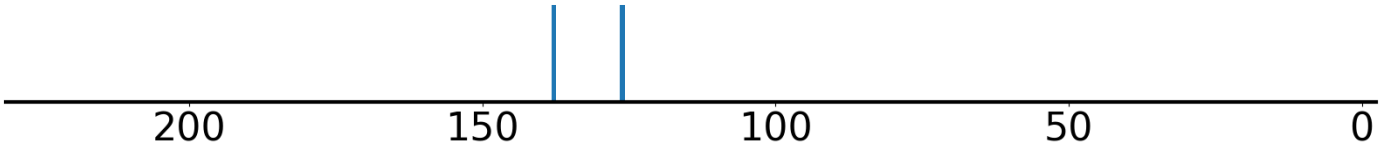
best positives	prob	best negatives	prob
[#6H3][#6][#6]	0.9943	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3]	0.9938	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[CX4H3][#6]	0.9934	[CX3H2]=[CX3H0][OX2H0][CX4H2]	0.0
[#6]#[#7]	0.6312	[OX2H0][CX4H2][CX3H0][OX2H0]	0.0
[#6H1]	0.6278	[CX3H0](=[CX3H2])([OX2H0])[CX3H0]	0.0
[CX4H3][CX4H1]	0.5524	[OX2H0]1[CX4H2][CX4H1][CX3H0]=[CX3H1]1	0.0
[CHX4]([CH3X4])[CH3X4]	0.2266	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6X2][#6X4H1]	0.1628	[OX2H0r6][CX4H2r6][OX2H0r6]	0.0
[CX2H0](#[NX1H0])[CX4H1]	0.1586	[CX3H2]=[CX3H0][CX4H2][OX2H0]	0.0
[#7]#[#6H0][#6H1]	0.1467	[CX4H3][OX2H0][CX3H1]=[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]([#6])[#6]	0.5225	[#7]#[#6H0][#6H1]	0.1467
[#6H3][#6H0]	0.3286	[CX2H0](#[NX1H0])[CX4H1]	0.1586
[#7X3H1]	0.266	[#6X2][#6X4H1]	0.1628
[#7X3H2]	0.2599	[CHX4]([CH3X4])[CH3X4]	0.2266
[cH]	0.2112	[CX4H3][CX4H1]	0.5524
[#6H3][#6H0][#6H1][#7]	0.2108	[#6H1]	0.6278
[#6H1][#6H1]	0.1935	[#6]#[#7]	0.6312
[#6H3][#6][#6][#6H3]	0.1894	[CX4H3][#6]	0.9934
[#6H2][#6X2]	0.1679	[CX4H3]	0.9938
[CX4H3][CX4H0][CX4H3]	0.165	[#6H3][#6][#6]	0.9943

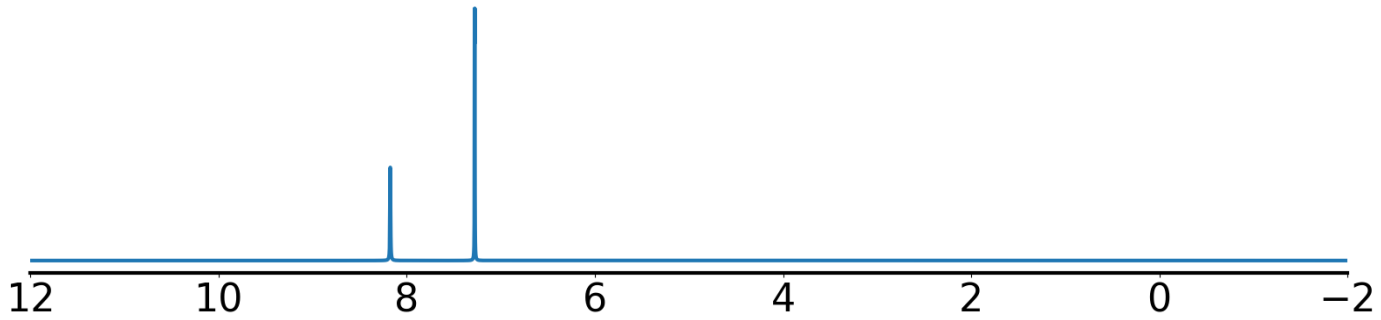
Example 91 true smiles: c1c[nH]cn1 formula: C3H4N2
Index of correct structure: 0 of 26
True structure loss: 0.026969
True structure:



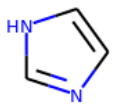
Experimental 13C NMR (solvent: CDCl3)



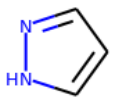
Experimental 1H NMR (solvent: D2O)



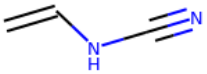
Top predicted structures (loss):



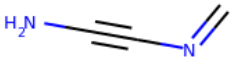
0.026969



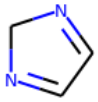
0.033607



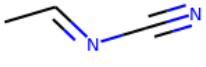
0.062508



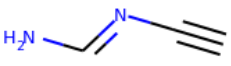
0.068495



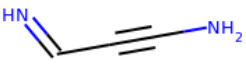
0.082974



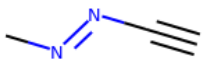
0.094676



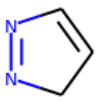
0.095782



0.100306



0.100809



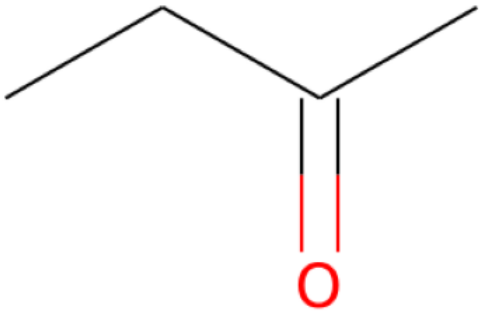
0.10102

Top predicted substructures	prob		
[#6H1]	0.9973	[#7][#6][#6][#6X3]	0.8934
[#6X3][#6X3]	0.9912	[#6H1][#7][#6H1]	0.8373
[cH]	0.9798	[cH][cH]	0.8314
[#7][#6][#6X3]	0.924	[#7X3H2]	0.7951
[#6X3H1][#6X3H0]	0.9195	[#6X3][#7][#6X3]	0.6831

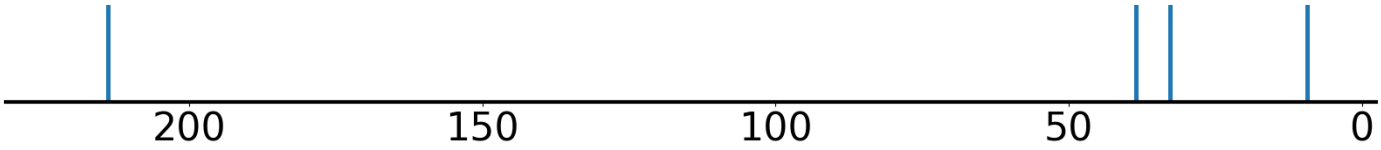
best positives	prob	best negatives	prob
[#6H1]	0.9973	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#6X3]	0.9912	[OX2H1][CX4H1]1[CX4H1][CX4H2][CX4H1]1	0.0
[cH]	0.9798	[CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]	0.0
[#7][#6][#6X3]	0.924	[OX1H0]=[CX3H0]1[CX4H1][CX4H1][CX4H2]1	0.0
[#6H1][#7][#6H1]	0.8373	[OX2H0][CX4H1][CX4H1]([CX4H2][CX4H1])[CX4H1]	0.0
[cH][cH]	0.8314	[CX4H1]([OX2H1])([CX4H2])[CX2H0]	0.0
[#6X3][#7][#6X3]	0.6831	[#8][#6H1][#6H2][#6H1]=[#8]	0.0
[#6H1][#6H1]	0.6524	[OX2H0]1[CX4H2][CX4H1][CX4H1]1	0.0
[#6X3][#7X3][#6X3]	0.595	[CX4H1]([OX2H0])([CX4H2])[CX2H0]	0.0
[#7][#6][#6][#7]	0.5501	[CX4H0]([OX2H0])([CX4H3])([CX4H2])[CX3H1]	0.0

worst negatives	prob	worst positives	prob
[#6X3H1][#6X3H0]	0.9195	[cX3H1]([nX3H1])[cX3H1]	0.1051
[#7][#6][#6][#6X3]	0.8934	[cX3H1]([nX2H0])[cX3H1]	0.2178
[#7X3H2]	0.7951	[#7H][#6X3H1]	0.3892
[#7][#6X3H0][#6X3H1]	0.6115	[#6H1r5][#7]	0.4605
[#6X3][#6X3][#6X3][#6X3]	0.599	[#6]1[#6][#7][#6][#7]1	0.4696
[#7][#6H0][#6H1]	0.5889	[#7X3H1]	0.4857
[cX3H1]([nX2H0])[cX3H0]	0.4794	[#7][#6H1][#7]	0.4911
[#7H2][#6H0]	0.373	[#7][#6][#7]	0.5165
[#6X3H1][#6X3H1][#6X3H0][#6X3H1]	0.3574	[#7][#6][#6][#7]	0.5501
[cX3H1]([cX3H1])[cX3H0]	0.3482	[#6X3][#7X3][#6X3]	0.595

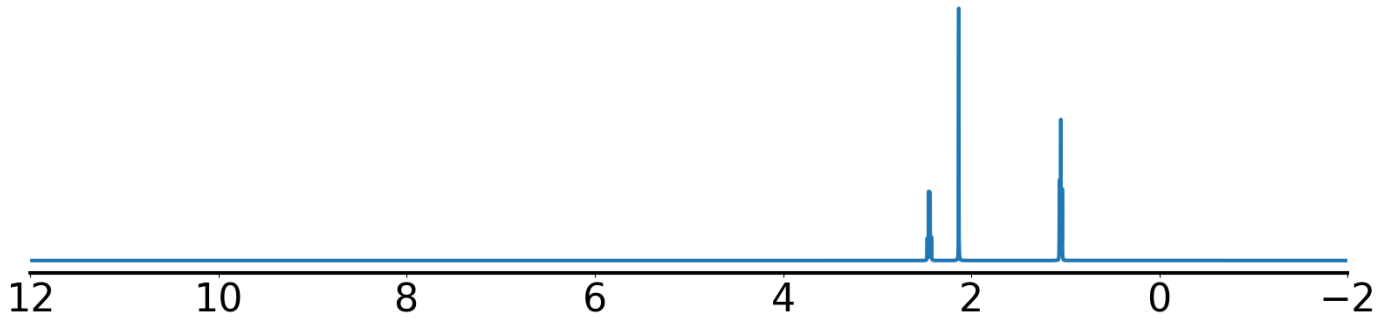
Example 92 true smiles: CCC(C)=O formula: C4H8O
Index of correct structure: 0 of 22
True structure loss: 0.006633
True structure:



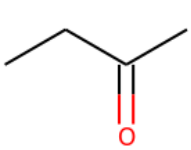
Experimental 13C NMR (solvent: CDCl3)



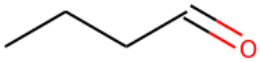
Experimental 1H NMR (solvent: CDCl3)



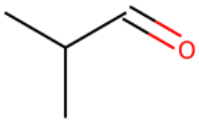
Top predicted structures (loss):



0.006633

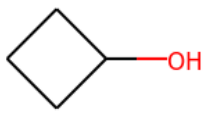


0.092054

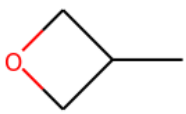


0.144201

0.209105

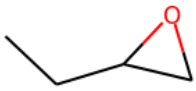


0.209332



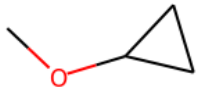
0.218539

0.23338



0.256734

0.268562



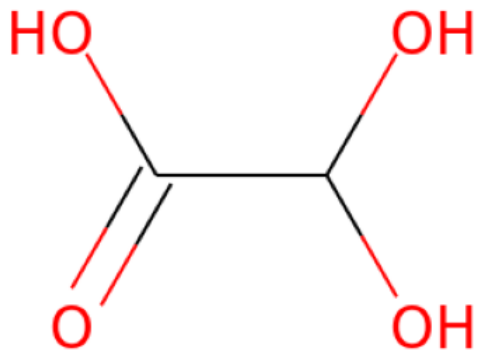
0.269362

Top predicted substructures	prob		
[CX4H3]	0.9999	[CX4H2]([CX4H3])[CX3H0]	0.9972
[CX3](=[OX1])C	0.9998	[OX1H0]=[CX3H0]([#6])[CX4H2]	0.997
[CX4H3][#6]	0.9997	[CX4H2]([#6])[#6]	0.9969
[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9996	[CX4H3][CX4H2]	0.9949
[#6H3][#6][#6]	0.9995	[CX4H3][CX3]	0.9879

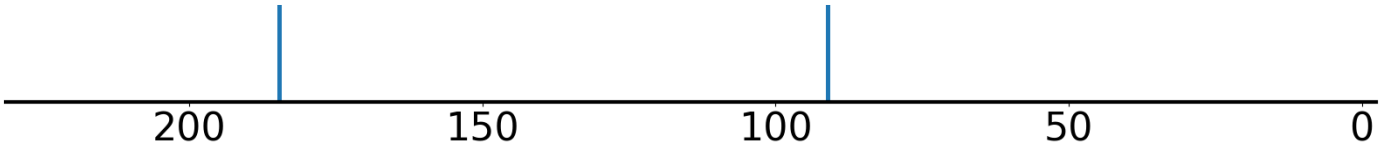
best positives	prob	best negatives	prob
[CX4H3]	0.9999	CCC=CC#C	0.0
[CX3](=[OX1])C	0.9998	[CX2H0](#[CX2H1])[CX2H0]	0.0
[CX4H3][#6]	0.9997	C=CC=CC#C	0.0
[OX1H0]=[CX3H0][CX4H2][CX4H3]	0.9996	C=CCCC#C	0.0
[#6H3][#6][#6]	0.9995	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX4H2]([CX4H3])[CX3H0]	0.9972	[CX3H1](=[CX3H2])[CX2H0]	0.0
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.997	[CX2H0](#[CX2H1])[CX3H1]	0.0
[CX4H2]([#6])[#6]	0.9969	CCC#CC#C	0.0
[CX4H3][CX4H2]	0.9949	CCC#CC=C	0.0
[CX4H3][CX3]	0.9879	[CX2H0](#[CX2H1])[CX3H0]	0.0

worst negatives	prob	worst positives	prob
[CX4H2]CC=O	0.522	[#6H3][#6][#6][#6H3]	0.0783
CCCCCC	0.2344	[#6H3][#6X3H0][#6H2]	0.7131
[#8][#6][#6H2]	0.1886	[#6H3][#6][#6X3]	0.9038
[#6X3][#6][#6][#6H3]	0.1871	[CX3H0](=[OX1H0])([CX4H3])[CX4H2]	0.9154
[CX4H2]([CX4H2])[CX3H0]	0.1862	[#6H3][#6H0]	0.9377
O=[CX3H0][CX4H2][CX4H2]	0.1615	[CX4H3][CX3H0]	0.9668
[CX4H2][CX4H2]	0.1608	[OX1H0]=[CX3H0][CX4H3]	0.975
[#6H2][#6X3H0][#6H2]	0.144	[CX4H2][CX3]=O	0.9784
[#8]=[#6H0][#6H1]	0.0776	[CX4H3][CX3]	0.9879
[CX3H0](=[OX1H0])([CX4H2])[CX4H2]	0.0757	[CX4H3][CX4H2]	0.9949

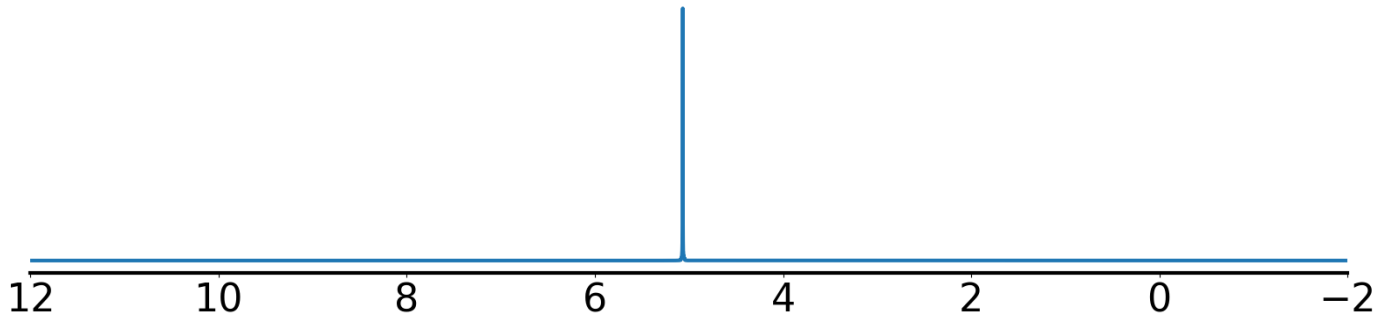
Example 93 true smiles: O=C(O)C(O)O formula: C2H4O4
Index of correct structure: 2 of 20
True structure loss: 0.032534
True structure:



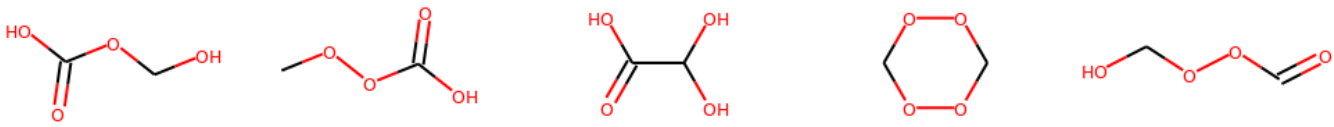
Experimental 13C NMR (solvent: D2O)



Experimental 1H NMR (solvent: D2O)



Top predicted structures (loss):



0.021618 0.027758 0.032534 0.033064 0.035346

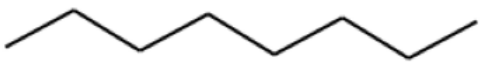
Top predicted substructures	prob		
[CX3](=[OX1])C	0.987	[#8]=[#6][#6H2][#8]	0.7207
[OX2H1]	0.9604	[CX4H2][CX3]=O	0.6389
[#8][#6][#6]=[#8]	0.833	[CX3](=O)[OX2H1]	0.554
[#8]=[#6][#8]	0.7686	[CX3](=[OX1])O	0.5335
[#8][#6][#6][#8]	0.723	[CX4H2][OX2H0][CX4H2]	0.4869

best positives	prob	best negatives	prob
[CX3](=[OX1])C	0.987	[#6X2][#6H1][#6X2]	0.0
[OX2H1]	0.9604	CCC#CC#C	0.0
[#8][#6][#6]=[#8]	0.833	[#7][#6][#6]#[#7]	0.0
[#8]=[#6][#8]	0.7686	CC=CCC#C	0.0
[#8][#6][#6][#8]	0.723	[OX2H0]1[CX4H2][CX4H2][CX4H1][CX4H1]1	0.0

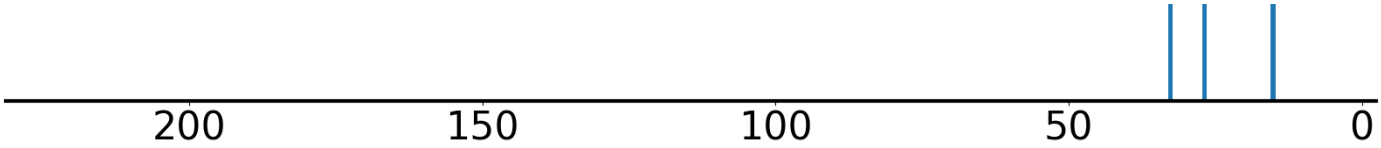
[CX3](=O)[OX2H1]	0.554	[CX3H0](=[CX3H1])([CX4H1])[CX2H0]	0.0
[CX3](=[OX1])O	0.5335	C=CC=CC#C	0.0
[#8]=[#6H0][#6H1]	0.4743	[CX3H1](=[CX3H1])[CX2H0]	0.0
[#8][#6H0][#6H1]	0.439	[CX4H1]([CX4H2])([CX4H1])[CX2H0]	0.0
[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.1852	CC=CC#CC	0.0

worst negatives	prob	worst positives	prob
[#8]=[#6][#6H2][#8]	0.7207	[#8H][#6X4H1][#6X3H0]	0.0427
[CX4H2][CX3]=O	0.6389	[OH][CX4H]	0.0469
[CX4H2][OX2H0][CX4H2]	0.4869	O=[CX3][CX4H]	0.0563
[#8][#6][#6][#6X3]	0.4487	[#6H1]	0.0906
[OX1H0]=[CX3H0]([#6])[CX4H2]	0.3157	[CX4H](O)CO	0.1059
[OX2H0][CX4H2][#6H0]	0.3001	[CX4H]O	0.1062
[CX3H0](=[OX1H0])([OX2H1])[CX4H2]	0.2852	[CX3H0](=[OX1H0])([OX2H1])[CX4H1]	0.1852
[CX4H2]([OX2H0])[OX2H0]	0.2841	[#8][#6H0][#6H1]	0.439
[CX4H2]([#6])[O]	0.2507	[#8]=[#6H0][#6H1]	0.4743
[CX4H3]	0.2375	[CX3](=[OX1])O	0.5335

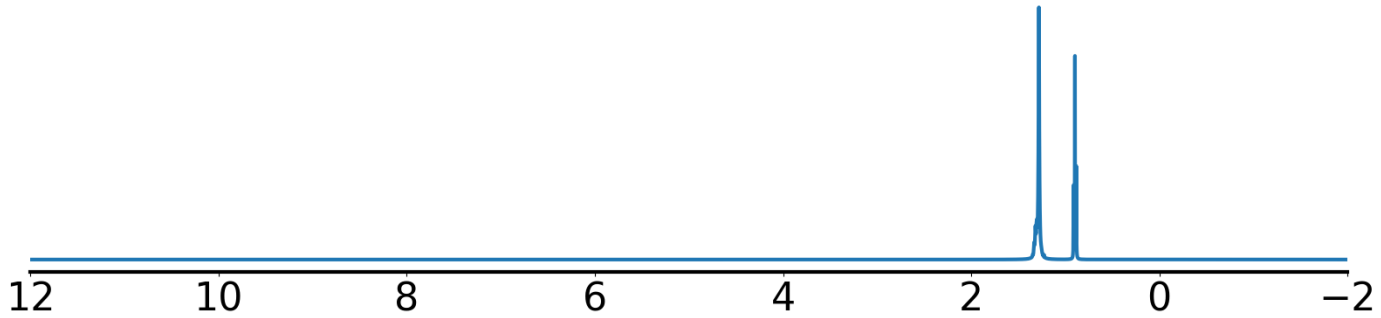
Example 94 true smiles: CCCCCCCC formula: C8H18
Index of correct structure: 0 of 18
True structure loss: 0.007935
True structure:



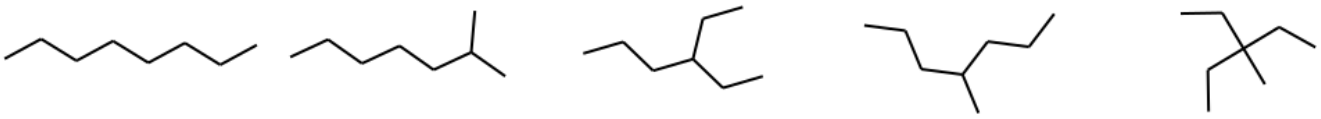
Experimental 13C NMR (solvent: CDCl3)



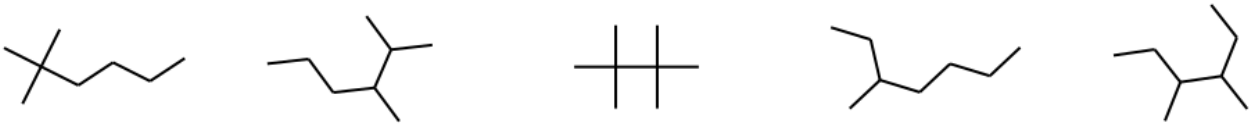
Experimental 1H NMR (solvent: CDCL3)



Top predicted structures (loss):



0.007935 0.018618 0.0269 0.02816 0.028807



0.029564 0.030285 0.031262 0.031736 0.032579

Top predicted substructures	prob		
[CX4H3]	1.0	[CX4H2]([CX4H3])[CX4H2]	0.7286
[CX4H3][#6]	0.9999	[#6H1]	0.5866
[#6H3][#6][#6]	0.9999	[CHX4]([CH3X4])[CH3X4]	0.5649
[CX4H3][CX4H2]	0.9938	[CX4H2]([CX4H2])[CX4H2]	0.5328
[CX4H2]([#6])[#6]	0.9644	CCCCCC	0.4769

best positives	prob	best negatives	prob

[CX4H3]	1.0	[CX2H0](#[CX2H1])[cX3H0]	0.0
[CX4H3][#6]	0.9999	CCC=CC#C	0.0
[#6H3][#6][#6]	0.9999	CC=CC#CC	0.0
[CX4H3][CX4H2]	0.9938	CC=CCC#C	0.0
[CX4H2]([#6])[#6]	0.9644	[CX2H0](#[CX2H1])[CX3H0]	0.0
[CX4H2]([CX4H3])[CX4H2]	0.7286	[CX2H0](#[CX2H1])[CX4H2]	0.0
[CX4H2]([CX4H2])[CX4H2]	0.5328	[CX2H0](#[CX2H1])[CX3H1]	0.0
CCCCCC	0.4769	[#7][#6]=[#6][#6]#[#7]	0.0
[CX4H2][CX4H2]	0.4536	[#6X2][#6H1][#6X2]	0.0
[CX4H2][CX4H2][CX4H2][CX4H2]	0.3337	[CX4H1]([OX2H0])([CX4H1])[CX2H0]	0.0

worst negatives	prob	worst positives	prob
[#6H1]	0.5866	[CX4H2][CX4H2][CX4H2][CX4H2]	0.3337
[CHX4]([CH3X4])[CH3X4]	0.5649	[CX4H2][CX4H2]	0.4536
[CX4H3][CX4H1]	0.3963	CCCCCC	0.4769
[#6H3][#6][#6][#6H3]	0.2745	[CX4H2]([CX4H2])[CX4H2]	0.5328
[#6H1][#6H2]	0.1841	[CX4H2]([CX4H3])[CX4H2]	0.7286
[CX4H3][CX4]O	0.1667	[CX4H2]([#6])[#6]	0.9644
[#6H3][#6H0]	0.1047	[CX4H3][CX4H2]	0.9938
[#6H1][#6H1]	0.0712	[#6H3][#6][#6]	0.9999
[#6H2][#6H1r3]	0.0709	[CX4H3][#6]	0.9999
[CX4H2]([CX4H3])[CX4H1]	0.0703	[CX4H3]	1.0
