Electronic Supplementary Material (ESI) for Chemical Science.
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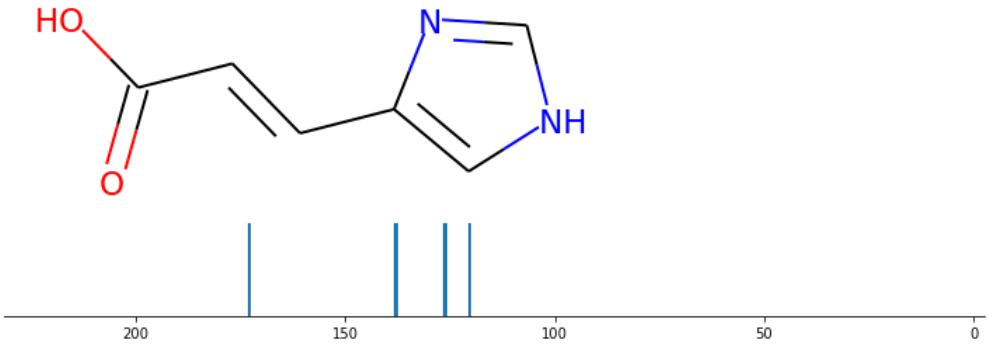
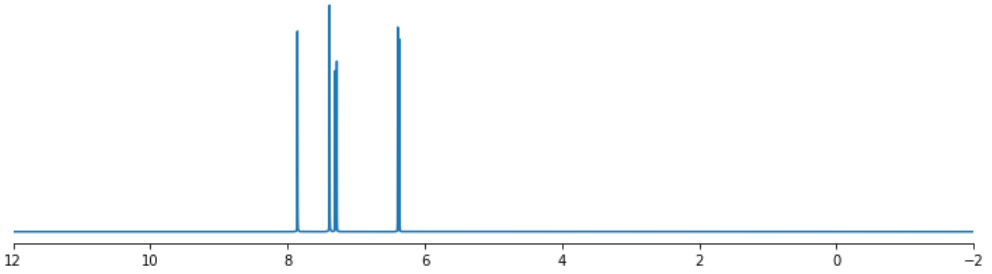
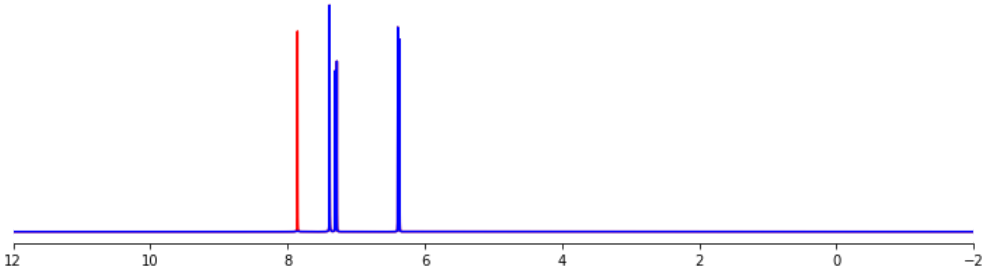
In [374…

True structure: O=C(O)C=Cc1c[nH]cn1

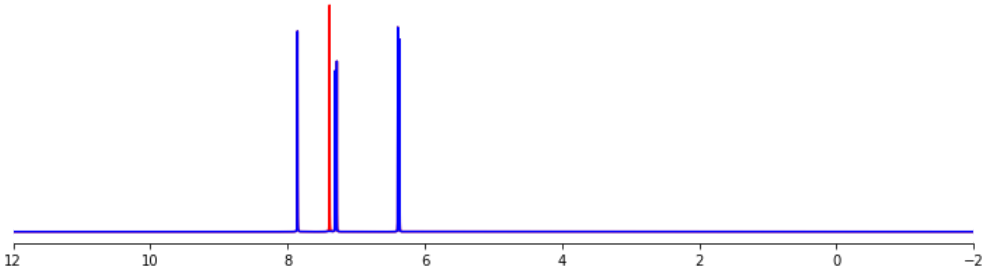






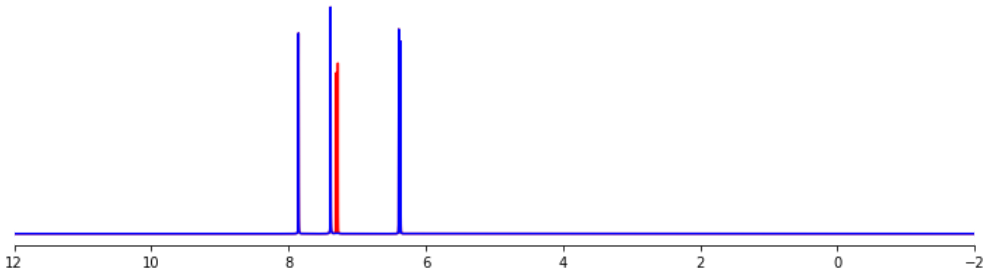
Top predicted substructures for the masked region(red):

0.4197 [#6X3H2]
0.271 [#8]=[#6H0][#6H1]
0.2503 [#6H1r5][#7]
0.2108 [#6X3H1][#7X3H0]
0.2042 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1954 [#7][#6H1][#7]
0.1879 O=[#6][#6]=[#6X3]
0.1838 [OX1H0]=[cX3H0][cX3H1]

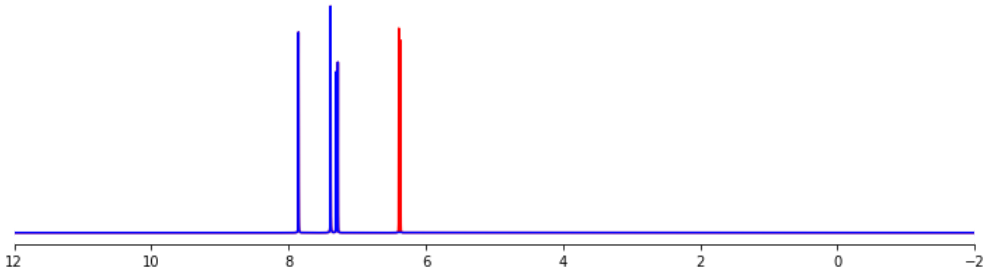


Top predicted substructures for the masked region(red):

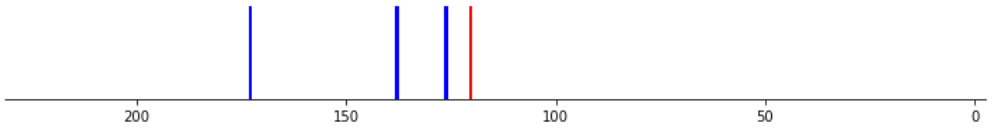
0.2094 [#8]=[#6H0][#6H1]
0.206 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1845 [#6X3][#6X3][#6X3][#6X3]
0.1844 [#6X3H2]
0.1718 O=[#6][#6]=[#6X3]
0.1712 [OX1H0]=[cX3H0][cX3H1]
0.1588 [CX3H2]=[CX3H0]([#6])[#6]
0.1586 [cX3H1]([nX2H0])[cX3H0]



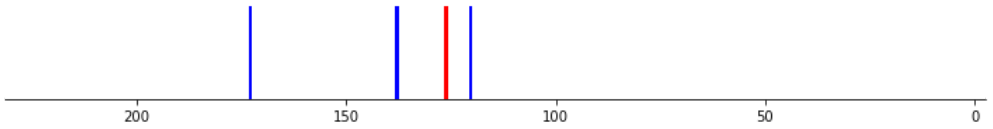
Top predicted substructures for the masked region(red):
0.3003 [#8]=[#6H0][#6H1]
0.2389 [#6X3H2]
0.227 [OX1H0]=[cX3H0][cX3H1]
0.1526 [#6H1r5][#7]
0.1392 [CHX3]=[CHX3]
0.1278 [#7][#6][#6][#6X3]
0.1258 [cX3H1]([nX2H0])[cX3H0]
0.1237 [CX3](=[OX1])O



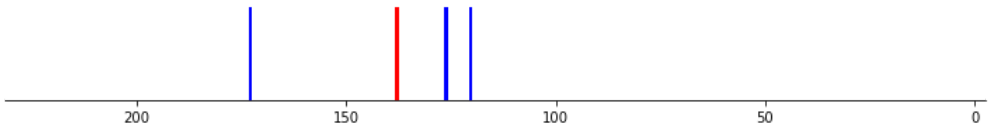
Top predicted substructures for the masked region(red):
0.3658 [#8]=[#6H0][#6H1]
0.3381 [#6X3H2]
0.2658 [cX3H1]([cX3H1])[cX3H0]
0.2354 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.227 [OX1H0]=[cX3H0][cX3H1]
0.2047 [#6X3H1][#7X3H0]
0.1991 [#6H1][#6H1]
0.1938 O=[#6][#6]=[#6X3]



Top predicted substructures for the masked region(red):
0.2322 [#8]=[#6H0][#6H1]
0.2256 [OX1H0]=[cX3H0][cX3H1]
0.2224 [#7][#6][#6][#6X3]
0.1745 [#6X3H1][#7X3H0]
0.1734 [#6X3][#6X3][#6X3][#6X3]
0.1652 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1507 [CX3H2]=[CX3H0]([#6])[#6]
0.1494 [#6H1r5][#7]

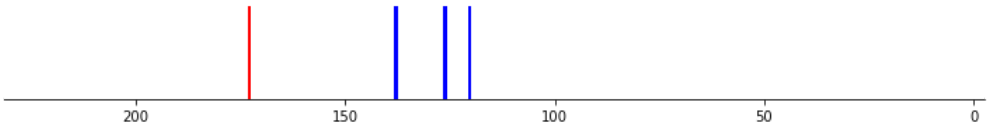


Top predicted substructures for the masked region(red):
0.2585 [#8]=[#6H0][#6H1]
0.1998 [#6H1r5][#7]
0.1961 [#7][#6][#6][#6X3]
0.196 [OX1H0]=[cX3H0][cX3H1]
0.1592 [#6X3][#6X3][#6X3][#6X3]
0.1559 [#6X3H2]
0.1521 [CX3H2]=[CX3H0]([#6])[#6]
0.146 [#6X3][#6X3][#6X3]=[#6X3]



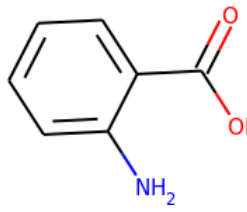
Top predicted substructures for the masked region(red):
0.3315 [#8]=[#6H0][#6H1]
0.2285 [OX1H0]=[cX3H0][cX3H1]
0.202 [#7][#6][#6][#6X3]

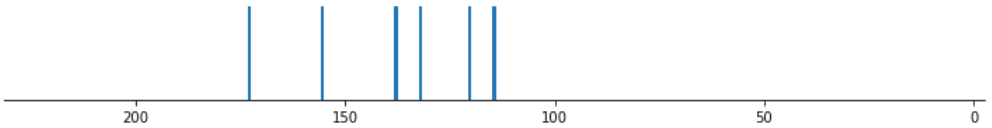
0.192 [CX3H2]=[CX3H0]([#6])[#6]
0.1686 [cX3H1]([nX2H0])[cX3H0]
0.157 [#6X3][#6X3][#6X3][#6X3]
0.1501 [#6X3][#6X3][#6X3]=[#6X3]
0.1496 [CX3](=[OX1])O

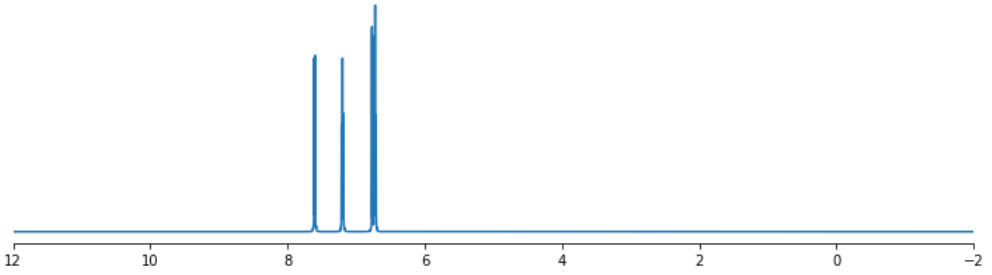


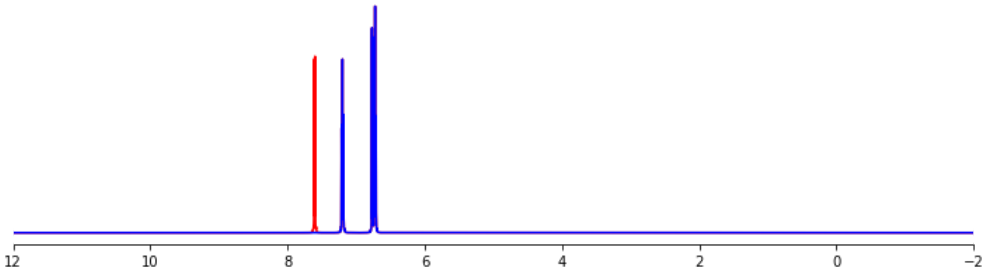
Top predicted substructures for the masked region(red):
0.7703 O=[#6][#6][#6X3]
0.6488 [#8]=[#6H0][#6H1]
0.312 [#6X3H2]
0.2999 [#8]=[#6][#8]
0.2907 [OX1H0]=[cX3H0][cX3H1]
0.2853 O=[#6][#6]=[#6X3]
0.2582 O=C[CX3H]
0.2416 [CX3H2]=[CX3H0]([#6])[#6]

True structure: Nc1ccccc1C(=O)O

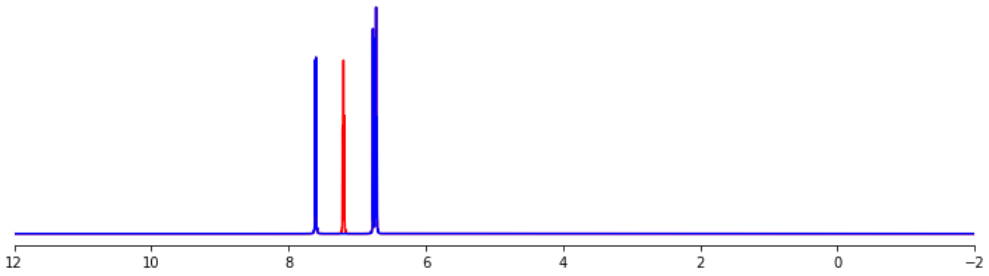




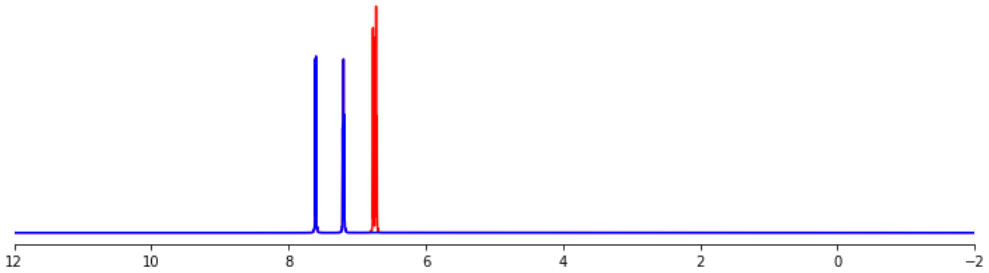




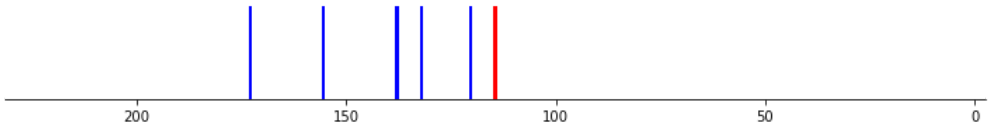
Top predicted substructures for the masked region(red):
0.2661 [OX2H][cX3]:[c]
0.2073 [#6]1[#6][#6][#6][#6][#7]1
0.2053 [#8][#6H1][#6H1]
0.19 [#7][#6][#6X3]
0.1862 [cX3H1]([oX2H0])[cX3H1]
0.1799 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1467 [#6H1][#6H1]
0.1401 [#8]=[#6][#6H1][#6H1]



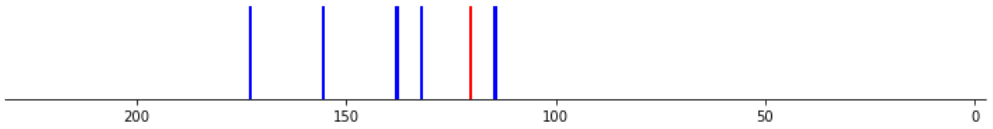
Top predicted substructures for the masked region(red):
0.3665 [OX2H][cX3]:[c]
0.247 [#7][#6][#6X3]
0.238 [cH]cO
0.2178 [#6]1[#6][#6][#6][#6][#7]1
0.1429 [OX1H0]=[cX3H0][cX3H1]
0.1379 [#6X3][#7][#6X3]
0.1239 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.12 [cX3H1]([oX2H0])[cX3H1]



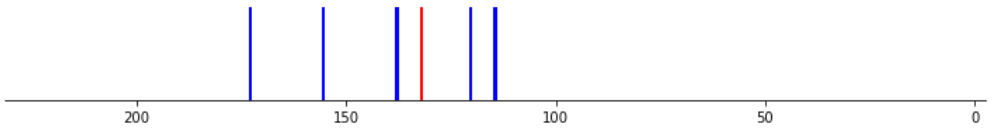
Top predicted substructures for the masked region(red):
0.4477 [#7][#6][#6X3]
0.3883 [OX2H][cX3]:[c]
0.2806 [cH]cO
0.197 [#7][#6][#6][#6X3]
0.1324 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1019 O=[#6][#6]=[#6X3]
0.092 [#6H1][#6H1]
0.0904 o[cH]



Top predicted substructures for the masked region(red):
0.2875 [OX2H][cX3]:[c]
0.1815 [cH]cO
0.1694 [#7][#6][#6][#6X3]
0.1684 [cX3H1]([oX2H0])[cX3H1]
0.1684 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1583 [#7][#6][#6X3]
0.1499 o[cH]
0.1428 [#6X3][#7][#6X3]

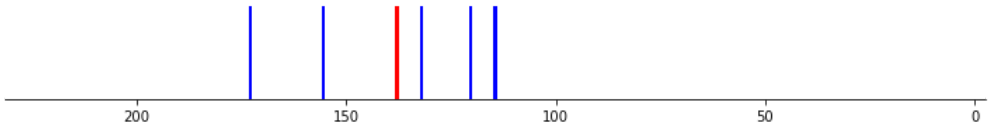


Top predicted substructures for the masked region(red):
0.312 [OX2H][cX3]:[c]
0.176 [#7][#6][#6][#6X3]
0.1739 [#7][#6][#6X3]
0.1427 [cH]cO
0.1191 [#7X3H2]
0.1113 [#7H][#6X3H1]
0.1059 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1009 [#6X3][#7][#6X3]

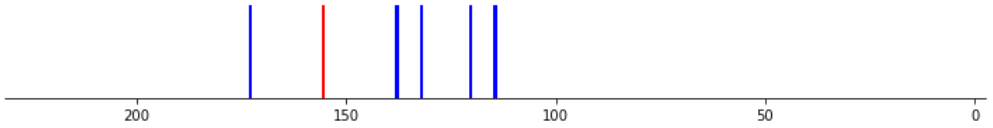


Top predicted substructures for the masked region(red):
0.4149 [#7][#6][#6X3]
0.3351 [OX2H][cX3]:[c]
0.1991 [#6]1[#6][#6][#6][#6][#7]1

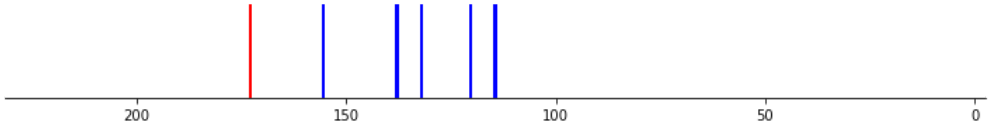
0.1852 [#7][#6][#6][#6X3]
0.164 [#6X3][#7][#6X3]
0.141 [cH]cO
0.104 o[cH]
0.1023 O=[#6][#6]=[#6X3]



Top predicted substructures for the masked region(red):
0.3573 [#7][#6][#6X3]
0.3187 [OX2H][cX3]:[c]
0.2484 [#6]1[#6][#6][#6][#6][#7]1
0.1318 [#7][#6][#6][#6X3]
0.1315 [cH]cO
0.1261 [#7X3H2]
0.1216 o[cH]
0.1049 O=[#6][#6]=[#6X3]

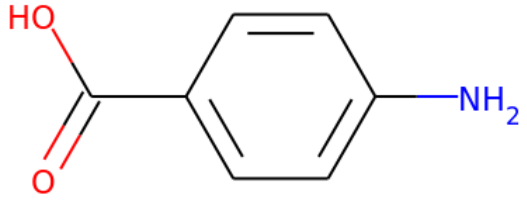


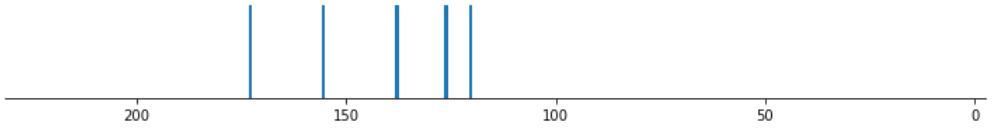
Top predicted substructures for the masked region(red):
0.3496 [#6]1[#6][#6][#6][#6][#7]1
0.3336 [OX2H][cX3]:[c]
0.2216 [#7X3H2]
0.1975 [#7][#6][#6][#6X3]
0.1605 [cH]cO
0.1548 [#7][#6][#6][#6X3]
0.1543 o[cH]
0.1477 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]

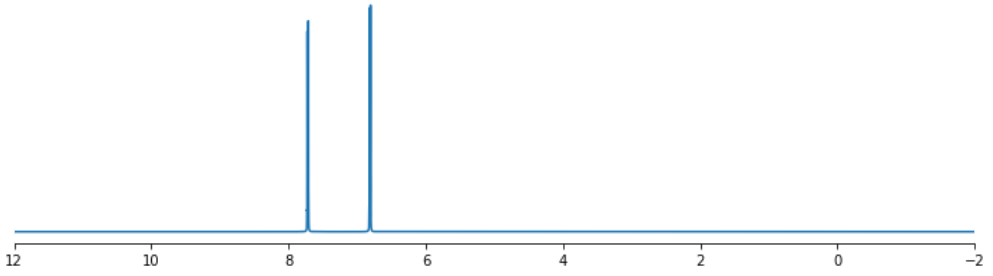


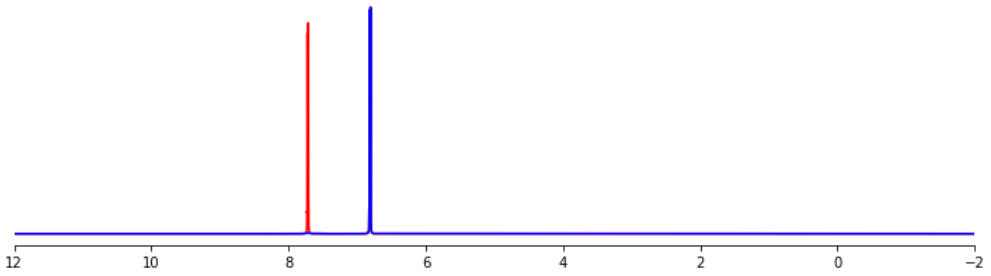
Top predicted substructures for the masked region(red):
0.6546 O=[#6][#6][#6X3]
0.3924 [#6]1[#6][#6][#6][#6][#7]1
0.3501 [#8]=[#6H0][#6H1]
0.3267 [OX1H0]=[cX3H0][cX3H1]
0.3259 [#8]=[#6][#6H1][#6H1]
0.2906 O=[cX3]
0.2703 [#7X3H2]
0.1435 [#7][#6][#6X3]

True structure: Nc1ccc(C(=O)O)cc1

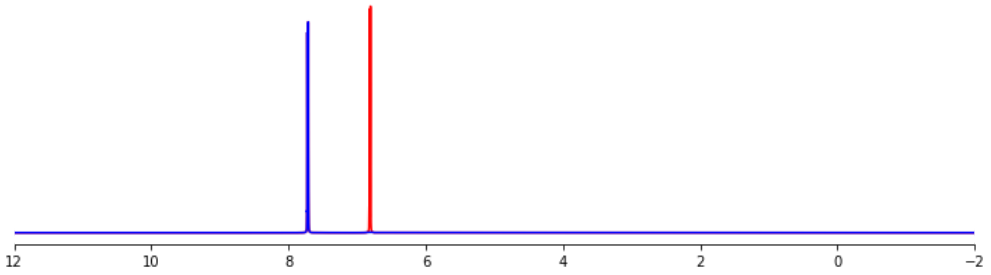




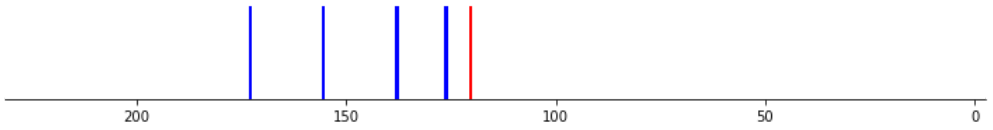




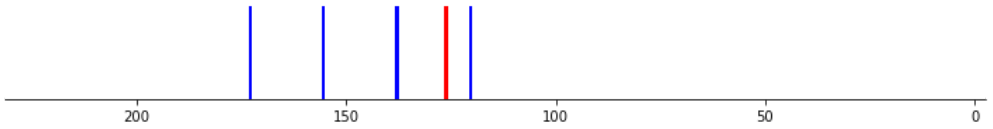
Top predicted substructures for the masked region(red):
0.381 [OX2H][cX3]:[c]
0.3137 [cX3H1]([cX3H1])[cX3H1]
0.2496 [#6]1[#6][#6][#6][#6][#7]1
0.2133 [#7][#6][#6][#6X3]
0.2 [#7][#6][#6X3]
0.1981 [#6H1][#6H1]
0.1946 [cH]
0.193 [#8][#6H1][#6H1]



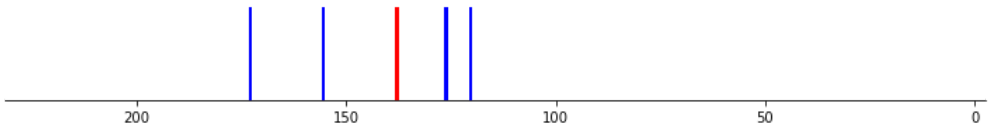
Top predicted substructures for the masked region(red):
0.4432 [OX2H][cX3]:[c]
0.2905 [cX3H1]([cX3H1])[cX3H1]
0.2625 [cH]cO
0.2309 [#7][#6][#6X3]
0.2152 [#7X3H1]
0.1859 [cX3H0][cX3H1][cX3H0][OX2H1]
0.1444 O=[#6][#6]=[#6X3]
0.1188 [cX3H1]([oX2H0])[cX3H1]



Top predicted substructures for the masked region(red):
0.3154 [OX2H][cX3]:[c]
0.2232 [#7X3H1]
0.2024 [#7X3H2]
0.1785 [#8][#6][#6][#6X3]
0.1635 [cX3H0][cX3H1][cX3H0][OX2H1]
0.1627 [#7][#6][#6X3]
0.1302 [#7][#6][#6][#6X3]
0.12 [#6X3][#7X3][#6X3]

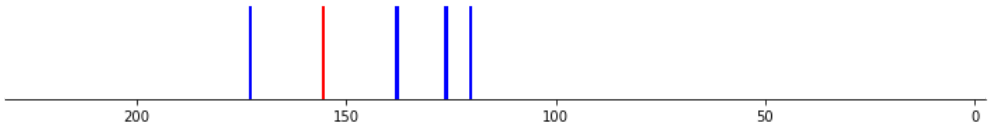


Top predicted substructures for the masked region(red):
0.316 [OX2H][cX3]:[c]
0.2283 [#7X3H2]
0.2272 [#7X3H1]
0.1632 [cX3H0][cX3H1][cX3H0][OX2H1]
0.1414 [#7][#6][#6X3]
0.1319 [#8][#6][#6][#6X3]
0.1207 [cX3H1]([cX3H1])[cX3H1]
0.1159 [#6X3][#7X3][#6X3]

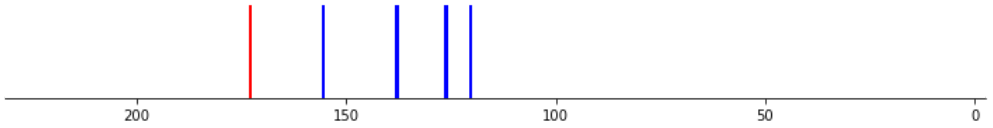


Top predicted substructures for the masked region(red):
0.3207 [OX2H][cX3]:[c]
0.2491 [#7X3H2]
0.2197 [#7X3H1]

0.1588 [#7][#6][#6X3]
0.1534 [cX3H0][cX3H1][cX3H0][OX2H1]
0.1208 [#6]1[#6][#6][#6][#6][#7]1
0.1152 [OX2H1]
0.1068 [#7][#6][#6][#6X3]

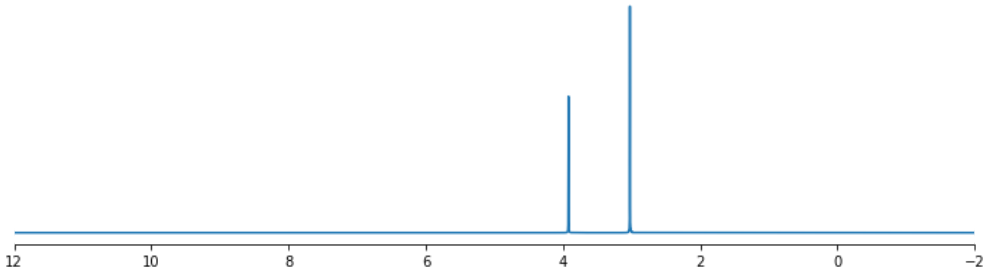


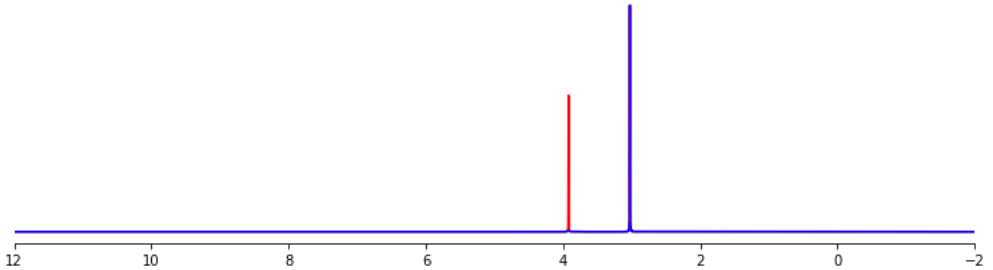
Top predicted substructures for the masked region(red):
0.3902 [OX2H][cX3]:[c]
0.2631 [#6]1[#6][#6][#6][#6][#7]1
0.2422 [#7X3H2]
0.2207 [#7][#6][#6X3]
0.1866 [#8][#6H0][#6H1]
0.1864 [#7][#6][#6][#6X3]
0.186 [cX3H0][cX3H1][cX3H0][OX2H1]
0.1664 [#7X3H1]



Top predicted substructures for the masked region(red):
0.7232 O=[#6][#6][#6X3]
0.3226 [#7X3H2]
0.2833 O=[cX3]
0.271 [OX1H0]=[cX3H0][cX3H1]
0.267 [#7X3H1]
0.2249 [#7][#6][#6][#6X3]
0.1912 [CX3](=[OX1])C
0.1869 O=[#6][#6]=[#6X3]

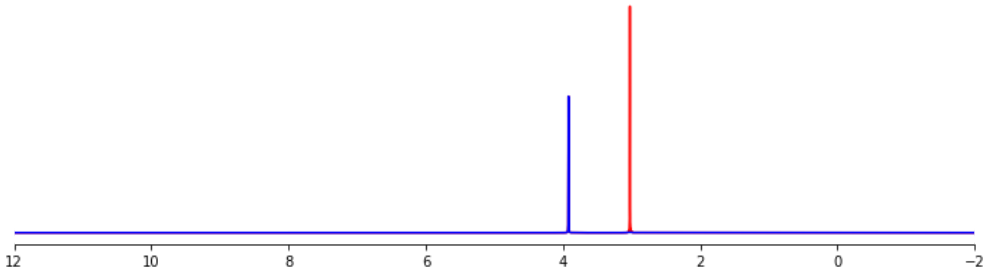
True structure: CN(CC(=O)O)C(=N)N



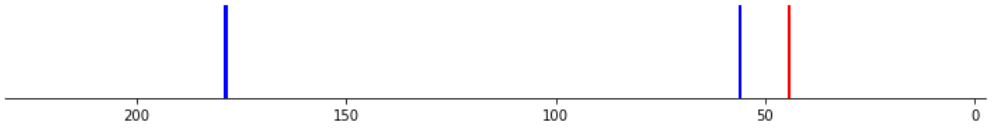


Top predicted substructures for the masked region(red):
0.4186 [#7X3][#6H2]
0.4132 [#7][#6H2]
0.3281 [#6H3][#7][#6X3]

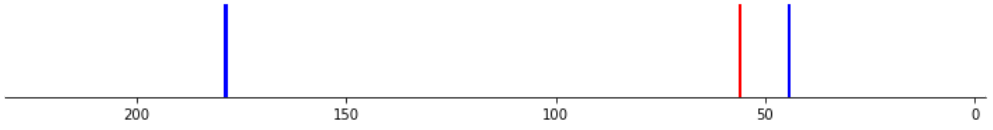
0.3023 [#7][#6]=[#7]
0.2506 [#7][#6H0]=[#7]
0.2473 [#7H2][#6X4H1][#6X3]
0.1992 [#7][#6][#6][#7]
0.182 [#7][#6H1r3]



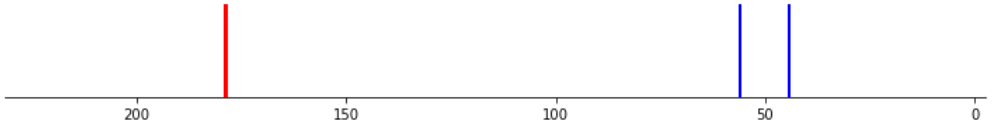
Top predicted substructures for the masked region(red):
0.7117 [#7X3][#6H3]
0.6616 [#6H3][#7][#6X3]
0.5696 [#6H3][#7]
0.5282 [CX4H3][NX3H0]
0.4032 [#7X3H0]
0.3622 [#7][#6]=[#7]
0.3101 [#7][#6H0]=[#7]
0.1971 O=[CX3][CX4H]



Top predicted substructures for the masked region(red):
0.4609 [CX4H3][NX3H0]
0.4469 [#6H3][#7][#6X3]
0.3986 [#7X3][#6H3]
0.3083 [#6H3][#7]
0.2731 [#7H2][#6X4H1][#6X3]
0.2609 [#7][#6][#6][#6][#7]
0.2467 [#7X3H0]
0.2275 [#7H2][#6H2]

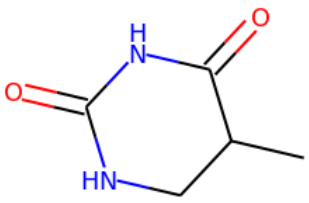


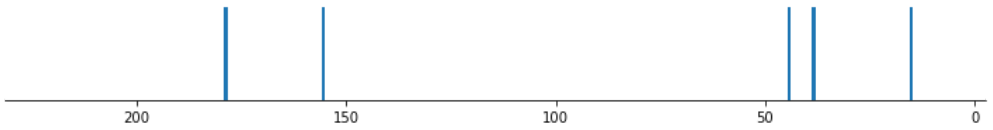
Top predicted substructures for the masked region(red):
0.3574 [#7H2][#6X4H1][#6X3]
0.3047 [#7][#6]=[#7]
0.2365 O=[CX3][CX4H]
0.2036 [#7H2][#6H1]
0.1856 [#7][#6H1r3]
0.171 [#7][#6H0]=[#7]
0.1613 [#6H3][#7][#6X3]
0.1555 [CX4H3][NX3H0]

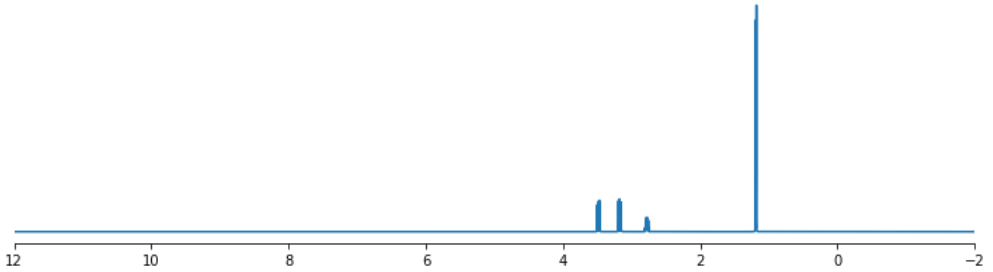


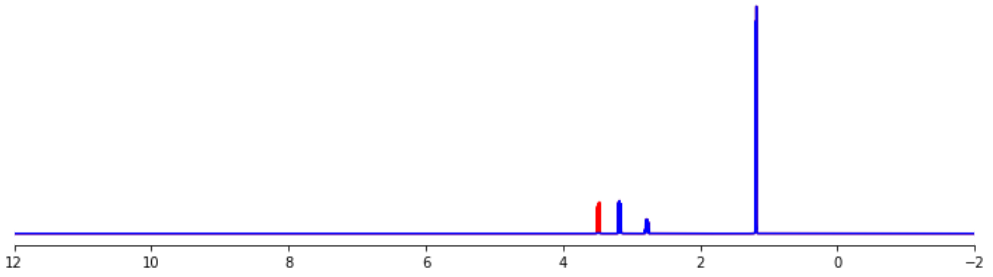
Top predicted substructures for the masked region(red):
0.8466 [CX3](=[OX1])C
0.7917 [#7X3][#6H3]
0.7402 [#7][#6][#6X3]
0.6855 [CX4H3][NX3H0]
0.679 [#6H3][#7][#6X3]
0.565 [#7X3H0]
0.5296 [#6H3][#7]
0.4578 O=[CX3][CX4H]

True structure: CC1CNC(=O)NC1=O

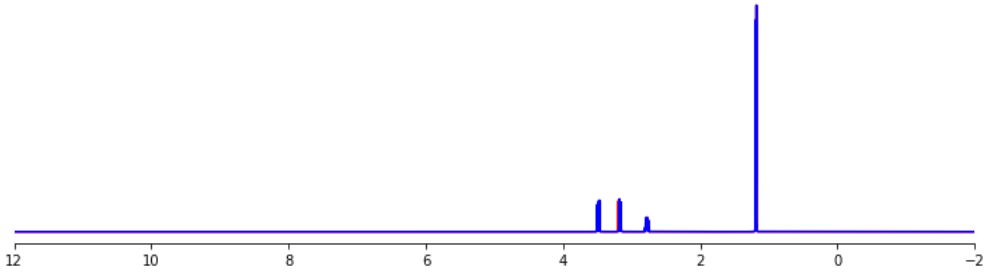




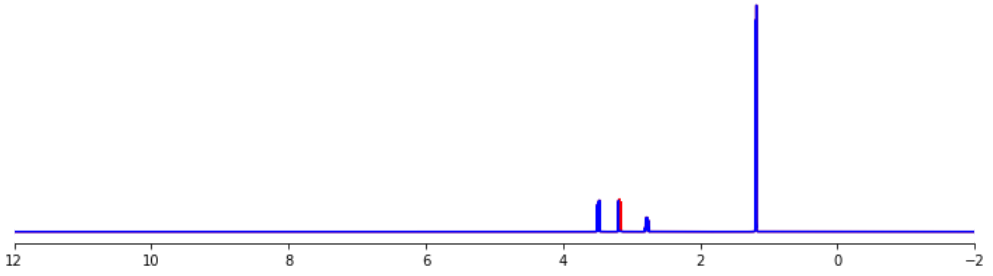




Top predicted substructures for the masked region(red):
0.6929 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.6783 [CHX4]([CH3X4])[CH2X4]
0.4786 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3775 [#7][#6H2]
0.329 [CX4H3][CX4H1]
0.3256 [#6H1][#6H2]
0.2981 [CX4H2]CC=O
0.2797 [#7X3][#6H2]

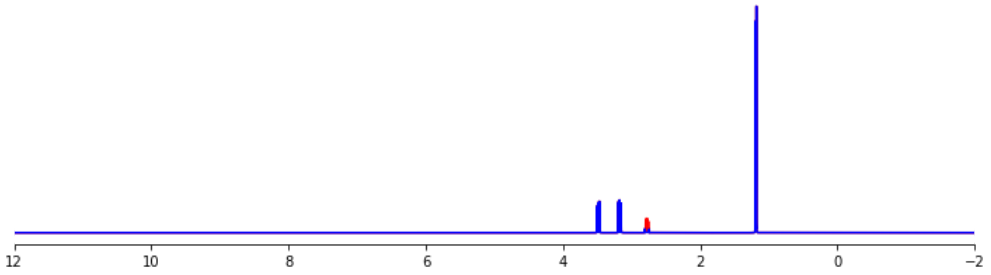


Top predicted substructures for the masked region(red):
0.5468 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.354 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3376 [CX4H3][CX4H1]
0.2759 [CHX4]([CH3X4])[CH2X4]
0.2749 [CX4H2]CC=O
0.2335 [CX4H2]([NX3H0])[CX4H1]
0.2314 [#6H3][#6][#6X3]
0.193 [#6H1]

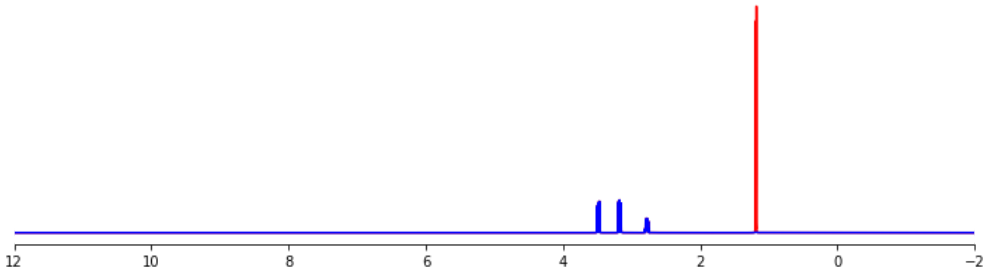


Top predicted substructures for the masked region(red):
0.6944 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.5153 [CHX4]([CH3X4])[CH2X4]
0.4287 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.4213 [CX4H3][CX4H1]
0.3429 [CX4H2]CC=O
0.3221 [CX4H2]([NX3H0])[CX4H1]
0.2943 [#6H1]

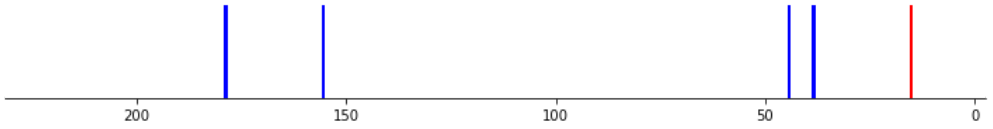
0.2334 [#6H1][#6H2]



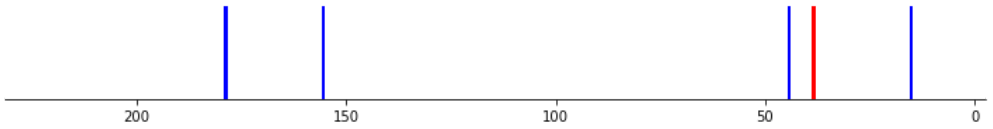
Top predicted substructures for the masked region(red):
0.801 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.499 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.4608 [CHX4]([CH3X4])[CH2X4]
0.392 [CX4H3][CX4H1]
0.3499 [CX4H2]CC=O
0.2976 [CX4H2]([NX3H0])[CX4H1]
0.2287 [#6H3][#6][#6X3]
0.1919 [#6H1][#6H2]



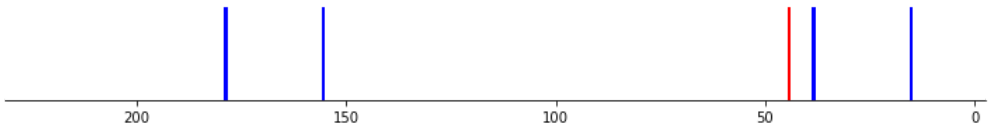
Top predicted substructures for the masked region(red):
0.8726 [CX4H3][CX4H1]
0.8708 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.8695 [CHX4]([CH3X4])[CH2X4]
0.7752 [#6H3][#6][#6]
0.6358 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.5745 [#6H3][#6][#6X3]
0.3998 [#6H1]
0.3974 [#6H3][#6H1r5]



Top predicted substructures for the masked region(red):
0.715 [CX4H3][#6]
0.7044 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.6425 [CX4H3][CX4H1]
0.5904 [#6H3][#6][#6X3]
0.5078 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3958 [#7][#6][#6H3]
0.3926 [CHX4]([CH3X4])[CH2X4]
0.3222 [#6H3][#6H1r5]

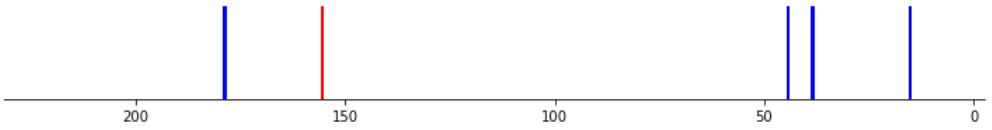


Top predicted substructures for the masked region(red):
0.5826 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.4492 [CX4H3][CX4H1]
0.3778 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.35 [CHX4]([CH3X4])[CH2X4]
0.3233 [CX4H2]CC=O
0.2962 [CX4H2]([NX3H0])[CX4H1]
0.2841 O=[CX3][CX4H]
0.2214 [#6H3][#6][#6X3]

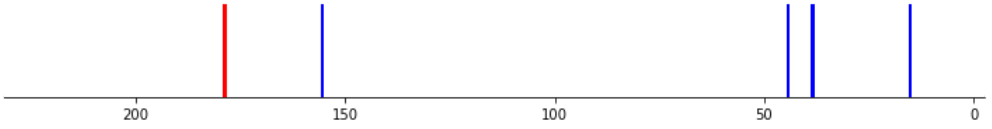


Top predicted substructures for the masked region(red):
0.6718 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]

0.4436 [CX4H3][CX4H1]
0.4221 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3793 [CHX4]([CH3X4])[CH2X4]
0.2971 [CX4H2]CC=O
0.2856 [#7][#6H2]
0.282 [#7][#6][#6H3]
0.2729 O=[CX3][CX4H]

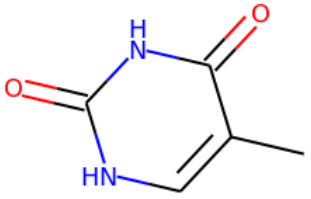


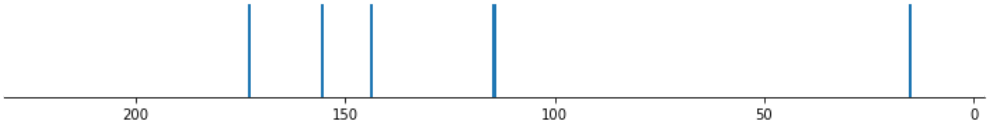
Top predicted substructures for the masked region(red):
0.651 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.5735 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.5347 [CX4H3][CX4H1]
0.4752 [CHX4]([CH3X4])[CH2X4]
0.4458 [#7][#6][#7]
0.3879 [#6X3][#7][#6X3]
0.355 [CX4H2]CC=O
0.3463 [#6X3][#7X3][#6X3]

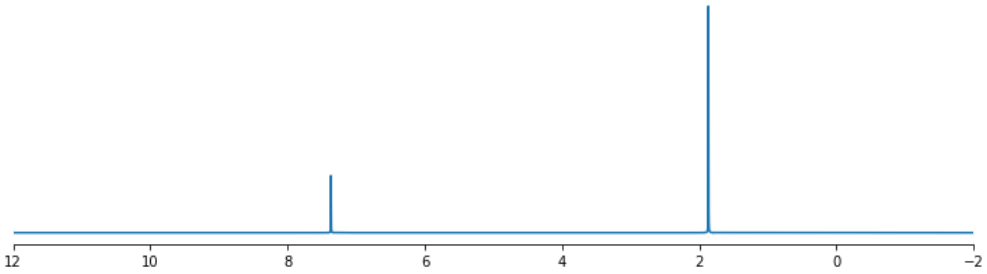


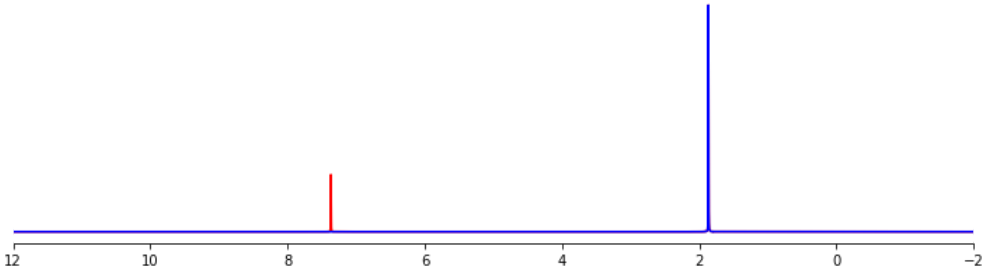
Top predicted substructures for the masked region(red):
0.8827 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.8056 O=[CX3][CX4H]
0.7711 [CX4H2]CC=O
0.7052 [#8]=[#6H0][#6H1]
0.6894 [CX3](=[OX1])C
0.6848 [#6H3][#6][#6X3]
0.6779 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.4688 [CX4H3][CX4H1]

True structure: Cc1c[nH]c(=O)[nH]c1=O



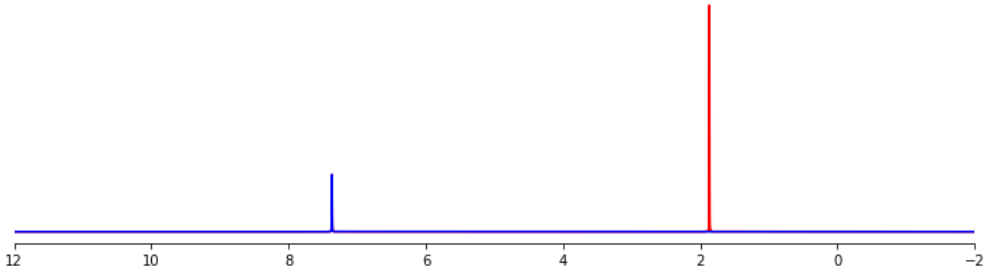




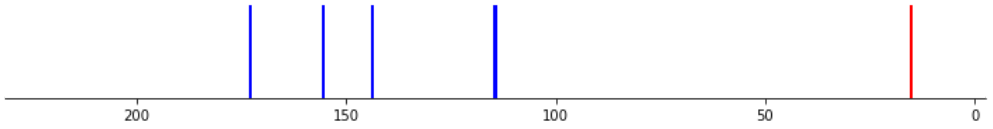


Top predicted substructures for the masked region(red):
0.5412 [#6H1]

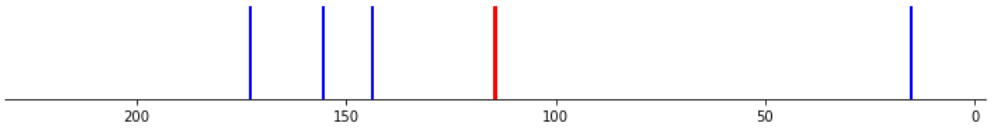
0.5215 [cH]
0.5166 [#6X3H1][#6X3H0]
0.4108 [cX3H0]([cX3H1])([cX3H0])[CX4H3]
0.3401 [#7]=[#6H1]
0.2872 [#6H3][#6H0][#6H1][#7]
0.2772 [#7][#6H0][#6H1]
0.2365 [#7][#6][#6H3]



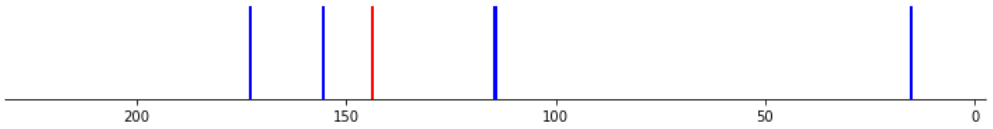
Top predicted substructures for the masked region(red):
0.5898 [OX1H0]=[CX3H0][CX3H0][CX4H3]
0.5615 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.5468 [CX4H3][CX3H0][CX3]=O
0.4981 [CX4H3][CX3H0]
0.4772 [CX4H3][CX3]
0.4061 [cX3H0]([cX3H1])([cX3H0])[CX4H3]
0.4034 [#6H3][#6H0]
0.35 [#6H3][#6]=[#6X3]



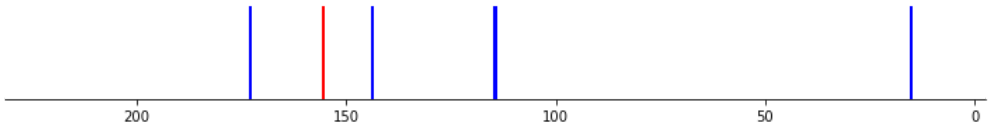
Top predicted substructures for the masked region(red):
0.7996 [CX4H3][#6]
0.7421 [#6H3][#6][#6X3]
0.7065 [CX4H3][cX3H0]
0.5759 [CX4H3][CX3]
0.5538 [CX4H3][CX3H0]
0.5456 [#6H3][#6][#6]
0.5444 [#6X3][#6][#6][#6H3]
0.5182 [CX4H3][CX3H0][CX3]=O



Top predicted substructures for the masked region(red):
0.3887 [#6X3][#6][#6][#6H3]
0.3239 [cX3H0]([cX3H1])([cX3H0])[CX4H3]
0.2993 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.2807 [#6H3][#6]=[#6X3]
0.2731 [#7X3H2]
0.2154 [#7][#6][#6H3]
0.212 [#7][#6][#6][#6X3]
0.205 O=[cX3]

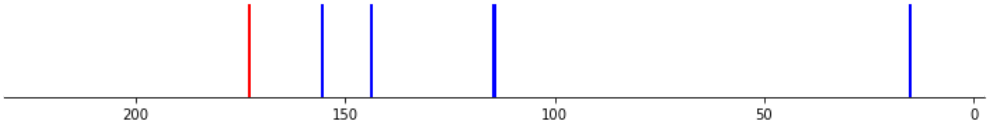


Top predicted substructures for the masked region(red):
0.3495 [CX4H3][CX3H0][CX3]=O
0.2912 [#6X3][#6][#6][#6H3]
0.2629 [OX1H0]=[CX3H0][CX3H0][CX4H3]
0.2539 O=[#6][#6]=[#6X3]
0.2477 [#7]=[#6H1]
0.2304 [#6H3][#6]=[#6X3]
0.227 [#7X3H2]
0.2203 [#7][#6][#6H3]



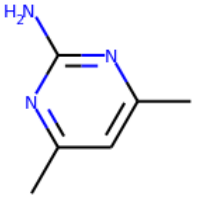
Top predicted substructures for the masked region(red):
0.3677 [CX4H3][CX3H0][CX3]=O
0.2874 [OX1H0]=[CX3H0][CX3H0][CX4H3]

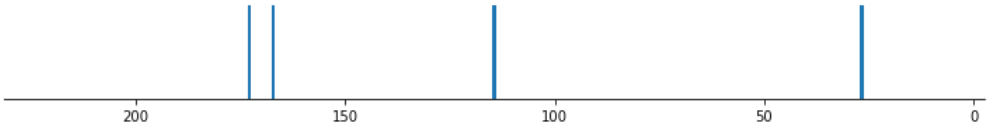
0.2598 [#7]=[#6H1]
0.258 [#7X3H2]
0.2491 [#6X3][#6][#6][#6H3]
0.2454 [CX4H3][CX3]
0.2134 [#7][#6][#6H3]
0.211 O=[#6][#6]=[#6X3]

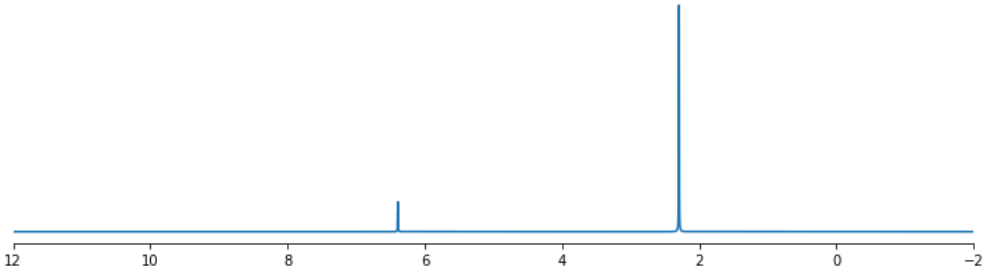


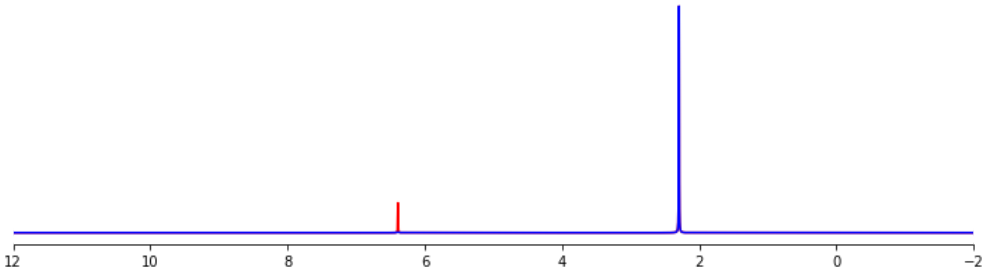
Top predicted substructures for the masked region(red):
0.6269 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.5857 [OX1H0]=[CX3H0][CX3H0][CX4H3]
0.5527 [CX4H3][CX3H0][CX3]=O
0.3957 [CX4H3][CX3H0]
0.3407 [CX3](=[OX1])C
0.3285 O=[#6][#6]=[#6X3]
0.3231 O=[#6][#6][#6X3]
0.3163 [#7X3H2]

True structure: Cc1cc(C)nc(N)n1

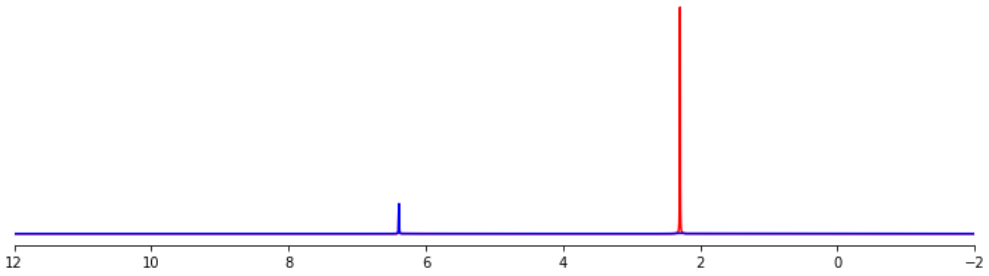




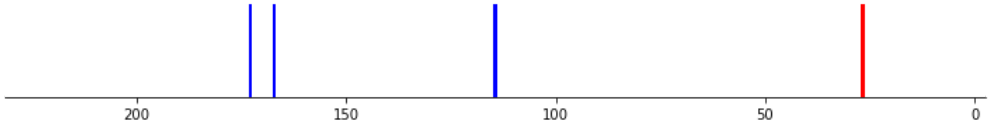




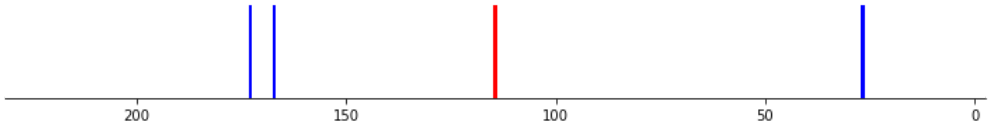
Top predicted substructures for the masked region(red):
0.3662 [#6X3H1][#6X3H0]
0.3461 [#6H1]
0.3147 [#7][#6][#6][#6X3]
0.31 [#6X3][#7][#6X3]
0.3003 [#7][#6X3H0][#6X3H1]
0.2625 [#7][#6H0][#6H1]
0.2224 [#7][#6]=[#7]
0.219 [#7H][#6X3H1]



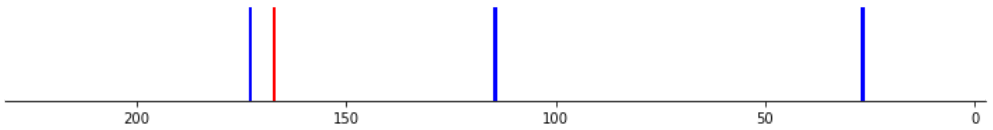
Top predicted substructures for the masked region(red):
0.4662 [#6H3][#6H0]
0.3996 [CX4H3][CX3]
0.3947 [CX4H3][CX3H0]
0.3719 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.3481 [#7][#6][#6H3]
0.3191 [CHX3](=C)C
0.2533 O=[#6][#6]=[#6X3]
0.2481 [#6H3][#6]=[#6X3]



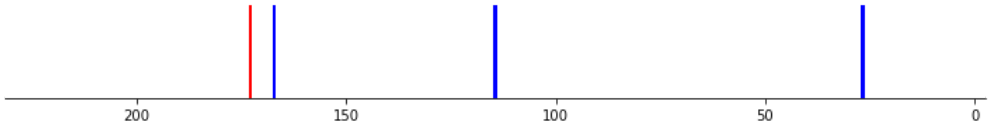
Top predicted substructures for the masked region(red):
0.9456 [CX4H3][#6]
0.6394 [#7][#6][#6H3]
0.5401 [CX4H3][CX3H0]
0.4689 [#6H3][#6H0]
0.4482 [CX4H3][CX3]
0.3967 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.374 [#6H3][#6][#6]
0.3044 [#6X3][#7][#6X3]



Top predicted substructures for the masked region(red):
0.4877 [CX4H3][#6]
0.4232 [#6X3][#6X3]
0.4153 [#6H3][#6][#6]
0.3741 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.3274 [CHX3](=C)C
0.308 [#7]#[#6][#6X3]
0.304 [#7][#6][#6][#6X3]
0.2874 [#7H2][#6H0]

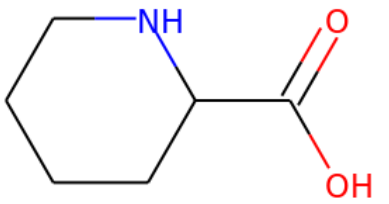


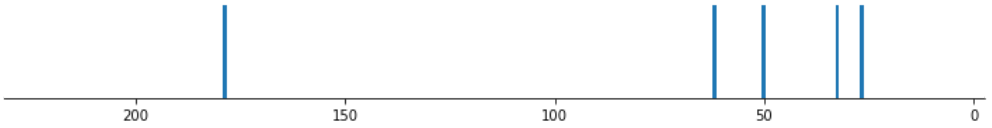
Top predicted substructures for the masked region(red):
0.3784 [#6H3][#6][#6]
0.3681 [CX4H3][#6]
0.356 [#7][#6]=[#7]
0.323 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.3203 [CHX3](=C)C
0.3202 [#7][#6H0]=[#7]
0.3149 [#7][#6][#6][#6X3]
0.2955 [#6X3][#7][#6X3]

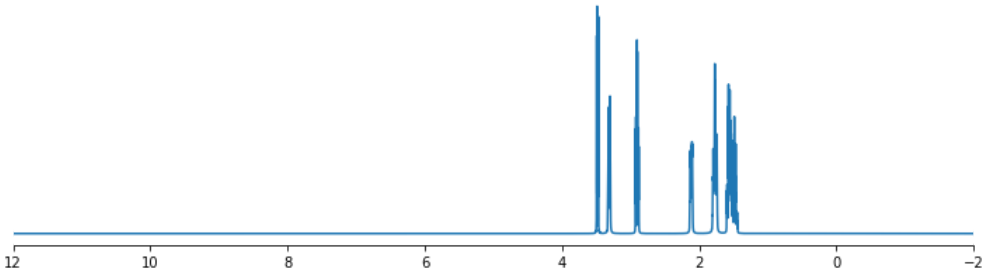


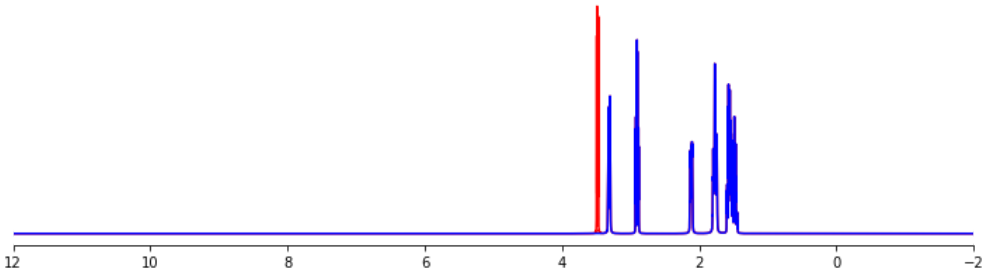
Top predicted substructures for the masked region(red):
0.4416 [CX4H3][#6]
0.3911 [#7][#6]=[#7]
0.384 [CHX3](=C)C
0.3607 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.344 [#6H3][#6][#6]
0.3285 O=[#6][#6]=[#6X3]
0.2729 [#7][#6][#6][#6X3]
0.2681 [#7][#6H0]=[#7]

True structure: O=C(O)C1CCCCN1



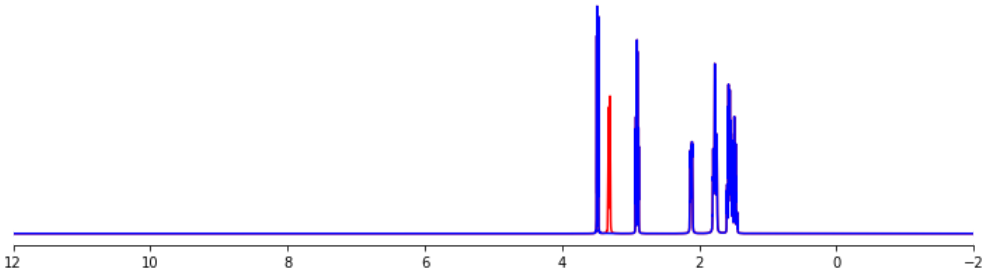






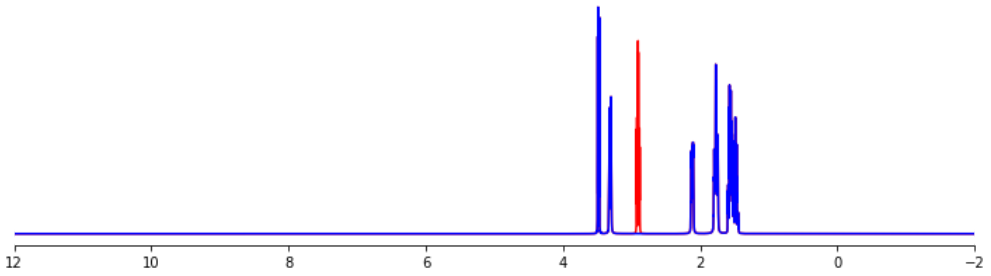
Top predicted substructures for the masked region(red):

0.3076 [#6]1[#6][#6][#6][#7]1
0.3031 [CX4H2]([NX3H1])[CX4H1]
0.2141 [#7X3H1]
0.2036 [CX3](=[OX1])O
0.1615 [#7][#6H2][#6H2]
0.1511 [#7][#6H2][#6H1]
0.1328 [#6H2][#7][#6X3]
0.1205 [CX4H1]([CX4H2])([CX4H2])[CX3H0]



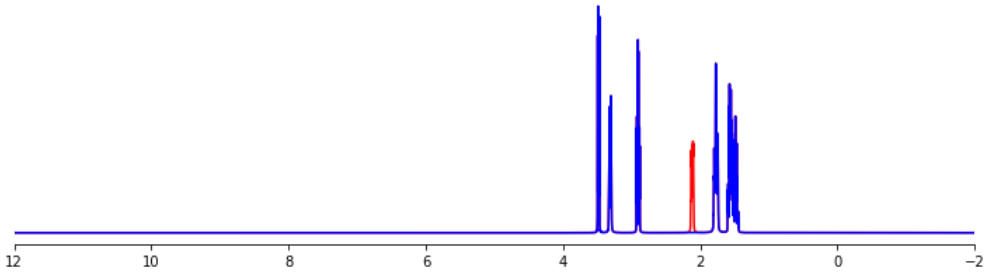
Top predicted substructures for the masked region(red):

0.3669 [#7][#6H2][#6H2]
0.3132 [CX4H2]([NX3H1])[CX4H1]
0.3014 [#6]1[#6][#6][#6][#7]1
0.236 [CX4H2]([NX3H1])[CX4H2]
0.2259 [#7X3H1]
0.2192 [CX3](=[OX1])O
0.1751 [#7][#6H2]
0.1704 [#7X3][#6H2]



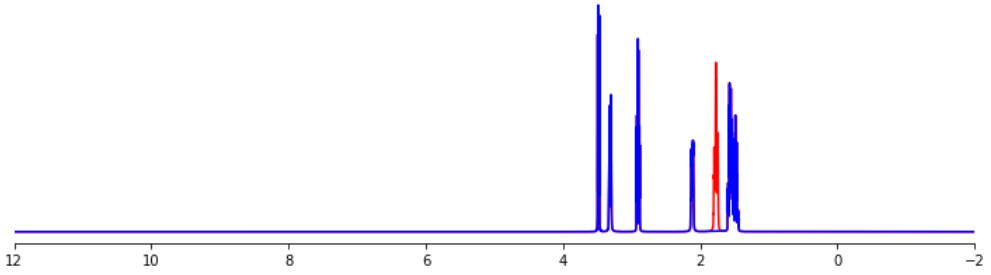
Top predicted substructures for the masked region(red):

0.4273 [#7][#6H2][#6H2]
0.3177 [#7X3][#6H2]
0.2963 [CX3](=[OX1])O
0.2931 [#6]1[#6][#6][#6][#7]1
0.2469 [CX4H2]([NX3H1])[CX4H1]
0.2337 [#7][#6H2]
0.2312 [CX4H2]([NX3H1])[CX4H2]
0.2048 [#7X3H1]



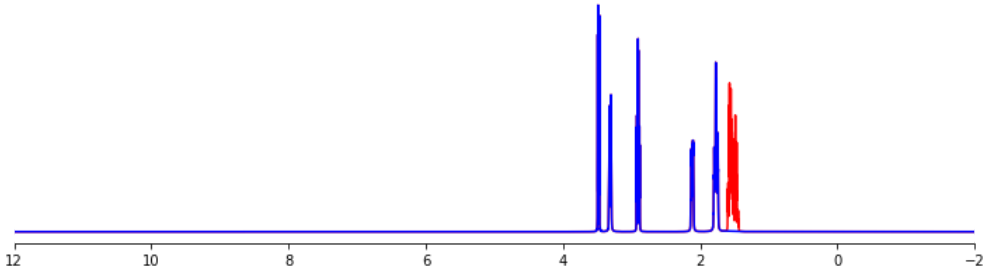
Top predicted substructures for the masked region(red):

0.3152 [CX3](=[OX1])O
0.256 [CX4H2]([NX3H1])[CX4H1]
0.2422 [#6]1[#6][#6][#6][#7]1
0.2373 [#7X3H2]
0.1698 [#7][#6H1][#6H2r5]
0.1683 [#6H1][#6H2][#6H2][#6H1]
0.1459 [CX4H2]CC=O
0.1412 [#8]=[#6H0][#6H1]



Top predicted substructures for the masked region(red):

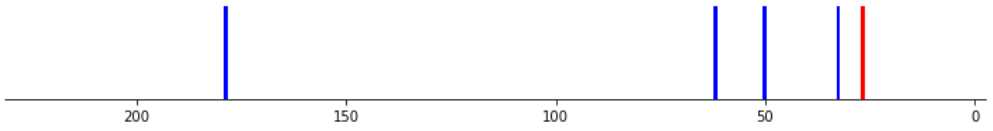
0.2786 [CX3](=[OX1])O
0.2534 [#8]=[#6H0][#6H1]
0.2039 [CX4H2]([NX3H1])[CX4H1]
0.1914 [#8][#6H0][#6H1]
0.1814 [#7X3H2]
0.1675 [CX4H2]CC=O
0.1453 [#7X3H1]
0.1438 [#6H1][#6H2][#6H2][#6H1]



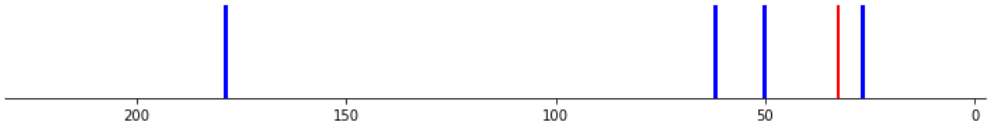
Top predicted substructures for the masked region(red):

0.3039 [CX3](=[OX1])O
0.2888 [#7X3H2]
0.2448 [CX4H2]([NX3H1])[CX4H1]
0.1706 [#6H1][#6H2][#6H2][#6H1]
0.1541 [CX4H2]([CX4H2])[CX4H2]

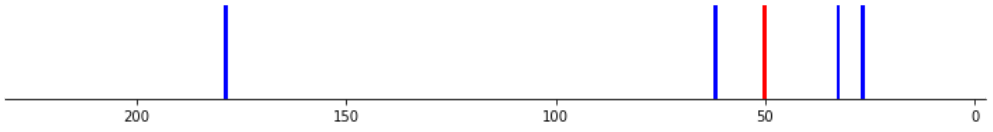
0.153 [#8]=[#6H0][#6H1]
0.132 CCCCCC
0.1217 [#7X3H1]



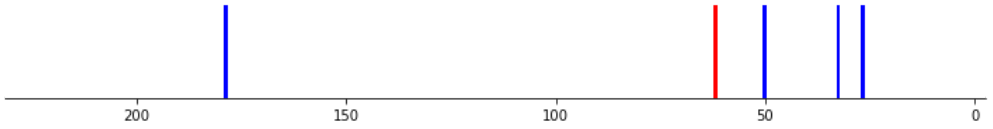
Top predicted substructures for the masked region(red):
0.6533 [CX4H2]([CX4H2])[CX4H2]
0.3355 [#7][#6H2][#6H2]
0.3339 [CX3](=[OX1])O
0.2445 [CX4H2][CX4H2][CX4H2][CX4H2]
0.1824 [#7X3H1]
0.1675 [CX4H2]CC=O
0.1608 [#8]=[#6H0][#6H1]
0.1526 [CX4H2]([NX3H1])[CX4H1]



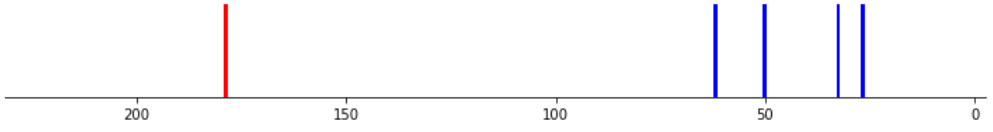
Top predicted substructures for the masked region(red):
0.3336 [CX3](=[OX1])O
0.2661 [CX4H2]([CX4H2])[CX4H2]
0.2184 [CX4H2]([NX3H1])[CX4H1]
0.1924 [CX4H2]([NX3H1])[CX4H2]
0.1792 [#7X3H1]
0.1757 [#7][#6H2][#6H2]
0.1598 [#7X3H2]
0.1361 [CX4H2]CC=O



Top predicted substructures for the masked region(red):
0.4344 [CX3](=[OX1])O
0.4247 [#7][#6H2][#6H2]
0.3547 [CX4H2]([NX3H1])[CX4H2]
0.3371 [#8]=[#6H0][#6H1]
0.3169 [#6]1[#6][#6][#6][#7]1
0.3164 [CX4H2]([NX3H1])[CX4H1]
0.3045 [#8][#6H0][#6H1]
0.2005 [#7X3H1]

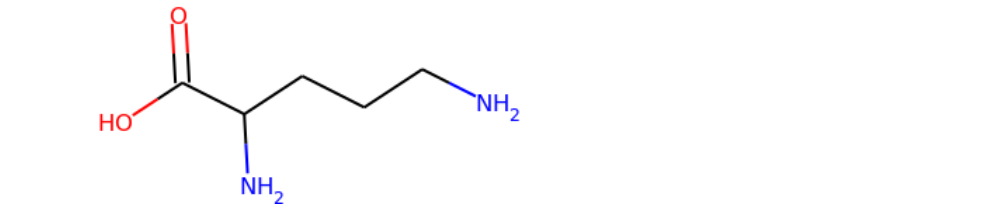


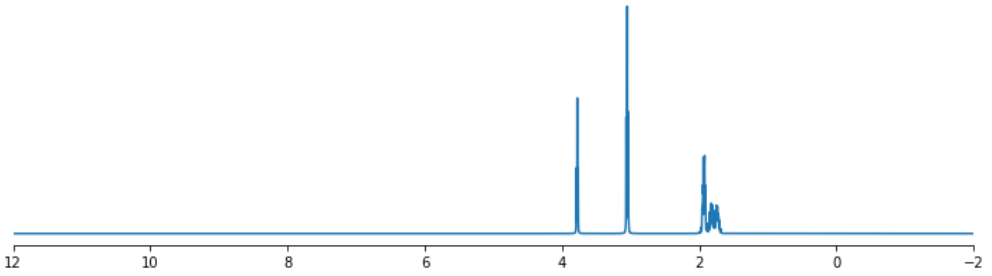
Top predicted substructures for the masked region(red):
0.4376 [#6]1[#6][#6][#6][#7]1
0.4366 [#7][#6H1][#6H2r5]
0.2035 [#8][#6H0][#6H1]
0.1911 [CX4H2]([NX3H1])[CX4H1]
0.1731 [#6H1r5][#7]
0.1405 [OX2H0][CX4H1][CX4H2][CX4H2]
0.1387 [#8]=[#6H0][#6H1]
0.1384 [CX4H1]([NX3H1])([CX4H2])[CX3H0]

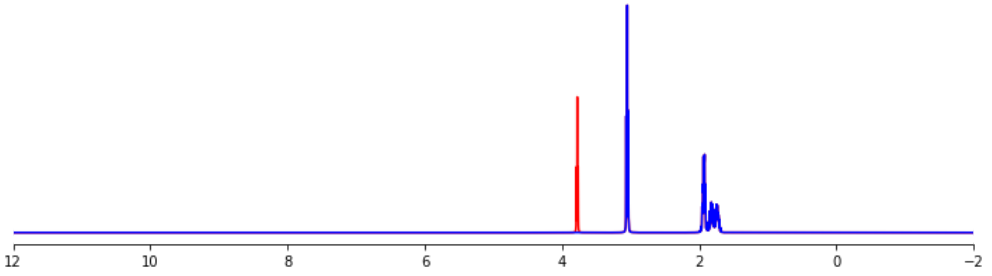


Top predicted substructures for the masked region(red):
0.986 [CX3](=[OX1])C
0.959 [CX4H2]CC=O
0.8705 [CX3](=O)[OX2H1]
0.8671 [CX3](=[OX1])O
0.8666 [#8]=[#6][#8]
0.8435 O=[CX3][CX4H]
0.8048 [#8]=[#6H0][#6H1]
0.7033 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]

True structure: NCCCC(N)C(=O)O

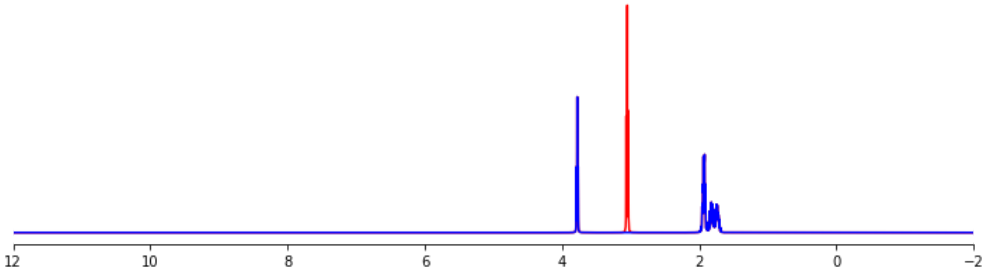






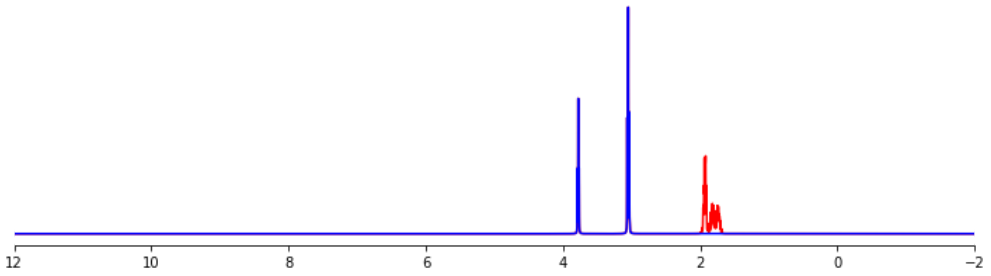
Top predicted substructures for the masked region(red):

0.3087 [CX4H2]([NX3H1])[CX4H2]
0.3074 [#7H2][#6X4H1][#6X3]
0.2856 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.179 [#7H2][#6H1]
0.1696 [CX4H2][CX3]=O
0.1581 [#8][#6][#6H2]
0.1476 [#6H2][#7][#6X3]
0.1432 [CX4H2]([OX2H1])[CX4H2]

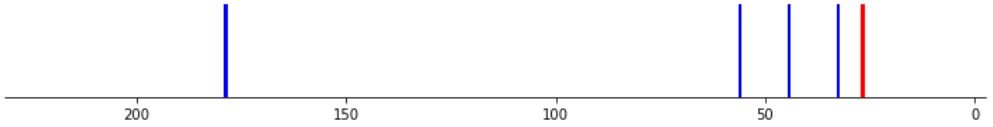


Top predicted substructures for the masked region(red):

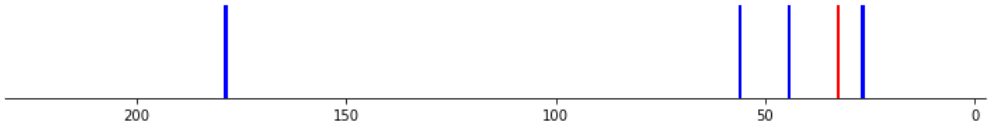
0.6764 [#7X3][#6H2]
0.6059 [CX4H2]([NX3H2])[CX4H2]
0.4909 [#7H2][#6H2]
0.4874 [#7][#6H2]
0.4864 [CX4H2]([NX3H1])[CX4H2]
0.4037 [CX4H2][CX3]=O
0.325 [#7][#6H2][#6H2]
0.2827 [CX4H2]([CX4H2])[CX3H0]



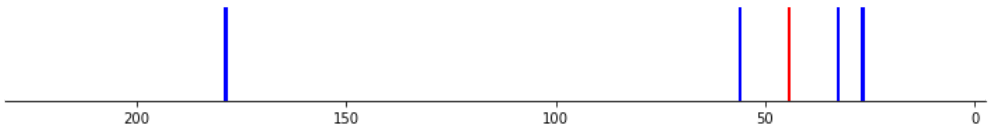
Top predicted substructures for the masked region(red):
0.5775 [#7H2][#6X4H1][#6X3]
0.515 [CX4H2]([CX4H2])[CX4H1]
0.4833 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.4512 [#7H2][#6H1]
0.4159 O=[CX3][CX4H]
0.3928 OCC[CH2]
0.2548 [#7][#6][#6X3]
0.2544 [#6H1]



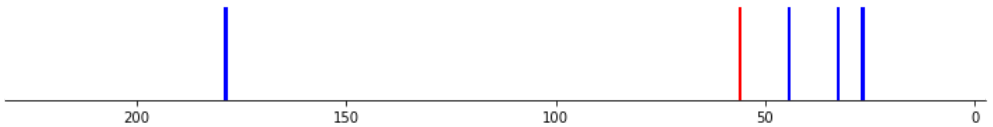
Top predicted substructures for the masked region(red):
0.3021 [CX4H2][CX4H2][CX4H2][CX4H2]
0.2826 [CX4H2]([NX3H1])[CX4H2]
0.2378 [CX4H2]([CX4H2])[CX4H2]
0.1415 [CX4H2]([CX4H2])[CX3H0]
0.1266 [#7X3][#6H2]
0.1072 [CX4H2][CX3]=O
0.1 OCC[CH2]
0.0865 [CX4H2]CC=O



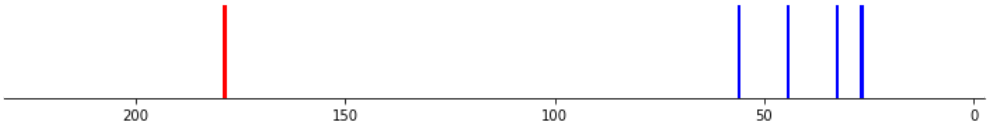
Top predicted substructures for the masked region(red):
0.3268 [CX4H2]([NX3H1])[CX4H2]
0.2395 [CX4H2]([CX4H2])[CX4H2]
0.2369 [CX4H2]([CX4H2])[CX3H0]
0.2249 [CX4H2]([NX3H2])[CX4H2]
0.1661 [CX4H2][CX3]=O
0.144 [#8][#6][#6H2]
0.1372 [CX4H2][CX4H2]
0.1207 [CX4H1]([NX3H2])([CX4H2])[CX3H0]



Top predicted substructures for the masked region(red):
0.5927 [CX4H2]([NX3H2])[CX4H2]
0.5408 [CX4H2]([NX3H1])[CX4H2]
0.4846 [#7H2][#6H2]
0.4127 [#7X3][#6H2]
0.3068 [#7][#6H2]
0.254 [CX4H2][CX3]=O
0.2097 [#7][#6H2][#6H2]
0.1833 [CX4H2]([CX4H2])[CX4H2]

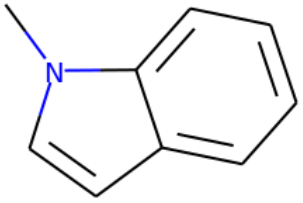


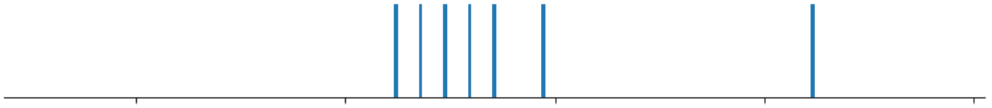
Top predicted substructures for the masked region(red):
0.6023 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.558 [#7H2][#6H1]
0.519 [#7H2][#6X4H1][#6X3]
0.3368 [CX4H2]([NX3H1])[CX4H2]
0.3057 [#7][#6][#6X3]
0.1903 O=[CX3][CX4H]
0.1593 [CX4H2]([CX4H2])[CX4H1]
0.142 [#8]=[#6][#8]

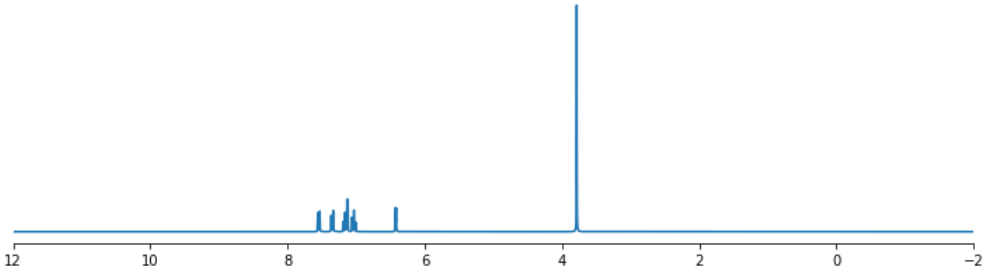


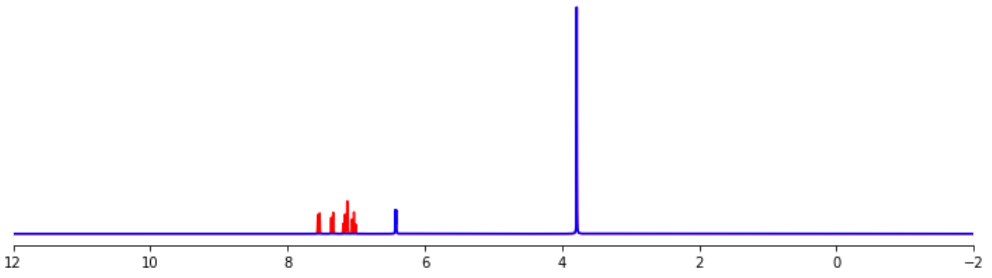
Top predicted substructures for the masked region(red):
0.9705 [CX3](=[OX1])C
0.9527 [CX4H2]CC=O
0.694 [#7][#6][#6X3]
0.6684 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.6607 [#7H2][#6X4H1][#6X3]
0.6442 [CX3](=O)[OX2H1]
0.6392 [CX4H2][CX3]=O
0.5991 [#8]=[#6][#8]

True structure: Cn1ccc2ccccc21

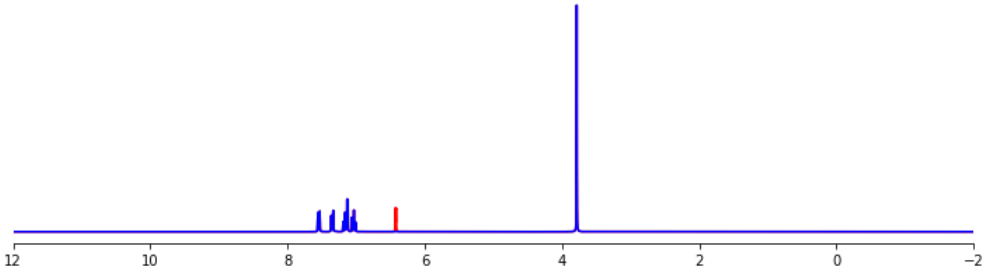






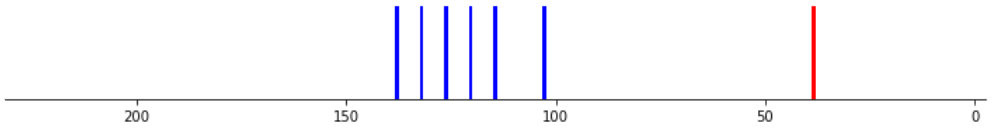


Top predicted substructures for the masked region(red):
0.8074 [cX3H1]([nX3H0])[cX3H1]
0.7428 [#7X3H0]
0.7365 [#6X3H1][#7X3H0]
0.7016 [#7X3][#6H3]
0.6907 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.6432 [#6H3][#7][#6X3]
0.5964 [cX3H1]([cX3H1])[cX3H1]
0.4237 [#7][#6X3H0][#6X3H1]

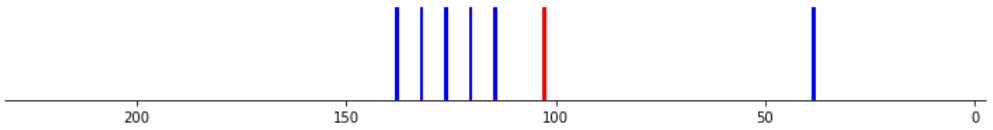


Top predicted substructures for the masked region(red):
0.5044 [cX3H1]([nX3H0])[cX3H1]
0.3561 [#6X3H1][#7X3H0]

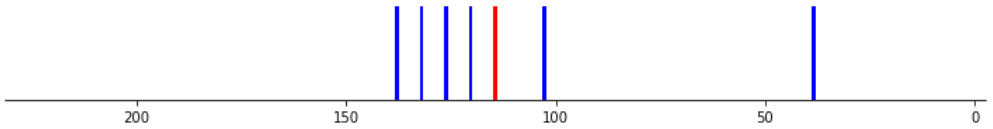
0.3094 [CX3H1](=[CX3H1])[cX3H0]
0.1971 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1549 [#7][#6X3H0][#6X3H1]
0.1497 [cX3H1]([nX2H0])[cX3H1]
0.1425 [#6H3][#7][#6X3]
0.1111 [#6]1[#6][#6][#6][#7]1



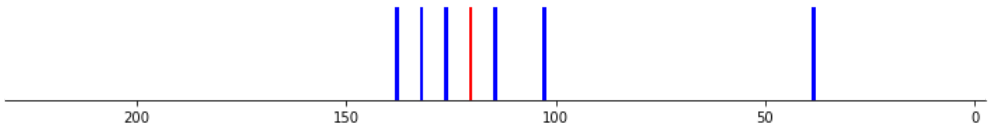
Top predicted substructures for the masked region(red):
0.8989 [#6H3][#7][#6X3]
0.8378 [#7X3][#6H3]
0.5483 [#6X3H1][#7X3H0]
0.508 [CX4H3][nX3H0]
0.4821 [cX3H1]([nX3H0])[cX3H1]
0.4297 [#6H3][#7]
0.3179 [#6X3][#6H2][#6X3]
0.3128 [CX3H1](=[CX3H1])[cX3H0]



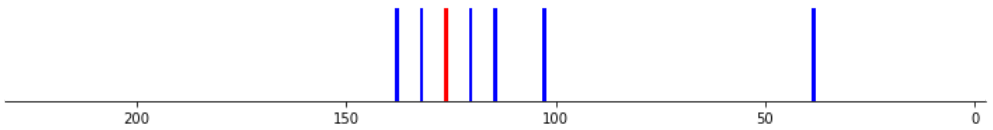
Top predicted substructures for the masked region(red):
0.5081 [cX3H1]([nX3H0])[cX3H1]
0.4291 [#6X3H1][#7X3H0]
0.4207 [#6H3][#7][#6X3]
0.3108 [#7][#6X3H0][#6X3H1]
0.2865 [#7X3][#6H3]
0.2763 [#6]1[#6][#6][#6][#7]1
0.2396 [#7H][#6X3H1]
0.239 [#6H1r5][#7]



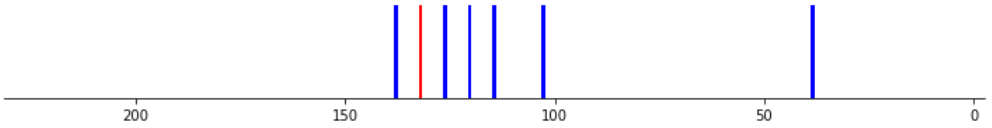
Top predicted substructures for the masked region(red):
0.5027 [cX3H1]([nX3H0])[cX3H1]
0.3199 [#6H3][#7][#6X3]
0.2763 [#6X3H1][#7X3H0]
0.2298 [#7][#6X3H0][#6X3H1]
0.219 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.2009 [#6]1[#6][#6][#6][#7]1
0.199 [#7X3][#6H3]
0.1816 [CX3H1](=[CX3H1])[cX3H0]



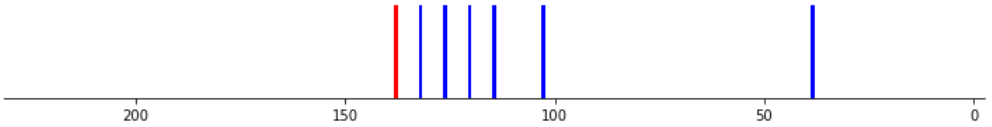
Top predicted substructures for the masked region(red):
0.4611 [cX3H1]([nX3H0])[cX3H1]
0.2652 [#6X3H1][#7X3H0]
0.2012 [CX3H1](=[CX3H1])[cX3H0]
0.164 [#7H][#6X3H1]
0.1584 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1405 [#6H3][#7][#6X3]
0.1292 [#6]1[#6][#6][#6][#7]1
0.1189 [cX3H1]([nX2H0])[cX3H1]



Top predicted substructures for the masked region(red):
0.4875 [cX3H1]([nX3H0])[cX3H1]
0.2561 [CX3H1](=[CX3H1])[cX3H0]
0.236 [#6X3H1][#7X3H0]
0.2359 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1733 [#6H3][#7][#6X3]
0.1704 [#7][#6X3H0][#6X3H1]
0.1665 [#6]1[#6][#6][#6][#6][#7]1
0.1571 [cX3H1]([nX2H0])[cX3H1]

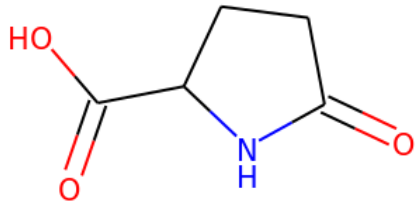


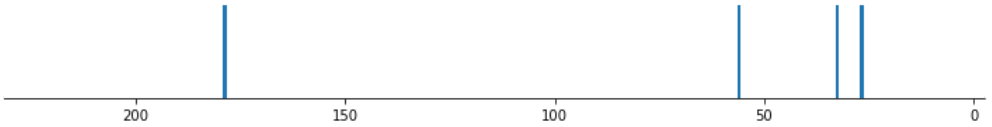
Top predicted substructures for the masked region(red):
0.4819 [cX3H1]([nX3H0])[cX3H1]
0.2897 [CX3H1](=[CX3H1])[cX3H0]
0.2489 [#6]1[#6][#6][#6][#6][#7]1
0.2434 [#7X3][#6H3]
0.24 [#6X3H1][#7X3H0]
0.236 [#6H3][#7][#6X3]
0.2068 [#7][#6X3H0][#6X3H1]
0.1656 [cX3H1]([nX2H0])[cX3H1]

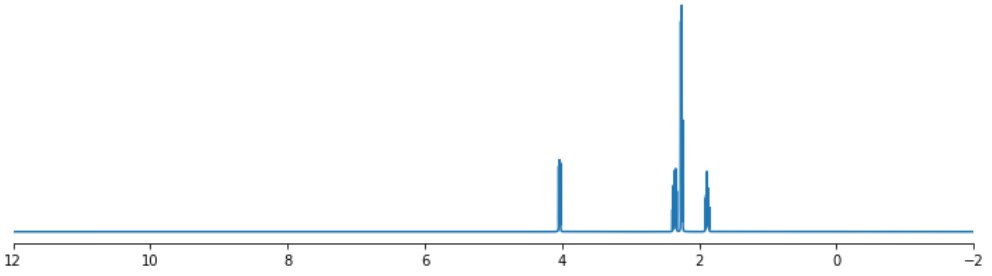


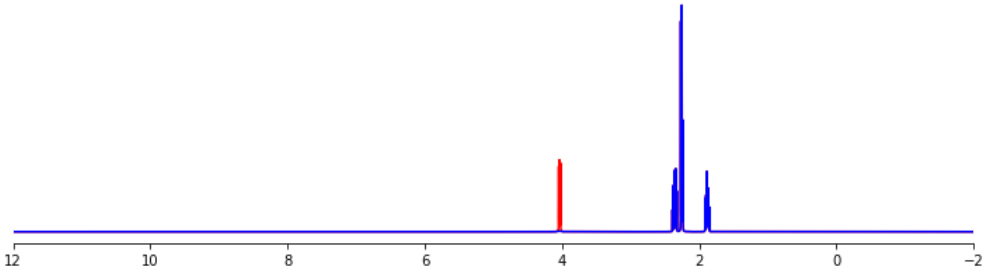
Top predicted substructures for the masked region(red):
0.4568 [cX3H1]([nX3H0])[cX3H1]
0.3189 [CX3H1](=[CX3H1])[cX3H0]
0.2989 [#6]1[#6][#6][#6][#6][#7]1
0.218 [#7][#6X3H0][#6X3H1]
0.2175 [#6H3][#7][#6X3]
0.2054 [#6X3H1][#7X3H0]
0.1683 [cX3H1]([nX2H0])[cX3H1]
0.1531 [#7X3][#6H3]

True structure: O=C1CCC(C(=O)O)N1

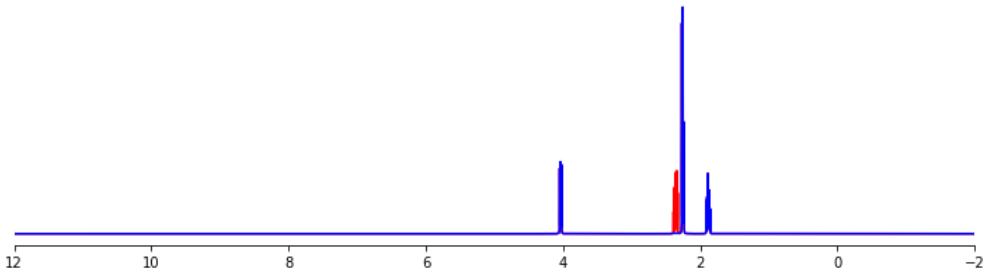






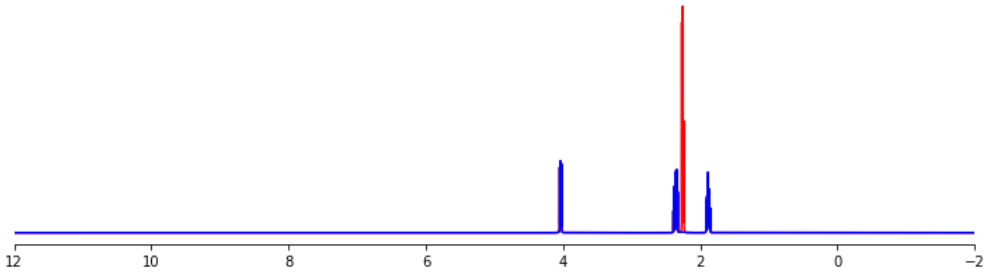


Top predicted substructures for the masked region(red):
0.4835 O=[CX3][CX4H]
0.4746 [#8]=[#6][#6H1][#6H1]
0.459 [CX4H](O)([CH])[CH]
0.4431 C1CC1O
0.4014 [#8]=[#6H0][#6H1]
0.3878 [#6X4H1][#6X4H1][#6X4H1]
0.3072 [#6H1][#6H1]
0.3057 [#8][#6][#6][#6][#6]=[#8]



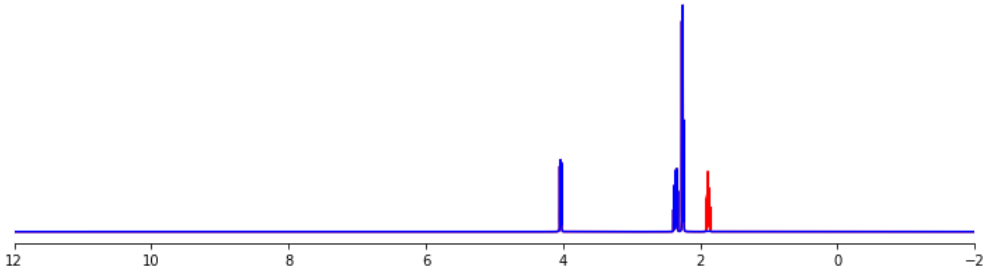
Top predicted substructures for the masked region(red):

0.3722 O=[CX3H0][CX4H2][CX4H2]
0.2984 [CX4H2]([CX4H2])[CX3H0]
0.2344 [#6H1][#6H2][#6][#6][#7]
0.2344 [OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H1]
0.2291 C1CC1O
0.2236 CCCCCC
0.2221 [#6X4H1][#6X4H1][#6X4H1]
0.1861 [#8][#6][#6][#6][#6]=[#8]



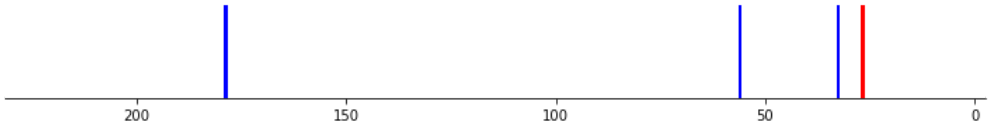
Top predicted substructures for the masked region(red):

0.4879 C1CC1O
0.3153 [#6X4H1][#6X4H1][#6X4H1]
0.2537 C1CC1
0.2417 O=[CX3H0][CX4H2][CX4H2]
0.2389 [OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H1]
0.2288 [#7][#6H1r3]
0.2274 [CX4H1]([CX4H1])([CX4H1])[CX3H0]
0.2245 CCCCCC



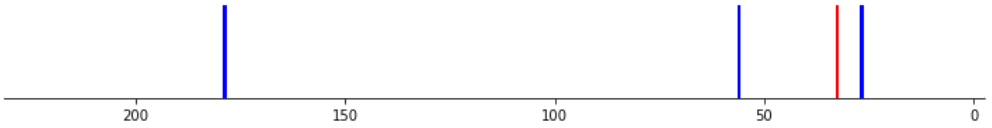
Top predicted substructures for the masked region(red):

0.3383 C1CC1O
0.3028 [CX4H2][CX4H2]
0.2952 [CX4H2]([CX4H2])[CX4H1]
0.2658 [#6H2][#6H1r3]
0.2601 [OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H1]
0.2597 CCCCCC
0.2443 [CX4H1]([CX4H1])([CX4H1])[CX3H0]
0.2286 [#8]=[#6][#6H1][#6H1]

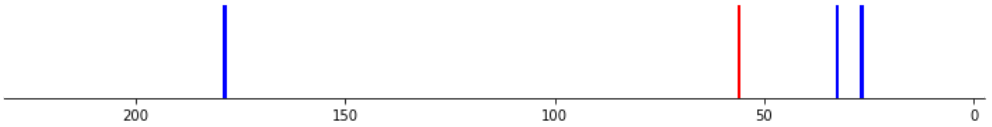


Top predicted substructures for the masked region(red):

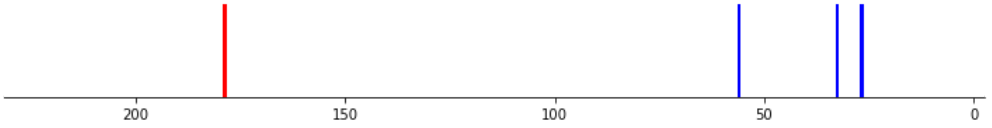
0.4927 C1CC1O
0.346 [#6X4H1][#6X4H1][#6X4H1]
0.3103 C1CC1
0.3046 O=[CX3H0][CX4H2][CX4H2]
0.2948 [CX4H2][CX4H2]
0.2726 [CX4H1]([CX4H1])([CX4H1])[CX3H0]
0.2591 [#8]=[#6][#6H1][#6H1]
0.24 CCCCCC



Top predicted substructures for the masked region(red):
0.4728 C1CC1O
0.3828 [#6X4H1][#6X4H1][#6X4H1]
0.2881 [#8]=[#6][#6H1][#6H1]
0.2784 [CX4H1]([CX4H1])([CX4H1])[CX3H0]
0.2774 [#7H2][#6H1]
0.2729 [#8][#6][#6][#6][#6]=[#8]
0.2645 [OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H1]
0.2603 C1CC1

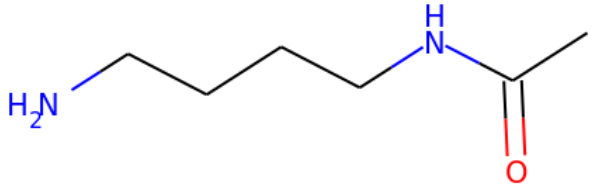


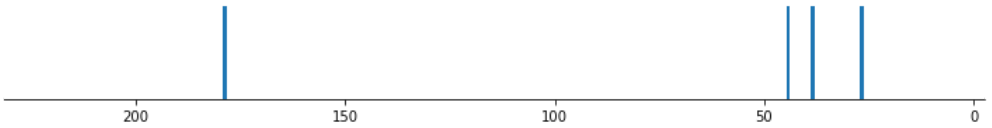
Top predicted substructures for the masked region(red):
0.5751 C1CC1O
0.3625 [#7H2][#6H1]
0.3559 [#6X4H1][#6X4H1][#6X4H1]
0.3275 [OX2H1][CX4H1]1[CX4H1][CX4H1]1
0.3226 [CX4H](O)([CH])[CH]
0.2811 [CX4H1]([CX4H1])([CX4H1])[CX3H0]
0.2809 [#8][#6][#6][#6][#6]=[#8]
0.246 [CX4H]O

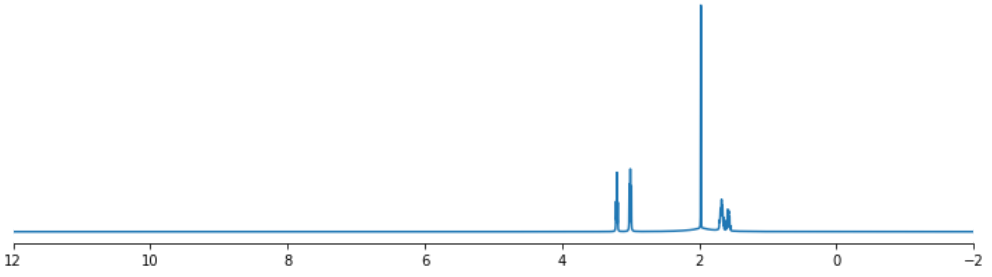


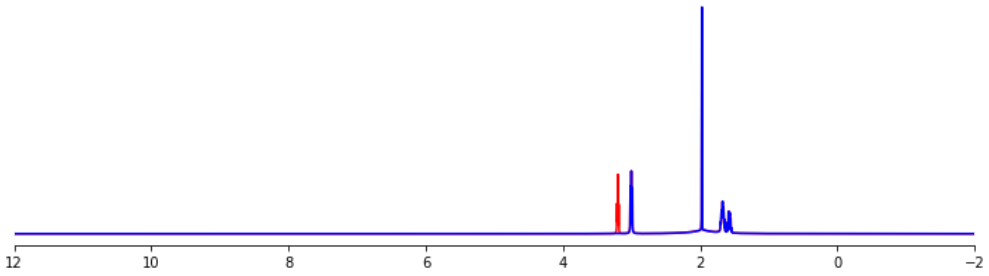
Top predicted substructures for the masked region(red):
0.9668 [CX3](=[OX1])C
0.9187 [CX3](=[OX1])O
0.9111 [#8]=[#6][#8]
0.8514 [CX4H2]CC=O
0.7581 O=[CX3][CX4H]
0.7448 [#8]=[#6H0][#6H1]
0.6172 [#7][#6][#6X3]
0.5962 [#8][#6][#6][#6][#6]=[#8]

True structure: CC(=O)NCCCCN

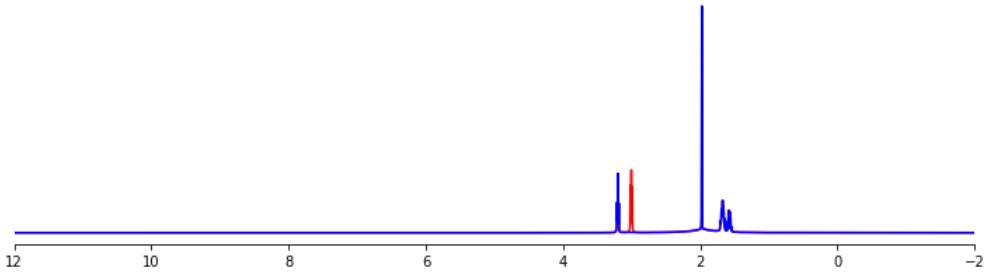




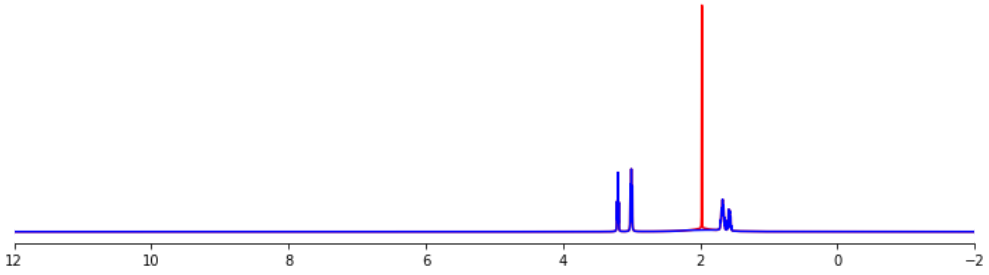




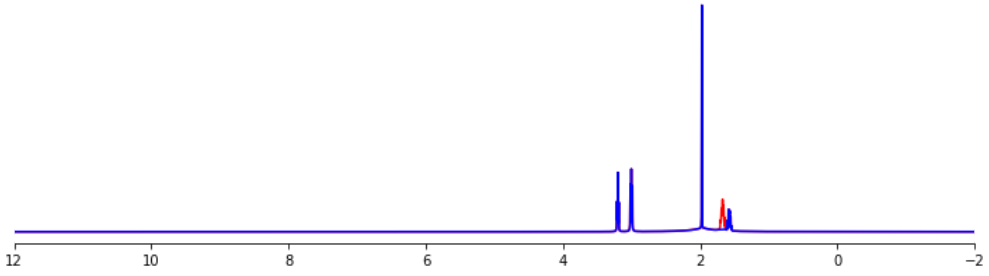
Top predicted substructures for the masked region(red):
0.4895 [CX4H2]CC=O
0.3635 [#7][#6][#6][#6][#7]
0.3062 [#7][#6][#6][#6][#6][#7]
0.3056 [#7][#6H2][#6H2][#6H1]
0.2836 [#6H1]
0.2624 [CX4H2]([NX3H1])[CX4H2]
0.2275 [CX4H3][CX3H0]
0.219 [#6H3][#7X3H0][#6X4H2][#6X4H2]



Top predicted substructures for the masked region(red):
0.495 [CX4H2]CC=O
0.3552 [#7H2][#6H2]
0.2959 [#7][#6][#6][#6][#6][#7]
0.2944 [#7][#6][#6][#6][#7]
0.2336 [#7][#6H2][#6H2][#6H1]
0.2242 O=[CX3H0][CX4H2][CX4H2]
0.216 [#6H3][#7X3H0][#6X4H2][#6X4H2]
0.2032 [#7X3][#6H3]

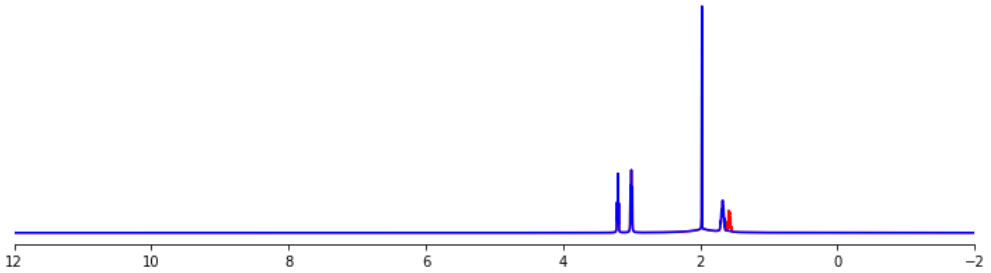


Top predicted substructures for the masked region(red):
0.9037 [CX4H3][CX3H0]
0.5562 [CX4H3][CX3]
0.4717 [OX1H0]=[CX3H0][CX4H3]
0.4686 [#6H3][#6H0]
0.3778 [#7][#6][#6H3]
0.3531 [#7][#6][#6][#6][#7]
0.2692 [#7][#6H2][#6H2][#6H1]
0.2267 [#7][#6][#6][#6][#6][#7]

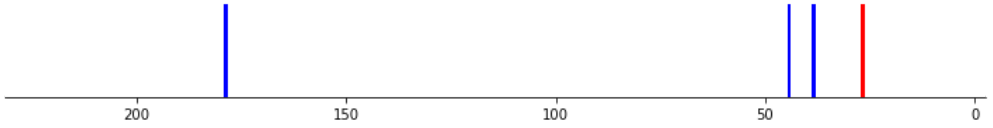


Top predicted substructures for the masked region(red):
0.3031 [CX4H2]CC=O
0.2383 [#7][#6][#6][#6][#6][#7]
0.2187 [#7][#6][#6][#6][#7]
0.2057 [#6H3][#7X3H0][#6X4H2][#6X4H2]
0.171 [#7X3][#6H3]

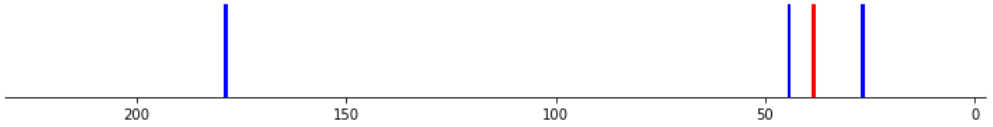
0.1408 [CX4H2]([CX4H2])[CX4H2]
0.1379 O=[CX3H0][CX4H2][CX4H2]
0.1309 [#6H1]



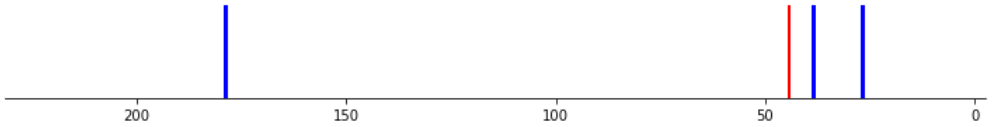
Top predicted substructures for the masked region(red):
0.2888 [CX4H2]CC=O
0.2523 [#7][#6][#6][#6][#6][#7]
0.2218 [#7][#6][#6][#6][#7]
0.2072 [#6H3][#7X3H0][#6X4H2][#6X4H2]
0.1571 [CX4H3][CX3H0]
0.1523 [#6H1]
0.1402 [#7X3][#6H3]
0.1362 O=[CX3H0][CX4H2][CX4H2]



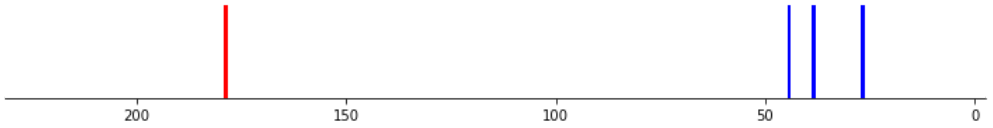
Top predicted substructures for the masked region(red):
0.8868 [CX4H3][CX3H0]
0.554 [CX4H2]([CX4H2])[CX4H2]
0.5235 [CX4H3][CX3]
0.397 [#6H3][#6H0]
0.3899 [CX4H2]CC=O
0.3841 [OX1H0]=[CX3H0][CX4H3]
0.3655 [#7][#6][#6H3]
0.3158 [CX4H3][#6]



Top predicted substructures for the masked region(red):
0.4266 [CX4H2]CC=O
0.3376 [#7][#6][#6][#6][#7]
0.3289 [#7][#6][#6][#6][#6][#7]
0.2855 [CX4H2]([NX3H2])[CX4H2]
0.2721 [#7][#6H2][#6H2][#6H1]
0.2503 O=[CX3H0][CX4H2][CX4H2]
0.241 [#7H2][#6H2]
0.2152 [#6H3][#7X3H0][#6X4H2][#6X4H2]



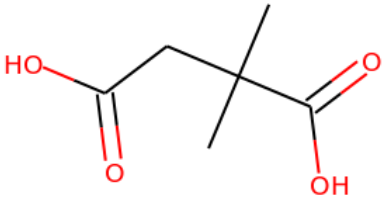
Top predicted substructures for the masked region(red):
0.5935 [#7H2][#6H2]
0.4263 [CX4H2]([NX3H2])[CX4H2]
0.3963 [#7][#6][#6][#6][#7]
0.3678 [#7][#6][#6][#6][#6][#7]
0.3637 [CX4H2]CC=O
0.3221 [CX4H2]([NX3H1])[CX4H2]
0.3189 [#7][#6H2][#6H2][#6H1]
0.2252 [#6H3][#7X3H0][#6X4H2][#6X4H2]

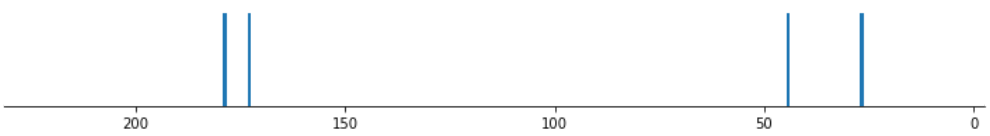


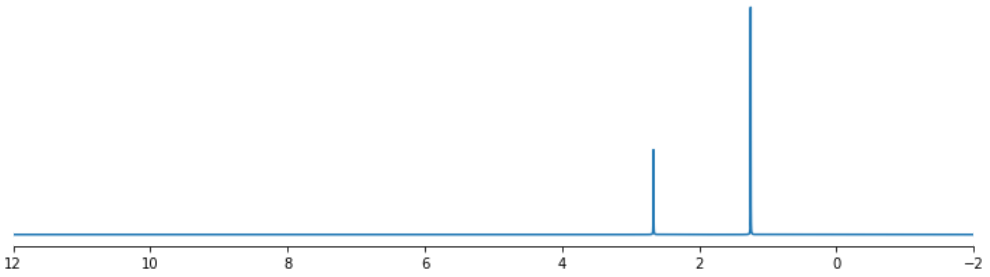
Top predicted substructures for the masked region(red):
0.9572 [CX3](=[OX1])C
0.907 [CX4H3][CX3H0]
0.8975 [CX4H2]CC=O
0.5935 [CX4H2][CX3]=O
0.5559 [CX4H3][CX3]
0.5483 O=[CX3H0][CX4H2][CX4H2]

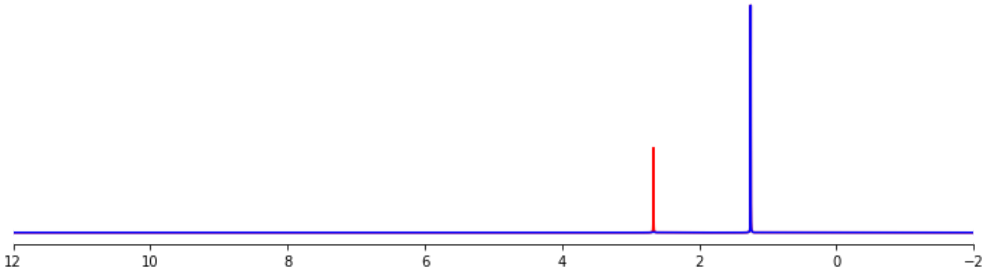
0.4937 [CX4H2]([CX4H2])[CX4H2]
0.4718 [OX1H0]=[CX3H0][CX4H3]

True structure: CC(C)(CC(=O)O)C(=O)O

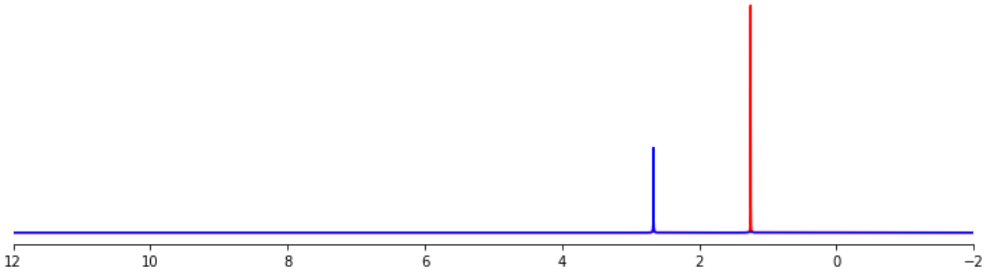




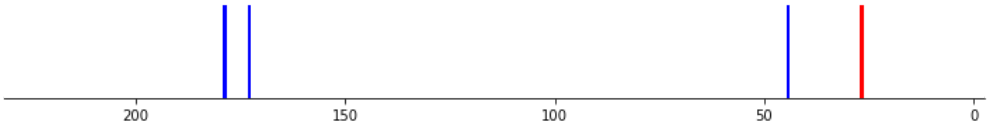




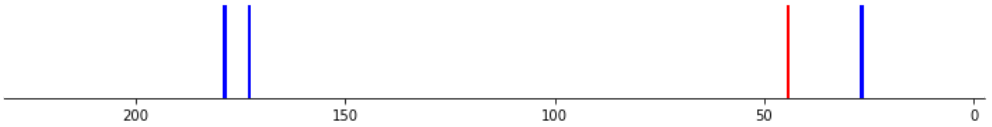
Top predicted substructures for the masked region(red):
0.5201 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.4718 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.4692 [CX4H2]([#6])[#6]
0.4628 [#8X1]=[#6X3][#6H2][#6H0]
0.3702 [#8][#6][#6H2]
0.3471 [OX2H0][CX3H0][CX4H2]
0.3169 [#8][#6][#6][#6][#6]=[#8]
0.3094 [CX4H2][CX3]=O



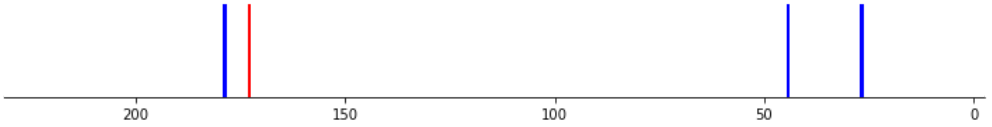
Top predicted substructures for the masked region(red):
0.9359 [CX4H3][CX4H0]
0.7808 [CX4H3][CX4H0][CX4H3]
0.7002 [#6H3][#6][#6X3]
0.5708 [#6X3][#6][#6][#6H3]
0.5633 [#6H3][#6H0]
0.5173 [#6H3][#6][#6]
0.424 [OX1H0]=[CX3H0][CX4H2][CX4H0]
0.3856 [CH3]CC[OH]



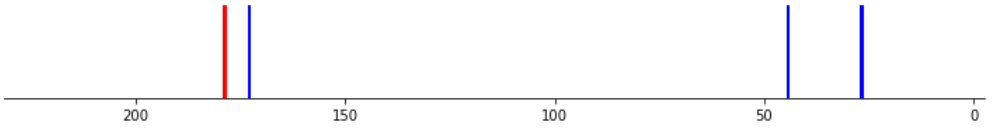
Top predicted substructures for the masked region(red):
0.3718 [CX4H3][#6]
0.3595 [#6H3][#6][#6X3]
0.2895 [CH3]CC[OH]
0.2437 [CX4H2]CC=O
0.2186 [CH3][#6][#8]
0.2066 [#8][#6][#6][#6][#6]=[#8]
0.1703 [#6X3][#6][#6][#6H3]
0.1306 [#8][#6H0][#6H1]



Top predicted substructures for the masked region(red):
0.3429 [#8][#6][#6][#6][#6]=[#8]
0.2773 [CX4H2]([#6])[#6]
0.2695 [CX4H2]CC=O
0.2693 [#6H3][#6][#6X3]
0.2309 [#8X1]=[#6X3][#6H2][#6H0]
0.2169 OCC[CH2]
0.2146 [#8]=[#6][#6][#6][#6]=[#8]
0.1977 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]

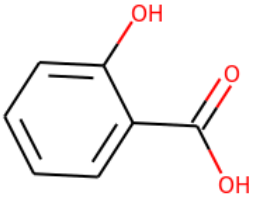


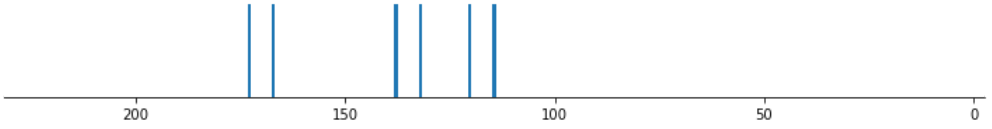
Top predicted substructures for the masked region(red):
0.584 [#6H3][#6][#6X3]
0.5151 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.298 [CX4H3][CX4H0][CX4H3]
0.2968 [OX2H0][CX3H0][CX4H2]
0.1852 [#6X3][#6][#6][#6H3]
0.1623 [CX4H3][#6]
0.1537 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.1326 [#8X1]=[#6X3][#6H2][#6H0]

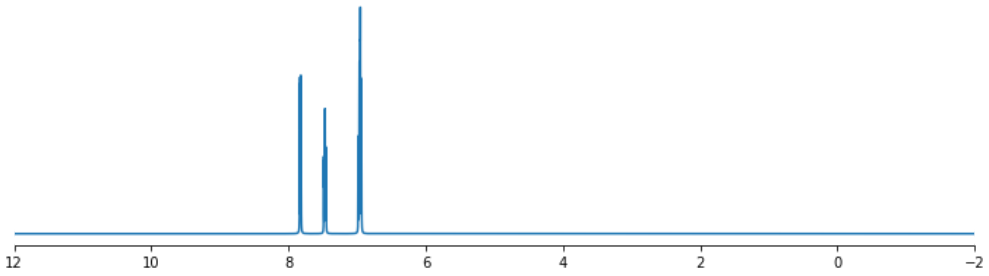


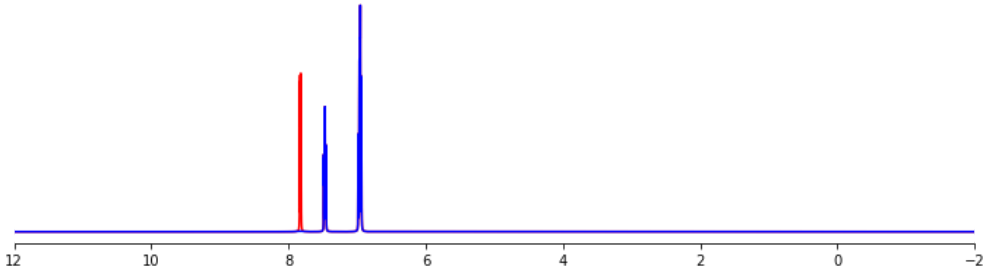
Top predicted substructures for the masked region(red):
0.6554 [#6H3][#6][#6X3]
0.4915 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.2633 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.2307 [CX4H3][CX4H0][CX4H3]
0.1951 [#6X3][#6][#6][#6H3]
0.1927 [CX4H2]CC=O
0.174 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.1558 [#8]=[#6][#6][#6][#6]=[#8]

True structure: O=C(O)c1ccccc1O



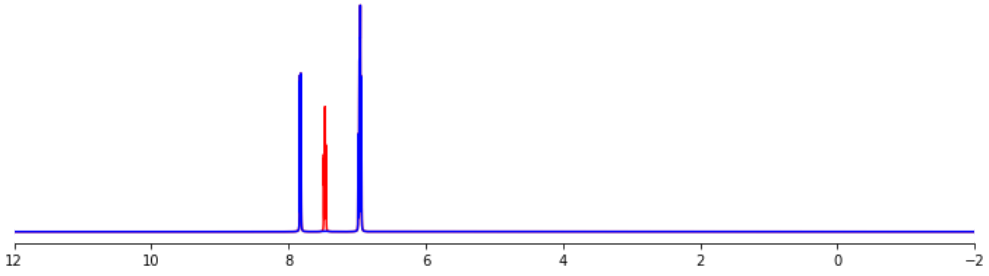






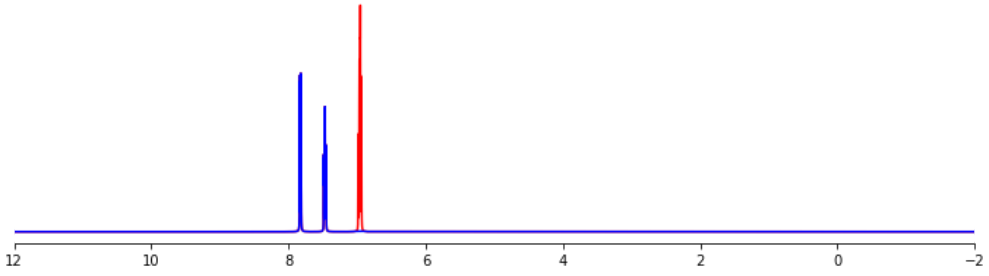
Top predicted substructures for the masked region(red):

0.2822 [OX2H][cX3]:[c]
0.2732 [#8]=[#6H0][#6H1]
0.2559 [#8]1[#6][#6][#6][#6][#6]1
0.1982 [cX3H1]([oX2H0])[cX3H1]
0.1964 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1669 [#8]=[#6][#6H1][#6H1]
0.1631 [#6H1][#6H1]
0.1548 [cH]cO



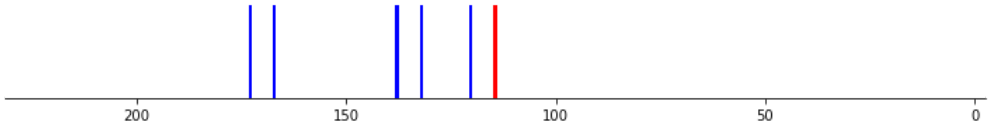
Top predicted substructures for the masked region(red):

0.4429 [#8]=[#6][#6H1][#6H1]
0.3669 [OX2H][cX3]:[c]
0.3236 [OX1H0]=[cX3H0][cX3H1]
0.288 [#8]1[#6][#6][#6][#6][#6]1
0.28 [cH]cO
0.2551 [cX3H1]([oX2H0])[cX3H1]
0.2493 [#8]=[#6H0][#6H1]
0.1824 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]

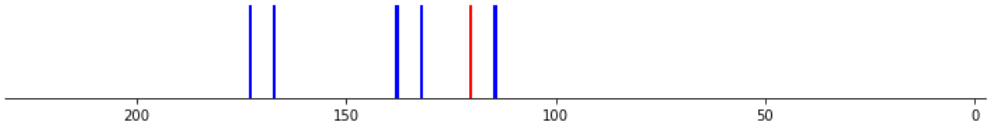


Top predicted substructures for the masked region(red):

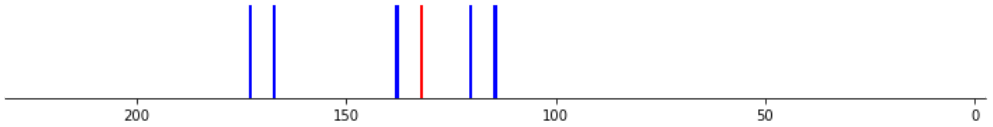
0.5027 [OX2H][cX3]:[c]
0.4455 [cH]cO
0.2668 [#8]1[#6][#6][#6][#6][#6]1
0.2413 [cX3H1]([oX2H0])[cX3H1]
0.2308 [#8]=[#6][#6H1][#6H1]
0.2249 [#8]=[#6H0][#6H1]
0.2121 [#6]1[#6][#6][#6][#6][#6]1
0.2056 [OX1H0]=[cX3H0][cX3H1]



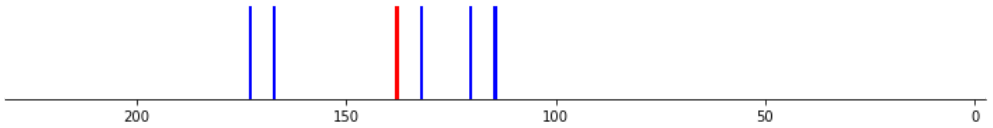
Top predicted substructures for the masked region(red):
0.444 [OX2H][cX3]:[c]
0.3274 [cX3H1]([oX2H0])[cX3H1]
0.2792 [#8]1[#6][#6][#6][#6][#6]1
0.274 [cH]cO
0.1819 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1772 [#6H1][#6H1]
0.1713 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1566 [#6]1[#6][#6][#6][#6][#6]1



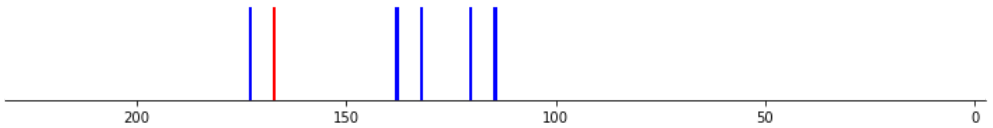
Top predicted substructures for the masked region(red):
0.3887 [OX2H][cX3]:[c]
0.2677 [#8]1[#6][#6][#6][#6][#6]1
0.2393 [cH]cO
0.2301 [cX3H1]([oX2H0])[cX3H1]
0.1827 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1581 [#6H1][#6H1]
0.1519 [#8]=[#6H0][#6H1]
0.1109 [cX3H0][cX3H1][cX3H0][OX2H1]



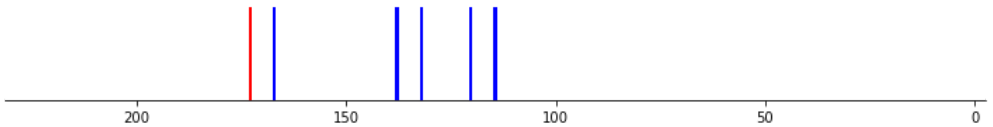
Top predicted substructures for the masked region(red):
0.4008 [OX2H][cX3]:[c]
0.2574 [cH]cO
0.2558 [#8]1[#6][#6][#6][#6][#6]1
0.1619 [#8]=[#6H0][#6H1]
0.1618 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1363 [cX3H1]([oX2H0])[cX3H1]
0.1183 O=[#6][#6]=[#6X3]
0.1183 [#6H1][#6H1]



Top predicted substructures for the masked region(red):
0.376 [OX2H][cX3]:[c]
0.2692 [#8]1[#6][#6][#6][#6][#6]1
0.2237 [cH]cO
0.1917 [cX3H1]([oX2H0])[cX3H1]
0.1555 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1343 [#8]=[#6H0][#6H1]
0.1289 [#6H1][#6H1]
0.1188 O=[#6][#6]=[#6X3]



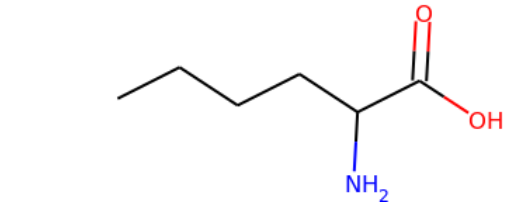
Top predicted substructures for the masked region(red):
0.4651 [OX1H0]=[cX3H0][cX3H1]
0.3558 [#8]=[#6H0][#6H1]
0.3534 [#8]1[#6][#6][#6][#6][#6]1
0.3067 [OX2H][cX3]:[c]
0.2493 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.2342 [cX3H1]([oX2H0])[cX3H1]
0.224 [#8]=[#6][#6H1][#6H1]
0.2238 O=[cX3]

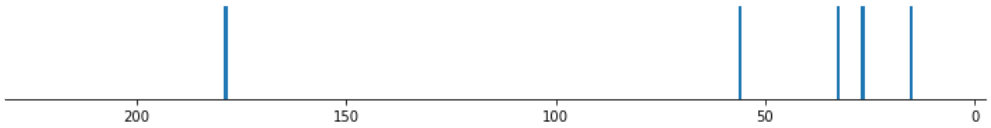


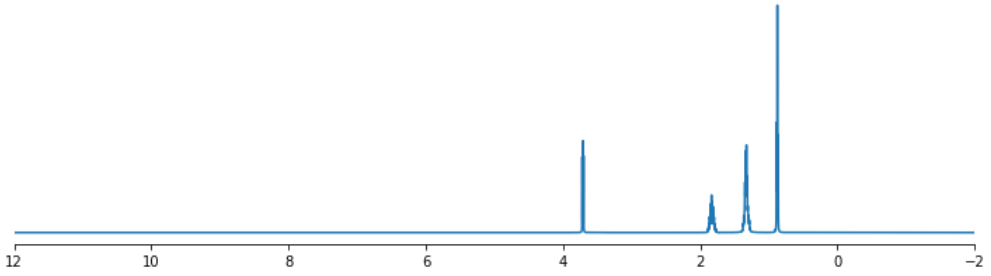
Top predicted substructures for the masked region(red):

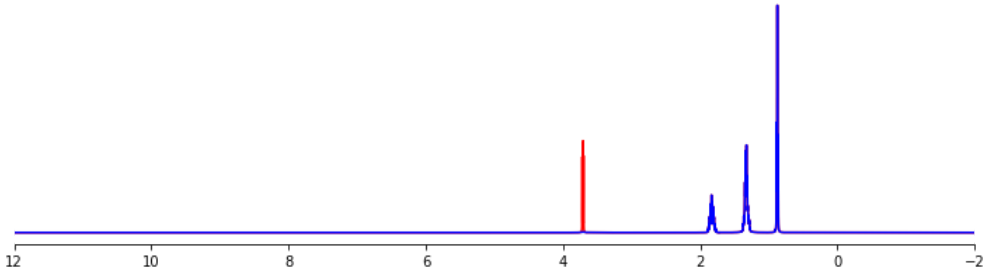
```
0.5661   [#8]=[#6H0][#6H1]
0.5525   [OX1H0]=[cX3H0][cX3H1]
0.5054   [#8]=[#6][#6H1][#6H1]
0.4268   [CX3](=[OX1])C
0.3178   [#8]1[#6][#6][#6][#6][#6]1
0.2122   O=[cX3]
0.2007   [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1882   [CX3](=O)[OX2H1]
```

True structure: CCCCC(N)C(=O)O



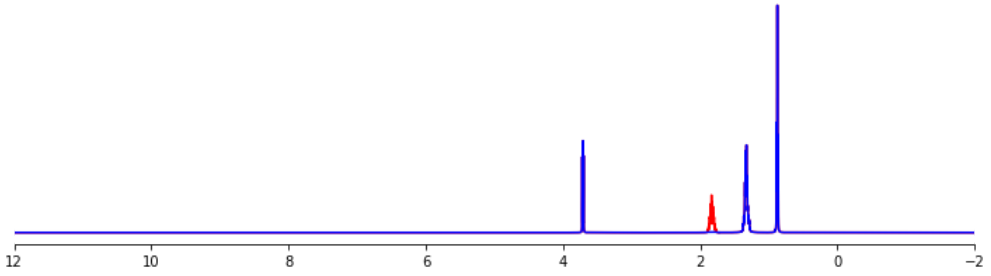






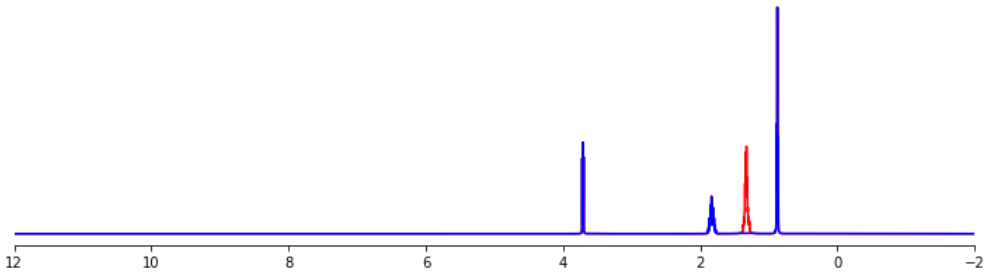
Top predicted substructures for the masked region(red):

```
0.3595   [CX4H2][CX4H2]
0.3338   [#7H2][#6X4H1][#6X3]
0.3337   [CX4H2]([CX4H2])[CX4H1]
0.234    [CX4H2]([CX4H2])[CX4H2]
0.2106   [#7H2][#6H1]
0.1858   [CX4H1]([CX4H2])([CX4H2])[CX3H0]
0.1855   [CX4H2]([CX4H3])[CX4H2]
0.1529   [#8]=[#6H0][#6H1]
```

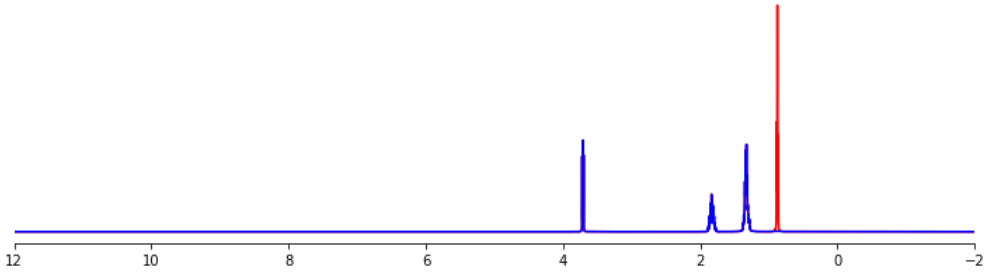


Top predicted substructures for the masked region(red):

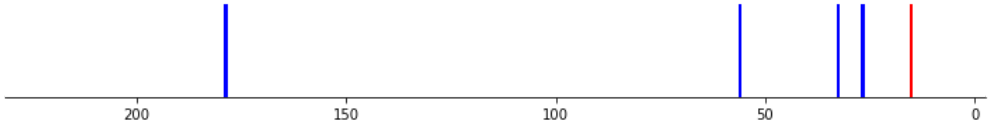
```
0.5636   [CX4H2]([CX4H2])[CX4H1]
0.3829   [CX4H2][CX4H2]
0.264    [#7H2][#6H1]
0.2455   [CX4H2]([CX4H2])[CX4H2]
0.2388   [#6H1][#6H2]
0.2379   [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.1908   [CX4H2]([CX4H3])[CX4H1]
0.1792   [#7H2][#6X4H1][#6X3]
```



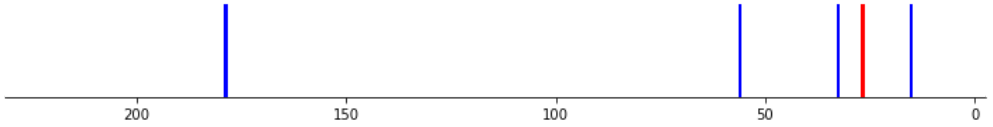
Top predicted substructures for the masked region(red):
0.5498 [CX4H2]([CX4H2])[CX4H1]
0.4826 [CX4H2][CX4H2]
0.4395 OCC[CH2]
0.4098 [CX4H2]([CX4H3])[CX4H2]
0.2866 [CX4H2]([CX4H2])[CX4H2]
0.2325 [#7H2][#6H1]
0.2302 [#6H1][#6H2]
0.1834 [CX4H1]([CX4H2])([CX4H2])[CX3H0]



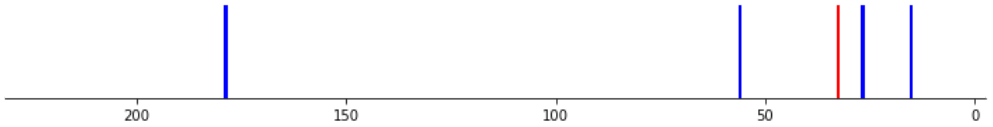
Top predicted substructures for the masked region(red):
0.5666 [CX4H2]([CX4H3])[CX4H1]
0.5223 [#6H3][#6][#6]
0.487 [#7H2][#6X4H1][#6X3]
0.4693 [#7H2][#6H1]
0.4365 [#6X3][#6][#6][#6H3]
0.3926 [#6H1][#6H2]
0.3638 [#6H1]
0.3183 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]



Top predicted substructures for the masked region(red):
0.8582 [CX4H3][CX4H2]
0.6298 [CX4H2]([CX4H3])[CX4H1]
0.5504 [CX4H2]([CX4H3])[CX4H2]
0.2658 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.2633 [#8]=[#6H0][#6H1]
0.2009 [#8]=[#6][#6H1][#6H1]
0.1912 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.1894 [CX4H1]([CX4H2])([CX4H2])[CX3H0]

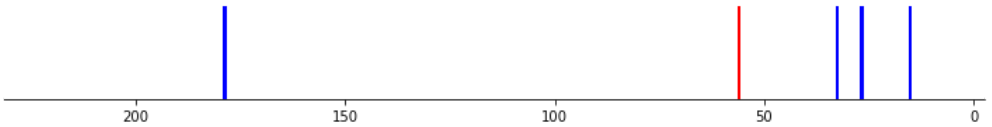


Top predicted substructures for the masked region(red):
0.4732 [CX4H2][CX4H2]
0.4222 [CX4H2]([CX4H3])[CX4H2]
0.3438 [CX4H2]([CX4H2])[CX4H2]
0.2116 [CX4H2]([CX4H2])[CX4H1]
0.1847 OCC[CH2]
0.156 [#8]=[#6][#6H1][#6H1]
0.1437 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.1428 [CX4H1]([CX4H2])([CX4H2])[CX3H0]

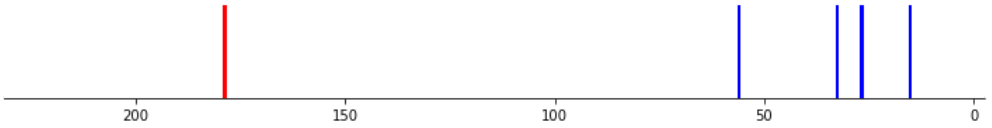


Top predicted substructures for the masked region(red):
0.5929 [CX4H2][CX4H2]
0.5008 [CX4H2]([CX4H2])[CX4H1]
0.4306 [CX4H2]([CX4H2])[CX4H2]

0.2621 [CX4H2]([CX4H3])[CX4H2]
0.1698 [#7H2][#6H1]
0.1632 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.1386 [OX2H1]
0.116 [CX3](=[OX1])O

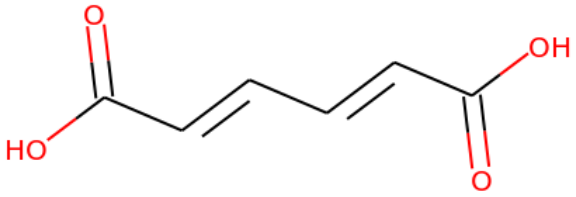


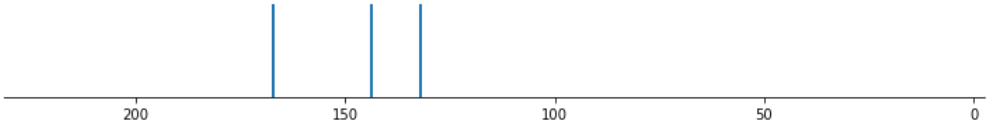
Top predicted substructures for the masked region(red):
0.8324 [#7H2][#6X4H1][#6X3]
0.8318 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.6287 [#7H2][#6H1]
0.3045 [CX4H2]([CX4H2])[CX4H1]
0.2983 [#8]=[#6H0][#6H1]
0.2562 [#7][#6][#6X3]
0.2539 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.2384 O=[CX3][CX4H]

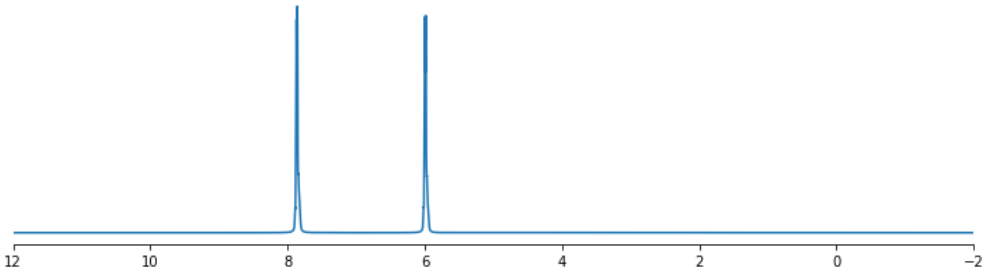


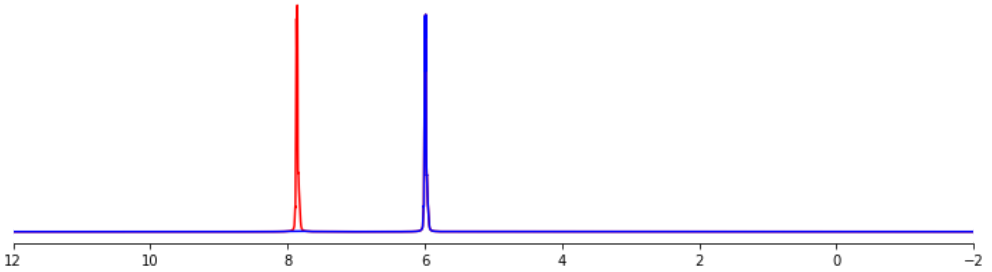
Top predicted substructures for the masked region(red):
0.9859 [CX3](=[OX1])C
0.9759 [#7H2][#6X4H1][#6X3]
0.9736 [#8]=[#6H0][#6H1]
0.9705 O=[CX3][CX4H]
0.926 [CX4H2]CC=O
0.9155 [CX3](=[OX1])O
0.8962 [#8]=[#6][#8]
0.8868 [CX4H1]([NX3H2])([CX4H2])[CX3H0]

True structure: O=C(O)C=CC=CC(=O)O



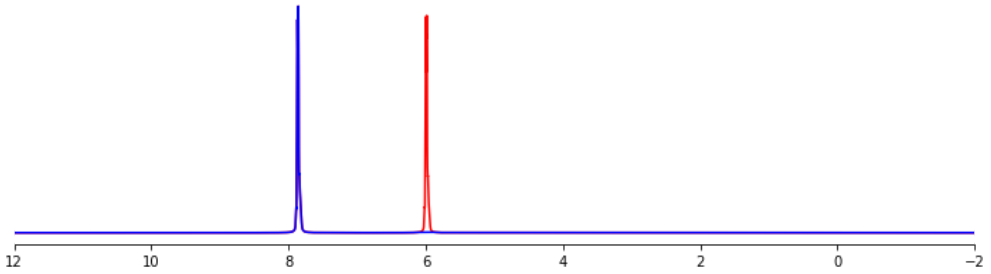




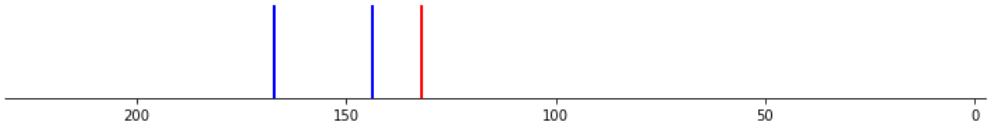


Top predicted substructures for the masked region(red):
0.4287 [#8][#6H1][#6H1]
0.3993 [#6H1][#6H1]
0.3612 O=C[CX3H]

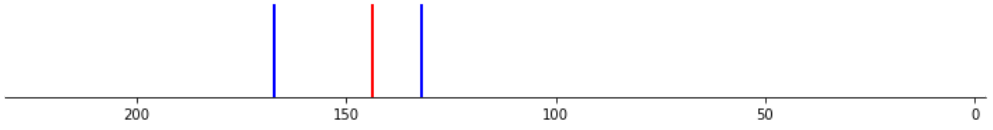
0.2987 [#8]=[#6][#6H1]=[#6H1]
0.2613 [OX2H1]
0.2571 [CX4H](O)CO
0.2048 [CX4H]O
0.186 [CX3H1](=[NX2H0])[CX3H1]



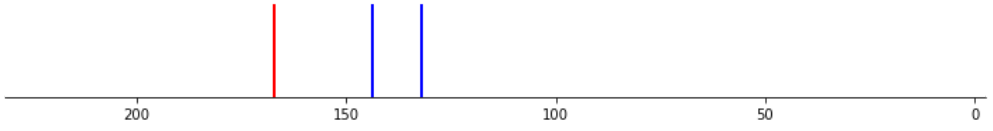
Top predicted substructures for the masked region(red):
0.7601 [CHX3](=C)C
0.7399 [#8][#6][#6]=[#6X3]
0.7232 [CHX3]=[CHX3]
0.5668 [#8][#6H1][#6H1]
0.5423 O=[#6][#6]=[#6X3]
0.4011 [#8]=[#6][#6H1]=[#6H1]
0.3322 [#6H1][#6H1]
0.2974 [CX4H](O)CO



Top predicted substructures for the masked region(red):
0.2494 [#8][#6H1][#6H1]
0.2346 [OX2H1]
0.1937 [#8][#6H0][#6H1]
0.1876 [#8][#6][#6]=[#6X3]
0.1857 [CX3H1](=[NX2H0])[CX3H1]
0.1668 [#6H1][#6H1]
0.1612 [CHX3]=[CHX3]
0.1244 [CX3](=O)[OX2H1]

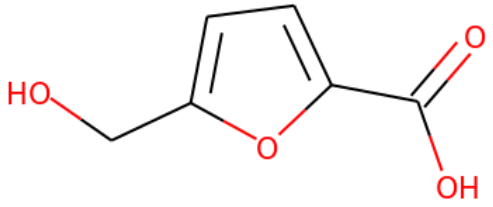


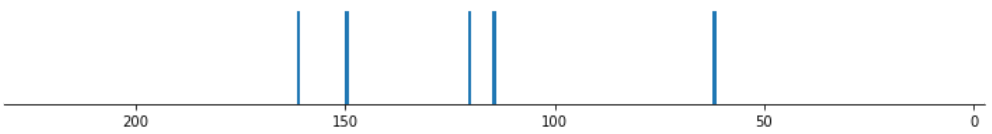
Top predicted substructures for the masked region(red):
0.2743 [#8][#6H0][#6H1]
0.2699 [#8][#6H1][#6H1]
0.1966 [OX2H1]
0.185 [CX3H1](=[NX2H0])[CX3H1]
0.1832 [#6H1][#6H1]
0.1644 [#8][#6][#6]=[#6X3]
0.1456 [CX3](=O)[OX2H1]
0.1041 [CHX3]=[CHX3]

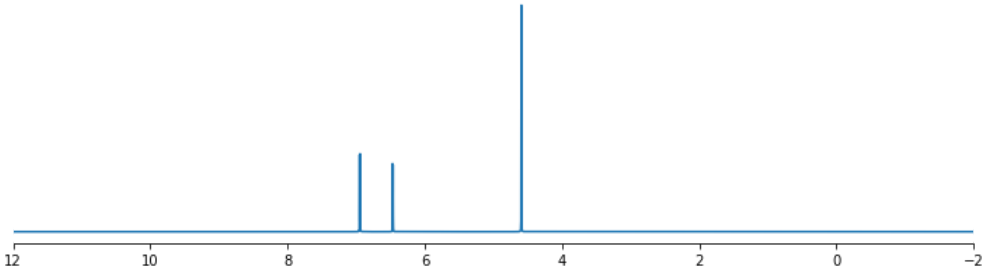


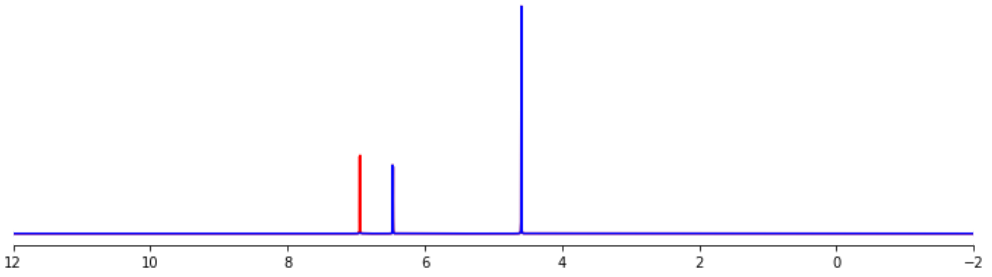
Top predicted substructures for the masked region(red):
0.6136 O=[#6][#6]=[#6X3]
0.5556 [CX3](=[OX1])C
0.5291 [CX3](=O)[OX2H1]
0.4429 O=C[CX3H]
0.4116 [#8]=[#6][#6H1]=[#6H1]
0.3175 [#8][#6][#6]=[#6X3]
0.3063 [#8][#6H0][#6H1]
0.2844 [#8]=[#6][#8]

True structure: O=C(O)c1ccc(CO)o1

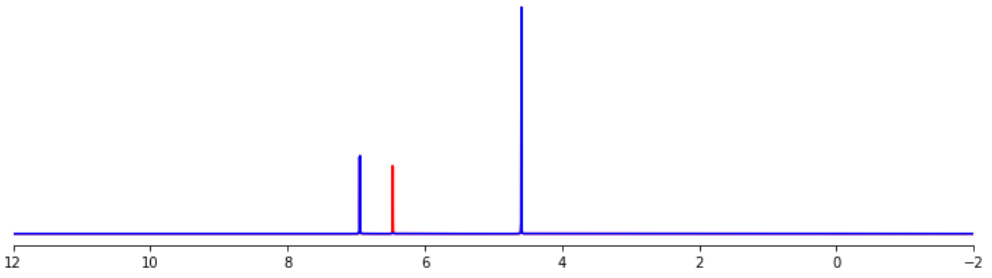




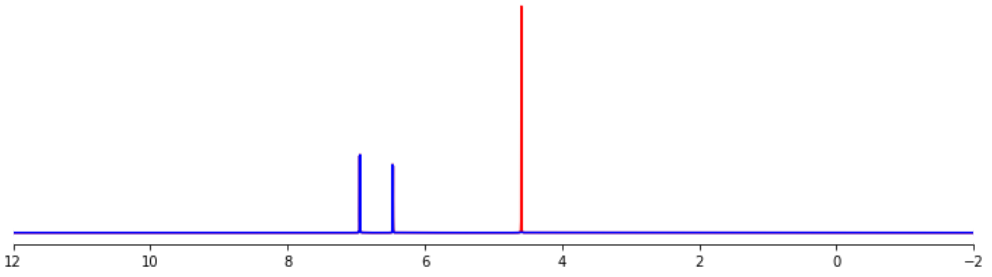




Top predicted substructures for the masked region(red):
0.3964 [cH][cH]
0.3416 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.3037 [#6H1][#6H1]
0.2941 [#8][#6H1][#6H1]
0.2334 [cX3H1]([cX3H1])[cX3H0]
0.1873 [#8][#6][#6]=[#8]
0.1705 [cX3H1]([oX2H0])[cX3H1]
0.1696 [CX3](=O)[OX2H1]

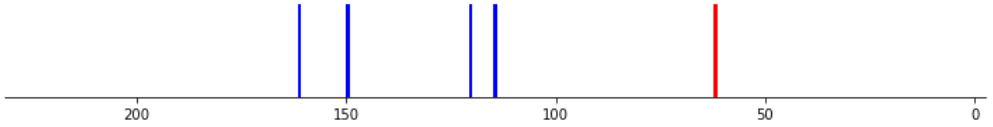


Top predicted substructures for the masked region(red):
0.3404 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.2442 [#8][#6][#6]=[#6X3]
0.2409 [#8][#6H1][#6H1]
0.2103 [#6H1][#6H1]
0.1935 [#8][#6][#6H2]
0.1882 [#8][#6][#6]=[#8]
0.1689 [CX3](=O)[OX2H1]
0.1433 [#8][#6][#6][#6][#6]=[#8]

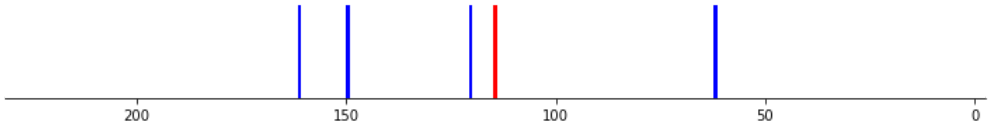


Top predicted substructures for the masked region(red):
0.8532 [OX2H1][CX4H2][#6X3H0]
0.7032 [CX4H2]([#6])[O]
0.6255 [CX4H2]([OX2H1])[cX3H0]
0.5606 [#6X3][#6H2][#8]
0.4937 [#8][#6][#6H2]
0.3987 [OX2H1][CX4H2][#6X3H0][#8X2H0]
0.3949 [#8][#6][#6H2][#8]

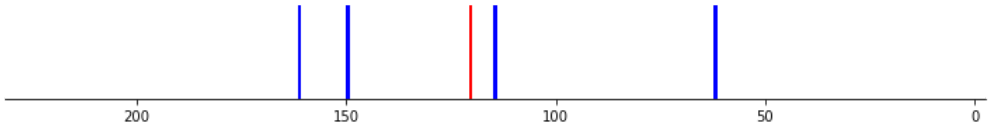
0.3177 [#8][#6][#6]=[#6X3]



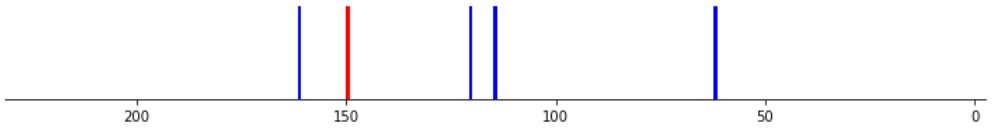
Top predicted substructures for the masked region(red):
0.7551 [CX4H2]([#6])[O]
0.5624 [#6X3][#6H2][#8]
0.4167 [#6H1][#6H1]
0.3944 [#8][#6][#6H2]
0.3397 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.3149 [OX2H1][CX4H2][#6X3H0][#8X2H0]
0.265 [#8][#6H1][#6H1]
0.2548 [OX2H1][CX4H2][#6X3H0]



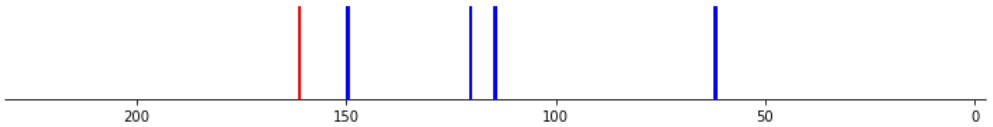
Top predicted substructures for the masked region(red):
0.3423 [#6H1][#6H1]
0.3405 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.3171 [#8][#6][#6H2]
0.2515 [cH][cH]
0.2263 [#8][#6H1][#6H1]
0.1787 [cX3H0][cX3H1][cX3H0][OX2H1]
0.1757 [#8][#6][#6]=[#8]
0.1646 [CX3](=O)[OX2H1]



Top predicted substructures for the masked region(red):
0.3258 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.2824 [#8][#6][#6H2]
0.2202 [#8][#6][#6]=[#6X3]
0.1837 [#8][#6][#6]=[#8]
0.168 [#6H1][#6H1]
0.1654 [CX3](=O)[OX2H1]
0.161 [cX3H0][cX3H1][cX3H0][OX2H1]
0.1459 [#8][#6][#6][#6][#6]=[#8]

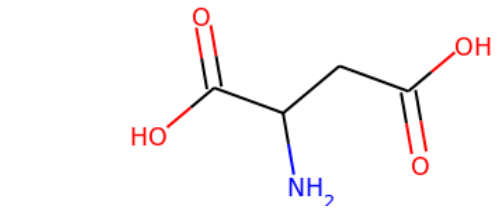


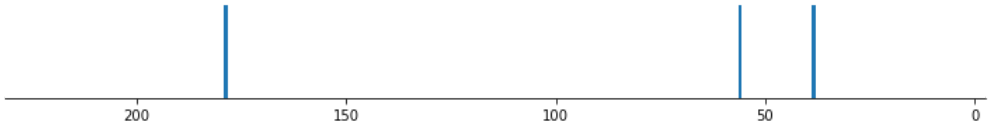
Top predicted substructures for the masked region(red):
0.3416 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.3153 [cH][cH]
0.2629 [#8][#6][#6]=[#6X3]
0.2355 [#6H1][#6H1]
0.193 [#8][#6][#6]=[#8]
0.182 [CX3](=O)[OX2H1]
0.1759 [cX3H1]([oX2H0])[cX3H1]
0.1564 [#8][#6H1][#6H1]

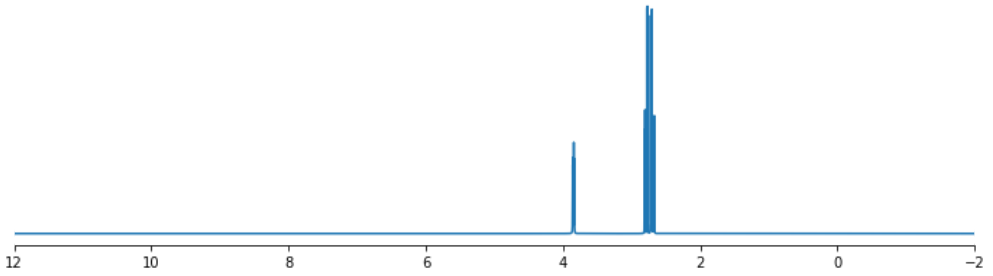


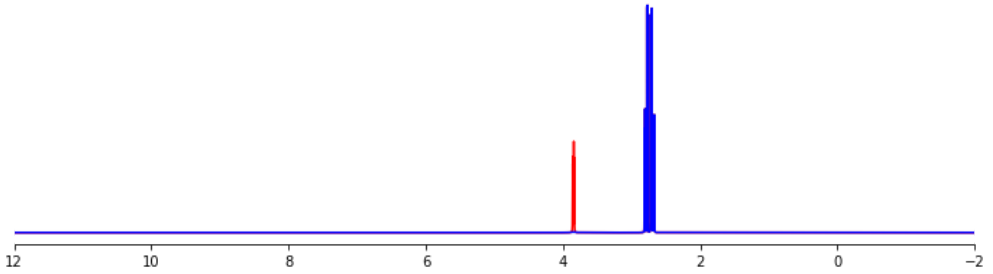
Top predicted substructures for the masked region(red):
0.4778 [cH][cH]
0.3412 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.2323 [#8][#6][#6]=[#6X3]
0.2012 [cX3H0][cX3H1][cX3H1][cX3H0]
0.2 [CX3](=O)[OX2H1]
0.1982 [#8][#6][#6]=[#8]
0.1891 [CX3](=[OX1])O
0.1791 [#6H1][#6H1]

True structure: NC(CC(=O)O)C(=O)O

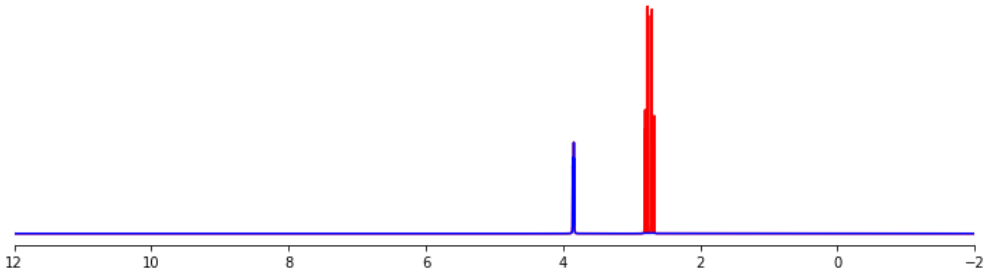




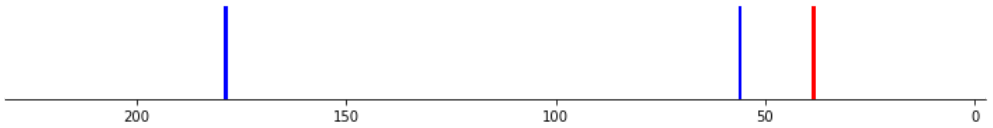




Top predicted substructures for the masked region(red):
0.5902 [#8]=[#6][#6H2][#6H1]
0.5474 O[CX4H]([CX4H2])[CX4H1]
0.4531 [CX4H1]([OX2H0])([CX4H2])[CX4H1]
0.3847 [CX4H2]([CX4H1])[CX3H0]
0.3844 O=[CX3H0][CX4H2][CX4H1]
0.3392 [#7H2][#6X4H1][#6X3]
0.3244 [#6H1][#6H2]
0.2968 C1OC1

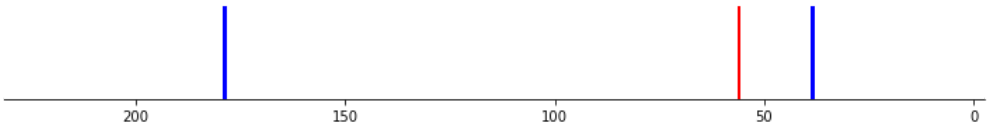


Top predicted substructures for the masked region(red):
0.7457 O=[CX3H0][CX4H2][CX4H1]
0.7182 [#8][#6][#6H2]
0.6788 [CX4H2]([CX4H1])[CX3H0]
0.6648 [#8]=[#6][#6H2][#6H1]
0.605 OCC[CH2]
0.5641 O[CX4H]([CX4H2])[CX4H1]
0.5628 [CX4H2][CX3]=O
0.5139 [#8][#6][#6][#6][#6]=[#8]



Top predicted substructures for the masked region(red):
0.6576 [#8]=[#6][#6H2][#6H1]
0.522 O=[CX3H0][CX4H2][CX4H1]
0.462 [CX4H2]([CX4H1])[CX3H0]
0.3414 [#8][#6][#6][#6][#6]=[#8]

```
0.2862   [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.2805   [CX4H1]([OX2H0])([CX4H2])[CX4H1]
0.2576   O[CX4H]([CX4H2])[CX4H1]
0.2162   [OX1H0]=[CX3H0]([#8])[CX4H2]
```

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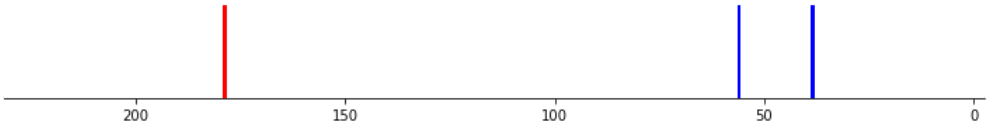
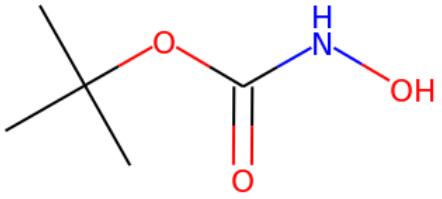
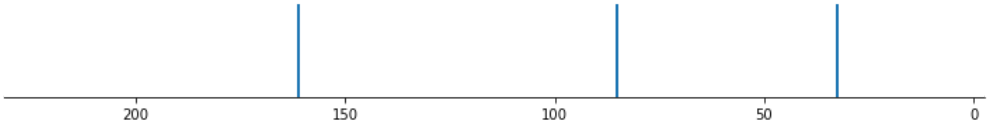
Top predicted substructures for the masked region(red):
0.52     O[CX4H]([CX4H2])[CX4H1]
0.4945   [CX4H1]([OX2H0])([CX4H2])[CX4H1]
0.4349   C1OC1
0.3619   [#7H2][#6H1]
0.3527   [OX2H0]1[CX4H2][CX4H1]1[CX4H1]
0.3509   [#8][#6][#6H2]
0.3407   [#8][#6][#6][#6][#6]=[#8]
0.3379   [#8][#6][#6][#6X3]
```

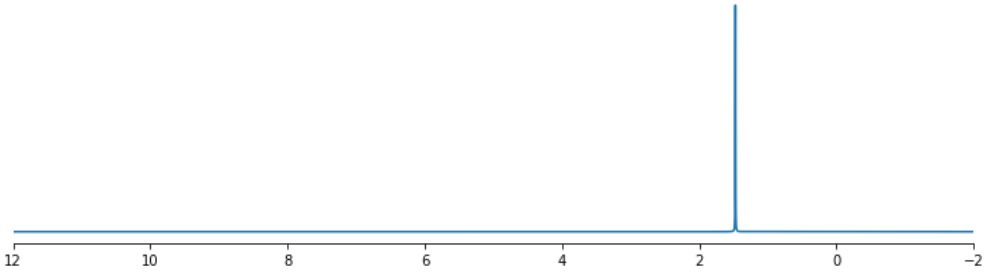


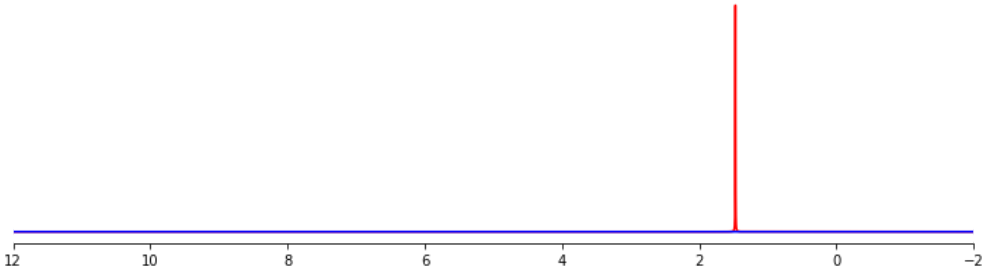

```
Top predicted substructures for the masked region(red):
0.9766   [CX3](=[OX1])C
0.8727   [CX3](=[OX1])O
0.8383   [#8]=[#6][#8]
0.7851   [CX3](=O)[OX2H1]
0.7543   O=[CX3H0][CX4H2][CX4H1]
0.7452   [CX4H2][CX3]=O
0.7319   [#8]=[#6][#6H2][#6H1]
0.6985   [#8][#6][#6][#6][#6]=[#8]
```

```
True structure: CC(C)(C)OC(=O)NO
```



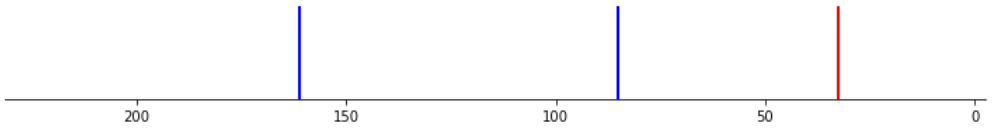




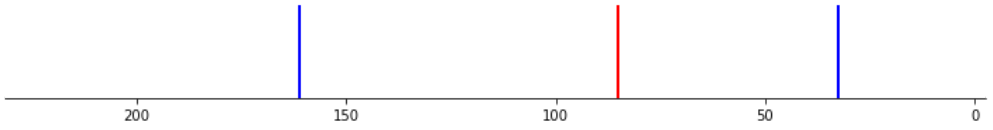



```
Top predicted substructures for the masked region(red):
0.7995   [CH3][#6][#8]
0.7624   [#6H3][#6][#6]
0.6698   [#6H3][#6H0]
0.6508   [#8][#6H0][#6H1]
```

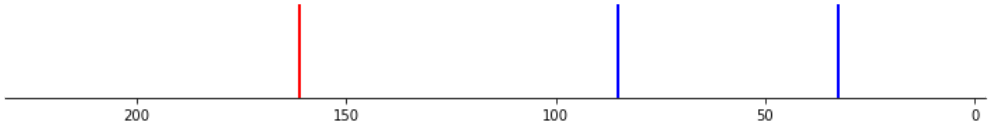
0.637 [CX4H3][CX4]O
0.6265 [CX4H3][CX4H0]
0.6155 [CX4H3][#6]
0.4455 [#6H0]([#6H3])([#6H3])[#8]



Top predicted substructures for the masked region(red):
0.419 [#8][#6H0][#6H1]
0.3815 [CH3][#6][#8]
0.3199 [#8]=[#6][#8]
0.3164 [CX3](=[OX1])O
0.307 [CX4]([CX4H3])([CX4H3])[CX4H3]
0.28 [CX3](=O)[OX2H1]
0.2789 [#6H0]([#6H3])([#6H3])[#8]
0.2202 [CX4H3][#6]

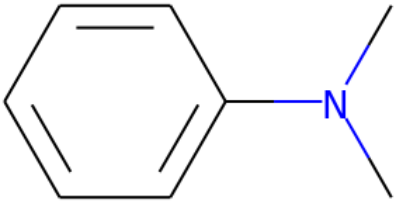


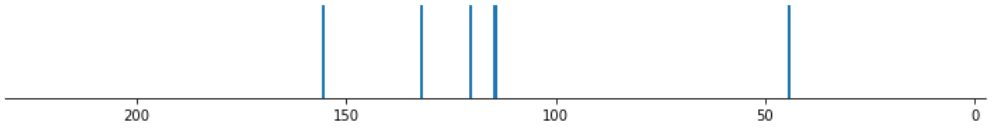
Top predicted substructures for the masked region(red):
0.7129 [CX4H3][CX4H0]([CX4H3])[OX2H0]
0.5829 [#8][#6H0][#6H1]
0.5384 [#6H0]([#6H3])([#6H3])[#8]
0.5067 [CH3][#6][#8]
0.4062 [#8][#6][#6][#8]
0.386 [#7X3H2]
0.3497 [#6H1]
0.2276 [#6H3][#6][#6X3]

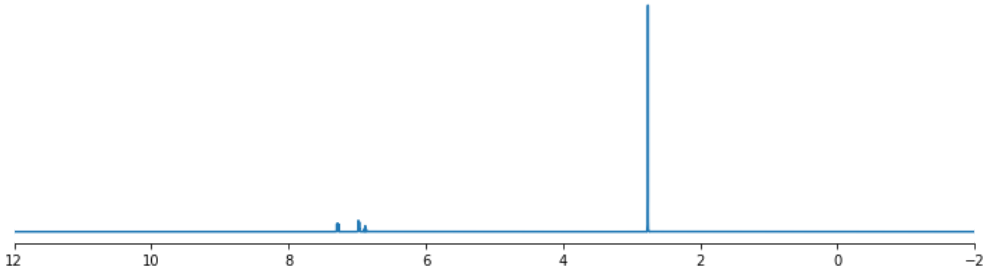


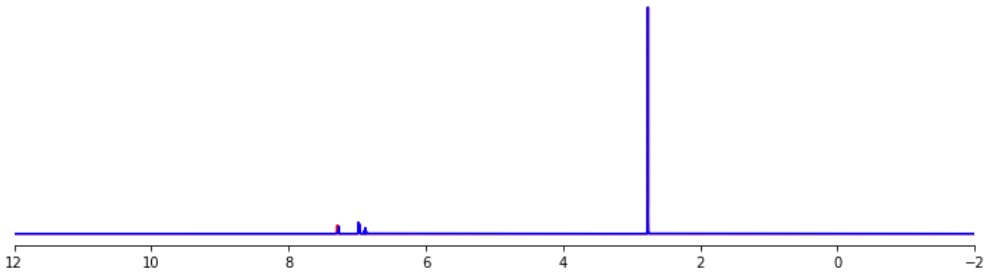
Top predicted substructures for the masked region(red):
0.8499 [CX3](=[OX1])O
0.8292 [#6H0]([#6H3])([#6H3])[#8]
0.7903 [#8]=[#6][#8]
0.7567 [CX4H3][CX4H0]([CX4H3])[OX2H0]
0.5069 [CX4H3][CX4H0][CX4H3]
0.3795 [CX3](=O)[OX2H1]
0.3221 [CX4]([CX4H3])([CX4H3])[CX4H3]
0.2898 [#6H3][#6][#6X3]

True structure: CN(C)c1ccccc1

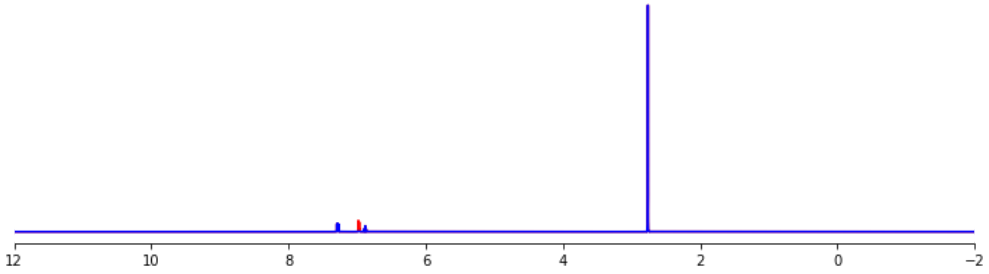




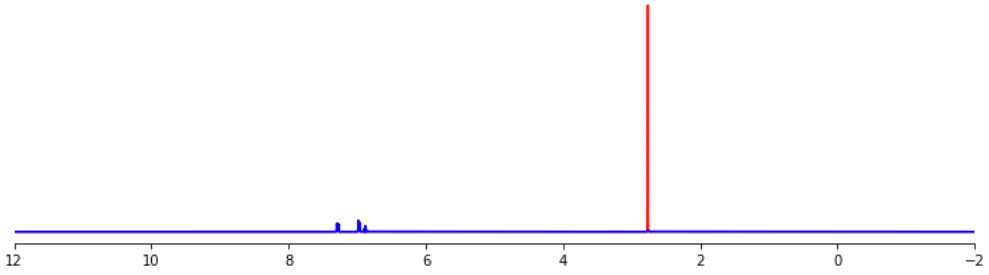




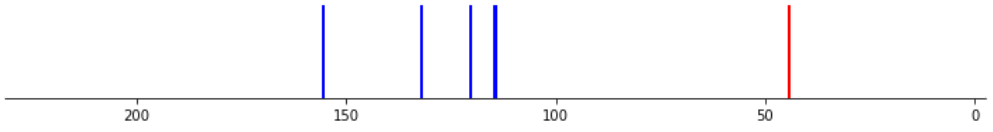
Top predicted substructures for the masked region(red):
0.3686 [#6]1[#6][#6][#6][#6][#7]1
0.3607 [#6H3][#7][#6X3]
0.334 [#6H1][#6H1]
0.247 [cX3H1]([cX3H1])[cX3H1]
0.2381 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.2343 [#7][#6X3H0][#6X3H1]
0.223 [#7X3H0]
0.2148 [#6X3][#7][#6X3]



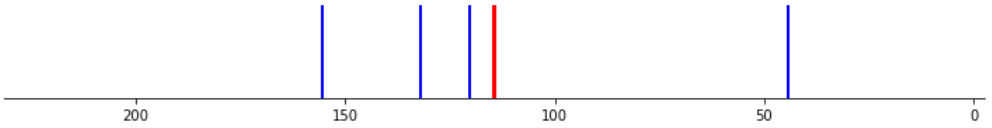
Top predicted substructures for the masked region(red):
0.4056 [#6H1][#6H1]
0.3787 [#6H3][#7][#6X3]
0.3559 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.3481 [#6]1[#6][#6][#6][#6][#7]1
0.333 [cX3H1]([cX3H1])[cX3H1]
0.261 [#7][#6X3H0][#6X3H1]
0.2605 [cH][cH]
0.2396 [cX3H1]([cX3H1])[cX3H0]



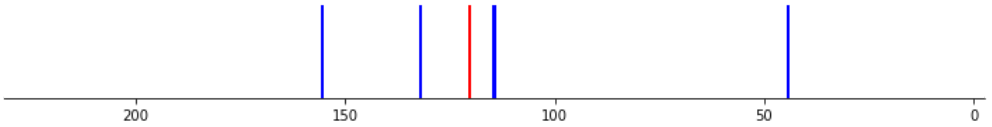
Top predicted substructures for the masked region(red):
0.7569 [#6H3][#7][#6X3]
0.7378 [#7X3][#6H3]
0.5428 [#6H3][#7]
0.3083 [#6]1[#6][#6][#6][#6][#7]1
0.2646 [CX4H3][NX3H0]
0.2603 [#7X3H0]
0.2394 [#7][#6X3H0][#6X3H1]
0.2311 [CX4H3]



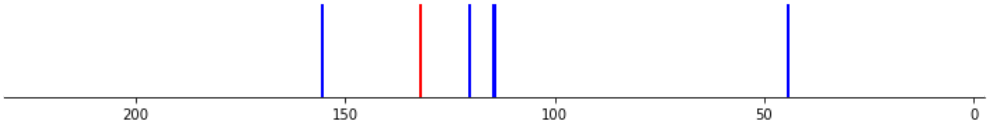
Top predicted substructures for the masked region(red):
0.7363 [#6H3][#7][#6X3]
0.6502 [#7X3][#6H3]
0.4777 [#6H3][#7]
0.332 [#6X3][#6H2][#6X3]
0.3145 [CX4H3][NX3H0]
0.3124 [#7X3H0]
0.2309 [#7X3][#6H2]
0.1701 [#6H3][#7][#6H2]



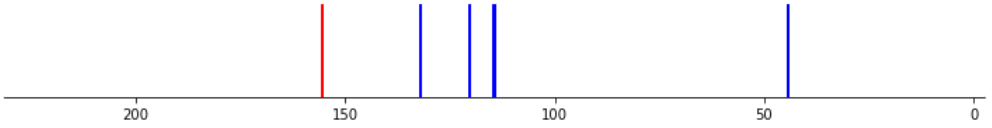
Top predicted substructures for the masked region(red):
0.4119 [#6H3][#7][#6X3]
0.3069 [#6]1[#6][#6][#6][#6][#7]1
0.2711 [#6X3][#7][#6X3]
0.2615 [#7][#6X3H0][#6X3H1]
0.2327 [#7X3H0]
0.2286 [cX3H1]([cX3H1])[cX3H0]
0.2163 [#7][#6][#6X3]
0.2115 [#6]1[#6][#6][#6][#7]1



Top predicted substructures for the masked region(red):
0.3514 [#6H3][#7][#6X3]
0.2552 [#7X3H0]
0.2543 [#6]1[#6][#6][#6][#6][#7]1
0.221 [#6X3][#7][#6X3]
0.2128 [#7][#6X3H0][#6X3H1]
0.2026 [#7H][#6X3H1]
0.1758 [#6H1][#6H1]
0.1726 [#7][#6][#6X3]

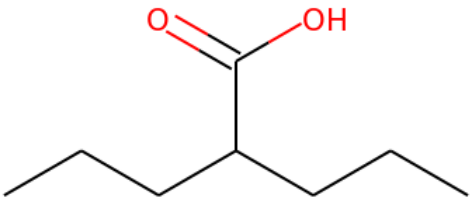


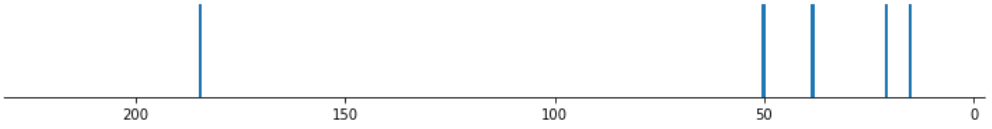
Top predicted substructures for the masked region(red):
0.3574 [#6H1][#6H1]
0.356 [#6]1[#6][#6][#6][#6][#7]1
0.3304 [#6H3][#7][#6X3]
0.3242 [#7][#6X3H0][#6X3H1]
0.2577 [#7][#6][#6X3]
0.2323 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.2183 [#6X3][#7][#6X3]
0.2177 [#7][#6H0][#6H1]

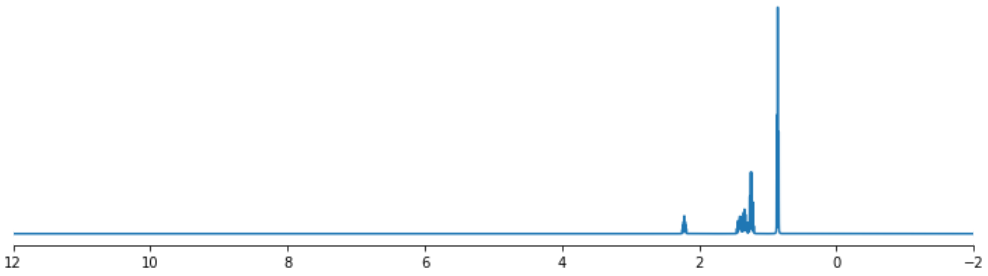


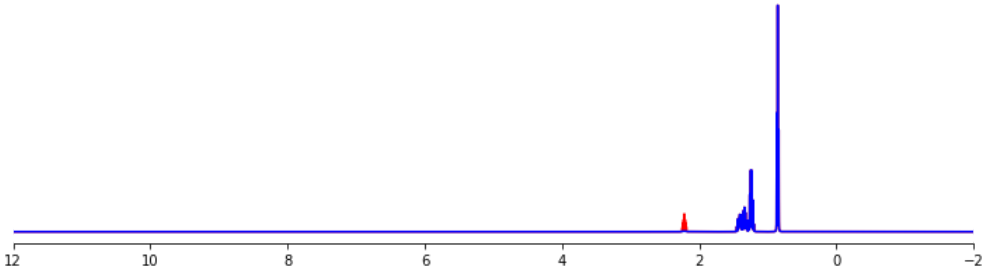
Top predicted substructures for the masked region(red):
0.4302 [#6]1[#6][#6][#6][#6][#7]1
0.4138 [#6H3][#7][#6X3]
0.3361 [#7][#6X3H0][#6X3H1]
0.2878 [#6H1][#6H1]
0.2285 [#7][#6H0][#6H1]
0.1799 [cX3H1]([cX3H1])[cX3H0]
0.1502 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.137 [CX4H3]

True structure: CCCC(CCC)C(=O)O



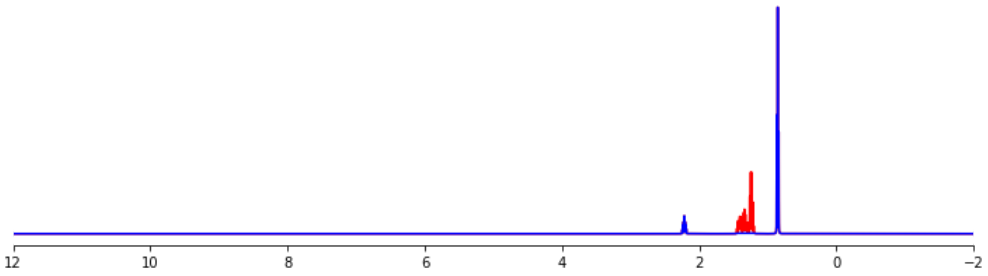






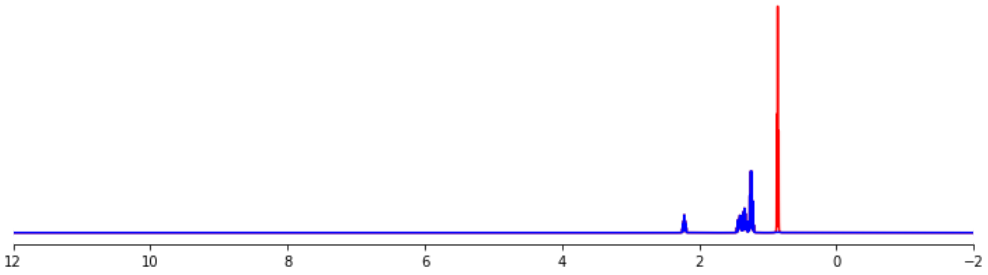
Top predicted substructures for the masked region(red):

0.1979 [CX4H2]CC=O
0.1674 [#6H1]([#6H2])[#6H2]
0.145 [#6H1]
0.1381 [OX1H0]=[CX3H0][CX4H1]([CX4H2])[CX4H2]
0.1118 [#8]=[#6H0][#6H1]
0.0971 [CX4H2][CX3]=O
0.0888 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.0841 CCCCCC



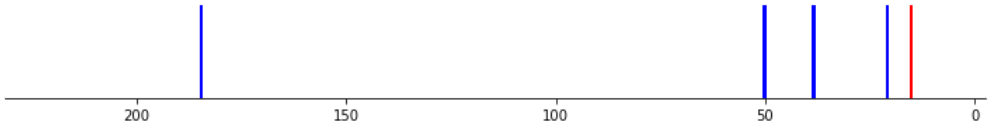
Top predicted substructures for the masked region(red):

0.7596 [CX4H2]([CX4H3])[CX4H2]
0.5662 [CX4H2][CX4H2]
0.4545 OCC[CH2]
0.3718 [CX4H2]([CX4H2])[CX4H1]
0.2793 [#6H1][#6H2]
0.2774 CCCCCC
0.2751 [#8]=[#6H0][#6H1]
0.2384 O=[CX3][CX4H]

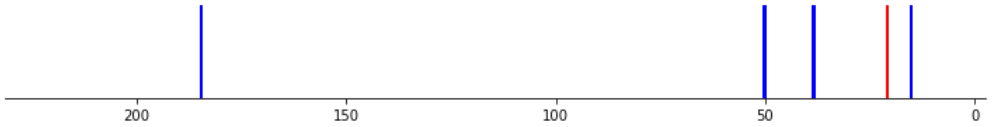


Top predicted substructures for the masked region(red):

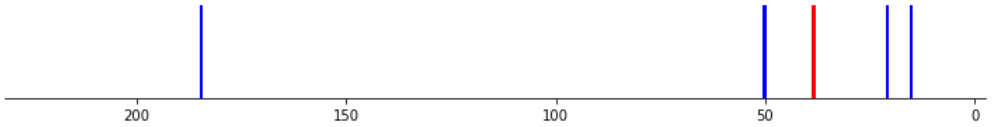
0.4082 [CX4H2]([CX4H3])[CX4H2]
0.2131 [#6X3][#6][#6][#6H3]
0.2011 CCCCCC
0.1883 [#8]=[#6H0][#6H1]
0.1601 [OX1H0]=[CX3H0][CX4H1]([CX4H2])[CX4H2]
0.1422 [CX4H2]CC=O
0.1374 [#6H1][#6H2]
0.0847 [CX4H2][CX4H2]



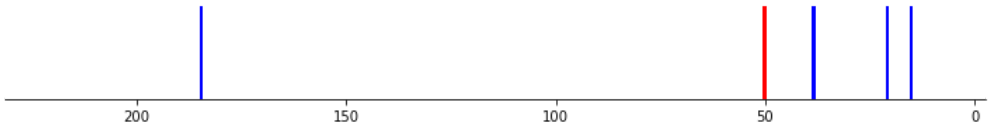
Top predicted substructures for the masked region(red):
0.9185 [CX4H2]([CX4H3])[CX4H2]
0.8197 [CX4H3][CX4H2]
0.3635 [CX4H2][CX4H2]
0.2659 [#8]=[#6H0][#6H1]
0.2191 O=[CX3][CX4H]
0.2049 [CX4H2]CC=O
0.1316 [CX4H2]([CX4H3])[CX4H1]
0.0672 [#6H3][#6][#6X3]



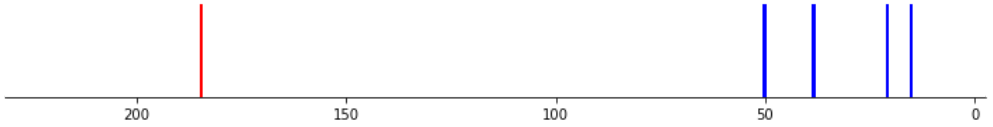
Top predicted substructures for the masked region(red):
0.7842 [CX4H2]([CX4H3])[CX4H2]
0.2256 [CX4H2][CX4H2]
0.2169 [#8]=[#6H0][#6H1]
0.1876 [CX4H2]CC=O
0.1843 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.177 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.1253 O=[CX3][CX4H]
0.0826 OCC[CH2]



Top predicted substructures for the masked region(red):
0.3174 [CX4H2]([CX4H3])[CX4H2]
0.2931 [CX4H2][CX4H2]
0.2244 CCCCCC
0.2215 [CX4H2]CC=O
0.1425 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.1068 [#8]=[#6H0][#6H1]
0.0846 [CX4H2][CX3]=O
0.0824 [#6H1][#6H2]

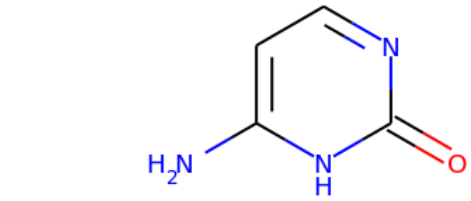


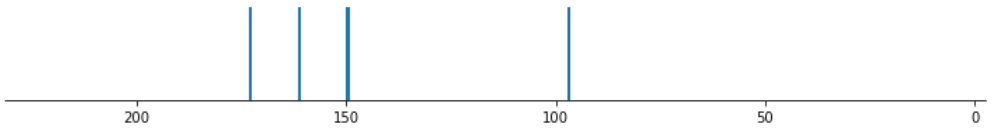
Top predicted substructures for the masked region(red):
0.2177 [#8]=[#6H0][#6H1]
0.2074 [#6H1][#6H2]
0.1686 [#6H1]
0.1554 [OX1H0]=[CX3H0][CX4H1]([CX4H2])[CX4H2]
0.1364 [CX4H2]CC=O
0.1304 [#6H1]([#6H2])[#6H2]
0.1096 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.101 [CX4H1]([CX4H2])([CX4H2])[CX3H0]

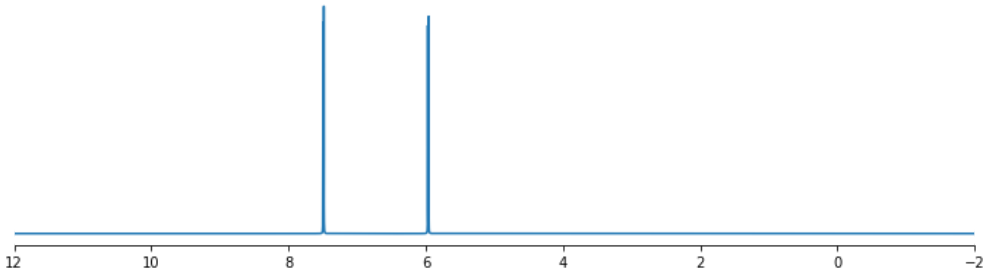


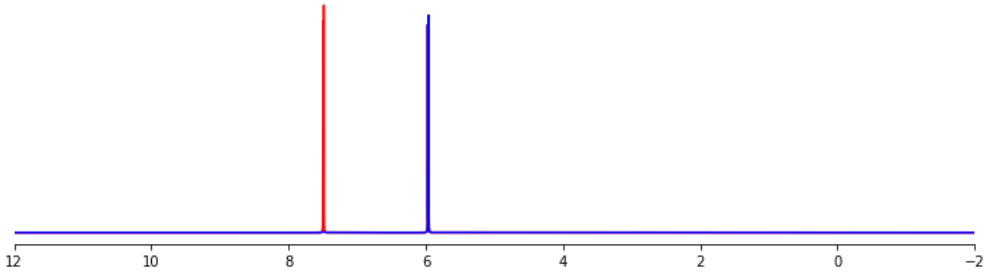
Top predicted substructures for the masked region(red):
0.9982 [CX3](=[OX1])C
0.9822 [CX3](=O)[OX2H1]
0.9815 [#8]=[#6][#8]
0.9772 [#8]=[#6H0][#6H1]
0.9741 [CX3](=[OX1])O
0.8787 O=[CX3][CX4H]
0.8706 [CX4H2]CC=O
0.6721 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]

True structure: Nc1ccnc(=O)[nH]1

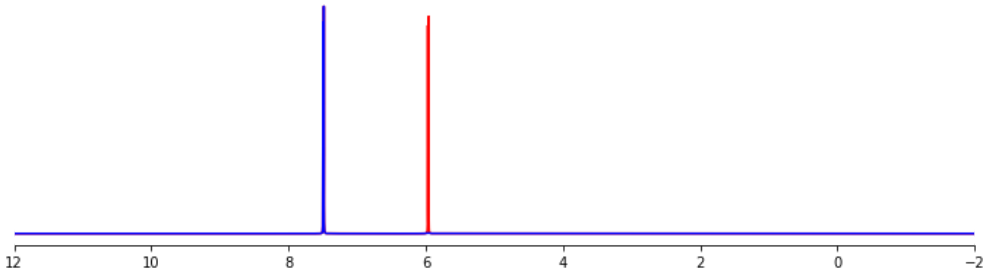




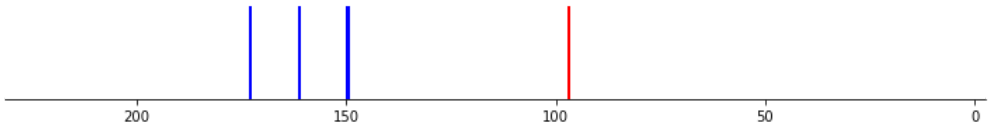




Top predicted substructures for the masked region(red):
0.4462 [#6H1][#6H1]
0.413 [#7][#7]
0.3196 O=[#6][#6]=[#6X3]
0.3173 [#8]=[#6][#6H1]=[#6H1]
0.315 [cX3H1]([cX3H1])[cX3H1]
0.2948 [cH][cH]
0.2458 [CX3H1](=[CX3H1])[CX3H0]
0.1813 O=C[CX3H]

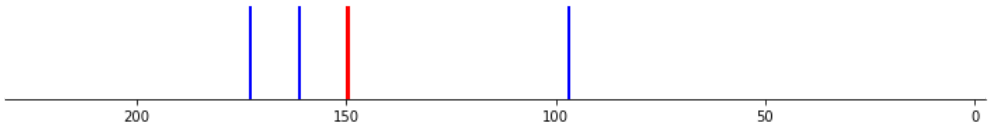


Top predicted substructures for the masked region(red):
0.3466 O=[#6][#6]=[#6X3]
0.2977 [#8]=[#6][#6H1]=[#6H1]
0.2591 [CX3H1](=[CX3H1])[CX3H0]
0.2286 [#6H1][#6H1]
0.2234 [#8][#6][#6][#6X3]
0.2144 [cX3H1]([cX3H1])[cX3H1]
0.2041 [CHX3]=[CHX3]
0.195 [#6X3][#7][#6X3]

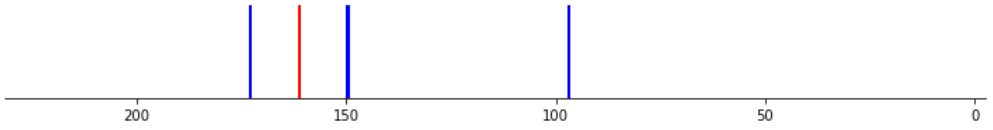


Top predicted substructures for the masked region(red):
0.298 O=[#6][#6]=[#6X3]
0.2403 [#7][#6X3H0][#6X3H1]
0.2285 [cX3H1]([cX3H1])[cX3H1]
0.2212 [#8][#6][#6][#6X3]

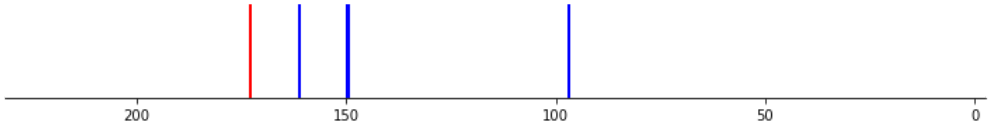
0.196 [#6X3][#7X3][#6X3]
0.1751 [#7][#6][#6][#6X3]
0.1713 [#8]=[#6][#6H1]=[#6H1]
0.1689 [#7][#7]



Top predicted substructures for the masked region(red):
0.3834 O=[#6][#6]=[#6X3]
0.3059 [#8]=[#6][#6H1]=[#6H1]
0.2976 [CX3H1](=[CX3H1])[CX3H0]
0.214 [#7][#6X3H0][#6X3H1]
0.191 [cX3H1]([cX3H1])[cX3H1]
0.1658 [CHX3]=[CHX3]
0.1583 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.1535 [#6H1][#6H1]

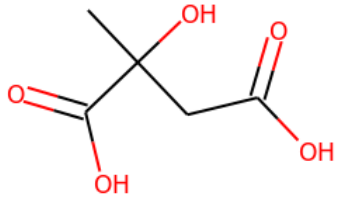


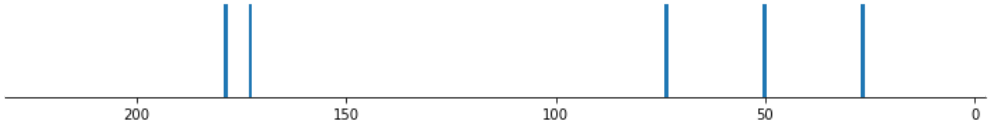
Top predicted substructures for the masked region(red):
0.371 O=[#6][#6]=[#6X3]
0.2854 [#8]=[#6][#6H1]=[#6H1]
0.2529 [#7][#6X3H0][#6X3H1]
0.2229 [CX3H1](=[CX3H1])[CX3H0]
0.169 [#7X3H2]
0.165 [#6X3][#7][#6X3]
0.1566 [cX3H1]([cX3H1])[cX3H1]
0.1534 [#6]=[#7H]

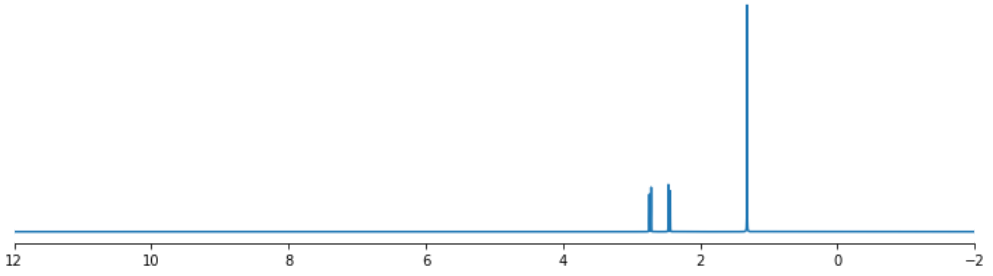


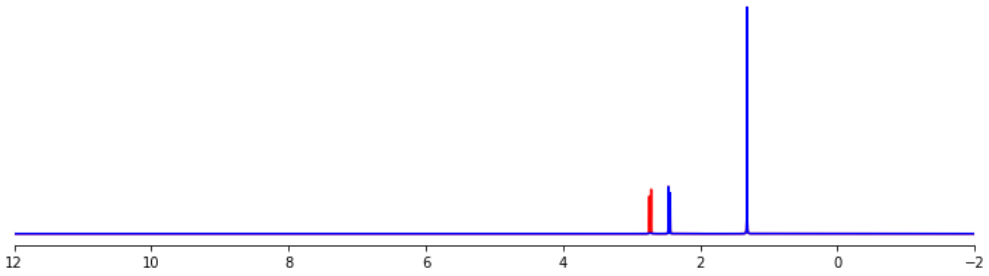
Top predicted substructures for the masked region(red):
0.4301 O=[#6][#6]=[#6X3]
0.3627 [#8]=[#6][#6H1]=[#6H1]
0.3492 [CX3H1](=[CX3H1])[CX3H0]
0.2707 O=[#6][#6][#6X3]
0.2648 O=C[CX3H]
0.2601 [#8]=[#6H0][#6H1]
0.2135 [#7][#6X3H0][#6X3H1]
0.1999 [CHX3]=[CHX3]

True structure: CC(O)(CC(=O)O)C(=O)O



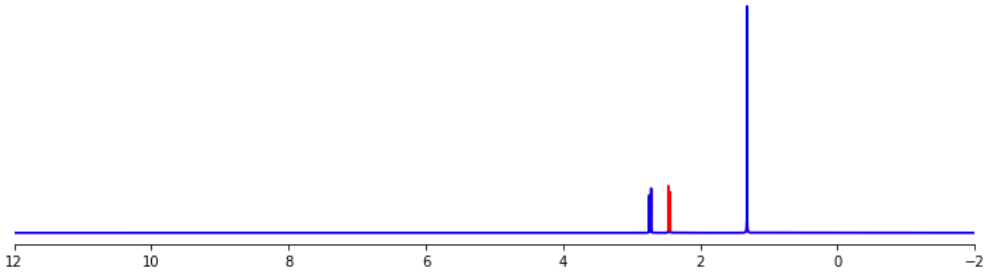






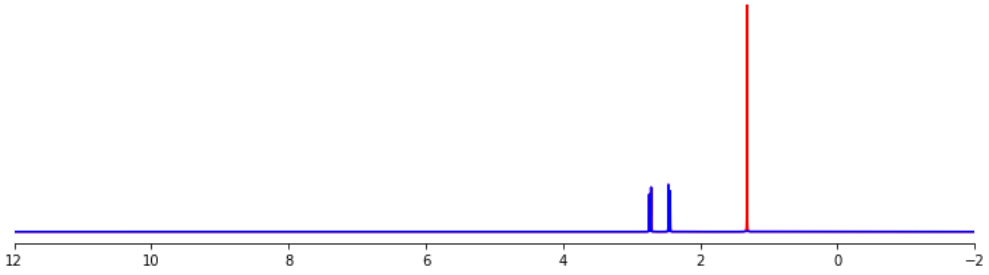
Top predicted substructures for the masked region(red):

0.6223 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.3804 [#8][#6][#6][#6][#6]=[#8]
0.232 [CX4H2]CC=O
0.228 C1OCCC1
0.2246 [CX3H0](=[OX1H0])([OX2H0])[CX4H0]
0.1172 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.1059 O[CX4H][CX4H2]
0.1027 [CX4H2][CX3]=O



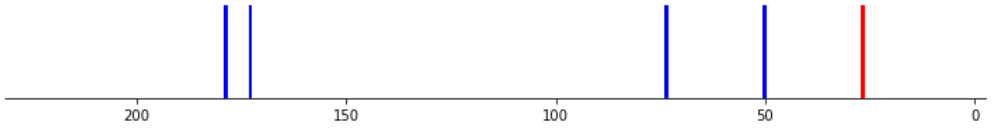
Top predicted substructures for the masked region(red):

0.6675 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.3392 [#8][#6][#6][#6][#6]=[#8]
0.23 [#6H3][#6H0]([#6H2])[#6H2]
0.2202 C1OCCC1
0.2178 [CX3H0](=[OX1H0])([OX2H0])[CX4H0]
0.204 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.1905 [CX4H2]CC=O
0.1346 [OX2H1][CX4H0][CX4H3]



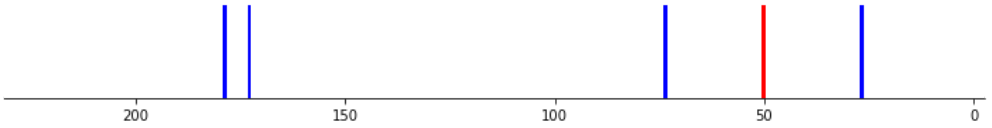
Top predicted substructures for the masked region(red):

0.7882 [CX4H3][CX4H0]
0.6574 [OX2H1][CX4H0][CX4H3]
0.6298 [#6X4H3][#6][#8H]
0.5414 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.4431 [#6H3][#6H0]
0.3997 [CX3H0](=[OX1H0])([OX2H0])[CX4H0]
0.3118 [#6H3][#6H0]([#6H2])[#6H2]
0.2882 [CX4H3][CX4]O

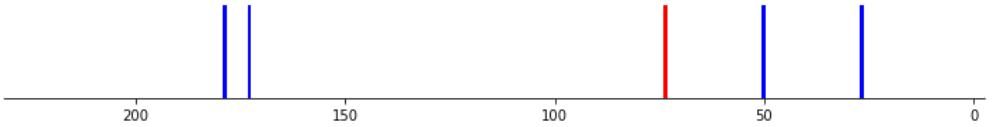


Top predicted substructures for the masked region(red):

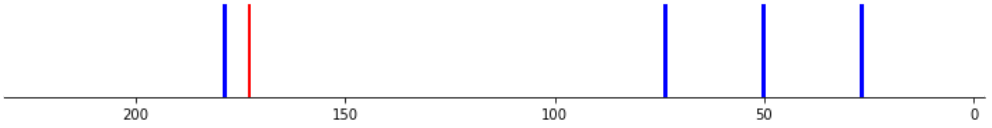
0.4793 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.4496 [CX4H3][#6]
0.3289 C1OCCC1
0.297 [#6H3][#6H0]
0.2746 [CX4H2]CC=O
0.2667 [OX2H1][CX4H0][CX4H3]
0.2424 [CX3H0](=[OX1H0])([OX2H0])[CX4H0]
0.199 [CH3][#6][#8]



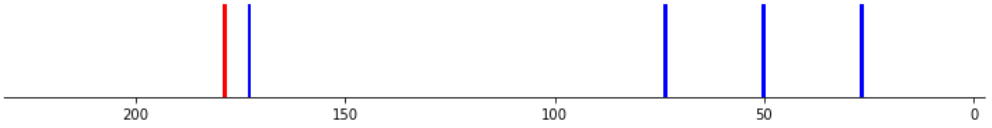
Top predicted substructures for the masked region(red):
0.4631 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.387 [#8][#6][#6][#6][#6]=[#8]
0.3197 [CX3H0](=[OX1H0])([OX2H0])[CX4H0]
0.3039 [#8][#6][#6][#6X3]
0.2114 [CX4H2]CC=O
0.1952 C1OCCC1
0.1534 [CX3](=O)[OX2H1]
0.1334 [#6X3][#6][#6][#6H3]



Top predicted substructures for the masked region(red):
0.573 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.3756 C1OCCC1
0.353 [#6X4H3][#6][#8H]
0.33 [OX2H1][CX4H0][CX4H3]
0.2898 [CX3H0](=[OX1H0])([OX2H0])[CX4H0]
0.2328 [CX4H2]CC=O
0.2051 [#8][#6][#6][#6][#6]=[#8]
0.1414 [#8][#6H0][#6H1]

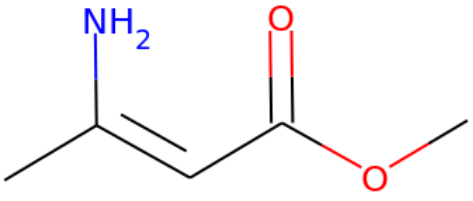


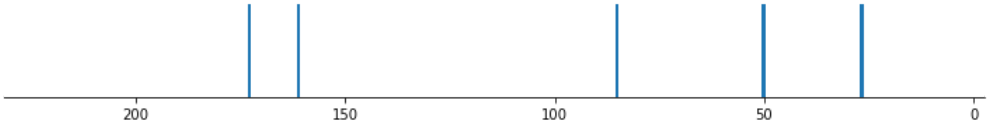
Top predicted substructures for the masked region(red):
0.7438 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.513 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.3457 C1OCCC1
0.3449 [OX2H0][CX3H0][CX4H2]
0.3402 [CX3H0](=[OX1H0])([OX2H0])[CX4H0]
0.3179 [CX4H2]CC=O
0.2389 [CX4H2][CX3]=O
0.2268 [CX3](=O)[OX2H1]

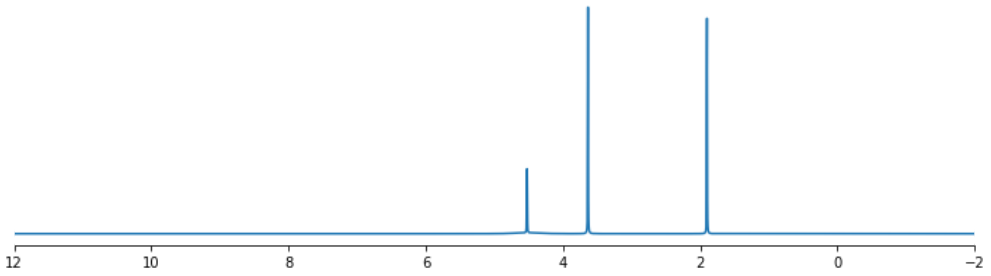


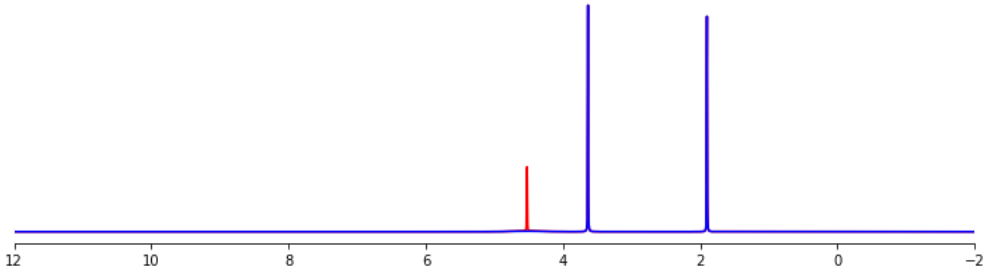
Top predicted substructures for the masked region(red):
0.7202 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.5537 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.4418 [CX4H2]CC=O
0.3739 C1OCCC1
0.3698 [CX3H0](=[OX1H0])([OX2H0])[CX4H0]
0.3521 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.3364 [CX3](=O)[OX2H1]
0.2819 [#8][#6][#6][#6][#6]=[#8]

True structure: COC(=O)C=C(C)N

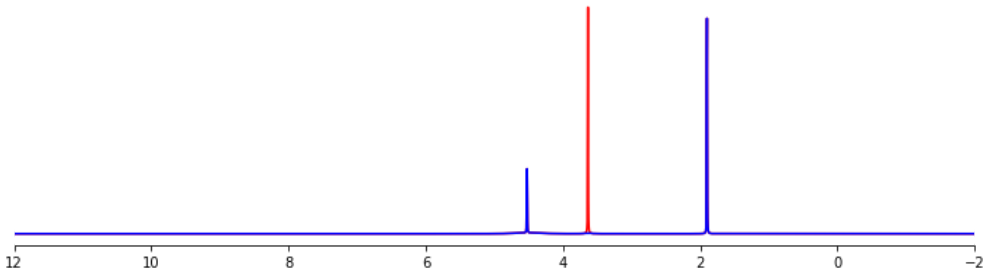




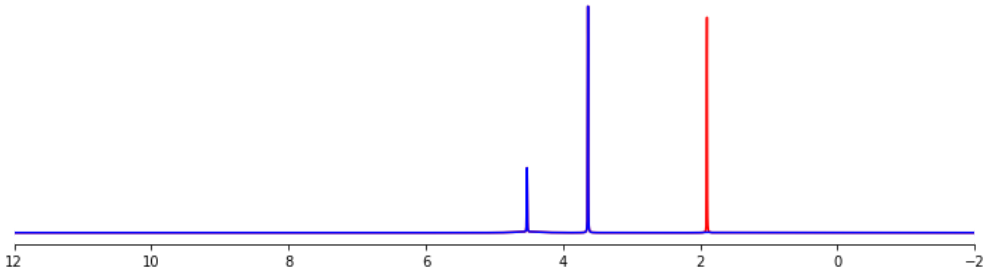




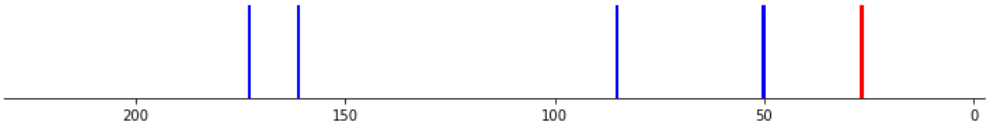
Top predicted substructures for the masked region(red):
0.7615 [#6X3H2]
0.7159 [CX3H2]=[CX3H0]
0.5638 [CH2X3](=C)
0.4391 [#8][#6]=[#6H2]
0.3877 [CX3H0](=[CX3H2])([OX2H0])[CX4H3]
0.3736 [CX3H2]=CO
0.3621 [#8]=[#6H0][#6H1]
0.3553 [#7][#6][#6X3]



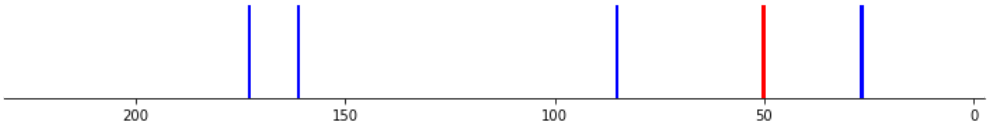
Top predicted substructures for the masked region(red):
0.6702 [#7][#6H2]
0.6691 [#7X3][#6H2]
0.6318 [CH2X3](=C)
0.5745 [#6X3H2]
0.4363 [#6X3][#6H2][#7]
0.4094 [#7][#6][#6X3]
0.3617 [CX3H2]=[CX3H0]
0.3513 [#7H2][#6H2]



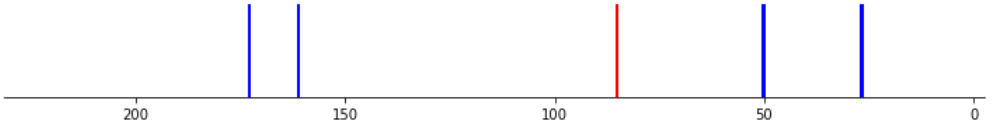
Top predicted substructures for the masked region(red):
0.9451 [#6H3][#6]=[#6X3]
0.8436 [CX4H3][CX3H0]
0.804 [CX4H3][CX3]
0.6735 [#6H3][#6H0]
0.6079 [CX4H3][#6]
0.4656 [CX4H3][CX3H0]=[CX3H2]
0.4321 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.4158 [OX2H0][CX3H0][CX4H3]



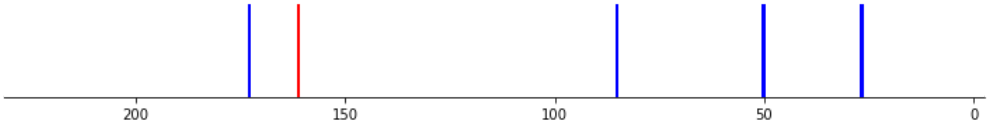
Top predicted substructures for the masked region(red):
0.9722 [CX4H3][#6]
0.8051 [CX4H3][CX3]
0.7642 [CX4H3][CX3H0]
0.7371 [#6H3][#6]=[#6X3]
0.5283 [#6H3][#6H0]
0.5114 [CH3][#6][#8]
0.4569 [CX3H0](=[CX3H2])([OX2H0])[CX4H3]
0.4259 [OX2H0][CX3H0][CX4H3]



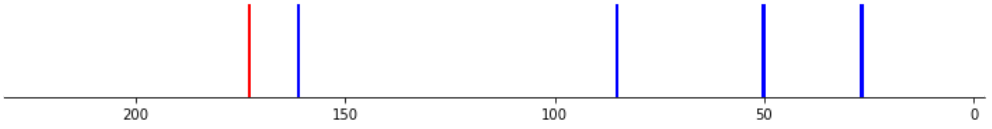
Top predicted substructures for the masked region(red):
0.8253 [#7][#6H2]
0.7045 [#7X3][#6H2]
0.4969 [#7][#6][#6X3]
0.4825 [#6X3][#6H2][#7]
0.4111 [#7H2][#6H2]
0.4045 [#8][#6H0][#6H1]
0.341 [CX4H2][CX3]=O
0.3325 [#8]=[#6H0][#6H1]



Top predicted substructures for the masked region(red):
0.7125 [#6X3H2]
0.6793 [CX3H2]=CO
0.669 [CX3H2]=[CX3H0]
0.5887 [#8][#6]=[#6H2]
0.475 [OX2H0][CX3H0]=[CX3H2]
0.47 [CH3][#6][#8]
0.4694 [#8]=[#6H0][#6H1]
0.4576 [CX3H0](=[CX3H2])([OX2H0])[CX4H3]

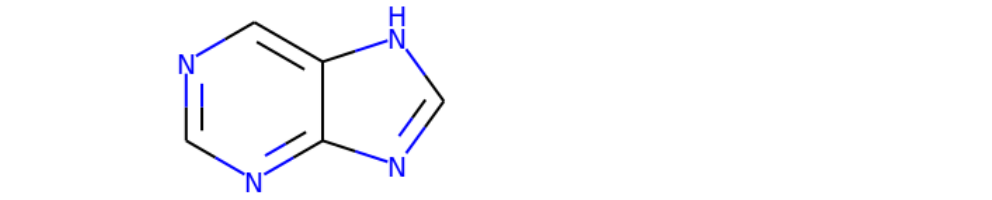


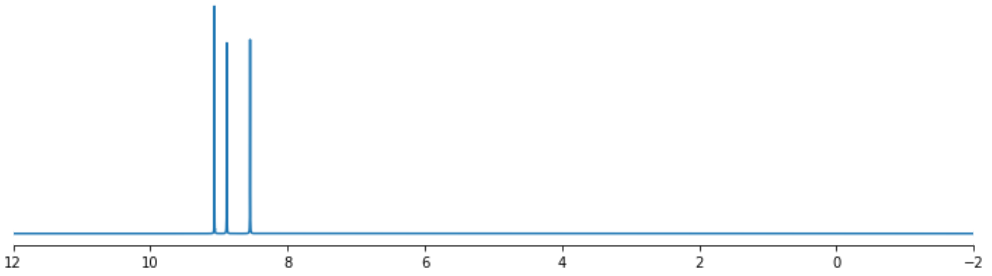
Top predicted substructures for the masked region(red):
0.823 [#6X3H2]
0.7905 [CX3H2]=[CX3H0]
0.769 [#6H3][#6]=[#6X3]
0.7632 [CH2X3](=C)
0.6639 [CX3H2]=CO
0.5679 [#8][#6]=[#6H2]
0.4826 [#8][#6X3][#6X3]=[#6X3][#6H3]
0.4641 O=[#6][#6]=[#6X3]

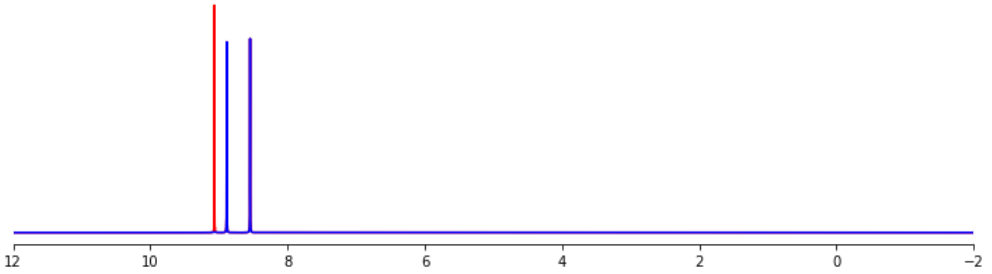


Top predicted substructures for the masked region(red):
0.8279 [CX3](=[OX1])C
0.6814 [CH2X3](=C)
0.6737 [#8]=[#6H0][#6H1]
0.6507 [#6X3H2]
0.6231 [CX3H2]=[CX3H0]
0.5853 O=[#6][#6]=[#6X3]
0.5597 [#7][#6][#6X3]
0.5307 [#6H3][#6]=[#6X3]

True structure: c1ncc2[nH]cnc2n1

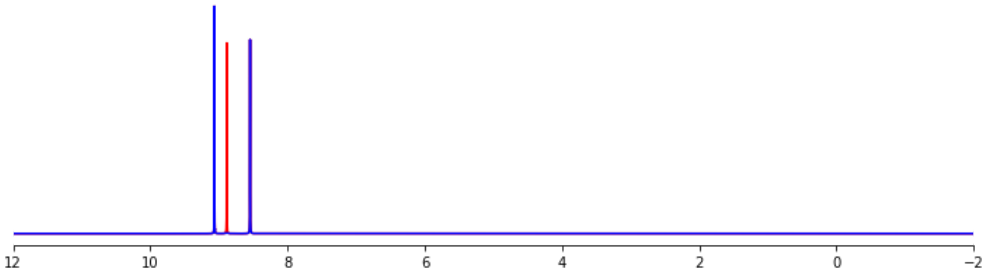






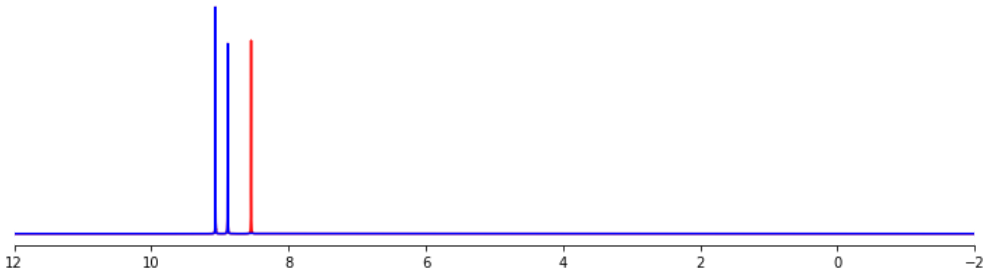
Top predicted substructures for the masked region(red):

0.2806 [#7][#6H1][#7]
0.1817 [cX3H1]([nX3H1])[cX3H0]
0.1562 [#7][#6][#6][#7]
0.1519 [#7][#6X3H0][#6X3H1]
0.151 [#8][#6][#6][#6X3]
0.149 [#7][#6H0][#7]
0.1379 [cX3H1]([nX2H0])[cX3H0]
0.1015 [#7][#6H0][#6H1]

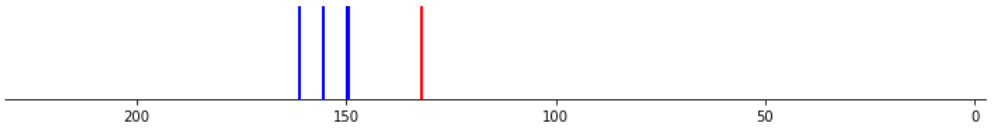


Top predicted substructures for the masked region(red):

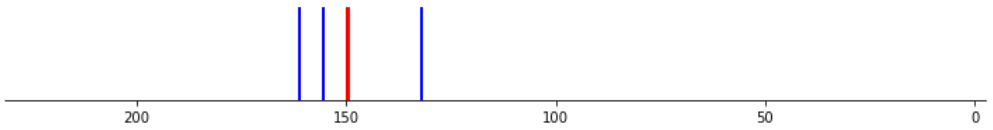
0.1677 [cX3H1]([nX3H1])[cX3H0]
0.1477 [#7][#6H1][#7]
0.134 [#8][#6][#6][#6X3]
0.1284 [#7][#6H0][#7]
0.1038 [cX3H1]([nX2H0])[cX3H0]
0.0826 [cX3H1]([nX3H1])[cX3H1]
0.0763 [#7][#6X3H0][#6X3H1]
0.073 [cX3H1]([cX3H1])[cX3H1]



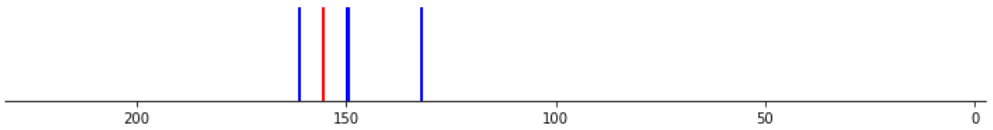
Top predicted substructures for the masked region(red):
0.2305 [#8][#6][#6][#6X3]
0.18 [cX3H1]([nX3H1])[cX3H0]
0.1599 [#7][#6][#6][#7]
0.1407 [#7][#6H0][#6H1]
0.1259 [#6H1r5][#7]
0.1068 [#6]1[#6][#6][#6][#6][#7]1
0.1043 [#6]1[#6][#7][#6][#6][#7]1
0.0818 [cX3H1]([nX3H1])[cX3H1]



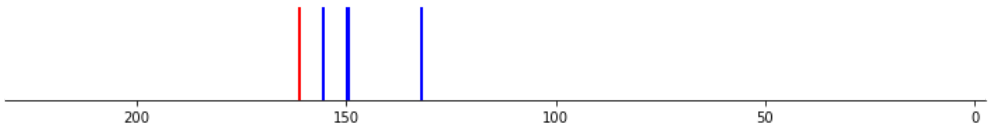
Top predicted substructures for the masked region(red):
0.2012 [#7][#6H0][#7]
0.1975 [cX3H1]([nX3H1])[cX3H0]
0.1369 [#7][#6][#6][#7]
0.1329 [#7][#6H0][#6H1]
0.1327 [#7][#6X3H0][#6X3H1]
0.1265 [#8][#6][#6][#6X3]
0.1137 [#7X3H2]
0.0973 [#6]1[#6][#6][#6][#6][#7]1



Top predicted substructures for the masked region(red):
0.2076 [#8][#6][#6][#6X3]
0.1838 [#7][#6H0][#7]
0.1786 [cX3H1]([nX3H1])[cX3H0]
0.1303 [#7][#6H0][#6H1]
0.1279 [#7][#6][#6][#7]
0.1166 [#7X3H2]
0.0989 [#7][#6][#6][#6][#7]
0.0988 [#6]1[#6][#6][#6][#6][#7]1

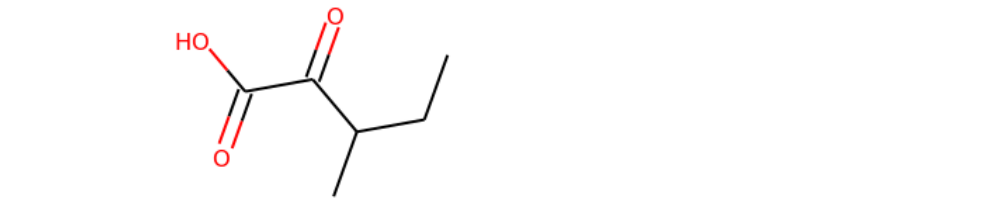


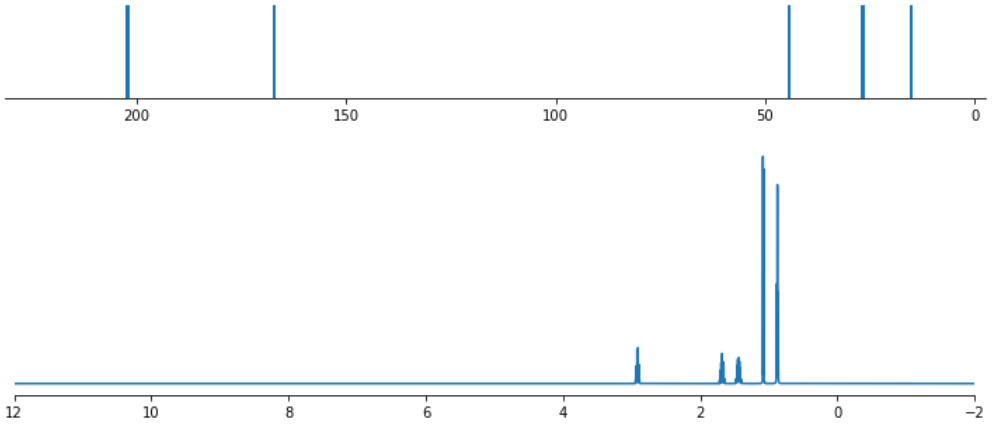
Top predicted substructures for the masked region(red):
0.221 [#8][#6][#6][#6X3]
0.2013 [#7][#6H0][#7]
0.1731 [cX3H1]([nX3H1])[cX3H0]
0.1545 [#7X3H2]
0.1199 [#7][#6H0][#6H1]
0.1022 [#6]1[#6][#6][#6][#6][#7]1
0.088 [#7][#6][#6][#6][#7]
0.0791 [cX3H1]([nX3H1])[cX3H1]

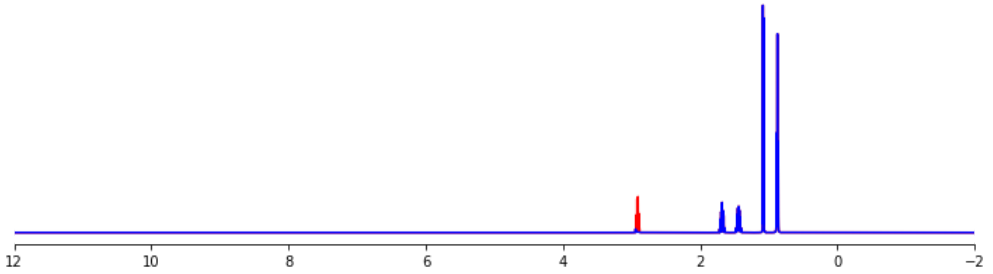


Top predicted substructures for the masked region(red):
0.2173 [#7][#6H0][#7]
0.188 [#8][#6][#6][#6X3]
0.1712 [#7X3H2]
0.1633 [cX3H1]([nX3H1])[cX3H0]
0.1328 [#7][#6H0][#6H1]
0.0995 [#6]1[#6][#6][#6][#6][#7]1
0.0817 [#7][#6][#6][#6][#7]
0.08 [#7][#6X3H0][#6X3H1]

True structure: CCC(C)C(=O)C(=O)O

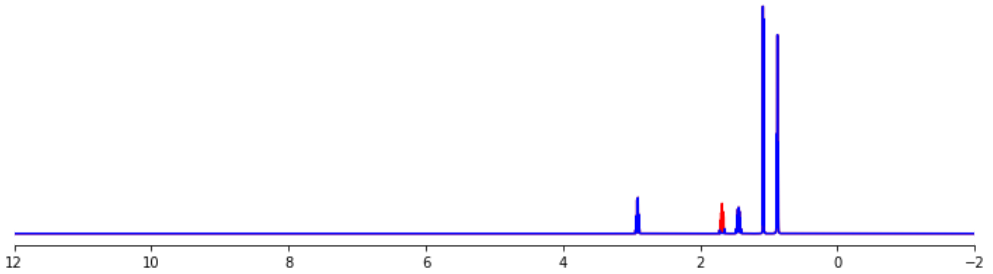






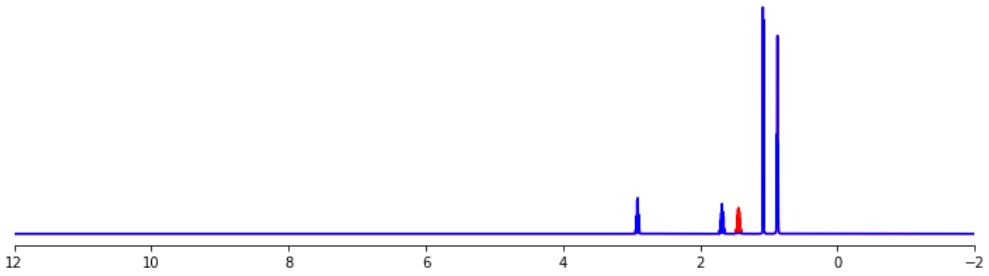
Top predicted substructures for the masked region(red):

0.4321 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.4252 [CX4H3][CX4H1]
0.3774 [#6H3][#6][#6X3]
0.3703 O=[CX3][CX4H]
0.3671 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.3663 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.2896 OCC[CH2]
0.2877 [CHX4]([CH3X4])[CH2X4]



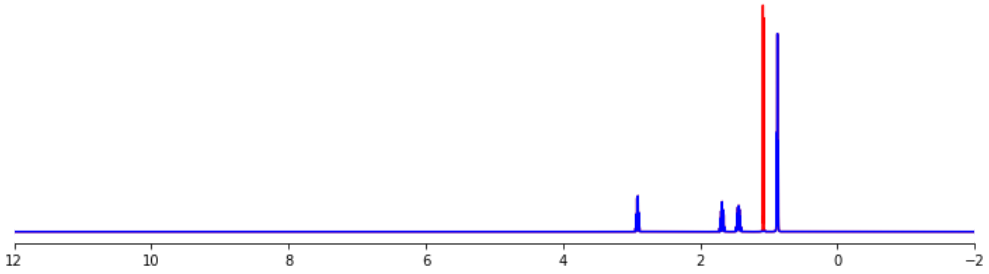
Top predicted substructures for the masked region(red):

0.4215 O=[CX3][CX4H]
0.4161 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3722 [CX4H3][CX4H1]
0.3029 [CHX4]([CH3X4])[CH2X4]
0.2925 [#8][#6H0][#6H1]
0.283 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.2682 [CX3H0](=[OX1H0])([CX4H1])[CX3H0]
0.2653 [#8]=[#6H0][#6H1]



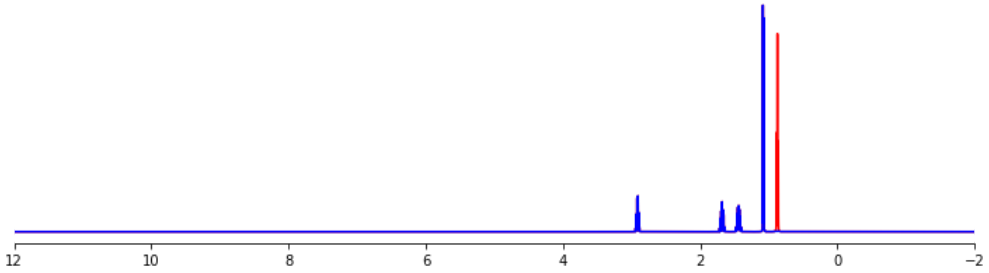
Top predicted substructures for the masked region(red):

0.4871 [CHX4]([CH3X4])[CH2X4]
0.4039 O=[CX3][CX4H]
0.3995 [CX4H3][CX4H1]
0.382 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3489 OCC[CH2]
0.3351 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.2936 [CX3H0](=[OX1H0])([CX4H1])[CX3H0]
0.2896 [#8][#6H0][#6H1]



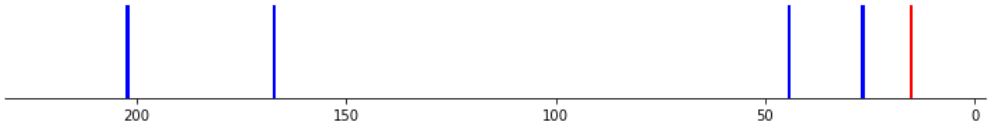
Top predicted substructures for the masked region(red):

0.9355 [CHX4]([CH3X4])[CH2X4]
0.8988 [CX4H3][CX4H1]
0.7132 [#6H3][#6][#6X3]
0.5169 O=[CX3][CX4H]
0.4835 [#6H1]
0.48 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3794 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.358 [#8][#6H0][#6H1]



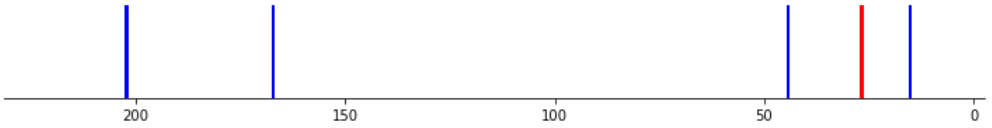
Top predicted substructures for the masked region(red):

0.3523 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.347 [CX4H3][CX4H1]
0.2961 [CHX4]([CH3X4])[CH2X4]
0.29 [#8]=[#6H0][#6H1]
0.2832 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.2611 [#8][#6H0][#6H1]
0.2566 O=[CX3][CX4H]
0.2549 [CX3H0](=[OX1H0])([CX4H1])[CX3H0]

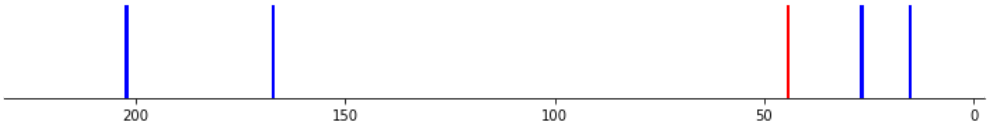


Top predicted substructures for the masked region(red):

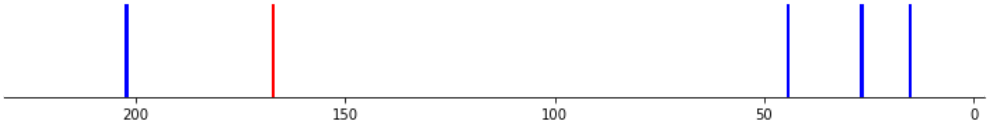
0.8358 [CX4H3][CX4H2]
0.5779 O=[CX3][CX4H]
0.5132 [CX3H0](=[OX1H0])([CX4H1])[CX3H0]
0.4504 [#6H3][#6][#6X3]
0.391 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3835 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.3337 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3276 [#8]=[#6H0][#6H1]



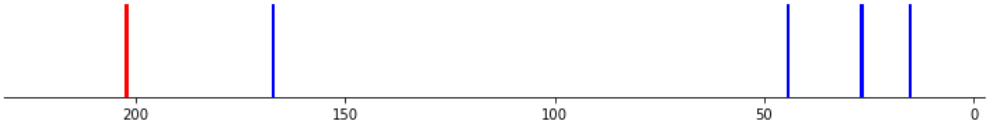
Top predicted substructures for the masked region(red):
0.3314 [CHX4]([CH3X4])[CH2X4]
0.3184 O=[CX3][CX4H]
0.3094 [CX3H0](=[OX1H0])([CX4H1])[CX3H0]
0.2928 [#6H3][#6][#6X3]
0.2741 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.2709 OCC[CH2]
0.2708 [CHX4]([CH3X4])[CH3X4]
0.2698 [CX4H1]([CX4H3])([CX4H2])[CX3H0]



Top predicted substructures for the masked region(red):
0.71 [CX4H3][CX4H1]
0.4922 O=[CX3][CX4H]
0.4609 [CHX4]([CH3X4])[CH2X4]
0.4167 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3744 [CX3H0](=[OX1H0])([CX4H2])[CX3H0]
0.3644 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3543 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.3261 [#8][#6H0][#6H1]

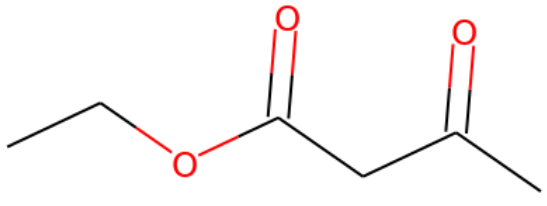


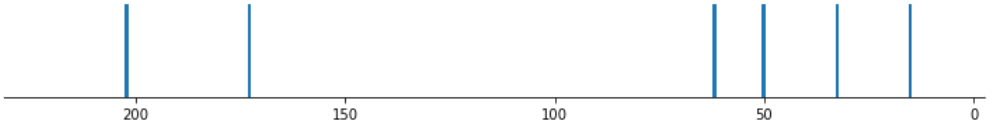
Top predicted substructures for the masked region(red):
0.9425 [CX3H0](=[OX1H0])([OX2H1])[CX3H0]
0.736 [CX3](=[OX1])O
0.6114 [#6H3][#6][#6X3]
0.5549 [CX3H0](=[OX1H0])([CX4H1])[CX3H0]
0.4923 [CHX4]([CH3X4])[CH2X4]
0.4804 [#8]=[#6][#8]
0.4452 [CX4H3][CX4H1]
0.4283 [CX4H1]([CX4H3])([CX4H2])[CX3H0]

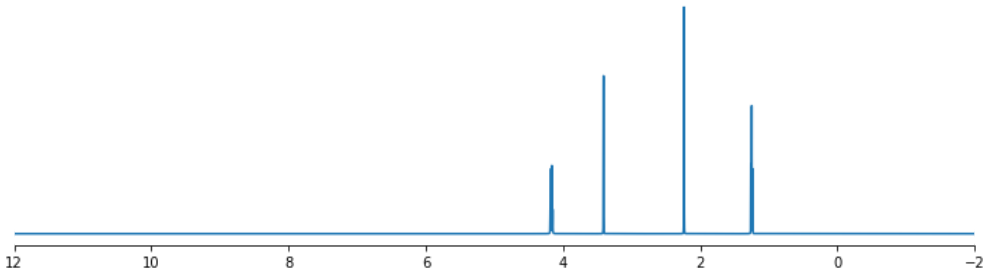


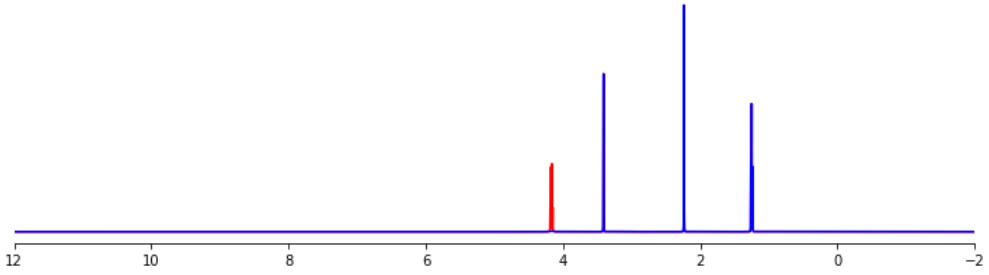
Top predicted substructures for the masked region(red):
0.9803 [#6X3][#6X3]
0.9377 [CX3H0](=[OX1H0])([CX4H1])[CX3H0]
0.9124 [#8]=[#6][#6]=[#8]
0.8696 [#6H3][#6][#6X3]
0.8364 O=CC=O
0.7254 O=[CX3][CX4H]
0.7098 [CX3H0](=[OX1H0])([OX2H1])[CX3H0]
0.5673 [CX3H0](=[OX1H0])([CX4H2])[CX3H0]

True structure: CCOC(=O)CC(C)=O



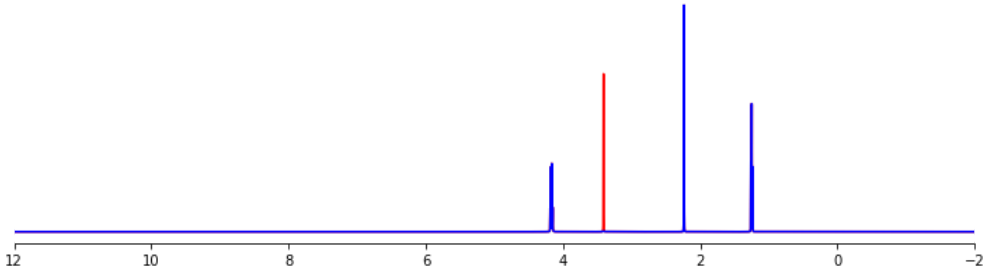






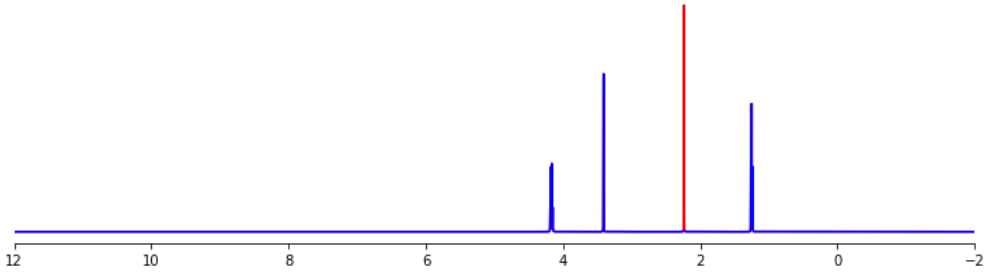
Top predicted substructures for the masked region(red):

0.6901 [CX4H3][CX4H2]
0.6167 [CX4H2]([OX2H0])[CX4H3]
0.4509 [OX2H0][CX3H0][CX4H2]
0.4021 [CH3][#6][#8]
0.267 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.2148 [#6H1]
0.184 [OX1H0]=[CX3H0][OX2H0][CX4H3]
0.1568 [#8][#6][#6][#6][#6]=[#8]



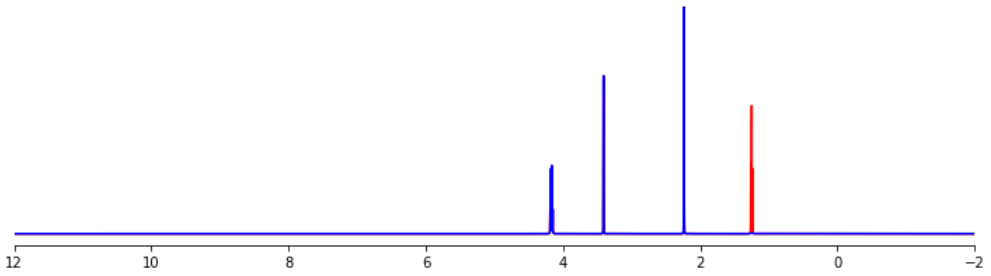
Top predicted substructures for the masked region(red):

0.919 [CX4H2]([CX3H0])[CX3H0]
0.9121 [OX1H0]=[CX3H0][CX4H2][CX3H0]
0.7989 [#8X1]=[#6X3][#6H2][#6H0]
0.7138 [OX2H0][CX3H0][CX4H2]
0.6919 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.6589 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.6468 [#6X3][#6H2][#6X3]
0.6091 [CX4H3][OX2H0]

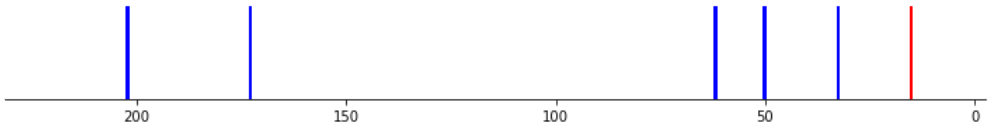


Top predicted substructures for the masked region(red):

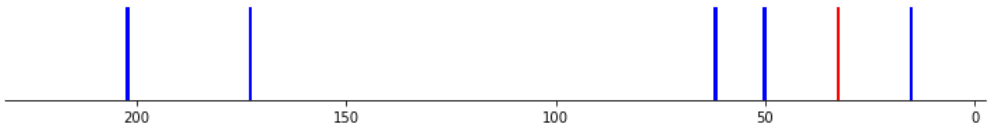
0.9933 [CX4H3][CX3]
0.9913 [CX4H3][CX3H0]
0.972 [#6H3][#6H0]
0.9301 [OX1H0]=[CX3H0][CX4H3]
0.6764 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.5907 [CH3][#6][#8]
0.4571 [OX2H0][CX3H0][CX4H2]
0.2776 [#6H3][#6][#6]



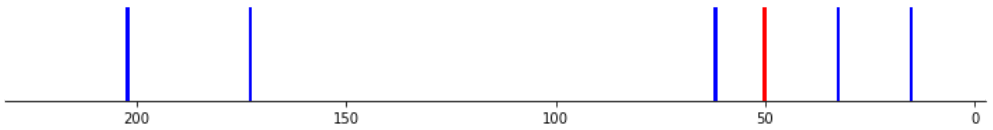
Top predicted substructures for the masked region(red):
0.8194 [CX4H3][CX4H2]
0.6314 [OX2H0][CX3H0][CX4H2]
0.6286 [CX4H2]([OX2H0])[CX4H3]
0.5536 [CH3][#6][#8]
0.532 [#6X3][#6][#6][#6H3]
0.3748 [CX4H3][CX4]O
0.3649 [#6H1]
0.3611 [#8X1]=[#6X3][#6H2][#6H0]



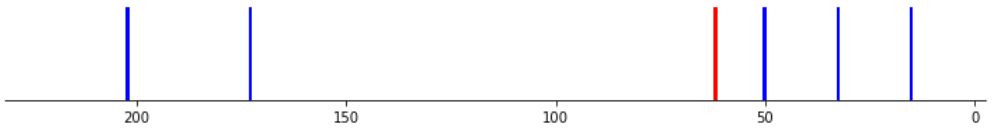
Top predicted substructures for the masked region(red):
0.8386 [CX4H3][CX4H2]
0.5298 [CH3][#6][#8]
0.5018 [OX2H0][CX3H0][CX4H2]
0.4831 [CX4H2]([OX2H0])[CX4H3]
0.3024 O=CC=O
0.1894 [#6X3][#6][#6][#6H3]
0.161 [CX3H0](=[OX1H0])([OX2H0])[CX3H0]
0.1608 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]



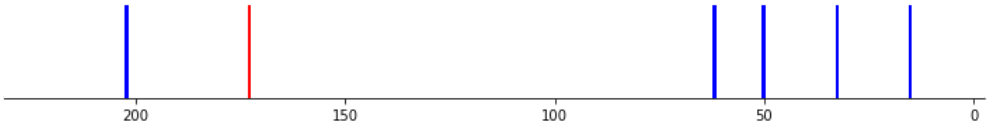
Top predicted substructures for the masked region(red):
0.6775 [CX4H3][CX4H2]
0.6202 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.5123 [OX2H0][CX3H0][CX4H2]
0.3535 [#6H3][#6][#6]
0.3209 [#6X3][#6][#6][#6H3]
0.3077 [OX1H0]=[CX3H0][OX2H0][CX4H3]
0.277 [OX1H0]=[CX3H0][CX4H3]
0.2403 [#8][#6][#6][#6][#6]=[#8]



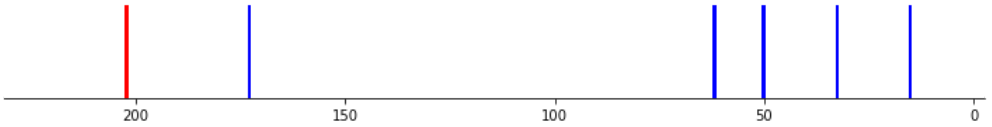
Top predicted substructures for the masked region(red):
0.5929 [OX2H0][CX3H0][CX4H2]
0.5589 [#8X1]=[#6X3][#6H2][#6H0]
0.4677 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.4656 [CX4H2]([CX3H0])[CX3H0]
0.4585 [OX1H0]=[CX3H0][CX4H2][CX3H0]
0.3811 [CX4H3][CX4H2]
0.3709 [#6X3][#6H2][#6X3]
0.3657 [OX1H0]=[CX3H0]([#8])[CX4H2]



Top predicted substructures for the masked region(red):
0.5864 [CX4H3][OX2H0]
0.5015 [OX2H0][CX3H0][CX4H2]
0.4169 [CX4H3][CX4H2]
0.3833 [CX4H2]([OX2H0])[CX4H3]
0.2764 O=CC=O
0.2735 [OX1H0]=[CX3H0][OX2H0][CX4H3]
0.2623 [#6X3][#6][#6][#6H3]
0.2537 [#6X3][#6X3]

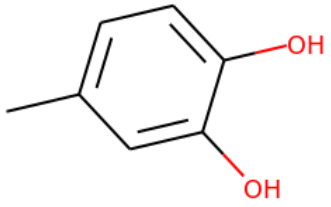


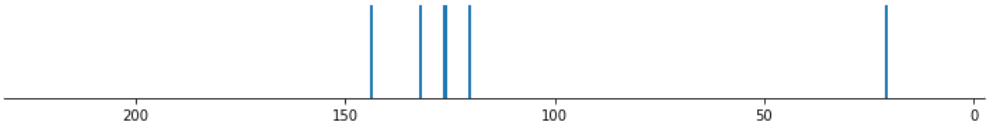
Top predicted substructures for the masked region(red):
0.8311 [CX4H3][CX4H2]
0.8252 [CX3](=[OX1])O
0.8013 [#8]=[#6][#8]
0.7629 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.7625 [OX2H0][CX3H0][CX4H2]
0.6266 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.6067 [#6X3][#6H2][#6X3]
0.5637 [#8X1]=[#6X3][#6H2][#6H0]

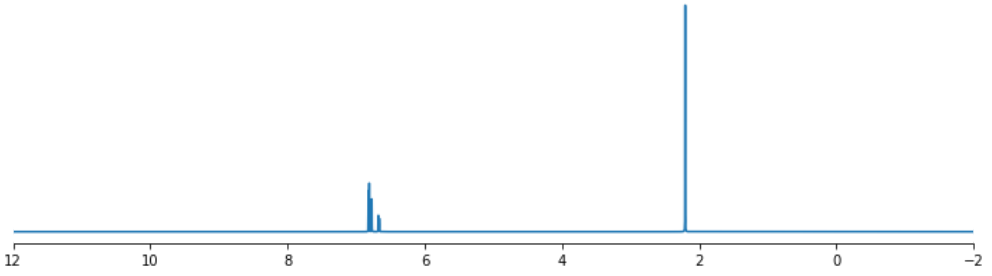


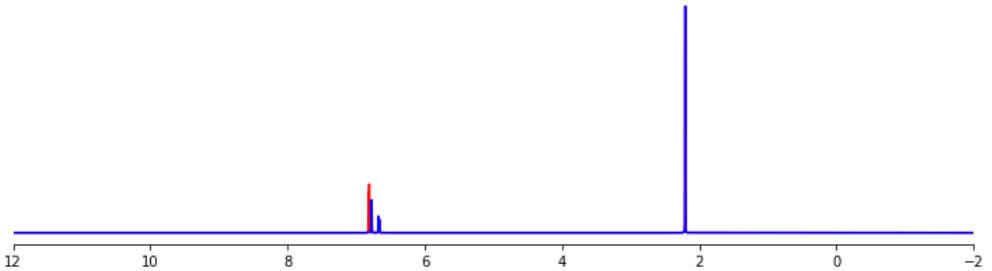
Top predicted substructures for the masked region(red):
0.7597 [OX1H0]=[CX3H0][CX4H2][CX3H0]
0.7426 [CX4H3][CX4H2]
0.7123 [#6X3][#6H2][#6X3]
0.6674 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.6129 O=[#6][#6][#6X3]
0.5931 [CX4H2]([CX3H0])[CX3H0]
0.5799 [#6X3][#6][#6][#6H3]
0.5719 [CX4H3][CX3]

True structure: Cc1ccc(O)c(O)c1

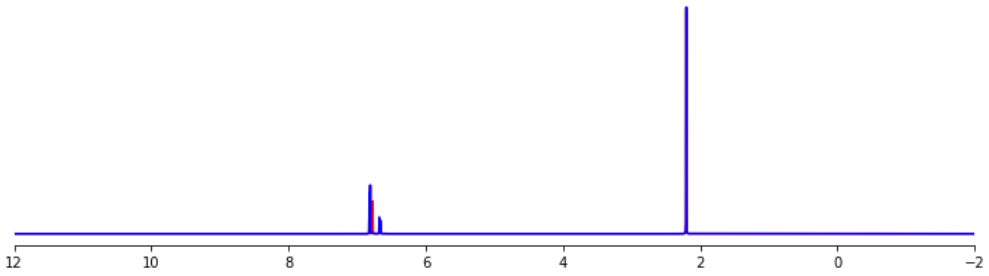






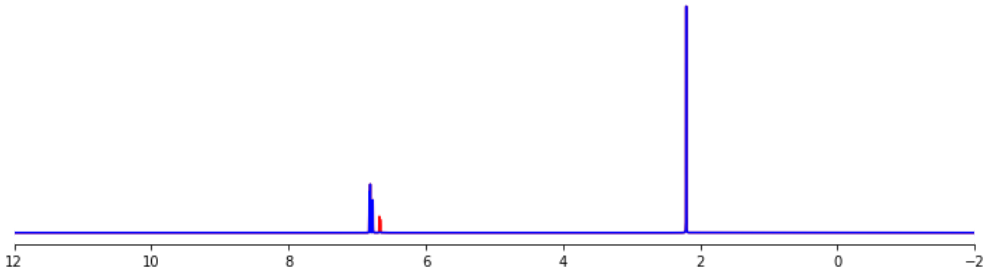


Top predicted substructures for the masked region(red):
0.372 [#6H1][#6H1]
0.2196 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.2139 [OX2H][cX3]:[c]
0.1945 [cX3H1]([cX3H1])[cX3H0]
0.1839 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1582 [#8][#6H1][#6H1]
0.1547 [cH]cO
0.148 [cX3H1]([cX3H1])[cX3H1]



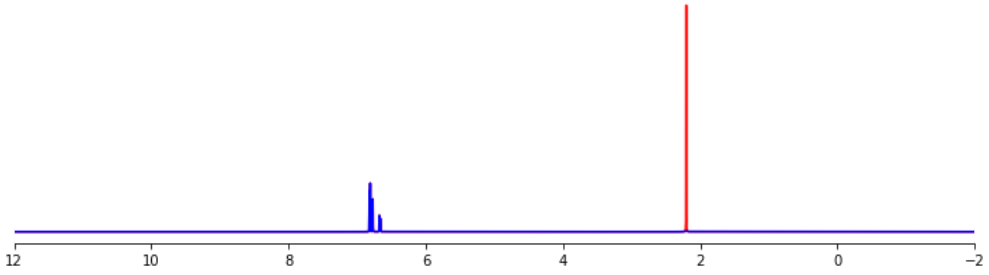
Top predicted substructures for the masked region(red):

0.2266 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.188 [OX2H][cX3]:[c]
0.1594 [cH]cO
0.154 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1495 [#8][#6H1][#6H1]
0.1411 [cX3H1]([oX2H0])[cX3H0]
0.1388 [CX4H3][cX3H0]
0.1097 [#8][#6][#6]=[#6X3]



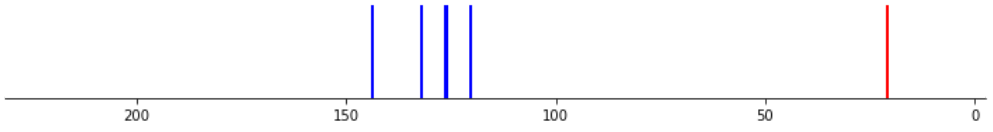
Top predicted substructures for the masked region(red):

0.2748 [#6H1][#6H1]
0.198 [OX2H][cX3]:[c]
0.1837 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1689 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1473 [#8][#6H1][#6H1]
0.14 [CX4H3][cX3H0]
0.1314 [cH]cO
0.1217 [cX3H0][cX3H1][cX3H0][OX2H1]



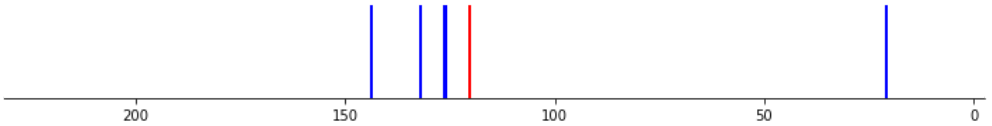
Top predicted substructures for the masked region(red):

0.6317 [CX4H3][cX3H0]
0.563 [#6H3][#6H0]
0.4296 [#8][#6X3][#6X3][#6X3][#6H3]
0.3704 [cX3H0]([cX3H1])([cX3H0])[CX4H3]
0.3142 [#6H3][#6][#6X3]
0.2429 [OX2H][cX3]:[c]
0.2267 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1719 [#8][#6H1][#6H1]

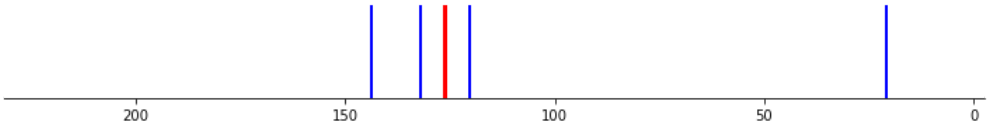


Top predicted substructures for the masked region(red):

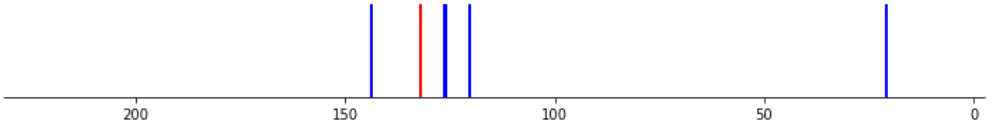
0.7269 [CX4H3][#6]
0.6913 [#6X3][#6][#6][#6H3]
0.6088 [CX4H3][cX3H0]
0.6064 [#6H3][#6][#6X3]
0.385 [#8][#6X3][#6X3][#6X3][#6H3]
0.3801 [#6H3][#6][#6]
0.3673 [#6H3][#6H0]
0.3122 [cX3H0]([cX3H1])([cX3H0])[CX4H3]



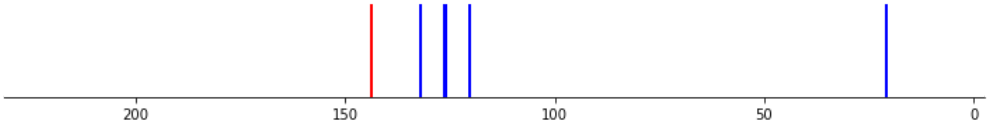
Top predicted substructures for the masked region(red):
0.5068 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.502 [OX2H][cX3]:[c]
0.295 [cH]cO
0.2581 [#6H1][#6H1]
0.2502 [CX4H3][cX3H0]
0.2496 [#8][#6X3][#6X3][#6X3][#6H3]
0.2341 [OX2H1]
0.2023 [#8][#6][#6][#6X3]



Top predicted substructures for the masked region(red):
0.3522 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.2988 [OX2H][cX3]:[c]
0.2892 [cH]cO
0.237 [OX2H1]
0.2194 [#6H1][#6H1]
0.1802 [cX3H0][cX3H1][cX3H0][OX2H1]
0.1657 [CX4H3][cX3H0]
0.1634 [#8][#6H0][#6H1]

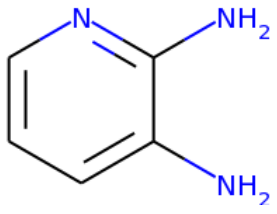


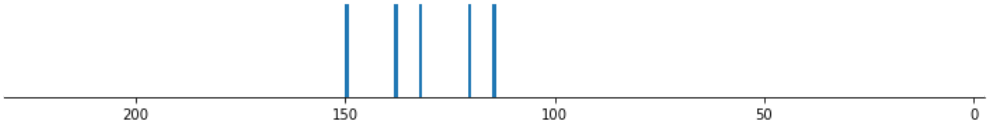
Top predicted substructures for the masked region(red):
0.2905 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.2528 [OX2H][cX3]:[c]
0.1975 [OX2H1]
0.1908 [cH]cO
0.1586 [CX4H3][cX3H0]
0.1556 [#6H1][#6H1]
0.144 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1436 [cX3H1]([oX2H0])[cX3H0]

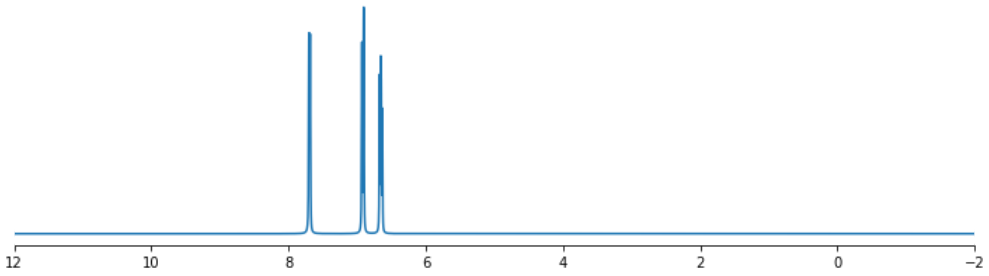


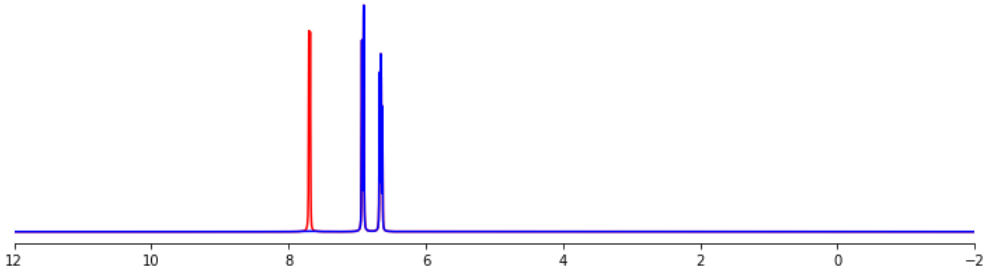
Top predicted substructures for the masked region(red):
0.3818 [#8][#6X3][#6X3][#6X3][#6H3]
0.3786 [#6H1][#6H1]
0.3421 [OX2H][cX3]:[c]
0.3325 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.2473 [cX3H0]([cX3H1])([cX3H0])[CX4H3]
0.2215 [CX4H3][cX3H0]
0.2173 [#6H3][#6][#6X3]
0.2163 [cH]cO

True structure: Nc1cccnc1N

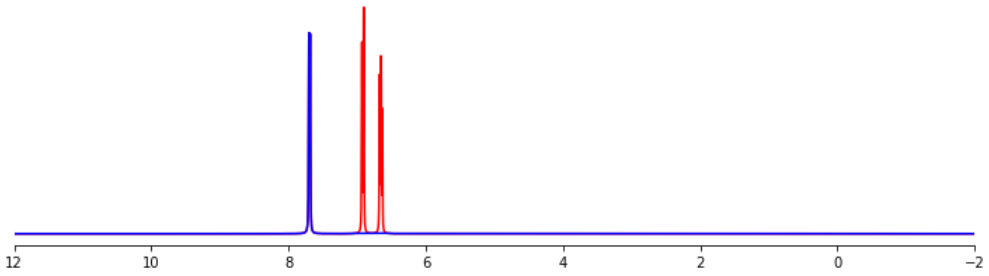




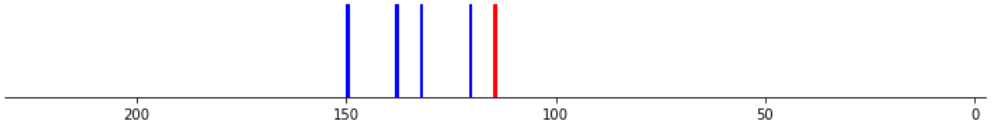




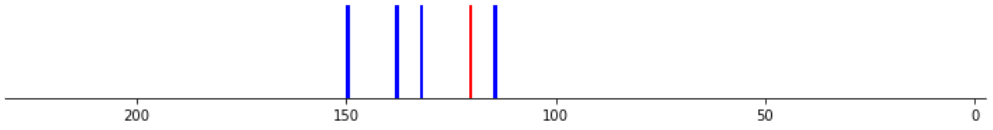
Top predicted substructures for the masked region(red):
0.3644 [#6]1[#6][#6][#6][#6][#7]1
0.1333 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.0803 [#6H1][#6H1]
0.0587 [OX2H1]
0.0561 [#7][#6H0]=[#7]
0.0546 [#7]=[#6][#6X3]
0.0499 [#6H1][#7][#6H1]
0.0475 [#7][#6H0][#6H1]



Top predicted substructures for the masked region(red):
0.3349 [cX3H1]([cX3H1])[cX3H1]
0.3114 [#7][#7]
0.2364 [#6]1[#6][#6][#6][#6][#6]1
0.1615 [cX3H1]([nX3H1])[cX3H1]
0.1451 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1041 [#6]1[#6][#6][#6][#6][#7]1
0.0861 [#7][#6X3H0][#6X3H1]
0.086 [#6H1][#6H1]

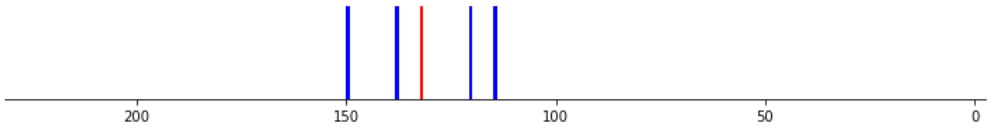


Top predicted substructures for the masked region(red):
0.227 [#6]=[#7H]
0.1901 [#7H][#6X3H1]
0.1477 [cX3H1]([nX3H1])[cX3H1]
0.141 [#7H2][#6H0]
0.1407 [#7][#6H0]=[#7]
0.1383 [#7][#6]=[#7]
0.1196 [#7][#6H0][#7]
0.1067 [#6X3][#7][#6X3]

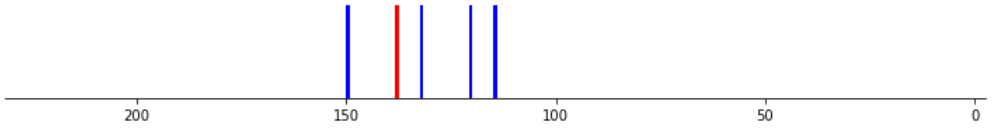


Top predicted substructures for the masked region(red):
0.1771 [#7H][#6X3H1]
0.1585 [#6]=[#7H]
0.1434 [#7][#6H0]=[#7]
0.1364 [cX3H1]([nX3H1])[cX3H1]
0.1236 [#7H2][#6H0]

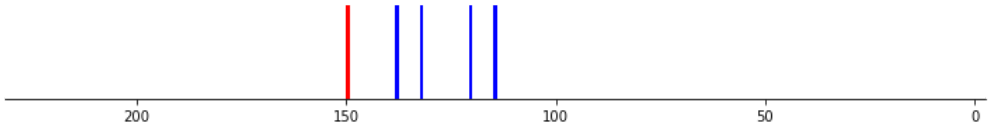
0.1031 [#7][#6H0][#7]
0.0893 [#6H1][#6H1]
0.0592 [#7][#6H0][#6H1]



Top predicted substructures for the masked region(red):
0.2524 [#6]=[#7H]
0.1758 [#7][#6H0]=[#7]
0.1094 [#7][#7]
0.0853 [#6H1][#6H1]
0.0621 [#7][#6H0][#6H1]
0.0593 [#7]=[#6][#6X3]
0.0583 [OX2H1]
0.0575 [#7H2][#6H0]

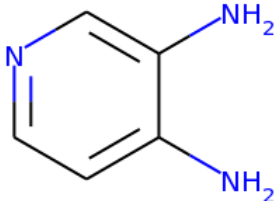


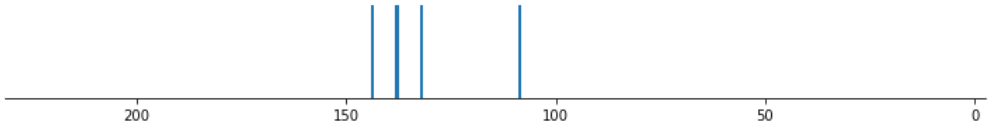
Top predicted substructures for the masked region(red):
0.2399 [#6]=[#7H]
0.1849 [#7][#6H0]=[#7]
0.1548 [#7][#7]
0.1058 [#6]1[#6][#6][#6][#6][#7]1
0.0946 [#7H2][#6H0]
0.0896 [#6H1][#6H1]
0.0675 [NH1]=[#6][#7]
0.0648 [#7]=[#6][#6X3]

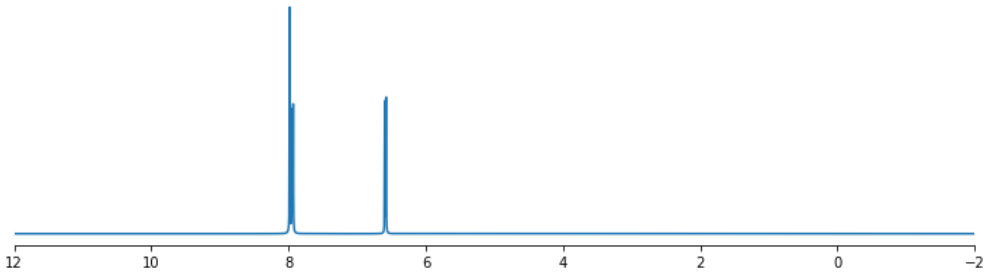


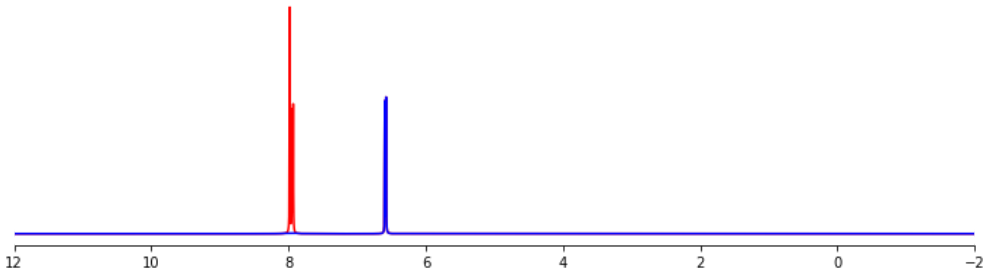
Top predicted substructures for the masked region(red):
0.3078 [#7][#6H0]=[#7]
0.284 [#6]=[#7H]
0.2354 [#6]1[#6][#6][#6][#6][#7]1
0.1472 [#7H2][#6H0]
0.1393 [NH1]=[#6][#7]
0.0846 [#6]1[#6][#6][#6][#6][#6]1
0.0826 [#6H1][#6H1]
0.0753 [#7]=[#6][#6X3]

True structure: Nc1ccncc1N

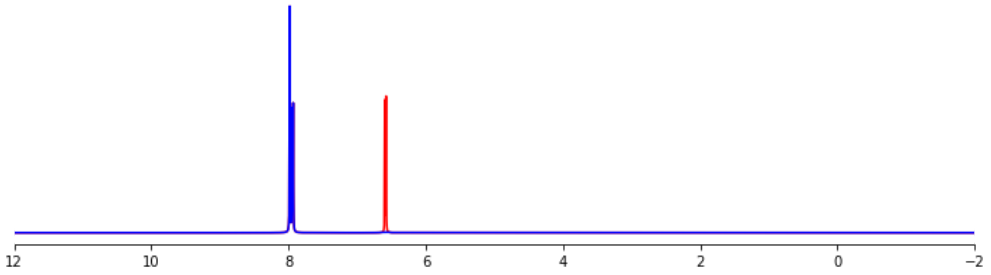




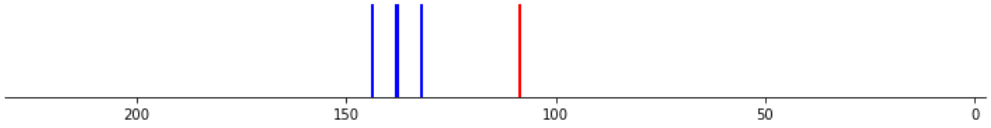




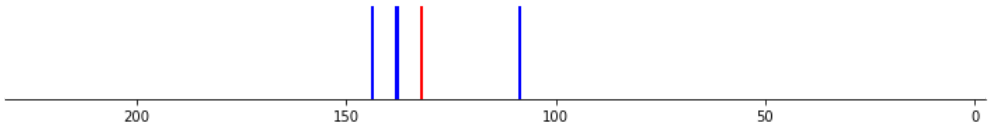
Top predicted substructures for the masked region(red):
0.33 [#6H1][#7][#6H1]
0.2943 [#7]=[#6H1]
0.2384 [CX4H3]
0.2336 [#7][#6H1][#7]
0.2002 [#6]1[#6][#6][#6][#6][#7]1
0.1951 [CX3H1](=[NX2H0])[CX3H1]
0.1788 [#7][#7]=[#6]
0.1681 [cX3H1]([cX3H1])[cX3H1]



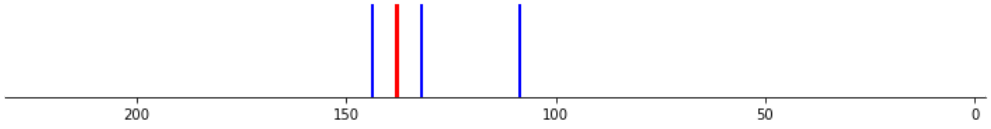
Top predicted substructures for the masked region(red):
0.4245 [cX3H1]([cX3H1])[cX3H1]
0.2489 [#7][#7]
0.2221 [#6H1][#6H1]
0.2022 [#7]=[#6H1]
0.1928 [CX3H1](=[NX2H0])[CX3H1]
0.1619 [#7][#7]=[#6]
0.1288 [cX3H1]([cX3H1])[cX3H0]
0.1227 [#7][#6H0][#6H1]



Top predicted substructures for the masked region(red):
0.2955 [#6X3][#7X3][#6X3]
0.2925 [CX4H3]
0.205 [#7H2][#6H0]
0.1696 [#7H][#6X3H1]
0.1692 [cX3H1]([cX3H1])[cX3H1]
0.1661 [#7]=[#6H1]
0.1437 [#7X3H0]
0.1411 [#6X3][#7][#6X3]

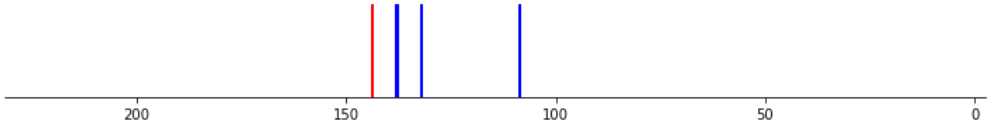


Top predicted substructures for the masked region(red):
0.263 [#7]=[#6H1]
0.2076 [CX4H3]
0.1688 [CX3H1](=[NX2H0])[CX3H1]
0.1531 [#7H2][#6H0]
0.1421 [cX3H1]([cX3H1])[cX3H1]
0.1269 [#7X3H2]
0.1103 [#7][#6H0][#6H1]
0.1061 [#7X3][#6H3]



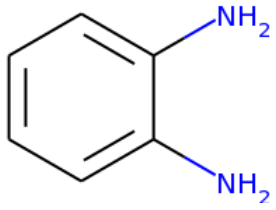
Top predicted substructures for the masked region(red):
0.2296 [CX4H3]
0.1993 [#7]=[#6H1]
0.1842 [CX3H1](=[NX2H0])[CX3H1]

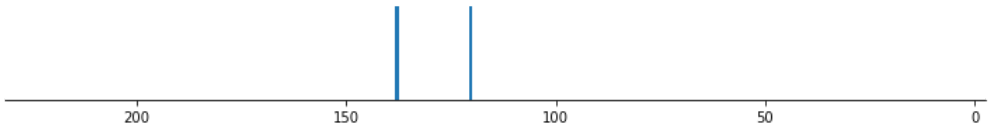
0.1764 [#7H2][#6H0]
0.1395 [#7X3H2]
0.1334 [#6]1[#6][#6][#6][#6][#7]1
0.1176 [#7][#6H0][#6H1]
0.1077 [#7][#6]=[#6][#6]=[#7]

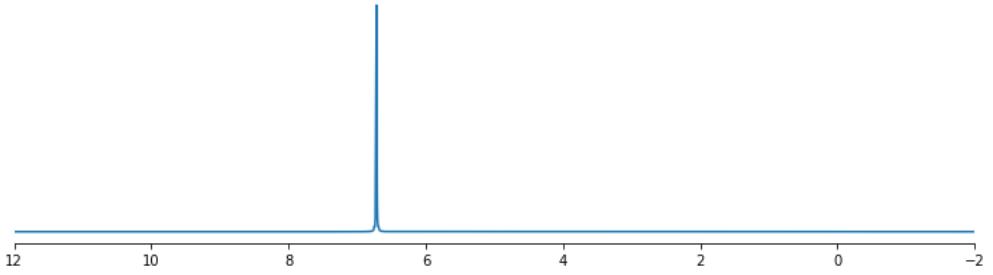


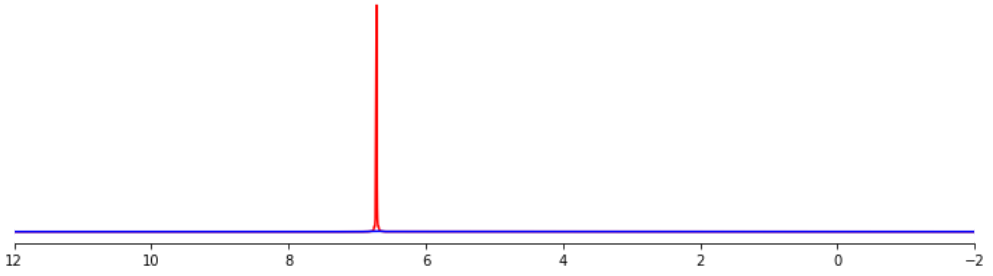
Top predicted substructures for the masked region(red):
0.2408 [CX4H3]
0.215 [#7]=[#6H1]
0.2097 [#7H2][#6H0]
0.1824 [CX3H1](=[NX2H0])[CX3H1]
0.1649 [#7X3H2]
0.1418 [#6]1[#6][#6][#6][#6][#7]1
0.1367 [#7][#6H0][#6H1]
0.1121 [cX3H1]([cX3H1])[cX3H1]

True structure: Nc1ccccc1N

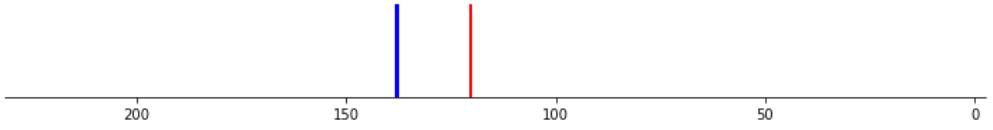






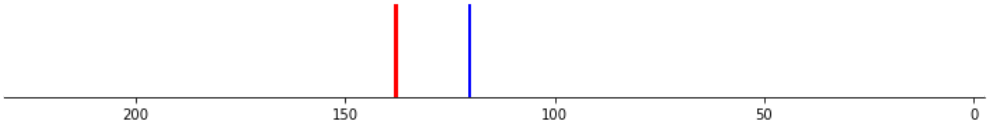


Top predicted substructures for the masked region(red):
0.7005 [cH][cH]
0.6641 [#6H1][#6H1]
0.6456 [cX3H1]([cX3H1])[cX3H1]
0.636 [cX3H1]([cX3H1])[cX3H0]
0.5318 [#6H1]
0.441 [#6X3H1][#6X3H0]
0.424 [cH]
0.4193 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]



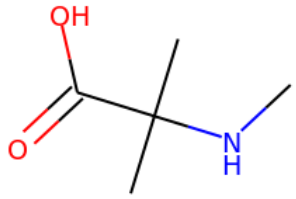
Top predicted substructures for the masked region(red):
0.3258 [#6X3][#7][#6X3]
0.3006 [#7H][#6X3H1]
0.2478 [#6X3][#7X3][#6X3]

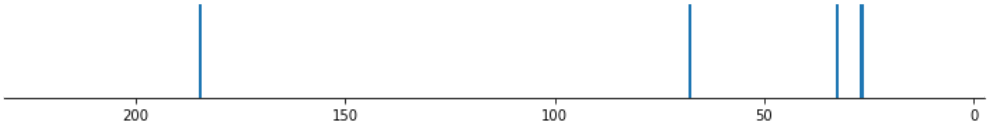
0.2081 [cX3H1]([nX3H1])[cX3H0]
0.1868 [#7H2][#6H0]
0.1666 [#7][#6H0][#6H1]
0.1639 [#6X3H1][#6X3H0]
0.1581 [#7][#6][#6X3]

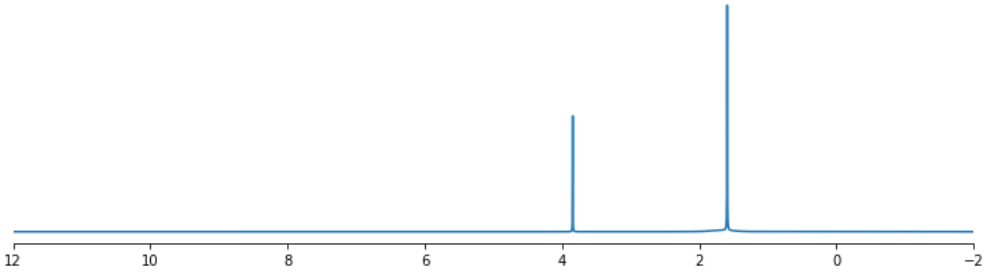


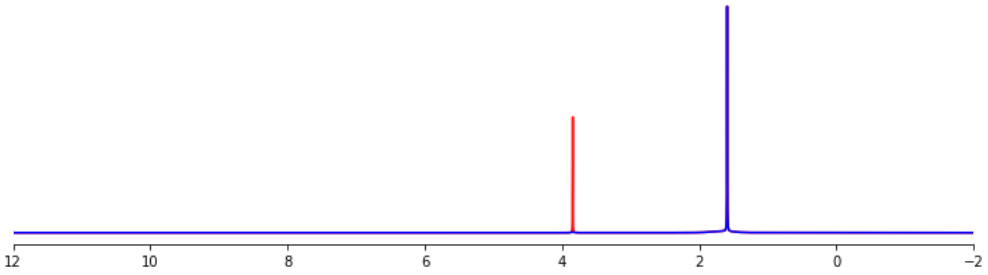
Top predicted substructures for the masked region(red):
0.2799 [#7][#6H0][#6H1]
0.2098 [#7][#6][#7]
0.2079 [#7H2][#6H0]
0.1982 [#7][#6][#6][#7]
0.1702 [#6X3H1][#6X3H0]
0.1624 [#6]=[#7H]
0.1622 [#7][#6X3H0][#6X3H1]
0.161 [#6]1[#6][#6][#6][#6][#7]1

True structure: CNC(C)(C)C(=O)O

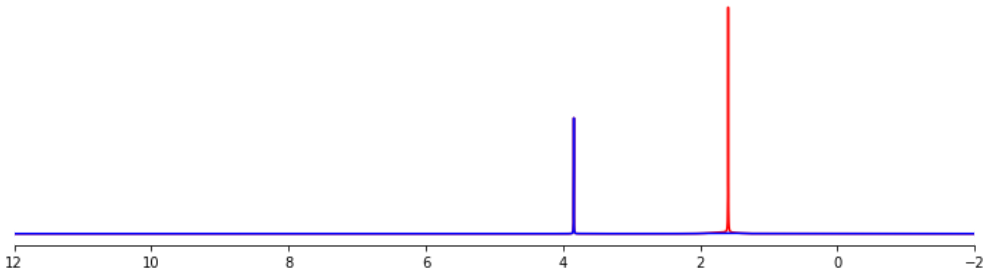




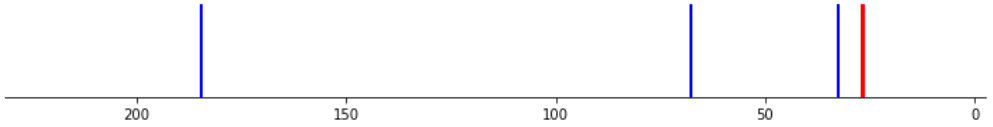




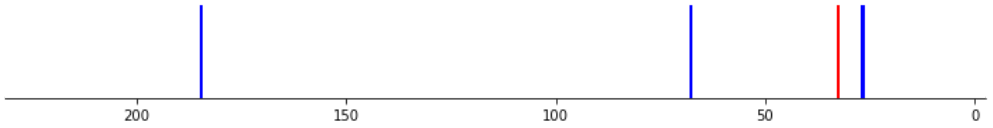
Top predicted substructures for the masked region(red):
0.7005 [CX4H2]([CX4H2])[CX4H2]
0.6587 [CX4H2]([#6])[O]
0.5393 [CX4H2][CX4H2]
0.4906 [CH2X4](O)[CX4H2][CX4H2]
0.4807 [CX4H3][CX3H0]
0.4648 [CH2X4](O)[CX4H2]
0.3547 [CX4H2]([OX2H1])[CX3H0]
0.2554 [CX4H3][CX3]



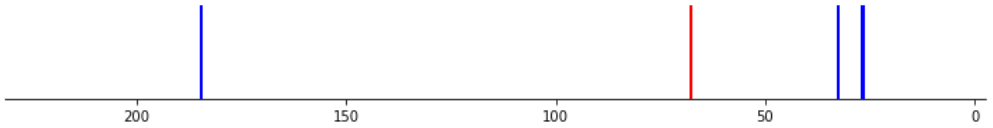
Top predicted substructures for the masked region(red):
0.6701 [CX4H2]([CX4H2])[CX4H2]
0.6462 [#6H3][#6][#6]
0.6354 [CX4H3][CX4H0]
0.6143 [#6H3][#6H0]
0.57 [OX1H0]=[CX3H0][CX4H0][CX4H3]
0.4982 [CX4H3][#6]
0.461 [CX4H2][CX4H2]
0.4176 [CH2X4](O)[CX4H2]



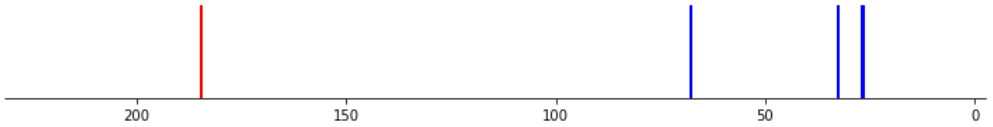
Top predicted substructures for the masked region(red):
0.7991 [CX4H2]([CX4H2])[CX4H2]
0.5339 [CX4H2][CX4H2]
0.5187 [CX4H3][CX3H0]
0.3948 [CH2X4](O)[CX4H2]
0.2796 [CX4H2]([#6])[#6]
0.2627 [CX4H2][CX4H2][CX4H2][CX4H2]
0.2599 [CH2X4](O)[CX4H2][CX4H2]
0.2541 [CX4H3][CX3]



Top predicted substructures for the masked region(red):
0.8582 [CX4H2]([CX4H2])[CX4H2]
0.6813 [CX4H2][CX4H2]
0.5544 [CH2X4](O)[CX4H2][CX4H2]
0.5036 [CH2X4](O)[CX4H2]
0.2826 [CX4H2]([#6])[#6]
0.2647 [CX4H3][CX3H0]
0.2624 [CX4H2][CX4H2][CX4H2][CX4H2]
0.262 OCC[CH2]

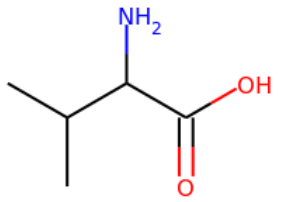


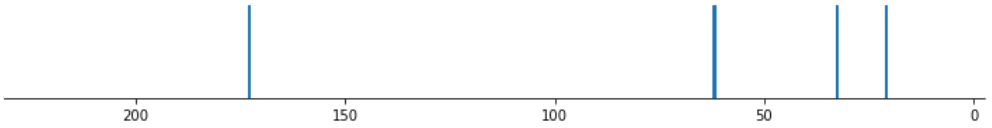
Top predicted substructures for the masked region(red):
0.7621 [CX4H2]([CX4H2])[CX4H2]
0.7403 [CX4H2]([#6])[O]
0.5928 [CX4H2][CX4H2]
0.5627 [CH2X4](O)[CX4H2][CX4H2]
0.5485 [CH2X4](O)[CX4H2]
0.4217 [CX4H3][CX3H0]
0.4109 [#8][#6][#6]=[#8]
0.3499 [CX4H2]([OX2H1])[CX3H0]

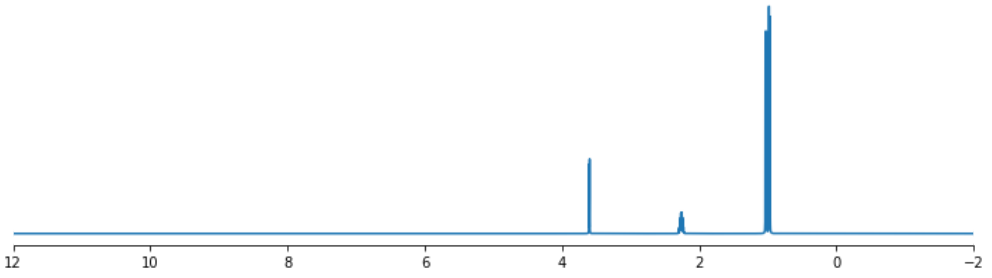


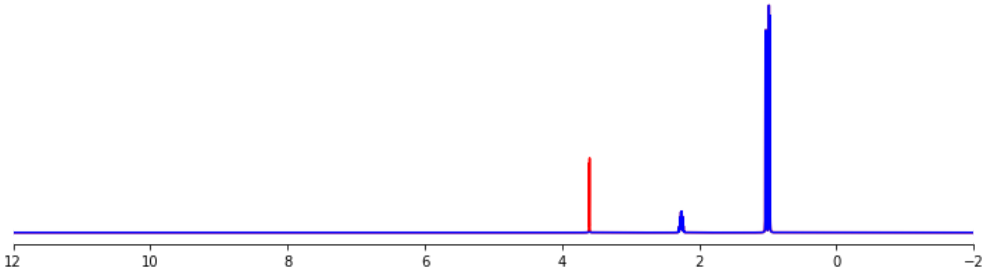
Top predicted substructures for the masked region(red):
0.9768 [CX3](=[OX1])C
0.6017 [OX1H0]=[CX3H0][CX4H0][CX4H3]
0.5397 [#8][#6][#6]=[#8]
0.5334 [CX4H3][CX3H0]
0.5028 [CX4H2]([CX4H2])[CX4H2]
0.4412 [#6H3][#6][#6]
0.4377 [#6H3][#6][#6X3]
0.4356 [CX4H2][CX3]=O

True structure: CC(C)C(N)C(=O)O



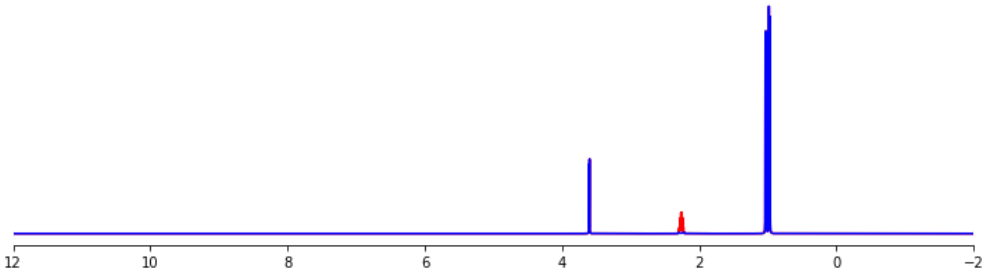






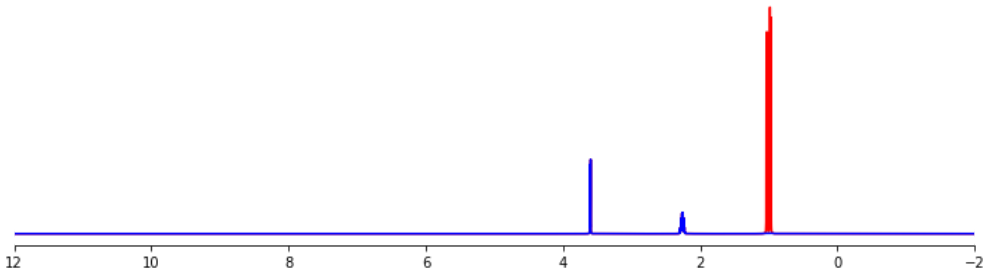
Top predicted substructures for the masked region(red):

0.3744 [#7][#6][#6X3]
0.2874 [CX4H1]([CX4H3])([CX4H3])[CX4H2]
0.262 [#7H2][#6X4H1][#6X3]
0.2379 O=[CX3][CX4H]
0.1986 [#6H3][#6][#6X3]
0.1602 [CHX4]([CH3X4])[CH2X4]
0.1376 [#8][#6H0][#6H1]
0.1103 [CX4H2]([#6])[O]

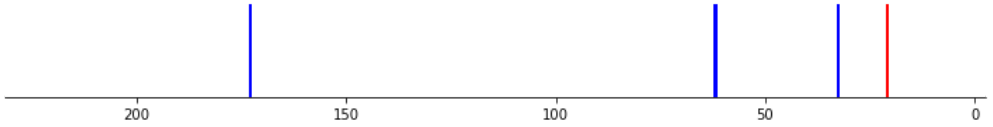


Top predicted substructures for the masked region(red):

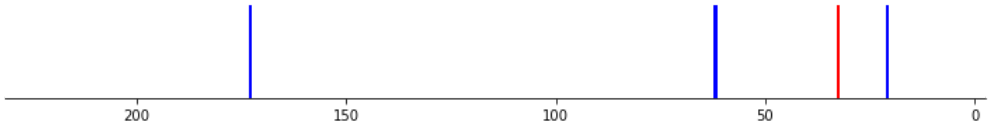
0.3756 [#6H3][#6][#6X3]
0.3448 [#7][#6][#6X3]
0.2297 [#7H2][#6X4H1][#6X3]
0.2213 [#8][#6H0][#6H1]
0.193 [CX4H1]([CX4H3])([CX4H3])[CX4H2]
0.1841 [CX4H1]([CX4H3])([CX4H3])[CX4H1]
0.1719 [CHX4]([CH3X4])[CH2X4]
0.168 O=[CX3][CX4H]



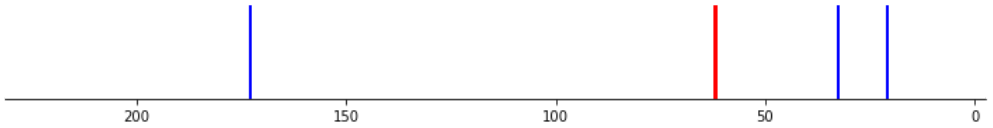
Top predicted substructures for the masked region(red):
0.9815 [CHX4]([CH3X4])[CH3X4]
0.8851 [#6H3][#6][#6]
0.8714 [#6H1]
0.8526 [CX4H3][CX4H1]
0.6712 [#6H3][#6][#6X3]
0.6013 [CX4H1]([CX4H3])([CX4H3])[CX3H0]
0.5066 [#8][#6H0][#6H1]
0.4522 [#7][#6][#6X3]



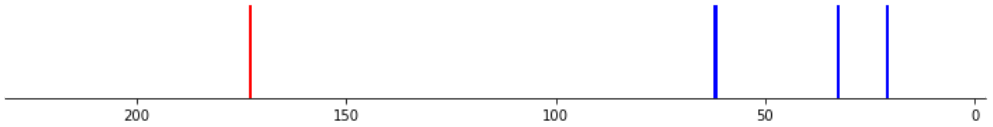
Top predicted substructures for the masked region(red):
0.4269 [#8][#6H0][#6H1]
0.3715 [#6H3][#6][#6X3]
0.3465 O=[CX3][CX4H]
0.3339 [CX4H1]([CX4H3])([CX4H3])[CX3H0]
0.3107 [CX4H3][CX4H1]
0.2991 [#7][#6][#6H3]
0.2846 [#7][#6][#6X3]
0.2827 [CHX4]([CH3X4])[CH3X4]



Top predicted substructures for the masked region(red):
0.2898 [#7][#6][#6X3]
0.2632 [#8][#6H0][#6H1]
0.2224 [CX4H1]([CX4H3])([CX4H3])[CX3H0]
0.2196 [CX4H1]([CX4H3])([CX4H3])[CX4H1]
0.2132 O=[CX3][CX4H]
0.2095 [#6H3][#6][#6X3]
0.1997 [CX4H1]([CX4H3])([CX4H3])[CX4H2]
0.1515 [OX2H1]

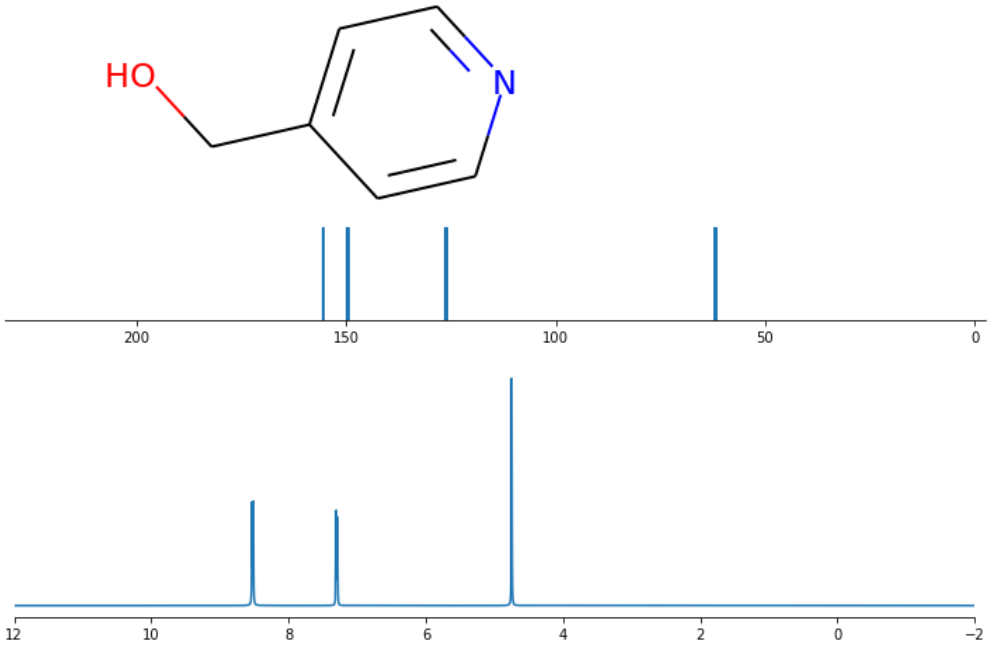


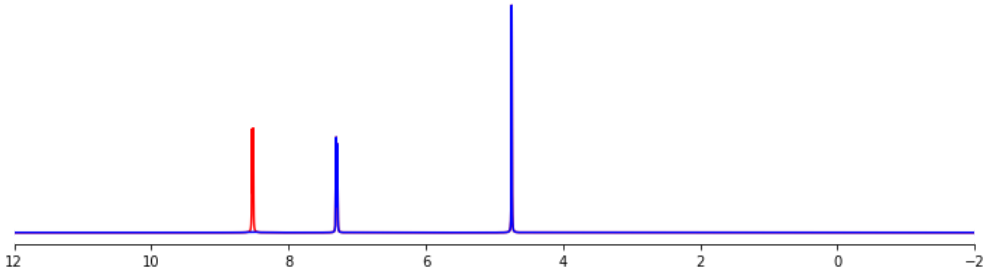
Top predicted substructures for the masked region(red):
0.4472 [#7][#6][#6X3]
0.422 [#8][#6H0][#6H1]
0.3526 [#7][#6][#6H3]
0.3251 O=[CX3][CX4H]
0.2876 [#7H2][#6X4H1][#6X3]
0.2153 [#6H3][#6][#6X3]
0.2049 [CX4H1]([CX4H3])([CX4H3])[CX4H1]
0.1735 [#6H3][#6H1][#6H1][#7]



Top predicted substructures for the masked region(red):
0.8283 [CX3](=[OX1])C
0.768 [#8]=[#6][#8]
0.7563 [#6H3][#6][#6X3]
0.7094 [CX3](=[OX1])O
0.629 [CX4H1]([CX4H3])([CX4H3])[CX3H0]
0.6038 [#7][#6][#6X3]
0.5171 [CHX4]([CH3X4])[CH3X4]
0.4449 O=[CX3][CX4H]

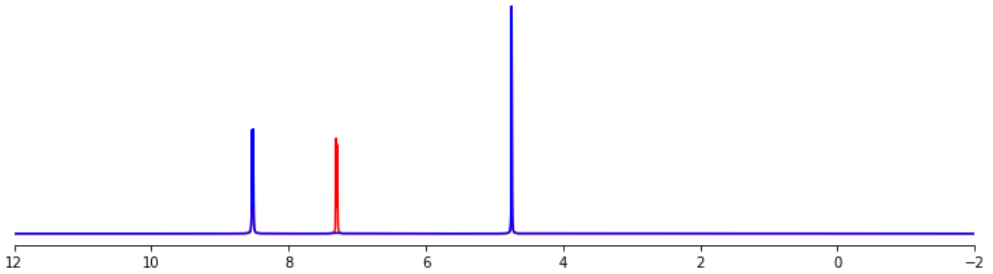
True structure: OCc1ccncc1





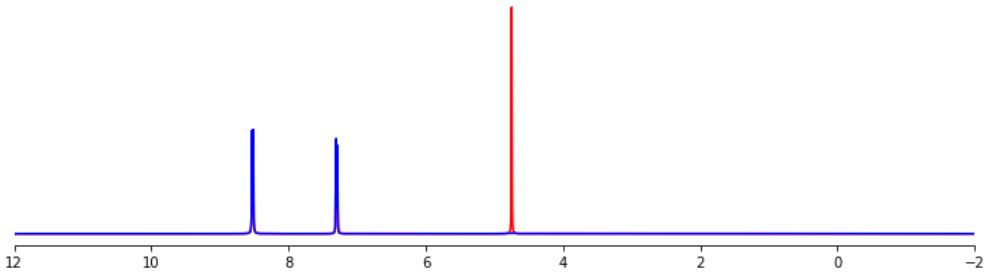
Top predicted substructures for the masked region(red):

0.3576 [#8][#6H2][#6H]=[#6X3]
0.341 [cX3H1]([cX3H1])[cX3H1]
0.2758 [CX3H1](=[NX2H0])[CX4H2]
0.2631 [#7]=[#6H1]
0.2538 [#6H1][#6H1]
0.2276 [cH][cH]
0.2223 [CX4H2]([OX2H0])[CX3H1]
0.1965 [CX3H1](=[CX3H1])[CX4H2]

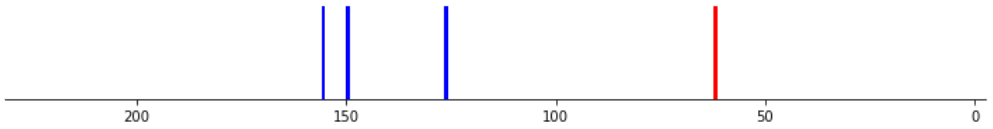


Top predicted substructures for the masked region(red):

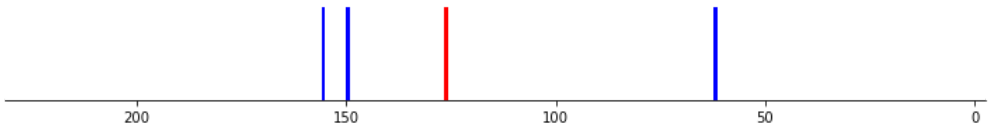
0.4961 [cX3H1]([cX3H1])[cX3H1]
0.4208 [cH][cH]
0.3128 [#6H1][#6H1]
0.272 [#7][#6H0][#6H1]
0.2719 [cH]
0.2641 [CX3H1](=[NX2H0])[CX4H2]
0.2562 [cX3H1]([cX3H1])[cX3H0]
0.1947 [CX3H2]=[CX3H1]



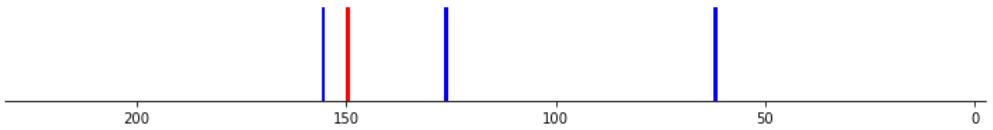
Top predicted substructures for the masked region(red):
0.6737 [CX4H2]([#6])[O]
0.6654 [#6X3][#6H2][#8]
0.5045 [CX4H2]([OX2H0])[CX3H1]
0.4352 [#8][#6H2][#6H]=[#6X3]
0.3944 [#7]=[#6H1]
0.3389 [CHX3](=C)C
0.3372 [#6H1][#6H2]
0.3224 O[CX4H2][CX3H1]



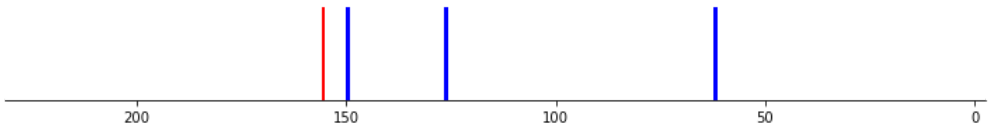
Top predicted substructures for the masked region(red):
0.5829 [#6X3][#6H2][#8]
0.4643 [CX4H2]([OX2H0])[CX3H1]
0.4374 [CX4H2]([#6])[O]
0.4264 [#8][#6H2][#6H]=[#6X3]
0.3179 [#7]=[#6H1]
0.276 [CX3H1](=[NX2H0])[CX4H2]
0.2442 [OX2H1][CX4H2][#6X3H0]
0.2206 [#6H1][#6H2]



Top predicted substructures for the masked region(red):
0.4298 [#8][#6H2][#6H]=[#6X3]
0.2936 [#6X3][#6X3][#6X3][#6X3]
0.2847 [#7][#6H0][#6H1]
0.2762 [#6X3H1][#6X3H0]
0.2542 [CX3H1](=[NX2H0])[CX4H2]
0.2252 [cX3H1]([cX3H1])[cX3H1]
0.2232 [#6H1][#6H2]
0.2124 [#6H1][#6H1]

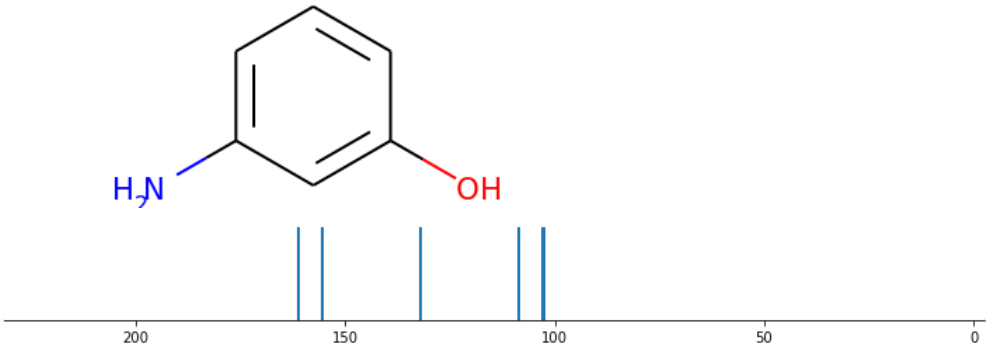


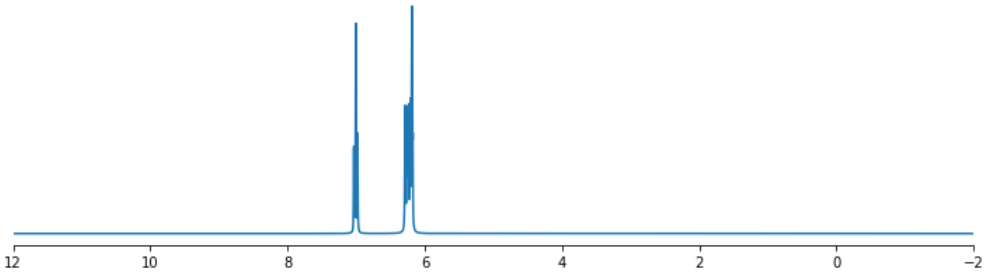
Top predicted substructures for the masked region(red):
0.4089 [#8][#6H2][#6H]=[#6X3]
0.3328 [#7]=[#6H1]
0.2736 [CX3H1](=[NX2H0])[CX4H2]
0.2716 [#6H1][#6H2]
0.251 [#6X3H1][#6X3H0]
0.2476 [CX4H2]([OX2H0])[CX3H1]
0.2141 [#7][#6H0][#6H1]
0.1961 [CX3H1](=[CX3H1])[CX4H2]

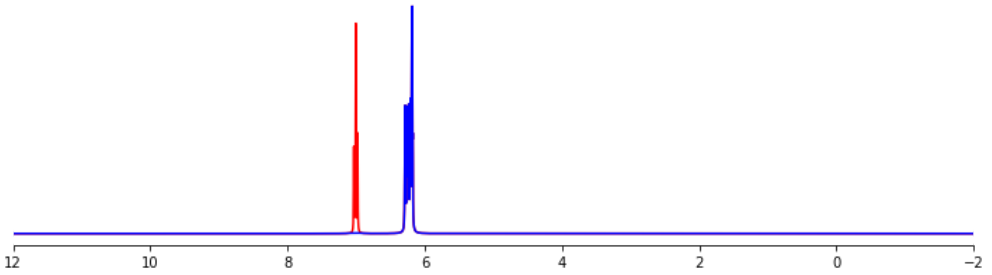


Top predicted substructures for the masked region(red):
0.4079 [#8][#6H2][#6H]=[#6X3]
0.3054 [#7]=[#6H1]
0.2812 [CX4H2]([OX2H0])[CX3H1]
0.2729 [CX3H1](=[NX2H0])[CX4H2]
0.2644 [#6H1][#6H2]
0.2594 [#6X3H1][#6X3H0]
0.2158 [#7][#6H0][#6H1]
0.195 [CX3H1](=[CX3H1])[CX4H2]

True structure: Nc1cccc(O)c1

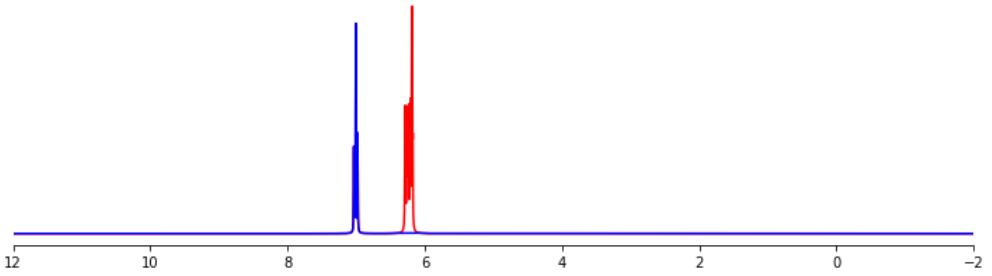






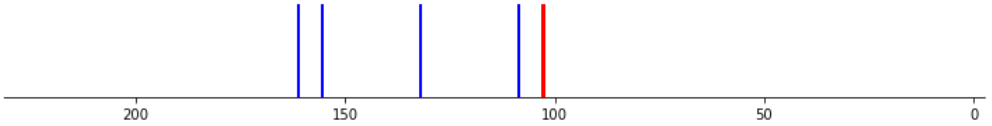
Top predicted substructures for the masked region(red):

0.1972 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1739 [#6]1[#6][#6][#6][#6][#7]1
0.1482 [cH]cO
0.1362 O=[cX3]
0.1195 [cX3H1]([cX3H1])[cX3H0]
0.0916 [#7][#6X3H0][#6X3H1]
0.0901 [#8][#6H1][#6H1]
0.0885 [cX3H1]([cX3H1])[cX3H1]



Top predicted substructures for the masked region(red):

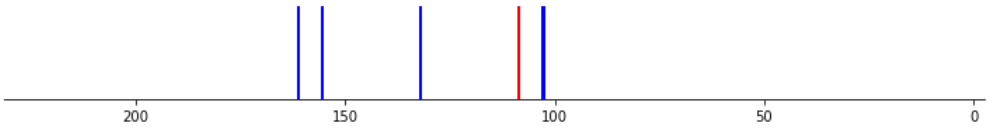
0.2038 [CHX3]=[CHX3]
0.173 [#7][#6X3H0][#6X3H1]
0.1521 [CX3H1](=[CX3H1])[CX3H1]
0.1127 [CHX3](=C)C
0.0949 [cX3H1]([cX3H1])[cX3H1]
0.0629 O=[cX3]
0.061 [#8][#6][#6]=[#8]
0.0591 [#6X3]=[#6X3][#6X3]=[#6X3]



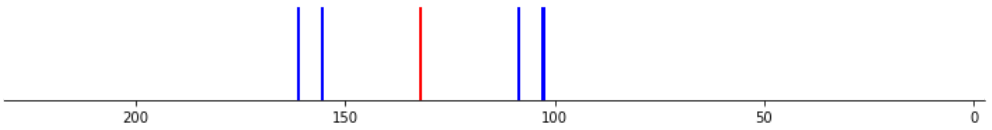
Top predicted substructures for the masked region(red):

0.1635 [CHX3]=[CHX3]
0.1619 [#7][#6X3H0][#6X3H1]

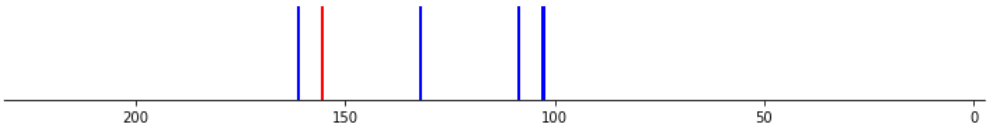
0.1493 [#7H][#6X3H1]
0.1467 [#6X3][#7][#6X3]
0.1382 [cH]cO
0.1337 [#8][#6][#6][#6X3]
0.1132 [cX3H1]([nX3H1])[cX3H1]
0.1102 [#7][#6H0][#6H1]



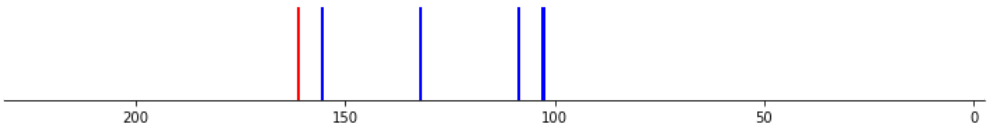
Top predicted substructures for the masked region(red):
0.2222 [#6X3][#7][#6X3]
0.179 [#7][#6X3H0][#6X3H1]
0.1521 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1362 [#6]1[#6][#6][#6][#6][#6]1
0.1304 [#8][#6][#6][#6X3]
0.1283 [#7H][#6X3H1]
0.1163 [CHX3]=[CHX3]
0.1033 [cX3H1]([nX3H1])[cX3H1]



Top predicted substructures for the masked region(red):
0.225 [#7][#6X3H0][#6X3H1]
0.2206 [CHX3]=[CHX3]
0.1228 [#7][#6H0][#6H1]
0.1222 O=[cX3]
0.107 [#6X3][#7][#6X3]
0.0926 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.0771 [#8][#6H0][#6H1]
0.0737 [#7H2][#6H0]

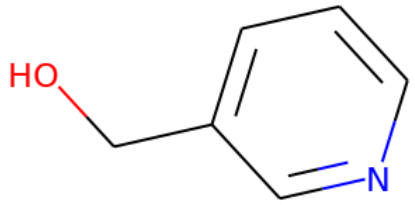


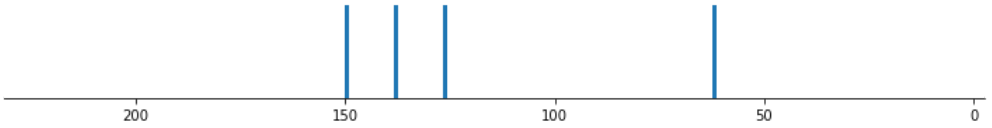
Top predicted substructures for the masked region(red):
0.2407 [#8][#6H0][#6H1]
0.1939 [CHX3]=[CHX3]
0.1885 [#7X3H2]
0.1859 [#6]1[#6][#6][#6][#6][#7]1
0.1522 [#7H2][#6H0]
0.1452 O=[cX3]
0.138 [#7][#6X3H0][#6X3H1]
0.0985 [#7][#6H0][#6H1]

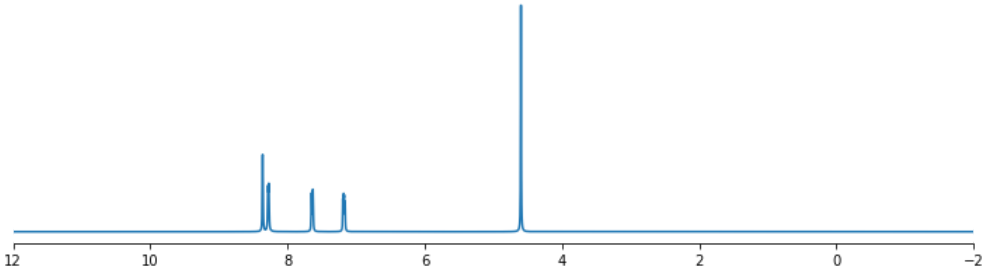


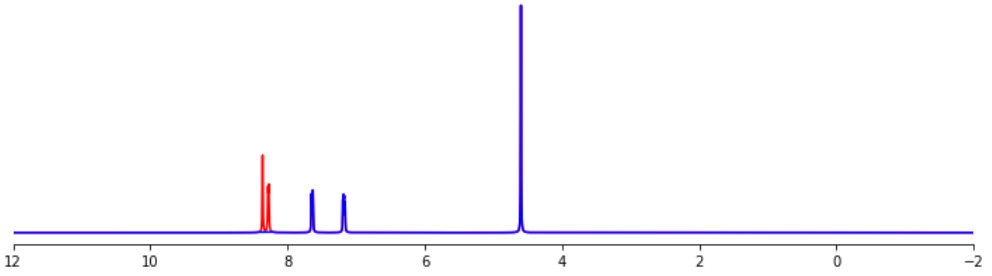
Top predicted substructures for the masked region(red):
0.3119 [#8][#6H0][#6H1]
0.2512 [#7X3H2]
0.25 [#6]1[#6][#6][#6][#6][#7]1
0.1932 [CHX3]=[CHX3]
0.1673 [#7][#6X3H0][#6X3H1]
0.155 O=[cX3]
0.1521 [#7][#6H0][#6H1]
0.1353 [#7H2][#6H0]

True structure: OCc1cccnc1

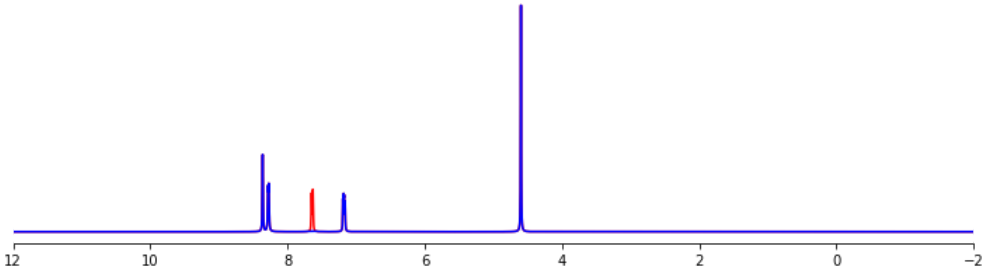




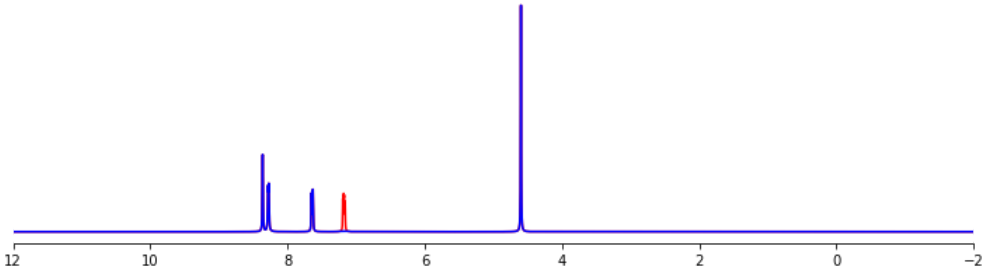




Top predicted substructures for the masked region(red):
0.4797 [#6H1][#7][#6H1]
0.4039 [cX3H1]([nX2H0])[cX3H1]
0.2023 [cX3H1]([cX3H1])[cX3H1]
0.1696 [#6X3][#7X3][#6X3]
0.145 [OX2H1][CX4H2][#6X3H0]
0.1326 [#7][#6H0][#6H1]
0.0958 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.0929 [#6X3][#6H2][#8]

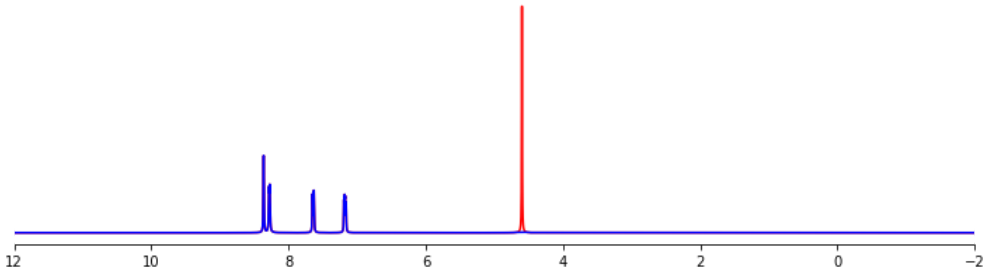


Top predicted substructures for the masked region(red):
0.213 [#8][#6H2][#6H]=[#6X3]
0.1734 [cX3H1]([nX2H0])[cX3H1]
0.1536 [#7][#6H0][#6H1]
0.1409 [cX3H1]([cX3H1])[cX3H1]
0.1206 [#6X3][#7X3][#6X3]
0.0915 [#6X3][#6H2][#8]
0.0892 [CHX3](=C)C
0.0831 [cX3H1]([nX3H1])[cX3H1]

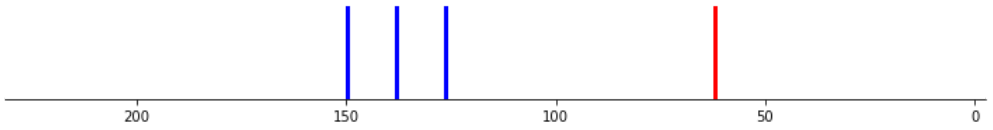


Top predicted substructures for the masked region(red):
0.3945 [#6H1][#7][#6H1]
0.226 [cX3H1]([nX2H0])[cX3H1]
0.1877 [#8][#6H2][#6H]=[#6X3]
0.1643 [#6X3][#7X3][#6X3]
0.1593 [cX3H1]([cX3H1])[cX3H1]
0.1554 [#7][#6H0][#6H1]
0.1044 [OX2H1][CX4H2][#6X3H0]

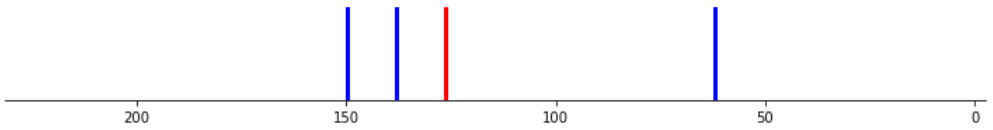
0.0972 [#6X3][#6H2][#8]



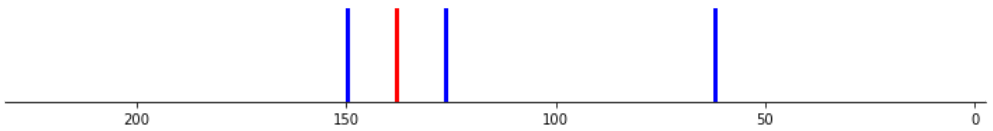
Top predicted substructures for the masked region(red):
0.7434 [#6X3][#6H2][#8]
0.6483 [OX2H1][CX4H2][#6X3H0]
0.6406 [CX4H2]([#6])[O]
0.2734 [#8][#6H2][#6H]=[#6X3]
0.1874 [#6H1][#6H2]
0.1567 [CHX3](=C)C
0.1529 [#6X3][#7X3][#6X3]
0.1443 [CX4H2]([OX2H1])[cX3H0]



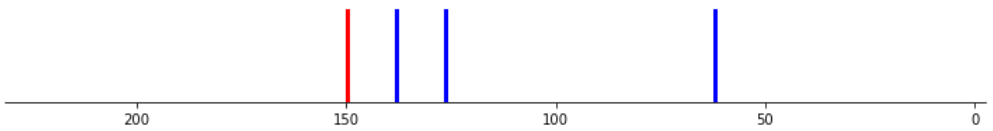
Top predicted substructures for the masked region(red):
0.6675 [#6X3][#6H2][#8]
0.6024 [CX4H2]([#6])[O]
0.5295 [OX2H1][CX4H2][#6X3H0]
0.2672 [#8][#6H2][#6H]=[#6X3]
0.2474 [cX3H1]([nX2H0])[cX3H1]
0.2471 [#6H1][#7][#6H1]
0.1906 [#8][#6][#6][#6X3]
0.1894 [OX2H1]



Top predicted substructures for the masked region(red):
0.2662 [#8][#6H2][#6H]=[#6X3]
0.2623 [#6H1][#7][#6H1]
0.2489 [OX2H1][CX4H2][#6X3H0]
0.2183 [#6X3][#7X3][#6X3]
0.2018 [#6X3H1][#6X3H0]
0.1962 [#7][#6H0][#6H1]
0.1869 [#6X3][#6H2][#8]
0.1732 [cX3H1]([nX2H0])[cX3H1]

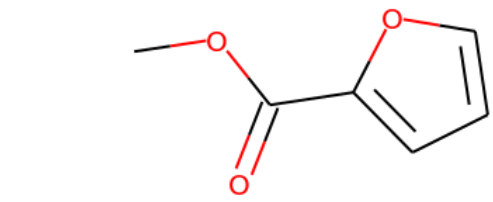


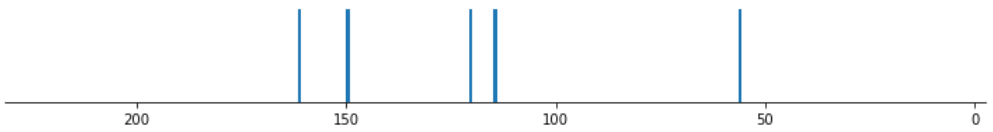
Top predicted substructures for the masked region(red):
0.2571 [#8][#6H2][#6H]=[#6X3]
0.2187 [#6H1][#7][#6H1]
0.2183 [#6X3H1][#6X3H0]
0.212 [OX2H1][CX4H2][#6X3H0]
0.1802 [#7][#6H0][#6H1]
0.1757 [#6X3][#7X3][#6X3]
0.1684 [cX3H1]([nX2H0])[cX3H1]
0.1683 [#6X3][#6H2][#8]

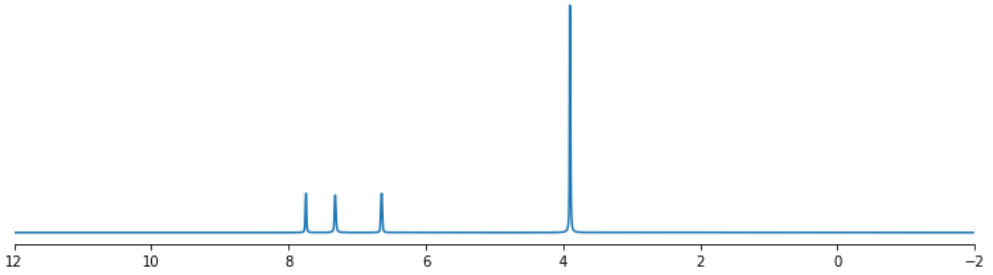


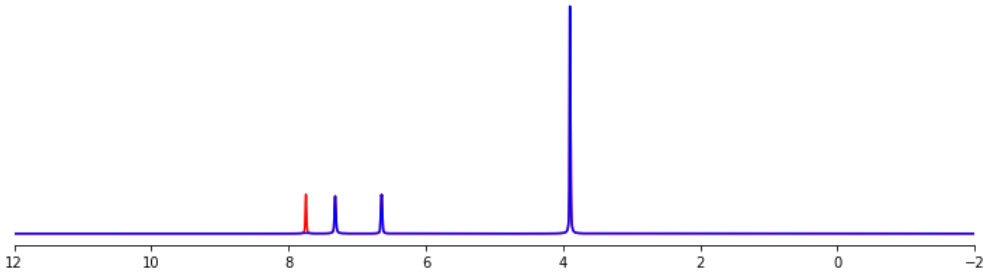
Top predicted substructures for the masked region(red):
0.2423 [cX3H1]([nX2H0])[cX3H1]
0.2297 [#8][#6H2][#6H]=[#6X3]
0.2141 [OX2H1][CX4H2][#6X3H0]
0.1877 [#6X3H1][#6X3H0]
0.1624 [#7][#6H0][#6H1]
0.1254 [#6X3][#6H2][#8]
0.1231 [CHX3](=C)C
0.1025 [#6H1][#7][#6H1]

True structure: COC(=O)c1ccco1

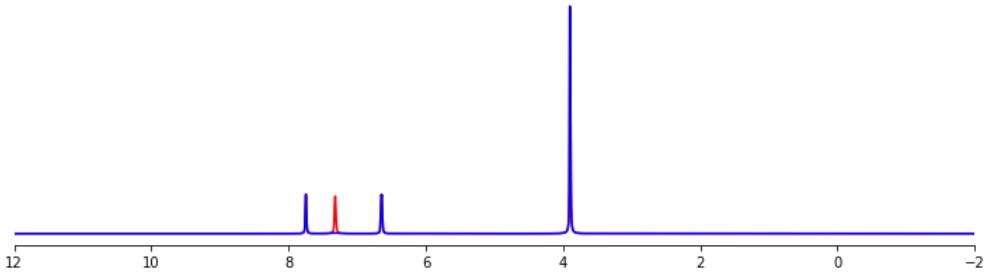




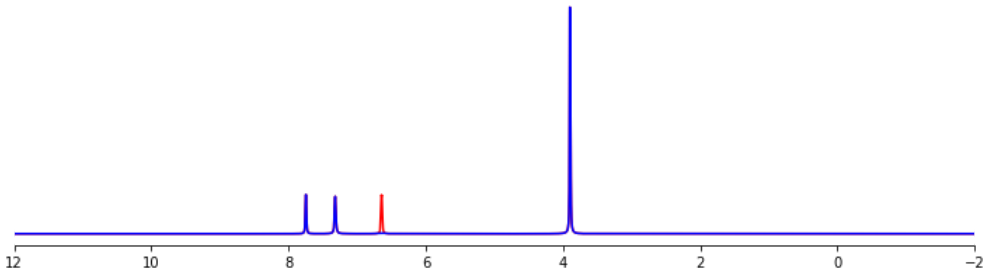




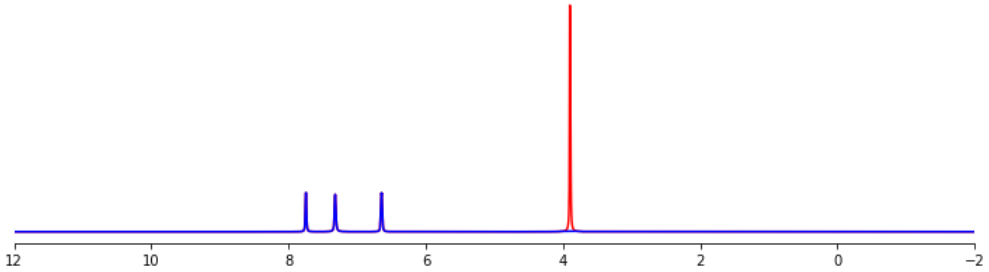
Top predicted substructures for the masked region(red):
0.3841 [cX3H1]([cX3H1])[cX3H1]
0.3431 [CX3H1](=[CX3H1])[CX4H1]
0.2957 [CX4H](O)CO
0.2511 [CX3H][CX4H]
0.2437 O=[#6][#6]=[#6X3]
0.2337 [CX3](=O)[OX2H1]
0.2312 [CX3H0](=[OX1H0])([OX2H0])[CX3H1]
0.2235 [CX4H](O)([CH])[CH]



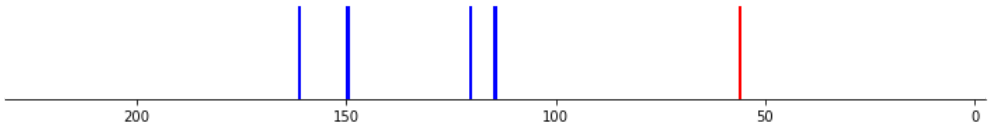
Top predicted substructures for the masked region(red):
0.4243 [CX3H1](=[CX3H1])[CX4H1]
0.3945 [cX3H1]([cX3H1])[cX3H1]
0.2784 [CX3](=O)[OX2H1]
0.2593 [CX4H](O)CO
0.2548 O=[#6][#6]=[#6X3]
0.2323 [CX3](=[OX1])O
0.2293 [#8]=[#6H0][#6H1]
0.1971 [CX4H](O)([CH])[CH]



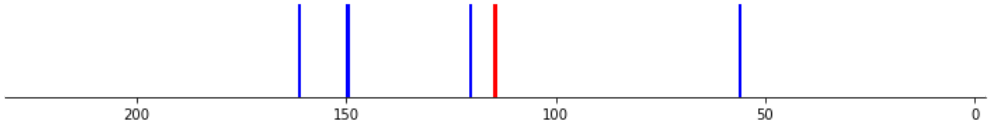
Top predicted substructures for the masked region(red):
0.4513 [CX3H1](=[CX3H1])[CX4H1]
0.3092 [CX3](=[OX1])O
0.3006 [CX4H](O)CO
0.293 [CX3](=O)[OX2H1]
0.2811 [CX3H][CX4H]
0.265 [cX3H1]([cX3H1])[cX3H1]
0.2614 [CX3H0](=[OX1H0])([OX2H0])[CX3H1]
0.2547 O=[#6][#6]=[#6X3]



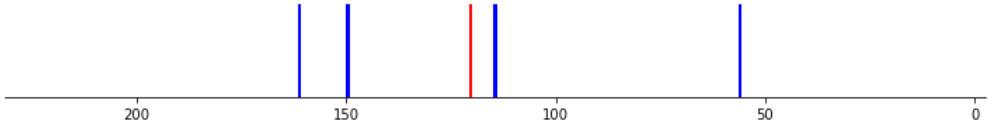
Top predicted substructures for the masked region(red):
0.4641 [CX3H1](=[CX3H1])[CX4H1]
0.4485 [#8][#6][#6][#8]
0.3489 [CX4H](O)CO
0.3202 [CX3H][CX4H]
0.2826 [CX3H0](=[OX1H0])([OX2H0])[CX3H1]
0.256 O=[#6][#6]=[#6X3]
0.2474 [#8]=[#6H0][#6H1]
0.2449 [CX4H](O)([CH])[CH]



Top predicted substructures for the masked region(red):
0.4663 [CX3H1](=[CX3H1])[CX4H1]
0.4449 [CX4H3][OX2H0]
0.3443 [CX4H](O)CO
0.3175 [CX3H][CX4H]
0.311 [CX3](=[OX1])O
0.2881 [#8][#6H1][#6H1]
0.257 [CX3H0](=[OX1H0])([OX2H0])[CX3H1]
0.255 O=[#6][#6]=[#6X3]

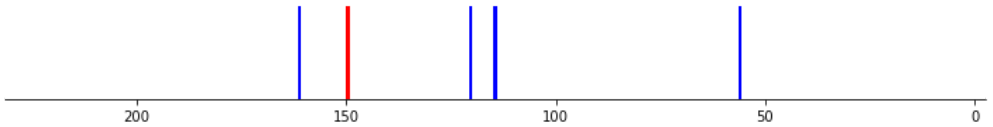


Top predicted substructures for the masked region(red):
0.3893 [CX3H1](=[CX3H1])[CX4H1]
0.2887 [#8][#6][#6][#8]
0.2278 o[cH]
0.2247 [CX3](=O)[OX2H1]
0.2236 O=[#6][#6]=[#6X3]
0.1952 [CX4H](O)CO
0.1889 [CX3H][CX4H]
0.1756 [#8][#6][#6]=[#6X3]

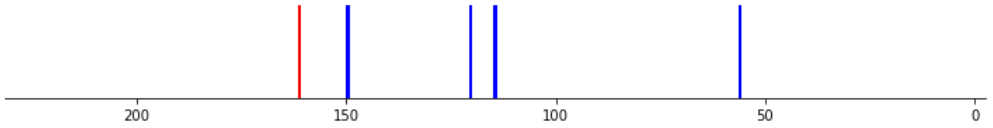


Top predicted substructures for the masked region(red):
0.41 [CX3H1](=[CX3H1])[CX4H1]
0.2459 O=[#6][#6]=[#6X3]
0.2311 [CX3H0](=[OX1H0])([OX2H0])[CX3H1]

0.2292 [CX3H][CX4H]
0.2264 [CX4H](O)CO
0.2221 [CX3](=O)[OX2H1]
0.201 [#8][#6][#6]=[#6X3]
0.19 [#8][#6][#6][#8]

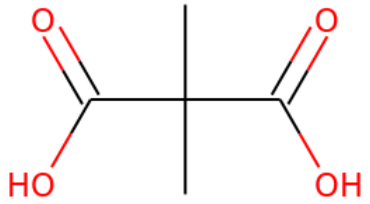


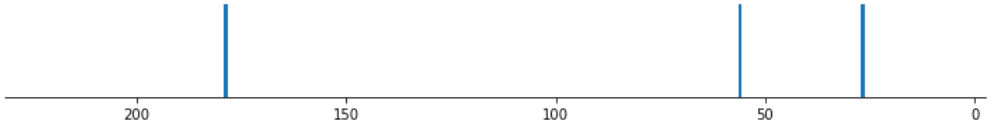
Top predicted substructures for the masked region(red):
0.4254 [CX3H1](=[CX3H1])[CX4H1]
0.3591 [CX3](=[OX1])O
0.2677 [CX3](=O)[OX2H1]
0.2554 O=[#6][#6]=[#6X3]
0.2535 [CX3H0](=[OX1H0])([OX2H0])[CX3H1]
0.2363 [CX4H](O)CO
0.2359 [cX3H1]([cX3H1])[cX3H1]
0.2256 [CX3H][CX4H]

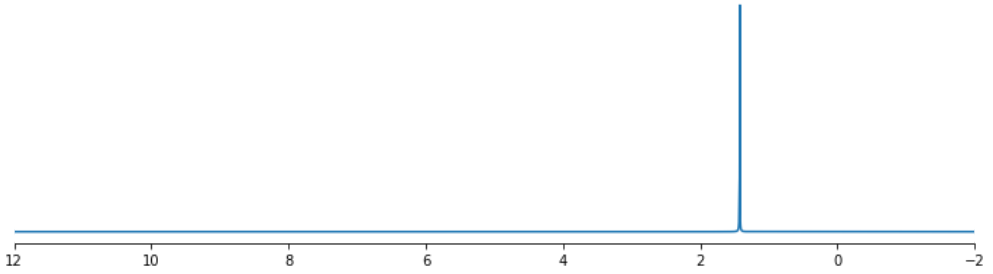


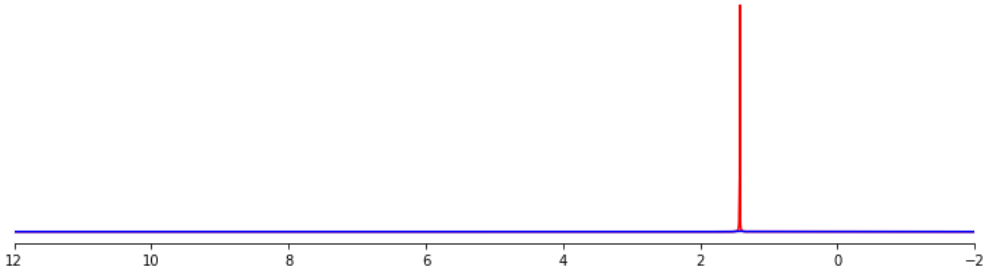
Top predicted substructures for the masked region(red):
0.621 [CX3](=[OX1])O
0.5079 [#8]=[#6][#8]
0.4377 [CX3H1](=[CX3H1])[CX4H1]
0.3435 [CX3](=O)[OX2H1]
0.2953 [#8]=[#6H0][#6H1]
0.2811 [CX3H0](=[OX1H0])([OX2H0])[CX3H1]
0.2603 [#8]=[#6][#6H1][#6H1]
0.2599 [cX3H1]([cX3H1])[cX3H1]

True structure: CC(C)(C(=O)O)C(=O)O



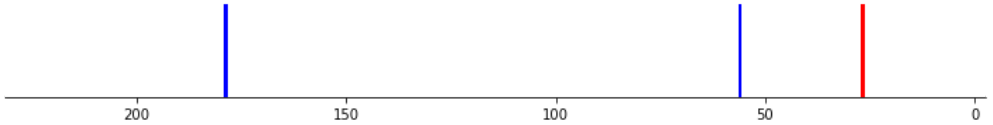




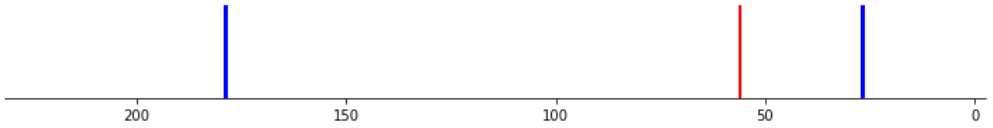


Top predicted substructures for the masked region(red):
0.8244 [CX4H3][#6]
0.7378 [CX4H3][CX4H0]
0.6875 [OX1H0]=[CX3H0][CX4H0][CX4H3]

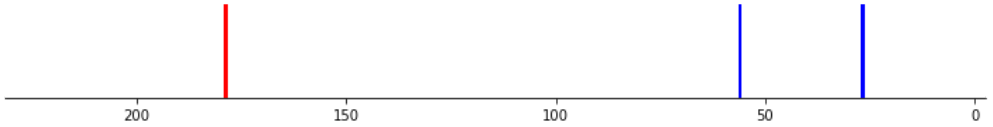
0.6833 [CH3][#6][#8]
0.6224 [#6H3][#6][#6]
0.6158 [CX4H3][CX4]O
0.5658 [#6H3][#6H0]
0.5269 [#6H3][#6][#6X3]



Top predicted substructures for the masked region(red):
0.5819 [CX4H3][#6]
0.4495 [CH3][#6][#8]
0.4312 [#8][#6H0][#6H1]
0.3826 [#6H3][#6][#6]
0.3378 [CH3]CC[OH]
0.3208 [#6H3][#6][#6X3]
0.2908 [CX4H3][CX4]O
0.279 [#6]1[#6]([#6H3])[#6]1

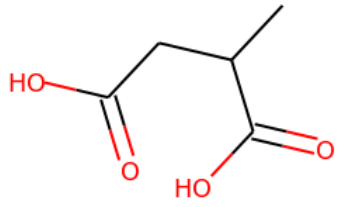


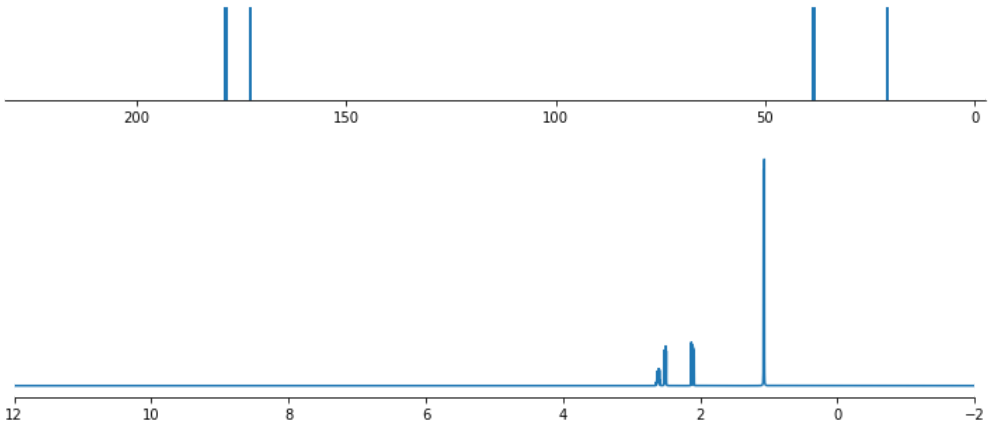
Top predicted substructures for the masked region(red):
0.4666 [#8][#6H0][#6H1]
0.283 O=[CX3][CX4H]
0.2365 [#8][#6][#6][#6][#6]=[#8]
0.2147 [#6]1[#6]([#6H3])[#6]1
0.2142 C1CC1O
0.2093 [#6H3][#6][#6X3]
0.1994 [OX1H0]=[CX3H0][CX4H0][CX4H3]
0.1884 [#6X3][#6][#6][#6H3]

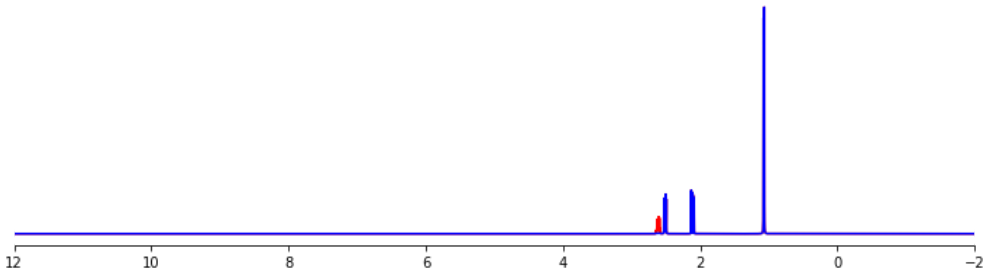


Top predicted substructures for the masked region(red):
0.9535 [CX3](=[OX1])C
0.9237 [CX3](=O)[OX2H1]
0.916 [CX3](=[OX1])O
0.8011 [OX1H0]=[CX3H0][CX4H0][CX4H3]
0.7437 [#8]=[#6][#8]
0.6034 [#6H3][#6][#6X3]
0.5392 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.4389 [#8]=[#6H0][#6H1]

True structure: CC(CC(=O)O)C(=O)O

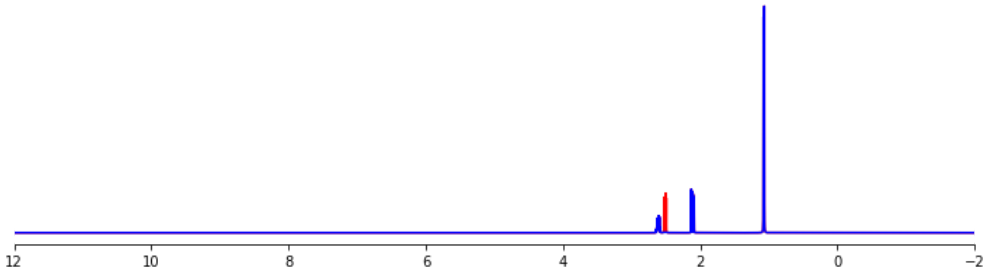






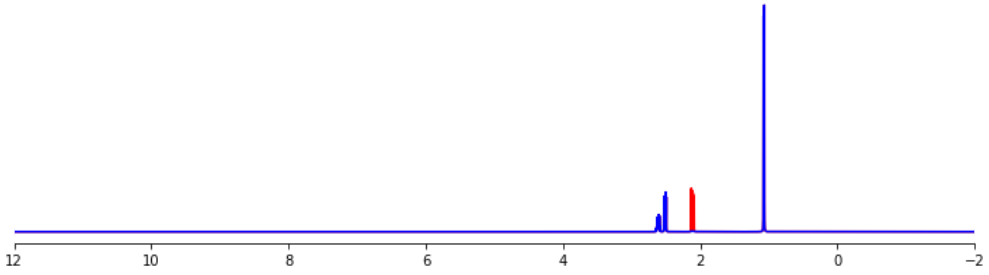
Top predicted substructures for the masked region(red):

0.4787 [CX4H2]CC=O
0.468 O=[CX3][CX4H]
0.4076 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3424 [#8]=[#6H0][#6H1]
0.2473 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.2091 [#8][#6H0][#6H1]
0.1998 [#6H1][#6H2]
0.186 [CHX4]([CH3X4])[CH2X4]



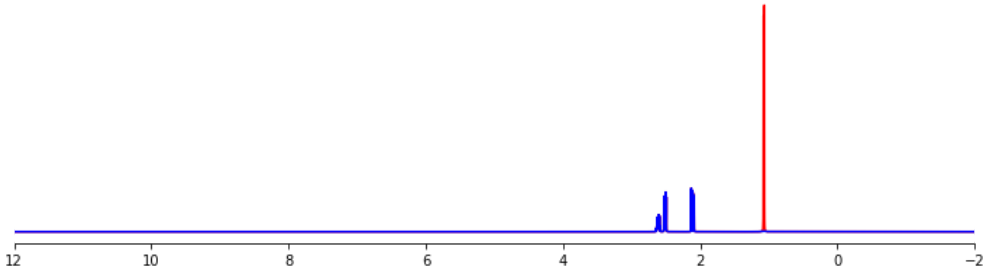
Top predicted substructures for the masked region(red):

0.4599 [CX4H2]CC=O
0.392 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.2636 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.2594 O=[CX3][CX4H]
0.1857 [CHX4]([CH3X4])[CH2X4]
0.1706 [#6H1][#6H2]
0.1664 [#8]=[#6H0][#6H1]
0.1481 [#8][#6][#6][#6][#6]=[#8]



Top predicted substructures for the masked region(red):

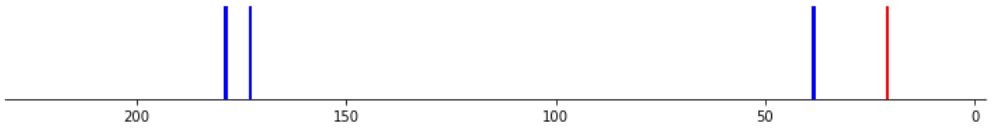
0.5127 [CX4H2]CC=O
0.4024 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3001 [#6H1][#6H2]
0.2964 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.2163 [CHX4]([CH3X4])[CH2X4]
0.2075 O=[CX3][CX4H]
0.1917 [#8][#6][#6][#6][#6]=[#8]
0.1905 [#8]=[#6H0][#6H1]



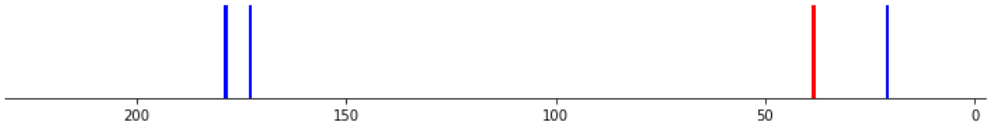
Top predicted substructures for the masked region(red):

0.9034 [CX4H3][CX4H1]
0.8253 [CHX4]([CH3X4])[CH2X4]
0.6985 [#6H3][#6][#6]
0.5294 O=[CX3][CX4H]
0.4826 [#6H1]

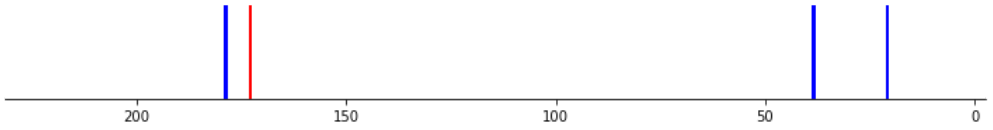
0.4201 [#6X3][#6][#6][#6H3]
0.4099 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3996 [#8]=[#6H0][#6H1]



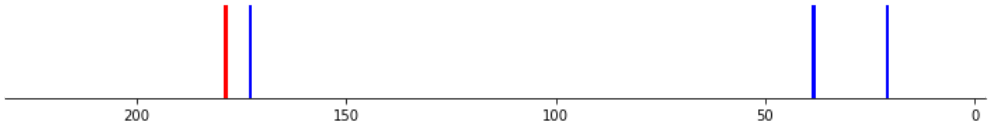
Top predicted substructures for the masked region(red):
0.4532 O=[CX3][CX4H]
0.4341 [CX4H3][#6]
0.4155 [CX4H3][CX4H1]
0.41 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.4084 [#8]=[#6H0][#6H1]
0.396 [CX4H2]CC=O
0.3697 [#8][#6H0][#6H1]
0.3271 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]



Top predicted substructures for the masked region(red):
0.5957 [CX4H2]CC=O
0.4717 O=[CX3][CX4H]
0.4098 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3141 [#8]=[#6H0][#6H1]
0.2834 [#6H1][#6H2]
0.2343 [#8][#6H0][#6H1]
0.2236 [#8]=[#6][#6H2][#6H1]
0.2107 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]

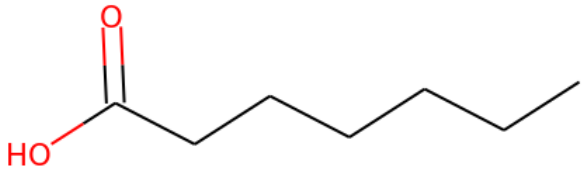


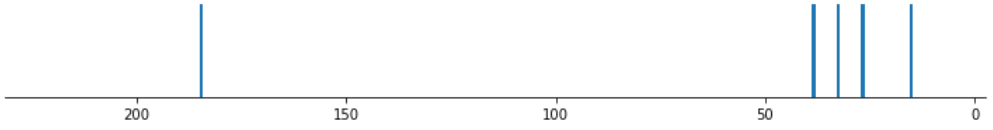
Top predicted substructures for the masked region(red):
0.5042 O=[CX3][CX4H]
0.446 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.4163 [CX4H2]CC=O
0.4096 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3665 [#8]=[#6H0][#6H1]
0.2195 [CHX4]([CH3X4])[CH2X4]
0.2127 [#6H3][#6][#6X3]
0.198 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]

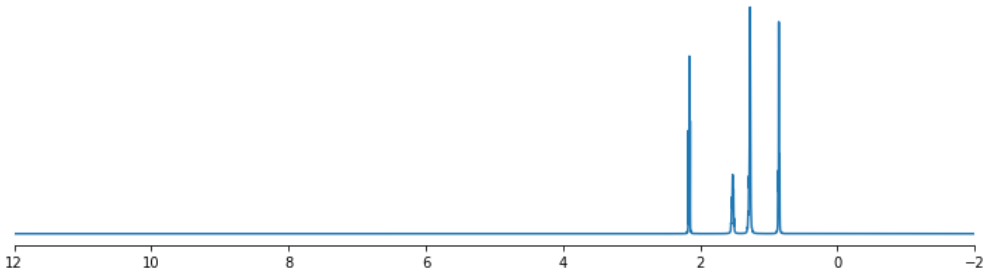


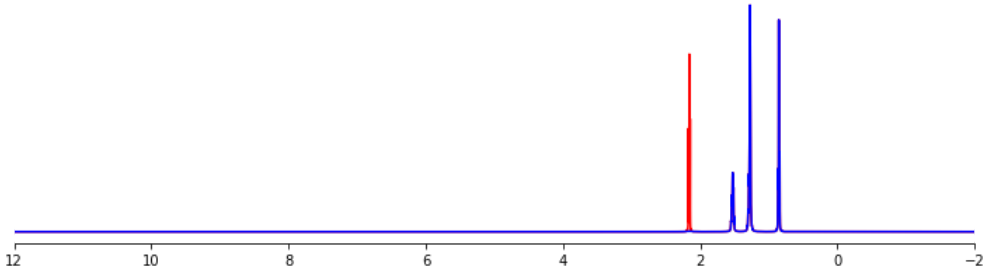
Top predicted substructures for the masked region(red):
0.5721 O=[CX3][CX4H]
0.5559 [CX4H2]CC=O
0.4852 [#8]=[#6H0][#6H1]
0.4419 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.4349 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.4098 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.2367 [CHX4]([CH3X4])[CH2X4]
0.2361 [#6H3][#6][#6X3]

True structure: CCCCCCC(=O)O



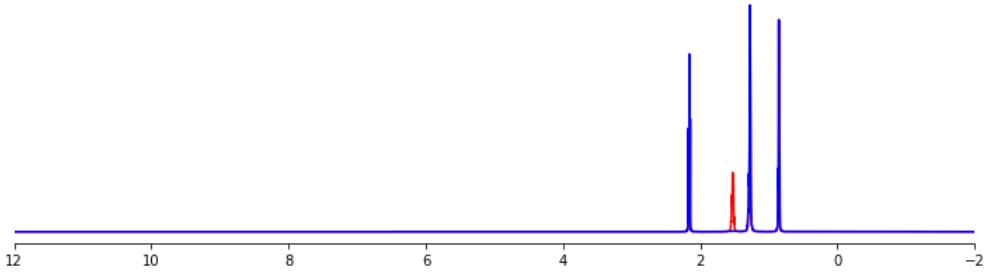






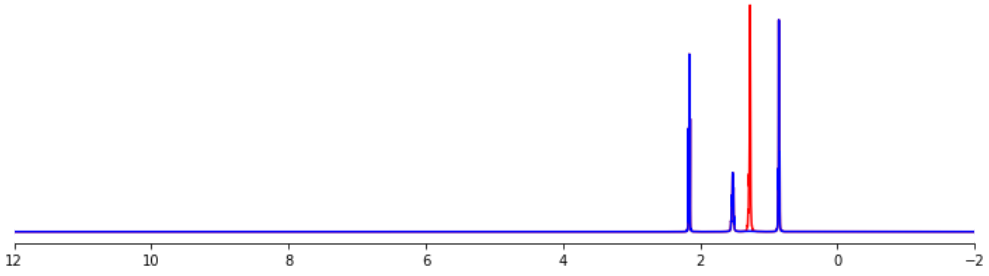
Top predicted substructures for the masked region(red):

0.8104 [CX4H2]([CX4H2])[CX3H0]
0.6796 O=[CX3H0][CX4H2][CX4H2]
0.4791 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.4773 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.4118 CCCCCC
0.3989 [CX4H2][CX3]=O
0.238 [CX4H2]([CX4H2])[CX4H2]
0.1672 [#8][#6][#6H2]



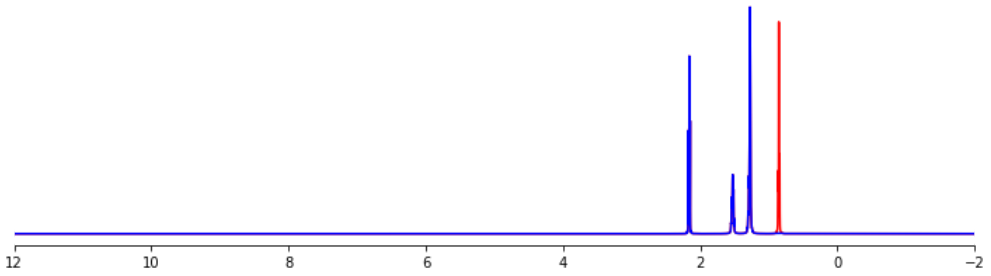
Top predicted substructures for the masked region(red):

0.4983 CCCCCC
0.4278 [CX4H2]([CX4H2])[CX4H2]
0.3972 [CX4H2]([CX4H2])[CX3H0]
0.3517 [CX4H2][CX4H2][CX4H2][CX4H2]
0.3397 [CX4H2]([CX4H3])[CX4H2]
0.2842 OCC[CH2]
0.247 [#6H1][#6H2]
0.2141 [CX4H2][CX4H2]

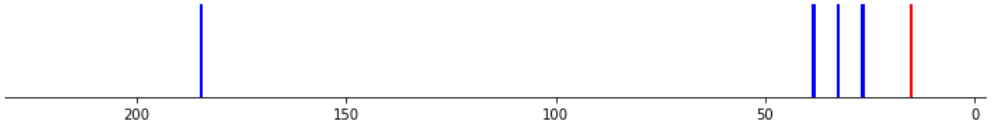


Top predicted substructures for the masked region(red):

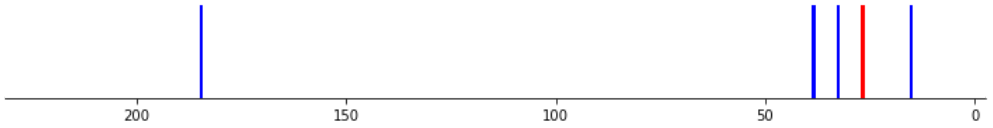
0.3699 CCCCCC
0.3652 [#6H1][#6H2]
0.3513 [#8][#6H0][#6H1]
0.2681 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.2472 [#6H1]
0.2186 [CX4H2]([CX4H2])[CX4H2]
0.1895 [CX4H2][CX4H2][CX4H2][CX4H2]
0.1885 [CX4H2]([CX4H2])[CX3H0]



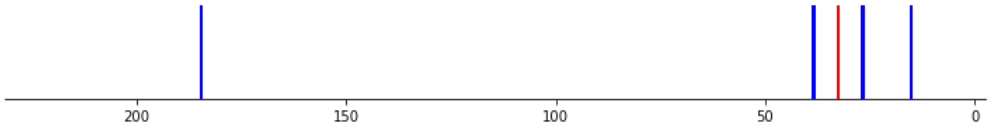
Top predicted substructures for the masked region(red):
0.4929 [CX4H2]([CX4H3])[CX4H2]
0.3613 [#6H1][#6H2]
0.359 CCCCCC
0.2975 [#8][#6H0][#6H1]
0.251 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.2407 [#6H1]
0.1216 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.1029 [CX4H2]([CX4H2])[CX3H0]



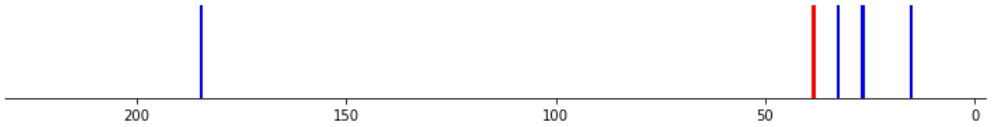
Top predicted substructures for the masked region(red):
0.8692 [CX4H2]([CX4H3])[CX4H2]
0.8026 [CX4H3][CX4H2]
0.3178 [#8][#6H0][#6H1]
0.1684 CCCCCC
0.138 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.116 [CX4H2]([CX4H2])[CX3H0]
0.1154 [#8]=[#6H0][#6H1]
0.1029 [CX4H2]([CX4H3])[CX4H1]



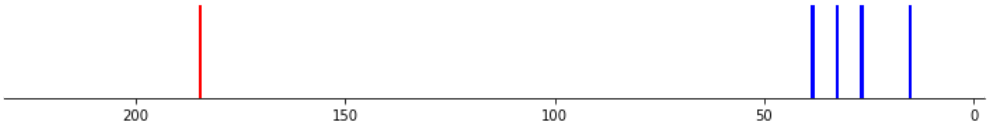
Top predicted substructures for the masked region(red):
0.4313 [CX4H2]([CX4H2])[CX3H0]
0.4231 CCCCCC
0.3959 [CX4H2]([CX4H3])[CX4H2]
0.3281 [CX4H2]([CX4H2])[CX4H2]
0.2679 [#8][#6H0][#6H1]
0.2205 [CX4H2][CX4H2][CX4H2][CX4H2]
0.212 O=[CX3H0][CX4H2][CX4H2]
0.1752 [#6H1][#6H2]



Top predicted substructures for the masked region(red):
0.4851 CCCCCC
0.4837 [CX4H2]([CX4H2])[CX3H0]
0.3756 [CX4H2]([CX4H2])[CX4H2]
0.2979 O=[CX3H0][CX4H2][CX4H2]
0.2275 [CX4H2][CX3]=O
0.1666 [#6H1][#6H2]
0.1663 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.1483 [#8][#6H0][#6H1]

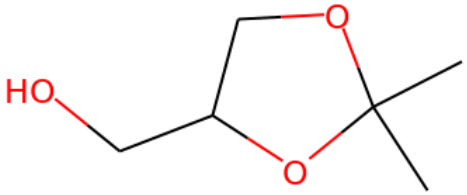


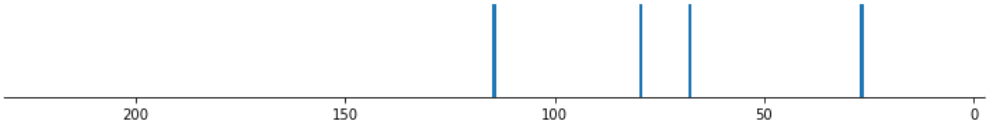
Top predicted substructures for the masked region(red):
0.5684 [CX4H2]([CX4H2])[CX3H0]
0.4726 CCCCCC
0.4353 O=[CX3H0][CX4H2][CX4H2]
0.3777 [CX4H2][CX3]=O
0.2528 [CX4H2]([CX4H2])[CX4H2]
0.249 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.232 [#8][#6H0][#6H1]
0.2024 [#6H1][#6H2]

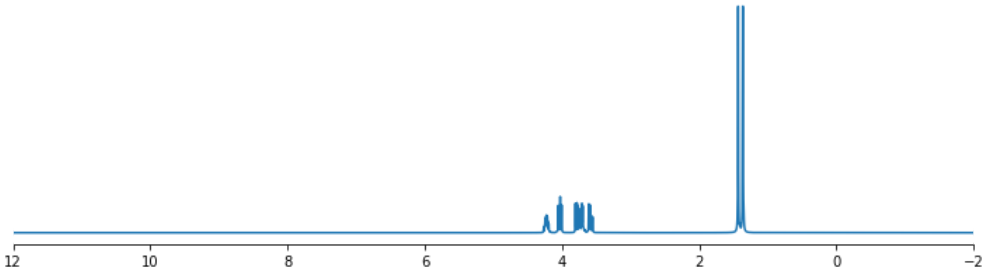


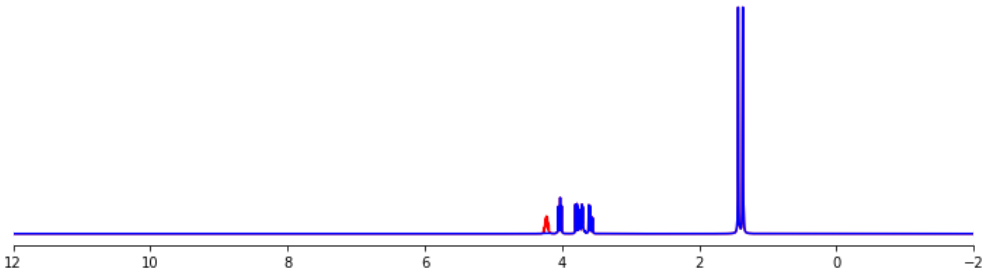
Top predicted substructures for the masked region(red):
0.993 [CX3](=[OX1])C
0.9912 [CX3](=O)[OX2H1]
0.984 [CX3](=[OX1])O
0.9662 [#8]=[#6][#8]
0.9553 [CX4H2]([CX4H2])[CX3H0]
0.9548 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.7528 [CX4H2]CC=O
0.7261 O=[CX3H0][CX4H2][CX4H2]

True structure: CC1(C)OCC(CO)O1

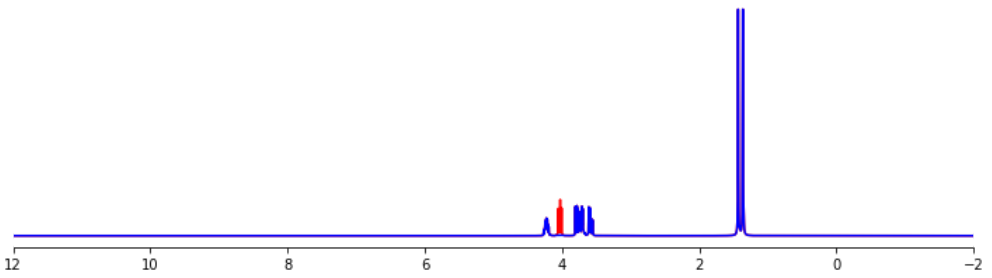






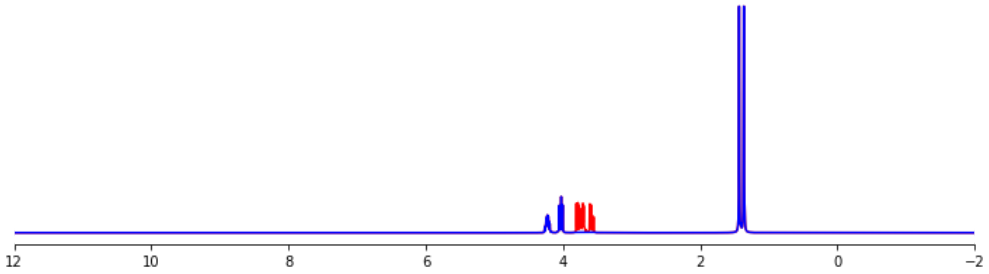


Top predicted substructures for the masked region(red):
0.4552 [CH3]CC[OH]
0.3407 [#6H2][#8][#6H1]
0.3286 [CH2X4](O)[CX4H2]
0.2629 [#8][#6H0][#6H1]
0.1888 [CX4H2][CX4H2]
0.16 [CX4H2]([#6])[#6]
0.1475 [#6X4H2][#6H1][#8H]
0.1348 [CX4H1]([OX2H1])([CX4H2])[CX4H0]

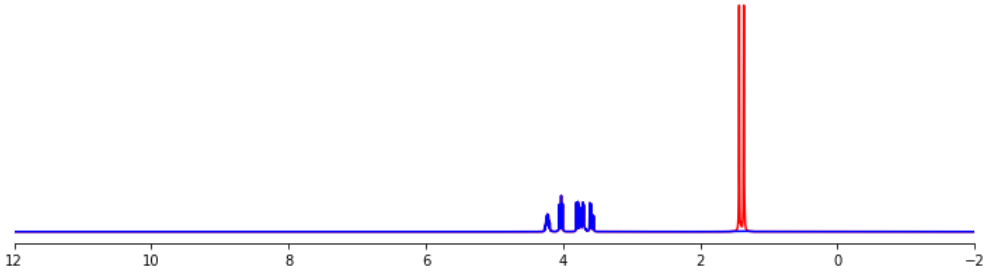


Top predicted substructures for the masked region(red):
0.4541 [CH2X4](O)[CX4H2]
0.3776 [CH3]CC[OH]

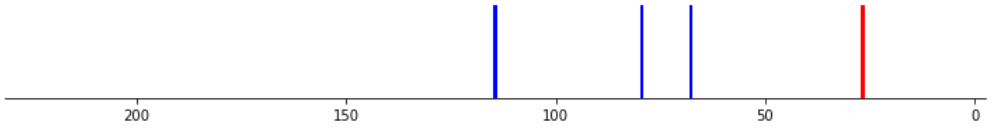
0.333 C1OCCC1
0.3101 [#6H2][#8][#6H1]
0.3 [OX2H0][CX4H2][#6H0]
0.2804 [#8][#6H0][#6H1]
0.2175 [CX4H2]([OX2H0])[CX4H2]
0.1655 [CX4H2]([OX2H0])[CX4H1]



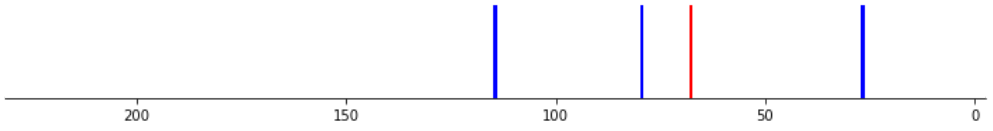
Top predicted substructures for the masked region(red):
0.5509 [CH2X4](O)[CX4H2]
0.423 [CH3]CC[OH]
0.3656 [#6H2][#8][#6H1]
0.3324 [OX2H0][CX4H2][#6H0]
0.2484 [CX4H2](O)[CHX4]
0.2111 [CX4H2]([OX2H0])[CX4H1]
0.211 [CX4H2]([OX2H1])[CX4H1]
0.1913 [#8][#6H0][#6H1]



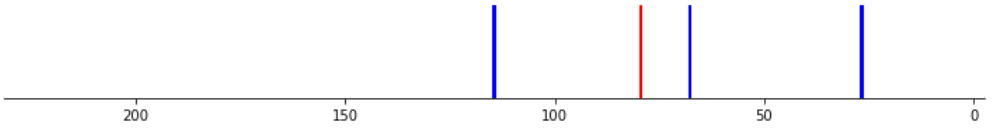
Top predicted substructures for the masked region(red):
0.8755 [#8][#6H0][#6H1]
0.8575 [#6H3][#6H0]
0.7971 [CX4H3][CX4H0]
0.7136 [CH3]CC[OH]
0.6365 [#6X4H3][#6][#8H]
0.629 [#6H3][#6][#6]
0.3658 [OX2H1][CX4H0][CX4H3]
0.363 [CH2X4](O)[CX4H2]



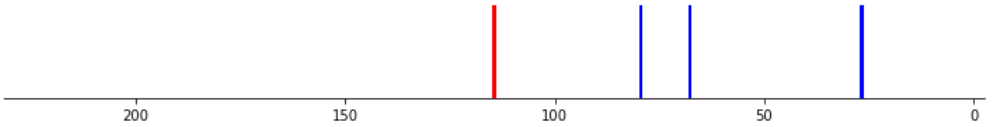
Top predicted substructures for the masked region(red):
0.5668 [CH2X4](O)[CX4H2]
0.5533 [CH3]CC[OH]
0.4454 [CX4H3][CX4H0]
0.4292 [#8][#6H0][#6H1]
0.3828 [#6H3][#6H0]
0.3415 [CX4H2][CX4H2]
0.3402 [CX4H2]([OX2H0])[CX4H2]
0.3351 [#6H2][#8][#6H1]



Top predicted substructures for the masked region(red):
0.8643 [CH2X4](O)[CX4H2]
0.5299 [CX4H2]([OX2H0])[CX4H2]
0.2834 [CX4H2][CX4H2]
0.2761 [#8][#6H0][#6H1]
0.2707 [CH3]CC[OH]
0.2509 [#6H2][#8][#6H1]
0.2494 [CX4H2]([OX2H1])[CX4H1]
0.2258 [OX2H0][CX4H2][CX4H2][OX2H0]

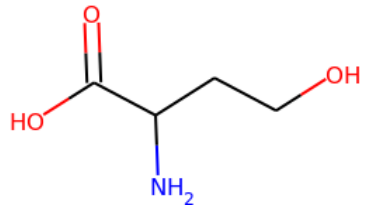


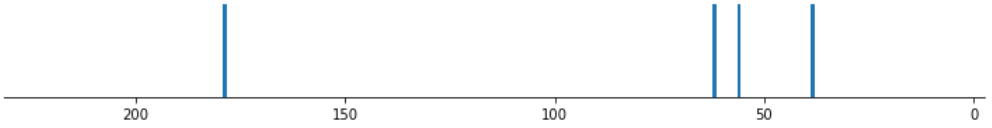
Top predicted substructures for the masked region(red):
0.5664 [CH3]CC[OH]
0.4014 C1OCCC1
0.3623 [CX4H](O)CO
0.3543 [#8][#6H0][#6H1]
0.3526 [OX2H0][CX4H2][#6H0]
0.3242 [#6H2][#8][#6H1]
0.2687 [#6X4H2][#6H1][#8H]
0.2485 [CX4H1]([OX2H1])([CX4H2])[CX4H0]

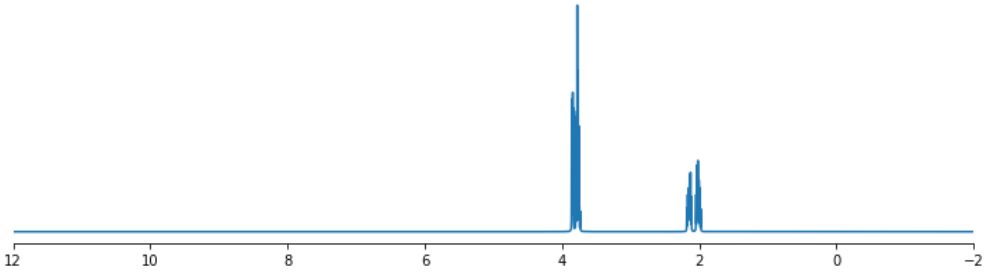


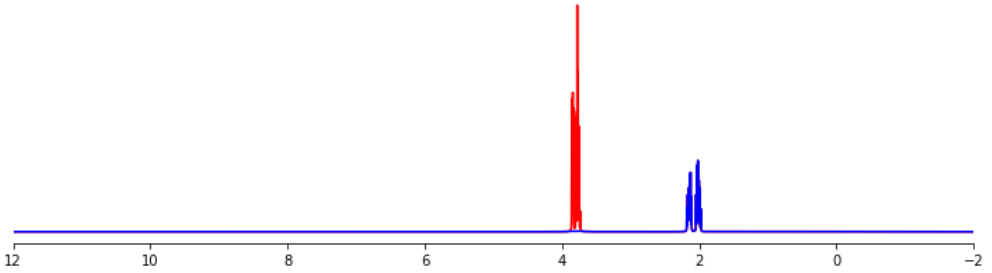
Top predicted substructures for the masked region(red):
0.4376 [CH2X4](O)[CX4H2]
0.3571 [#6H2][#8][#6H1]
0.3517 [CX4H2]([OX2H0])[CX4H2]
0.2425 [CH3]CC[OH]
0.2197 [OX2H0][CX4H2][CX4H2][OX2H0]
0.2175 [CX4H2][CX4H2]
0.1503 [CX4H2]([#6])[#6]
0.1346 [CX4H3][CX4H0]

True structure: NC(CCO)C(=O)O

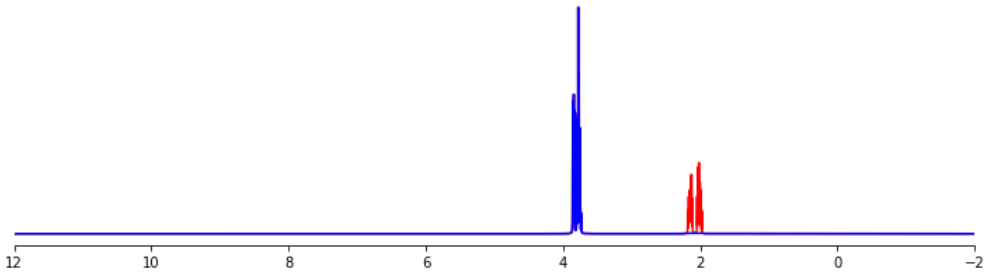




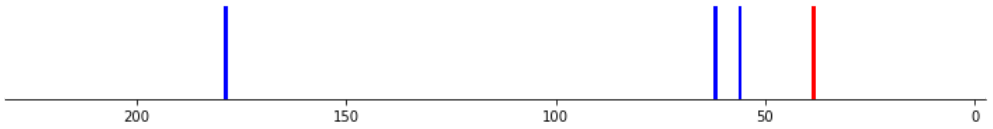




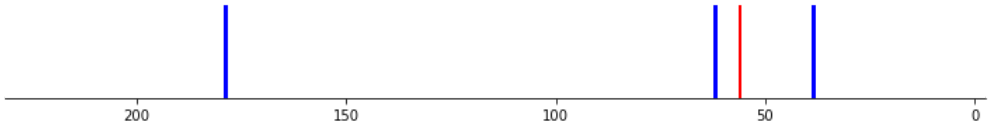
Top predicted substructures for the masked region(red):
0.8134 [CX4H2]([#6])[O]
0.8132 [CH2X4](O)[CX4H2]
0.5199 [CX4H2]([OX2H1])[CX4H2]
0.488 [#7H2][#6X4H1][#6X3]
0.3841 [#6H1]
0.3617 [#8]=[#6H0][#6H1]
0.3557 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.3513 [CX4H2]([CX4H2])[CX4H1]



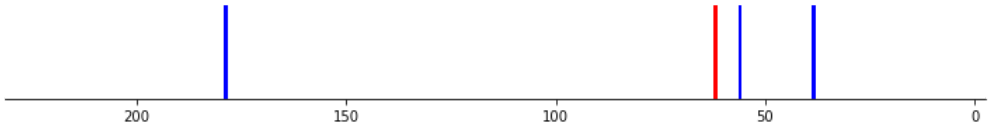
Top predicted substructures for the masked region(red):
0.5733 [CX4H2]([#6])[#6]
0.4916 [#6H1][#6H2]
0.4853 [#7H2][#6H1]
0.4781 OCC[CH2]
0.4702 [#6H1]
0.455 [CX4H2]([CX4H2])[CX4H1]
0.43 O=[CX3][CX4H]
0.4266 [CX4H1]([NX3H2])([CX4H2])[CX3H0]



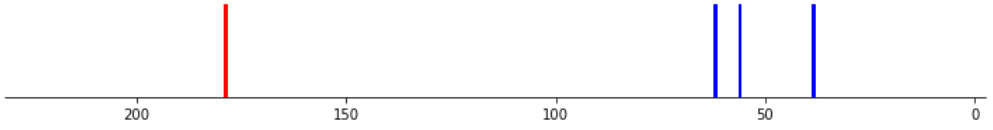
Top predicted substructures for the masked region(red):
0.4302 [CH2X4](O)[CX4H2]
0.2269 [CX4H2][CX4H2]
0.2268 [CX4H2]([OX2H1])[CX4H2]
0.1932 [#8][#6][#6][#6][#6]=[#8]
0.1625 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.1302 [CX4H2][CX3]=O
0.1266 [CX4H2]CC=O
0.1251 [CX4H2]([CX4H2])[CX3H0]



Top predicted substructures for the masked region(red):
0.4104 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.3677 [#7H2][#6X4H1][#6X3]
0.2937 [#8][#6H0][#6H1]
0.2765 [#7H2][#6H1]
0.2162 O=[CX3][CX4H]
0.1909 [#7][#6][#6X3]
0.1787 [#6H1r5][#7]
0.1721 [CH2X4](O)[CX4H2]

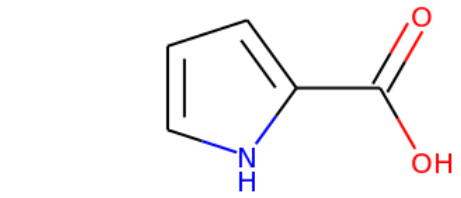


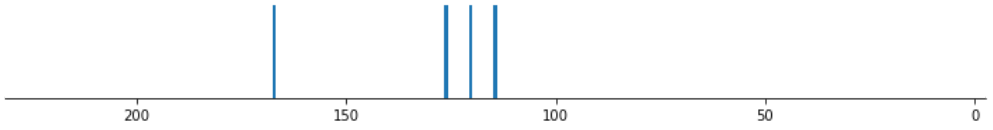
Top predicted substructures for the masked region(red):
0.7428 [CH2X4](O)[CX4H2]
0.6675 [CX4H2]([#6])[O]
0.5616 [CX4H2]([OX2H1])[CX4H2]
0.2472 [#8][#6][#6H2]
0.2261 [#8][#6H0][#6H1]
0.2163 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.2143 [CX4H2][CX4H2]
0.2111 [#6H1r5][#7]

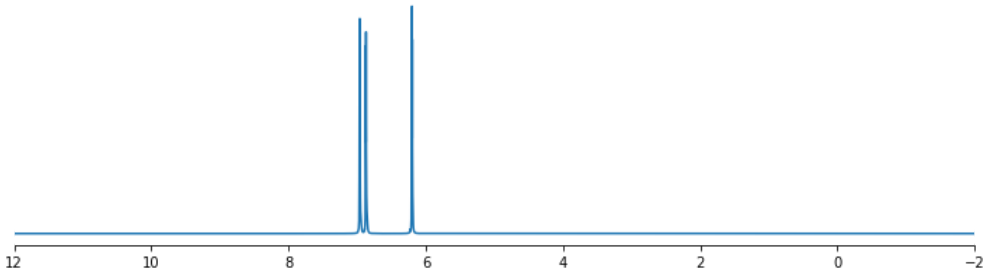


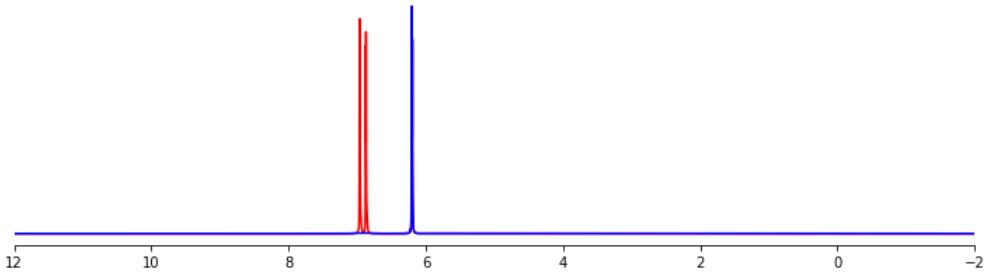
Top predicted substructures for the masked region(red):
0.9886 [CX3](=[OX1])C
0.9653 [CX4H2]CC=O
0.9434 O=[CX3][CX4H]
0.9324 [#7H2][#6X4H1][#6X3]
0.9301 [#8]=[#6][#8]
0.9244 [CX3](=[OX1])O
0.9167 [CX4H1]([NX3H2])([CX4H2])[CX3H0]
0.9092 [#8]=[#6H0][#6H1]

True structure: O=C(O)c1ccc[nH]1



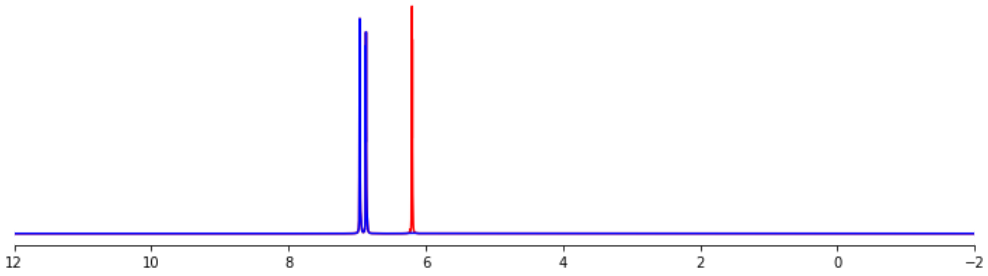






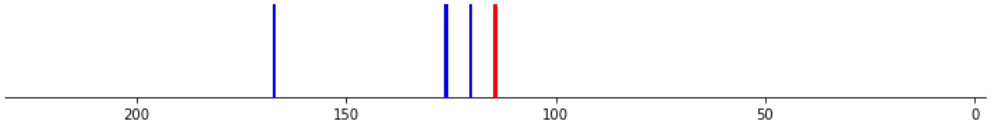
Top predicted substructures for the masked region(red):

0.4443 [OX2H][cX3]:[c]
0.4409 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.4129 [#6]1[#6][#6][#6][#7]1
0.4063 [#6H1r5][#7]
0.4022 [cH]cO
0.3433 [#8][#6H1][#6H1]
0.2879 [cX3H1]([cX3H1])[cX3H1]
0.2744 [cX3H1]([nX3H0])[cX3H1]



Top predicted substructures for the masked region(red):

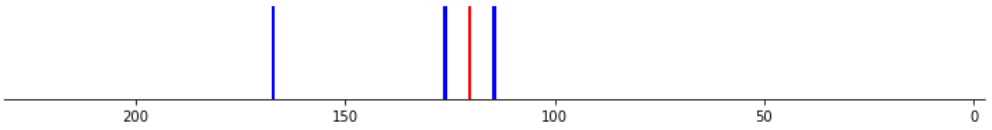
0.3727 O=[#6][#6][#6X3]
0.2862 [#8][#6H1][#6H1]
0.2822 [cX3H1]([nX3H0])[cX3H1]
0.2529 [#6H1r5][#7]
0.199 [#6H1][#7][#6H1]
0.1806 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1741 [cX3H1]([oX2H0])[cX3H1]
0.1494 [#6]1[#6][#6][#6][#7]1



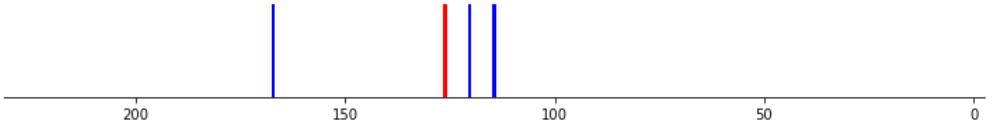
Top predicted substructures for the masked region(red):

0.4783 [#6]1[#6][#6][#6][#7]1
0.4522 [OX2H][cX3]:[c]

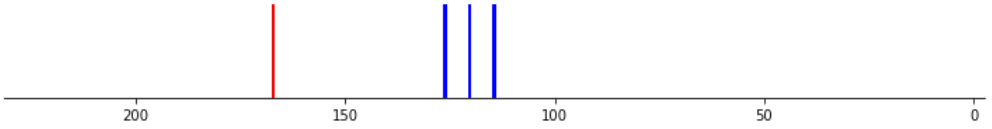
0.4072 [#6H1r5][#7]
0.3845 O=[#6][#6][#6X3]
0.3366 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.3321 [#8][#6][#6][#6X3]
0.3265 [cX3H1]([nX3H0])[cX3H1]
0.3018 [#7X3H2]



Top predicted substructures for the masked region(red):
0.4405 [OX2H][cX3]:[c]
0.4378 O=[#6][#6][#6X3]
0.3499 [#6]1[#6][#6][#6][#7]1
0.3467 [#6H1r5][#7]
0.3037 [cX3H1]([nX3H0])[cX3H1]
0.2804 [#7X3H2]
0.2332 [#8][#6][#6][#6X3]
0.2318 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]

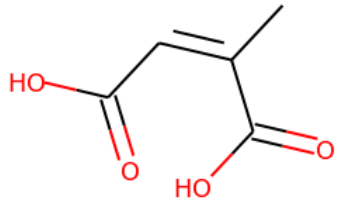


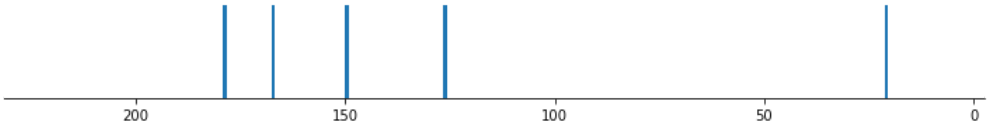
Top predicted substructures for the masked region(red):
0.5526 O=[#6][#6][#6X3]
0.4195 [#6H1r5][#7]
0.3737 [OX2H][cX3]:[c]
0.2977 [#6]1[#6][#6][#6][#7]1
0.2936 [#7X3H2]
0.2908 [cX3H1]([nX3H0])[cX3H1]
0.2222 [#6H1][#7][#6H1]
0.1855 [cX3H0][cX3H1][cX3H0][OX2H1]

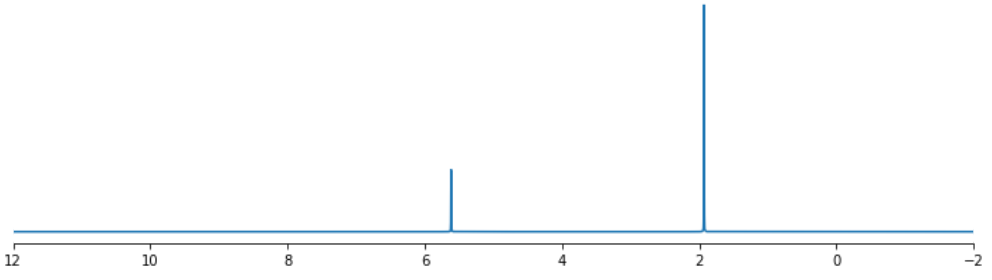


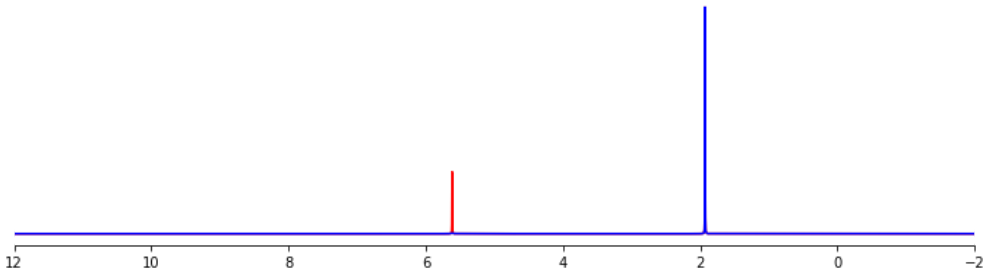
Top predicted substructures for the masked region(red):
0.7364 O=[#6][#6][#6X3]
0.3937 [OX2H][cX3]:[c]
0.3383 [#7X3H2]
0.2464 [CX3](=O)[OX2H1]
0.2292 [cX3H0][cX3H1][cX3H0][OX2H1]
0.2214 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.2191 [#7X3H1]
0.219 [#8]=[#6][#6H1][#6H1]

True structure: CC(=CC(=O)O)C(=O)O

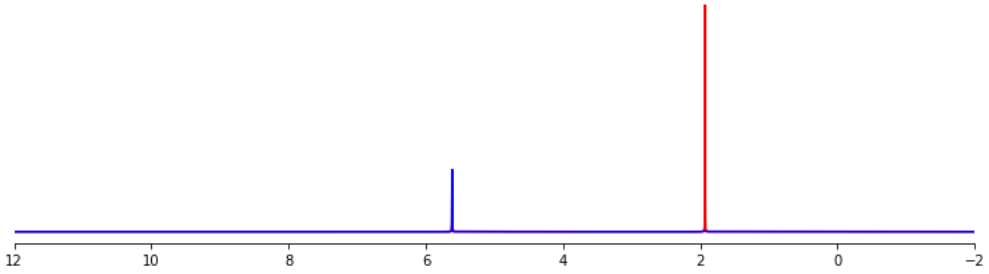




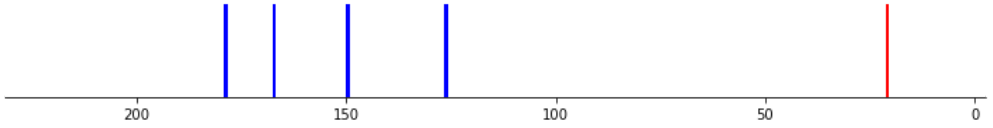




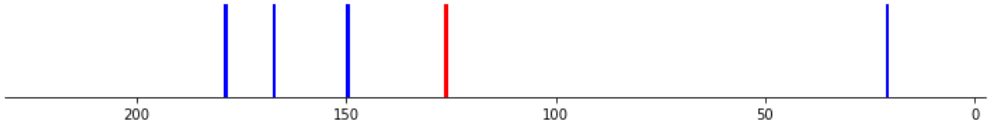
Top predicted substructures for the masked region(red):
0.4557 [CX3H1](=[CX3H0])[CX3H0]
0.4211 [#8]=[#6H0][#6H1]
0.4002 O=C[CX3H]
0.3959 [OX1H0]=[CX3H0][CX3H1]=[CX3H0]
0.3491 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.3089 [CHX3](=C)C
0.2955 [CX3H2]=[CX3H0]
0.2844 [#8][#6H0][#6H1]



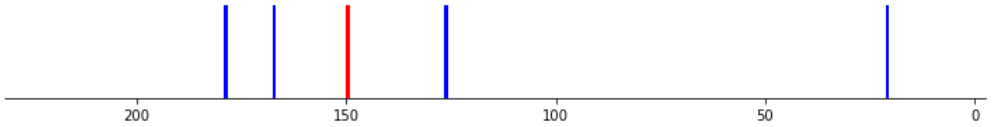
Top predicted substructures for the masked region(red):
0.7007 [#6H3][#6H0]
0.6295 [CX4H3][CX3H0]
0.624 [CX4H3][CX3H0][CX3]=O
0.5529 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.5472 [OX1H0]=[CX3H0][CX3H0][CX4H3]
0.4662 [CX4H3][CX3]
0.4439 [#6H3][#6][#6]
0.4232 [#6X3][#6]=[#6][#6H3]



Top predicted substructures for the masked region(red):
0.7432 [CX4H3][CX3]
0.6467 [CX4H3][CX3H0]
0.523 [#6X3][#6]=[#6][#6H3]
0.5139 [CX4H3][CX3H0][CX3]=O
0.4536 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.4498 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.4422 [CX4H3][#6]
0.363 [#8][#6X3][#6X3]=[#6X3][#6H3]

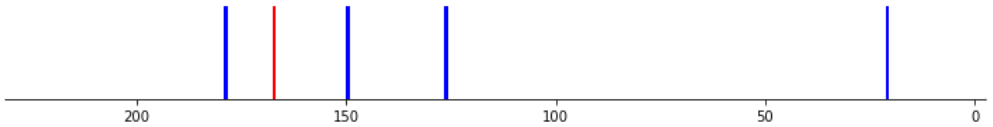


Top predicted substructures for the masked region(red):
0.4706 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.3686 [OX1H0]=[CX3H0][CX3H1]=[CX3H0]
0.3632 [CX3H1](=[CX3H0])[CX3H0]
0.2965 [#6H3][#6][#6]
0.2922 [#8][#6][#6]=[#6][#6]=[#8]
0.2855 [#6X3H1][#6X3H0]
0.2778 [#8][#6][#6]=[#6X3]
0.2749 [#8]=[#6H0][#6H1]

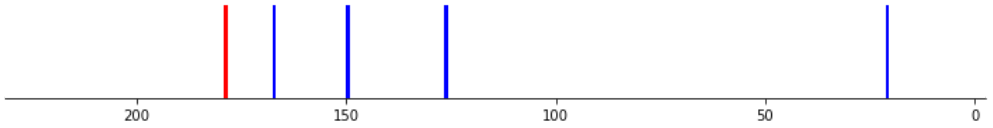


Top predicted substructures for the masked region(red):
0.4939 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.4675 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.3959 [#6X3][#6]=[#6][#6H3]

0.3725 [CX3H1](=[CX3H0])[CX3H0]
0.3646 [OX1H0]=[CX3H0][CX3H1]=[CX3H0]
0.343 [#8][#6][#6]=[#6][#6]=[#8]
0.3075 [CHX3](=C)C
0.2968 [#6X3H1][#6X3H0]

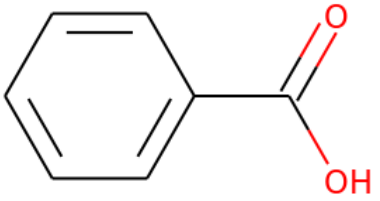


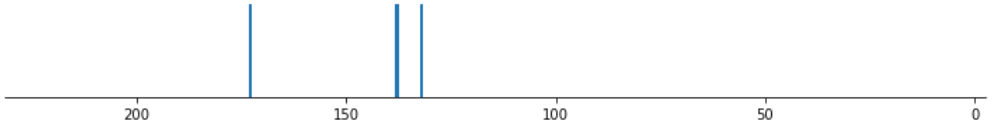
Top predicted substructures for the masked region(red):
0.6353 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.5363 [#6X3][#6]=[#6][#6H3]
0.4615 [CX3H1](=[CX3H0])[CX3H0]
0.4127 O=C[CX3H]
0.4117 [#8]=[#6H0][#6H1]
0.4032 [#6X3H1][#6X3H0]
0.3904 [OX1H0]=[CX3H0][CX3H1]=[CX3H0]
0.3685 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]

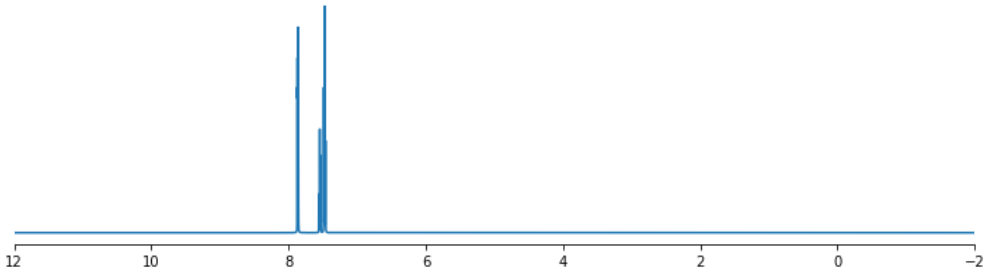


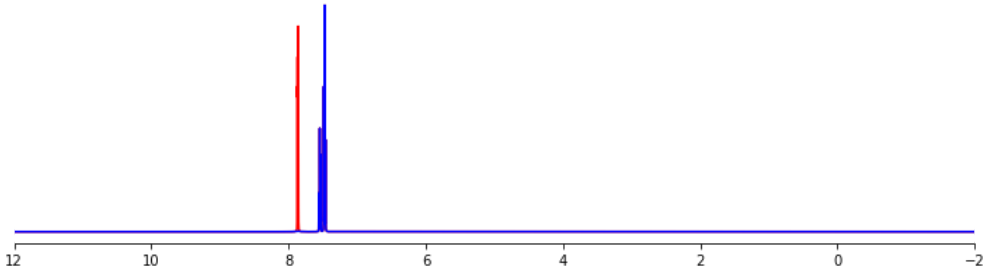
Top predicted substructures for the masked region(red):
0.6808 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.5499 [#8]=[#6H0][#6H1]
0.5466 [#6X3][#6]=[#6][#6H3]
0.5021 [CX3H0](=[CX3H1])([CX4H3])[CX3H0]
0.4672 [CX3H1](=[CX3H0])[CX3H0]
0.4024 [OX1H0]=[CX3H0][CX3H1]=[CX3H0]
0.3736 [#8][#6][#6]=[#6][#6]=[#8]
0.3699 O=C[CX3H]

True structure: O=C(O)c1ccccc1



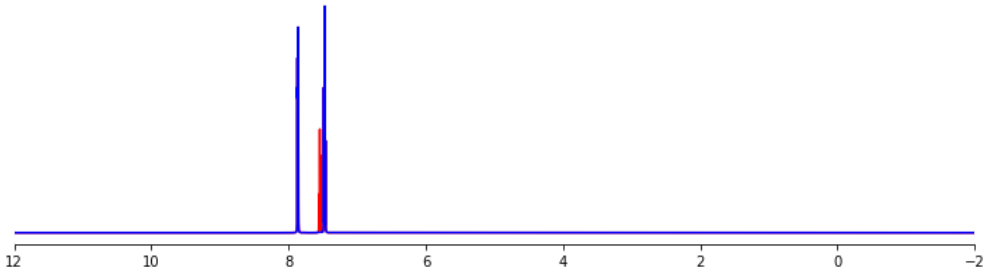




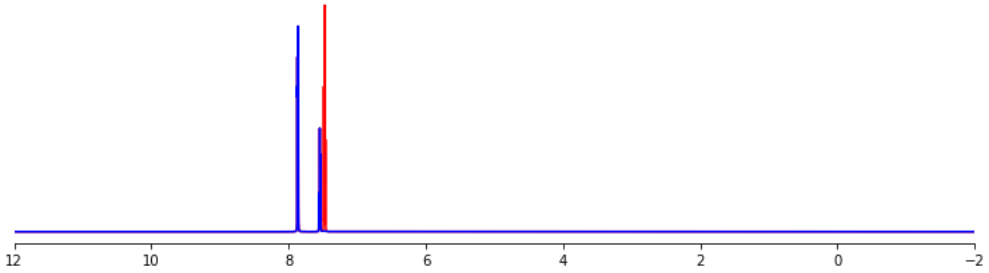


Top predicted substructures for the masked region(red):
0.229 [#6H][#8][#6H]
0.2251 [cX3H1]([oX2H0])[cX3H1]
0.2153 [#8][#6H1][#6H1]

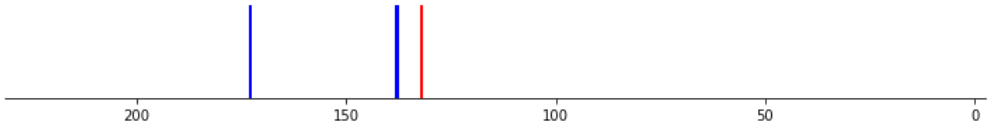
0.1802 [#8]1[#6][#6][#6][#6][#6]1
0.176 [#8][#6][#6][#6X3]
0.1641 o[cH]
0.1565 [#6X3][#7][#6X3]
0.1421 [#6H1][#6H1]



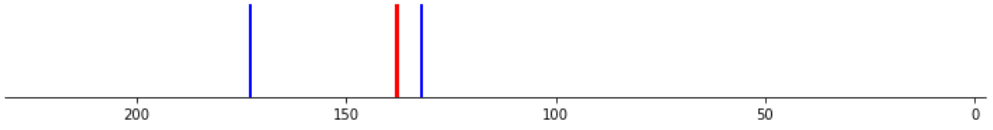
Top predicted substructures for the masked region(red):
0.2072 [#8][#6H1][#6H1]
0.1965 [cX3H1]([oX2H0])[cX3H1]
0.186 O=[#6][#6]=[#6X3]
0.1561 [#6X3][#7][#6X3]
0.1413 [#8]1[#6][#6][#6][#6][#6]1
0.133 [#8]=[#6][#6H1][#6H1]
0.1189 [CHX3](=C)C
0.103 [#8][#6H0][#6H1]



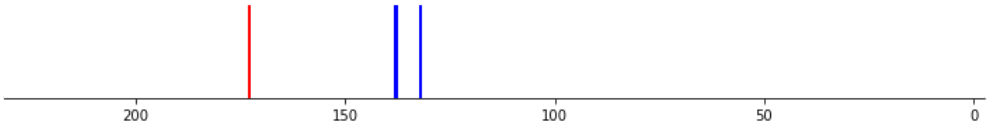
Top predicted substructures for the masked region(red):
0.2068 [cX3H1]([oX2H0])[cX3H1]
0.1787 [#8]=[#6][#6H1][#6H1]
0.1773 [#8][#6H1][#6H1]
0.1593 O=[#6][#6]=[#6X3]
0.1563 [#6X3][#7][#6X3]
0.1458 [#8]1[#6][#6][#6][#6][#6]1
0.1442 [#6H1][#6H1]
0.1281 [#8]=[#6][#6H1]=[#6H1]



Top predicted substructures for the masked region(red):
0.178 [cX3H1]([oX2H0])[cX3H1]
0.1562 [#6X3][#7][#6X3]
0.156 [#8]1[#6][#6][#6][#6][#6]1
0.1516 [#8][#6][#6][#6X3]
0.1509 [#8][#6H1][#6H1]
0.1388 O=[#6][#6]=[#6X3]
0.1373 [#8][#6H0][#6H1]
0.1017 [#8][#6H][#6X3][#6X3H]

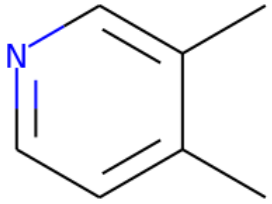


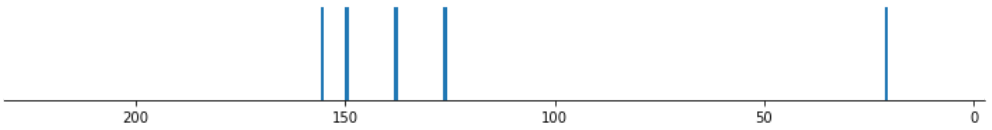
Top predicted substructures for the masked region(red):
0.2387 [#8][#6][#6][#6X3]
0.1875 [cX3H1]([oX2H0])[cX3H1]
0.1714 [#8]1[#6][#6][#6][#6][#6]1
0.1556 [#6X3][#7][#6X3]
0.1542 [#8][#6H1][#6H1]
0.1418 O=[cX3]
0.1307 [#8][#6H0][#6H1]
0.1198 [#8]=[#6][#6H1][#6H1]

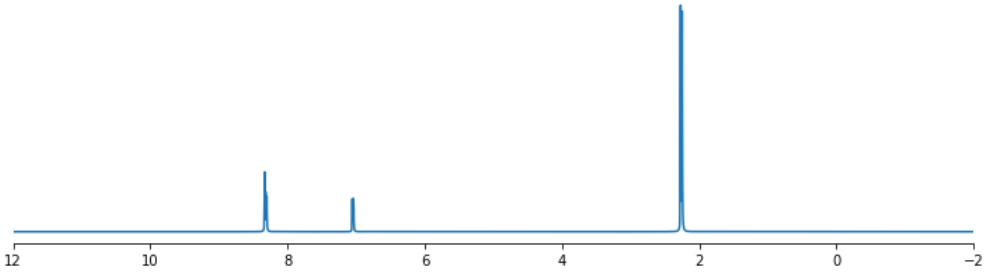


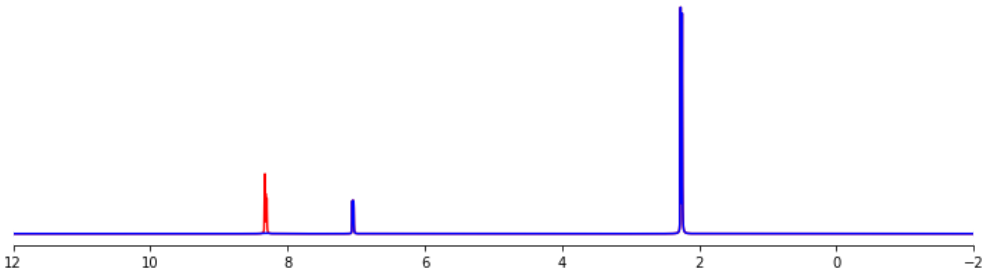
Top predicted substructures for the masked region(red):
0.8184 O=[#6][#6][#6X3]
0.578 [CX3](=[OX1])O
0.4629 [#8]=[#6][#8]
0.4286 [#8]=[#6H0][#6H1]
0.426 [CX3](=[OX1])C
0.3163 O=[#6][#6]=[#6X3]
0.3029 O=[cX3]
0.2933 [#8]=[#6][#6H1][#6H1]

True structure: Cc1ccncc1C

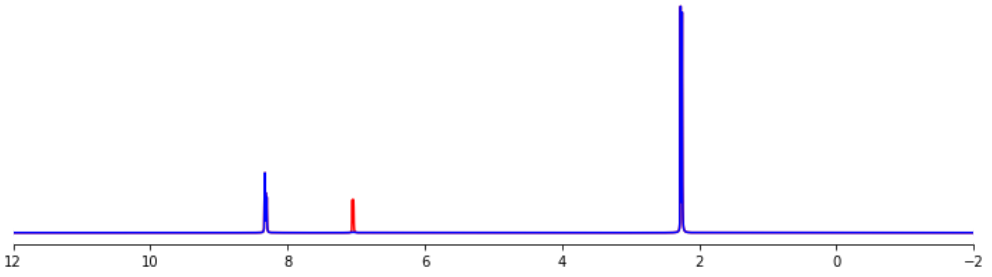






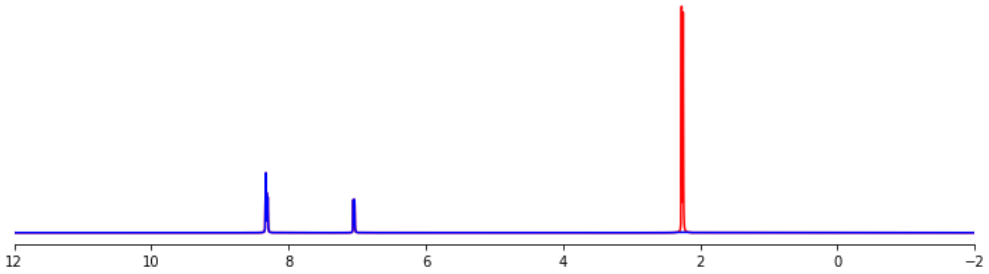


Top predicted substructures for the masked region(red):
0.4437 [cX3H0][cX3H1][cX3H1][cX3H0]
0.2897 [cX3H1]([cX3H1])[cX3H1]
0.2489 [cX3H1]([nX2H0])[cX3H0]
0.2432 [cX3H1]([nX2H0])[cX3H1]
0.2303 [#6X3][#7][#6X3]
0.2066 [#7][#6][#6][#6X3]
0.1627 [#6]1[#6][#6][#6][#6][#7]1
0.1541 [cH]

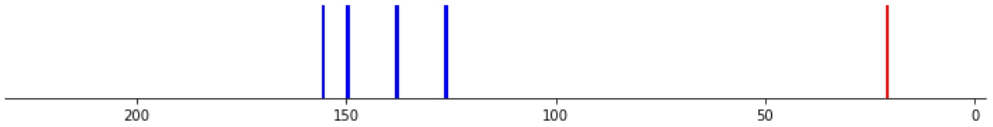


Top predicted substructures for the masked region(red):
0.3527 [cX3H1]([cX3H1])[cX3H1]
0.238 [cX3H0][cX3H1][cX3H1][cX3H0]

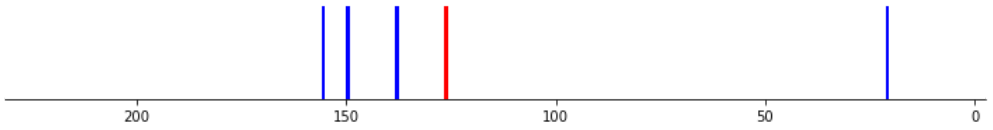
0.2105 [CX4H2][CX3H]
0.1875 [CX4H2]([CX4H2])[CX3H1]
0.1215 [#6X3H1]=[#6X3H0]
0.0982 [CX4H2][CX4H2]
0.0955 [#7][#6][#6H3]
0.0904 [#6X3][#7X3][#6X3]



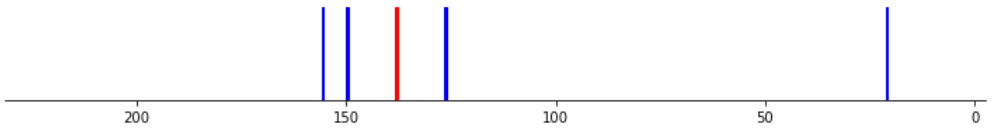
Top predicted substructures for the masked region(red):
0.3438 [CX4H2]([#6])[#6]
0.2904 [cX3H0][cX3H1][cX3H1][cX3H0]
0.2747 [#6H3][#6H0]
0.2723 [CX4H2][CX3H]
0.2308 [CX4H2]([CX4H2])[CX3H1]
0.2299 [#7][#6][#6H3]
0.2162 [CHX3](=C)C
0.136 [CX4H3][cX3H0]



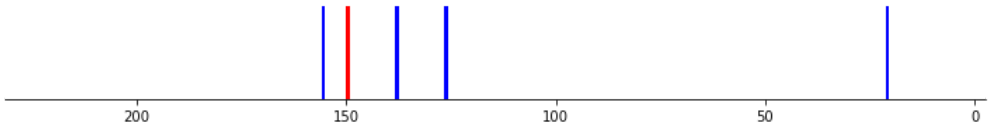
Top predicted substructures for the masked region(red):
0.98 [CX4H3][#6]
0.7858 [#6H3][#6][#6X3]
0.7761 [#6X3][#6][#6][#6H3]
0.6174 [CX4H3][cX3H0]
0.5584 [#6H3][#6H0]
0.4534 [#6H3][#6][#6]
0.3257 [cX3H0][cX3H1][cX3H1][cX3H0]
0.2771 [CX4H3]



Top predicted substructures for the masked region(red):
0.3585 [cX3H0][cX3H1][cX3H1][cX3H0]
0.2093 [#6X3][#7][#6X3]
0.1486 [#7X3H2]
0.1443 [#7][#6][#6H3]
0.1326 [CX4H2]([CX4H2])[CX3H1]
0.1301 [#7][#6X3H0][#6X3H1]
0.1138 [#7][#6][#6][#6X3]
0.1094 [#6X3][#7X3][#6X3]

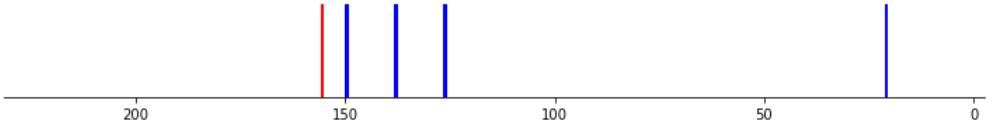


Top predicted substructures for the masked region(red):
0.3033 [cX3H0][cX3H1][cX3H1][cX3H0]
0.1507 [#7][#6][#6H3]
0.1324 [CX4H2][CX3H]
0.1223 [CX4H2]([CX4H2])[CX3H1]
0.1177 [#6X3H1]=[#6X3H0]
0.1081 [CHX3](=C)C
0.0936 [#6X3][#7X3][#6X3]
0.0883 [#7H2][#6H0]



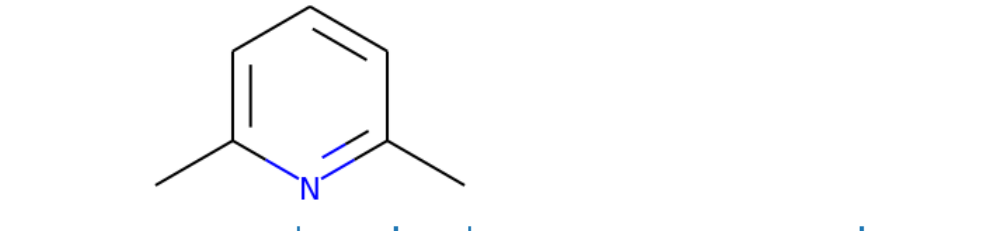
Top predicted substructures for the masked region(red):
0.2341 [cX3H0][cX3H1][cX3H1][cX3H0]
0.1598 [#7][#6][#6H3]
0.1562 [CX4H2]([CX4H2])[CX3H1]

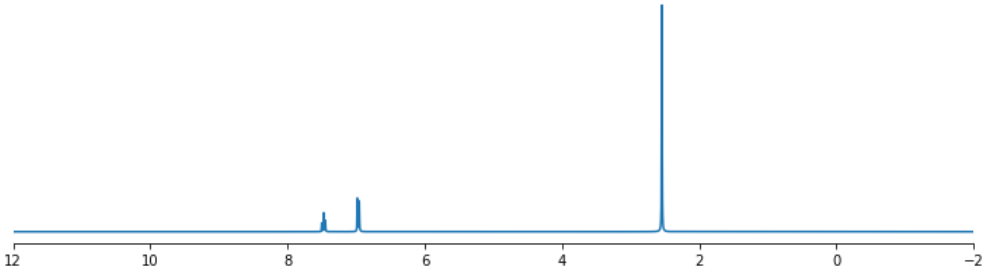
0.1313 [CX4H2][CX3H]
0.1188 [#6X3H1]=[#6X3H0]
0.1083 [CHX3](=C)C
0.0926 [CX4H2][CX4H2]
0.0765 [#7H2][#6H0]

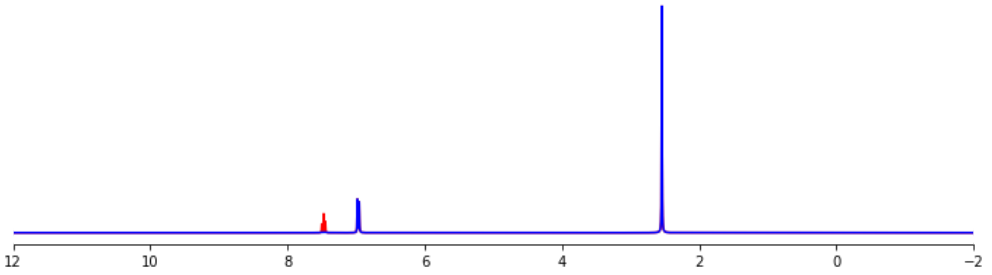


Top predicted substructures for the masked region(red):
0.1973 [cX3H0][cX3H1][cX3H1][cX3H0]
0.1844 [#7][#6][#6H3]
0.1686 [CX4H2]([CX4H2])[CX3H1]
0.1275 [CX4H2][CX3H]
0.1181 [CHX3](=C)C
0.1172 [#6X3H1]=[#6X3H0]
0.0984 [CX4H2][CX4H2]
0.0901 [#7H2][#6H0]

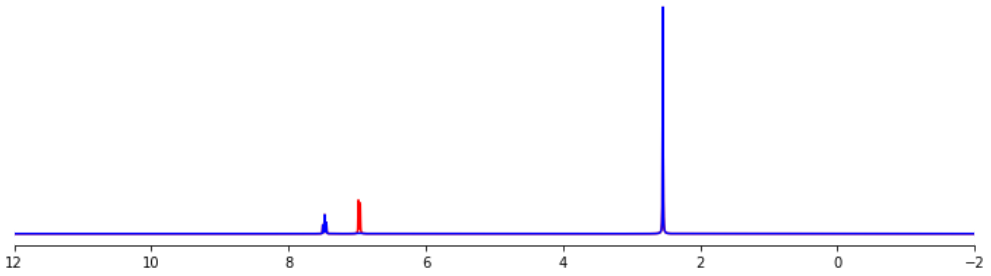
True structure: Cc1cccc(C)n1



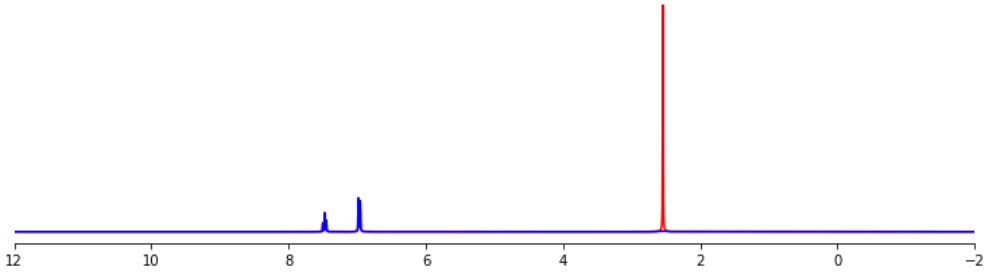




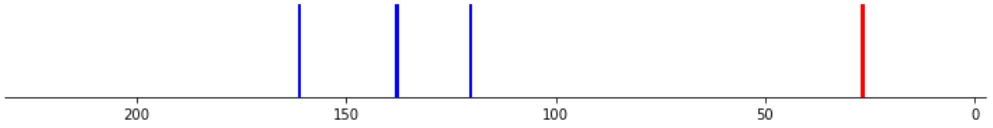
Top predicted substructures for the masked region(red):
0.3861 [CX4H2]([CX4H2])[cX3H0]
0.3403 [cX3H1]([cX3H1])[cX3H1]
0.2173 [#6]1[#6][#6][#6][#6][#7]1
0.1694 [CX4H2]([#6])[#6]
0.1305 [#7][#6][#6H3]
0.1305 [cX3H1]([cX3H1])[cX3H0]
0.1007 [#6H3][#6][#6X3]
0.097 [#7][#6][#6][#6X3]



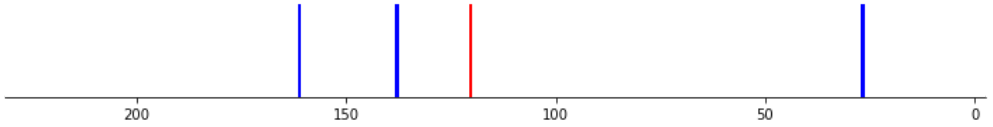
Top predicted substructures for the masked region(red):
0.3784 [cX3H1]([cX3H1])[cX3H1]
0.3721 [CX4H2]([CX4H2])[cX3H0]
0.29 [CX4H2]([#6])[#6]
0.2068 [cX3H1]([cX3H1])[cX3H0]
0.181 [#6]1[#6][#6][#6][#6][#7]1
0.1532 [#7][#6][#6H3]
0.1417 [cX3H0][cX3H1][cX3H1][cX3H0]
0.1282 [#6]1[#6][#6][#6][#6][#6]1



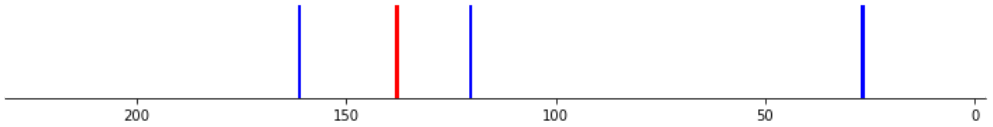
Top predicted substructures for the masked region(red):
0.7603 [CX4H2]([#6])[#6]
0.7269 [CX4H2][CX4H2]
0.6529 [CX4H2]([CX4H2])[cX3H0]
0.2376 [CX4H3][cX3H0]
0.156 [#6X3H0][CX4H2][CX4H2][#6X3H0]
0.1434 [#7][#6][#6H3]
0.1386 [CX4H2]([CX4H2])[CX3H0]
0.1225 [#6H3][#6H0]



Top predicted substructures for the masked region(red):
0.7229 [CX4H2]([#6])[#6]
0.6822 [CX4H2][CX4H2]
0.6527 [CX4H2]([CX4H2])[cX3H0]
0.6224 [CX4H3][cX3H0]
0.615 [#6X3][#6][#6][#6H3]
0.5221 [#6H3][#6H0]
0.5203 [#6H3][#6][#6X3]
0.4975 [#6H3][#6][#6]

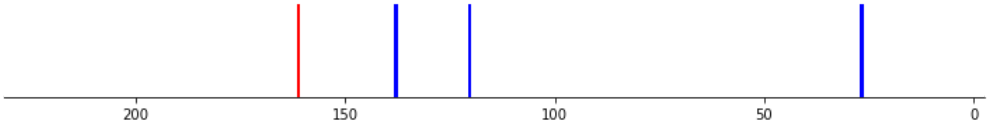


Top predicted substructures for the masked region(red):
0.3423 [CX4H2]([CX4H2])[cX3H0]
0.2777 [CX4H2]([#6])[#6]
0.1036 [#7H2][#6H0]
0.0875 [#6X3][#7X3][#6X3]
0.0861 [#6X3H1]=[#6X3H0]
0.085 [cX3H1]([nX3H1])[cX3H1]
0.0758 [cX3H1]([cX3H1])[cX3H1]
0.0744 [#6]#[#7]



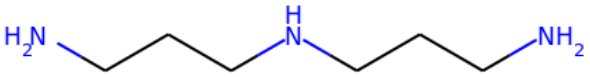
Top predicted substructures for the masked region(red):
0.5394 [CX4H2]([CX4H2])[cX3H0]
0.3367 [#6]1[#6][#6][#6][#6][#7]1
0.2285 [#6H3][#6H0]

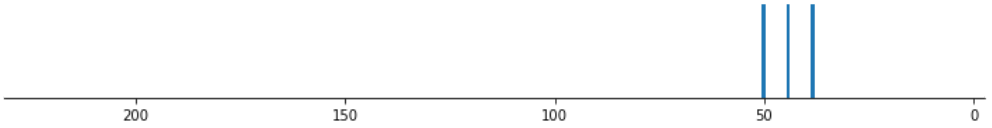
0.2249 [CX4H2]([#6])[#6]
0.187 [#6H3][#6][#6X3]
0.1675 [#7][#6H0][#6H1]
0.1674 [#6]1[#6][#6][#6][#6][#6]1
0.1479 [cX3H1]([cX3H1])[cX3H1]

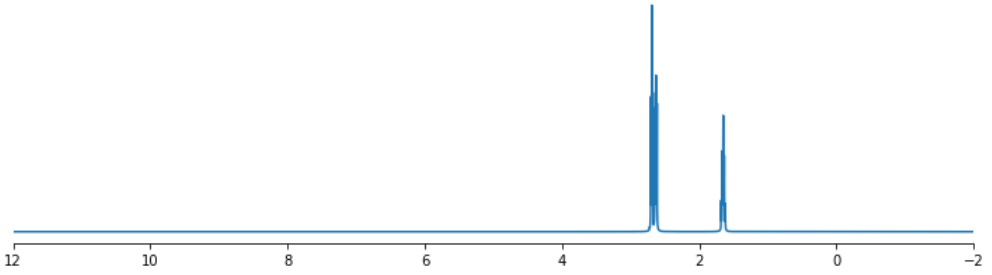


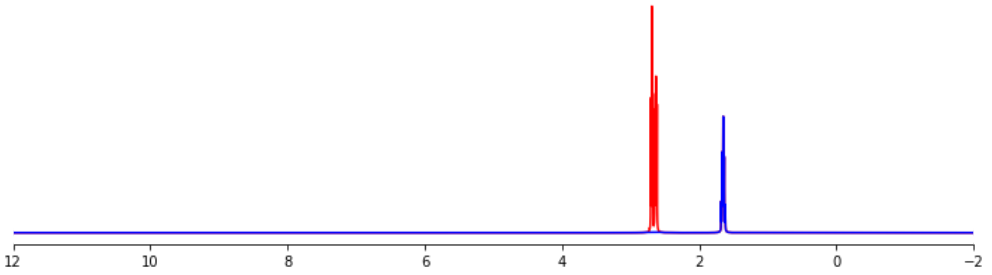
Top predicted substructures for the masked region(red):
0.3967 [#6]1[#6][#6][#6][#6][#7]1
0.3449 [CX4H2]([CX4H2])[cX3H0]
0.333 [#6H3][#6H0]
0.2026 [#7][#6][#6H3]
0.1869 [#7][#6H0][#6H1]
0.1828 [#6]1[#6][#6][#6][#6][#6]1
0.1758 [CX4H3][cX3H0]
0.1743 [#6H3][#6][#6X3]

True structure: NCCCNCCCN

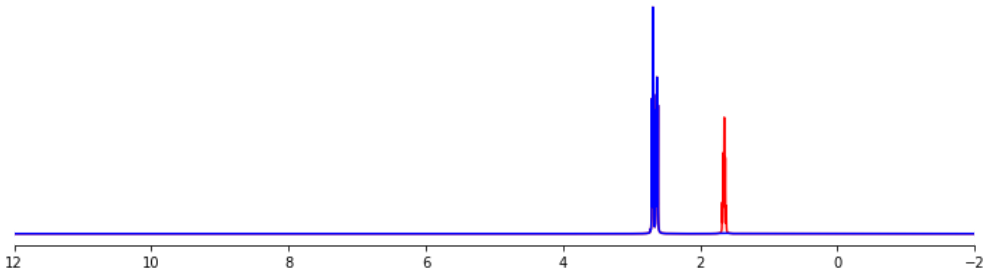




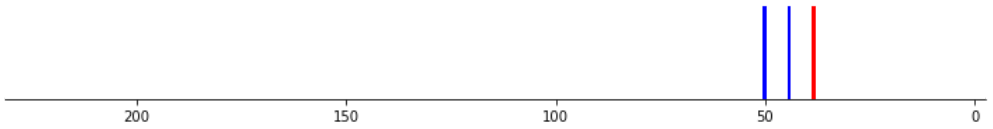




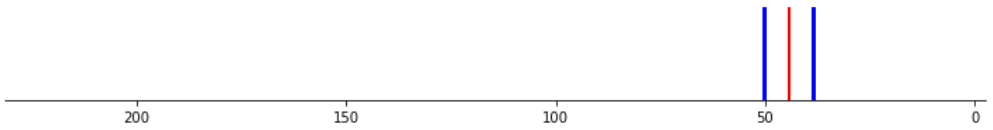
Top predicted substructures for the masked region(red):
0.574 [CX4H2]([NX3H1])[CX4H2]
0.4941 [CX4H2]([CX4H2])[CX4H2]
0.4466 [#6H2][#7][#6H2]
0.4447 [#7][#6H2][#6H2][#7]
0.3583 [#7H2][#6H2]
0.2951 [CX4H2]([NX3H2])[CX4H2]
0.2542 [#7][#6H2][#6H2]
0.249 [#7X3][#6H2]



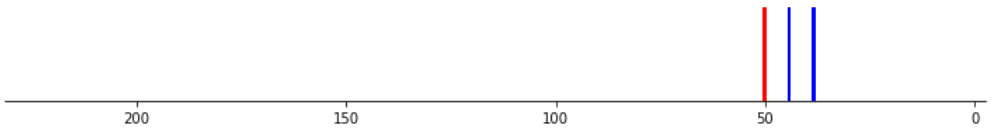
Top predicted substructures for the masked region(red):
0.7135 [CX4H2]([CX4H2])[CX4H2]
0.3857 [CX4H2]([#6])[#6]
0.2345 [#6H1]
0.2045 [#7][#6][#6][#6][#7]
0.1927 [CX4H2][CX4H2][CX4H2][CX4H2]
0.1746 [#7][#6][#6][#6][#6][#7]
0.1722 [#6H1]([#6H2])[#6H2]
0.084 [CX4H2][CX4H2]



Top predicted substructures for the masked region(red):
0.5221 [CX4H2]([CX4H2])[CX4H2]
0.1847 [#7][#6][#6][#6][#7]
0.1798 [CX4H2][CX4H2]
0.1669 [#7][#6H2][#6H2][#6H1]
0.1389 [#7X3H1]
0.1322 [#6H1]
0.1022 [#7][#6][#6][#6][#6][#7]
0.0769 [CX4H2]([#6])[#6]

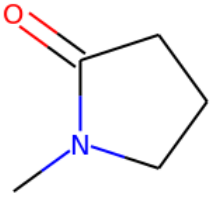


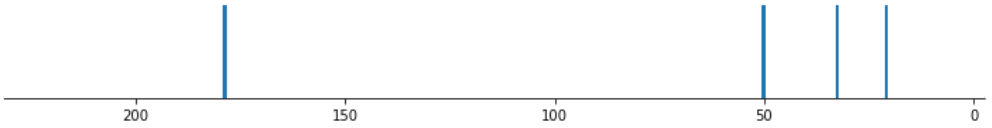
Top predicted substructures for the masked region(red):
0.4103 [CX4H2]([CX4H2])[CX4H2]
0.1482 [CX4H2][CX4H2]
0.1378 [CX4H2]([NX3H2])[CX4H2]
0.127 [#6H1]
0.1222 [#7][#6H2][#6H2][#6H1]
0.0835 [#7][#6][#6][#6][#7]
0.0781 [#6H2][#7][#6H2]
0.0656 [CX4H2]([CH])[CH]

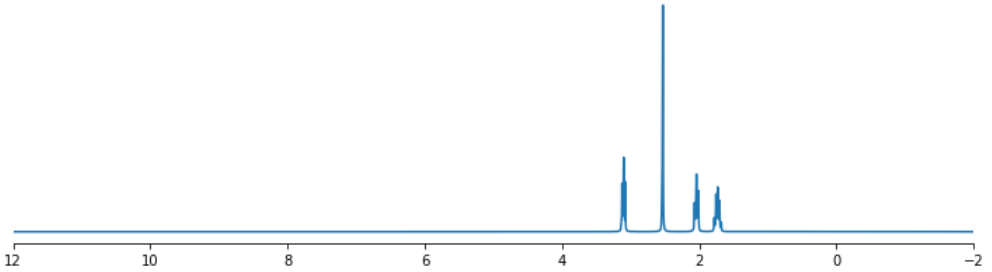


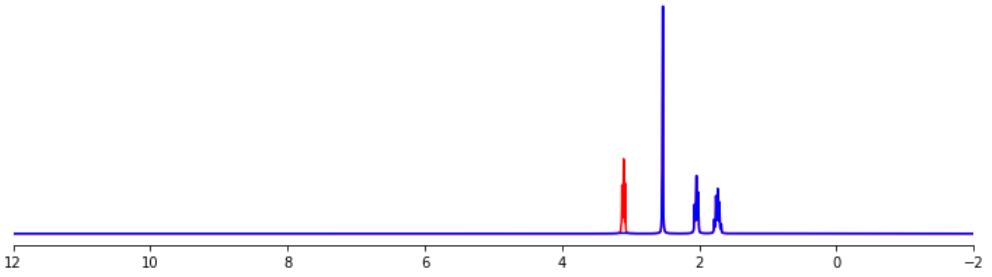
Top predicted substructures for the masked region(red):
0.4557 [CX4H2]([CX4H2])[CX4H2]
0.4266 [CX4H2]([NX3H1])[CX4H2]
0.3029 [#6H2][#7][#6H2]
0.2174 [#7][#6H2][#6H2][#7]
0.1278 [CX4H2][CX4H2]
0.126 [#6H1]
0.106 [#7][#6H2][#6H2][#6H1]
0.0809 [#7][#6][#6][#7]

True structure: CN1CCCC1=O

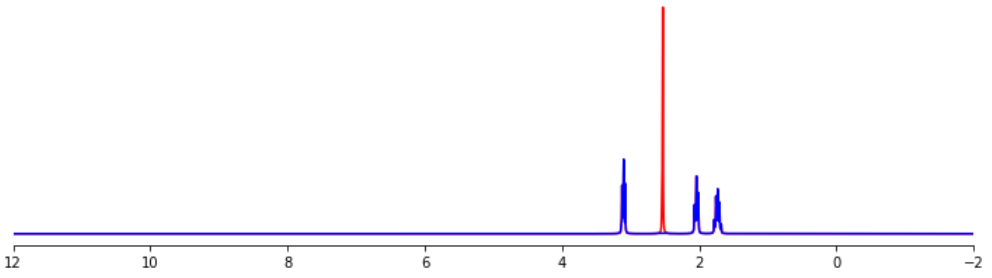




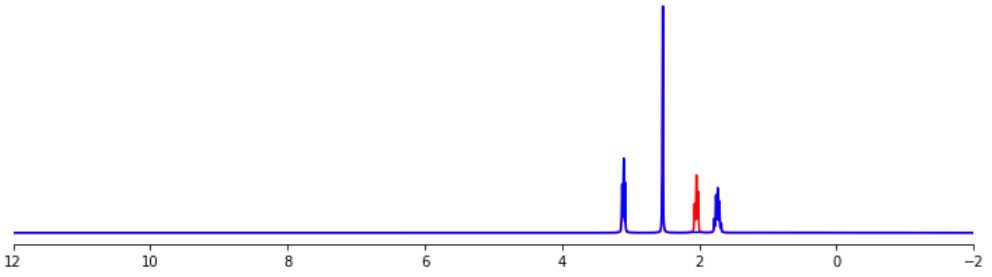




Top predicted substructures for the masked region(red):
0.609 [#7X3][#6H2]
0.5644 O=[CX3][CX4H]
0.3626 [CX4H2]([CX4H2])[CX4H1]
0.3544 [CX4H1]([CX4H2])([CX4H2])[CX3H0]
0.3491 [#6]1[#6][#6][#6][#7]1
0.2976 [#7X3][#6H3]
0.2831 [#7][#6][#6][#6X3]
0.2828 [#7][#6H2]

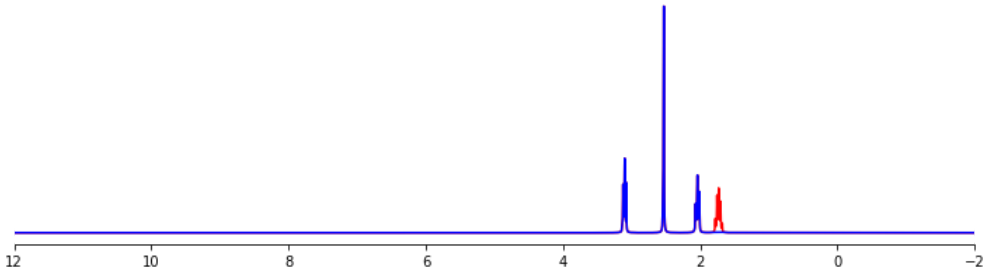


Top predicted substructures for the masked region(red):
0.4423 [#7X3][#6H3]
0.2669 [#6]1[#6][#6][#6][#7]1
0.2445 [CX4H1]([CX4H2])([CX4H2])[CX3H0]
0.2251 [#7][#6][#6][#6X3]
0.2208 [#6H3][#7]
0.1926 [CX4H2]([CX4H2])[CX3H0]
0.1752 [#6H3][#7][#6H2]
0.1736 [#6H3][#7X3H0][#6X4H2][#6X4H2]

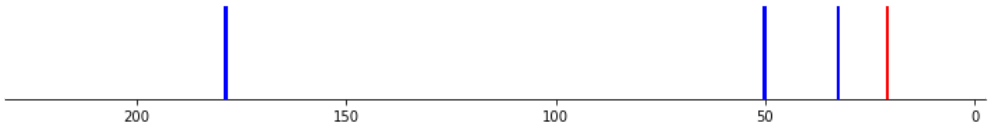


Top predicted substructures for the masked region(red):
0.3528 O=[CX3][CX4H]
0.2527 [CX4H2]([CX4H2])[CX4H1]
0.242 [#6]1[#6][#6][#6][#7]1
0.2307 [CX4H1]([CX4H2])([CX4H2])[CX3H0]
0.2036 [#7X3H2]
0.173 [#7][#6][#6][#6X3]
0.1482 [CX4H2]([NX3H1])[CX4H1]

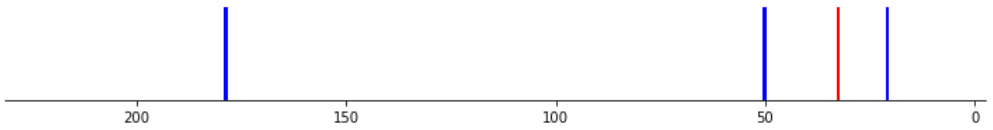
0.1404 [#6H1]



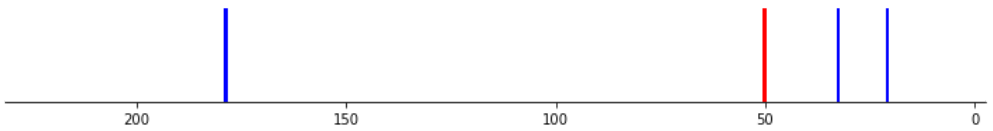
Top predicted substructures for the masked region(red):
0.5079 [CX4H2]([CX4H2])[CX4H1]
0.488 O=[CX3][CX4H]
0.2879 [CX4H1]([CX4H2])([CX4H2])[CX3H0]
0.2609 [#7X3H2]
0.1892 [CX4H2]([CX4H2])[CX4H2]
0.1875 [#8]=[#6H0][#6H1]
0.1785 [#6H1]
0.1687 [#6]1[#6][#6][#6][#7]1



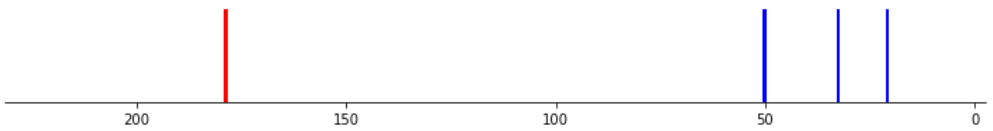
Top predicted substructures for the masked region(red):
0.4666 O=[CX3][CX4H]
0.3926 [CX4H2]([CX4H2])[CX4H2]
0.3223 [CX4H3]
0.2837 [#7X3][#6H3]
0.269 [CX4H1]1[CX4H2][CX4H2][CX4H2]1
0.2436 [#6]1[#6][#6][#6][#7]1
0.1908 [#7][#6][#6][#6X3]
0.1811 [#8]=[#6H0][#6H1]



Top predicted substructures for the masked region(red):
0.3286 [#7X3][#6H3]
0.3124 O=[CX3][CX4H]
0.2598 [#6]1[#6][#6][#6][#7]1
0.2577 [CX4H2]([CX4H2])[CX4H2]
0.2324 [CX4H2]([NX3H1])[CX4H2]
0.1953 [CX4H2][CX4H2]
0.185 [CX4H2]([CX4H2])[CX4H1]
0.1669 [#6H3][#7X3H0][#6X4H2][#6X4H2]

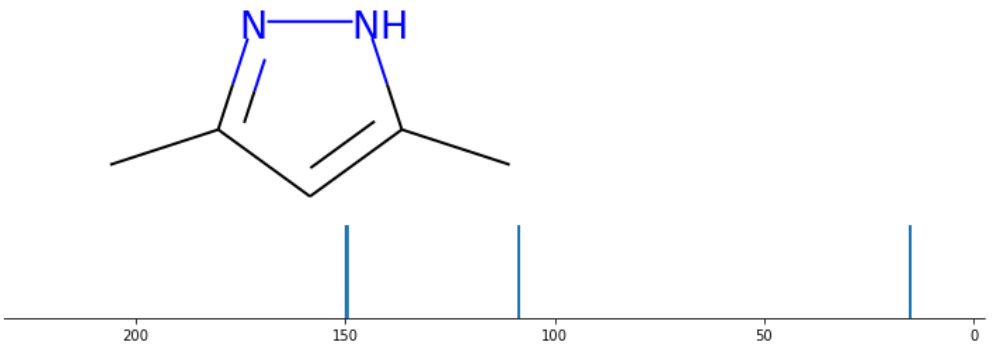


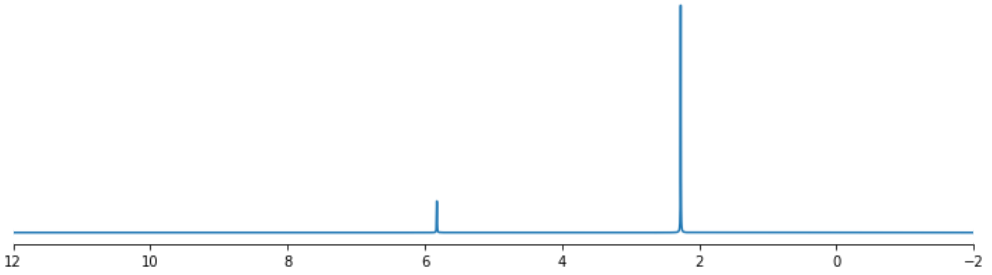
Top predicted substructures for the masked region(red):
0.5414 [#7X3][#6H2]
0.51 O=[CX3][CX4H]
0.3861 [#7][#6H2][#6H2]
0.3839 [CX4H2]([NX3H1])[CX4H2]
0.3781 [CX4H1]([CX4H2])([CX4H2])[CX3H0]
0.3423 [#6]1[#6][#6][#6][#7]1
0.3059 [#7][#6][#6][#6X3]
0.3028 [#7][#6H2]

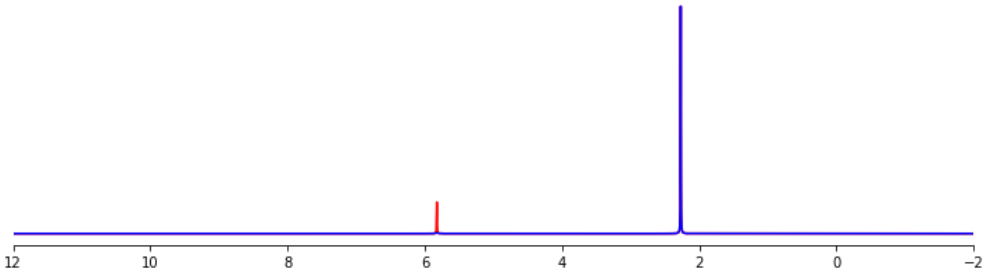


Top predicted substructures for the masked region(red):
0.9566 [CX3](=[OX1])C
0.9027 [CX4H2]CC=O
0.745 O=[CX3][CX4H]
0.5604 [#8]=[#6H0][#6H1]
0.4718 [CX4H1]([CX4H2])([CX4H2])[CX3H0]
0.4287 [CX4H2][CX3]=O
0.427 [CX4H2]([CX4H2])[CX4H2]
0.4003 [#7X3][#6H3]

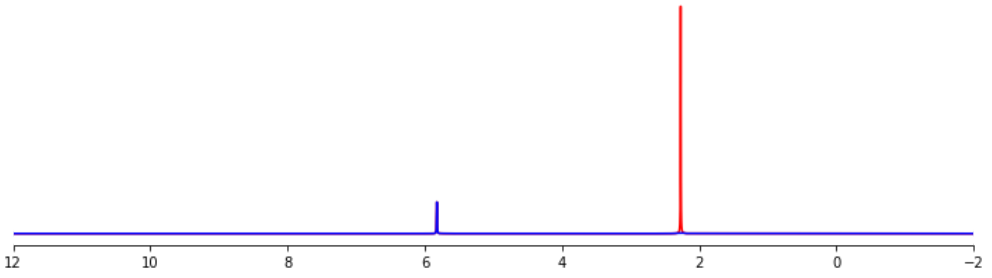
True structure: Cc1cc(C)[nH]n1



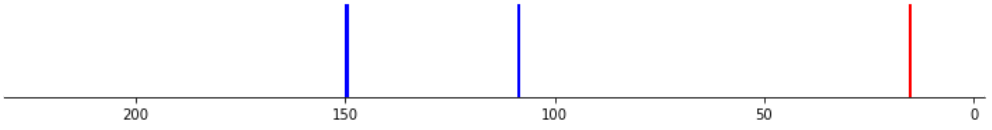




Top predicted substructures for the masked region(red):
0.6073 [#6H1]
0.579 [#6X3H1][#6X3H0]
0.5112 [cX3H1]([cX3H1])[cX3H0]
0.4292 [#6X3][#6X3][#6X3][#6X3]
0.3637 [#7][#6X3H0][#6X3H1]
0.3523 [#7][#6H0][#6H1]
0.3476 [cX3H0][cX3H1][cX3H1][cX3H0]
0.3373 [cH][cH]

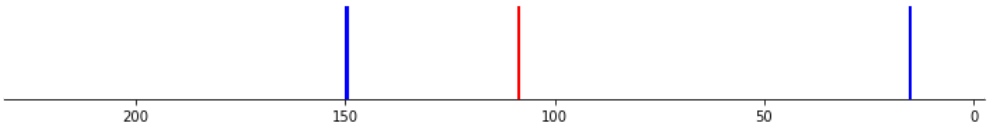


Top predicted substructures for the masked region(red):
0.5563 [#7][#6][#6H3]
0.4006 [#6H3][#6H0][#7H0][#6H0]
0.3733 [#6H3][#6H0]
0.2235 [#6H3][#6H0][#6H1][#7]
0.1952 [cX3H1]([cX3H0])[cX3H0]
0.1418 [CX4H3][#6]
0.1395 [#7X3H0]
0.1349 [#7][#6]=[#7]

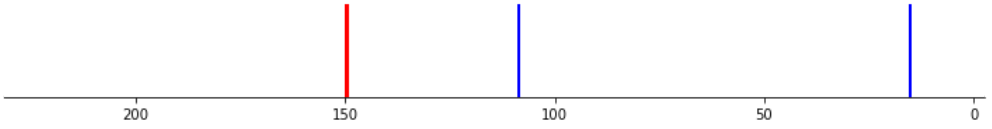


Top predicted substructures for the masked region(red):
0.9954 [CX4H3][#6]

0.8736 [#6H3][#6][#6X3]
0.8584 [CX4H3][cX3H0]
0.7953 [#7][#6][#6H3]
0.776 [#6H3][#6][#6]
0.6298 [#6X3][#6][#6][#6H3]
0.6086 [#6H3][#6H0]
0.4996 [#6H3][#6H0][#7H0][#6H0]

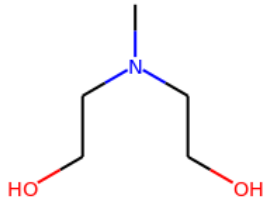


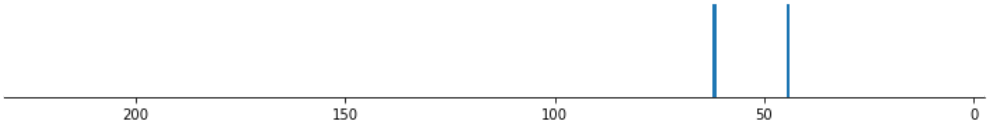
Top predicted substructures for the masked region(red):
0.4583 [#6X3][#6X3][#6X3][#6X3]
0.3752 [cX3H1]([cX3H1])[cX3H0]
0.2815 [cX3H1]([cX3H0])[cX3H0]
0.2532 [cH]
0.2529 [#7H2][#6H0]
0.2494 [#7][#6H0][#7]
0.2441 [#7X3H2]
0.2409 [cX3H1]([nX3H1])[cX3H0]

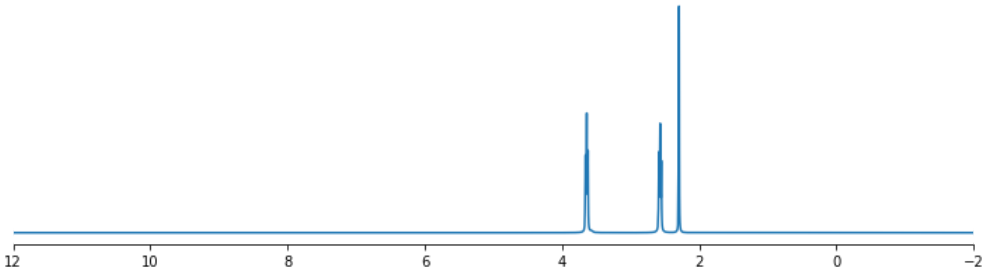


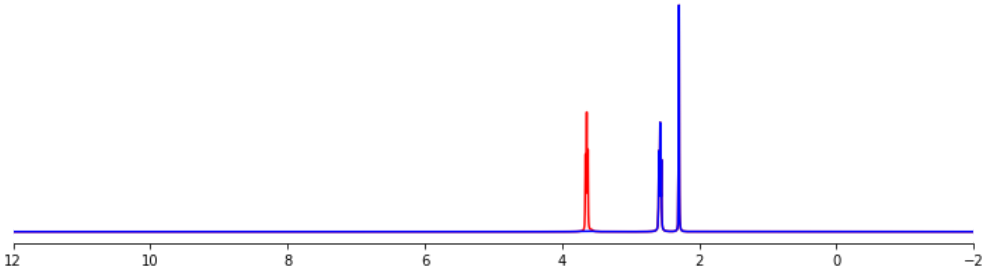
Top predicted substructures for the masked region(red):
0.3636 [#7][#6H0][#7]
0.3296 [#6H3][#6H0][#7H0][#6H0]
0.3081 [#7][#6][#7]
0.2904 [#6H3][#6][#6X3]
0.2626 [cX3H1]([cX3H0])[cX3H0]
0.2491 [#7][#6]=[#7]
0.2441 [cX3H1]([cX3H1])[cX3H0]
0.2048 [#6X3H1][#6X3H0]

True structure: CN(CCO)CCO



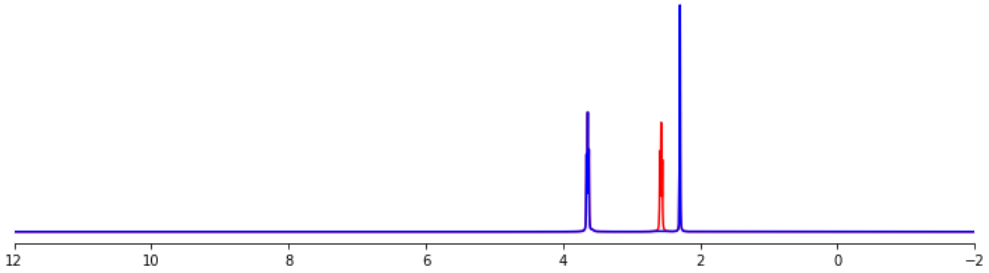




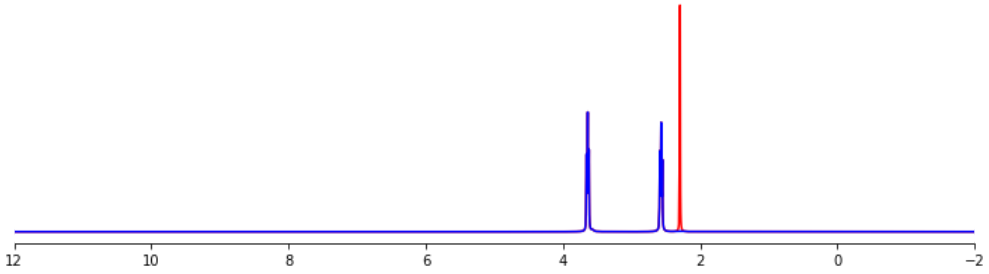


Top predicted substructures for the masked region(red):
0.4959 [CX4H2]([OX2H1])[CX4H2]

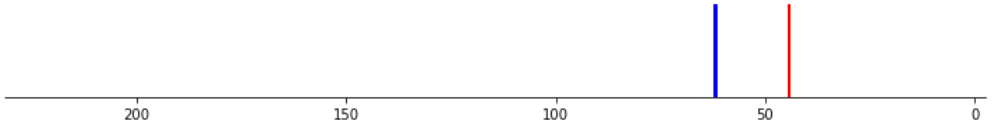
0.463 [CX4H2][CX4H2]
0.4436 [CX4H2]([#6])[O]
0.4267 [CH2X4](O)[CX4H2]
0.317 [CX4H3]
0.3103 [#7X3H2]
0.3026 [#8H][#6H2][#6H1]
0.196 [#7H2][#6H1]



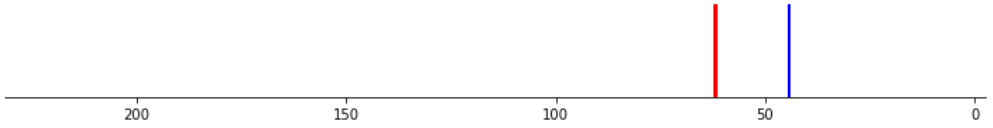
Top predicted substructures for the masked region(red):
0.7102 [#7X3H2]
0.4064 [#6H1][#6H2]
0.3827 [CX4H2]([#6])[#6]
0.3448 [#7H2][#6H2]
0.2467 [#8H][#6H2][#6H1]
0.2077 [#6H1]
0.1833 [#7H2][#6H1]
0.1699 [#6H1]([#6H2])[#6H2]



Top predicted substructures for the masked region(red):
0.7621 [#7X3][#6H3]
0.5386 [#6H3][#7]
0.4682 [CX4H3]
0.3696 [#6H1][#6H2]
0.2862 [CX4H2]([#6])[#6]
0.2757 [#8H][#6H2][#6H1]
0.2439 [CX4H3][NX3H0]
0.2135 [#7X3H2]

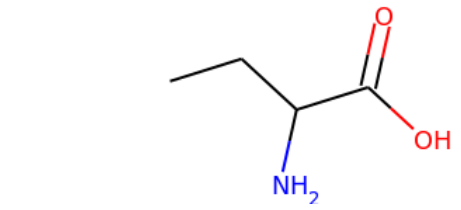


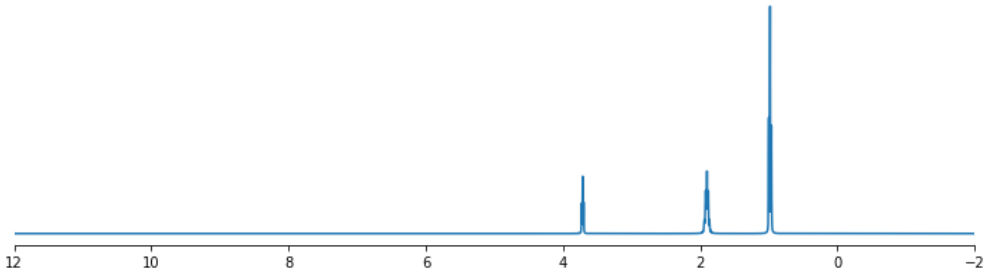
Top predicted substructures for the masked region(red):
0.4472 [CX4H3]
0.4265 [#6H3][#7]
0.4165 [#7X3][#6H3]
0.3824 [#7X3H2]
0.3709 [#7H2][#6H2]
0.3594 [#7][#6H2]
0.2905 [#7X3][#6H2]
0.2296 [#6H1][#6H2]

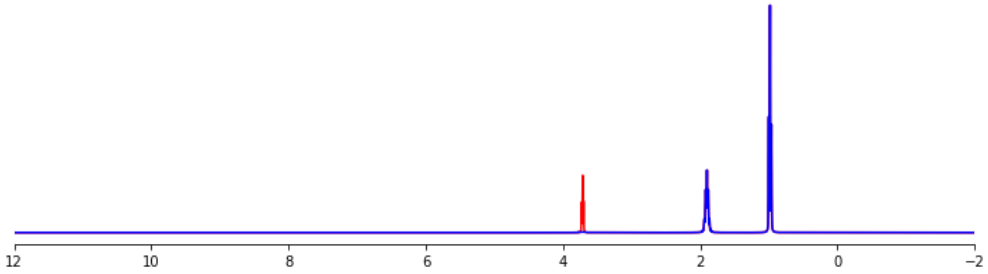


Top predicted substructures for the masked region(red):
0.7897 [CX4H2]([OX2H1])[CX4H2]
0.6659 [CH2X4](O)[CX4H2]
0.5427 [CX4H2]([#6])[O]
0.5043 [CX4H3]
0.4891 [#7X3][#6H3]
0.2766 [CX4H2][CX4H2]
0.2758 [#6H3][#7]
0.2249 [#8H][#6H2][#6H1]

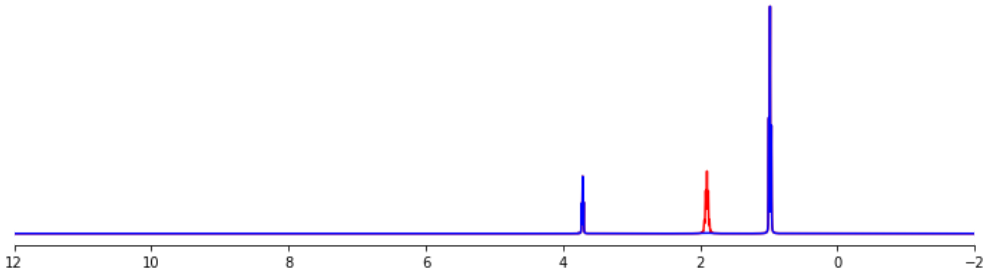
True structure: CCC(N)C(=O)O



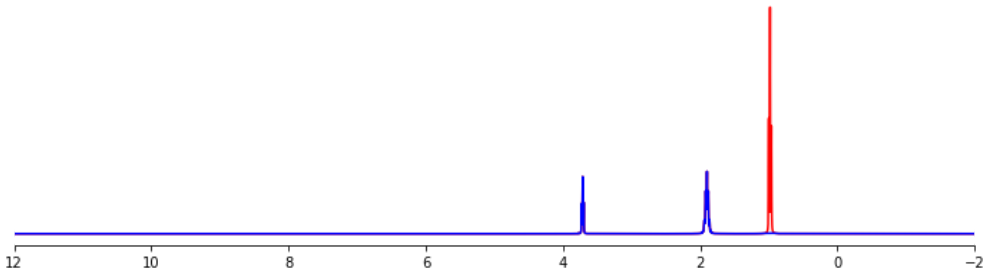




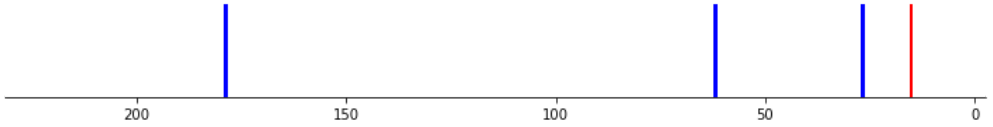
Top predicted substructures for the masked region(red):
0.4157 [#6H1][#6H1]
0.3814 [#7H2][#6H1]
0.2509 [#8]=[#6][#6H1][#6H1]
0.2347 [OH][CX4H]
0.1848 [#7H2][#6X4H1][#6X3]
0.1399 [CX3](=[OX1])O
0.1148 [CX4H]O
0.113 [#6H1]



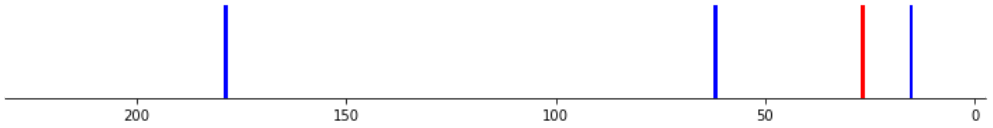
Top predicted substructures for the masked region(red):
0.5001 [#7H2][#6H1]
0.4187 [CX4H2]([CX4H3])[CX4H1]
0.3722 [#6H1][#6H2]
0.3476 [#6X3][#6][#6][#6H3]
0.3431 [#6H1][#6H1]
0.2182 [CX4H3][CX4H2]
0.174 [CX3](=[OX1])O
0.1694 [#7H2][#6X4H1][#6X3]



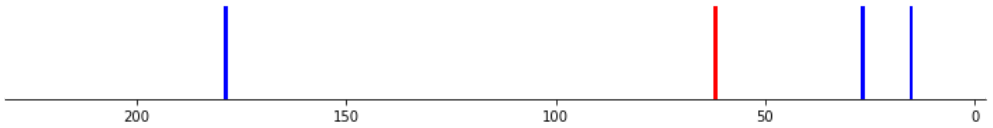
Top predicted substructures for the masked region(red):
0.735 [#6H1]
0.72 [#6X3][#6][#6][#6H3]
0.6919 [#6H3][#6][#6]
0.6328 [#7H2][#6H1]
0.5779 [CX4H3][CX4H2]
0.5543 [CX4H2]([CX4H3])[CX4H1]
0.5253 [#8]=[#6][#6H1][#6H1]
0.4942 [#6H1][#6H1]



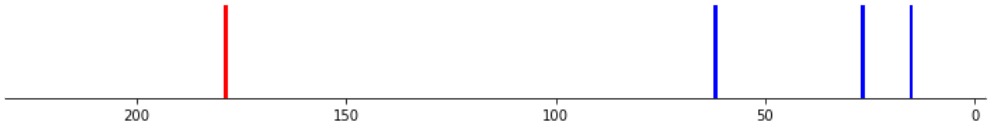
Top predicted substructures for the masked region(red):
0.957 [CX4H3][CX4H2]
0.5097 [CX4H2]([CX4H3])[CX4H1]
0.3445 [#6H1][#6H1]
0.2306 [#7H2][#6H1]
0.2304 [CH3]CC[OH]
0.194 [#6X3][#6][#6][#6H3]
0.1813 [#6H3][#6H1][#6H1][#7]
0.1475 [#6H3][#6H2][#6H1][#7]



Top predicted substructures for the masked region(red):
0.4145 [#7H2][#6H1]
0.187 [CX4H3][CX4H2]
0.186 [#6H1][#6H1]
0.1812 [#6X3][#6][#6][#6H3]
0.1744 [#6H1][#6H2]
0.1354 [CX4H2]([CX4H3])[CX4H1]
0.1289 [CX3](=[OX1])O
0.1258 [#6H3][#6H2][#6H1][#7]

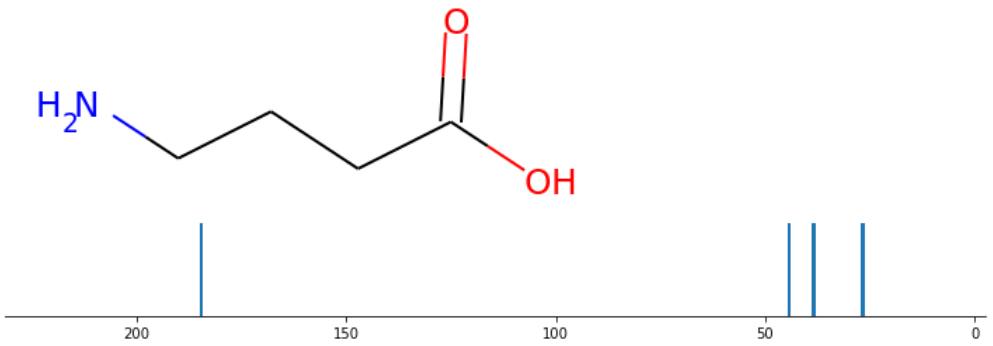


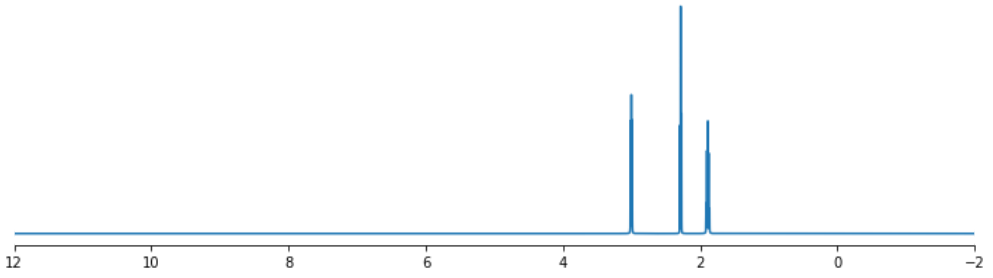
Top predicted substructures for the masked region(red):
0.5506 [#7H2][#6X4H1][#6X3]
0.5419 [#7H2][#6H1]
0.3788 [#6H1][#6H1]
0.2727 [#8][#6H0][#6H1]
0.2407 [OH][CX4H]
0.236 [#8]=[#6][#6H1][#6H1]
0.2305 [#6X3][#6][#6][#6H3]
0.2188 [CX4H1]([NX3H2])([CX4H2])[CX3H0]

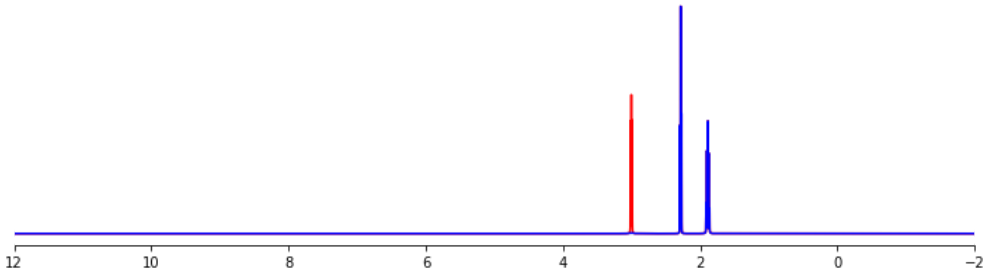


Top predicted substructures for the masked region(red):
0.9597 [CX3](=[OX1])C
0.9158 [CX3](=O)[OX2H1]
0.9096 [CX3](=[OX1])O
0.8904 [#8]=[#6][#8]
0.8849 O=[CX3][CX4H]
0.8726 [#8]=[#6H0][#6H1]
0.8124 [#6X3][#6][#6][#6H3]
0.7642 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]

True structure: NCCCC(=O)O

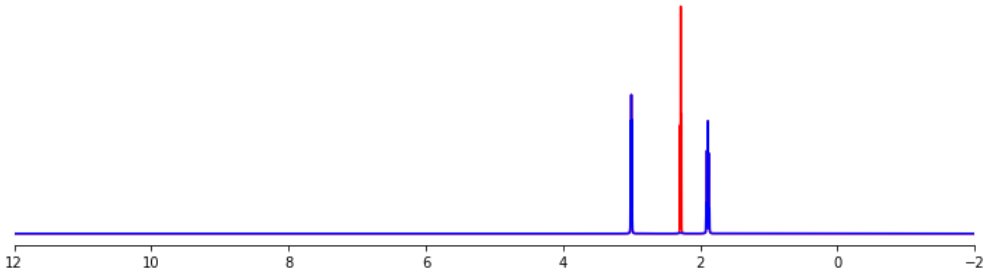






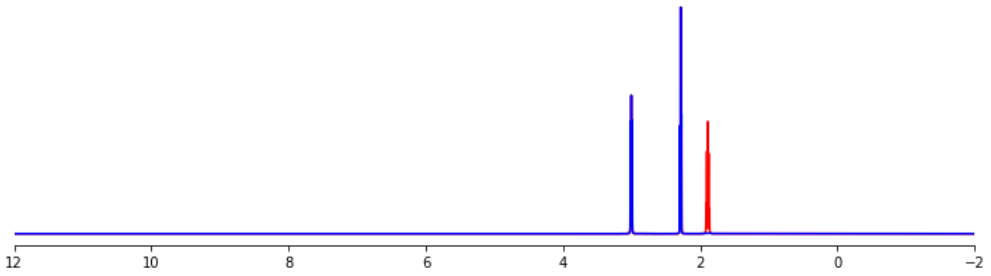
Top predicted substructures for the masked region(red):

0.7148 [#7H2][#6H2]
0.5176 [CX4H2]([NX3H2])[CX4H2]
0.4149 [#7X3][#6H2]
0.3063 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.2632 [#7][#6H2]
0.1873 OCC[CH2]
0.1692 [CX4H2]([CX4H2])[CX4H2]
0.1689 [#7][#6H2][#6H2]

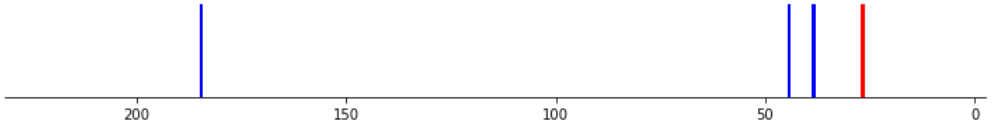


Top predicted substructures for the masked region(red):

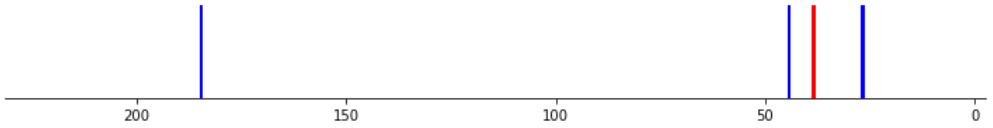
0.4383 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.2209 [CX4H2]([CX4H2])[CX3H0]
0.2055 [CX4H2][CX3]=O
0.2043 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.1934 [CX4H2]([NX3H2])[CX4H2]
0.1508 [CX4H2]([CX4H2])[CX4H2]
0.1298 O=[CX3H0][CX4H2][CX4H2]
0.0766 [#8][#6][#6H2]



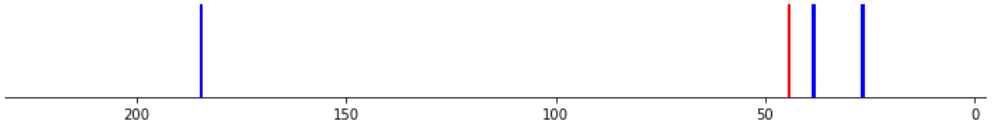
Top predicted substructures for the masked region(red):
0.3875 [CX4H2]([CX4H2])[CX4H2]
0.2899 [#7X3H2]
0.2285 [CX4H2]([NX3H2])[CX4H2]
0.2134 [CX4H2][CX4H2][CX4H2][CX4H2]
0.1906 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.1745 OCC[CH2]
0.146 [#8]=[#6][#8]
0.1219 [#7H2][#6H0]



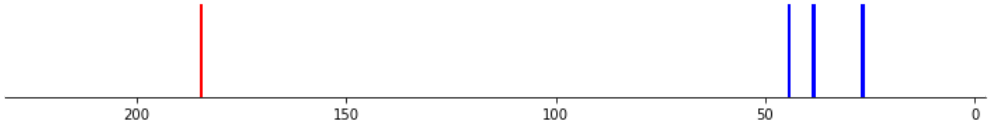
Top predicted substructures for the masked region(red):
0.6145 [CX4H2]([CX4H2])[CX4H2]
0.3151 [CX4H2][CX4H2][CX4H2][CX4H2]
0.2407 [CX4H2]([CX4H2])[CX3H0]
0.2352 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.2019 [CX4H2]([NX3H2])[CX4H2]
0.1757 [CX4H2][CX4H2]
0.1625 [#7H2][#6H2]
0.1362 [CX4H2][CX3]=O



Top predicted substructures for the masked region(red):
0.3766 [CX4H2]([NX3H2])[CX4H2]
0.3746 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.2908 [#7H2][#6H2]
0.2438 [CX4H2]([CX4H2])[CX4H2]
0.2437 [CX4H2]([CX4H2])[CX3H0]
0.2065 [CX4H2][CX3]=O
0.1955 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.1783 [CX4H2][CX4H2]

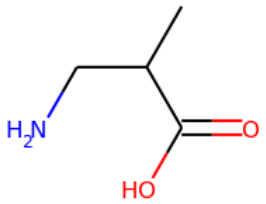


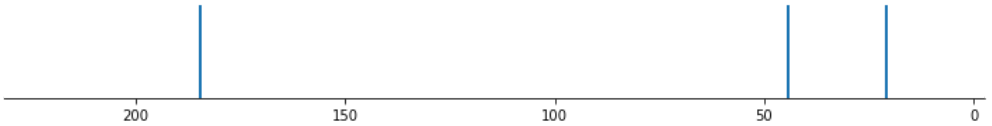
Top predicted substructures for the masked region(red):
0.6394 [CX4H2]([NX3H2])[CX4H2]
0.6287 [#7H2][#6H2]
0.3393 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.249 [#7][#6H2]
0.239 [#7X3][#6H2]
0.2347 [CX4H2]([CX4H2])[CX4H2]
0.2229 [#8]=[#6][#8]
0.1928 [CX4H2][CX4H2]

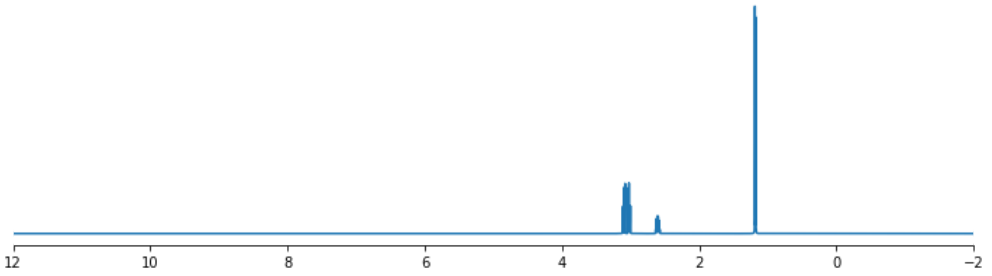


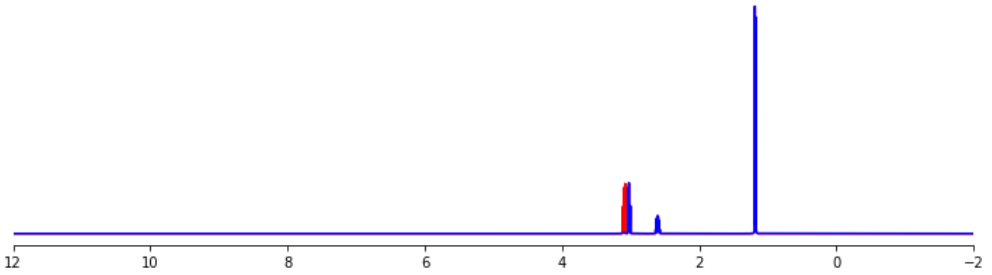
Top predicted substructures for the masked region(red):
0.9845 [CX3](=[OX1])C
0.9785 [CX4H2]CC=O
0.9683 O=[CX3H0][CX4H2][CX4H2]
0.9671 [CX4H2]([CX4H2])[CX3H0]
0.9631 [CX3](=O)[OX2H1]
0.9003 [CX4H2][CX3]=O
0.8938 [#8]=[#6][#8]
0.8882 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]

True structure: CC(CN)C(=O)O



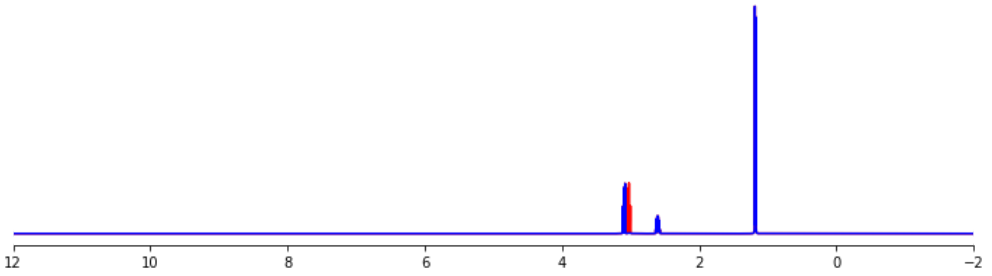






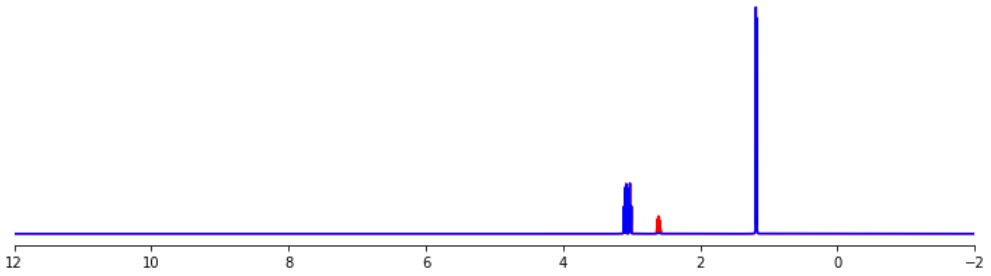
Top predicted substructures for the masked region(red):

0.5135 [CX4H2]([NX3H2])[CX4H1]
0.4898 [#7][#6H2]
0.4407 [CHX4]([CH3X4])[CH2X4]
0.4264 [#6H1][#6H2]
0.4234 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.4096 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3978 [CX4H2]CC=O
0.3574 [CH3]CC[OH]

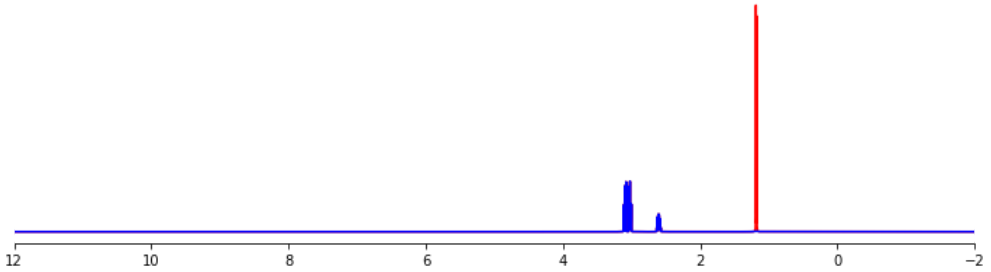


Top predicted substructures for the masked region(red):

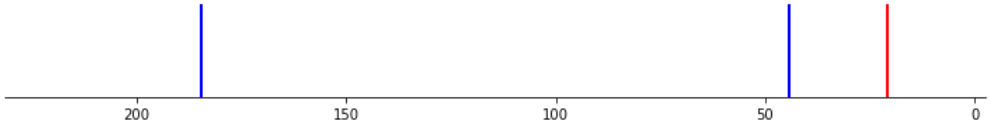
0.4689 [CX4H2]([NX3H2])[CX4H1]
0.457 [CHX4]([CH3X4])[CH2X4]
0.4131 [#6H1][#6H2]
0.382 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.3784 [#7][#6H2]
0.3719 [#7][#6][#6][#6X3]
0.3692 [CX4H2]CC=O
0.3681 [CH3]CC[OH]



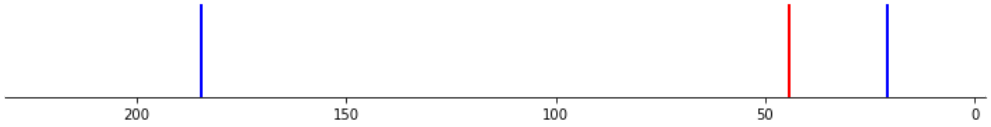
Top predicted substructures for the masked region(red):
0.4978 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.4831 [CX4H2]([NX3H2])[CX4H1]
0.4817 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.4301 [CHX4]([CH3X4])[CH2X4]
0.4248 [#6H1][#6H2]
0.3772 [CX4H2]CC=O
0.3691 [#7][#6H2]
0.3197 [CH3]CC[OH]



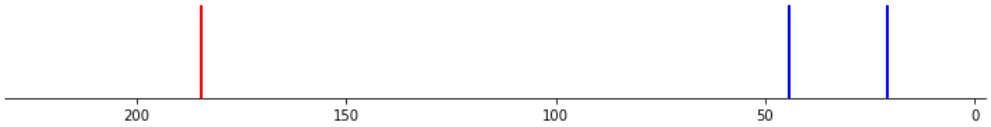
Top predicted substructures for the masked region(red):
0.8627 [CHX4]([CH3X4])[CH2X4]
0.6009 [#6H3][#6][#6X3]
0.5503 [#6H3][#6][#6]
0.5241 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.5034 [CX4H3][CX4H1]
0.4756 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.4642 [CH3]CC[OH]
0.3501 [CX4H2]([NX3H2])[CX4H1]



Top predicted substructures for the masked region(red):
0.7002 [CH3]CC[OH]
0.5877 [#6H3][#6][#6X3]
0.5871 [CX4H3][CX4H1]
0.4642 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.4303 [CHX4]([CH3X4])[CH2X4]
0.4219 [CX4H3][#6]
0.4212 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.3212 [#6X3][#6][#6][#6H3]



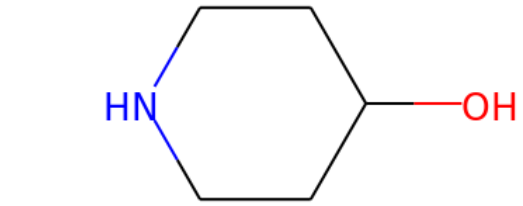
Top predicted substructures for the masked region(red):
0.6409 [#7][#6H2]
0.6344 [CX4H2]([NX3H2])[CX4H1]
0.6189 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.6126 [#7H2][#6H2]
0.5688 [CX4H2]CC=O
0.5437 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.4555 [#7X3][#6H2]
0.4528 [CHX4]([CH3X4])[CH2X4]

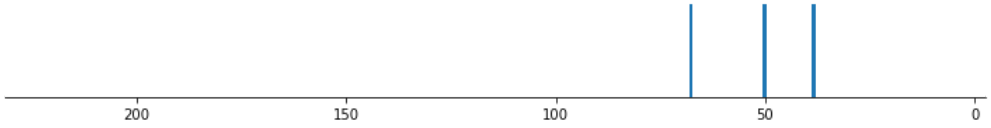


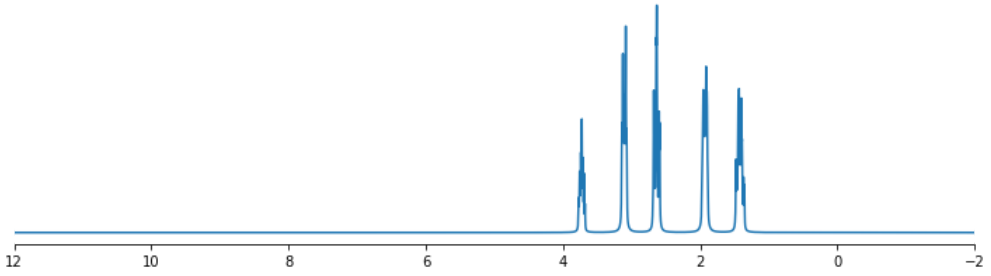
Top predicted substructures for the masked region(red):
0.979 [CX3](=[OX1])C
0.97 [#8]=[#6H0][#6H1]
0.9457 [CX3](=O)[OX2H1]

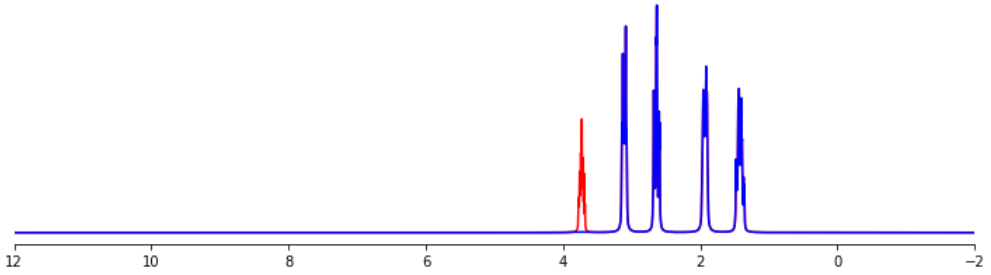
0.9304 [#6H3][#6][#6X3]
0.9278 [CX4H2]CC=O
0.9201 O=[CX3][CX4H]
0.7694 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.7516 [#8]=[#6][#8]

True structure: OC1CCNCC1

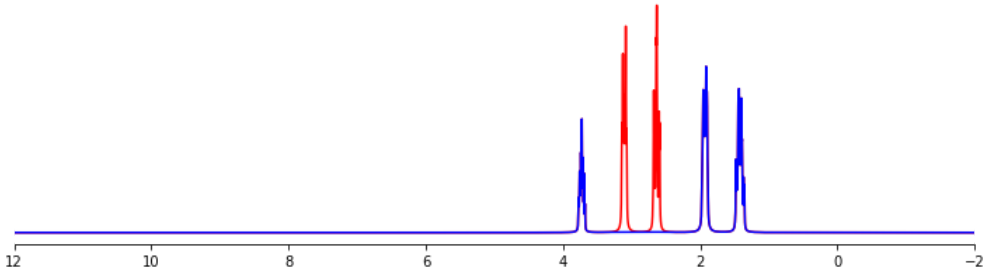




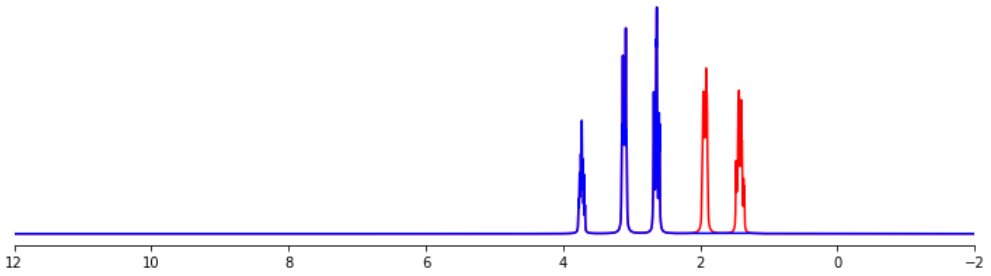




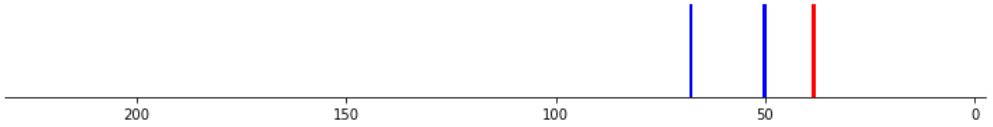
Top predicted substructures for the masked region(red):
0.5421 [CH2X4](O)[CX4H2]
0.5087 [CX4H2]([#6])[O]
0.4201 [#6H1r5][#7]
0.394 [CX4H2]([NX3H0])[CX4H2]
0.366 [#6]1[#6][#6][#6][#7]1
0.35 [CX4H1]([NX3H1])([CX4H2])[CX4H2]
0.3182 [CX4H2]([CX4H2])[CX4H2]
0.2937 [#7][#6H1][#6H2r5]



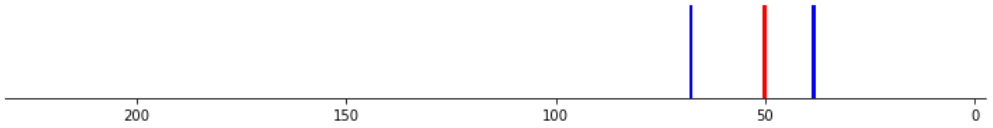
Top predicted substructures for the masked region(red):
0.913 [#7X3][#6H2]
0.8447 [#7][#6H2]
0.8053 [#7][#6H2][#6H2]
0.6773 [#7][#6H2][#6H2][#6H1]
0.6651 [CX4H2]([NX3H1])[CX4H2]
0.5554 [#6]1[#6][#6][#6][#7]1
0.5368 [#6H1r5][#7]
0.4779 [#6H2][#7][#6H2]



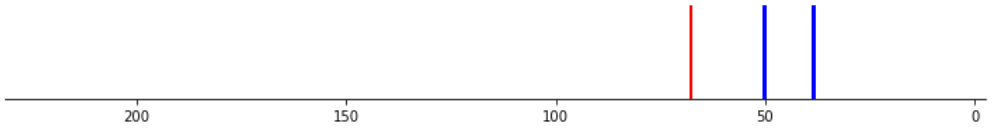
Top predicted substructures for the masked region(red):
0.6432 [#7][#6H1][#6H2r5]
0.616 [CX4H2]([CX4H2])[CX4H1]
0.5581 [#6H1r5][#7]
0.4989 [#6]1[#6][#6][#6][#7]1
0.4603 [CX4H1]([OX2H1])([CX4H2])[CX4H2]
0.4447 [CX4H2]([CX4H2])[CX4H2]
0.4345 [#6X4H2][#6H1][#8H]
0.4223 [OH][CX4H]



Top predicted substructures for the masked region(red):
0.3846 [CH2X4](O)[CX4H2]
0.3608 [CX4H2]([NX3H0])[CX4H2]
0.3562 [#7][#6H1][#6H2r5]
0.3152 [CX4H2]([CX4H2])[CX4H2]
0.2898 [CX4H1]([NX3H1])([CX4H2])[CX4H2]
0.2721 [CX4H1]([OX2H1])([CX4H2])[CX4H2]
0.2633 [#6H1r5][#7]
0.2596 CCCCCC

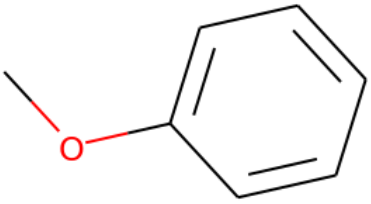


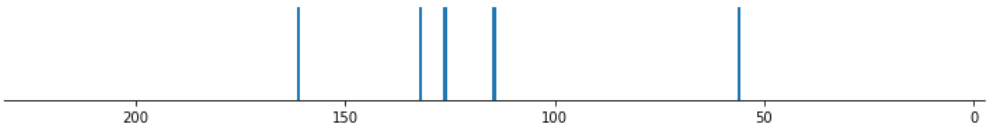
Top predicted substructures for the masked region(red):
0.3977 [CX4H2]([NX3H0])[CX4H2]
0.3815 [#6]1[#6][#6][#6][#7]1
0.3501 [CX4H2]([CX4H2])[CX4H2]
0.3064 [#7][#6H1][#6H2r5]
0.2526 [#6H1r5][#7]
0.2419 [#6H2][#7][#6H2]
0.2293 [OH][CX4H]
0.2273 [CH2X4](O)[CX4H2]

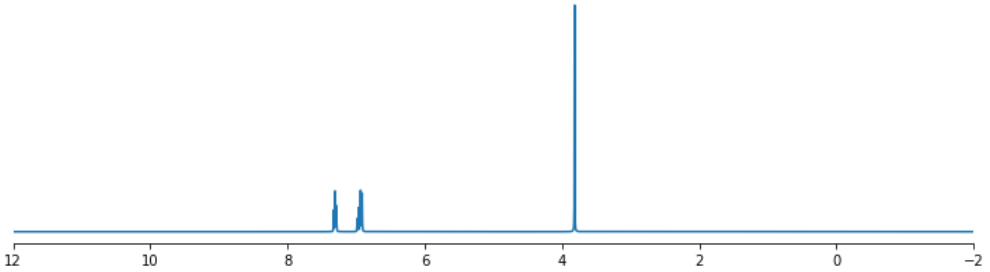


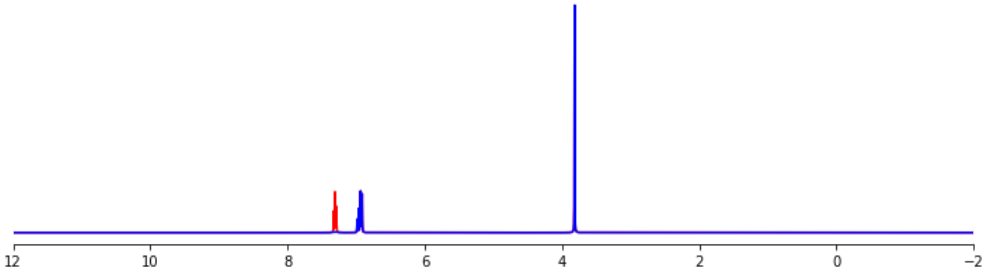
Top predicted substructures for the masked region(red):
0.5369 [#7][#6H1][#6H2r5]
0.5277 [#6H1r5][#7]
0.5046 [CH2X4](O)[CX4H2]
0.4963 [#6]1[#6][#6][#6][#7]1
0.4582 [CX4H1]([OX2H1])([CX4H2])[CX4H2]
0.4176 [#6X4H2][#6H1][#8H]
0.3796 [CX4H2]([NX3H0])[CX4H2]
0.3769 [CX4H1]([NX3H1])([CX4H2])[CX4H2]

True structure: COc1ccccc1

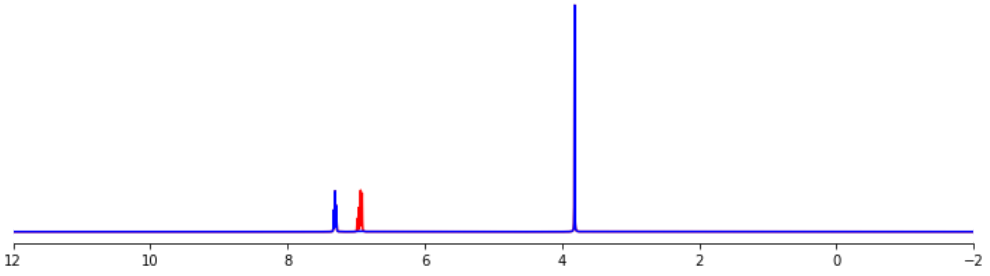




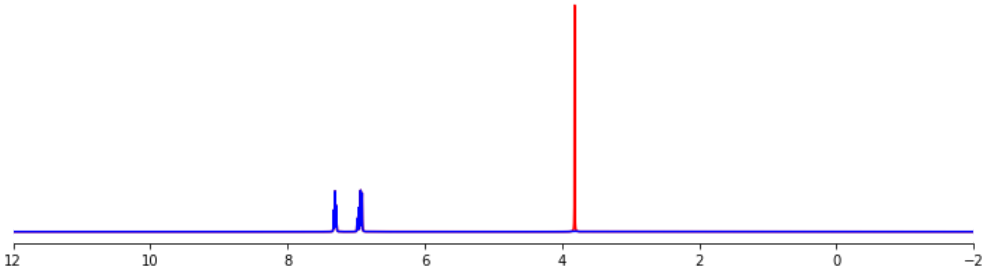




Top predicted substructures for the masked region(red):
0.4875 [OX2H][cX3]:[c]
0.2235 [#7][#6][#6][#6X3]
0.2222 [cH]cO
0.196 [#6X3][#7][#6X3]
0.1887 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1554 [#7][#6H0][#6H1]
0.151 [#7][#6][#6X3]
0.102 [cX3H1]([cX3H1])[cX3H1]

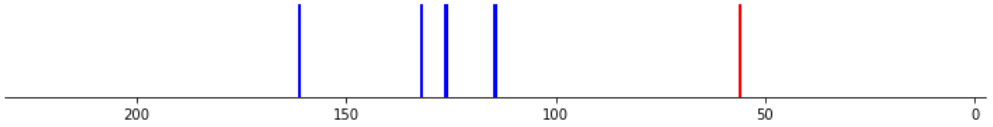


Top predicted substructures for the masked region(red):
0.463 [OX2H][cX3]:[c]
0.2989 [cH]cO
0.2081 [#7][#6][#6][#6X3]
0.1905 [#6X3][#7][#6X3]
0.1493 [#7][#6H0][#6H1]
0.1453 [#7][#6][#6X3]
0.1409 [cX3H1]([cX3H1])[cX3H1]
0.1121 [OX2H1]

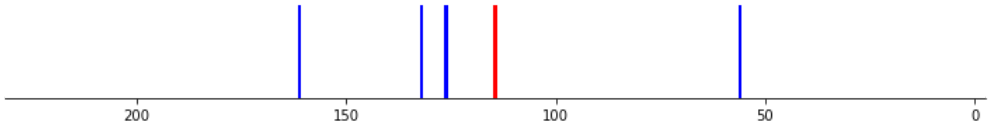


Top predicted substructures for the masked region(red):
0.3501 [CX4H3][OX2H0]
0.2766 [OX2H][cX3]:[c]
0.1657 [CX4H3]
0.1575 [cH]cO
0.1352 [#6X3][#7][#6X3]
0.1197 [#7][#6][#6][#6X3]
0.1119 [#7][#6][#6X3]

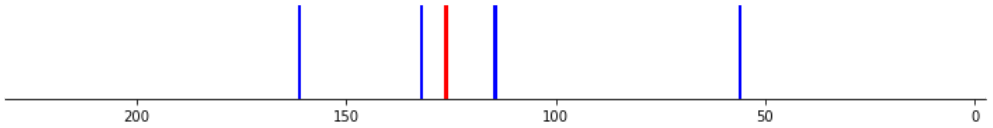
0.1119 [#7][#6H0][#6H1]



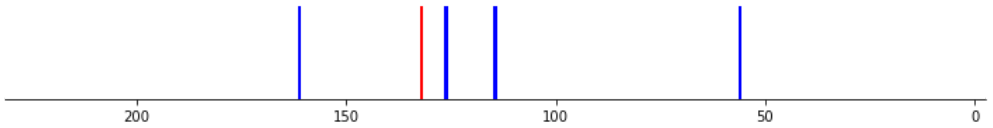
Top predicted substructures for the masked region(red):
0.6701 [CX4H3][OX2H0]
0.2298 [CX4H3]
0.1482 [#6X3][#7][#6X3]
0.1309 [#7][#6][#6][#6X3]
0.129 [#7][#6][#6X3]
0.1287 [#7][#6H0][#6H1]
0.0796 [CX3H1](=[CX3H1])[CX3H1]
0.0793 [cX3H1]([oX2H0])[cX3H1]



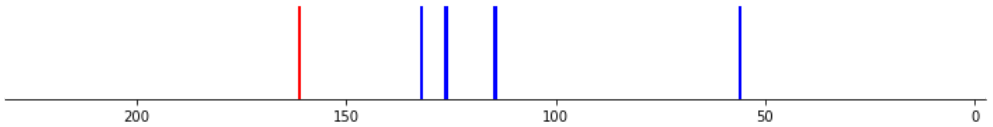
Top predicted substructures for the masked region(red):
0.465 [OX2H][cX3]:[c]
0.2052 [#7][#6][#6][#6X3]
0.1852 [#6X3][#7][#6X3]
0.1471 [#7][#6H0][#6H1]
0.1417 [cH]cO
0.14 [#7][#6][#6X3]
0.1199 o[cH]
0.0994 [cX3H1]([oX2H0])[cX3H1]



Top predicted substructures for the masked region(red):
0.4817 [OX2H][cX3]:[c]
0.1829 [#7][#6][#6][#6X3]
0.177 [#6X3][#7][#6X3]
0.1478 [#7][#6][#6X3]
0.1446 [#7][#6H0][#6H1]
0.1231 [cH]cO
0.1182 [OX2H1]
0.0854 o[cH]

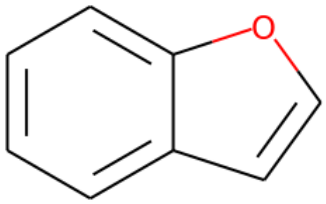


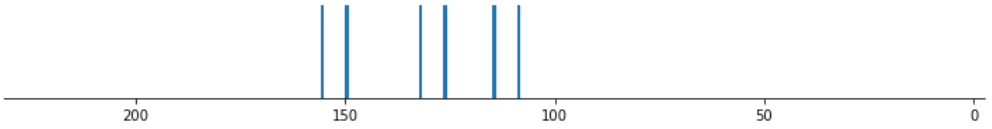
Top predicted substructures for the masked region(red):
0.4958 [OX2H][cX3]:[c]
0.1876 [#7][#6][#6][#6X3]
0.1736 [cH]cO
0.1718 [#6X3][#7][#6X3]
0.1501 [#7][#6][#6X3]
0.147 [#7][#6H0][#6H1]
0.1217 [OX2H1]
0.0777 [CX3H1](=[CX3H1])[CX3H1]

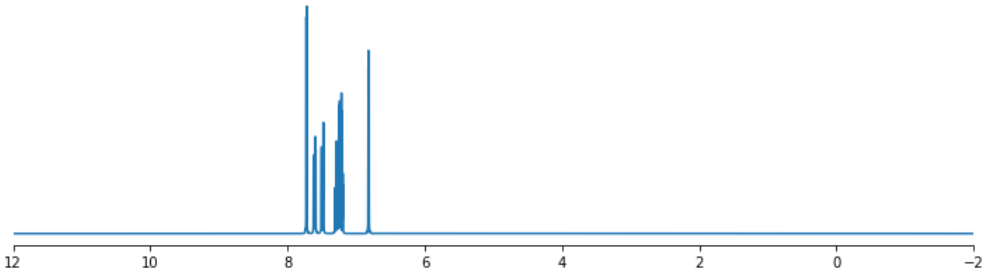


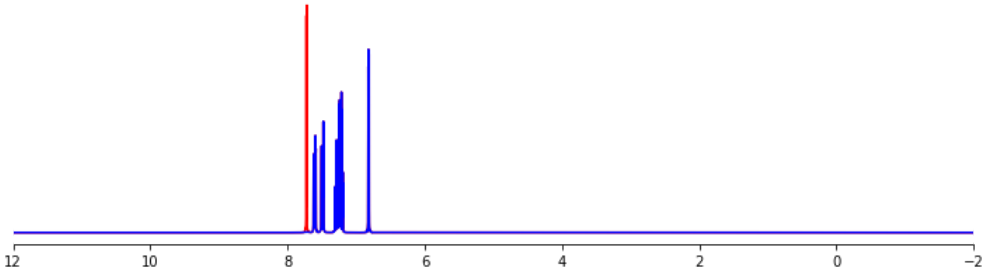
Top predicted substructures for the masked region(red):
0.5142 [OX2H][cX3]:[c]
0.3101 [cH]cO
0.1826 [#7][#6][#6][#6X3]
0.1634 [#6X3][#7][#6X3]
0.1556 [CX4H3][OX2H0]
0.1553 [#7][#6H0][#6H1]
0.1527 [#8][#6H0][#6H1]
0.141 [#7][#6][#6X3]

True structure: c1ccc2occc2c1

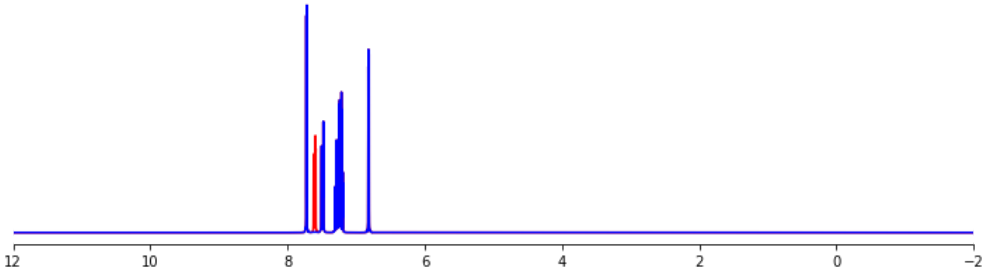




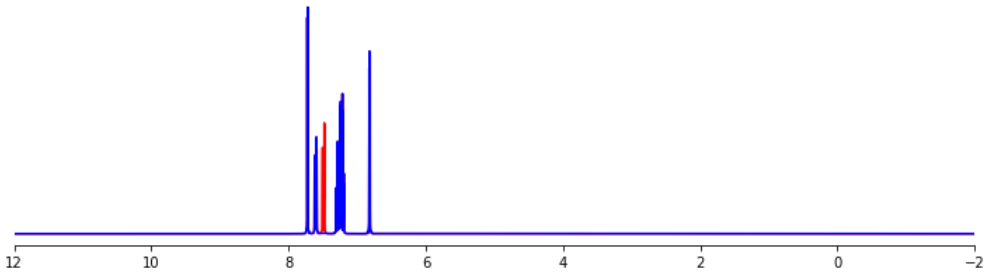




Top predicted substructures for the masked region(red):
0.3844 [OX2H][cX3]:[c]
0.3038 [OX2H1]
0.2448 [#7][#6][#6X3]
0.1575 [#6X3][#7][#6X3]
0.1456 [#8][#6H][#6X3][#6X3H]
0.11 [#7][#6H0][#6H1]
0.1045 [cX3H1]([oX2H0])[cX3H1]
0.0863 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]

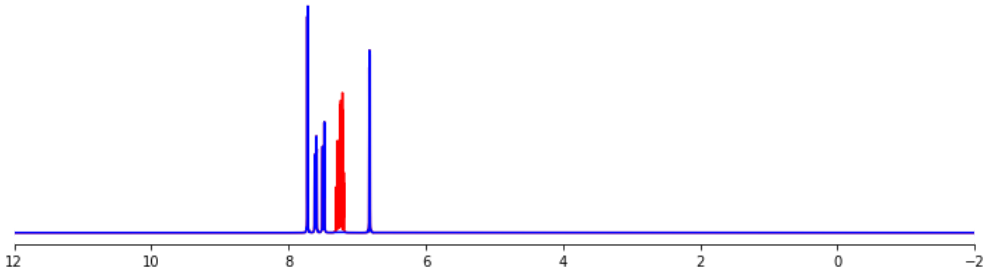


Top predicted substructures for the masked region(red):
0.426 [OX2H][cX3]:[c]
0.2978 [OX2H1]
0.2448 [#7][#6][#6X3]
0.1368 [#6X3][#7][#6X3]
0.1338 [#8][#6H][#6X3][#6X3H]
0.1158 [#7][#6H0][#6H1]
0.0964 [cX3H1]([oX2H0])[cX3H1]
0.0864 [cX3H1]([nX3H1])[cX3H1]



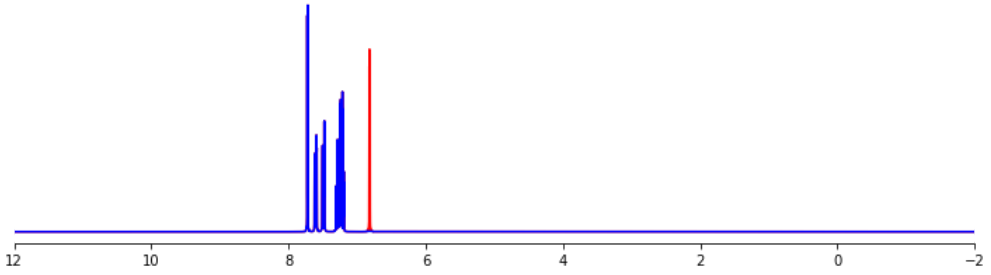
Top predicted substructures for the masked region(red):

0.4208 [OX2H][cX3]:[c]
0.29 [OX2H1]
0.2448 [#7][#6][#6X3]
0.1563 [#8][#6H][#6X3][#6X3H]
0.124 [#6X3][#7][#6X3]
0.1049 [#7][#6H0][#6H1]
0.0977 [cX3H1]([oX2H0])[cX3H1]
0.0864 [cX3H1]([nX3H1])[cX3H1]



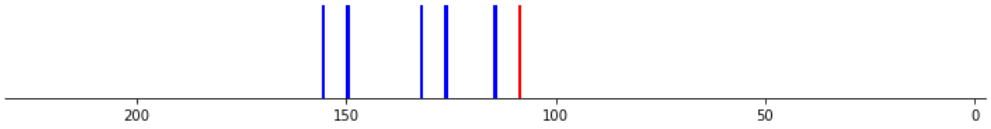
Top predicted substructures for the masked region(red):

0.4308 [OX2H][cX3]:[c]
0.2561 [OX2H1]
0.2448 [#7][#6][#6X3]
0.1783 [#6X3][#7][#6X3]
0.1411 [#7][#6H0][#6H1]
0.0879 [cX3H1]([nX3H1])[cX3H1]
0.0818 [#6X3][#7X3][#6X3]
0.0793 [cX3H1]([oX2H0])[cX3H1]



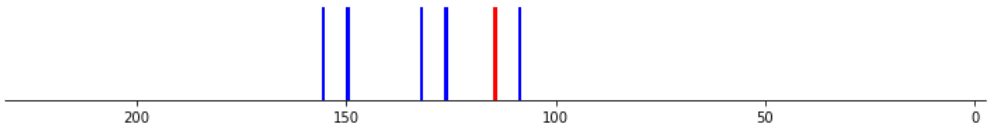
Top predicted substructures for the masked region(red):

0.5224 [OX2H][cX3]:[c]
0.3227 [OX2H1]
0.2448 [#7][#6][#6X3]
0.1544 [#6X3][#7][#6X3]
0.1299 [#8][#6H][#6X3][#6X3H]
0.11 [#7][#6H0][#6H1]
0.0884 [cX3H1]([nX3H1])[cX3H1]
0.0796 [#6X3][#7X3][#6X3]

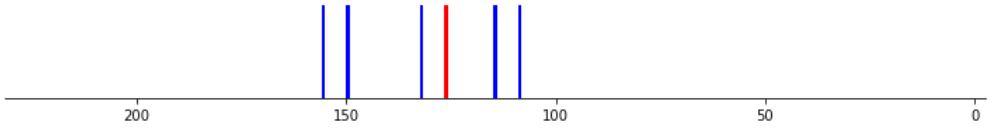


Top predicted substructures for the masked region(red):

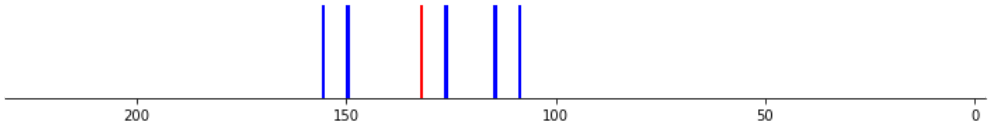
0.3441 [OX2H][cX3]:[c]
0.2448 [#7][#6][#6X3]
0.2354 [cX3H1]([oX2H0])[cX3H1]
0.2299 [OX2H1]
0.1633 [#6X3][#7][#6X3]
0.1327 [#8][#6H][#6X3][#6X3H]
0.1314 [#7][#6H0][#6H1]
0.0899 [cX3H1]([nX3H1])[cX3H1]



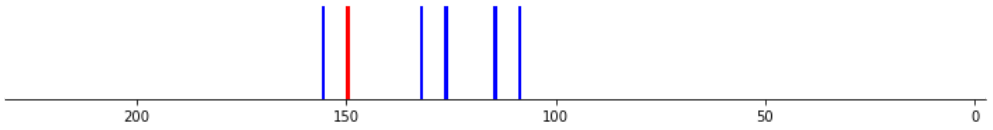
Top predicted substructures for the masked region(red):
0.3982 [OX2H][cX3]:[c]
0.2636 [OX2H1]
0.2448 [#7][#6][#6X3]
0.2106 [cX3H1]([oX2H0])[cX3H1]
0.1687 [#8][#6H][#6X3][#6X3H]
0.1538 [#6X3][#7][#6X3]
0.13 [#7][#6H0][#6H1]
0.088 [cX3H1]([nX3H1])[cX3H1]



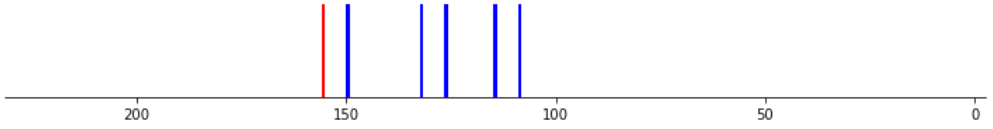
Top predicted substructures for the masked region(red):
0.516 [OX2H][cX3]:[c]
0.3696 [OX2H1]
0.2448 [#7][#6][#6X3]
0.1688 [#6X3][#7][#6X3]
0.1304 [#7][#6H0][#6H1]
0.1296 [#8][#6H][#6X3][#6X3H]
0.088 [cX3H1]([nX3H1])[cX3H1]
0.0819 [#6X3][#7X3][#6X3]



Top predicted substructures for the masked region(red):
0.4664 [OX2H][cX3]:[c]
0.3615 [OX2H1]
0.2448 [#7][#6][#6X3]
0.1731 [#6X3][#7][#6X3]
0.1317 [#7][#6H0][#6H1]
0.1215 [#8][#6H][#6X3][#6X3H]
0.0871 [cX3H1]([nX3H1])[cX3H1]
0.0836 [#6X3][#7X3][#6X3]

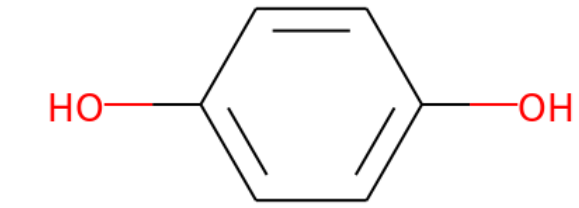


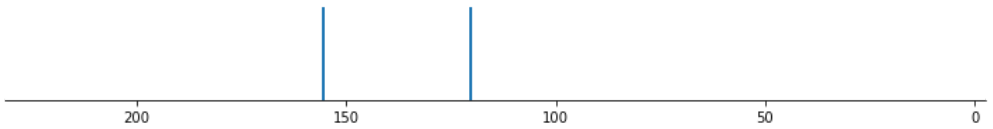
Top predicted substructures for the masked region(red):
0.4621 [OX2H][cX3]:[c]
0.2448 [#7][#6][#6X3]
0.2376 [OX2H1]
0.2154 [cX3H1]([oX2H0])[cX3H1]
0.1588 [#8][#6H][#6X3][#6X3H]
0.1257 [#7][#6H0][#6H1]
0.1162 [#6X3][#7][#6X3]
0.0772 [#6X3][#7X3][#6X3]

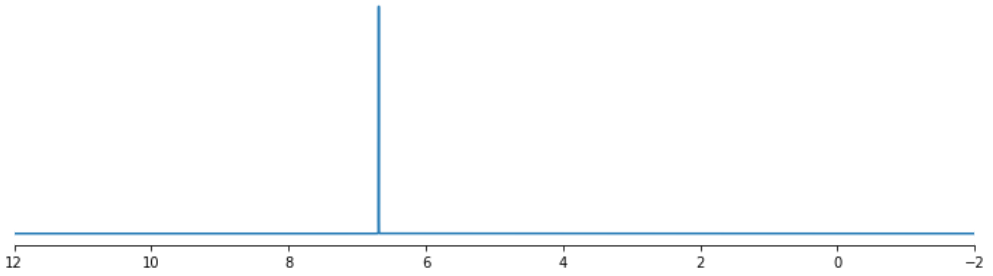


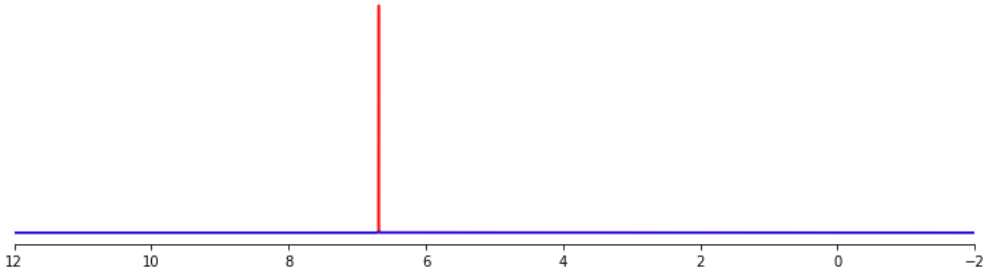
Top predicted substructures for the masked region(red):
0.4799 [OX2H][cX3]:[c]
0.2448 [#7][#6][#6X3]
0.2392 [OX2H1]
0.199 [cX3H1]([oX2H0])[cX3H1]
0.1316 [#7][#6H0][#6H1]
0.1267 [#8][#6H][#6X3][#6X3H]
0.123 [#6X3][#7][#6X3]
0.0771 [#6X3][#7X3][#6X3]

True structure: Oc1ccc(O)cc1

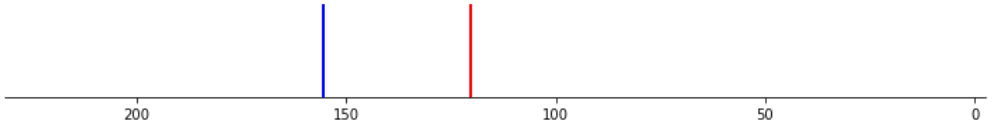




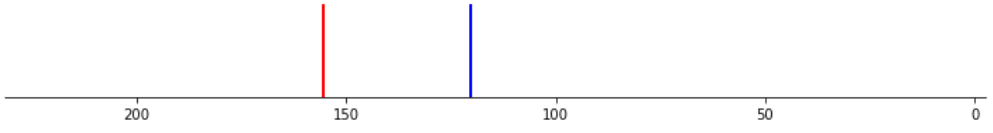




Top predicted substructures for the masked region(red):
0.605 [#6X3H1][#6X3H0]
0.5022 [cX3H0][cX3H1][cX3H1][cX3H0]
0.4934 [#6H1]
0.4747 [cX3H1]([cX3H1])[cX3H0]
0.4325 [cH]
0.4146 [#8][#6H0][#6H1]
0.3654 [cH]cO
0.2576 [cH][cH]

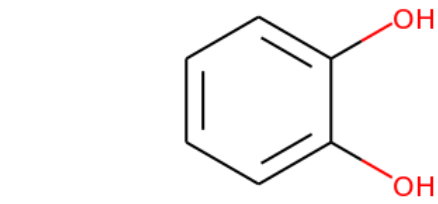


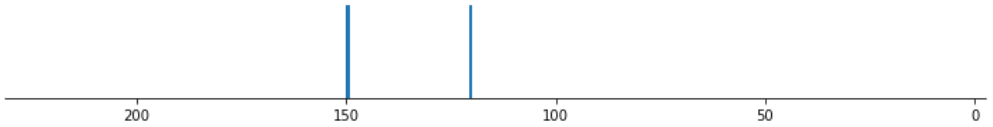
Top predicted substructures for the masked region(red):
0.4139 [#6X3][#6X3][#6X3][#6X3]
0.3387 [cX3H1]([cX3H1])[cX3H0]
0.3039 [OX2H][cX3]:[c]
0.2726 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.2635 [cH]cO
0.2488 [#8][#6][#6][#6X3]
0.2348 [#8][#6H0][#6H1]
0.2331 [#6X3H1][#6X3H0]

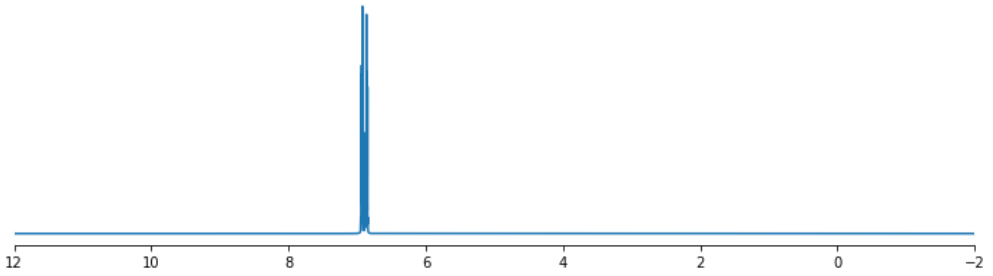


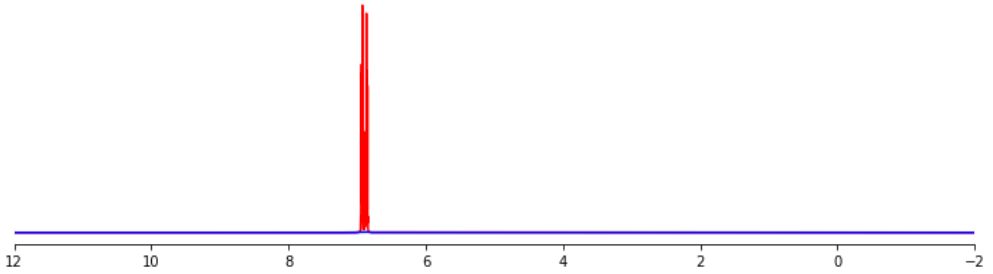
Top predicted substructures for the masked region(red):
0.5261 [cX3H0][cX3H1][cX3H1][cX3H0]
0.4943 [#6X3H1][#6X3H0]
0.4705 [cX3H1]([cX3H1])[cX3H0]
0.4367 [OX2H][cX3]:[c]
0.4042 [cH]cO
0.4039 [#6X3][#6X3][#6X3][#6X3]
0.4031 [cH]
0.3648 [#8][#6H0][#6H1]

True structure: Oc1ccccc1O

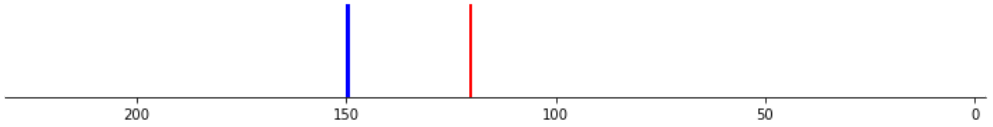




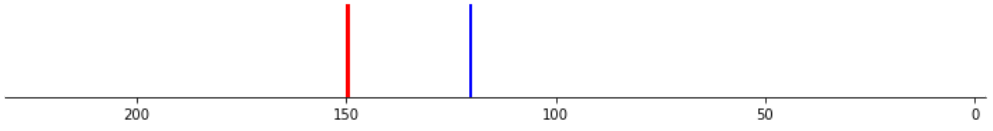




Top predicted substructures for the masked region(red):
0.8594 [cH][cH]
0.7824 [cX3H1]([cX3H1])[cX3H0]
0.7788 [#6H1][#6H1]
0.7341 [cH]cO
0.7278 [cX3H1]([cX3H1])[cX3H1]
0.6339 [OX2H1]
0.5494 [#6X3H1][#6X3H0]
0.5442 [#6H1]

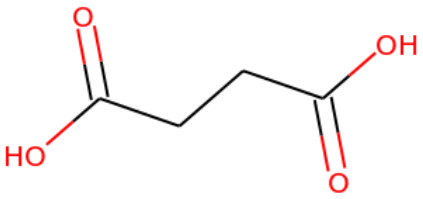


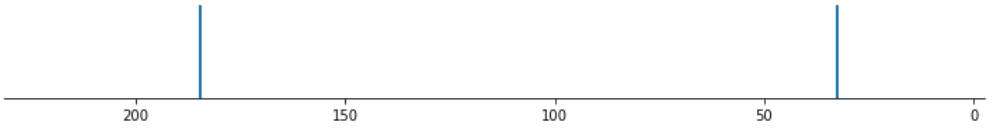
Top predicted substructures for the masked region(red):
0.6038 [OX2H][cX3]:[c]
0.5364 [OX2H1]
0.4265 [cH]cO
0.3835 [#6X3H1][#6X3H0]
0.3108 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.2962 [cX3H0][cX3H1][cX3H0][OX2H1]
0.2337 [#8][#6H1][#6H1]
0.2319 [cX3H1]([cX3H1])[cX3H1]

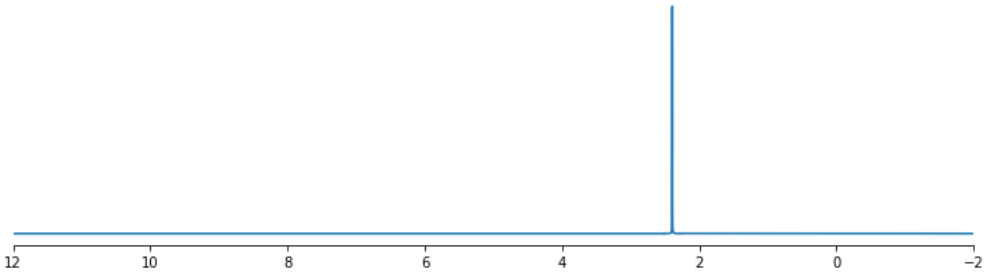


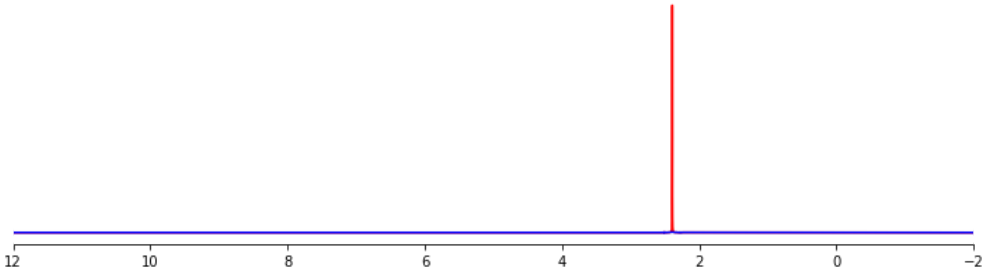
Top predicted substructures for the masked region(red):
0.6253 [OX2H][cX3]:[c]
0.5352 [OX2H1]
0.5239 [cH]cO
0.4154 [#6X3H1][#6X3H0]
0.3689 [cX3H0][cX3H1][cX3H1][cX3H0]
0.3013 [cX3H1]([cX3H1])[cX3H1]
0.2925 [cX3H0][cX3H1][cX3H0][OX2H1]
0.2312 [cX3H0]([cX3H1])([cX3H0])[OX2H1]

True structure: O=C(O)CCC(=O)O

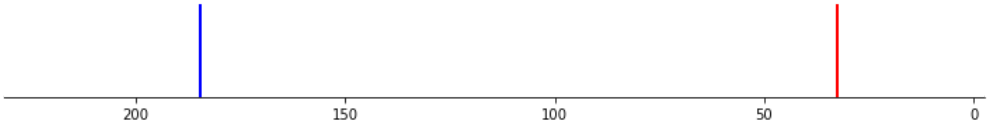




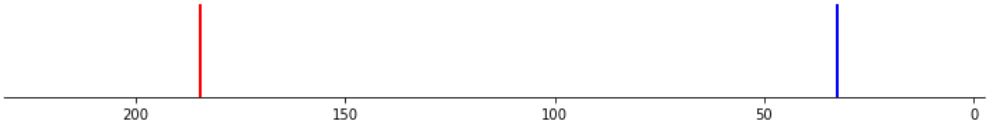




Top predicted substructures for the masked region(red):
0.8461 [OX1H0]=[CX3H0][CX4H3]
0.5245 [CX4H3][#6]
0.518 [CX4H3]
0.4909 [#6H3][#6H0]
0.3854 [#6X3][#6X3]
0.2918 [CX4H3][CX3H0]
0.2482 [#6H3][#6][#6]
0.2462 O=CC=O

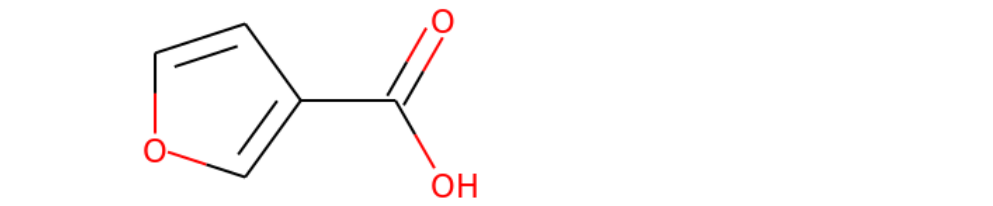


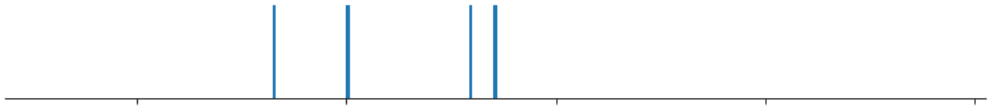
Top predicted substructures for the masked region(red):
0.6574 [OX1H0]=[CX3H0][CX4H3]
0.5483 [CX4H3][#6]
0.4112 [#6H3][#6][#6]
0.4029 [CX4H3]
0.3657 [#6H3][#6H0]
0.2991 [#6X3][#6X3]
0.2484 [#6H3][#6][#6X3]
0.2383 [CX4H3][CX3H0]

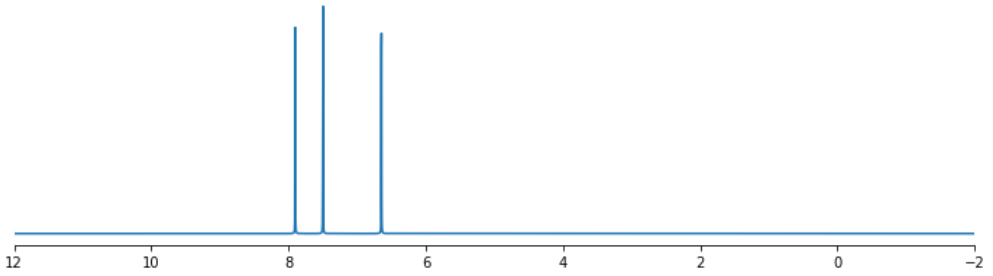


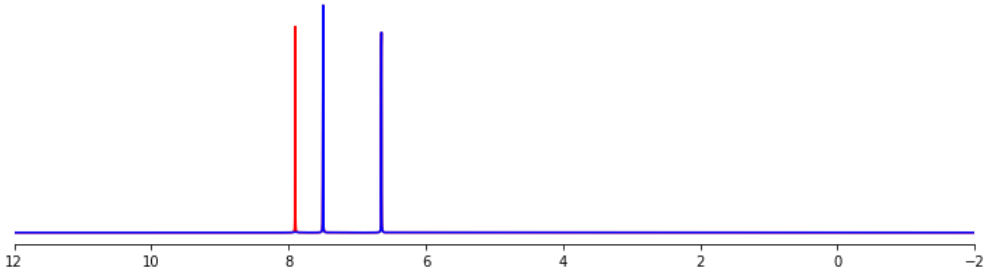
Top predicted substructures for the masked region(red):
0.8801 [CX3](=[OX1])C
0.8736 [CX3](=[OX1])O
0.8662 [OX1H0]=[CX3H0][CX4H3]
0.7846 [CX3](=O)[OX2H1]
0.6867 [CX4H3]
0.6415 [#8]=[#6][#8]
0.5358 [CX4H3][#6]
0.5279 [#6H3][#6H0]

True structure: O=C(O)c1ccoc1

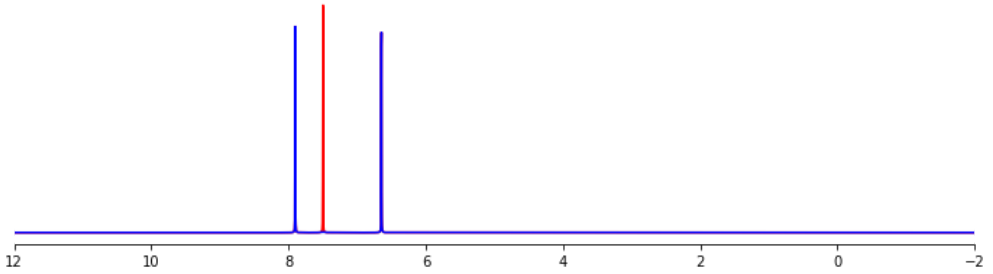




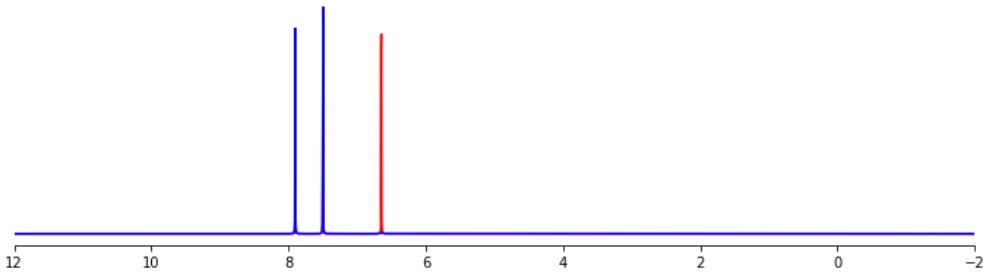




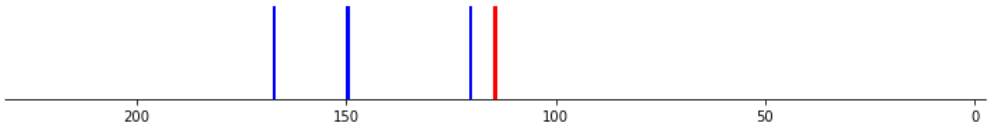
Top predicted substructures for the masked region(red):
0.6976 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.4168 [cX3H1]([oX2H0])[cX3H0]
0.2387 [cX3H1]([cX3H1])[cX3H1]
0.2309 [#8][#6][#6]=[#6X3]
0.1654 [#8][#6H1][#6H1]
0.1461 [#6H][#8][#6H]
0.1452 o[cH]
0.0946 [#6X3][#7][#6X3]



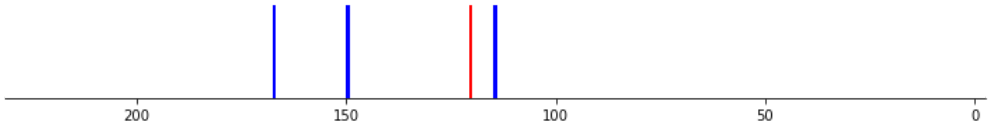
Top predicted substructures for the masked region(red):
0.8301 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.5825 [cX3H1]([oX2H0])[cX3H0]
0.3981 [#8][#6H1][#6H1]
0.396 [cX3H1]([oX2H0])[cX3H1]
0.2827 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.2663 [cX3H1]([cX3H1])[cX3H1]
0.2413 [#6H][#8][#6H]
0.1855 [#8][#6][#6]=[#6X3]



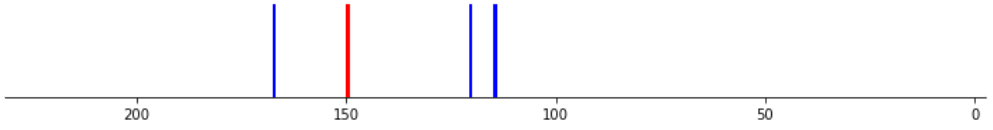
Top predicted substructures for the masked region(red):
0.7203 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.5147 [cX3H1]([oX2H0])[cX3H0]
0.2652 [#8][#6][#6]=[#6X3]
0.2233 [cX3H1]([oX2H0])[cX3H1]
0.2166 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.19 [#8][#6H1][#6H1]
0.1591 o[cH]
0.1451 O=[#6][#6][#6X3]



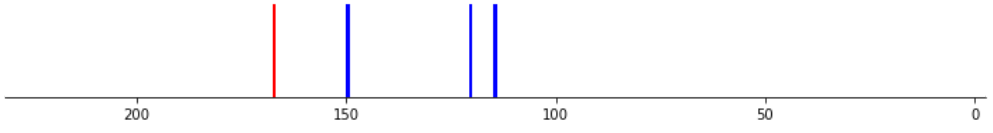
Top predicted substructures for the masked region(red):
0.6993 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.4851 [cX3H1]([oX2H0])[cX3H0]
0.2636 [OX2H][cX3]:[c]
0.235 [cX3H1]([cX3H1])[cX3H1]
0.2342 [#8][#6H1][#6H1]
0.2269 o[cH]
0.2198 [#8][#6][#6]=[#6X3]
0.1934 [cX3H0]([cX3H1])([cX3H0])[OX2H1]



Top predicted substructures for the masked region(red):
0.6199 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.4693 [cX3H1]([oX2H0])[cX3H0]
0.3217 [OX2H][cX3]:[c]
0.2484 [#8][#6][#6]=[#6X3]
0.2072 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.2029 o[cH]
0.2006 [cX3H1]([cX3H1])[cX3H1]
0.2006 [cH]cO

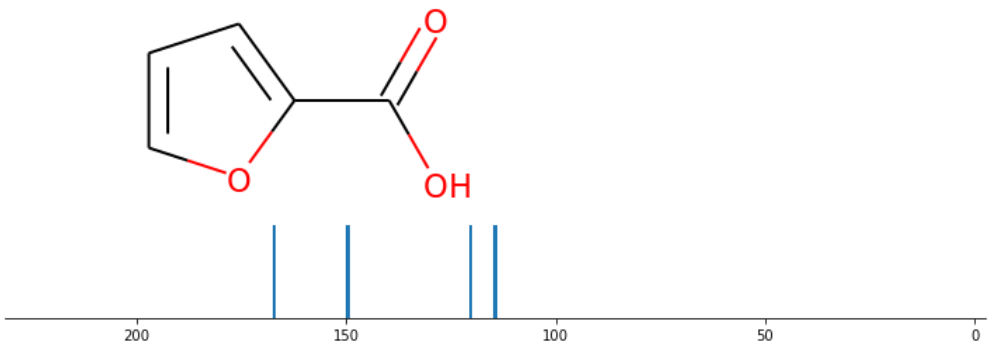


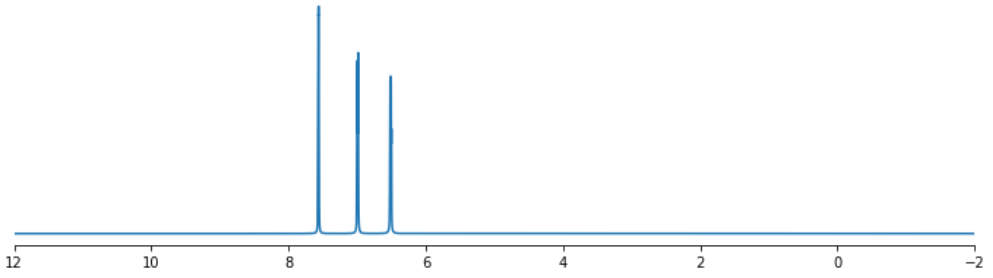
Top predicted substructures for the masked region(red):
0.6807 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.4361 [cX3H1]([oX2H0])[cX3H0]
0.2997 O=[#6][#6][#6X3]
0.2553 [#8][#6][#6]=[#6X3]
0.2469 [cX3H1]([cX3H1])[cX3H1]
0.2005 o[cH]
0.1975 [#8][#6H1][#6H1]
0.1972 [cX3H1]([oX2H0])[cX3H1]

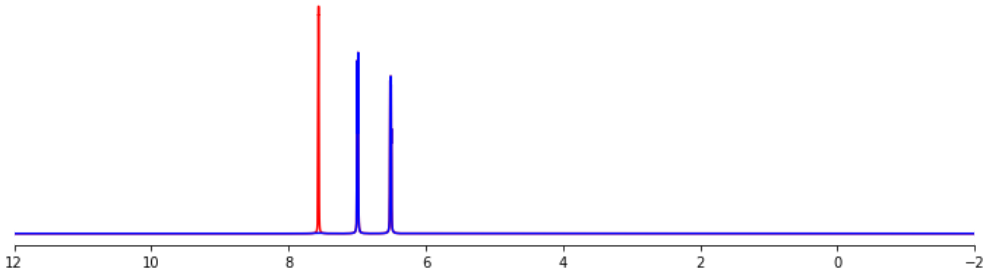


Top predicted substructures for the masked region(red):
0.6669 [#8X2H0][#6X3H1][#6X3H1][#6X3H0]
0.561 O=[#6][#6][#6X3]
0.4958 [#8]=[#6][#8]
0.4147 [cX3H1]([oX2H0])[cX3H0]
0.3591 [CX3](=[OX1])O
0.2635 [#8][#6][#6]=[#6X3]
0.2354 [cX3H1]([cX3H1])[cX3H1]
0.2084 [CX3](=O)[OX2H1]

True structure: O=C(O)c1ccco1

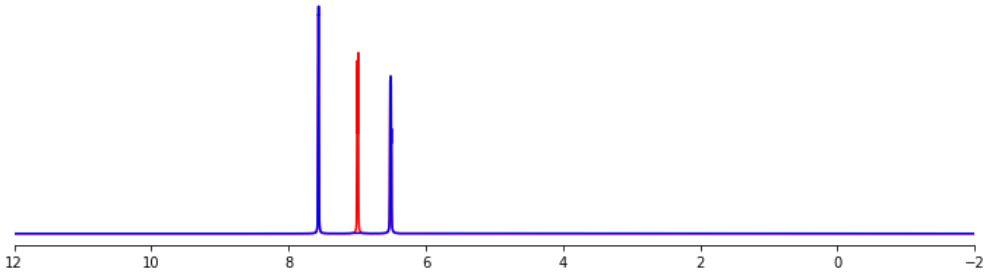






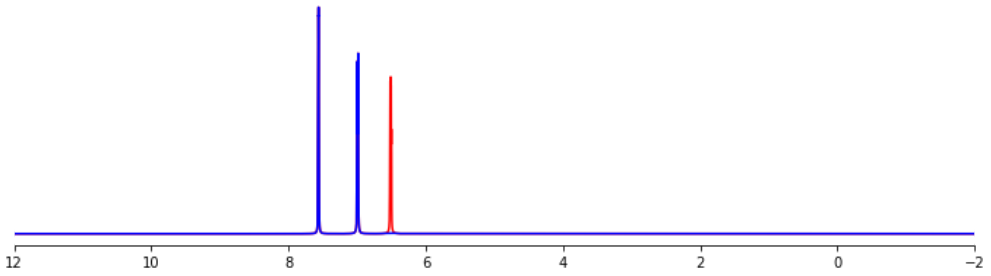
Top predicted substructures for the masked region(red):

0.301 [#8][#6H1][#6H1]
0.2977 [cX3H1]([oX2H0])[cX3H1]
0.1952 o[cH]
0.1646 [#8]=[#6][#6H1][#6H1]
0.1538 O=[#6][#6][#6X3]
0.1057 [#8][#6H][#6X3][#6X3H]
0.1013 [#8]1[#6][#6][#6][#6][#6]1
0.0961 [#6H1][#6H1]

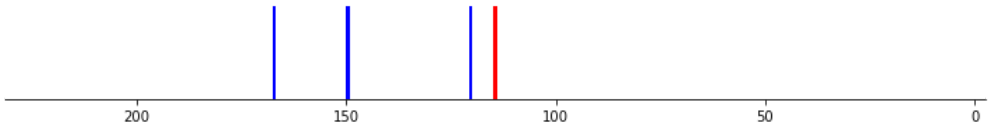


Top predicted substructures for the masked region(red):

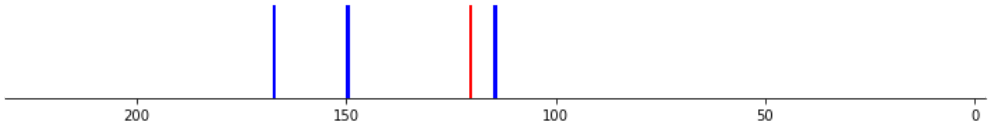
0.3719 [#8]=[#6][#6H1][#6H1]
0.2541 O=[#6][#6][#6X3]
0.1645 [cX3H1]([oX2H0])[cX3H1]
0.1206 [#8][#6H1][#6H1]
0.1051 o[cH]
0.105 [cH]cO
0.1046 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.104 [#8]=[#6H0][#6H1]



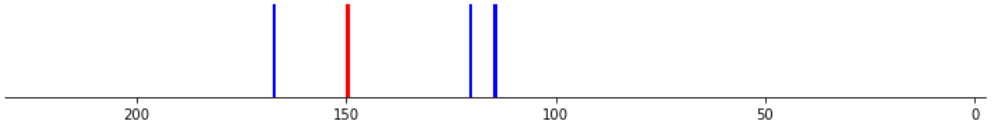
Top predicted substructures for the masked region(red):
0.3531 [#8]=[#6][#6H1][#6H1]
0.2632 O=[#6][#6][#6X3]
0.2019 [#8]=[#6H0][#6H1]
0.1372 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1312 [#8][#6][#6]=[#6X3]
0.1089 [CX3](=O)[OX2H1]
0.0963 [#6H1][#6H1]
0.0906 [cX3H1]([oX2H0])[cX3H1]



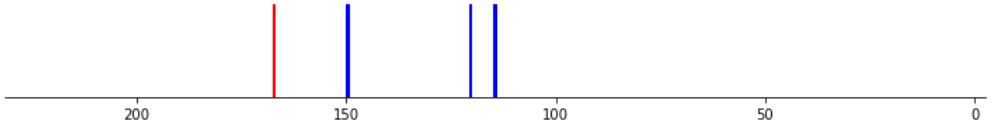
Top predicted substructures for the masked region(red):
0.3095 [#8]=[#6][#6H1][#6H1]
0.2383 [cX3H1]([oX2H0])[cX3H1]
0.2345 O=[#6][#6][#6X3]
0.1935 [#8][#6][#6][#8]
0.1906 o[cH]
0.1453 [#8][#6H1][#6H1]
0.1355 [#6H1][#6H1]
0.1349 [CX3](=O)[OX2H1]



Top predicted substructures for the masked region(red):
0.2293 O=[#6][#6][#6X3]
0.2259 [OX2H][cX3]:[c]
0.1998 [#8]=[#6][#6H1][#6H1]
0.1703 [cX3H0]([cX3H1])([cX3H0])[OX2H1]
0.1696 [#8][#6][#6][#8]
0.1498 o[cH]
0.136 [CX3](=O)[OX2H1]
0.1022 [cH]cO

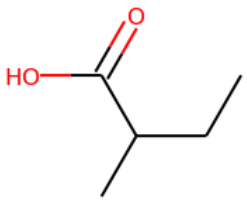


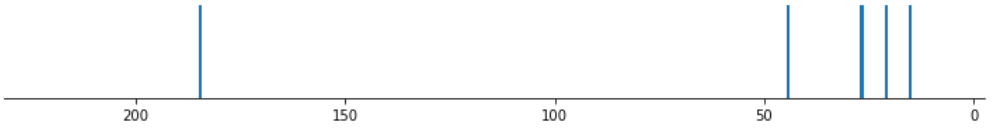
Top predicted substructures for the masked region(red):
0.3877 O=[#6][#6][#6X3]
0.2927 [#8]=[#6][#6H1][#6H1]
0.2916 [cX3H1]([oX2H0])[cX3H1]
0.2079 o[cH]
0.1748 [#8]=[#6H0][#6H1]
0.1662 O=[cX3]
0.1396 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1374 [#8][#6H1][#6H1]

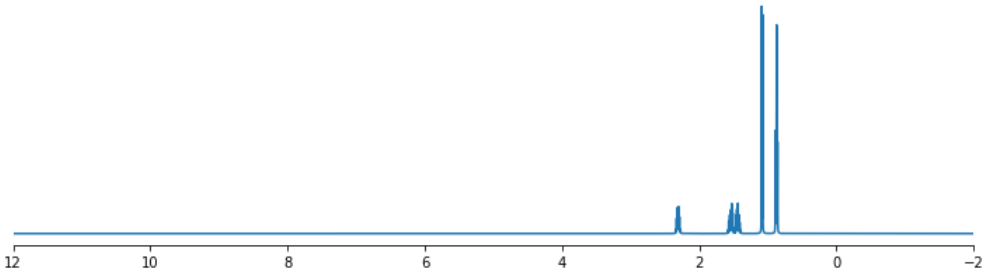


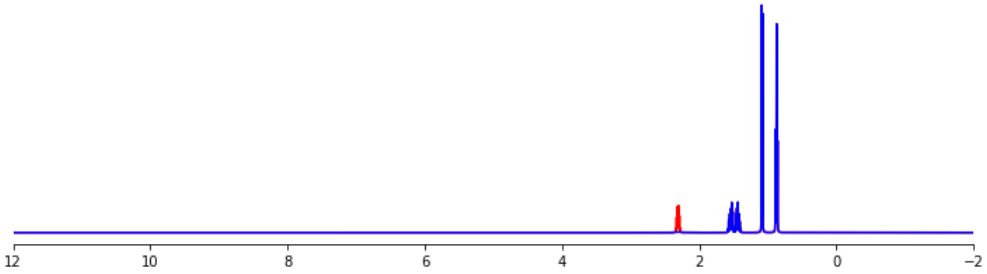
Top predicted substructures for the masked region(red):
0.9242 O=[#6][#6][#6X3]
0.5723 [#8]=[#6][#6H1][#6H1]
0.5348 [#8]=[#6][#8]
0.4969 [CX3](=[OX1])O
0.4371 [CX3](=O)[OX2H1]
0.3968 O=[cX3]
0.3416 [#8]=[#6H0][#6H1]
0.2348 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]

True structure: CCC(C)C(=O)O



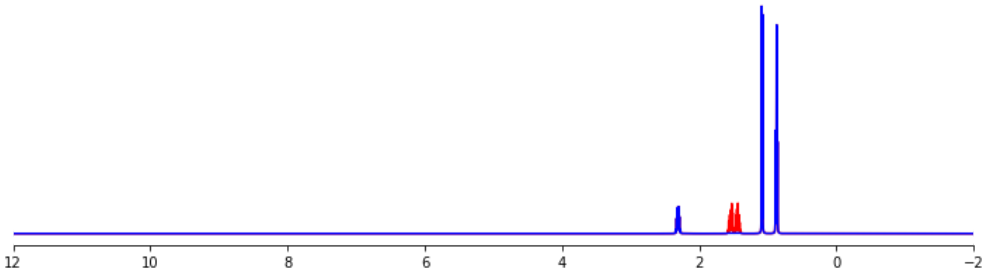






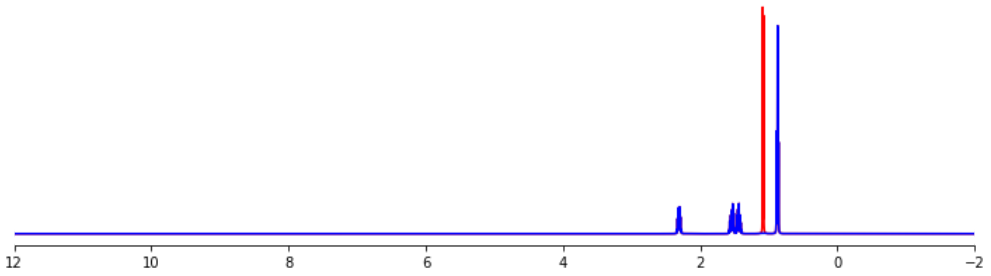
Top predicted substructures for the masked region(red):

0.3154 [#6H3][#6][#6X3]
0.2359 [CX4H3][CX4H1]
0.2324 [CHX4]([CH3X4])[CH2X4]
0.1664 OCC[CH2]
0.1517 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.1185 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.1043 [CX4H2]CC=O
0.0943 [#8][#6][#6]=[#8]

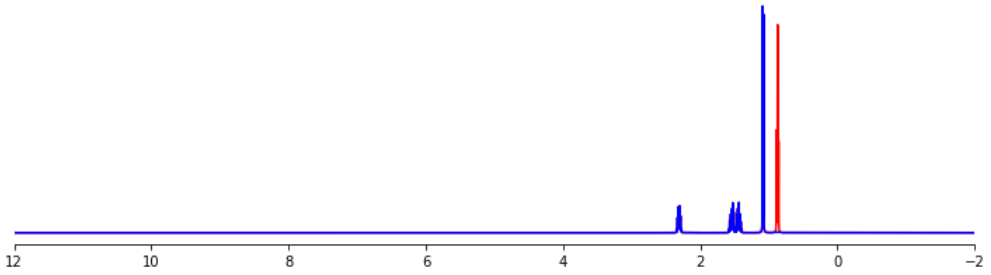


Top predicted substructures for the masked region(red):

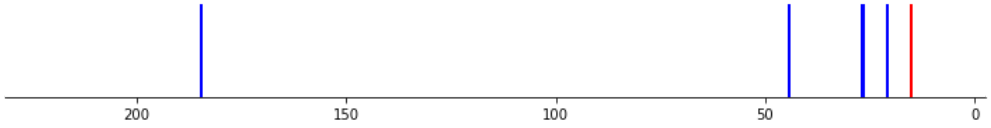
0.751 [CX4H2]([#6])[#6]
0.6055 [CHX4]([CH3X4])[CH2X4]
0.5355 OCC[CH2]
0.3973 [#6H1][#6H2]
0.3511 [CX4H2]([CX4H3])[CX4H2]
0.3096 [CX4H2]CC=O
0.1609 [#6H3][#6][#6X3]
0.1605 [CX4H3][CX4H2]



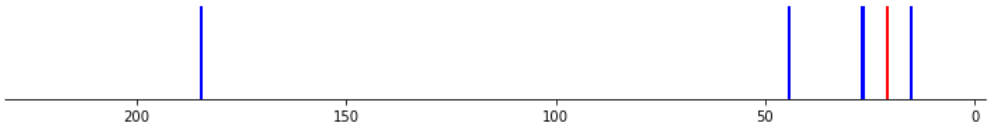
Top predicted substructures for the masked region(red):
0.7828 [CHX4]([CH3X4])[CH2X4]
0.7793 [#6H3][#6][#6X3]
0.7443 [CX4H3][CX4H1]
0.4994 [#6H3][#6][#6][#6H3]
0.3331 [#8]=[#6][#6H1][#6H1]
0.309 [#6H1]
0.3064 [CH3]CC[OH]
0.1601 [CX4H1]([CX4H3])([CX4H2])[CX3H0]



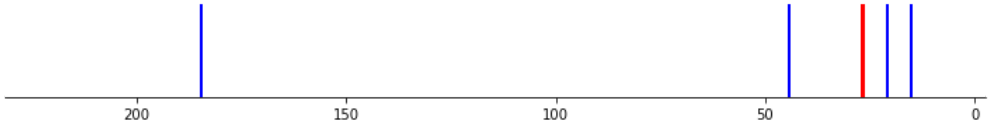
Top predicted substructures for the masked region(red):
0.3057 [#6X3][#6][#6][#6H3]
0.1921 [CHX4]([CH3X4])[CH2X4]
0.1713 [CX4H2]([CX4H3])[CX4H2]
0.1533 [#6H3][#6][#6X3]
0.1443 [CX4H3][CX4H1]
0.138 [#6H3][#6][#6][#6H3]
0.1199 [#8][#6][#6]=[#8]
0.085 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]



Top predicted substructures for the masked region(red):
0.718 [CX4H3][CX4H2]
0.395 [CX4H2]([CX4H3])[CX4H2]
0.3318 [CX4H2]([CX4H3])[CX4H1]
0.3315 [#6H3][#6][#6][#6H3]
0.3014 [#6H3][#6][#6X3]
0.2369 [#6X3][#6][#6][#6H3]
0.1377 [#8]=[#6H0][#6H1]
0.1183 [CHX4]([CH3X4])[CH2X4]

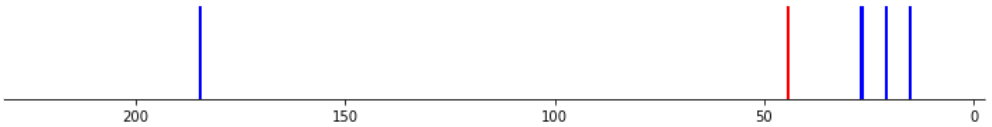


Top predicted substructures for the masked region(red):
0.3095 [#6H3][#6][#6][#6H3]
0.2971 [CX4H3][CX4H1]
0.2402 OCC[CH2]
0.2322 [#6H3][#6][#6X3]
0.2197 [CHX4]([CH3X4])[CH2X4]
0.2072 [CX4H2]([CX4H3])[CX4H2]
0.1686 [#6X3][#6][#6][#6H3]
0.1629 [CX4H1]([CX4H3])([CX4H2])[CX3H0]

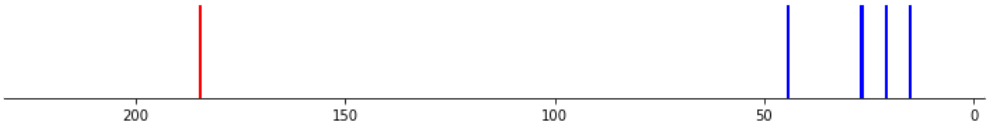


Top predicted substructures for the masked region(red):
0.2297 [CHX4]([CH3X4])[CH2X4]
0.2295 [CX4H2]CC=O
0.2 OCC[CH2]

0.1621 [#6H3][#6][#6X3]
0.1227 [#6H1][#6H2]
0.1179 [CX4H3][CX4H1]
0.1151 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]
0.0906 [CX4H2]([CX4H3])[CX4H2]

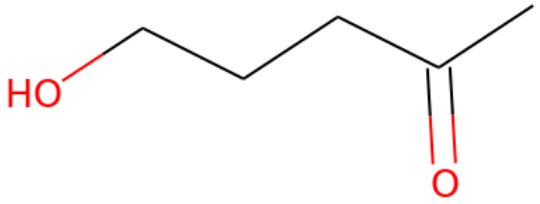


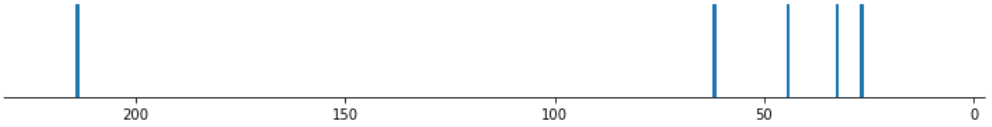
Top predicted substructures for the masked region(red):
0.3926 [CHX4]([CH3X4])[CH2X4]
0.3553 [CX4H3][CX4H1]
0.3246 [#6H3][#6][#6X3]
0.3157 [#6H3][#6][#6][#6H3]
0.2303 OCC[CH2]
0.1933 [#6X3][#6][#6][#6H3]
0.1901 [CX4H1]([CX4H3])([CX4H2])[CX3H0]
0.1392 [OX1H0]=[CX3H0][CX4H1]([CX4H3])[CX4H2]

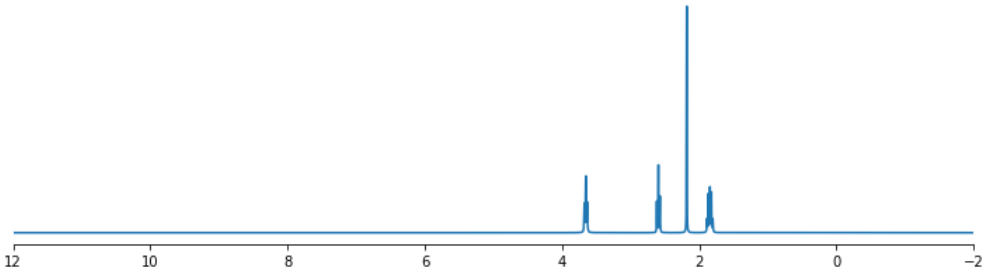


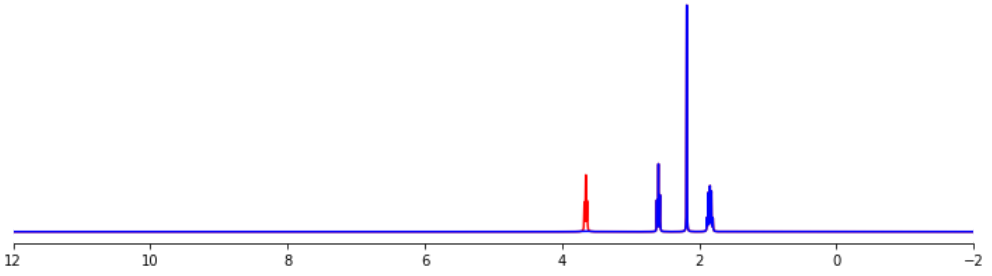
Top predicted substructures for the masked region(red):
0.9723 [#8]=[#6H0][#6H1]
0.971 [#6H3][#6][#6X3]
0.9705 [CX3](=[OX1])C
0.9469 O=[CX3][CX4H]
0.9428 [CX3](=[OX1])O
0.8916 [CX3H0](=[OX1H0])([OX2H1])[CX4H1]
0.8902 [CX3](=O)[OX2H1]
0.8376 [#6X3][#6][#6][#6H3]

True structure: CC(=O)CCCO



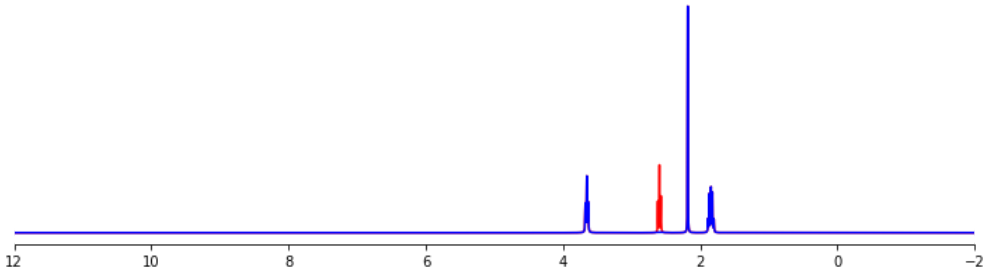




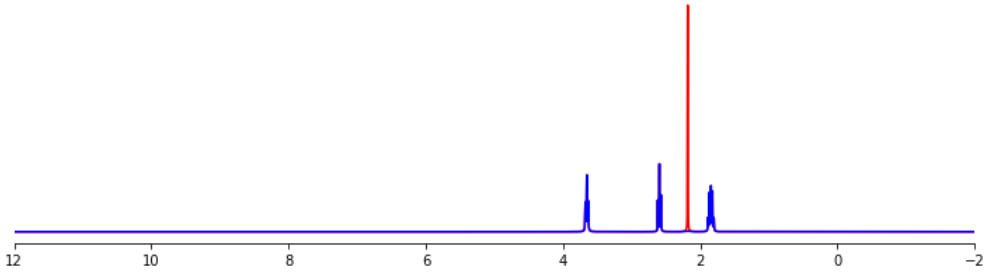


Top predicted substructures for the masked region(red):
0.5586 [CX4H2]([OX2H1])[CX4H1]
0.4562 [CX4H2](O)[CHX4]
0.4235 [#6H1]

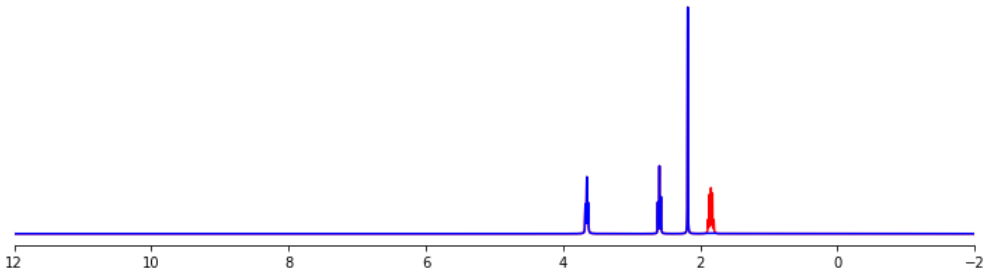
0.4142 [#8H][#6H2][#6H1]
0.3912 [CX4H2]([CX4H2])[CX4H1]
0.3878 [#6H1][#6H2]
0.3452 [CX4H2]([#6])[O]
0.3309 O=[CX3][CX4H]



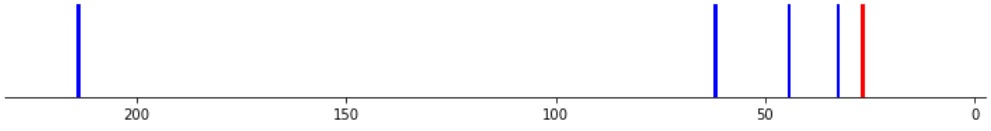
Top predicted substructures for the masked region(red):
0.5579 [CX4H2]([OX2H1])[CX4H1]
0.4268 [CX4H2](O)[CHX4]
0.3927 [CX4H2][CX3]=O
0.3921 [#6H1]
0.36 [#6H1][#6H2]
0.3465 [#8H][#6H2][#6H1]
0.3363 [CX4H2]([CX4H2])[CX3H0]
0.3038 O=[CX3H0][CX4H2][CX4H2]



Top predicted substructures for the masked region(red):
0.5476 [CX4H2]([OX2H1])[CX4H1]
0.4722 [#6H1]
0.4636 [CX4H3][CX3]
0.4452 [#6H1][#6H2]
0.4401 [#6H3][#6H0]
0.4205 [CX4H2](O)[CHX4]
0.3015 [#8H][#6H2][#6H1]
0.2835 [#8]=[#6H0][#6H1]

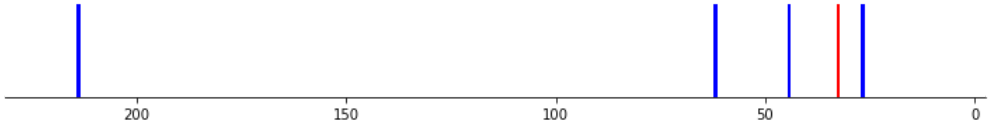


Top predicted substructures for the masked region(red):
0.5401 [CX4H2]([CX4H2])[CX4H1]
0.464 [CX4H2]([OX2H1])[CX4H1]
0.4497 [#6H1][#6H2]
0.3815 [CX4H2](O)[CHX4]
0.3477 [#6H1]
0.2394 CCCCCC
0.2228 [#8]=[#6H0][#6H1]
0.1926 O[CX4H][CX4H2]

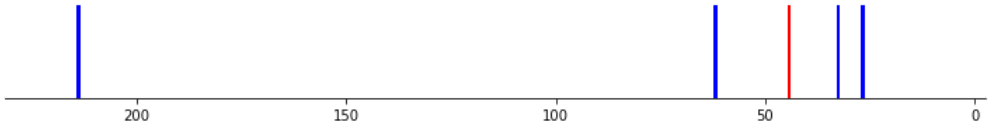


Top predicted substructures for the masked region(red):
0.5071 [CX4H2]([OX2H1])[CX4H1]
0.3781 [#6H1][#6H2]
0.3743 [CX4H2](O)[CHX4]
0.2417 [#6H1]
0.2059 CCCCCC
0.2019 [CX4H]O

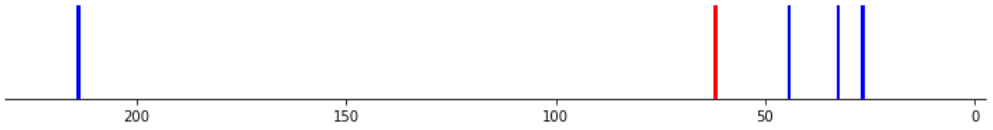
0.1984 O[CX4H][CX4H2]
0.1776 [CX4H3][#6]



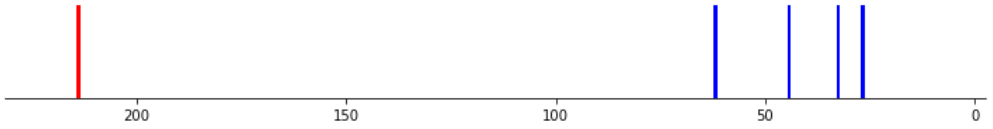
Top predicted substructures for the masked region(red):
0.4687 [CX4H2]([OX2H1])[CX4H1]
0.3776 [CX4H2](O)[CHX4]
0.2891 [#6H1][#6H2]
0.2257 [CX4H2]([CX4H2])[CX4H1]
0.2176 CCCCCC
0.2016 [#6H1]
0.1939 [CX3H0](=[OX1H0])([CX4H3])[CX4H1]
0.1816 O[CX4H][CX4H2]



Top predicted substructures for the masked region(red):
0.5286 [CX4H2]([OX2H1])[CX4H1]
0.4127 [CX4H2](O)[CHX4]
0.3005 O=[CX3H0][CX4H2][CX4H2]
0.2935 [#6H1]
0.2688 [CX4H2]([CX4H2])[CX3H0]
0.2657 [#6H1][#6H2]
0.2598 [#8H][#6H2][#6H1]
0.2533 CCCCCC

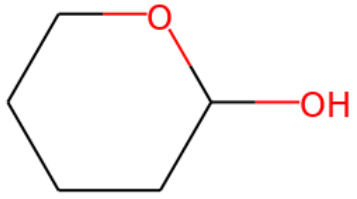


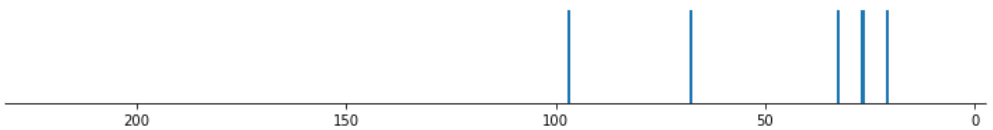
Top predicted substructures for the masked region(red):
0.6882 [CX4H2]([#6])[O]
0.632 [CX4H2]([OX2H1])[CX4H2]
0.558 [CX4H2]([OX2H1])[CX4H1]
0.4115 [CX4H2](O)[CHX4]
0.3764 [#6H1][#6H2]
0.3489 [CH2X4](O)[CX4H2]
0.3119 [#6H1]
0.2321 O=[CX3][CX4H]

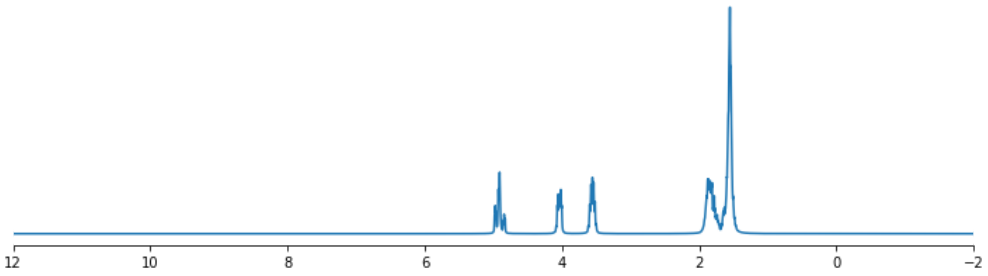


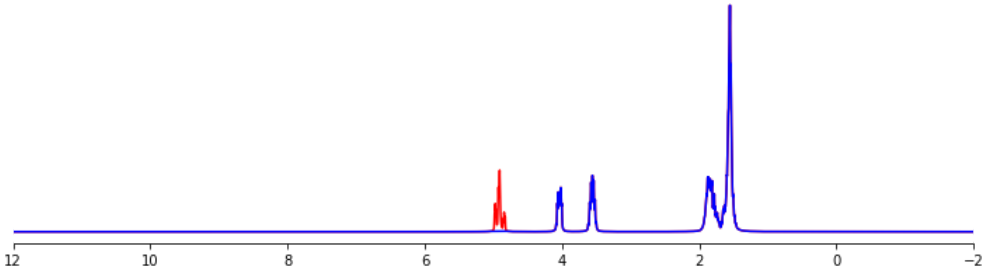
Top predicted substructures for the masked region(red):
0.9984 [CX3](=[OX1])C
0.9894 [CX4H3][CX3]
0.9864 [CX4H3][CX3H0]
0.9803 [CX4H2]CC=O
0.9166 [OX1H0]=[CX3H0][CX4H3]
0.8744 [#6H3][#6][#6]
0.8497 [CX4H2][CX3]=O
0.8009 [CX4H3][#6]

True structure: OC1CCCCO1



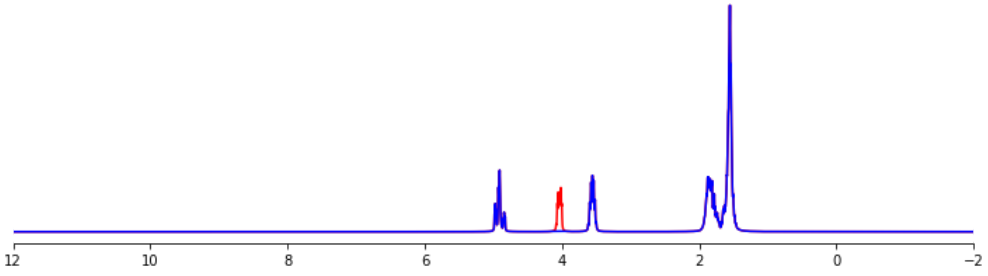






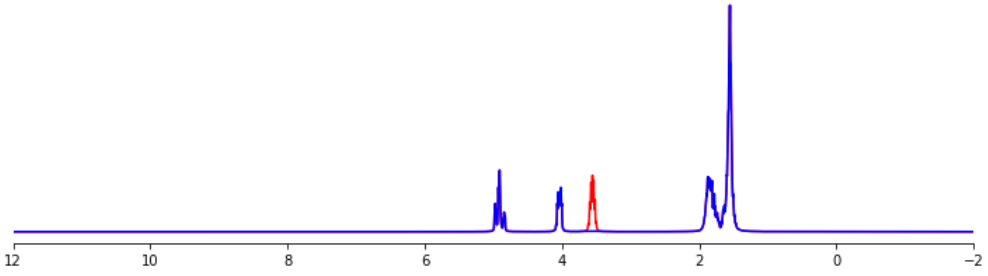
Top predicted substructures for the masked region(red):

0.4232 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.3957 CCCCCC
0.3857 [OX2H0][CX4H1][CX4H2][CX4H2]
0.239 [CX4H2]([OX2H0])[CX4H2]
0.1749 [CH2X4](O)[CX4H2]
0.1674 [OX2H1]
0.1485 [#6H2][#8][#6H1]
0.1353 [CX4H2]([CX4H2])[CX4H2]



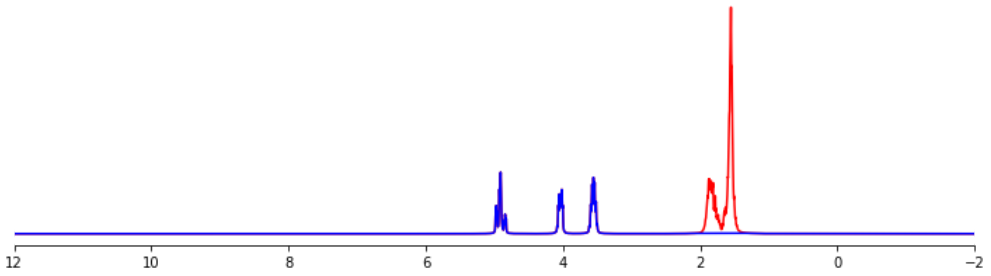
Top predicted substructures for the masked region(red):

0.5661 [CX4H2]([OX2H0])[CX4H2]
0.5079 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.4388 [OX2H0][CX4H2][CX4H2][CX4H2]
0.2733 [OX2H0][CX4H1][CX4H2][CX4H2]
0.2549 CCCCCC
0.2289 [CH2X4](O)[CX4H2]
0.1494 C1OCCC1
0.1454 [#6H2][#8][#6H1]

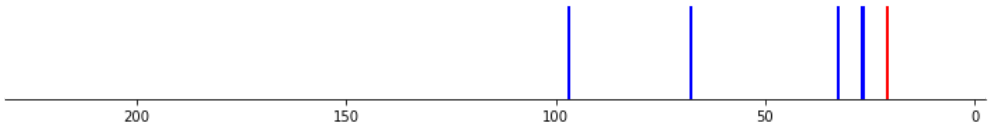


Top predicted substructures for the masked region(red):

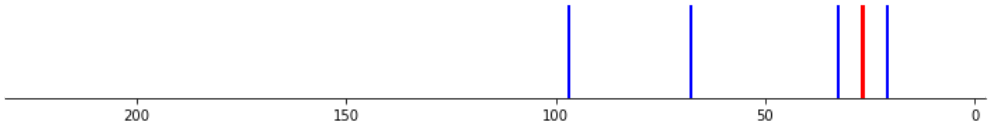
0.5501 [OX2H0][CX4H2][CX4H2][CX4H2]
0.5264 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.2955 [OX2H0][CX4H1][CX4H2][CX4H2]
0.2882 CCCCCC
0.2667 [CX4H2]([OX2H0])[CX4H2]
0.2086 [CX4H2][CX4H2][CX4H2][CX4H2]
0.1888 [#6H2][#8][#6H1]
0.179 [CH2X4](O)[CX4H2]



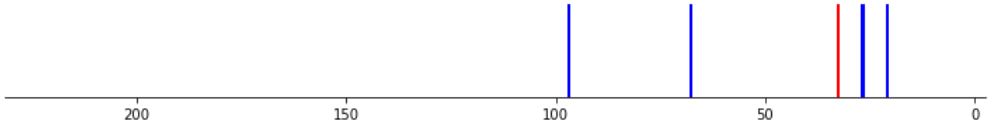
Top predicted substructures for the masked region(red):
0.7312 [OX2H0][CX4H2][CX4H2][CX4H2]
0.5535 [CH2X4](O)[CX4H2][CX4H2]
0.5446 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.5441 CCCCCC
0.5252 [OX2H1]
0.5237 [CX4H2]([CX4H2])[CX4H1]
0.522 [OX2H0][CX4H1][CX4H2][CX4H2]
0.5 [CX4H2]([CX4H2])[CX4H2]



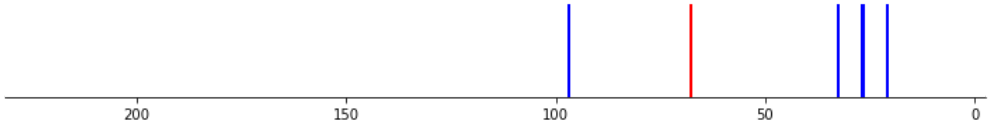
Top predicted substructures for the masked region(red):
0.3977 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.3632 [CX4H3]
0.3245 CCCCCC
0.3159 [OX2H1]
0.2322 [OX2H0][CX4H1][CX4H2][CX4H2]
0.2254 [OX2H0][CX4H2][CX4H2][CX4H2]
0.136 [OH][CX4H]
0.127 [#8][#6H0][#6H1]



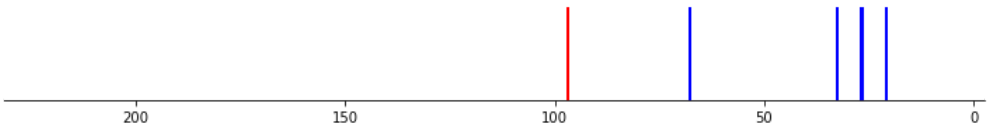
Top predicted substructures for the masked region(red):
0.4901 [OX2H0][CX4H2][CX4H2][CX4H2]
0.4714 CCCCCC
0.3889 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.3644 [CX4H2][CX4H2][CX4H2][CX4H2]
0.3372 [OX2H1]
0.2134 [CH2X4](O)[CX4H2][CX4H2]
0.2003 [OX2H0][CX4H1][CX4H2][CX4H2]
0.1821 [CX4H2]([CX4H2])[CX4H2]



Top predicted substructures for the masked region(red):
0.4748 CCCCCC
0.4453 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.3246 [OX2H0][CX4H1][CX4H2][CX4H2]
0.3103 [OX2H1]
0.2703 [OX2H0][CX4H2][CX4H2][CX4H2]
0.2609 [CX4H2]([OX2H0])[CX4H2]
0.1912 [CH2X4](O)[CX4H2][CX4H2]
0.1898 [CX4H2][CX4H2][CX4H2][CX4H2]

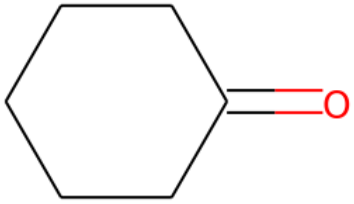


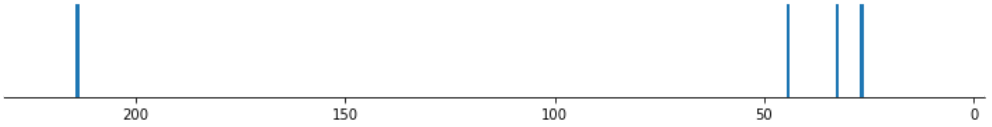
Top predicted substructures for the masked region(red):
0.8816 [CX4H2]([OX2H0])[CX4H2]
0.5822 [OX2H0][CX4H2][CX4H2][CX4H2]
0.5617 [CH2X4](O)[CX4H2]
0.5482 [CX4H2]([#6])[O]
0.4486 [CH2X4](O)[CX4H2][CX4H2]
0.4372 CCCCCC
0.3749 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.271 [#6H2][#8][#6H1]

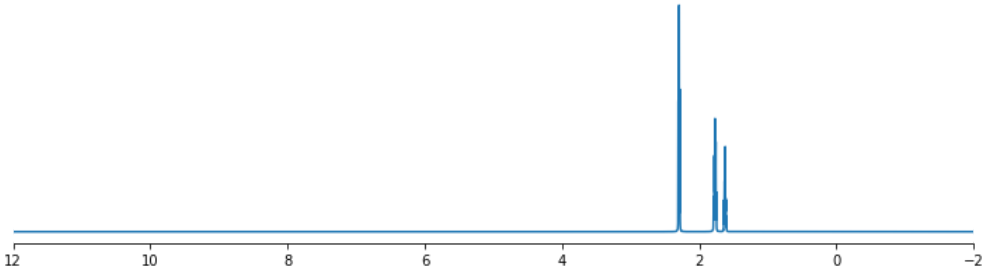


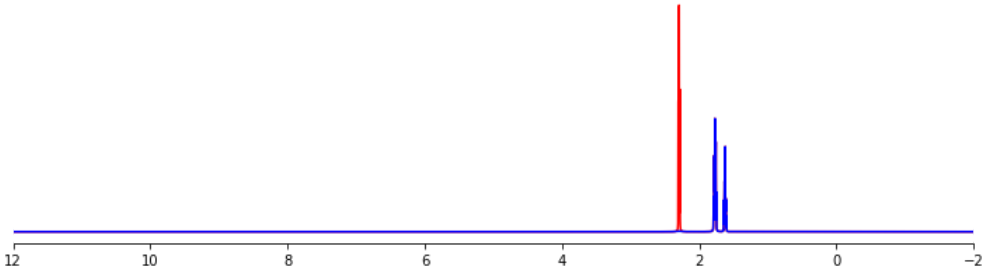
Top predicted substructures for the masked region(red):
0.6256 [CX4H2]([OX2H0])[CX4H2]
0.6163 [CX4H1]([OX2H0])([OX2H0])[CX4H2]
0.4865 [OX2H0][CX4H1][CX4H2][CX4H2]
0.4484 [OX2H0][CX4H2][CX4H2][CX4H2]
0.3342 [#6H2][#8][#6H1]
0.3075 [CH2X4](O)[CX4H2]
0.2675 [OX2H0][CX4H1][OX2H0]
0.2263 [CX4H3]

True structure: O=C1CCCCC1

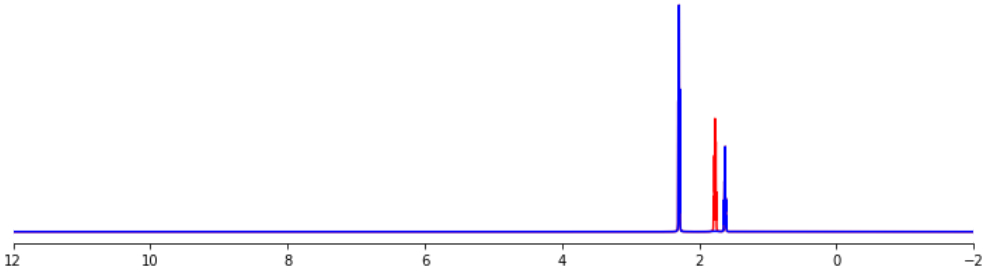






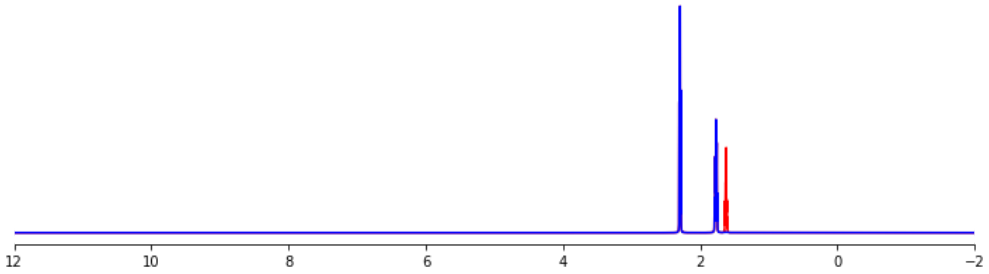


Top predicted substructures for the masked region(red):
0.8082 [CX3H0](=[OX1H0])([CX4H2])[CX4H2]
0.4461 [#6H2][#6X3H0][#6H2]
0.202 [CX4H2][CX3]=O
0.1899 [#6]1[#6][#6][#6][#6]1
0.1553 [#6H1]
0.1155 [CX4H2]([CX4H2])[CX4H1]
0.1067 [CX4H2]([CX4H2])[CX3H0]
0.0976 [#6H2][#6H1][#6H1][#6H2]

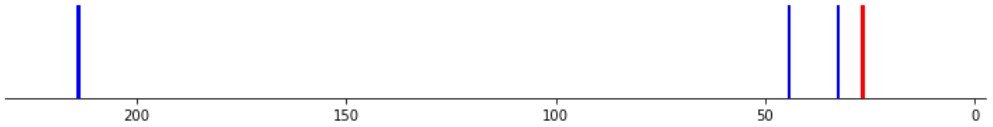


Top predicted substructures for the masked region(red):
0.2406 [#6]1[#6][#6][#6][#6]1
0.2283 [#6H2][#6X3H0][#6H2]

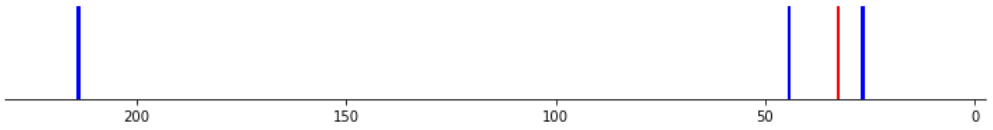
0.2078 C1CCCC1
0.1984 [CX4H2]([CX4H2])[CX4H1]
0.1892 [CX3H0](=[OX1H0])([CX4H2])[CX4H2]
0.1646 [#6H1]
0.1074 [#6H1]([#6H2])[#6H2]
0.0938 [#6H2][#6H1][#6H1][#6H2]



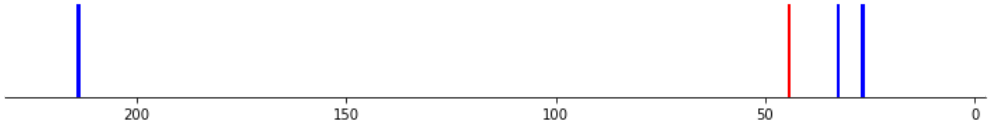
Top predicted substructures for the masked region(red):
0.2525 [#6]1[#6][#6][#6][#6]1
0.2357 [#6H1]
0.22 [CX3H0](=[OX1H0])([CX4H2])[CX4H2]
0.2162 C1CCCC1
0.2029 [CX4H2]([CX4H2])[CX4H1]
0.2023 [#6H2][#6X3H0][#6H2]
0.103 [#6H1]([#6H2])[#6H2]
0.0989 CCCCCC



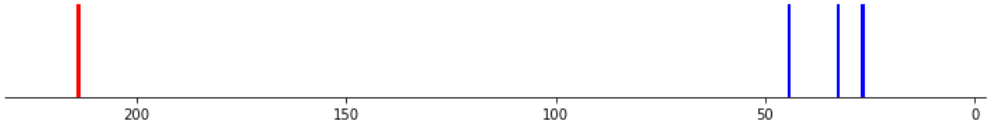
Top predicted substructures for the masked region(red):
0.2716 [CX4H2]([CX4H2])[CX4H2]
0.2306 [#6]1[#6][#6][#6][#6]1
0.147 [CX4H2][CX4H2][CX4H2][CX4H2]
0.1174 [CX3H0](=[OX1H0])([CX4H2])[CX4H2]
0.0969 CCCCCC
0.0964 [CX4H2]([CX4H2])[CX4H1]
0.0955 [#6H2][#6H1][#6H1][#6H2]
0.0923 [#6H2][#6X3H0][#6H2]



Top predicted substructures for the masked region(red):
0.2244 [#6]1[#6][#6][#6][#6]1
0.206 [CX3H0](=[OX1H0])([CX4H2])[CX4H2]
0.1298 [#6H2][#6X3H0][#6H2]
0.1199 [CX4H2]([CX4H2])[CX4H1]
0.1077 C1CCCC1
0.0886 [#6H2][#6H1][#6H1][#6H2]
0.0825 CCCCCC
0.0791 [CX4H2]([CX4H2])[CX4H2]



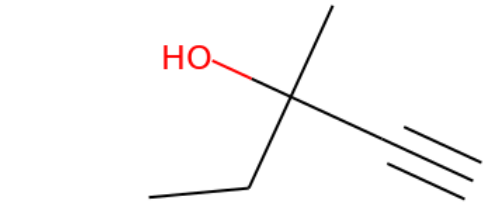
Top predicted substructures for the masked region(red):
0.7314 [CX3H0](=[OX1H0])([CX4H2])[CX4H2]
0.3294 [#6H2][#6X3H0][#6H2]
0.2396 [#6]1[#6][#6][#6][#6]1
0.1875 C1CCCC1
0.186 [OX1H0]=[CX3H0]([#6])[CX4H2]
0.1847 [CX4H2][CX3]=O
0.1076 [#6H1]([#6H2])[#6H2]
0.1056 CCCCCC

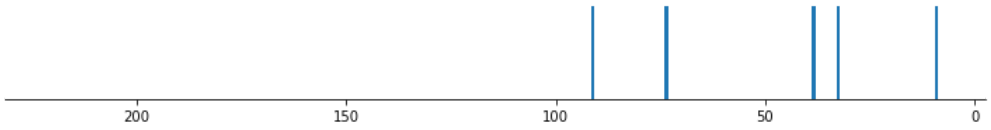


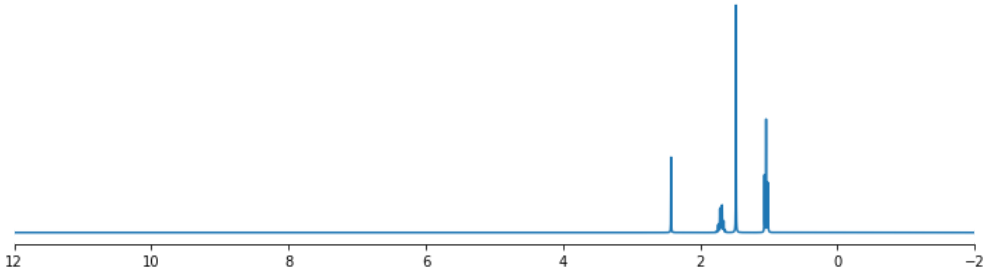
Top predicted substructures for the masked region(red):
0.9967 [OX1H0]=[CX3H0]([#6])[CX4H2]
0.9959 [CX3](=[OX1])C
0.9943 [CX4H2]([CX4H2])[CX3H0]

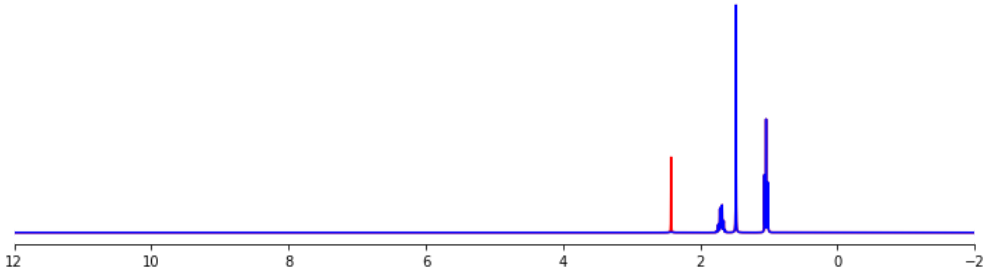
0.9683 O=[CX3H0][CX4H2][CX4H2]
0.9651 [CX4H2][CX3]=O
0.9614 [#6H2][#6X3H0][#6H2]
0.9581 [CX4H2]CC=O
0.9446 [CX3H0](=[OX1H0])([CX4H2])[CX4H2]

True structure: C#CC(C)(O)CC

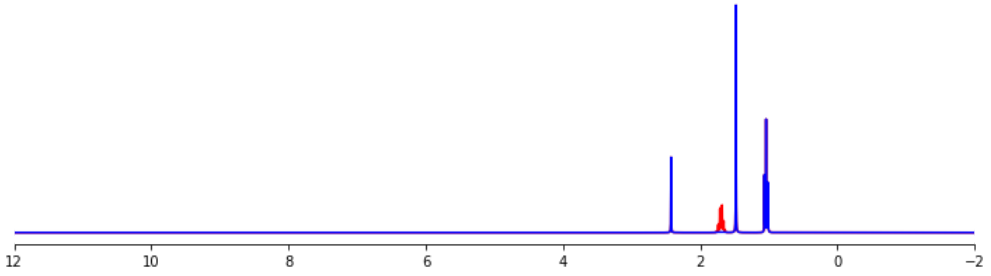




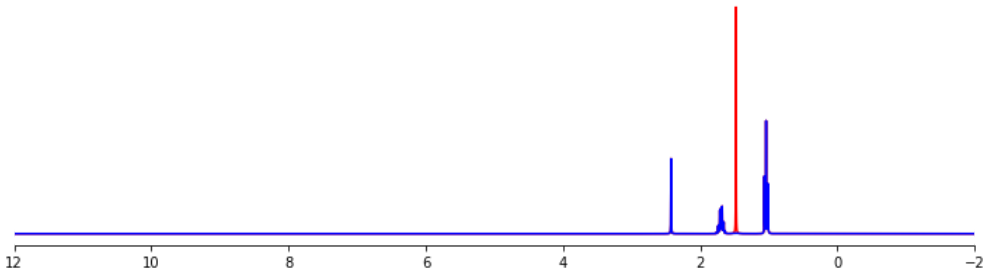




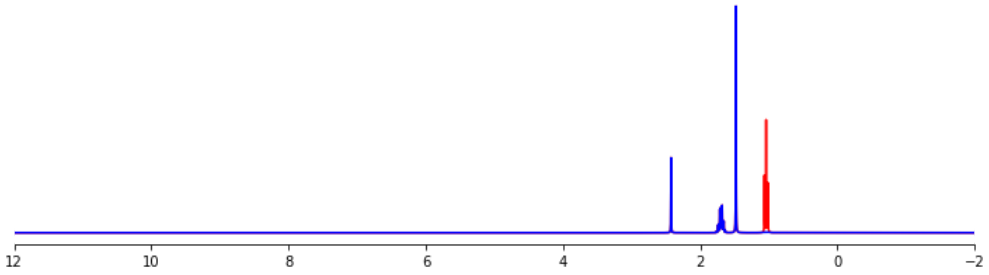
Top predicted substructures for the masked region(red):
0.4905 CCCCCC
0.406 [#6]1[#6][#6][#6][#6]1
0.3819 [#8][#6H0][#6H1]
0.2728 C1CCCC1
0.257 [CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]
0.1976 [CH3][#6][#8]
0.1709 [#6X2][#6X4H1]
0.1631 [#6H3][#6][#6][#6H3]



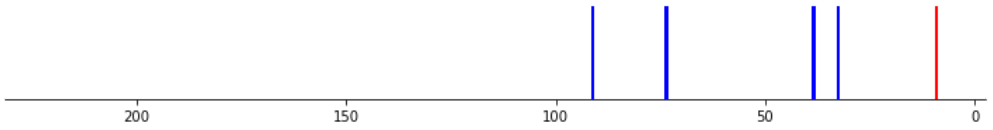
Top predicted substructures for the masked region(red):
0.734 CCCCCC
0.5801 [#8][#6H0][#6H1]
0.463 OCC[CH2]
0.4618 [#6]1[#6][#6][#6][#6]1
0.457 C1CCCC1
0.3693 [CX4H2]([#6])[#6]
0.2486 [CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]
0.2227 [#6]1[#6][#6][#6][#6][#6]1



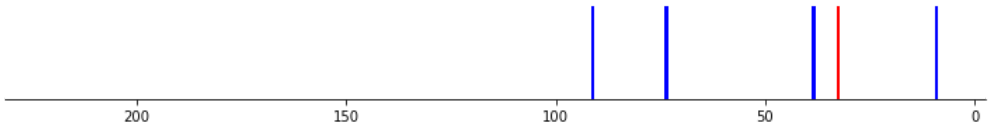
Top predicted substructures for the masked region(red):
0.9059 [CX4H3][CX4]O
0.9043 [CH3][#6][#8]
0.7998 [OX2H1][CX4H0][CX4H3]
0.7007 [#8][#6H0][#6H1]
0.6616 [#6X4H3][#6][#8H]
0.5538 CCCCCC
0.5426 [CX4H3][CX4H0]
0.504 [#6H3][#6][#6][#6H3]



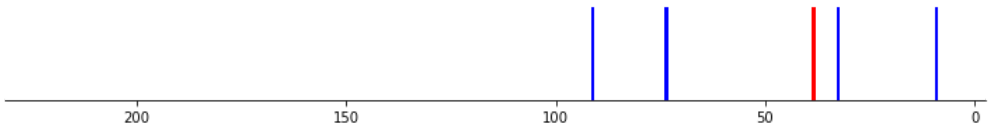
Top predicted substructures for the masked region(red):
0.7446 CCCCCC
0.7325 [#8][#6H0][#6H1]
0.4389 [#6H3][#6][#6][#6H3]
0.4362 [#6]1[#6][#6][#6][#6]1
0.4104 C1CCCC1
0.3445 C1CC1
0.283 [CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]
0.2479 [#6H1]



Top predicted substructures for the masked region(red):
0.5625 [#8][#6H0][#6H1]
0.5335 [#6H3][#6][#6][#6H3]
0.5072 [OX2H1][CX4H0][CX4H2][CX4H3]
0.4405 CCCCCC
0.2978 [#6]1[#6][#6][#6][#6]1
0.2835 C1CC1
0.2372 C1CCCC1
0.2353 [CH3][#6][#8]

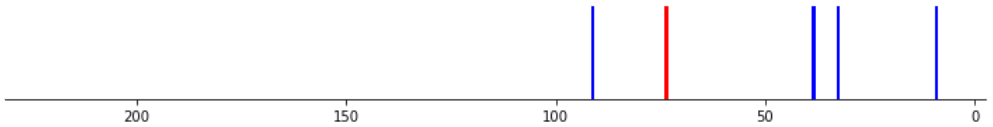


Top predicted substructures for the masked region(red):
0.5627 CCCCCC
0.4654 [#8][#6H0][#6H1]
0.4332 [#6]1[#6][#6][#6][#6]1
0.3548 C1CCCC1
0.3357 [#6H3][#6][#6][#6H3]
0.2629 [CH3][#6][#8]
0.2574 [CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]
0.1777 [#6]1[#6][#6][#6][#6][#6]1

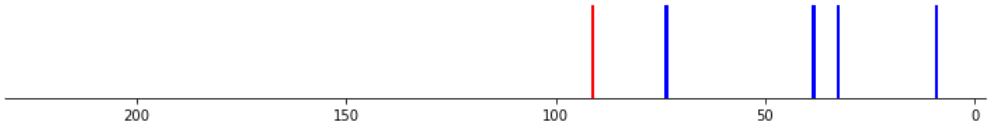


Top predicted substructures for the masked region(red):
0.7153 CCCCCC
0.4627 [#8][#6H0][#6H1]
0.4569 [#6]1[#6][#6][#6][#6]1

0.4248 C1CCCC1
0.2431 [CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]
0.2389 [#6H3][#6][#6][#6H3]
0.2175 [#6]1[#6][#6][#6][#6][#6]1
0.2068 [CH3][#6][#8]

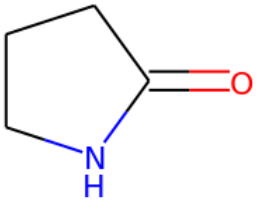


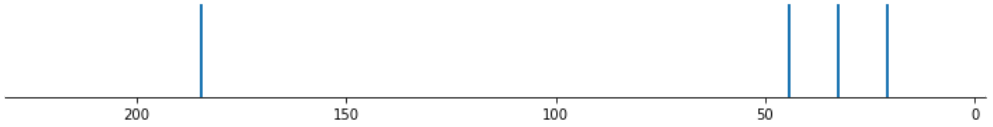
Top predicted substructures for the masked region(red):
0.5363 [#8][#6H0][#6H1]
0.3571 [$([CX2]#C)]
0.3494 [#6X4H3][#6][#8H]
0.3491 [CH3][#6][#8]
0.3356 [OX2H1][CX4H0][CX4H3]
0.3299 [OX2H1]
0.3071 C1CCCC1
0.3007 [#6]1[#6][#6][#6][#6]1

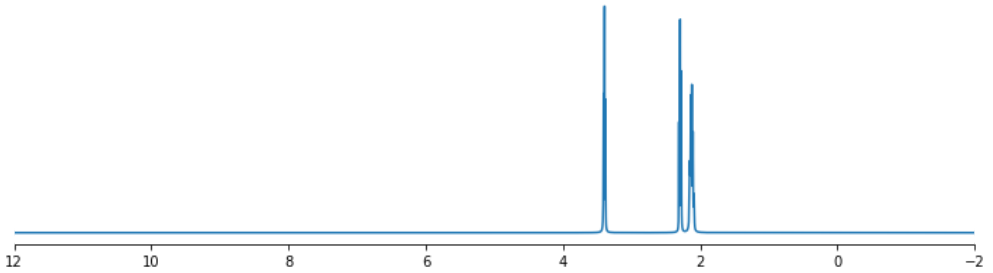


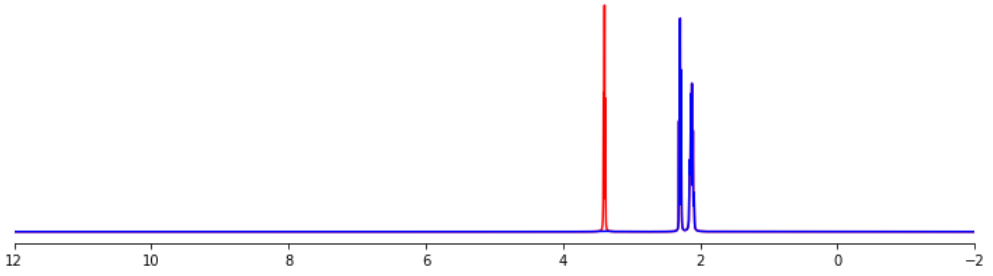
Top predicted substructures for the masked region(red):
0.4574 [$([CX2]#C)]
0.3397 [#6H3][#6][#6][#6H3]
0.309 [#8][#6H0][#6H1]
0.2708 [#6X2][#6X4H1]
0.2572 [CH3][#6][#8]
0.253 [CX4H0]([OX2H1])([CX4H3])([CX4H2])[CX4H1]
0.2355 [#6]1[#6][#6][#6][#6]1
0.2183 [#6X4H3][#6][#8H]

True structure: O=C1CCCN1



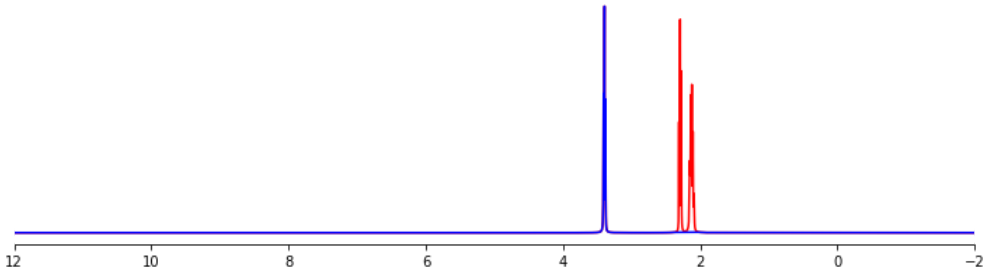




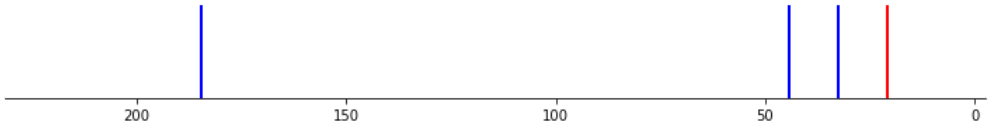


Top predicted substructures for the masked region(red):
0.7286 [#7X3][#6H2]
0.6634 [#6H2][#7][#6X3]
0.5113 [#7][#6H2]

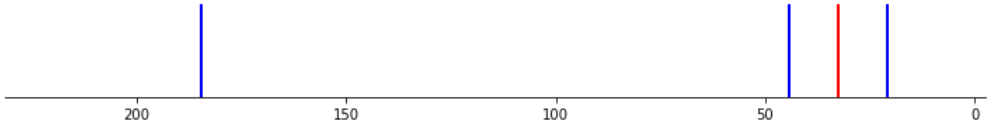
0.3684 [CX4H2]([NX3H1])[CX4H2]
0.3278 [#6]1[#6][#6][#6][#7]1
0.2909 [#7][#6H2][#6H2]
0.2222 CCCCCC
0.2206 [#7][#6][#6][#6X3]



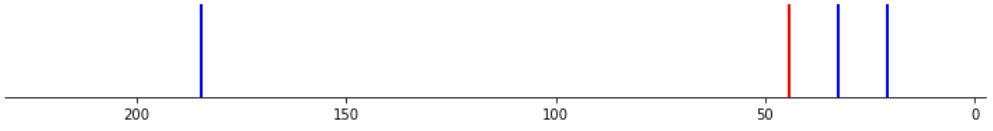
Top predicted substructures for the masked region(red):
0.4816 [CX4H2]([CX4H2])[CX4H2]
0.4713 O=[CX3H0][CX4H2][CX4H2]
0.4167 [CX4H2]([#6])[#6]
0.3873 [CX4H2]([CX4H2])[CX3H0]
0.3802 [CX4H2]CC=O
0.2942 CCCCCC
0.2937 [CX4H2][CX4H2]
0.2578 [#7X3H2]



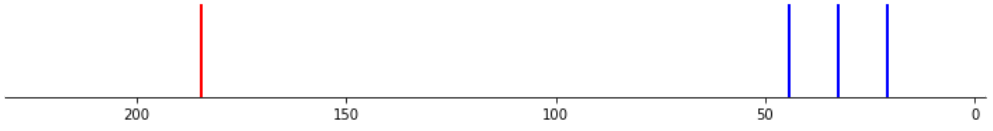
Top predicted substructures for the masked region(red):
0.3909 [CX4H2]([CX4H2])[CX4H2]
0.2716 [OX2H1]
0.2585 CCCCCC
0.1979 [#7][#6][#6][#6X3]
0.1847 [#7][#6][#6X3]
0.1502 [CX4H2][CX4H2]
0.1464 [#6H2][#7][#6X3]
0.1203 [CX4H2]CC=O



Top predicted substructures for the masked region(red):
0.3353 O=[CX3H0][CX4H2][CX4H2]
0.2751 CCCCCC
0.2623 [#6H2][#7][#6X3]
0.2456 [CX4H2]([CX4H2])[CX3H0]
0.2106 [OX2H1]
0.1965 [CX4H2]CC=O
0.1953 [#7][#6][#6][#6X3]
0.1763 [CX4H2][CX4H2]



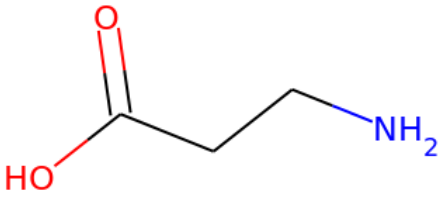
Top predicted substructures for the masked region(red):
0.4532 [#6H2][#7][#6X3]
0.3507 [CX4H2]([NX3H1])[CX4H2]
0.281 CCCCCC
0.267 [#7][#6H2][#6H2]
0.2499 [#7][#6][#6][#6X3]
0.2288 [#7X3H1]
0.202 O=[CX3H0][CX4H2][CX4H2]
0.1727 [OX2H1]

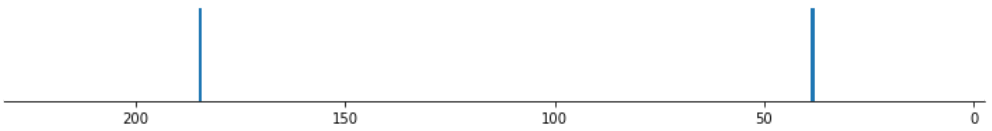


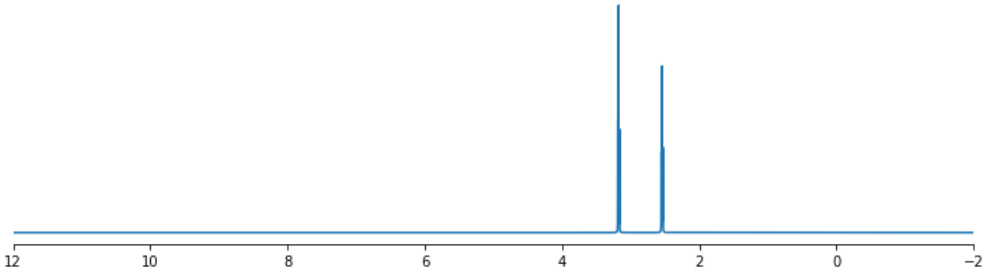
Top predicted substructures for the masked region(red):
0.9732 [CX3](=[OX1])C
0.8865 [CX4H2]CC=O
0.8137 O=[CX3H0][CX4H2][CX4H2]
0.7753 [#6H2][#7][#6X3]

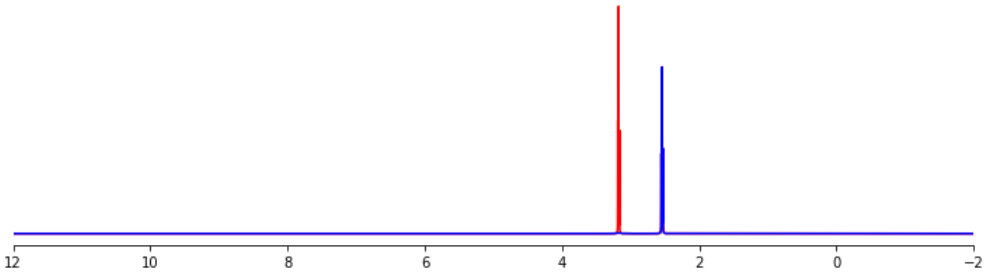
0.6907 [CX4H2]([CX4H2])[CX3H0]
0.6488 [CX4H2][CX3]=O
0.6277 [CX4H2]([CX4H2])[CX4H2]
0.3721 O=[CX3][CX4H]

True structure: NCCC(=O)O

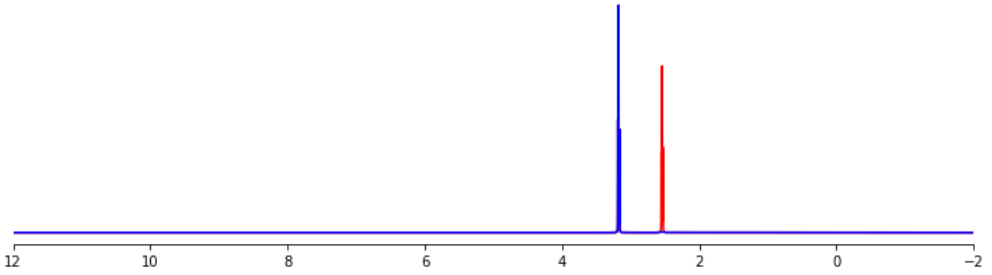




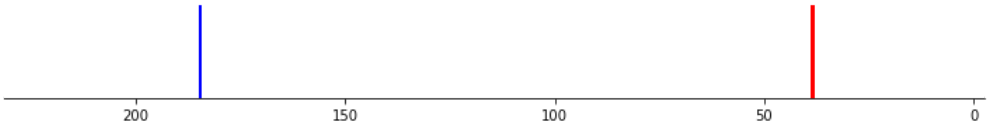




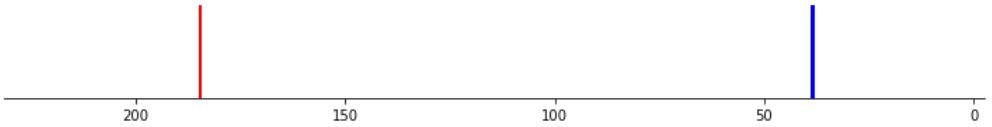
Top predicted substructures for the masked region(red):
0.8041 [#7][#6H2]
0.6775 [#7X3][#6H2]
0.5725 [#7H2][#6H2]
0.448 [CX4H2]([NX3H2])[CX4H2]
0.4426 [#7][#6H2][#6H2]
0.3882 [#7][#6][#6][#6X3]
0.2587 [#7X3H2]
0.2415 [CX4H2][CX4H2]



Top predicted substructures for the masked region(red):
0.5643 [CX4H2]([CX4H2])[CX3H0]
0.4864 [CX4H2][CX4H2]
0.4515 O=[CX3H0][CX4H2][CX4H2]
0.4206 [CX4H2]([NX3H2])[CX4H2]
0.3809 OCC[CH2]
0.3103 [CX4H2]([#6])[#6]
0.2987 [CX4H2]CC=O
0.266 [#7][#6][#6][#6X3]

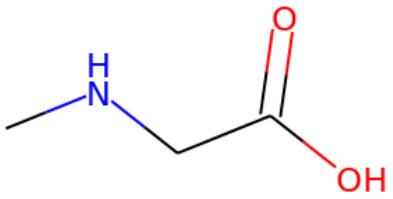


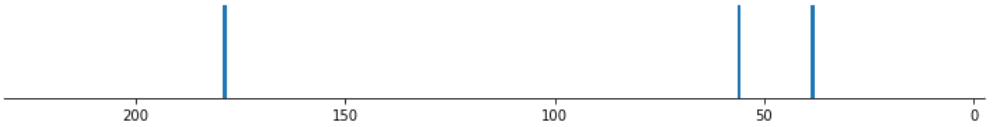
Top predicted substructures for the masked region(red):
0.6807 [CX4H2]([CX4H2])[CX3H0]
0.6578 [#7][#6H2]
0.5421 [CX4H2][CX4H2]
0.5348 [#7X3][#6H2]
0.4833 [CX4H2]([NX3H2])[CX4H2]
0.4781 [#7H2][#6H2]
0.4524 O=[CX3H0][CX4H2][CX4H2]
0.4162 [CX4H2]([#6])[#6]

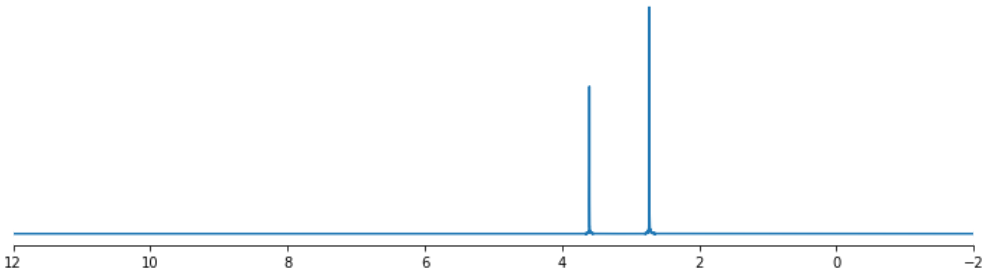


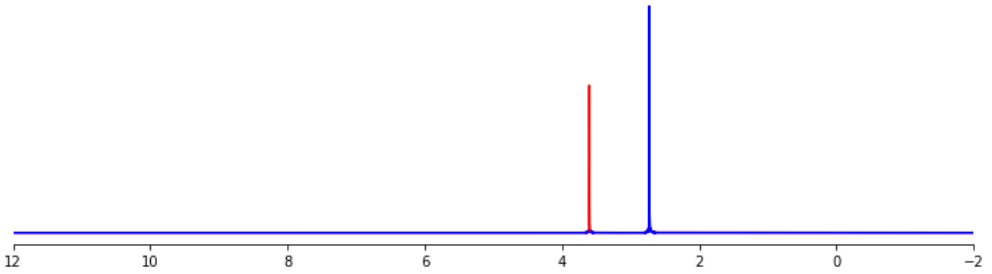
Top predicted substructures for the masked region(red):
0.9809 [CX4H2]([CX4H2])[CX3H0]
0.9696 [CX3](=[OX1])C
0.9647 [CX4H2]CC=O
0.9582 O=[CX3H0][CX4H2][CX4H2]
0.8997 [CX3](=O)[OX2H1]
0.8179 [CX4H2][CX3]=O
0.7277 [CX4H2][CX4H2]
0.6957 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]

True structure: CNCC(=O)O

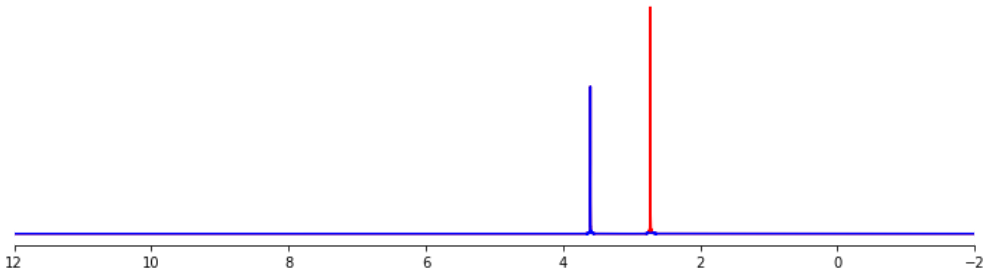




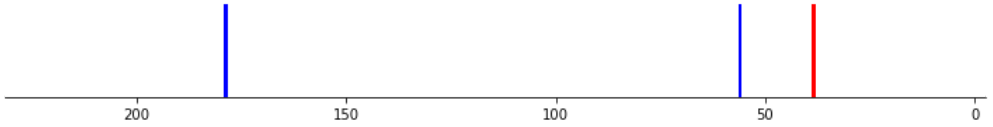




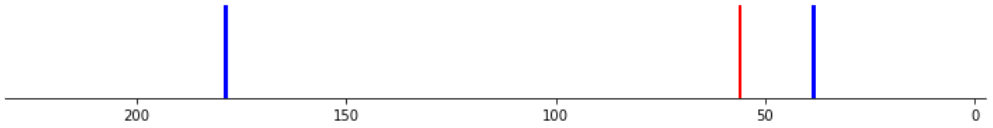
Top predicted substructures for the masked region(red):
0.602 [#7X3][#6H2]
0.4822 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.4779 [#7][#6H2]
0.3228 [#7][#6][#6X3]
0.2669 [OX1H0]=[CX3H0][OX2H0][CX4H3]
0.2437 [#8][#6][#6H2]
0.2405 [OX2H0][CX3H0][CX4H2]
0.2103 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]



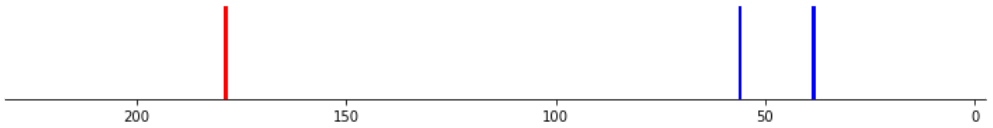
Top predicted substructures for the masked region(red):
0.8252 [#7X3][#6H3]
0.5781 [#6H3][#7]
0.5752 [CX4H3][NX3H1]
0.4211 [#6H3][#7][#6H2]
0.4081 [#7X3H1]
0.4044 [#6H3][#7][#6X3]
0.3159 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.3008 [CX4H3][NX3H0]



Top predicted substructures for the masked region(red):
0.63 [CX4H3][NX3H1]
0.444 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.4213 [#6H3][#7]
0.3516 O=[CX3H0][CX4H2][CX4H2]
0.3383 [CX4H2]([#6])[#6]
0.2971 [#6H3][#7][#6X3]
0.2779 [CX4H2][CX4H2]
0.2631 [OX1H0]=[CX3H0]([#8])[CX4H2]

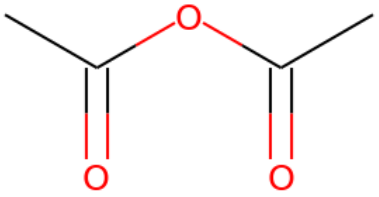


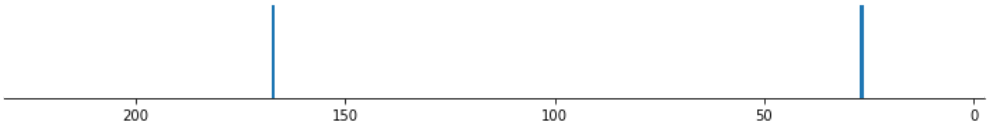
Top predicted substructures for the masked region(red):
0.4268 [OX1H0]=[CX3H0][OX2H0][CX4H3]
0.3372 [CX4H3][NX3H1]
0.33 [#7][#6H2]
0.3227 [#6H3][#7][#6H2]
0.2697 [#7X3H1]
0.2555 [#7][#6][#6][#6X3]
0.2383 [CX4H3][OX2H0]
0.2275 [OX2H0][CX3H0][CX4H2]

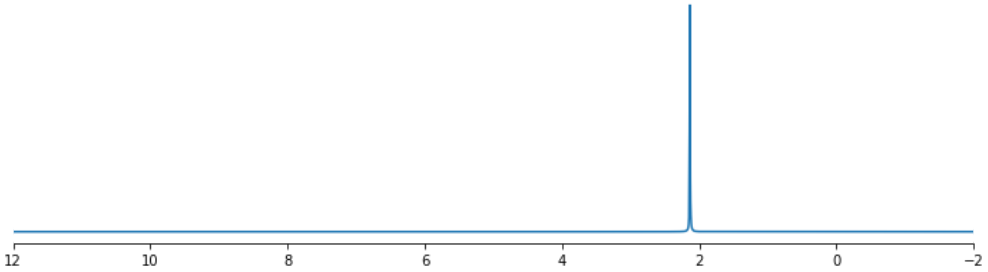


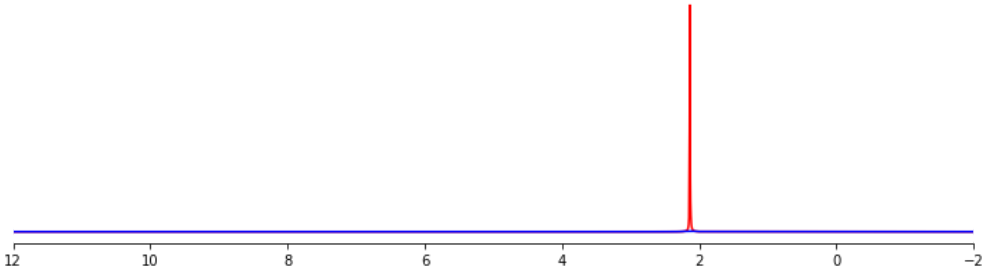
Top predicted substructures for the masked region(red):
0.9784 [CX3](=[OX1])C
0.8634 [CX3](=[OX1])O
0.8617 [#8]=[#6][#8]
0.8315 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.8211 [CX4H2][CX3]=O
0.7521 [CX3H0](=[OX1H0])([OX2H1])[CX4H2]
0.5905 [#7][#6][#6X3]
0.5296 [CX3](=O)[OX2H1]

True structure: CC(=O)OC(C)=O

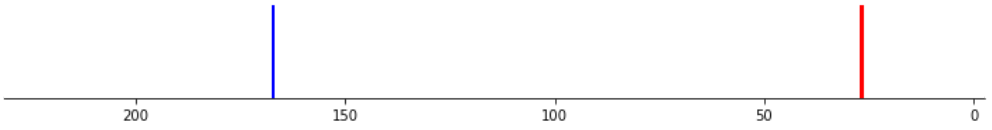




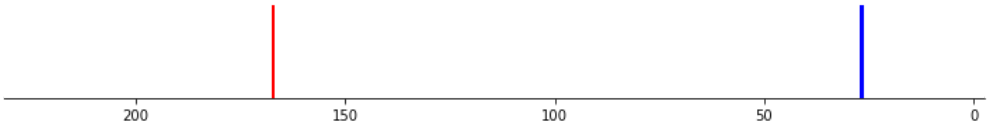




Top predicted substructures for the masked region(red):
0.6946 [CX4H2][CX4H2]
0.671 [CX4H2]([#6])[#6]
0.5742 [CX4H2]([CX4H2])[CX3H0]
0.5359 [CX4H2]([CX4H2])[CX4H2]
0.5208 O=[CX3H0][CX4H2][CX4H2]
0.5202 [#6H3][#6H0]
0.4011 OCC[CH2]
0.3638 [#8][#6][#6H2]

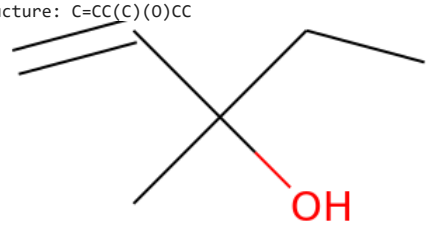


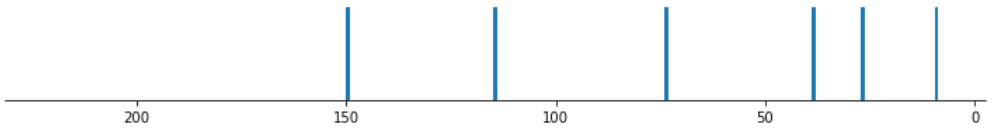
Top predicted substructures for the masked region(red):
0.7349 [CX4H2]([CX4H2])[CX4H2]
0.6429 [CX4H2][CX4H2]
0.5567 [CX4H2]([#6])[#6]
0.5261 O=[CX3H0][CX4H2][CX4H2]
0.4889 [CX4H2]([CX4H2])[CX3H0]
0.3669 [#6H3][#6H0]
0.3045 [CX4H2][CX4H2][CX4H2][CX4H2]
0.2996 [CX3H0](=[OX1H0])([OX2H1])[CX3H0]

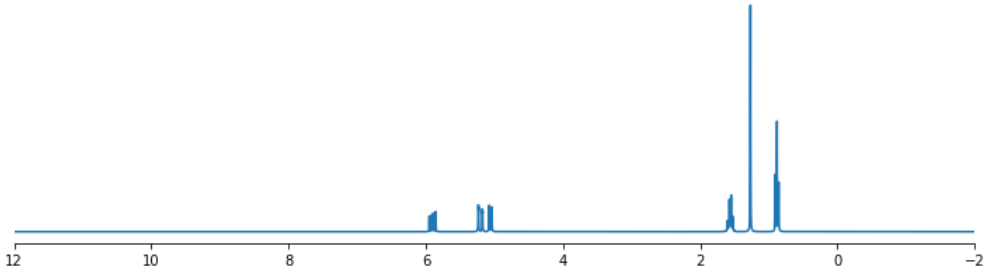


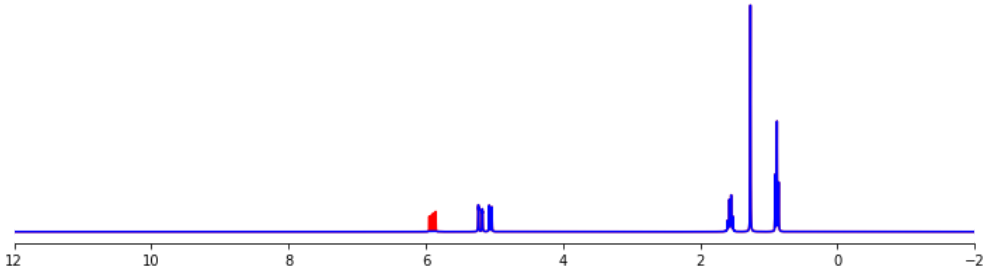
Top predicted substructures for the masked region(red):
0.8688 [CX3](=[OX1])C
0.8655 [CX3](=O)[OX2H1]
0.8618 [CX3](=[OX1])O
0.7548 [#8]=[#6][#8]
0.6319 [CX4H2]([CX4H2])[CX3H0]
0.5688 O=[CX3H0][CX4H2][CX4H2]
0.5211 [#6H3][#6H0]
0.5112 [CX4H2][CX4H2]

True structure: C=CC(C)(O)CC

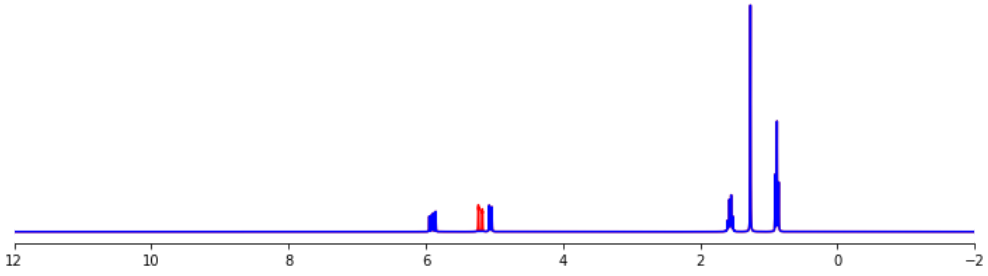




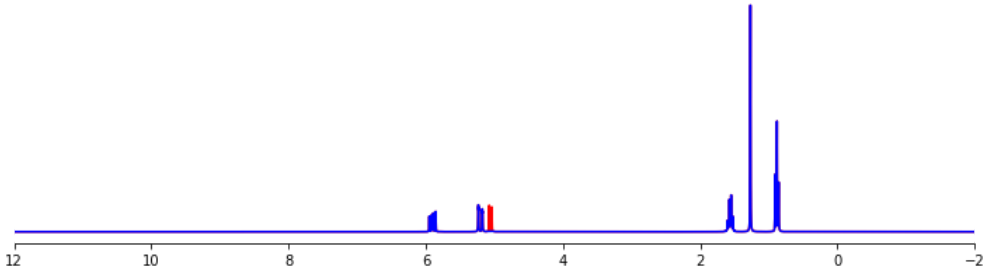




Top predicted substructures for the masked region(red):
0.4282 [CHX4]([CH3X4])[CH2X4]
0.4053 CCCCC=C
0.3668 [CHX3](=C)C
0.3247 [CX3H2]=[CX3H1]
0.2918 [CX3H2]=[CX3H1][CX4H0][OX2H1]
0.2001 [CX4H]O
0.1772 [CX4H3][CX4H1]
0.1608 [OX2H1][CX4H0][CX4H2][CX4H3]

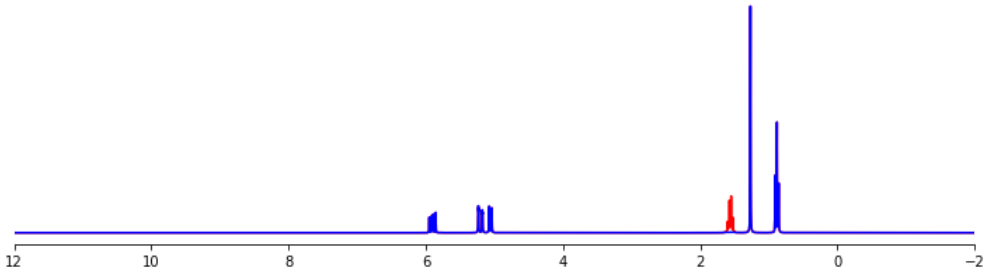


Top predicted substructures for the masked region(red):
0.3384 [CX4H]O
0.3241 CCCCC=C
0.2617 [CHX4]([CH3X4])[CH2X4]
0.2363 [CX3H2]=[CX3H1][CX4H0][OX2H1]
0.2259 [CX4H3][CX4H1]
0.2051 [OH][CX4H]
0.204 OCC[CH2]
0.1432 [CH2X3](=C)

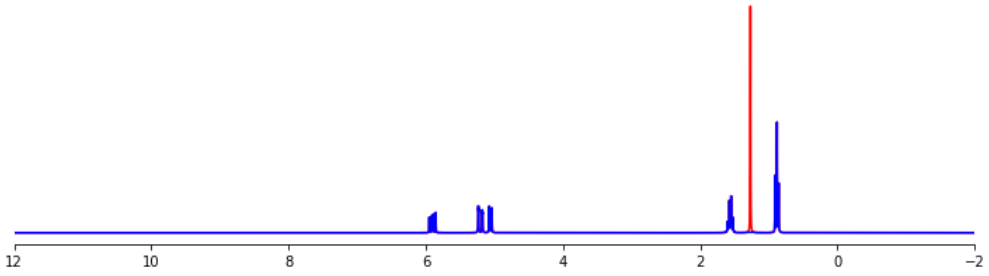


Top predicted substructures for the masked region(red):
0.3358 CCCCC=C
0.3329 [CX4H]O
0.288 [CHX4]([CH3X4])[CH2X4]
0.2326 [CX4H3][CX4H1]
0.1998 OCC[CH2]
0.1242 [CH3]CC[OH]
0.1211 [CH3][#6][#8]

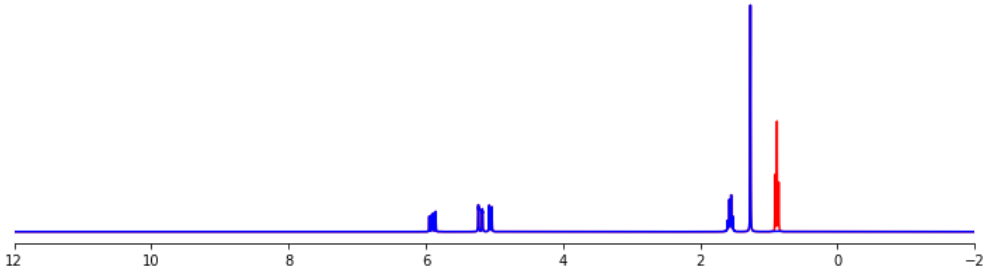
0.1081 [OH][CX4H]



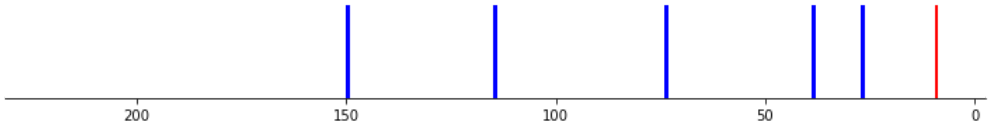
Top predicted substructures for the masked region(red):
0.6575 [CX4H2]([#6])[#6]
0.5378 [CHX4]([CH3X4])[CH2X4]
0.4121 [OX2H1][CX4H0][CX4H2][CX4H3]
0.3793 CCCCC=C
0.3306 [#8][#6][#6H2]
0.2887 [CX4H]O
0.2379 OCC[CH2]
0.1643 [CX4H3][CX4H1]



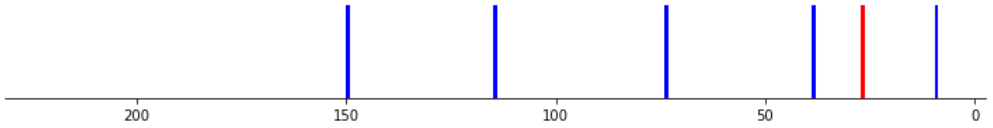
Top predicted substructures for the masked region(red):
0.8547 [CX4H3][CX4]O
0.8464 [#6X4H3][#6][#8H]
0.7512 [CH3][#6][#8]
0.6083 [#6X3]=[#6][#6][#6H3]
0.6041 [OX2H1][CX4H0][CX4H3]
0.5397 [CX4H3][CX4H0]
0.4379 [#6H3][#6][#6X3]
0.4014 [#8][#6H0][#6H1]



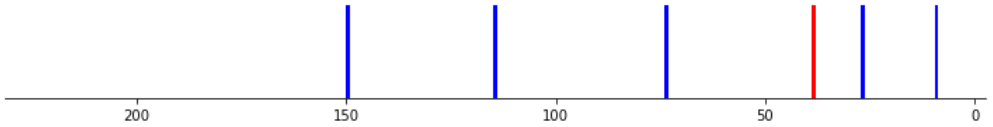
Top predicted substructures for the masked region(red):
0.55 [CHX4]([CH3X4])[CH2X4]
0.4022 [CX4H2]([#6])[#6]
0.3692 CCCCC=C
0.3666 [OX2H1][CX4H0][CX4H2][CX4H3]
0.2799 [CX4H3][CX4H1]
0.2672 [CX4H]O
0.2595 [#8][#6][#6H2]
0.2562 [CH3]CC[OH]



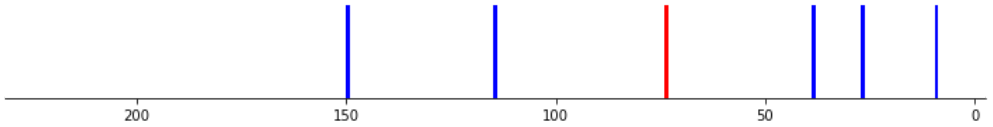
Top predicted substructures for the masked region(red):
0.921 [CX4H3][CX4H2]
0.8843 [CX4H2]([CX4H3])[CX4H0]
0.7237 [OX2H1][CX4H0][CX4H2][CX4H3]
0.614 [#6H3][#6][#6][#6H3]
0.4498 [CH3]CC[OH]
0.371 [#6X3][#6][#6][#6H3]
0.3217 [CX4H2]([#6])[#6]
0.2261 [CX4H]O



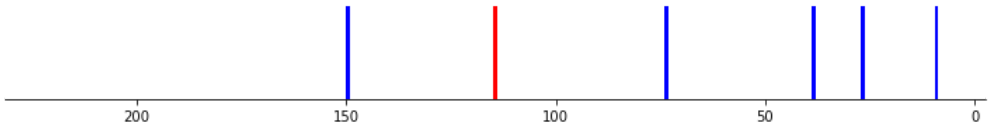
Top predicted substructures for the masked region(red):
0.3791 CCCCC=C
0.2811 [CX4H]O
0.2561 [CX4H3][CX4H1]
0.2332 [CX4H2]([#6])[#6]
0.2323 [CHX4]([CH3X4])[CH2X4]
0.2283 OCC[CH2]
0.2254 [CH3][#6][#8]
0.1815 [#6H3][#6][#6][#6H3]



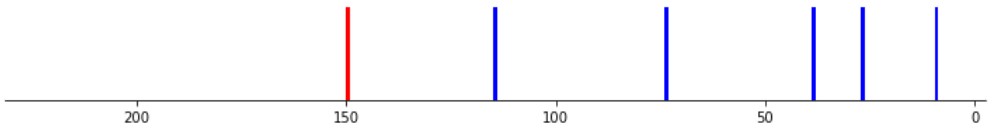
Top predicted substructures for the masked region(red):
0.4419 CCCCC=C
0.4194 [CHX4]([CH3X4])[CH2X4]
0.3501 [OX2H1][CX4H0][CX4H2][CX4H3]
0.2604 [CX4H2]([CX4H3])[CX4H0]
0.2427 [CX4H3][CX4H1]
0.2052 [#8][#6][#6H2]
0.1798 OCC[CH2]
0.1496 CCCCCC



Top predicted substructures for the masked region(red):
0.4708 CCCCC=C
0.4461 [CX4H]O
0.4457 [#6X4H3][#6][#8H]
0.4048 [CHX4]([CH3X4])[CH2X4]
0.3155 [OH][CX4H]
0.3128 [OX2H1][CX4H0][CX4H3]
0.3061 [OX2H1][CX4H0][CX4H2][CX4H3]
0.2947 [CX3H2]=[CX3H1][CX4H0][OX2H1]

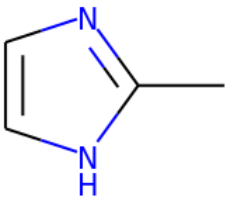


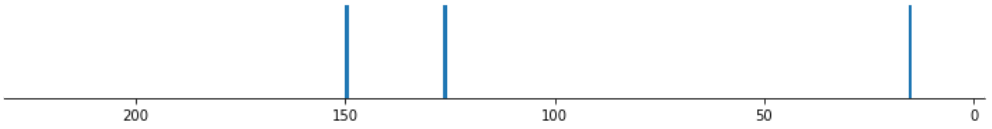
Top predicted substructures for the masked region(red):
0.661 [CX3H1](=[CX3H2])[CX4H0]
0.5374 [CX3H2]=[CX3H1][CX4H0][OX2H1]
0.4105 CCCCC=C
0.3334 [CX3H2]=[CX3H1]
0.3308 [CX4H]O
0.2916 [#6X3H2]
0.2593 [OX2H1][CX4H0][CX4H2][CX4H3]
0.2183 [CHX4]([CH3X4])[CH2X4]

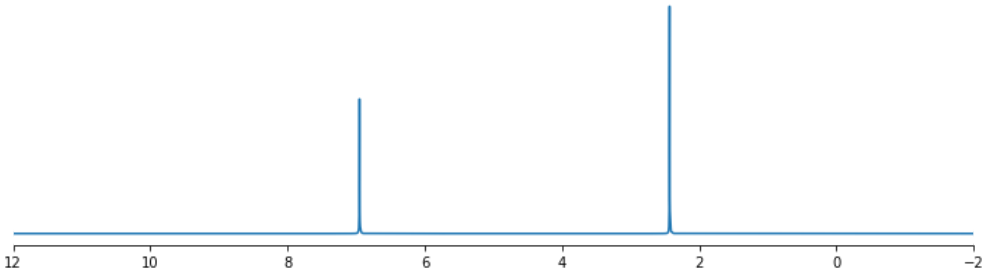


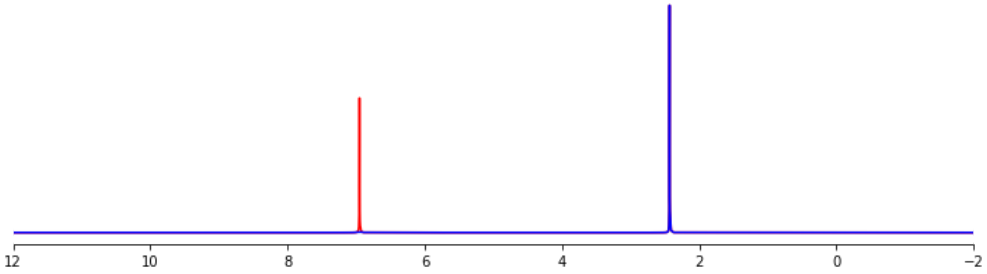
Top predicted substructures for the masked region(red):
0.8787 [#6H3][#6][#6X3]
0.8775 [CX3H1](=[CX3H2])[CX4H0]
0.751 [#6X3]=[#6][#6][#6H3]
0.7059 [CX3H2]=[CX3H1][CX4H0][OX2H1]
0.647 [#8][#6][#6]=[#6X3]
0.5707 [CHX3](=C)C
0.5434 [#6X3][#6][#6][#6H3]
0.4938 CCCCC=C

True structure: Cc1ncc[nH]1

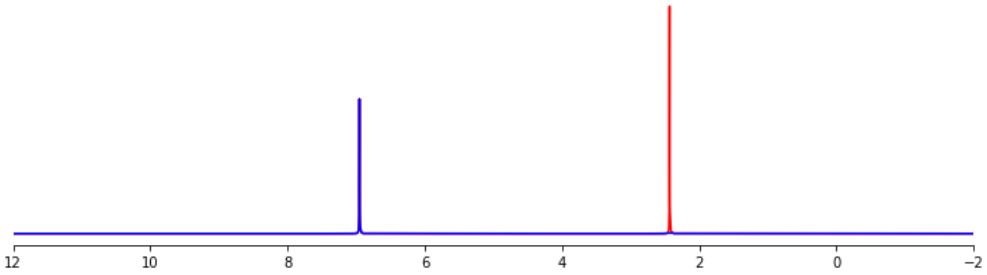




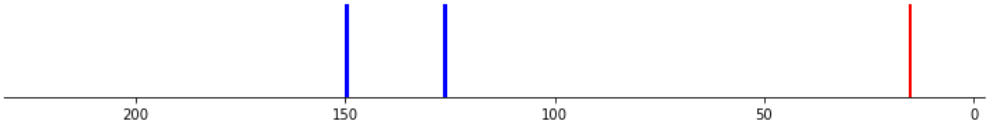




Top predicted substructures for the masked region(red):
0.6685 [#6X3H1][#6X3H0]
0.6531 [#6H1]
0.4817 [#6H1r5][#7]
0.4631 [cH]
0.4534 [#6H3][#6H0][#6H1][#7]
0.4223 [#7][#6X3H0][#6X3H1]
0.3738 [#7][#6H0][#6H1]
0.2984 [#6X3][#6X3][#6X3][#6X3]

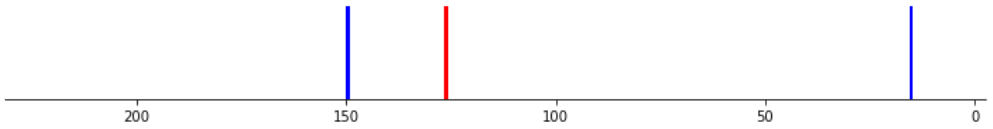


Top predicted substructures for the masked region(red):
0.6319 [#7][#6][#6H3]
0.4568 [#6H3][#6H0]
0.4342 [#6H3][#6][#6]
0.4208 [CX4H3][cX3H0]
0.4086 [#6H3][#6H0][#6H1][#7]
0.2676 [#6X3][#6][#6][#6H3]
0.2363 [#6H3][#6][#6X3]
0.2139 [#6]1[#6][#7][#6][#7]1

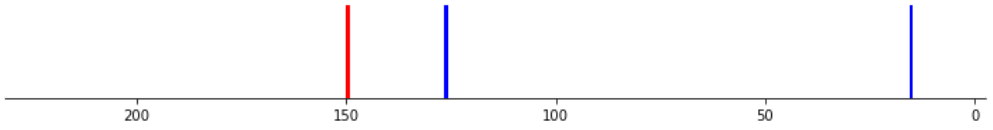


Top predicted substructures for the masked region(red):
0.9936 [CX4H3][#6]
0.9475 [#6H3][#6][#6X3]
0.9392 [#6H3][#6][#6]
0.906 [CX4H3][cX3H0]

0.7525 [#7][#6][#6H3]
0.7277 [#6H3][#6H0]
0.5897 [#6]1[#6][#7][#6][#7]1
0.5893 [#6H3][#6H0][#6H1][#7]

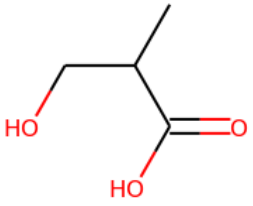


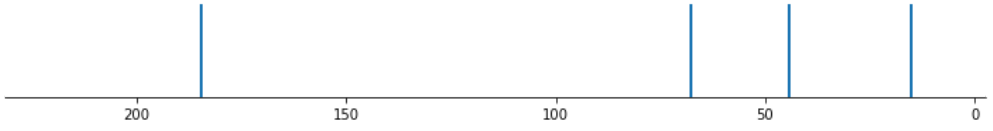
Top predicted substructures for the masked region(red):
0.4034 [cX3H1]([nX3H1])[cX3H0]
0.3785 [#6X3][#6X3][#6X3][#6X3]
0.3039 [#6]1[#6][#7][#6][#7]1
0.3022 [#6H1r5][#7]
0.2658 [#7][#6][#6][#7]
0.2382 [#6X3H1][#6X3H0]
0.228 [#7X3H2]
0.1973 [#7H2][#6H0]

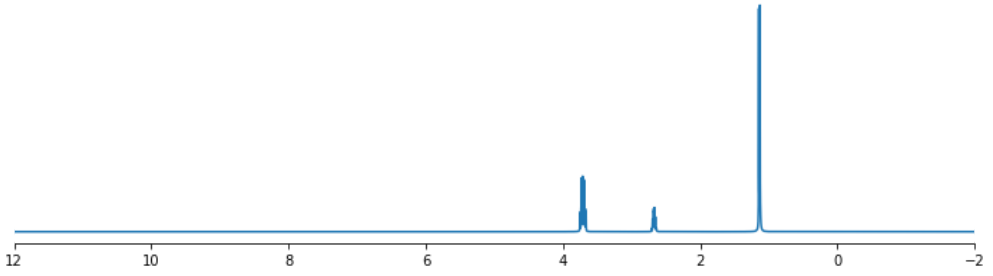


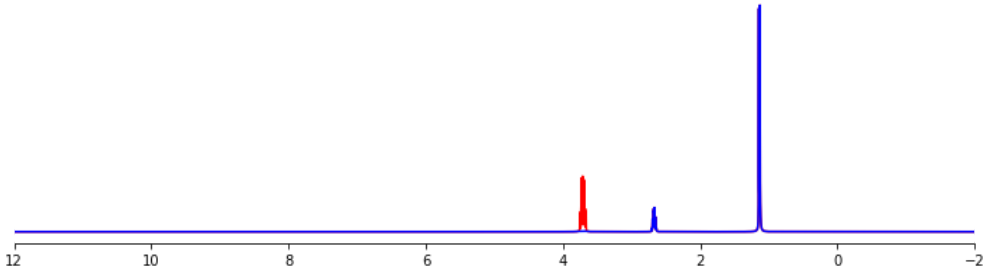
Top predicted substructures for the masked region(red):
0.2717 [#7][#6][#6H3]
0.2681 [cX3H1]([nX3H1])[cX3H0]
0.2405 [#7X3H2]
0.2375 [#7][#6H0][#7]
0.2156 [#6X3][#6X3][#6X3][#6X3]
0.1979 [#7][#6][#7]
0.194 [#7H2][#6H0]
0.1422 [#7][#6H0][#6H1]

True structure: CC(CO)C(=O)O



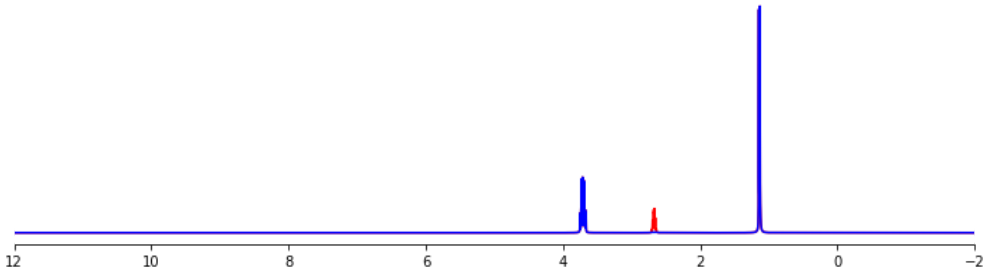




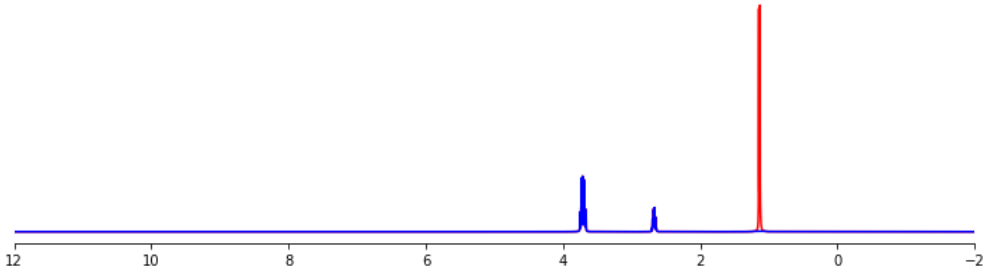


Top predicted substructures for the masked region(red):
0.6432 [CX4H2]([#6])[O]
0.419 [CX4H2](O)[CHX4]
0.3498 [#8H][#6H2][#6H1]
0.3497 [CX4H1]([CX4H3])([CX4H1])[CX3H0]

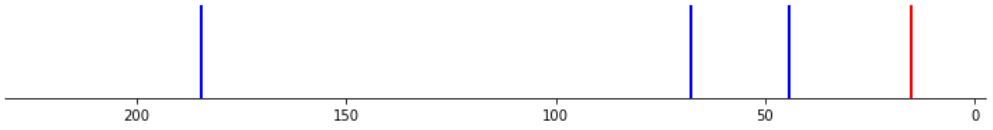
0.3251 [#6H1][#6H1]
0.3137 [CX4H2]([OX2H1])[CX4H1]
0.2169 [#8][#6H1][#6H1][#6H3]
0.2031 [CX4H3][CX4H1][OX2H1]



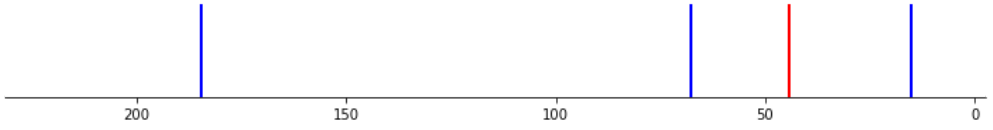
Top predicted substructures for the masked region(red):
0.4409 [#8][#6H1][#6H1][#6H3]
0.3204 [CX4H1]([CX4H3])([CX4H1])[CX3H0]
0.2878 [CX4H3][CX4H1][OX2H1]
0.2828 [#6H1][#6H1]
0.2397 [CX4H2](O)[CHX4]
0.2196 [CX4H1]([OX2H1])([CX4H3])[CX4H1]
0.2187 [#6H3][#6][#6][#6H3]
0.204 [#6H3][#6][#6X3]



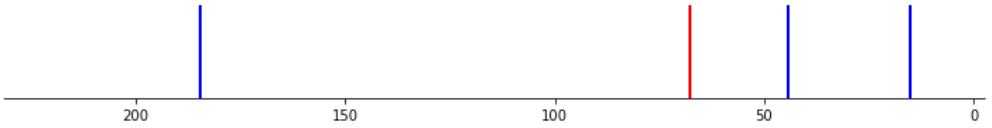
Top predicted substructures for the masked region(red):
0.8676 [#6H1][#6H1]
0.857 [#6H3][#6][#6]
0.8536 [CX4H1]([CX4H3])([CX4H1])[CX3H0]
0.8443 [#8]=[#6][#6H1][#6H1]
0.8147 [CX4H3][CX4H1]
0.7496 [#8][#6H1][#6H1][#6H3]
0.6023 [#6H3][#6][#6X3]
0.5871 [OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H3]



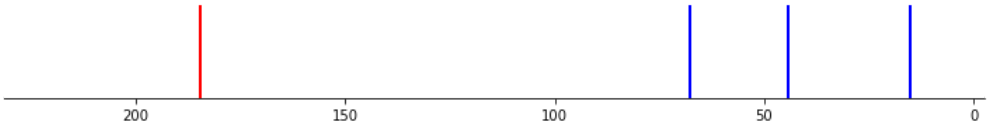
Top predicted substructures for the masked region(red):
0.8404 [CX4H1]([CX4H3])([CX4H1])[CX3H0]
0.7438 [#8][#6H1][#6H1][#6H3]
0.6453 [#6H1][#6H1]
0.6147 [CH3]CC[OH]
0.534 [OX1H0]=[CX3H0][CX4H1]([CX4H1])[CX4H3]
0.47 [#6H3][#6][#6X3]
0.4228 [#6H3][#6][#6][#6H3]
0.3991 [CX4H3][CX4H1]



Top predicted substructures for the masked region(red):
0.6069 [CX4H1]([CX4H3])([CX4H1])[CX3H0]
0.3782 [#6H3][#6][#6][#6H3]
0.3697 [#6H3][#6][#6X3]
0.3176 [CX4H3][CX4H1]
0.3135 [#6H1][#6H1]
0.281 [CX4H2]([OX2H1])[CX4H1]
0.2705 [CX4H3][CX4H1][OX2H1]
0.2696 [#8][#6H1][#6H1][#6H3]

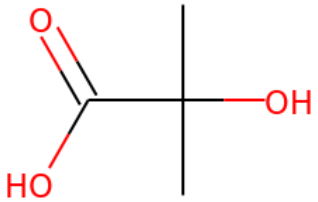


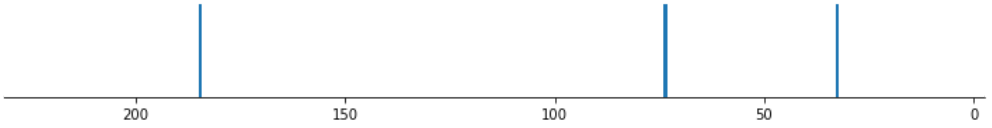
Top predicted substructures for the masked region(red):
0.637 [CX4H2]([#6])[O]
0.4925 [CX4H2]([OX2H1])[CX4H1]
0.4652 [CX4H3][CX4H1][OX2H1]
0.4082 [#8][#6H1][#6H1][#6H3]
0.3921 [CX4H1]([CX4H3])([CX4H1])[CX3H0]
0.368 [CX4H1]([OX2H1])([CX4H3])[CX4H1]
0.364 [OH][CX4H]
0.3563 [CX4H2](O)[CHX4]

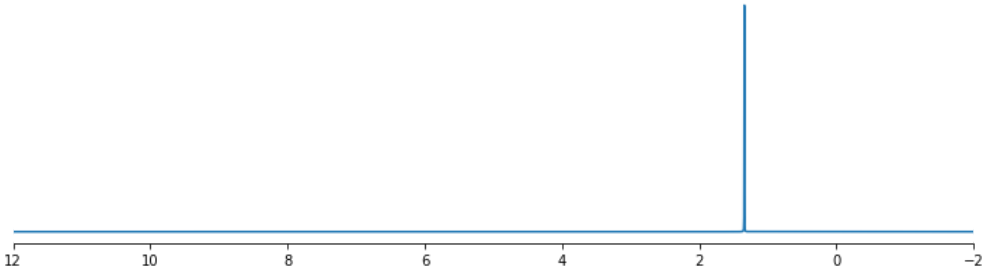


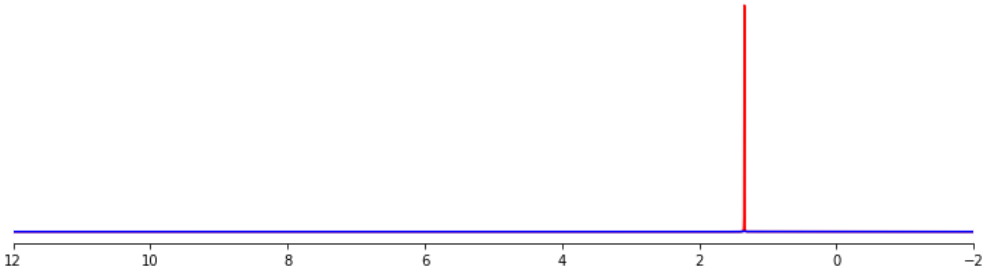
Top predicted substructures for the masked region(red):
0.9897 [#8]=[#6H0][#6H1]
0.9696 [CX3](=[OX1])C
0.9559 [CX3](=[OX1])O
0.9472 [CX3](=O)[OX2H1]
0.946 O=[CX3][CX4H]
0.9388 [#6H3][#6][#6X3]
0.9305 [#8]=[#6][#8]
0.8793 [CX4H1]([CX4H3])([CX4H1])[CX3H0]

True structure: CC(C)(O)C(=O)O

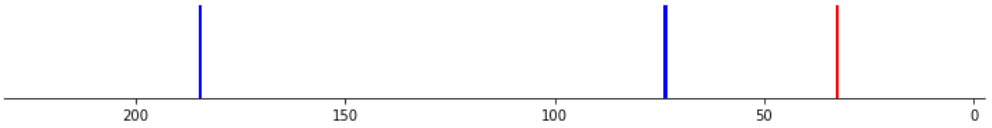




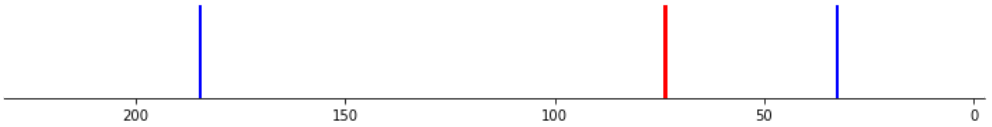




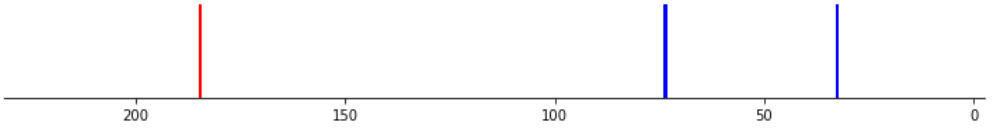
Top predicted substructures for the masked region(red):
0.7726 [#6H0]([#6H3])([#6H3])[#8]
0.7596 [#6X4H3][#6][#8H]
0.75 [OX2H1][CX4H0][CX4H3]
0.7275 [CX4H3][CX4H0]
0.706 [CH3][#6][#8]
0.6613 [#6H3][#6][#6X3]
0.5805 [OX1H0]=[CX3H0][CX4H0][CX4H3]
0.5196 [#6H3][#6H0]



Top predicted substructures for the masked region(red):
0.5746 [#6H3][#6][#6X3]
0.5253 [CX4]([CX4H3])([CX4H3])[CX4H3]
0.507 [CH3][#6][#8]
0.4938 [OX2H1][CX4H0][CX4H3]
0.4171 [#6H3][#6H0]
0.3682 [#6H3][#6][#6]
0.2638 [#6H0]([#6H3])([#6H3])[#8]
0.2593 [CX3](=O)[OX2H1]

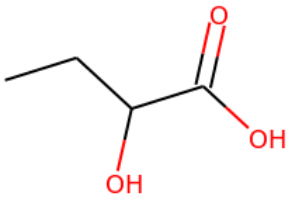


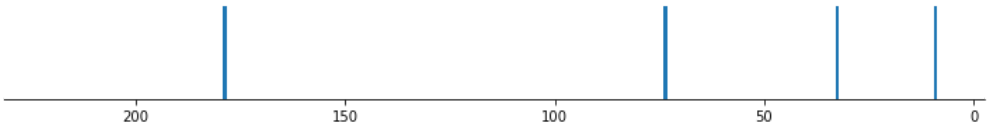
Top predicted substructures for the masked region(red):
0.8461 [CH3][#6][#8]
0.7406 [#6H0]([#6H3])([#6H3])[#8]
0.7402 [OX2H1][CX4H0][CX4H3]
0.7229 [#6X4H3][#6][#8H]
0.653 [CX4H3][CX4]O
0.4848 [#8][#6][#6]=[#8]
0.3455 [#8][#6][#6][#8]
0.2272 [#8][#6H0][#6H1]

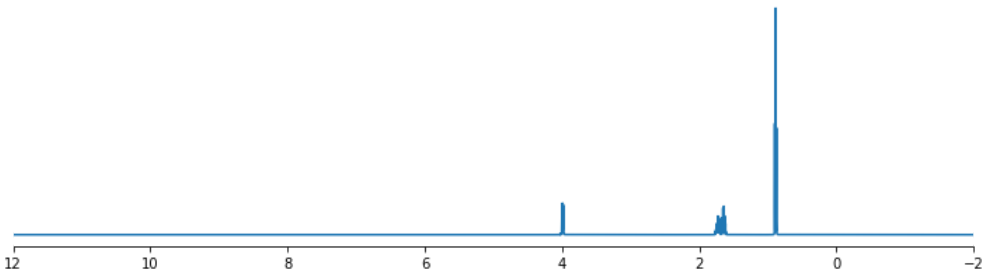


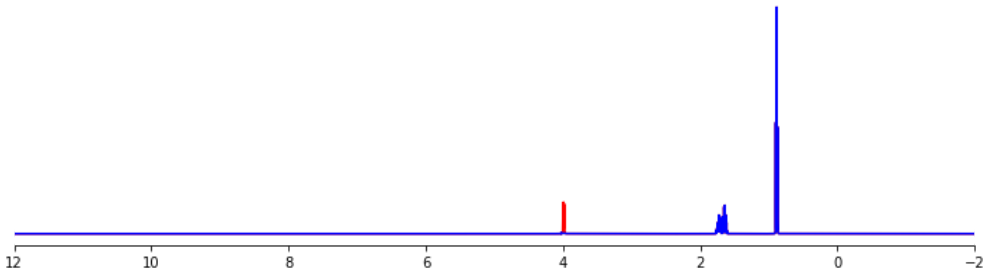
Top predicted substructures for the masked region(red):
0.9796 [CX3](=[OX1])C
0.9272 [CX3](=O)[OX2H1]
0.9265 [CX3](=[OX1])O
0.8094 [#8]=[#6][#8]
0.7692 [#6H3][#6][#6X3]
0.6594 [OX1H0]=[CX3H0][CX4H0][CX4H3]
0.6474 [CX4]([CX4H3])([CX4H3])[CX4H3]
0.5649 [#8][#6][#6]=[#8]

True structure: CCC(O)C(=O)O



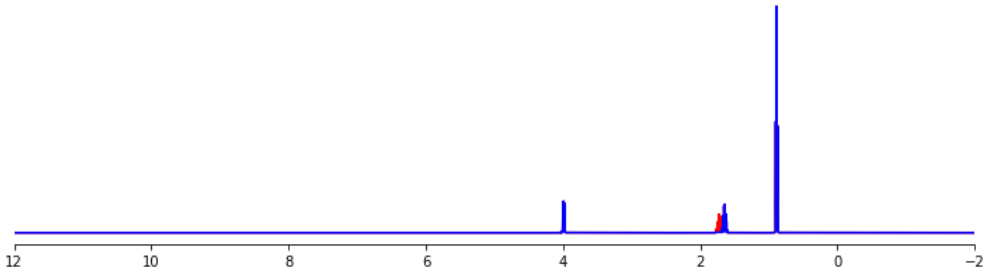






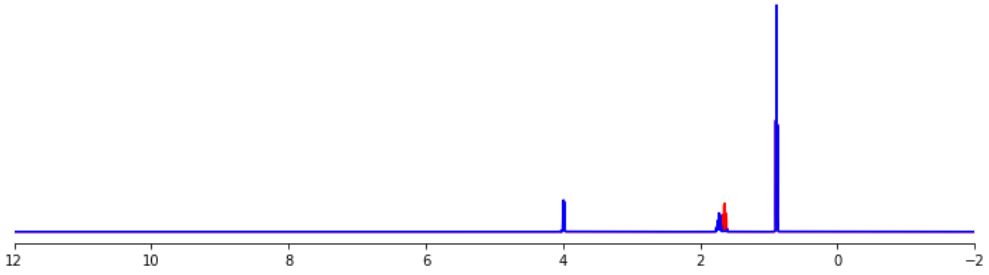
Top predicted substructures for the masked region(red):

0.7063 [OX1H0]=[CX3H0][CX4H1]([OX2H1])[CX4H2]
0.5337 [#8]=[#6H0][#6H1]
0.5138 O=[CX3][CX4H]
0.4557 [OH][CX4H]
0.4533 [#6X4H2][#6H1][#8H]
0.4459 [#8H][#6X4H1][#6X3H0]
0.4116 [CX4H](O)CO
0.4012 O[CX4H][CX4H2]



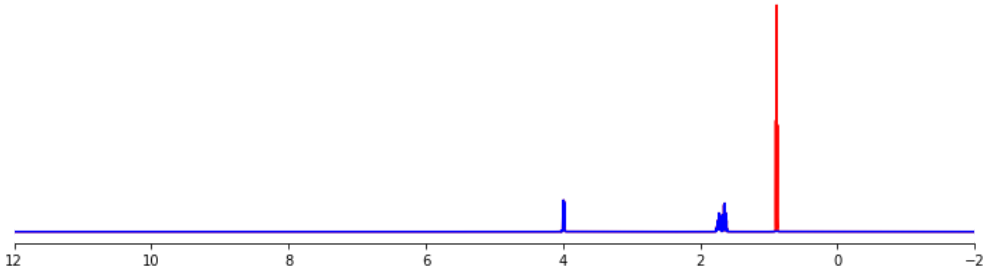
Top predicted substructures for the masked region(red):

0.3928 [#8][#6H0][#6H1]
0.3426 O=[#6][#6H][#6H0]
0.338 [#8]=[#6H0][#6H1]
0.2972 O=[CX3][CX4H]
0.281 [CX4H2]([CX4H3])[CX4H0]
0.2582 [OX1H0]=[CX3H0][CX4H1]([OX2H1])[CX4H2]
0.238 [#6X3][#6][#6][#6H3]
0.2287 [CX4H2]([CX4H3])[CX4H1]



Top predicted substructures for the masked region(red):

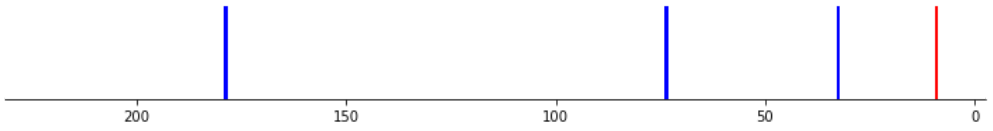
0.3901 [CX4H2]([CX4H3])[CX4H0]
0.385 [#8][#6H0][#6H1]
0.3412 [#8]=[#6H0][#6H1]
0.3305 O=[#6][#6H][#6H0]
0.2928 O=[CX3][CX4H]
0.2198 [CX3](=O)[OX2H1]
0.2138 [CX4H2]([CX4H3])[CX4H1]
0.1815 [#6X3][#6][#6][#6H3]



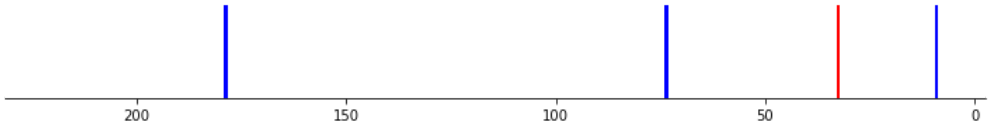
Top predicted substructures for the masked region(red):

0.7663 [CX4H2]([CX4H3])[CX4H0]
0.753 [#6X3][#6][#6][#6H3]
0.6936 [OX2H1][CX4H0][CX4H2][CX4H3]
0.5954 [#6H3][#6][#6]
0.5442 [#8][#6H0][#6H1]

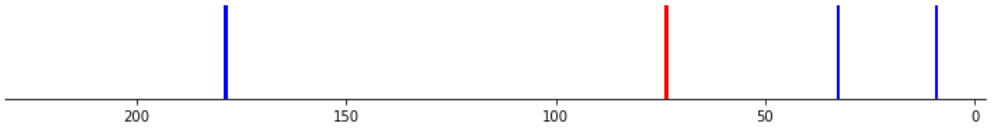
0.443 [#8]=[#6H0][#6H1]
0.4349 O=[CX3][CX4H]
0.4132 [#6H1]



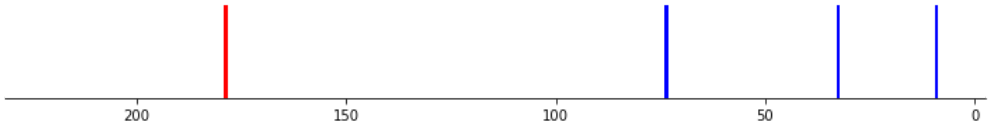
Top predicted substructures for the masked region(red):
0.9958 [CX4H3][CX4H2]
0.8962 [CX4H2]([CX4H3])[CX4H0]
0.8912 [OX2H1][CX4H0][CX4H2][CX4H3]
0.7309 [CH3]CC[OH]
0.6348 [#6X3][#6][#6][#6H3]
0.4581 [#8][#6H0][#6H1]
0.3565 O=[#6][#6H][#6H0]
0.3268 [CX4H3][#6]



Top predicted substructures for the masked region(red):
0.7247 [CX4H2]([CX4H3])[CX4H0]
0.3962 [#6X3][#6][#6][#6H3]
0.3542 [OX1H0]=[CX3H0][CX4H1]([OX2H1])[CX4H2]
0.2985 O=[#6][#6H][#6H0]
0.2963 OCC[CH2]
0.2667 [#8][#6H0][#6H1]
0.2536 [CX4H2]([CX4H3])[CX4H1]
0.243 [CX3](=O)[OX2H1]

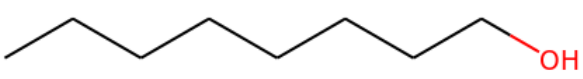


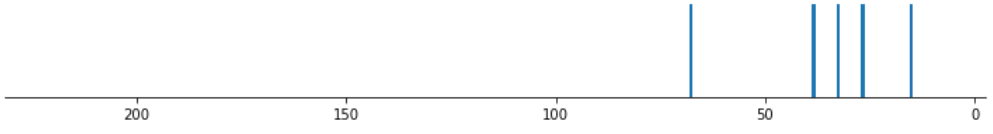
Top predicted substructures for the masked region(red):
0.7757 [OX1H0]=[CX3H0][CX4H1]([OX2H1])[CX4H2]
0.5567 [CX4H2]([CX4H3])[CX4H0]
0.5544 [#8][#6H0][#6H1]
0.5219 [#8H][#6X4H1][#6X3H0]
0.4856 [OH][CX4H]
0.4475 [#6X4H2][#6H1][#8H]
0.4382 [CX4H1]([OX2H1])([CX4H2])[CX3H0]
0.4311 [#8][#6][#6][#8]

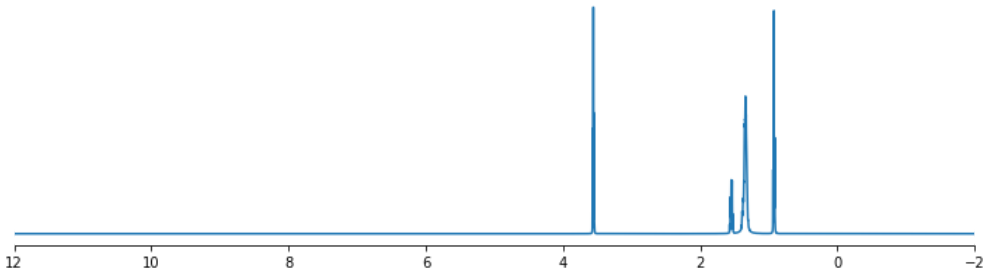


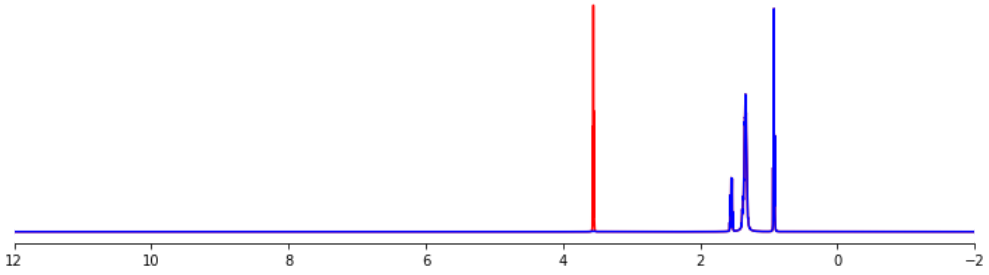
Top predicted substructures for the masked region(red):
0.9671 [CX3](=[OX1])C
0.967 [CX3](=[OX1])O
0.9309 [CX3](=O)[OX2H1]
0.9221 [#8]=[#6][#8]
0.9067 [CX4H2]CC=O
0.8891 [#6X3][#6][#6][#6H3]
0.8678 [OX1H0]=[CX3H0][CX4H1]([OX2H1])[CX4H2]
0.8249 [#8]=[#6H0][#6H1]

True structure: CCCCCCCCO



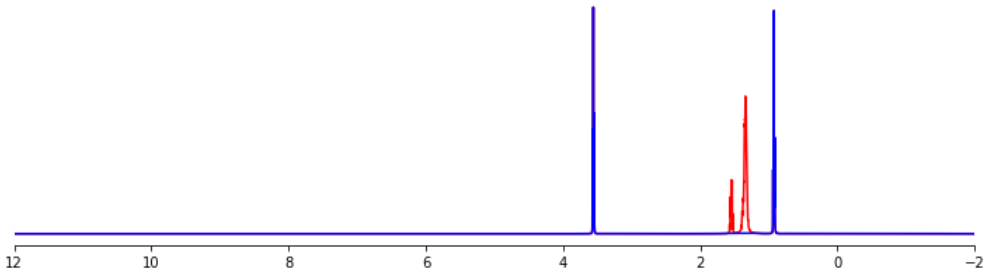






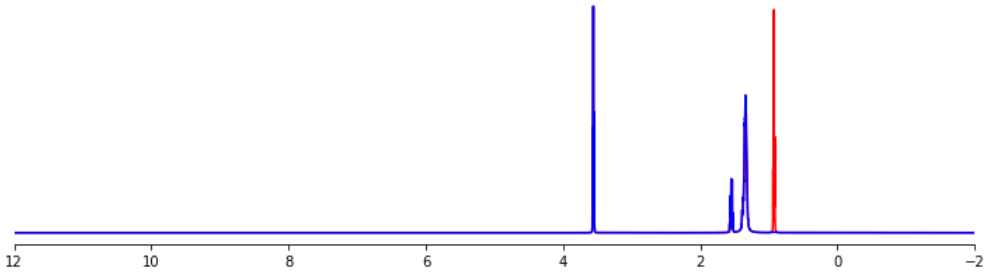
Top predicted substructures for the masked region(red):

0.7785 [CH2X4](O)[CX4H2]
0.7611 [CH2X4](O)[CX4H2][CX4H2]
0.6176 [CX4H2]([#6])[O]
0.5329 [CX4H2]([OX2H1])[CX4H2]
0.1896 [CX4H2]([OX2H0])[CX4H2]
0.1524 [#6H1]([#6H2])[#6H2]
0.1465 [CX4H2]([CX4H3])[CX4H1]
0.1453 [#8H][#6H2][#6H1]



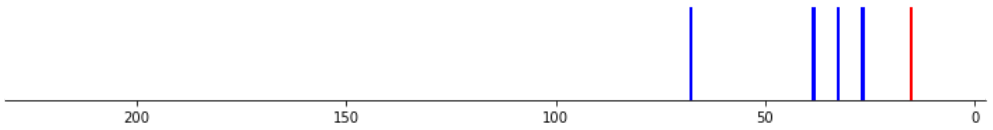
Top predicted substructures for the masked region(red):

0.911 [CH2X4](O)[CX4H2][CX4H2]
0.8764 [CX4H2][CX4H2][CX4H2][CX4H2]
0.7809 [#8][#6][#6H2]
0.7216 [CX4H2]([CX4H3])[CX4H2]
0.6333 [CH2X4](O)[CX4H2]
0.5879 OCC[CH2]
0.5725 CCCCCC
0.5267 [CX4H2]([OX2H1])[CX4H2]

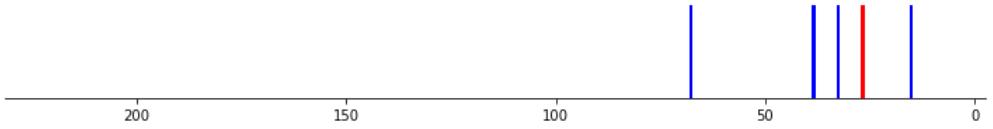


Top predicted substructures for the masked region(red):

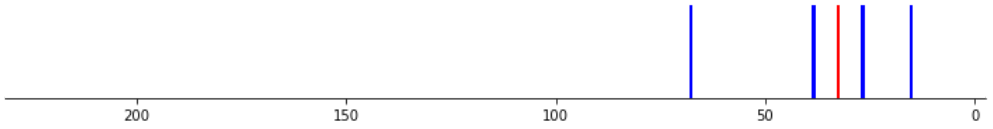
0.8039 [#6H3][#6][#6]
0.3537 [CX4H2]([CX4H3])[CX4H2]
0.3505 [#6H1]
0.2943 [CX4H3]
0.289 [CX4H2]([OX2H1])[CX4H2]
0.2328 [#8][#6][#6H2]
0.2071 [CX4H2]([CX4H3])[CX4H1]
0.1774 CCCCCC



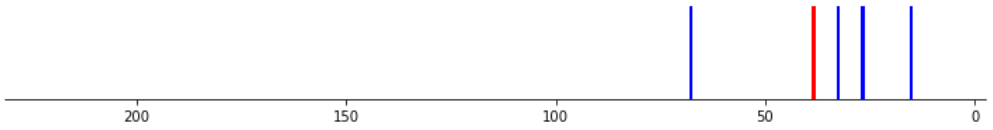
Top predicted substructures for the masked region(red):
0.9461 [CX4H3][CX4H2]
0.8283 [CX4H2]([CX4H3])[CX4H2]
0.3686 [#8][#6][#6H2]
0.2217 [CH2X4](O)[CX4H2]
0.22 [CX4H2]([CX4H3])[CX4H1]
0.1794 [CX4H2]([OX2H0])[CX4H2]
0.1577 [CX4H2]([OX2H1])[CX4H2]
0.1474 [CH2X4](O)[CX4H2][CX4H2]



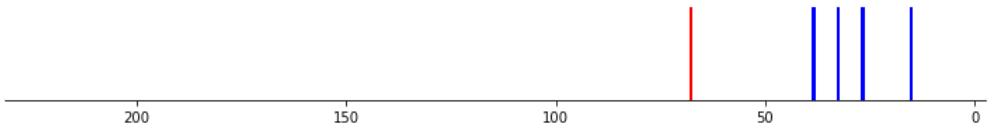
Top predicted substructures for the masked region(red):
0.4064 [#8][#6][#6H2]
0.3934 [CX4H2]([OX2H1])[CX4H2]
0.3593 [CX4H2]([CX4H3])[CX4H2]
0.3141 [CH2X4](O)[CX4H2]
0.2841 CCCCCC
0.2439 [CH2X4](O)[CX4H2][CX4H2]
0.1546 [CX4H2]([OX2H0])[CX4H2]
0.1007 [CX4H2][CX4H2]



Top predicted substructures for the masked region(red):
0.6146 [#8][#6][#6H2]
0.5707 [CX4H2]([OX2H1])[CX4H2]
0.5481 [CH2X4](O)[CX4H2][CX4H2]
0.5041 [CH2X4](O)[CX4H2]
0.2591 CCCCCC
0.1712 [CX4H2]([OX2H0])[CX4H2]
0.1312 [CX4H2]([CX4H2])[CX4H2]
0.1025 [CX4H2]([CX4H3])[CX4H1]

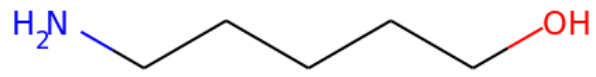


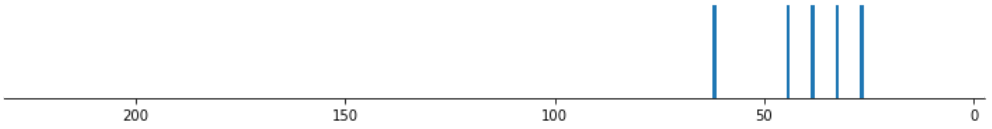
Top predicted substructures for the masked region(red):
0.4737 [CX4H2]([OX2H1])[CX4H2]
0.3555 [CH2X4](O)[CX4H2]
0.2552 [#8][#6][#6H2]
0.2289 CCCCCC
0.1865 [CX4H2]([CX4H3])[CX4H1]
0.1658 [#6H1]([#6H2])[#6H2]
0.1305 [CX4H2]([OX2H0])[CX4H2]
0.1136 [CX4H2][CX4H2]

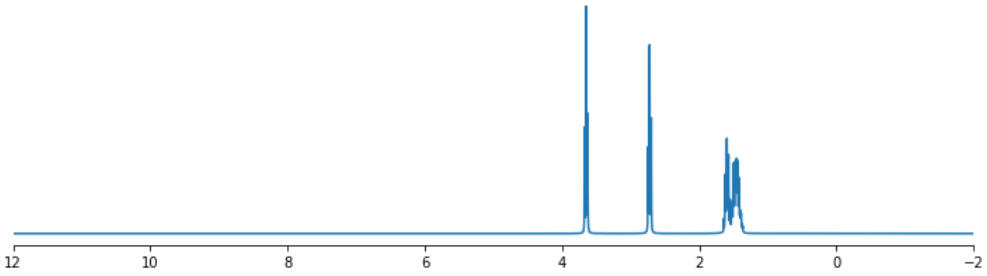


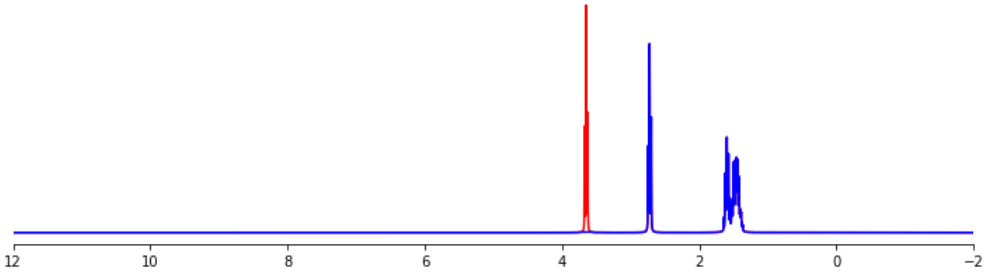
Top predicted substructures for the masked region(red):
0.8219 [CH2X4](O)[CX4H2][CX4H2]
0.7756 [CH2X4](O)[CX4H2]
0.552 [CX4H2]([OX2H1])[CX4H2]
0.4129 [#8][#6][#6H2]
0.3004 [CX4H2]([#6])[O]
0.1973 [CX4H2]([OX2H0])[CX4H2]
0.176 [CX4H2]([CX4H3])[CX4H1]
0.1399 CCCCCC

True structure: NCCCCCO



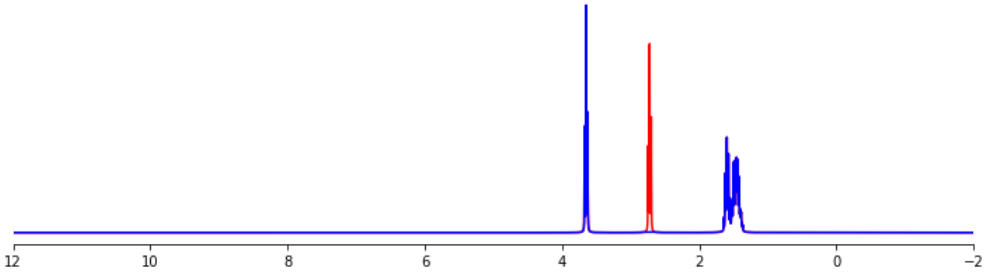






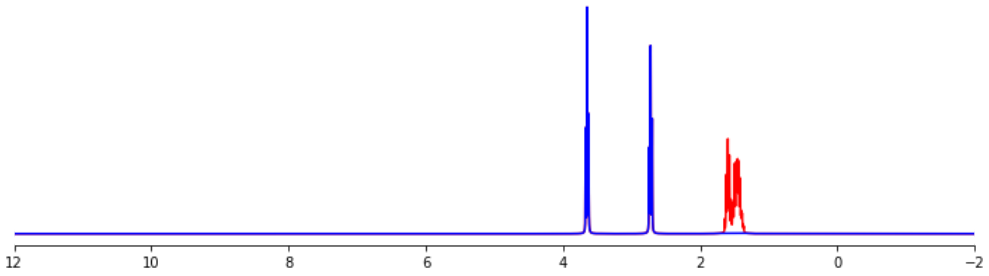
Top predicted substructures for the masked region(red):

0.4644 [CX4H2]([#6])[O]
0.4423 [CX4H2]([CX4H2])[CX4H1]
0.3152 [CX4H2]([OX2H1])[CX4H1]
0.2914 [CH2X4](O)[CX4H2]
0.256 [CH2X4](O)[CX4H2][CX4H2]
0.2405 [#6H1]([#6H2])[#6H2]
0.2325 [CX4H2]([OX2H1])[CX4H2]
0.2191 [CX4H2](O)[CHX4]

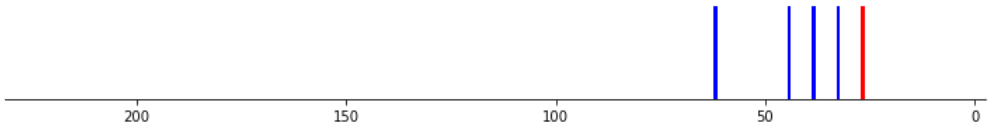


Top predicted substructures for the masked region(red):

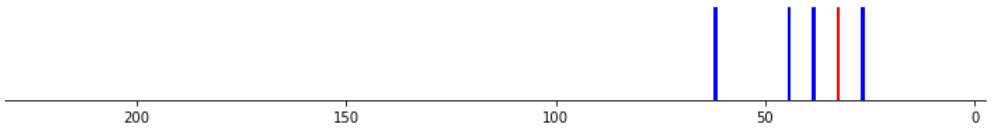
0.5028 [#7X3][#6H2]
0.438 [#7H2][#6H2]
0.3935 [CX4H2]([NX3H2])[CX4H2]
0.3837 [#7][#6H2][#6H2]
0.3734 [#7][#6H2]
0.2743 [#6H1]([#6H2])[#6H2]
0.2558 [CX4H2]([OX2H1])[CX4H1]
0.2194 [#6H1]



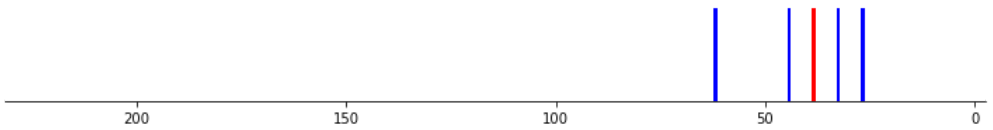
Top predicted substructures for the masked region(red):
0.749 [CX4H2]([CX4H2])[CX4H1]
0.6038 [#7X3H2]
0.4253 OCC[CH2]
0.3157 [CX4H2][CX4H2][CX4H2][CX4H2]
0.3036 [CX4H2]([OX2H1])[CX4H1]
0.282 [#6H1][#6H2]
0.2786 [#6H1]
0.2763 CCCCCC



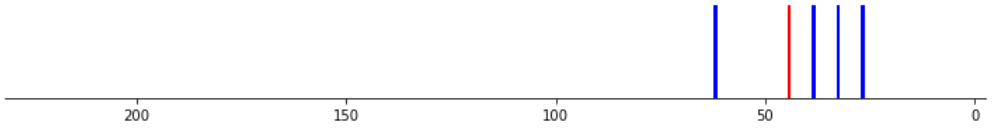
Top predicted substructures for the masked region(red):
0.2487 OCC[CH2]
0.2237 [CX4H2]([OX2H1])[CX4H1]
0.1926 CCCCCC
0.1415 [CX4H2]([CX4H2])[CX4H2]
0.0893 [#7X3H1]
0.0884 [CX4H3]
0.0863 [CH2X4](O)[CX4H2][CX4H2]
0.0804 [CX4H2](O)[CHX4]



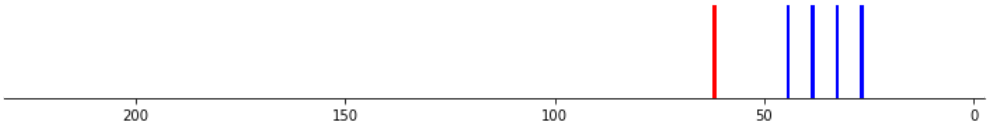
Top predicted substructures for the masked region(red):
0.2259 [CH2X4](O)[CX4H2][CX4H2]
0.178 CCCCCC
0.1714 [CX4H2]([OX2H1])[CX4H1]
0.1595 OCC[CH2]
0.1587 [CX4H2]([CX4H2])[CX4H2]
0.1192 [CX4H2]([CX4H2])[CX4H1]
0.0892 [#7X3H1]
0.0757 [CX4H2](O)[CHX4]



Top predicted substructures for the masked region(red):
0.2743 [CX4H2]([CX4H2])[CX4H1]
0.145 [CX4H1]([CX4H2])([CX4H2])[CX4H2]
0.1348 [#6H1]([#6H2])[#6H2]
0.1334 [#6H1]
0.126 [CX4H3]
0.1251 CCCCCC
0.1028 [#6H1][#6H2]
0.1023 [#7X3H1]

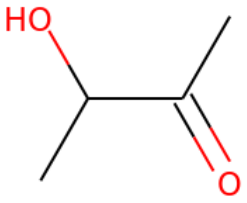


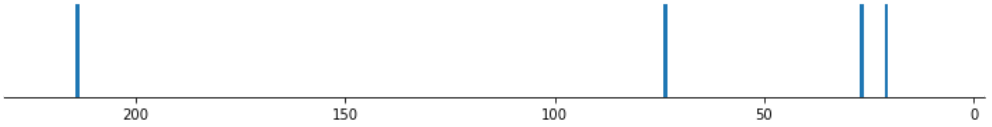
Top predicted substructures for the masked region(red):
0.3436 [CX4H2]([NX3H2])[CX4H2]
0.1967 [CX4H2]([CX4H2])[CX4H1]
0.1639 [#6H1]([#6H2])[#6H2]
0.1588 [CX4H1]([CX4H2])([CX4H2])[CX4H2]
0.1461 [#7X3][#6H2]
0.1312 [#7H2][#6H2]
0.1185 [CX4H3]
0.1104 [#6H1]

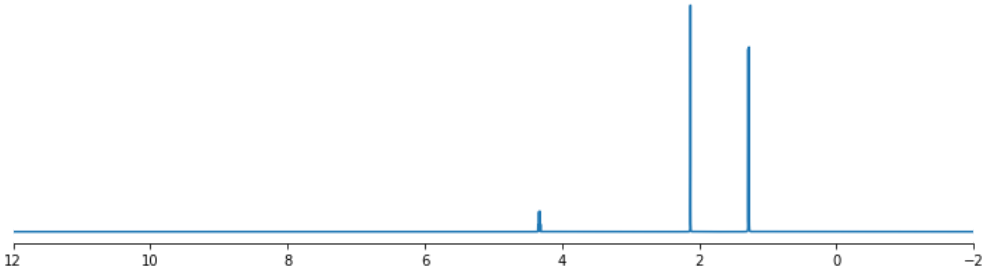


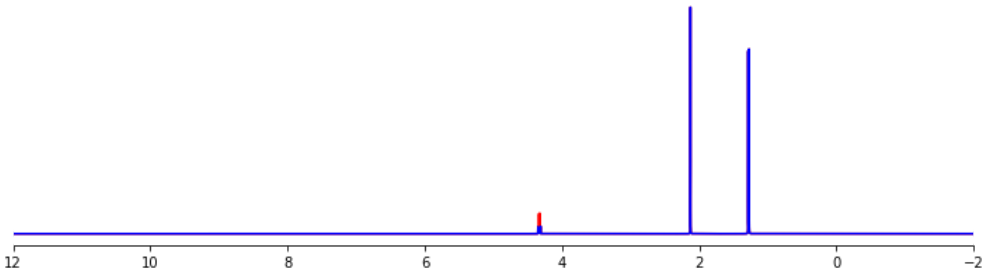
Top predicted substructures for the masked region(red):
0.681 [CH2X4](O)[CX4H2]
0.518 [CX4H2]([OX2H1])[CX4H2]
0.3083 [CX4H2]([#6])[O]
0.2907 [CX4H2]([OX2H1])[CX4H1]
0.1579 [CX4H2]([NX3H1])[CX4H2]
0.136 [#7X3H1]
0.124 [CX4H3]
0.1172 [CH2X4](O)[CX4H2][CX4H2]

True structure: CC(=O)C(C)O

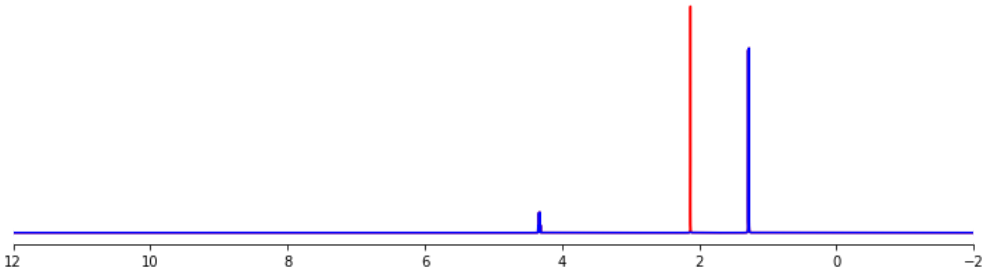






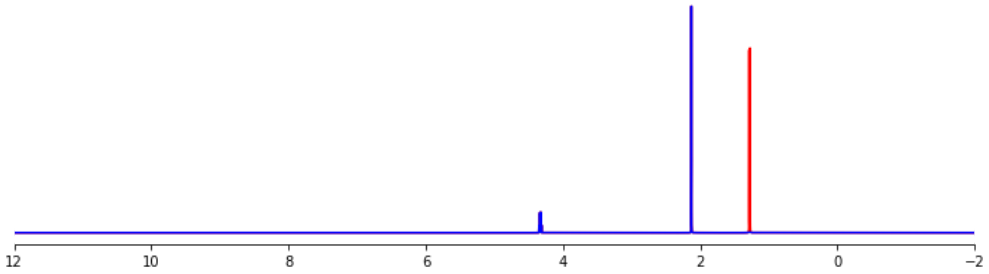


Top predicted substructures for the masked region(red):
0.3262 O=[CX3][CX4H]
0.2904 [CX3H0](=[OX1H0])([CX4H3])[CX4H1]
0.2559 [CX4H1]([OX2H1])([CX4H3])[CX3H0]
0.2263 [#8]=[#6H0][#6H1]
0.2013 [OH][CX4H]
0.1605 [CH3][#6][#8]
0.1431 [#6H3][#6][#6X3]
0.1401 [CX4H3][CX4H1]

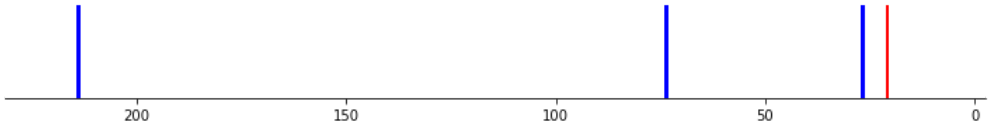


Top predicted substructures for the masked region(red):
0.9958 [CX4H3][CX3]
0.9755 [CX4H3][CX3H0]

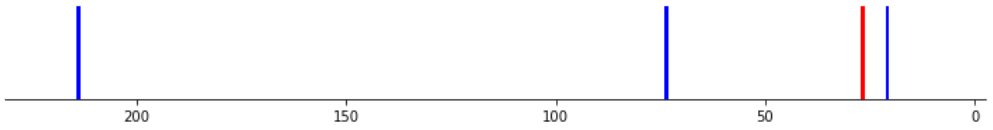
0.9677 [OX1H0]=[CX3H0][CX4H3]
0.6732 [#6H3][#6H0]
0.5331 [#6H3][#6][#6][#6H3]
0.4252 [CX3H0](=[OX1H0])([CX4H3])[CX4H1]
0.2062 [CH3]CC[OH]
0.1263 [CX3H0](=[OX1H0])([CX4H3])[CX4H0]



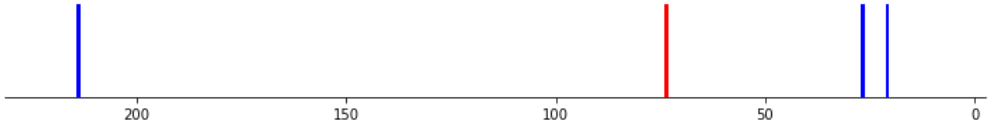
Top predicted substructures for the masked region(red):
0.7374 [#6X4H3][#6][#8H]
0.5493 [CX4H3][CX4H1][OX2H1]
0.5129 [CH3][#6][#8]
0.5095 [#6H3][#6][#6X3]
0.4762 [CX4H3][CX4H1]
0.4355 [CX4H1]([OX2H1])([CX4H3])[CX3H0]
0.4331 [CX4H3][CX4]O
0.4235 [#6H3][#6][#6][#6H3]



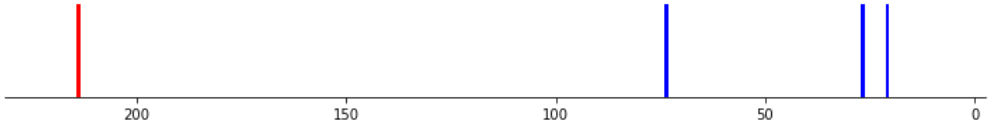
Top predicted substructures for the masked region(red):
0.3833 [#6H3][#6][#6][#6H3]
0.3044 [#6H3][#6][#6X3]
0.2727 [CX4H3][CX4H1]
0.2632 [#8]=[#6H0][#6H1]
0.2075 [#6X4H3][#6][#8H]
0.1929 [CH3][#6][#8]
0.1768 O=[CX3][CX4H]
0.1712 [CX4H3][CX4H1][OX2H1]



Top predicted substructures for the masked region(red):
0.2314 [#6H3][#6][#6X3]
0.1839 [#6H3][#6][#6][#6H3]
0.1573 [CHX4]([CH3X4])[CH3X4]
0.1268 [CX4H1]([OX2H0])([CX4H3])[CX4H3]
0.117 [CX4H1]([CX4H3])([CX4H3])[CX3H0]
0.1078 [#6X4H3][#6][#8H]
0.1074 [CX4H3][CX4H1][OX2H1]
0.0937 [#8H][#6X4H1][#6X3H0]



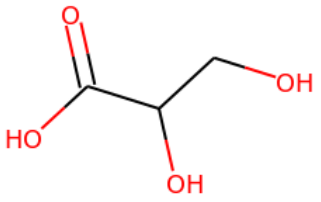
Top predicted substructures for the masked region(red):
0.6866 [#8H][#6X4H1][#6X3H0]
0.6512 [CX4H1]([OX2H1])([CX4H3])[CX3H0]
0.6411 [#6X4H3][#6][#8H]
0.5999 [CX4H3][CX4H1][OX2H1]
0.5312 [CH3][#6][#8]
0.408 [OH][CX4H]
0.389 [CX4H3][CX4]O
0.3744 [#8][#6][#6]=[#8]

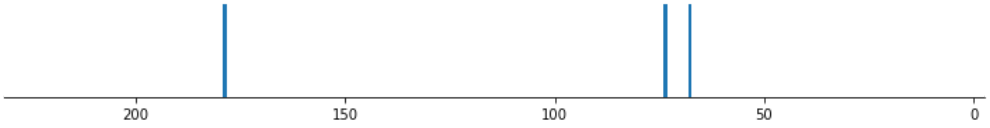


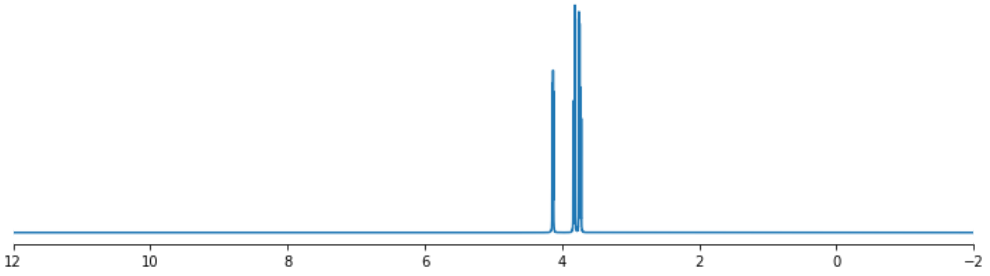
Top predicted substructures for the masked region(red):
0.9952 [CX4H3][CX3]
0.9789 [OX1H0]=[CX3H0][CX4H3]
0.9753 [CX3](=[OX1])C

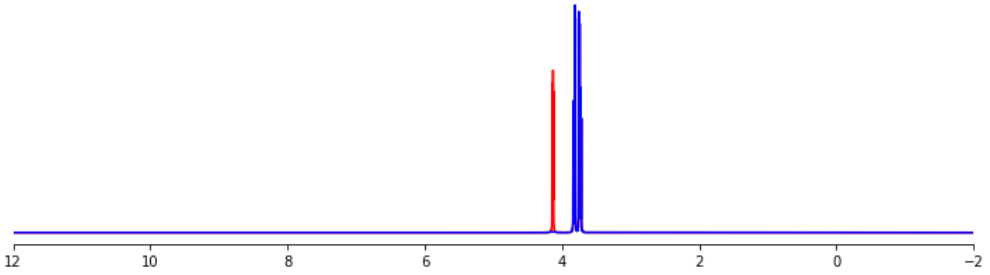
0.9409 [CX4H3][CX3H0]
0.9131 [#6H3][#6][#6X3]
0.8983 [CX4H1]([OX2H1])([CX4H3])[CX3H0]
0.8918 [#8][#6][#6]=[#8]
0.8584 O=[CX3][CX4H]

True structure: O=C(O)C(O)CO

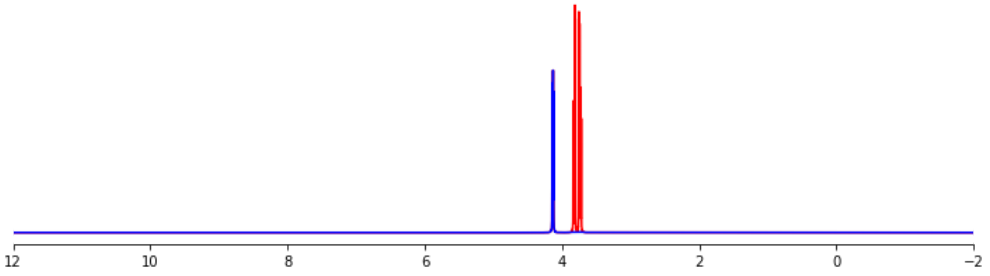




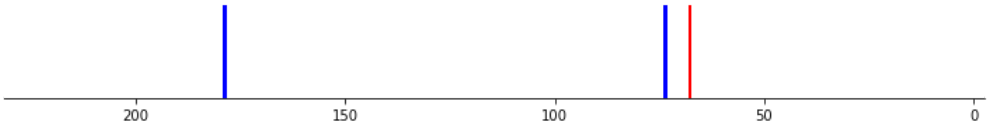




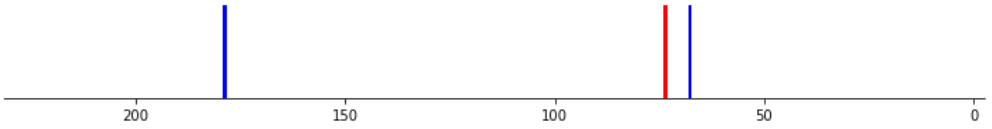
Top predicted substructures for the masked region(red):
0.491 [#8][#6H2][#6H][#6X3]
0.4165 [CX4H2]([OX2H1])[CX4H1]
0.3691 [#8][#6][#6][#6X3]
0.3396 [#8][#6][#6][#6][#6][#8]
0.3008 [#8][#6H0][#6H1]
0.2847 [#8][#6H2][#6H1][#6H0]
0.266 [#8]=[#6H0][#6H1]
0.2589 O=[CX3][CX4H]



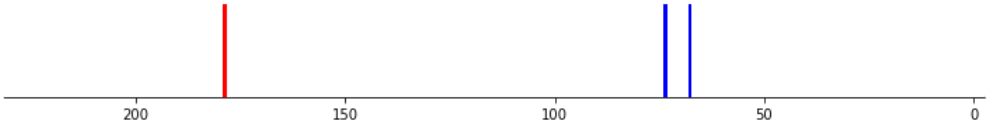
Top predicted substructures for the masked region(red):
0.777 [#8][#6H2][#6H][#6X3]
0.7611 [CX4H2](O)[CHX4]
0.7135 [CX4H2]([OX2H1])[CX4H1]
0.6783 [#8][#6H2][#6H1][#6H0]
0.5435 O=[CX3][CX4H]
0.5228 [CX4H](O)CO
0.5214 [#8][#6][#6][#6X3]
0.5153 [#6H1][#6H2]



Top predicted substructures for the masked region(red):
0.6311 [CX4H2]([OX2H1])[CX4H1]
0.4041 [#8][#6H2][#6H1][#6H0]
0.3906 [CX4H2]([OX2H0])[CX4H2]
0.3746 [#8][#6H2][#6H][#6X3]
0.3326 [#8][#6][#6][#6X3]
0.3004 [#8][#6][#6][#6][#6][#8]
0.2756 [#8][#6H0][#6H1]
0.1949 O=[CX3][CX4H]

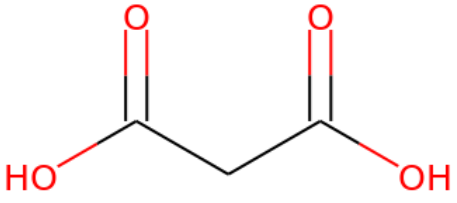


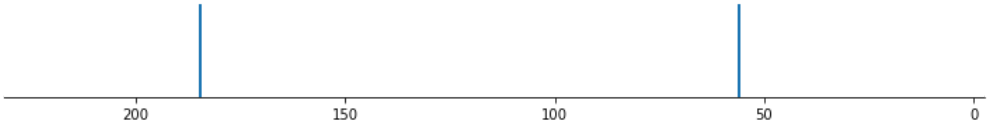
Top predicted substructures for the masked region(red):
0.4099 [#8][#6][#6][#6X3]
0.399 [#8H][#6X4H1][#6X3H0]
0.3821 [#8][#6H2][#6H][#6X3]
0.3039 [#8][#6][#6][#6][#6][#8]
0.2456 [CX4H1]([OX2H1])([CX4H2])[CX4H1]
0.2258 [CX4H2]([OX2H0])[CX4H2]
0.217 [OH][CX4H]
0.2094 [#8][#6H0][#6H1]

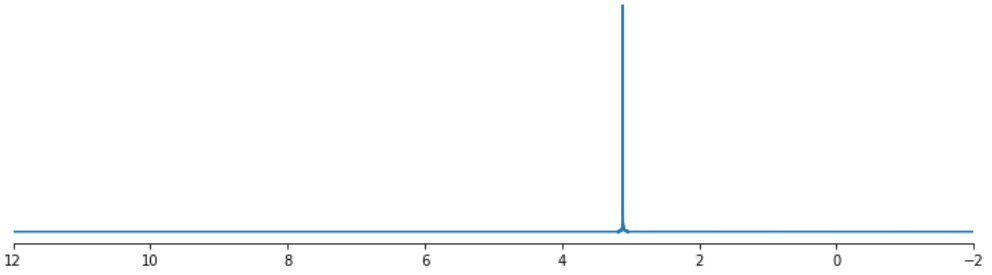


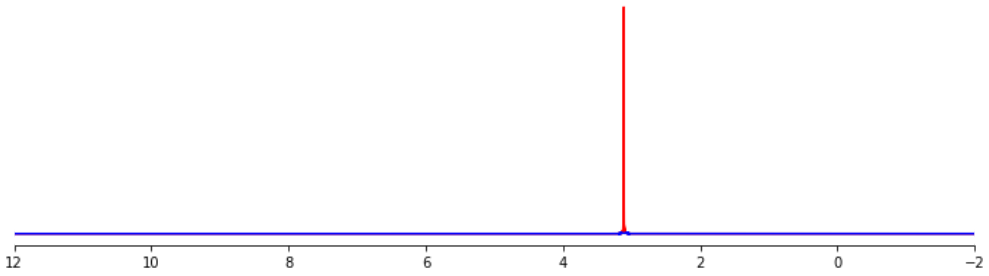
Top predicted substructures for the masked region(red):
0.9698 [CX3](=[OX1])C
0.845 [CX3](=[OX1])O
0.8099 [#8][#6H2][#6H][#6X3]
0.7822 [#8]=[#6][#8]
0.7808 [#8]=[#6H0][#6H1]
0.7321 O=[CX3][CX4H]
0.6969 [#8][#6][#6]=[#8]
0.6791 [#8][#6][#6][#6X3]

True structure: O=C(O)CC(=O)O

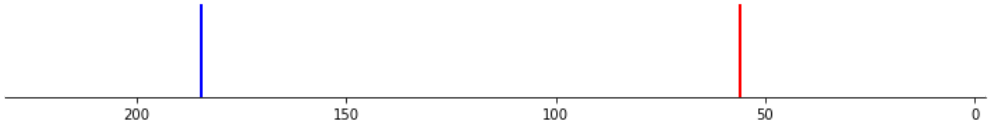




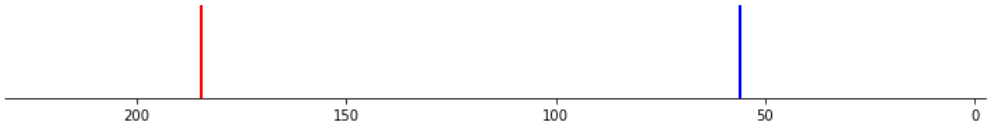




Top predicted substructures for the masked region(red):
0.1777 [CX4H2][CX3]=O
0.1722 [#6]1[#6]([#8])[#6]1[#8]
0.1709 [#7X3H0]
0.1227 [#8][#6][#6][#6][#6]=[#8]
0.1173 [#8][#6][#6][#8]
0.1116 [OX2H0]1[CX4H1][CX4H1]1
0.1097 C1OC1
0.1056 [CX4H3][NX3H0]

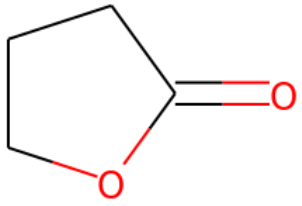


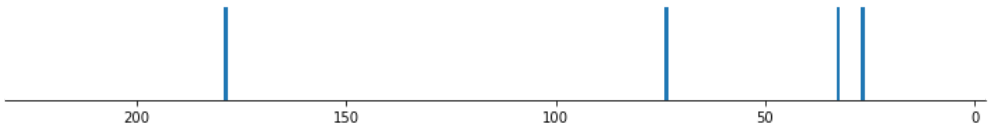
Top predicted substructures for the masked region(red):
0.2763 [#8][#6H0][#6H1]
0.2097 [#8][#6][#6]=[#8]
0.184 O=[CX3][CX4H]
0.1796 [#6]1[#6]([#8])[#6]1[#8]
0.1719 [CX4H3]
0.1405 [#8]=[#6H0][#6H1]
0.1344 [#7X3H0]
0.1214 C1CC1O

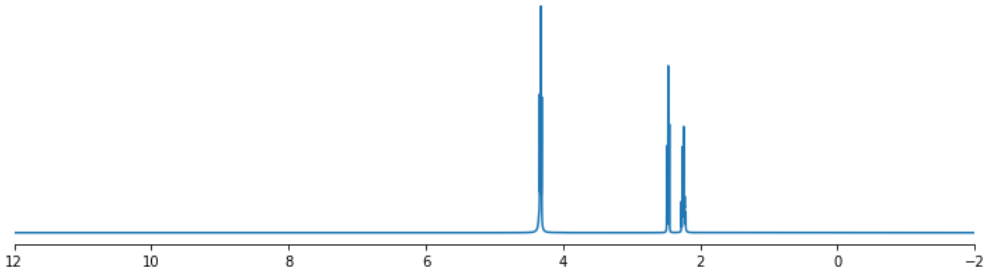


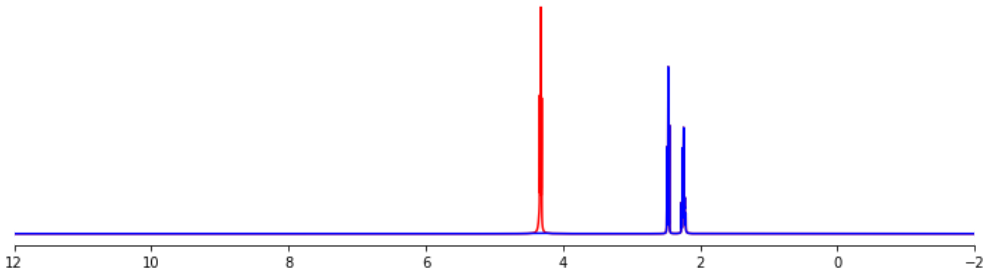
Top predicted substructures for the masked region(red):
0.904 [CX3](=[OX1])C
0.6744 [CX3](=[OX1])O
0.6635 [CX3](=O)[OX2H1]
0.5382 [#8][#6][#6]=[#8]
0.4975 [#8]=[#6][#8]
0.3251 [#8]=[#6H0][#6H1]
0.3182 [#8][#6][#6][#6X3]
0.3072 O=[CX3][CX4H]

True structure: O=C1CCCO1



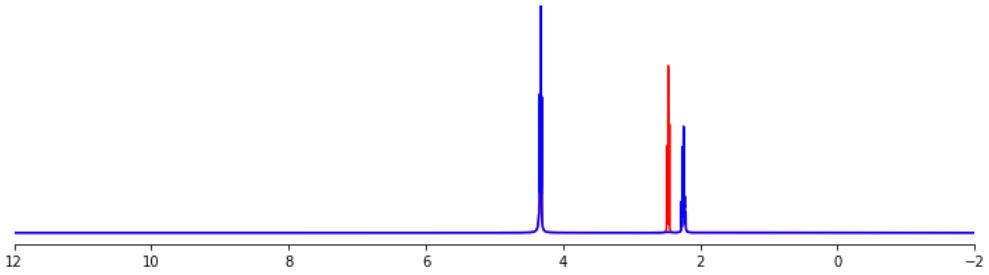






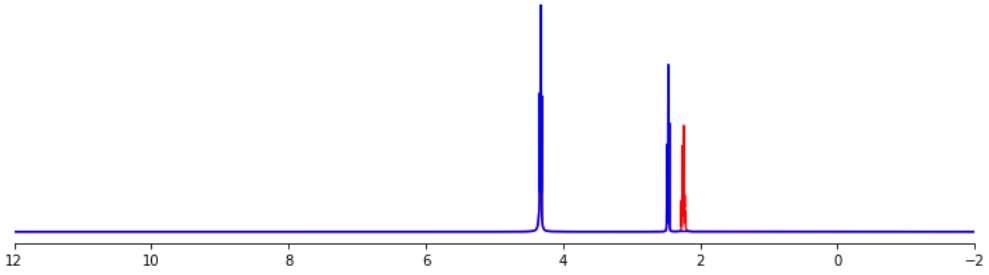
Top predicted substructures for the masked region(red):

0.7272 [CX4H2]([#6])[O]
0.5918 [CH2X4](O)[CX4H2]
0.4836 [OX2H0][CX4H2][CX4H2][CX4H2]
0.3186 [#8][#6][#6][#6][#6]=[#8]
0.3119 [#6H1]
0.31 [CX4H2]([OX2H0])[CX4H2]
0.2624 CCC=CCC
0.2555 [#6H1][#6H2]



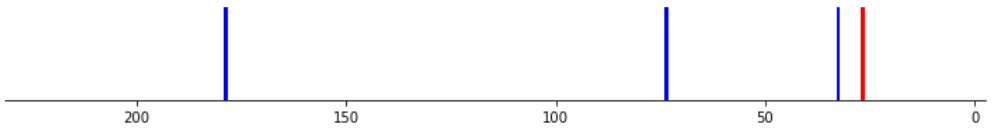
Top predicted substructures for the masked region(red):

0.4164 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.2783 [OX2H0][CX3H0][CX4H2]
0.2609 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.2445 CCC=CCC
0.1984 [CX4H2][CX3]=O
0.1874 [OX2H1]
0.179 [#8][#6][#6][#6][#6]=[#8]
0.1743 [#8][#6][#6][#8]



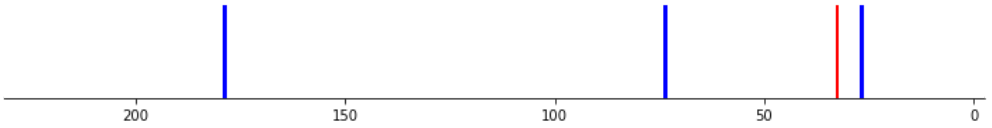
Top predicted substructures for the masked region(red):

0.2518 CCC=CCC
0.2254 [#6H1][#6H2]
0.2121 [#8][#6][#6][#6][#6]=[#8]
0.1929 [#8][#6][#6][#8]
0.1849 [#6H1]
0.1836 [CX4H2][CX3]=C
0.1752 [OX2H1]
0.1655 O[CX4H][CX4H2]

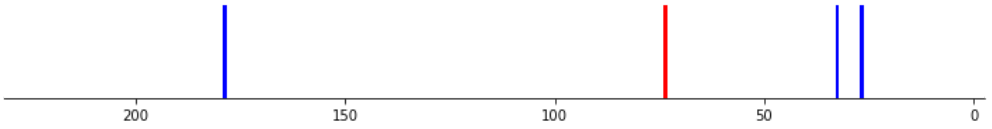


Top predicted substructures for the masked region(red):

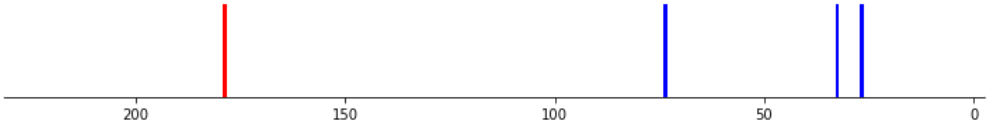
0.4629 [CX4H2]([CX4H2])[CX4H2]
0.3864 [CX4H2]([#6])[O]
0.3262 [OX2H0][CX4H2][CX4H2][CX4H2]
0.2699 [CH2X4](O)[CX4H2]
0.2584 CCC=CCC
0.1775 [CX4H2][CX3]=C
0.1651 [CH2X4](O)[CX4H2][CX4H2]
0.1409 [CX4H2][CX4H2][CX4H2][CX4H2]



Top predicted substructures for the masked region(red):
0.363 [CX4H2]([#6])[O]
0.3627 [CX4H2]([CX4H2])[CX4H2]
0.3316 [CH2X4](O)[CX4H2]
0.2874 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.2568 [#8][#6][#6][#6][#6]=[#8]
0.2533 CCC=CCC
0.2219 [OX2H0][CX4H2][CX4H2][CX4H2]
0.2077 [OX2H0][CX3H0][CX4H2]

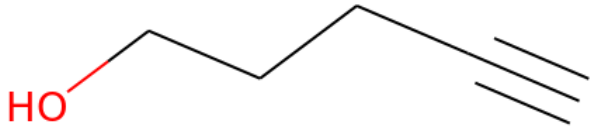


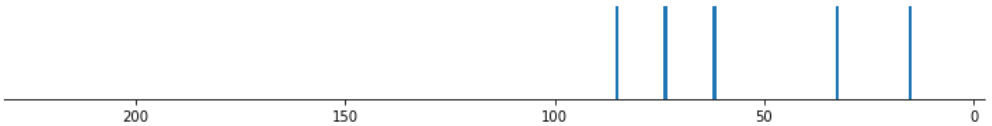
Top predicted substructures for the masked region(red):
0.7735 [CH2X4](O)[CX4H2]
0.7735 [CX4H2]([#6])[O]
0.5547 [CX4H2]([OX2H0])[CX4H2]
0.5066 [OX2H0][CX4H2][CX4H2][CX4H2]
0.2745 [#8][#6][#6][#6][#6]=[#8]
0.2559 [#8][#6][#6][#6X3]
0.2547 [#8][#6][#6][#8]
0.2416 [CH2X4](O)[CX4H2][CX4H2]

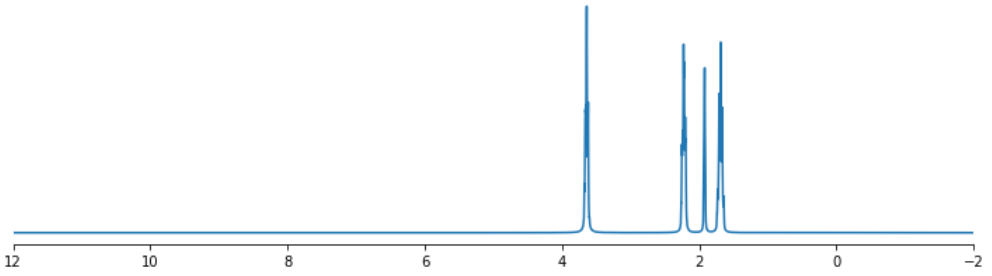


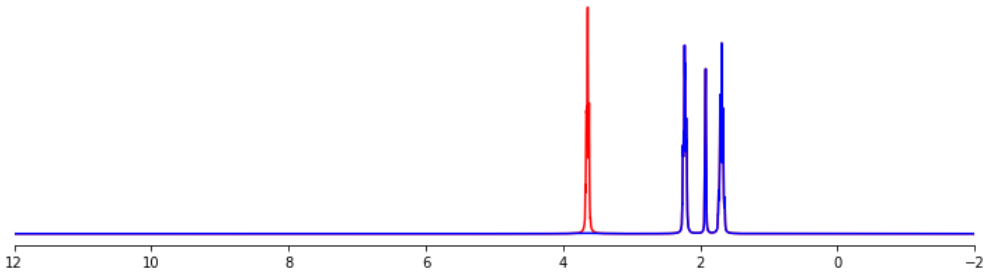
Top predicted substructures for the masked region(red):
0.9876 [CX3H0](=[OX1H0])([OX2H0])[CX4H2]
0.9621 [CX4H2]CC=O
0.9552 [#8]=[#6][#8]
0.9511 [OX1H0]=[CX3H0]([#8])[CX4H2]
0.9354 O=[CX3H0][CX4H2][CX4H2]
0.9297 [CX3](=[OX1])C
0.9287 [CX3](=[OX1])O
0.9277 [CX4H2]([CX4H2])[CX3H0]

True structure: C#CCCCO

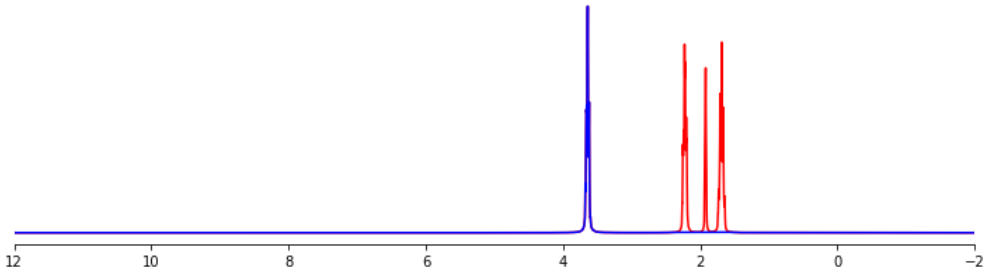




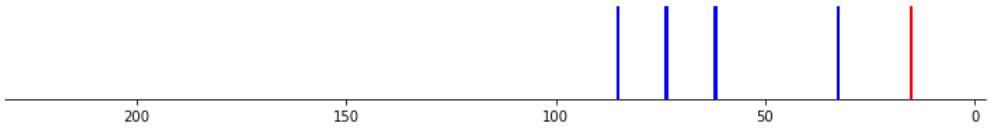




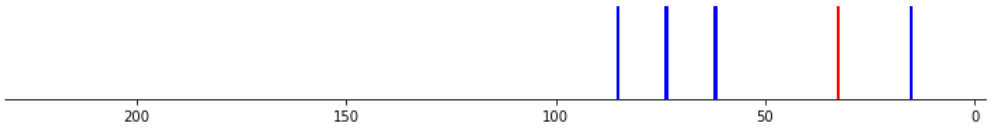
Top predicted substructures for the masked region(red):
0.7874 [CH2X4](O)[CX4H2]
0.6655 [CX4H2]([#6])[O]
0.5865 [CX4H2]([OX2H1])[CX4H2]
0.4582 [OX2H0][CX4H1][CX4H2][CX4H2]
0.4357 CCCCCC
0.4169 [#6H2][#6][#6X2]
0.3913 [CX4H2]([CX4H2])[CX4H1]
0.3642 [CX4H]O



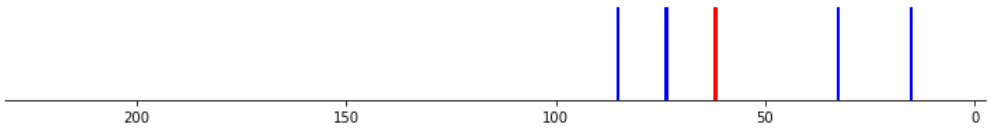
Top predicted substructures for the masked region(red):
0.8887 OCC[CH2]
0.6445 CCCCCC
0.5257 [OX2H0][CX4H1][CX4H2][CX4H2]
0.5245 [CX4H2]([CX4H2])[CX4H1]
0.4914 [CX4H]O
0.4159 [CX4H2]([CX4H2])[CX4H2]
0.359 [#6H1]
0.3545 [OH][CX4H]



Top predicted substructures for the masked region(red):
0.4555 CCCCCC
0.3844 [CX4H2]([CX4H2])[CX4H2]
0.2822 [CX4H]O
0.2647 [CX2H0](#[CX2H0])[CX4H2]
0.2596 [OX2H1]
0.2484 [OX2H0][CX4H1][CX4H2][CX4H2]
0.2237 [OH][CX4H]
0.2141 CCCC#CC

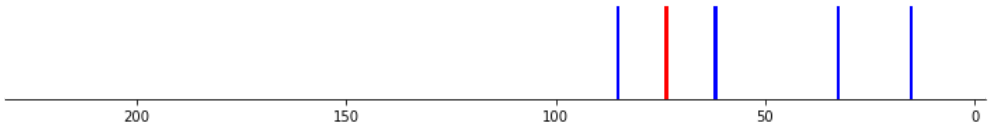


Top predicted substructures for the masked region(red):
0.5838 CCCCCC
0.45 [OX2H0][CX4H1][CX4H2][CX4H2]
0.2837 [CH2X4](O)[CX4H2]
0.2753 [#6H2][#6][#6X2]
0.2743 [CX4H]O
0.2572 [OX2H1]
0.2259 [CX4H2]([CX4H2])[CX4H1]
0.213 CCCC#CC

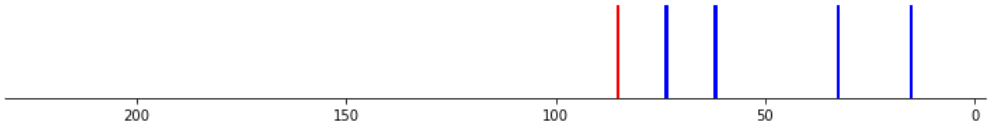


Top predicted substructures for the masked region(red):
0.7401 [CX4H2]([OX2H1])[CX4H2]
0.4613 CCCCCC
0.4521 [CH2X4](O)[CX4H2]

0.3579 [OX2H1]
0.3028 [#6H2][#6][#6X2]
0.2783 [OX2H0][CX4H1][CX4H2][CX4H2]
0.2053 CCCC#CC
0.1971 [CX2H0](#[CX2H0])[CX4H2]

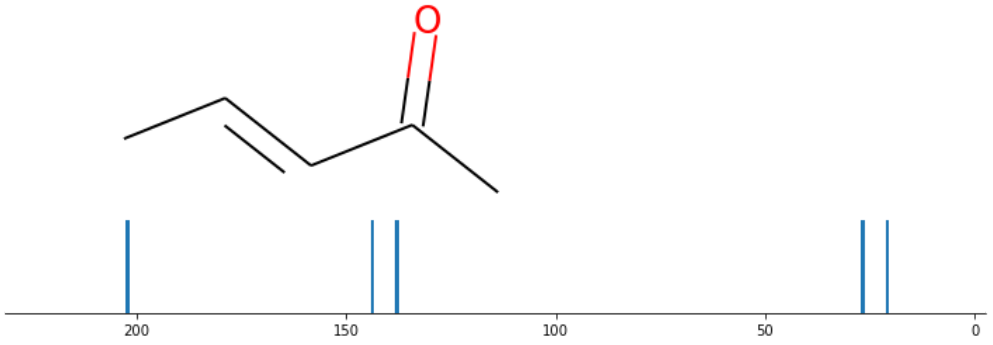


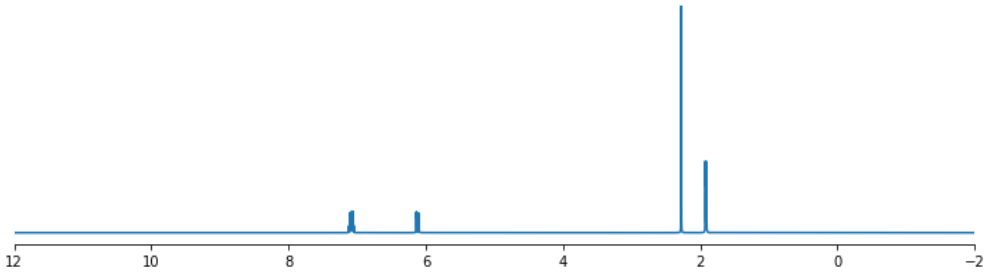
Top predicted substructures for the masked region(red):
0.4472 [CH2X4](O)[CX4H2]
0.3604 CCCCCC
0.3084 [#6H2][#6][#6X2]
0.2933 [OX2H0][CX4H2][CX4H2][CX4H2]
0.2474 [CH2X4](O)[CX4H2][CX4H2]
0.2383 [OX2H0][CX4H1][CX4H2][CX4H2]
0.2266 [CX2H1]#[CX2H0]
0.2116 [#6X4H2][#6H1][#8H]

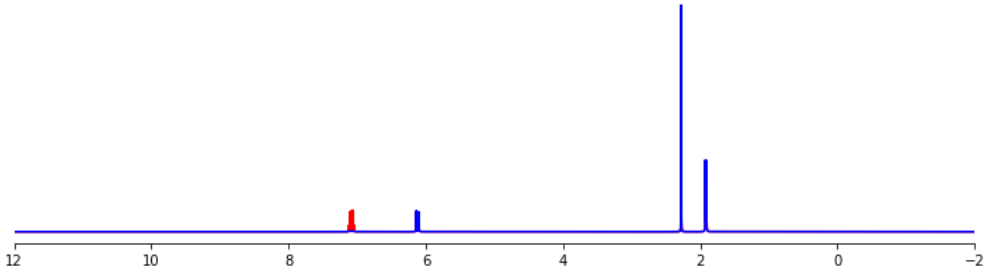


Top predicted substructures for the masked region(red):
0.7107 [#6H2][#6X2]
0.6696 [$([CX2]#C)]
0.5821 [#6H2][#6][#6X2]
0.5647 [#6H2][#6]#[#6X2]
0.4283 [OX2H1]
0.4168 [CX4H2]([OX2H1])[CX4H2]
0.3493 [OX2H0][CX4H1][CX4H2][CX4H2]
0.2931 [CX2H0](#[CX2H0])[CX4H2]

True structure: CC=CC(C)=O

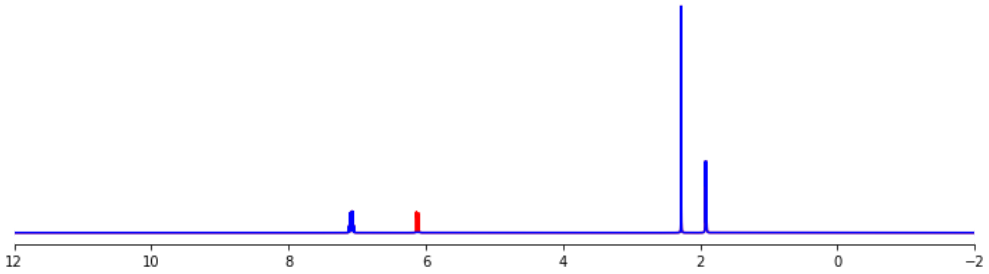




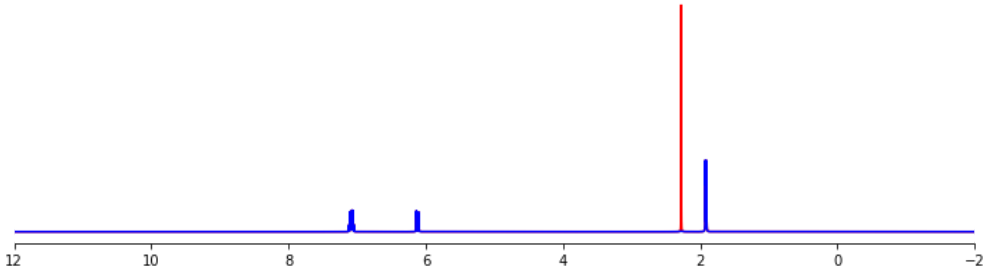


Top predicted substructures for the masked region(red):
0.7235 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.7201 [CX3H1](=[CX3H1])[CX3H0]
0.7115 [#8]=[#6][#6H1]=[#6H1]

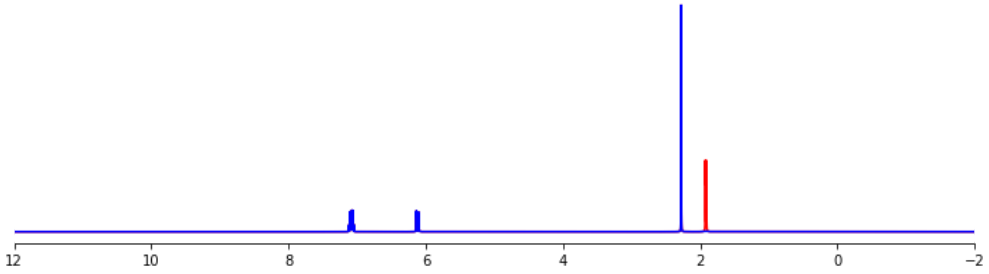
0.6412 [#8]=[#6H0][#6H1]
0.6124 [CHX3]=[CHX3]
0.4209 [CX3H1](=[CX3H1])[CX4H3]
0.383 O=C[CX3H]
0.3028 [CX4H3][CX3H1]



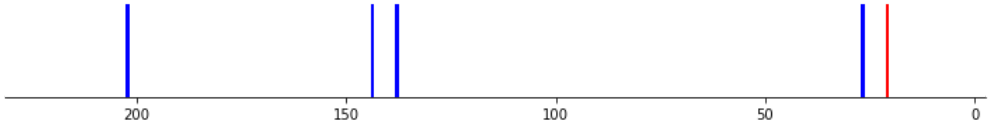
Top predicted substructures for the masked region(red):
0.9461 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.9109 [CX3H1](=[CX3H1])[CX3H0]
0.8396 [#8]=[#6H0][#6H1]
0.7196 O=C[CX3H]
0.6146 [#8]=[#6][#6H1]=[#6H1]
0.5882 [CHX3]=[CHX3]
0.4507 [#6X3H1][#6X3H0]
0.3946 [CX3H1](=[CX3H1])[CX4H3]



Top predicted substructures for the masked region(red):
0.8871 [#6X3]=[#6][#6][#6H3]
0.7493 [OX1H0]=[CX3H0][CX4H3]
0.6034 [CX4H3][CX3H0]
0.2845 [#8]=[#6H0][#6H1]
0.2327 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.2302 [#6H3][#6H0]
0.1934 O=C[CX3H]
0.1198 [#6H3][#6][#6X3]

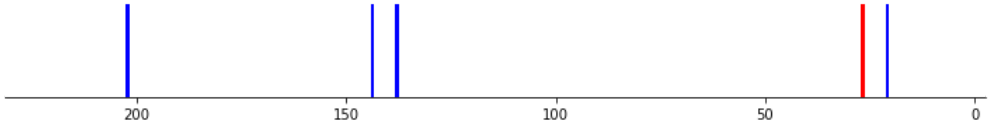


Top predicted substructures for the masked region(red):
0.8399 [CX4H3][CX3H1]
0.4563 [CX3H1](=[CX3H1])[CX4H3]
0.3535 [#8]=[#6H0][#6H1]
0.3375 [#6H3][#6]=[#6X3]
0.3336 [#6X3][#6]=[#6][#6H3]
0.2732 [#8]=[#6X3][#6X3]=[#6X3][#6H3]
0.2085 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.173 O=C[CX3H]

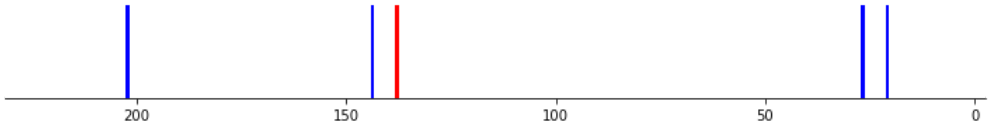


Top predicted substructures for the masked region(red):
0.4228 [CX3H1](=[CX3H1])[CX4H3]
0.3867 [CX4H3][CX3H1]
0.3759 [#8]=[#6H0][#6H1]
0.2612 [#6X3][#6]=[#6][#6H3]
0.2184 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.1691 [#6X3]=[#6][#6][#6H3]

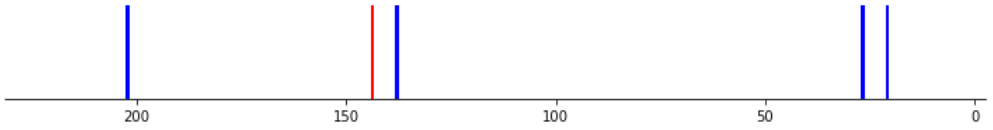
0.1504 [CX3H1](=[CX3H1])[CX3H0]
0.1275 [#8]=[#6X3][#6X3]=[#6X3][#6H3]



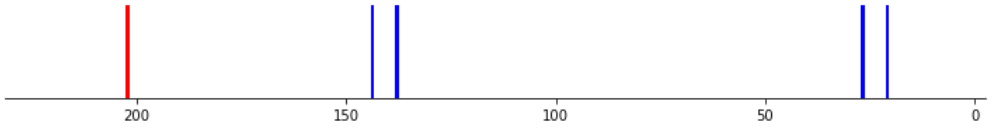
Top predicted substructures for the masked region(red):
0.3959 [#6X3]=[#6][#6][#6H3]
0.1982 [#8]=[#6H0][#6H1]
0.1221 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.1156 [CX4H3][CX3H1]
0.1088 [OX1H0]=[CX3H0][CX4H3]
0.1035 [CX4H2][CX3H]
0.0799 [#6H3][#6][#6X3]
0.0797 [CX3H1](=[CX3H1])[CX3H0]



Top predicted substructures for the masked region(red):
0.4645 [#8]=[#6H0][#6H1]
0.2571 [CX3H1](=[CX3H1])[CX3H0]
0.2442 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.218 O=C[CX3H]
0.2157 [CX4H3][CX3H1]
0.1869 [#6X3]=[#6][#6][#6H3]
0.1864 [CX3H1](=[CX3H1])[CX4H3]
0.1239 [#6X3][#6]=[#6][#6H3]

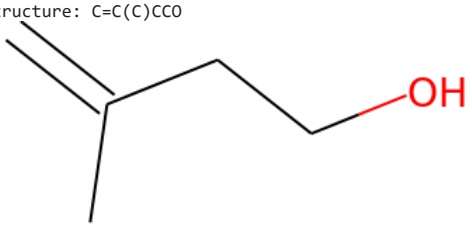


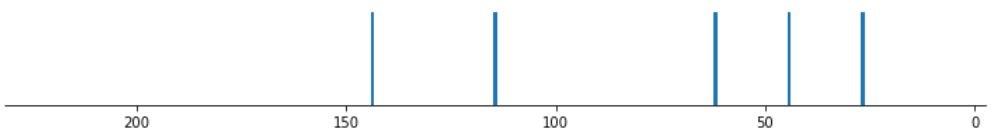
Top predicted substructures for the masked region(red):
0.3234 [#8]=[#6H0][#6H1]
0.2647 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.2618 [CX3H1](=[CX3H1])[CX3H0]
0.2349 [CX4H3][CX3H1]
0.2198 [CX3H1](=[CX3H1])[CX4H3]
0.2085 [#6X3]=[#6][#6][#6H3]
0.1778 O=C[CX3H]
0.1424 [CHX3]=[CHX3]

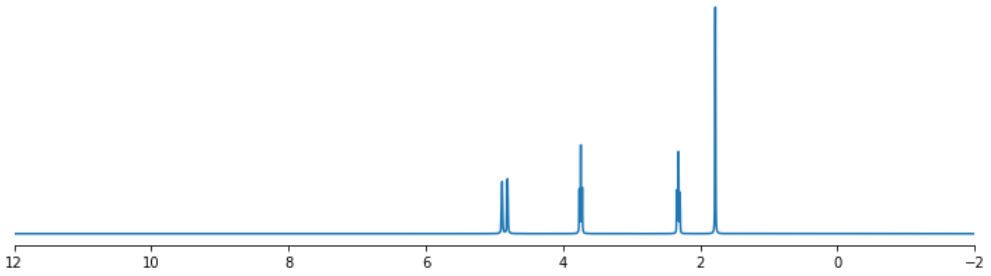


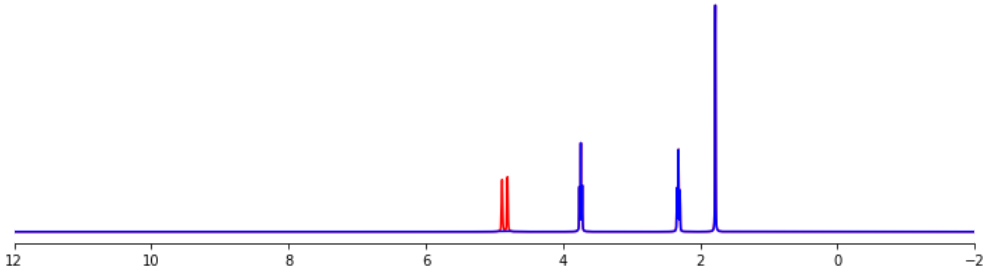
Top predicted substructures for the masked region(red):
0.9501 [#8]=[#6H0][#6H1]
0.9258 [OX1H0]=[CX3H0][CX3H1]=[CX3H1]
0.9221 [CX3](=[OX1])C
0.9214 O=C[CX3H]
0.8908 [OX1H0]=[CX3H0][CX4H3]
0.8446 [#8]=[#6][#6H1]=[#6H1]
0.7179 O=[#6][#6]=[#6X3]
0.6853 [CX3H1](=[CX3H1])[CX3H0]

True structure: C=C(C)CCO

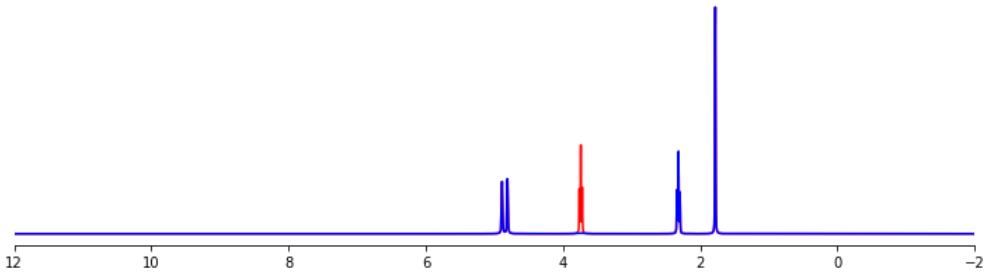




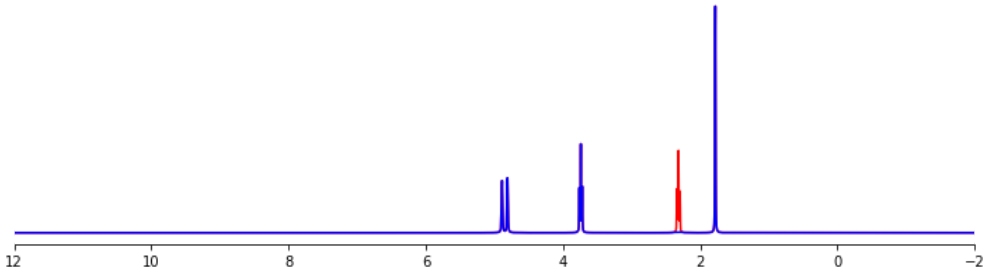




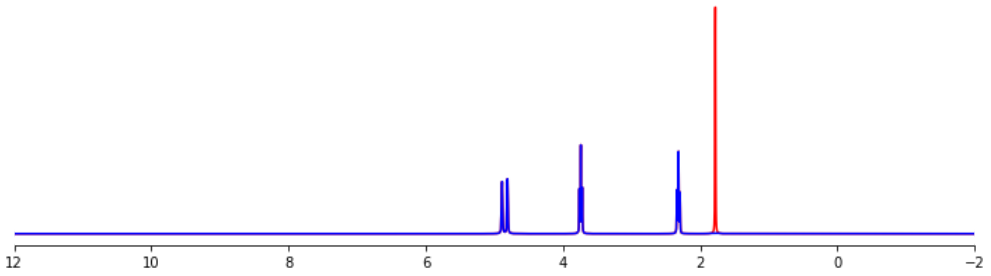
Top predicted substructures for the masked region(red):
0.7658 [CHX3](=C)C
0.7286 [#6H1][#6H2]
0.6776 [#6H1]
0.5786 [CX3H1](=[CX3H0])[CX4H2]
0.5257 [#6X3H1]=[#6X3H0]
0.4875 [CX3H0](=[CX3H1])([CX4H3])[CX4H3]
0.365 [CX4H2]([CX4H2])[CX4H1]
0.3321 [CX4H3][CX3H0][CX4H3]



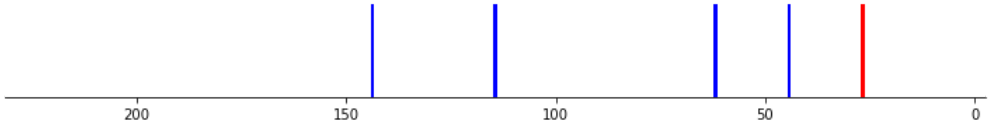
Top predicted substructures for the masked region(red):
0.4983 [CX4H3][CX3H0][CX4H3]
0.4585 [CX4H2]([#6])[O]
0.4264 [CH2X4](O)[CX4H2]
0.413 [CHX3](=C)C
0.3665 [CX3H1](=[CX3H0])[CX4H2]
0.3388 [CX4H2]([CX4H2])[CX4H1]
0.2923 [CX4H2]([OX2H1])[CX4H2]
0.2657 [#6X3H1]=[#6X3H0]



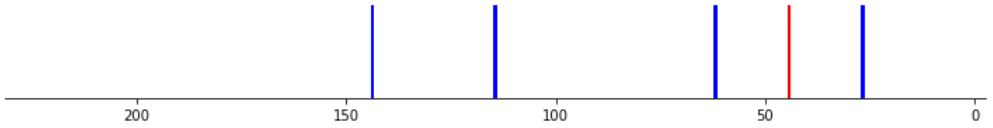
Top predicted substructures for the masked region(red):
0.6074 [CX4H2]([#6])[#6]
0.5727 [#6H1][#6H2]
0.5198 [CX3H1](=[CX3H0])[CX4H2]
0.5051 [CX4H2][CX3]=C
0.4226 [CX4H3][CX3H0][CX4H3]
0.2661 [CX4H2]([CX4H2])[CX4H1]
0.2327 [#6X3H1]=[#6X3H0]
0.201 OCC[CH2]



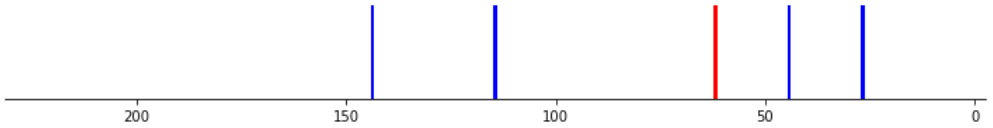
Top predicted substructures for the masked region(red):
0.9575 [CX4H3][CX3]
0.8529 [#6H3][#6]=[#6X3]
0.8394 [CX4H3][CX3H0][CX4H3]
0.8359 [#6H3][#6H0]
0.805 [CX4H3][CX3H0]
0.6597 [CX4H3][#6]
0.6322 [#6H3][#6][#6]
0.6125 [CX3H0](=[CX3H1])([CX4H3])[CX4H3]



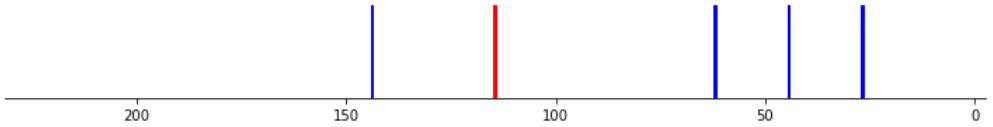
Top predicted substructures for the masked region(red):
0.8694 [CX4H3][CX3H0][CX4H3]
0.7846 [CX4H3][#6]
0.5248 [CX4H3][CX3H0]
0.4569 [CX3H1](=[CX3H0])[CX4H2]
0.4534 [CX3H0](=[CX3H1])([CX4H3])[CX4H3]
0.4065 [#6H3][#6][#6]
0.4015 [#6H3][#6H0]
0.3997 [CX4H3][CX3]



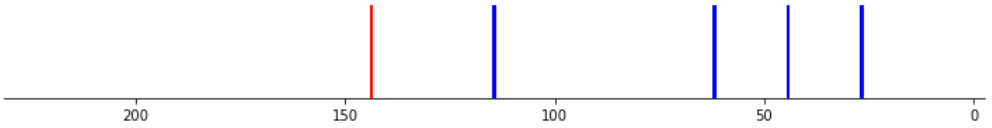
Top predicted substructures for the masked region(red):
0.4383 [#6H1][#6H2]
0.3587 [CX3H1](=[CX3H0])[CX4H2]
0.3563 [CX4H2]([CX4H2])[CX4H1]
0.2519 [CX4H2]([OX2H1])[CX4H2]
0.1871 [CX4H3][CX3H0][CX4H3]
0.1869 [#6X3H1]=[#6X3H0]
0.1845 CCCCC=C
0.1782 [#6H1]([#6H2])[#6H2]



Top predicted substructures for the masked region(red):
0.9233 [CX4H2]([OX2H1])[CX4H2]
0.8194 [CH2X4](O)[CX4H2]
0.7293 [CX4H2]([#6])[O]
0.462 [CHX3](=C)C
0.4184 [CX3H1](=[CX3H0])[CX4H2]
0.3519 [CX4H2]([CX4H2])[CX4H1]
0.3003 [#6H1][#6H2]
0.2949 [CX4H3][CX3H0][CX4H3]

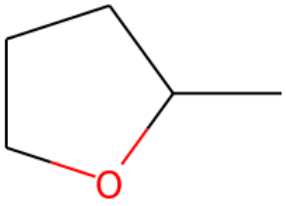


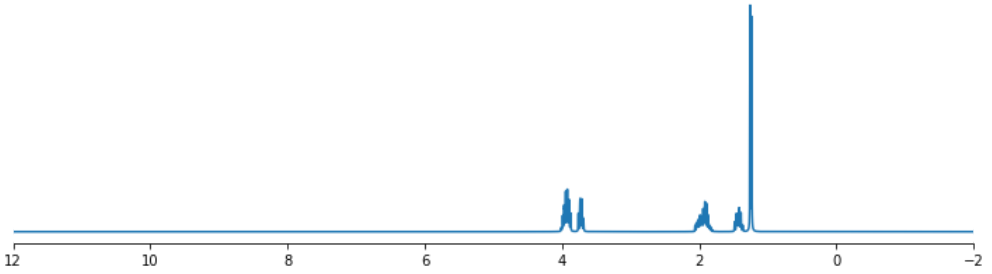
Top predicted substructures for the masked region(red):
0.5041 [CX4H3][CX3H0][CX4H3]
0.4596 [CX3H0](=[CX3H1])([CX4H3])[CX4H3]
0.3919 [CX3H1](=[CX3H0])[CX4H2]
0.2748 [CX3H2]=[CX3H0]([#6])[#6]
0.2344 [#6H1][#6H2]
0.2151 [CX4H2][CX3]=C
0.2139 [CX4H3][CX3H0]=[CX3H2]
0.199 [CX4H2]([CX4H2])[CX4H1]

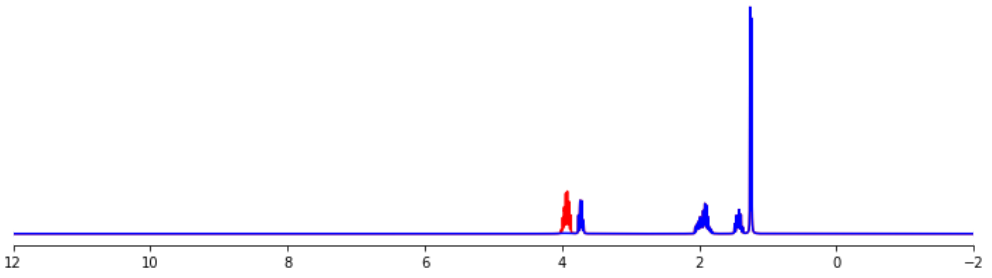


Top predicted substructures for the masked region(red):
0.8253 [CX4H3][CX3H0][CX4H3]
0.7597 [CHX3](=C)C
0.6672 [CX3H1](=[CX3H0])[CX4H2]
0.6197 [CX4H2][CX3]=C
0.5741 [#6X3H1]=[#6X3H0]
0.508 [CX3H0](=[CX3H1])([CX4H3])[CX4H3]
0.4122 [#8][#6][#6][#6X3]
0.3875 [OX2H1]

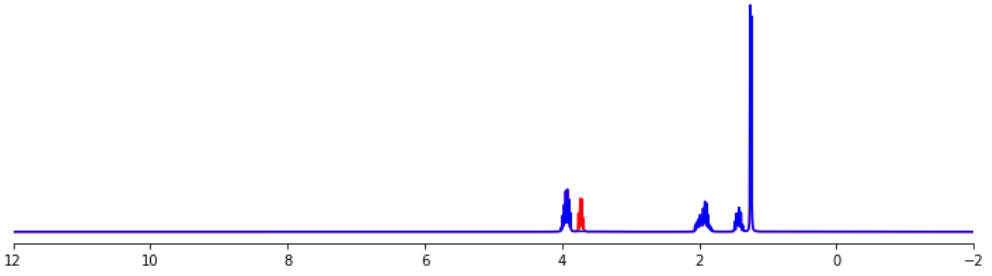
True structure: CC1CCCO1





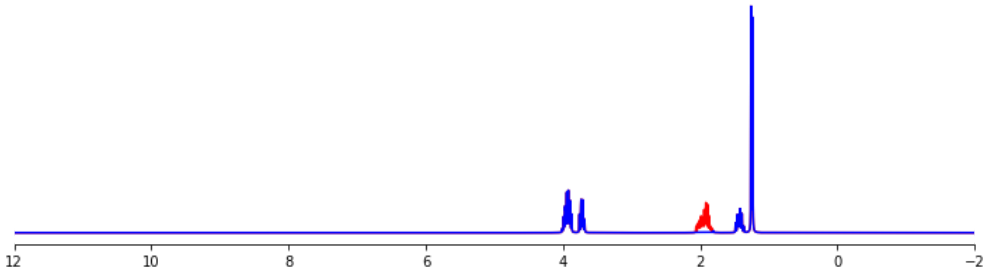


Top predicted substructures for the masked region(red):
0.6519 [CX4H2]([#6])[O]
0.6004 [CH2X4](O)[CX4H2]
0.5445 C1OCCC1
0.4984 [CX4H2][OX2H0][CX4H2]
0.481 [CX4H2](O)[CHX4]
0.4566 [OX2H0][CX4H2][CX4H2][CX4H2]
0.3899 [CX4H2]([OX2H0])[CX4H2]
0.3588 [OX2H0][CX4H2][CX4H1][CX4H2]

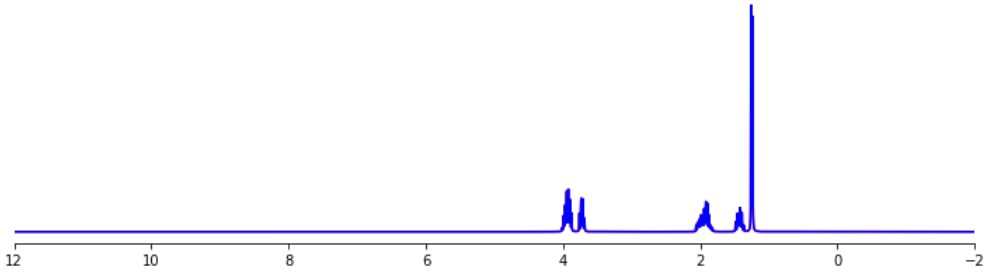


Top predicted substructures for the masked region(red):
0.5014 [CX4H2](O)[CHX4]
0.4921 [CX4H2][OX2H0][CX4H2]

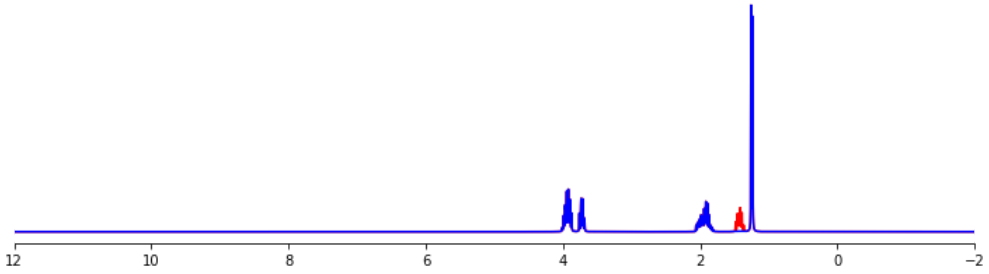
0.4183 [CX4H2]([#6])[O]
0.3706 [OX2H0][CX4H2][CX4H1][CX4H2]
0.2908 [CH2X4](O)[CX4H2]
0.2854 [CX4H2]([CX4H2])[CX4H2]
0.2169 [OX2H0][CX4H2][CX4H2][CX4H2]
0.1917 [#6H1]([#6H2])[#6H2]



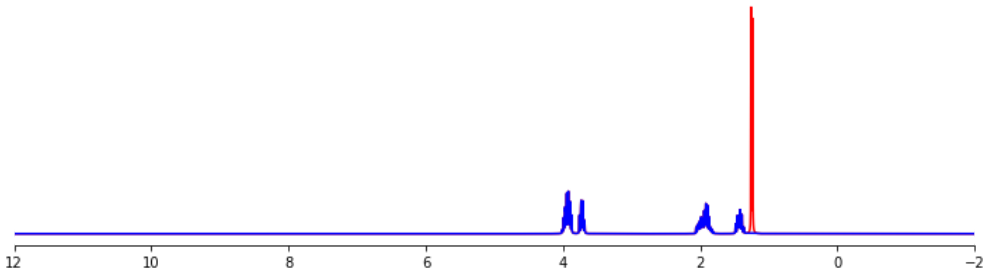
Top predicted substructures for the masked region(red):
0.5288 CCCCCC
0.3873 [CX4H2]([CX4H2])[CX4H2]
0.3184 O[CX4H][CX4H2]
0.3151 [#6H1]([#6H2])[#6H2]
0.3141 [OX2H0][CX4H2][CX4H1][CX4H2]
0.3093 [CX4H]O
0.2717 [CH2X4](O)[CX4H2]
0.2644 [#8][#6H0][#6H1]



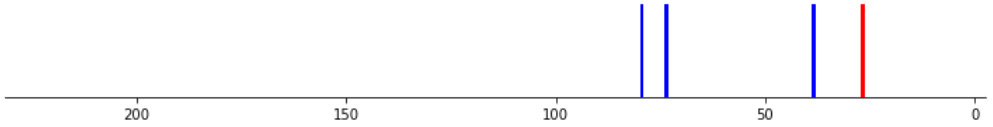
Top predicted substructures for the masked region(red):
0.3156 [CX4H2][OX2H0][CX4H2]
0.2589 [CH2X4](O)[CX4H2]
0.2583 [CX4H2]([CX4H2])[CX4H2]
0.2494 [#8][#6H0][#6H1]
0.229 CCCCCC
0.227 [OX2H0][CX4H2][CX4H1][CX4H2]
0.2099 C1OCCC1
0.1619 [OX2H0][CX4H2][CX4H2][CX4H2]



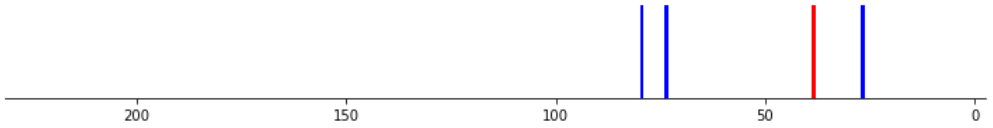
Top predicted substructures for the masked region(red):
0.3821 CCCCCC
0.3784 [CX4H2]([CX4H2])[CX4H2]
0.274 [CX4H2][OX2H0][CX4H2]
0.2678 [OX2H0][CX4H2][CX4H1][CX4H2]
0.2618 [#8][#6H0][#6H1]
0.2582 [CH2X4](O)[CX4H2]
0.2504 [CX4H2][CX4H2][CX4H2][CX4H2]
0.2374 [CH2X4](O)[CX4H2][CX4H2]



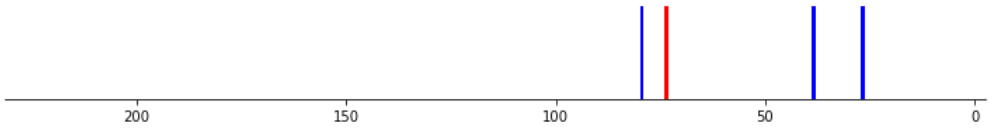
Top predicted substructures for the masked region(red):
0.6886 [#6H3][#6][#6]
0.6119 [CX4H3][#6]
0.4996 [CH3][#6][#8]
0.4342 [CX4H3][CX4]O
0.3845 [#8][#6H0][#6H1]
0.3684 CCCCCC
0.3474 [CX4H3]
0.3411 [CX4H]O



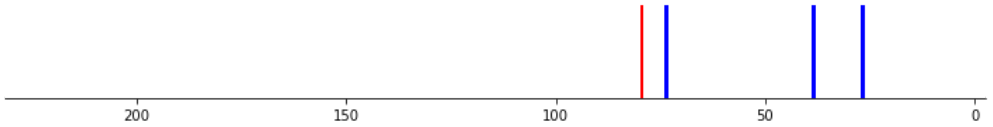
Top predicted substructures for the masked region(red):
0.7498 [CX4H2]([CX4H2])[CX4H2]
0.582 [OX2H0][CX4H2][CX4H2][CX4H2]
0.4863 CCCCCC
0.4545 [CH2X4](O)[CX4H2][CX4H2]
0.3283 [#8][#6H0][#6H1]
0.2812 [CX4H2][CX4H2][CX4H2][CX4H2]
0.2655 [CX4H]O
0.2647 C1OCCC1



Top predicted substructures for the masked region(red):
0.4833 CCCCCC
0.3926 [CX4H2][OX2H0][CX4H2]
0.3921 [CH2X4](O)[CX4H2]
0.3765 [OX2H0][CX4H2][CX4H1][CX4H2]
0.3178 [CX4H2]([CX4H2])[CX4H2]
0.2956 [CX4H2]([CX4H2])[CX4H0]
0.2377 [#6H1]([#6H2])[#6H2]
0.2343 [CX4H2](O)[CHX4]

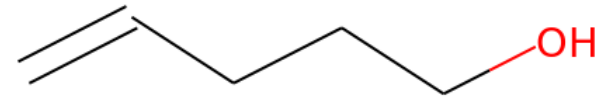


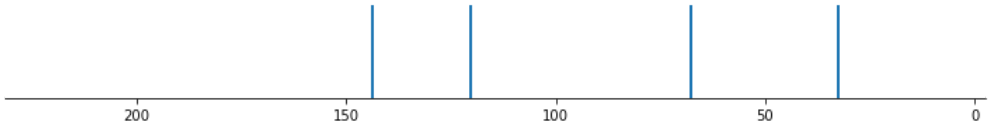
Top predicted substructures for the masked region(red):
0.6329 [CH2X4](O)[CX4H2]
0.5438 [CH2X4](O)[CX4H2][CX4H2]
0.5021 [OX2H0][CX4H2][CX4H2][CX4H2]
0.4908 [CX4H2]([OX2H0])[CX4H2]
0.3442 [CX4H2][OX2H0][CX4H2]
0.2786 [#8][#6H0][#6H1]
0.2775 C1OCCC1
0.2685 [CX4H2]([CX4H2])[CX4H2]

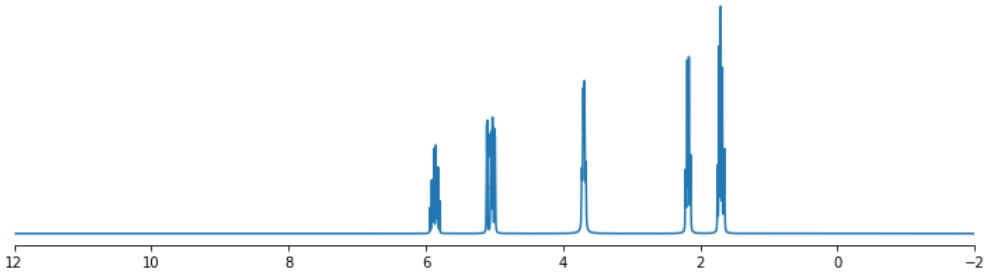


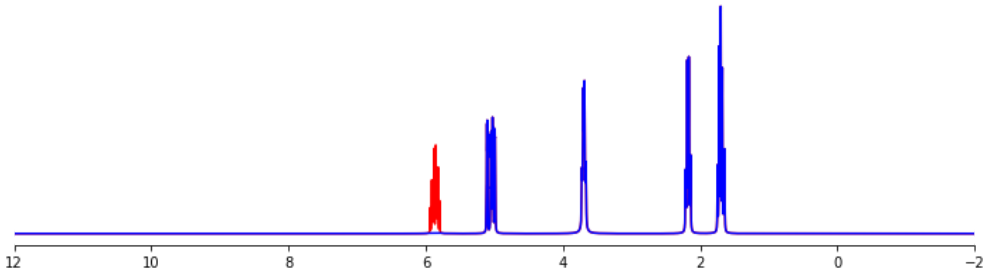
Top predicted substructures for the masked region(red):
0.5248 C1OCCC1
0.4279 [CH2X4](O)[CX4H2][CX4H2]
0.3828 [CX4H]O
0.3562 [OX2H0][CX4H2][CX4H2][CX4H2]
0.2995 [CX4H2]([CX4H2])[CX4H2]
0.2973 [#8][#6H0][#6H1]
0.2847 [CH2X4](O)[CX4H2]
0.2807 [OX2H0][CX4H2][CX4H1][CX4H2]

True structure: C=CCCCO



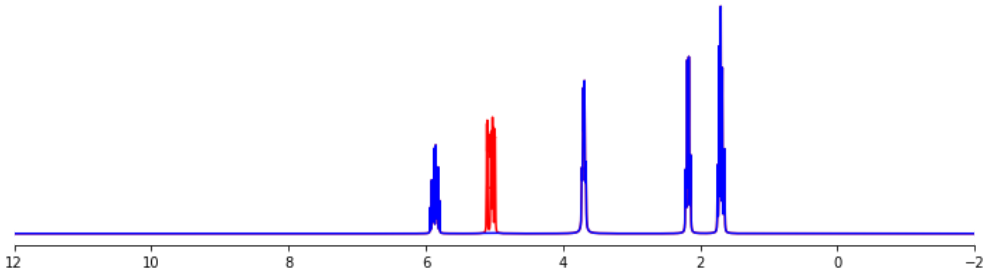






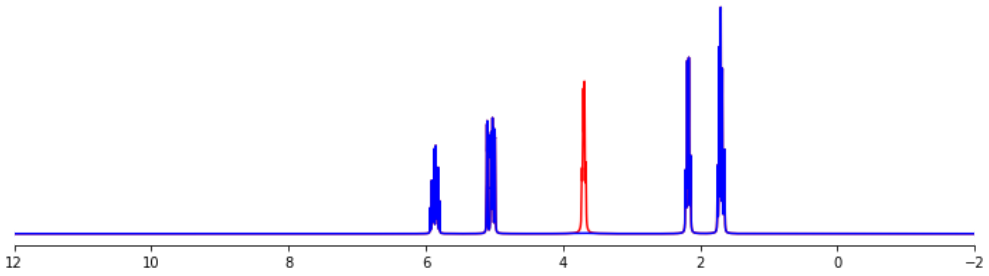
Top predicted substructures for the masked region(red):

0.815 [CX3H2]=[CX3H1]
0.6923 [CX3H1](=[CX3H2])[CX4H1]
0.6056 [#6X3H1][#6H1][#6H2]
0.5697 [#6H2][#6H1][#6H1]=[#6H2]
0.4881 [CHX3]=[CHX3]
0.458 [CX3H][CX4H]
0.4298 [CX4H]O
0.3378 [#6X3H2]



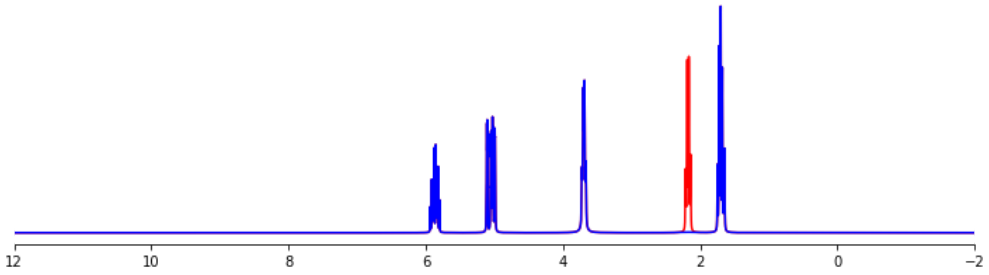
Top predicted substructures for the masked region(red):

0.8767 [CX3H1](=[CX3H2])[CX4H1]
0.8216 [CX3H2]=[CX3H1]
0.6291 [#6H2][#6H1][#6H1]=[#6H2]
0.6231 [CH2X3](=C)
0.615 [#6X3H2]
0.5588 [CX4H3][CX3]
0.5366 [#6X3H1][#6H1][#6H2]
0.5323 [CX4H2]([CX4H2])[CX4H1]



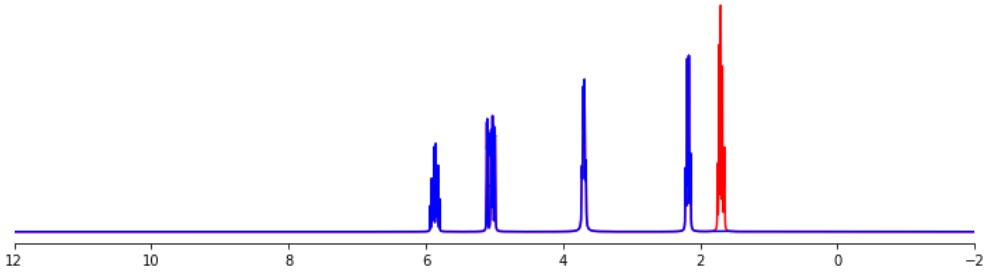
Top predicted substructures for the masked region(red):

0.84 [CX4H2]([#6])[O]
0.6955 [CH2X4](O)[CX4H2]
0.6272 [CX4H3][CX3]
0.4944 [#6X3H1][#6H1][#6H2]
0.445 [CX3H1](=[CX3H2])[CX4H1]
0.3944 [CHX3]=[CHX3]
0.3798 [#6H3][#6]=[#6X3]
0.3359 [CX4H2]([OX2H0])[CX4H2]



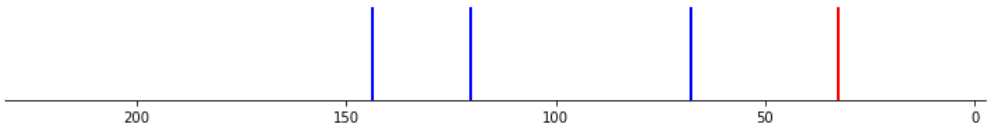
Top predicted substructures for the masked region(red):

0.5561 [CX4H3][CX3]
0.4927 [CX4H]O
0.4212 [CX4H2][CX3]=C
0.3602 [CX4H2][CX3H]
0.3392 [CHX3]=[CHX3]
0.3248 O[CX4H][CX4H2]
0.2877 [#6X4H2][#6H1][#8H]
0.2777 [CX4H2]([CX4H2])[CX4H1]



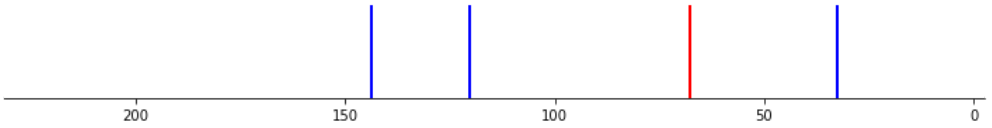
Top predicted substructures for the masked region(red):

0.7841 [#6H3][#6]=[#6X3]
0.6551 [CX4H2]([CX4H2])[CX4H1]
0.628 [CX4H3][CX3]
0.5727 [#6X3H1][#6H1][#6H2]
0.503 O[CX4H][CX4H2]
0.4928 [CX4H]O
0.4303 [CX4H3]
0.393 [CX3H0](=[CX3H1])([CX4H3])[CX4H3]

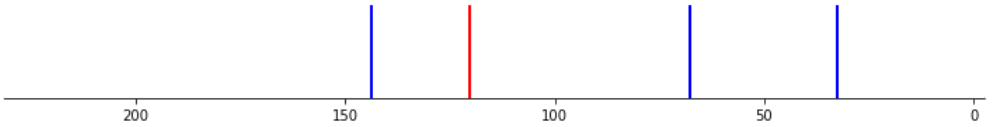


Top predicted substructures for the masked region(red):

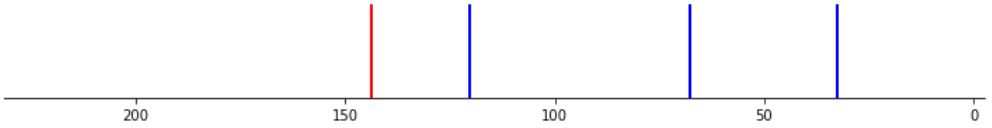
0.6278 [CX4H3][CX3]
0.5739 [CH2X4](O)[CX4H2][CX4H2]
0.5297 [CH2X4](O)[CX4H2]
0.4997 [CX4H2][CX4H2]
0.4969 [CX4H2]([CX4H2])[CX4H1]
0.3889 [CX4H2]([OX2H1])[CX4H2]
0.3535 [CHX3]=[CHX3]
0.3483 [CX4H2]([OX2H0])[CX4H2]



Top predicted substructures for the masked region(red):
0.9227 [CX4H2]([#6])[O]
0.8533 [CH2X4](O)[CX4H2]
0.6228 [CX4H3][CX3]
0.5992 [CX4H]O
0.5912 [#6X3H1][#6H1][#6H2]
0.5349 [CH2X4](O)[CX4H2][CX4H2]
0.5181 [CX3H1](=[CX3H2])[CX4H1]
0.4612 [CX4H2]([OX2H1])[CX4H2]

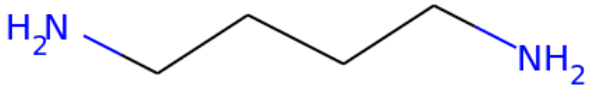


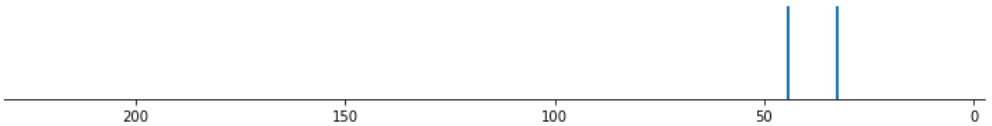
Top predicted substructures for the masked region(red):
0.9387 [CX3H2]=[CX3H1]
0.8557 [#6X3H2]
0.6612 [CX3H1](=[CX3H2])[CX4H1]
0.6279 [CX4H3][CX3]
0.5218 [CH2X3](=C)
0.4944 [CX4H]O
0.4068 [#6H2][#6H1][#6H1]=[#6H2]
0.3987 [#6H3][#6]=[#6X3]

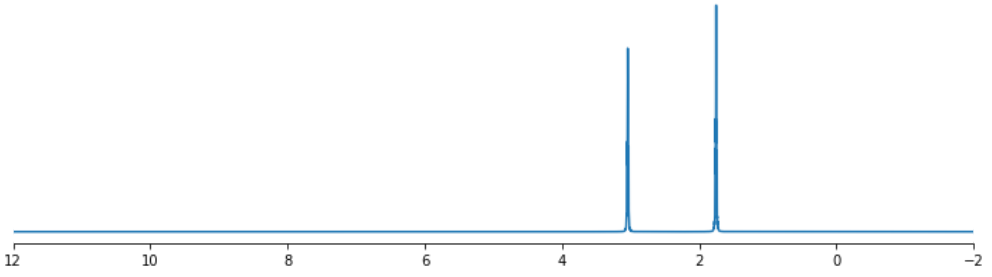


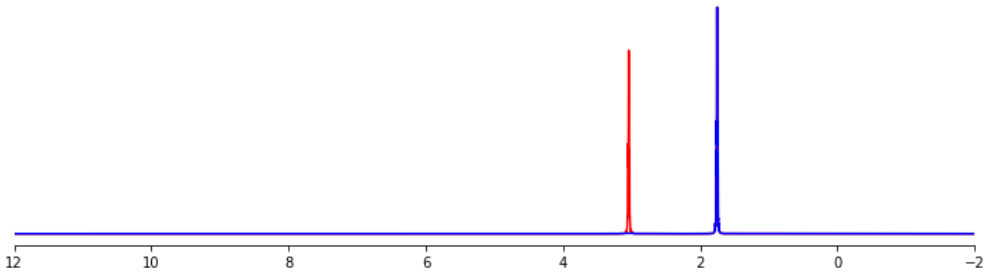
Top predicted substructures for the masked region(red):
0.7029 [CX3H1](=[CX3H2])[CX4H1]
0.6499 [#6X3H1][#6H1][#6H2]
0.6294 [#6H2][#6H1][#6H1]=[#6H2]
0.628 [CX4H3][CX3]
0.4867 [CX3H][CX4H]
0.4734 [#6H3][#6]=[#6X3]
0.3866 [CX4H2]([OX2H1])[CX4H2]
0.3829 [CH2X3](=C)

True structure: NCCCCN

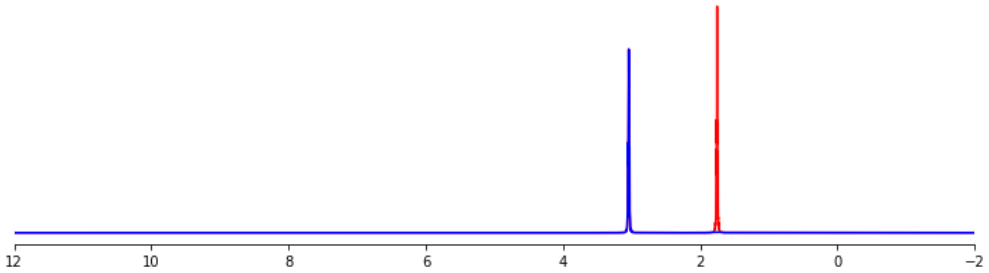




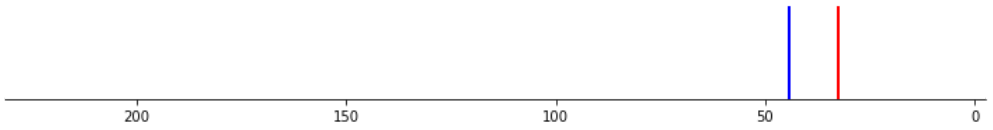




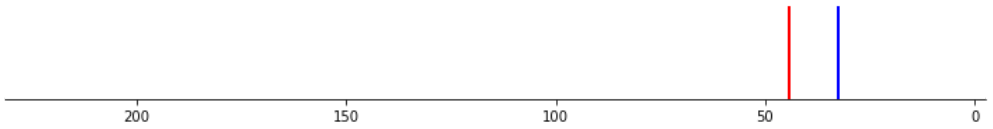
Top predicted substructures for the masked region(red):
0.3848 [#7][#6H2][#6H2]
0.383 [#6H1]
0.3829 [#7X3][#6H2]
0.3705 [CX4H2]([NX3H1])[CX4H2]
0.3606 [#7H2][#6H2]
0.3384 [#7][#6][#6][#6][#7]
0.2696 [#7][#6H2]
0.191 [CX4H2]([NX3H2])[CX4H2]



Top predicted substructures for the masked region(red):
0.4031 [CX4H2]([CX4H2])[CX4H2]
0.3937 [CX4H2]([#6])[#6]
0.3668 [#6H1]
0.2595 [CX4H2][CX4H2][CX4H2][CX4H2]
0.2524 [#7][#6][#6][#6][#7]
0.1716 [CX4H2][CX4H2]
0.147 [#6H1][#6H2]
0.1408 [#7][#6][#6][#6][#6][#7]

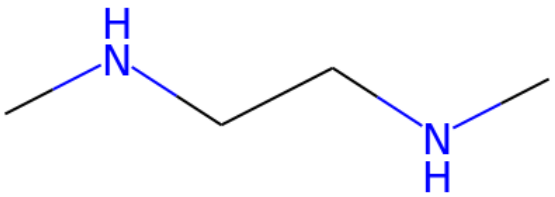


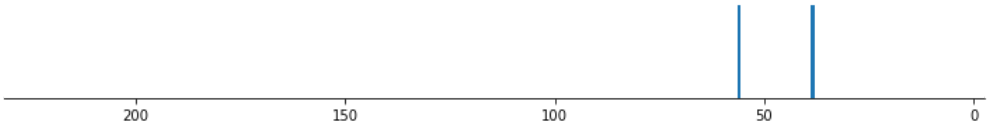
Top predicted substructures for the masked region(red):
0.5206 [CX4H2]([CX4H2])[CX4H2]
0.3852 [CX4H2][CX4H2][CX4H2][CX4H2]
0.3685 [CX4H2][CX4H2]
0.2654 [CX4H2]([NX3H1])[CX4H2]
0.239 [#7][#6][#6][#6][#7]
0.1782 [#6H1]
0.1282 [#7H2][#6H2]
0.0979 [#7X3][#6H2]

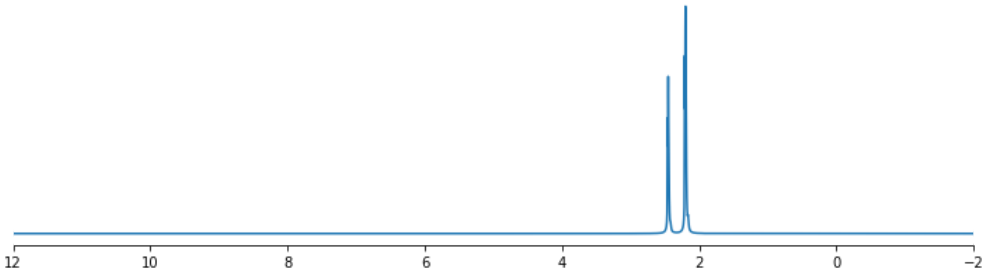


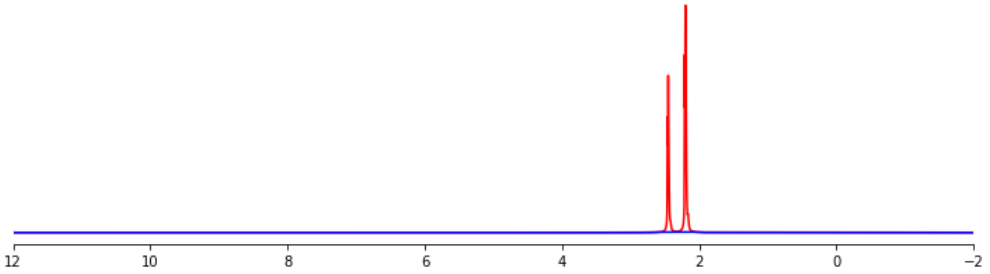
Top predicted substructures for the masked region(red):
0.448 [#7][#6][#6][#6][#7]
0.4065 [#7][#6H2]
0.3857 [#7X3][#6H2]
0.3425 [#7H2][#6H2]
0.3391 [CX4H2]([NX3H1])[CX4H2]
0.2498 [#6H1]
0.2275 [CX4H2]([CX4H2])[CX4H2]
0.2212 [CX4H2]([NX3H2])[CX4H2]

True structure: CNCCNC

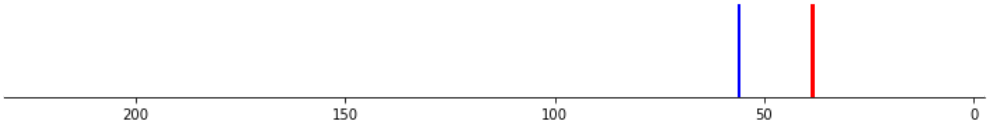




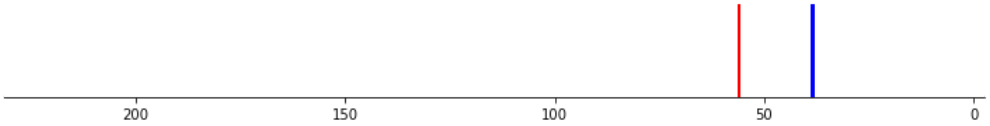




Top predicted substructures for the masked region(red):
0.986 [CX4H2]([#6])[#6]
0.5809 [#7X3][#6H3]
0.5685 [#6H1][#6H2]
0.5574 [#7H2][#6H1]
0.4427 [CX4H2]([CH])[CH]
0.4236 [#6H1]
0.3737 [#6H1]([#6H2])[#6H2]
0.3703 C1CCC1

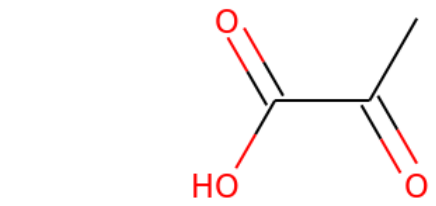


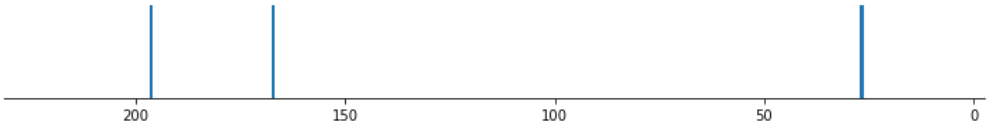
Top predicted substructures for the masked region(red):
0.3357 [CX4H2]([CH])[CH]
0.3354 [#7][#6][#6][#6][#7]
0.306 [CX4H3]
0.3009 [#7H2][#6H1]
0.2945 [#7H2][#6H2]
0.2592 [#6H3][#7]
0.255 C1CCC1
0.1764 [CX4H2][CX4H2]

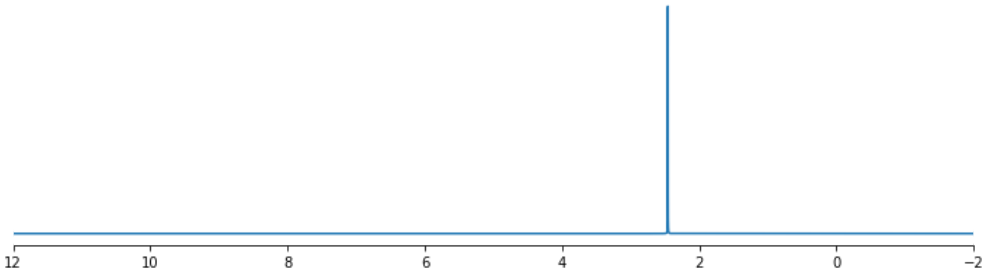


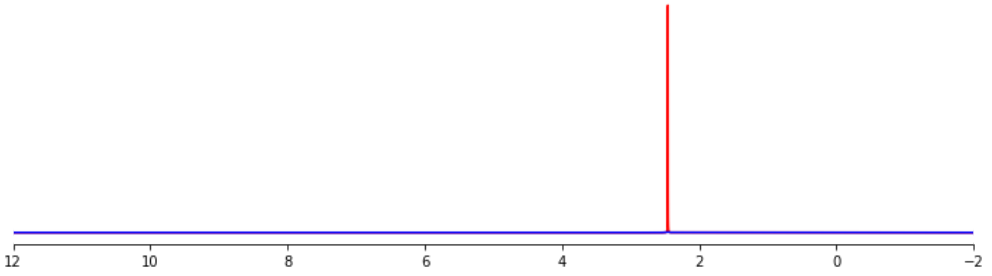
Top predicted substructures for the masked region(red):
0.6555 [#7H2][#6H1]
0.2828 [CX4H3]
0.2733 [CX4H2]([CH])[CH]
0.2512 [#7][#6][#6][#6][#7]
0.2391 [#6H2][#7][#6H2]
0.1709 [#7X3][#6H3]
0.1644 [CX4H3][NX3H0]
0.1544 C1CCC1

True structure: CC(=O)C(=O)O

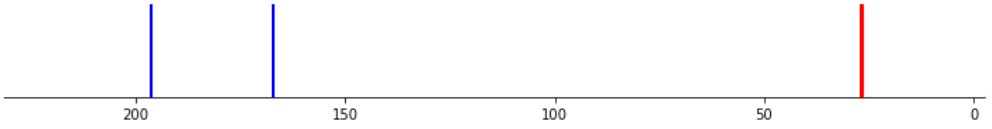




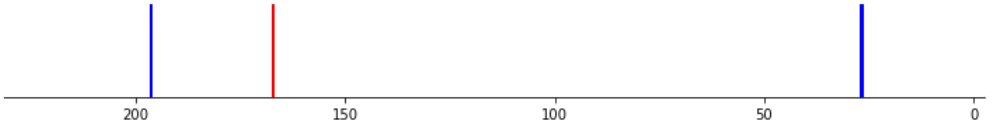




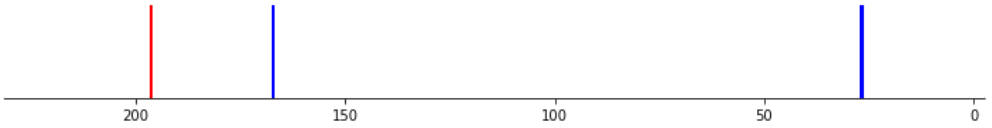
Top predicted substructures for the masked region(red):
0.7845 [CX4H3][CX3]
0.6779 [CX3H0](=[OX1H0])([CX4H3])[CX3H0]
0.545 [CX4H3][CX3H0]
0.4555 [#6H3][#6H0]
0.4197 [CX4H3][CX3H0][CX3]=O
0.3685 [OX1H0]=[CX3H0][CX4H3]
0.3322 [#6X3][#6][#6][#6H3]
0.3041 [#6H3][#6][#6X3]



Top predicted substructures for the masked region(red):
0.8235 [CX4H3][CX3]
0.6786 [CX3H0](=[OX1H0])([CX4H3])[CX3H0]
0.5197 [CX4H3][CX3H0]
0.4653 [#6H3][#6][#6X3]
0.4569 [CX4H3][#6]
0.4538 [#6H3][#6H0]
0.4373 [#6H3][#6][#6]
0.4331 [OX1H0]=[CX3H0][CX4H3]

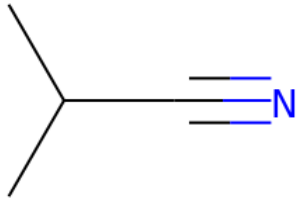


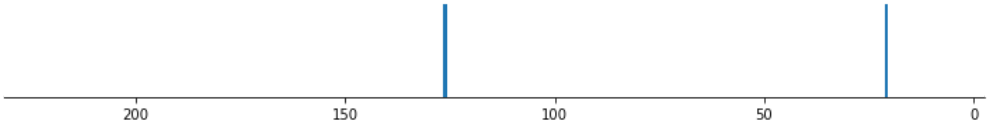
Top predicted substructures for the masked region(red):
0.7488 [CX3](=[OX1])O
0.6838 [CX3H0](=[OX1H0])([OX2H1])[CX3H0]
0.5382 [#8]=[#6][#8]
0.3789 [CX3H0](=[OX1H0])([CX4H3])[CX3H0]
0.2905 [#6X3][#6][#6][#6H3]
0.2799 [#8]=[#6][#6]=[#6][#6]=[#8]
0.2625 [CX3](=O)[OX2H1]
0.2167 [#6H3][#6][#6X3]

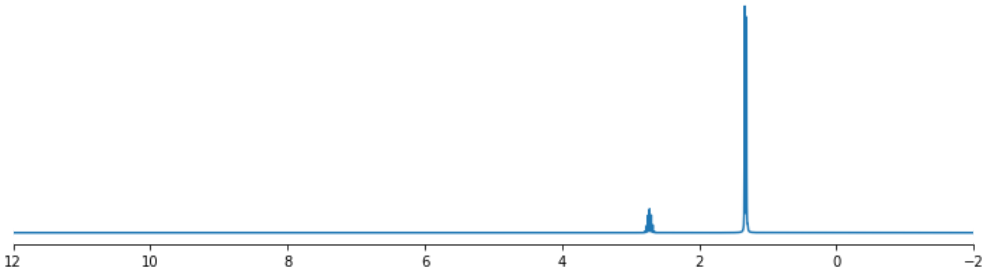


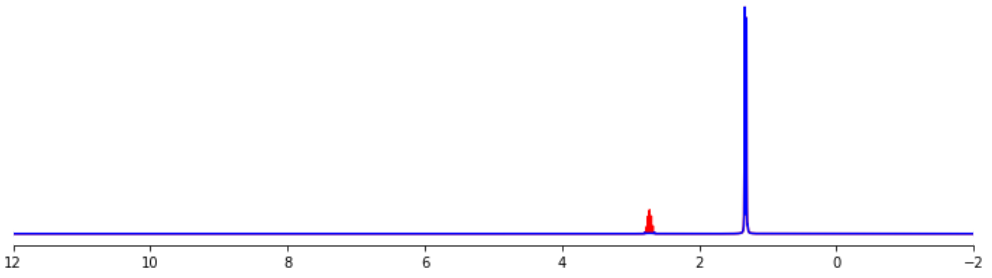
Top predicted substructures for the masked region(red):
0.9592 [CX3H0](=[OX1H0])([CX4H3])[CX3H0]
0.8569 [#6X3][#6X3]
0.8552 [OX1H0]=[CX3H0][CX3H0][CX4H3]
0.813 [#6H3][#6][#6X3]
0.7913 [CX4H3][CX3H0][CX3]=O
0.7751 [CX4H3][CX3]
0.6512 [OX1H0]=[CX3H0][CX4H3]
0.6453 [#8]=[#6][#6]=[#8]

True structure: CC(C)C#N

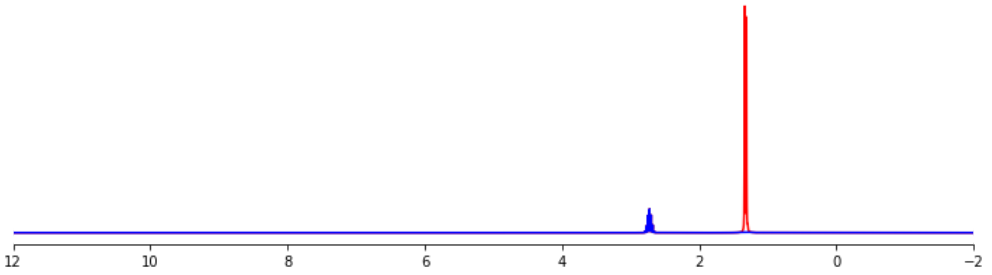






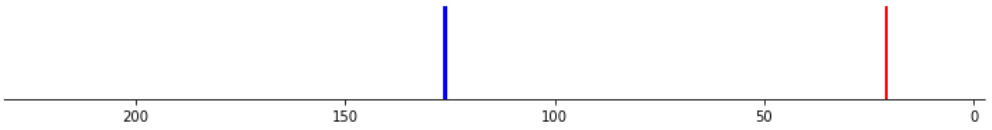


Top predicted substructures for the masked region(red):
0.439 [CX4H3][CX4H0r3]
0.294 [#6H3][#6][#6][#6H3]
0.2904 [CX4H2]([#6])[#6]
0.2615 [CX2H0](#[NX1H0])[CX4H1]
0.2514 [CX2H0](#[NX1H0])[CX4H2]
0.2487 [#6]#[#7]
0.2423 [#7]#[#6H0][#6H1]
0.228 [CX4H3][CX4H1]

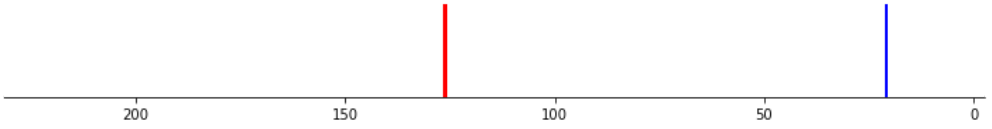


Top predicted substructures for the masked region(red):
0.5455 [#6H3][#6][#6][#6H3]
0.5196 [CX4H3][CX4H1]

0.5005 [#6H1]
0.4648 [#6]#[#7]
0.4471 [CX4H3][CX4H0r3]
0.4184 [CX4H3][#6]
0.3566 [CX2H0](#[NX1H0])[CX4H1]
0.3367 [CX4H3][CX4H0][CX4H3]

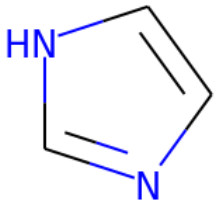


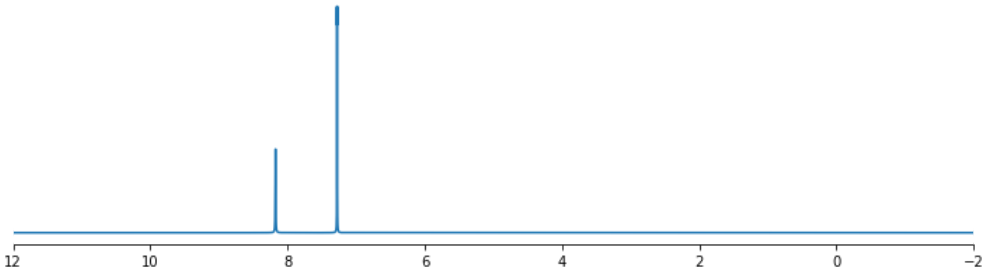
Top predicted substructures for the masked region(red):
0.7875 [CX4H3][#6]
0.6146 [CX4H3][CX4H1]
0.5643 [#6H3][#6][#6][#6H3]
0.5198 [CX4H3]
0.4438 [CX4H3][CX4H0r3]
0.4268 [#6H3][#6][#6]
0.3786 [#6]#[#7]
0.3336 [CX2H0](#[NX1H0])[CX4H1]

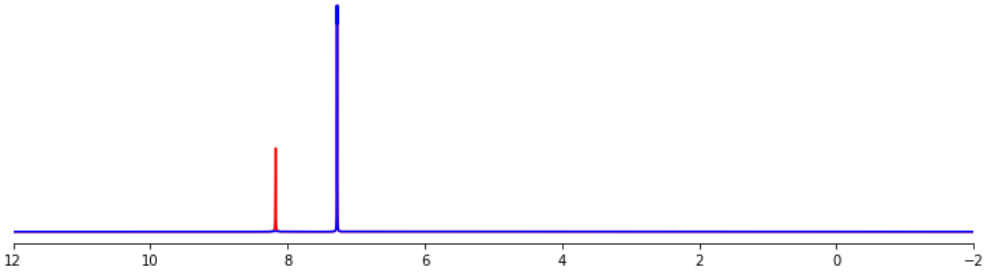


Top predicted substructures for the masked region(red):
0.7874 [#6]#[#7]
0.375 [#6H3][#6][#6][#6H3]
0.3647 [CX2H0](#[NX1H0])[CX4H1]
0.2902 [#7]#[#6H0][#6H1]
0.2624 [CX4H3][CX4H0][CX4H3]
0.2552 [cH]
0.2489 [CX2H0](#[NX1H0])[CX4H2]
0.2234 [CX4H3][CX4H1]

True structure: c1c[nH]cn1

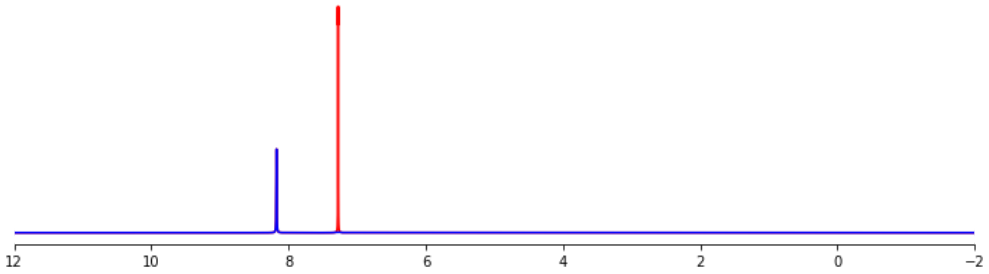




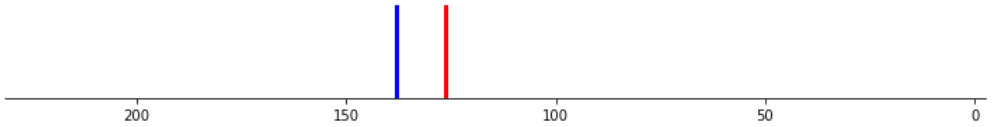


Top predicted substructures for the masked region(red):
0.2884 [#6H1][#7][#6H1]
0.2717 [#7][#6H1][#7]

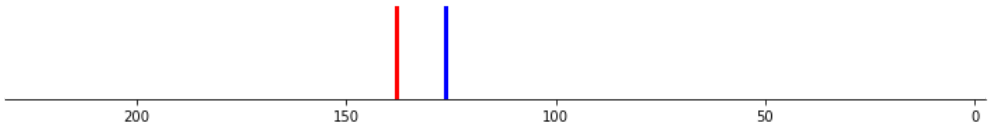
0.2261 [cX3H1]([nX2H0])[cX3H0]
0.214 [cX3H1]([cX3H1])[cX3H0]
0.1841 [cX3H1]([cX3H1])[cX3H1]
0.1749 [OX2H1]
0.1399 [cX3H1]([nX2H0])[cX3H1]
0.135 [#7X3H0]



Top predicted substructures for the masked region(red):
0.3081 [#7][#6H1][#7]
0.2974 [cX3H1]([cX3H1])[cX3H0]
0.2784 [#6H1][#6H1]
0.2277 [#7][#6H0][#6H1]
0.2036 [#6X3H1][#6X3H1][#6X3H0][#6X3H1]
0.1916 [cX3H1]([cX3H1])[cX3H1]
0.1895 [#7][#7]
0.1888 [cH][cH]

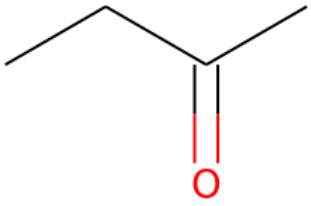


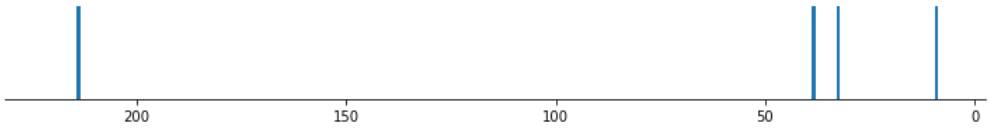
Top predicted substructures for the masked region(red):
0.3149 [#6X3][#6X3][#6X3][#6X3]
0.2604 [cX3H1]([cX3H1])[cX3H0]
0.2173 [#6H1][#6H1]
0.211 [cX3H1]([nX2H0])[cX3H0]
0.1869 [OX2H1]
0.1731 [cX3H1]([cX3H1])[cX3H1]
0.1513 [#7][#6][#6X3]
0.1396 [#7][#6][#6][#6][#7]

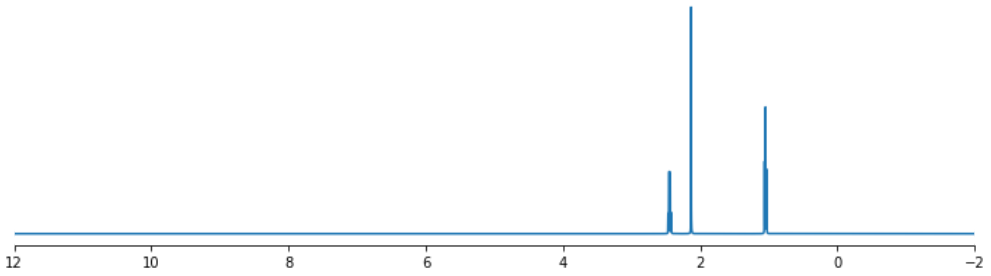


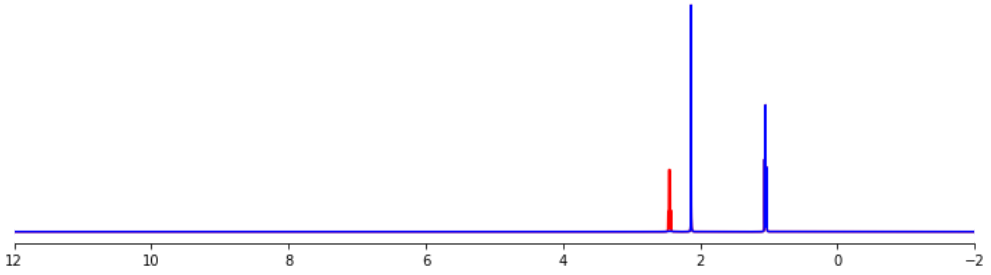
Top predicted substructures for the masked region(red):
0.3481 [cX3H1]([nX2H0])[cX3H0]
0.2787 [cX3H1]([cX3H1])[cX3H0]
0.2222 [#6X3][#6X3][#6X3][#6X3]
0.2145 [#6]1[#6][#6][#6][#6][#7]1
0.1917 [cX3H1]([cX3H1])[cX3H1]
0.1855 [OX2H1]
0.1816 [#7][#6X3H0][#6X3H1]
0.1755 [#7][#6H0][#6H1]

True structure: CCC(C)=O



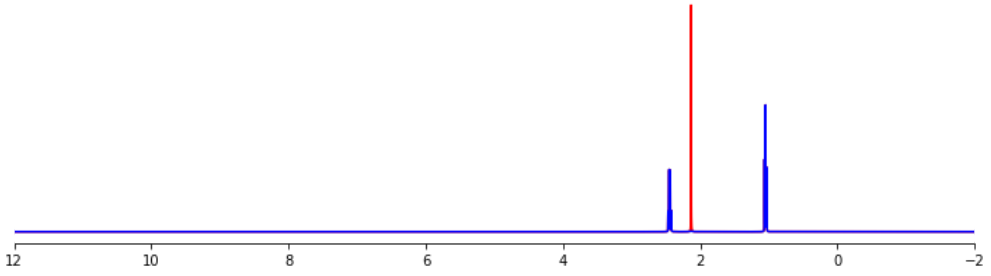






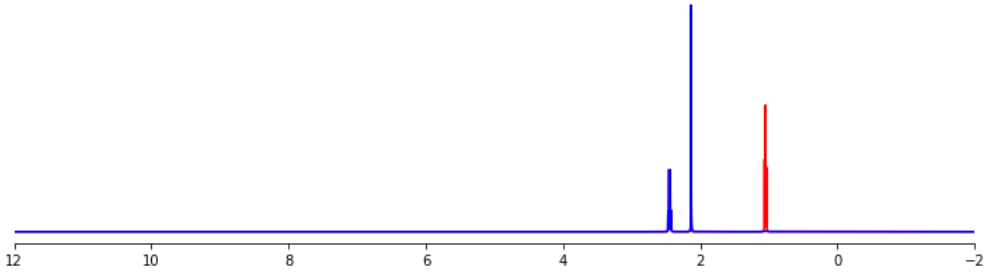
Top predicted substructures for the masked region(red):

0.5413 [CX4H2]([#6])[#6]
0.3597 O=[CX3H0][CX4H2][CX4H2]
0.3293 [#6H3][#6X3H0][#6H2]
0.2948 [CX4H2]CC=O
0.2803 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.2185 [CX4H2][CX3]=O
0.1783 [OX1H0]=[CX3H0]([#6])[CX4H2]
0.1714 CCCCCC



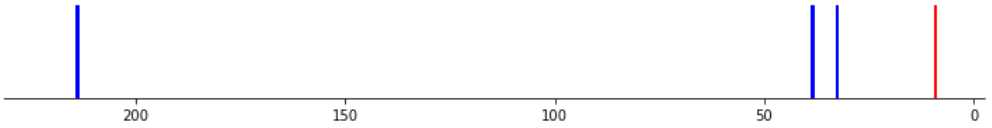
Top predicted substructures for the masked region(red):

0.9878 [CX4H3][CX3H0]
0.9831 [OX1H0]=[CX3H0][CX4H3]
0.9592 [CX4H3][CX3]
0.8837 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.8679 [#6H3][#6H0]
0.7187 [#6H3][#6X3H0][#6H2]
0.3055 [#6X3][#6][#6][#6H3]
0.081 O=[CX3H0][CX4H2][CX4H2]

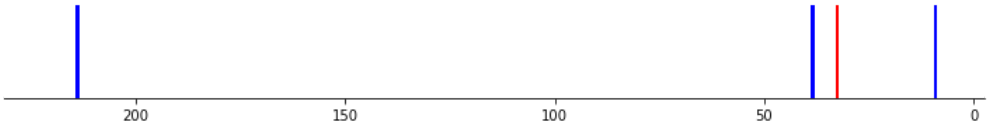


Top predicted substructures for the masked region(red):

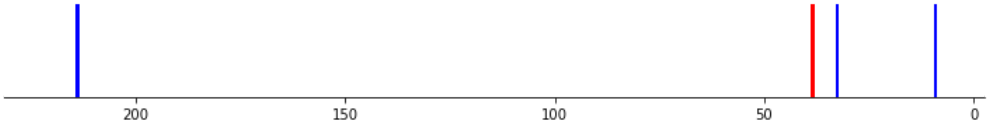
0.4349 [#6H3][#6][#6X3]
0.3872 [#6X3][#6][#6][#6H3]
0.3853 [CX4H3][CX4H2]
0.33 [CX4H2]([CX4H3])[CX3H0]
0.0949 CCCCCC
0.0836 [#6H1]
0.0591 [CX4H2]([CX4H3])[CX4H2]
0.0508 [#6H2][#6X3H0][#6H2]



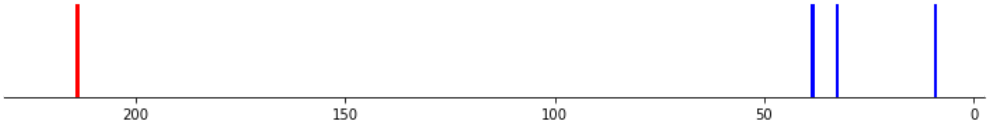
Top predicted substructures for the masked region(red):
0.9503 [CX4H3][CX4H2]
0.7941 [CX4H2]([CX4H3])[CX3H0]
0.6447 [OX1H0]=[CX3H0][CX4H2][CX4H3]
0.44 [#6H3][#6][#6X3]
0.2755 [#6X3][#6][#6][#6H3]
0.0936 [#6H2][#6X3H0][#6H2]
0.0441 [CX4H2]([CX4H3])[CX4H2]
0.0337 [#8]=[#6][#6]=[#8]



Top predicted substructures for the masked region(red):
0.2512 [#6H3][#6X3H0][#6H2]
0.2352 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.2163 O=[CX3H0][CX4H2][CX4H2]
0.2127 [#6X3][#6][#6][#6H3]
0.2049 [CX4H3][CX3H0]
0.1882 [CX4H2]CC=O
0.1205 [OX1H0]=[CX3H0][CX4H3]
0.0884 CCCCCC

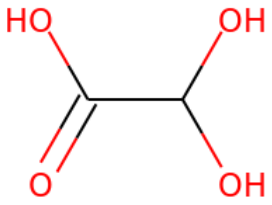


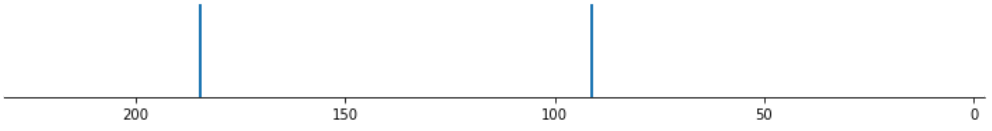
Top predicted substructures for the masked region(red):
0.3502 O=[CX3H0][CX4H2][CX4H2]
0.2575 [CX4H2]CC=O
0.2539 [#6X3][#6][#6][#6H3]
0.1689 [CX3H0](=[OX1H0])([CX4H3])[CX4H2]
0.1531 [CX4H2]([CX4H2])[CX3H0]
0.1393 CCCCCC
0.138 [#6H3][#6X3H0][#6H2]
0.126 [#6H2][#6X3H0][#6H2]

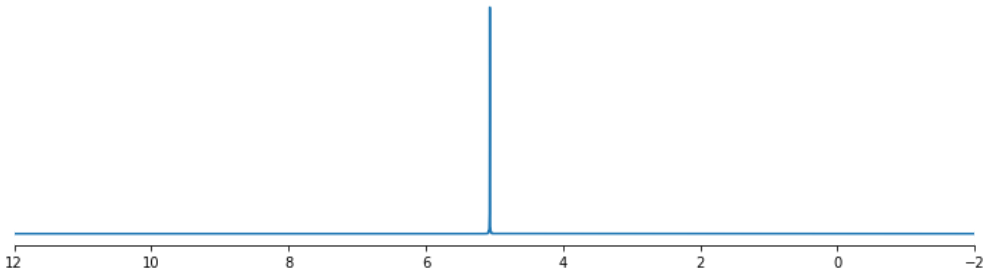


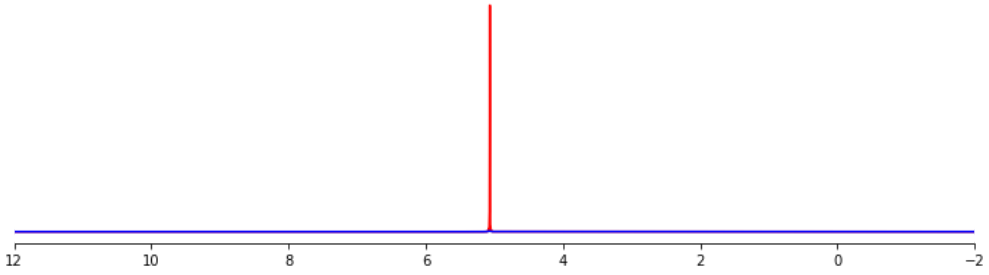
Top predicted substructures for the masked region(red):
0.9968 [OX1H0]=[CX3H0]([#6])[CX4H2]
0.9929 [CX4H2]([CX4H3])[CX3H0]
0.9927 [#6H3][#6][#6X3]
0.9854 [CX4H3][CX3H0]
0.9705 [OX1H0]=[CX3H0][CX4H3]
0.9649 [CX3](=[OX1])C
0.9577 [CX4H3][CX3]
0.9406 [OX1H0]=[CX3H0][CX4H2][CX4H3]

True structure: O=C(O)C(O)O

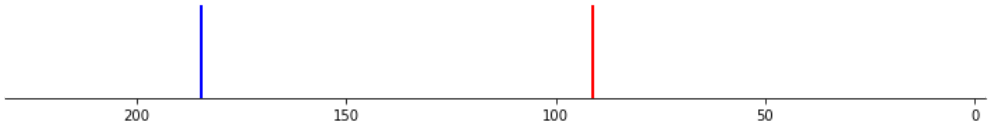




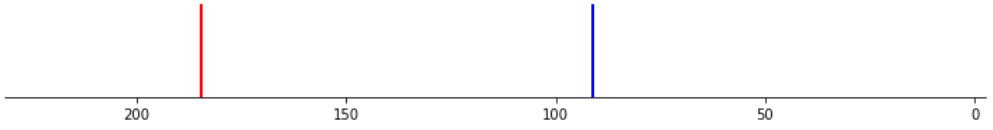




Top predicted substructures for the masked region(red):
0.8076 [#8]=[#6][#6H2][#8]
0.7352 [CX4H2][CX3]=O
0.708 [OX2H0][CX4H2][#6H0]
0.7077 [CX4H2]([OX2H0])[OX2H0]
0.5631 [#6X3][#6H2][#8]
0.5591 [CX4H2][OX2H0][CX4H2]
0.5149 [CX4H2]([#6])[O]
0.3321 [CX4H2]([OX2H0])[CX3H0]

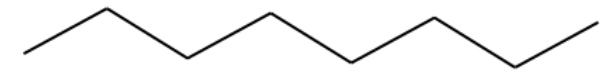


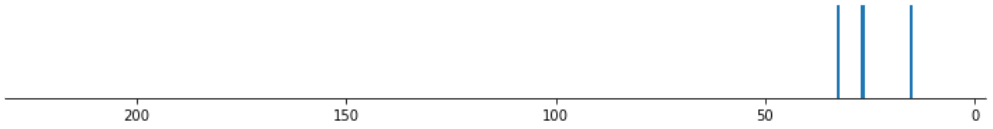
Top predicted substructures for the masked region(red):
0.709 [CX4H2]([OX2H0])[OX2H0]
0.6074 [OX2H0][CX4H2][#6H0]
0.4834 [CX4H2][OX2H0][CX4H2]
0.4344 [#6X3][#6H2][#8]
0.319 [CX4H2]([OX2H0])[CX3H0]
0.3055 [#8][#6H0][#6H1]
0.2769 [CX4H2]([#6])[O]
0.2013 [#8][#6][#6]=[#8]

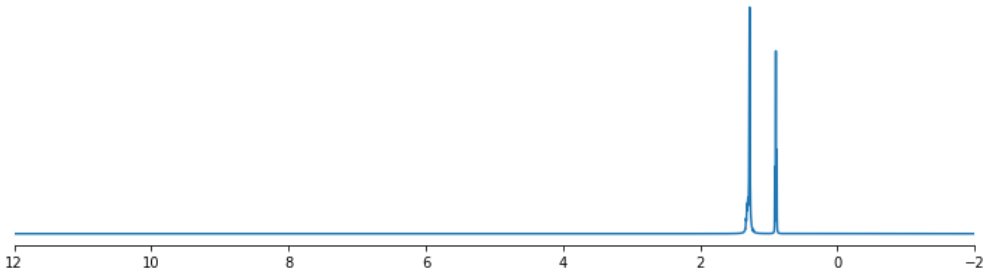


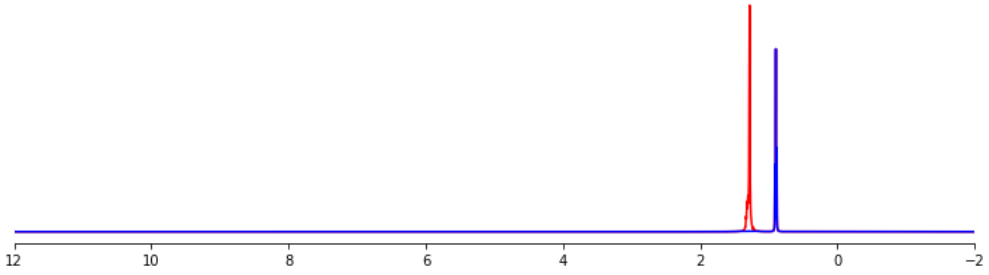
Top predicted substructures for the masked region(red):
0.9187 [CX3](=[OX1])C
0.8941 [#8][#6][#6]=[#8]
0.8112 [#8]=[#6][#6H2][#8]
0.8083 [CX4H2][CX3]=O
0.5652 [CX3](=[OX1])O
0.5651 [CX3](=O)[OX2H1]
0.5642 [#6X3][#6H2][#8]
0.4765 [OX2H0][CX4H2][#6H0]

True structure: CCCCCCCC

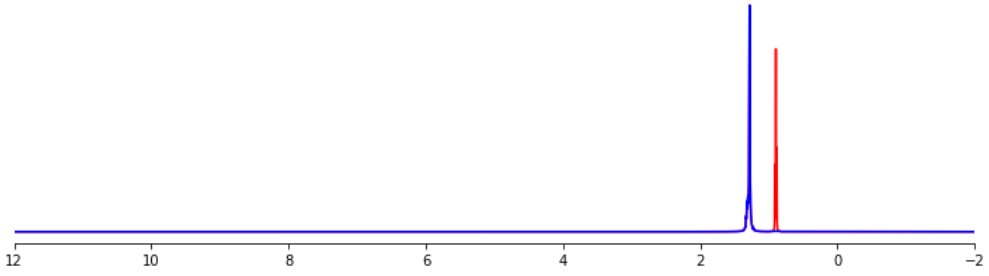




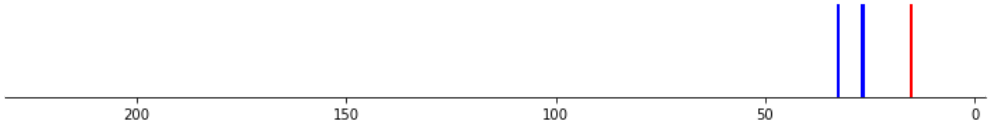




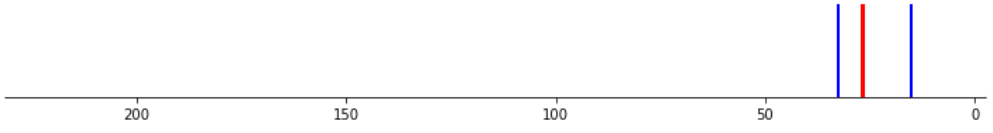
Top predicted substructures for the masked region(red):
0.7954 [CX4H2][CX4H2][CX4H2][CX4H2]
0.7352 [CX4H2]([CX4H2])[CX4H2]
0.6429 [CX4H2]([CX4H3])[CX4H2]
0.5987 [CX4H2][CX4H2]
0.2944 [CX4H2]([#6])[#6]
0.2727 [#6H1]
0.1789 CCCCCC
0.0984 [CX4H2]([CX4H2])[CX4H1]



Top predicted substructures for the masked region(red):
0.7404 [CX4H2]([CX4H3])[CX4H2]
0.5436 [#6H1]
0.4161 [CX4H2]([CX4H2])[CX4H2]
0.2806 [CX4H2]([#6])[#6]
0.2801 [CX4H2][CX4H2]
0.2377 CCCCCC
0.1745 [CX4H2]([CX4H3])[CX4H1]
0.14 [CX4H3][CX4H2]

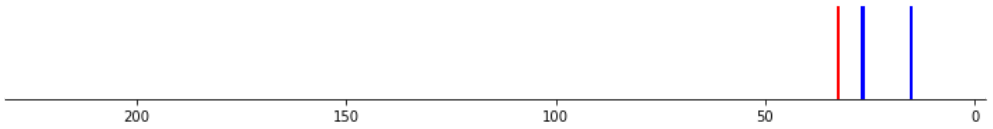


Top predicted substructures for the masked region(red):
0.7993 [CX4H3][CX4H2]
0.7205 [CX4H2]([CX4H3])[CX4H2]
0.3563 [CX4H2]([CX4H2])[CX4H2]
0.2426 [CX4H2][CX4H2]
0.1959 [CX4H2]([#6])[#6]
0.1882 [CX4H2]([CX4H3])[CX4H1]
0.1347 [#6H3][#6][#6][#6H3]
0.0947 [#6H1]



Top predicted substructures for the masked region(red):
0.6739 [CX4H2]([CX4H2])[CX4H2]
0.5799 [CX4H2][CX4H2][CX4H2][CX4H2]
0.4953 [CX4H2]([CX4H3])[CX4H2]
0.4226 [CX4H2][CX4H2]
0.2488 [#6H1]

```
0.1887   CCCCCC
0.0886   [#6H3][#6H0]
0.0883   [CX4H2]([#6])[#6]
```




```
Top predicted substructures for the masked region(red):
0.8427   [CX4H2]([CX4H2])[CX4H2]
0.6217   [CX4H2][CX4H2][CX4H2][CX4H2]
0.4257   [CX4H2][CX4H2]
0.3043   [CX4H2]([CX4H3])[CX4H2]
0.2981   CCCCCC
0.1795   [#6H1]
0.0711   [#6H3][#6H0]
0.07     [CX4H2]([CX4H2])[CX4H1]
```

In [ ]:

In [ ]: