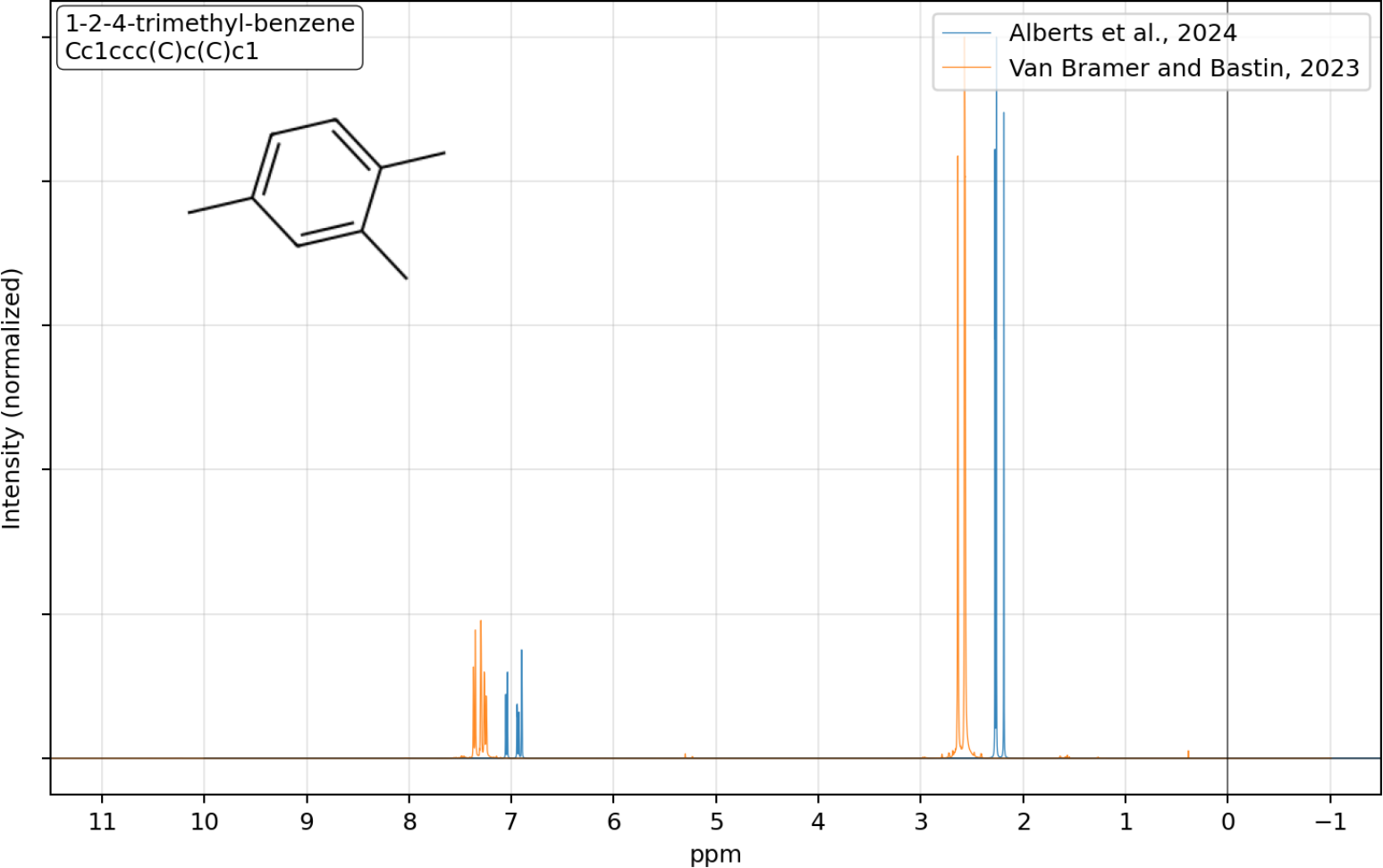
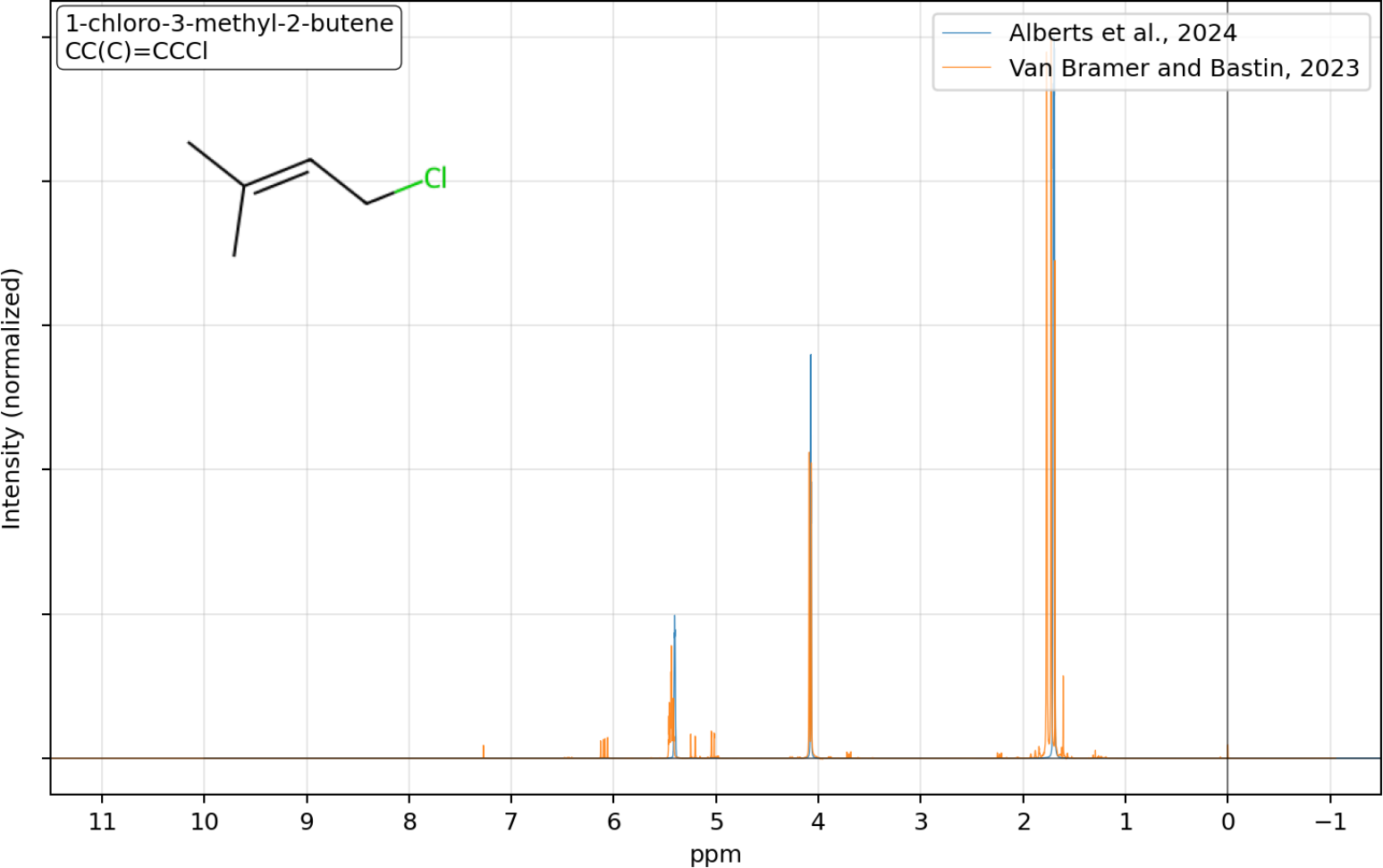
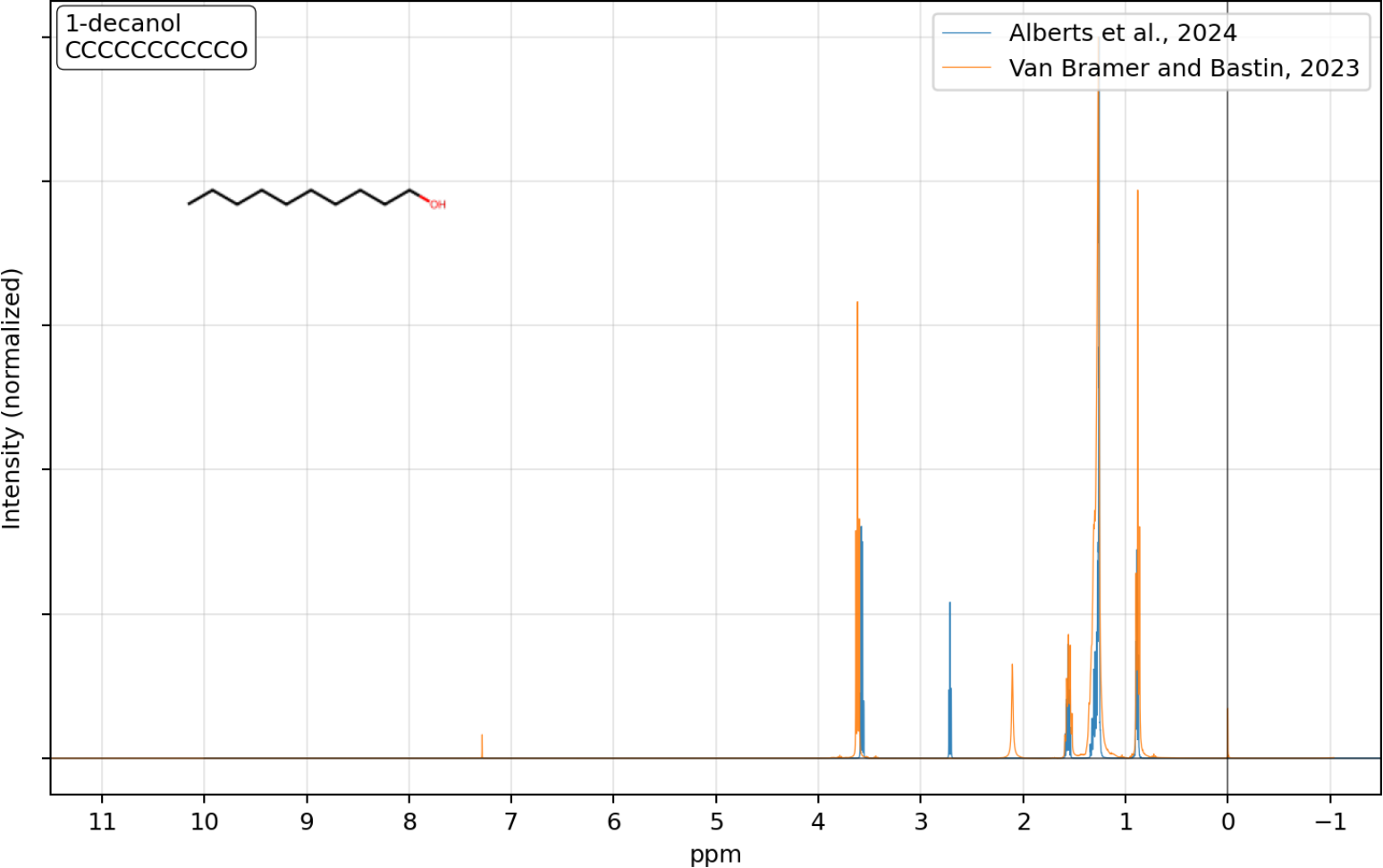
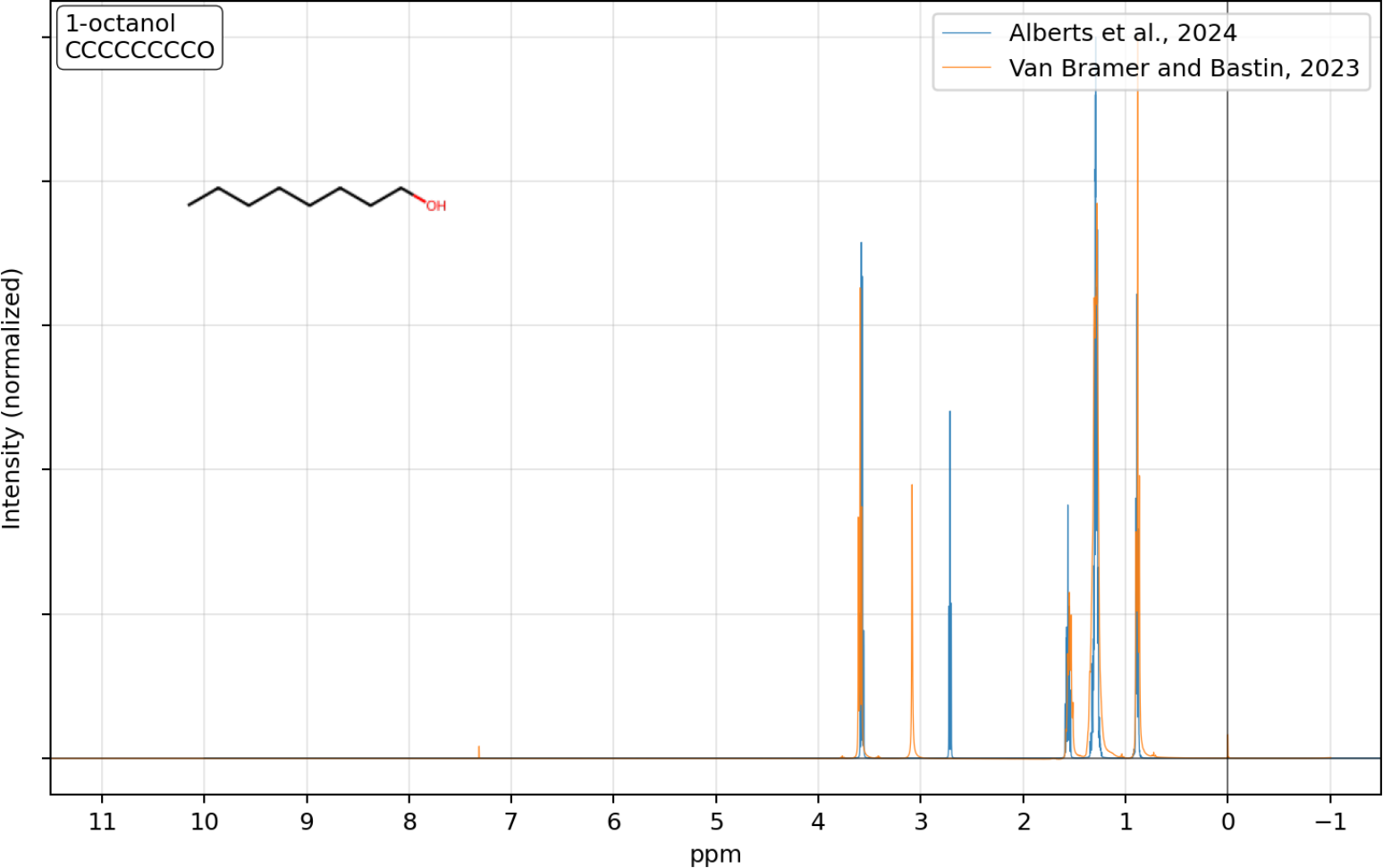
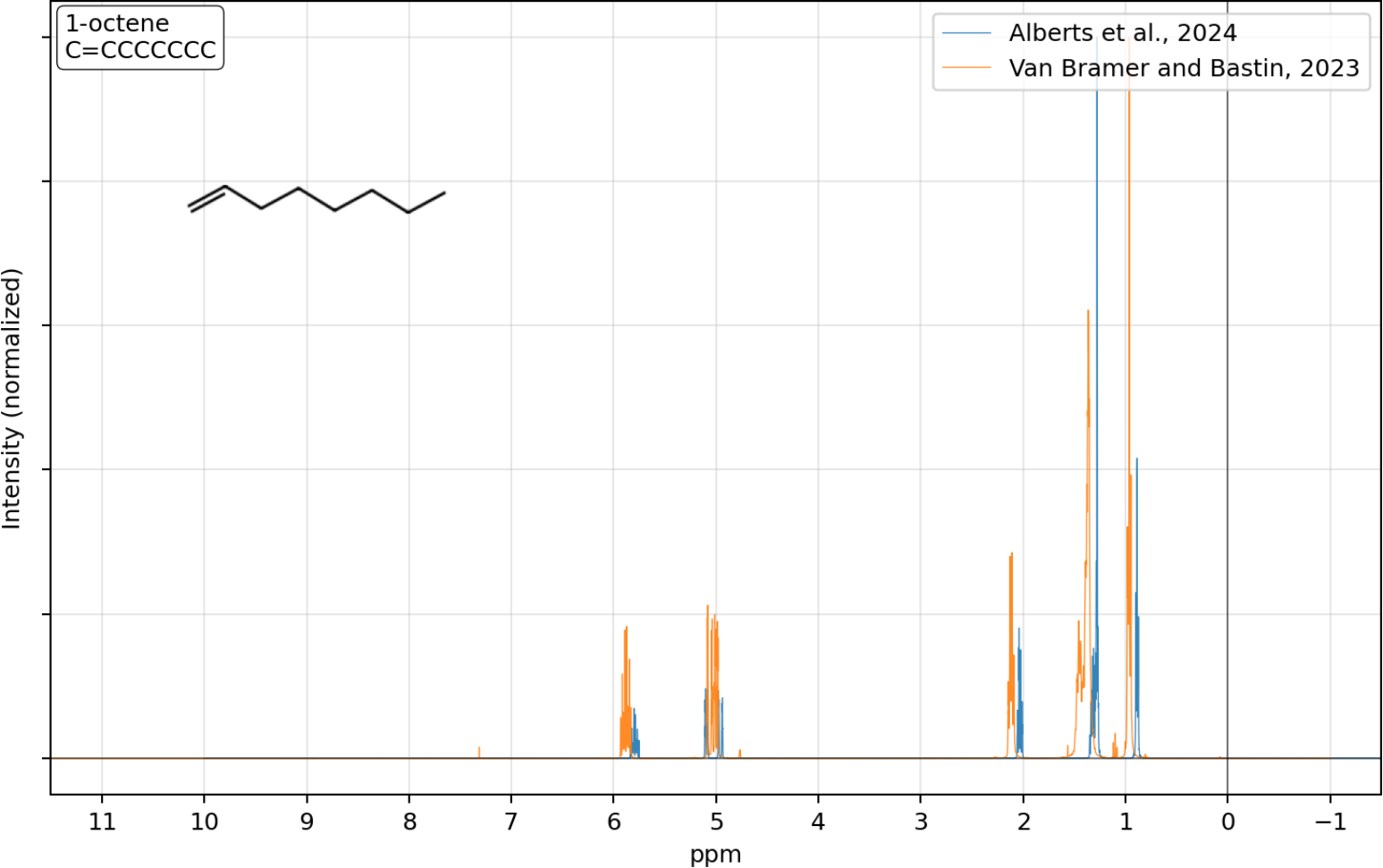
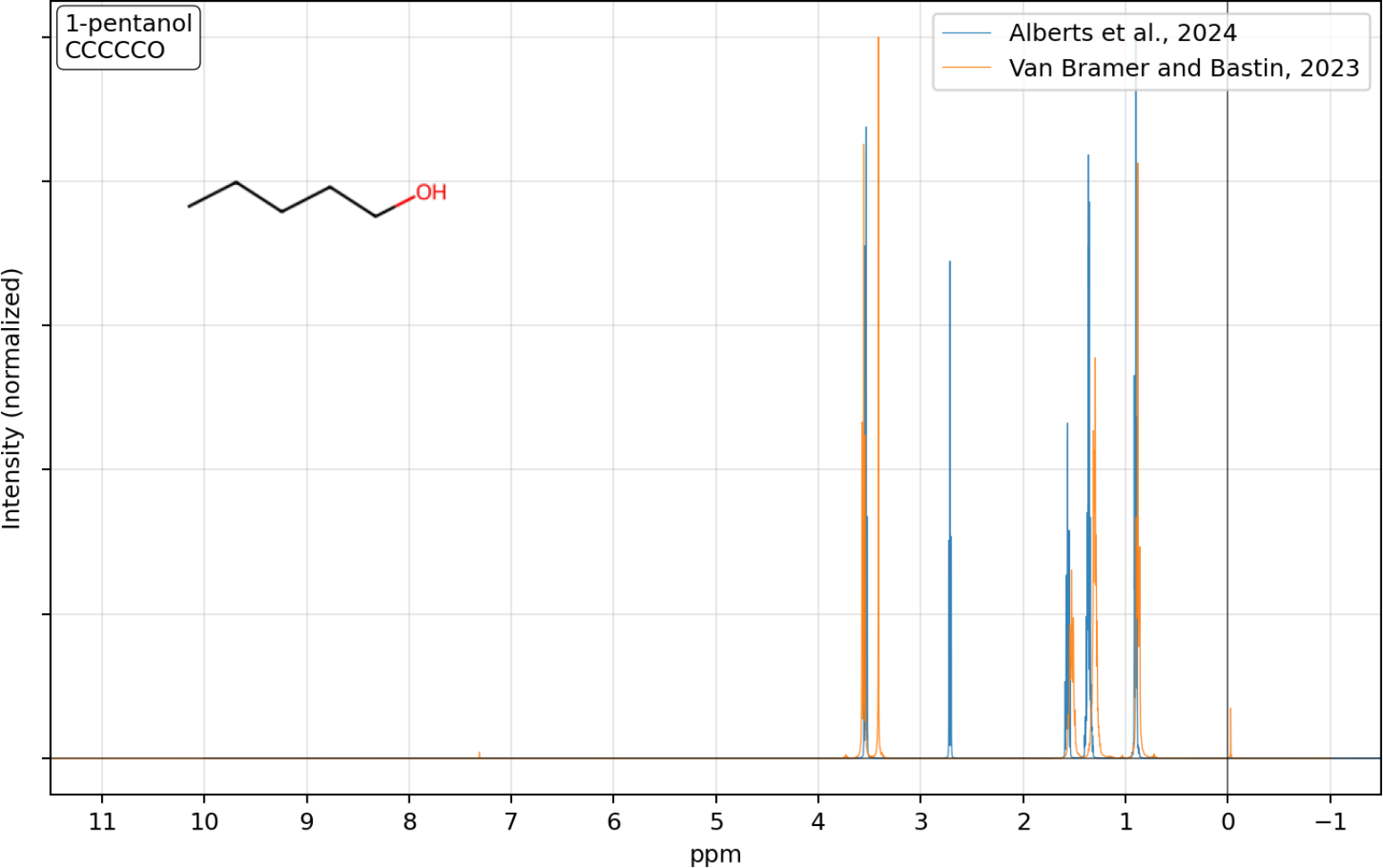

1-2-4-trimethyl-benzene
Cc1ccc(C)c(C)c1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

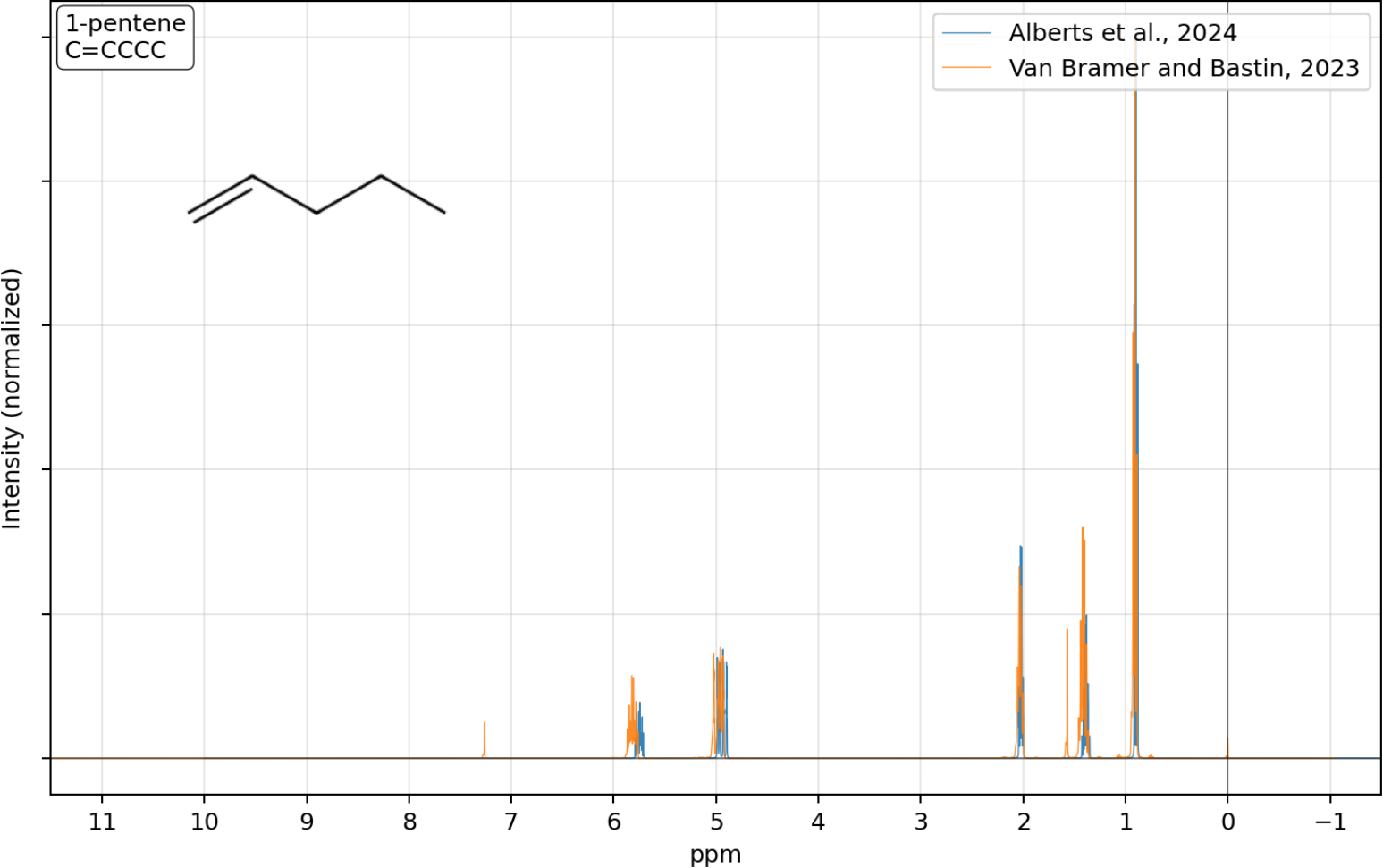

1-chloro-3-methyl-2-butene
CC(C)=CCCl
Cl
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

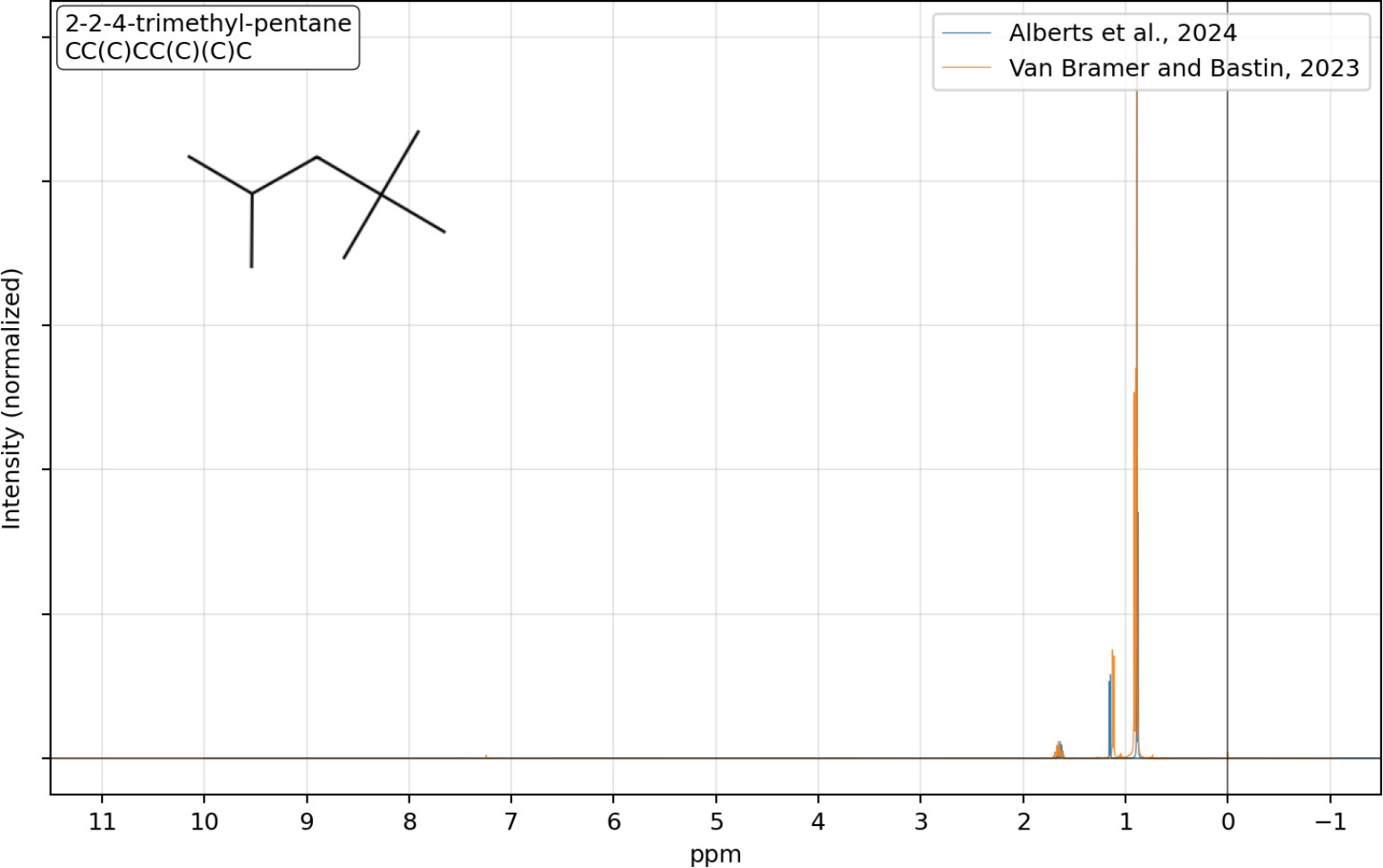

1-decanol
CCCCCCCCCCO
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

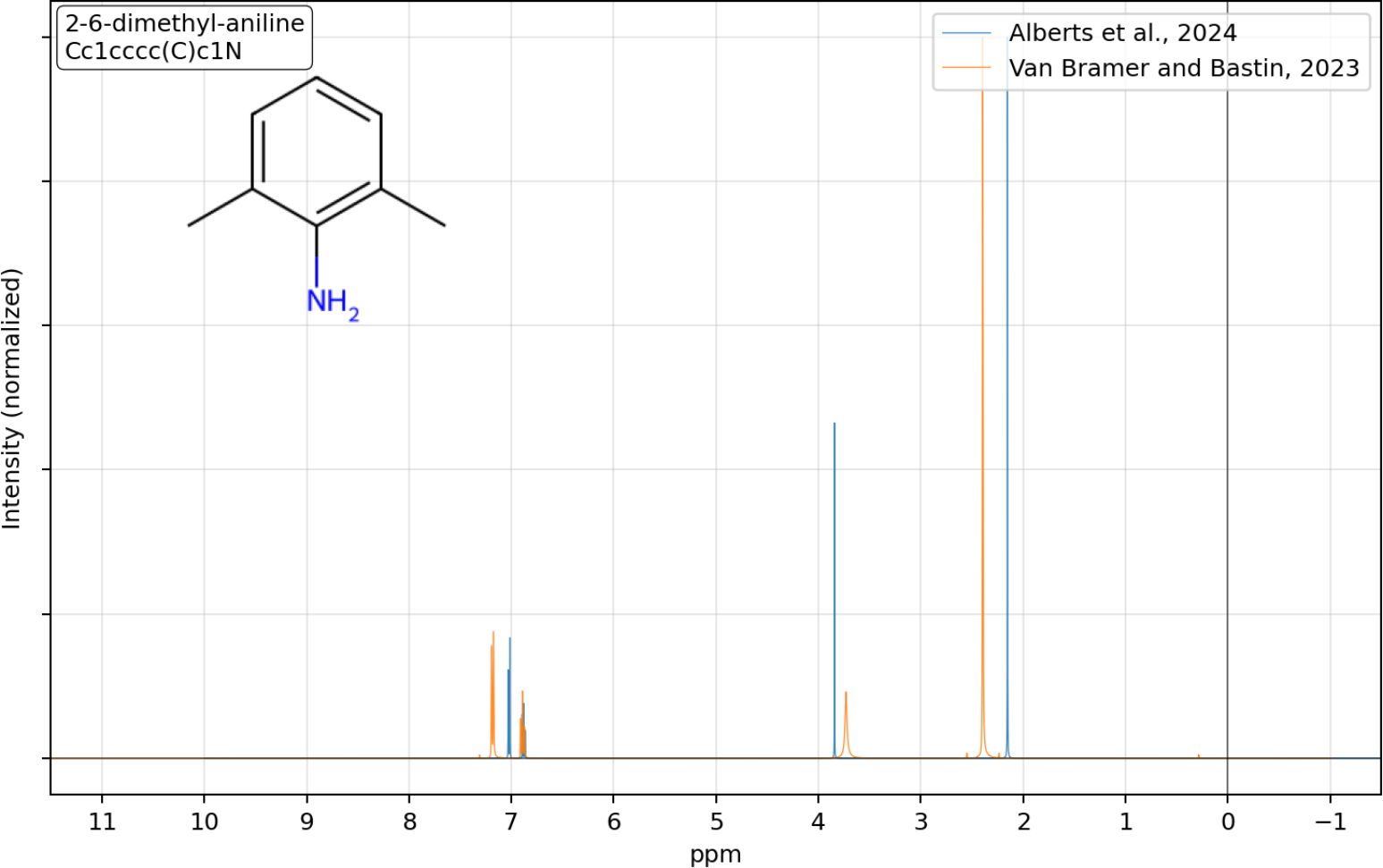

1-octanol
CCCCCCCCO
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

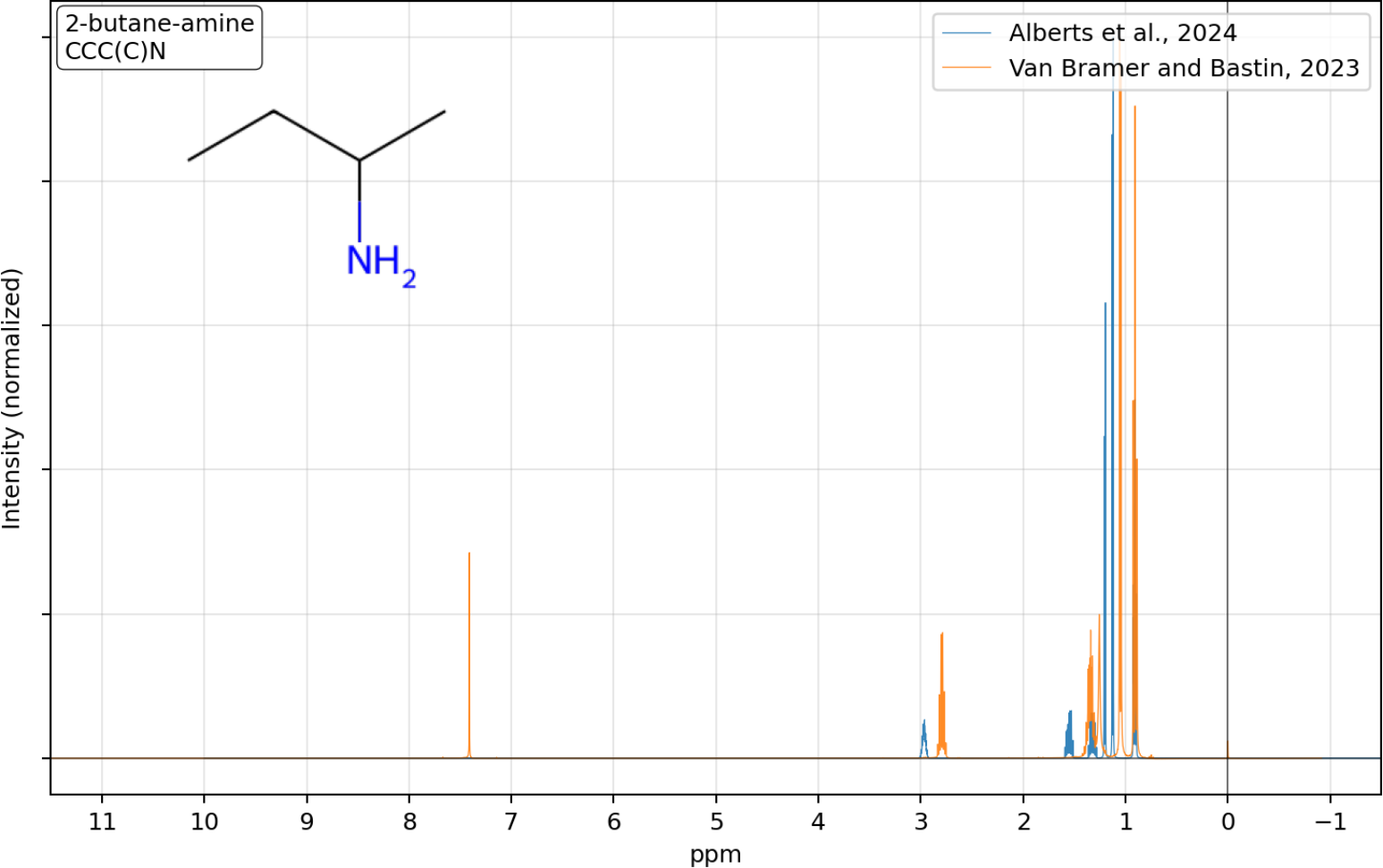

1-octene
C=CCCCCCC
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

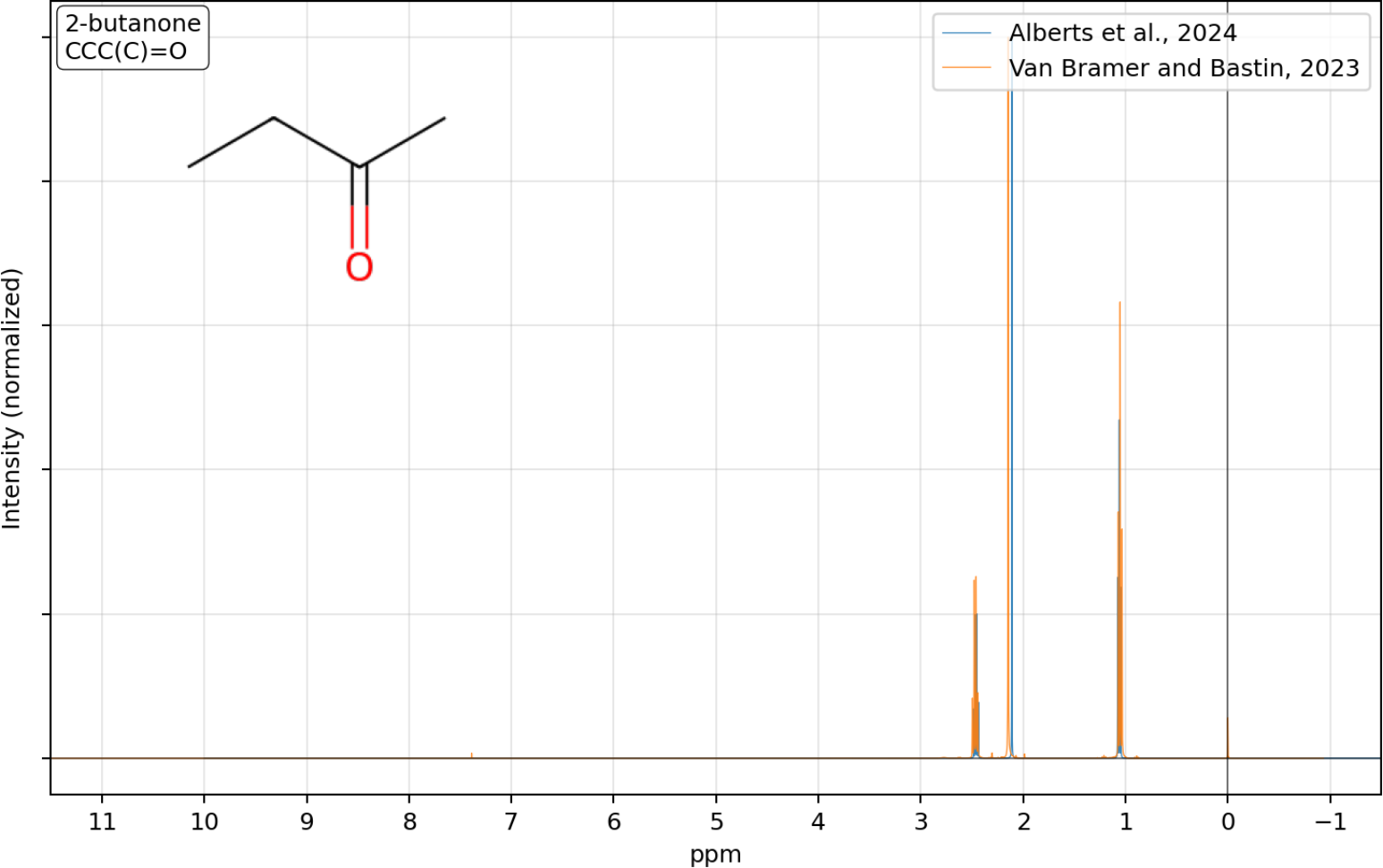

1-pentanol
CCCCCO
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

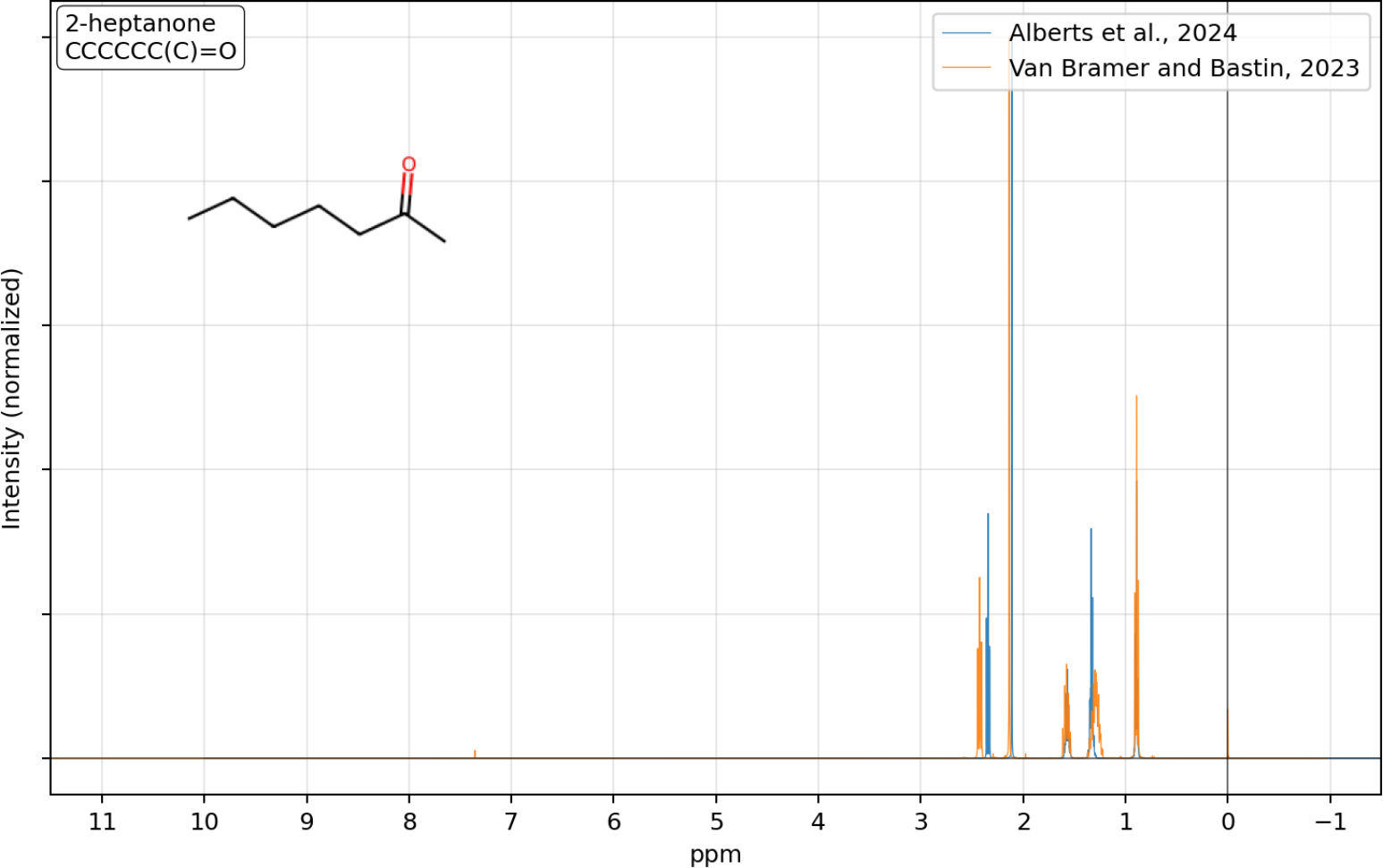

1-pentene
C=CCCC
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

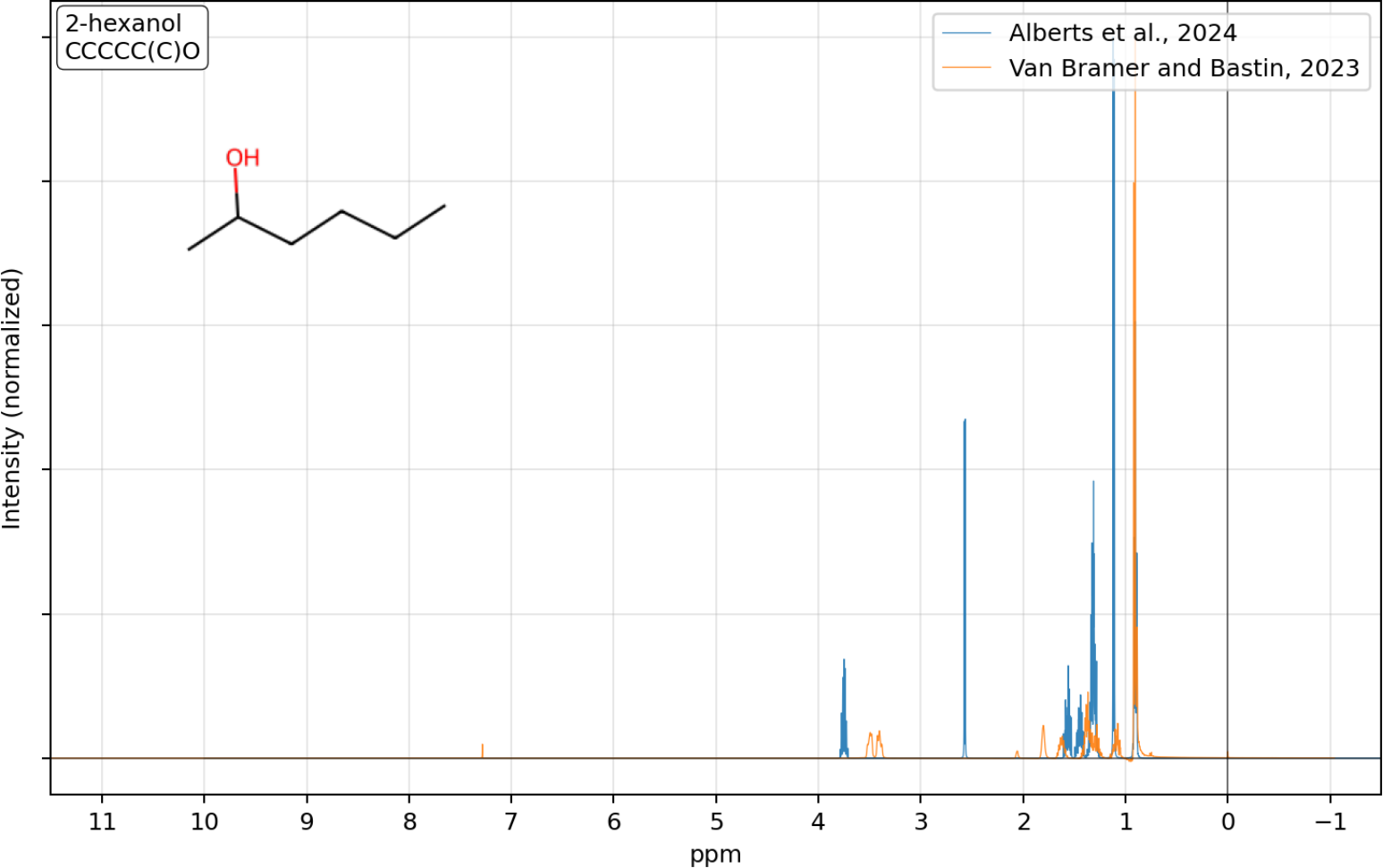

2-2-4-trimethyl-pentane
CC(C)CC(C)(C)C
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

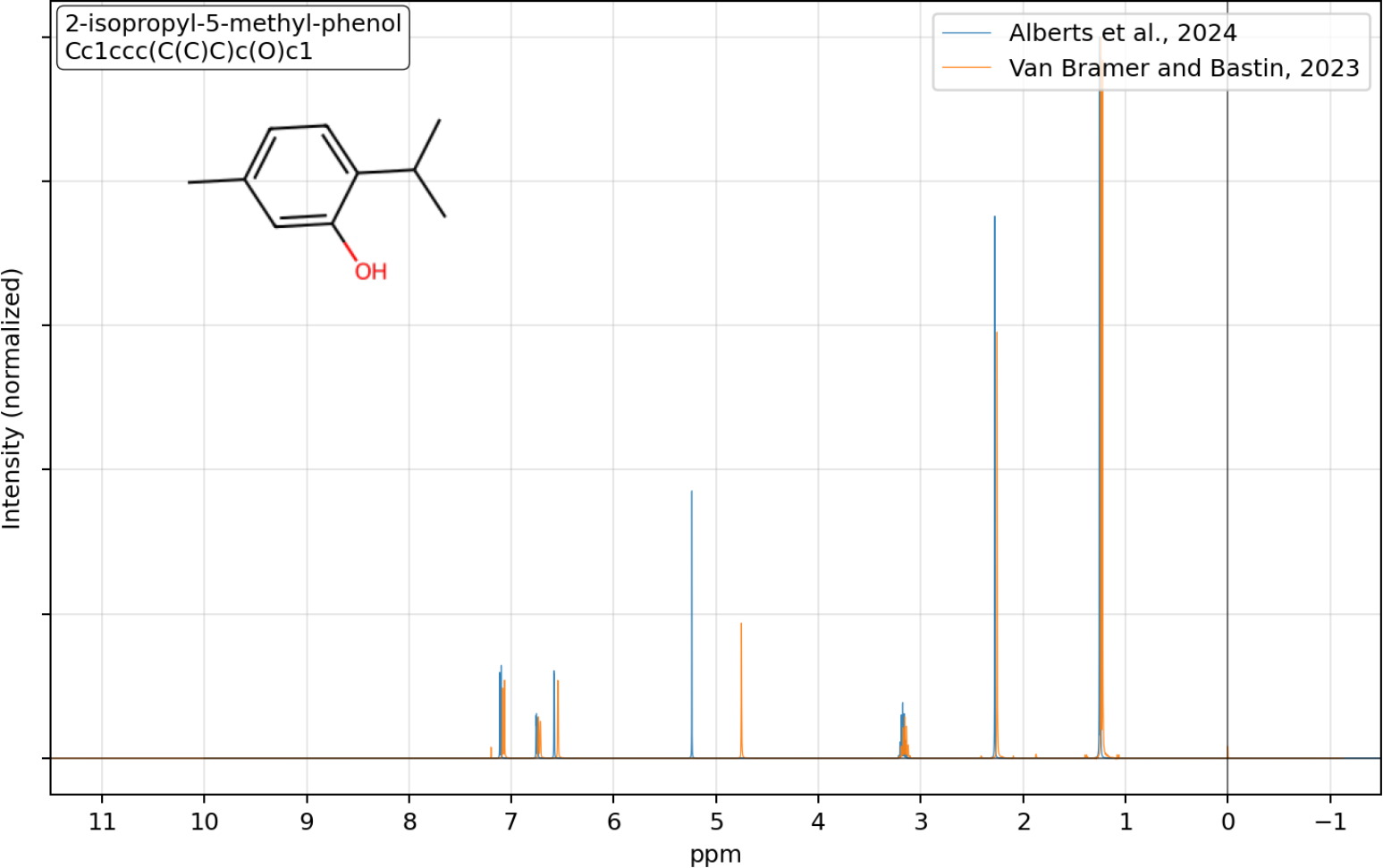

2-6-dimethyl-aniline
Cc1cccc(C)c1N
NH2
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

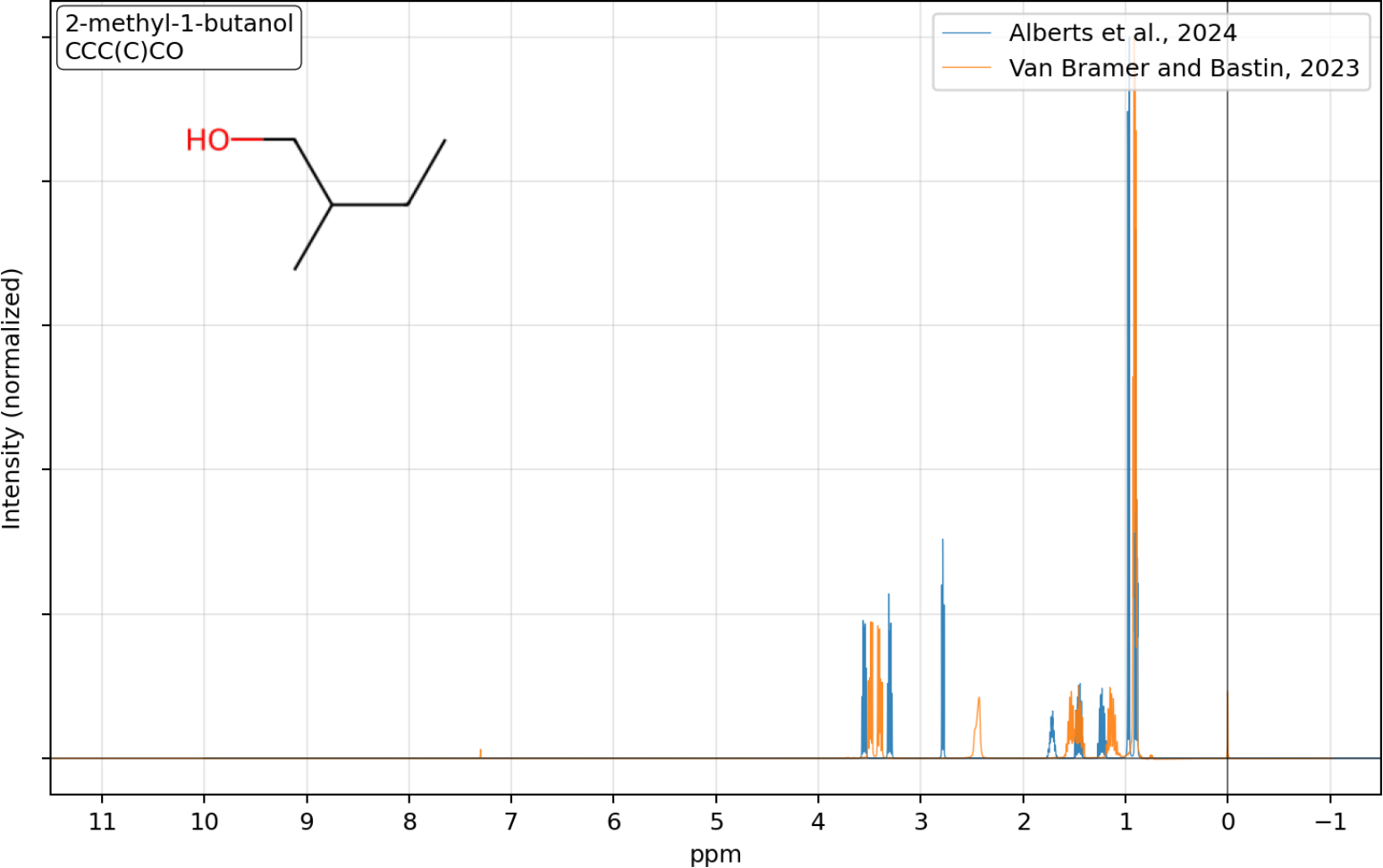

2-butane-amine
CCC(C)N
NH2
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

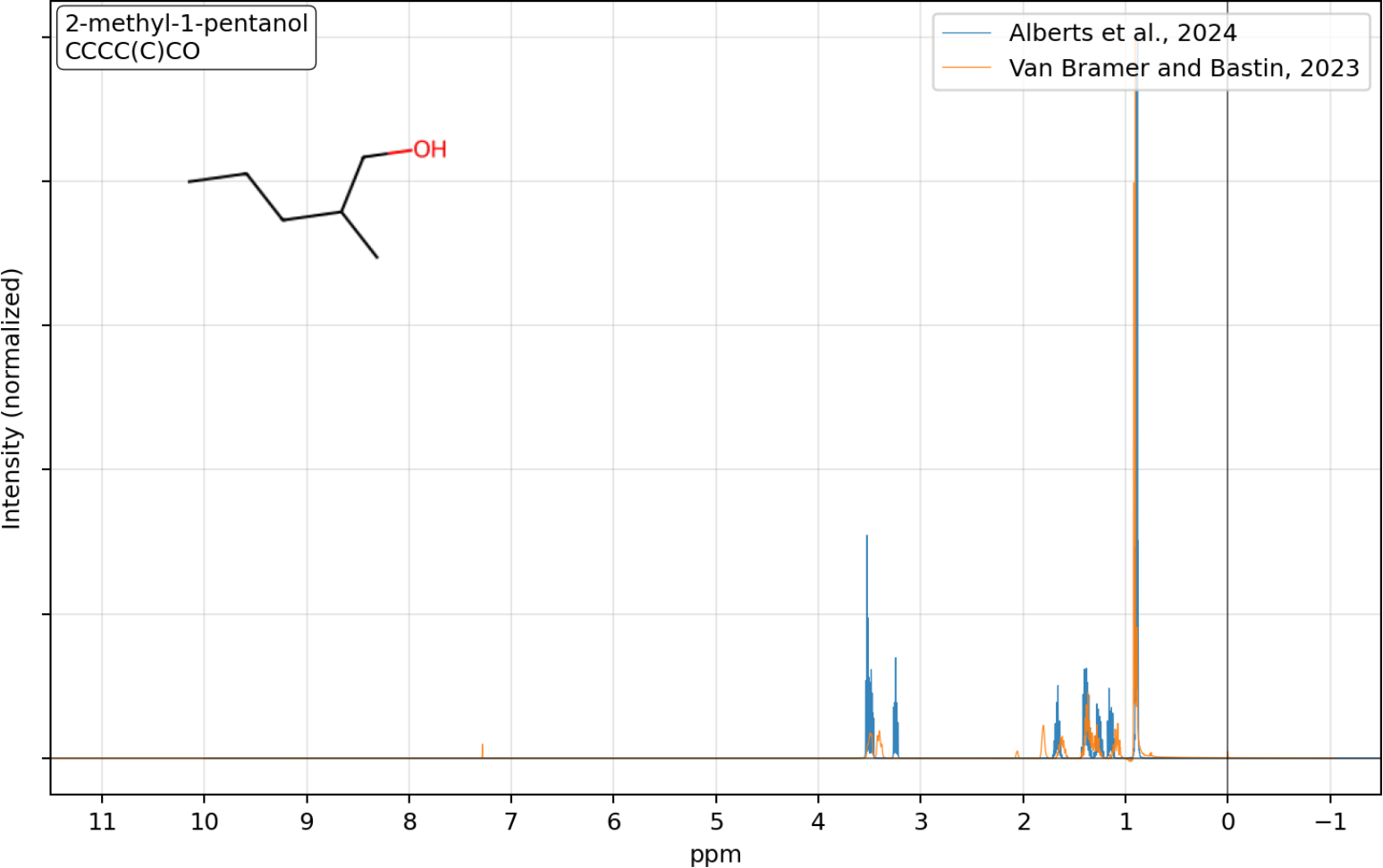

2-butanone
CCC(C)=O
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

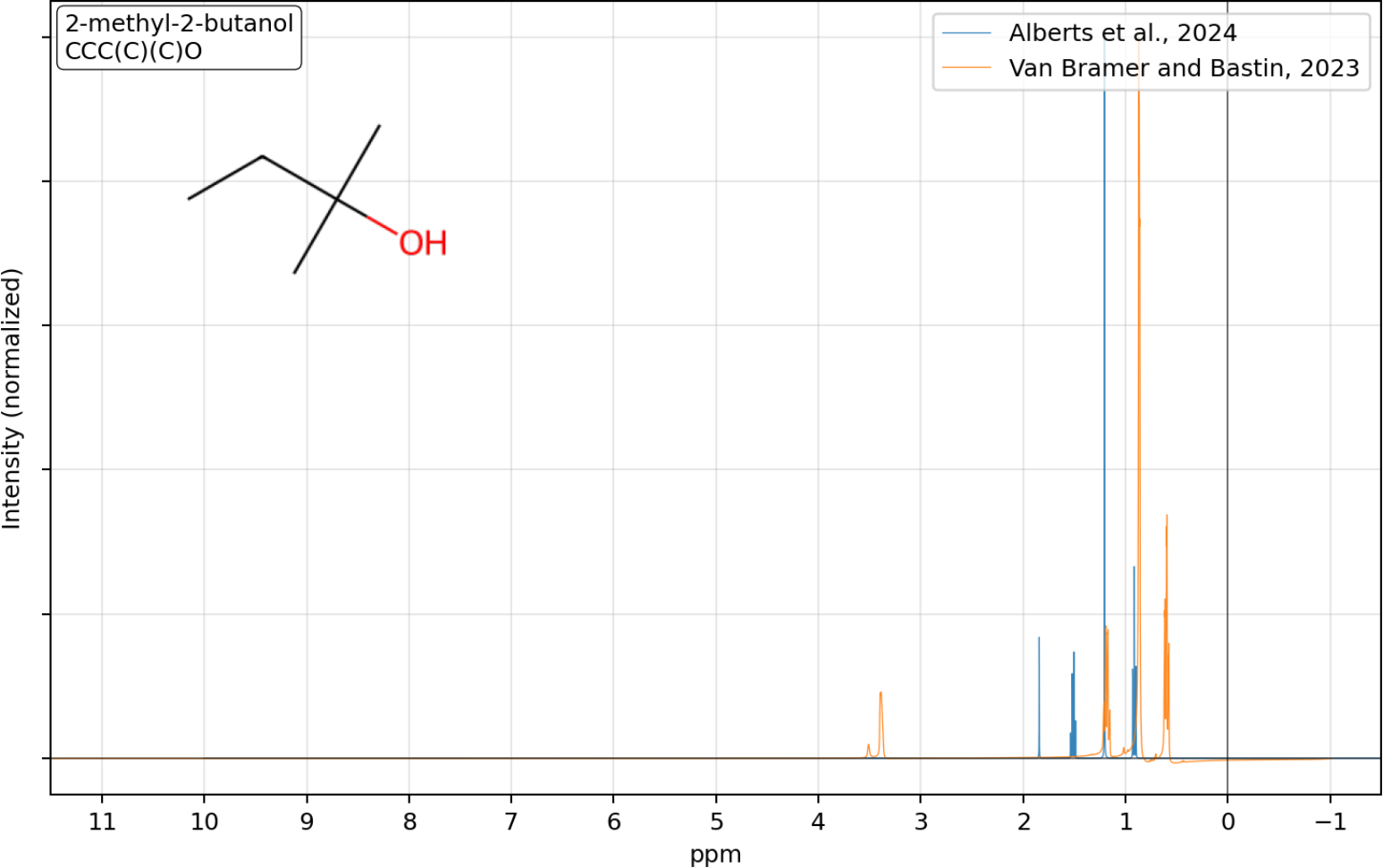

2-heptanone
CCCCCC(C)=O
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

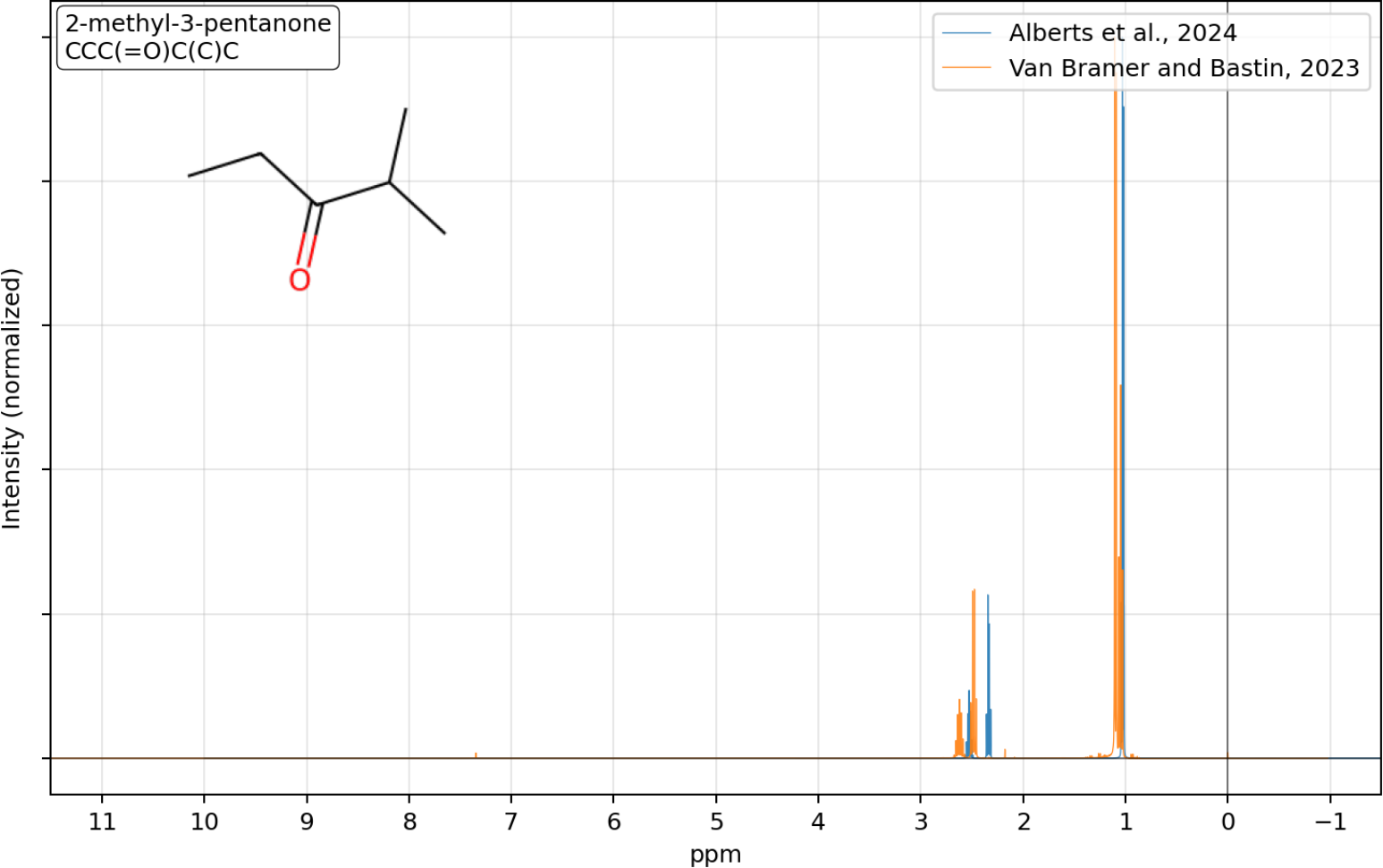

2-hexanol
CCCCC(C)O
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

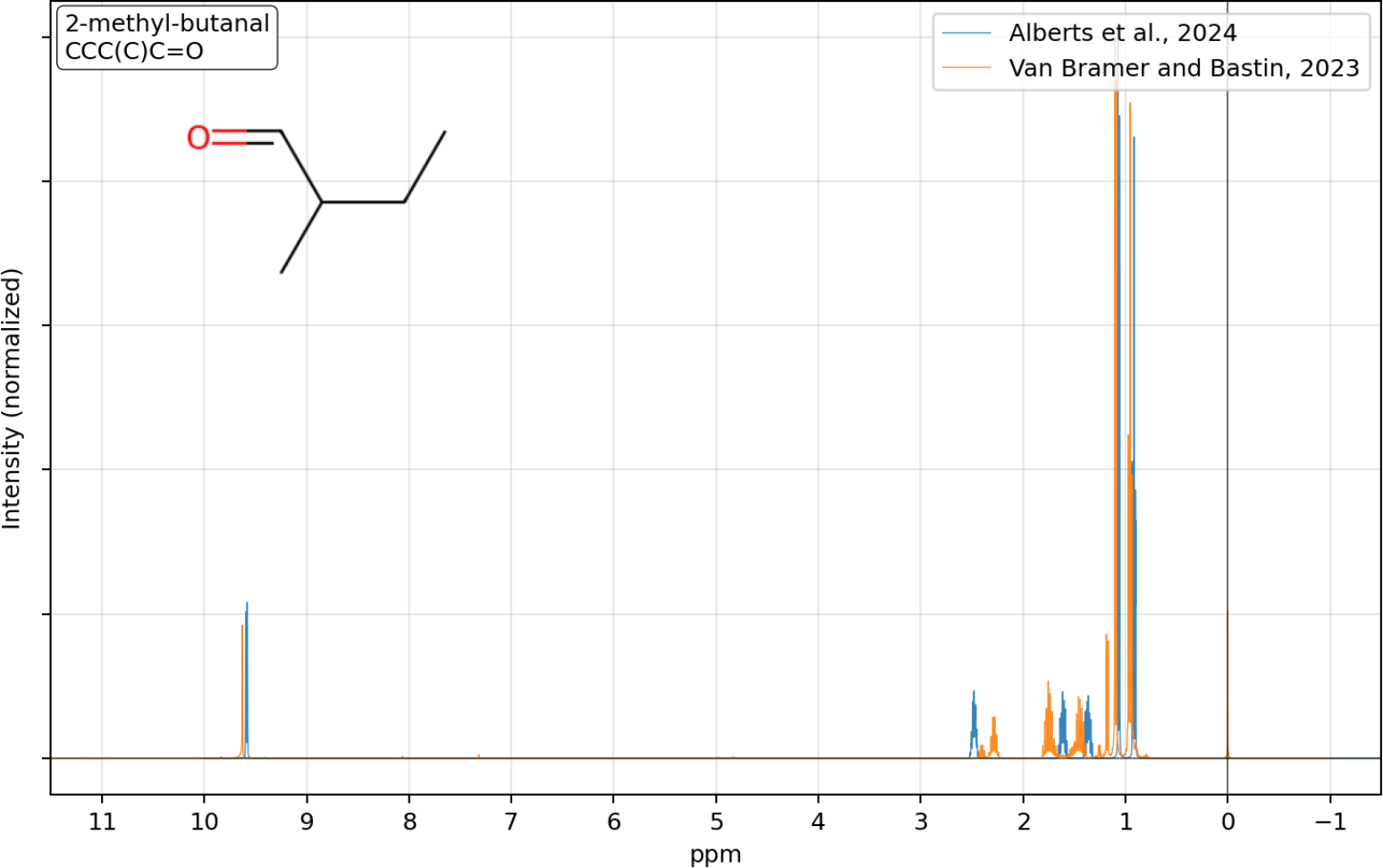

2-isopropyl-5-methyl-phenol
Cc1ccc(C(C)C)c(O)c1
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

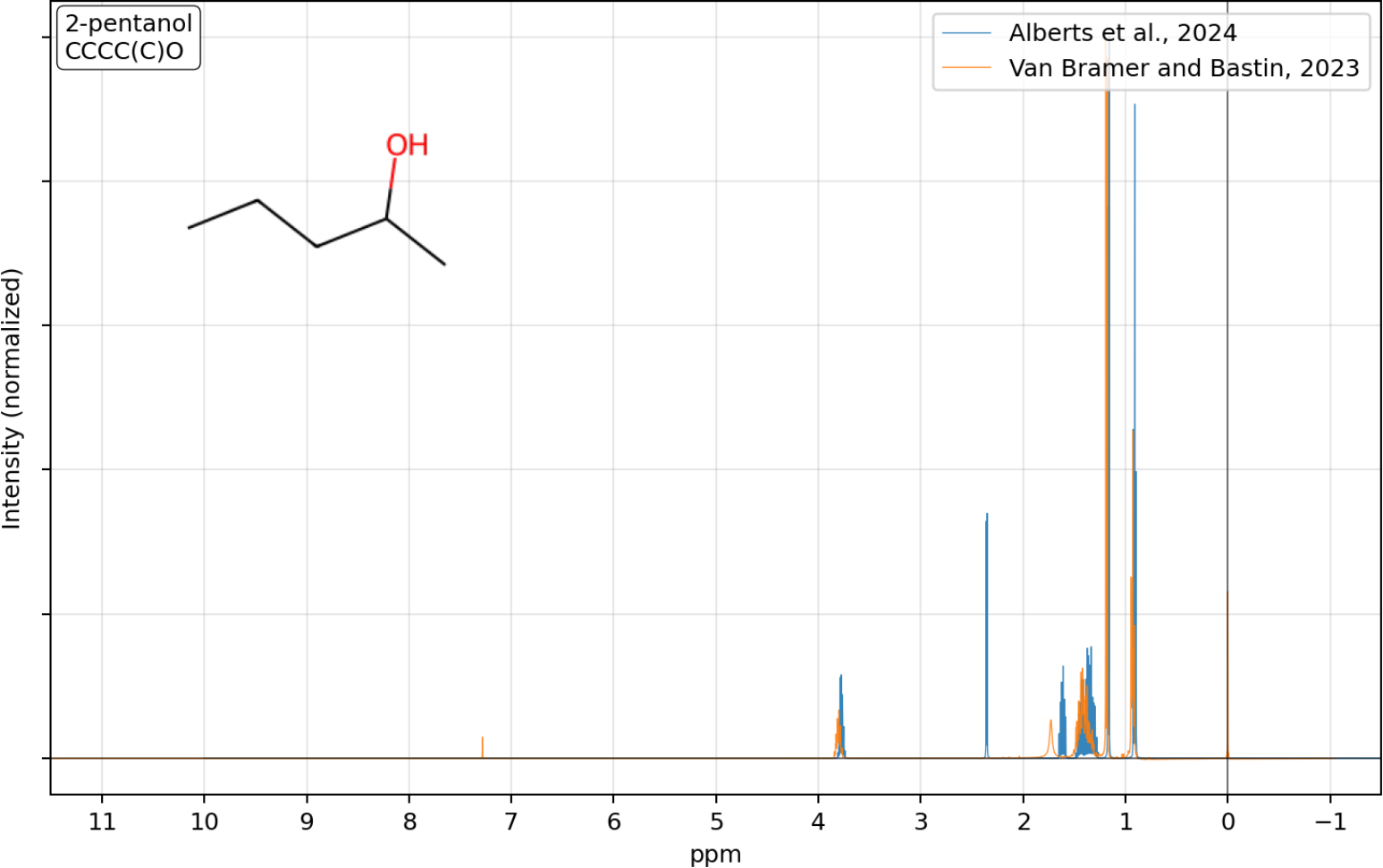

2-methyl-1-butanol
CCC(C)CO
HO
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

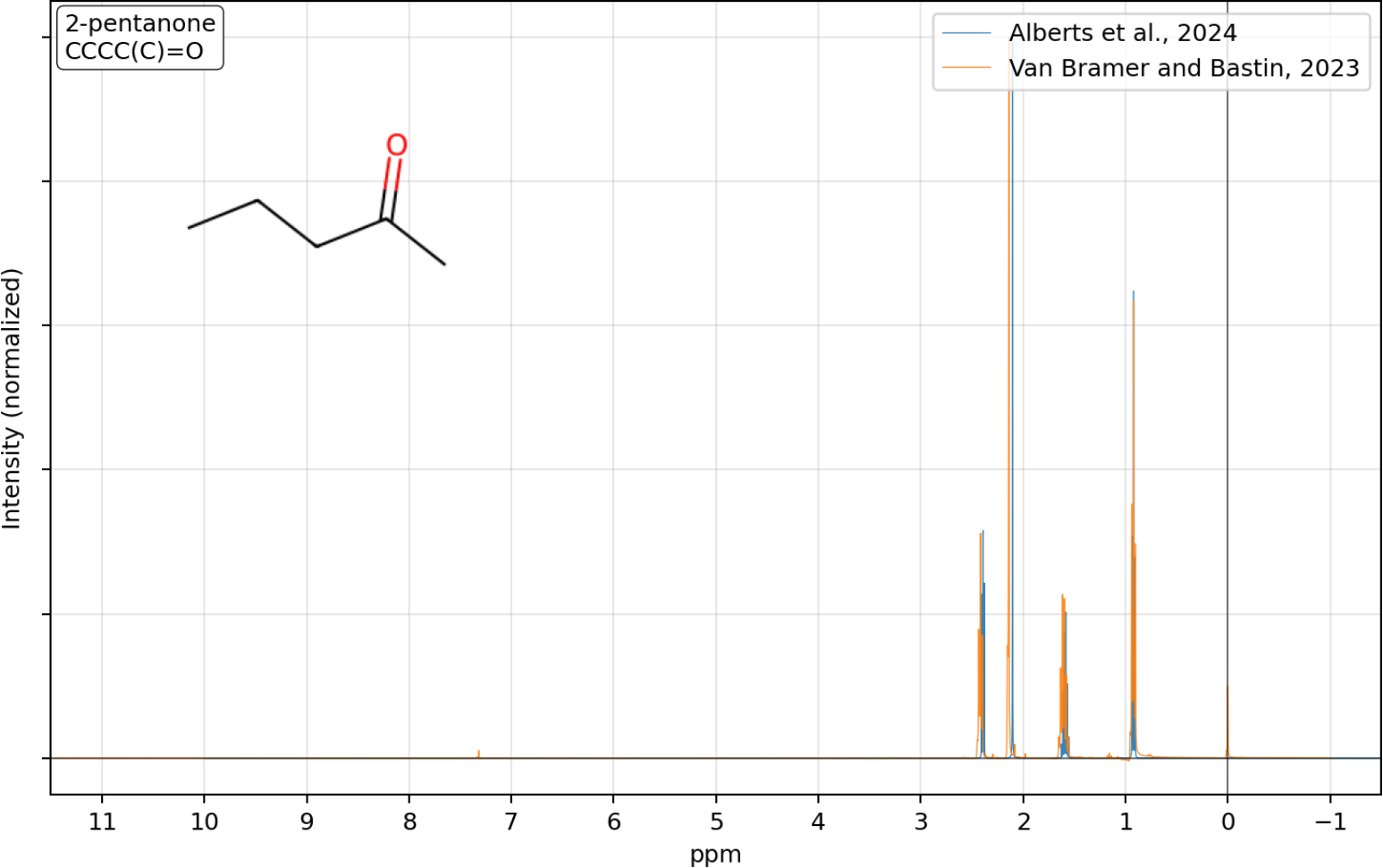

2-methyl-1-pentanol
CCCC(C)CO
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

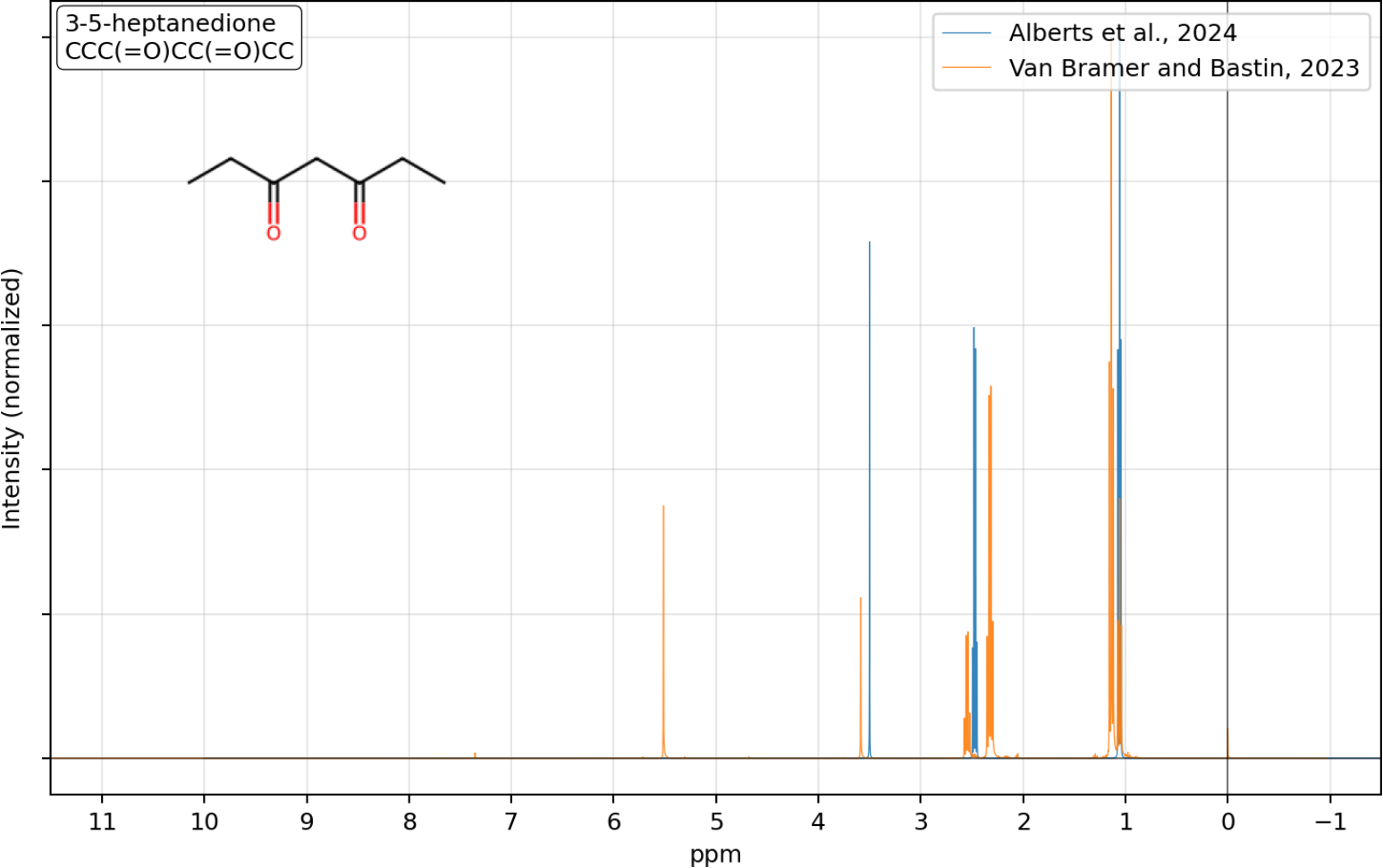

2-methyl-2-butanol
CCC(C)(C)O
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

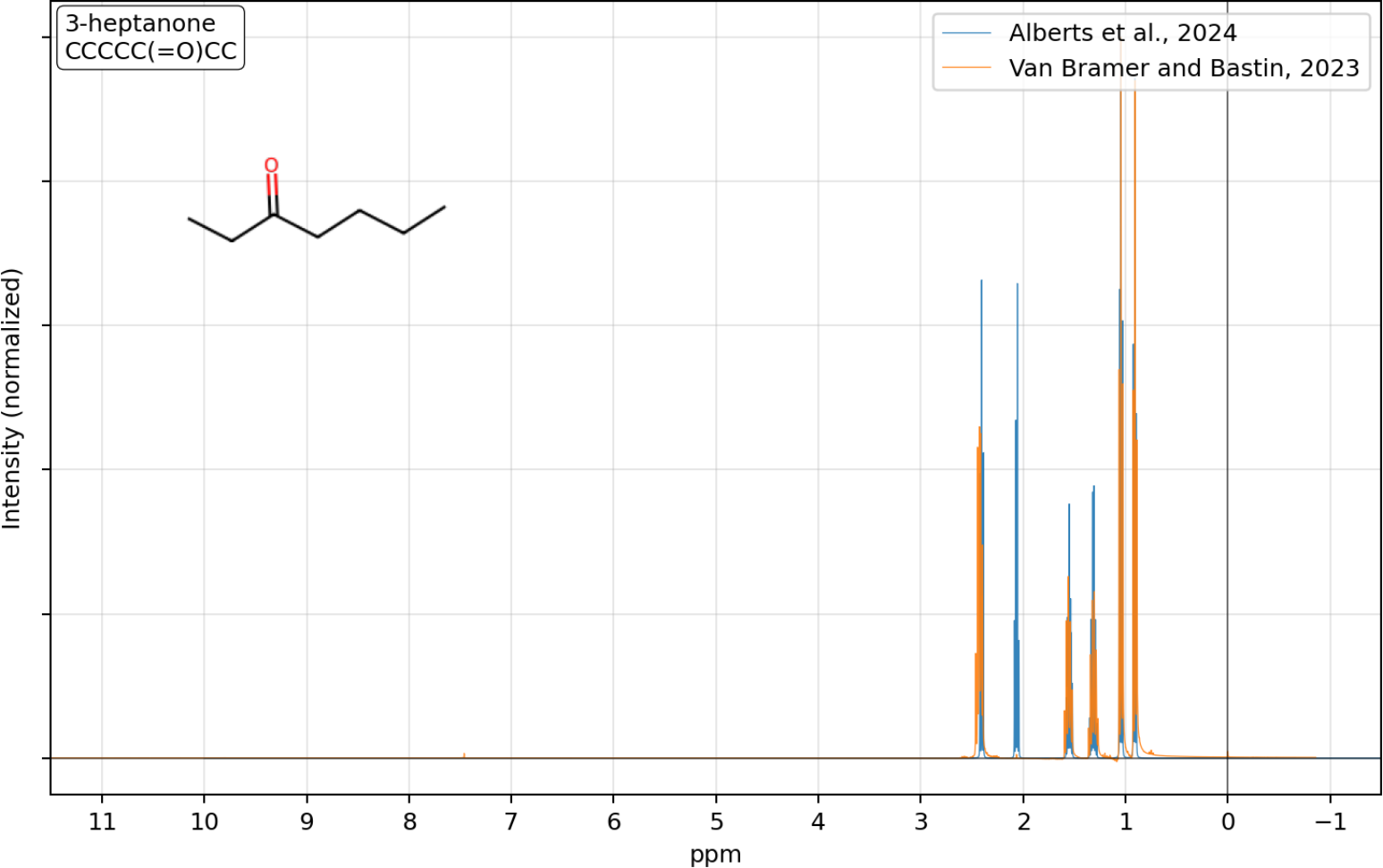

2-methyl-3-pentanone
CCC(=O)C(C)C
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

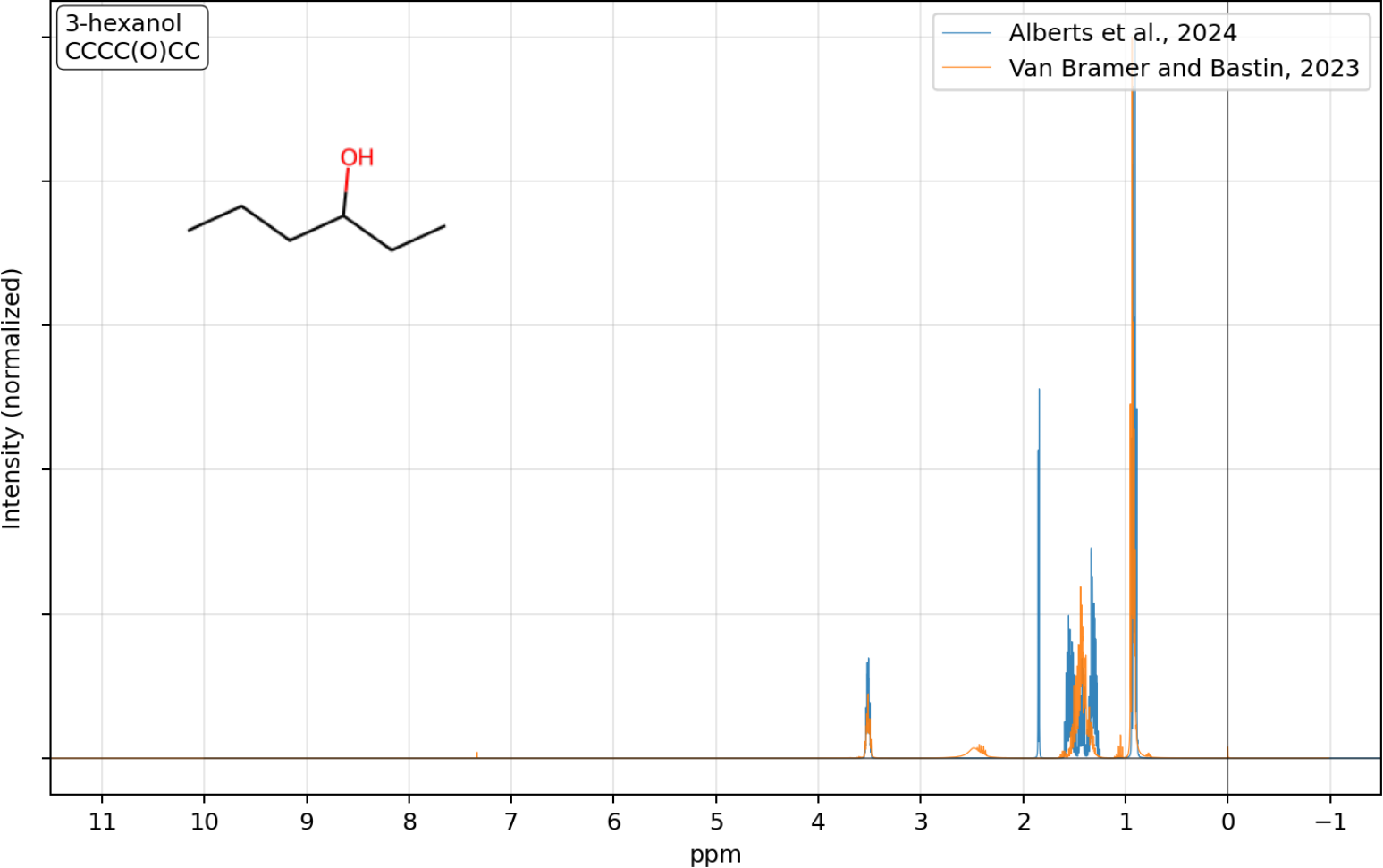

2-methyl-butanal
CCC(C)C=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

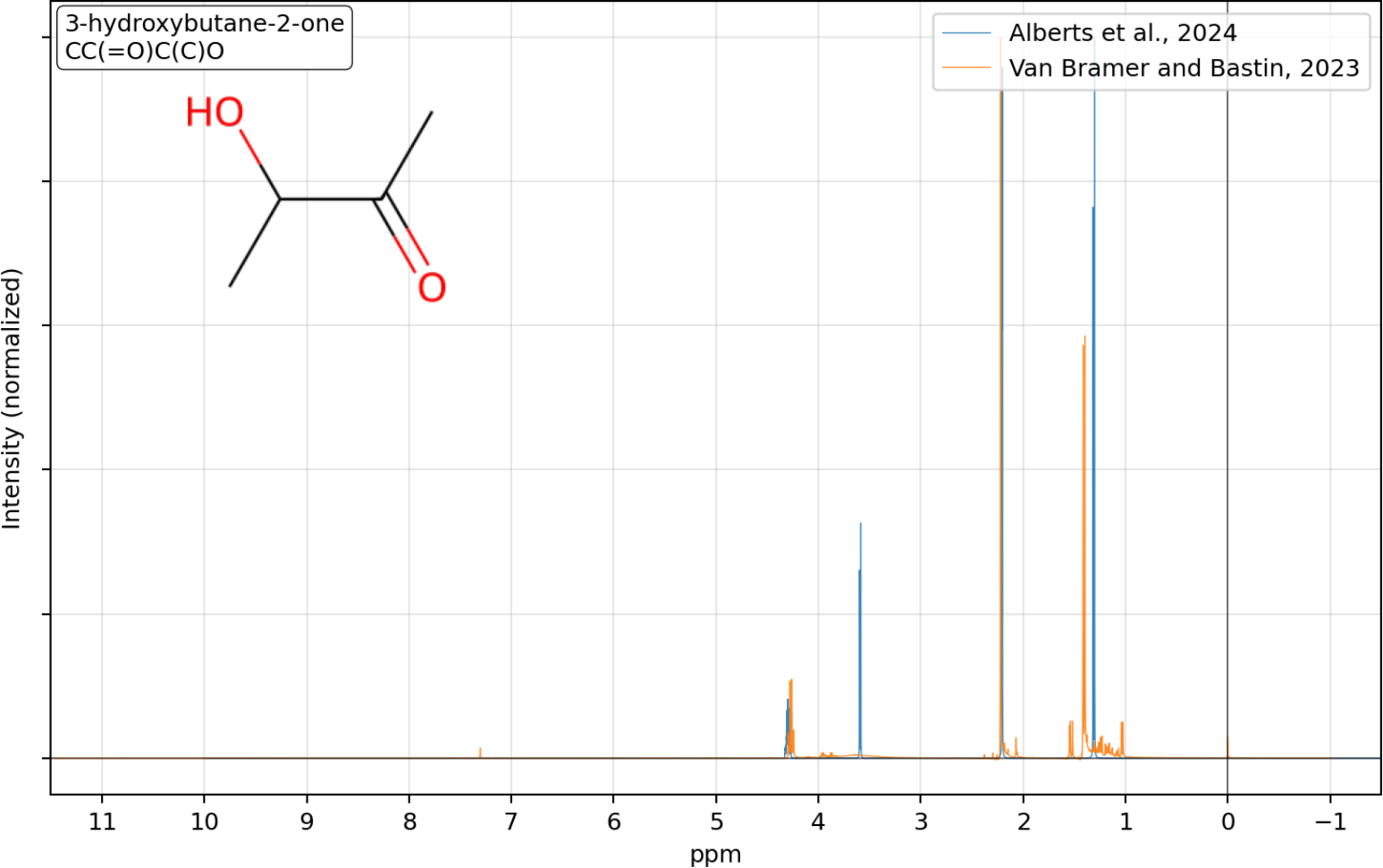

2-pentanol
CCCC(C)O
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

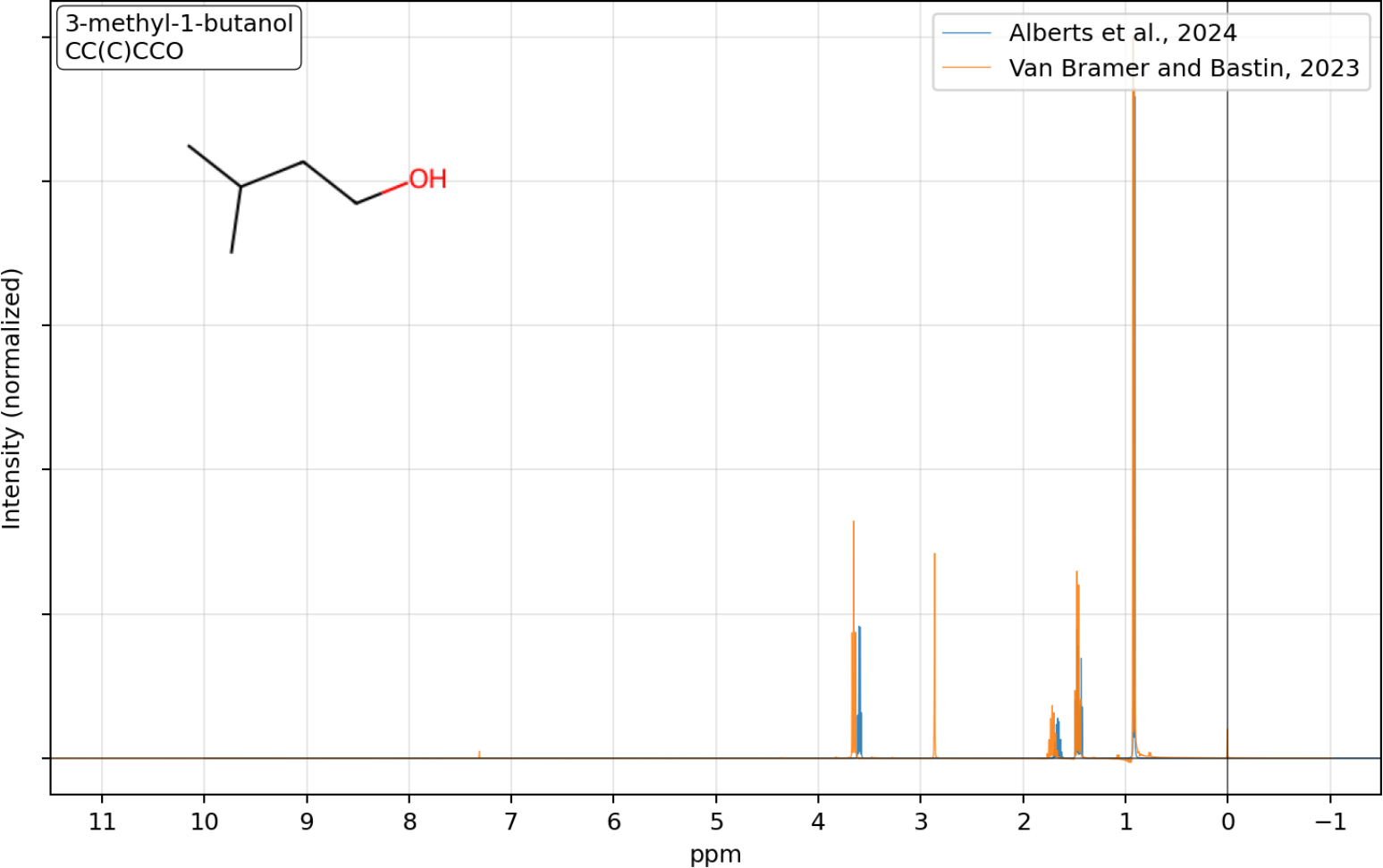

2-pentanone
CCCC(C)=O
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

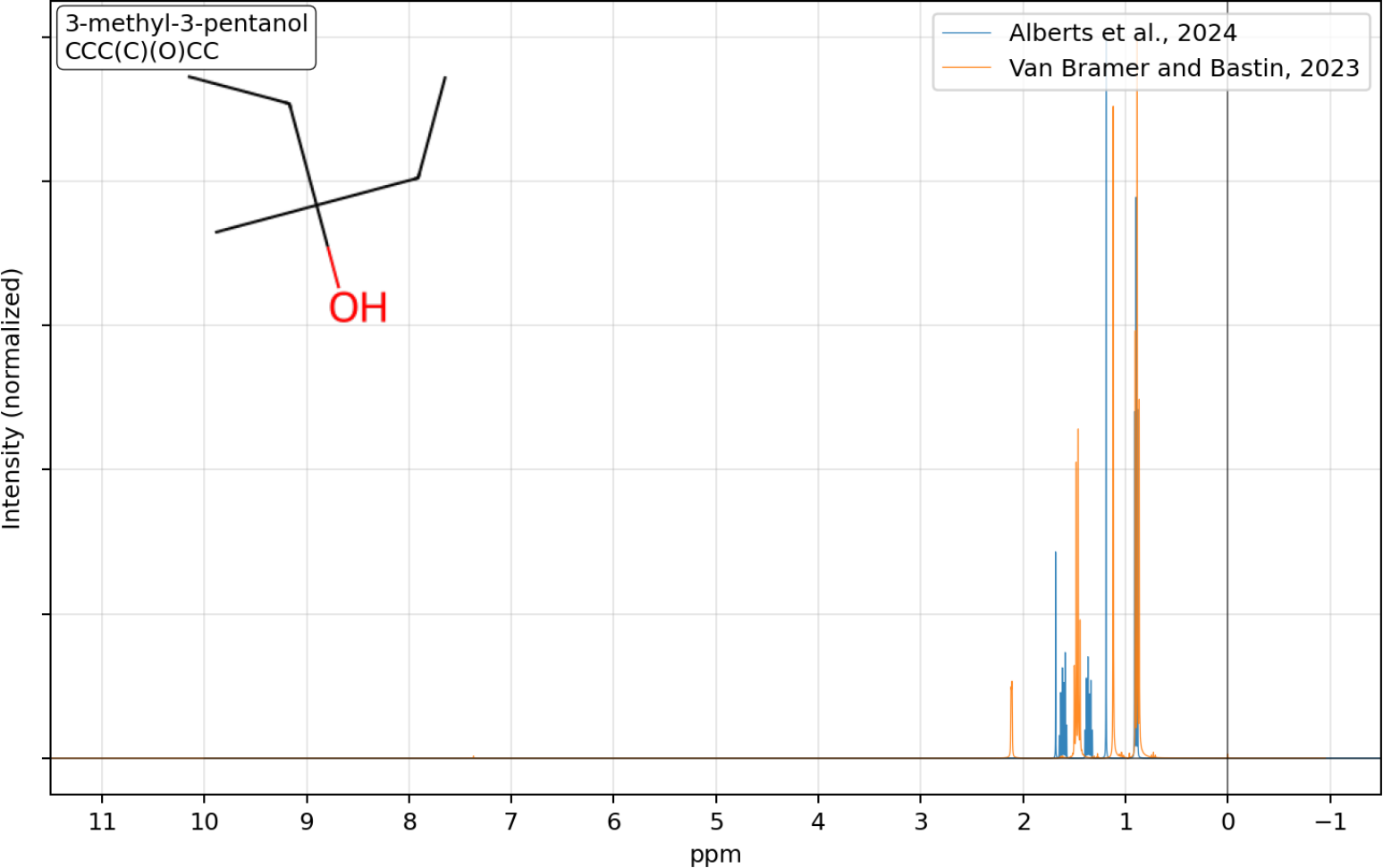

3-5-heptanedione
CCC(=O)CC(=O)CC
O
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

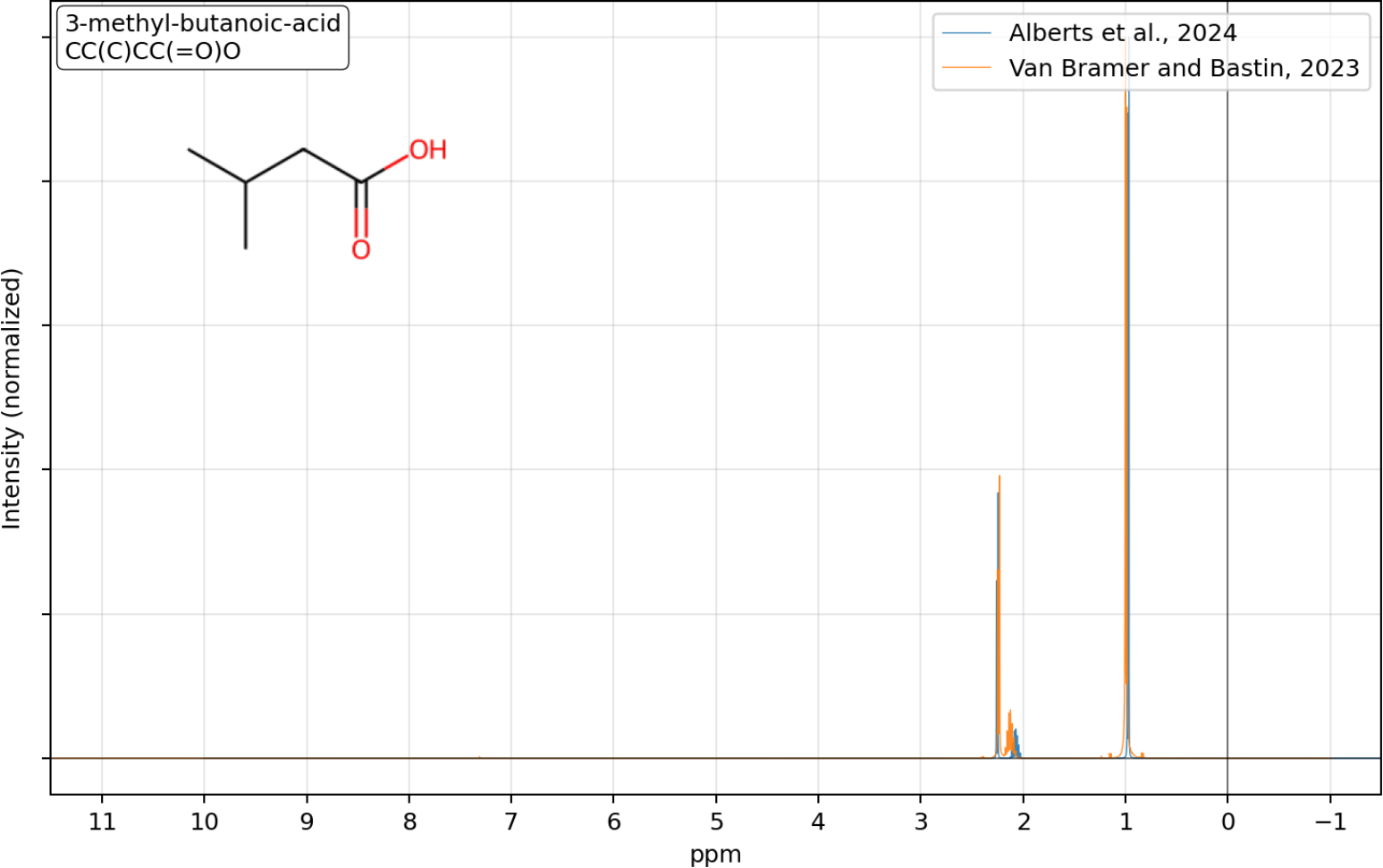

3-heptanone
CCCCC(=O)CC
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

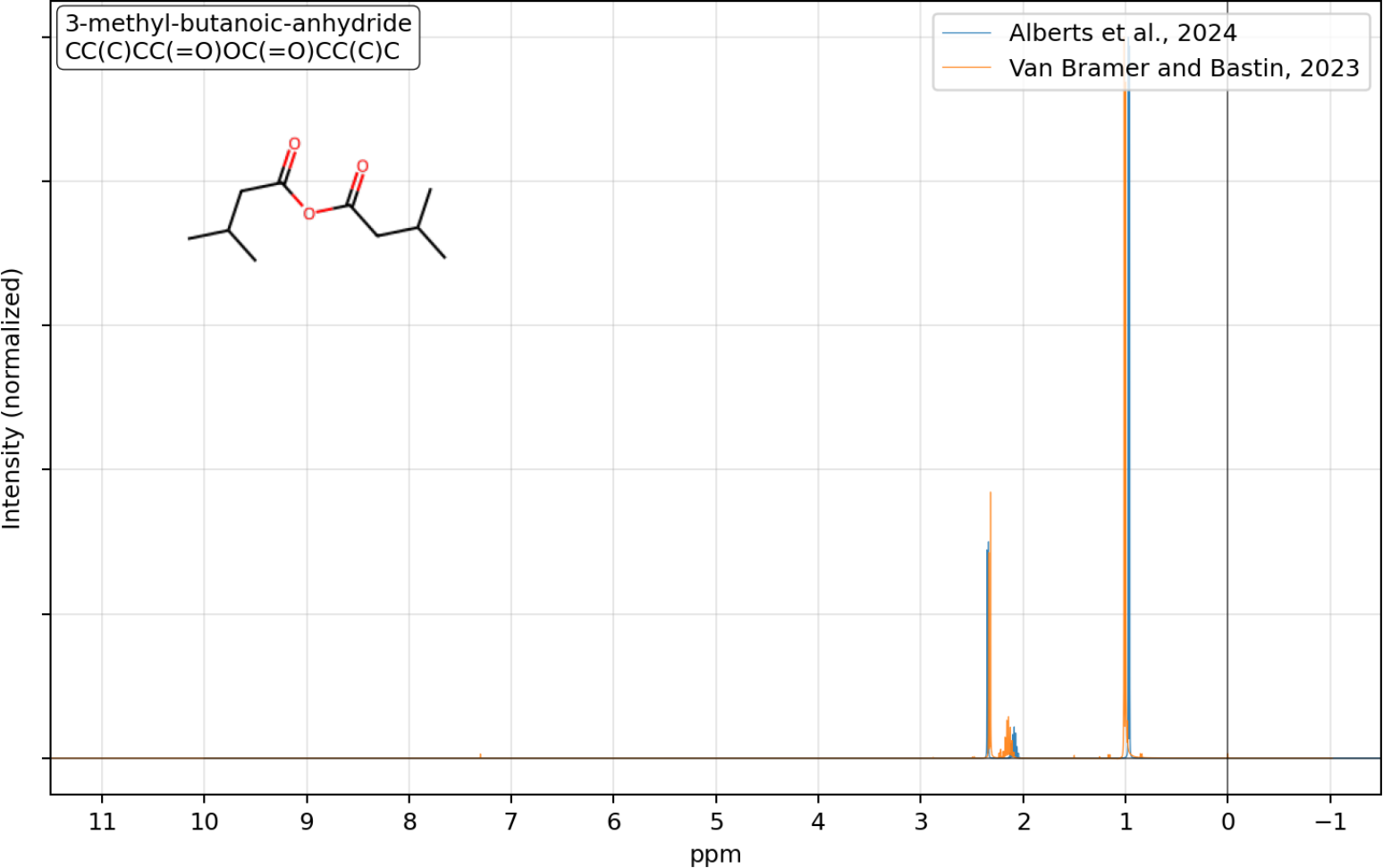

3-hexanol
CCCC(O)CC
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

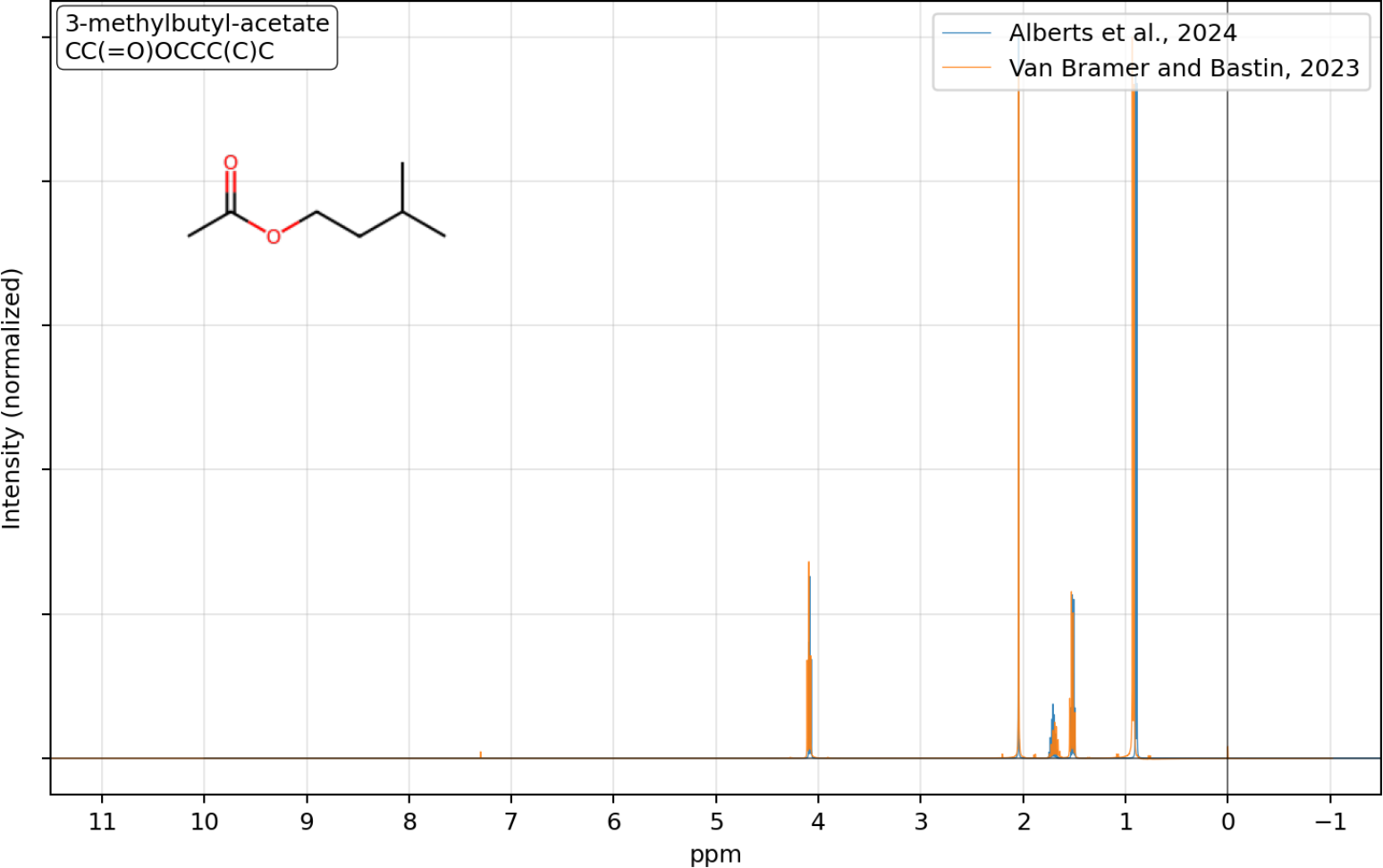

3-hydroxybutane-2-one
CC(=O)C(C)O
HO
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

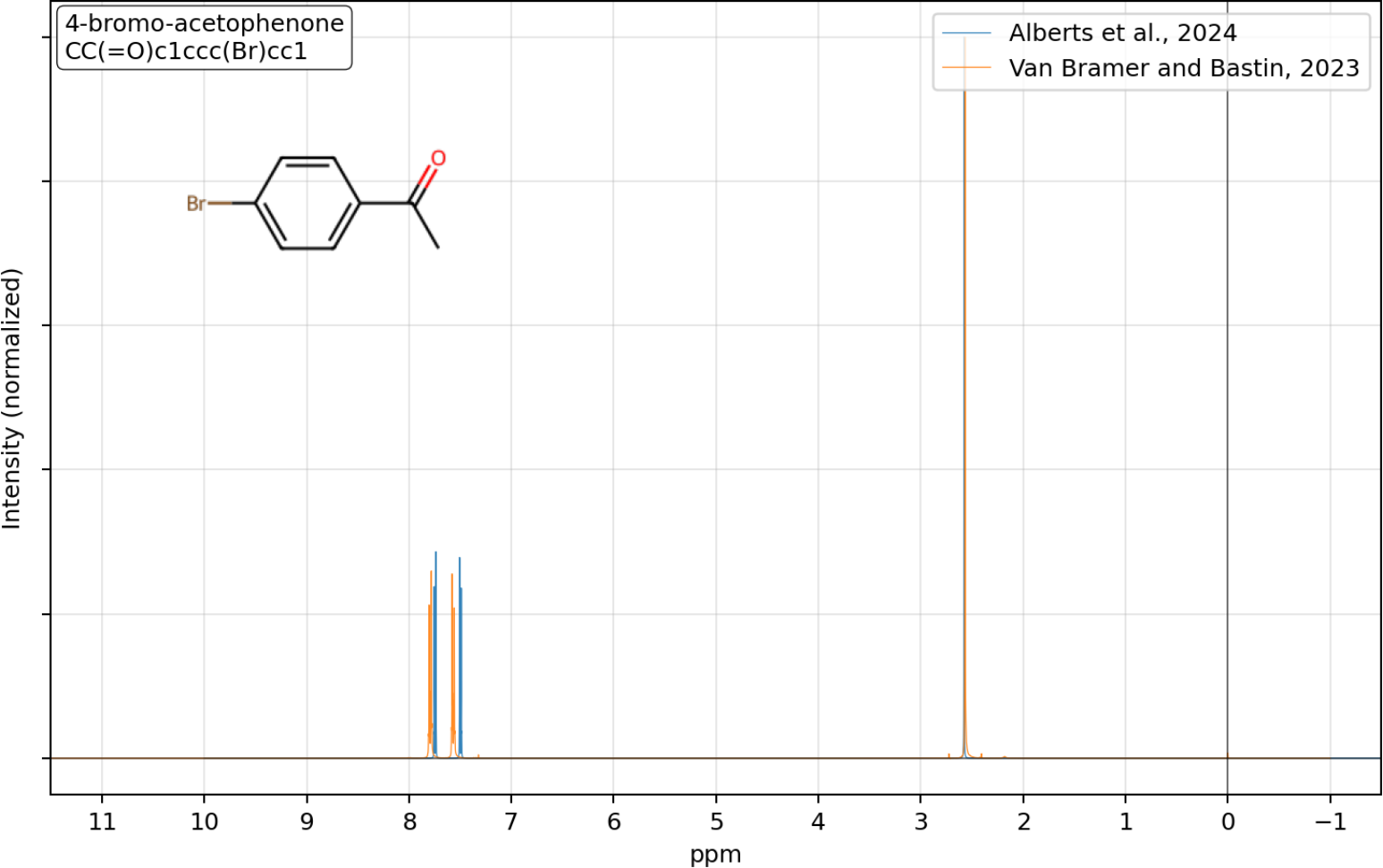

3-methyl-1-butanol
CC(C)CCO
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

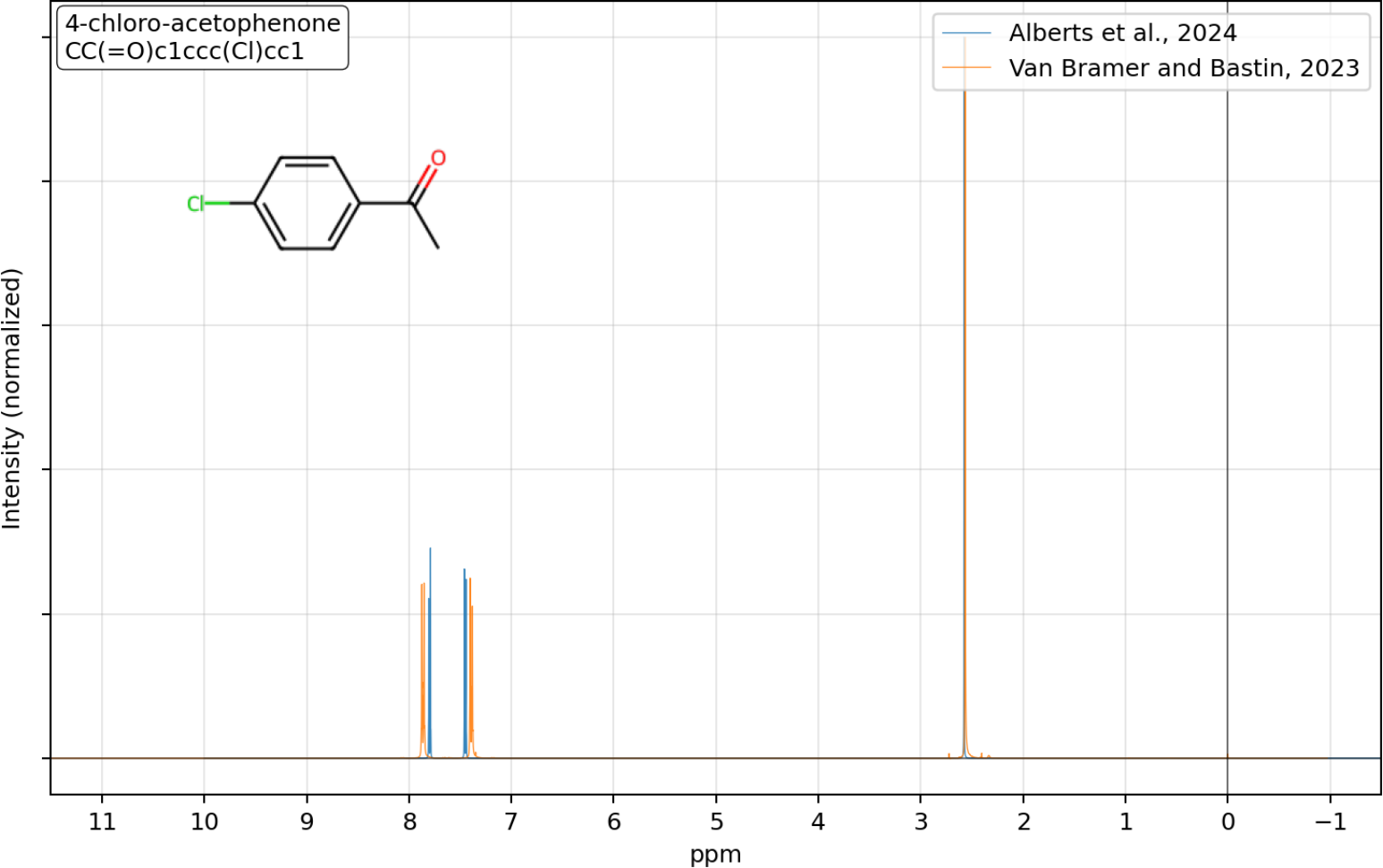

3-methyl-3-pentanol
CCC(C)(O)CC
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

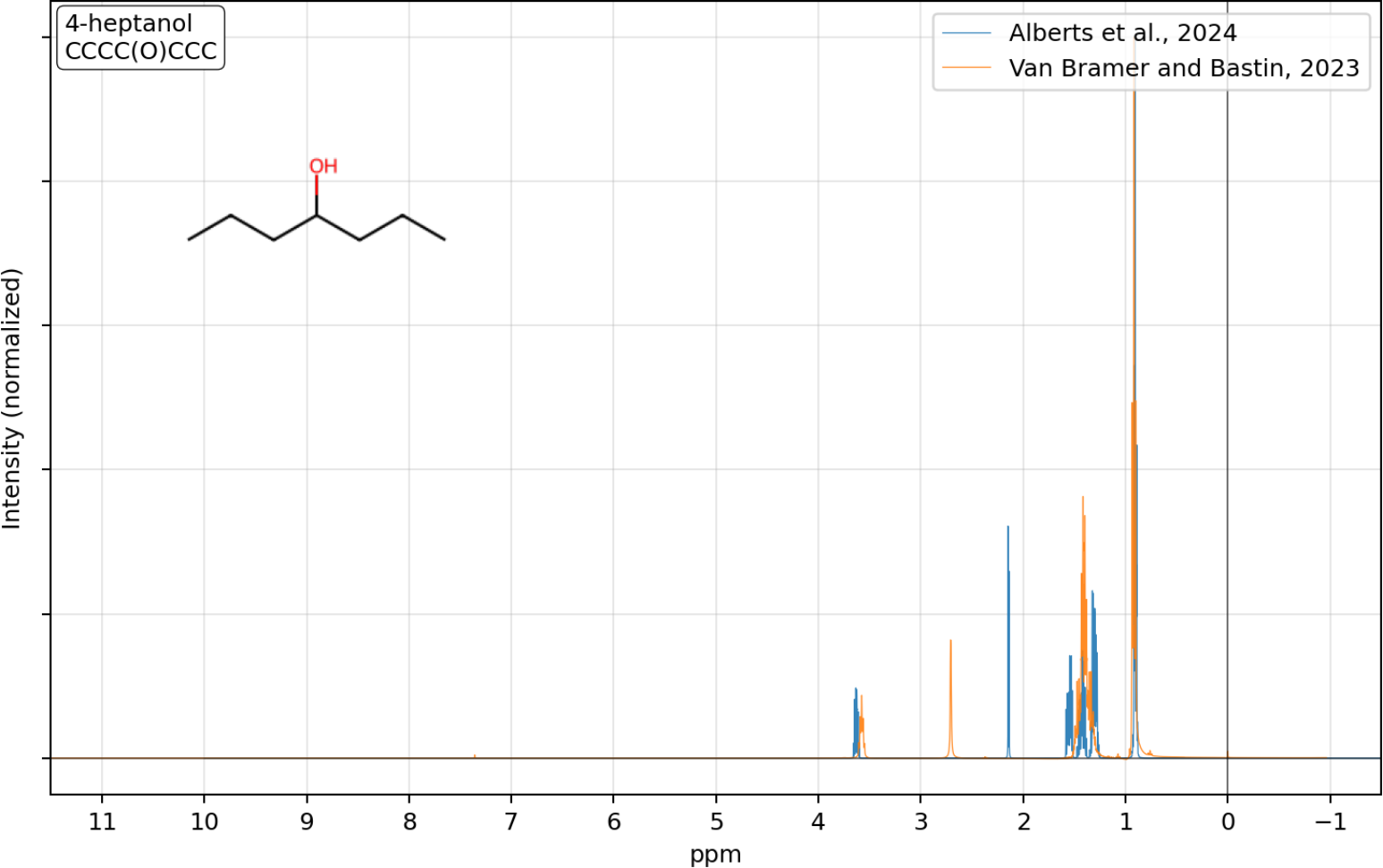

3-methyl-butanoic-acid
CC(C)CC(=O)O
OH
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

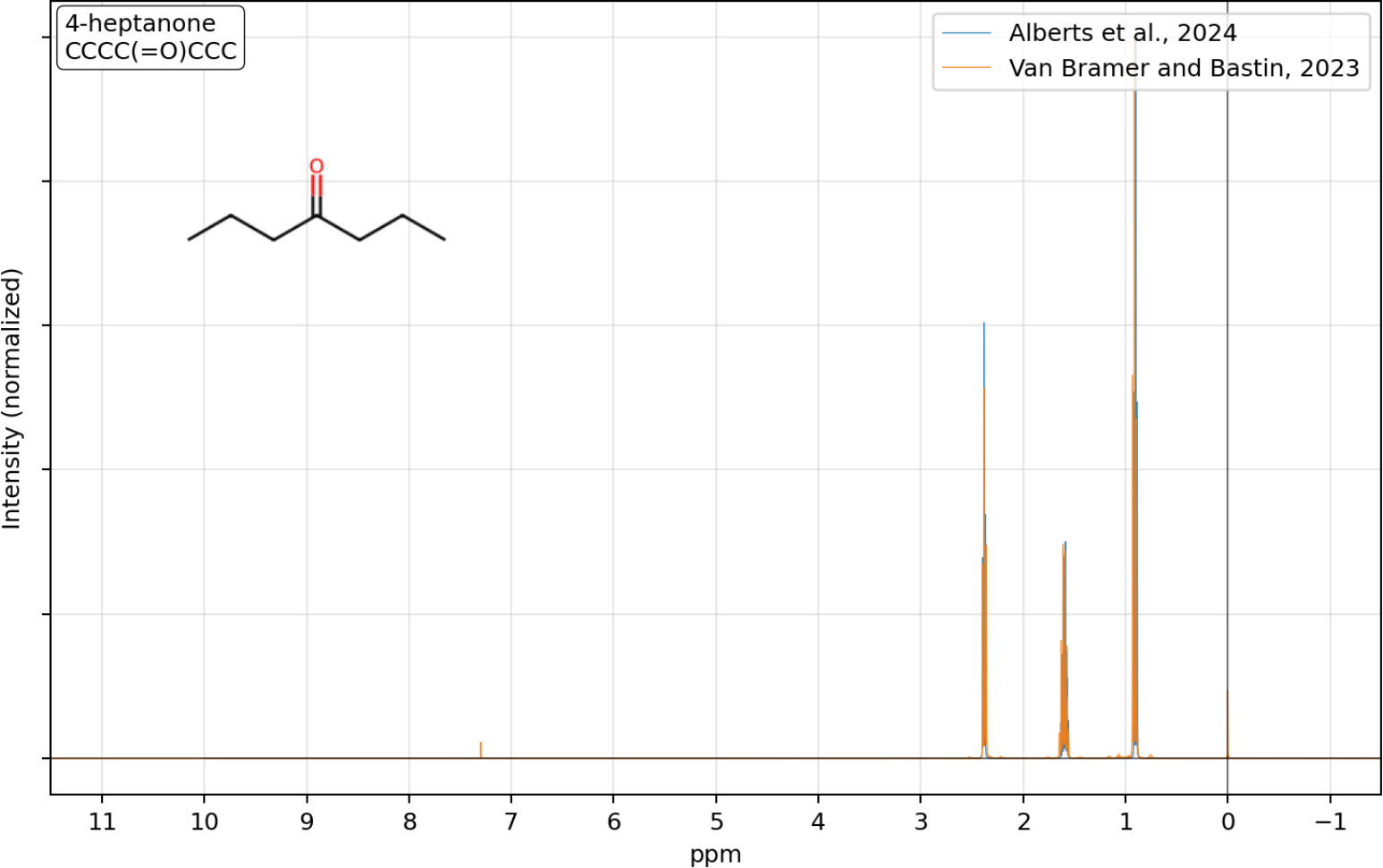

3-methyl-butanoic-anhydride
CC(C)CC(=O)OC(=O)CC(C)C
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

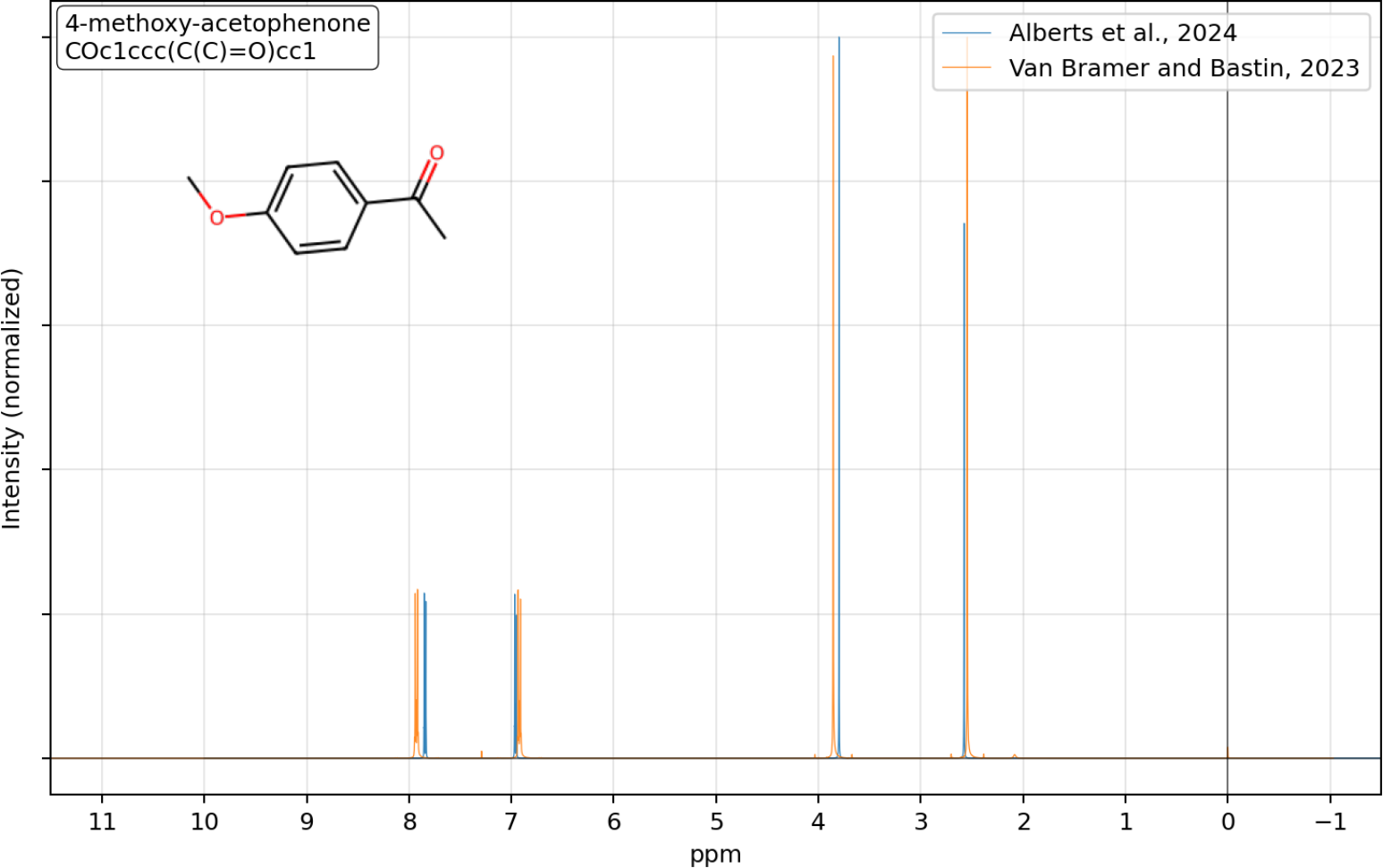

3-methylbutyl-acetate
CC(=O)OCCC(C)C
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

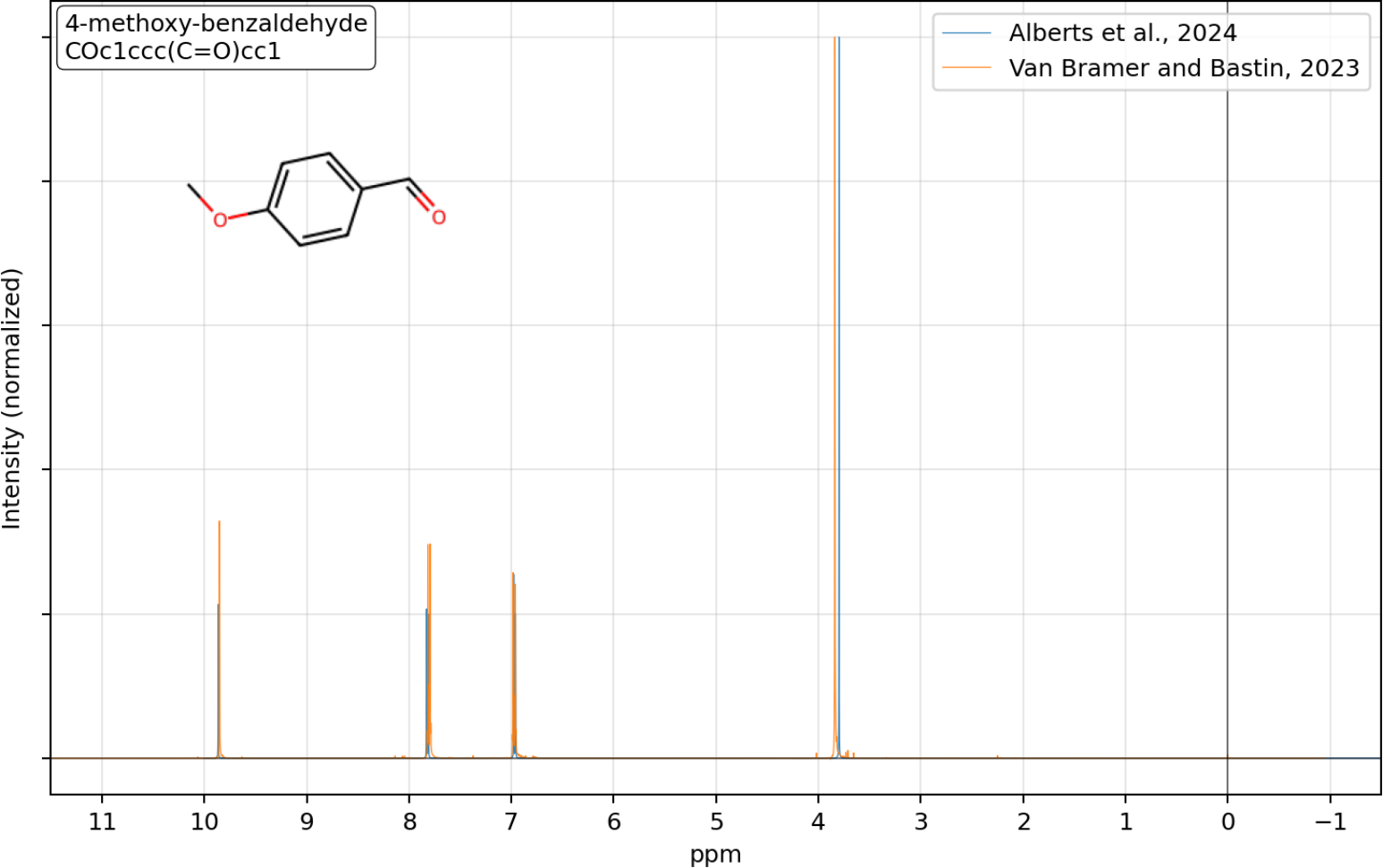

4-bromo-acetophenone
CC(=O)c1ccc(Br)cc1
Br
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

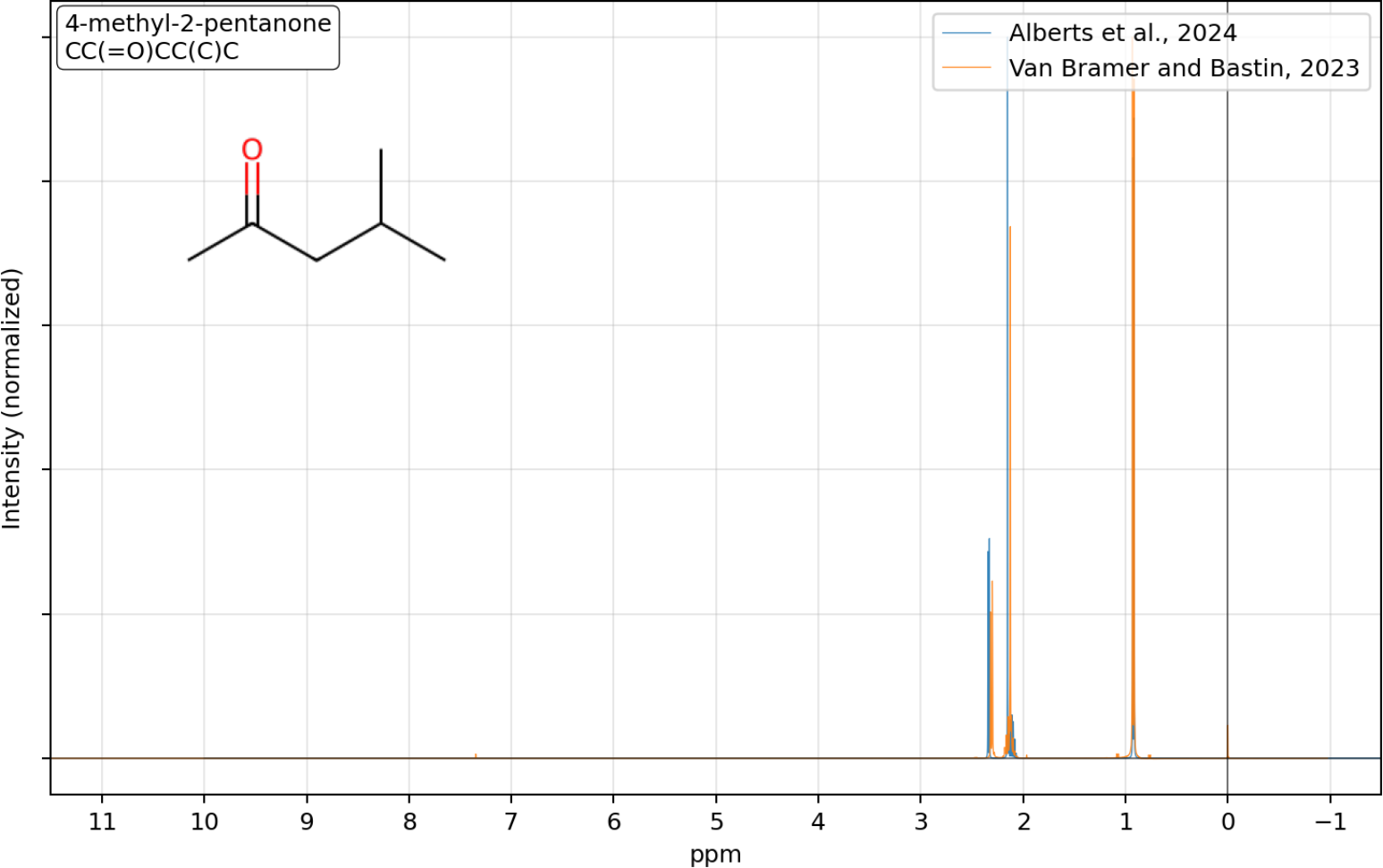

4-chloro-acetophenone
CC(=O)c1ccc(Cl)cc1
Cl
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

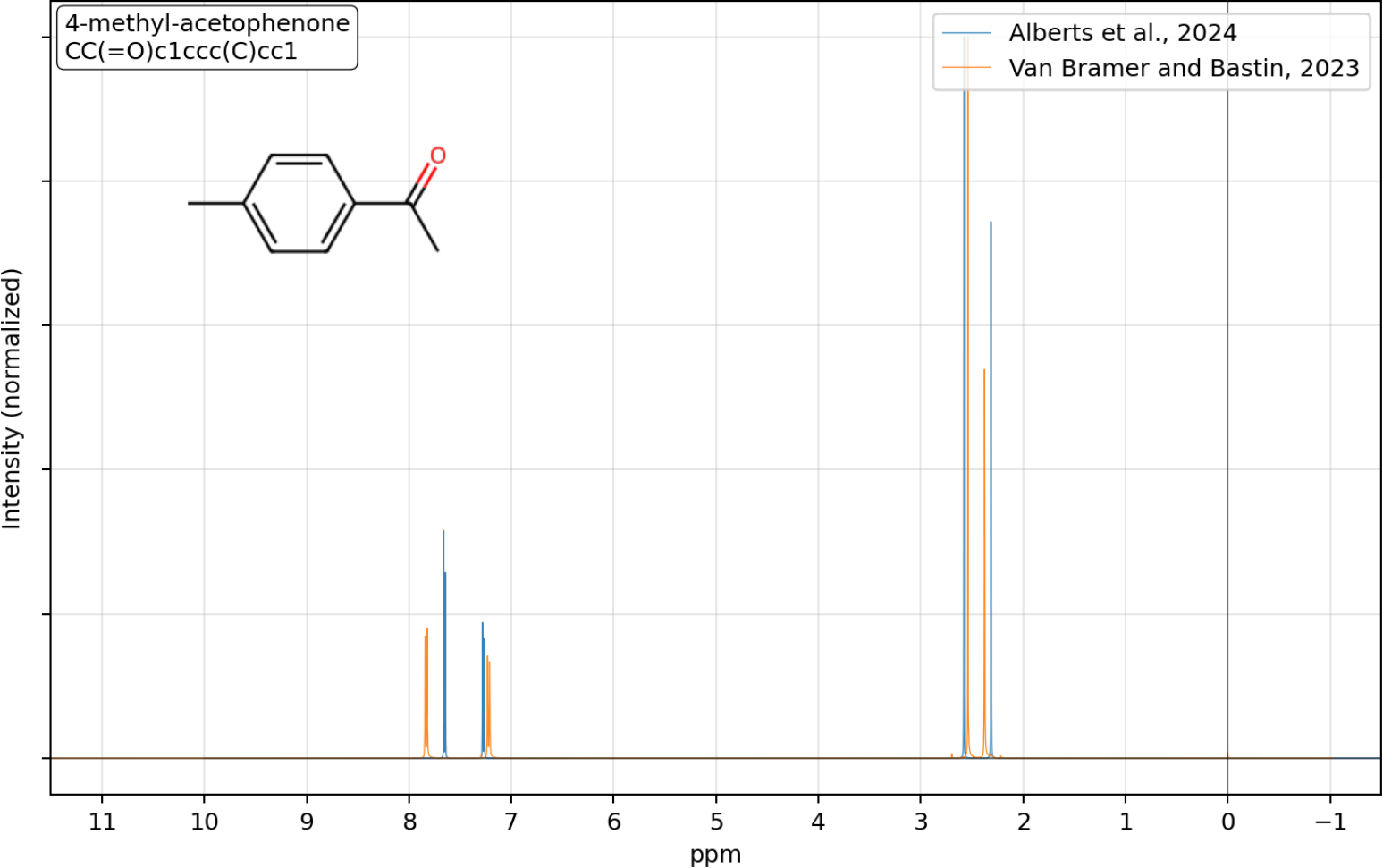

4-heptanol
CCCC(O)CCC
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

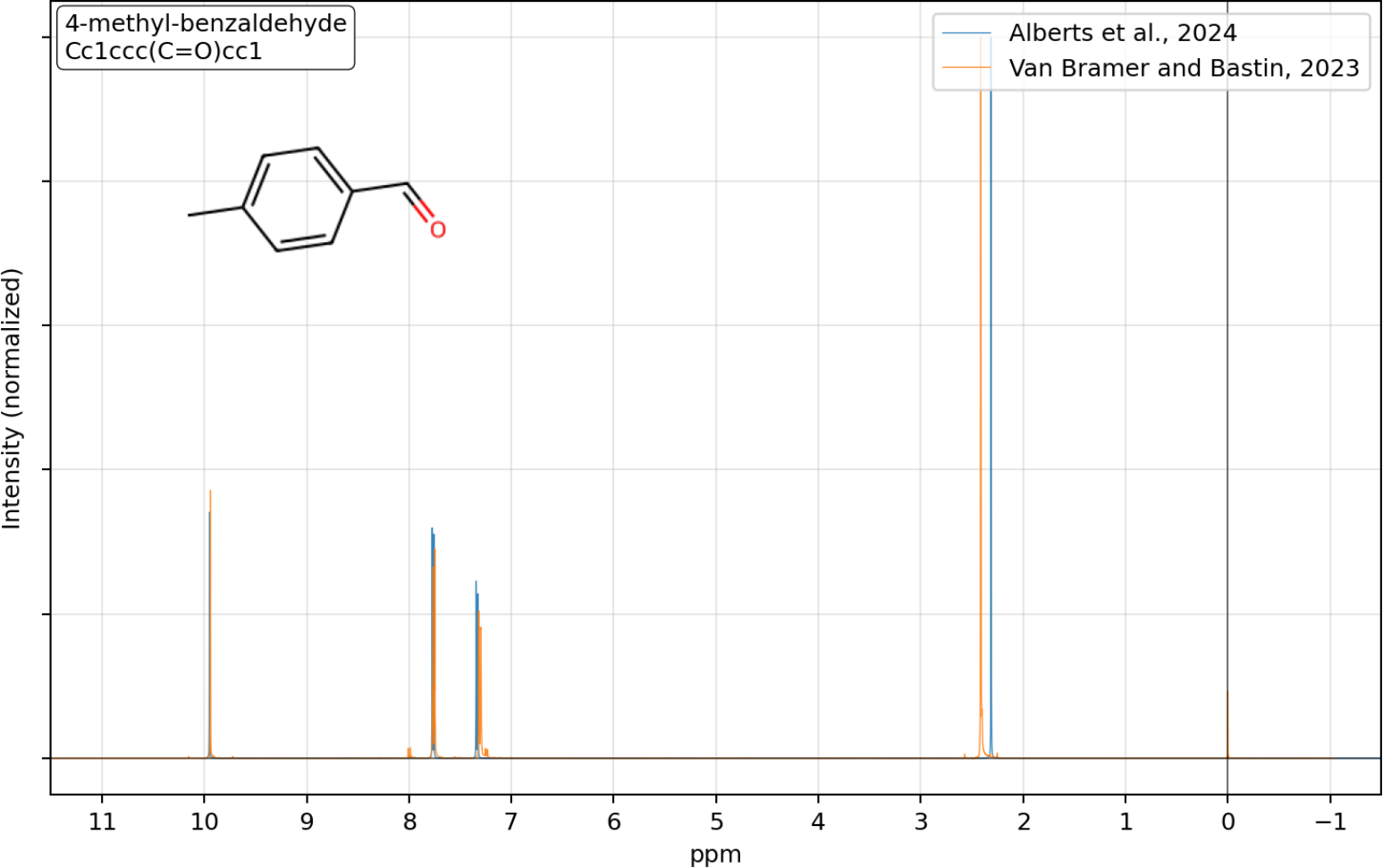

4-heptanone
CCCC(=O)CCC
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

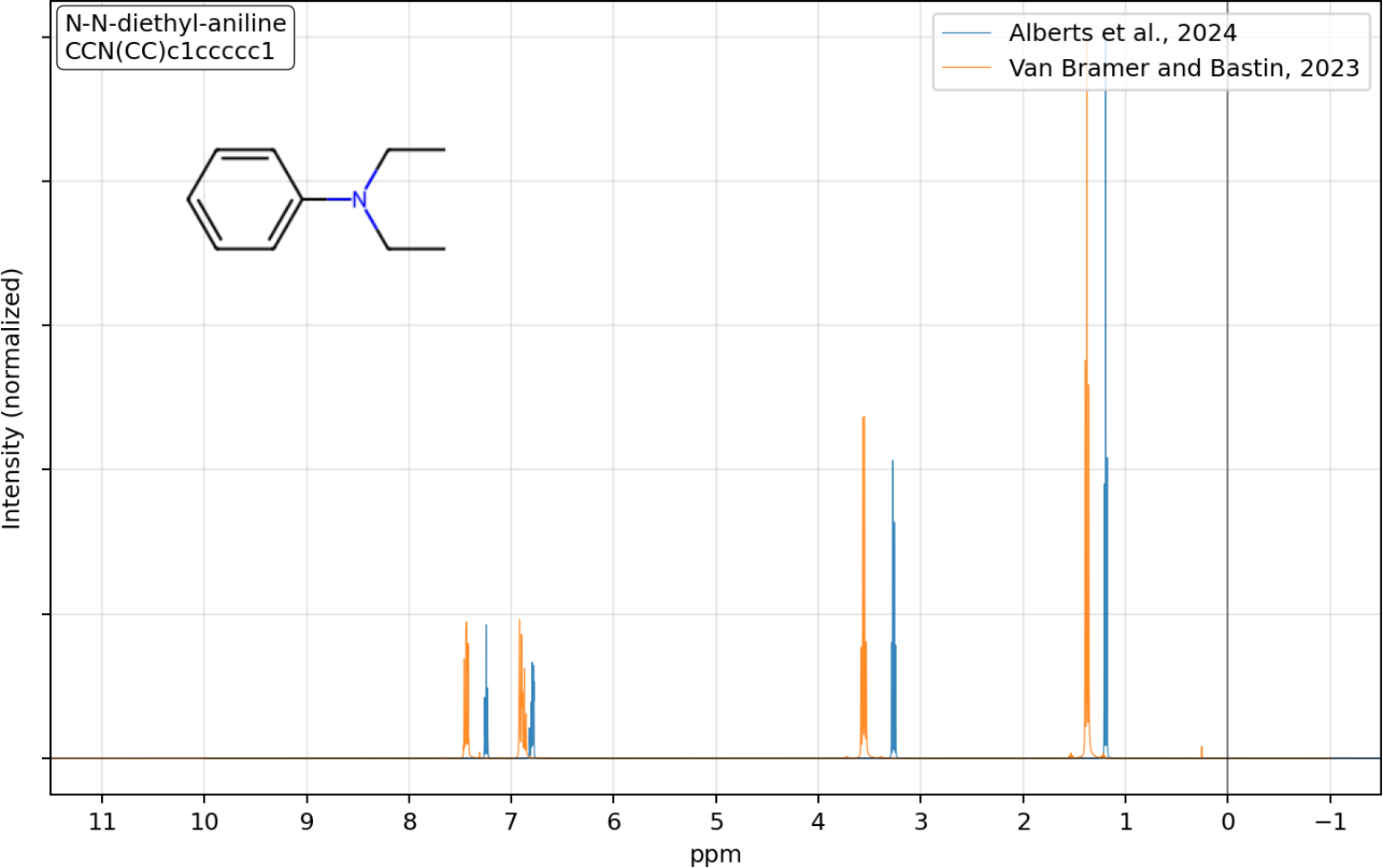

4-methoxy-acetophenone
COc1ccc(C(C)=O)cc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

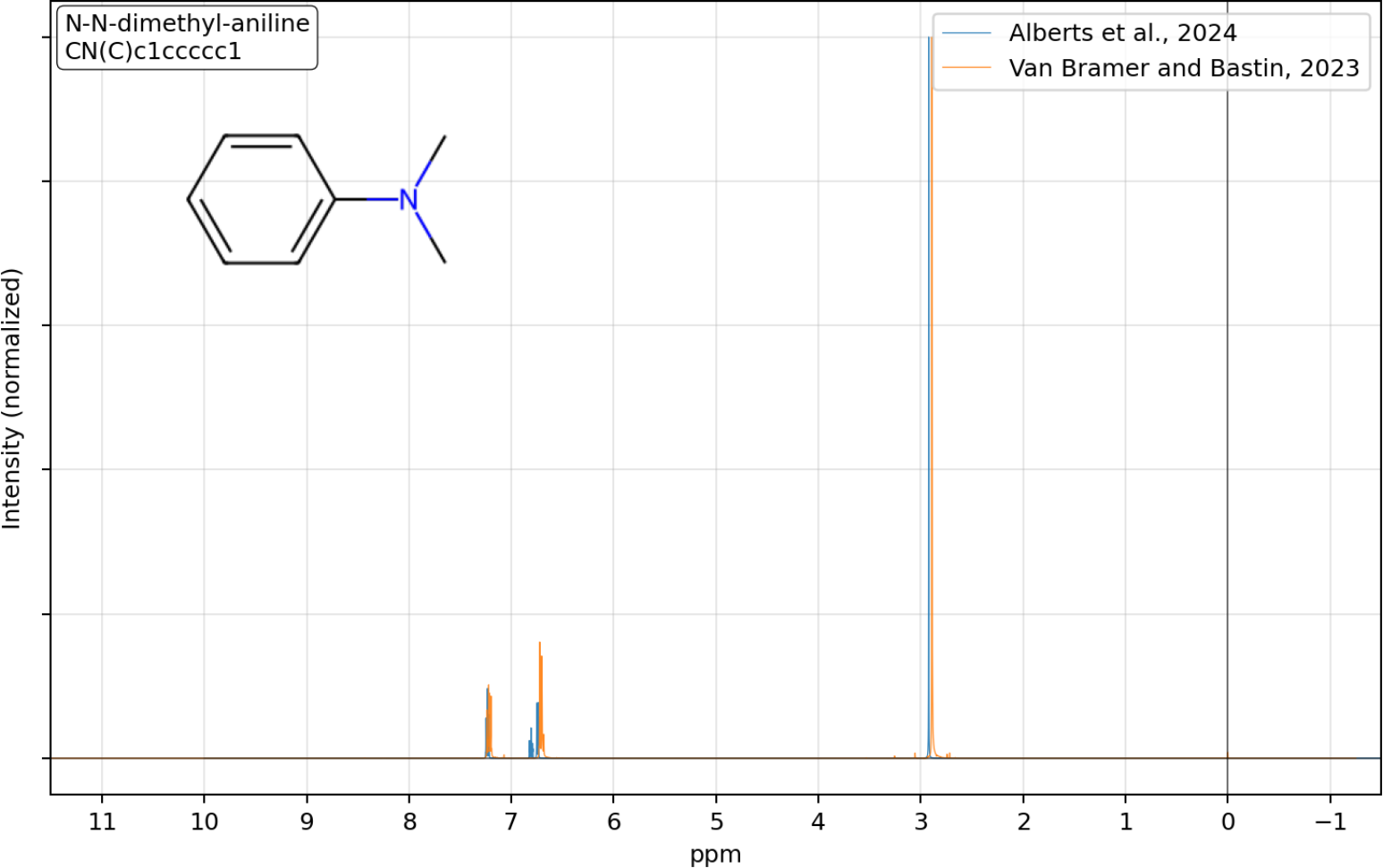

4-methoxy-benzaldehyde
COc1ccc(C=O)cc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

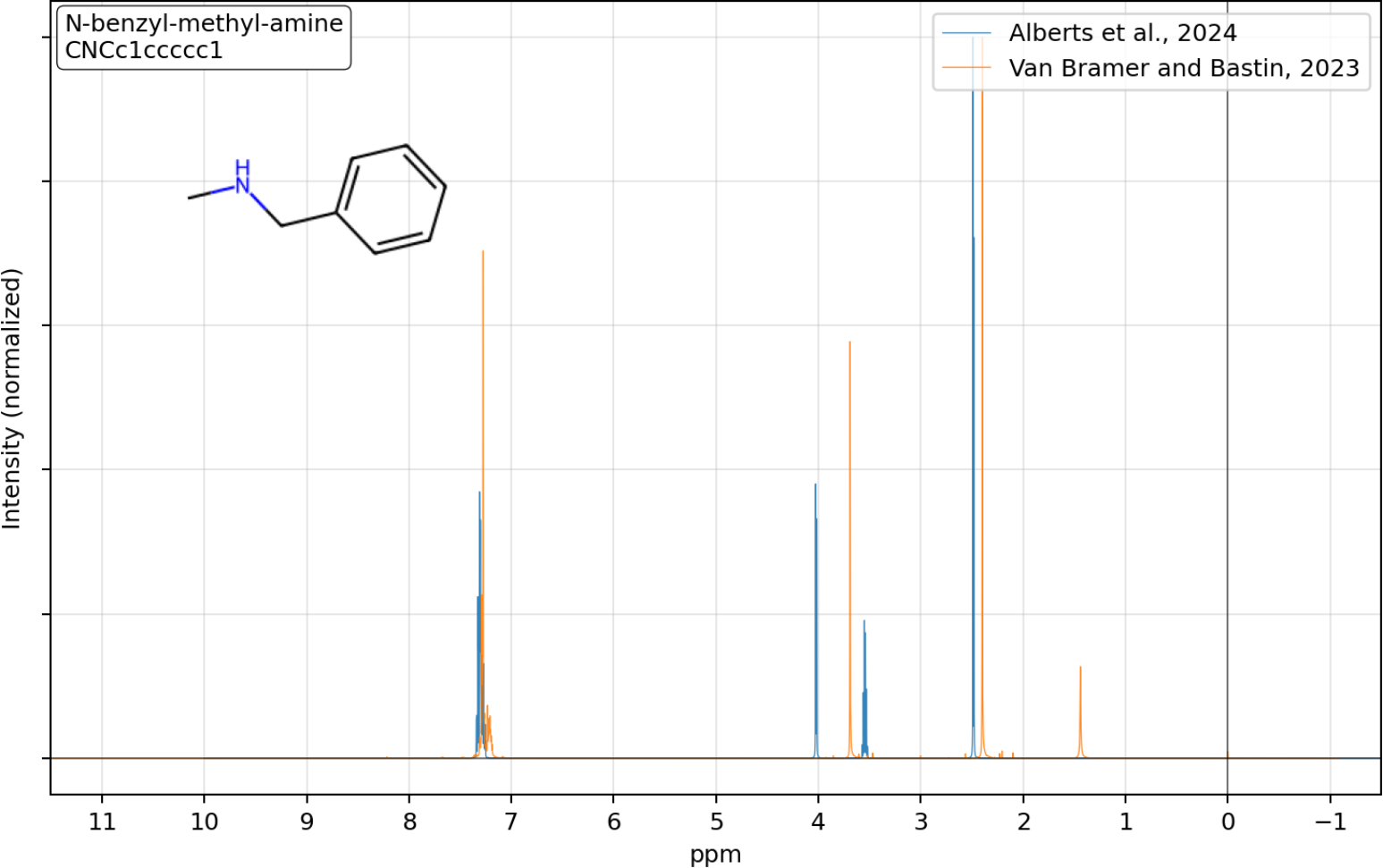

4-methyl-2-pentanone
CC(=O)CC(C)C
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

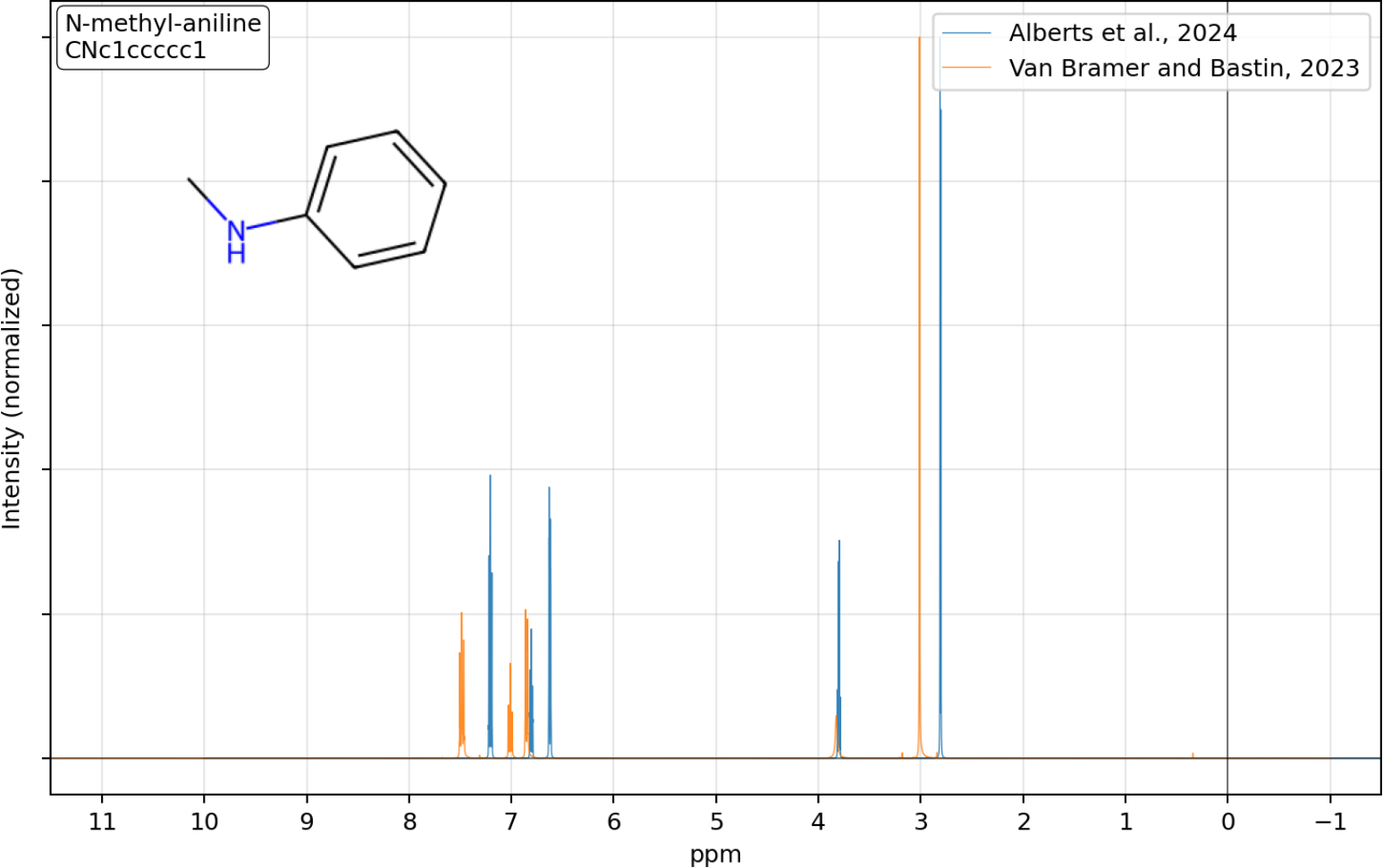

4-methyl-acetophenone
CC(=O)c1ccc(C)cc1
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

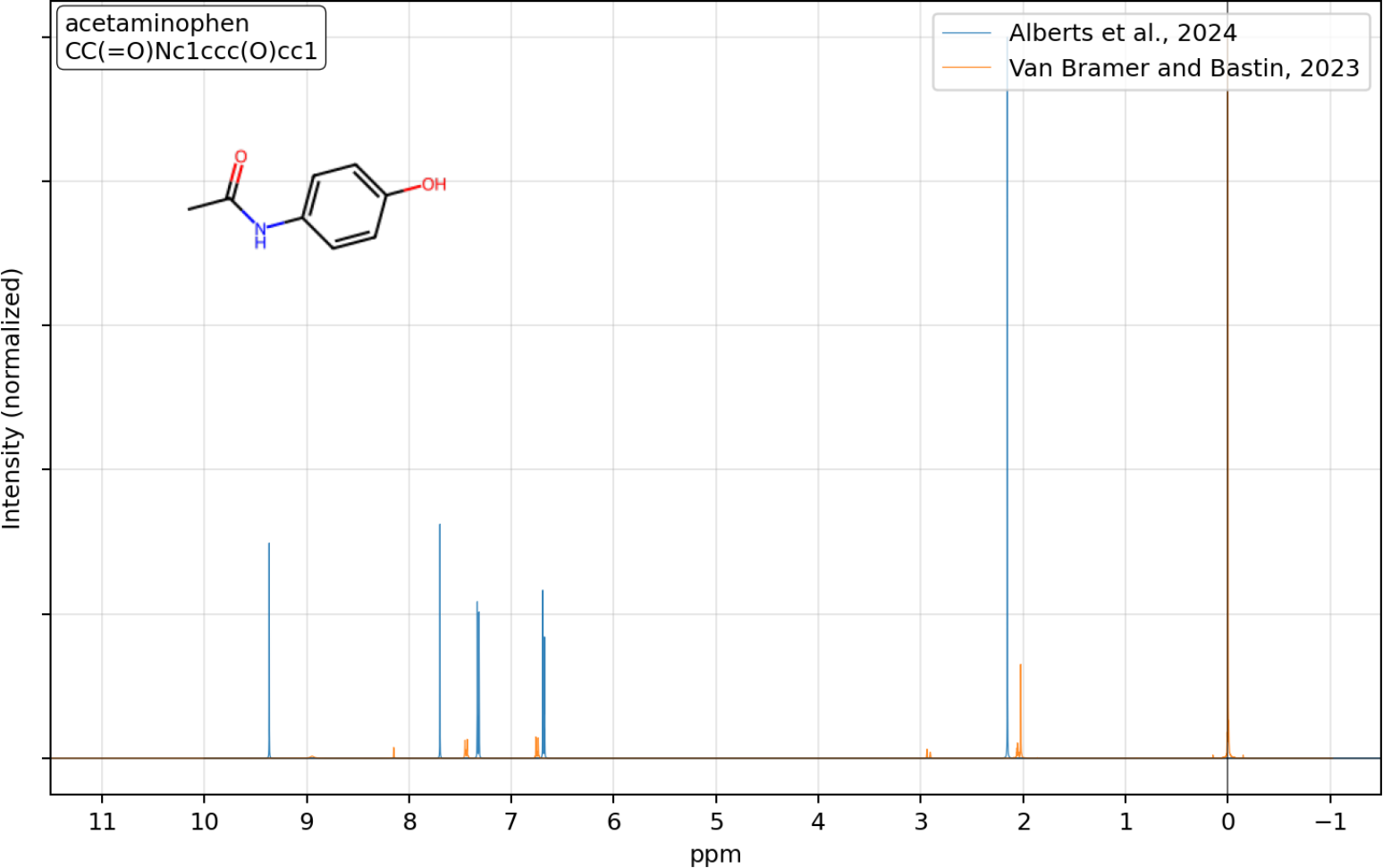

4-methyl-benzaldehyde
Cc1ccc(C=O)cc1
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

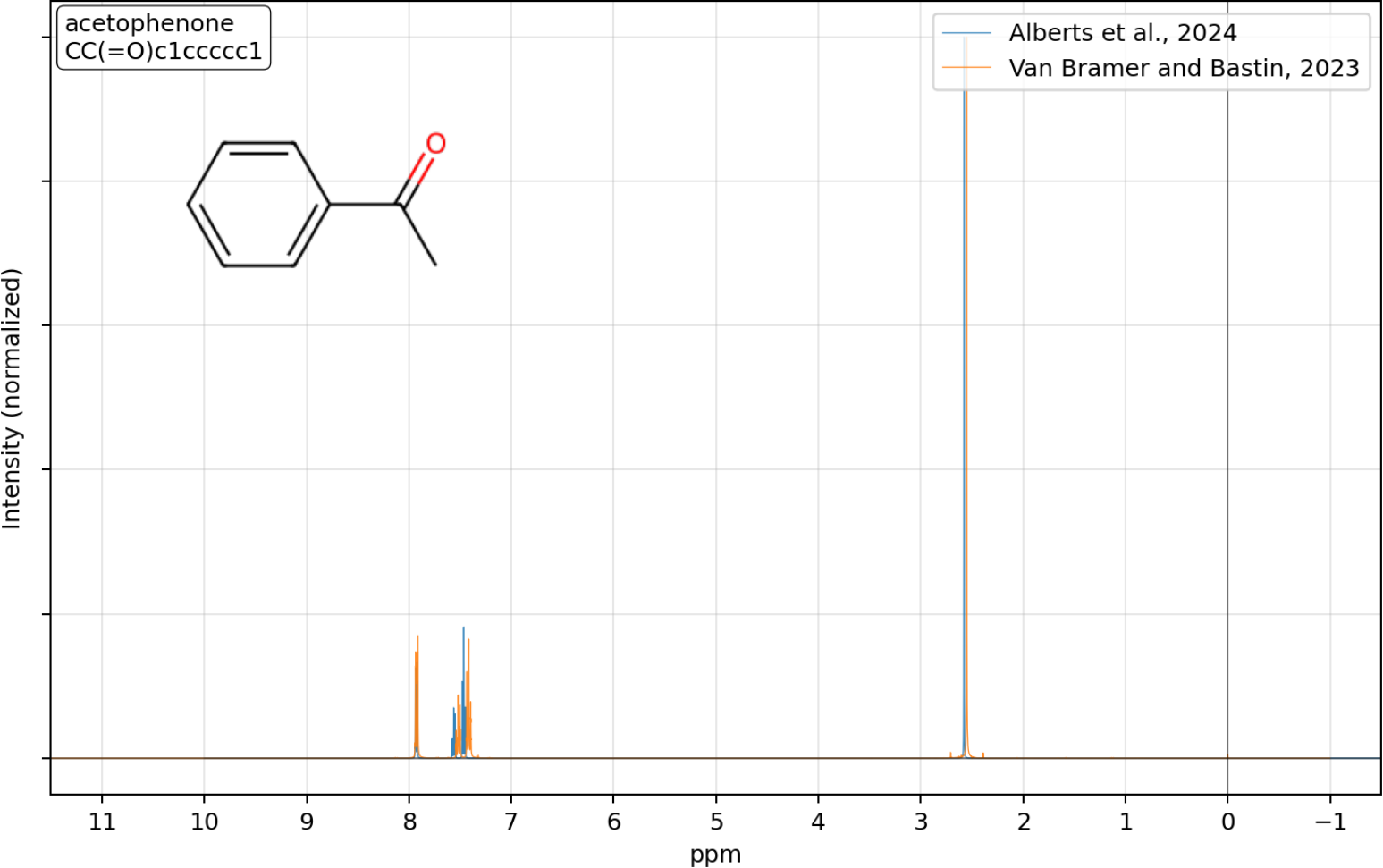

N-N-diethyl-aniline
CCN(CC)c1ccccc1
N
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

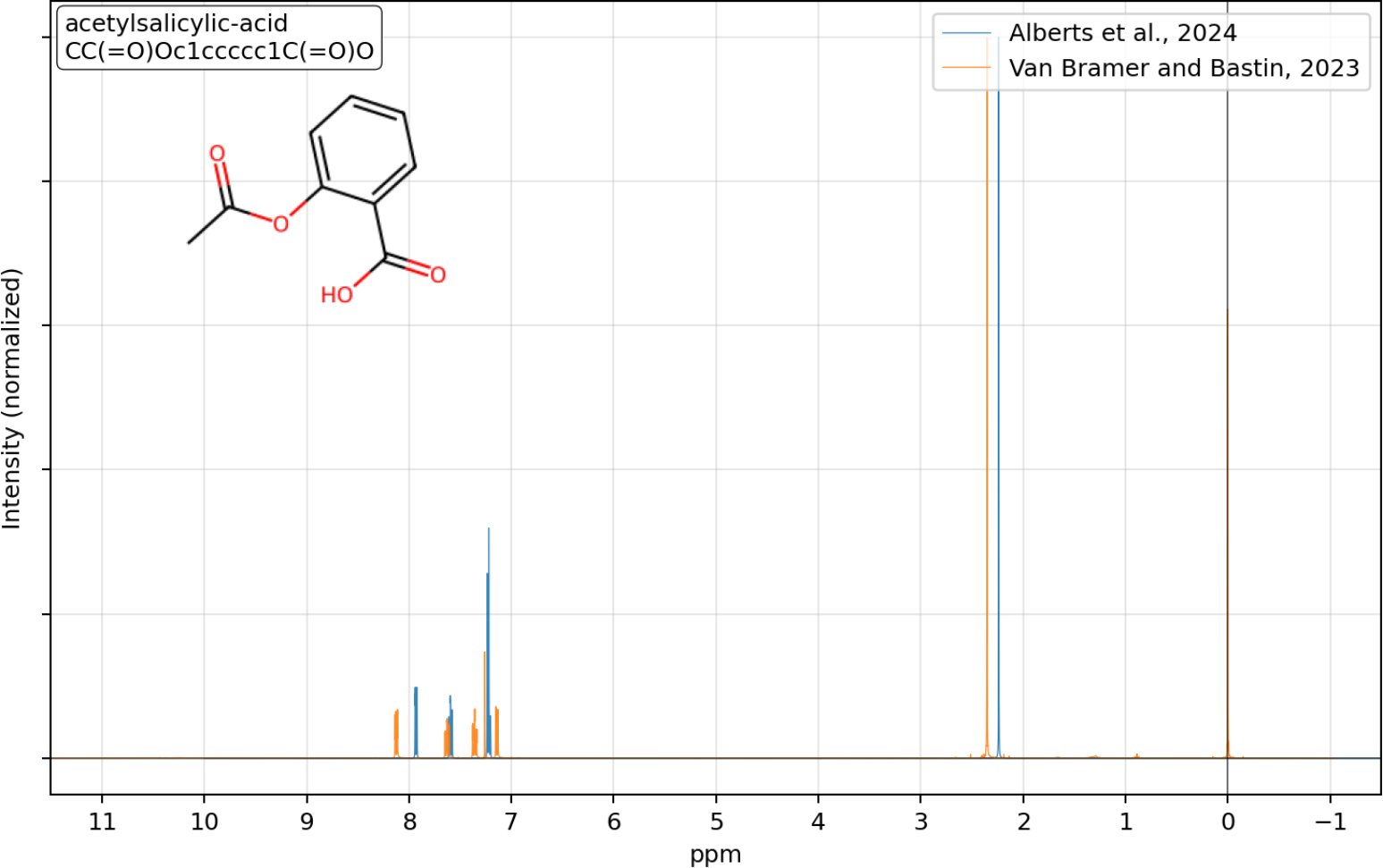

N-N-dimethyl-aniline
CN(C)c1ccccc1
N
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

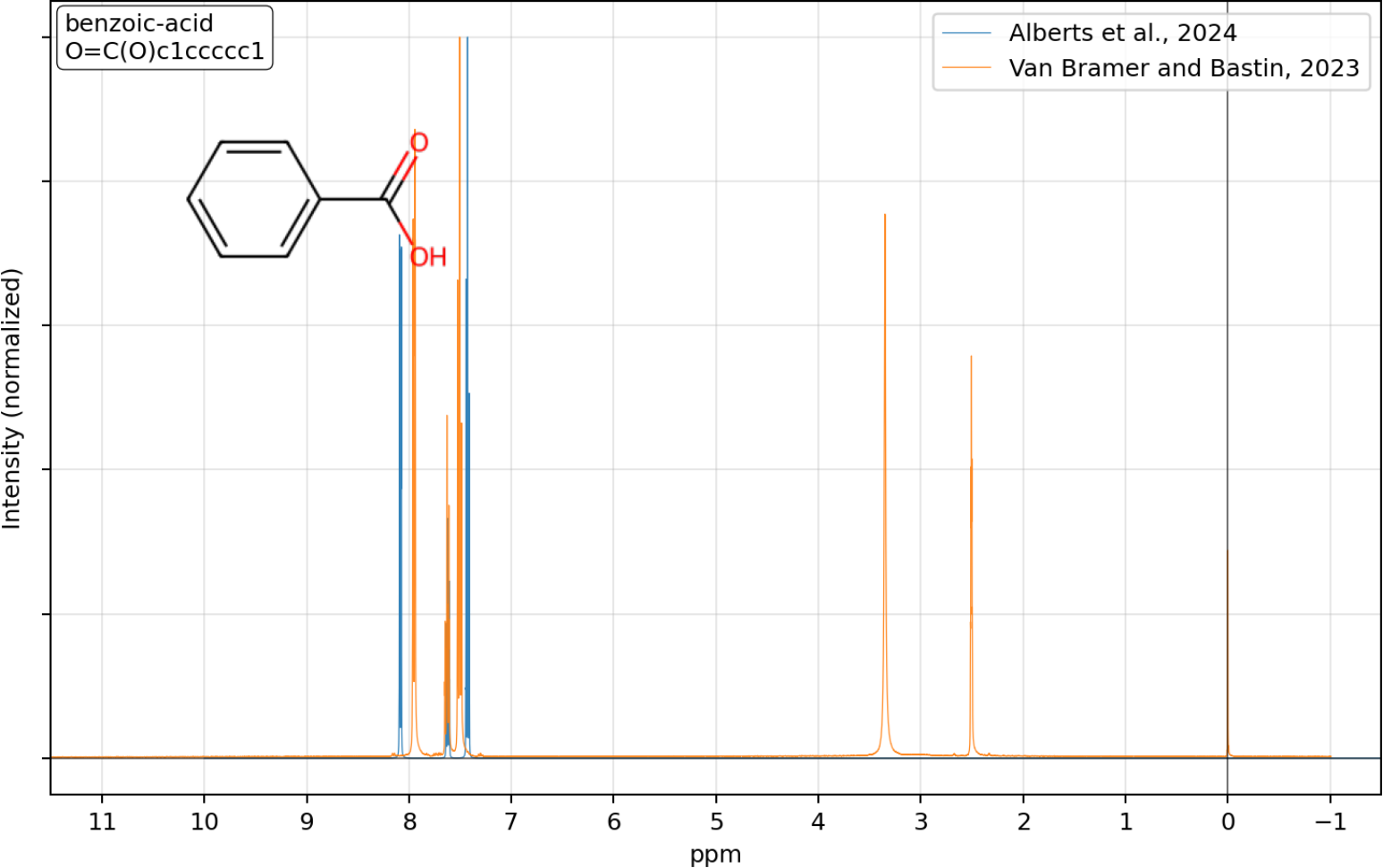

N-benzyl-methyl-amine
CNCc1ccccc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

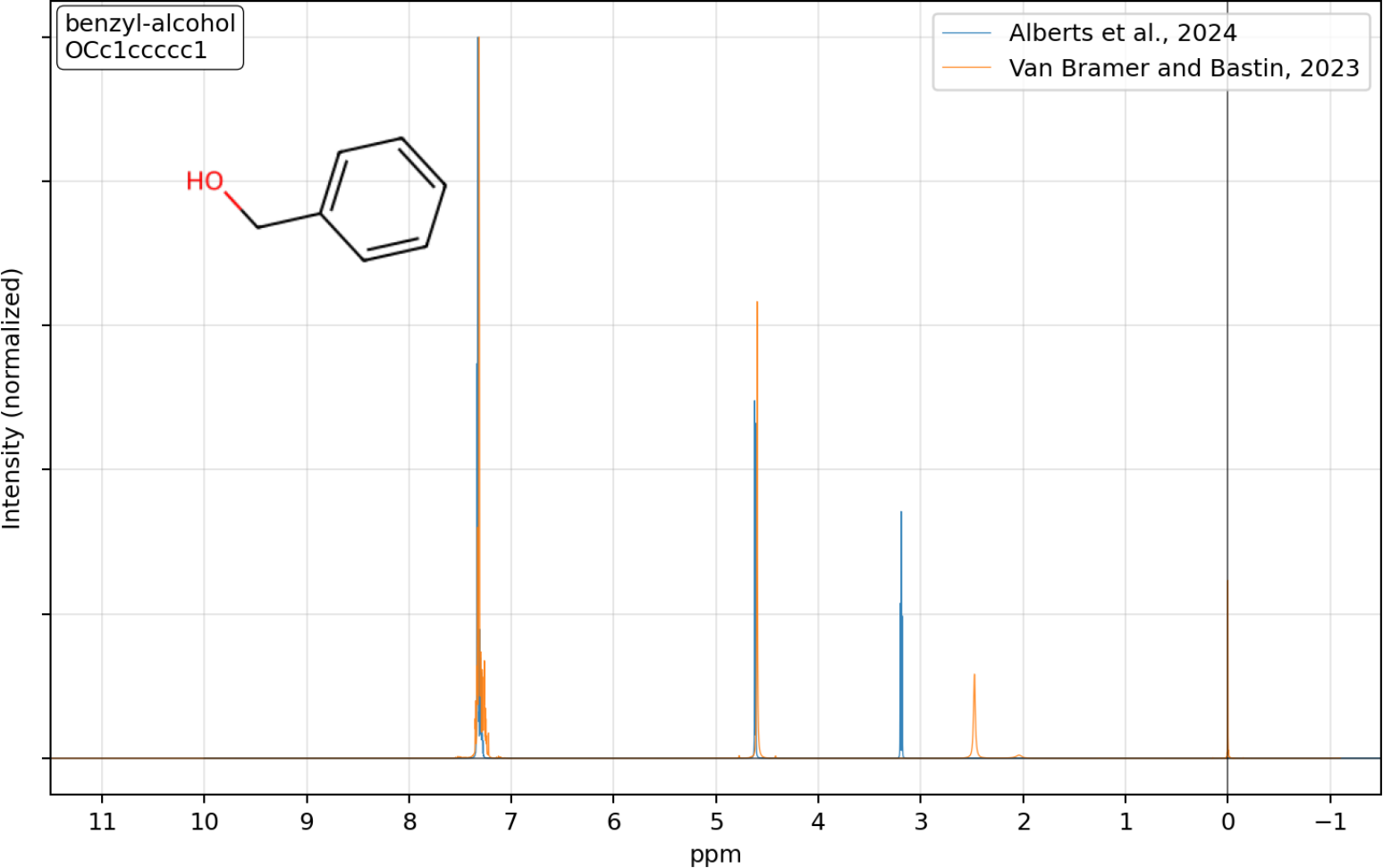

N-methyl-aniline
CNc1ccccc1
N
H
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

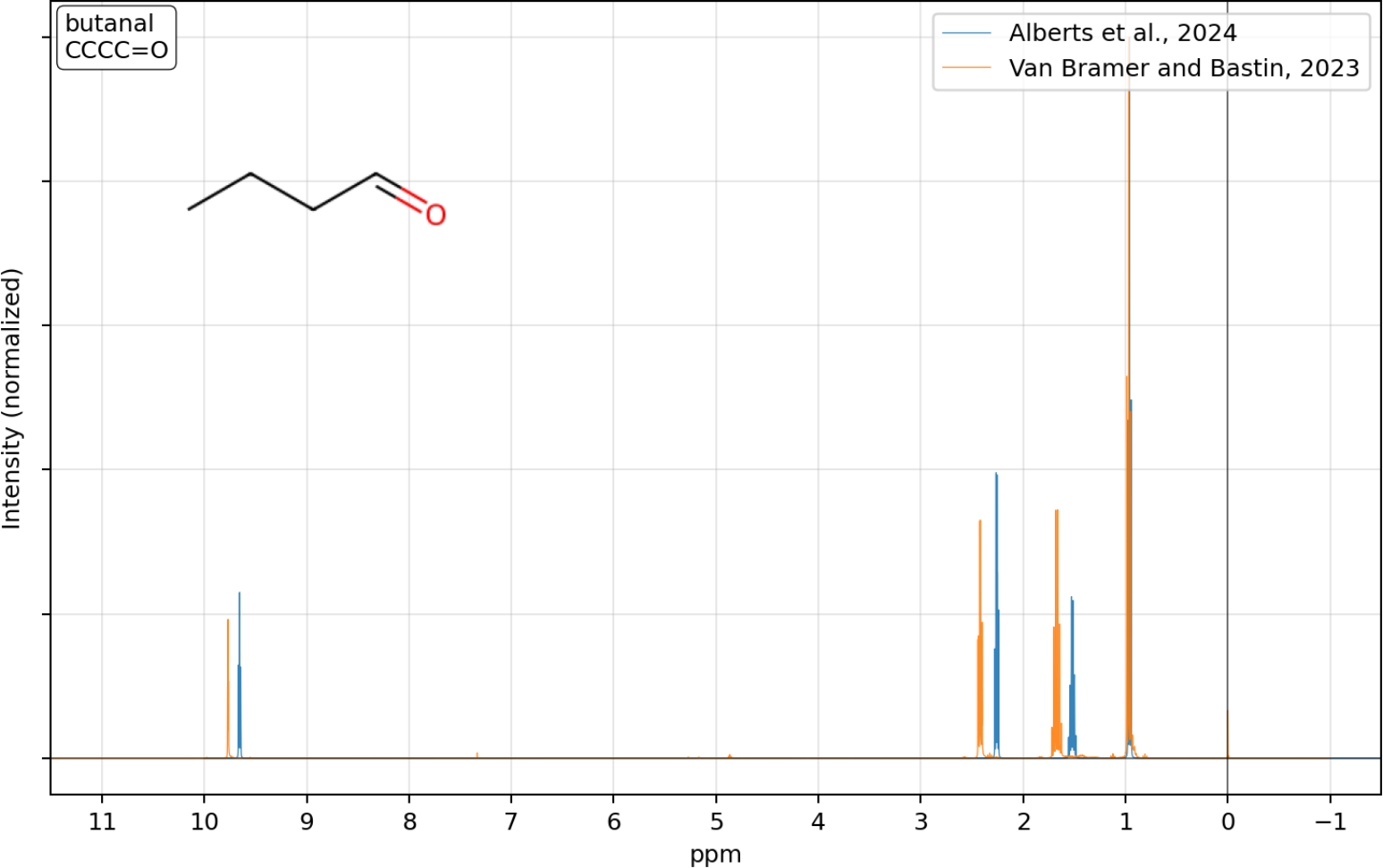

acetaminophen
CC(=O)Nc1ccc(O)cc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1
O
OH
N
H

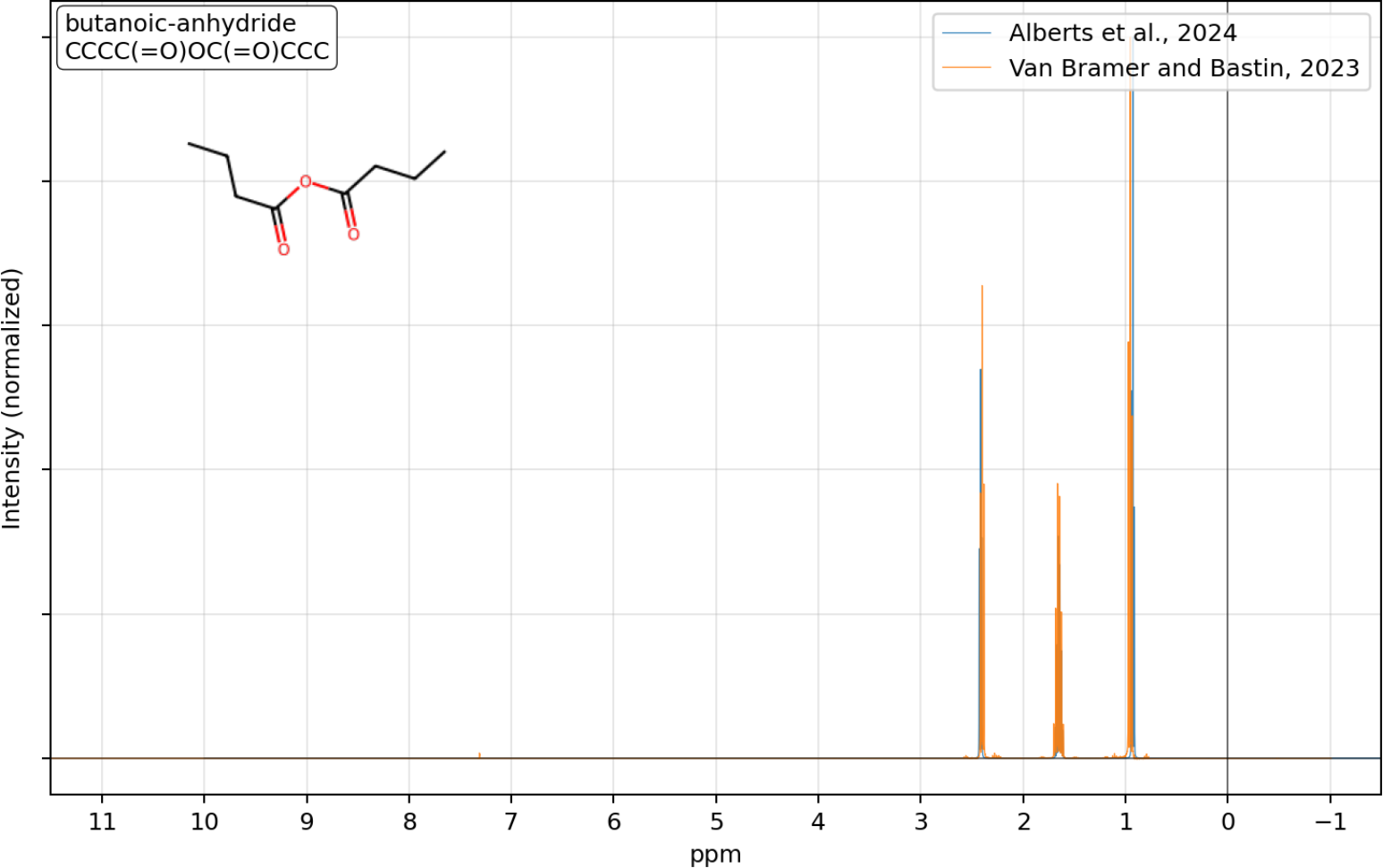

acetophenone
CC(=O)c1ccccc1
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

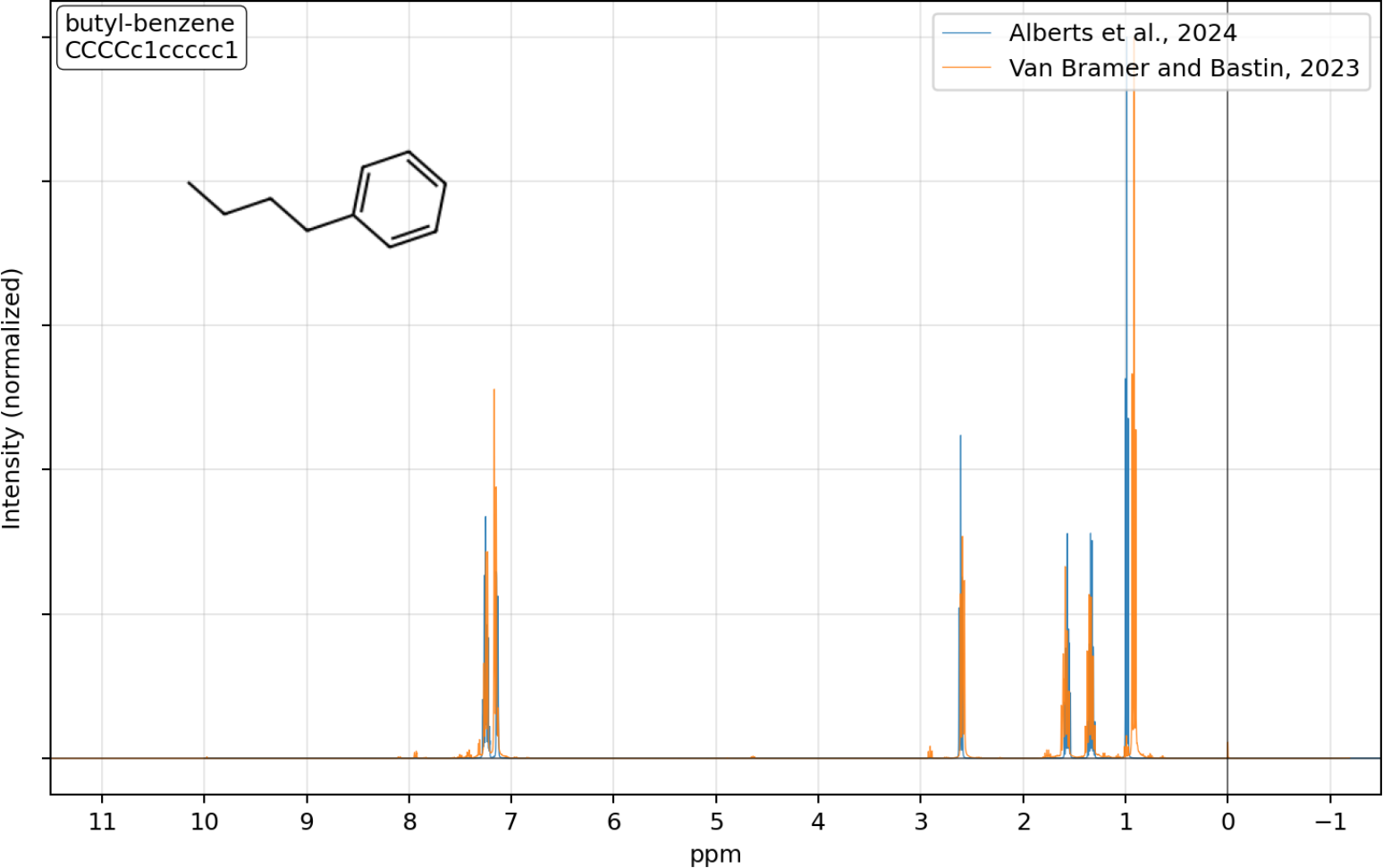

acetylsalicylic-acid
CC(=O)Oc1ccccc1C(=O)O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

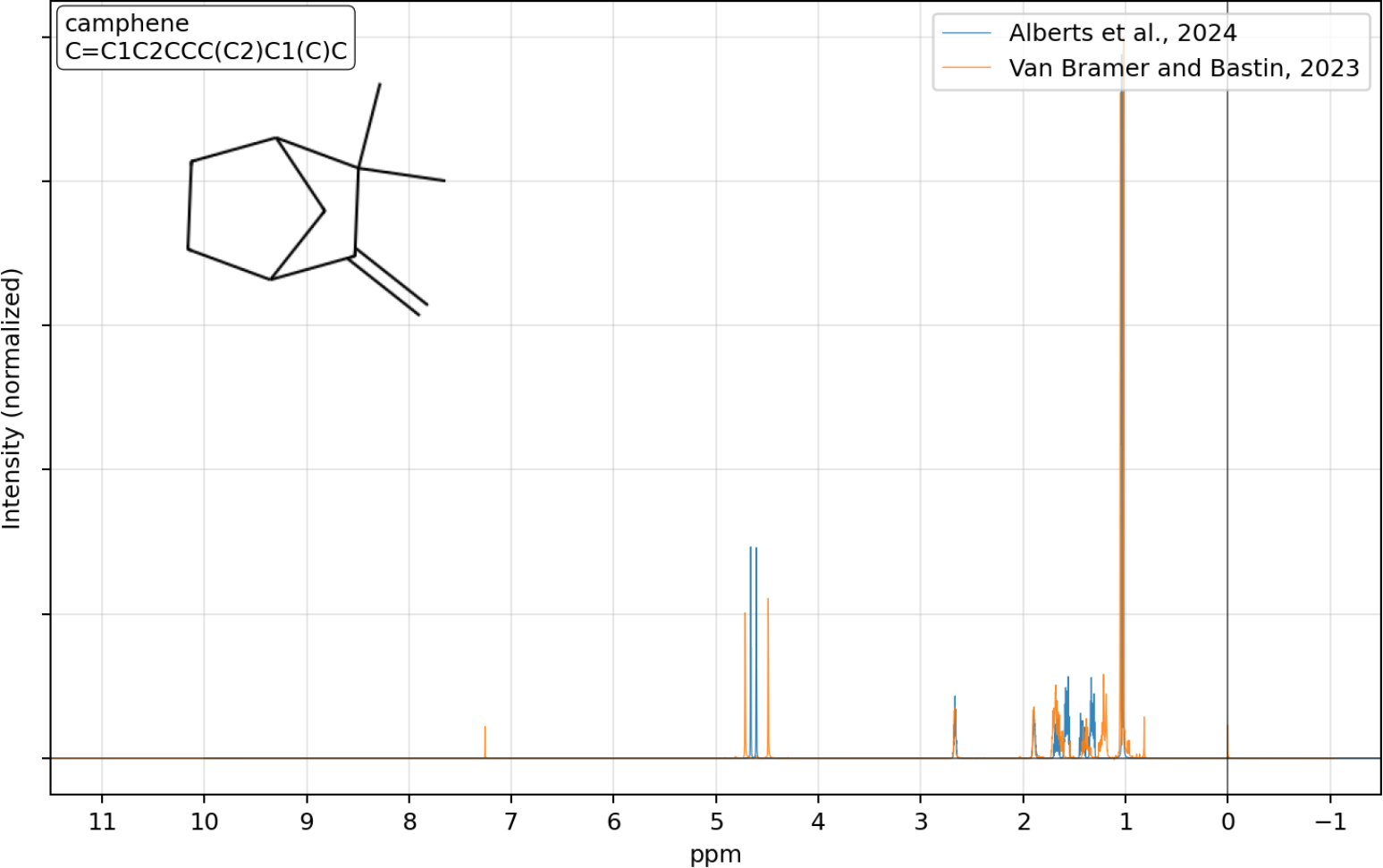

benzoic-acid
O=C(O)c1ccccc1
O
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

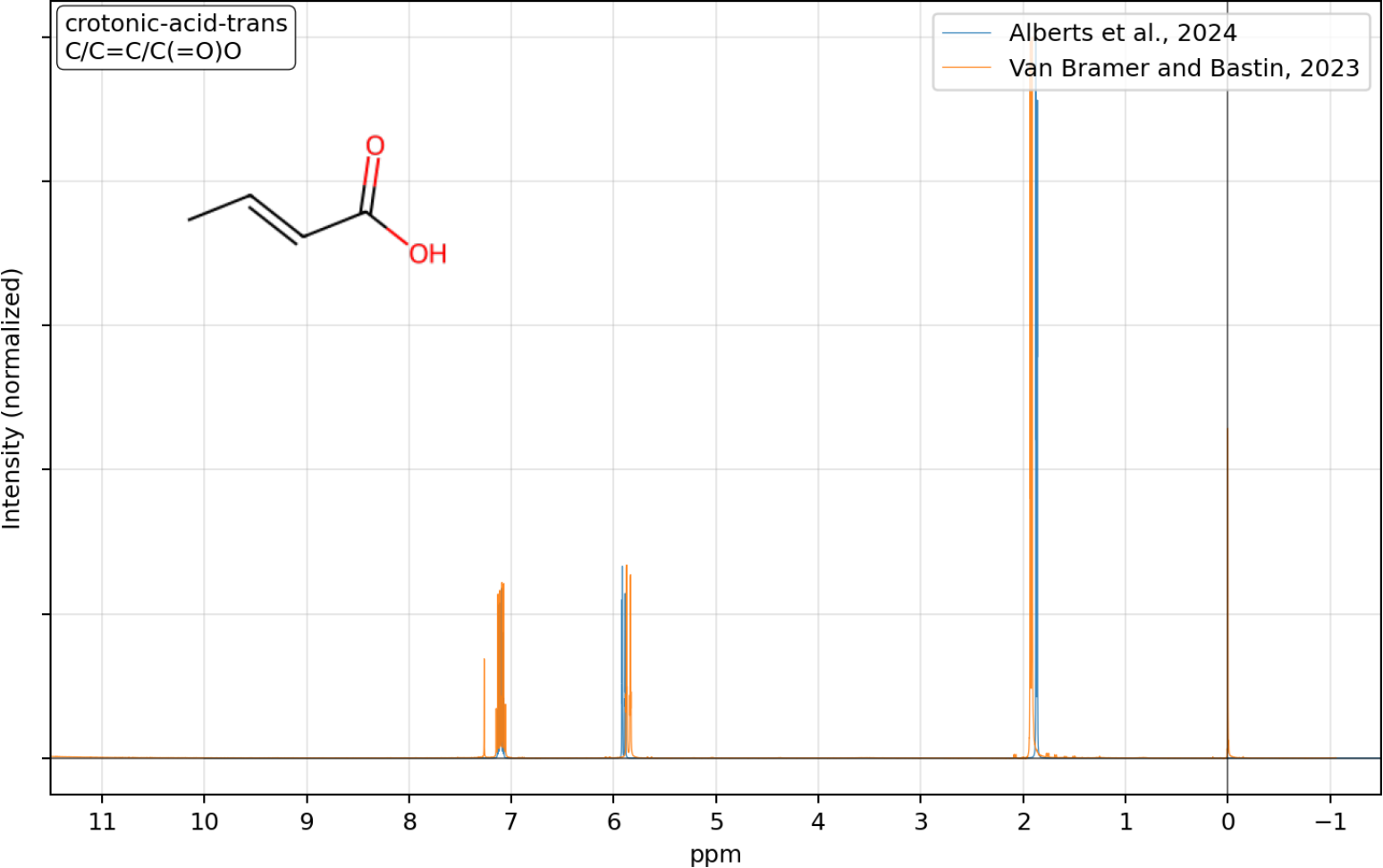

benzyl-alcohol
OCc1ccccc1
HO
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

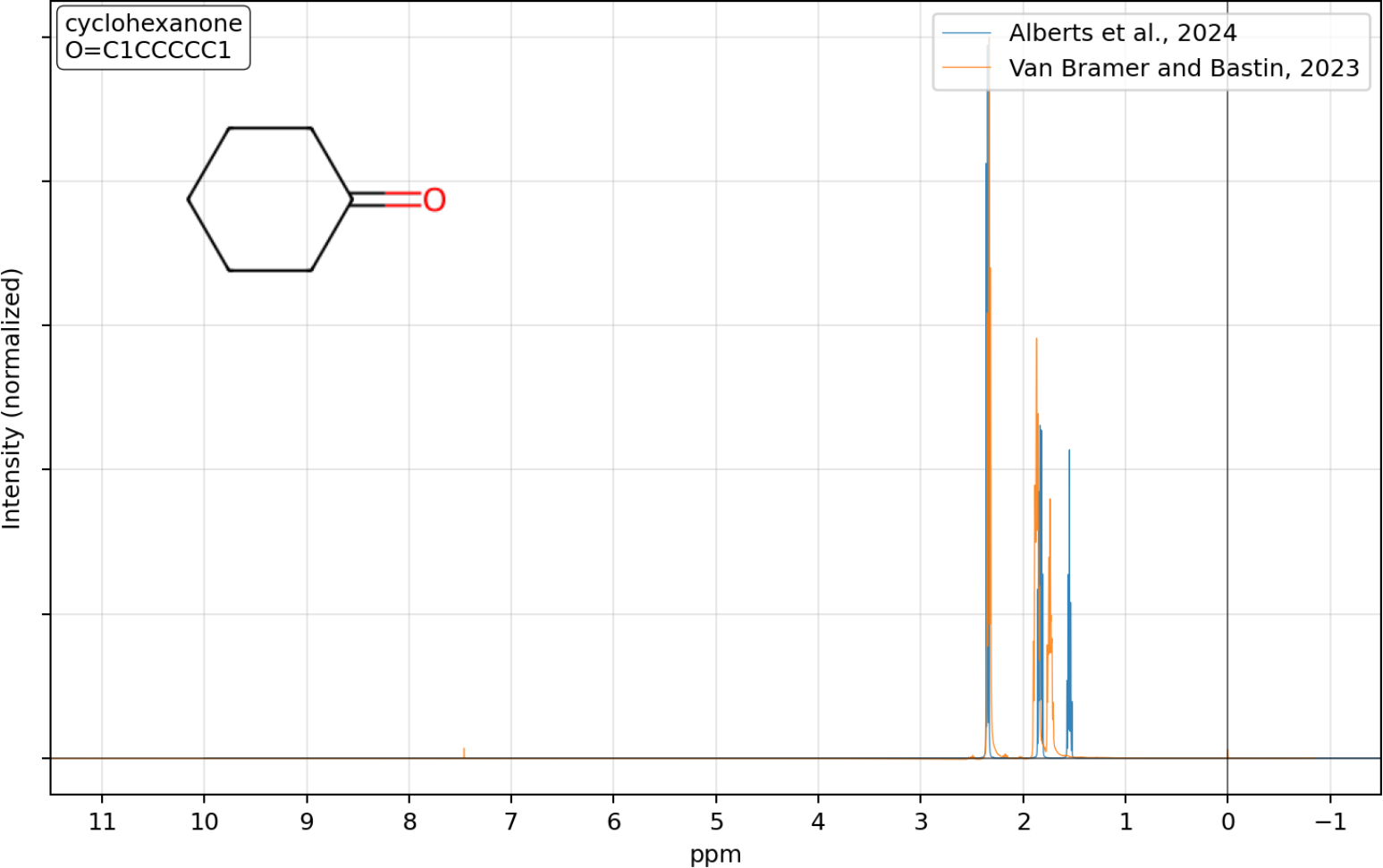

butanal
CCCC=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
O
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

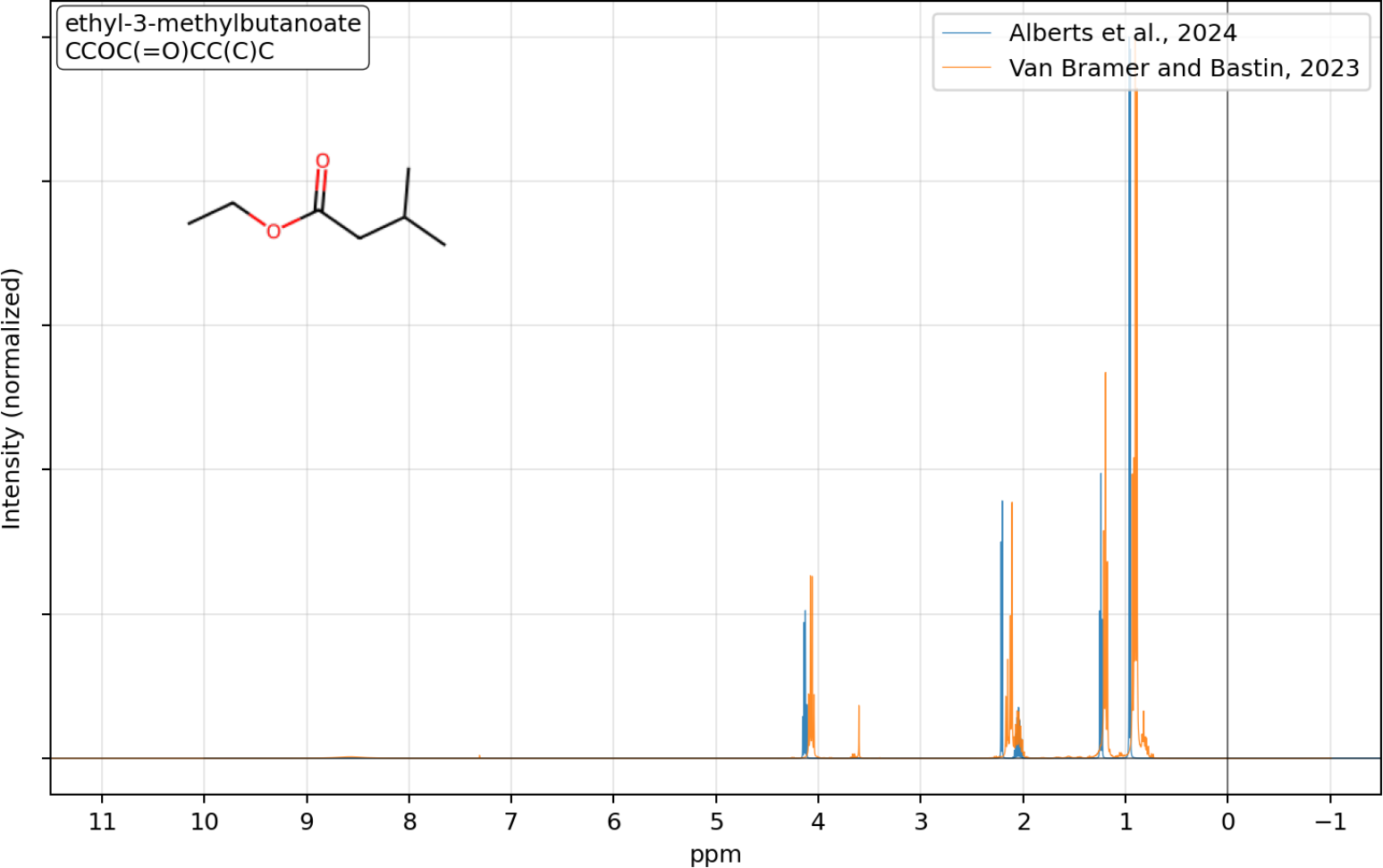

butanoic-anhydride
CCCC(=O)OC(=O)CCC
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

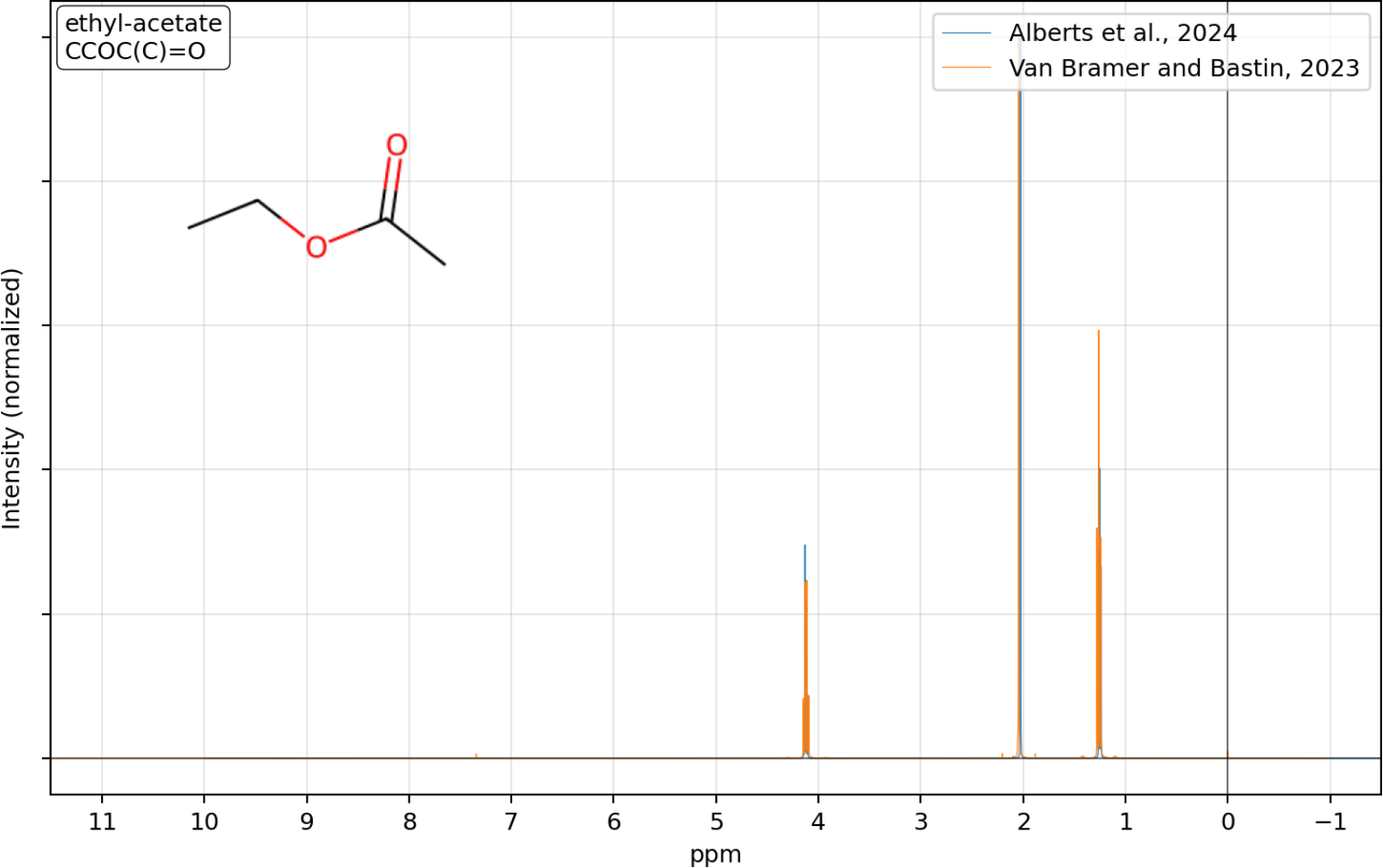

butyl-benzene
CCCCc1ccccc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

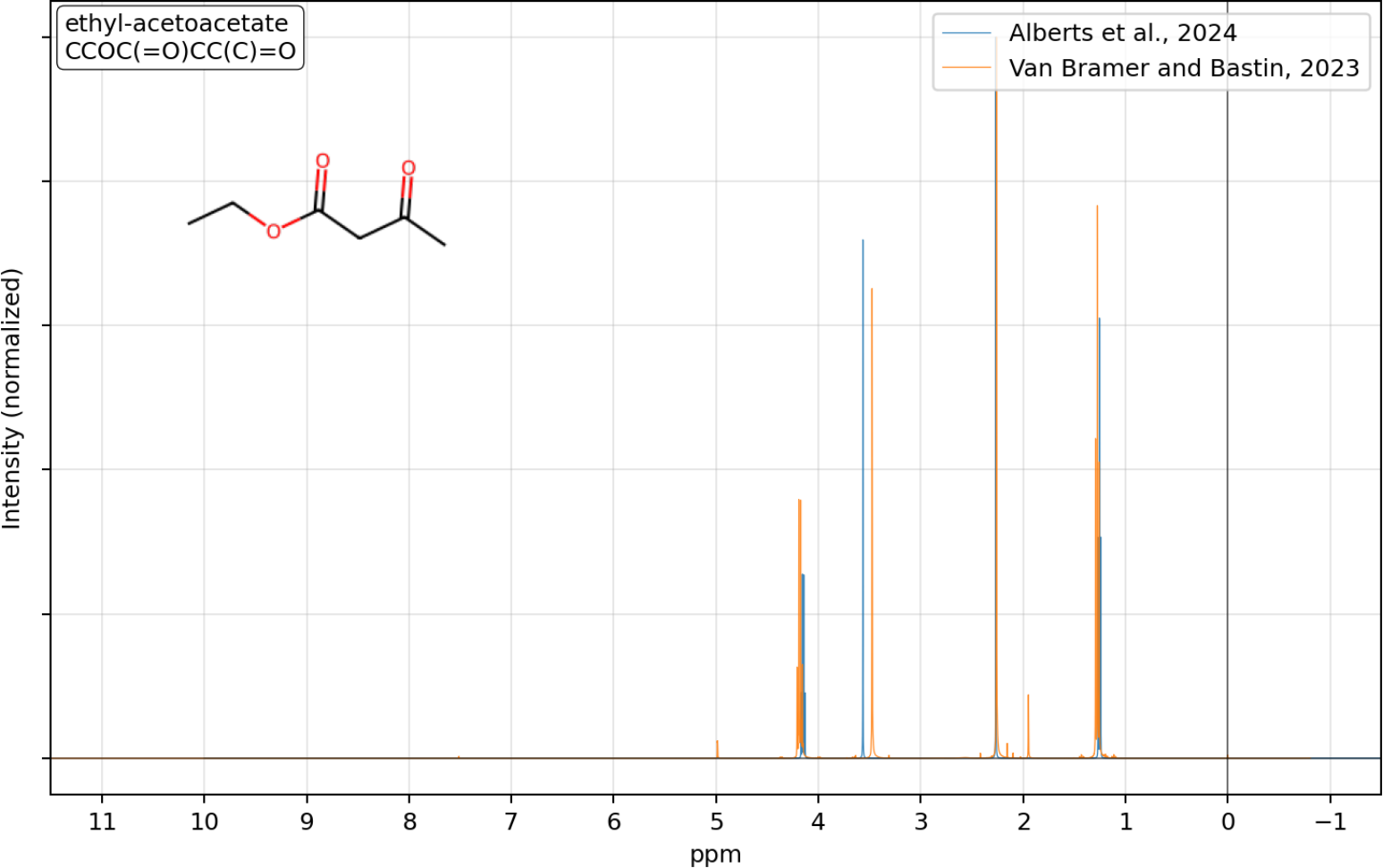

camphene
C=C1C2CCC(C2)C1(C)C
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

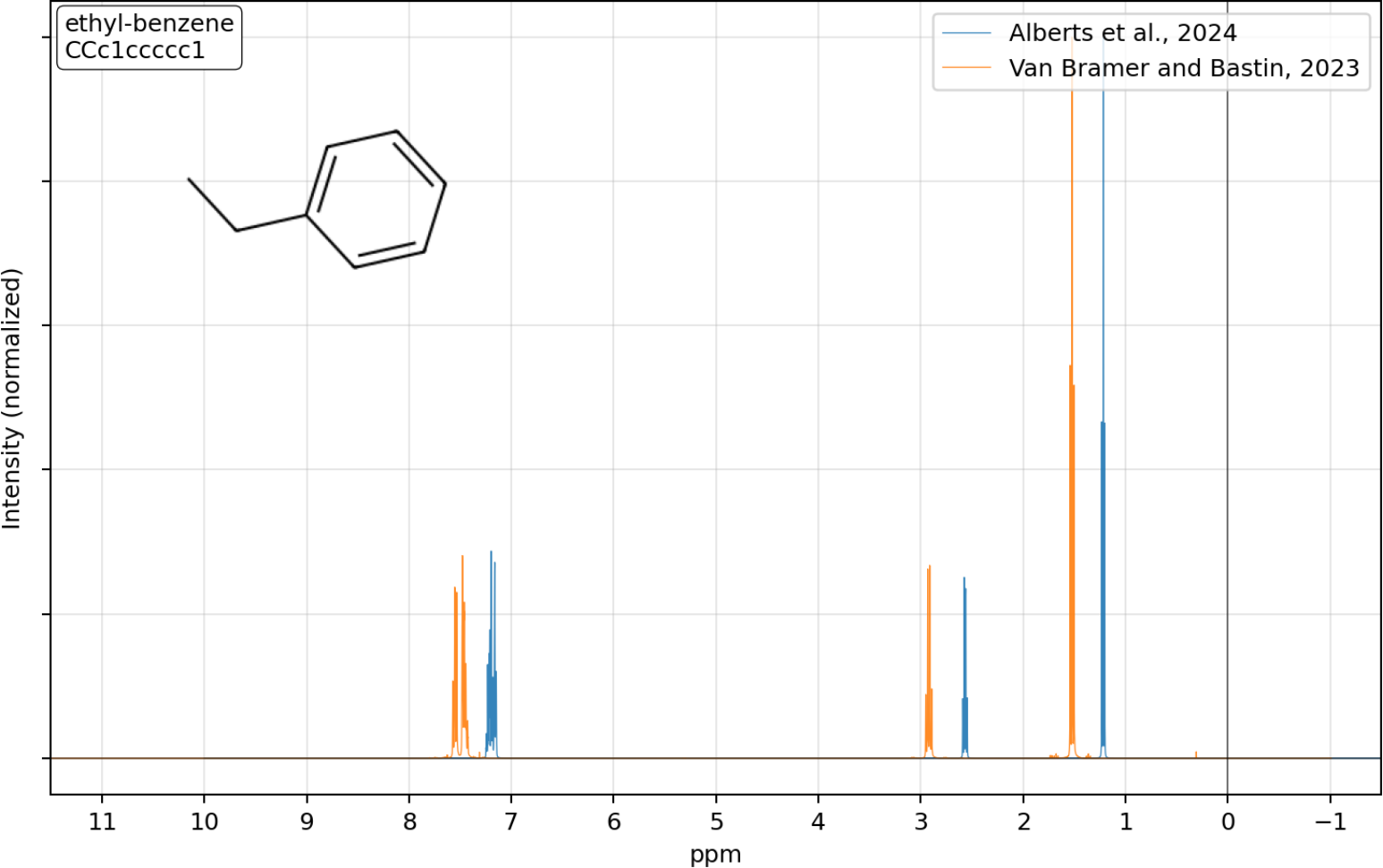

crotonic-acid-trans
C/C=C/C(=O)O
O
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

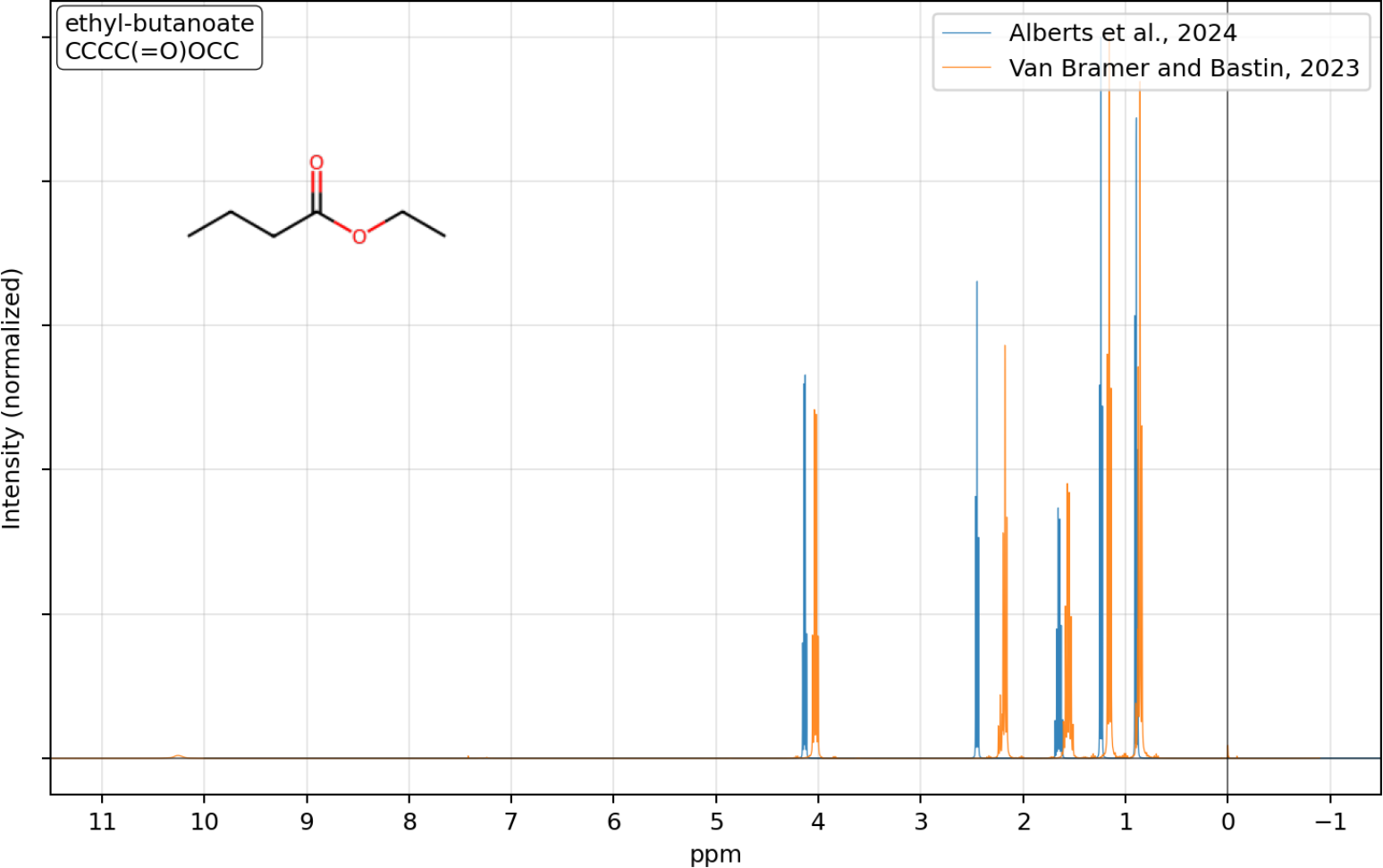

cyclohexanone
O=C1CCCCC1
O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

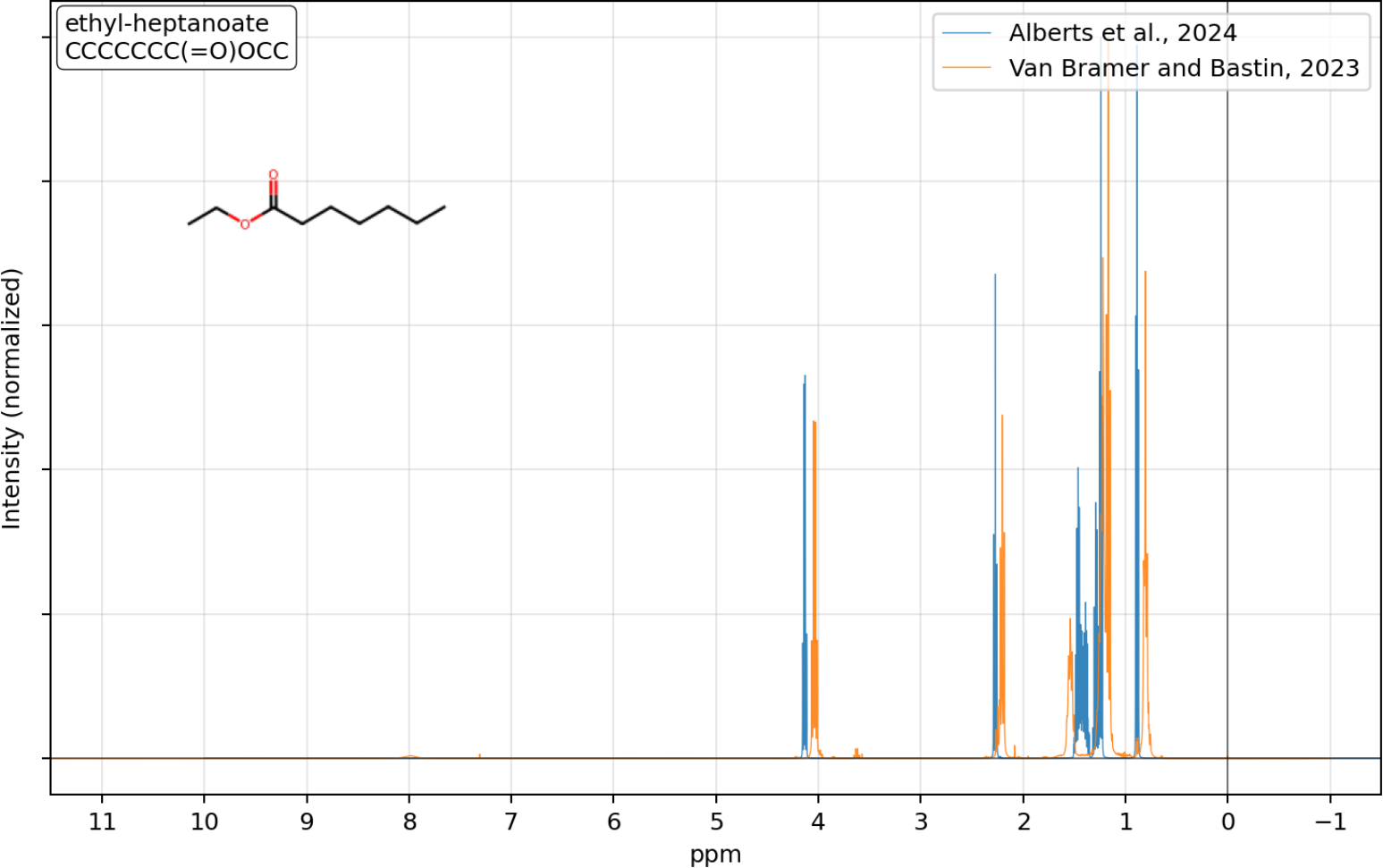

ethyl-3-methylbutanoate
CCOC(=O)CC(C)C
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

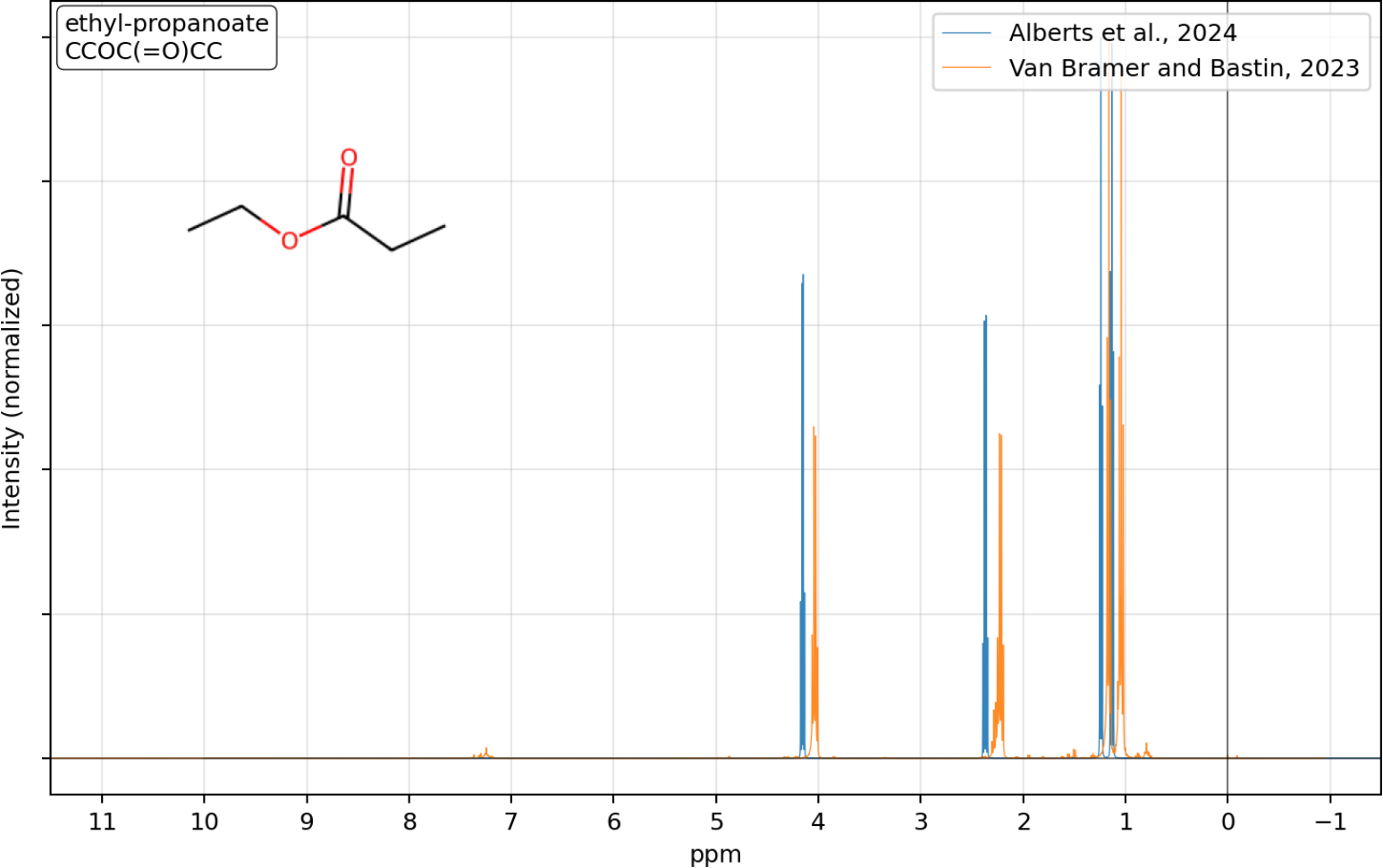

ethyl-acetate
CCOC(C)=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
O
O
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

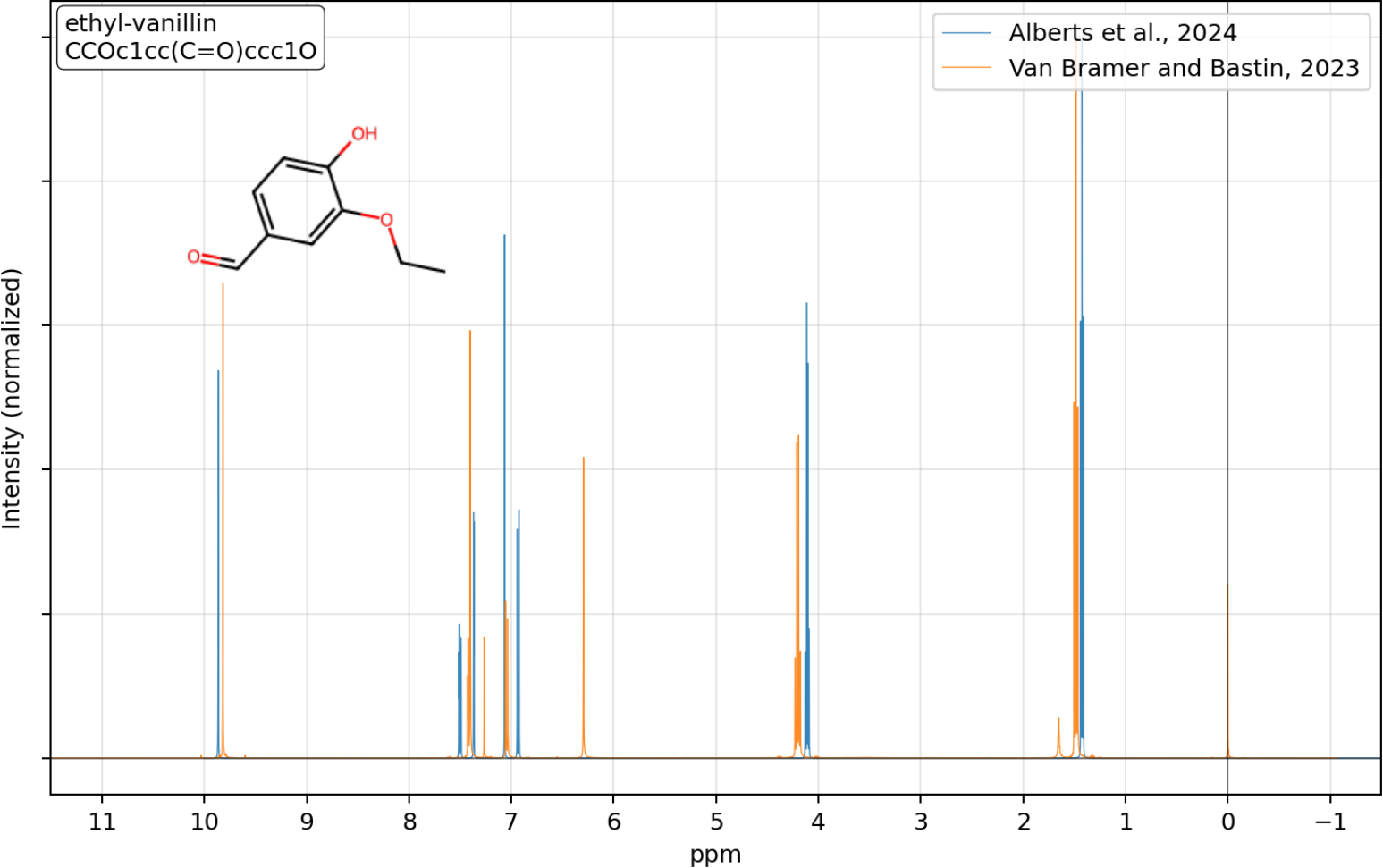

ethyl-acetoacetate
CCOC(=O)CC(C)=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

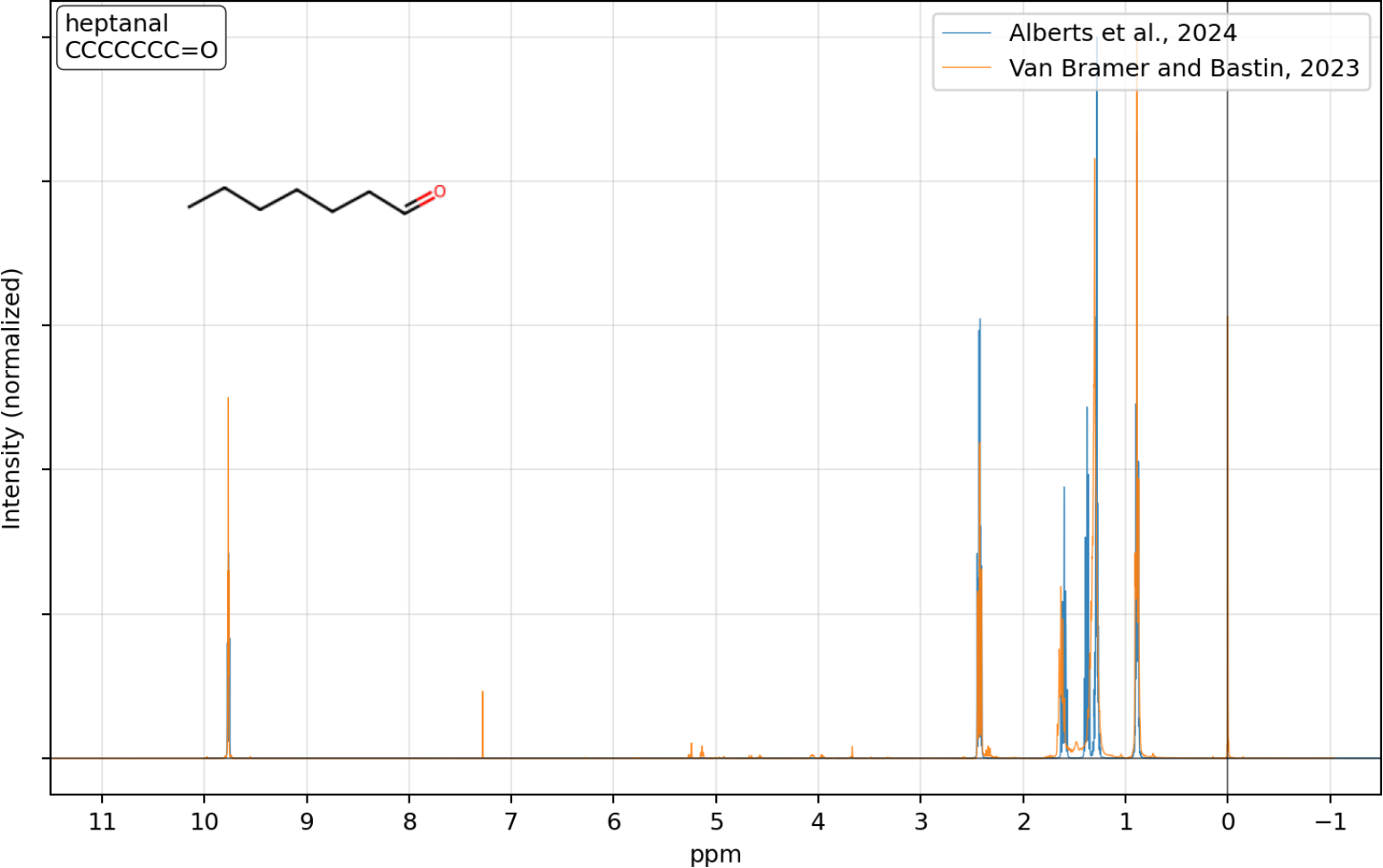

ethyl-benzene
CCc1ccccc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

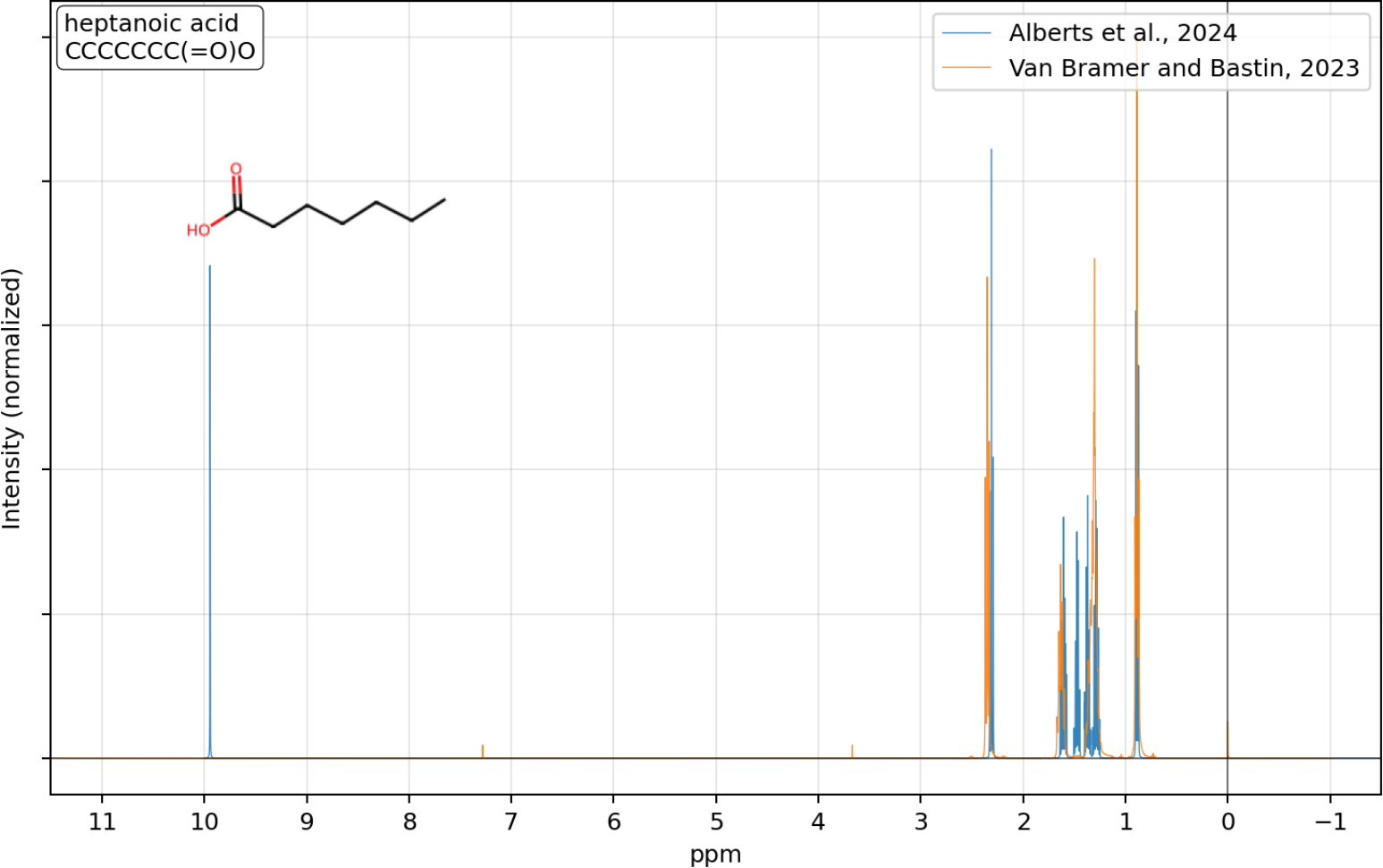

ethyl-butanoate
CCCC(=O)OCC
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

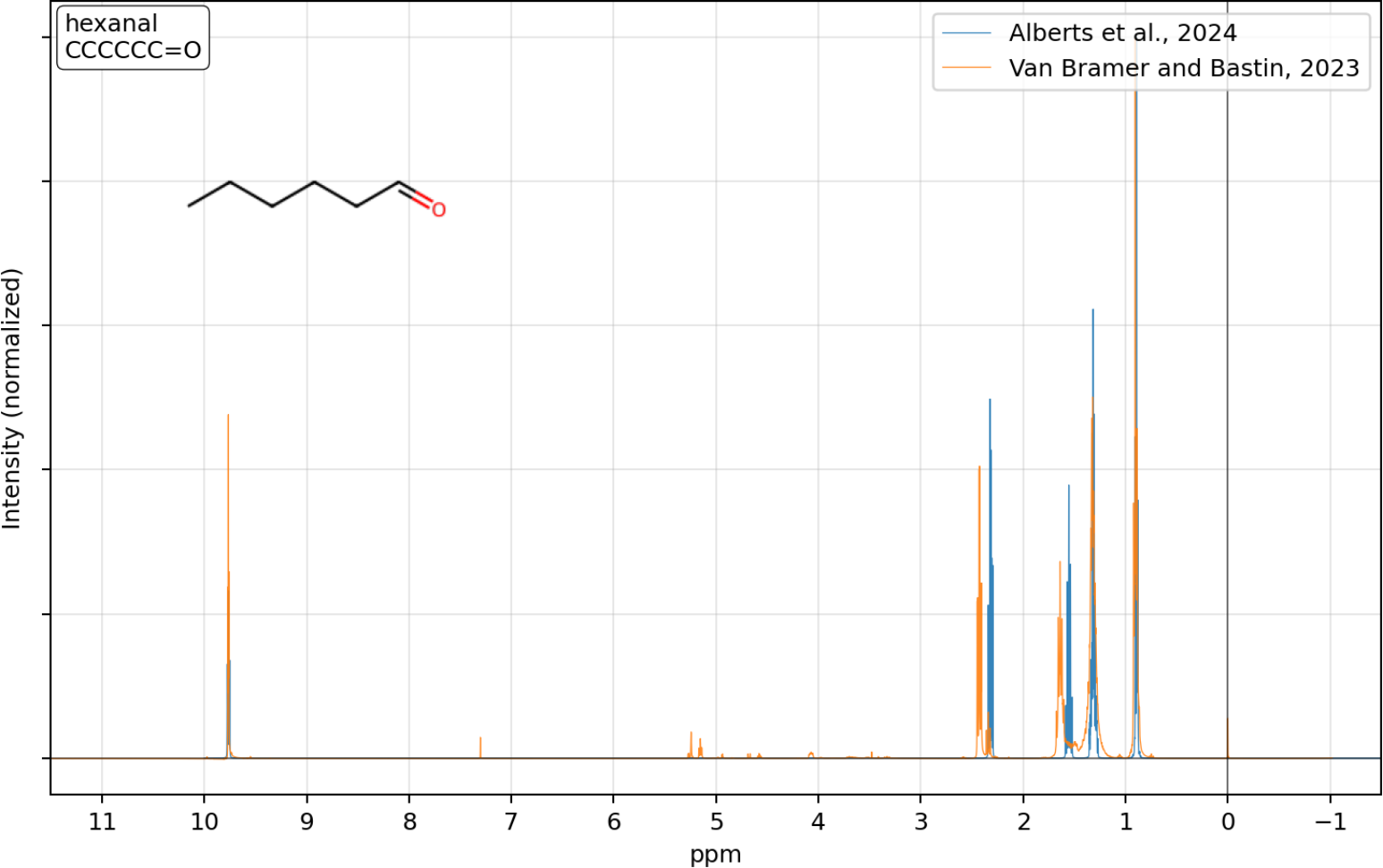

ethyl-heptanoate
CCCCCCC(=O)OCC
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

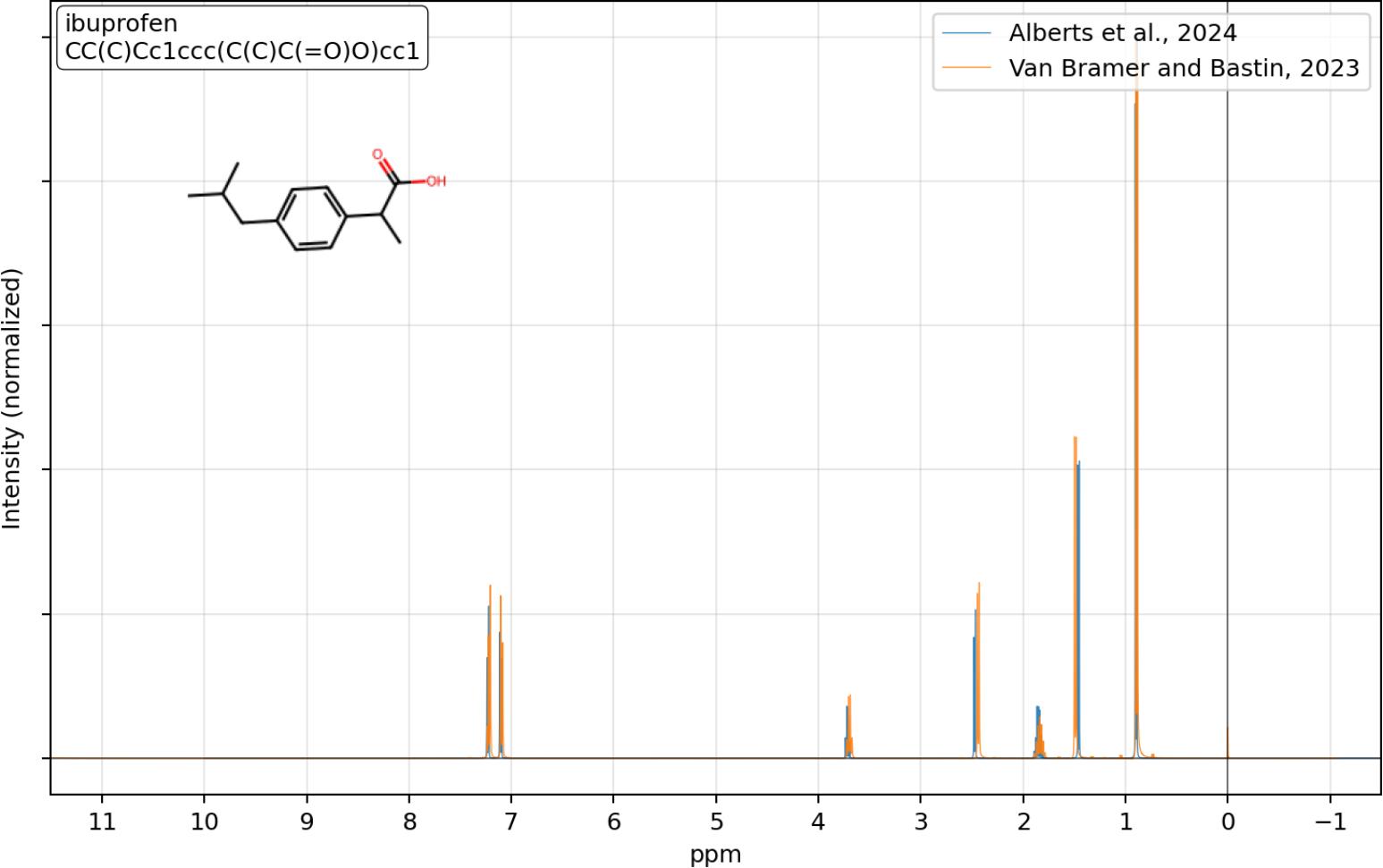

ethyl-propanoate
CCOC(=O)CC
Alberts et al., 2024
Van Bramer and Bastin, 2023
O
O
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

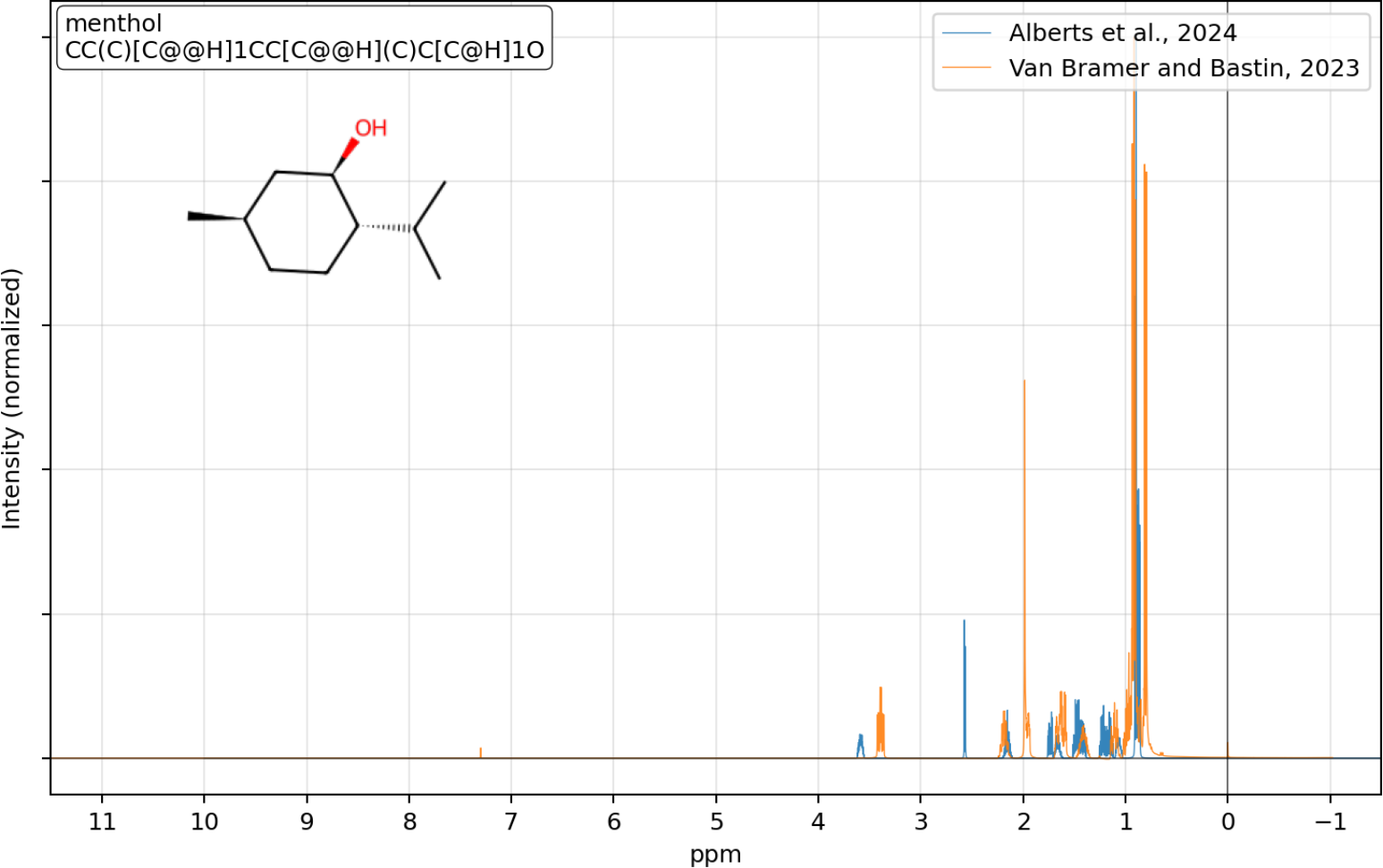

ethyl-vanillin
CCOc1cc(C=O)ccc1O
Alberts et al., 2024
Van Bramer and Bastin, 2023
OH
O
O
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

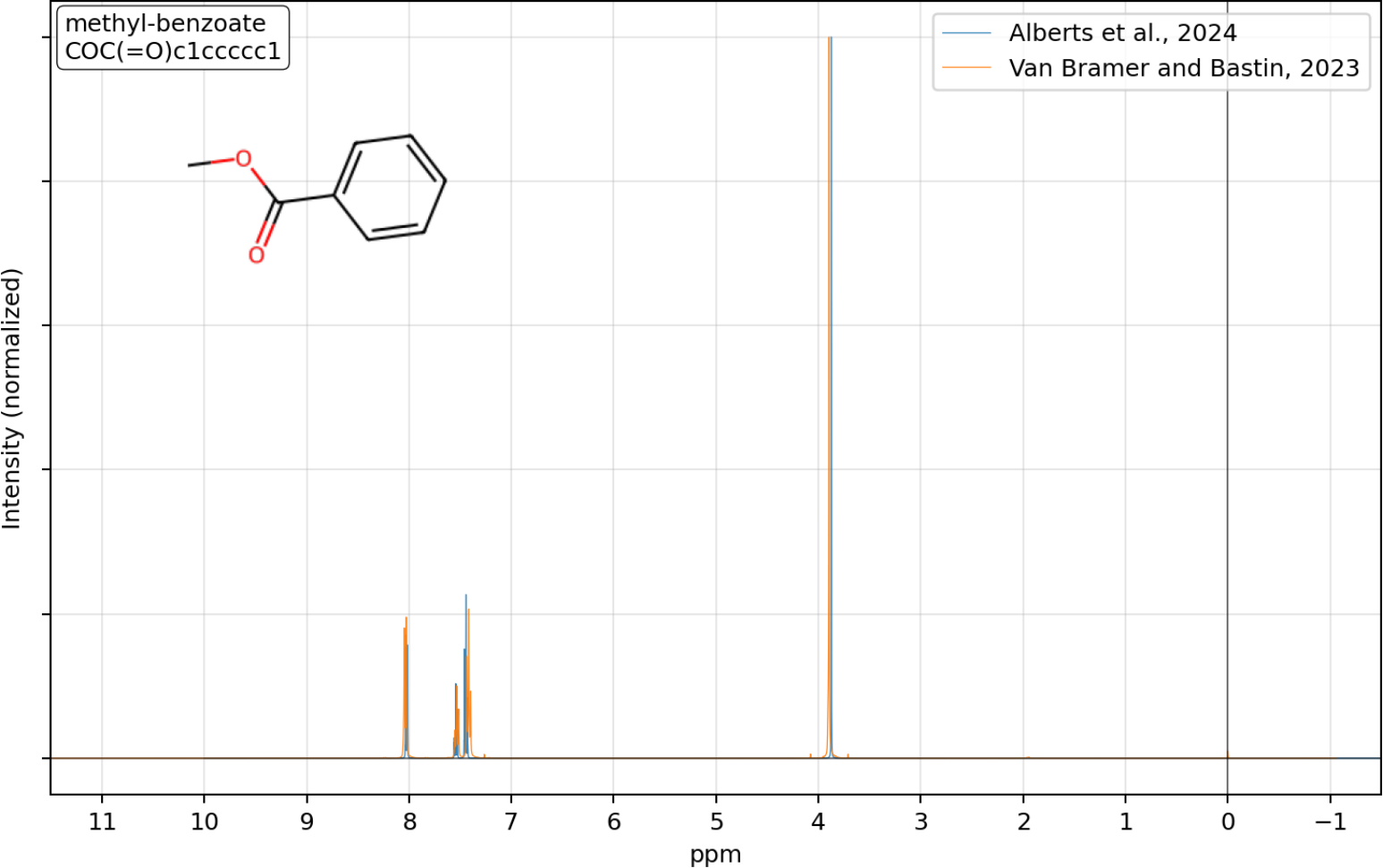

heptanal
CCCCCCC=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

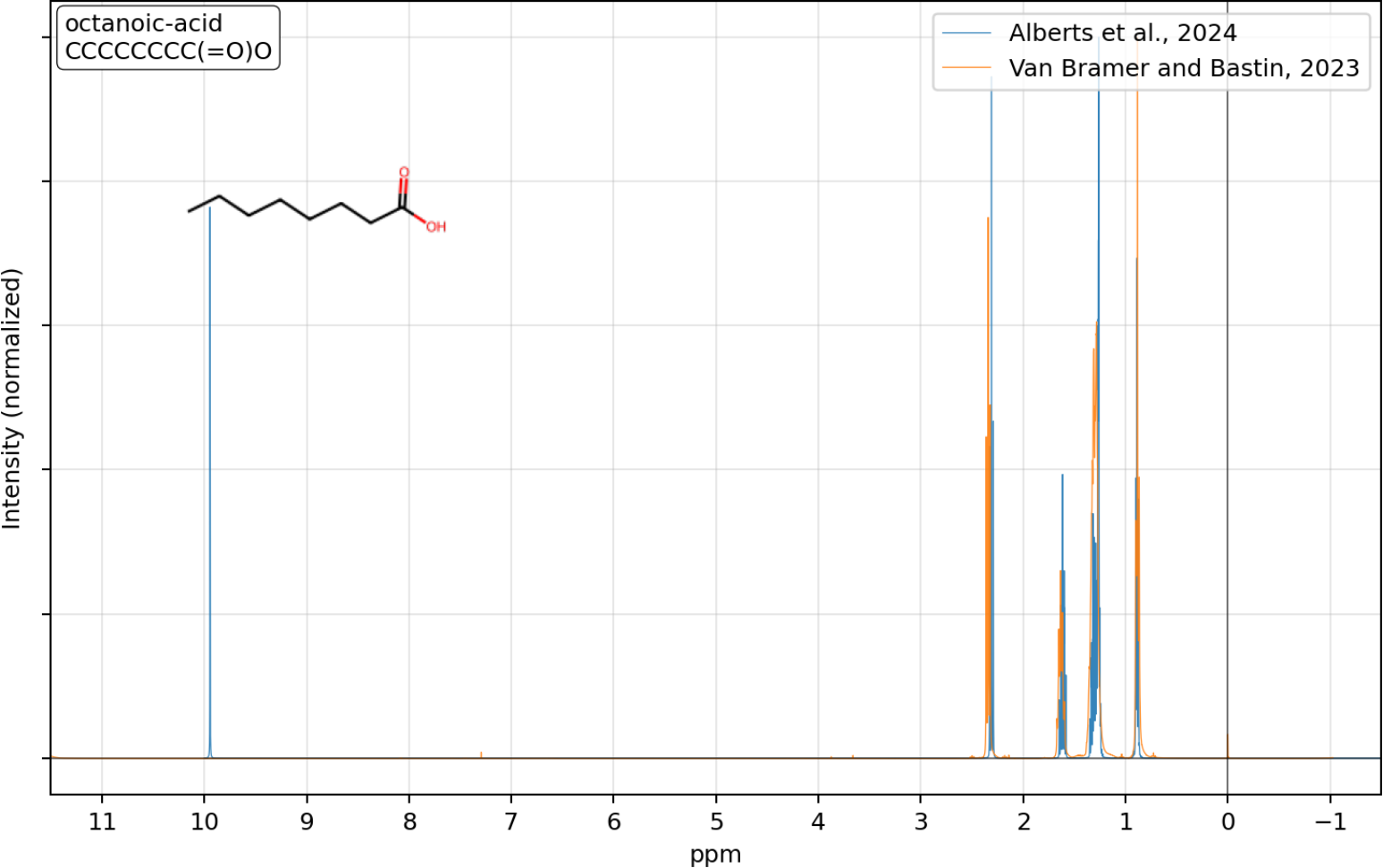

heptanoic acid
CCCCCCC(=O)O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

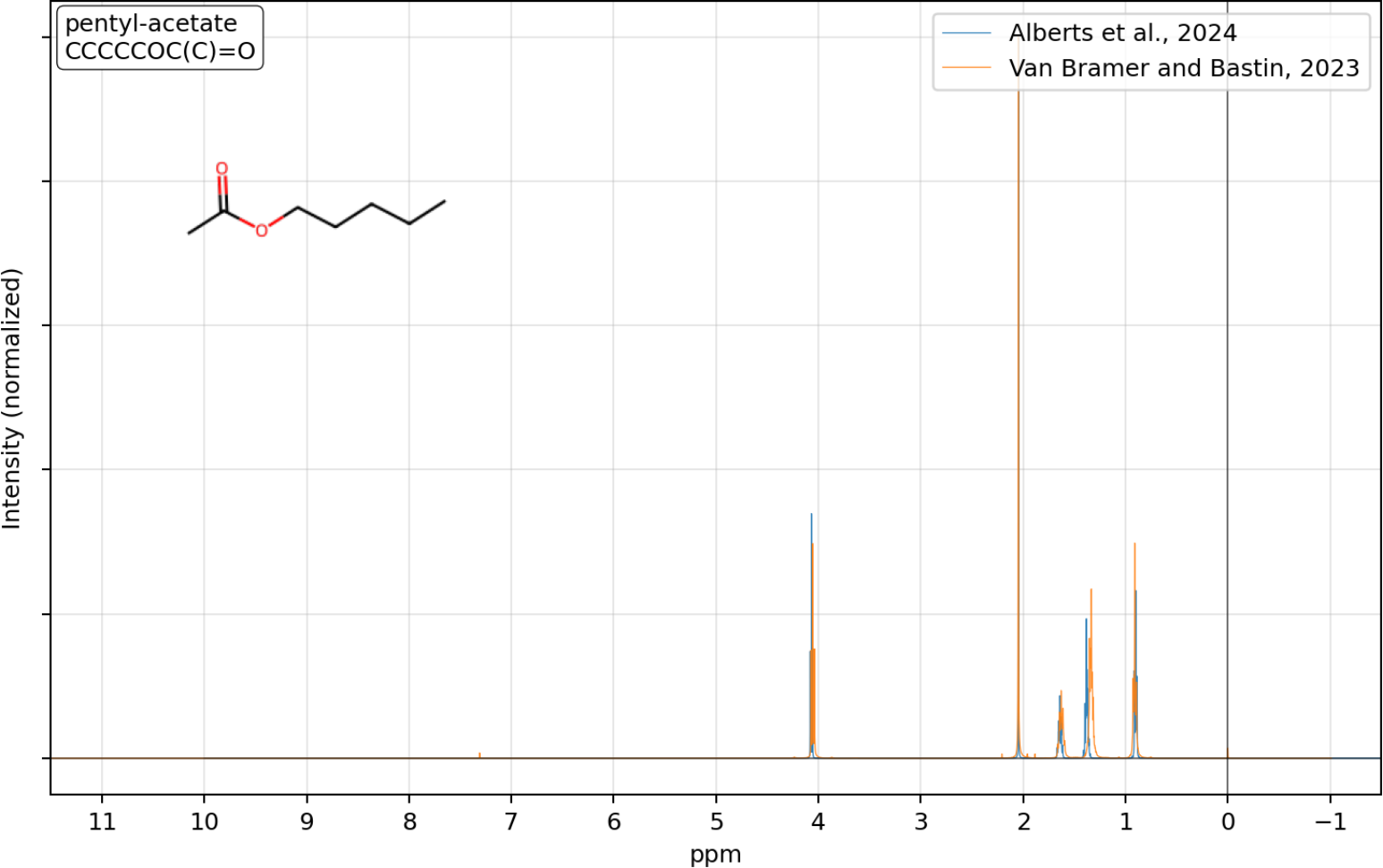

hexanal
CCCCCC=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
O
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

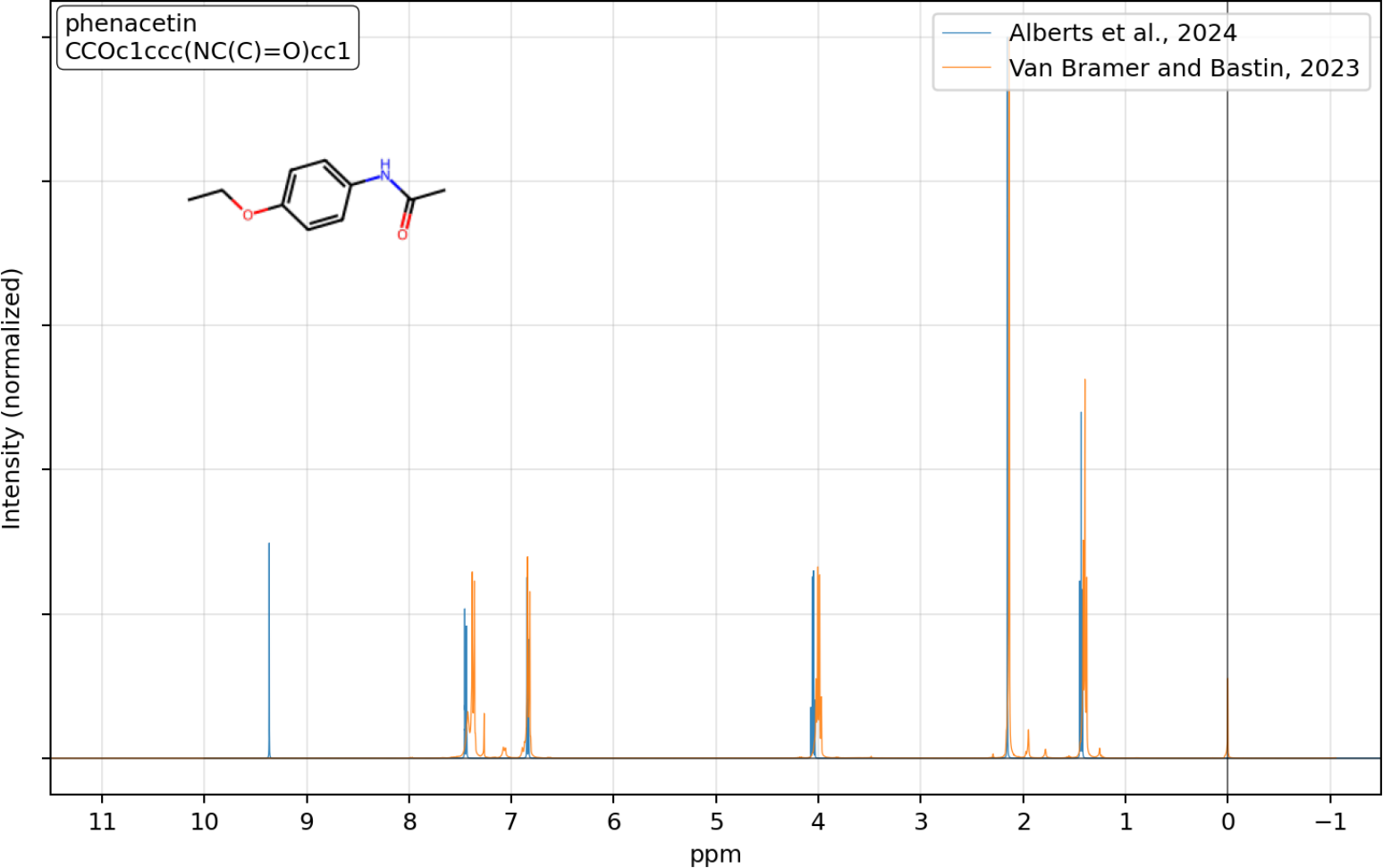

ibuprofen
CC(C)Cc1ccc(C(C)C(=O)O)cc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

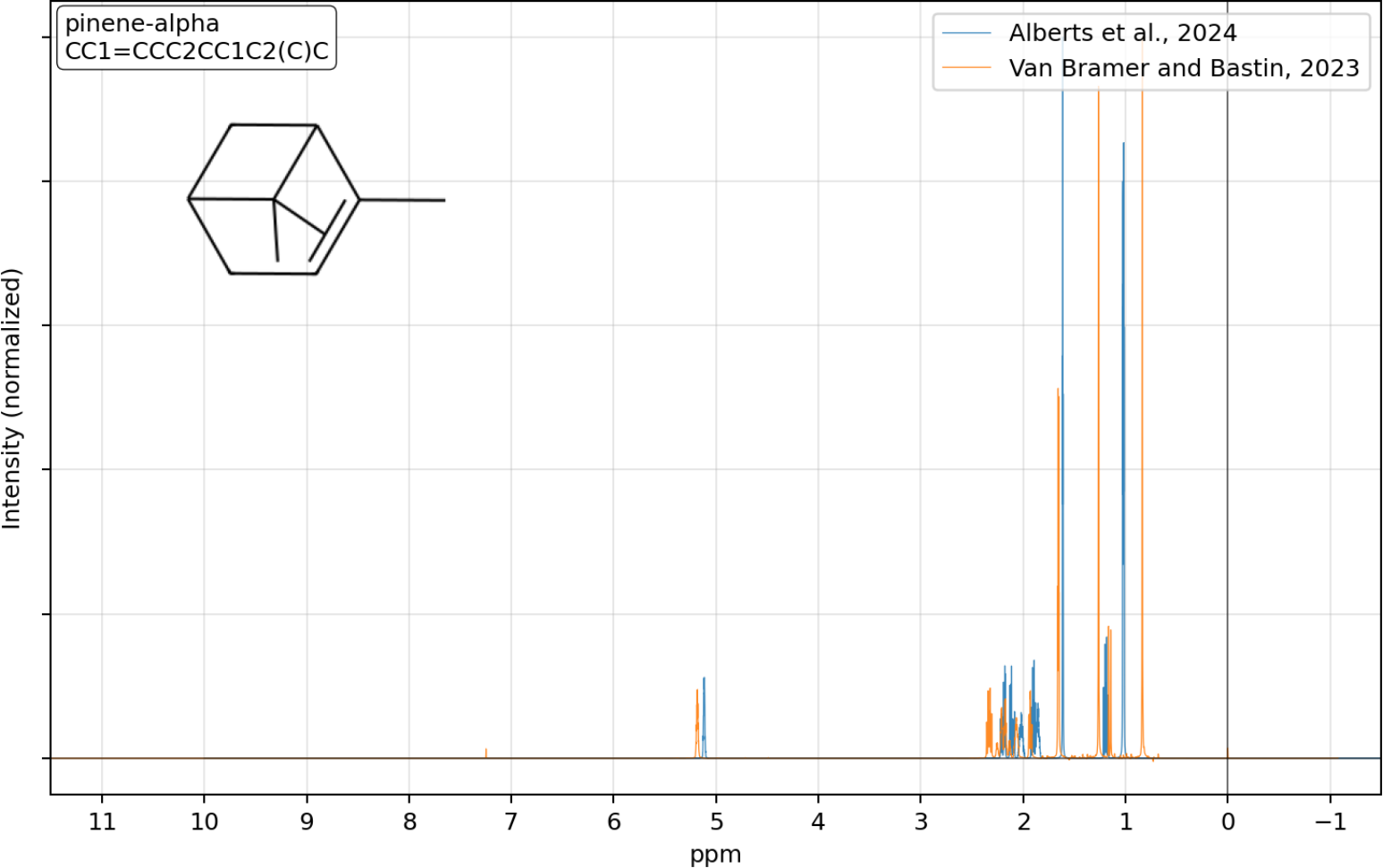

menthol
CC(C)[C@@H]1CC[C@@H](C)C[C@H]1O
OH
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

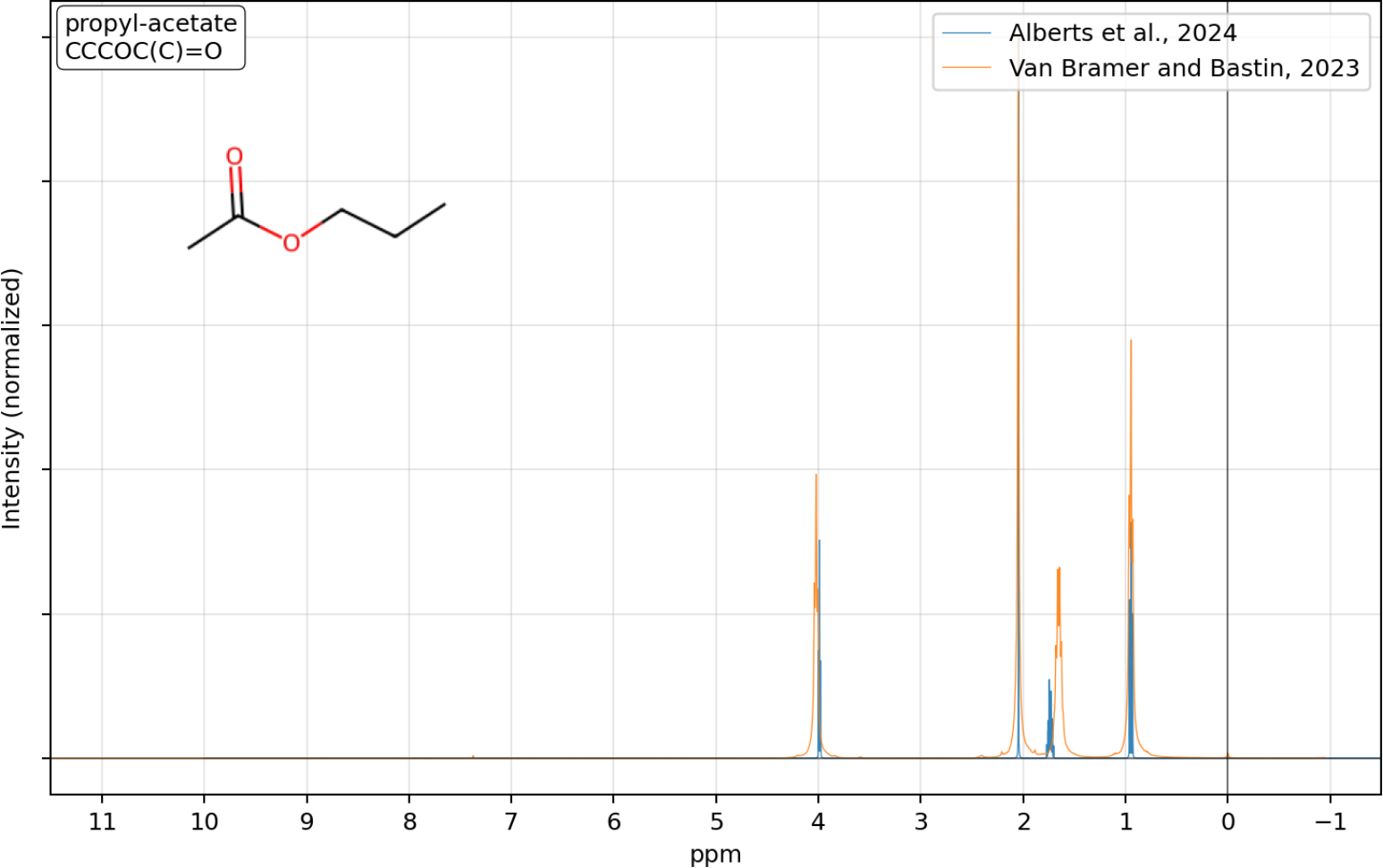

methyl-benzoate
COC(=O)c1ccccc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1

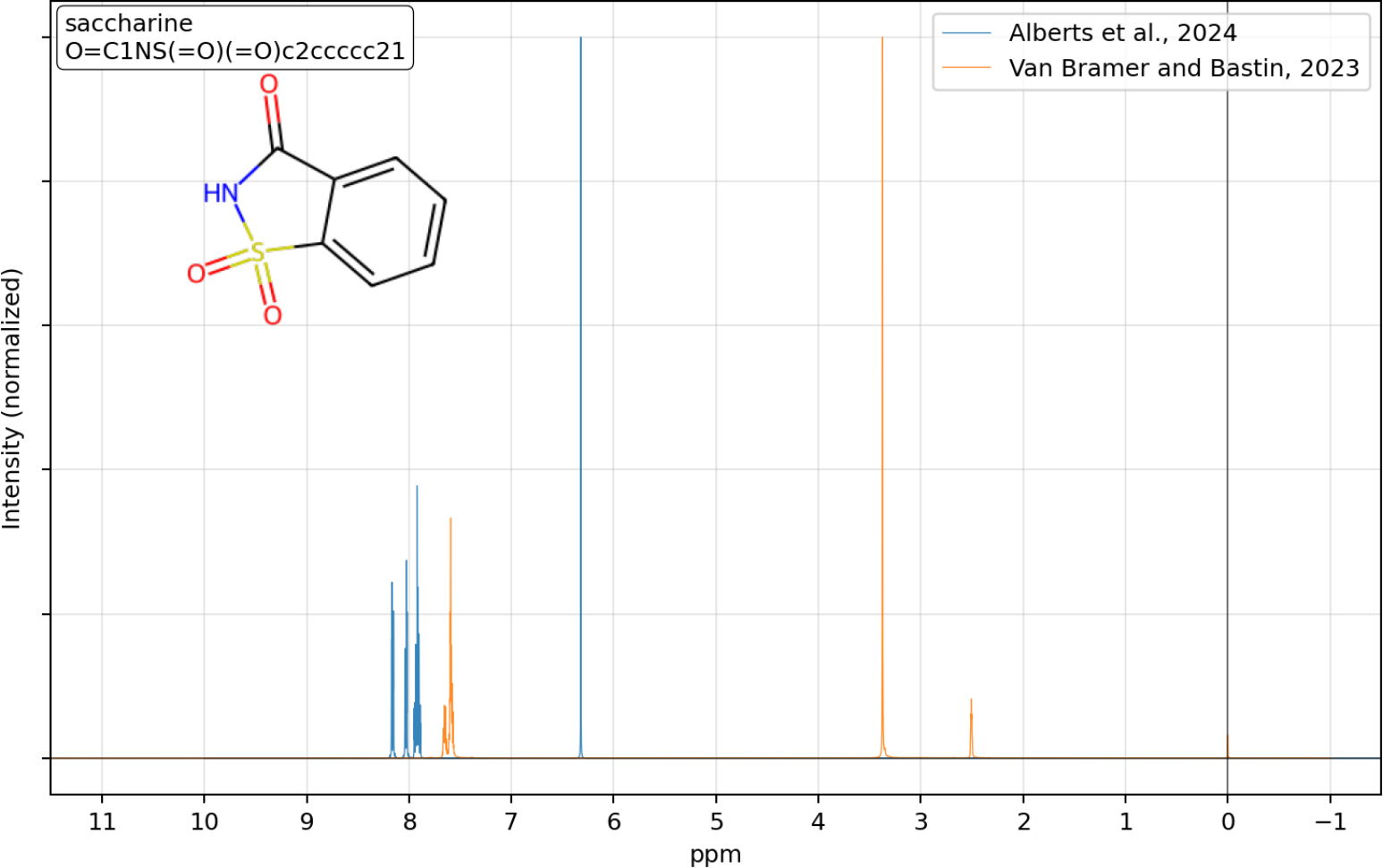

octanoic-acid
CCCCCCCC(=O)O
Alberts et al., 2024
Van Bramer and Bastin, 2023
O
OH
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm

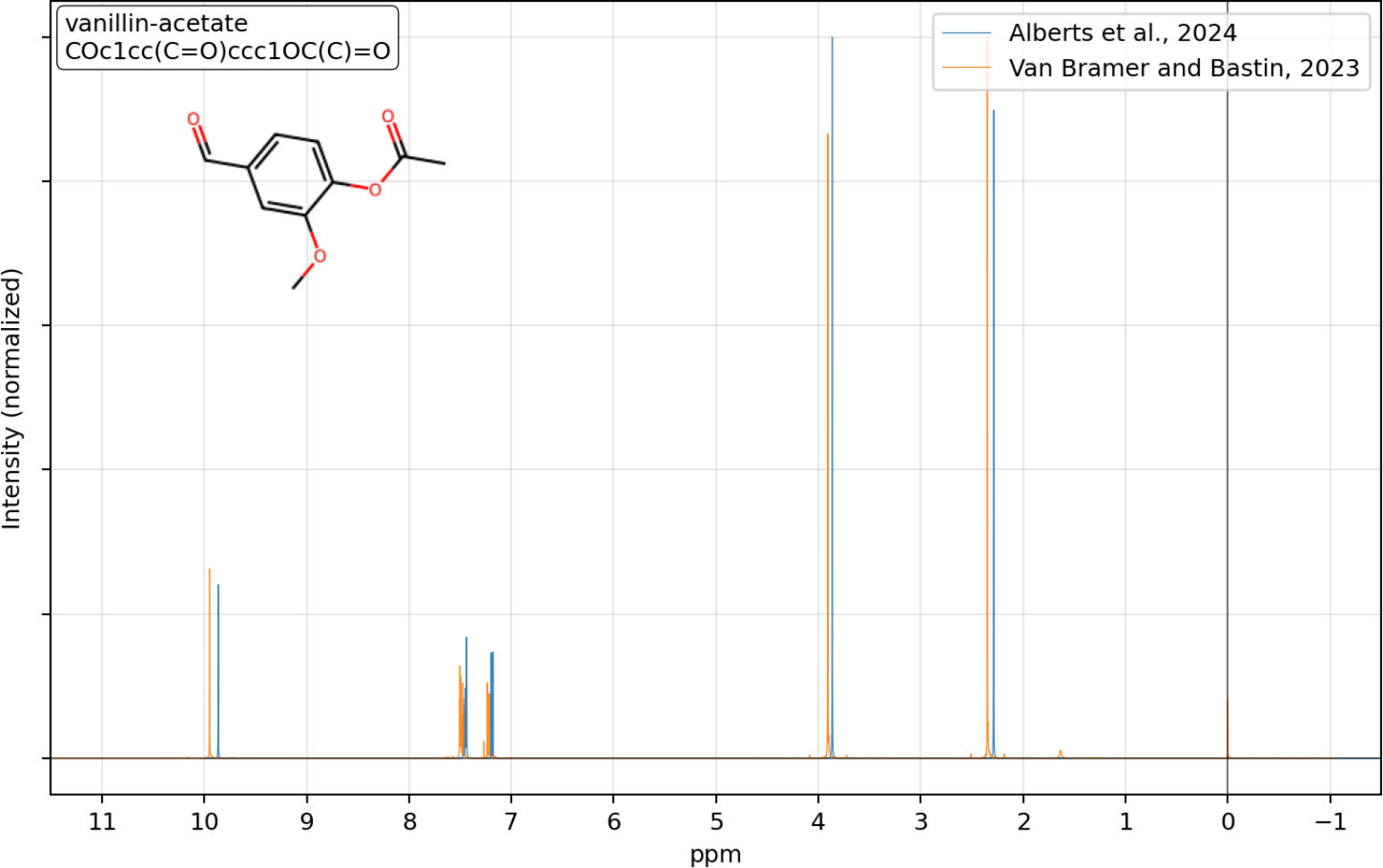

pentyl-acetate
CCCCCOC(C)=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1


phenacetin
CCOc1ccc(NC(C)=O)cc1
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1


pinene-alpha
CC1=CCC2CC1C2(C)C
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm


propyl-acetate
CCCOC(C)=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1


saccharine
O=C1NS(=O)(=O)c2ccccc21
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1
O
HN
S
O
O


vanillin-acetate
COc1cc(C=O)ccc1OC(C)=O
Alberts et al., 2024
Van Bramer and Bastin, 2023
Intensity (normalized)
ppm
11
10
9
8
7
6
5
4
3
2
1
0
−1