Electronic Supplementary Information

Mechanistic Investigation on Superelectrophilic Activation of 1,1'-Bi-2-naphthols in the Presence of Aluminum Halides

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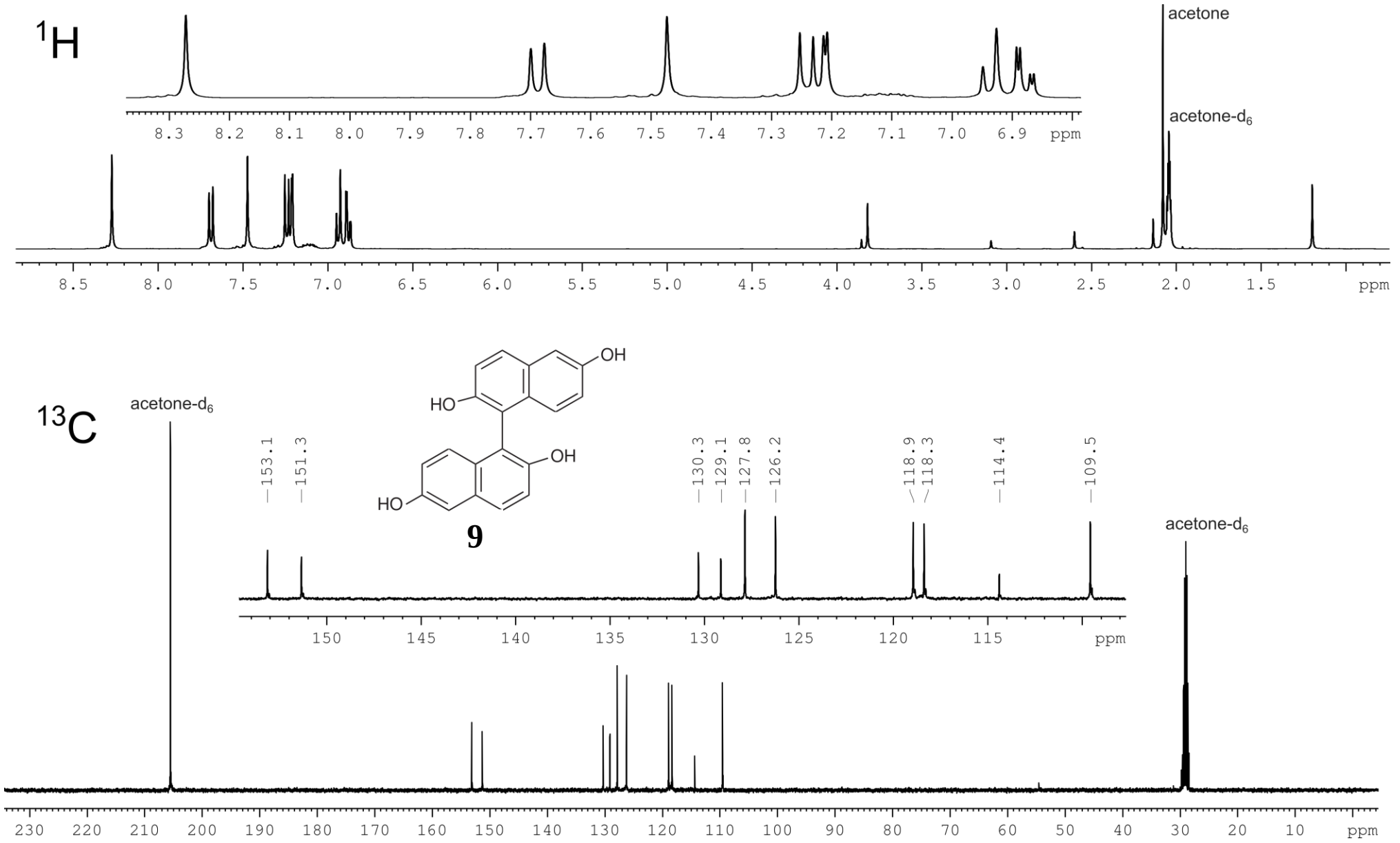
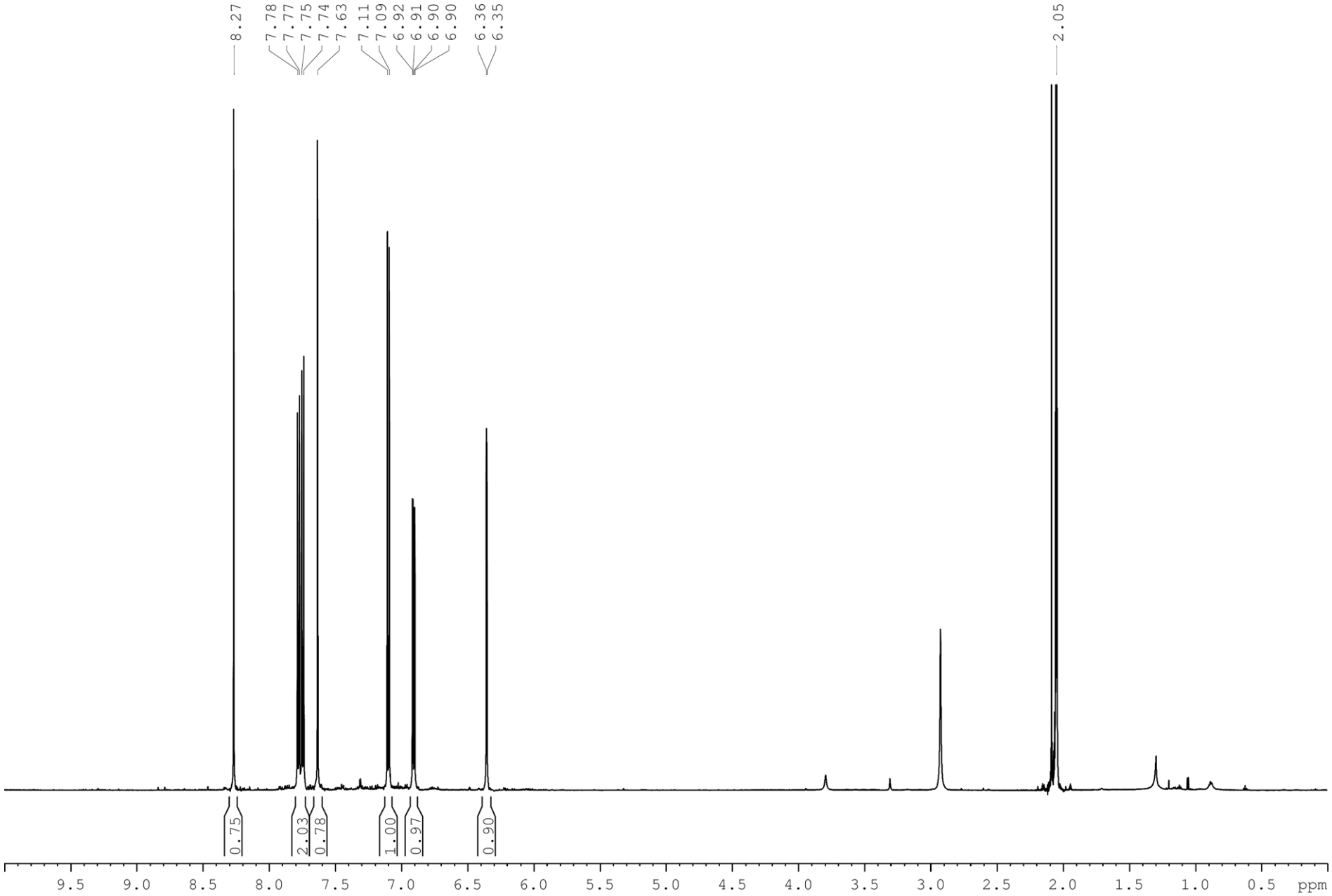
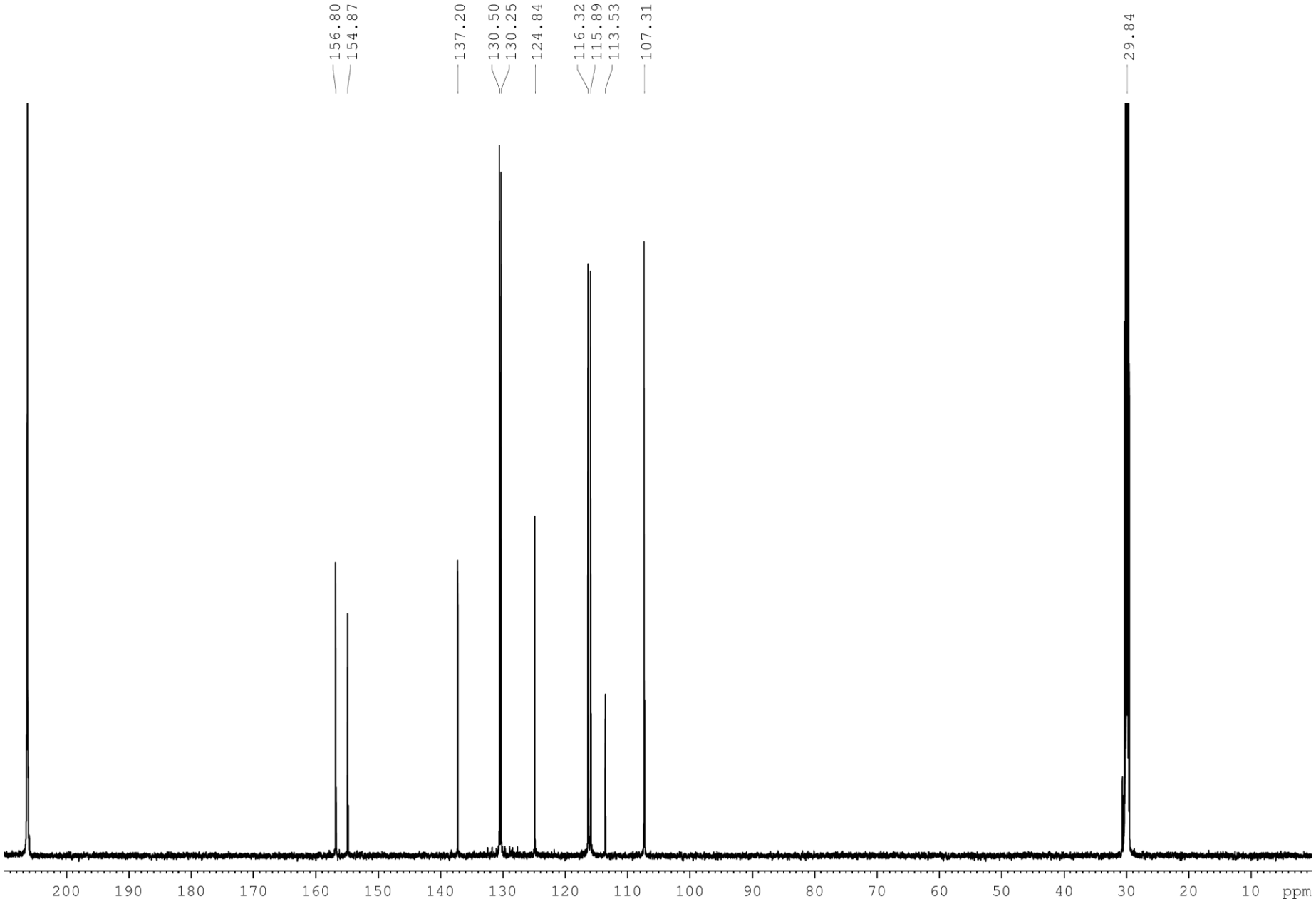
^{1}H (400 MHz) and ^{13}C{^{1}H} (100 MHz) NMR spectra of compound 9 in acetone-d_6 at 25 ^{o}C



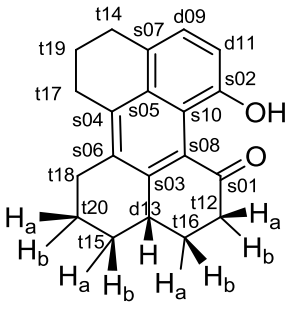
^{1}H NMR spectrum of compound 10 at 25 ^{o}C (600 MHz, acetone-d_6)



$^{13}C\{^{1}H\}$ NMR spectrum of compound 10 at 25 ^{o}C (151 MHz, acetone-d_6)



^{1}H and ^{13}C NMR signal assignments for compound 13



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Experiment Bruker_9, 1D 13C: 20 peaks
s01 205.8
s02 151.2
s03 149.6
s04 143.2
s05 130.8
s06 129.9
s07 128.6
s08 126.7
d09 126.1
s10 121.4
d11 116.4
t12 40.2
d13 38.4
t14 31.0
t15 29.9
t16 29.2
t17 29.2
t18 26.5
t19 22.6
t20 21.9

Experiment Bruker_10, 1D 1H: 20 peaks
d09-H 7.20
d11-H 7.08
d13-H 2.81 (t)
OH-H 8.77
t12-a 2.80 (t)
t12-b 2.97 (d)
t14-a 2.98
t14-b 3.00
t15-a 1.39 (q)
t15-b 2.08 (d)
t16-a 1.80 (q)
t16-b 2.11 (d)
t17-a 2.91 (d)
t17-b 3.00 (d)
t18-a 2.77 (m)
t18-b 2.91 (d)
t19-a 1.99
t19-b 2.03
t20-a 1.82
t20-b 2.09

Experiment Bruker_14, 2D 13C-1H via onebond (HSQC): 19 peaks
d09-H - d09
d11-H - d11
d13-H - d13
t12-a - t12
t12-b - t12
t14-a - t14
t14-b - t14
t15-a - t15
t15-b - t15
t16-a - t16
t16-b - t16
t17-a - t17
t17-b - t17
t18-a - t18
t18-b - t18
t19-a - t19
t19-b - t19
t20-a - t20
t20-b - t20

Experiment Bruker_15, 2D 13C-1H via onebond (HSQC): 16 peaks
d13-H - d13(t)
t12-a - t12(t)
t12-b - t12(d)
t14-a - t14
t14-b - t14
t15-a - t15(q)
t15-b - t15(d)
t16-a - t16(q)
t16-b - t16(d)
t17-a - t17(d)
t17-b - t17(d)
t18-a - t18(m)
t18-b - t18(d)
t19-a - t19
t19-b - t19
t20-a - t20
t20-b - t20

Experiment Bruker_17, 2D 1H-13C via onebond (H-C correlation): 17 peaks
d13 - d13-H
t12 - t12-a t12-b
t14 - t14-a t14-b
t15 - t15-a t15-b
t16 - t16-a t16-b
t17 - t17-a t17-b
t18 - t18-a t18-b
t19 - t19-a t19-b
t20 - t20-a t20-b

Experiment Bruker_6, 2D 1H-1H via Jcoupling (COSY): 39 peaks
d09-H - d11-H
d11-H - d09-H
d13-H - t15-a t16-a t16-b
t12-a - t12-b t16-a t16-b
t12-b - t12-a t16-a t16-b?
t14-a - t19-a t19-b
t14-b - t19-a t19-b
t15-a - d13-H t15-b t20-a
t15-b - t15-a
t16-a - d13-H t12-a t12-b t16-b
t16-b - d13-H t12-a t16-a
t17-a - t19-a? t19-b?
t17-b - t19-a t19-b
t18-a - t18-b t20-a? t20-b?
t18-b - t18-a t20-b?
t19-a - t14-a t14-b t17-b
t19-b - t14-a t14-b t17-b
t20-a - t15-a t18-b? t20-b
t20-b - t20-a

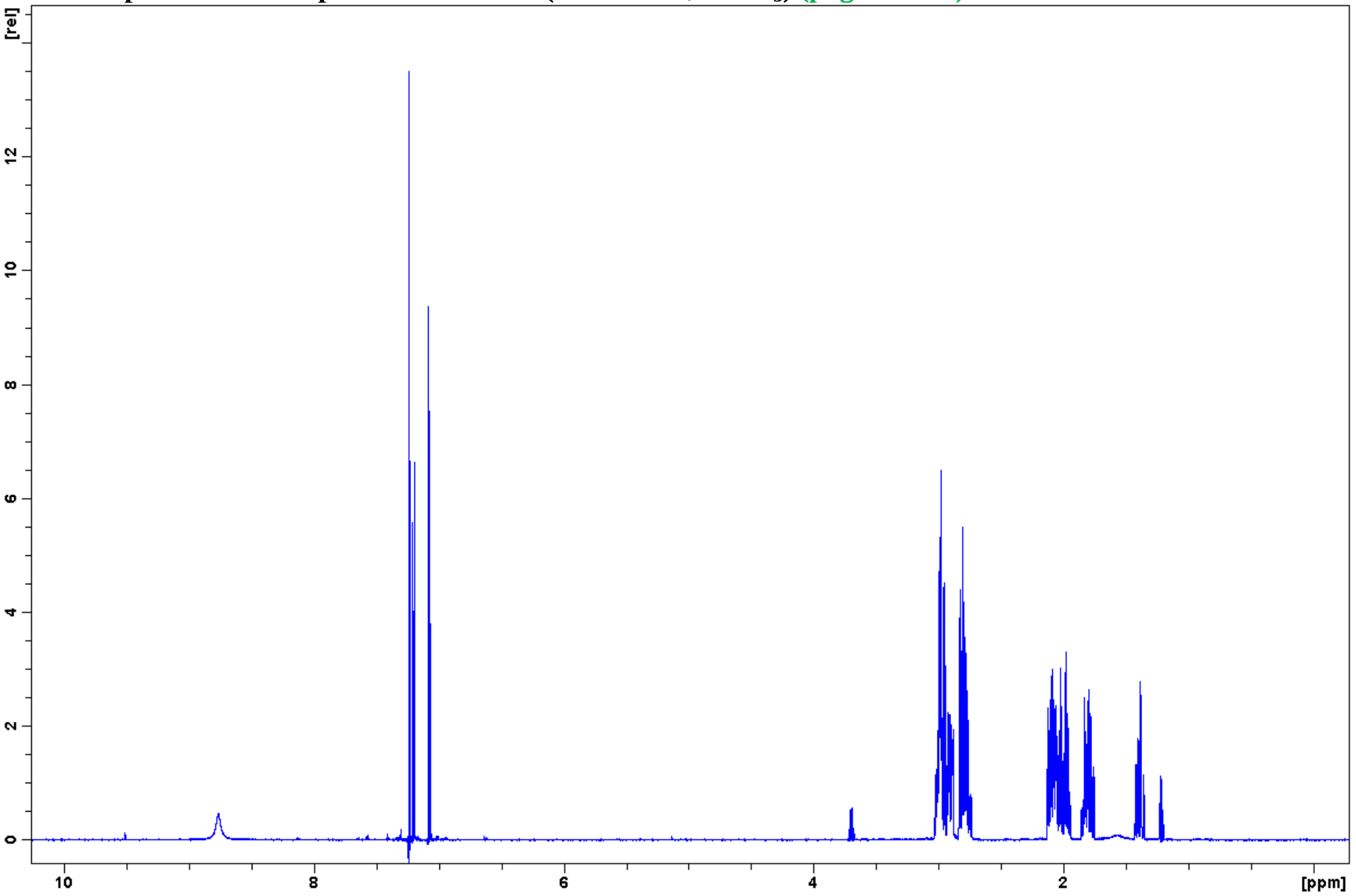
Experiment Bruker_7, 2D 1H-1H via Jcoupling (COSY): 23 peaks
t12-a - t12-b t16-a t16-b
t12-b - t12-a t16-a t16-b
t15-a - t15-b t20-a?
t15-b - t15-a
t16-a - t12-a t12-b t16-b
t16-b - t12-a t12-b t16-a
t19-a - t14-a? t14-b? t17-b?
t19-b - t14-a? t14-b? t17-a? t17-b?
t20-a - t18-a? t18-b?
t20-b - t18-b?

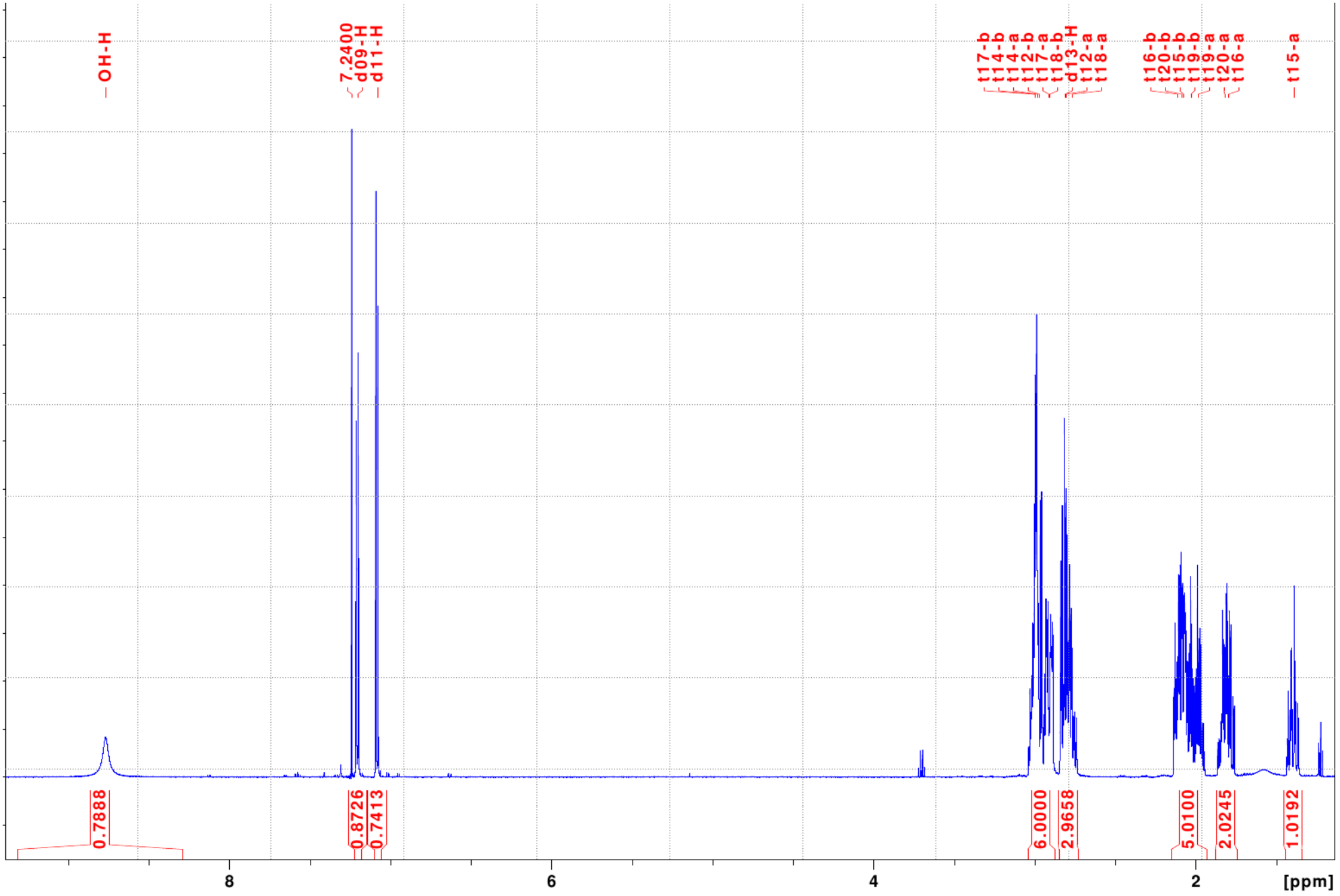
Experiment Bruker_11, 2D 1H-1H via through-space (NOESY): 6 peaks
d09-H - t14-a t14-b
OH-H - d11-H?
t14-a - d09-H
t14-b - d09-H
t15-a - t18-a
t18-a - t15-a

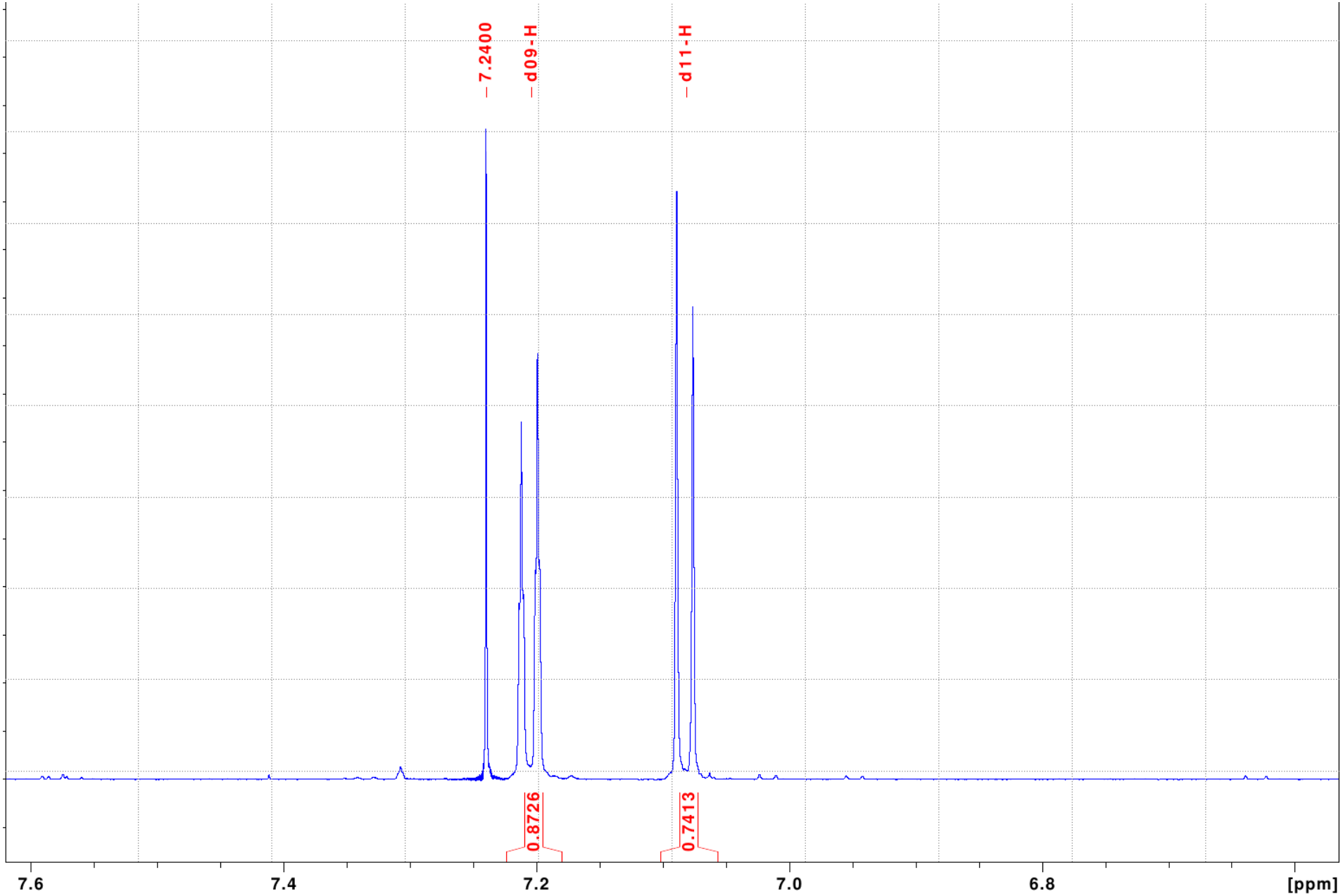
Experiment Bruker_12, 2D 13C-1H via Jcoupling (HMBC): 90 peaks
d09-H - s02 s04(weak) s05 s10(weak) t14
d11-H - s02(weak) s03(weak) s05(weak) s07 s10
d13-H - s03 s06 s08 s10(weak) t12 t16 t20
t12-a - d13 s01 s08 t16
t12-b - d13 s01 t16
t14-a - d09 d11(weak) s02(weak) s05 s07 t17 t19
t14-b - d09 d11(weak) s02(weak) s05 s07 t17 t19
t15-a - d13 s03 t16 t18 t20
t15-b - d13 s03 t16 t18 t20
t16-a - d13 s01 s03 t12 t15
t16-b - d13 s01 s03 t12 t15
t17-a - s04 s05 s06 t14 t19
t17-b - s04 s05 s06 t14 t19
t18-a - s03 s04 s06 t15 t20
t18-b - s03 s04 s06 t15 t20
t19-a - s04 s07 t14 t17
t19-b - s04 s07 t14 t17
t20-a - d13 s06 t15 t18
t20-b - d13 s06 t15 t18

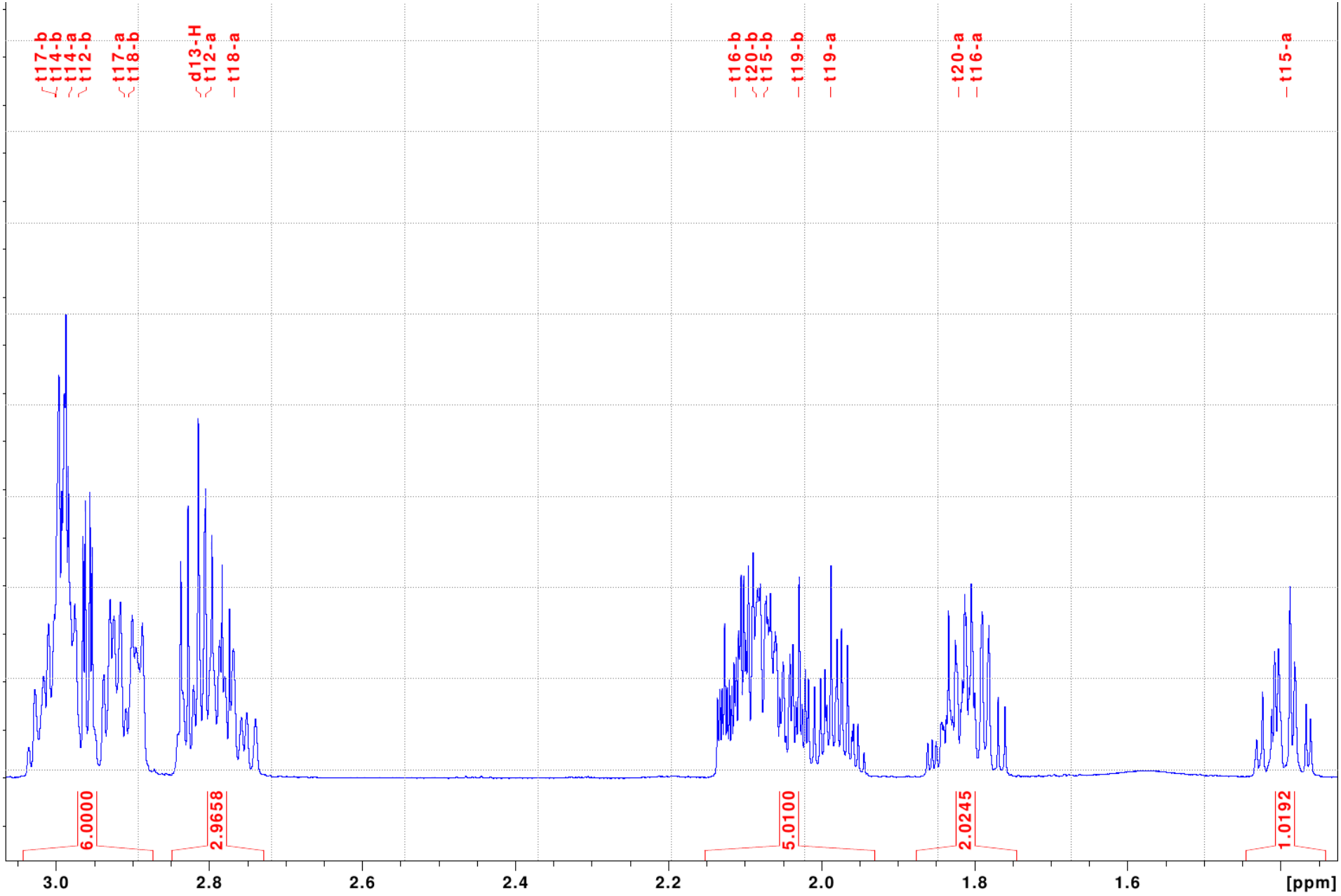
Experiment Bruker_13, 2D 13C-1H via Jcoupling (HMBC): 61 peaks
d13-H - s08 t12 t15 t16 t20
t12-a - d13 s01 s08 t16
t12-b - d13 s01 s08 t16
t14-a - d09 s05 s07 t17 t19
t14-b - d09 s05 s07 t17 t19
t15-a - d13 s03 t16 t18 t20
t15-b - d13 s03 t18 t20
t16-a - d13 s01 s03 t12 t15
t16-b - d13 s01 s03 t12 t15
t17-a - s04 s05 s06 t14 t19
t17-b - s04 s05 t14 t19
t18-b - s04 s06
t19-a - s04 s07 t14 t17
t19-b - s04 s07 t14 t17
t20-a - d13 s06 t15 t18
t20-b - d13 s06 t15 t18

^{1}H NMR spectrum of compound 13 at 25 ^{o}C (600.3 MHz, $CDCl_3$) **(pages S6-S9)**

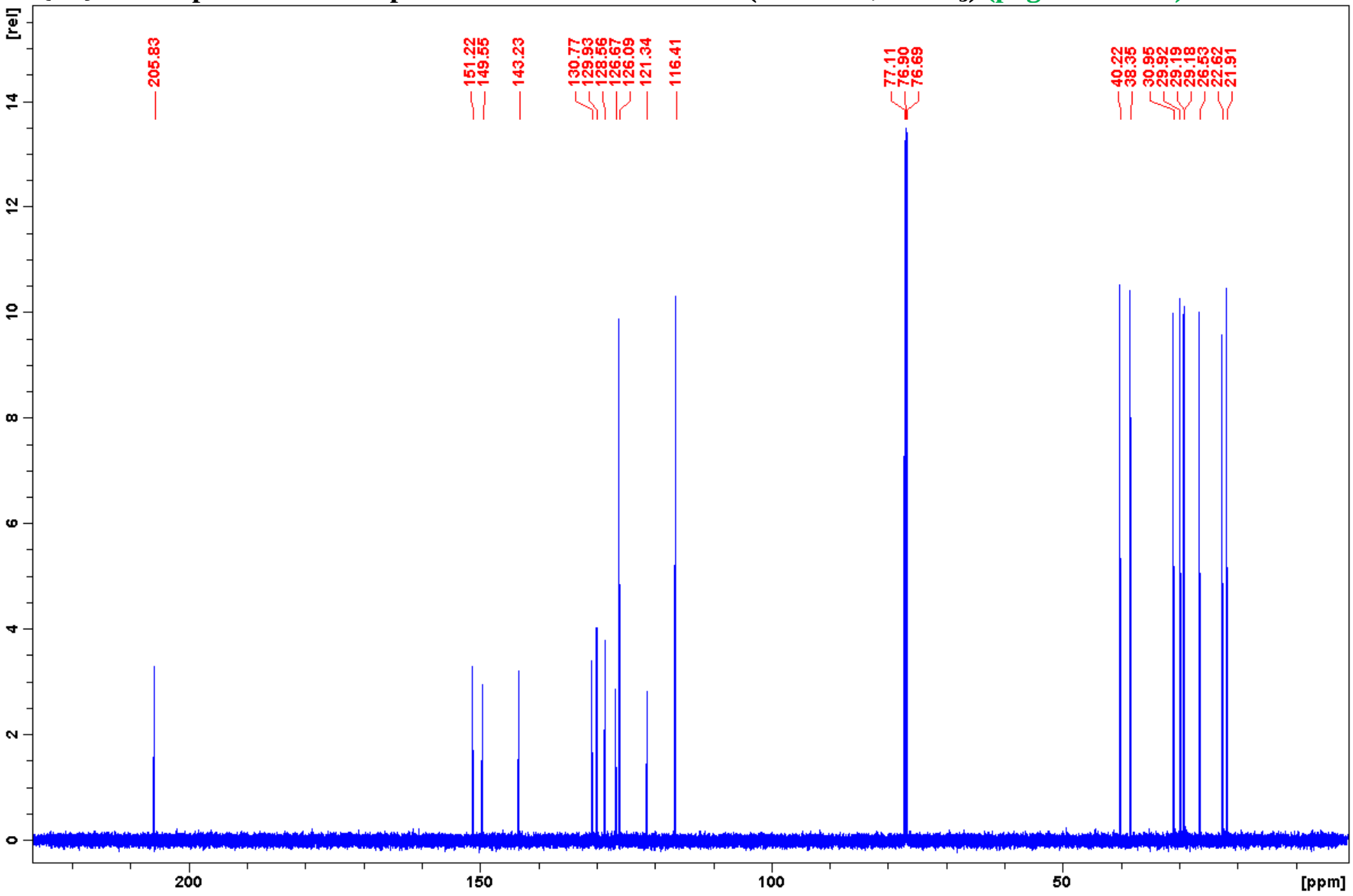


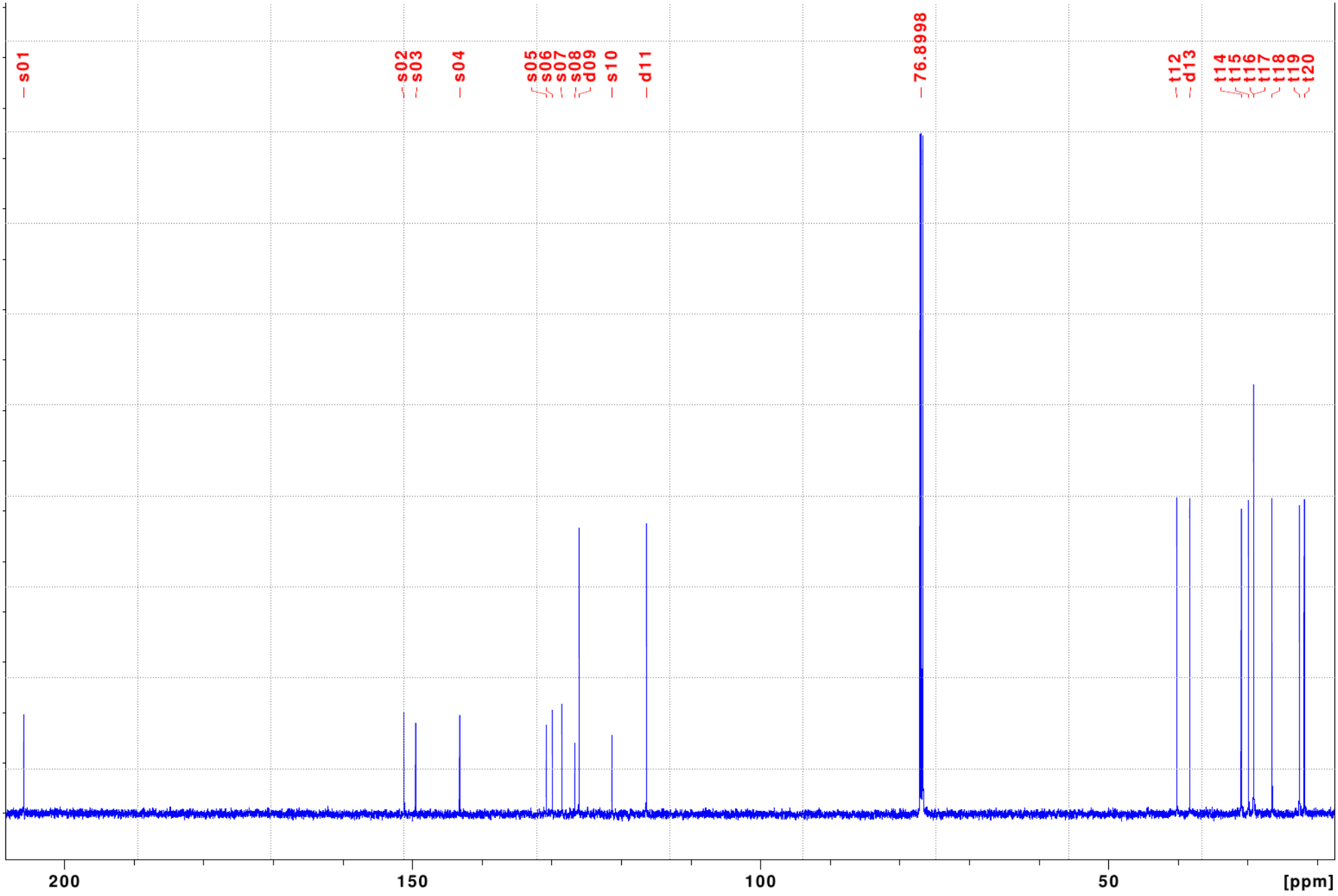

OH-H
7.2400
d09-H
d11-H
t17-b
t14-b
t14-a
t12-b
t17-a
t18-b
d13-H
t12-a
t18-a
t16-b
t20-b
t15-b
t19-b
t19-a
t20-a
t16-a
t15-a
0.7888
0.8726
0.7413
6.0000
2.9658
5.0100
2.0245
1.0192
8
6
4
2
[ppm]

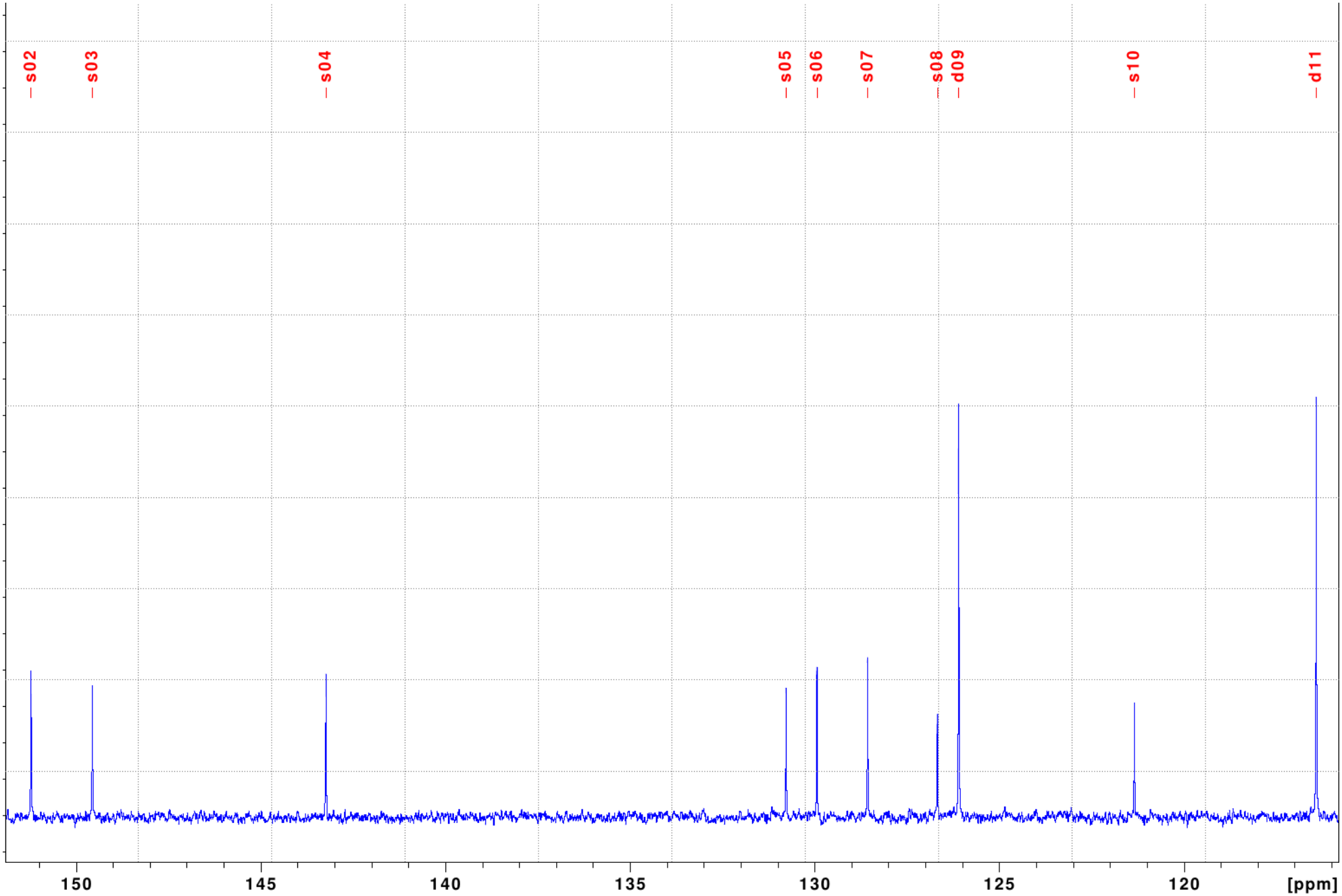

7.2400
d09-H
d11-H
0.8726
0.7413
7.6
7.4
7.2
7.0
6.8
[ppm]

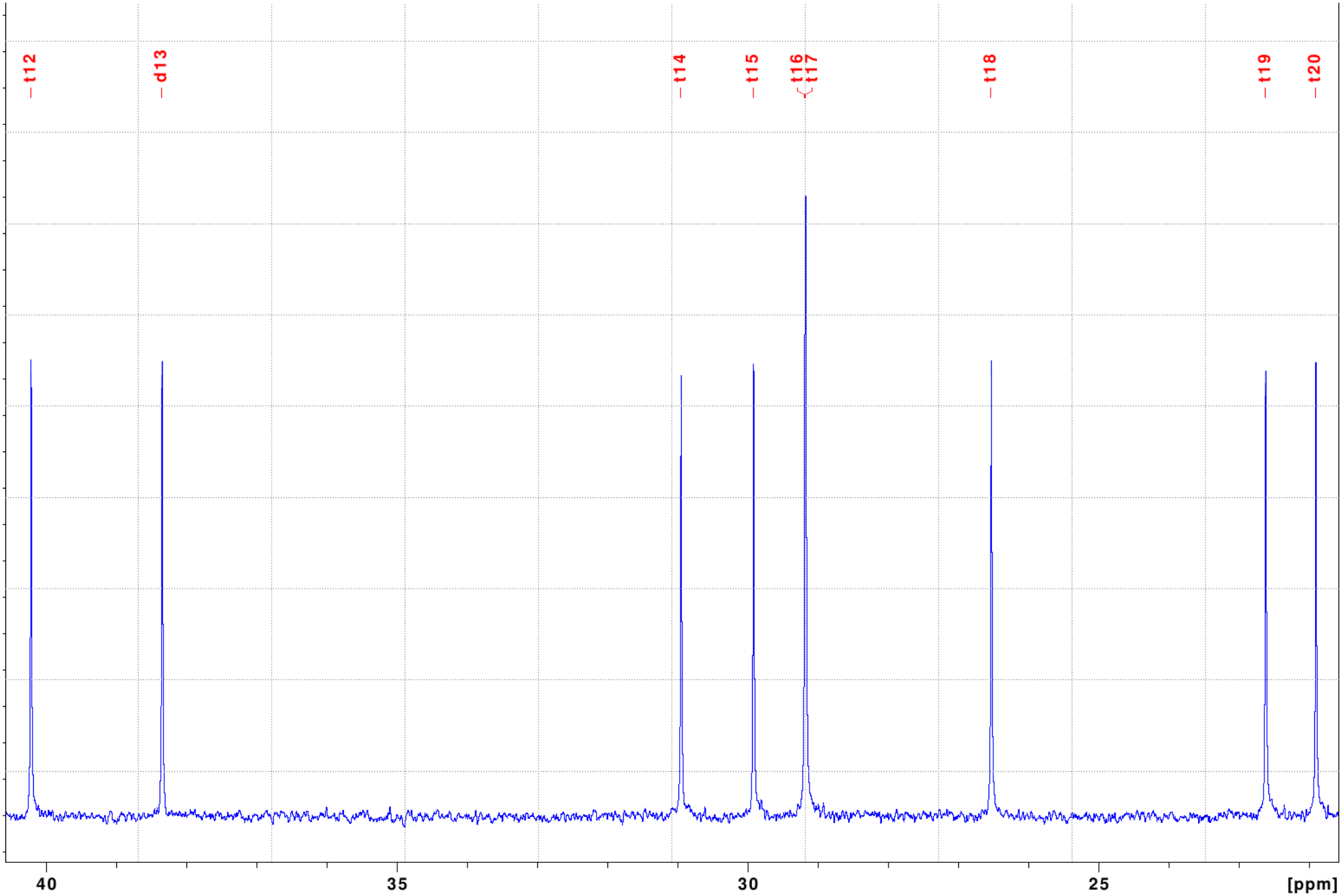

t17-b
t14-b
t14-a
t12-b
t17-a
t18-b
d13-H
t12-a
t18-a
t16-b
t20-b
t15-b
t19-b
t19-a
t20-a
t16-a
t15-a
6.0000
2.9658
5.0100
2.0245
1.0192
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
[ppm]

$^{13}C\{^{1}H\}$ NMR spectrum of compound 13 in CDCl3 at 25 ^{o}C (151 MHz, $CDCl_3$) (pages S10-S13)

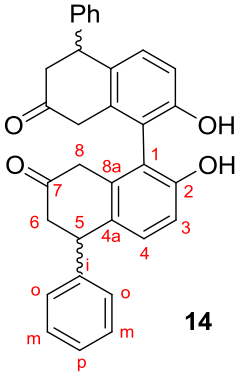



s01
s02
s03
s04
s05
s06
s07
s08
d09
s10
d11
76.8998
t12
d13
t14
t15
t16
t17
t18
t19
t20
200
150
100
50
[ppm]


s02
s03
s04
s05
s06
s07
s08
d09
s10
d11
150
145
140
135
130
125
120
[ppm]


t12
d13
t14
t15
t16
t17
t18
t19
t20
40
35
30
25
[ppm]

^{1}H and ^{13}C NMR signal assignments for compound 14 (pages S14-S17)



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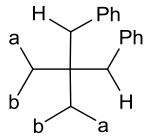
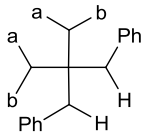
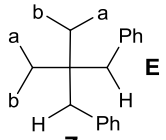


S

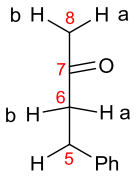


L



E

Z



fragment	S	L	E	Z	comment
1	s059	s058	s057	s060	C-1
2	s043	s042	s041	s044	C-OH
3	d012	d026	d013	d011	CH-3
4	d027	d008	d010	d009	CH-4
4a	s055	s054	s053	s056	C-4a
5	d025	d015	d016	d014	CH-aliph
6	t020	t017	t019	t018	CH2-6
7	s039	s038	s037	s040	C=O
8	t021	t023	t022	t024	CH2-8
8a	s051	s050	s049	s052	C-8a
i	s047	s046	s045	s048	Ph-i
o	d030	d007	d005	d006	Ph-o
m	d029	d031	d001	d002	Ph-m
p	d028	d032	d003	d004	Ph-p
OH	o036	o033	o034	o035	OH

S-S symmetric, lowest contribution
L-L symmetric, highest contribution
E-Z unsymmetric, medium contribution

S: H-6 equiv, H-8 far
L: H-6 far, H-8 near
E: H-6 equiv, H-8 far
Z: H-6 far, H-8 equiv

L: W-constant H-6a - H-8a
E: W-constant H-6a - H-8a
S,Z: no W-constant

S,E - similar shifts
L,Z - similar shifts

cross-NOE:
S:OH - S:H-8b
L:OH - L:H-8a
E:H-8a - Z:H-8b
E:OH - Z:H-8a
Z:OH - E:H-8b
E:Ph-o - Z:H-8a (weak)

Fragment: S

Experiment Bruker_2, 1D 13C: 44 peaks
d012 113.5
d025 43.9
d027 127.6
d028 126.6
d029 128.6 (*2)
d030 127.9 (*2)
s039 209.1
s043 153.4
s047 143.2
s051 133.5
s055 129.6
s059 122.5
t020 46.0
t021 42.3

Experiment Bruker_23, 1D 1H: 38 peaks
d012-H 6.77
d025-H 4.51
d027-H 6.72
d028-H 7.25
d029-H 7.34 (*2)
d030-H 7.18 (*2)
o036-H 9.17
t020-a 2.82
t020-b 2.82
t021-a 2.94
t021-b 3.34

Experiment Bruker_12, 2D 13C-1H via onebond (HSQC): 14 peaks
d027-H - d027
d028-H - d028
d029-H - d029
d030-H - d030

Experiment Bruker_13, 2D 13C-1H via onebond (HSQC): 16 peaks
d025-H - d025
t020-a - t020
t020-b - t020
t021-a - t021
t021-b - t021

Experiment Bruker_14, 2D 1H-13C via onebond (H-C correlation): 14 peaks
d012 - d012-H
d027 - d027-H
d029 - d029-H

Experiment Bruker_15, 2D 1H-13C via onebond (H-C correlation): 16 peaks
d025 - d025-H
t020 - t020-a t020-b
t021 - t021-a t021-b

Experiment Bruker_5, 2D 1H-1H via Jcoupling (COSY): 21 peaks
d012-H - t021-a?(weak) t021-b?(weak)
d025-H - d030-H?(weak)
d027-H - d025-H?(weak)

Experiment Bruker_6, 2D 1H-1H via Jcoupling (COSY): 34 peaks
d012-H - d027-H t021-a?(weak) t021-b?(weak)
d027-H - d012-H d025-H?(weak)
d028-H - d029-H
d029-H - d028-H d030-H
d030-H - d029-H

Experiment Bruker_7, 2D 1H-1H via Jcoupling (COSY): 34 peaks
d025-H - d027-H?(weak) d030-H?(weak)
t020-a t020-b
t020-a - d025-H
t020-b - d025-H
t021-a - d012-H?(weak) t021-b
t021-b - d012-H?(weak) t021-a

Experiment Bruker_21, 2D 1H-1H via through-space (NOESY): 63 peaks
d012-H - o036-H
d025-H - d027-H d030-H t020-b
d027-H - d025-H d030-H
d030-H - d025-H d027-H t020-a t021-a
o036-H - d012-H t021-b
t020-a - d030-H
t020-b - d025-H
t021-a - d030-H

t021-b - d025-H? o036-H

Experiment Bruker_11, 2D 13C-1H via Jcoupling (HMBC): 105 peaks
d012-H - s059
d025-H - d030 s047 s051 s055 t020
d027-H - s043 s059(weak)
d029-H - s047
o036-H - d012 s043 s051(weak) s059
t020-a - d025 s039 s047 s055
t020-b - d025 s039 s047 s055
t021-a - s039 s051 s059
t021-b - s039 s051 s055 s059

Experiment Bruker_16, 2D 13C-1H via Jcoupling (HMBC): 64 peaks
d012-H - s043(weak) s051(weak) s055 s059
d027-H - d025 s043 s051 s059(weak)
d028-H - d030
d029-H - d029 s047
d030-H - d025 d028 d030
o036-H - d012 s043 s051(weak) s059

Experiment Bruker_17, 2D 13C-1H via Jcoupling (HMBC): 70 peaks
d025-H - d027 d030 s039 s047 s051 s055 t020
t020-a - d025 s039 s047 s055
t020-b - d025 s039 s047 s055
t021-a - s039 s051 s055 s059
t021-b - s039 s051 s055 s059

Experiment Bruker_22, 2D 1H-13C via Jmultibond (COLOC): 29 peaks
d025 - t020-a t020-b
d029 - d030-H(weak)
s043 - d027-H
s051 - t021-b
s055 - t020-a t020-b

Fragment: L

Experiment Bruker_2, 1D 13C: 44 peaks
d007 127.6 (*2)
d008 127.9
d015 44.1
d026 113.6
d031 128.5 (*2)
d032 126.4
s038 209.3
s042 153.3
s046 143.5
s050 133.8
s054 129.0
s058 122.5
t017 46.3
t023 42.1

Experiment Bruker_23, 1D 1H: 38 peaks
d007-H 7.14 (*2)
d008-H 6.85
d015-H 4.53
d026-H 6.78
d031-H 7.31 (*2)
d032-H 7.22
o033-H 9.22
t017-a 2.71
t017-b 2.93
t023-a 3.16
t023-b 3.17

Experiment Bruker_12, 2D 13C-1H via onebond (HSQC): 14 peaks
d007-H - d007
d008-H - d008
d026-H - d026
d031-H - d031
d032-H - d032

Experiment Bruker_13, 2D 13C-1H via onebond (HSQC): 16 peaks
d015-H - d015
t017-a - t017
t017-b - t017
t023-a - t023
t023-b - t023

Experiment Bruker_14, 2D 1H-13C via onebond (H-C correlation): 14 peaks
d007 - d007-H
d008 - d008-H
d026 - d026-H
d031 - d031-H
d032 - d032-H

Experiment Bruker_15, 2D 1H-13C via onebond (H-C correlation): 16 peaks
d015 - d015-H
t017 - t017-a t017-b
t023 - t023-a t023-b

Experiment Bruker_5, 2D 1H-1H via Jcoupling (COSY): 21 peaks
d007-H - d015-H(weak)
d008-H - d015-H(weak) t023-a?(weak) t023-b?(weak)
d015-H - d007-H(weak) d008-H(weak)
d026-H - t023-a(weak) t023-b(weak)
t023-a - d026-H(weak)
t023-b - d026-H(weak)

Experiment Bruker_6, 2D 1H-1H via Jcoupling (COSY): 34 peaks
d007-H - d031-H
d008-H - d015-H?(weak) d026-H t023-a?(weak) t023-b?(weak)
d026-H - d008-H t023-a?(weak) t023-b?(weak)
d031-H - d007-H d032-H
d032-H - d031-H

Experiment Bruker_7, 2D 1H-1H via Jcoupling (COSY): 34 peaks
d015-H - d007-H?(weak) t017-a t017-b
t017-a - d015-H t017-b t023-a(weak)
t017-b - d015-H t017-a
t023-a - d008-H?(weak) d026-H?(weak) t017-a(weak)
t023-b - d008-H?(weak) d026-H?(weak)

Experiment Bruker_21, 2D 1H-1H via through-space (NOESY): 63 peaks
d007-H - d008-H d015-H t017-a t023-a
d008-H - d007-H d015-H
d015-H - d007-H d008-H t017-b t023-b
d026-H - o033-H
o033-H - d026-H t023-a
t017-a - d007-H
t017-b - d015-H
t023-a - d007-H o033-H
t023-b - d007-H?(weak) d015-H

Experiment Bruker_11, 2D 13C-1H via Jcoupling (HMBC): 105 peaks
d008-H - s042 s050 s058(weak)
d015-H - d007 s038 s046 s050 s054 t017
d026-H - s042(weak) s050(weak) s054 s058
d031-H - s046
o033-H - d026 s042 s050(weak) s058
t017-a - d015 s038 s046 s054
t017-b - d015 s038 s046 s054
t023-a - s038 s050 s054 s058
t023-b - s038 s050 s054 s058

Experiment Bruker_16, 2D 13C-1H via Jcoupling (HMBC): 64 peaks
d007-H - d007 d015 d032
d008-H - d015 s042 s050 s058(weak)
d026-H - s042(weak) s050(weak) s054 s058
d031-H - d031 s046
d032-H - d007
o033-H - d026 s042 s050(weak) s058

Experiment Bruker_17, 2D 13C-1H via Jcoupling (HMBC): 70 peaks
d015-H - d007 d008 s038 s046 s050 s054 t017
t017-a - d015 s038 s046 s054
t017-b - d015 s038 s046 s054
t023-a - s038 s050 s054 s058
t023-b - s038 s050 s054 s058

Experiment Bruker_22, 2D 1H-13C via Jmultibond (COLOC): 29 peaks
d015 - d007-H t017-b
d031 - d007-H(weak)
d032 - d007-H
s038 - d015-H t017-a t017-b
s046 - t017-b
s054 - d015-H t017-a

s058 - d026-H o033-H

Fragment: E

Experiment Bruker_2, 1D 13C: 44 peaks
d001 128.6 (*2)
d003 126.6
d005 127.9 (*2)
d010 127.6
d013 113.5
d016 43.9
s037 209.2
s041 153.3
s045 143.2
s049 133.5
s053 129.6
s057 122.5
t019 46.0
t022 42.2

Experiment Bruker_23, 1D 1H: 38 peaks
d001-H 7.33 (*2)
d003-H 7.24
d005-H 7.17 (*2)
d010-H 6.72
d013-H 6.76
d016-H 4.51
o034-H 9.21
t019-a 2.81
t019-b 2.81
t022-a 3.01
t022-b 3.35

Experiment Bruker_12, 2D 13C-1H via onebond (HSQC): 14 peaks
d001-H - d001
d003-H - d003
d005-H - d005
d010-H - d010
d013-H - d013

Experiment Bruker_13, 2D 13C-1H via onebond (HSQC): 16 peaks
d016-H - d016
t019-a - t019
t019-b - t019
t022-a - t022
t022-b - t022

Experiment Bruker_14, 2D 1H-13C via onebond (H-C correlation): 14 peaks
d001 - d001-H
d003 - d003-H
d005 - d005-H
d010 - d010-H
d013 - d013-H

Experiment Bruker_15, 2D 1H-13C via onebond (H-C correlation): 16 peaks
d016 - d016-H
t019 - t019-a t019-b
t022 - t022-a t022-b

Experiment Bruker_5, 2D 1H-1H via Jcoupling (COSY): 21 peaks
d010-H - d016-H?(weak)
d013-H - t022-a?(weak) t022-b?(weak)
d016-H - d005-H?(weak)

Experiment Bruker_6, 2D 1H-1H via Jcoupling (COSY): 34 peaks
d001-H - d003-H d005-H
d003-H - d001-H
d005-H - d001-H
d010-H - d013-H d016-H?(weak)
d013-H - d010-H t022-a?(weak) t022-b?(weak)

Experiment Bruker_7, 2D 1H-1H via Jcoupling (COSY): 34 peaks
d016-H - d005-H?(weak) d010-H?(weak)
t019-a t019-b
t019-a - d016-H t022-a(weak)
t019-b - d016-H
t022-a - d013-H? t019-a(weak) t022-b
t022-b - d013-H?(weak) t022-a

Experiment Bruker_21, 2D 1H-1H via through-space (NOESY): 63 peaks
d005-H - d010-H d016-H t019-a t022-a Z:t024-a?(weak)
d010-H - d005-H d016-H
d013-H - o034-H
d016-H - d005-H d010-H t019-b t022-b
o034-H - d013-H Z:t024-a?
t019-a - d005-H
t019-b - d016-H
t022-a - d005-H Z:t024-b?
t022-b - d016-H Z:o035-H?

Experiment Bruker_11, 2D 13C-1H via Jcoupling (HMBC): 105 peaks
d001-H - s045
d010-H - s041 s049 s057(weak)
d013-H - s041(weak) s049(weak) s053 s057
d016-H - d005 s037 s045 s049 s053 t019
o034-H - d013 s041 s049(weak) s057
t019-a - d016 s037 s045 s053
t019-b - d016 s037 s045 s053
t022-a - s037 s049 s053 s057
t022-b - s037 s049 s053 s057

Experiment Bruker_16, 2D 13C-1H via Jcoupling (HMBC): 64 peaks
d001-H - d001 s045
d003-H - d005
d005-H - d003 d005 d016
d010-H - d016 s041 s049 s057(weak)
d013-H - s041(weak) s049(weak) s053 s057
o034-H - d013 s041 s049(weak) s057

Experiment Bruker_17, 2D 13C-1H via Jcoupling (HMBC): 70 peaks
d016-H - d005 d010 s037 s045 s049 s053 t019
t019-a - d016 s037 s045 s053
t019-b - d016 s037 s045 s053
t022-a - s037 s049 s053 s057
t022-b - s037 s049 s053 s057

Experiment Bruker_22, 2D 1H-13C via Jmultibond (COLOC): 29 peaks
d001 - d005-H(weak)
d016 - t019-a t019-b
s037 - t022-a
s041 - d010-H
s045 - t019-a t019-b
s049 - t022-a t022-b
s053 - t019-a t019-b
s057 - o034-H

Fragment: Z

Experiment Bruker_2, 1D 13C: 44 peaks
d002 128.5 (*2)
d004 126.4
d006 127.7 (*2)
d009 127.9
d011 113.6
d014 44.0
s040 209.3
s044 153.3
s048 143.5
s052 133.8
s056 129.1
s060 122.4
t018 46.3
t024 42.1

Experiment Bruker_23, 1D 1H: 38 peaks
d002-H 7.31 (*2)
d004-H 7.22
d006-H 7.15 (*2)
d009-H 6.84
d011-H 6.79
d014-H 4.54
o035-H 9.18
t018-a 2.72
t018-b 2.94
t024-a 3.15
t024-b 3.15

Experiment Bruker_12, 2D 13C-1H via onebond (HSQC): 14 peaks
d002-H - d002
d004-H - d004
d006-H - d006
d009-H - d009
d011-H - d011

Experiment Bruker_13, 2D 13C-1H via onebond (HSQC): 16 peaks
d014-H - d014
t018-a - t018
t018-b - t018
t024-a - t024
t024-b - t024

Experiment Bruker_14, 2D 1H-13C via onebond (H-C correlation): 14 peaks
d002 - d002-H
d004 - d004-H
d006 - d006-H
d009 - d009-H
d011 - d011-H

Experiment Bruker_15, 2D 1H-13C via onebond (H-C correlation): 16 peaks
d014 - d014-H
t018 - t018-a t018-b
t024 - t024-a t024-b

Experiment Bruker_5, 2D 1H-1H via Jcoupling (COSY): 21 peaks
d006-H - d014-H(weak)
d009-H - d014-H(weak) t024-a?(weak) t024-b?(weak)
d011-H - t024-a(weak) t024-b(weak)
d014-H - d006-H(weak) d009-H(weak)
t024-a - d011-H(weak)
t024-b - d011-H(weak)

Experiment Bruker_6, 2D 1H-1H via Jcoupling (COSY): 34 peaks
d002-H - d004-H d006-H
d004-H - d002-H
d006-H - d002-H
d009-H - d011-H d014-H?(weak) t024-a?(weak) t024-b?(weak)
d011-H - d009-H t024-a?(weak) t024-b?(weak)

Experiment Bruker_7, 2D 1H-1H via Jcoupling (COSY): 34 peaks
d014-H - d006-H?(weak) t018-a t018-b
t018-a - d014-H t018-b
t018-b - d014-H t018-a
t024-a - d009-H?(weak) d011-H?(weak)
t024-b - d009-H?(weak) d011-H?(weak)

Experiment Bruker_21, 2D 1H-1H via through-space (NOESY): 63 peaks
d006-H - d009-H d014-H t018-a t024-a
d009-H - d006-H d014-H
d011-H - o035-H
d014-H - d006-H d009-H t018-b t024-b
o035-H - d011-H E:t022-b?
t018-a - d006-H
t018-b - d014-H
t024-a - d006-H E:o034-H?
t024-b - d014-H E:t022-a?

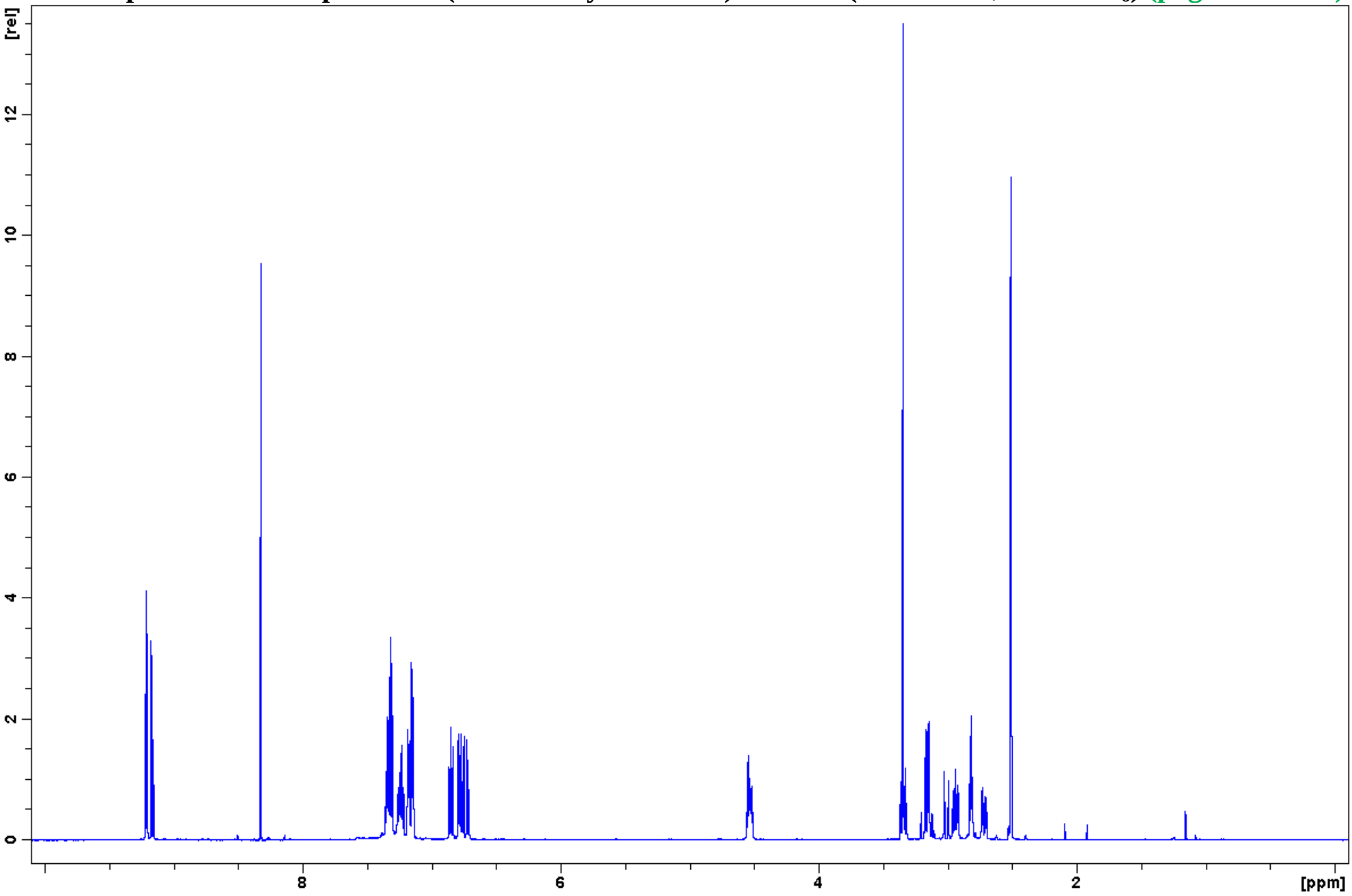
Experiment Bruker_11, 2D 13C-1H via Jcoupling (HMBC): 105 peaks
d002-H - s048
d009-H - s044 s052 s060(weak)
d011-H - s044(weak) s052(weak) s056 s060
d014-H - d006 s040 s048 s052 s056 t018
o035-H - d011 s044 s052(weak) s060
t018-a - d014 s040 s048 s056
t018-b - d014 s040 s048 s056
t024-a - s040 s052 s056 s060
t024-b - s040 s052 s056 s060

Experiment Bruker_16, 2D 13C-1H via Jcoupling (HMBC): 64 peaks
d002-H - d002 s048
d004-H - d006
d006-H - d004 d006 d014
d009-H - d014 s044 s052 s060(weak)
d011-H - s044(weak) s052(weak) s056 s060
o035-H - d011 s044 s052(weak) s060

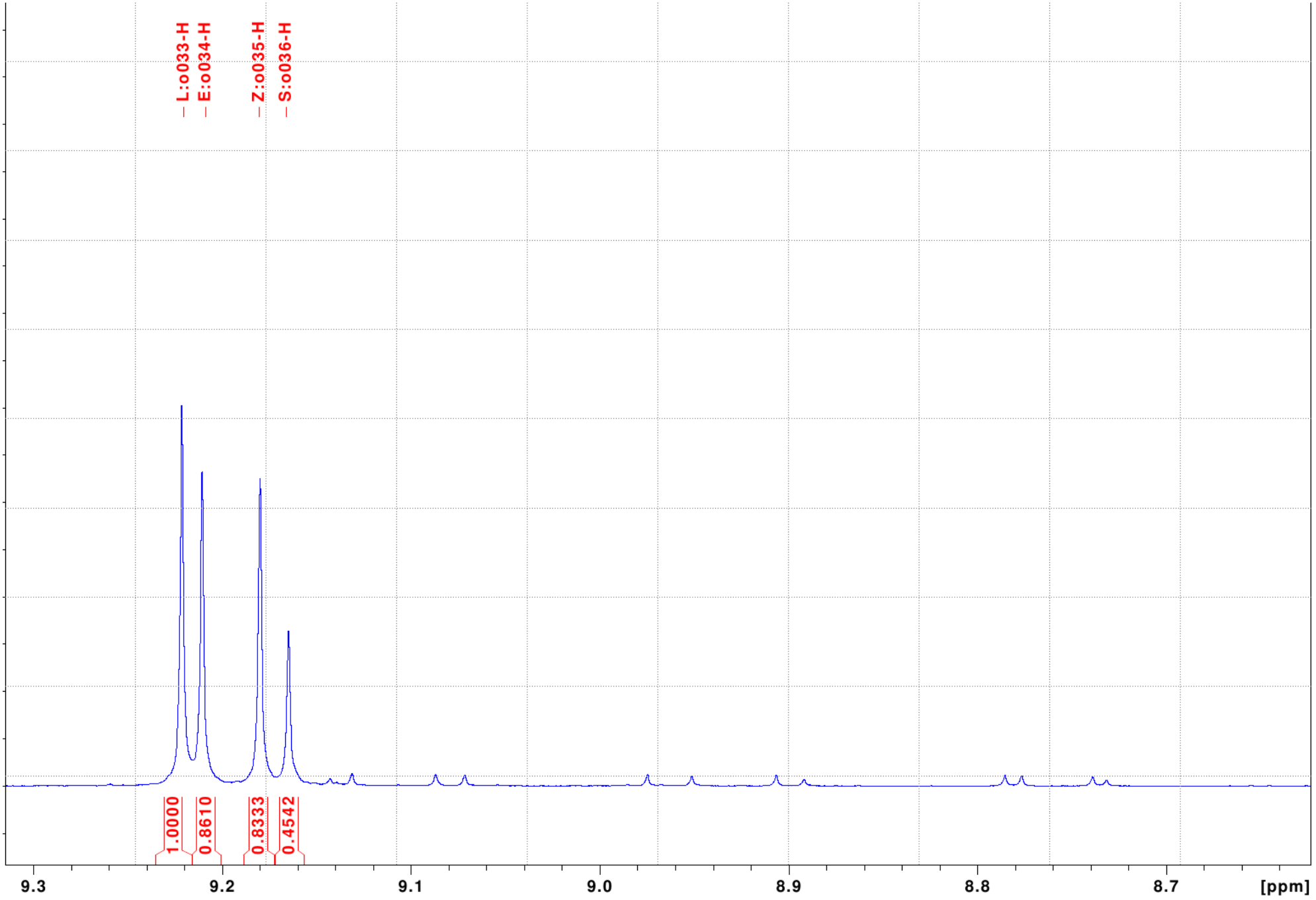
Experiment Bruker_17, 2D 13C-1H via Jcoupling (HMBC): 70 peaks
d014-H - d006 s040 s048 s052 s056 t018
t018-a - d014 s040 s048 s056
t018-b - d014 s040 s048 s056
t024-a - s040 s052 s056 s060
t024-b - s040 s052 s056 s060

Experiment Bruker_22, 2D 1H-13C via Jmultibond (COLOC): 29 peaks
d002 - d006-H(weak)
d004 - d006-H
d014 - d006-H t018-b
s040 - d014-H t018-a t018-b t024-a t024-b
s044 - d009-H
s048 - t018-b
s052 - t024-a t024-b
s056 - d014-H t018-a t024-a t024-b
s060 - o035-H t024-a t024-b

^{1}H NMR spectrum of compound 14 (obtained by method a) at 25 ^{o}C (600.3 MHz, DMSO-d_6) **(pages S18-S22)**




L:o033-H
E:o034-H
Z:o035-H
S:o036-H
S:d029-H
E:d001-H
Z:d002-H
L:d031-H
S:d028-H
E:d003-H
L:d032-H
S:d030-H
E:d005-H
Z:d006-H
L:d007-H
L:d008-H
Z:d009-H
Z:d011-H
L:d026-H
S:d012-H
E:d013-H
E:d010-H
S:d027-H
Z:d014-H
L:d015-H
S:d025-H
E:d016-H
E:t022-b
S:t021-b
L:t023-b
L:t023-a
Z:t024-*
E:t022-a
Z:t018-b
S:t021-a
L:t017-b
S:t020-*
E:t019-*
Z:t018-a
L:t017-a
2.5000
0.4542
0.5860
7.0004
4.3070
6.9522
1.9656
2.4622
1.3573
3.3563
6.3947
4.0443
0.4270
2.4936
2.6697
2.0294
9
8
7
6
5
4
3
[ppm]


L:o033-H
E:o034-H
Z:o035-H
S:o036-H
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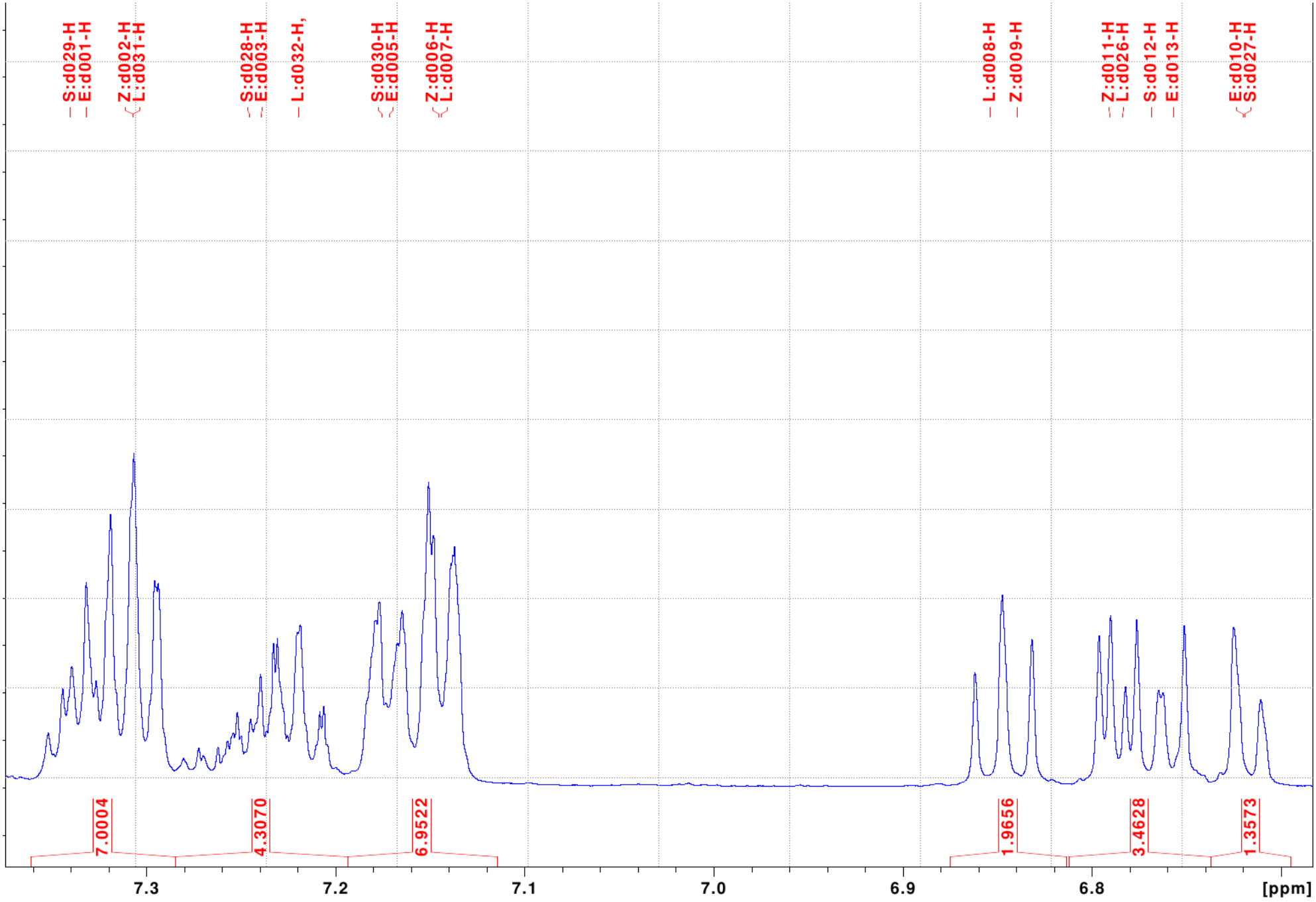
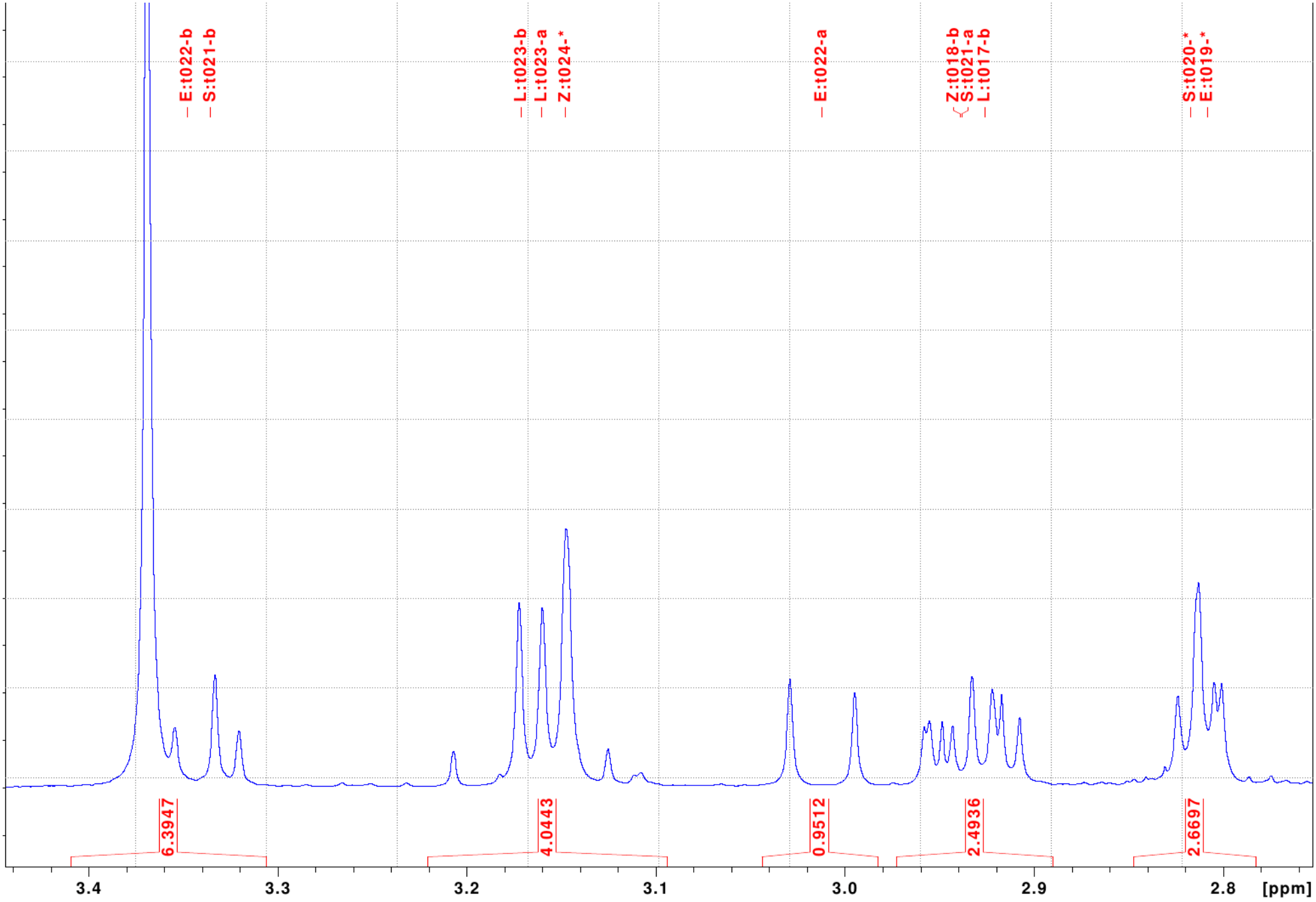
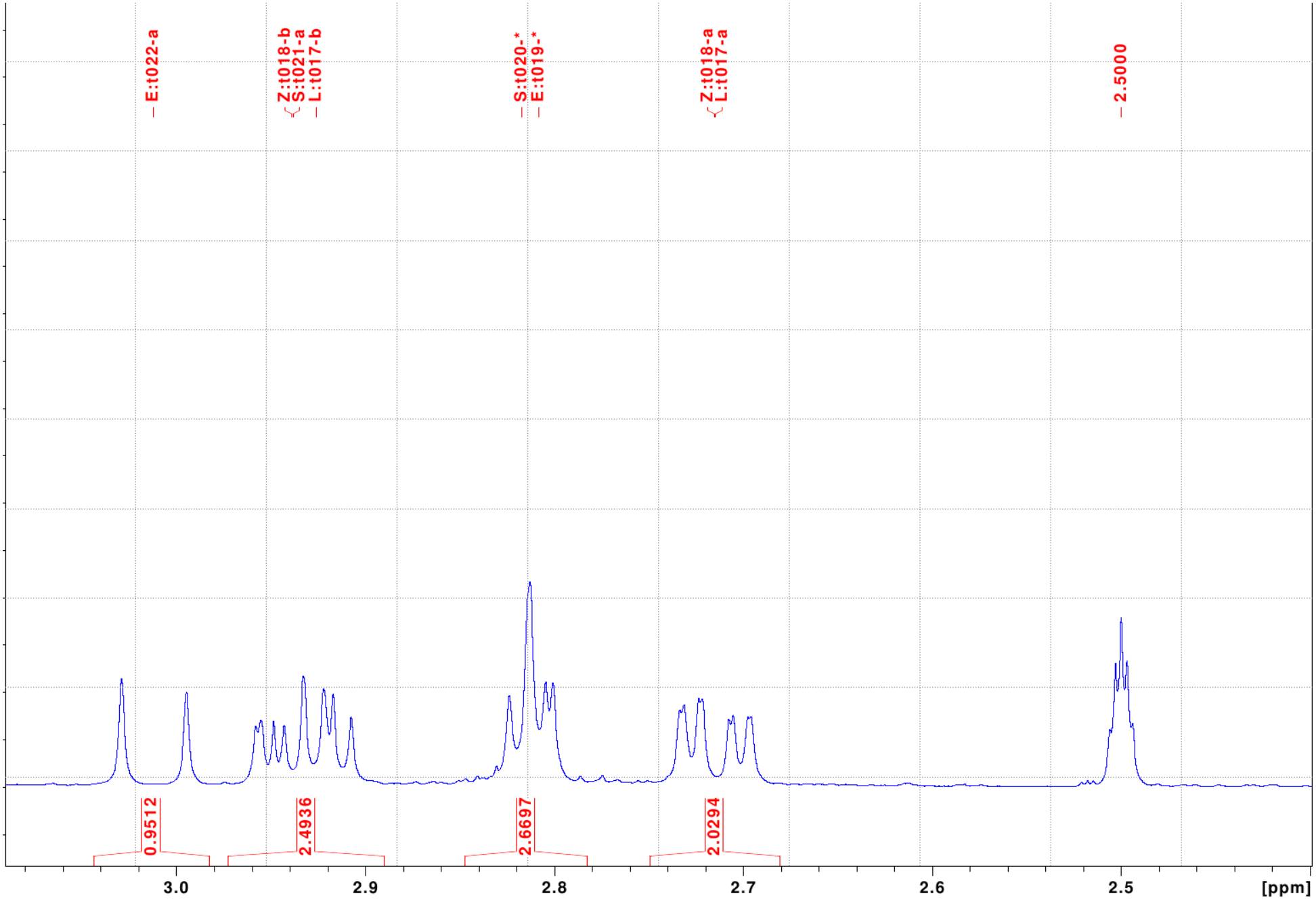
0.8610
0.8333
0.4542
9.3
9.2
9.1
9.0
8.9
8.8
8.7
[ppm]

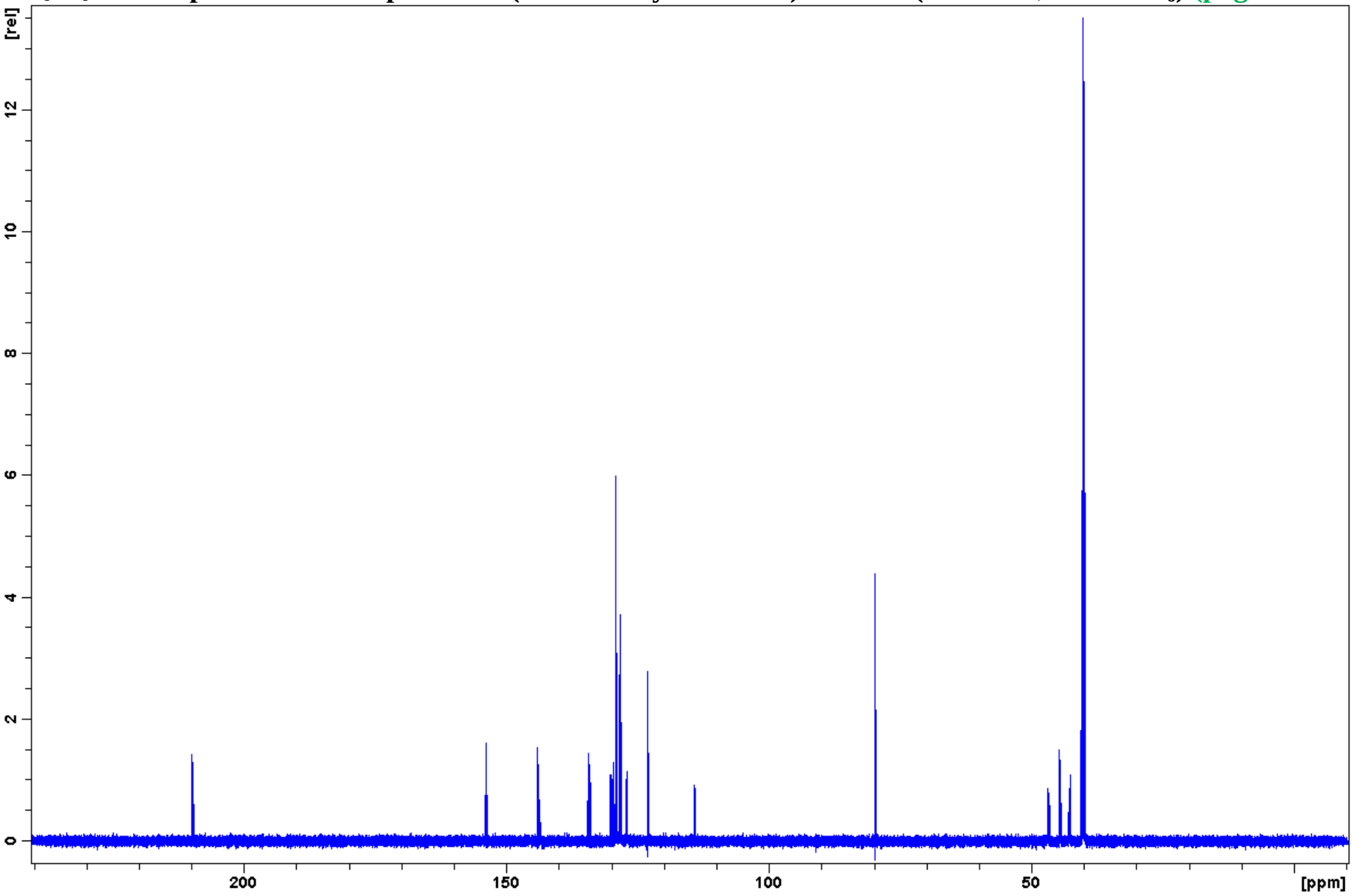

S:d029-H
E:d001-H
Z:d002-H
L:d031-H
S:d028-H
E:d003-H
L:d032-H,
S:d030-H
E:d005-H
Z:d006-H
L:d007-H
L:d008-H
Z:d009-H
Z:d011-H
L:d026-H
S:d012-H
E:d013-H
E:d010-H
S:d027-H
7.0004
4.3070
6.9522
1.9656
3.4628
1.3573
7.3
7.2
7.1
7.0
6.9
6.8
[ppm]

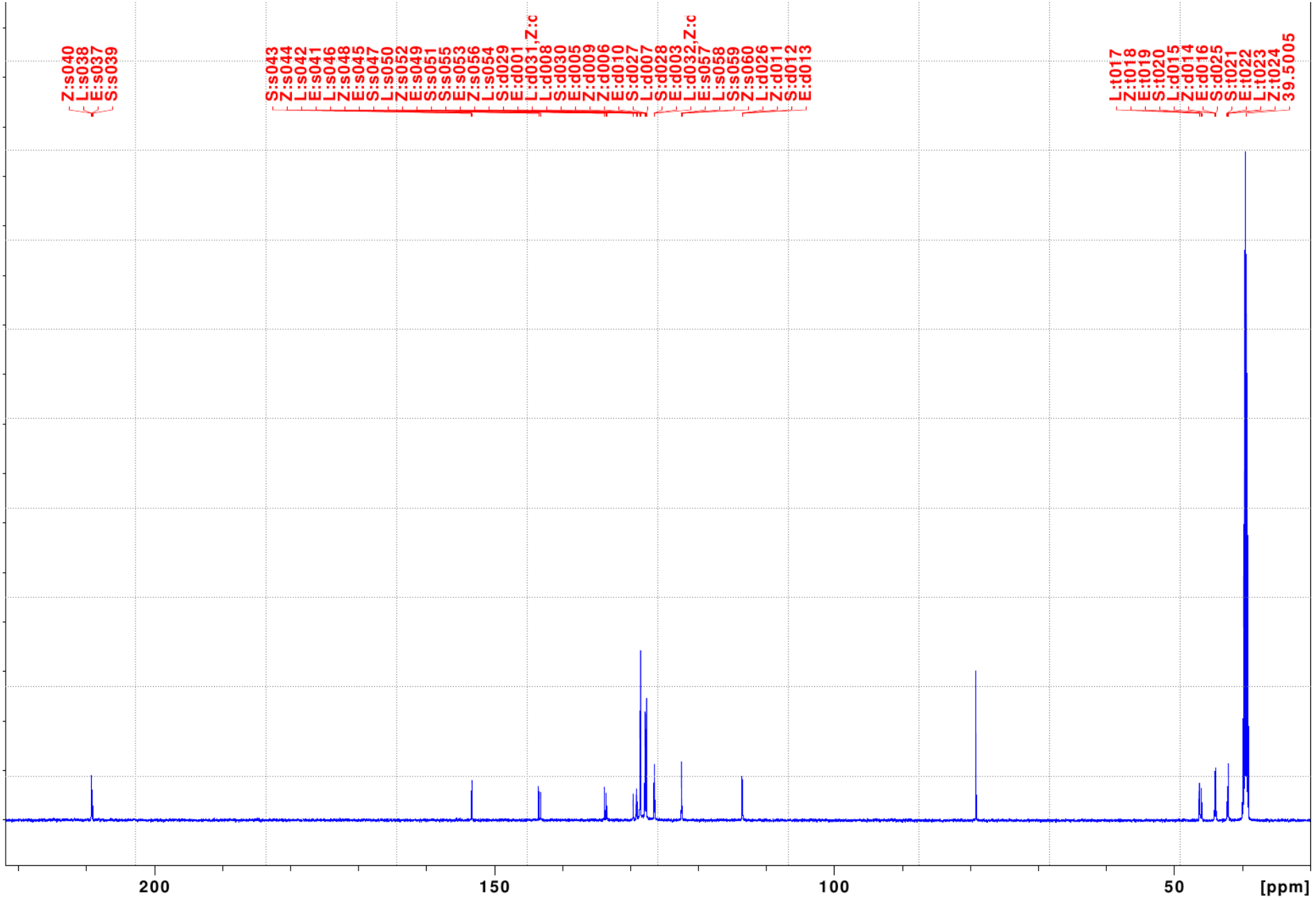

Z:d014-H
L:d015-H
S:d025-H
E:d016-H
3.3563
4.6
4.5
4.4
4.3
4.2
4.1
4.0
[ppm]


E:t022-b
S:t021-b
L:t023-b
L:t023-a
Z:t024-*
E:t022-a
Z:t018-b
S:t021-a
L:t017-b
S:t020-*
E:t019-*
6.3947
4.0443
0.9512
2.4936
2.6697
3.4
3.3
3.2
3.1
3.0
2.9
2.8
[ppm]


E:t022-a
Z:t018-b
S:t021-a
L:t017-b
S:t020-*
E:t019-*
Z:t018-a
L:t017-a
2.5000
0.9512
2.4936
2.6697
2.0294
3.0
2.9
2.8
2.7
2.6
2.5
[ppm]

$^{13}C\{^{1}H\}$ NMR spectrum of compound 14 (obtained by method a) at 25 ^{o}C (151 MHz, DMSO-d_6) **(pages S25-S31)**

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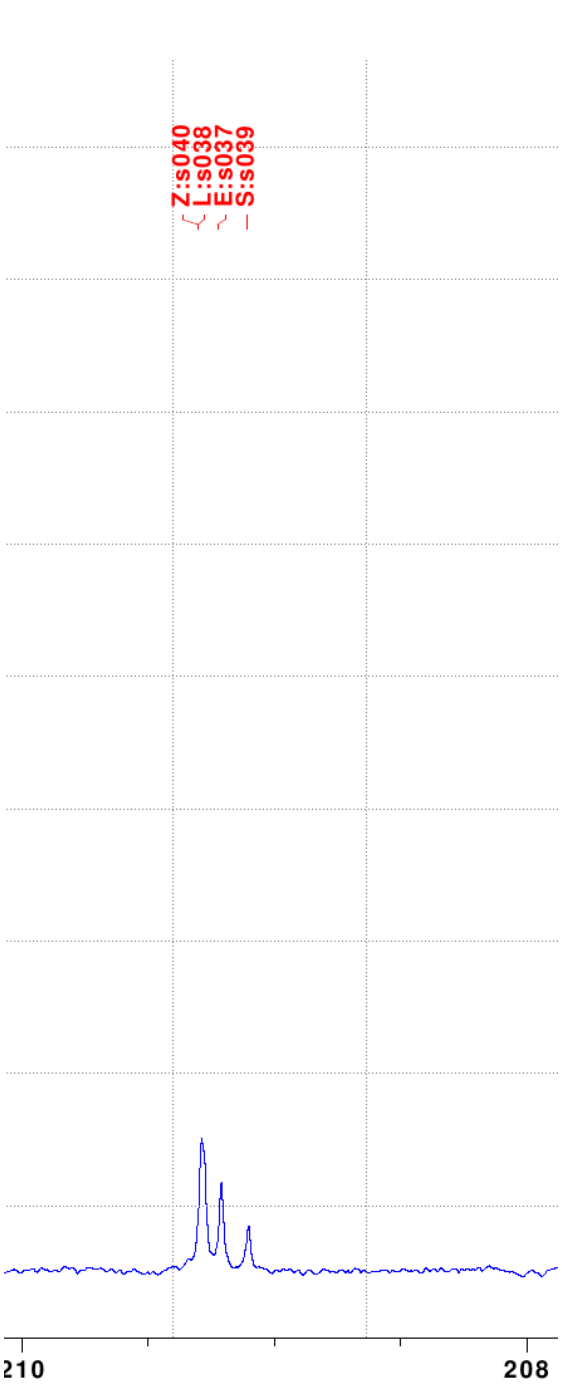
L:s038
E:s037
S:s039
S:s043
Z:s044
L:s042
E:s041
L:s046
Z:s048
E:s045
S:s047
L:s050
Z:s052
E:s049
S:s051
S:s055
E:s053
Z:s056
L:s054
S:d029
E:d001
L:d031,Z:c
L:d008
S:d030
E:d005
Z:d009
Z:d006
E:d010
S:d027
L:d007
S:d028
E:d003
L:d032,Z:c
E:s057
L:s058
S:s059
Z:s060
L:d026
Z:d011
S:d012
E:d013
L:t017
Z:t018
E:t019
S:t020
L:d015
Z:d014
E:d016
S:d025
S:t021
E:t022
L:t023
Z:t024
39.5005
200
150
100
50
[ppm]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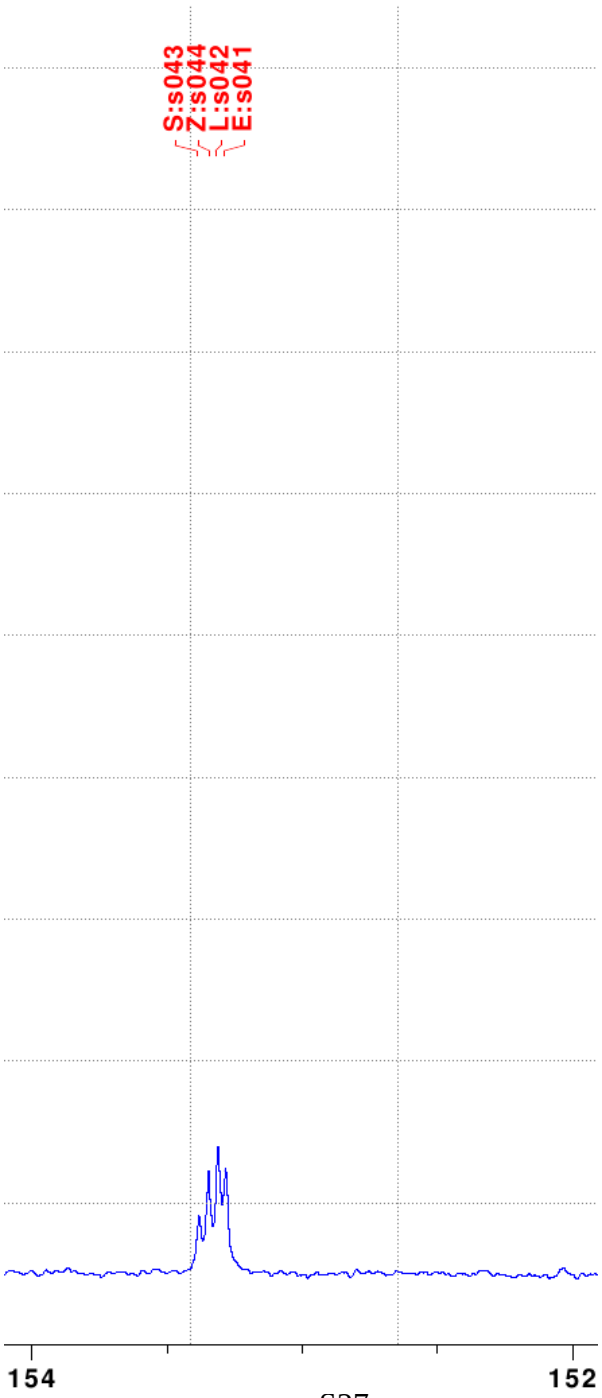
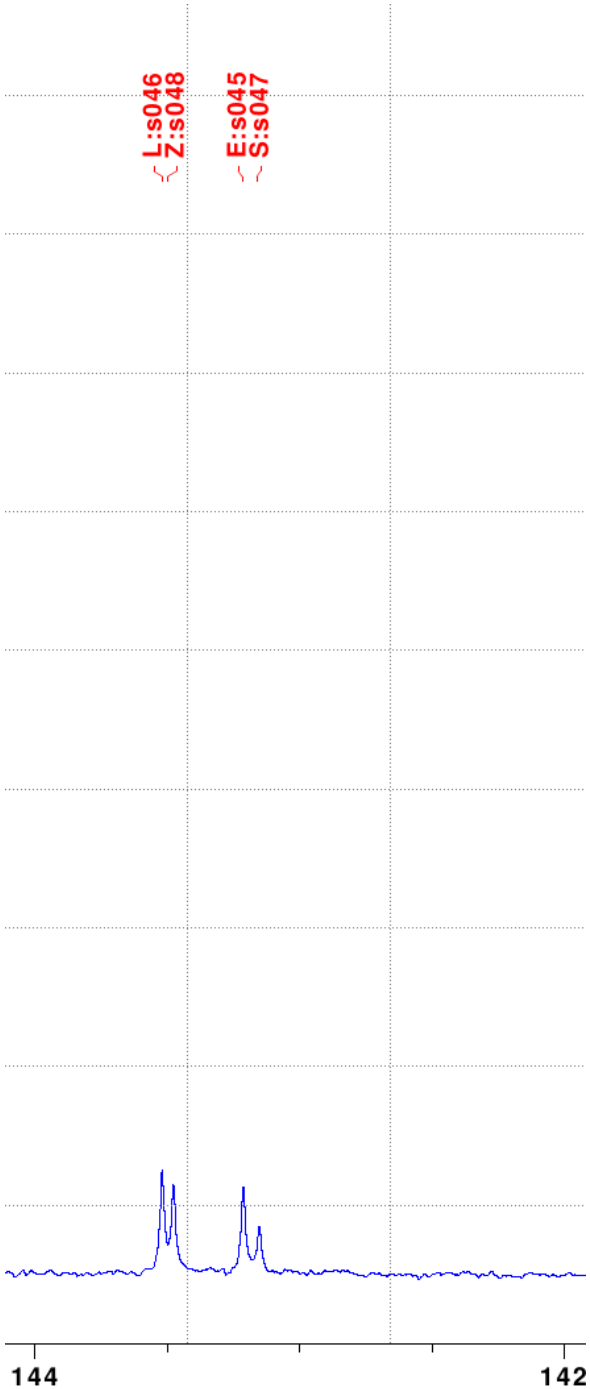
L:s038
E:s037
S:s039
210
208


S:s043
Z:s044
L:s042
E:s041
154
152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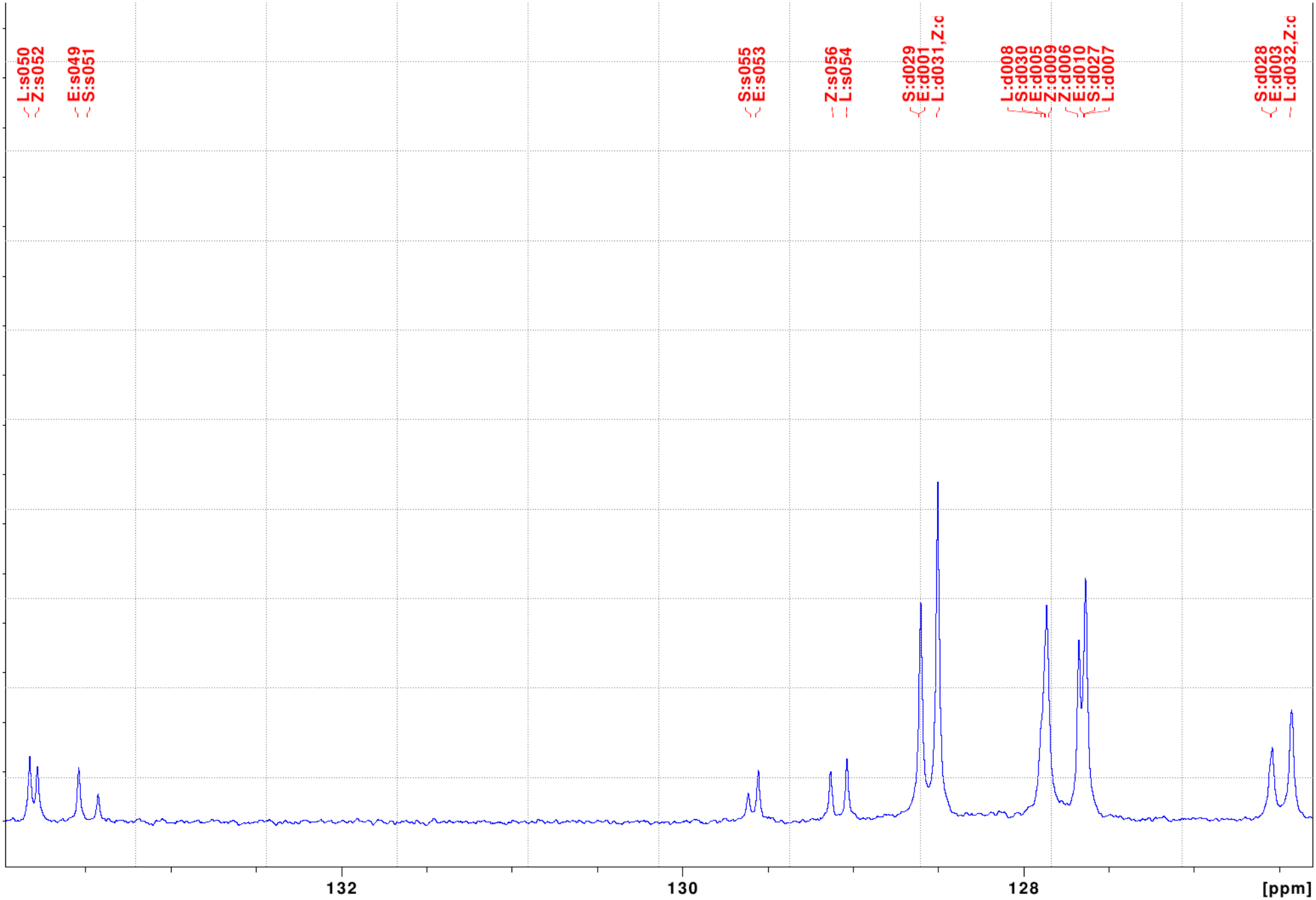
Z:s048
E:s045
S:s047
144
142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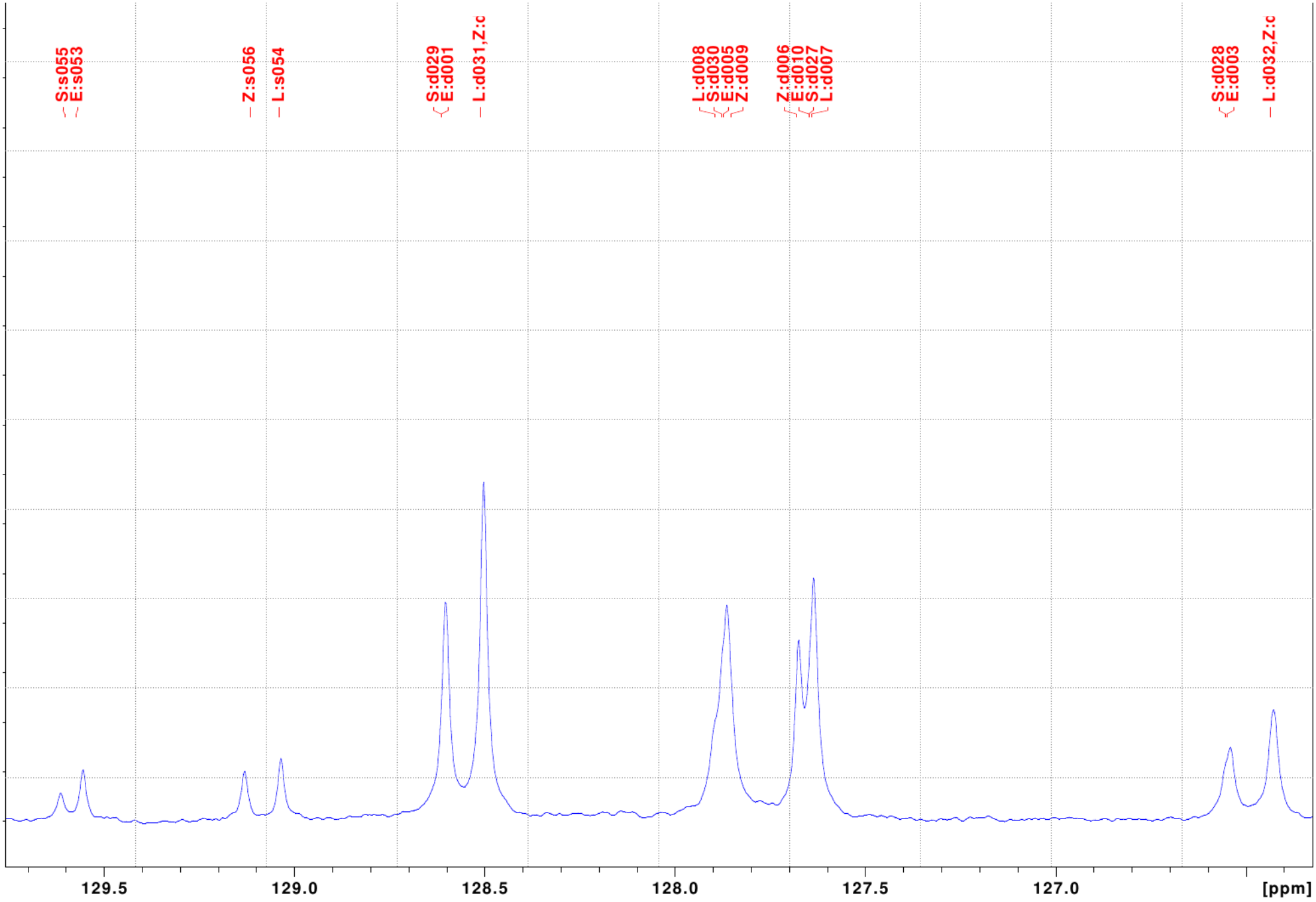
Z:s052
E:s049
S:s051
S:s055
E:s053
Z:s056
L:s054
S:d029
E:d001
L:d031,Z:c
L:d008
S:d030
E:d005
Z:d009
Z:d006
E:d010
S:d027
L:d007
S:d028
E:d003
L:d032,Z:c
132
130
128
[ppm]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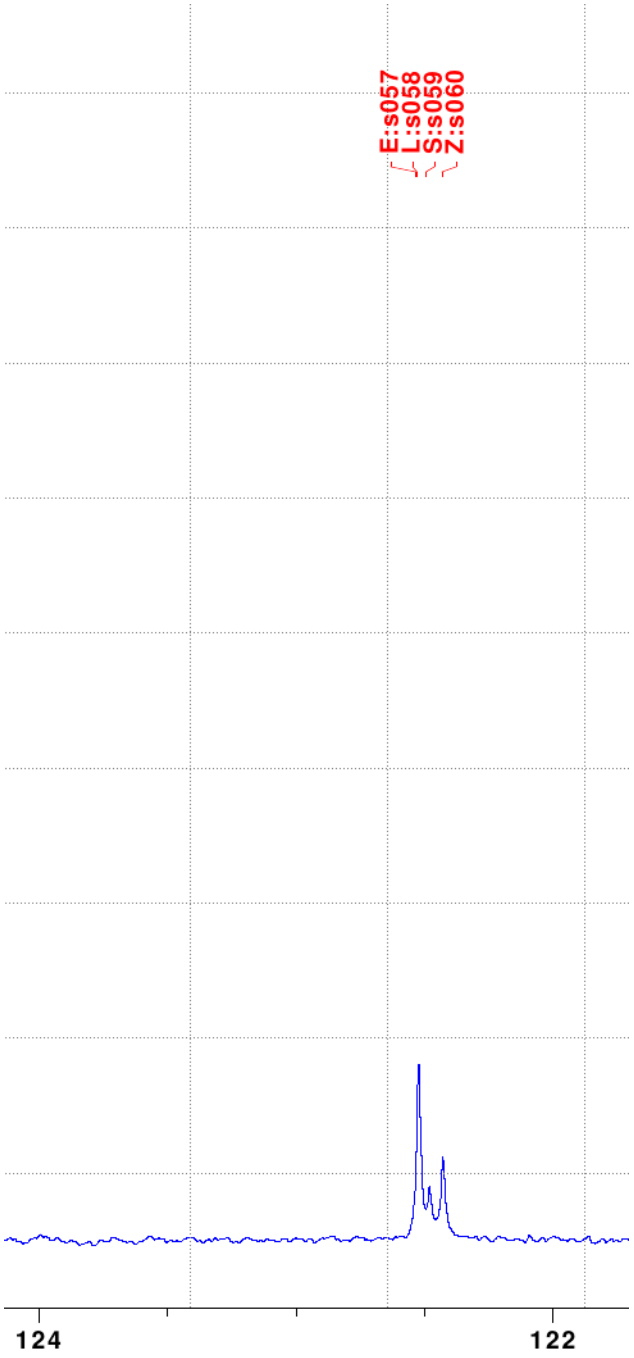
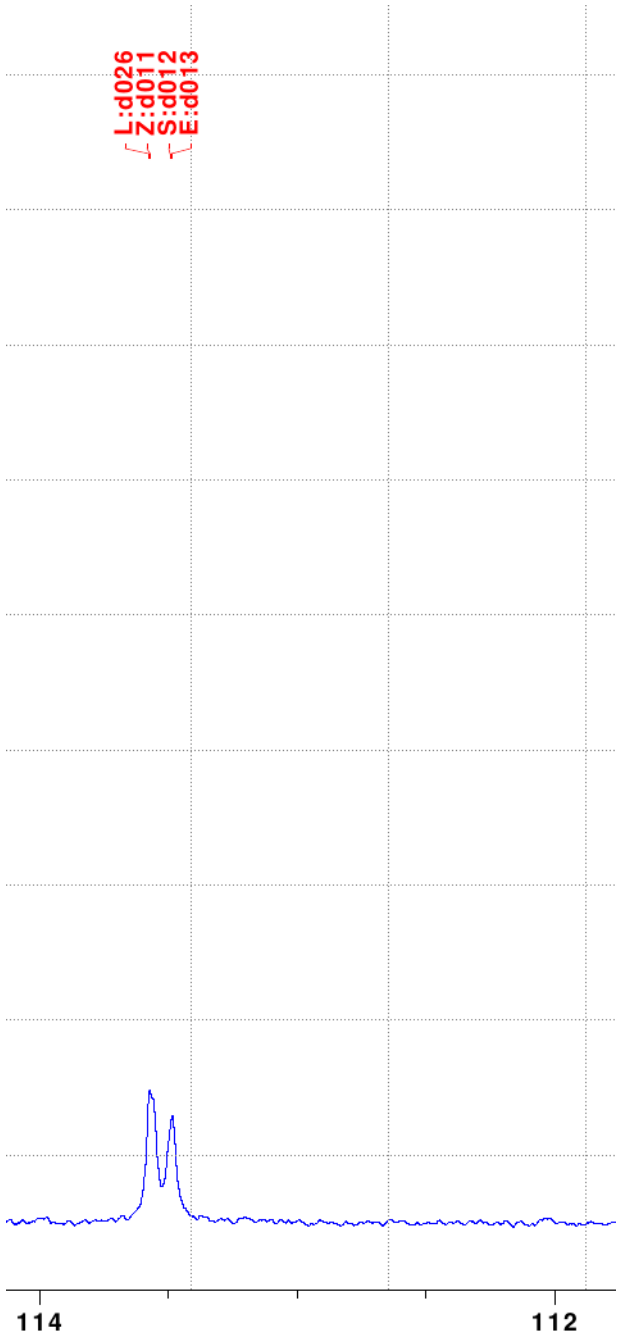
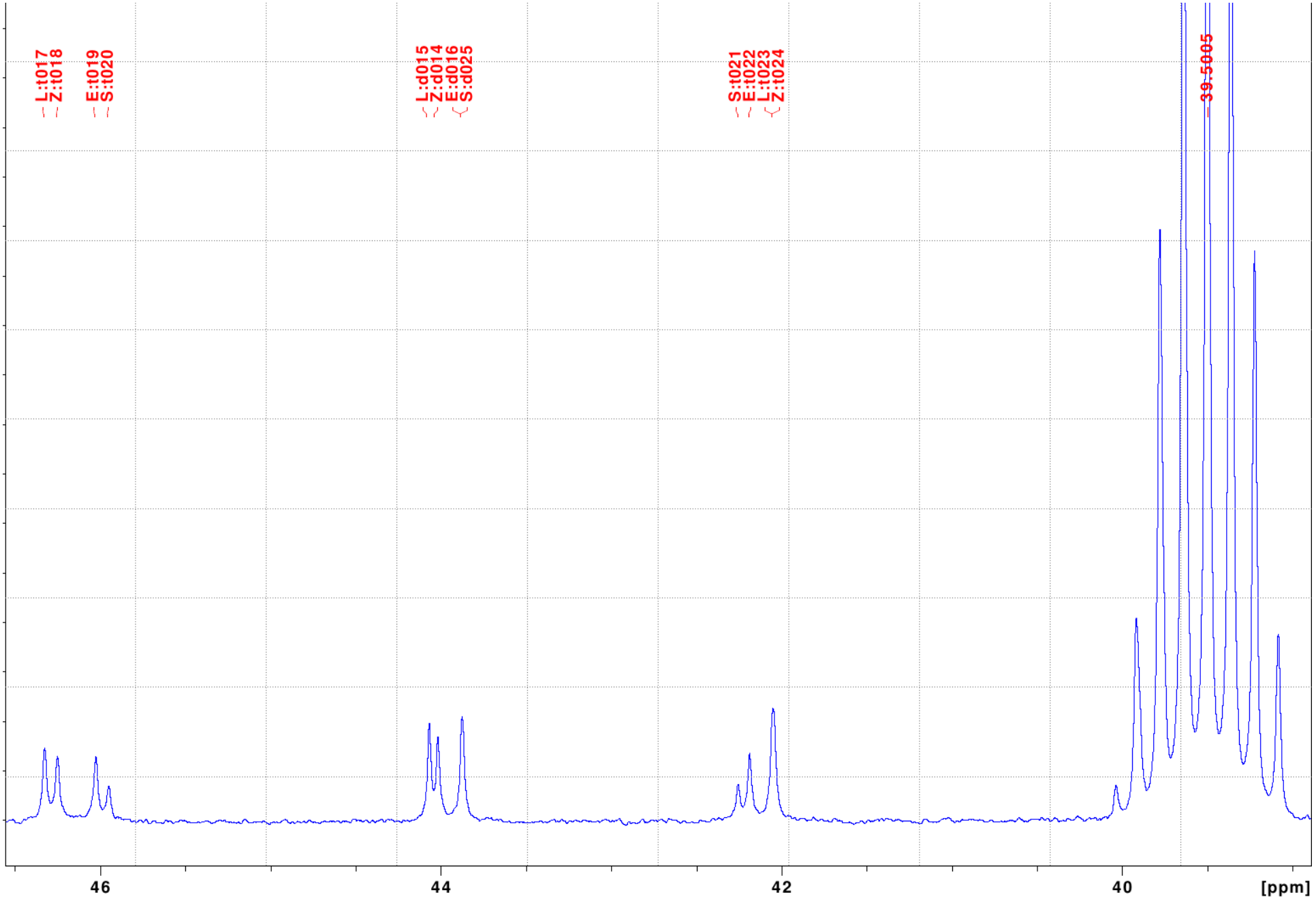
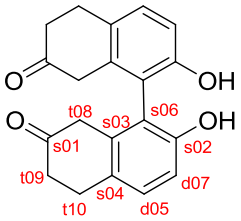
E:s053
Z:s056
L:s054
S:d029
E:d001
L:d031,Z:c
L:d008
S:d030
E:d005
Z:d009
Z:d006
E:d010
S:d027
L:d007
S:d028
E:d003
L:d032,Z:c
129.5
129.0
128.5
128.0
127.5
127.0
[ppm]


E:s057
L:s058
S:s059
Z:s060
124
122

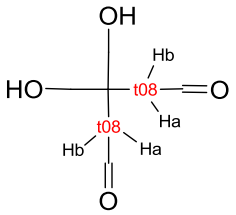

L:d026
Z:d011
S:d012
E:d013
114
112


L:t017
Z:t018
E:t019
S:t020
L:d015
Z:d014
E:d016
S:d025
S:t021
E:t022
L:t023
Z:t024
39.5005
46
44
42
40
[ppm]

^{1}H and ^{13}C NMR signal assignments for compound 15



15



Experiment Bruker_3, 1D 13C: 10 peaks

d05 128.1

d07 113.8

s01 209.3

s02 153.7

s03 134.3

s04 128.4

s06 121.9

t08 42.3

t09 38.3

t10 28.1

Experiment Bruker_4, 1D 1H: 7 peaks

d05-H 7.12

d07-H 6.82

OH-H 7.72

t08-a 3.04

t08-b 3.23

t09-a 2.43

t09-b 2.43

t10-a 3.03

t10-b 3.03

Experiment Bruker_9, 2D 13C-1H via onebond (HSQC): 6 peaks

d05-H - d05

d07-H - d07

t08-a - t08

t08-b - t08

t09-a - t09

t09-b - t09

t10-a - t10

t10-b - t10

Experiment Bruker_11, 2D 1H-1H via Jcoupling (COSY): 8 peaks

d05-H - d07-H t08-a?(weak)

d07-H - d05-H t08-b?(weak)

t08-a - t08-b

t08-b - t08-a

t09-a - t10-a? t10-b?

t09-b - t10-a? t10-b?

t10-a - t09-a? t09-b?

t10-b - t09-a? t09-b?

Experiment Bruker_10, 2D 13C-1H via Jcoupling (HMBC): 36 peaks

d05-H - d07(weak) s02 s03 s06(weak) t08(weak) t10

d07-H - s02(weak) s03(weak) s04 s06

OH-H - d07 s02 s03(weak) s06

t08-a - d07(weak) s01 s02(weak) s03 s04 s06 t09

t08-b - d07(weak) s01 s02(weak) s03 s04 s06 t09

t09-a - s01 s04 t08 t10

t09-b - s01 s04 t08 t10

t10-a - d05? s01 s03 s04? t09

t10-b - d05? s01 s03 s04? t09

Experiment Bruker_12, 2D 1H-1H via through-space (NOESY): 6 peaks

d05-H - t10-a t10-b

d07-H - OH-H

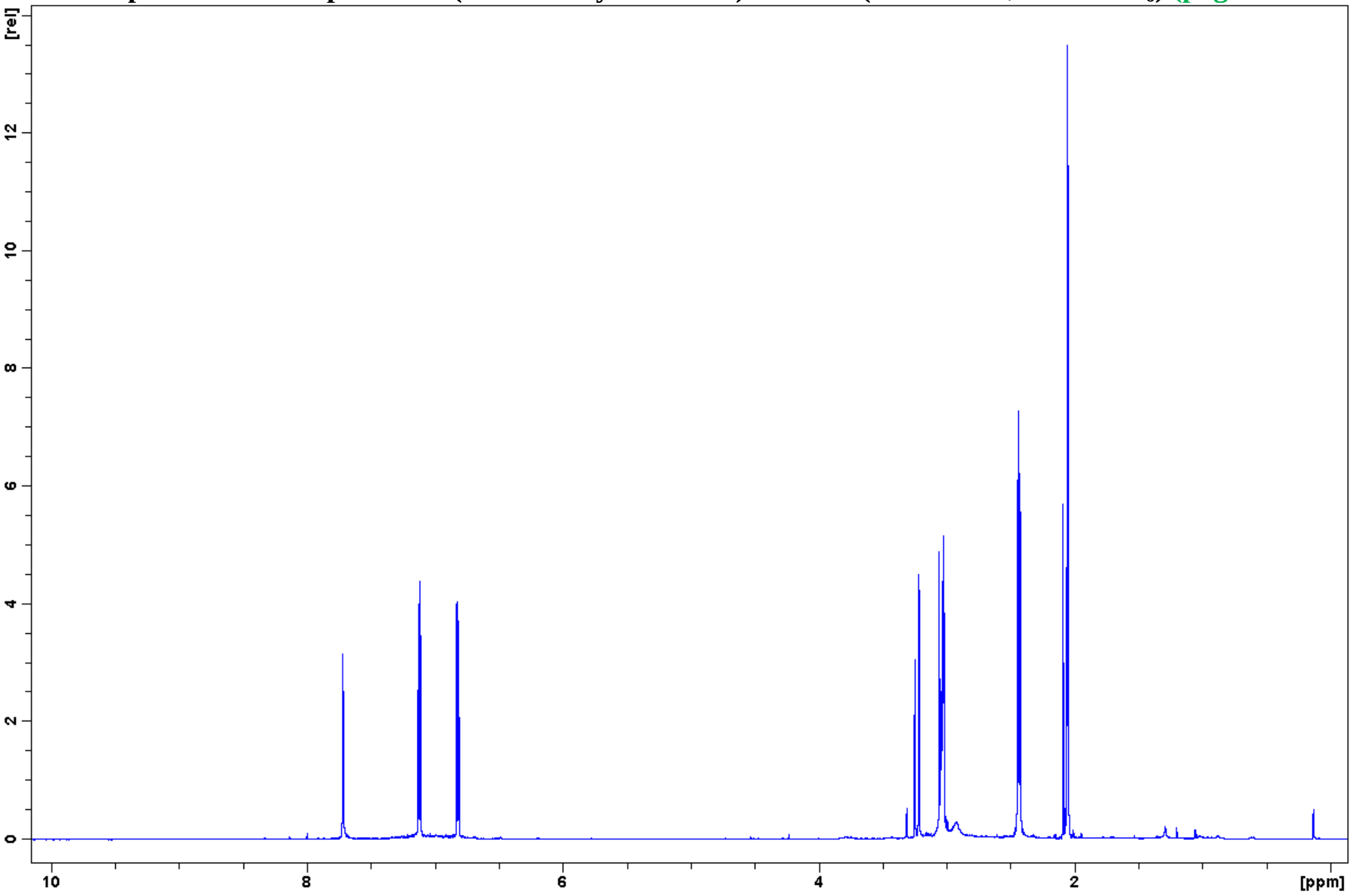
OH-H - d07-H t08-b?

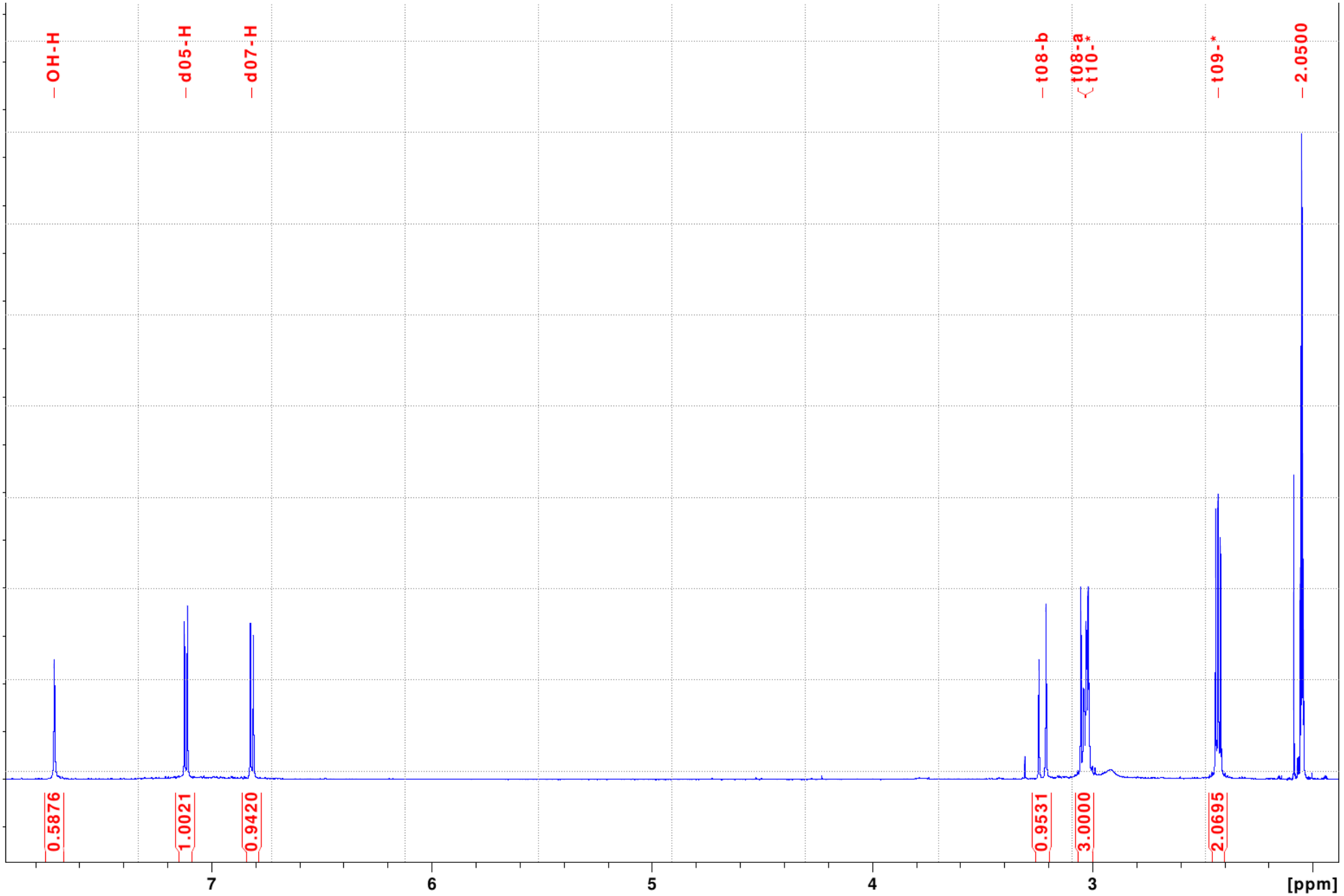
t08-b - t09-a? t09-b?

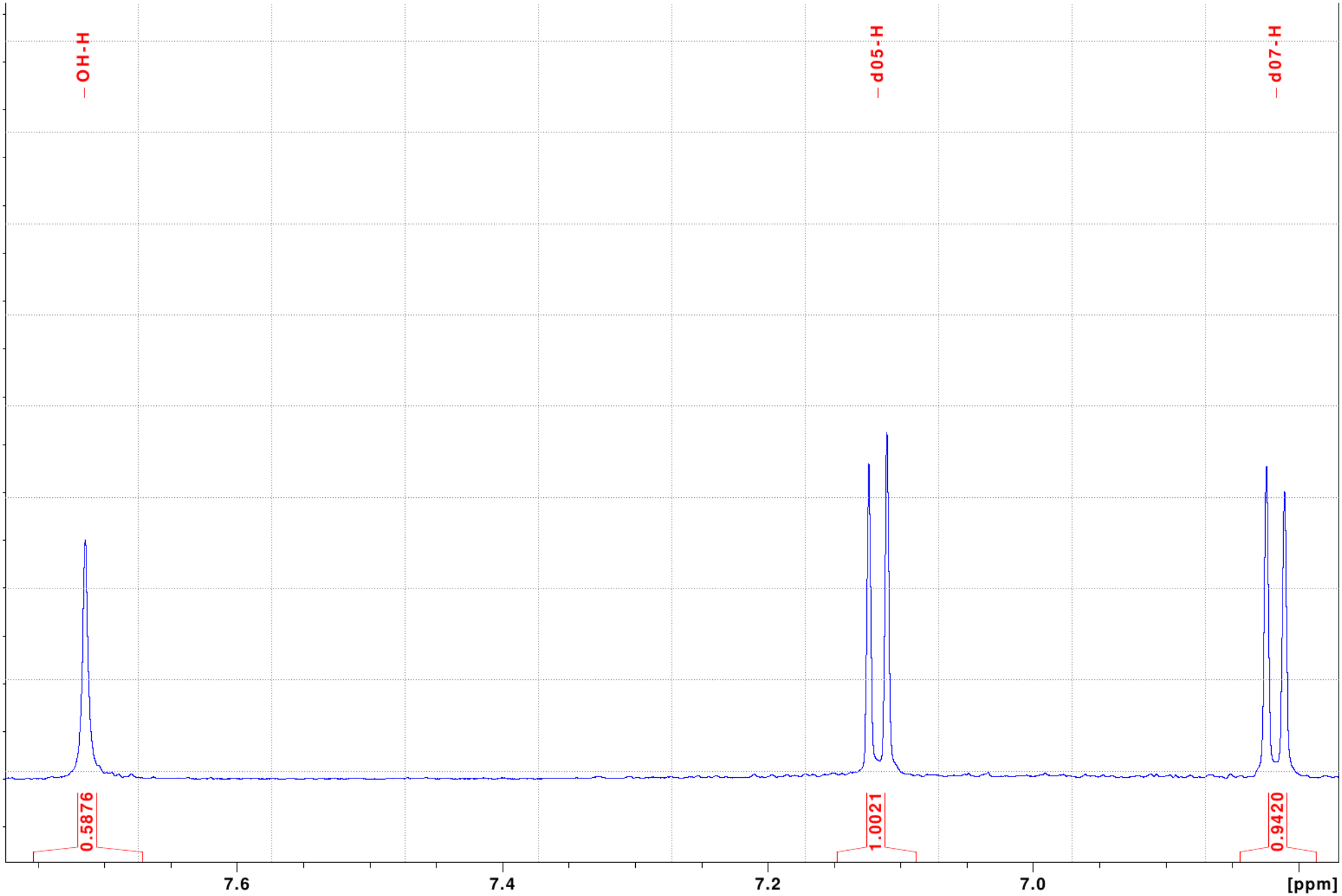
t10-a - d05-H

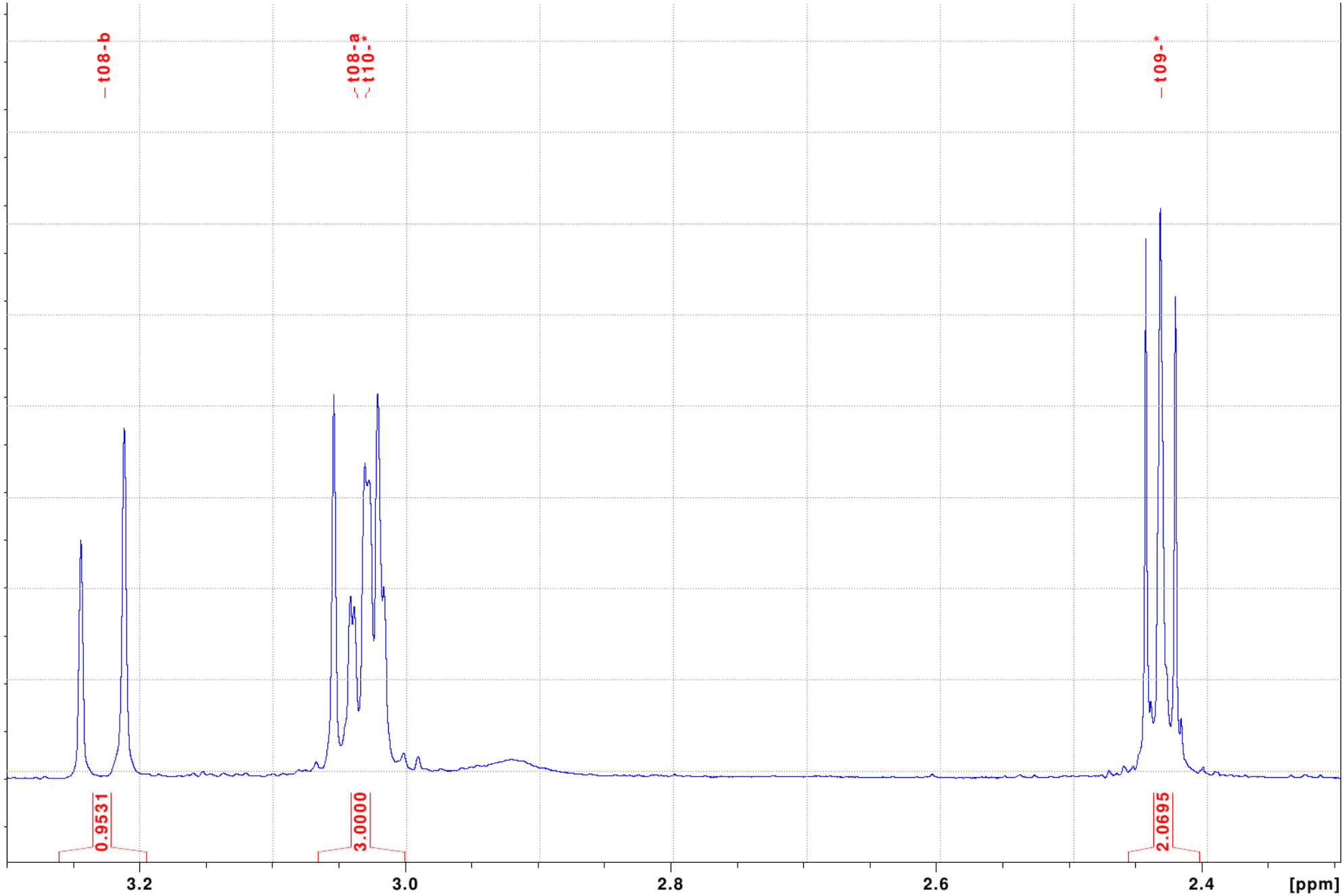
t10-b - d05-H

^{1}H NMR spectrum of compound 15 (obtained by method a) at 25 ^{o}C (600.3 MHz, acetone-d_6) **(pages S33-S36)**

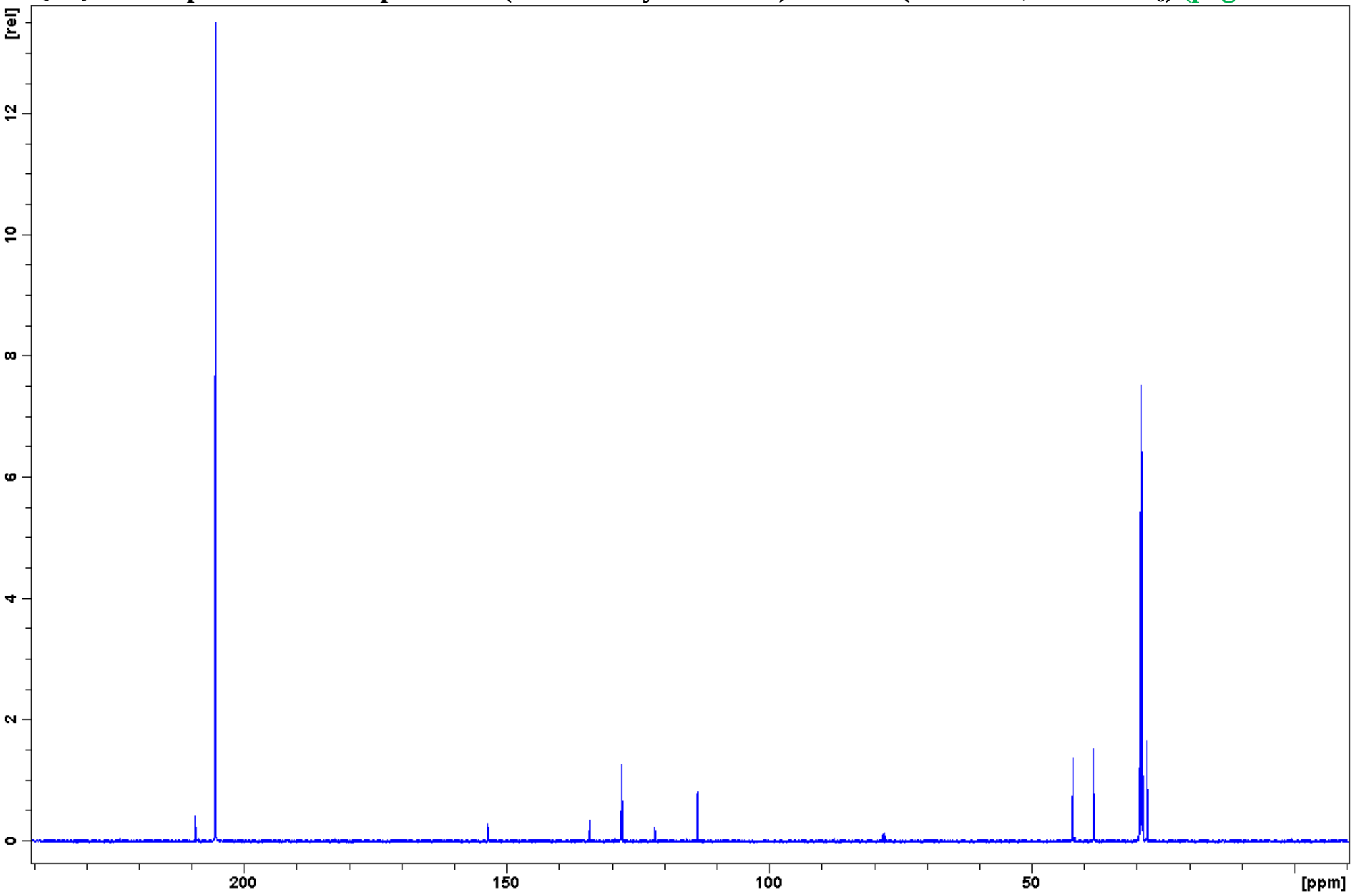


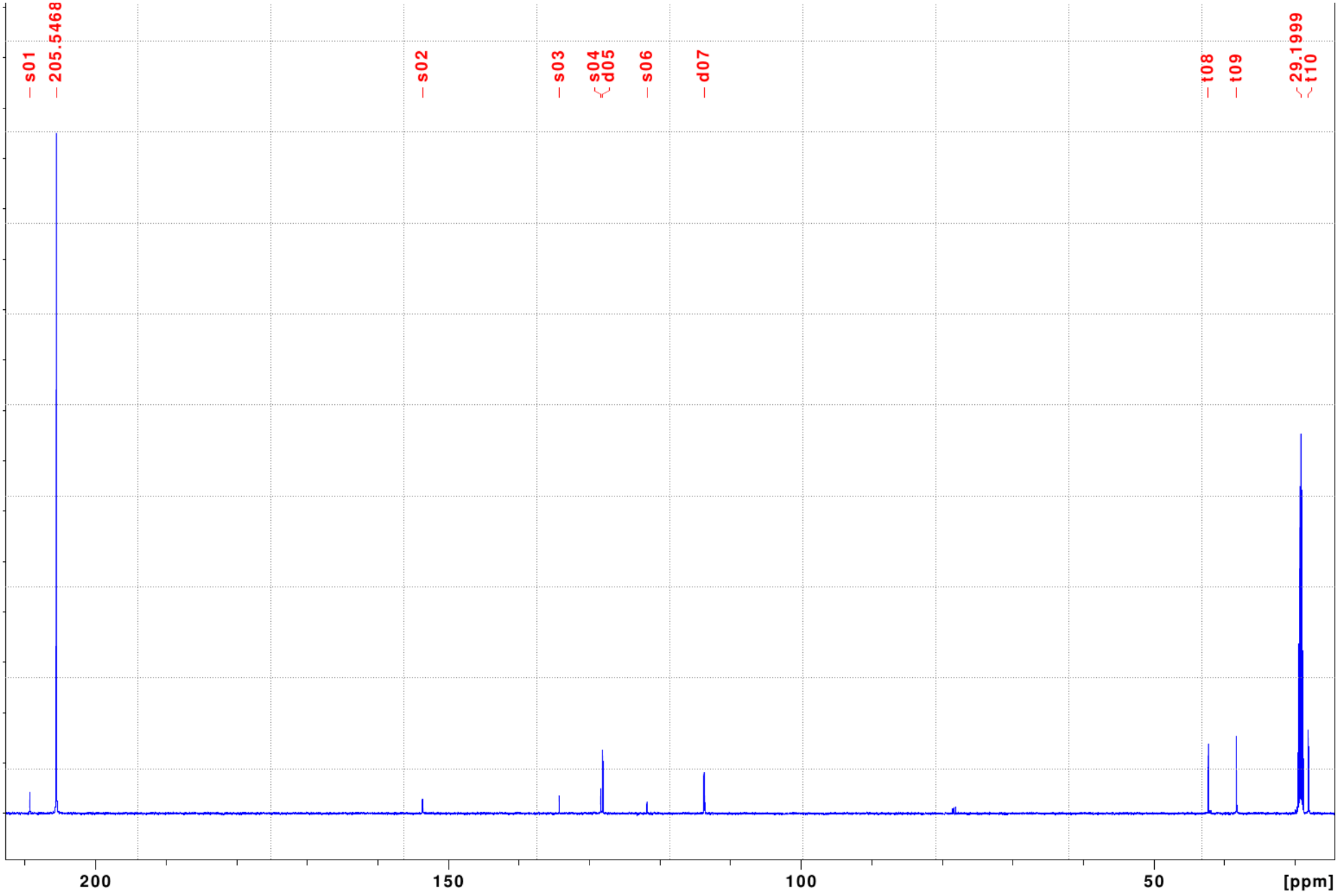

OH-H
d05-H
d07-H
t08-b
t08-a
t10-*
t09-*
2.0500
0.5876
1.0021
0.9420
0.9531
3.0000
2.0695
7
6
5
4
3
[ppm]

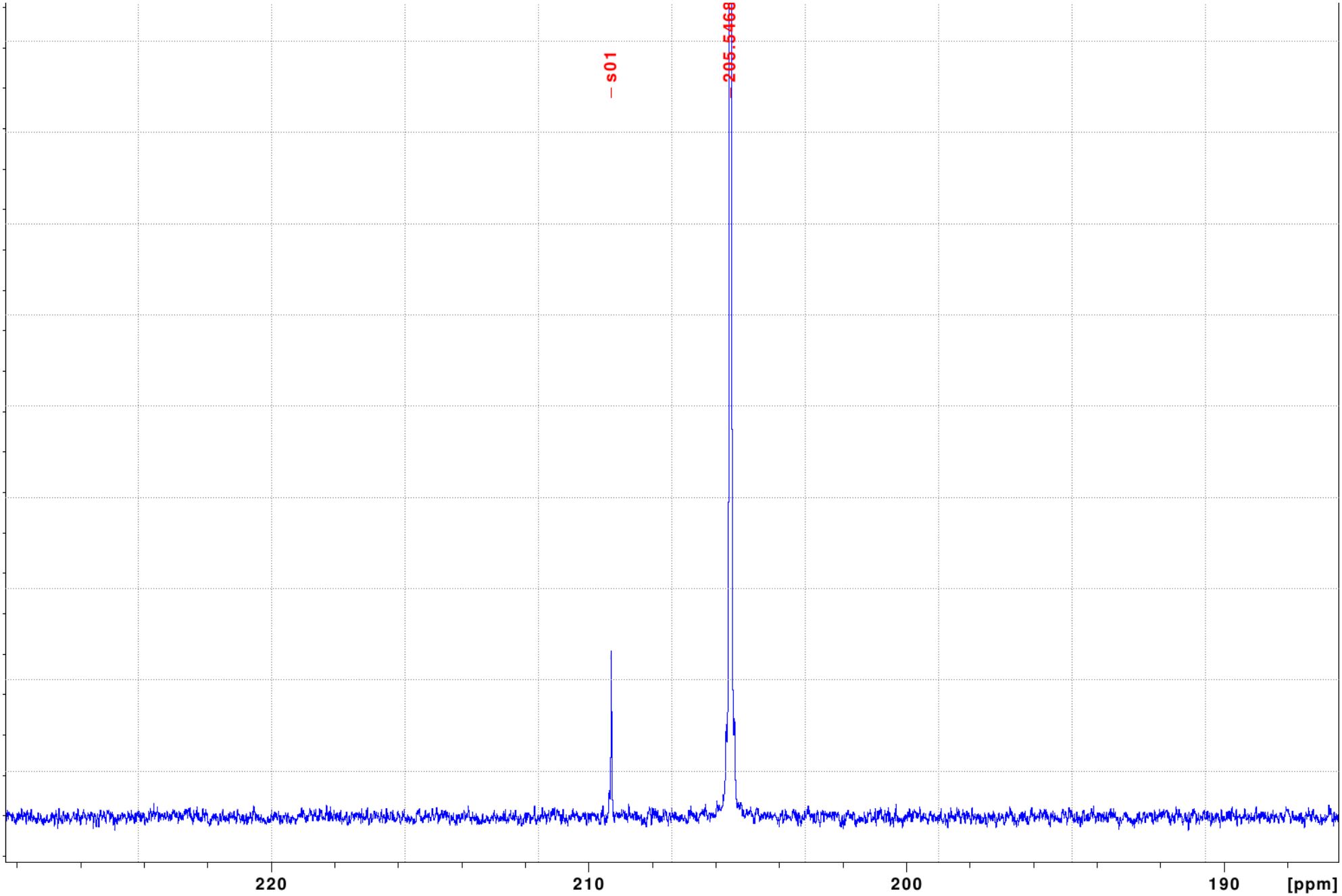

OH-H
d05-H
d07-H
0.5876
1.0021
0.9420
7.6
7.4
7.2
7.0
[ppm]

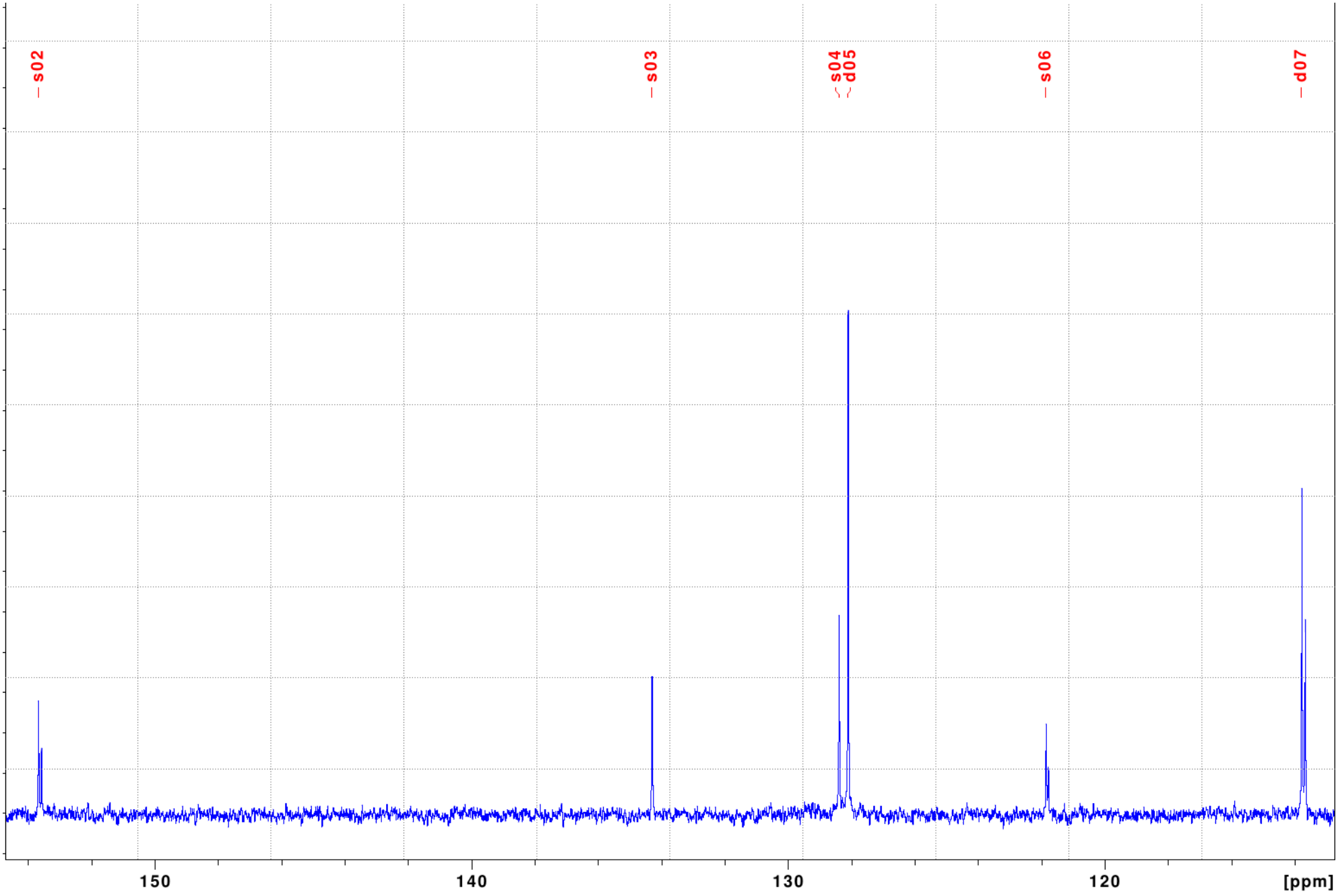

t08-b
t08-a
t10-*
t09-*
0.9531
3.0000
2.0695
3.2
3.0
2.8
2.6
2.4
[ppm]

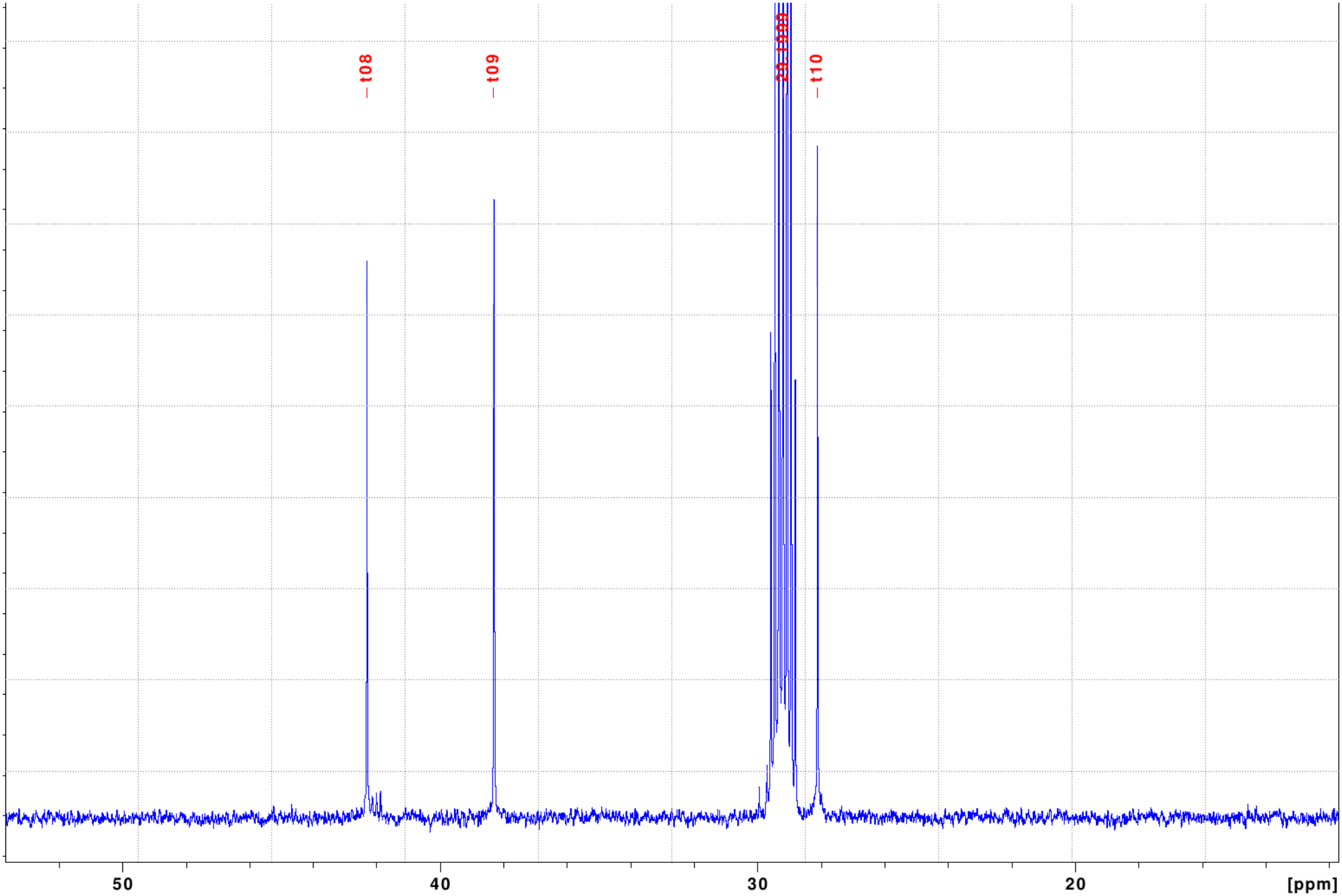
$^{13}C\{^{1}H\}$ NMR spectrum of compound 15 (obtained by method a) at 25 ^{o}C (151 MHz, acetone-d_6) **(pages S37-S41)**



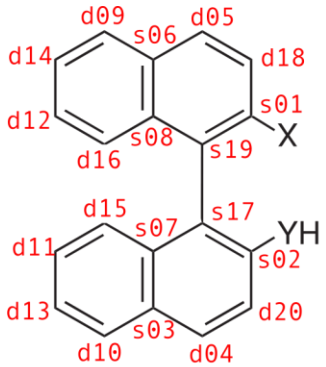

s01
205.5468
s02
s03
s04
d05
s06
d07
t08
t09
29.1999
t10
200
150
100
50
[ppm]


s01
205.5468
220
210
200
190
[ppm]


s02
s03
s04
d05
s06
d07
150
140
130
120
[ppm]


t08
t09
29.1999
t10
50
40
30
20
[ppm]

^{1}H NMR spectrum of complex 16 at –28 ^{o}C (600.3 MHz, CD_2Cl_2)

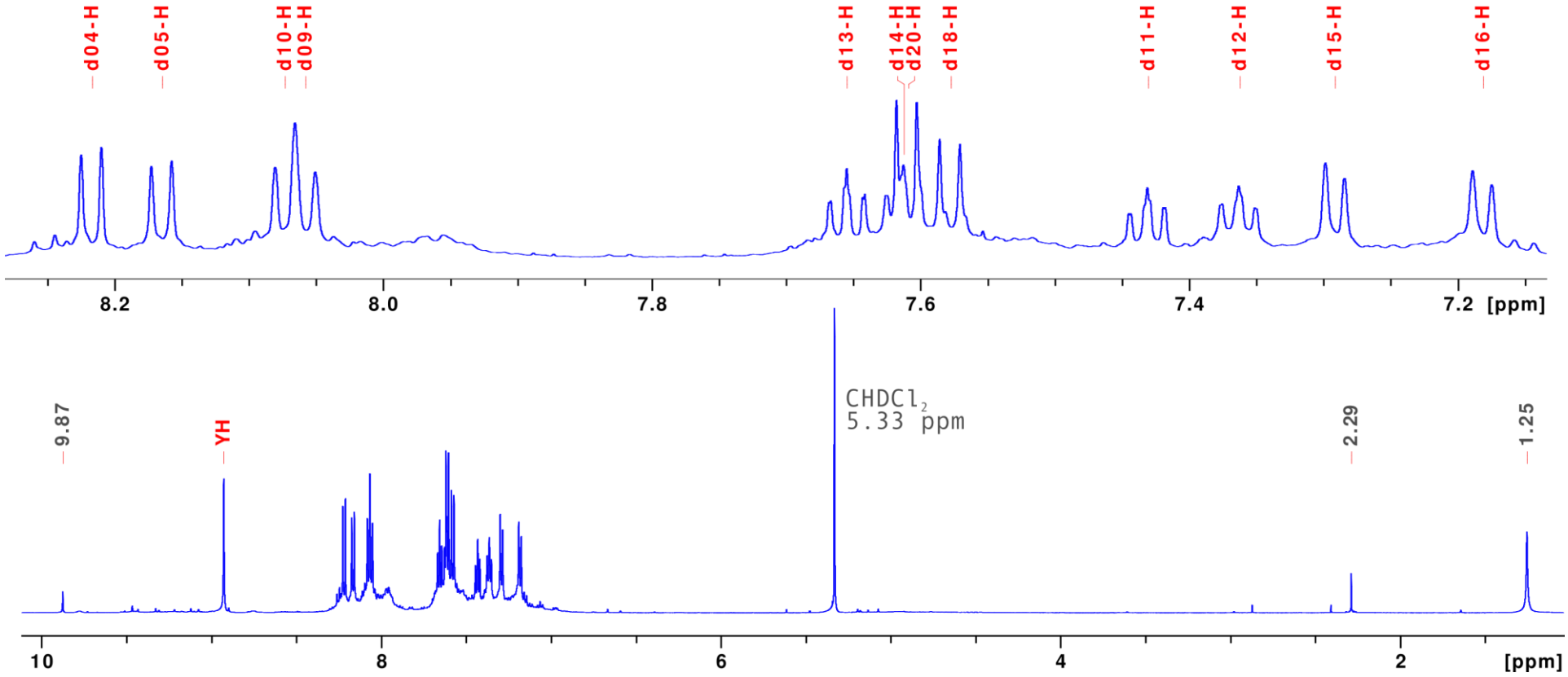


16

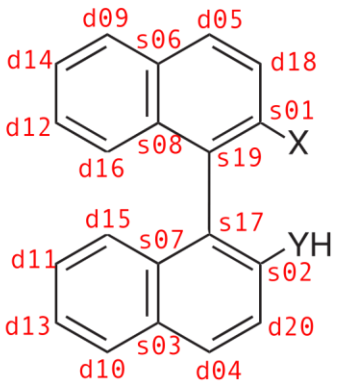
```
Experiment Bruker_32
1D 1H: 13 peaks
d04-H   H-C4'   8.22 d
d05-H   H-C4    8.16 d
d09-H   H-C5    8.06 d
d10-H   H-C5'   8.07 d
d11-H   H-C7'   7.43 t
d12-H   H-C7    7.36 t
d13-H   H-C6'   7.66 t
d14-H   H-C6    7.61 t
d15-H   H-C8'   7.29 d
d16-H   H-C8    7.18 d
d18-H   H-C3    7.58 d
d20-H   H-C3'   7.61 d
YH              8.93 s
```

```
Experiment Bruker_29
2D 1H-1H via Jcoupling
(COSY): 32 peaks
d04-H - d15-H d20-H
d05-H - d16-H d18-H
d09-H - d12-H d14-H
d10-H - d11-H d13-H d15-H
d11-H - d10-H d13-H d15-H
d12-H - d09-H d14-H d16-H
d13-H - d10-H d11-H d15-H
d14-H - d09-H d12-H d16-H
d15-H - d04-H d10-H d11-H d13-H
d16-H - d05-H d12-H d14-H
d18-H - d05-H
d20-H - d04-H YH
YH - d20-H
```

```
Experiment Bruker_31
2D 1H-1H via through-space
(NOESY): 6 peaks
d04-H - d10-H
d05-H - d09-H
d09-H - d05-H
d10-H - d04-H
d15-H - d16-H
d16-H - d15-H
```



$^{13}C\{^{1}H\}$ NMR spectrum of complex 16 at –28 ^{o}C (151 MHz, CD_2Cl_2)

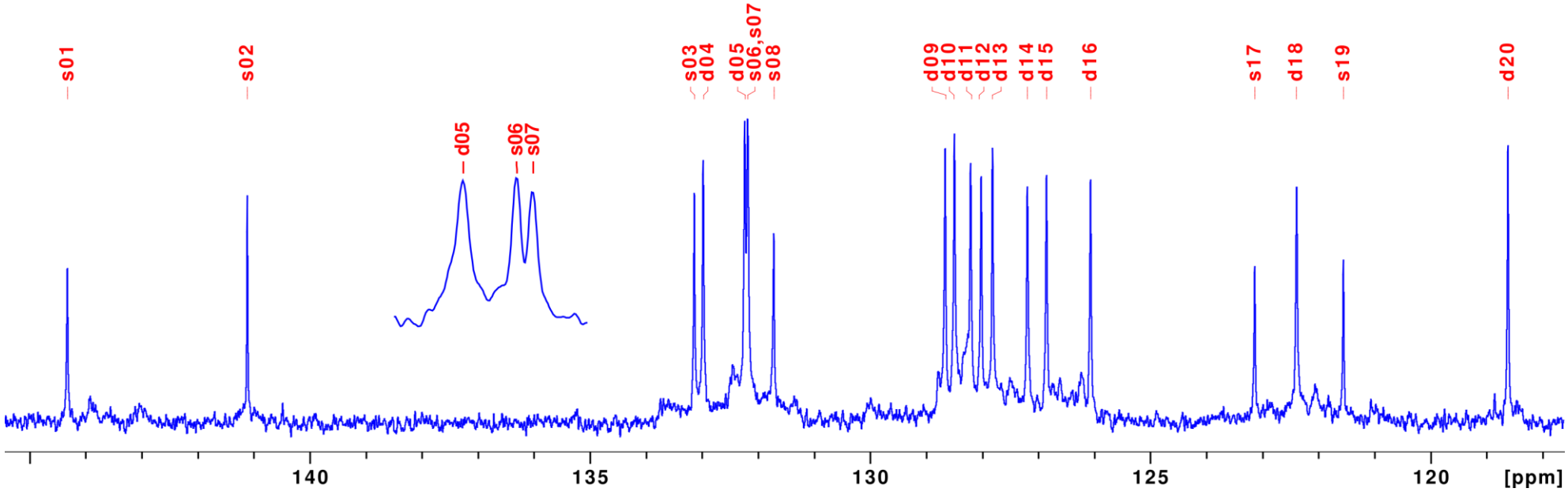


16

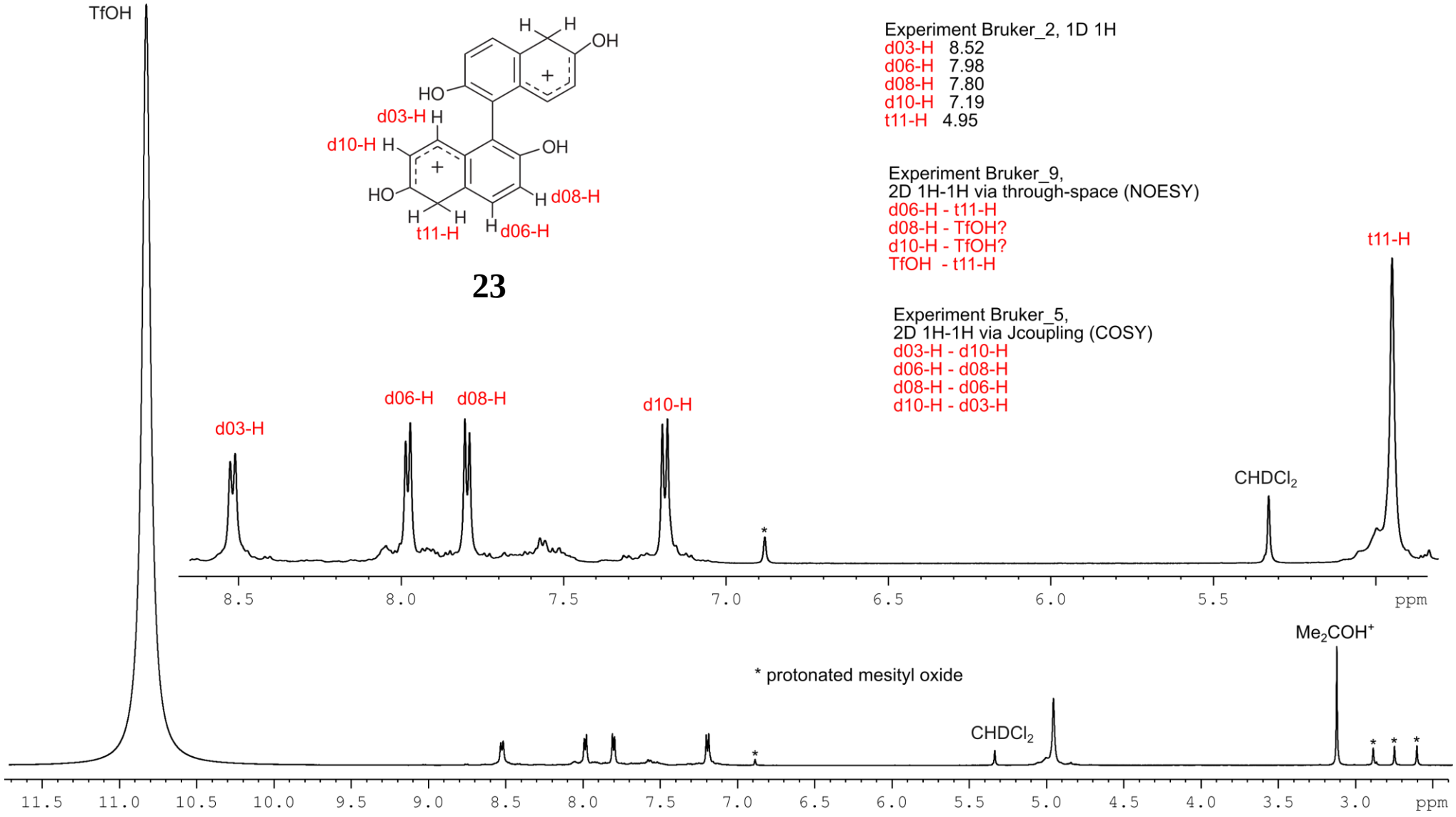
```
Experiment Bruker_22
  1D 13C: 19 peaks
  s01   C2     144.3
  s02   C2'    141.1
  s03   C4a'   133.1
  d04   C4'    133.0
  d05   C4     132.24
  s06   C4a    132.19
  s07   C8a'   132.19
  s08   C8a    131.7
  d09   C5     128.7
  d10   C5'    128.5
  d11   C7'    128.2
  d12   C7     128.1
  d13   C6'    127.8
  d14   C6     127.2
  d15   C8'    126.9
  d16   C8     126.1
  s17   C1'    123.1
  d18   C3     122.4
  s19   C1     121.6
  d20   C3'    118.6
```

```
Experiment Bruker_28
2D 13C-1H via one bond
   (HSQC): 12 peaks
      d04-H - d04
      d05-H - d05
      d09-H - d09
      d10-H - d10
      d11-H - d11
      d12-H - d12
      d13-H - d13
      d14-H - d14
      d15-H - d15
      d16-H - d16
      d18-H - d18
      d20-H - d20
```

```
Experiment Bruker_27
2D 13C-1H via Jcoupling
(HMBC): 38 peaks
d04-H - d10 s02 s06 s07 s17
d05-H - d09 s01 s08 s19
d09-H - d05 d12 s08
d10-H - d04 d11 s06 s07
d11-H - d10 s06 s07
d12-H - d09 s08
d13-H - d15 s03
d14-H - d16 s06 s07
d15-H - d13 s03 s17
d16-H - d14 s06 s07 s19
d18-H - s01 s06 s07 s17 s19
d20-H - s02 s03 s17 s19
   YH - s02 s17
```



^{1}H NMR spectrum of ion 23 at 0 ^{o}C [600.3 MHz, TfOH (825 mg)-CD_2Cl_2 (0.1 mL) + compound 9 (18 mg)]



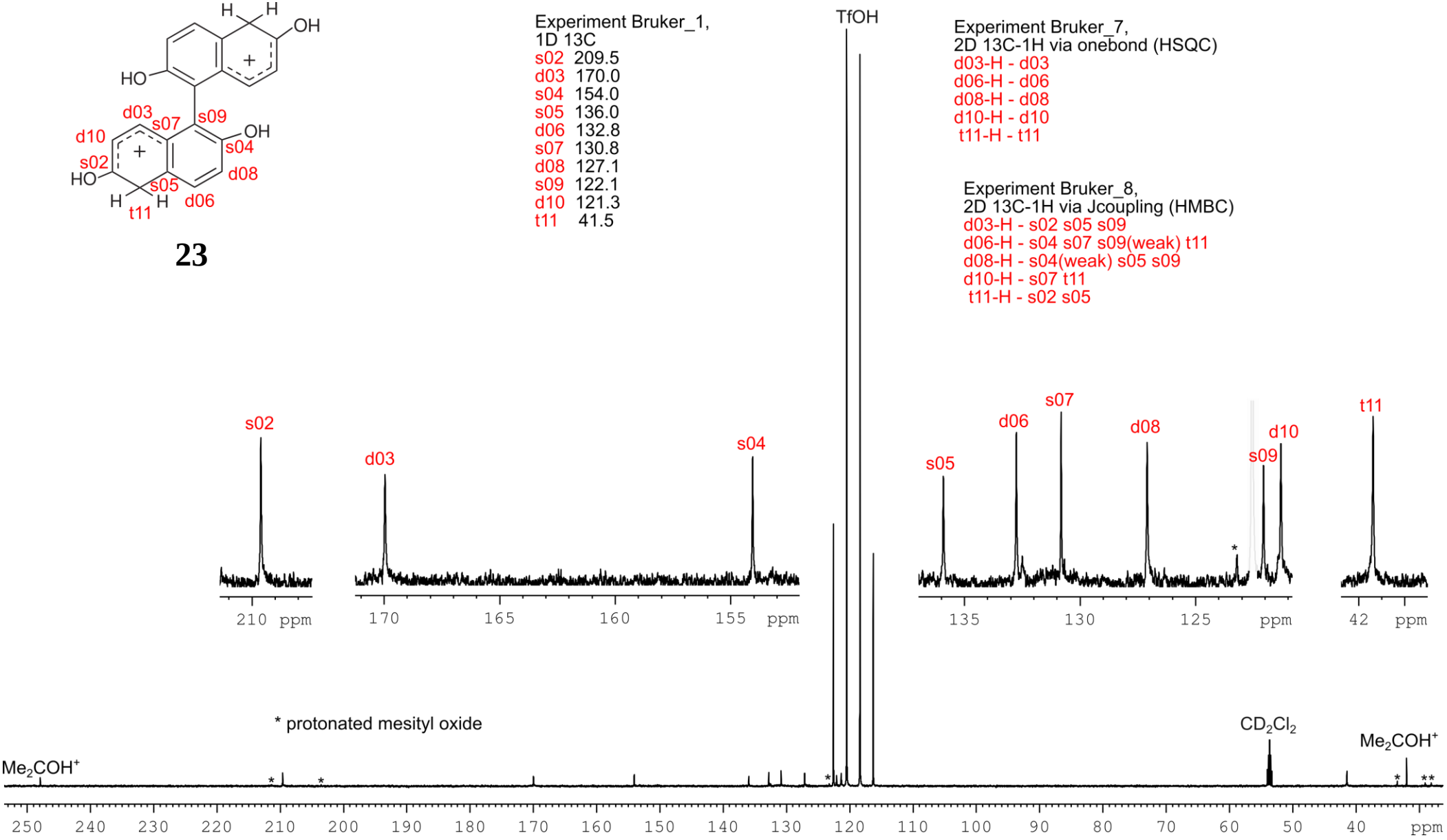
$^{13}C\{^{1}H\}$ NMR spectrum of ion 23 at 0 ^{o}C [600.3 MHz, TfOH (825 mg)-CD_2Cl_2 (0.1 mL) + compound 9 (18 mg)]

23

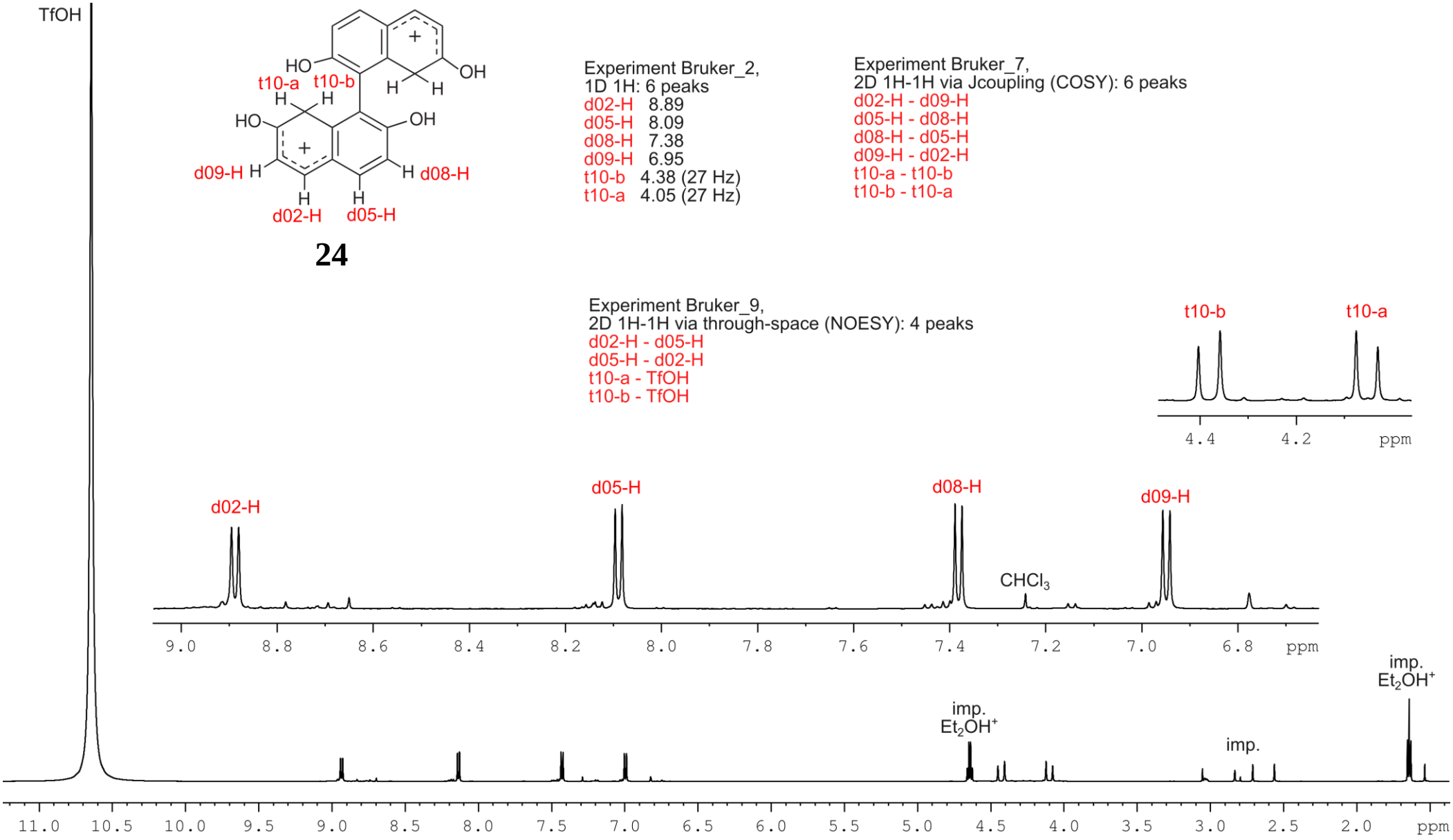
Experiment Bruker_1,
1D 13C
s02 209.5
d03 170.0
s04 154.0
s05 136.0
d06 132.8
s07 130.8
d08 127.1
s09 122.1
d10 121.3
t11 41.5

Experiment Bruker_7,
2D 13C-1H via onebond (HSQC)
d03-H - d03
d06-H - d06
d08-H - d08
d10-H - d10
t11-H - t11

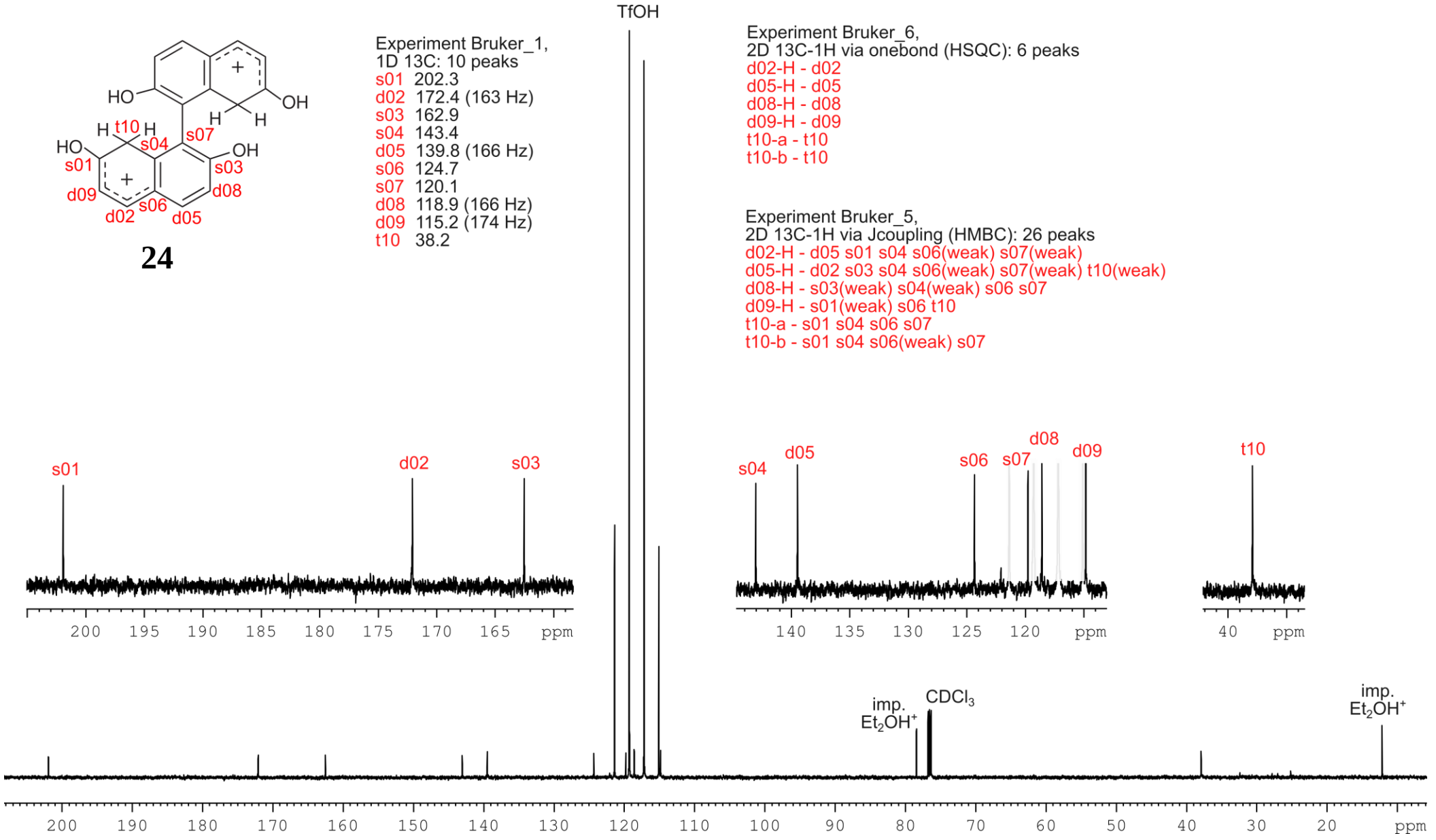
Experiment Bruker_8,
2D 13C-1H via Jcoupling (HMBC)
d03-H - s02 s05 s09
d06-H - s04 s07 s09(weak) t11
d08-H - s04(weak) s05 s09
d10-H - s07 t11
t11-H - s02 s05



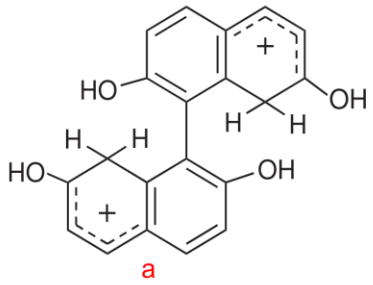
^{1}H NMR spectrum of ion 24 at 26 ^{o}C [600.3 MHz, TfOH (635 mg)-$CDCl_3$ (0.1 mL) + compound 10 (12 mg)]



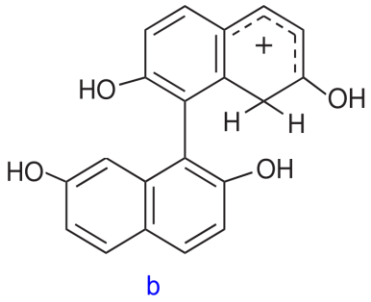
$^{13}C\{^{1}H\}$ NMR spectrum of ion 24 at 26 ^{o}C [151 MHz, TfOH (635 mg)-$CDCl_3$ (0.1 mL) + compound 10 (12 mg)]



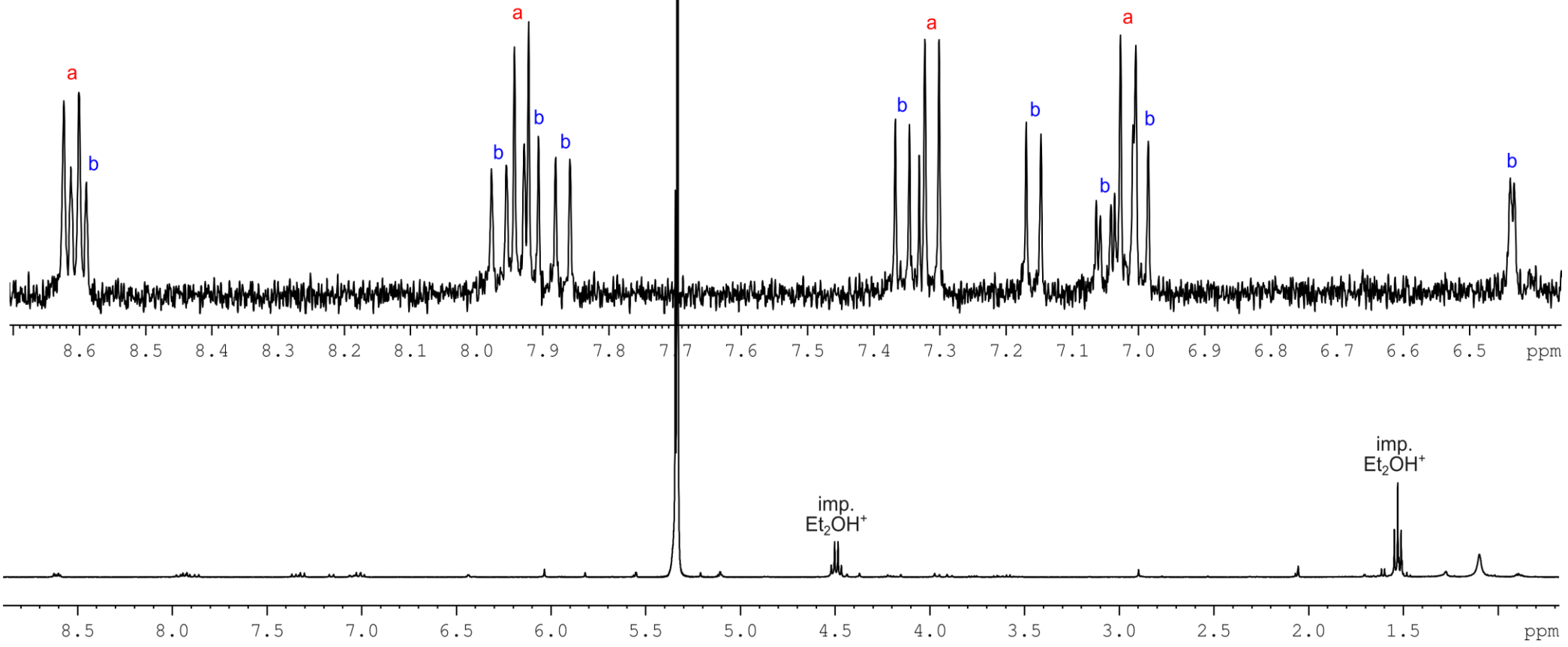
^{1}H NMR spectrum of complexes 24′ (a) and 24″ (b) at 20 ^{o}C [400 MHz, CD_2Cl_2 (0.5 mL) + compound 10 (7.5 mg) + $AlCl_3$ (16.5 mg)]



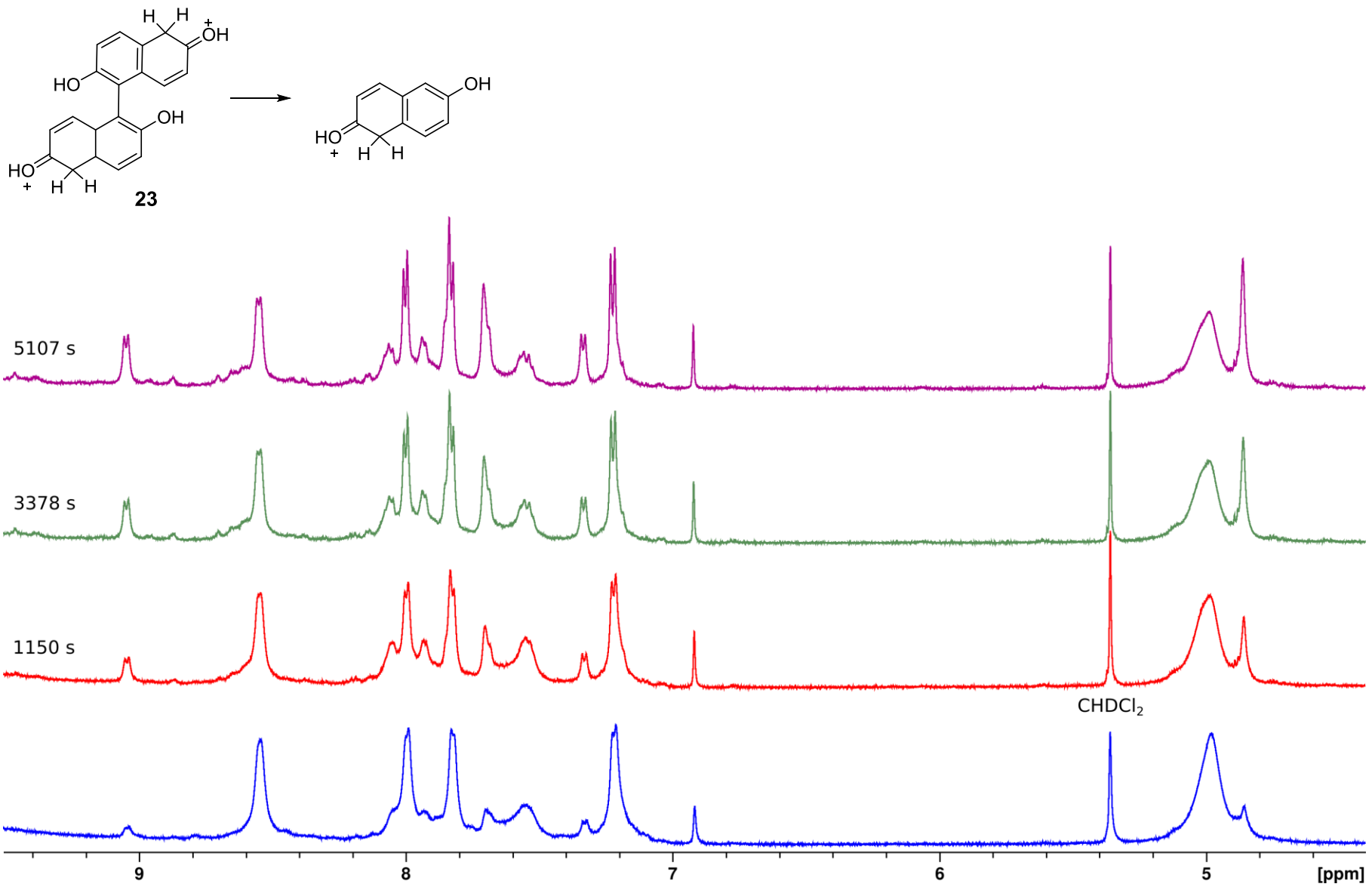
24′



24″

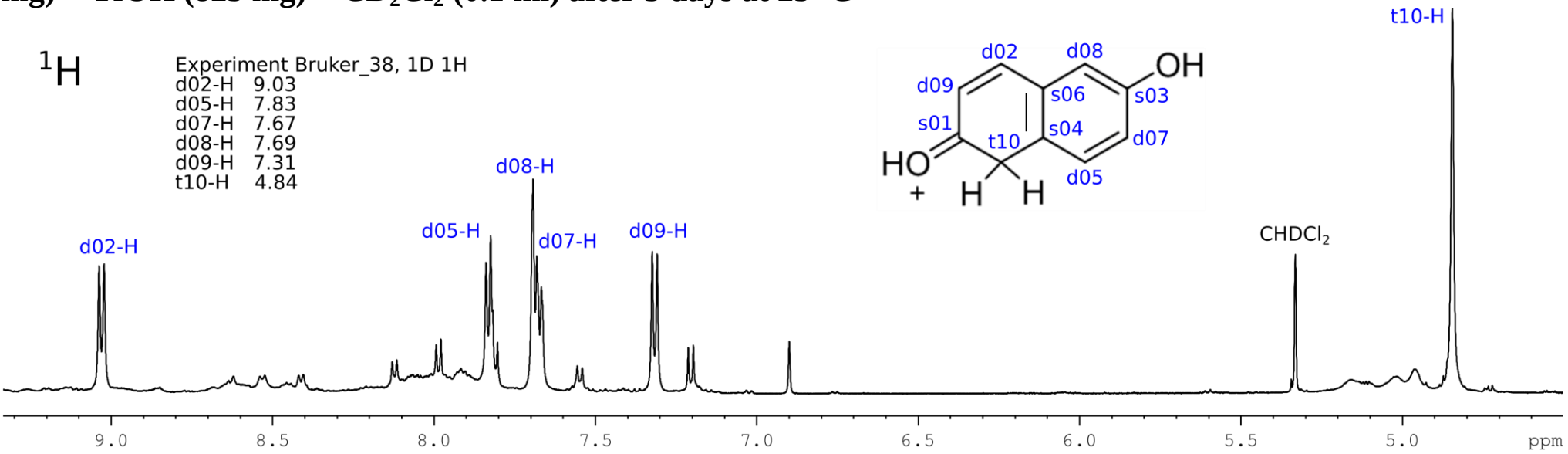


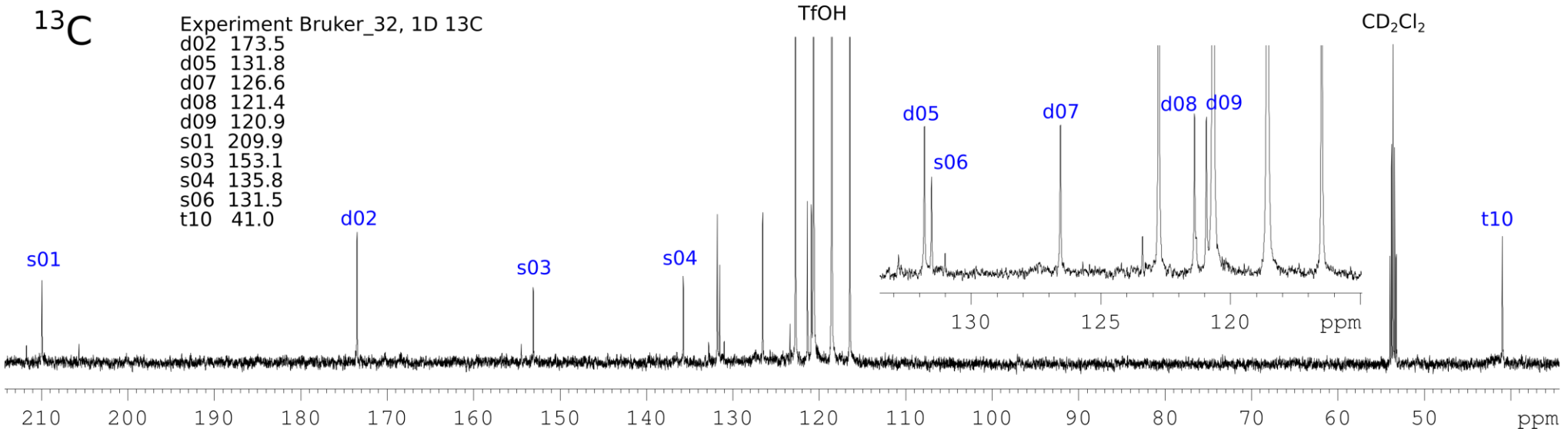
^{1}H NMR spectra of ion 23 [compound 9 (18 mg) + TfOH (825 mg) + CD_2Cl_2 (0.1 ml)]. Time course at 25 °C



$k = (2.40\pm0.14)\times10^{-5}$ s^{-1}, $t_{½}$ = 8 h, $\Delta G^{\#} = 24.8\pm0.1$ kcal/mol

^{1}H and ^{13}C{^{1}H} NMR spectra and the signal assignments for the product of the reaction of ion 23 (compound 9 (18 mg) + TfOH (825 mg) + CD_2Cl_2 (0.1 ml) after 3 days at 25 ^{o}C



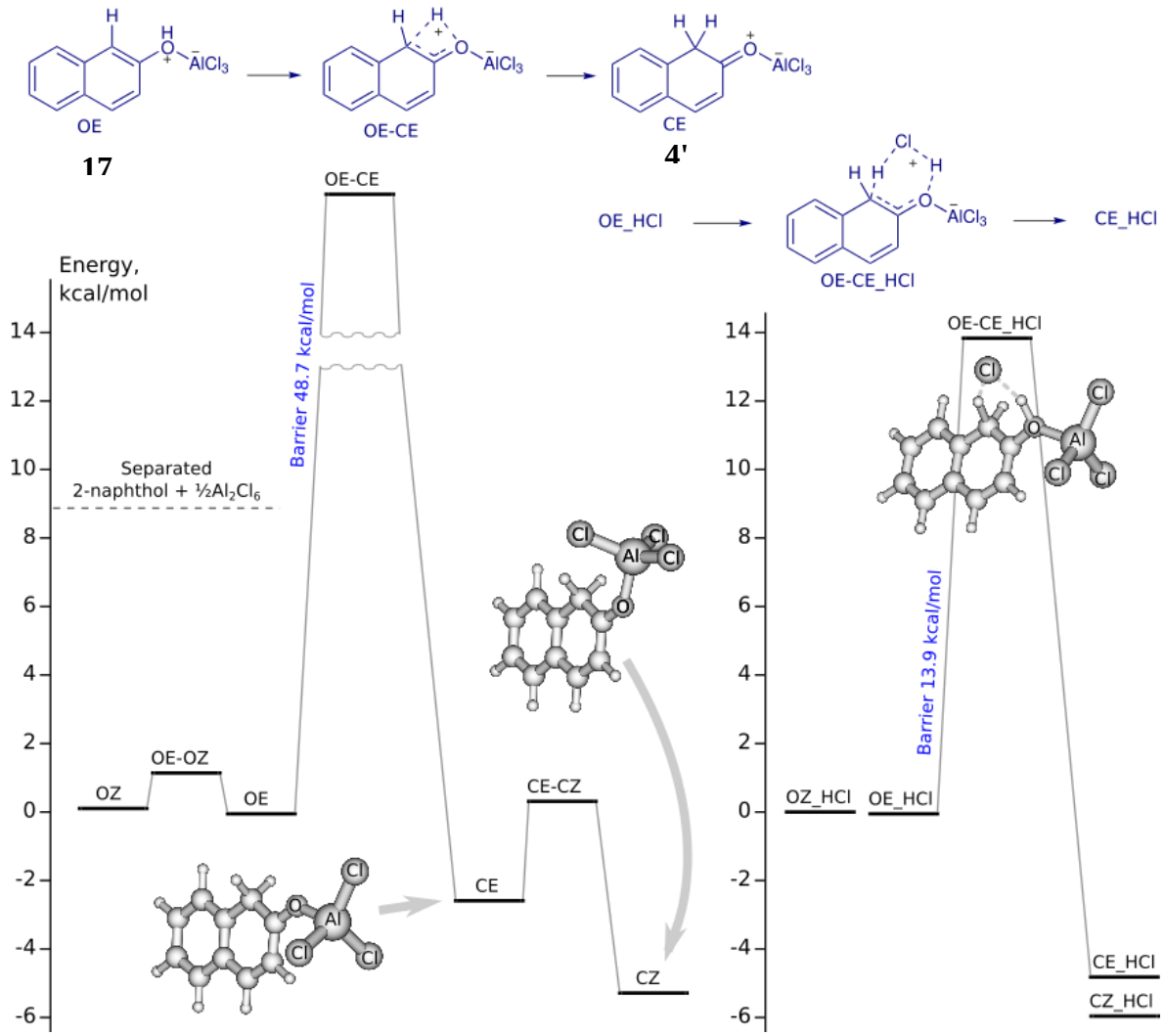


DFT calculations

The total number of all the molecular geometries is too big (130). Therefore all the files with cartesian coordinates (xyz-files) are packed into a single ZIP archive. The archive with cartesian coordinates is named “Binols_modification.zip”.

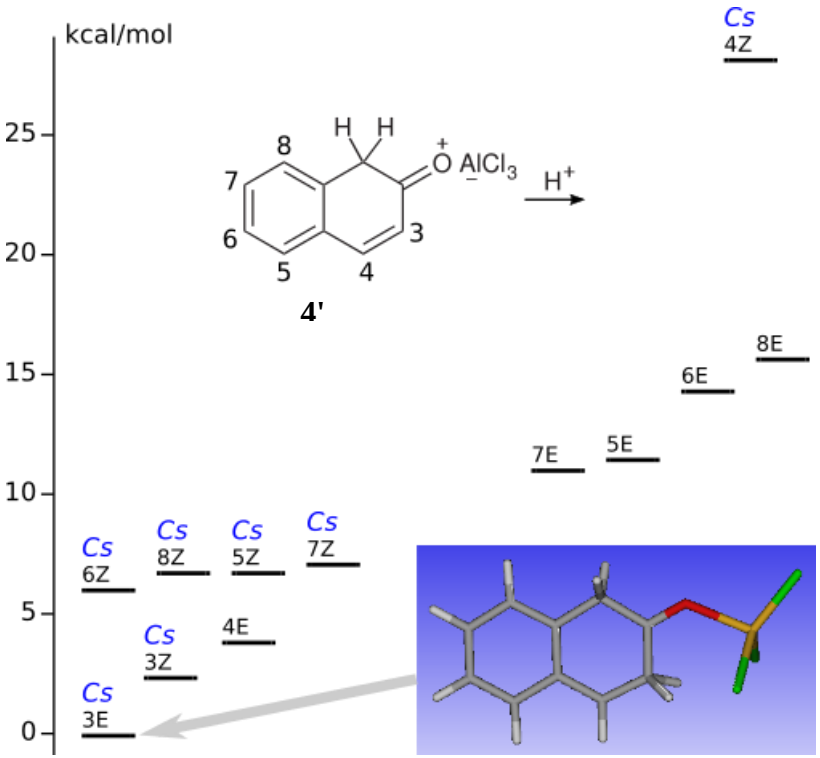
Relative energies and activation barriers of tautomerization of complexes 17 and 4' (DFT/PBE/Λ1).

For Cartesian coordinates see, please, zip-archive, folder tautomerization_17-4.



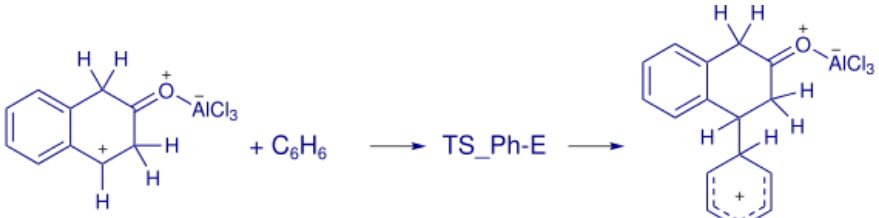
Protonation of 4' on atoms C3-C8 leading to dicationic species 5 (X = $AlCl_3^-$) and less stable isomers (DFT/PBE/Λ1).

For Cartesian coordinates see, please, zip-archive, folder protonation_4.

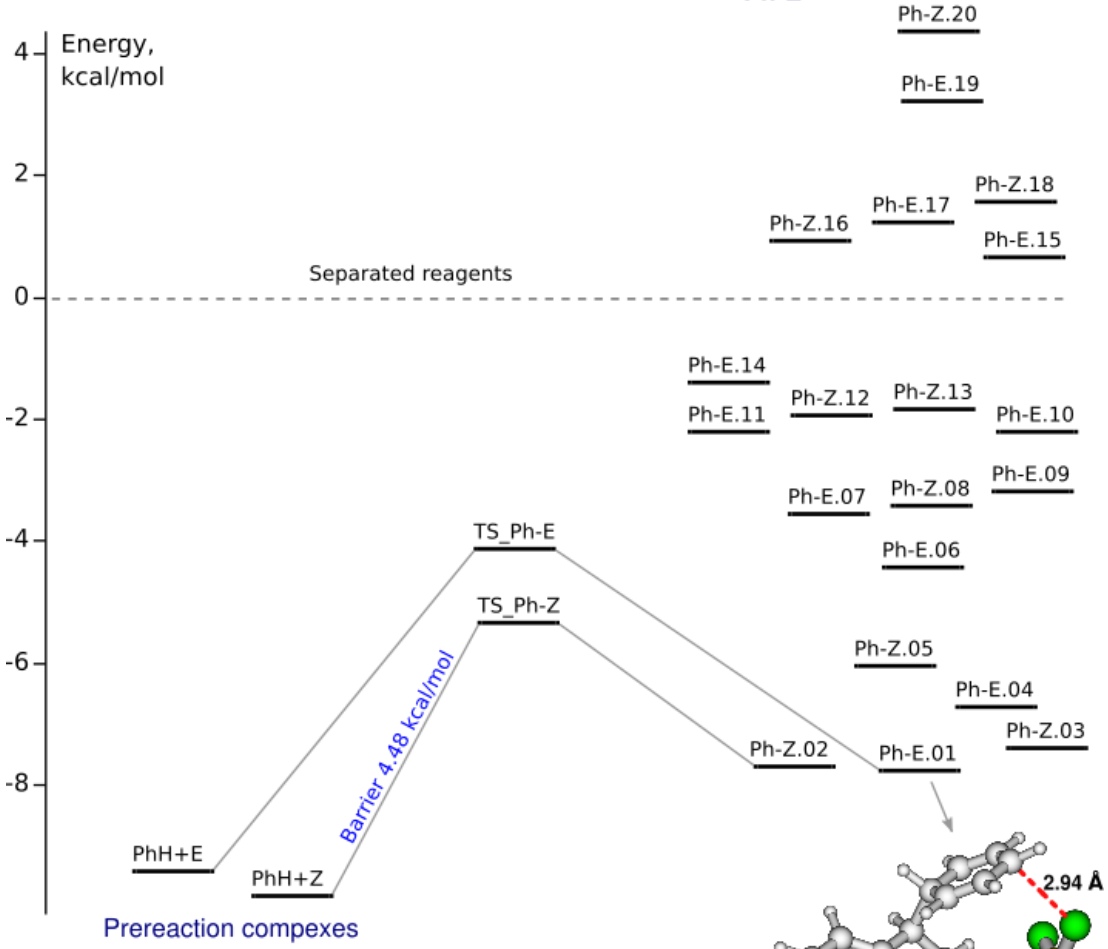


5 (X = $AlCl_3^-$) = *E*-isomer of C3-protonated complex **4'**

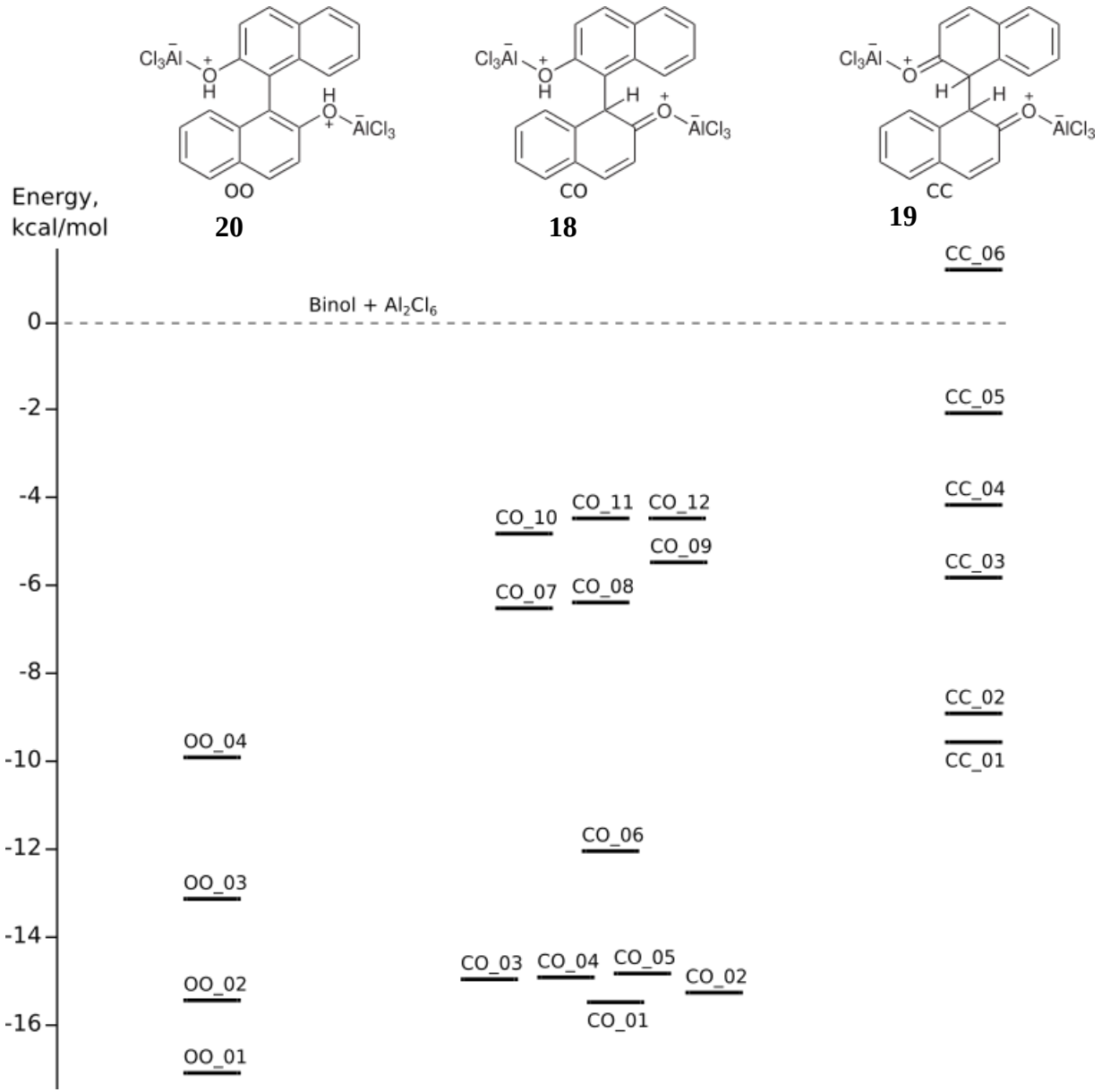
Reaction of 5 (X = $AlCl_3^-$) with benzene (DFT/PBE/Λ1). For Cartesian coordinates see, please, zip-archive, folder 5+benzene.



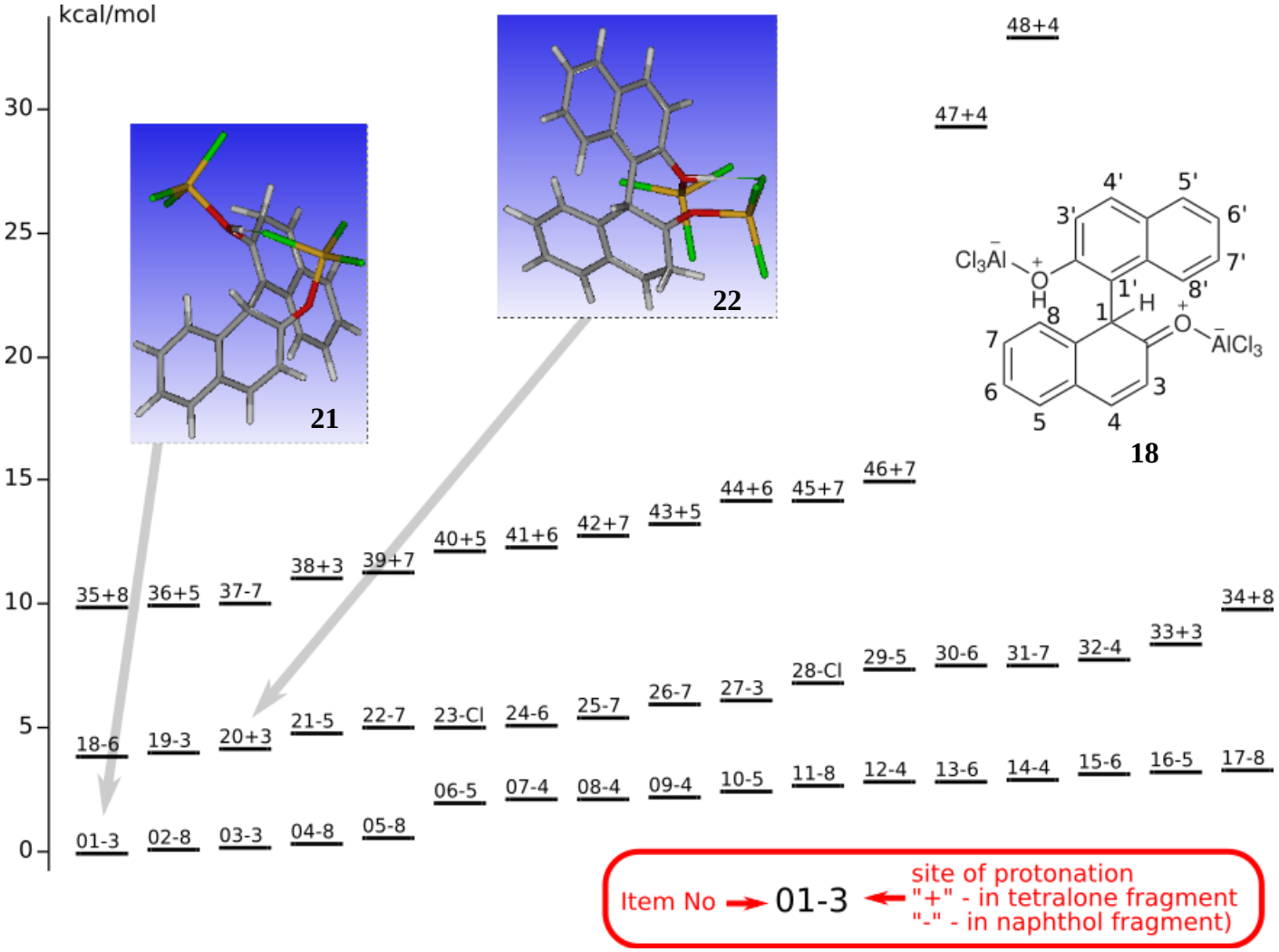
E5 (X = $AlCl_3^-$) **Ph-E**



Relative energies of tautomers 18-20 for a variety of conformers (DFT/PBE/Λ1). For Cartesian coordinates see, please, zip-archive, folder tautomers_18.

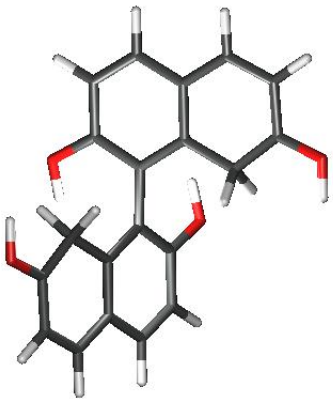


Protonation of 18 (DFT/PBE/Λ1). For Cartesian coordinates see, please, zip-archive, folder protonation_18.



DFT calculations of 24, 28', 25-28

24



```
40
Energy -1071.106858277  Charge 2  Dipole 3.452655  ZPE 0.307353  G(298.15)
C  -2.87113212   0.94375599   0.50197650
C  -3.63747395   1.17902953   1.67582468
C  -3.09420223   1.33304252   2.94259024
C  -1.71396607   1.26724336   3.09941042
C  -0.79453562   1.05532990   1.93806487
C  -1.45192298   0.86015963   0.58874950
C  -0.69254314   0.60336074  -0.56461460
C  -1.37248559   0.46675505  -1.81131026
C  -2.77707676   0.53996151  -1.89387382
C  -3.51076578   0.77451369  -0.75346940
C   1.46322869  -0.74445423  -0.70646028
C   0.79861753   0.48180439  -0.54083292
C   1.58046149   1.66075060  -0.35635478
C   2.98696695   1.60712032  -0.29380076
C   3.62527327   0.39674413  -0.44007807
C   2.88563073  -0.79550878  -0.65309018
C   3.55309954  -2.04228764  -0.79656160
C   2.90639511  -3.25463353  -0.98512848
C   1.51748685  -3.27743941  -1.05141312
C   0.69937376  -2.02908482  -0.94539033
O  -0.71246139   0.24894386  -2.96005479
O   1.01753179   2.87202530  -0.21989223
O  -1.22881887   1.41740360   4.31477514
O   0.93298714  -4.44406881  -1.23128179
H  -4.72635290   1.23585013   1.57001500
H  -3.72366273   1.50650892   3.81827779
H  -0.12688767   0.20077594   2.16435190
H  -3.25081521   0.42816405  -2.87204821
H  -4.60058966   0.84342552  -0.81121974
H   3.54076237   2.53793726  -0.15012741
H   4.71712347   0.34855861  -0.40345418
H   4.64754529  -2.04223946  -0.74890489
H   3.46139582  -4.19015963  -1.08464941
H   0.12284525  -1.94181260  -1.89070787
H   0.25349385   0.37394593  -2.82989329
H   0.05990876   2.83181440  -0.43663541
H  -0.24828969   1.37217294   4.35990367
H  -0.04711590  -4.39435880  -1.28075106
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H  -0.06477168  -2.17091932  -0.15592569
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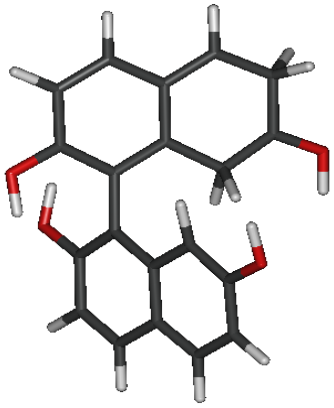
28'



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 40
Energy -1071.052285652  Charge 2  Dipole 8.137326  ZPE 0.304186  G(298.15)
C  -1.85973259   2.13065969   0.51257543
C  -3.20563587   2.02115530   0.25813367
C  -3.87430595   0.73175520  -0.02837228
C  -3.00553058  -0.46929902   0.01052200
C  -1.56236256  -0.38455157   0.12827557
C  -1.01359000   0.95879848   0.51274023
C   0.33901569   1.05515097   0.80835614
C   0.87584462   2.36684378   1.07512615
C   0.05063071   3.52928622   1.11429885
C  -1.27855386   3.41355727   0.83509317
C   1.39994342  -0.87681944  -0.44172309
C   1.23775711  -0.12442307   0.77006786
C   1.88701930  -0.56499659   1.95168888
C   2.71613567  -1.70646406   1.93299989
C   2.84411436  -2.44614232   0.77740838
C   2.18016617  -2.07439573  -0.41710667
C   2.28372415  -2.85751951  -1.60168352
C   1.66638215  -2.49268596  -2.77630738
C   0.94577258  -1.27853079  -2.83311476
C   0.78325400  -0.48890564  -1.67120958
O   2.16279973   2.55963646   1.26089092
O   1.75712175   0.04337739   3.15234541
O  -3.64509815  -1.59670426  -0.11278743
O   0.45629105  -0.93485048  -4.03289833
H  -3.84437071   2.91067670   0.27969546
H  -4.38068588   0.77972906  -1.02082845
H  -1.05058931  -0.67116083  -0.88277147
H   0.51836810   4.49008293   1.34392394
H  -1.92378233   4.29661565   0.84695920
H   3.20626752  -2.00304768   2.86319535
H   3.46079525  -3.34946343   0.78185311
H   2.88503890  -3.77093428  -1.57222596
H   1.76436932  -3.08718378  -3.68727213
H   0.38920029   0.52812665  -1.78169365
H   2.66769864   1.71309470   1.16506799
H   1.01653938   0.68120433   3.16181018
H  -3.06797060  -2.39704384  -0.08134237
H   0.08479611  -0.02967087  -4.03221143
H  -1.13163723  -1.18425344   0.77060067
H  -4.73520037   0.57929581   0.65992004
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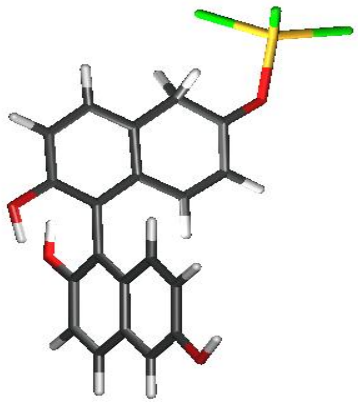
25 (n=1, Hal=Cl)



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 42
 Energy -2693.14280575  Dipole 11.154757  ZPE 0.289681  G(298.15) 144.43
 C   1.13769653  -3.55814088   1.06475910
 C   0.33038567  -3.85225484  -0.06472715
 C   0.67077487  -5.00561012  -0.85290691
 C   1.77746454  -5.80550037  -0.48826335
 C   2.54335656  -5.49199276   0.62224927
 C   2.21321759  -4.35499691   1.39983435
 C  -0.12682773  -5.30608361  -1.99376094
 C  -1.19794767  -4.52296968  -2.34560352
 C  -1.53927793  -3.38355384  -1.57057457
 C  -0.79263134  -3.04223762  -0.44155441
 C  -1.19470982  -1.84819539   0.35989921
 C  -0.71421859  -0.53787645   0.08011207
 C  -1.13606659   0.56882140   0.85498419
 C  -2.03333211   0.35545476   1.90752486
 C  -2.50468806  -0.91797794   2.19750061
 C  -2.08802159  -2.02385455   1.43246956
 C   0.22647857  -0.31438013  -0.99021845
 C   0.73323958   0.91467859  -1.31260597
 C   0.34287633   2.07693504  -0.57960474
 C  -0.62247142   1.94192678   0.54946703
 O   0.82465285   3.21054183  -0.89685704
Al   0.54896226   4.93950100  -0.16154181
Cl  -1.58505962   5.21124031  -0.36722728
 O  -2.57578203  -3.24149036   1.76803193
 O  -2.61496056  -2.66418429  -1.99299870
 O   3.60160011  -6.29945397   0.92831447
Cl   1.14577155   4.68139301   1.89989513
Cl   1.76853763   6.23528127  -1.32623663
 H  -1.45345110   2.65321679   0.34095825
 H  -0.13448500   2.40192626   1.43827554
 H   1.44706183   1.04582458  -2.12885258
 H   0.54480420  -1.19137601  -1.56316387
 H  -3.20243802  -1.08817675   3.02102527
 H  -2.36675143   1.20361642   2.51260545
 H  -1.81036053  -4.75044417  -3.22141197
 H   0.12835325  -6.18211360  -2.59700738
 H   2.03919363  -6.68227767  -1.08659600
 H   2.82125071  -4.10511701   2.27649119
 H   0.90179567  -2.68377502   1.67640666
 H  -2.17328638  -3.89482629   1.15353609
 H   4.04000387  -5.95100707   1.72633204
 H  -2.73349957  -1.91209768  -1.37574706
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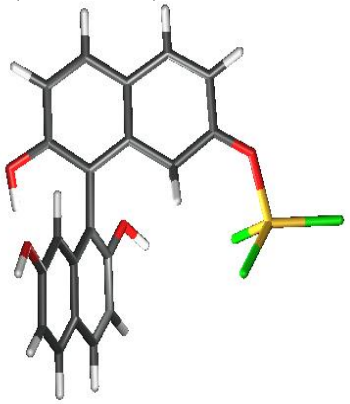
26 (n=1, Hal=Cl)



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 42
 Energy -2693.148685397  Dipole 9.633441  ZPE 0.289652  G(298.15) 145.69
 C  -0.50489428  -3.42424852  -0.93654609
 C  -0.98721457  -2.62395014   0.12843662
 C  -2.38898571  -2.68720913   0.45337552
 C  -3.22405936  -3.57062644  -0.27565111
 C  -2.72554541  -4.35425346  -1.29161499
 C  -1.35209617  -4.27218080  -1.63227501
 C  -2.90457498  -1.84287373   1.46675100
 C  -2.08906884  -0.97156057   2.14773339
 C  -0.70392094  -0.91851845   1.85625251
 C  -0.13515721  -1.72700519   0.86769150
 C   1.31759255  -1.62575690   0.54198725
 C   1.88679110  -0.46743021  -0.00260895
 C   3.26178553  -0.43254538  -0.35839400
 C   4.06541697  -1.57512659  -0.13693551
 C   3.52958354  -2.70872313   0.43643137
 C   2.16321471  -2.73832196   0.78196749
 C   1.06631435   0.76998104  -0.16968488
 C   1.71911462   1.97195351  -0.75651874
 C   3.07981921   1.90961762  -1.15141509
 C   3.79968964   0.75522358  -0.94151495
 O   1.06239724   3.06577977  -0.86625132
Al  -0.66882623   3.54133741  -0.30884223
Cl  -0.87307095   5.60202489  -0.80436424
 O   1.70157001  -3.86736461   1.35555033
 O   0.11677612  -0.07040301   2.54359923
 O  -0.81887390  -5.01053463  -2.64810063
Cl  -0.67039081   3.16608511   1.84611246
Cl  -1.98876544   2.18314796  -1.34021476
 H   4.85724968   0.73671051  -1.22863427
 H   3.53505423   2.80204404  -1.58554887
 H   0.11770265   0.57783939  -0.71322413
 H   0.71450337   1.07706982   0.84116506
 H   4.13516145  -3.59517294   0.63653501
 H   5.12275205  -1.54782891  -0.41562552
 H  -2.49529979  -0.31548852   2.92308300
 H  -3.97306040  -1.88522401   1.69701613
 H  -4.28722373  -3.61496500  -0.02244452
 H  -3.38613299  -5.02891214  -1.84665546
 H   0.54094213  -3.37095600  -1.24509066
 H   0.74084122  -3.74647127   1.52615351
 H  -0.41599586   0.66774835   2.90704160
 H  -1.53103786  -5.53442918  -3.05965575
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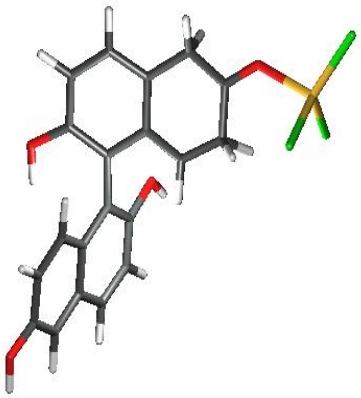
27 (n=1, Hal=Cl)



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 43
 Energy -2693.455033817  Charge 1  Dipole 14.599917  ZPE 0.298987  G(298.15) 150.54
 C    2.38785265  -0.36835351   0.38090707
 C    2.33455417  -1.86639191   0.28170025
 C    0.96753723  -2.47809136   0.20772832
 C   -0.21086421  -1.61876932  -0.09904143
 C    0.02913074  -0.17639045  -0.19930986
 C    1.26328751   0.43021877  -0.03919158
 C    1.35411529   1.87431635  -0.10533031
 C    2.50966582   2.48513002   0.41665992
 C    3.57001290   1.68237054   0.87971242
 C    3.51236290   0.28340451   0.85345614
 C   -0.41138307   3.69007425  -0.02863341
 C    0.30280555   2.67419741  -0.74982181
 C    0.07480327   2.52939457  -2.13847833
 C   -0.82469655   3.39379617  -2.80842120
 C   -1.48594227   4.38686267  -2.12679958
 C   -1.30814509   4.56863111  -0.72633445
 C   -2.01650755   5.56374146  -0.02013855
 C   -1.85967808   5.70671602   1.35626472
 C   -1.00040766   4.82270023   2.05534904
 C   -0.30903752   3.83898816   1.38397936
 O    2.71119583   3.81470635   0.44606937
 O   -2.49566132   6.63649566   2.10037449
 O    0.84903098  -3.70538931   0.36286460
Al   -0.76741794  -4.84130533   0.17241851
Cl   -1.31813546  -4.24282104  -1.83259787
Cl   -2.01752459  -3.91608548   1.65987559
Cl   -0.06787364  -6.80034989   0.47545460
 O    0.78978782   1.60308976  -2.81913283
 H    2.82887988  -2.18659037  -0.66342613
 H    2.90826972  -2.36648535   1.08092835
 H   -0.67902273  -2.04314542  -1.03341537
 H   -1.02557754  -1.86917586   0.62981329
 H   -0.84648854   0.46155338  -0.36399291
 H    4.47408365   2.19122443   1.22545149
 H    4.37659316  -0.28849917   1.20204666
 H   -0.97512277   3.27550860  -3.88646268
 H   -2.16815038   5.05044304  -2.66546998
 H   -2.70333843   6.21542774  -0.57042747
 H   -0.91867793   4.93103705   3.13933587
 H    0.31427068   3.14599877   1.95453590
 H    1.91789378   4.27508915   0.09753234
 H   -3.07617204   7.18529975   1.53713443
 H    0.58707707   1.67130417  -3.77255495
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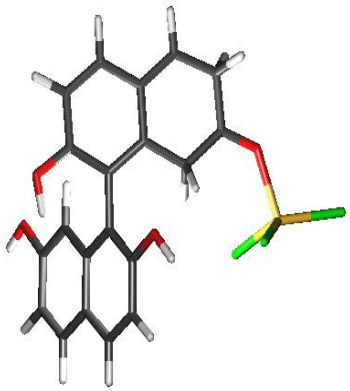
28 (n=1, Hal=Cl)



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 43
 Energy -2693.470440751  Charge 1  Dipole 12.980881  ZPE 0.299737  G(298.15) 151.19
 C    3.29427064  -0.36640876   0.33146257
 C    3.83974559   0.76718143   0.88124508
 C    3.08783855   2.01608205   1.13844784
 C    1.65465877   2.02574986   0.67976824
 C    1.05959334   0.82322719   0.05523093
 C    1.89053504  -0.41274125  -0.02550101
 C    1.32198424  -1.59242974  -0.48003607
 C    2.18154278  -2.72958794  -0.64674896
 C    3.57018692  -2.69849841  -0.31727015
 C    4.10944972  -1.54664784   0.16535112
 C   -0.97553844  -2.60519026  -0.10994700
 C   -0.10553050  -1.73295195  -0.86067278
 C   -0.61864502  -1.02469281  -1.95677002
 C   -1.96241470  -1.18085341  -2.36177375
 C   -2.78970415  -2.04496029  -1.67970140
 C   -2.33482132  -2.77082801  -0.55343757
 C   -3.19202461  -3.63326867   0.17671754
 C   -2.75375864  -4.29901555   1.29855109
 C   -1.42456286  -4.11236645   1.75469144
 C   -0.55681125  -3.27313687   1.06307017
 O    1.72898390  -3.85817600  -1.15338993
 O    0.23182042  -0.19317996  -2.62264556
 O    1.00912220   3.08014610   0.81690588
Al   -0.83421294   3.55249898   0.26470341
Cl   -0.64566701   3.19318126  -1.85731421
Cl   -1.04330430   5.54577073   0.90901409
Cl   -1.94343580   2.01116589   1.27281457
 O   -0.94736226  -4.71799438   2.86807155
 H    4.89534756   0.75924279   1.17643397
 H    3.60793314   2.88644456   0.68636035
 H    3.10694845   2.25513807   2.22411051
 H    0.76102826   1.13034675  -0.98177421
 H    0.06107294   0.63943701   0.51800474
 H    4.15840137  -3.60623692  -0.46701563
 H    5.16768436  -1.49752667   0.43574448
 H   -2.33483634  -0.61855610  -3.22315933
 H   -3.82686011  -2.16916751  -2.00351231
 H   -4.22410550  -3.75784211  -0.16198483
 H   -3.43211220  -4.95817238   1.84935464
 H    0.44323396  -3.12419645   1.47681648
 H    0.75574569  -3.76438261  -1.32502775
 H   -0.26883312   0.31746026  -3.29032931
 H   -1.65123265  -5.25723755   3.27762576
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