

Supporting Information

Chemical Constituents of the Deep-Sea-Derived *Penicillium solitum*

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Table S1. Energies analysis for 1*S*,2*S*,8*S*,8*aR*,11*R*,13*R*-1 at MMFF94 force field.

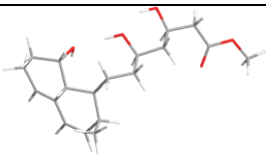
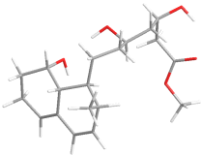
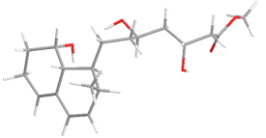
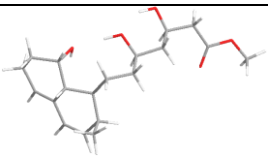
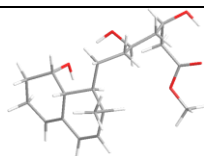
Configuration	Conformer	Structure	E (kcal/mol)	Population (%)
1 <i>S</i> ,2 <i>S</i> ,8 <i>S</i> ,8 <i>aR</i> ,11 <i>R</i> ,13 <i>R</i> -1	1		26.35	97.09
1 <i>S</i> ,2 <i>S</i> ,8 <i>S</i> ,8 <i>aR</i> ,11 <i>R</i> ,13 <i>R</i> -1	2		25.46	1.69
1 <i>S</i> ,2 <i>S</i> ,8 <i>S</i> ,8 <i>aR</i> ,11 <i>R</i> ,13 <i>R</i> -1	3		26.38	1.22

Table S2. Standard orientations at BP86/6-311G(d,p) level in MeOH..

Conformer 1 <i>S</i> ,2 <i>S</i> ,8 <i>S</i> ,8 <i>aR</i> ,11 <i>R</i> ,13 <i>R</i> -1-1					
					
SCF Energy (BP86): -1118.500294 Hartree: -701869.5253 kcal/mol					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.867822	3.147789	1.468235
2	6	0	2.154288	2.410052	0.312449
3	6	0	2.866963	2.688329	-0.988051
4	6	0	3.627330	1.781452	-1.621223
5	6	0	3.866983	0.435824	-1.102085
6	6	0	4.538898	-0.476190	-1.835442
7	6	0	4.835799	-1.883640	-1.395952
8	6	0	4.517470	-2.101492	0.090216
9	6	0	3.218984	-1.399546	0.500503
10	8	0	2.087476	-1.959657	-0.199993
11	6	0	3.319407	0.126992	0.293194
12	6	0	1.973675	0.877208	0.507142
13	6	0	1.242435	0.511979	1.818578
14	6	0	-0.289366	0.651626	1.756250
15	6	0	-0.970086	-0.337580	0.789780
16	6	0	-2.493979	-0.318807	0.935028
17	6	0	-3.215076	-1.244406	-0.058615
18	8	0	-2.964162	-2.614537	0.223438

19	6	0	-4.736768	-1.086073	-0.020417
20	6	0	-5.245648	0.213915	-0.601914
21	8	0	-4.570584	1.090367	-1.102697
22	8	0	-6.593754	0.288817	-0.503588
23	6	0	-7.185701	1.481575	-1.040589
24	8	0	-0.518550	-1.682859	1.023052
25	1	0	3.856446	2.720373	1.670365
26	1	0	2.285252	3.121739	2.394805
27	1	0	3.017402	4.201395	1.205739
28	1	0	1.147509	2.847274	0.235345
29	1	0	2.755253	3.685726	-1.411050
30	1	0	4.103981	2.035279	-2.567089
31	1	0	4.889192	-0.187847	-2.826857
32	1	0	4.260788	-2.592569	-2.013264
33	1	0	5.888437	-2.125783	-1.595819
34	1	0	4.441152	-3.170584	0.316177
35	1	0	5.330981	-1.695375	0.705607
36	1	0	3.018104	-1.621673	1.550683
37	1	0	2.139446	-1.658812	-1.122930
38	1	0	4.045536	0.495865	1.034615
39	1	0	1.332684	0.560686	-0.325590
40	1	0	1.627472	1.114780	2.648669
41	1	0	1.445042	-0.525530	2.095007
42	1	0	-0.582526	1.672375	1.473865
43	1	0	-0.691763	0.475800	2.762573
44	1	0	-0.730462	-0.056215	-0.248249
45	1	0	-2.761386	-0.623826	1.956497
46	1	0	-2.839091	0.710290	0.785806
47	1	0	-2.871775	-0.988277	-1.076301
48	1	0	-2.020015	-2.657169	0.476152
49	1	0	-5.186848	-1.914123	-0.582085
50	1	0	-5.109127	-1.189744	1.006527
51	1	0	-6.970952	1.572121	-2.108989
52	1	0	-8.258352	1.376731	-0.873914
53	1	0	-6.802461	2.367885	-0.527429
54	1	0	0.356085	-1.801874	0.596916

Conformer 1*S*,2*S*,8*S*,8*aR*,11*R*,13*R*-1-2

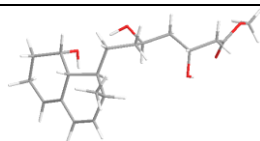


SCF Energy (BP86): -1118.496467 Hartree: -701867.1243 kcal/mol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.669851	1.432245	3.067910
2	6	0	1.822800	1.519218	1.777791
3	6	0	2.409206	2.554101	0.849211
4	6	0	3.068033	2.245260	-0.278862
5	6	0	3.311842	0.869909	-0.711483
6	6	0	3.864952	0.613157	-1.915196
7	6	0	4.154671	-0.762085	-2.451145
8	6	0	4.004478	-1.842918	-1.371362
9	6	0	2.785113	-1.587400	-0.479260

10	8	0	1.562491	-1.667090	-1.240491
11	6	0	2.909174	-0.238715	0.262806
12	6	0	1.616508	0.175593	1.021747
13	6	0	1.015388	-0.936870	1.908211
14	6	0	-0.503401	-0.827429	2.131971
15	6	0	-1.342711	-1.031201	0.851700
16	6	0	-2.836216	-1.124517	1.180975
17	6	0	-3.747601	-1.488228	-0.005631
18	8	0	-5.109599	-1.532637	0.401211
19	6	0	-3.576023	-0.575026	-1.239501
20	6	0	-3.898695	0.871330	-0.942833
21	8	0	-4.778809	1.247342	-0.186192
22	8	0	-3.106835	1.726199	-1.620175
23	6	0	-3.387661	3.123748	-1.422573
24	8	0	-0.976859	-2.221960	0.158758
25	1	0	3.659815	1.005065	2.872239
26	1	0	2.180961	0.829431	3.839811
27	1	0	2.825226	2.434239	3.484267
28	1	0	0.827144	1.876261	2.081404
29	1	0	2.292444	3.598961	1.134211
30	1	0	3.454868	3.037637	-0.918384
31	1	0	4.114883	1.455022	-2.561461
32	1	0	3.482996	-0.978387	-3.297571
33	1	0	5.165929	-0.793458	-2.878909
34	1	0	3.920805	-2.835236	-1.827607
35	1	0	4.897038	-1.851737	-0.731969
36	1	0	2.703646	-2.403018	0.242458
37	1	0	1.517757	-0.873196	-1.799412
38	1	0	3.721304	-0.359126	0.997026
39	1	0	0.883002	0.401182	0.237198
40	1	0	1.524827	-0.966812	2.878225
41	1	0	1.188338	-1.917497	1.458313
42	1	0	-0.768872	0.141635	2.578146
43	1	0	-0.798671	-1.597678	2.856313
44	1	0	-1.191478	-0.160487	0.190690
45	1	0	-2.993890	-1.890433	1.950048
46	1	0	-3.165246	-0.169775	1.613146
47	1	0	-3.496256	-2.502137	-0.326020
48	1	0	-5.374797	-0.604562	0.537728
49	1	0	-2.572751	-0.660197	-1.663509
50	1	0	-4.287042	-0.913848	-2.004460
51	1	0	-3.262454	3.395262	-0.371224
52	1	0	-2.668471	3.656026	-2.045502
53	1	0	-4.410540	3.356284	-1.729796
54	1	0	-0.131881	-2.065296	-0.307160

Conformer 1S,2S,8S,8aR,11R,13R-1-3

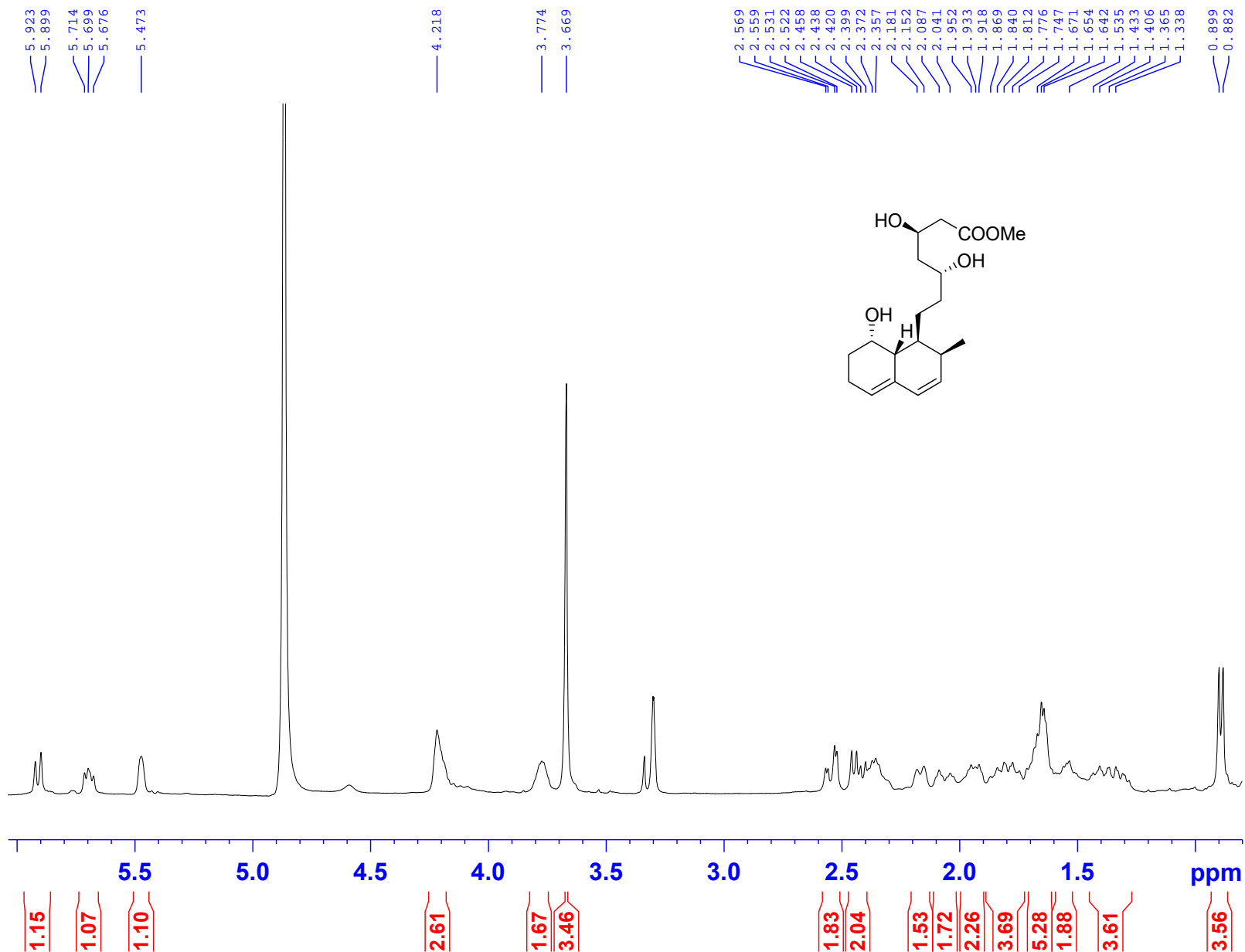


SCF Energy (BP86): -1118.496162 Hartree: -701866.9326 kcal/mol

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-2.760521	3.187630	-0.895459
2	6	0	-2.135658	2.216564	0.131906
3	6	0	-2.919893	2.261119	1.420076
4	6	0	-3.730086	1.271817	1.827684
5	6	0	-3.959709	0.055129	1.050474
6	6	0	-4.684279	-0.962555	1.560725
7	6	0	-4.973335	-2.254900	0.847848
8	6	0	-4.572201	-2.197670	-0.633142
9	6	0	-3.244357	-1.459881	-0.834333
10	8	0	-2.158889	-2.162583	-0.196885
11	6	0	-3.340756	0.002786	-0.347926
12	6	0	-1.974974	0.747136	-0.351348
13	6	0	-1.197796	0.623840	-1.680020
14	6	0	0.325056	0.798587	-1.546013
15	6	0	1.003282	-0.321060	-0.726669
16	6	0	2.532452	-0.288964	-0.832793
17	6	0	3.183897	1.002108	-0.313639
18	8	0	2.778499	1.322748	1.012258
19	6	0	4.724264	0.965137	-0.422555
20	6	0	5.354853	-0.081062	0.472290
21	8	0	4.898025	-0.454369	1.540272
22	8	0	6.511612	-0.546575	-0.029460
23	6	0	7.200978	-1.514468	0.783933
24	8	0	0.607244	-1.615183	-1.177730
25	1	0	-3.741637	2.837701	-1.236268
26	1	0	-2.119808	3.323601	-1.772749
27	1	0	-2.907355	4.174249	-0.440826
28	1	0	-1.126907	2.596552	0.350695
29	1	0	-2.815892	3.156508	2.031517
30	1	0	-4.256534	1.354657	2.777725
31	1	0	-5.085218	-0.858710	2.569428
32	1	0	-4.443032	-3.079920	1.350272
33	1	0	-6.038773	-2.506064	0.941603
34	1	0	-4.495380	-3.207392	-1.051082
35	1	0	-5.345019	-1.666201	-1.204141
36	1	0	-2.990746	-1.483102	-1.896337
37	1	0	-2.254230	-2.031470	0.761593
38	1	0	-4.021283	0.521175	-1.041947
39	1	0	-1.376254	0.256117	0.426086
40	1	0	-1.586689	1.339747	-2.413712
41	1	0	-1.354161	-0.363357	-2.120786
42	1	0	0.564580	1.770447	-1.094966
43	1	0	0.759689	0.798776	-2.555626
44	1	0	0.745661	-0.193165	0.334625
45	1	0	2.917140	-1.150284	-0.272634
46	1	0	2.813136	-0.442776	-1.884555
47	1	0	2.845557	1.844297	-0.927668
48	1	0	3.215417	0.664511	1.585351
49	1	0	5.051696	0.806247	-1.454630
50	1	0	5.118447	1.938780	-0.101750
51	1	0	6.579871	-2.401827	0.929130
52	1	0	8.106705	-1.764781	0.231545
53	1	0	7.448335	-1.088124	1.759439
54	1	0	-0.286544	-1.806261	-0.833217

Figure S1. ¹H NMR spectrum of 1 in MeOH-d₄.



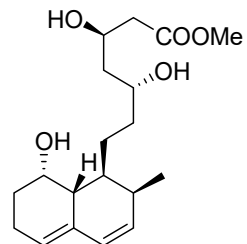
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 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
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 Time 13.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 19
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 13.90 usec
 PLW1 12.14299965 W

F2 - Processing parameters
 SI 32768
 SF 400.1300116 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S2. ¹³C NMR spectrum of 1 in MeOH-d₄.



Current Data Parameters
 NAME HB2-10 M 10mg
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
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 Time 13.38
 INSTRUM spect
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 PULPROG zgpg30
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 SOLVENT MeOD
 NS 482
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 296.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6228293 MHz
 NUC1 ¹³C
 P1 12.37 usec
 PLW1 28.13500023 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG[2] waltz16
 PCPD2 90.00 usec
 PLW2 12.14299965 W
 PLW12 0.28964999 W
 PLW13 0.23461001 W

F2 - Processing parameters
 SI 32768
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 WDW EM
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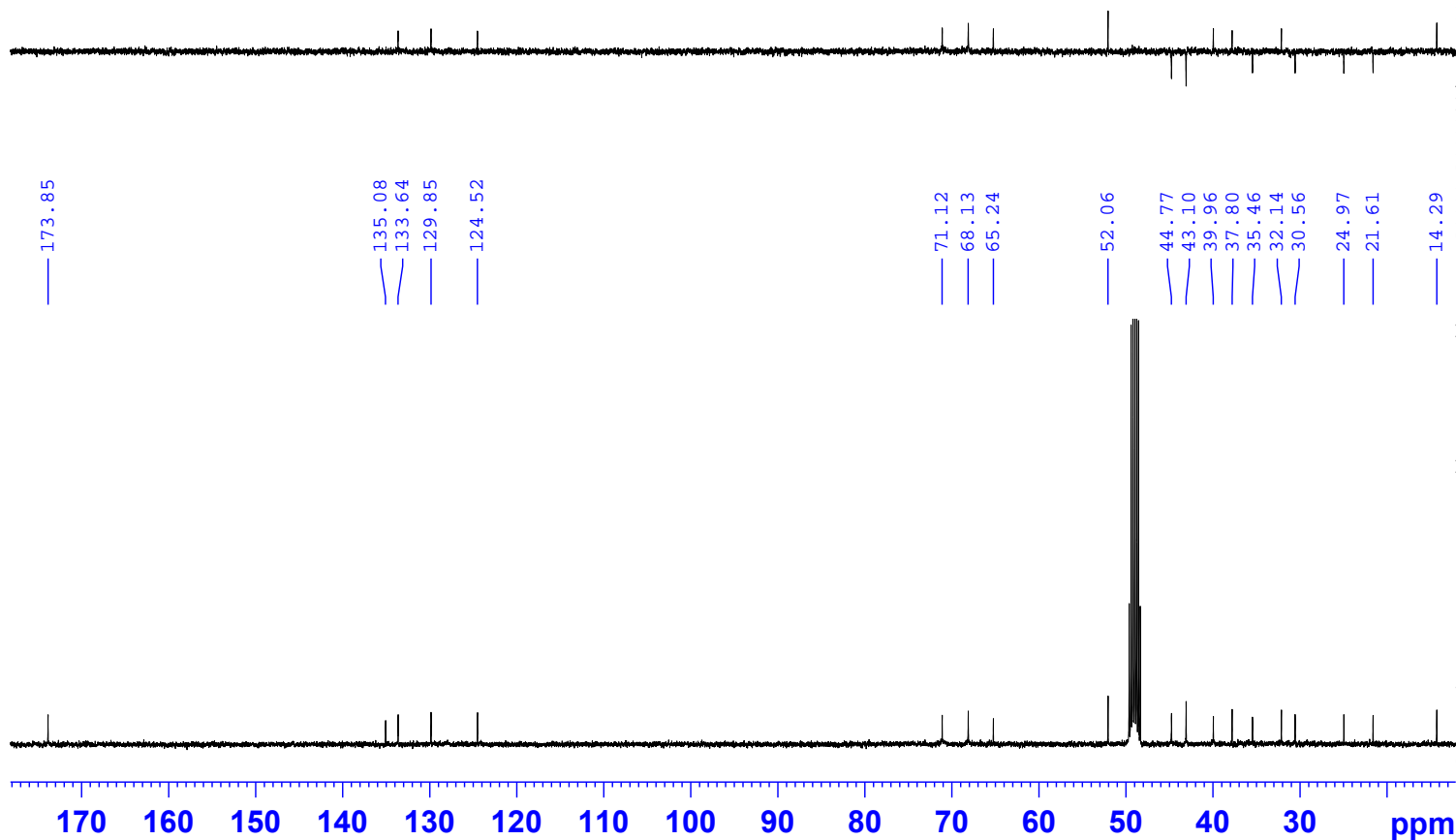
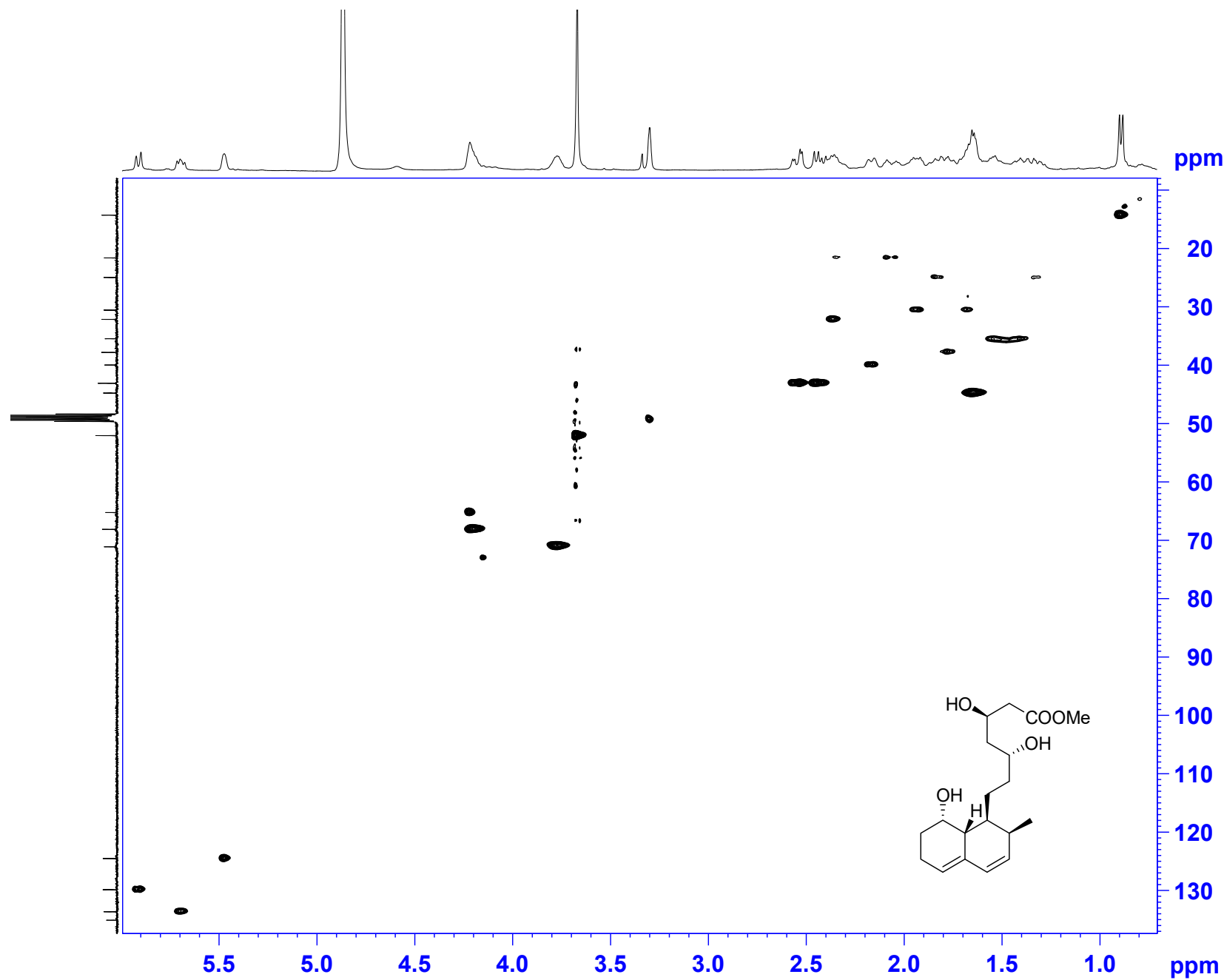


Figure S3. HSQC NMR spectrum of 1 in MeOH-d₄.



Current Data Parameters
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EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
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TD 1024
SOLVENT MeOD
NS 16
DS 32
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AQ 0.1599488 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 296.1 K
CNST2 145.000000
CNST17 -0.500000
D0 0.00000300 sec
D1 2.00000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00089000 sec
INO 0.0002480 sec

===== CHANNEL f1 =====
SFO1 400.1316005 MHz
NUC1 1H
P1 13.90 usec
P2 27.80 usec
P28 1000.00 usec
PLW1 12.14299965 W

===== CHANNEL f2 =====
SFO2 100.6228298 MHz
NUC2 13C
CPDPRG[2] garp
P3 12.37 usec
P14 500.00 usec
P24 2000.00 usec
PCPD2 70.00 usec
PLW0 0 W
PLW2 28.13500023 W
PLW12 0.87860000 W
SPNAM[3] Crp60,0.5,20.1
SPOAL3 0.500
SPOFFS3 0 Hz
SPW3 6.57779980 W
SPNAM[7] Crp60comp.4
SPOAL7 0.500
SPOFFS7 0 Hz
SPW7 6.57779980 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.6228 MHz
FIDRES 78.755043 Hz
SW 200.365 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300075 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6126294 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S4. COSY NMR spectrum of 1 in MeOH-d4.



Current Data Parameters
NAME HB2-10 M 10mg
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200813
Time 23.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfzf
TD 2048
SOLVENT MeOD
NS 8
DS 8
SWH 3201.024 Hz
FIDRES 1.563000 Hz
AQ 0.3198976 sec
RG 203
DW 156.200 usec
DE 6.50 usec
TE 296.2 K
D0 0.00000300 sec
D1 2.00000000 sec
D13 0.00000400 sec
D16 0.00020000 sec
INO 0.00031240 sec

===== CHANNEL f1 =====
SF01 400.1316005 MHz
NUC1 1H
P1 13.90 usec
PLW1 12.14299965 W

===== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPZ1 16.00 %
GPZ2 12.00 %
GPZ3 40.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SF01 400.1316 MHz
FIDRES 25.008003 Hz
SW 8.000 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300117 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300117 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

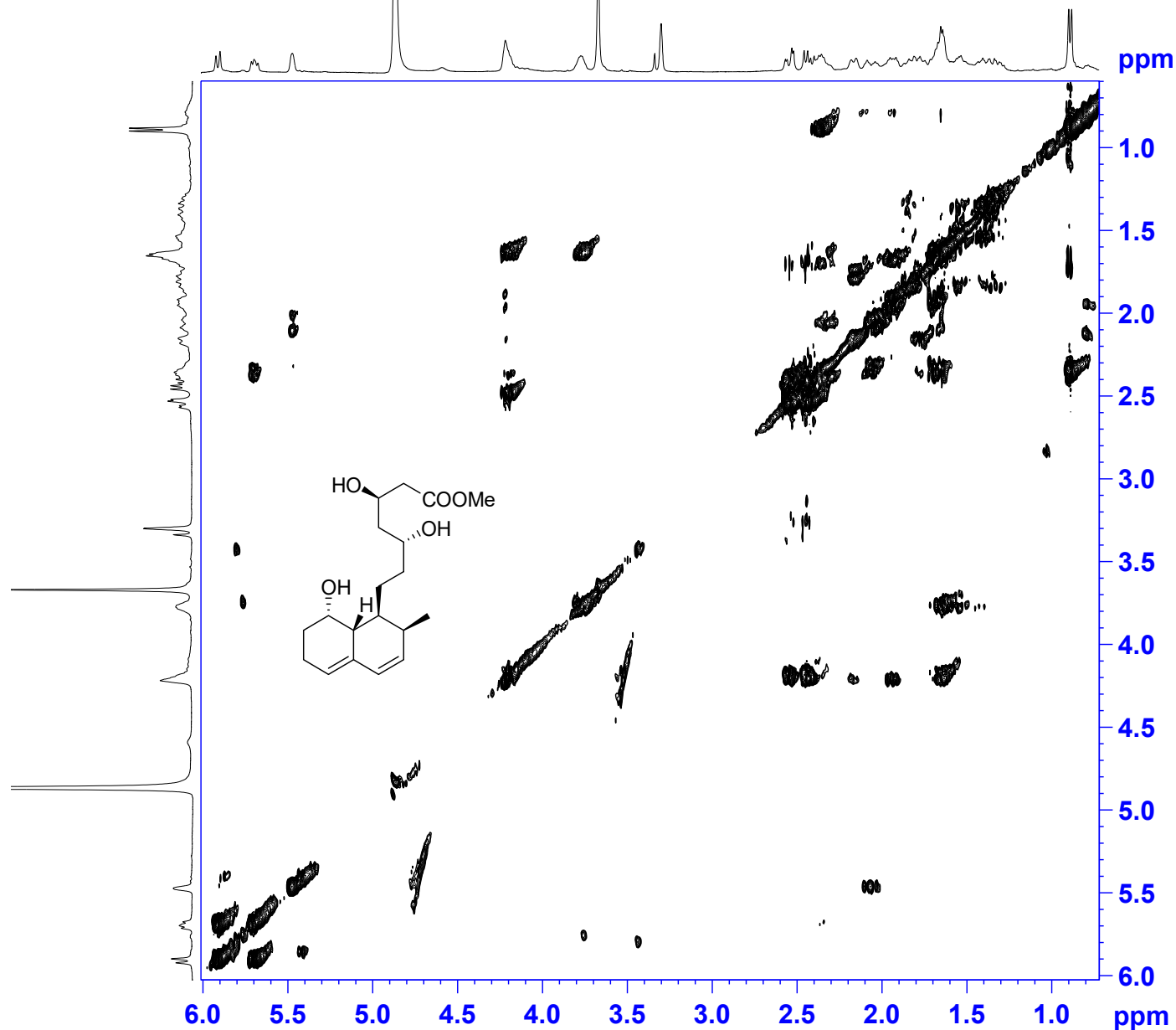
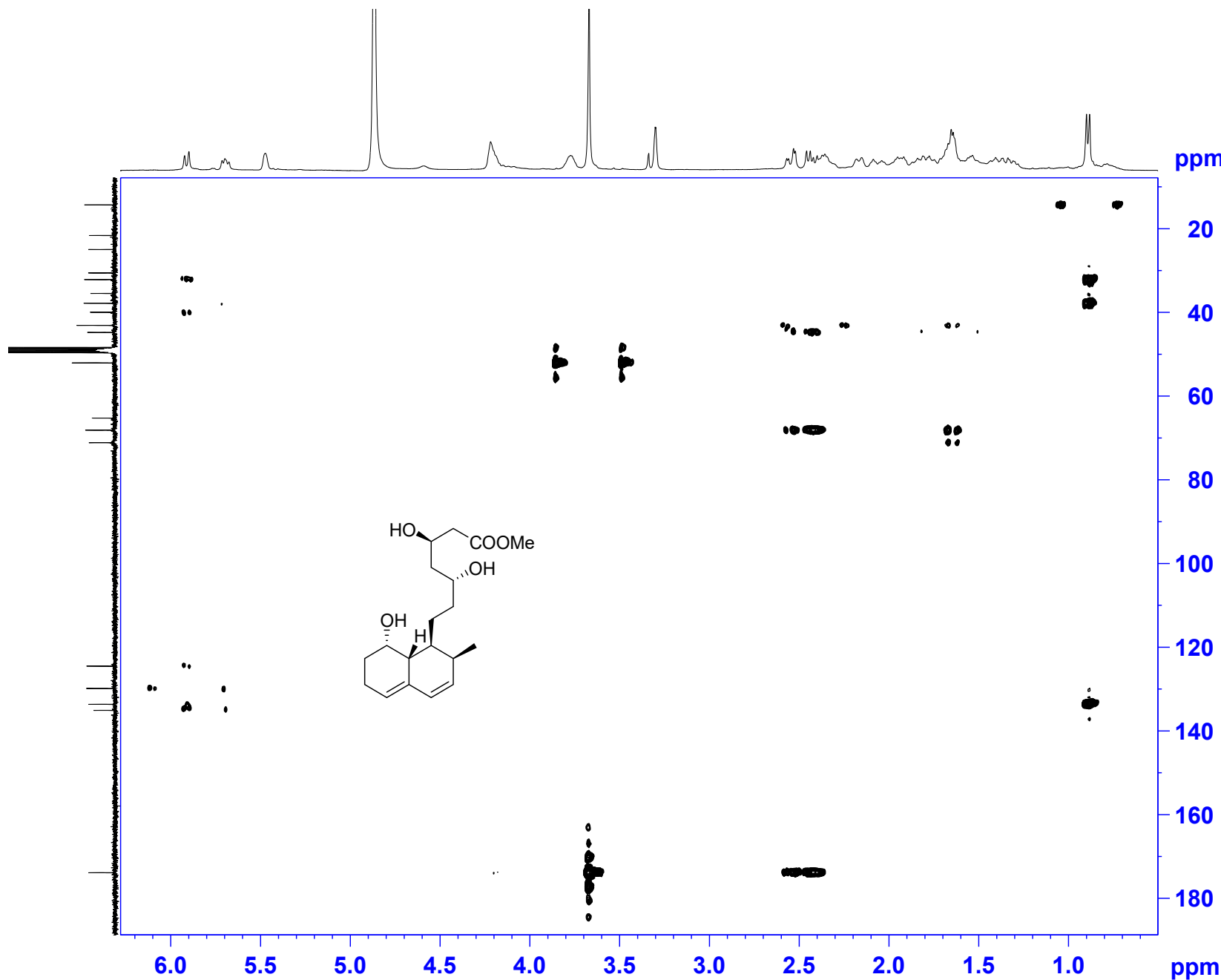


Figure S5. HMBC NMR spectrum of 1 in MeOH-d₄



Current Data Parameters
 NAME HB2-10 M 10mg
 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200814
 Time 0.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG hmbcgpndqf
 TD 4096
 SOLVENT MeOD
 NS 48
 DS 16
 SWH 3201.024 Hz
 FIDRES 0.781500 Hz
 AQ 0.6397952 sec
 RG 203
 DW 156.200 usec
 DE 6.50 usec
 TE 295.9 K
 CNST13 8.0000000
 D0 0.00000300 sec
 D1 1.50000000 sec
 D6 0.06250000 sec
 D16 0.00020000 sec
 IN0 0.00002480 sec

===== CHANNEL f1 =====
 SFO1 400.1316005 MHz
 NUC1 1H
 P1 13.90 usec
 P2 27.80 usec
 PLW1 12.14299965 W

===== CHANNEL f2 =====
 SFO2 100.6228298 MHz
 NUC2 13C
 P3 12.37 usec
 PLW2 28.13500023 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPNAM[2] SMSQ10.100
 GPNAM[3] SMSQ10.100
 GPZ1 50.00 %
 GPZ2 30.00 %
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 100.6228 MHz
 FIDRES 157.510086 Hz
 SW 200.365 ppm
 FnmODE QF

F2 - Processing parameters
 SI 1024
 SF 400.1300117 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.40

F1 - Processing parameters
 SI 1024
 MC2 QF
 SF 100.6126294 MHz
 WDW SINE
 SSB 0
 LB 0 Hz
 GB 0

Figure S6. NOESY NMR spectrum of 1 in MeOH-d₄



Current Data Parameters
 NAME HB2-10 M 10mg
 EXPNO 7
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20200814
 Time_ 4.16
 INSTRUM spect
 PROBD 5 mm PABBO BB-
 PULPROG noesygpph
 TD 2048
 SOLVENT MeOD
 NS 12
 DS 32
 SWH 3201.024 Hz
 FIDRES 1.563000 Hz
 AQ 0.3198976 sec
 RG 203
 DW 156.200 usec
 DE 6.50 usec
 TE 295.9 K
 D0 0.00013850 sec
 D1 2.00000000 sec
 D8 0.30000001 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 INO 0.00031240 sec

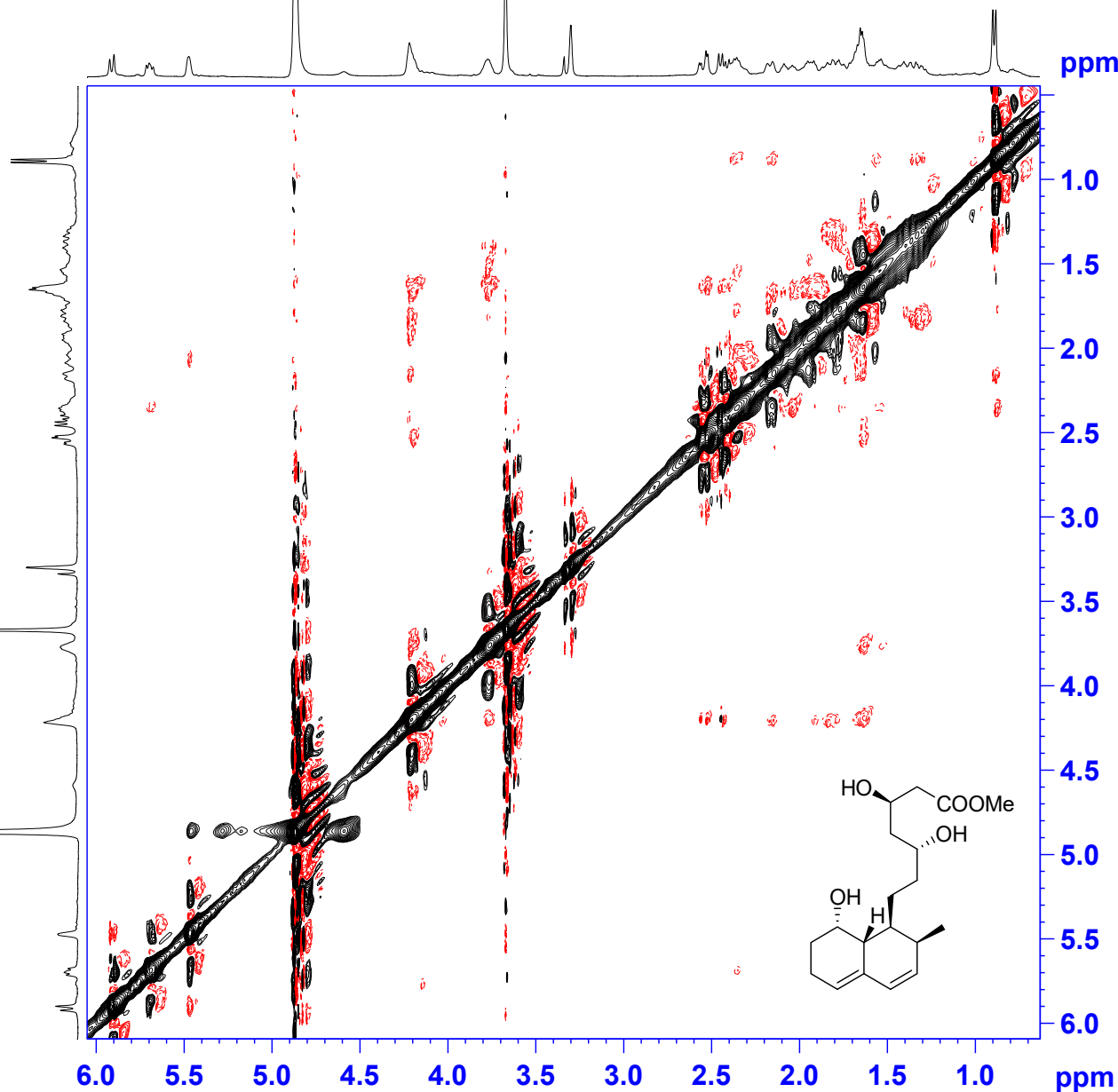
===== CHANNEL f1 =====
 SFO1 400.1316005 MHz
 NUC1 1H
 P1 13.90 usec
 P2 27.80 usec
 P17 2500.00 usec
 PLW1 12.14299965 W
 PLW10 3.47059989 W

===== GRADIENT CHANNEL =====
 GPNAM[1] SMSQ10.100
 GPZ1 40.00 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 256
 SFO1 400.1316 MHz
 FIDRES 12.504002 Hz
 SW 8.000 ppm
 FnmODE States-TPPI

F2 - Processing parameters
 SI 1024
 SF 400.1300117 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 1024
 MC2 States-TPPI
 SF 400.1300117 MHz
 WDW QSINE
 SSB 2
 LB 0 Hz
 GB 0



Single Mass Analysis

Tolerance = 20.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

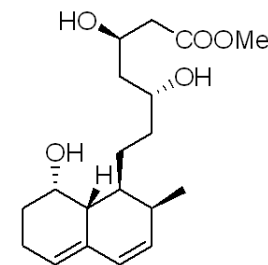
1726 formula(e) evaluated with 73 results within limits (up to 50 closest results for each mass)

Elements Used:

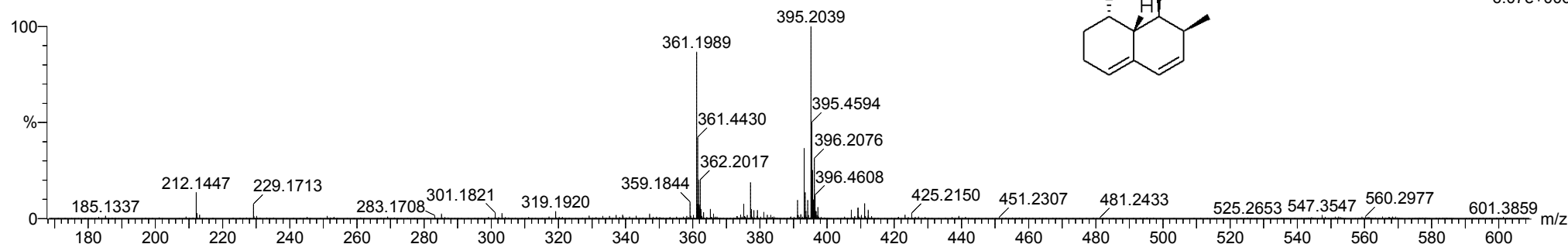
C: 0-50 H: 0-50 N: 0-50 O: 0-50 ²³Na: 0-1

HB 2-10-Aug 148 (0.580) Cm (126:167)

1: TOF MS ES+



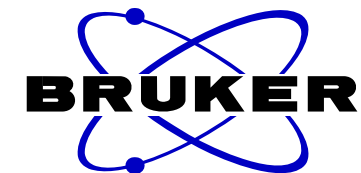
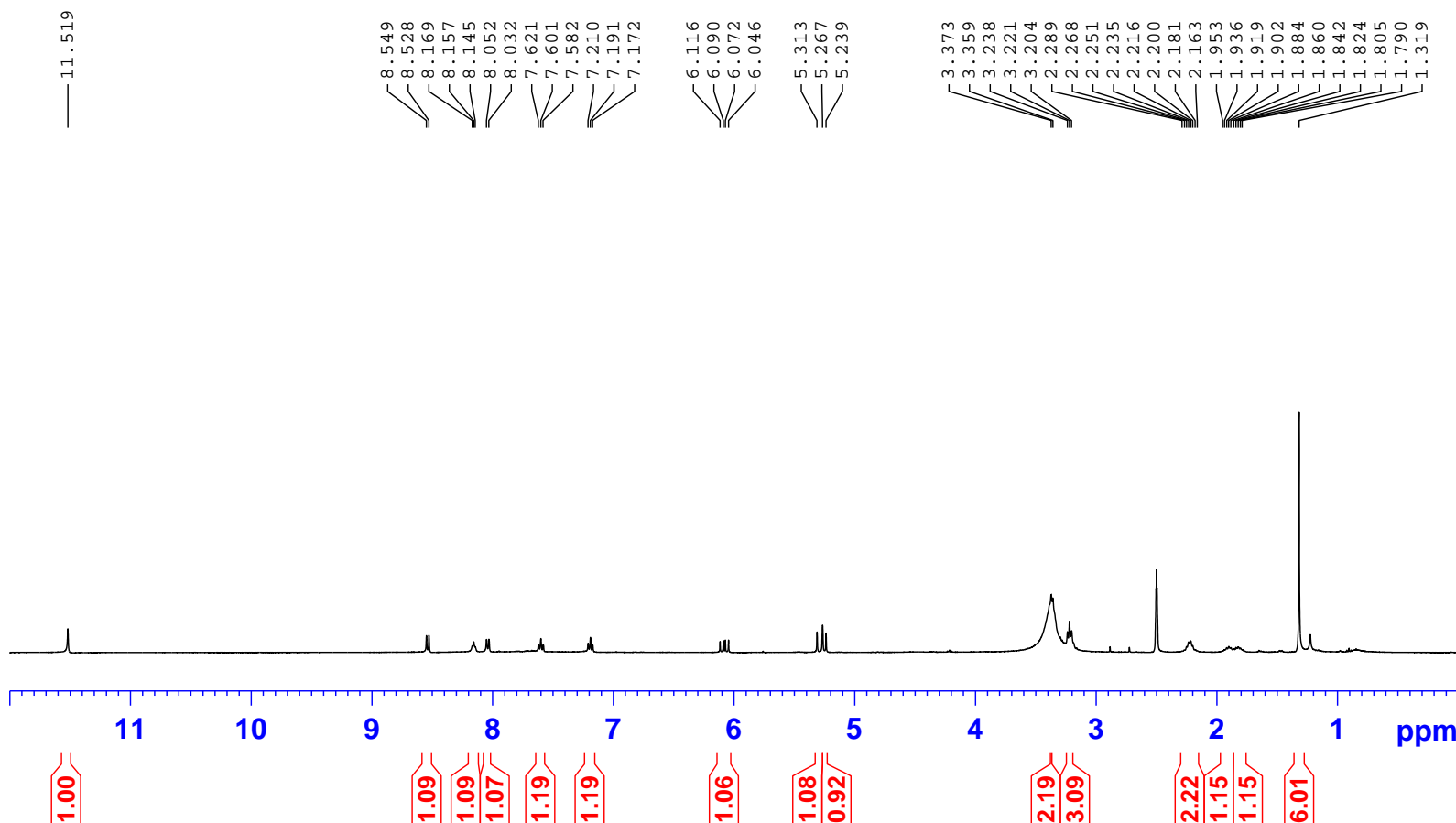
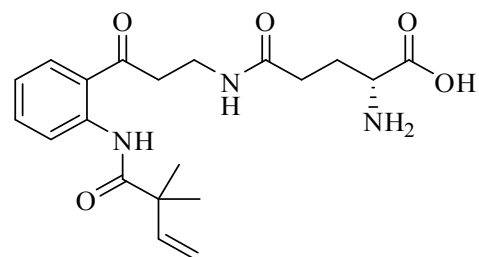
6.07e+006



Minimum: -1.5
Maximum: 20.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
361.1989	361.1988	0.1	0.3	8.5	1820.9	11.424	0.00	C17 H25 N6 O3
	361.1991	-0.2	-0.6	4.5	1819.2	9.639	0.01	C19 H30 O5 ²³ Na
	361.1993	-0.4	-1.1	1.5	1829.6	20.052	0.00	C2 H21 N18 O4
	361.1982	0.7	1.9	3.5	1832.5	22.942	0.00	C H18 N22 ²³ Na
	361.1975	1.4	3.9	3.5	1822.6	13.089	0.00	C16 H29 N2 O7
	361.2004	-1.5	-4.2	9.5	1818.9	9.344	0.01	C20 H26 N4 O ²³ Na
	361.2007	-1.8	-5.0	6.5	1831.2	21.703	0.00	C3 H17 N22
	361.1969	2.0	5.5	-1.5	1830.3	20.761	0.00	H22 N18 O4 ²³ Na
	361.2009	-2.0	-5.5	2.5	1829.1	19.615	0.00	C5 H22 N16 O2 ²³ Na
	361.1964	2.5	6.9	5.5	1823.3	13.822	0.00	C15 H26 N6 O3 ²³ Na
	361.2015	-2.6	-7.2	7.5	1809.5	0.001	99.93	C21 H29 O5
	361.1961	2.8	7.8	9.5	1824.8	15.318	0.00	C13 H21 N12 O
	361.2020	-3.1	-8.6	0.5	1827.9	18.329	0.00	C6 H25 N12 O6
	361.1956	3.3	9.1	16.5	1822.6	13.047	0.00	C28 H25
	361.1951	3.8	10.5	0.5	1824.4	14.914	0.00	C14 H30 N2 O7 ²³ Na
	361.2028	-3.9	-10.8	12.5	1819.6	10.036	0.00	C22 H25 N4 O
	361.1948	4.1	11.4	4.5	1825.2	15.633	0.00	C12 H25 N8 O5
	361.2033	-4.4	-12.2	5.5	1828.2	18.671	0.00	C7 H21 N16 O2
	361.2036	-4.7	-13.0	1.5	1827.0	17.427	0.00	C9 H26 N10 O4 ²³ Na
	361.1937	5.2	14.4	6.5	1826.3	16.798	0.00	C11 H22 N12 O ²³ Na
	361.1935	5.4	15.0	-0.5	1826.0	16.509	0.00	C11 H29 N4 O9
	361.1932	5.7	15.8	13.5	1821.2	11.701	0.00	C26 H26 ²³ Na
	361.2047	-5.8	-16.1	-0.5	1826.4	16.867	0.00	C10 H29 N6 O8
	361.2050	-6.1	-16.9	6.5	1827.2	17.710	0.00	C10 H22 N14 ²³ Na
	361.1924	6.5	18.0	1.5	1826.4	16.889	0.00	C10 H26 N8 O5 ²³ Na
	361.1921	6.8	18.8	5.5	1827.5	17.930	0.00	C8 H21 N14 O3
	361.2060	-7.1	-19.7	4.5	1825.8	16.301	0.00	C11 H25 N10 O4

Figure S8. ¹H NMR spectrum of 2 in DMSO-d₆.



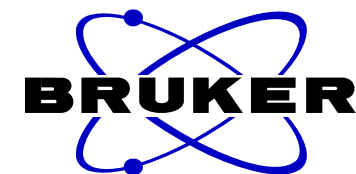
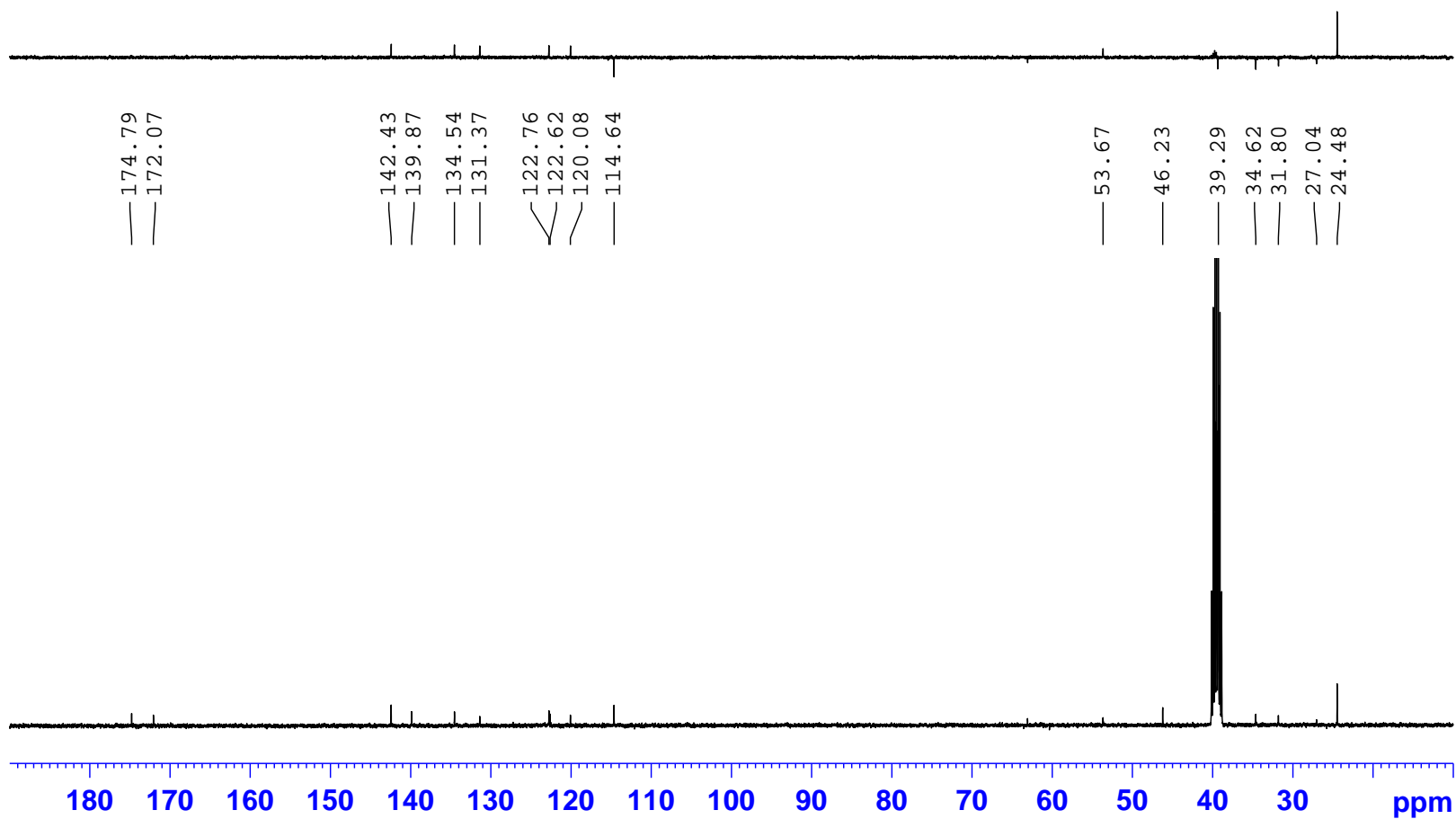
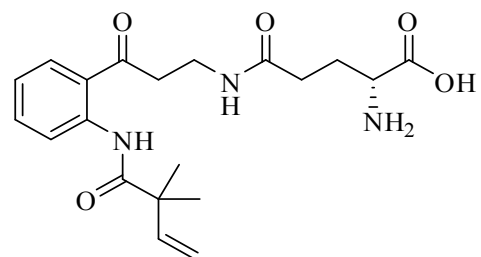
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NAME          HB4-6 D 5mg
EXPNO          1
PROCNO         1
Date_          20200108
Time           9.18
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zg30
TD             65536
SOLVENT        DMSO
NS             28
DS             2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ            4.0894966 sec
RG            203
DW            62.400 usec
DE            6.50 usec
TE            292.5 K
D1            1.00000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
SF01          400.1324710 MHz
NUC1           1H
P1            13.90 usec
SI            32768
SF            400.1300029 MHz
WDW            EM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00
  
```

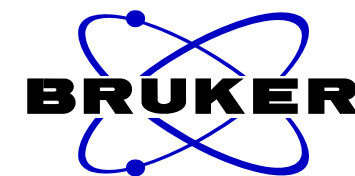
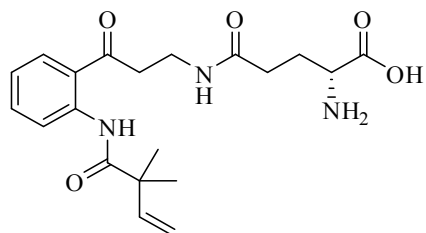
Figure S9. ^{13}C NMR spectrum of 2 in DMSO- d_6 .



NAME HB4-6 D 5mg
 EXPNO 2
 PROCNO 1
 Date_ 20200108
 Time 9.23
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1229
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 292.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 100.6228293 MHz
 NUC1 ^{13}C
 P1 12.37 usec
 SI 32768
 SF 100.6128134 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure S10. HSQC NMR spectrum of 2 in DMSO-d₆.



NAME HB4-6 D 5mg
 EXPNO 4
 PROCNO 1
 Date_ 20200111
 Time 18.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG hsqcetgpsisp2.2
 TD 1024
 SOLVENT DMSO
 NS 8
 DS 32
 SWH 5197.505 Hz
 FIDRES 5.075689 Hz
 AQ 0.0985588 sec
 RG 203
 DW 96.200 usec
 DE 6.50 usec
 TE 294.1 K
 CNST2 145.000000
 CNST17 -0.500000
 D0 0.00000300 sec
 D1 2.00000000 sec
 D4 0.00172414 sec
 D11 0.03000000 sec
 D16 0.00020000 sec
 D24 0.00089000 sec
 IN0 0.00002260 sec

===== CHANNEL f1 =====
 SFO1 400.1326008 MHz
 NUC1 1H
 P1 13.90 usec
 P2 27.80 usec
 P28 1000.00 usec
 ND0 2
 TD 256
 SFO1 100.6238 MHz
 FIDRES 86.421463 Hz
 SW 219.867 ppm
 FnmODE Echo-Antiecho
 SI 1024
 SF 400.1299999 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 echo-antiecho
 SF 100.6128137 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

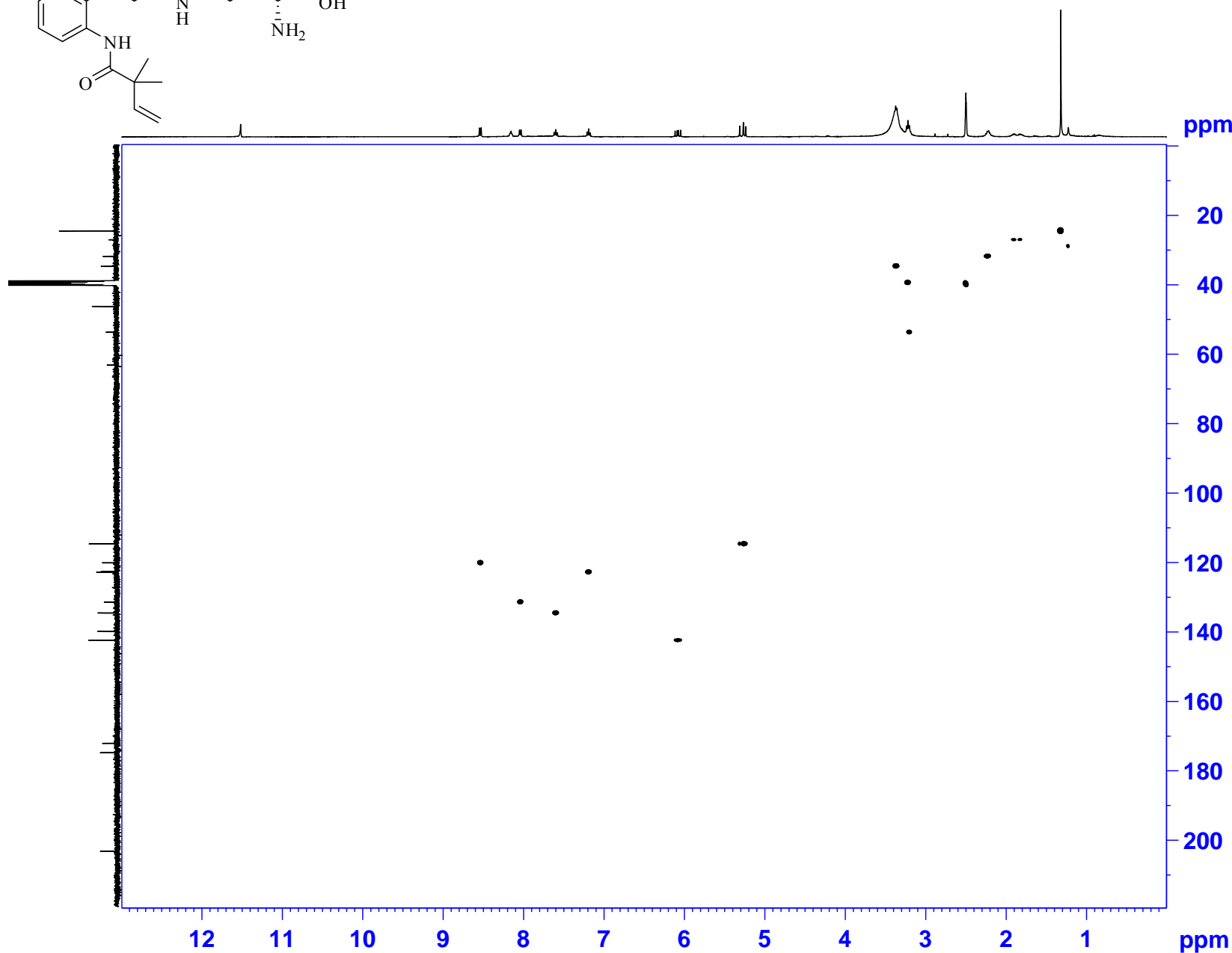
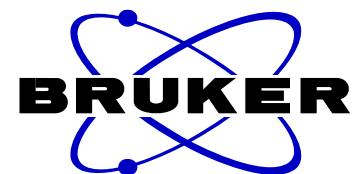
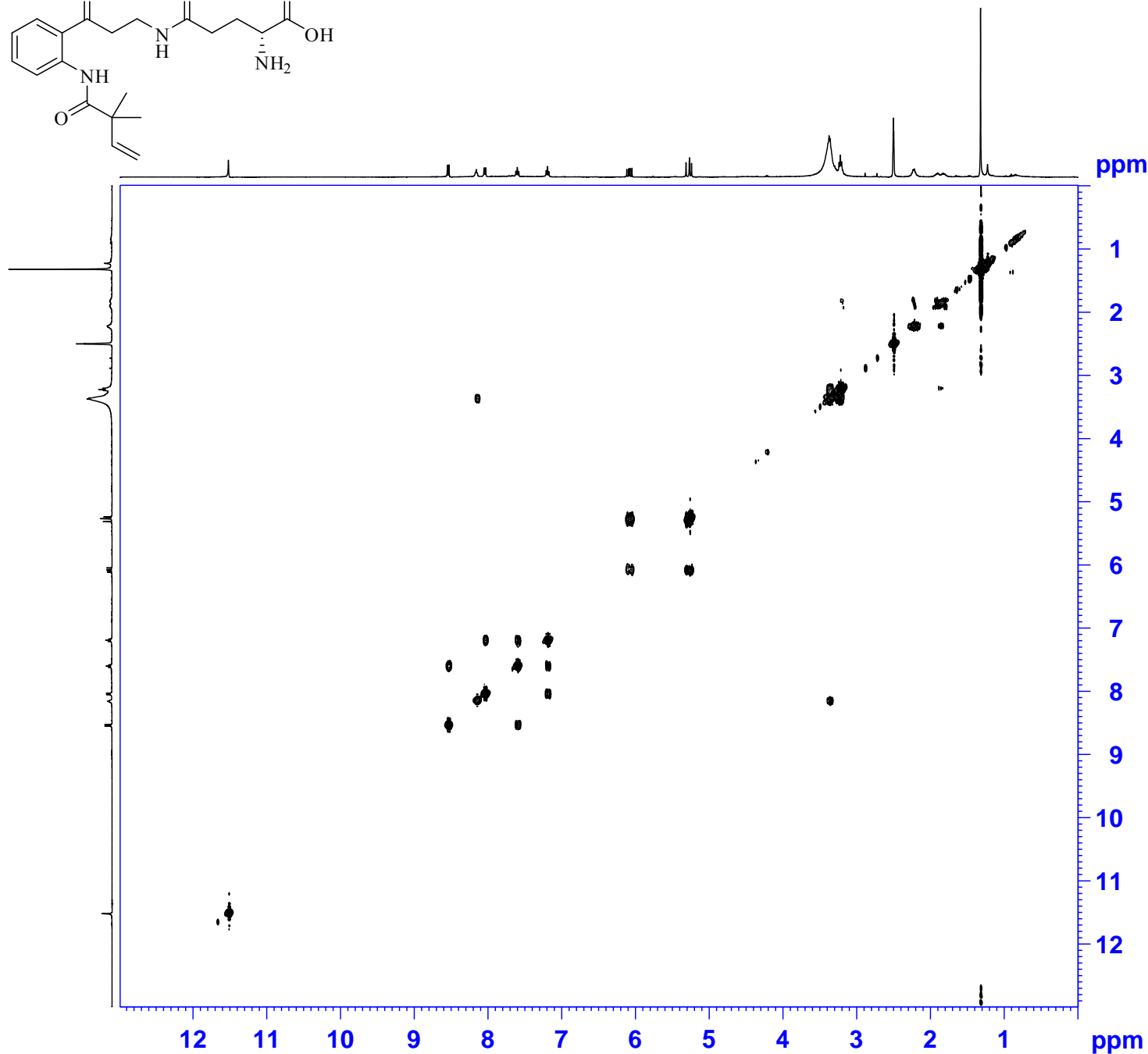
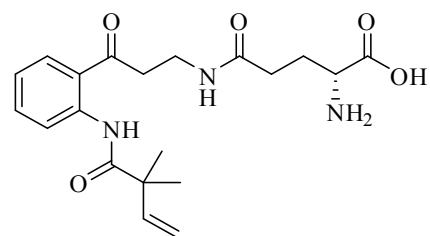


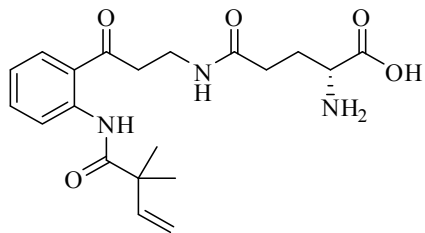
Figure S11. COSY NMR spectrum of 2 in DMSO-d6.



NAME HB4-6 D 5mg
 EXPNO 5
 PROCNO 1
 Date_ 20200111
 Time 10.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG cosygpgf
 TD 2048
 SOLVENT DMSO
 NS 16
 DS 8
 SWH 5197.505 Hz
 FIDRES 2.537844 Hz
 AQ 0.1970676 sec
 RG 203
 DW 96.200 usec
 DE 6.50 usec
 TE 293.8 K
 D0 0.00000300 sec
 D1 1.50000000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00019220 sec

===== CHANNEL f1 =====
 SF01 400.1326008 MHz
 NUC1 1H
 P0 13.90 usec
 P1 13.90 usec
 ND0 1
 TD 128
 SF01 400.1326 MHz
 FIDRES 40.647762 Hz
 SW 13.003 ppm
 FnMODE QF
 SI 1024
 SF 400.1300030 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 400.1300030 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

Figure S12. HMBC NMR spectrum of 2 in DMSO-d₆.



NAME HB4-6 D 5mg
 EXPNO 6
 PROCNO 1
 Date_ 20200111
 Time 11.20
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG hmbcgpndqf
 TD 4096
 SOLVENT DMSO
 NS 64
 DS 16
 SWH 5197.505 Hz
 FIDRES 1.268922 Hz
 AQ 0.3940852 sec
 RG 203
 DW 96.200 usec
 DE 6.50 usec
 TE 293.8 K
 CNST13 8.0000000
 D0 0.00000300 sec
 D1 1.50000000 sec
 D6 0.06250000 sec
 D16 0.00020000 sec
 IN0 0.00002260 sec

===== CHANNEL f1 =====
 SFO1 400.1326008 MHz
 NUC1 1H
 P1 13.90 usec
 P2 27.80 usec
 ND0 2
 TD 128
 SFO1 100.6238 MHz
 FIDRES 172.842926 Hz
 SW 219.867 ppm
 FnMODE QF
 SI 1024
 SF 400.1300030 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 100.6128137 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

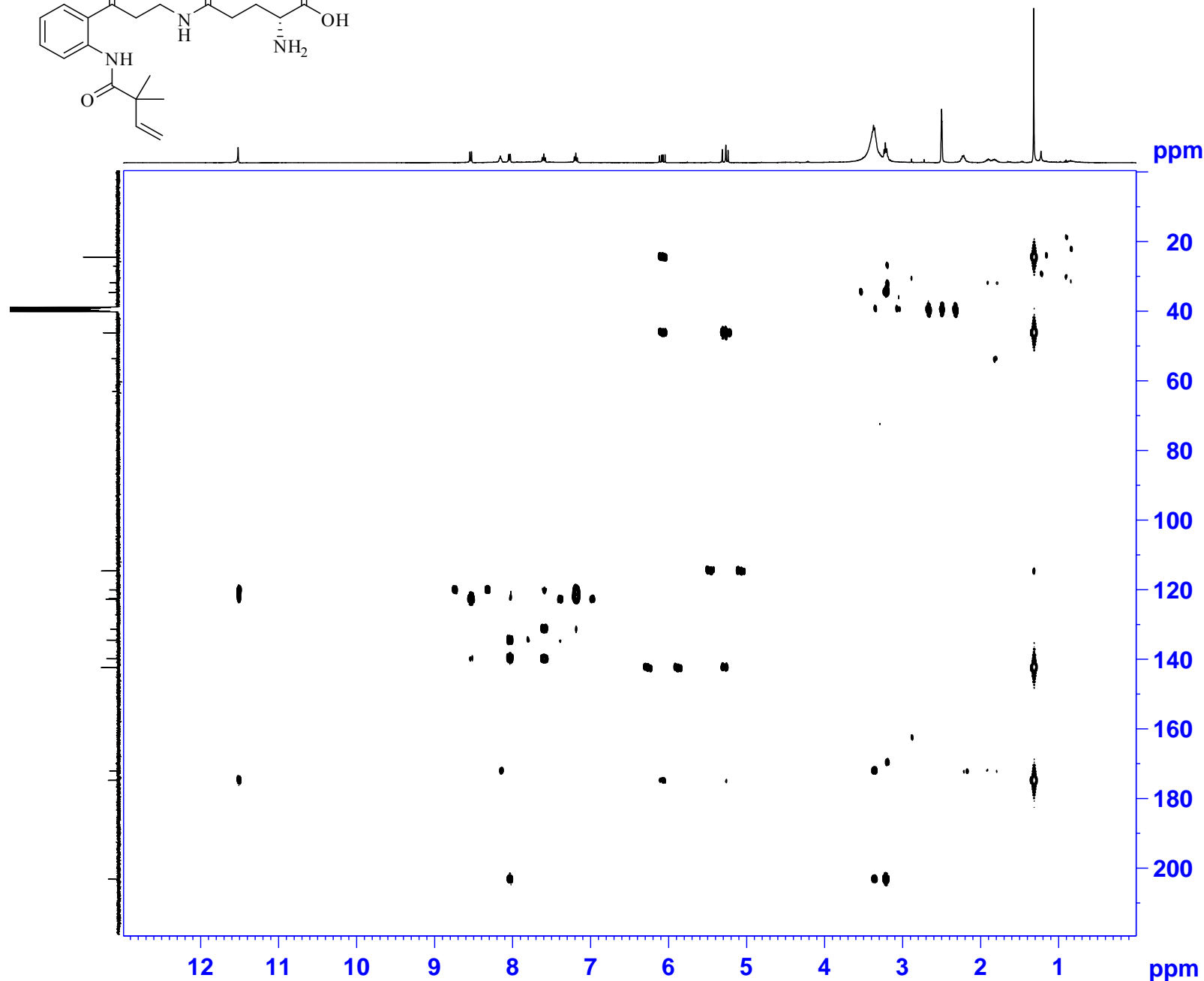
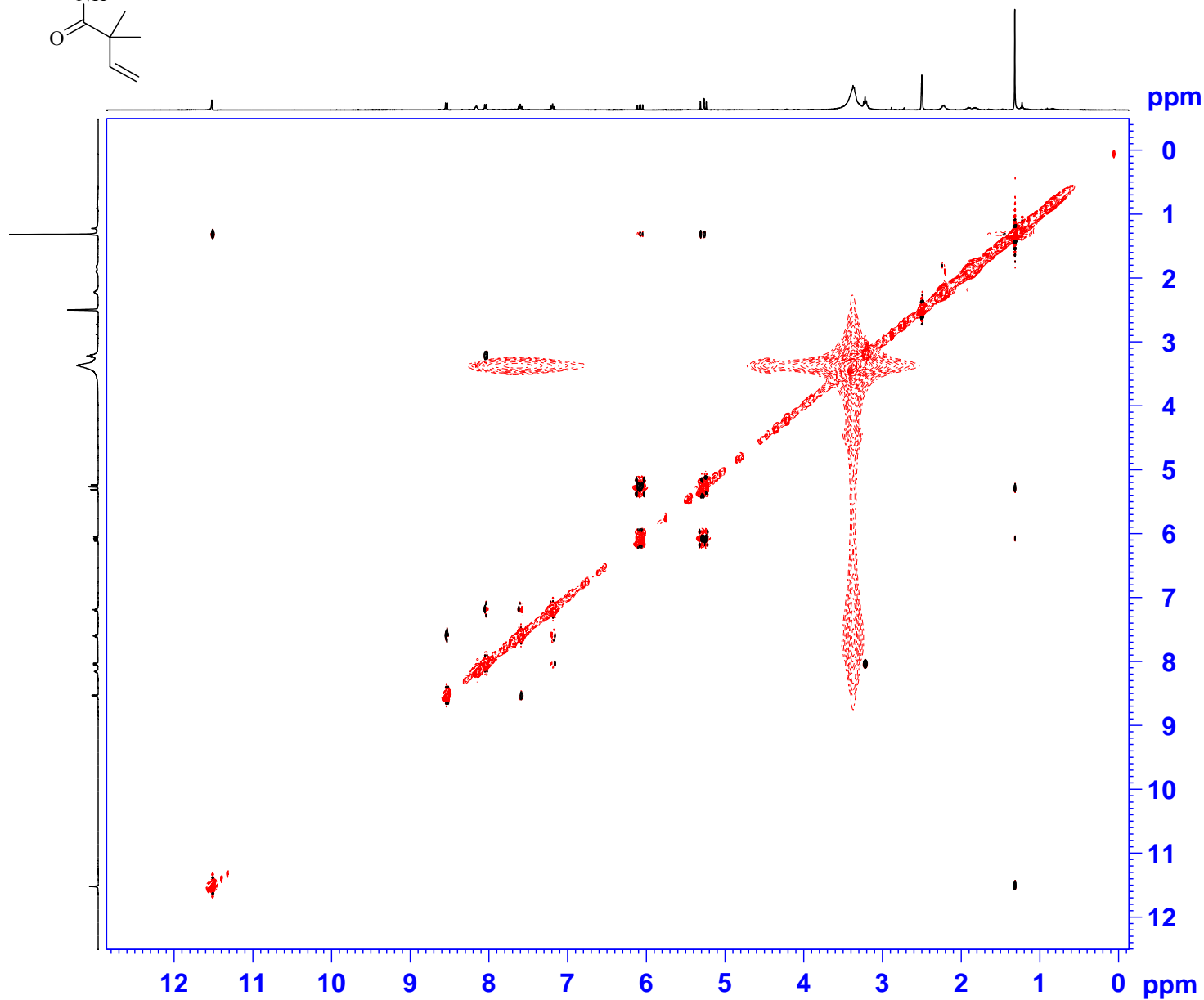
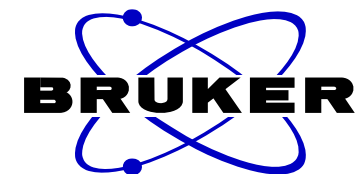
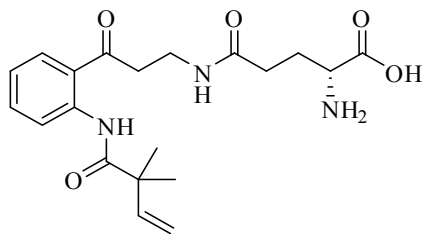


Figure S13. NOESY NMR spectrum of 2 in DMSO-d₆.



```

NAME           HB4-6 D 5mg
EXPNO           7
PROCNO          1
Date_           20200111
Time            15.49
INSTRUM         spect
PROBHD          5 mm PABBO BB-
PULPROG         noesygpphpp
TD              2048
SOLVENT         DMSO
NS               16
DS               32
SWH              5197.505 Hz
FIDRES          2.537844 Hz
AQ              0.1970676 sec
RG               203
DW              96.200 usec
DE               6.50 usec
TE              294.0 K
D0              0.00007840 sec
D1              2.00000000 sec
D8              0.30000001 sec
D11             0.03000000 sec
D12             0.00002000 sec
D16             0.00020000 sec
IN0             0.00019220 sec
  
```

```

===== CHANNEL f1 =====
SFO1           400.1326008 MHz
NUC1            1H
P1              13.90 usec
P2              27.80 usec
P17            2500.00 usec
ND0             1
TD              256
SFO1           400.1326 MHz
FIDRES          20.323881 Hz
SW              13.003 ppm
FnMODE          States-TPPI
SI              1024
SF             400.1300030 MHz
WDW             QSINE
SSB             2
LB              0.00 Hz
GB              0
PC              1.00
SI              1024
MC2            States-TPPI
SF             400.1300030 MHz
WDW             QSINE
SSB             2
LB              0.00 Hz
GB              0
  
```

Figure S14. The HR-ESI-MS spectrum of 2.

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

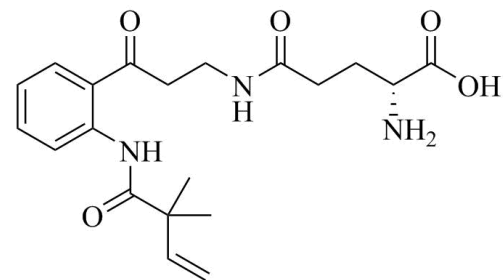
626 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 10-20 H: 1-100 N: 0-20 O: 0-30

HB 4-7-N 105 (0.415)

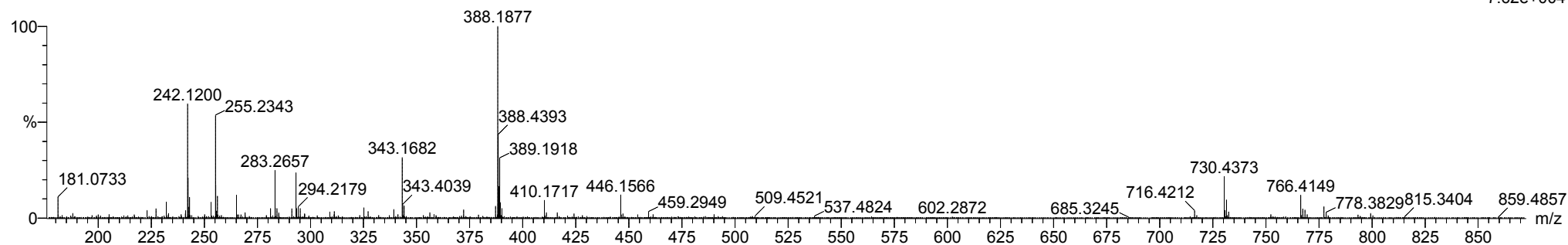
1: TOF MS ES-



Chemical Formula: C₂₀H₂₇N₃O₅

Molecular Weight: 389.4520

7.62e+004

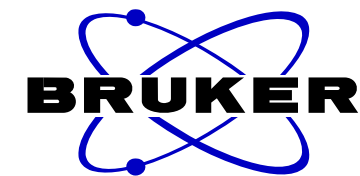
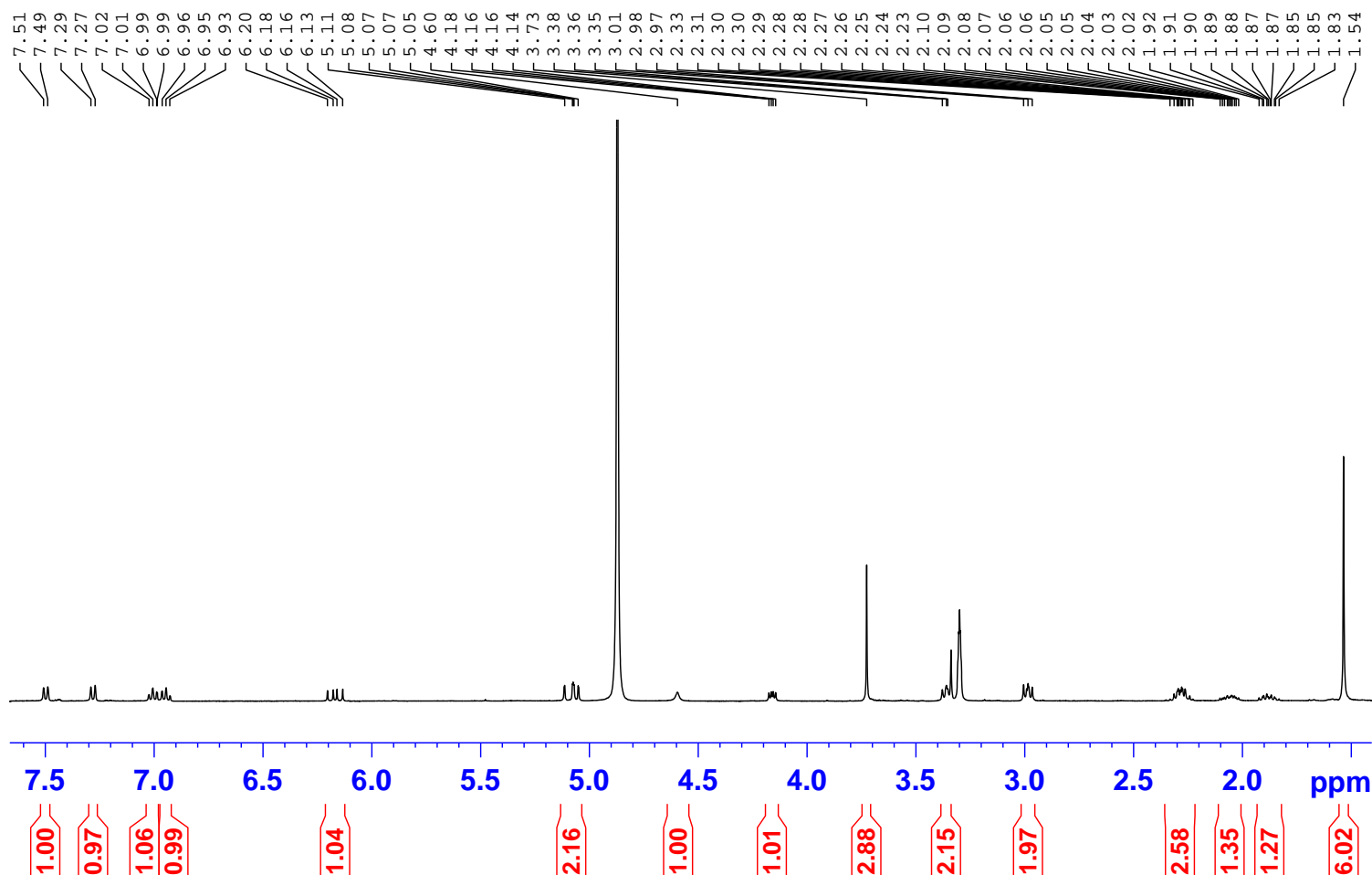
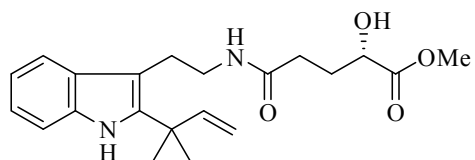


Minimum: -1.5

Maximum: 50.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
388.1877	388.1872	0.5	1.3	9.5	565.4	0.012	98.81	C20 H26 N3 O5
	388.1846	3.1	8.0	10.5	569.8	4.427	1.19	C16 H22 N9 O3

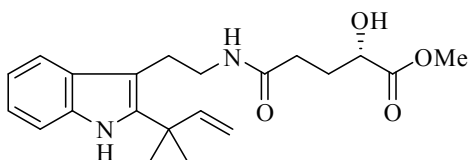
Figure S15. ¹H NMR spectrum of 3 in MeOH-d₄



NAME HB2-12 M 3mg
 EXPNO 1
 PROCNO 1
 Date_ 20200805
 Time 16.30
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 22
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 296.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 13.90 usec
 SI 32768
 SF 400.1300116 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S16. ¹³C NMR spectrum of 3 in MeOH-d₄



NAME HB2-12 M 3mg
 EXPNO 2
 PROCNO 1
 Date_ 20200805
 Time 16.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 1045
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 296.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 100.6228293 MHz
 NUC1 13C
 P1 12.37 usec
 SI 32768
 SF 100.6126277 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

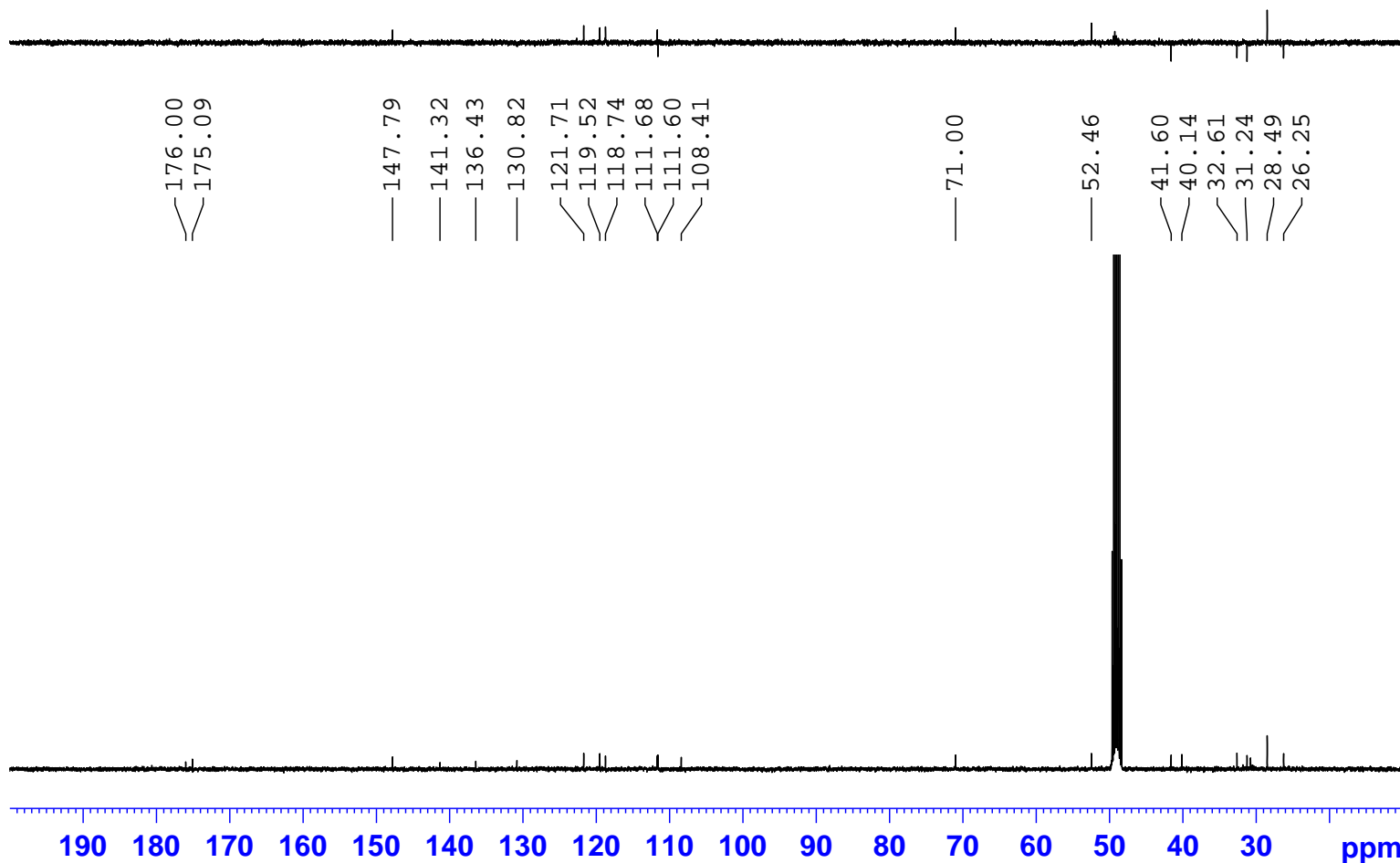
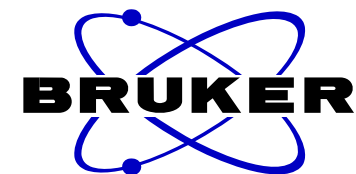
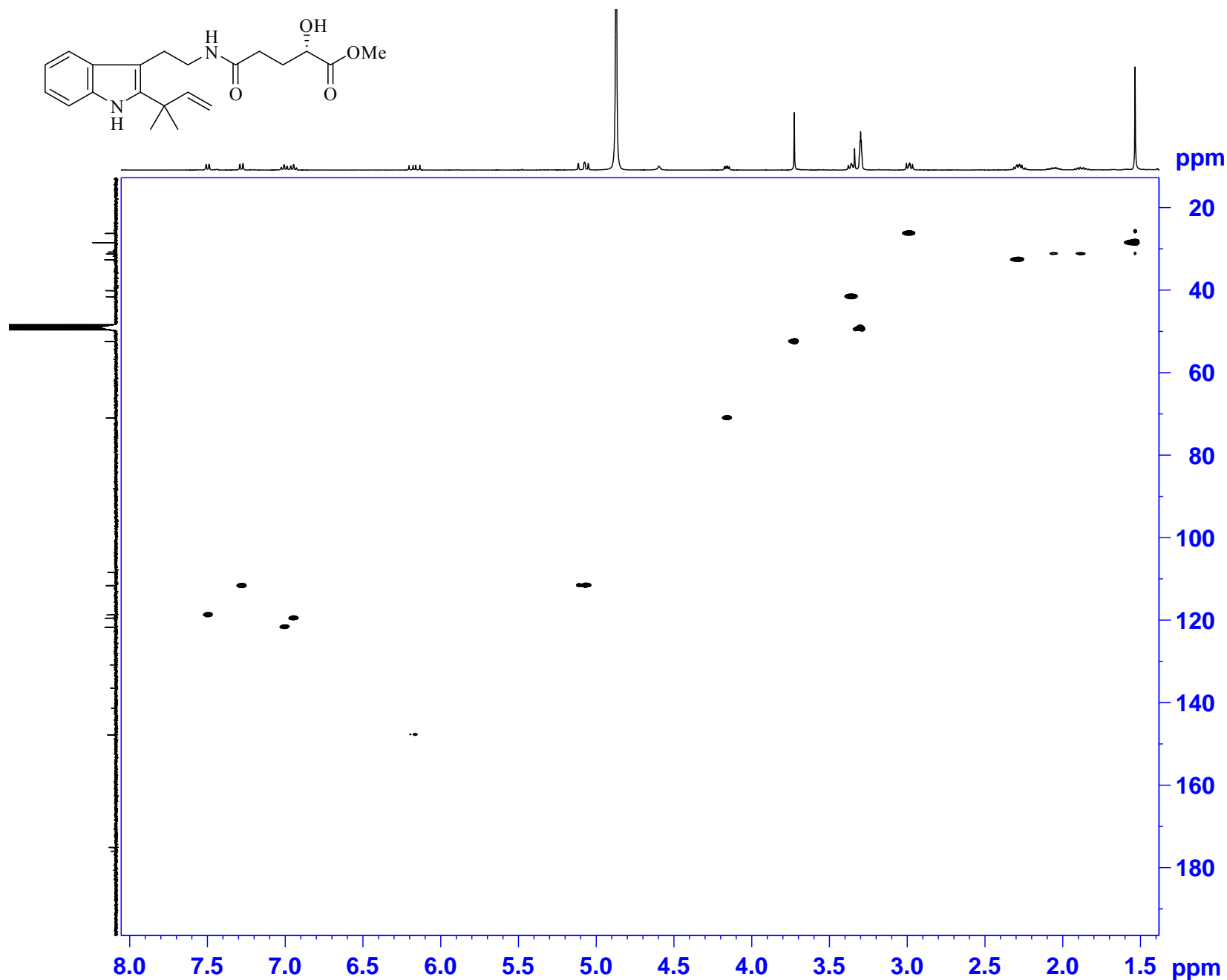
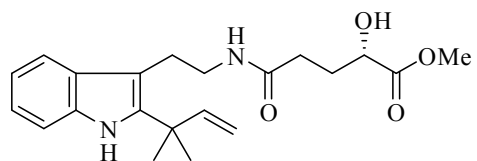


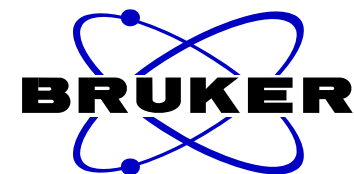
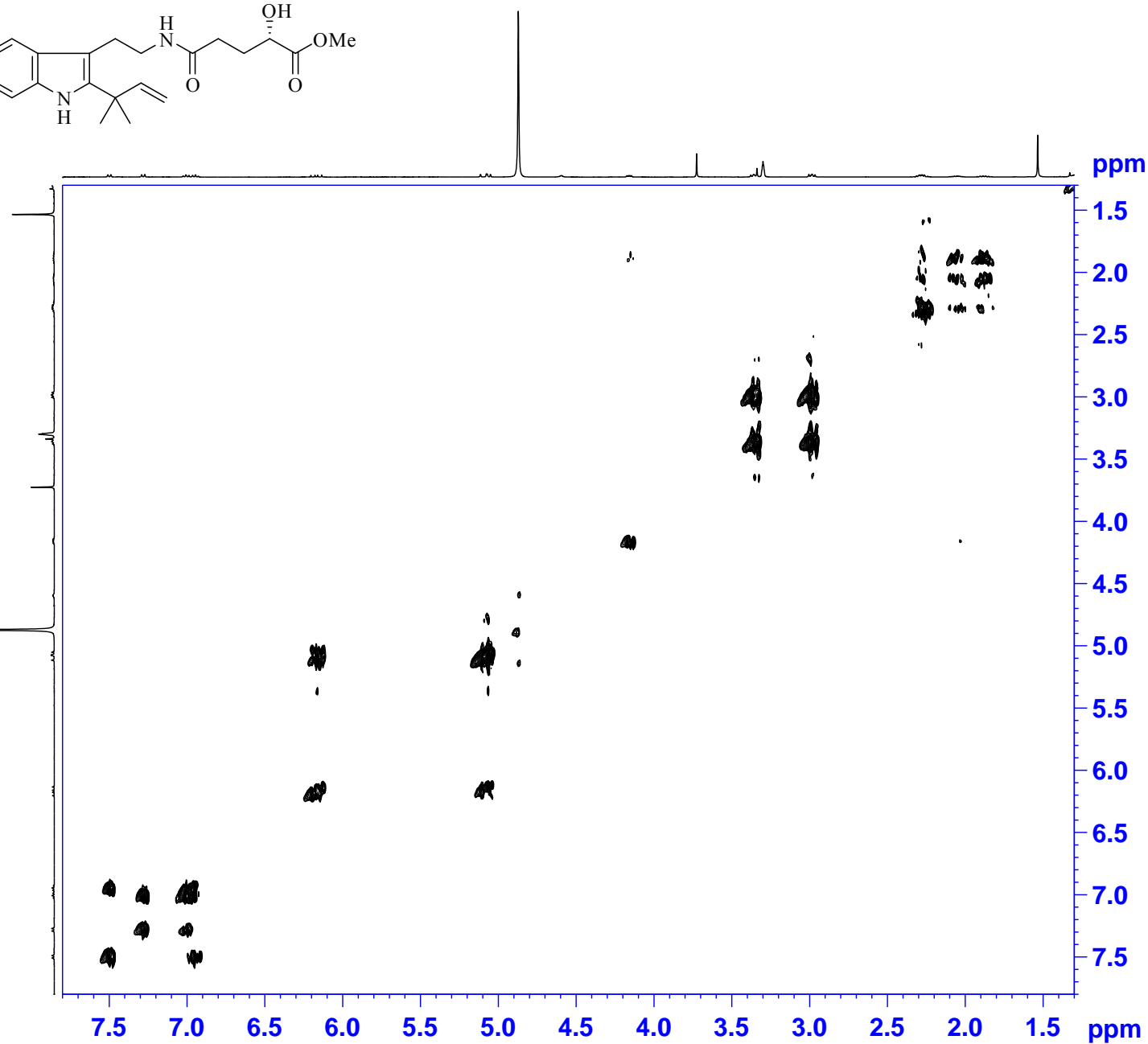
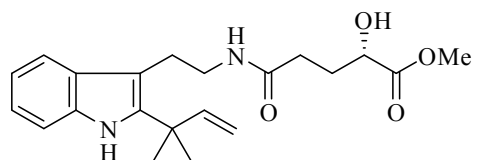
Figure S17. HSQC NMR spectrum of 3 in MeOH-d₄



NAME HB2-12 M 3mg
 EXPNO 4
 PROCNO 1
 Date_ 20200809
 Time 13.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG hsqcetgpsisp2.2
 TD 1024
 SOLVENT MeOD
 NS 32
 DS 32
 SWH 3597.122 Hz
 FIDRES 3.512815 Hz
 AQ 0.1423860 sec
 RG 203
 DW 139.000 usec
 DE 6.50 usec
 TE 296.6 K
 CNST2 145.0000000
 CNST17 -0.5000000
 D0 0.00000300 sec
 D1 2.00000000 sec
 D4 0.00172414 sec
 D11 0.03000000 sec
 D16 0.00020000 sec
 D24 0.00089000 sec
 IN0 0.00002480 sec

===== CHANNEL f1 =====
 SFO1 400.1318006 MHz
 NUC1 1H
 P1 13.90 usec
 P2 27.80 usec
 P28 1000.00 usec
 ND0 2
 TD 256
 SFO1 100.6228 MHz
 FIDRES 78.755043 Hz
 SW 200.365 ppm
 FnMODE Echo-Antiecho
 SI 1024
 SF 400.1300116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 echo-antiecho
 SF 100.6126277 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

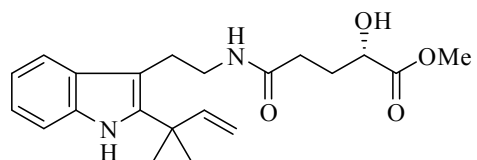
Figure S18. HSQC NMR spectrum of 3 in MeOH-d₄



NAME HB2-12 M 3mg
 EXPNO 5
 PROCNO 1
 Date_ 20200809
 Time 18.40
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG cosygpmfzf
 TD 2048
 SOLVENT MeOD
 NS 32
 DS 8
 SWH 3597.122 Hz
 FIDRES 1.756407 Hz
 AQ 0.2847220 sec
 RG 203
 DW 139.000 usec
 DE 6.50 usec
 TE 296.3 K
 D0 0.00000300 sec
 D1 2.00000000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 IN0 0.00027760 sec

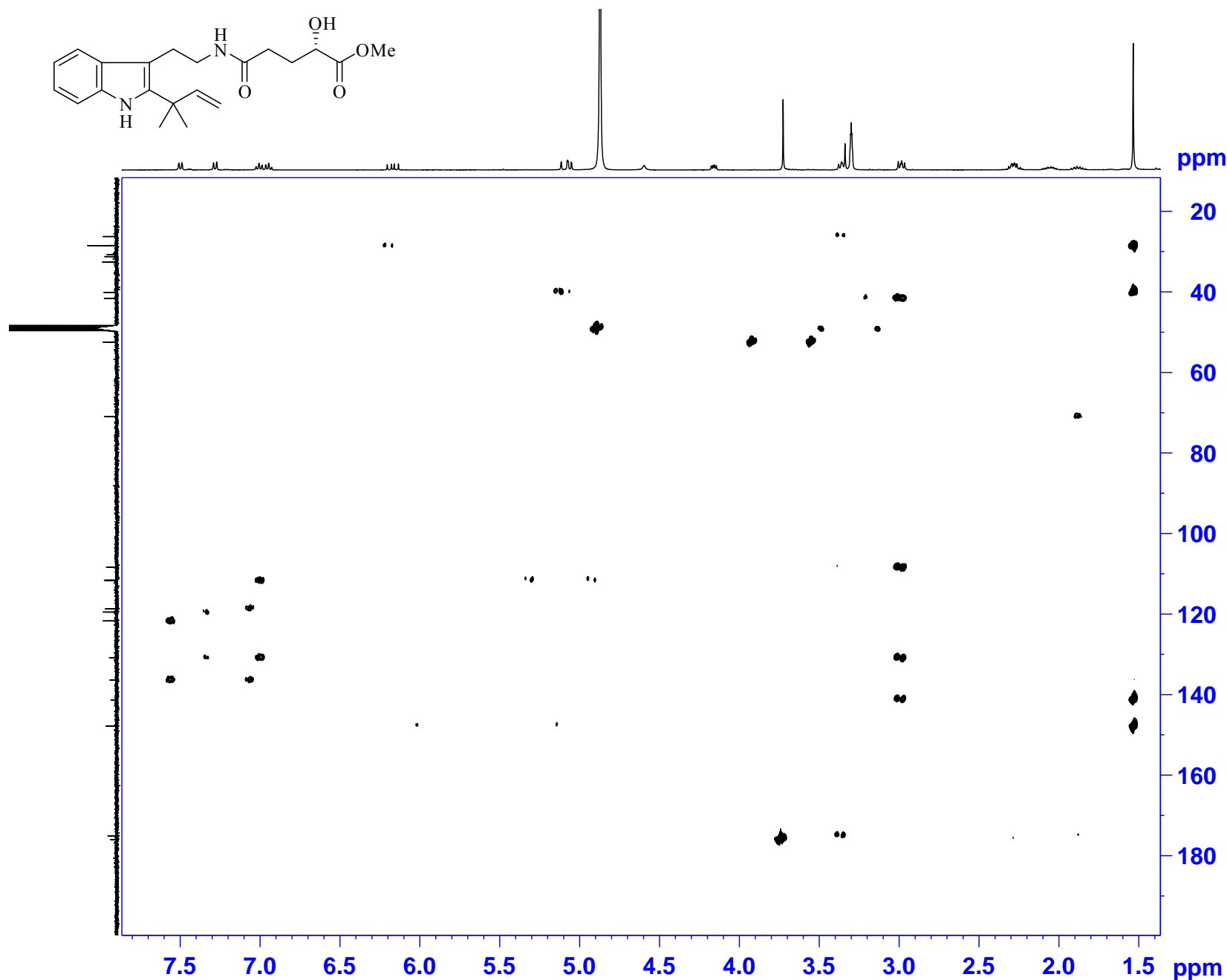
===== CHANNEL f1 =====
 SFO1 400.1318006 MHz
 NUC1 1H
 P1 13.90 usec
 ND0 1
 TD 128
 SFO1 400.1318 MHz
 FIDRES 28.143011 Hz
 SW 9.003 ppm
 FmMODE QF
 SI 1024
 SF 400.1300116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 400.1300116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0

Figure S19. HMBC NMR spectrum of 3 in MeOH-d₄

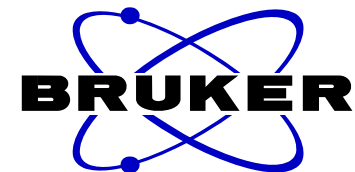
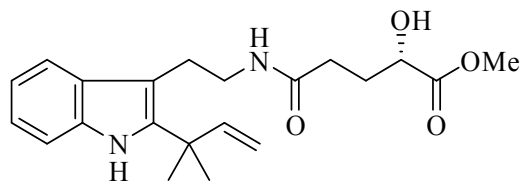


NAME HB2-12 M 3mg
 EXPNO 6
 PROCNO 1
 Date_ 20200809
 Time 21.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG hmbcgpndqf
 TD 4096
 SOLVENT MeOD
 NS 64
 DS 16
 SWH 3597.122 Hz
 FIDRES 0.878204 Hz
 AQ 0.5693940 sec
 RG 203
 DW 139.000 usec
 DE 6.50 usec
 TE 295.9 K
 CNST13 8.0000000
 D0 0.00000300 sec
 D1 1.50000000 sec
 D6 0.06250000 sec
 D16 0.00020000 sec
 IN0 0.00002480 sec

===== CHANNEL f1 =====
 SFO1 400.1318006 MHz
 NUC1 1H
 P1 13.90 usec
 P2 27.80 usec
 ND0 2
 TD 128
 SFO1 100.6228 MHz
 FIDRES 157.510086 Hz
 SW 200.365 ppm
 FnMODE QF
 SI 1024
 SF 400.1300116 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40
 SI 1024
 MC2 QF
 SF 100.6126277 MHz
 WDW SINE
 SSB 0
 LB 0.00 Hz
 GB 0



HB2-12 M 3mg NOE



NAME HB2-12 M 3mg
 EXPNO 7
 PROCNO 1
 Date_ 20200810
 Time 2.13
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG noesygpphpp
 TD 2048
 SOLVENT MeOD
 NS 32
 DS 32
 SWH 3597.122 Hz
 FIDRES 1.756407 Hz
 AQ 0.2847220 sec
 RG 203
 DW 139.000 usec
 DE 6.50 usec
 TE 296.0 K
 D0 0.00012110 sec
 D1 2.00000000 sec
 D8 0.30000001 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 D16 0.00020000 sec
 IN0 0.00027760 sec

===== CHANNEL f1 =====
 SFO1 400.1318006 MHz
 NUC1 1H
 P1 13.90 usec
 P2 27.80 usec
 P17 2500.00 usec
 ND0 1
 TD 256
 SFO1 400.1318 MHz
 FIDRES 14.071506 Hz
 SW 9.003 ppm
 FnmODE States-TPPI
 SI 1024
 SF 400.1300116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0
 PC 1.00
 SI 1024
 MC2 States-TPPI
 SF 400.1300116 MHz
 WDW QSINE
 SSB 2
 LB 0.00 Hz
 GB 0

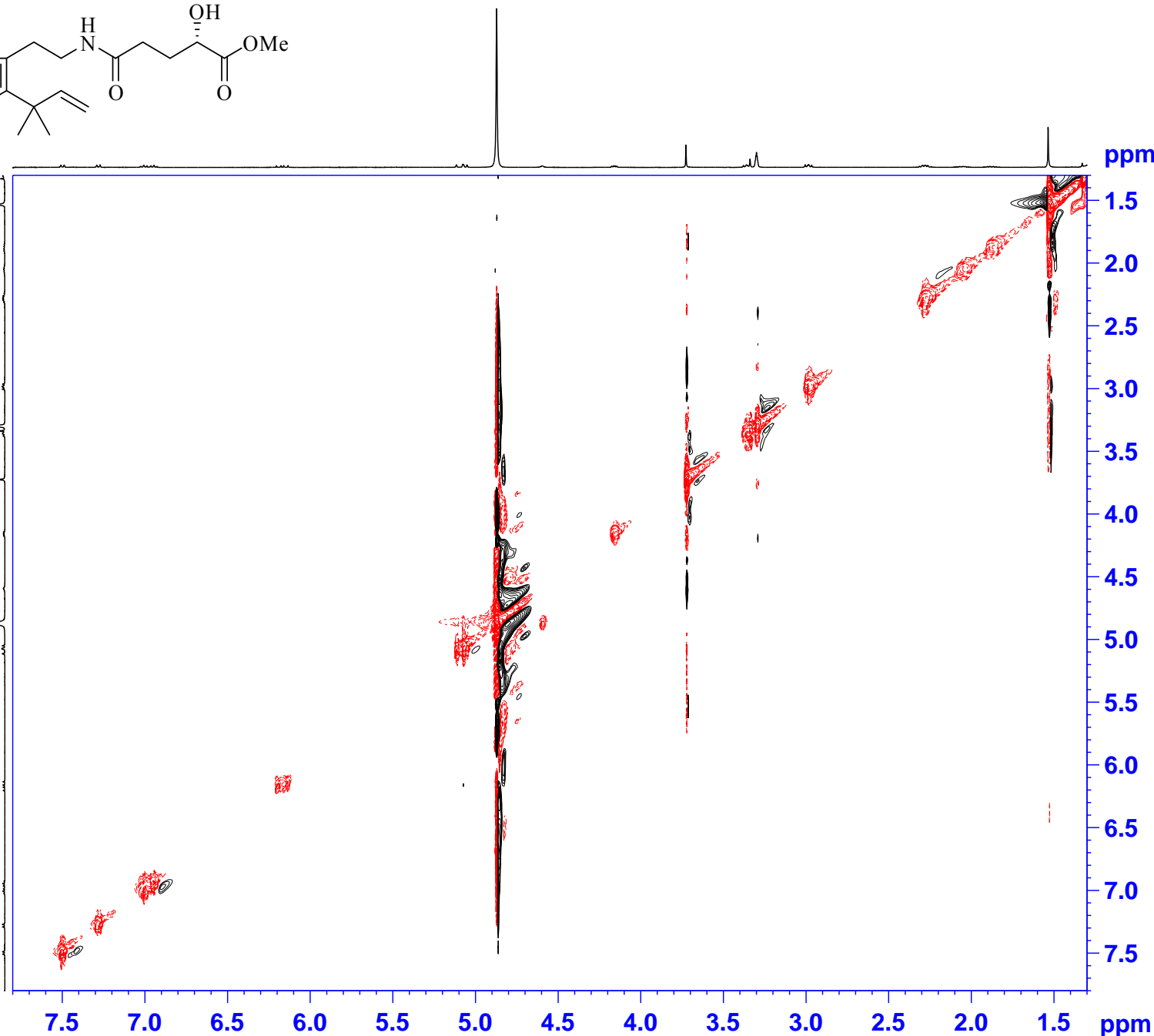


Figure S20. NOESY NMR spectrum of **3** in MeOH- d_4 .

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

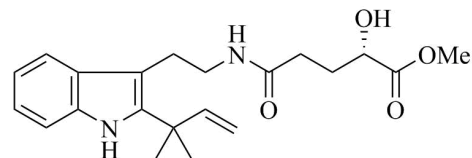
700 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

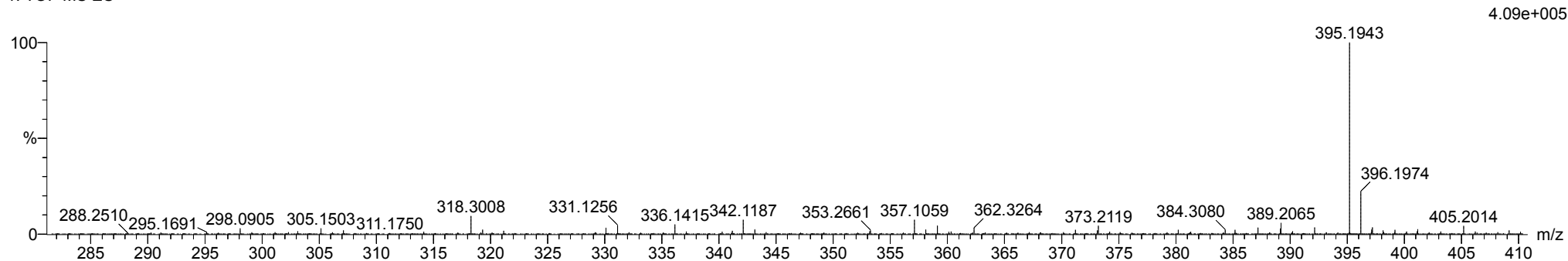
C: 19-20 H: 1-100 N: 0-20 O: 0-30 ²³Na: 0-1

HB 2-12-Oct 92 (0.368)

1: TOF MS ES+

Chemical Formula: C₂₁H₂₈N₂O₄

Molecular Weight: 372.4650

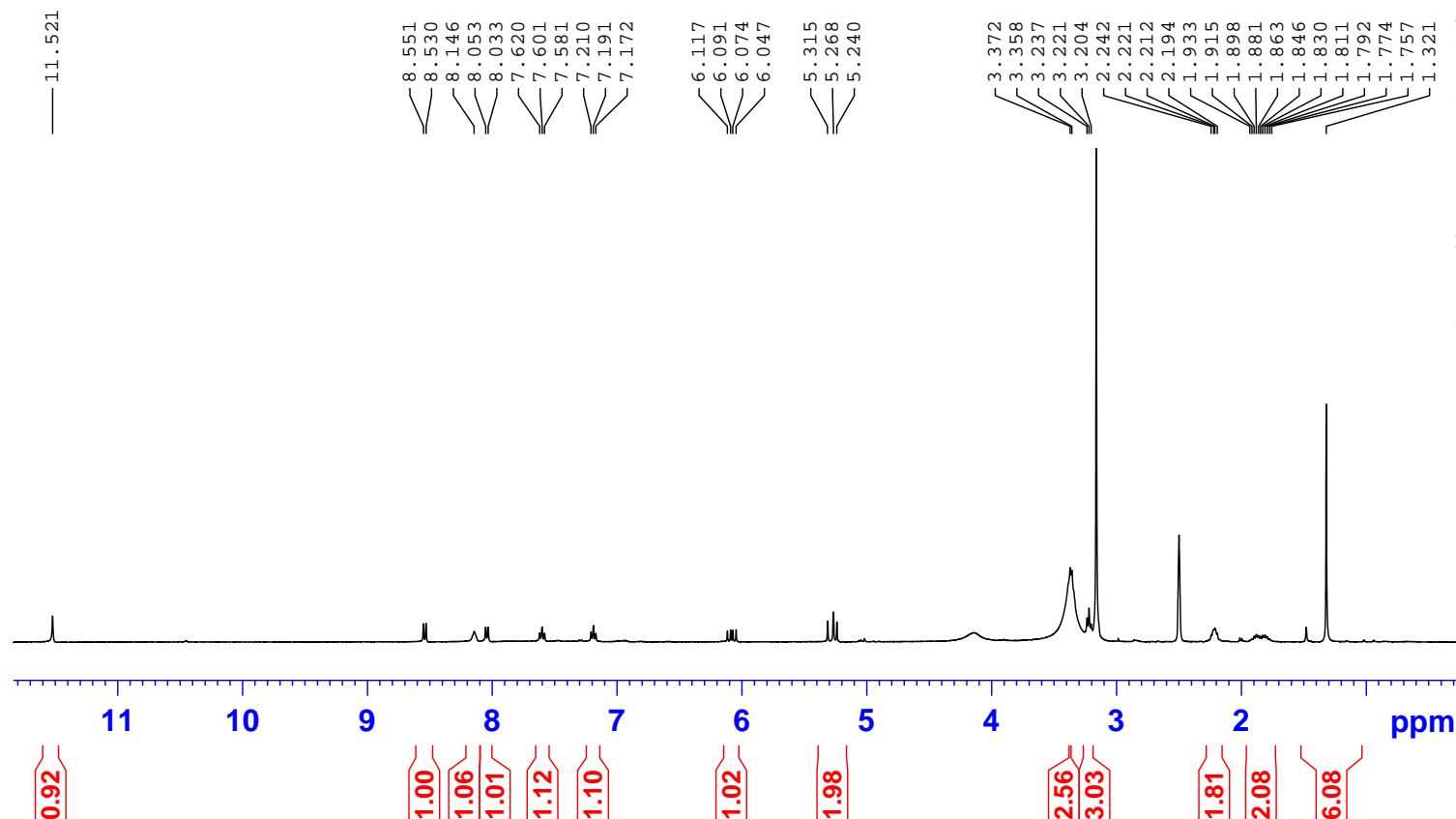
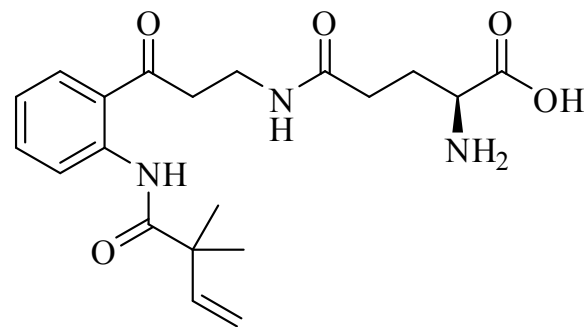
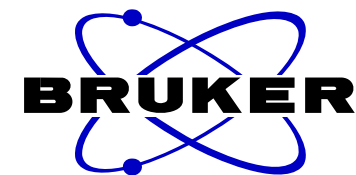


Minimum: -1.5
Maximum: 50.0 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
395.1943	395.1944	-0.1	-0.3	12.5	775.7	n/a	n/a	C19 H23 N8 O2

Figure S21. The HR-ESI-MS spectrum of **3**.

HB4-7 D 2mg H

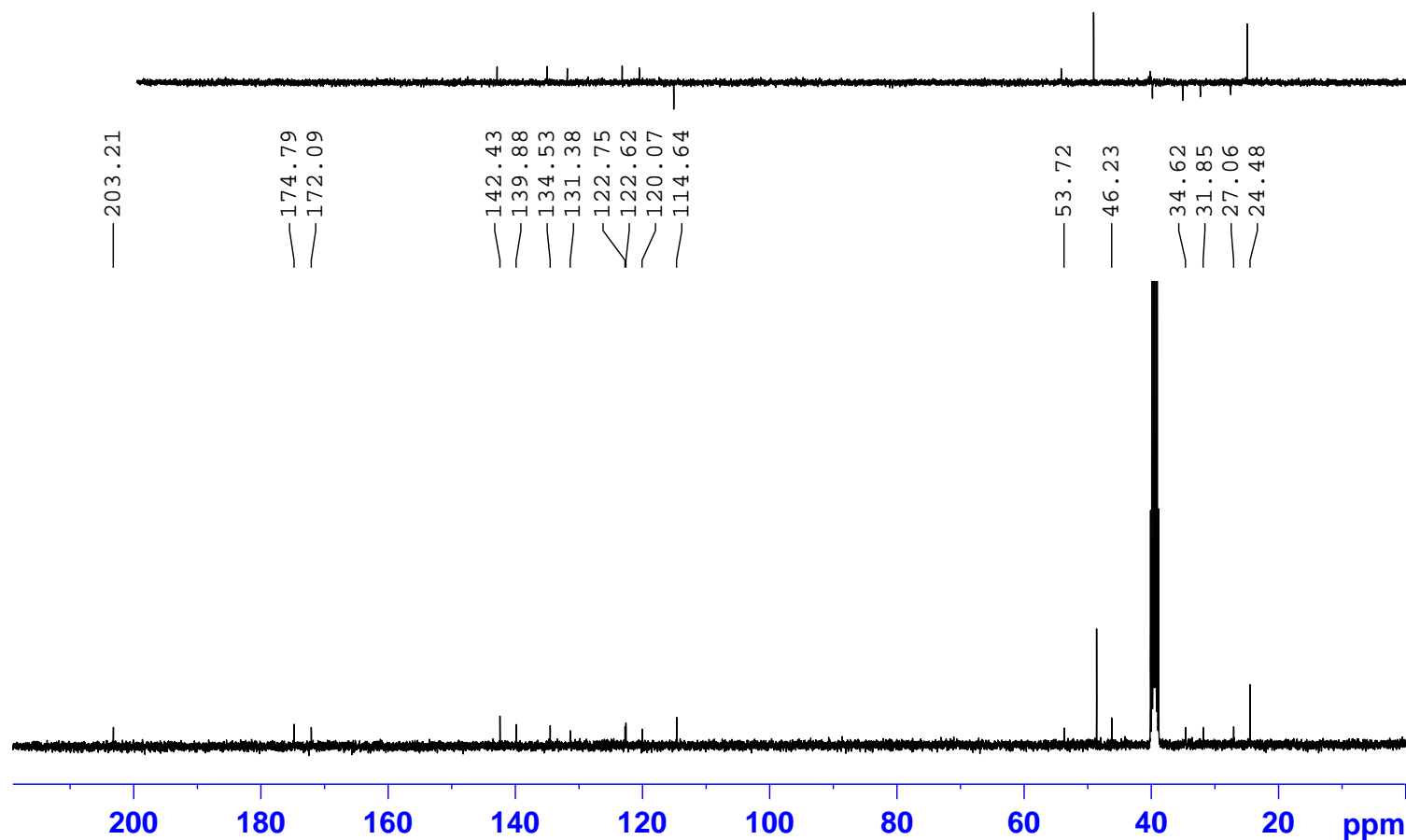
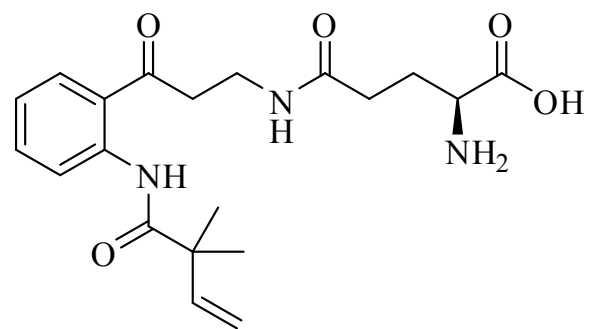
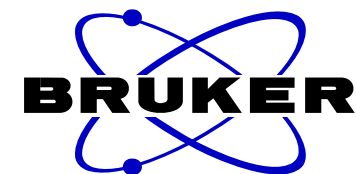


NAME HB4-7 D 2mg
 EXPNO 1
 PROCNO 1
 Date_ 20200108
 Time 20.35
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 19
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 292.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 13.90 usec
 SI 32768
 SF 400.1300028 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S22. ¹H NMR spectrum of 4.

HB4-7 D 2mg C

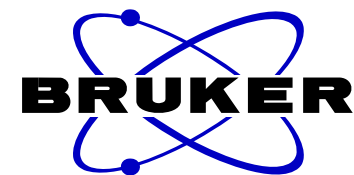


NAME HB4-7 D 2mg
EXPNO 2
PROCNO 1
Date_ 20200108
Time 20.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 711
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 292.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6128133 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S23. ¹³C NMR spectrum of 4.

HB2-13 C 5mg H



NAME HB2-13 C 5mg
EXPNO 1
PROCNO 1
Date_ 20200805
Time 18.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 21
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

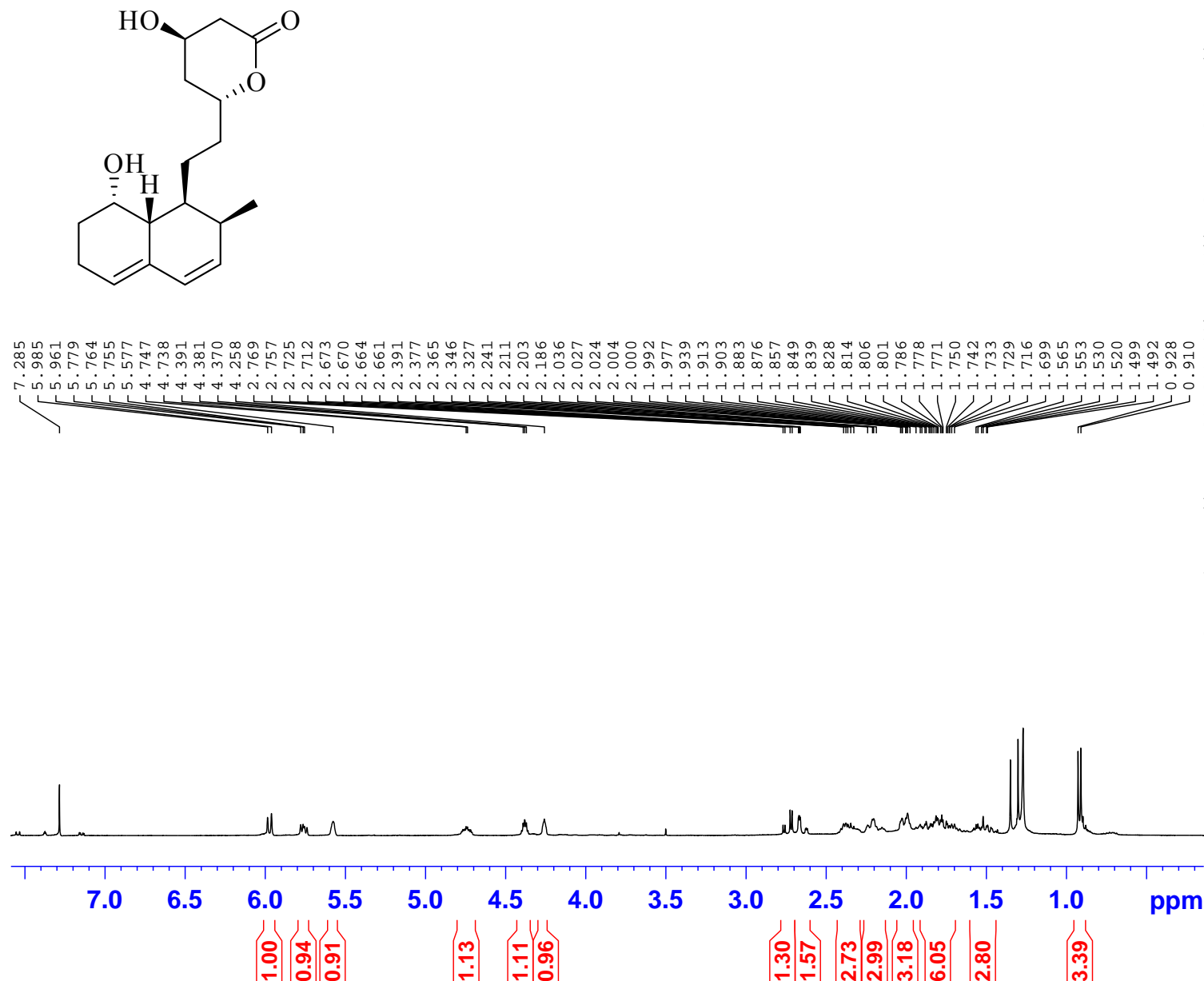
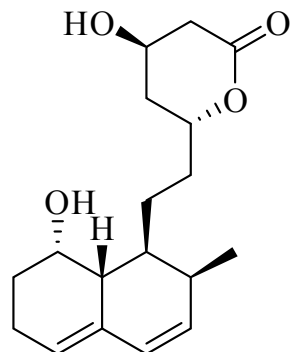
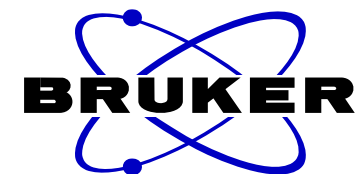


Figure S24. ¹H NMR spectrum of 5.

HB2-13 C 5mg C



NAME HB2-13 C 5mg
 EXPNO 2
 PROCNO 1
 Date_ 20200805
 Time 18.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 524
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 203
 DW 20.800 usec
 DE 6.50 usec
 TE 296.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 100.6228293 MHz
 NUC1 13C
 P1 12.37 usec
 SI 32768
 SF 100.6127717 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

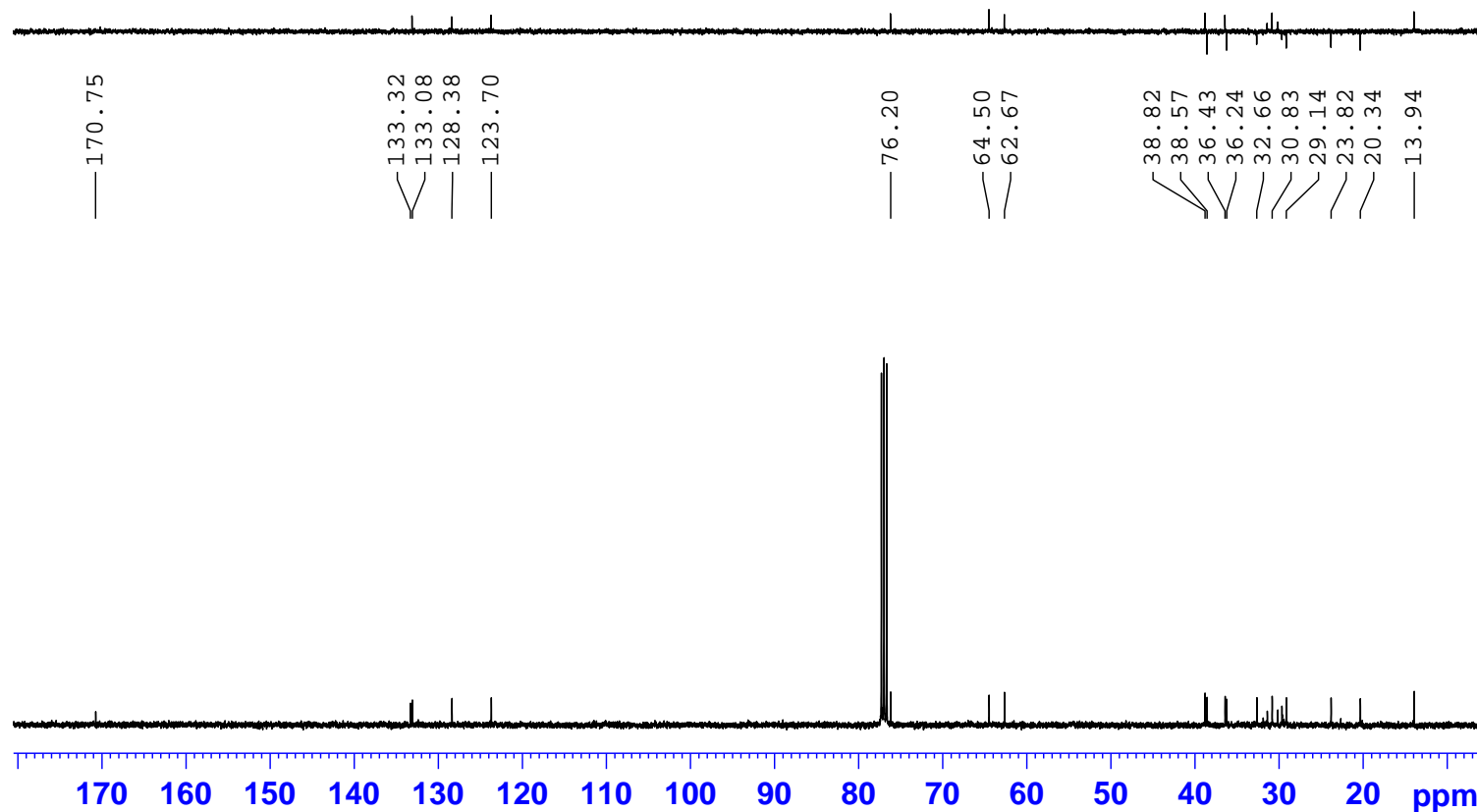
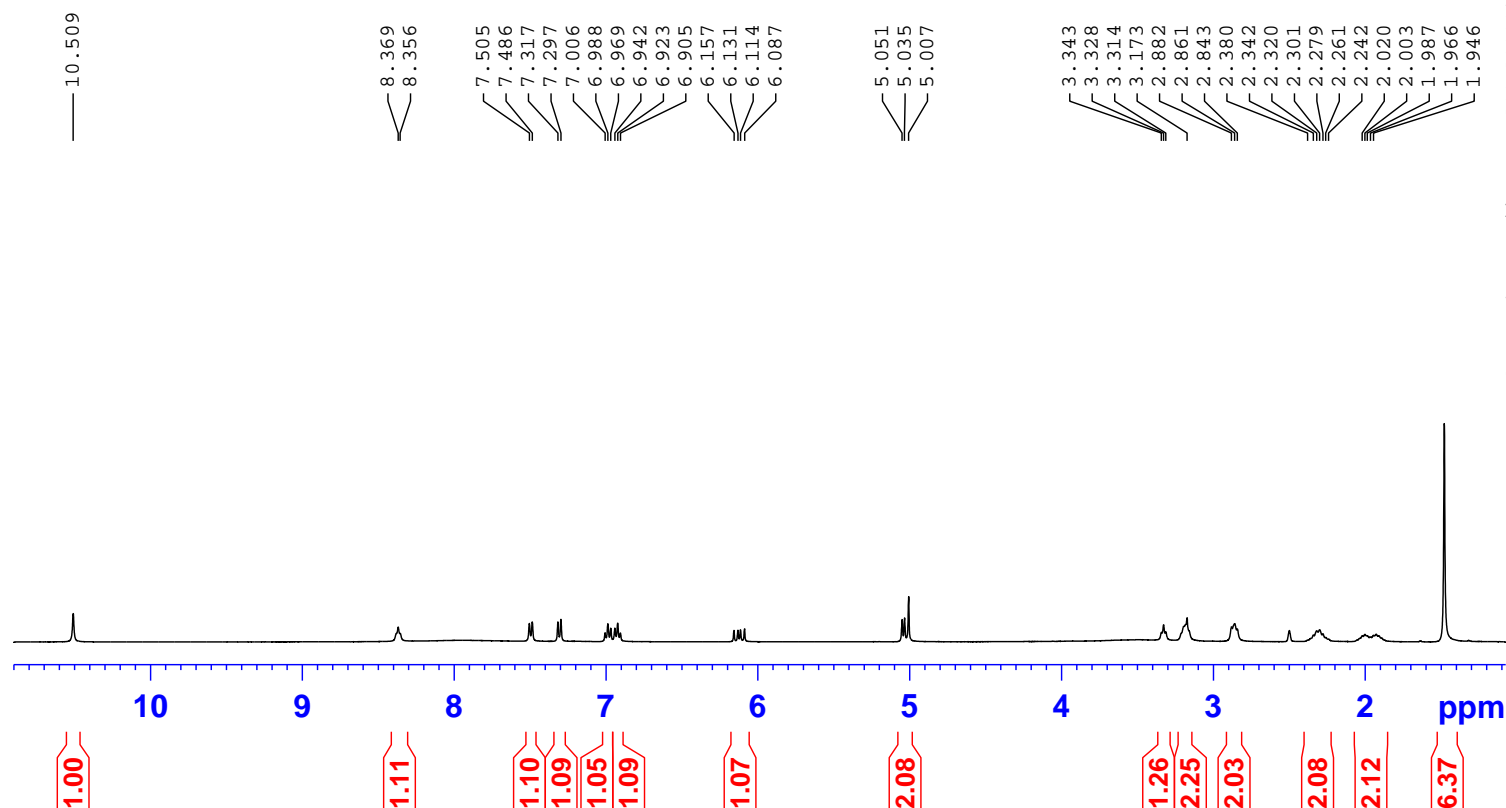
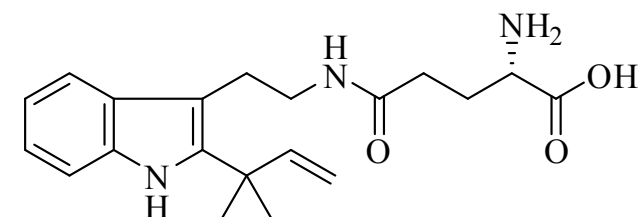
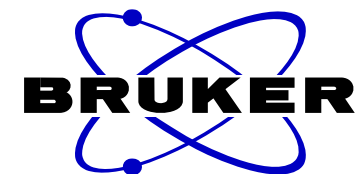


Figure S25. ¹³C NMR spectrum of 5.

HB4-3 D 30mg H

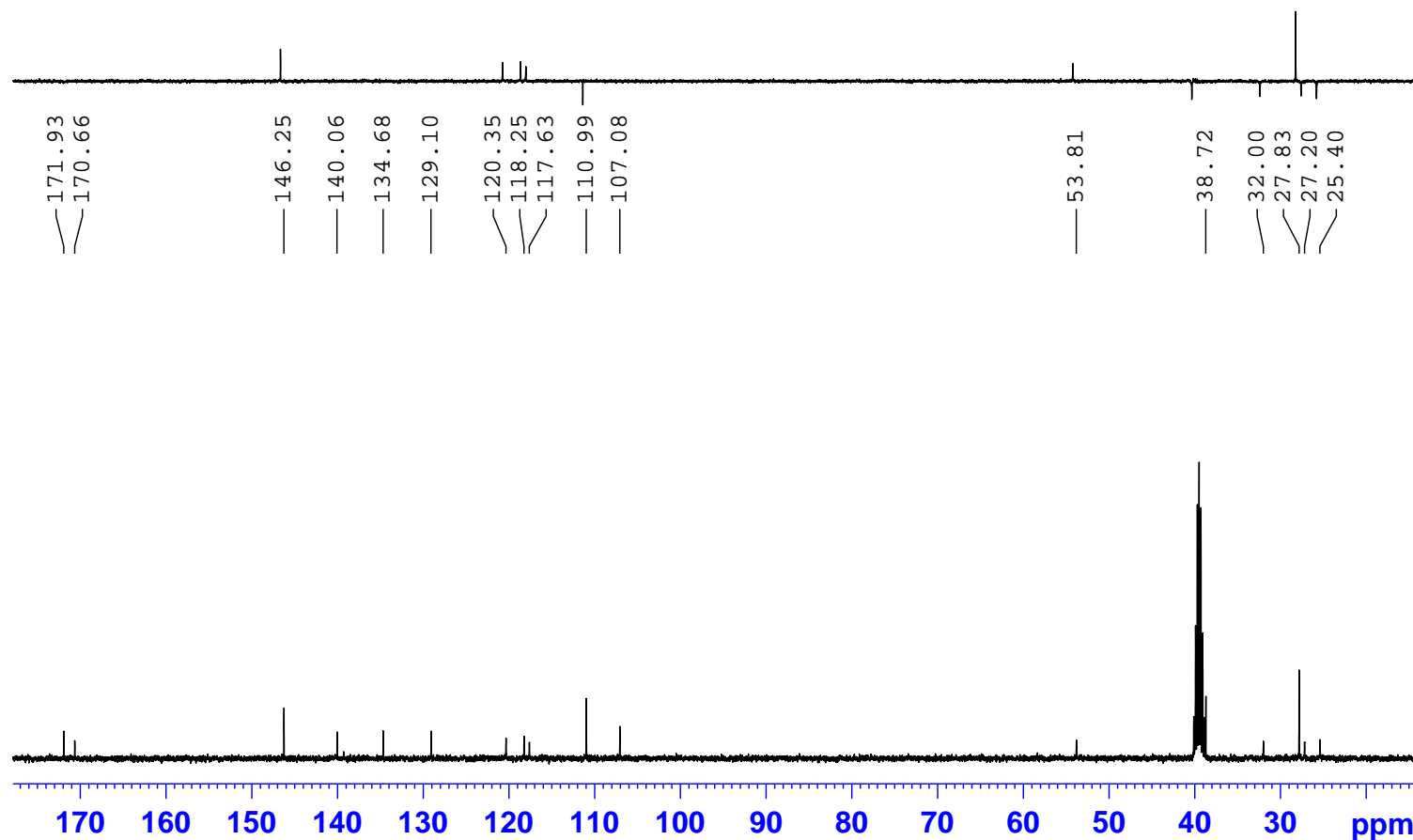
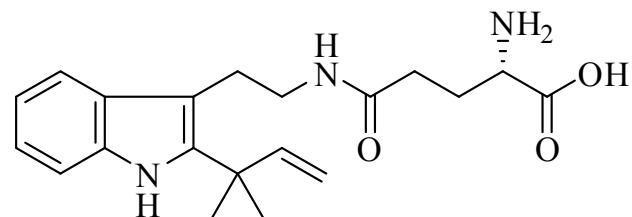
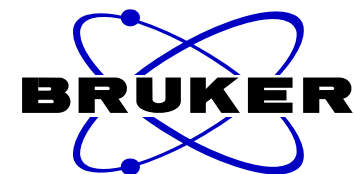


NAME HB4-5-2 D 30mg
 EXPNO 1
 PROCNO 1
 Date_ 20200108
 Time 21.38
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 23
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 71.8
 DW 62.400 usec
 DE 6.50 usec
 TE 292.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 13.90 usec
 SI 32768
 SF 400.1300026 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S26. ¹H NMR spectrum of **6**.

HB4-3 D 30mg C

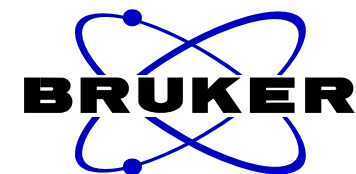
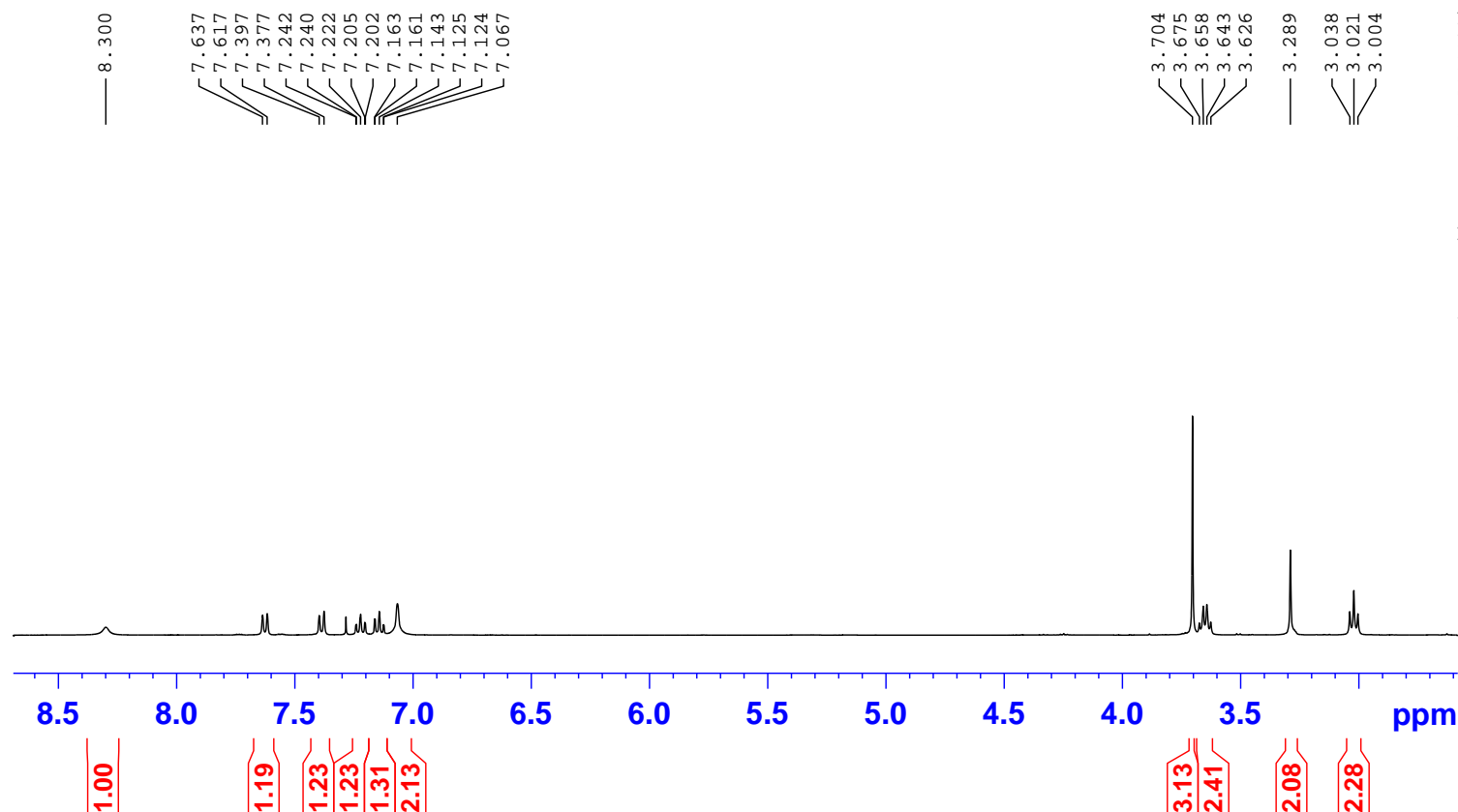
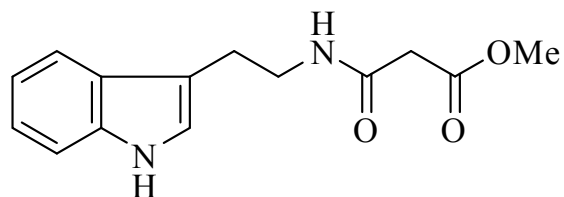


NAME HB4-5-2 D 30mg
EXPNO 2
PROCNO 1
Date_ 20200108
Time 21.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 59
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6128097 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S27. ¹³C NMR spectrum of **6**.

HB2-7 C 12mg H

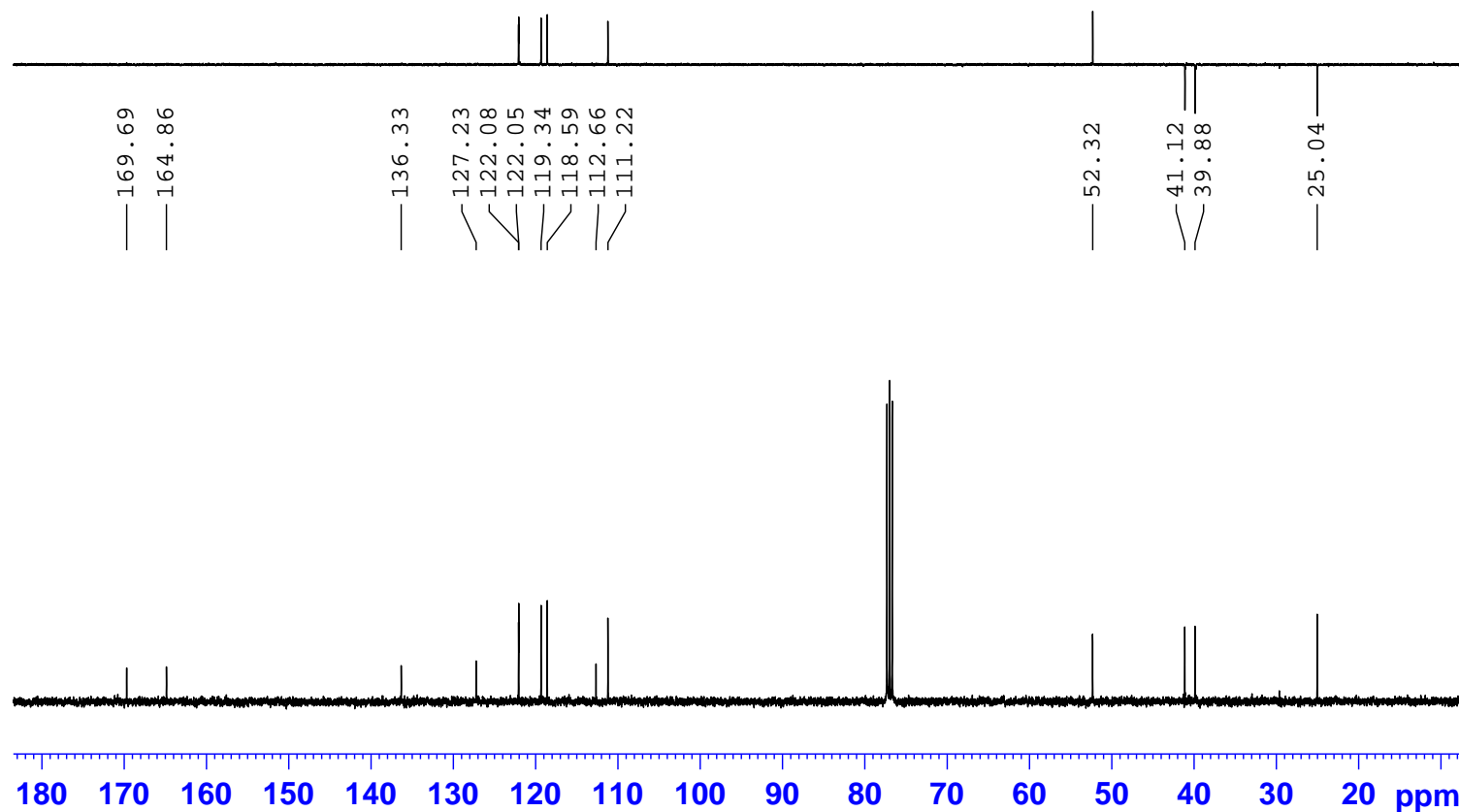
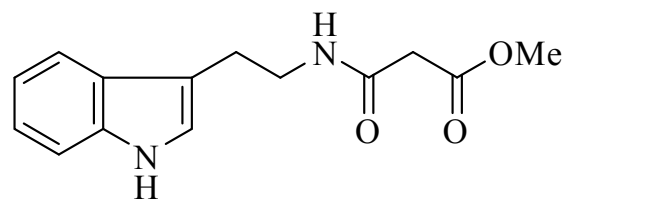
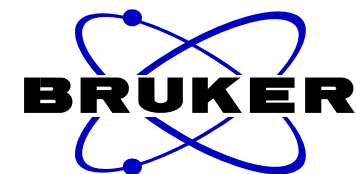


NAME HB2-7 C 12mg
EXPNO 1
PROCNO 1
Date_ 20200801
Time 9.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 18
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S28. ¹H NMR spectrum of 7.

HB2-7 C 12mg C

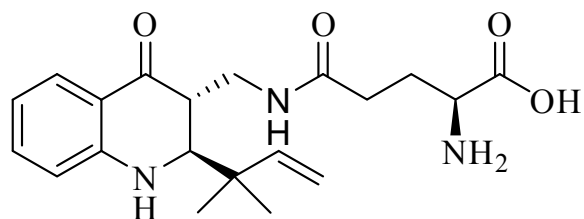
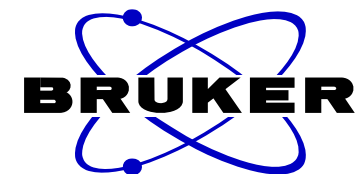


NAME HB2-7 C 12mg
EXPNO 2
PROCNO 1
Date_ 20200801
Time 9.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 102
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6127766 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S29. ¹³C NMR spectrum of 7.

HB5-6 M 10mg H



7.521
7.504
7.501
7.254
7.250
7.233
7.216
7.212
6.726
6.705
6.512
6.493
6.475

5.733
5.706
5.689
5.662

4.971
4.952
4.926

3.604
3.591
3.397
3.377
3.364
3.343
3.324
2.828
2.809
2.790
2.418
2.401
2.384
2.085
2.071

0.998
0.940

NAME HB5-6 M 10mg
EXPNO 1
PROCNO 1
Date_ 20200712
Time 13.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

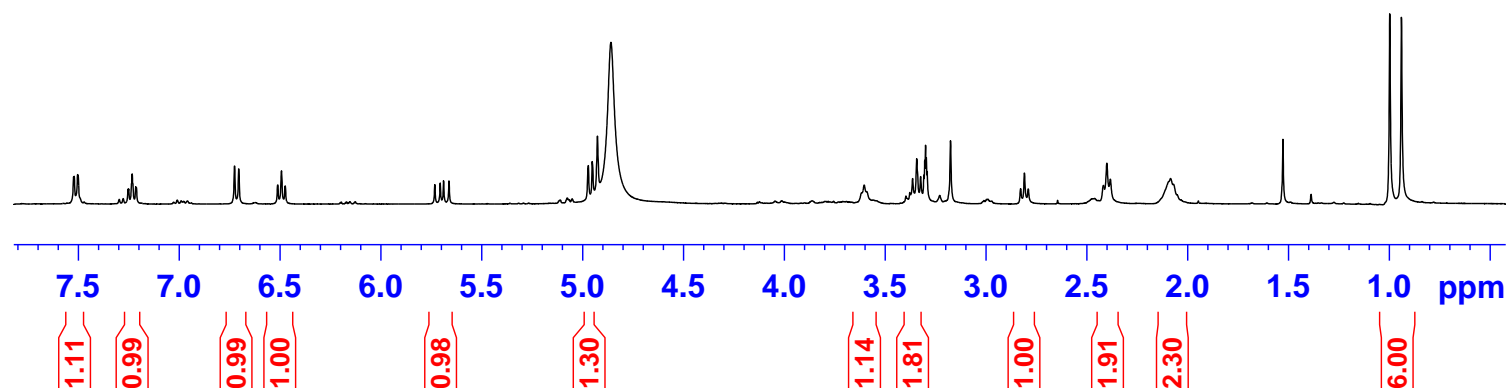
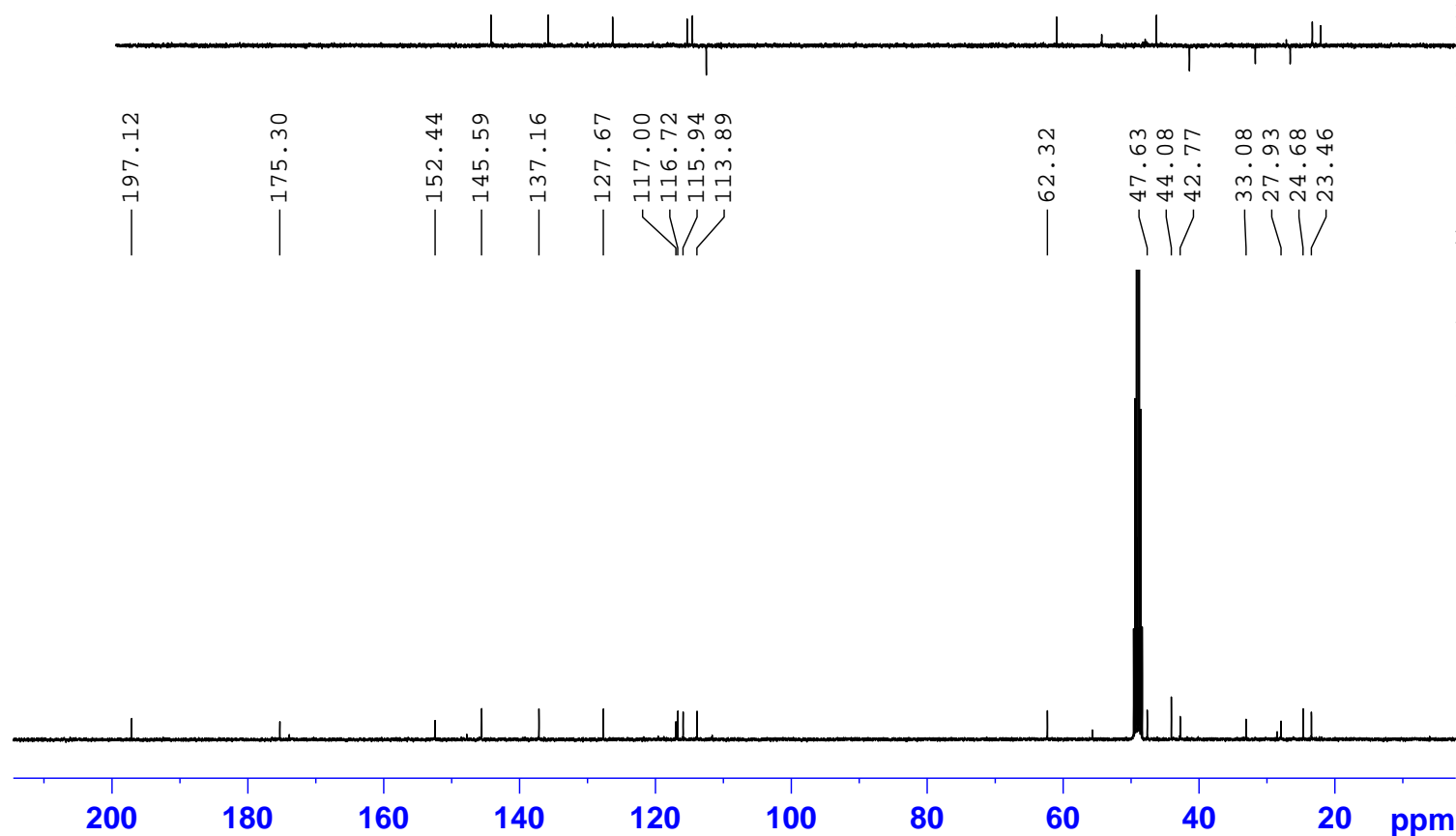
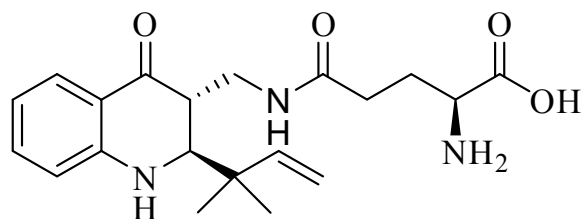
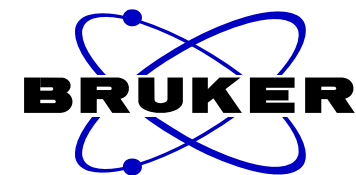


Figure S30. ¹H NMR spectrum of **8**.

HB5-6 M 10mg C

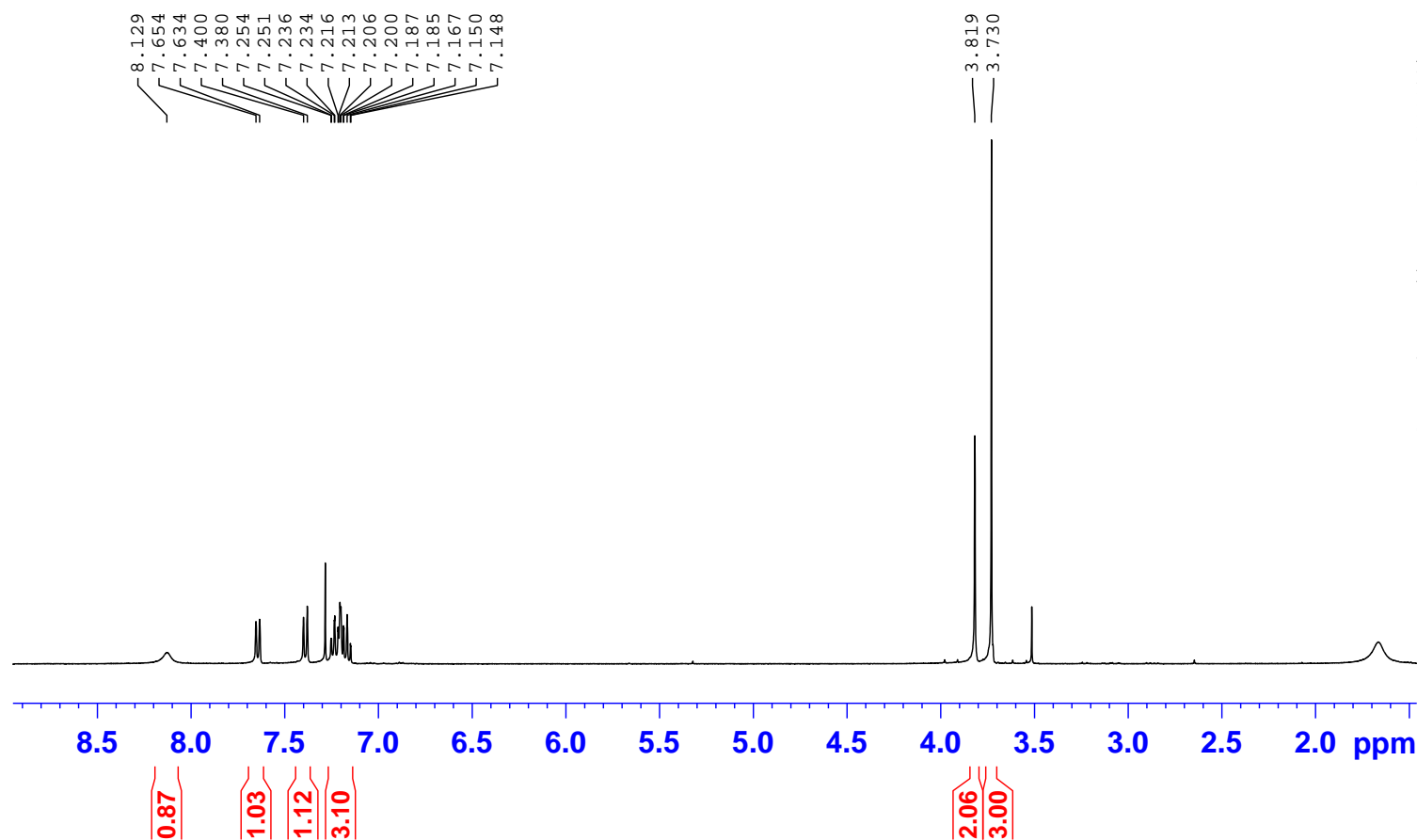
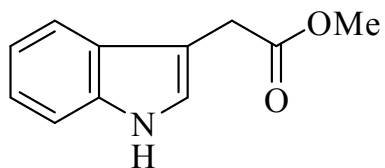
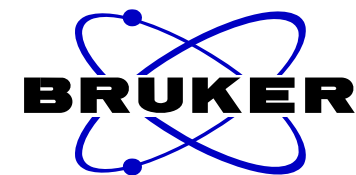


NAME HB5-6 M 10mg
EXPNO 2
PROCNO 1
Date_ 20200712
Time 13.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 424
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126303 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S31. ^{13}C NMR spectrum of **8**.

HB2-8 C 2mg H

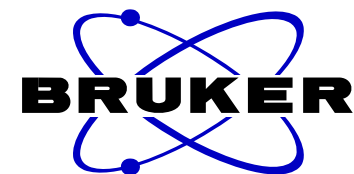
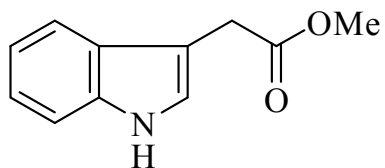


NAME HB2-8 C 2mg
EXPNO 1
PROCNO 1
Date_ 20200801
Time 10.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 15
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S32. ¹H NMR spectrum of **9**.

HB2-8 C 2mg C



NAME HB2-8 C 2mg
EXPNO 2
PROCNO 1
Date_ 20200801
Time 10.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 530
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

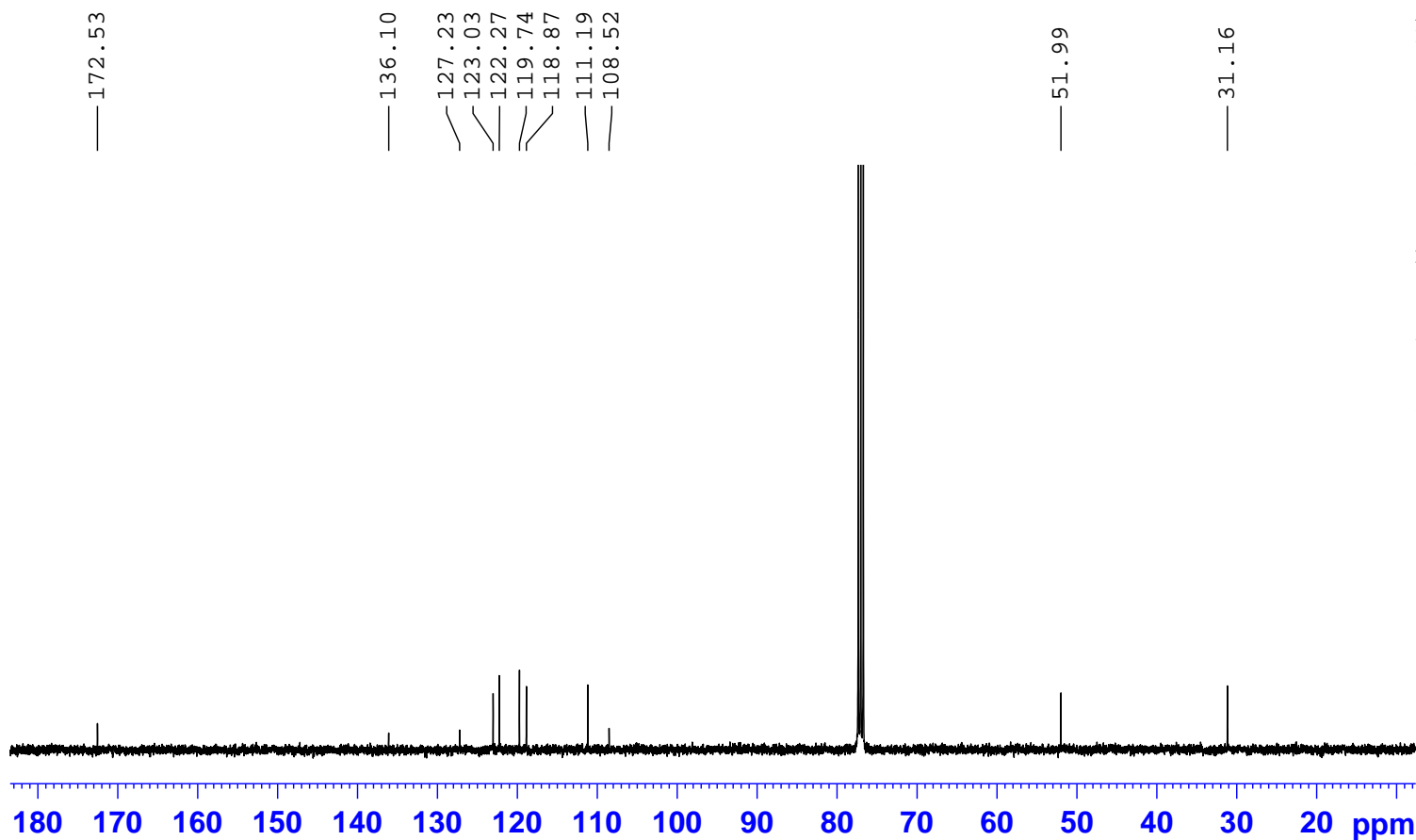
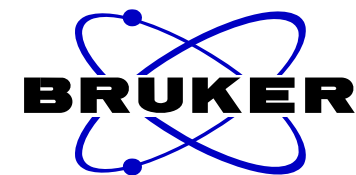
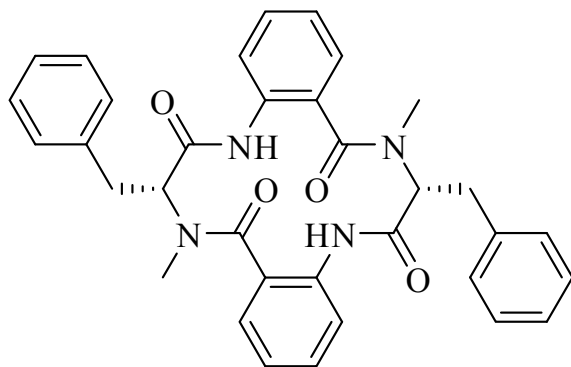


Figure S33. ^{13}C NMR spectrum of **9**.

HB-C14 M 127mg H



NAME HB-C14 M 127mg
 EXPNO 1
 PROCNO 1
 Date_ 20200910
 Time 20.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 10
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 32
 DW 62.400 usec
 DE 6.50 usec
 TE 296.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 13.90 usec
 SI 32768
 SF 400.1300113 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

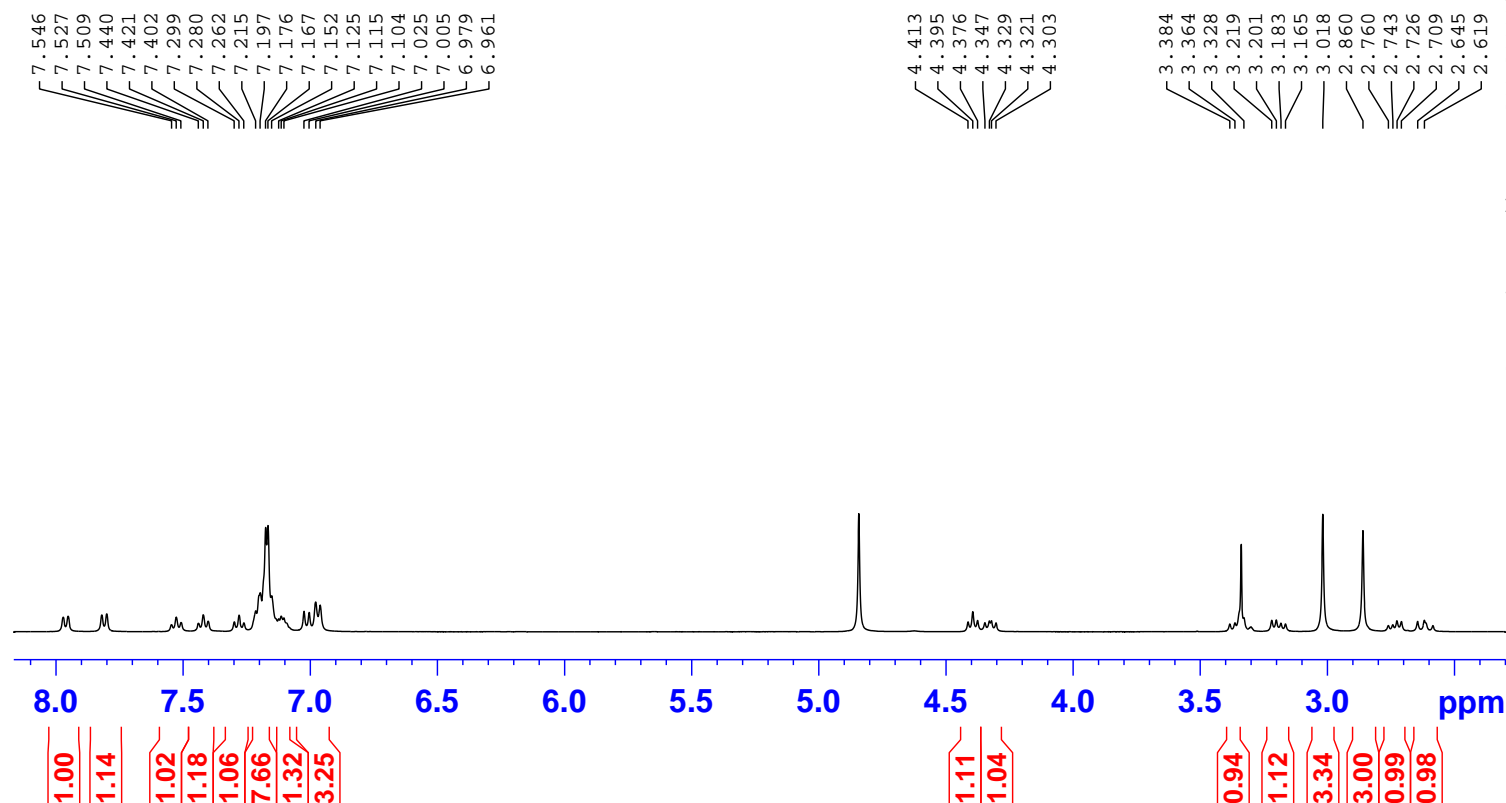
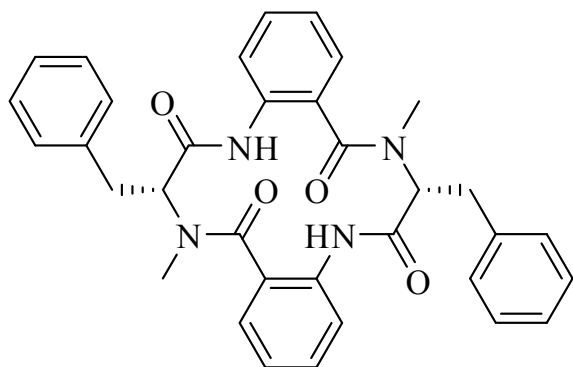
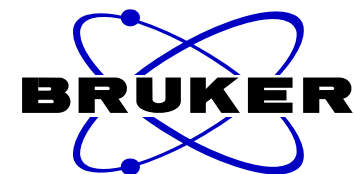
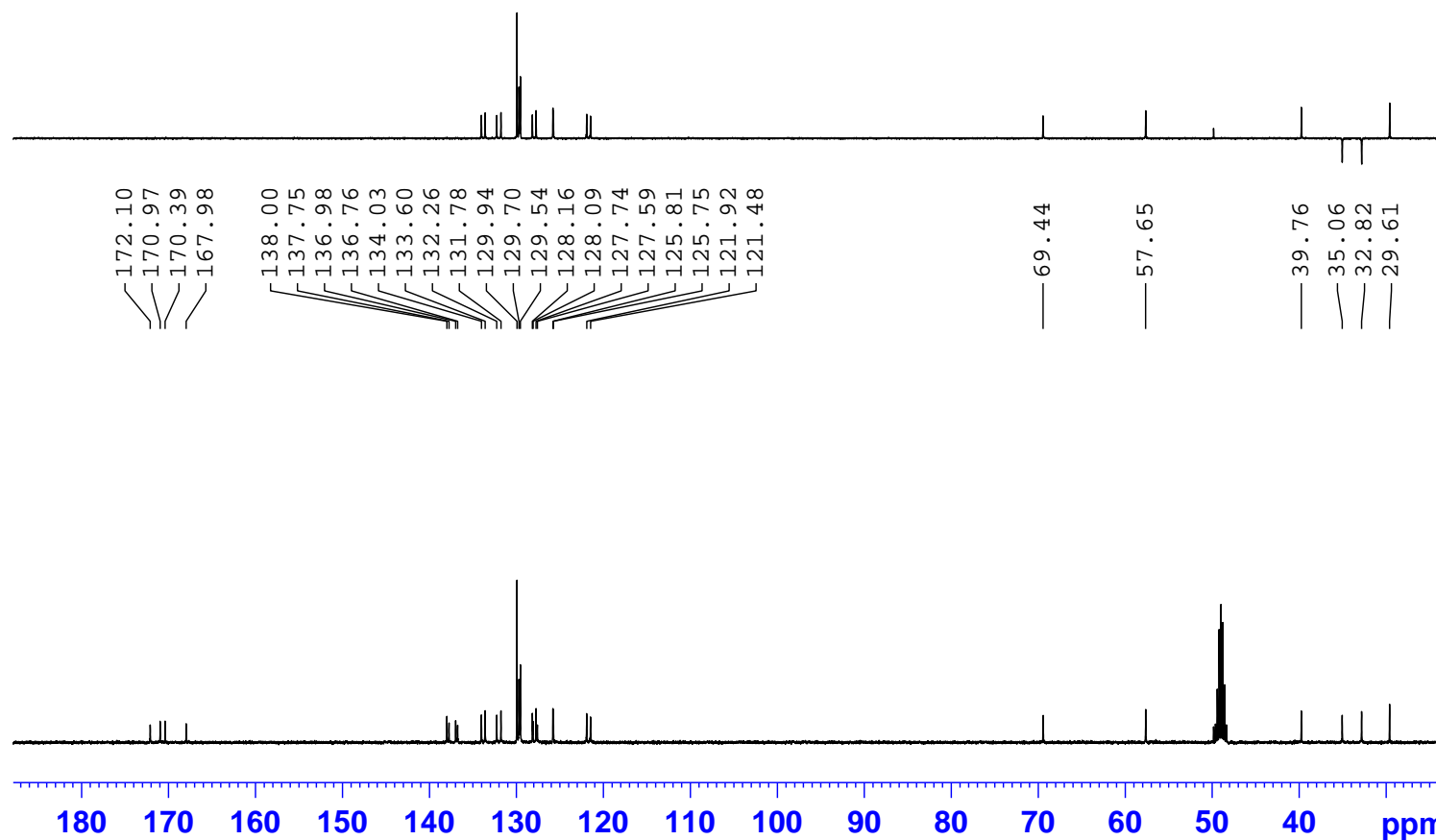


Figure S34. ¹H NMR spectrum of **10**.

HB-C14 M 127mg C



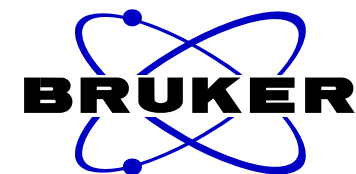
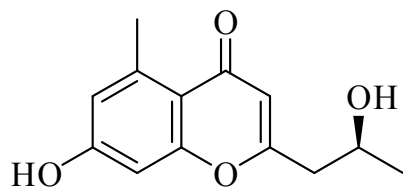
NAME HB-C14 M 127mg
EXPNO 2
PROCNO 1
Date_ 20200910
Time 20.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 46
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



===== CHANNEL f1 =====
SF01 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126497 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S35. ¹³C NMR spectrum of **10**.

HB-C8 M 2mg H



NAME HB-C8 M 2mg
EXPNO 1
PROCNO 1
Date_ 20200903
Time 20.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

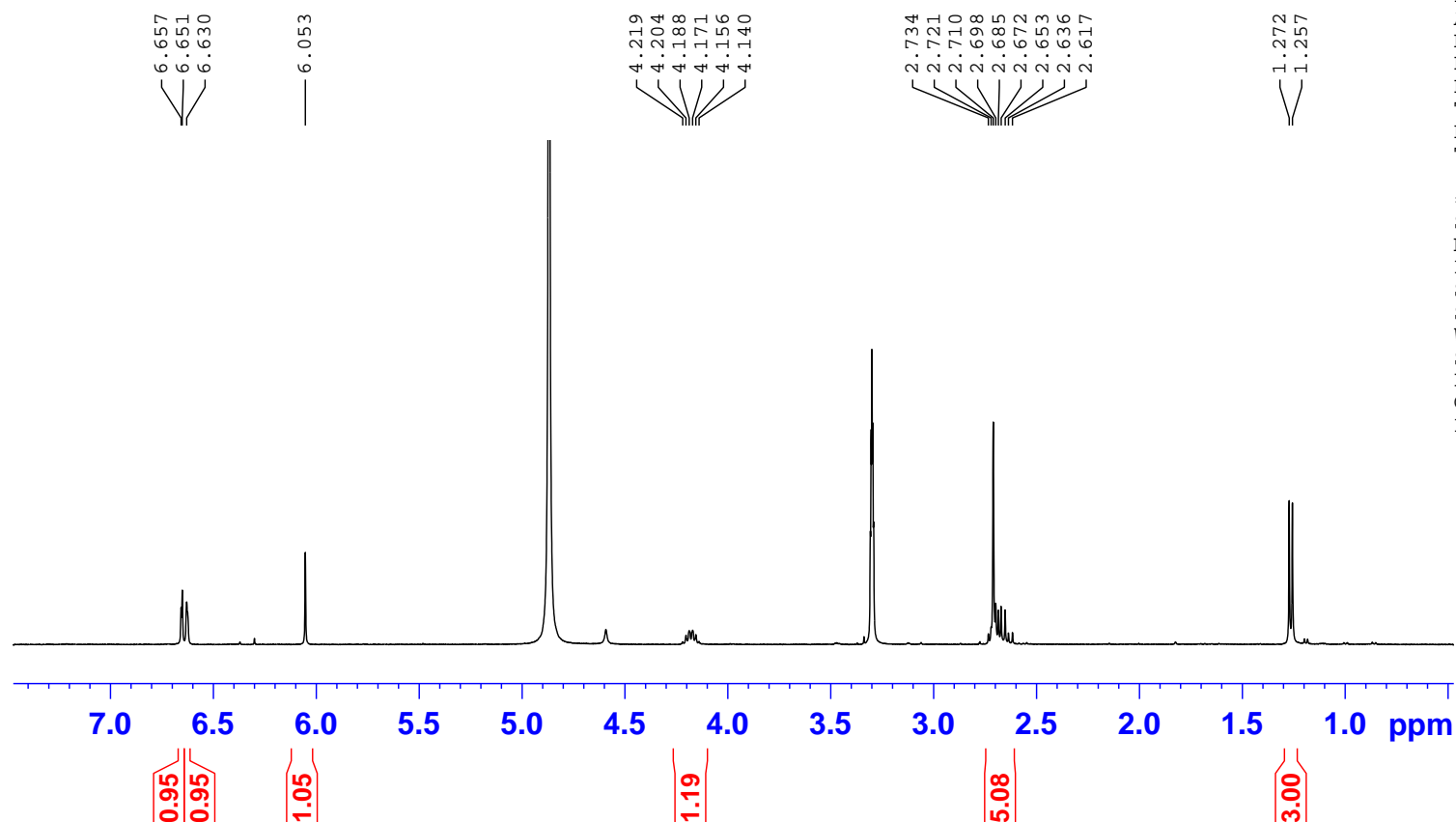
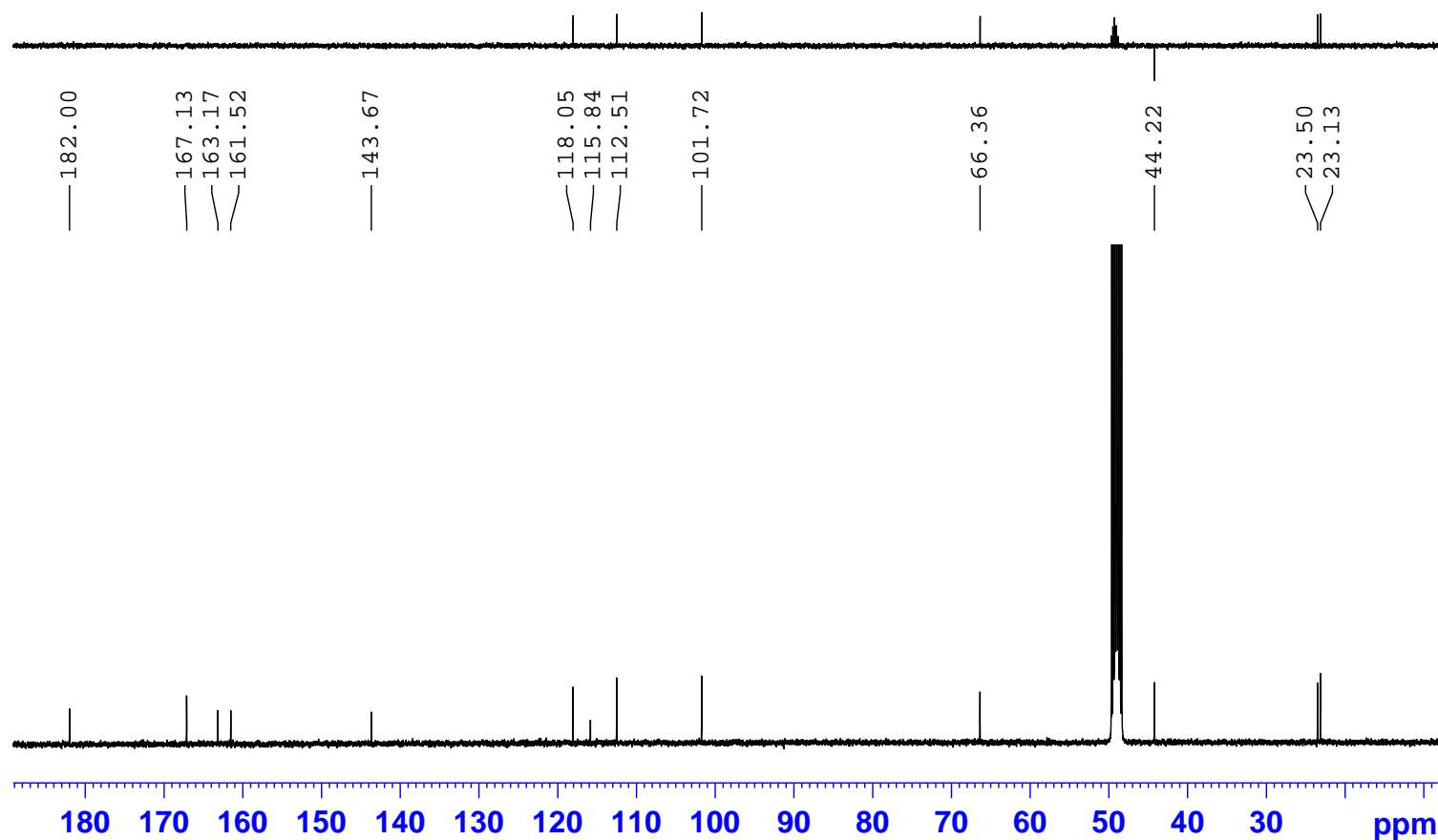
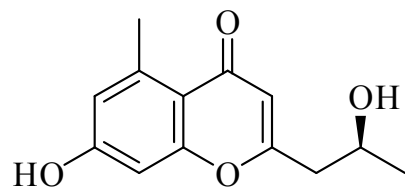
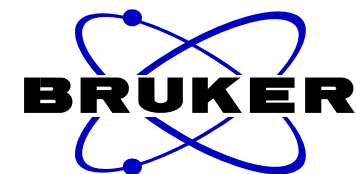


Figure S36. ¹H NMR spectrum of **11**.

HB-C8 M 2mg C

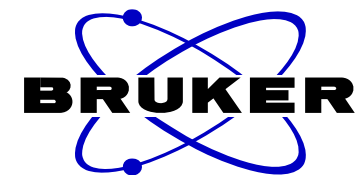
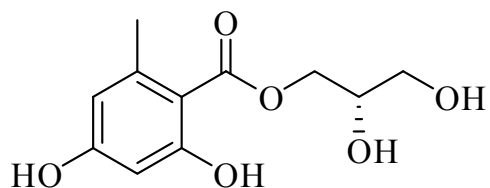


NAME HB-C8 M 2mg
EXPNO 2
PROCNO 1
Date_ 20200903
Time 21.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 10240
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126266 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S37. ¹³C NMR spectrum of **11**.

HB2-3 M 2mg H



NAME HB2-3 M 2mg
EXPNO 1
PROCNO 1
Date_ 20200726
Time 17.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 24
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

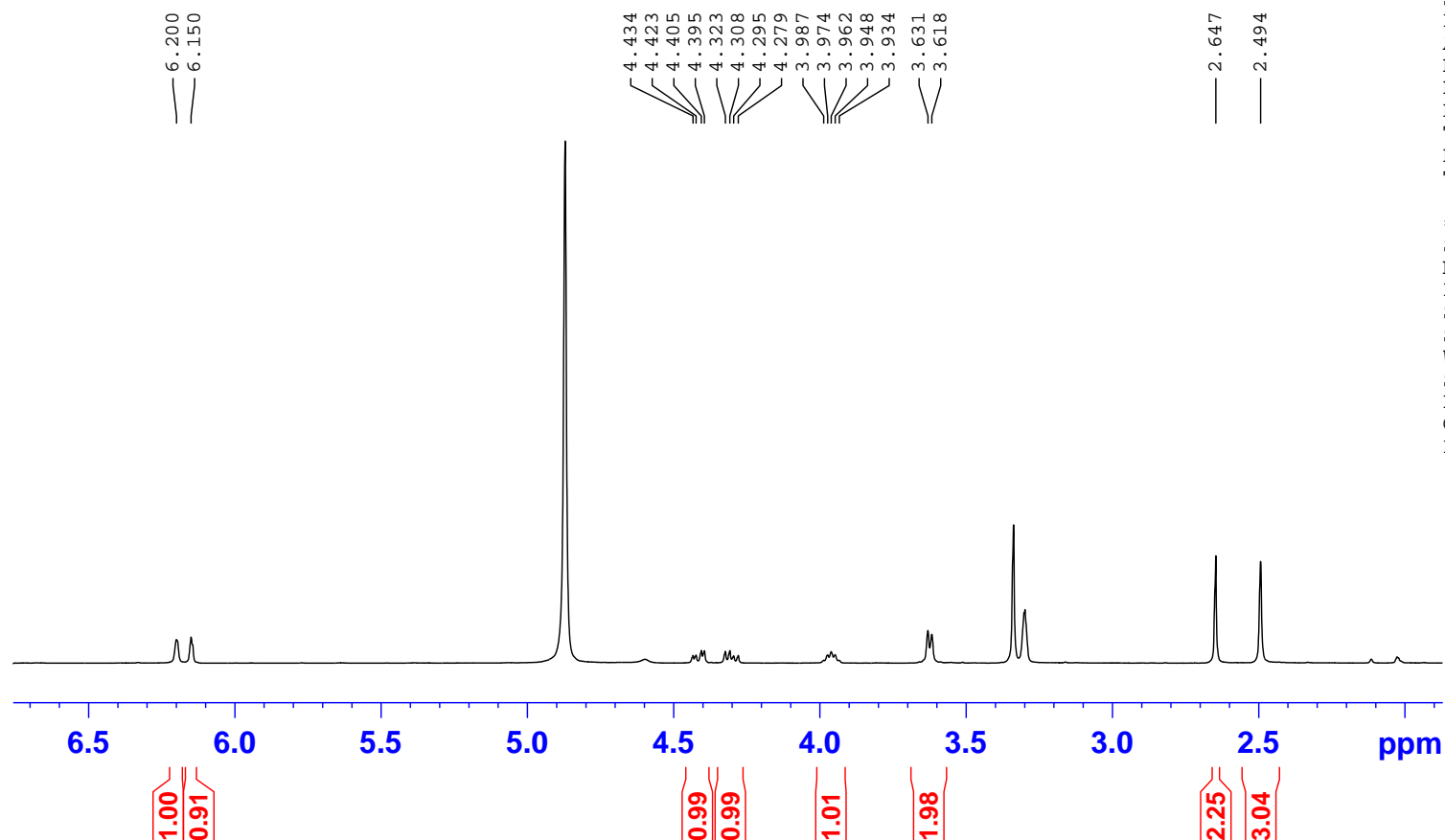
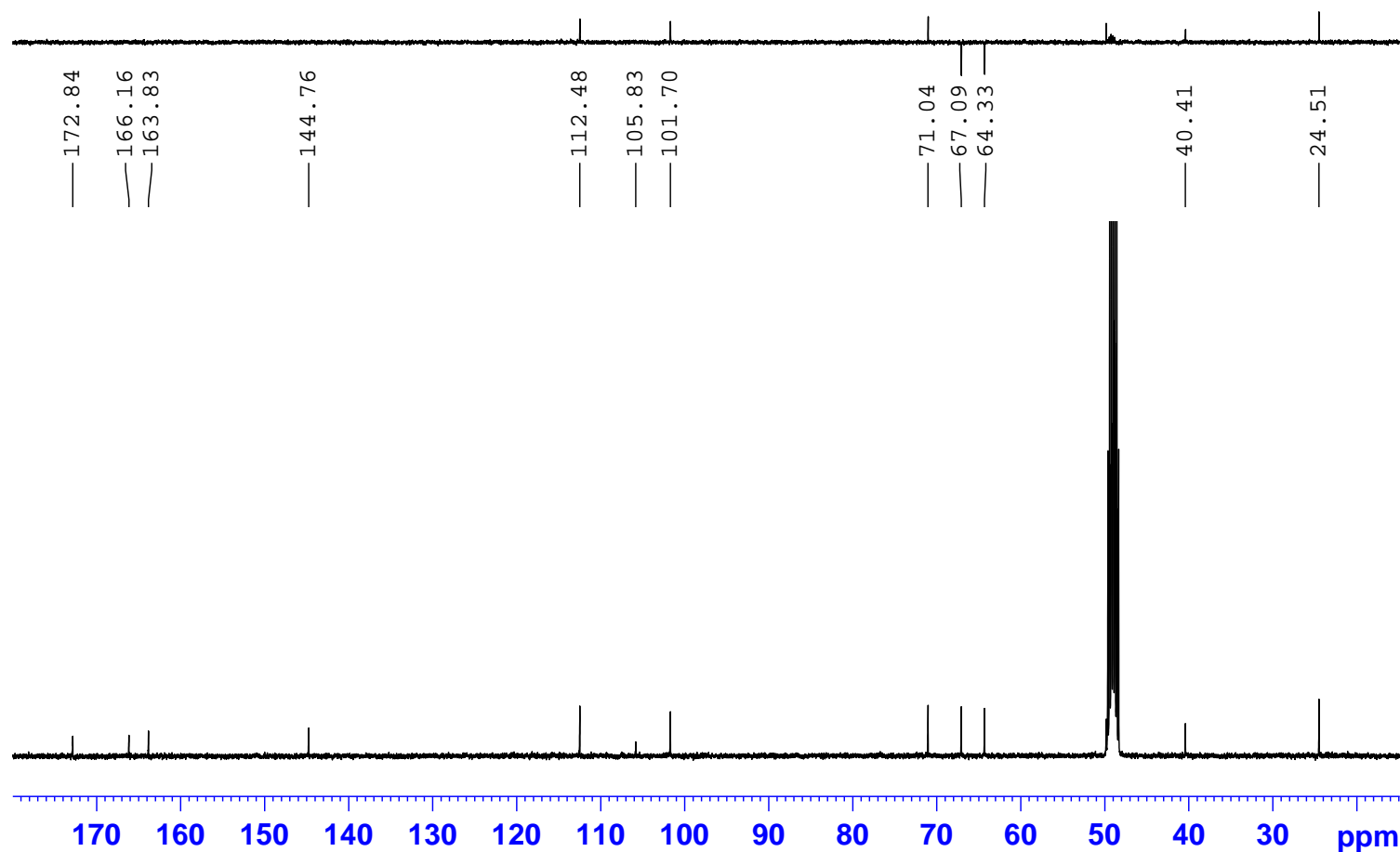
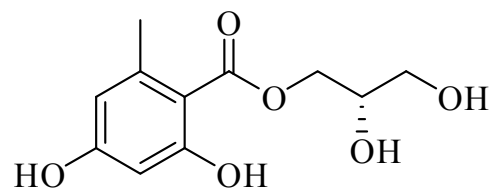
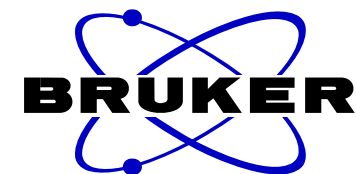


Figure S38. ¹H NMR spectrum of **12**.

HB2-3 M 2mg C

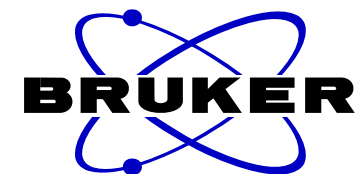
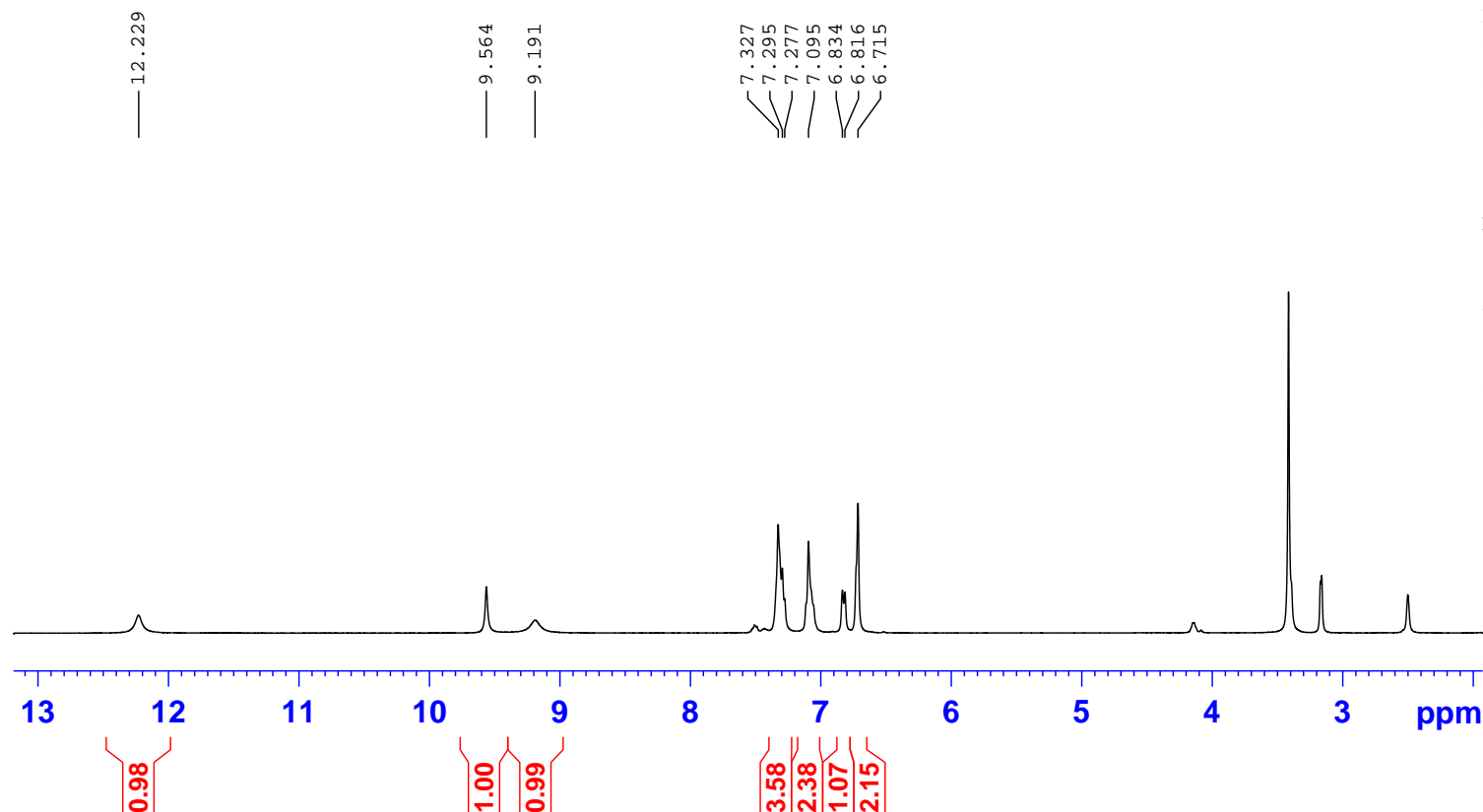
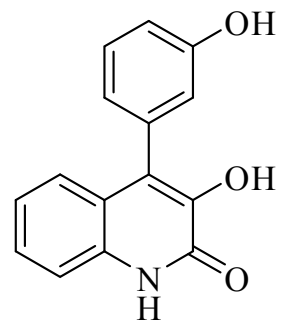


NAME HB2-3 M 2mg
EXPNO 2
PROCNO 1
Date_ 20200726
Time 17.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 2767
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126282 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S39. ¹³C NMR spectrum of **12**.

HB-1 D 16mg H

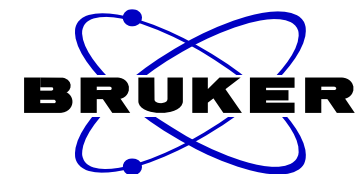
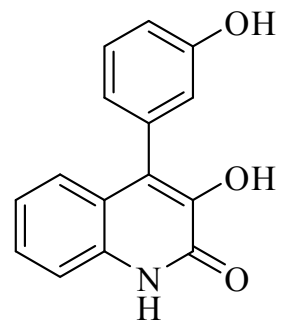


NAME HB1-1 D 16mg
EXPNO 1
PROCNO 1
Date_ 20191224
Time 18.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 15
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1

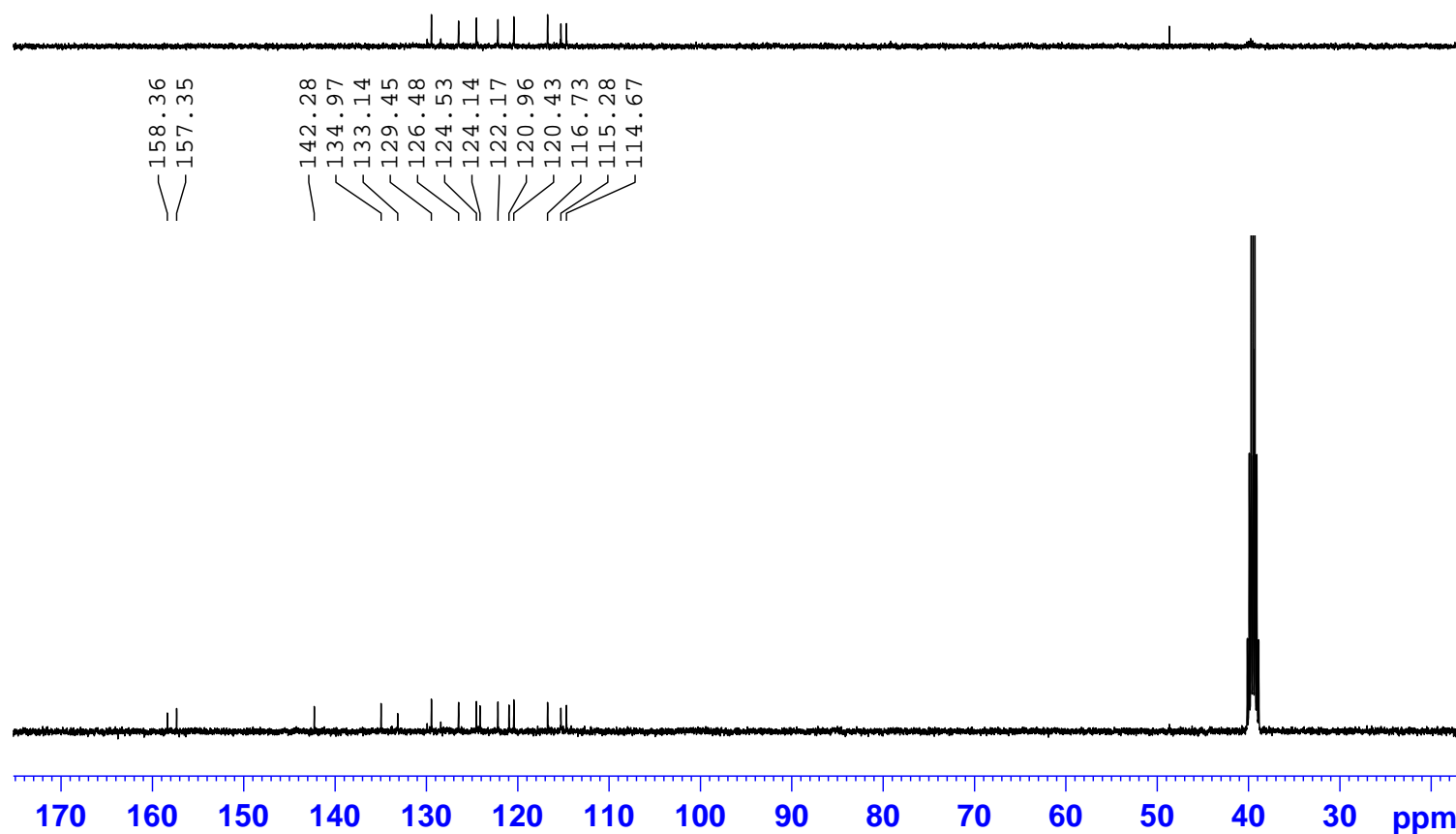
===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S40. ¹H NMR spectrum of **13**.

HB-1 D 16mg C



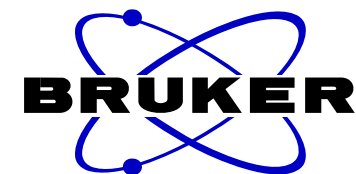
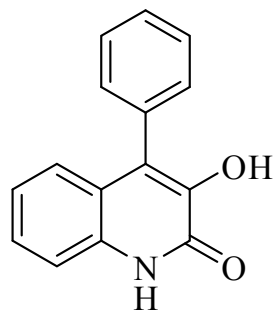
NAME HB1-1 D 16mg
EXPNO 2
PROCNO 1
Date_ 20191224
Time 18.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 72
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 292.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6128095 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S41. ¹³C NMR spectrum of **13**.

HB-2 D 50mg H



NAME HB1-2 D 50mg
EXPNO 1
PROCNO 1
Date_ 20191226
Time 19.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 90.5
DW 62.400 usec
DE 6.50 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300028 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

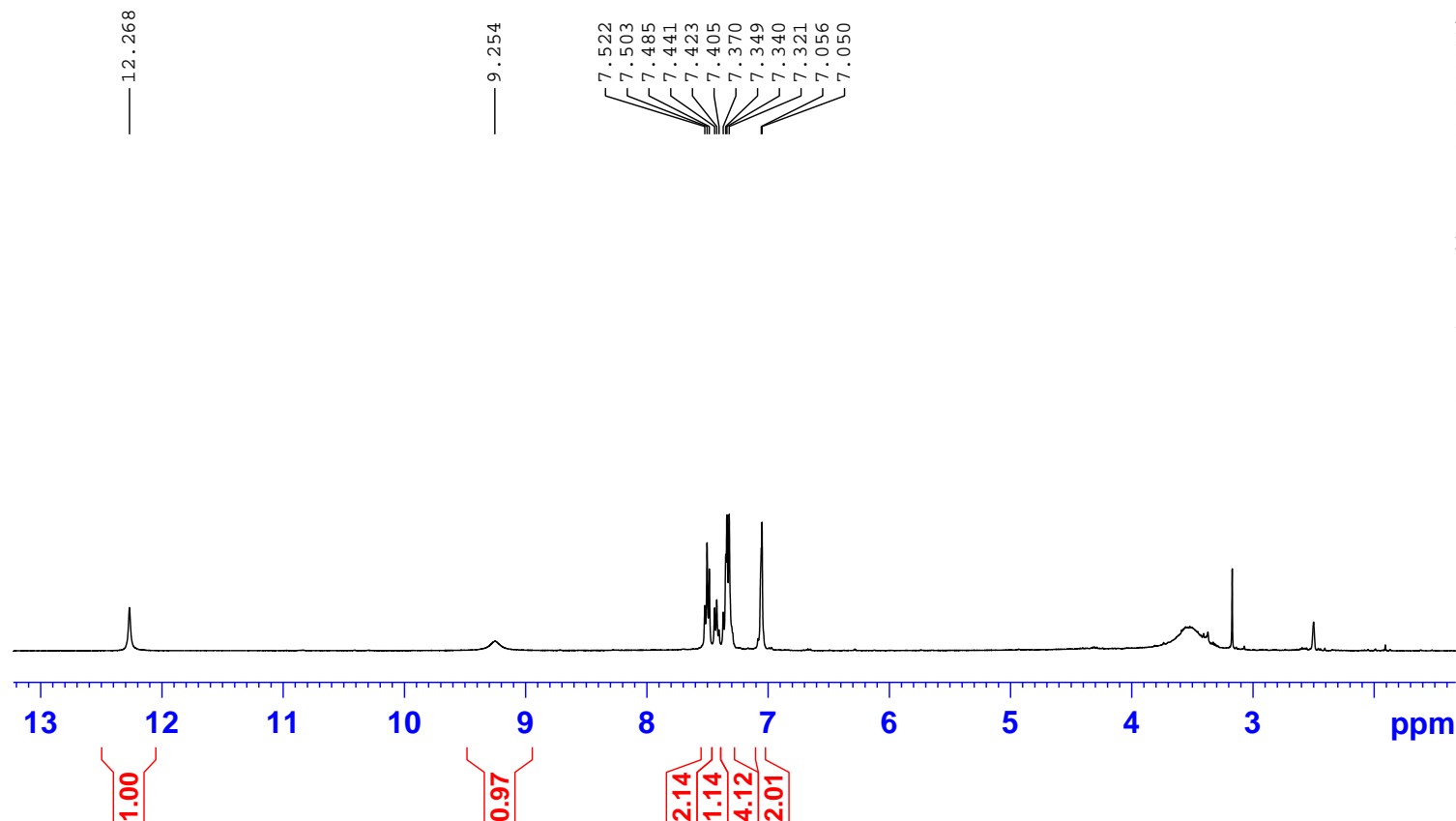
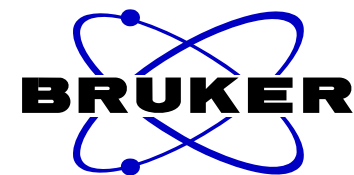
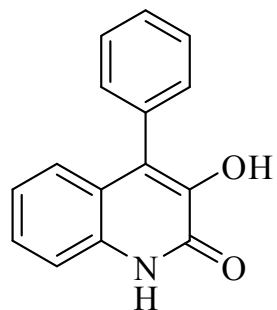


Figure S42. ¹H NMR spectrum of 14.

HB-2 D 50mg C



NAME HB1-2 D 50mg
EXPNO 2
PROCNO 1
Date_ 20191226
Time 19.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 92
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 292.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6128060 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

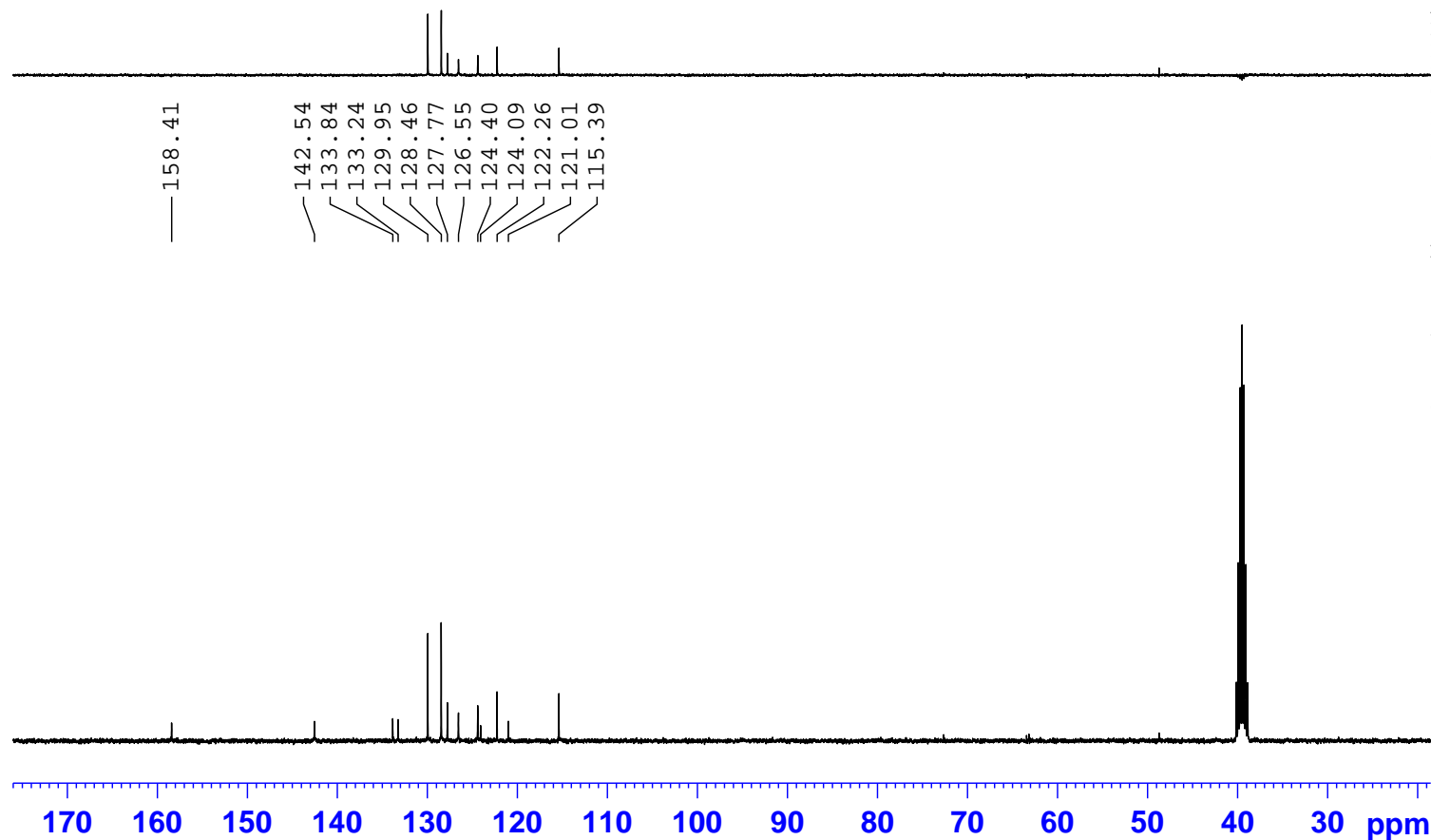
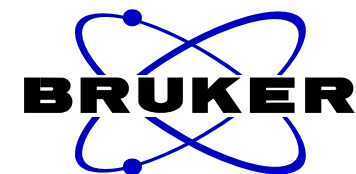
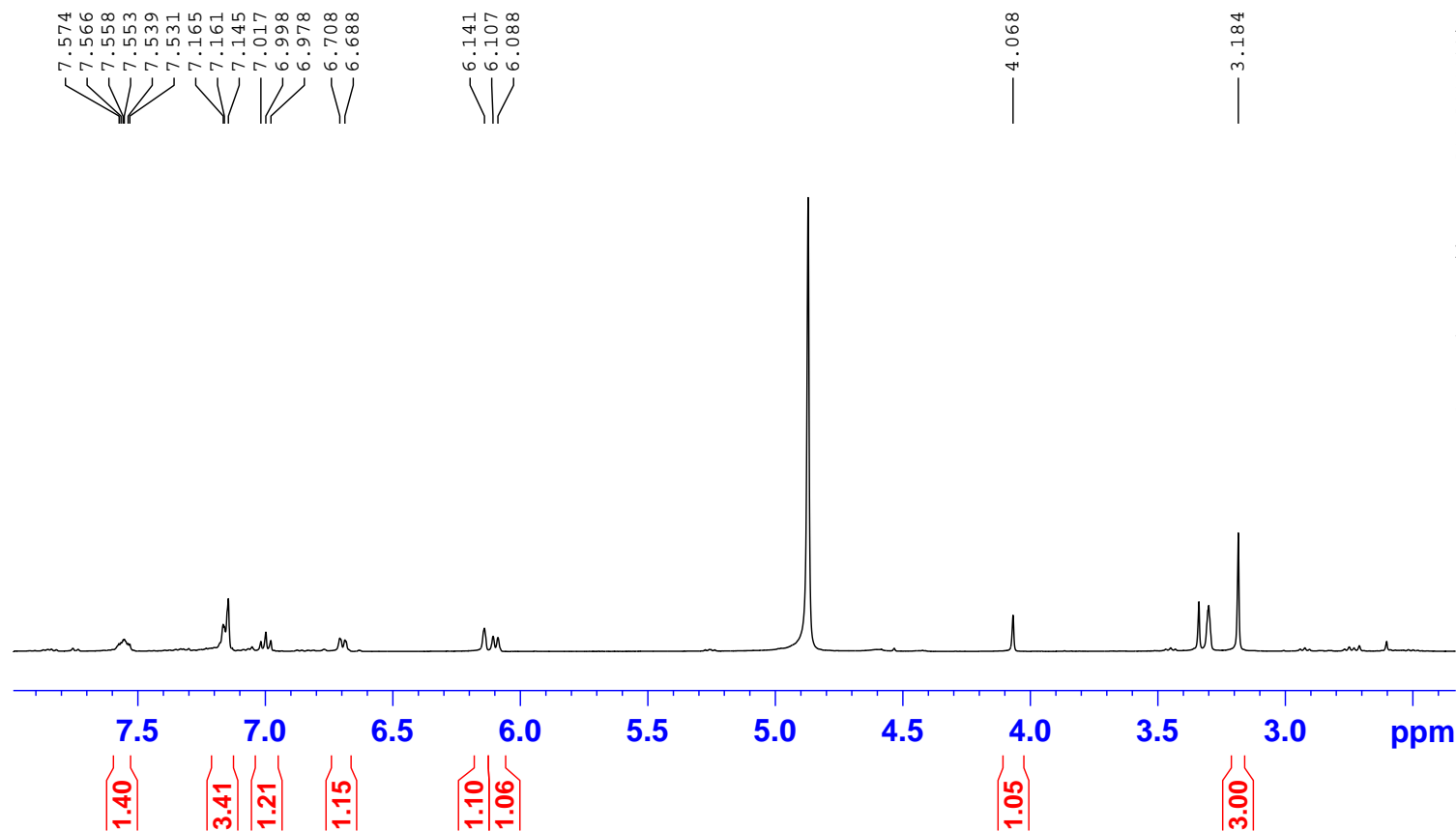
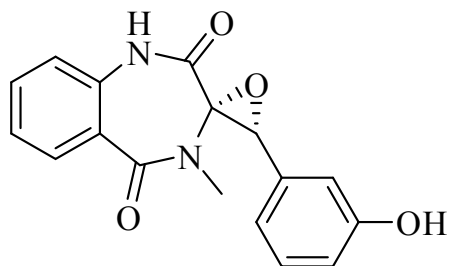


Figure S43. ¹³C NMR spectrum of 14.

HB2-2 M 3mg H

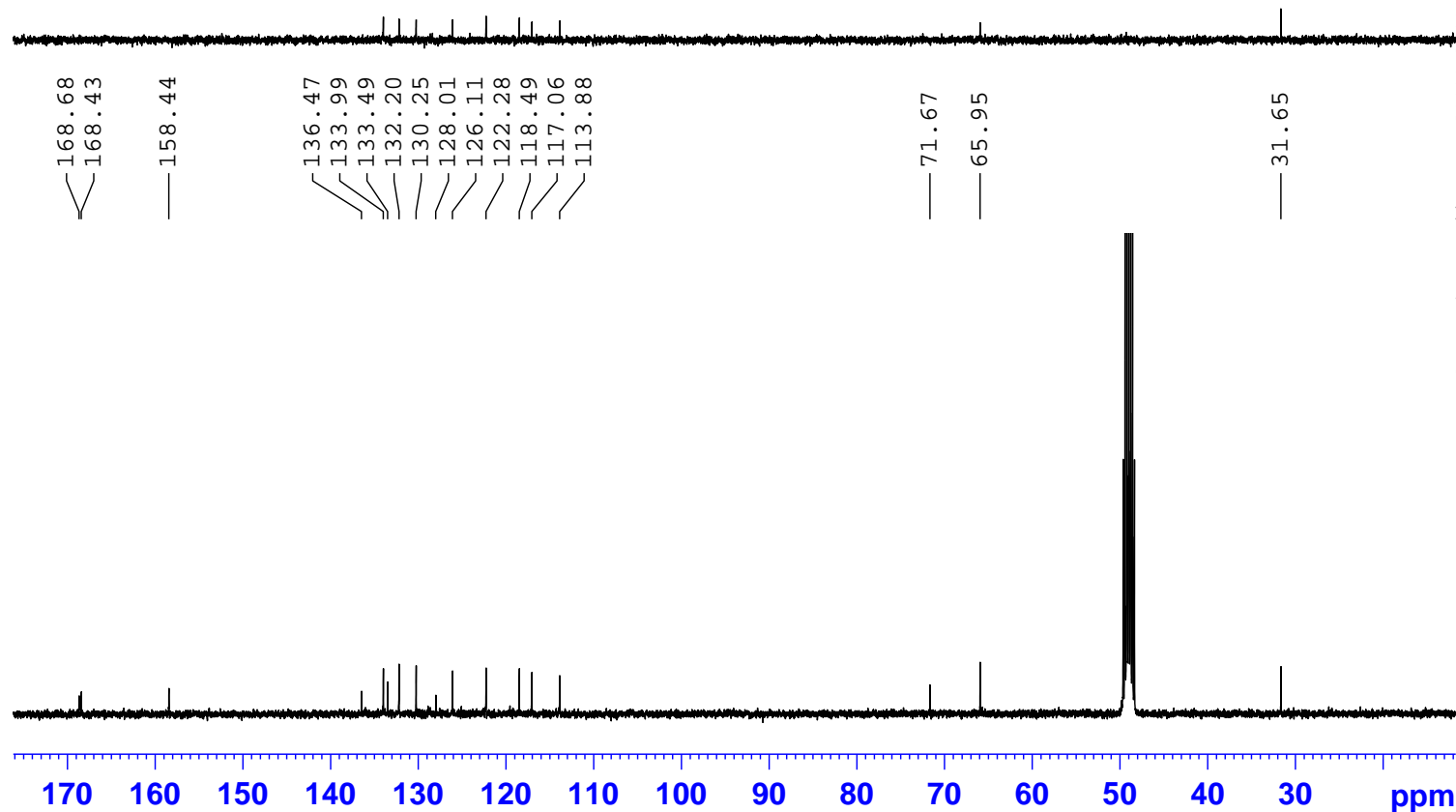
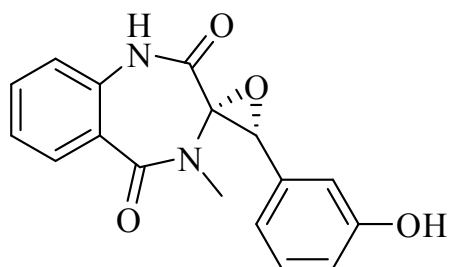
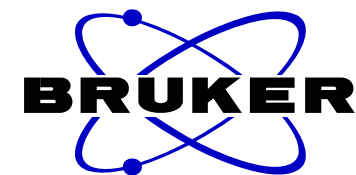


NAME HB2-2 M 3mg
EXPNO 1
PROCNO 1
Date_ 20200726
Time 13.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 17
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300113 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S44. ¹H NMR spectrum of **15**.

HB2-2 M 3mg C

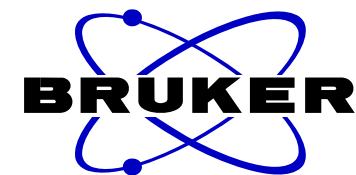
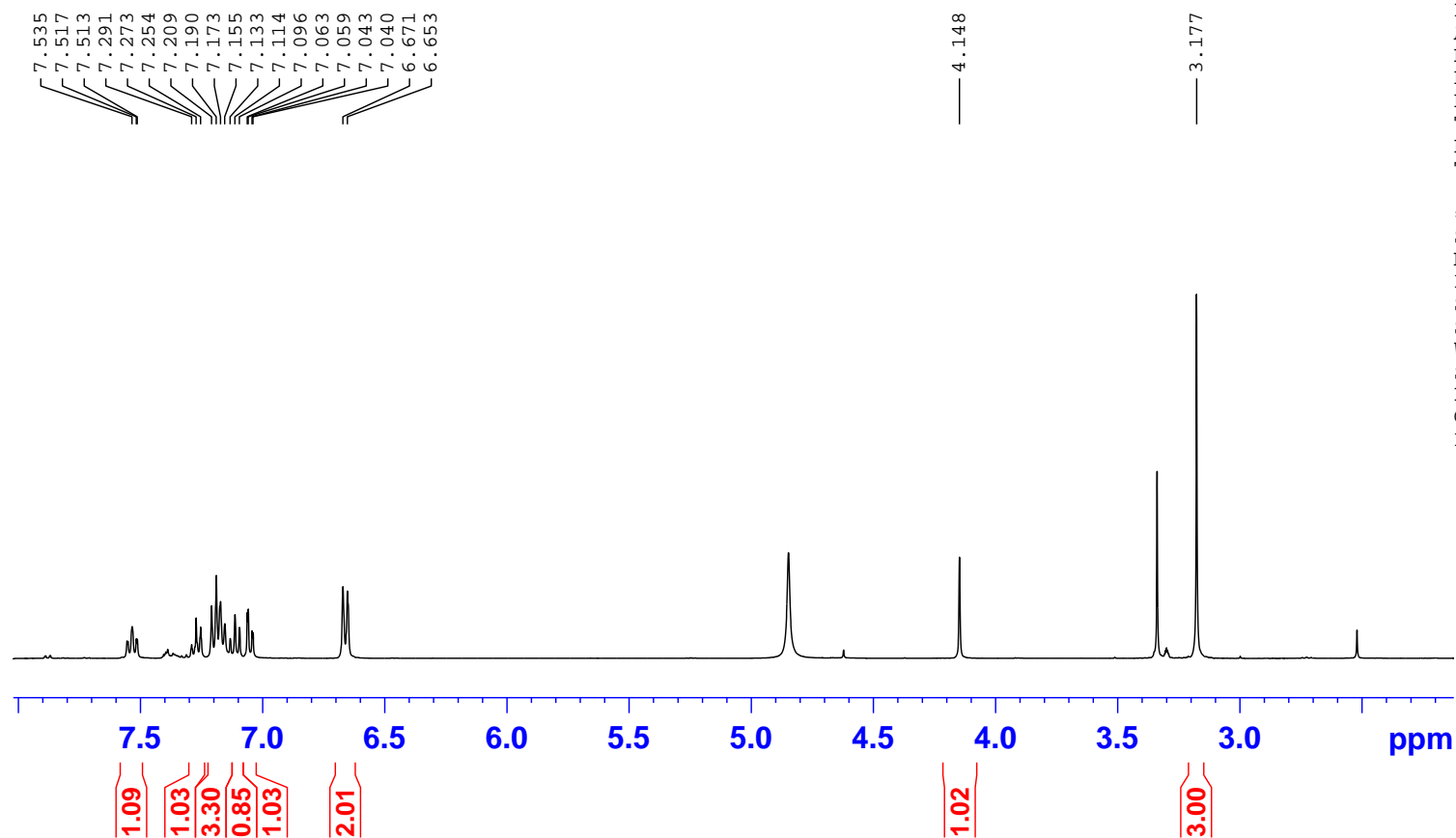
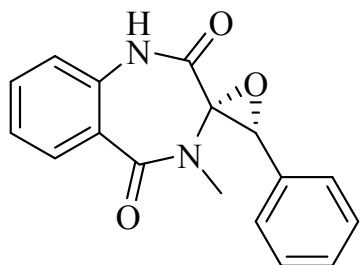


NAME HB2-2 M 3mg
EXPNO 2
PROCNO 1
Date_ 20200726
Time 13.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 649
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126288 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S45. ¹³C NMR spectrum of 15.

HB-C16 M 60mg H

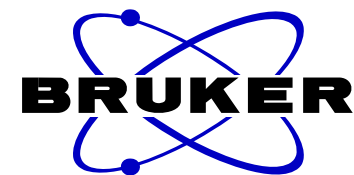
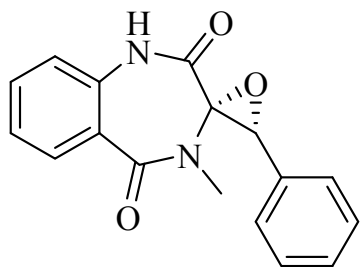


NAME HB-C16 M 60mg
EXPNO 1
PROCNO 1
Date_ 20200910
Time 20.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 9
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S46. ¹H NMR spectrum of **16**.

HB-C16 M 60mg C



NAME HB-C16 M 60mg
EXPNO 2
PROCNO 1
Date_ 20200910
Time 20.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 36
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126394 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

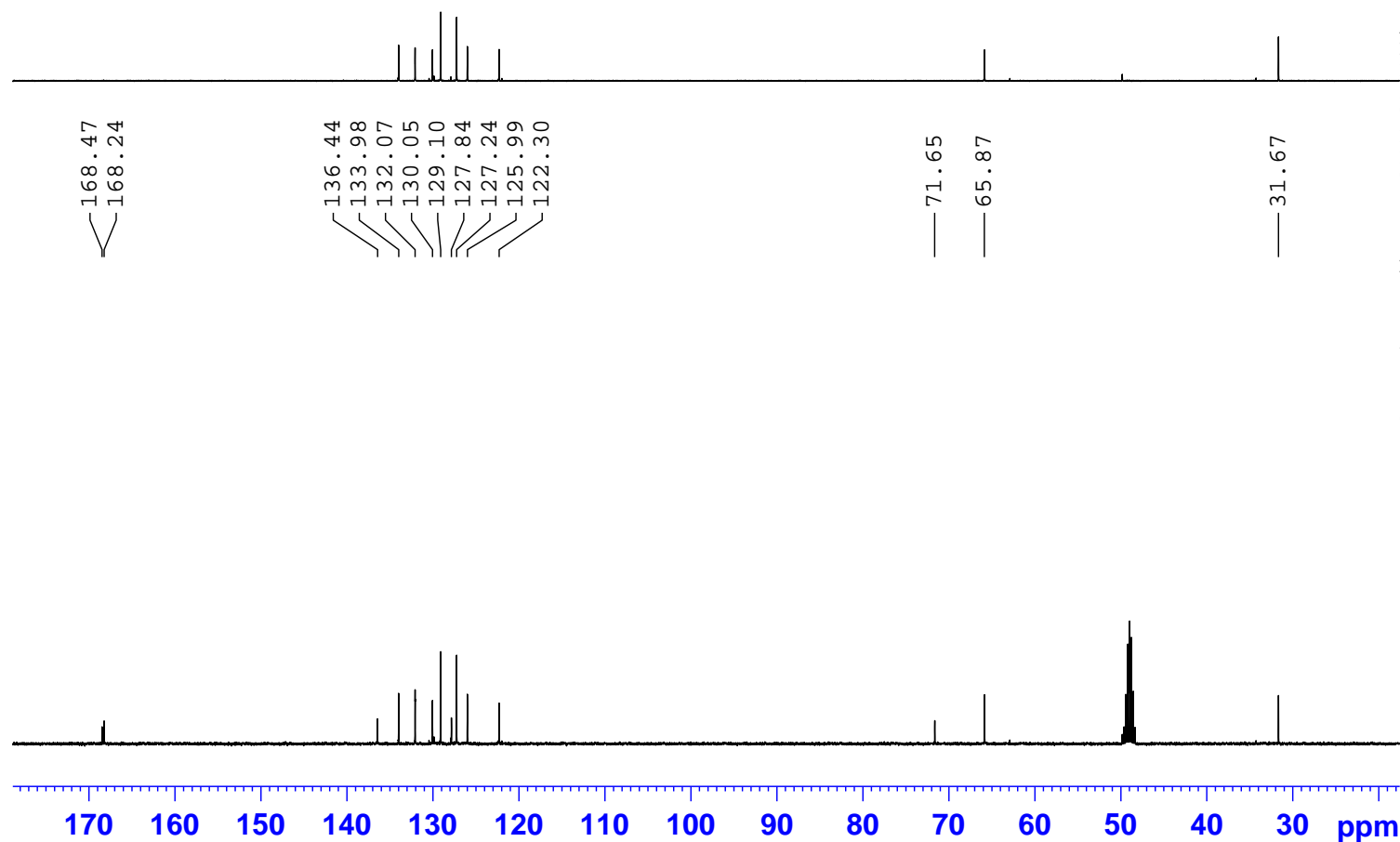
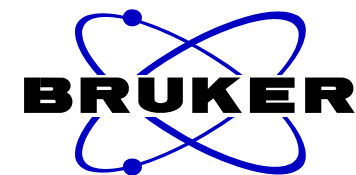
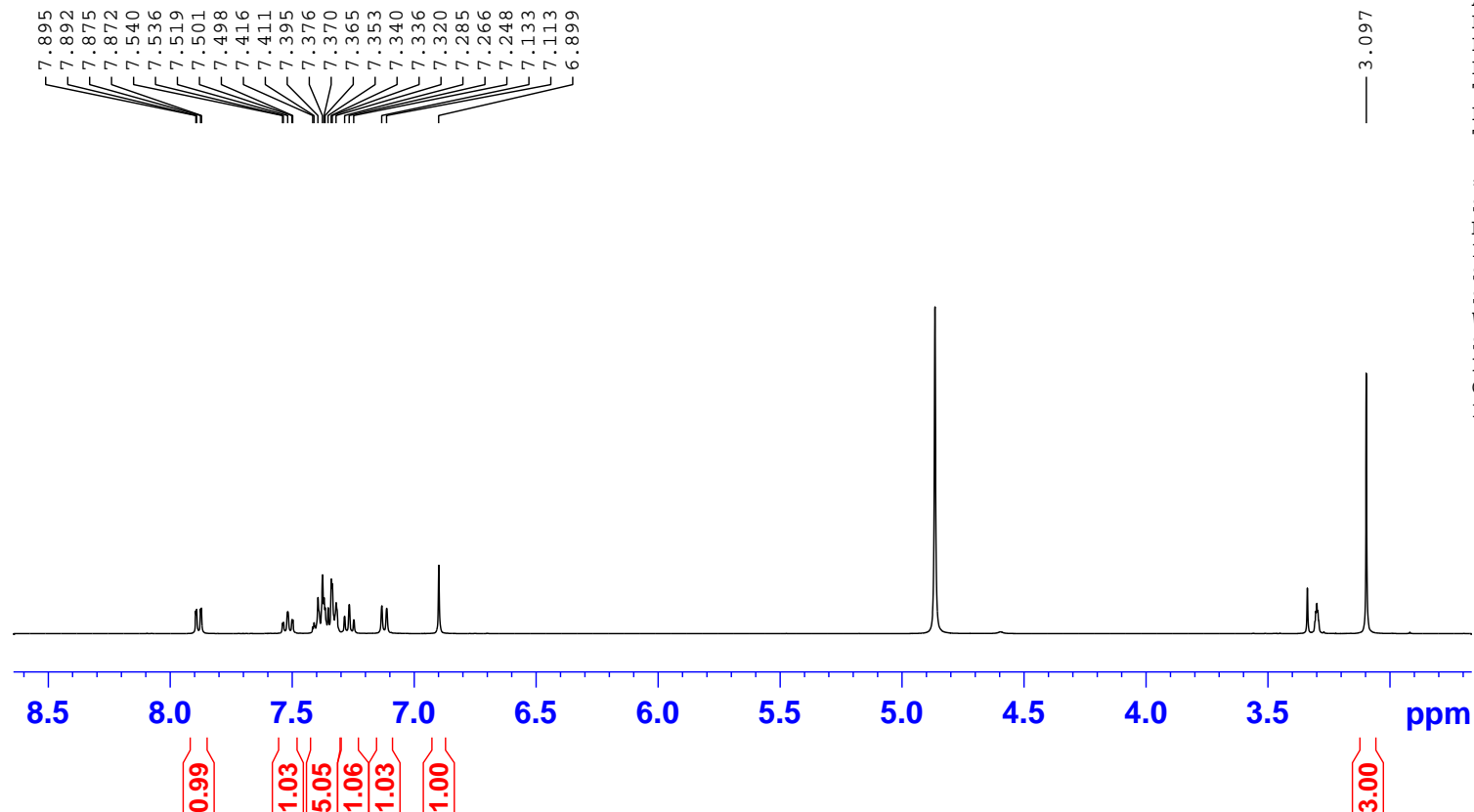
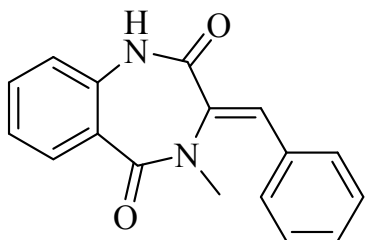


Figure S47. ¹³C NMR spectrum of **16**.

HB-C11 M 8mg H

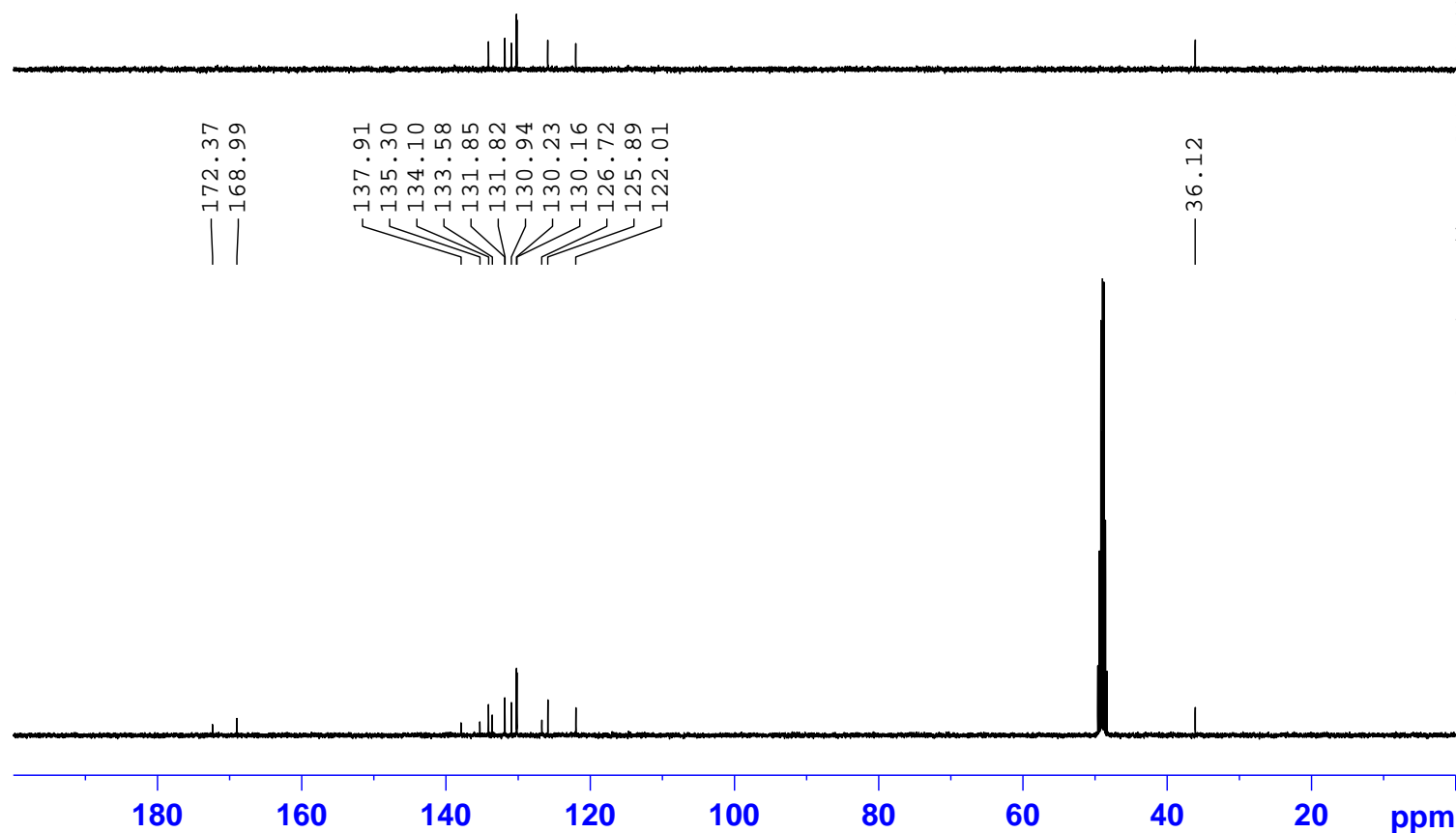
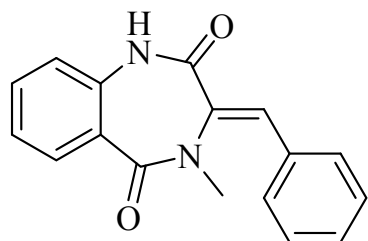
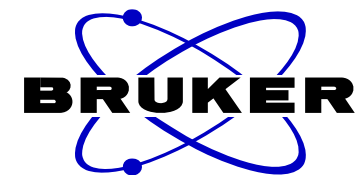


NAME HB-C11 M 8mg
EXPNO 1
PROCNO 1
Date_ 20200903
Time 19.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 18
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure S48. ¹H NMR spectrum of **17**.

HB-C11 M 8mg C

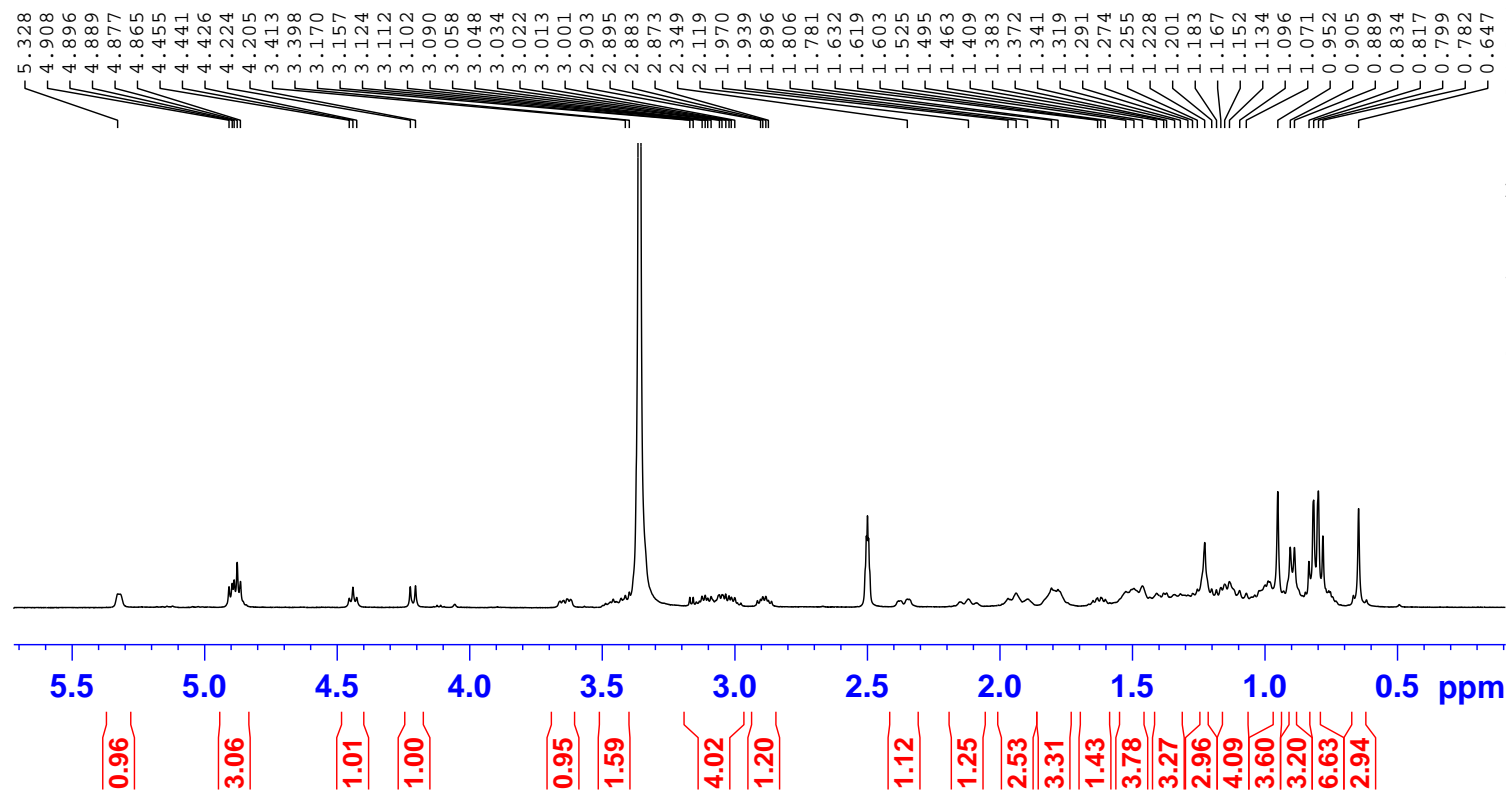
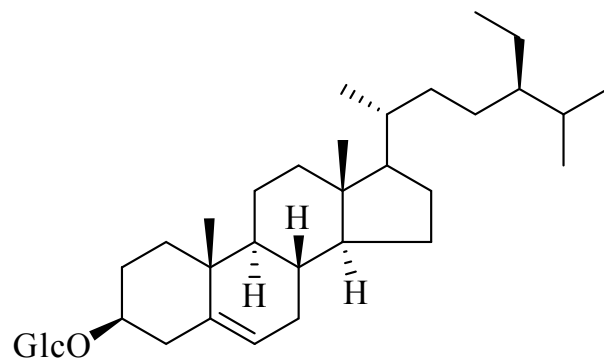
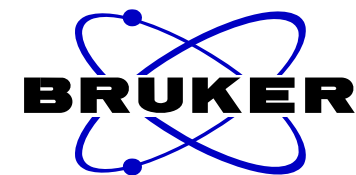


NAME HB-C11 M 8mg
EXPNO 2
PROCNO 1
Date_ 20200903
Time 19.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 68
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126292 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S49. ^{13}C NMR spectrum of **17**.

HB2-11 D 3mg H



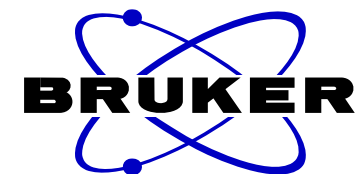
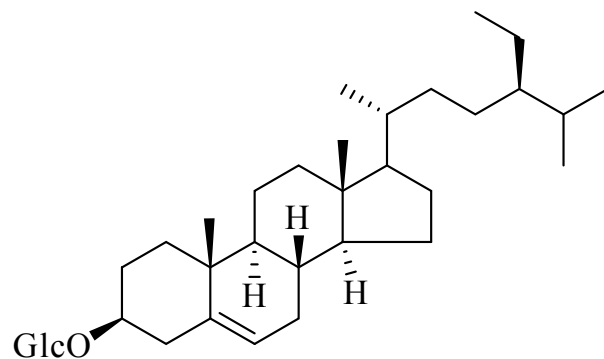
```

NAME      HB2-11 D 3mg
EXPNO      1
PROCNO      1
Date_      20200805
Time       10.32
INSTRUM     spect
PROBHD      5 mm PABBO BB-
PULPROG     zg30
TD          65536
SOLVENT      DMSO
NS           18
DS           2
SWH          8012.820 Hz
FIDRES       0.122266 Hz
AQ           4.0894966 sec
RG           181
DW           62.400 usec
DE           6.50 usec
TE           295.9 K
D1           1.00000000 sec
TD0          1

===== CHANNEL f1 =====
SFO1        400.1324710 MHz
NUC1         1H
P1           13.90 usec
SI           32768
SF           400.1300032 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00
  
```

Figure S50. ¹H NMR spectrum of **18**.

HB2-11 D 3mg C



NAME HB2-11 D 3mg
EXPNO 2
PROCNO 1
Date_ 20200805
Time 10.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3984
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6128135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

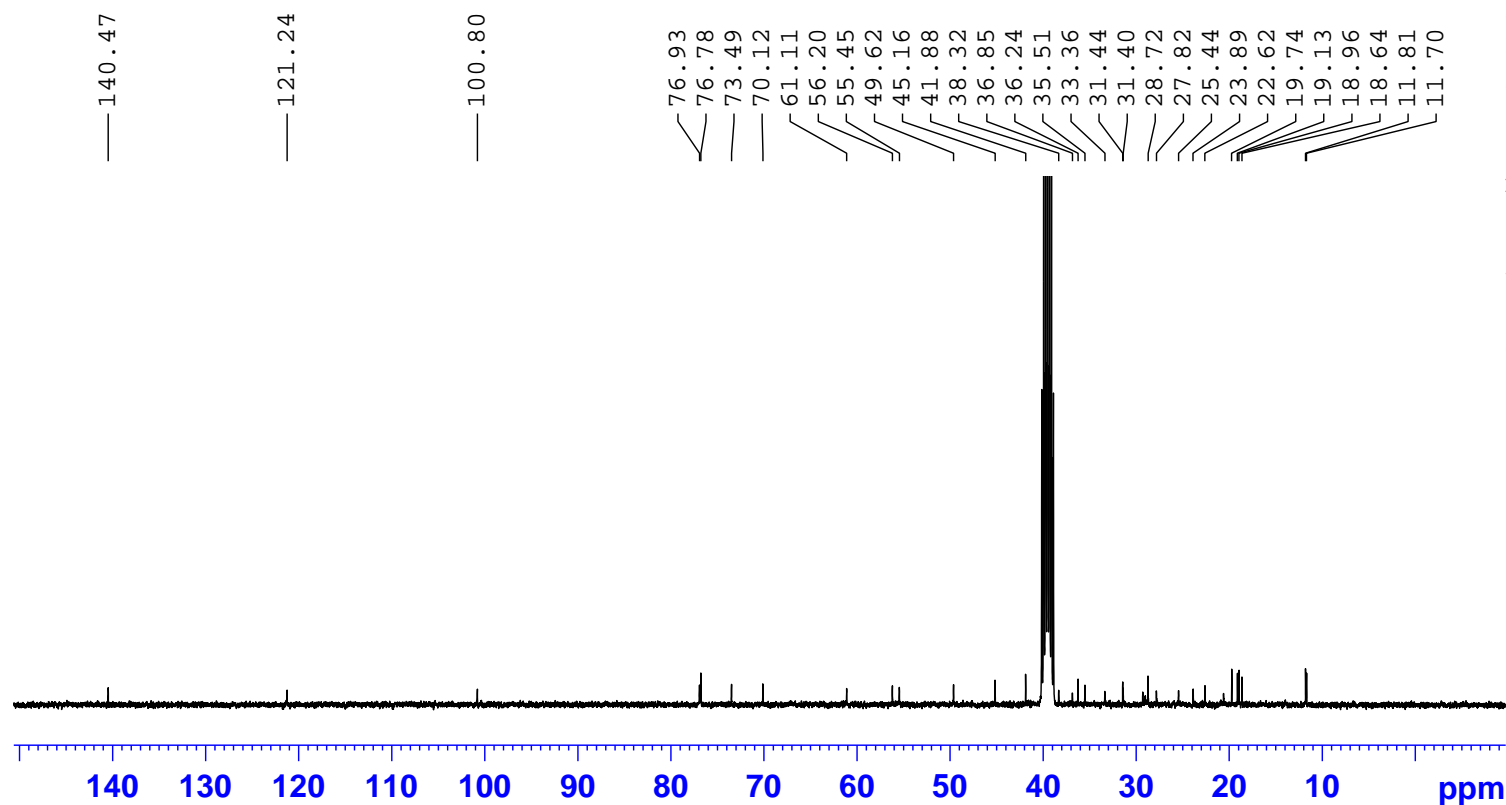
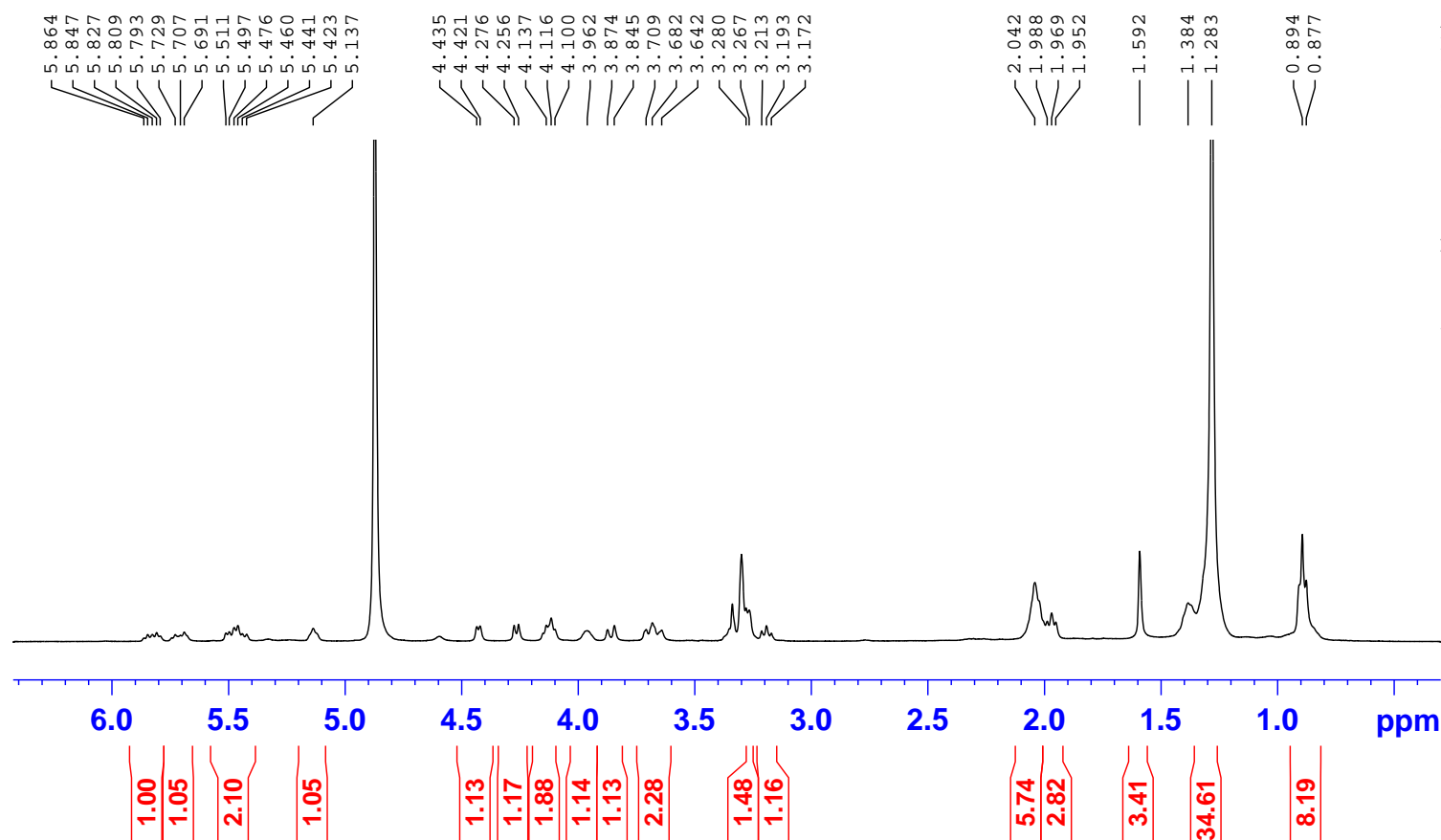
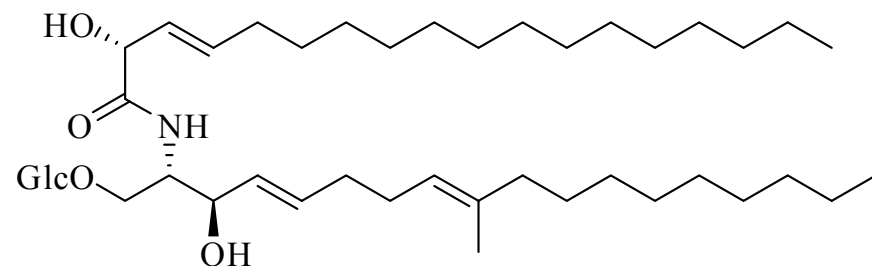
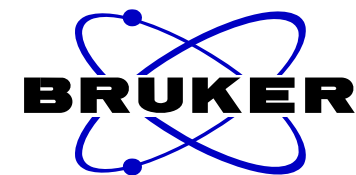


Figure S51. ¹³C NMR spectrum of 18.

HB2-1 M 7mg H

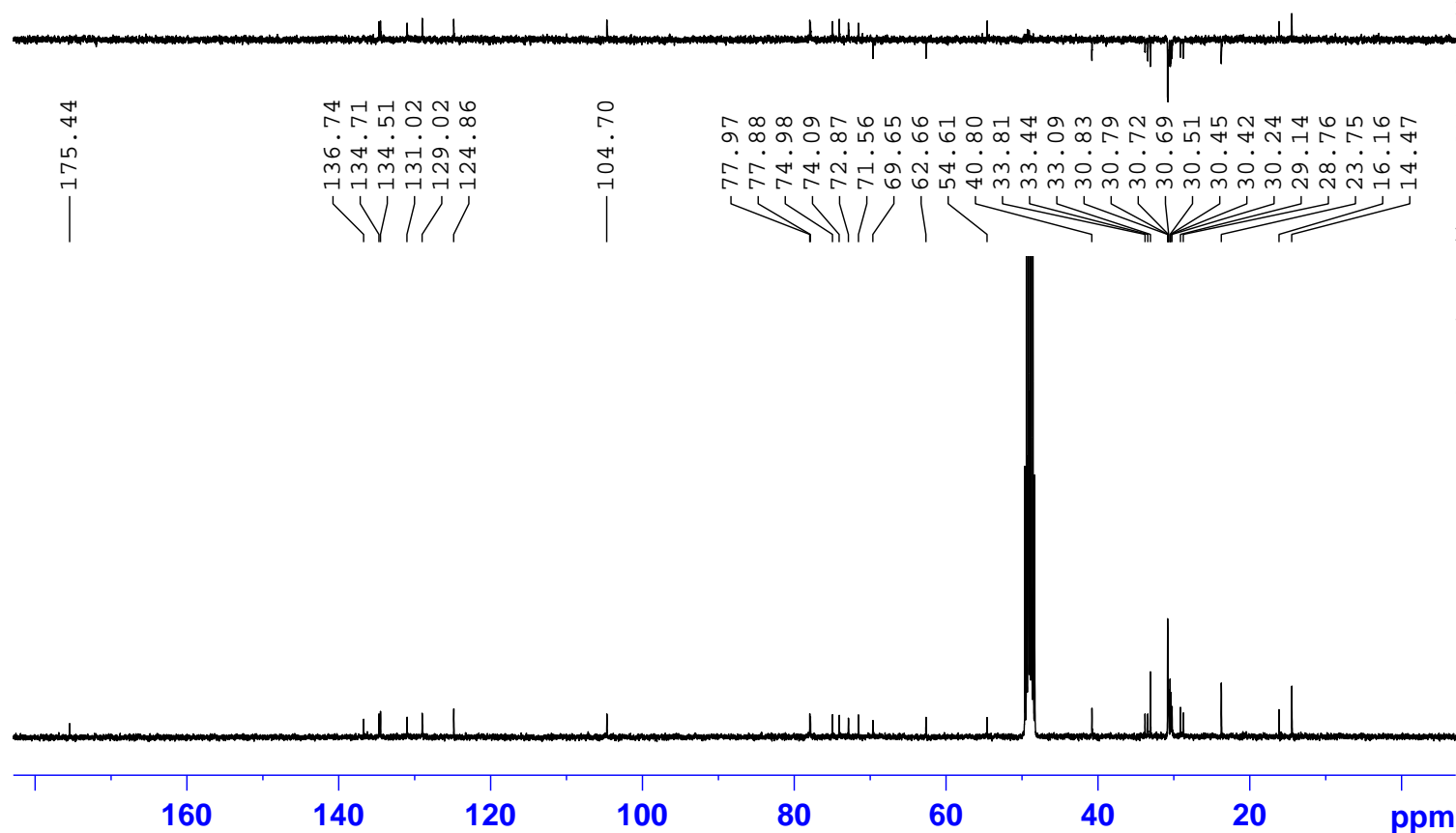
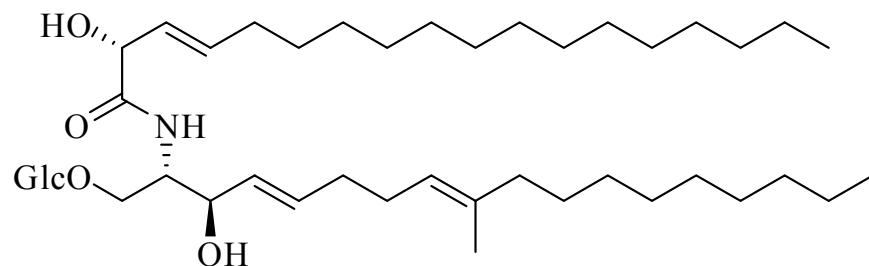
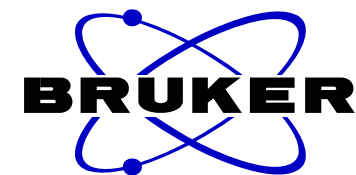


NAME HB2-1 M 7mg
 EXPNO 1
 PROCNO 1
 Date_ 20200723
 Time 19.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 19
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894966 sec
 RG 144
 DW 62.400 usec
 DE 6.50 usec
 TE 295.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 13.90 usec
 SI 32768
 SF 400.1300115 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S52. ¹H NMR spectrum of **19**.

HB2-1 M 7mg C

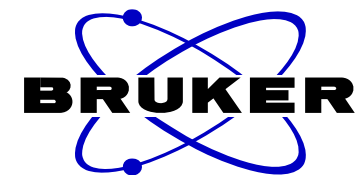
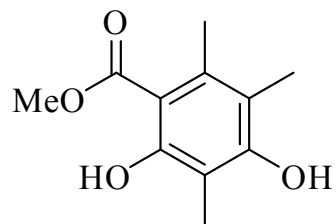


NAME HB2-1 M 7mg
EXPNO 2
PROCNO 1
Date_ 20200723
Time 19.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 1494
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126284 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S53. ^{13}C NMR spectrum of 19.

HB-C17 M 8mg H



NAME HB-C17 M 8mg
EXPNO 1
PROCNO 1
Date_ 20201203
Time 20.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 15
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

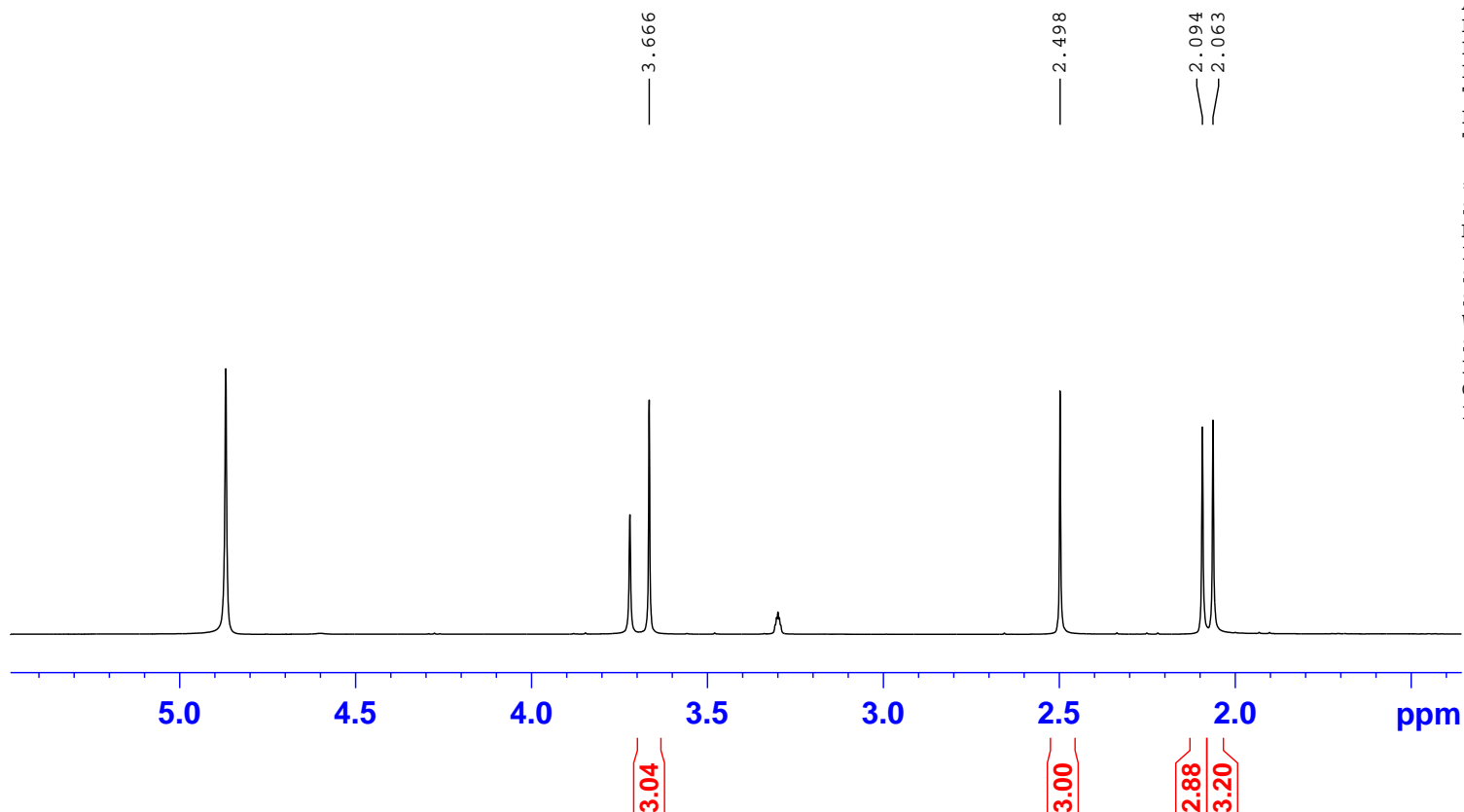
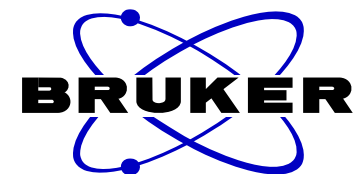
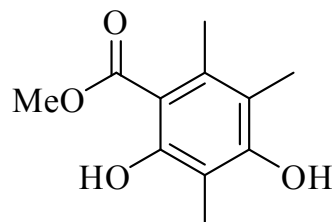
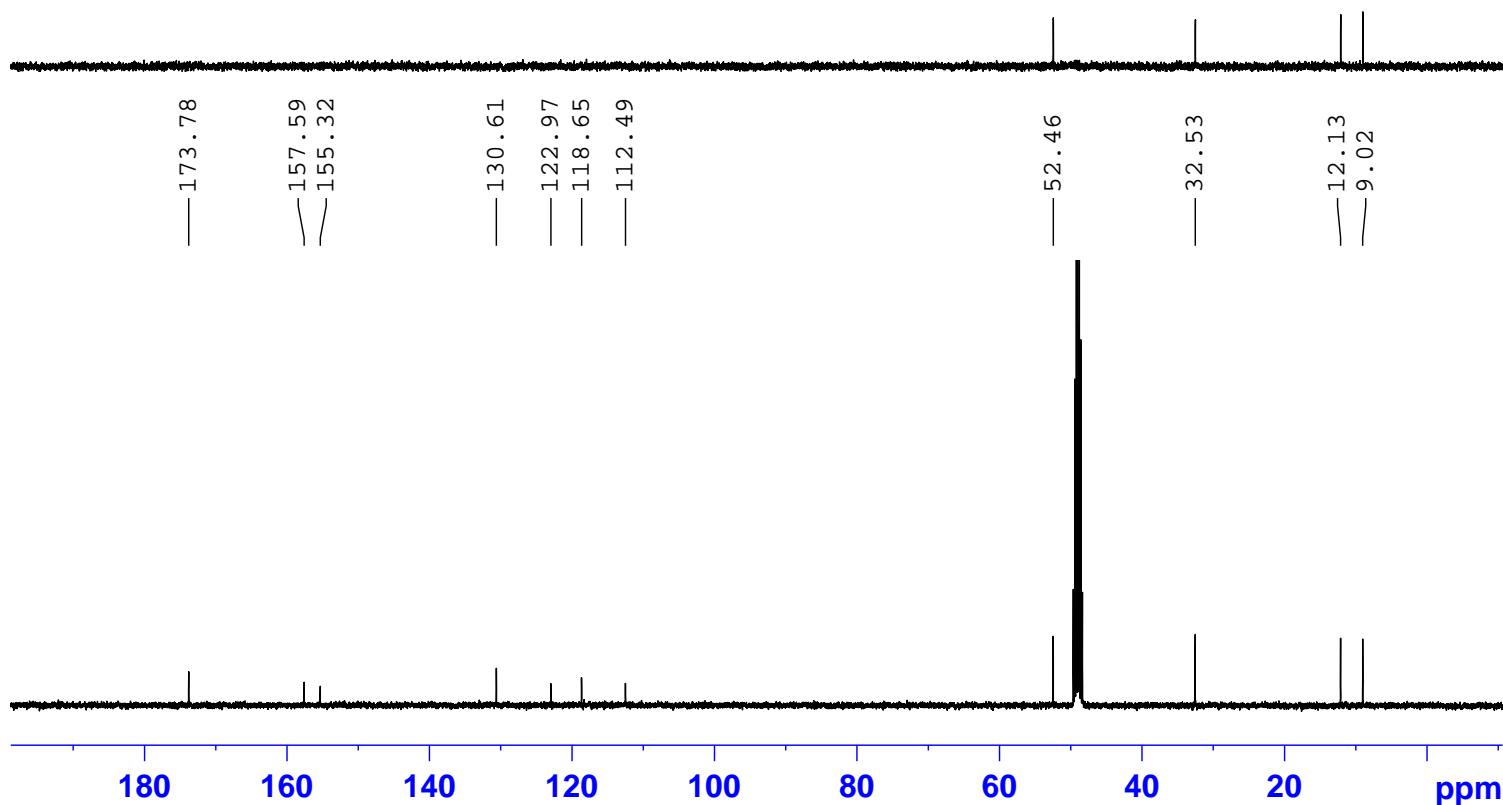


Figure S54. ¹H NMR spectrum of **20**.

HB-C17 M 8mg C



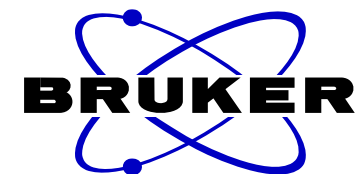
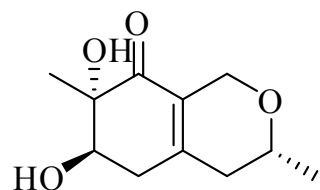
NAME HB-C17 M 8mg
EXPNO 2
PROCNO 1
Date_ 20201203
Time 20.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 137
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



===== CHANNEL f1 =====
SF01 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126292 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S55. ¹³C NMR spectrum of 20.

HB-C18 C 1mg H



```

NAME      HB-C18 C 2mg
EXPNO     1
PROCNO    1
Date_     20191204
Time      22.34
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   CDCl3
NS        512
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        203
DW        62.400 usec
DE        6.50 usec
TE        295.5 K
D1        1.00000000 sec
TD0       1
  
```

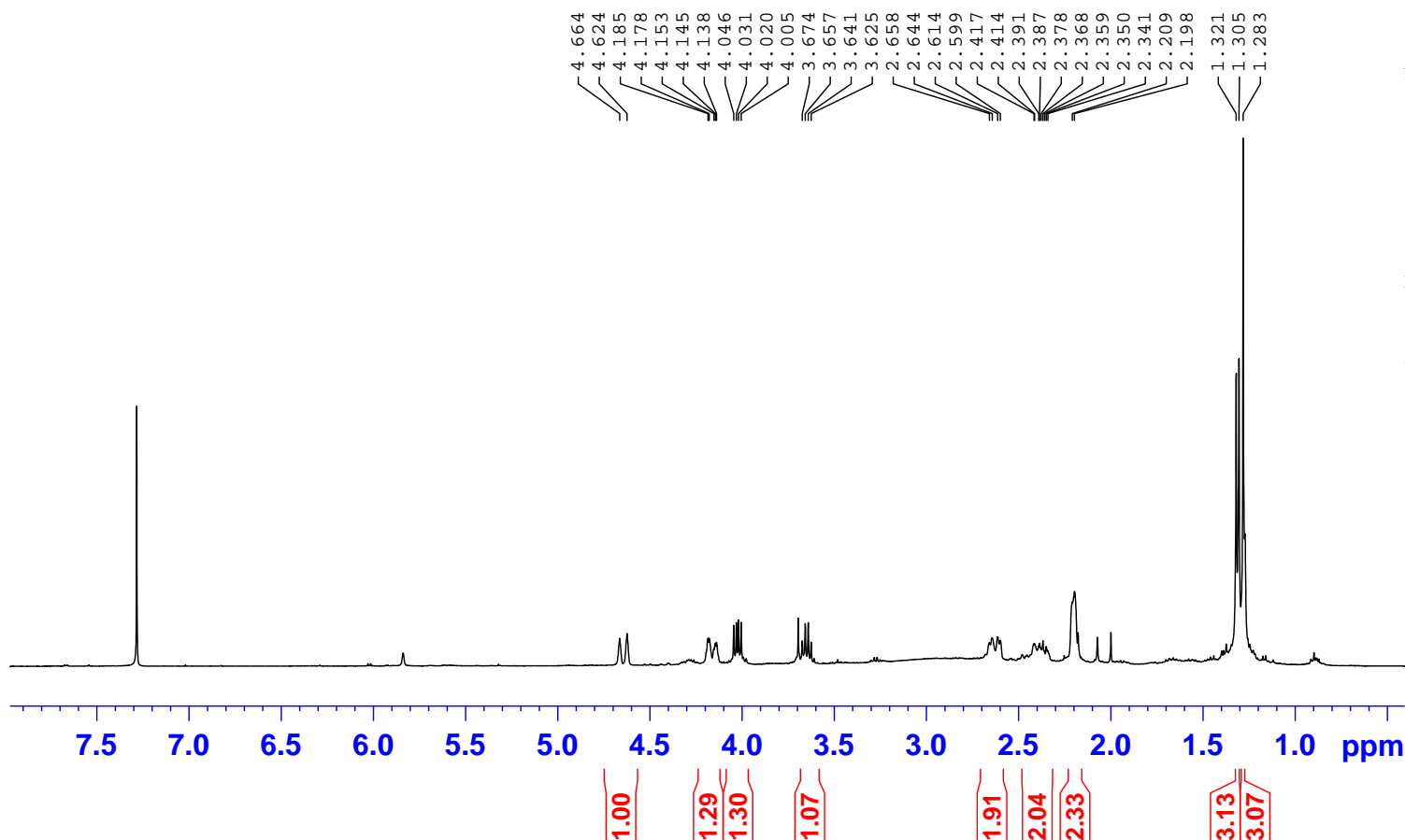
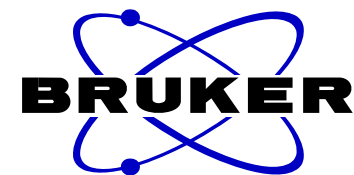
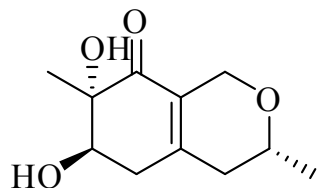


Figure S56. ¹H NMR spectrum of **21**.

HB-C18 C 1mg C



NAME HB-C18 C 2mg
EXPNO 2
PROCNO 1
Date_ 20191205
Time 8.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10240
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6127712 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

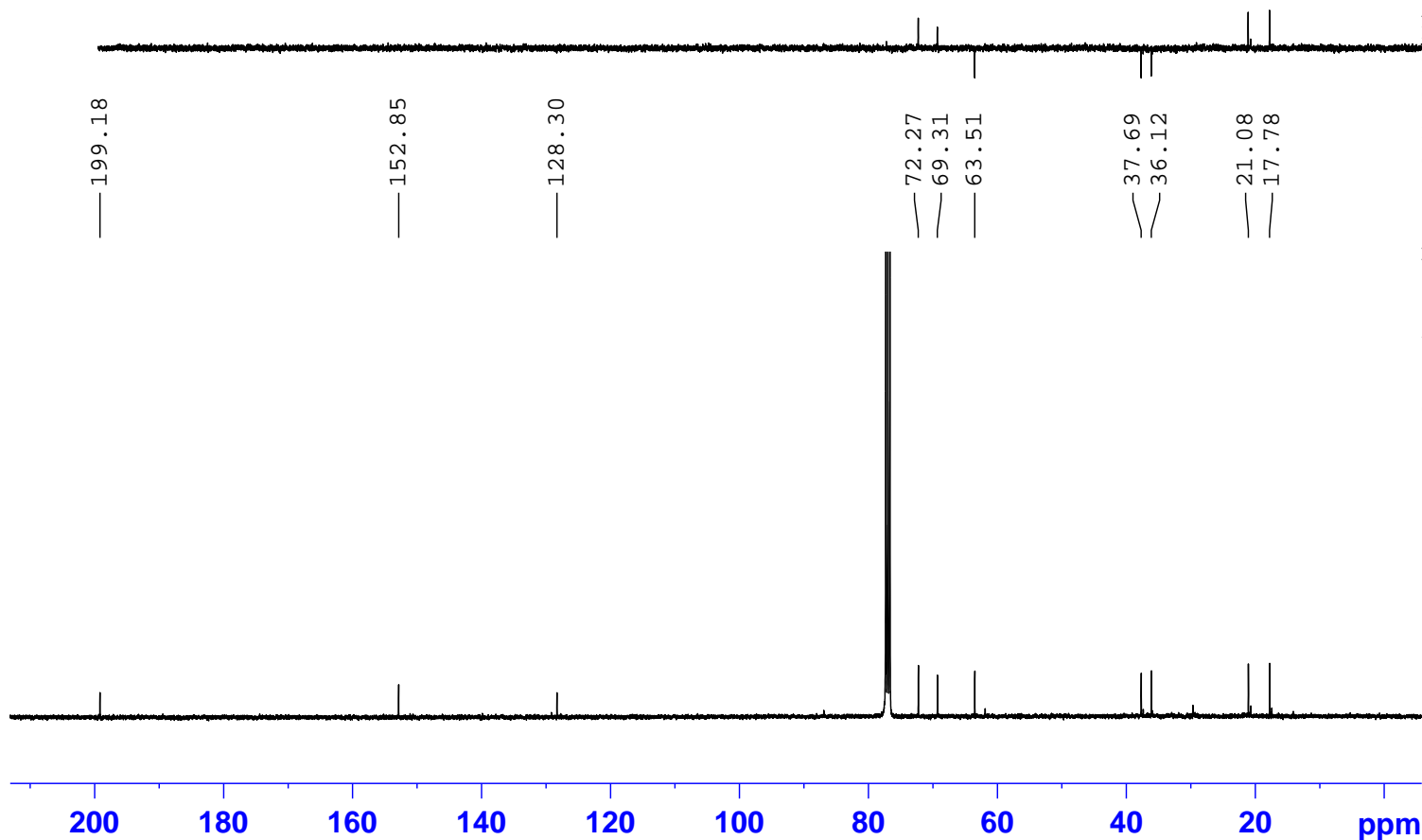
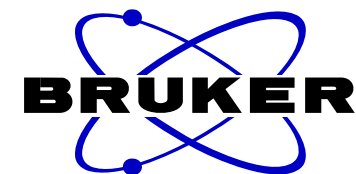
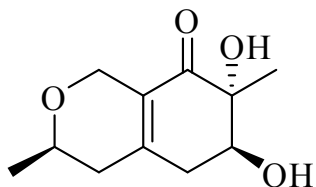


Figure S57. ¹³C NMR spectrum of 21.

HB-C19 C 1mg H



NAME HB-C19 C 1.5mg
EXPNO 1
PROCNO 1
Date_ 20200920
Time 14.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 27
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

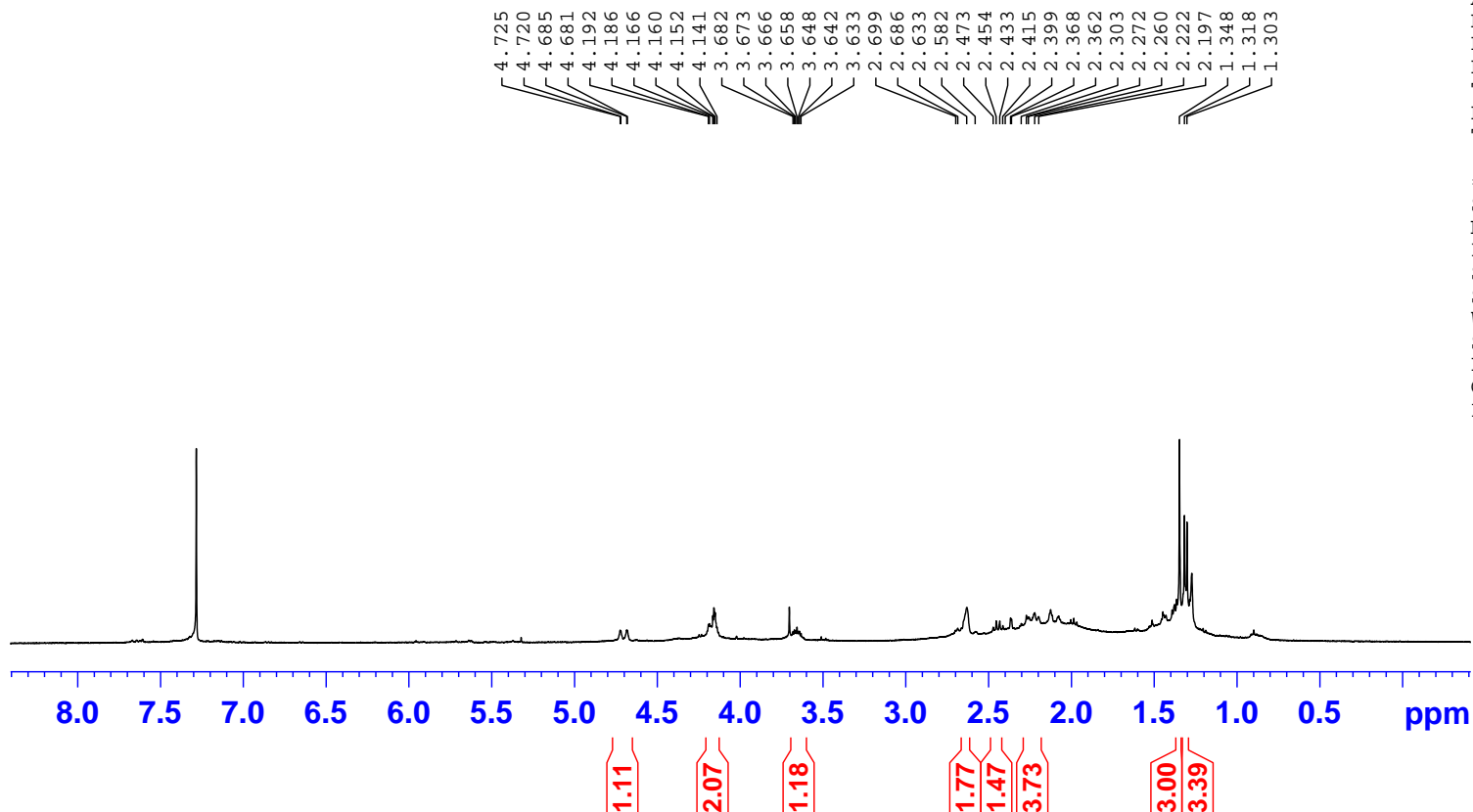
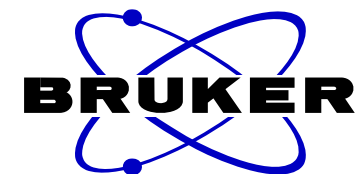
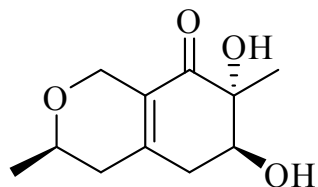
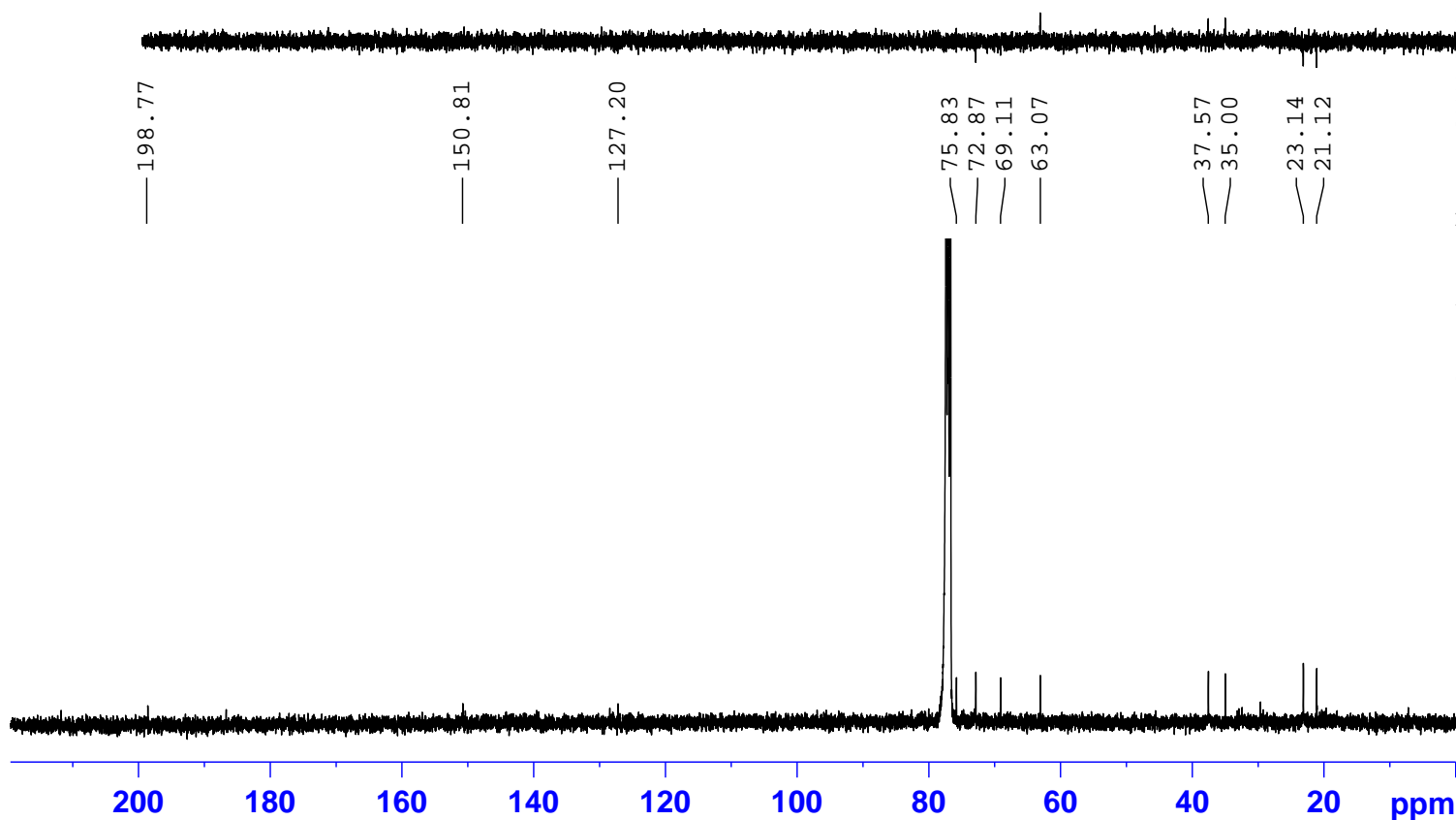


Figure S58. ¹H NMR spectrum of 22.

HB-C19 C 1mg C



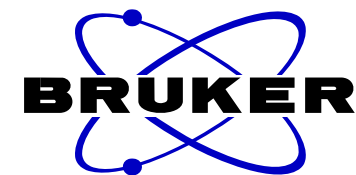
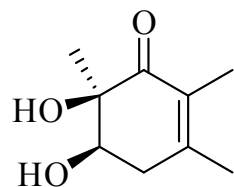
NAME HB-C19 C 1.5mg
EXPNO 2
PROCNO 1
Date_ 20200921
Time 6.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15360
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S59. ¹³C NMR spectrum of 22.

HB-C15 M 2mg H



NAME HB-C15 M 2mg
EXPNO 1
PROCNO 1
Date_ 20200910
Time 21.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 21
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

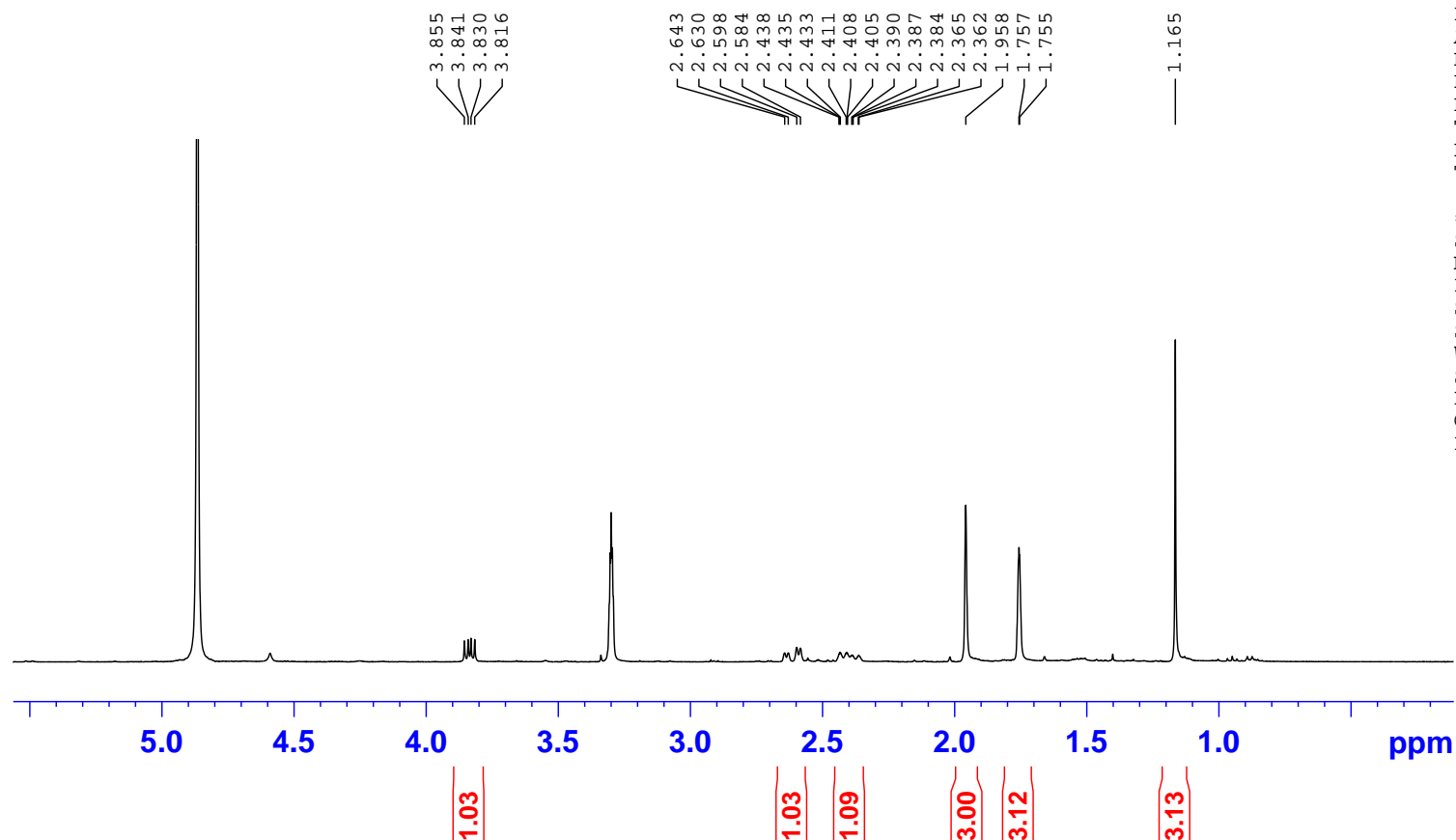
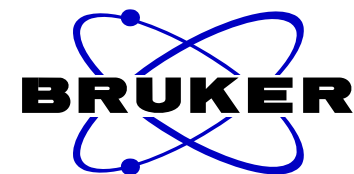
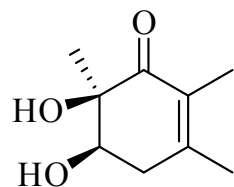


Figure S60. ¹H NMR spectrum of **23**.

HB-C15 M 2mg C



NAME HB-C15 M 2mg
EXPNO 2
PROCNO 1
Date_ 20200911
Time 6.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 10240
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126274 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

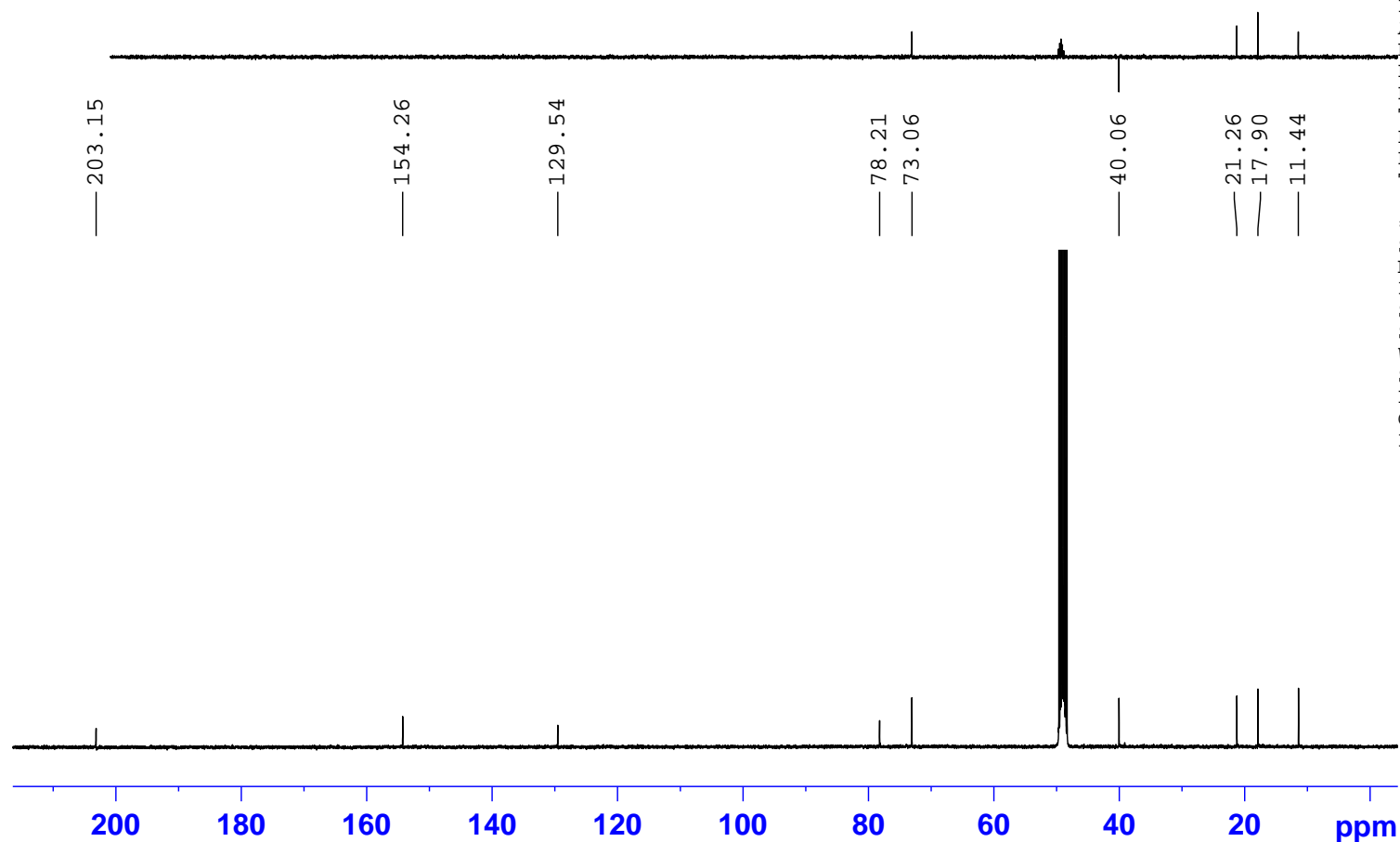
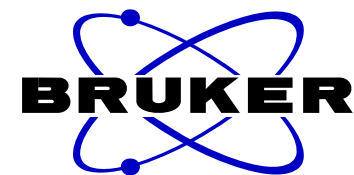
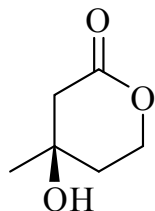


Figure S61. ¹³C NMR spectrum of **23**.

HB4-9 C 5mg H



NAME HB4-9 C 5mg
EXPNO 1
PROCNO 1
Date_ 20200611
Time 15.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 27
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

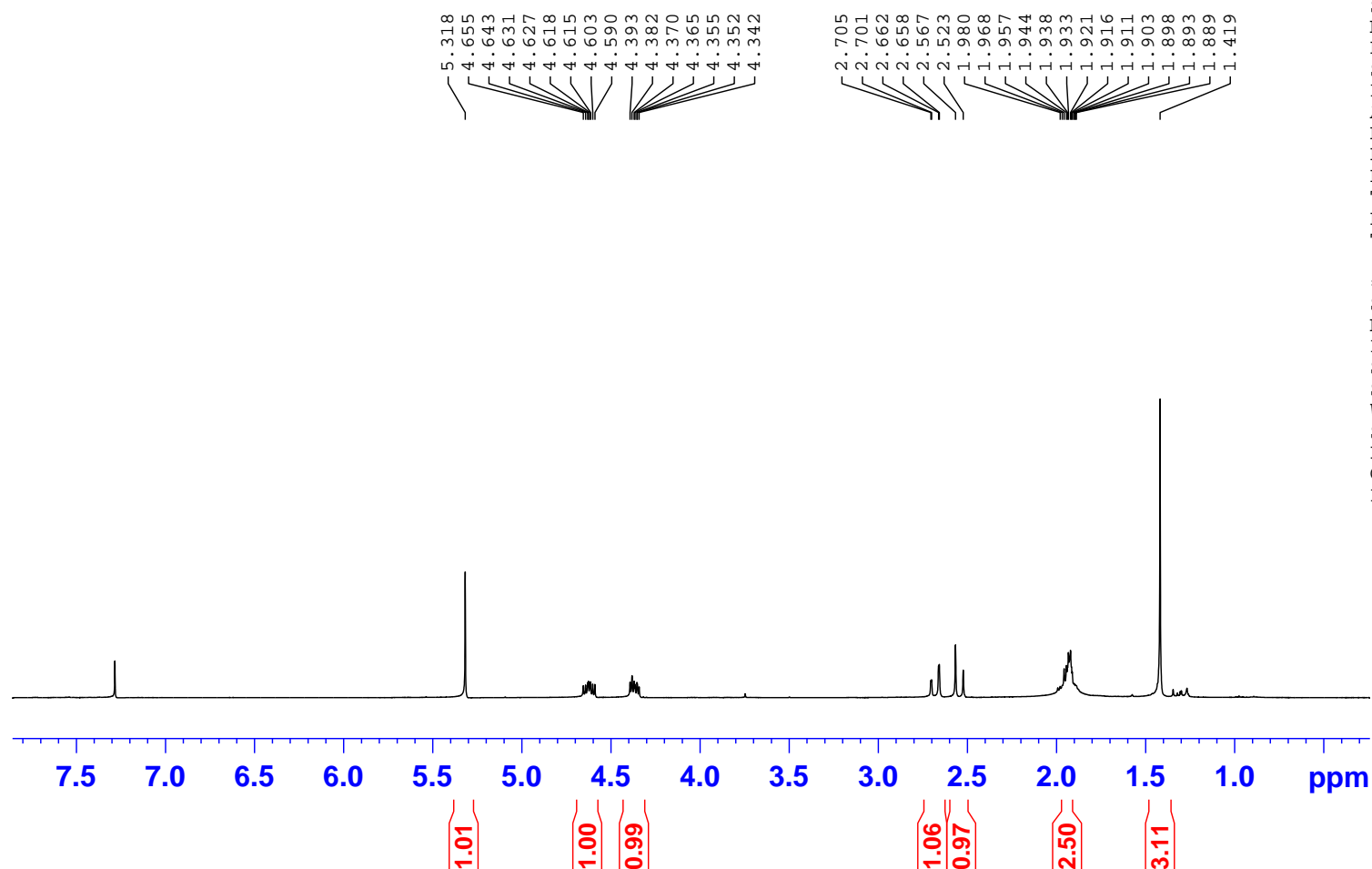
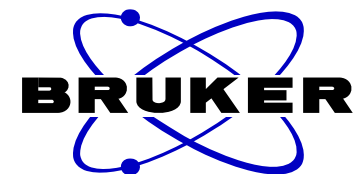
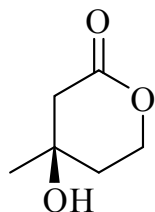


Figure S62. ¹H NMR spectrum of **24**.

HB4-9 C 5mg C



NAME HB4-9 C 5mg
EXPNO 2
PROCNO 1
Date_ 20200611
Time 15.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1020
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

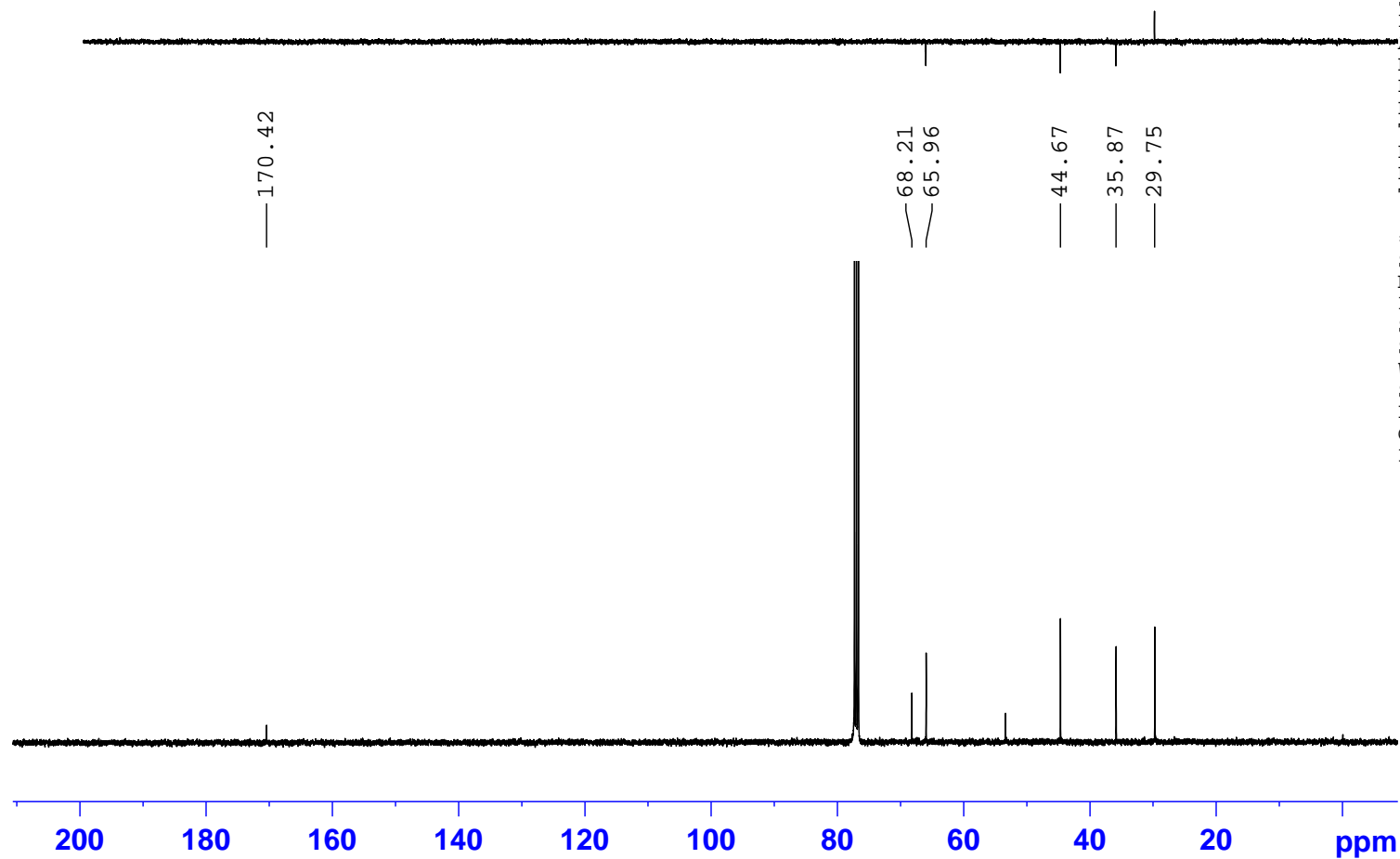
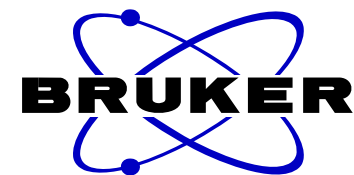


Figure S63. ^{13}C NMR spectrum of 24.

HB-C12 M 26mg H



NAME HB-C12 M 26mg
EXPNO 1
PROCNO 1
Date_ 20200906
Time 13.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 14
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 101
DW 62.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1324710 MHz
NUC1 1H
P1 13.90 usec
SI 32768
SF 400.1300117 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

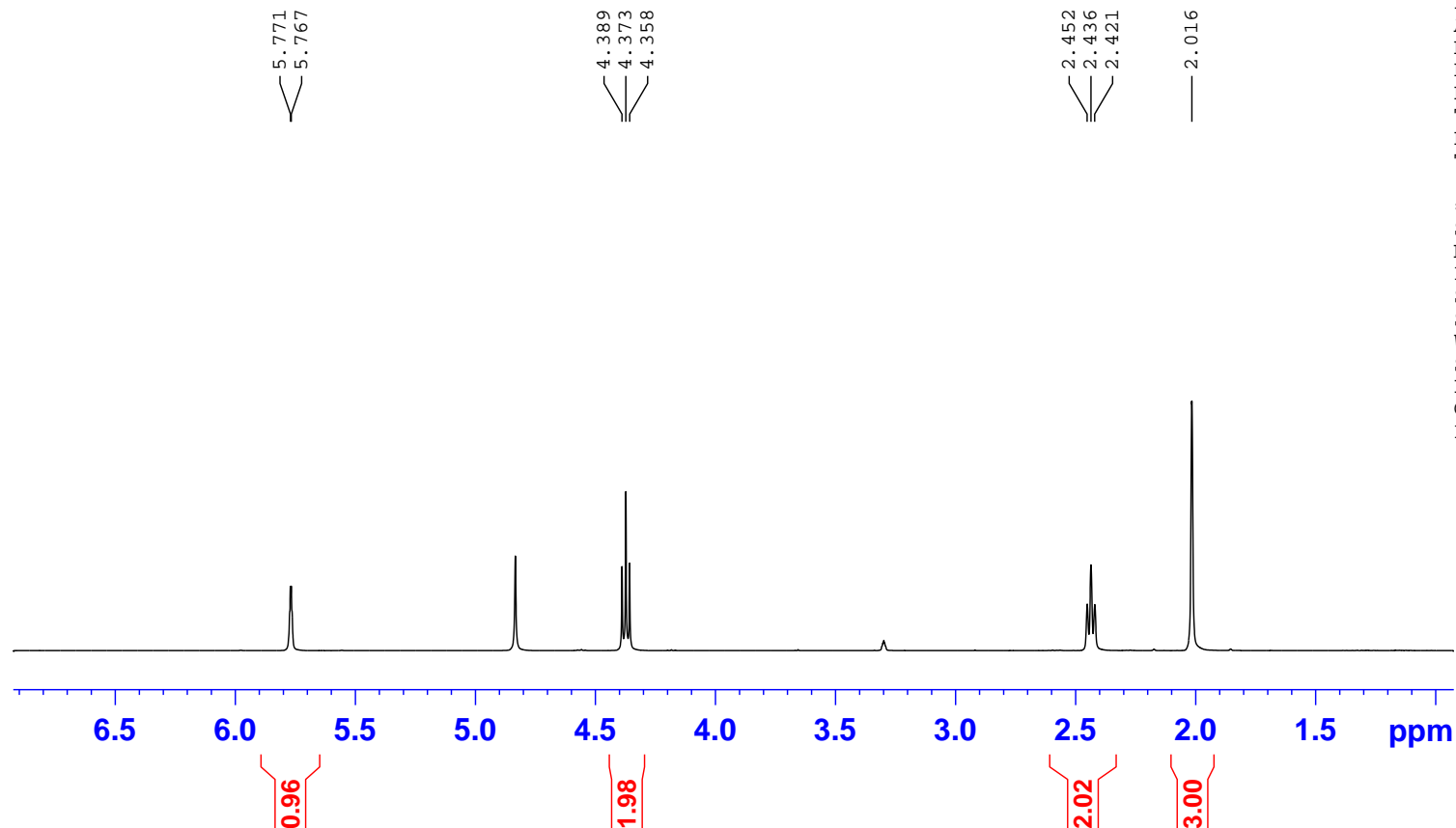
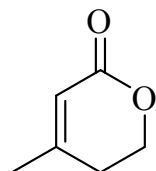
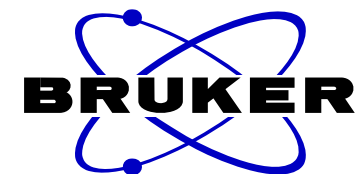


Figure S64. ¹H NMR spectrum of **25**.

HB-C12 M 26mg C



NAME HB-C12 M 26mg
EXPNO 2
PROCNO 1
Date_ 20200906
Time 13.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT MeOD
NS 11
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.6228293 MHz
NUC1 13C
P1 12.37 usec
SI 32768
SF 100.6126314 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

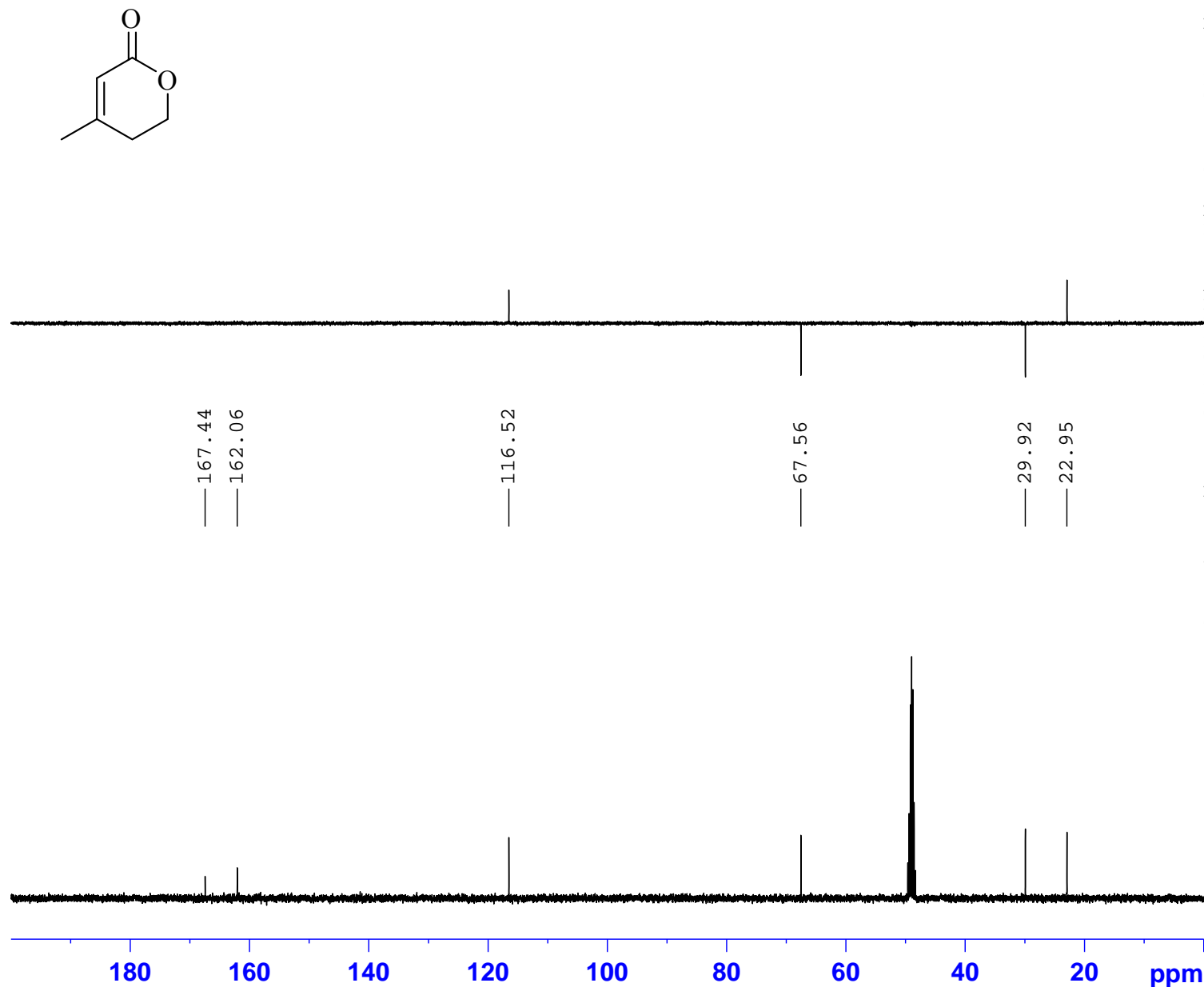


Figure S65. ¹³C NMR spectrum of **25**.