

SUPPLEMENTARY MATERIAL

New polyesterified ursane derivatives from leaves of *Maesa membranacea* and their cytotoxic activity

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Table S1. Viability of human normal and cancer cell lines treated for 24 h with 5-100 µg/mL of **1** or **2** (values are means of three measurements ± SD).

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -0.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

126 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-200 O: 0-15 Na: 1-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
739.4401	739.4397	0.4	0.5	9.5	C41 H64 O10 Na	184.1	n/a	n/a	41	64	10	1

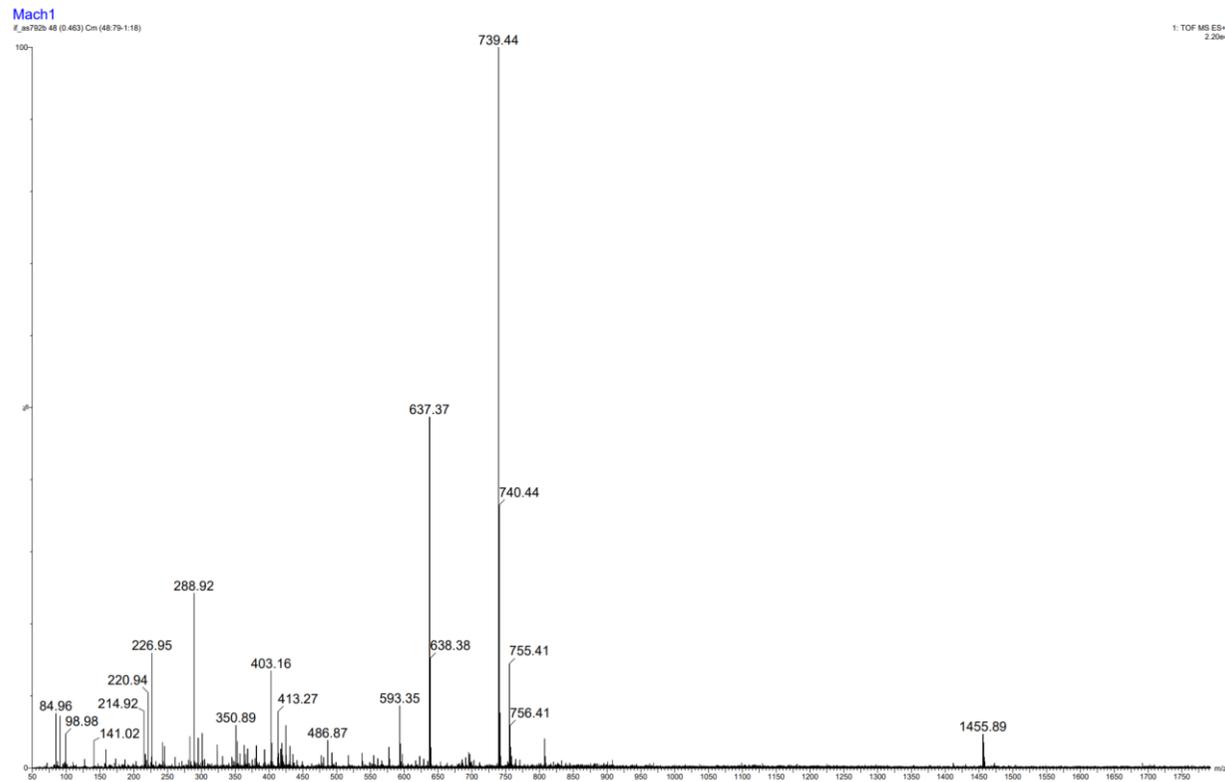


Figure S1. HR ESIMS spectrum of compound **1**.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1



Current Data Parameters
NAME 21-02-19-mach1
EXPNO 37
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210219
Time_ 18.17 h
INSTRUM spect
PROBHD Z108618_0682 (
PULPROG zg30
TD 32050
SOLVENT CDCl3
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 0.400016 Hz
AQ 2.4999001 sec
RG 140.97
DW 78.000 usec
DE 6.50 usec
TE 298.8 K
D1 1.0000000 sec
TD0 1
SFO1 400.1728012 MHz
NUC1 1H
P1 15.25 usec
PLW1 11.30000019 W

F2 - Processing parameters
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

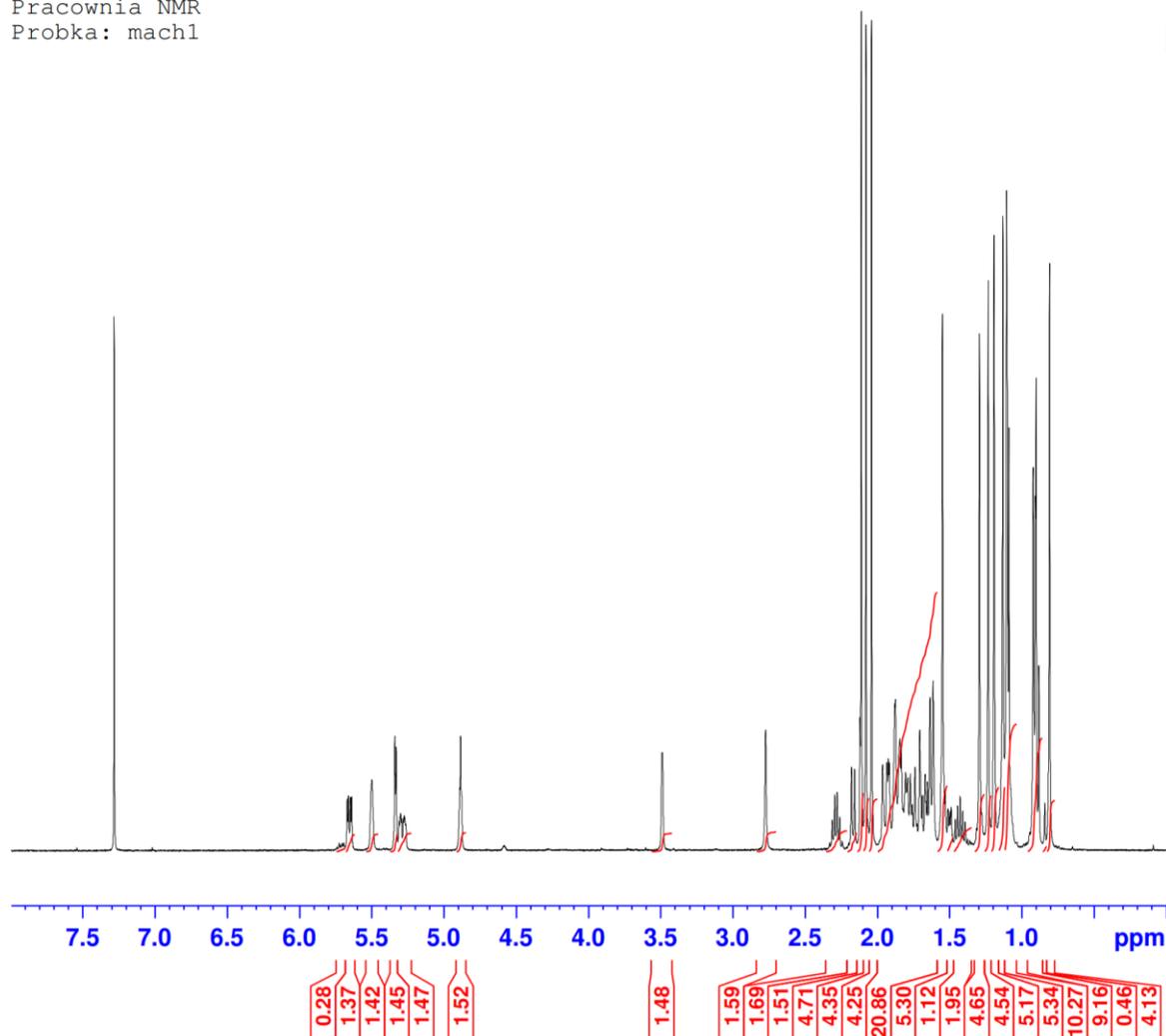


Figure S2. ¹H NMR spectrum of compound 1.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

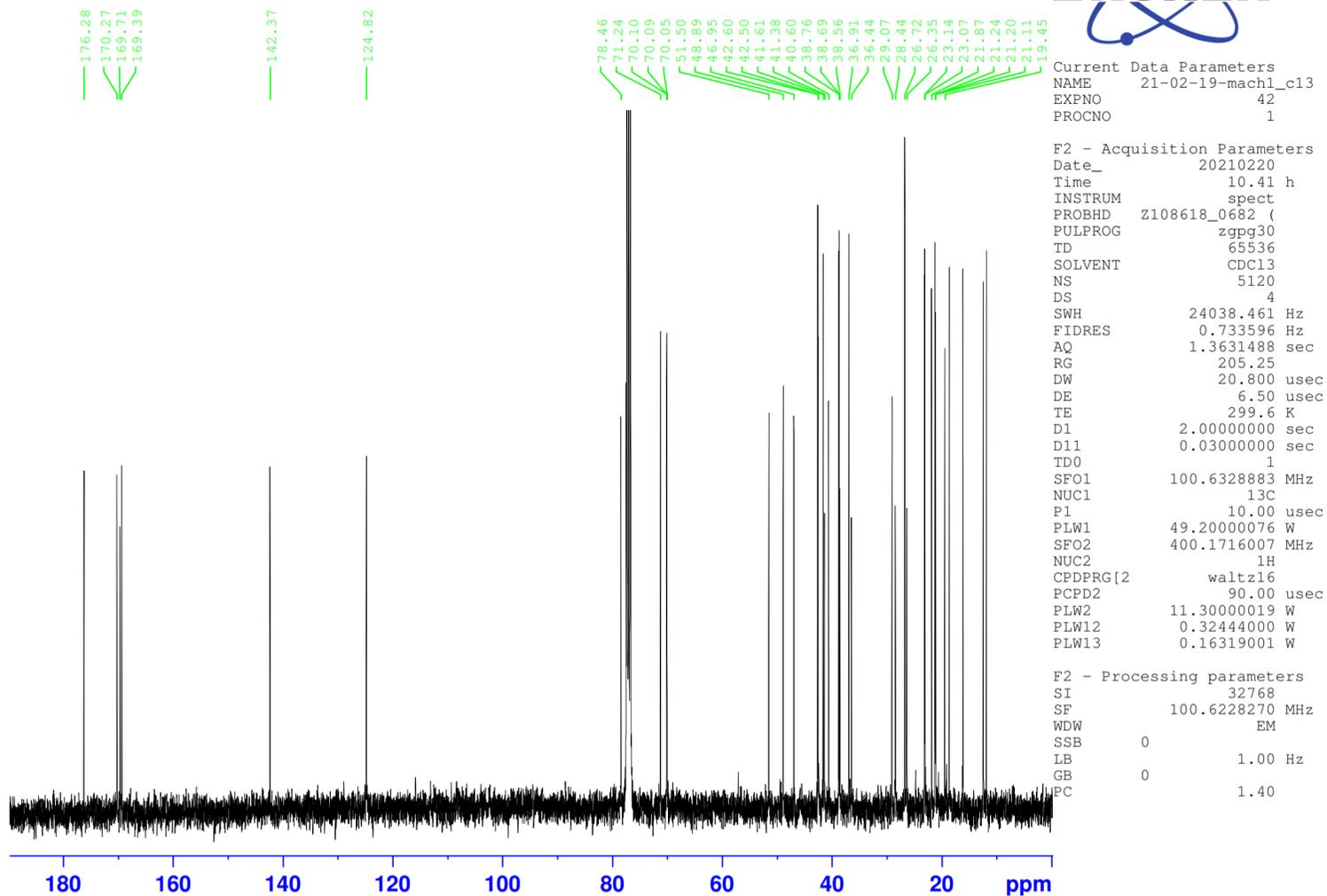


Figure S3. ¹³C NMR spectrum of compound 1.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

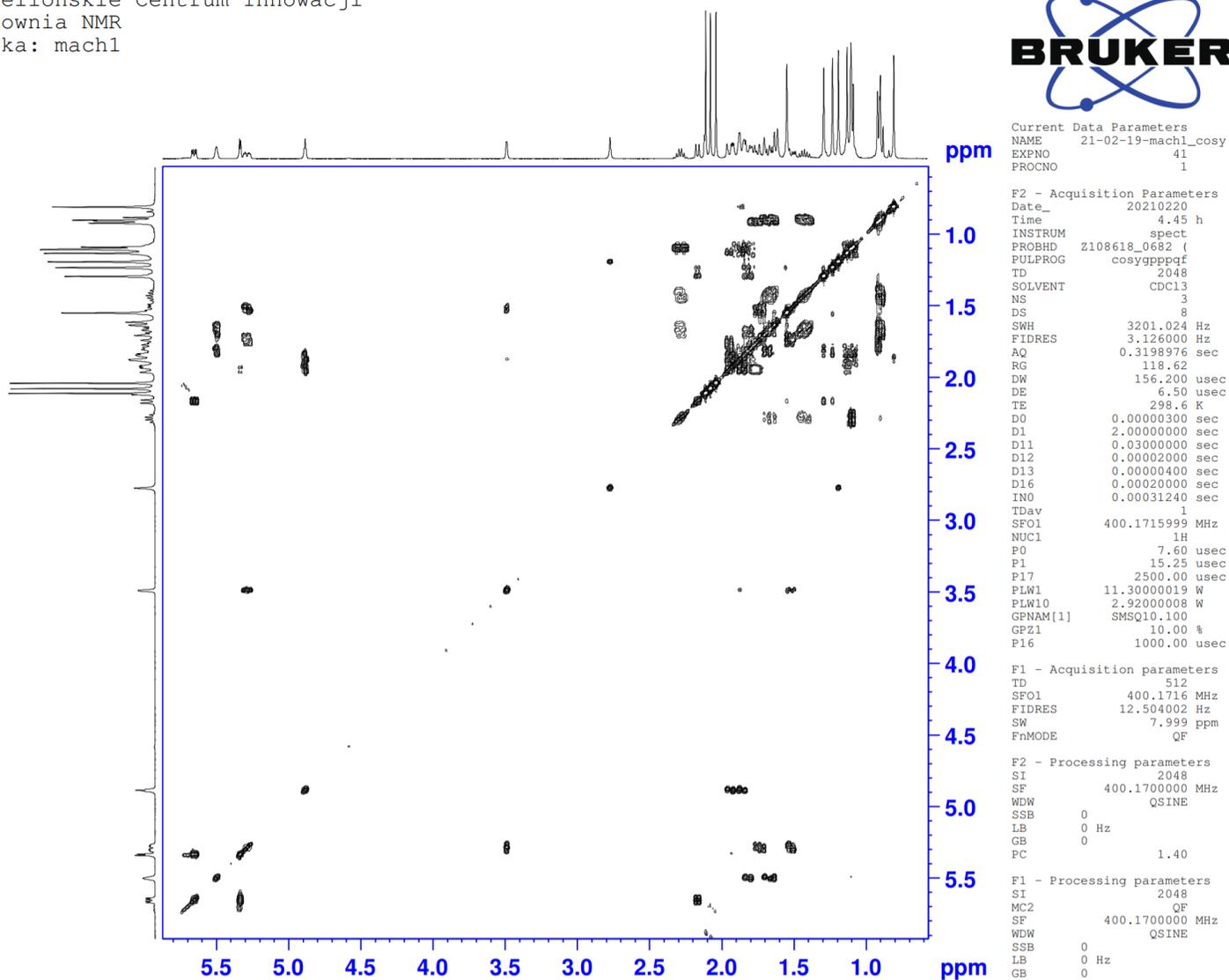


Figure S4. ^1H - ^1H COSY spectrum of compound 1.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

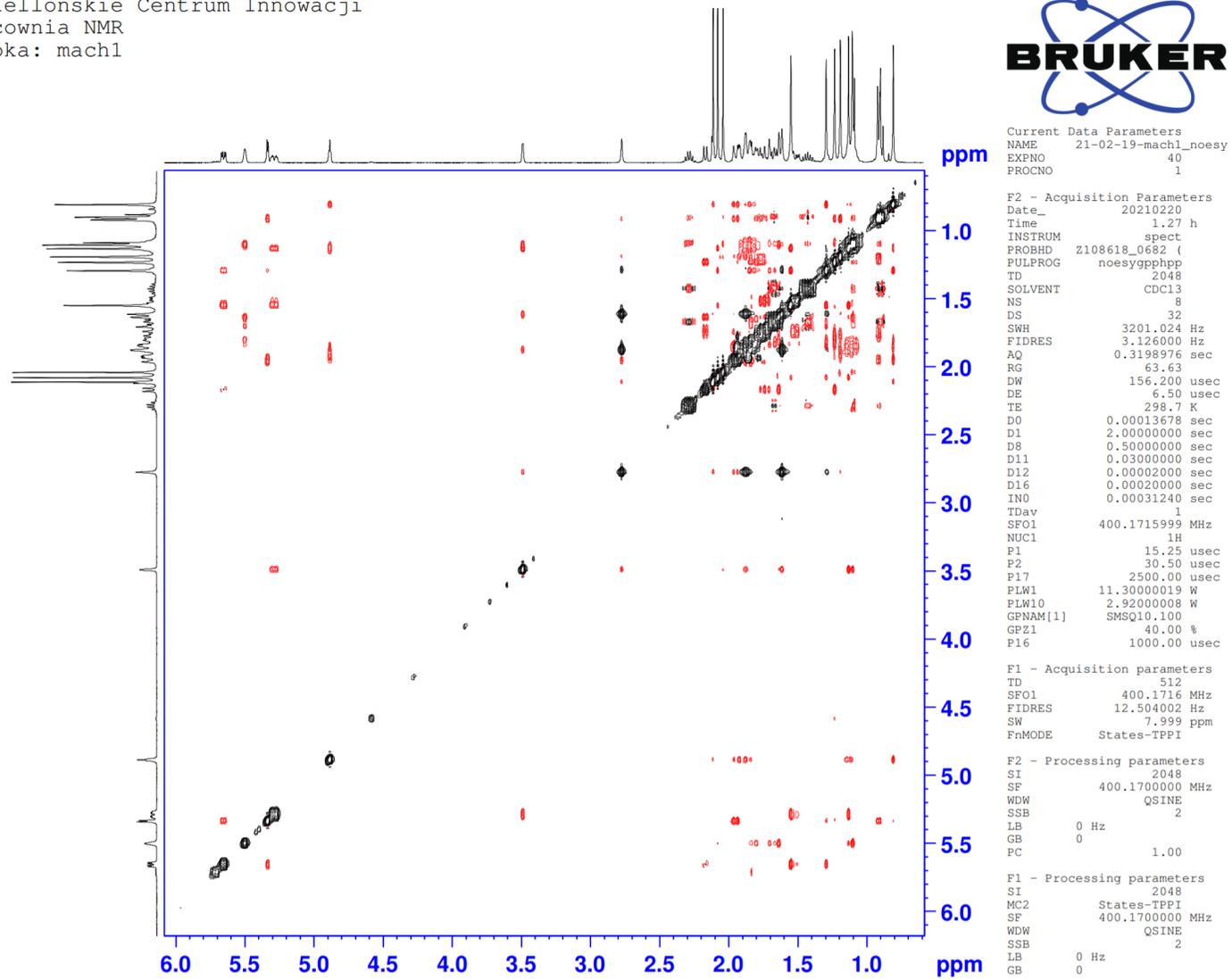


Figure S5. NOESY spectrum of compound 1.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

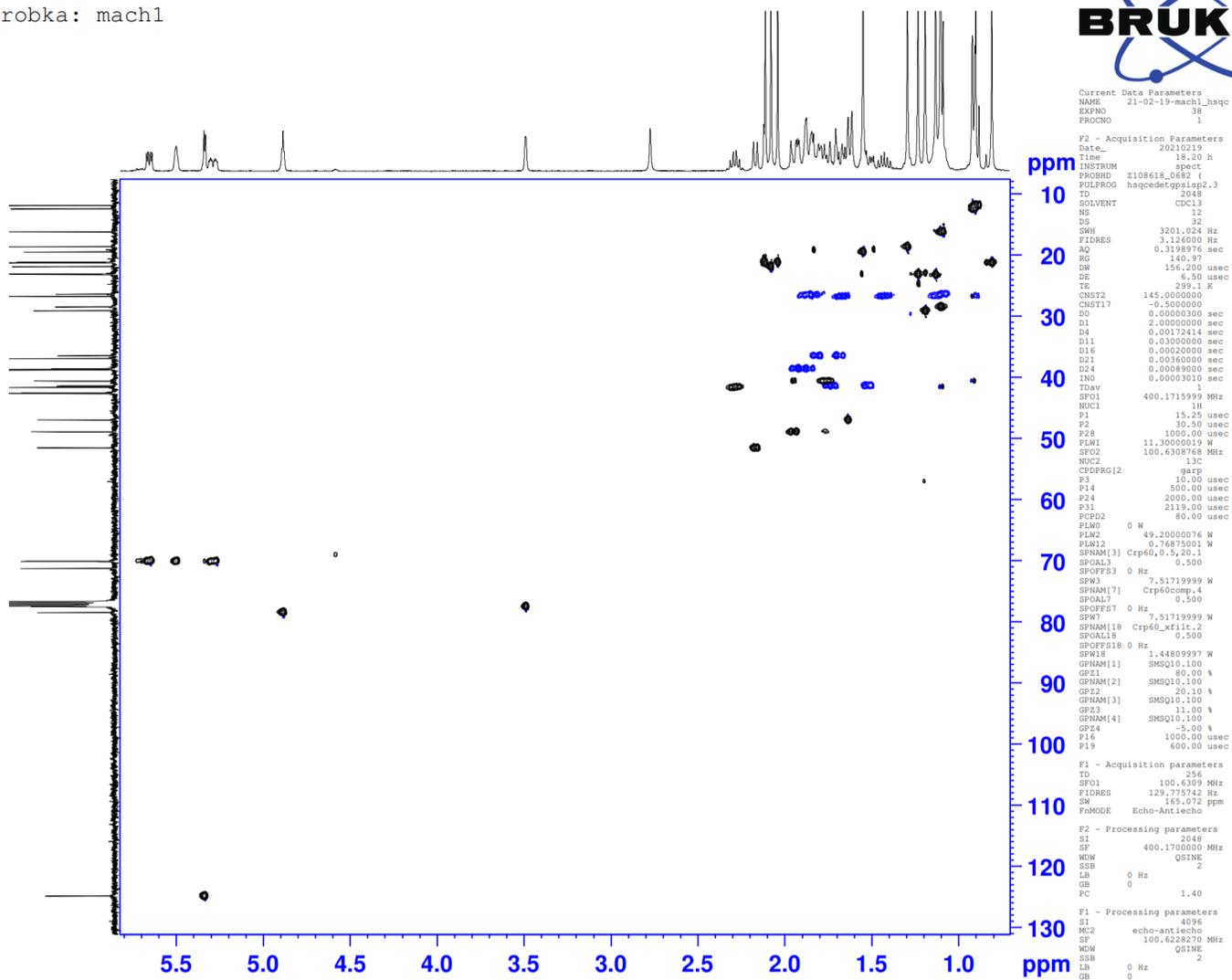


Figure S6. HSQC spectrum of compound 1.

Probka: mach1

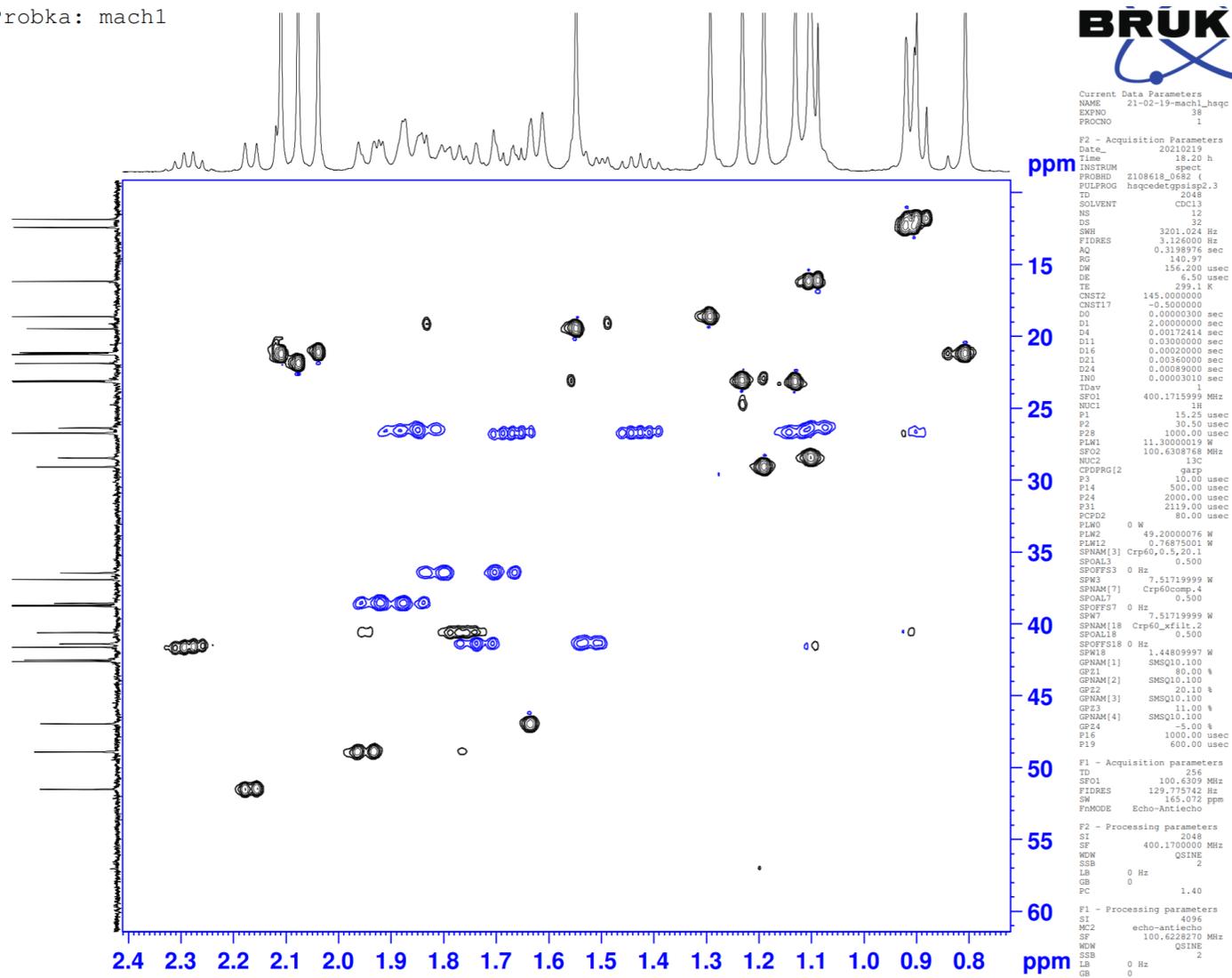


Figure S6a. Expansion of HSQC spectrum of compound 1.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

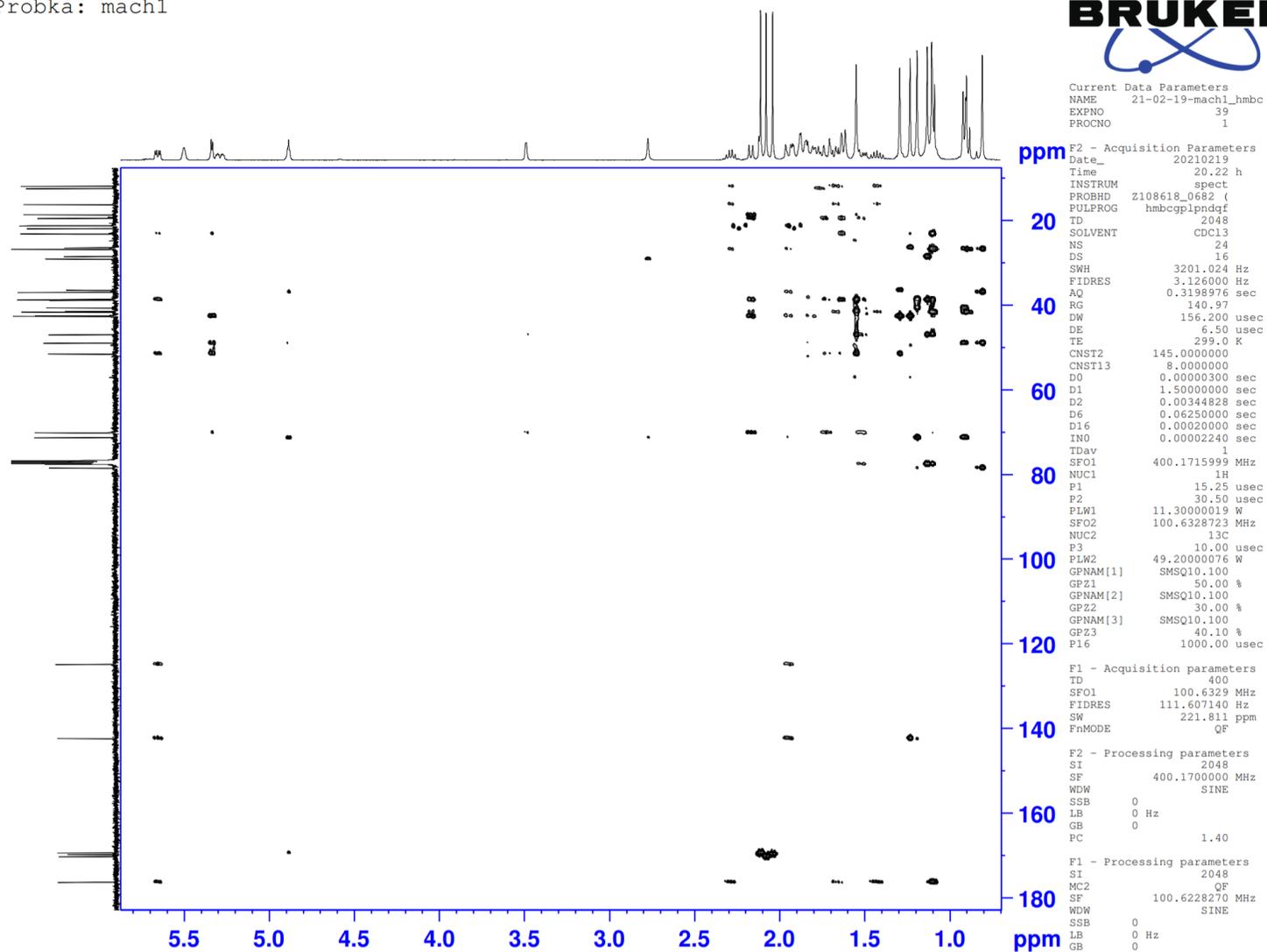


Figure S7. HMBC spectrum of compound 1.

Probka: mach1

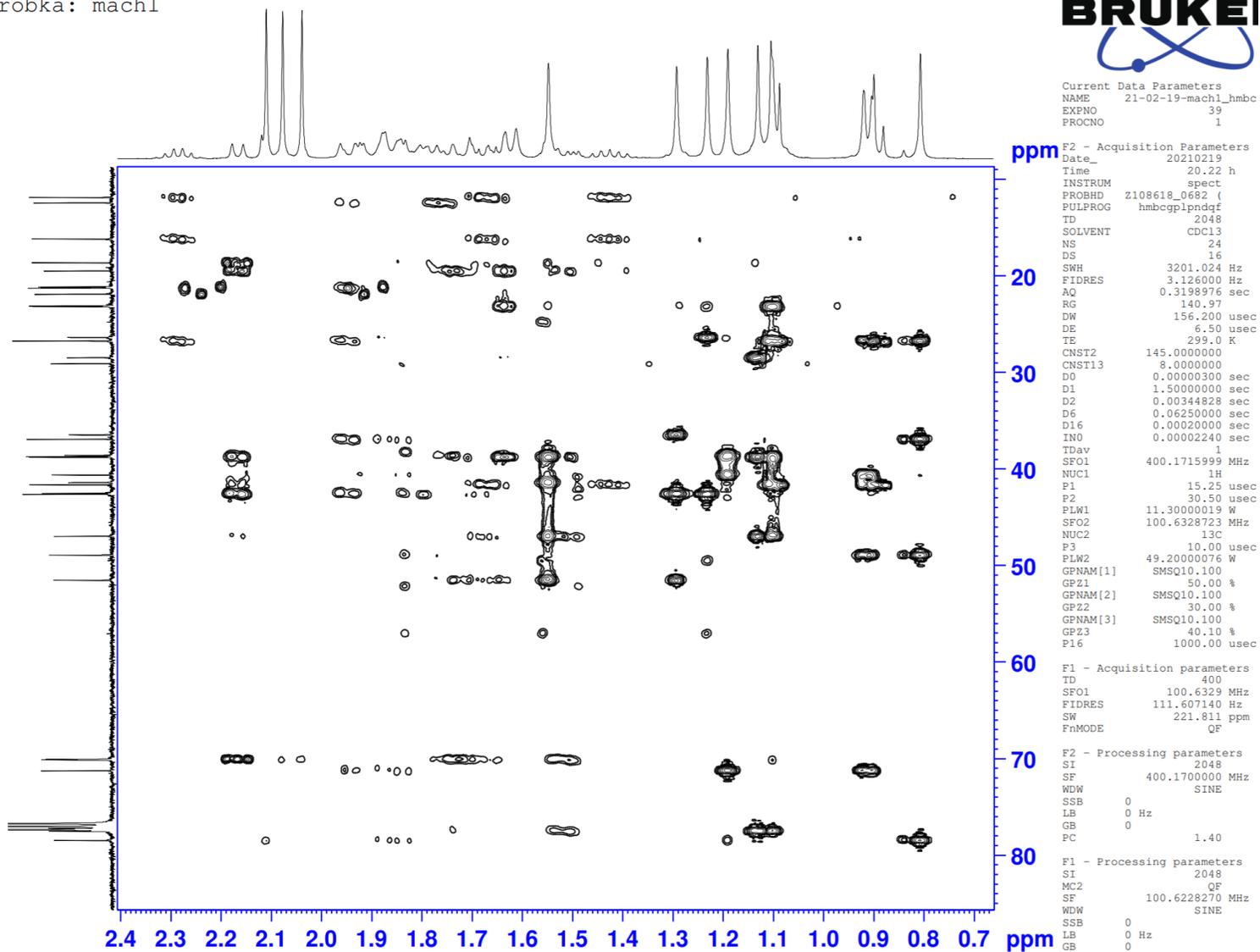


Figure S7a. Expansion of HMBC spectrum of compound 1.

Single Mass Analysis

Tolerance = 3.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

156 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-200 O: 0-9 Na: 0-1

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	O	Na
655.3824	655.3822	0.2	0.3	8.5	C36 H56 O9 Na	589.3	0.013	98.66	36	56	9	1
	655.3846	-2.2	-3.4	11.5	C38 H55 O9	593.6	4.315	1.34	38	55	9	

Mach 296-2

if_as2579a 10 (0.332) Cm (8:15-(7:9+12:15))

1: TOF MS ES+
7.52e4

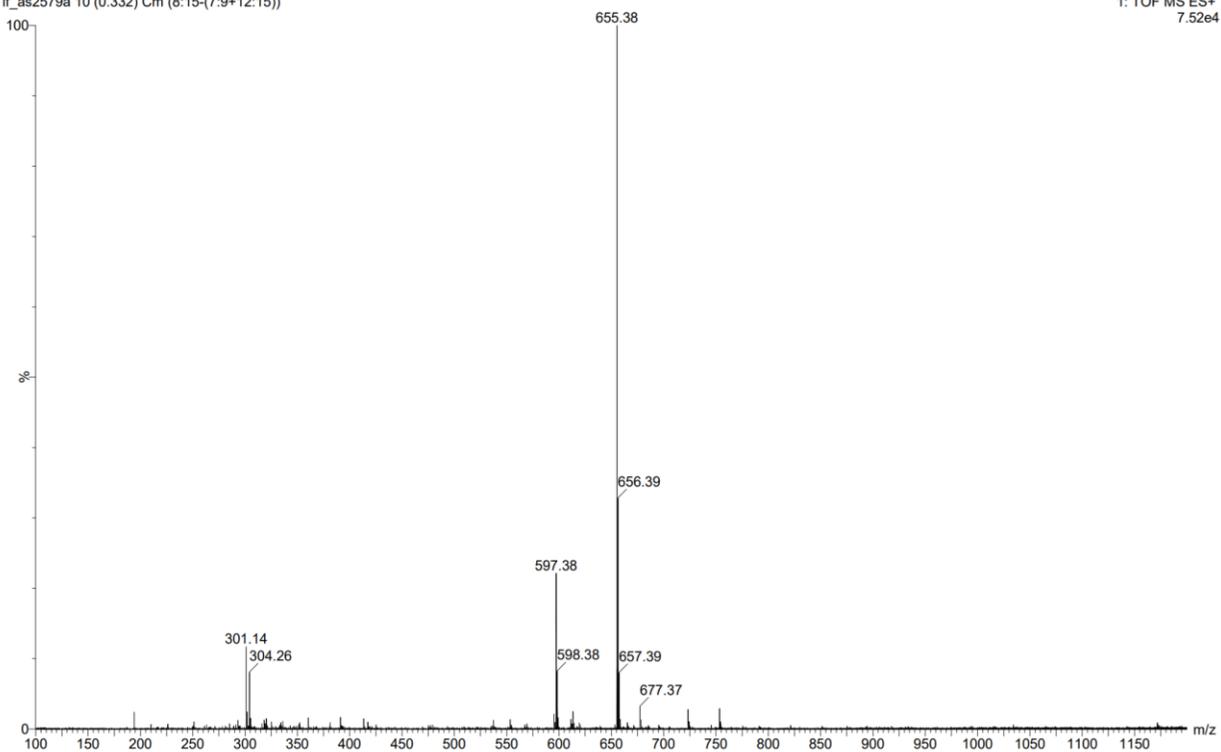


Figure S8. HR ESIMS spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2



Current Data Parameters
NAME 21-07-26-mach296-2
EXPNO 16
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210726
Time 12.09 h
INSTRUM spect
PROBHD Z108618_0682 (
PULPROG zg30
TD 32050
SOLVENT CDC13
NS 64
DS 0
SWH 7211.539 Hz
FIDRES 0.450018 Hz
AQ 2.2221334 sec
RG 140.97
DW 69.333 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.1732014 MHz
NUC1 1H
P1 15.25 usec
PLW1 11.30000019 W

F2 - Processing parameters
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

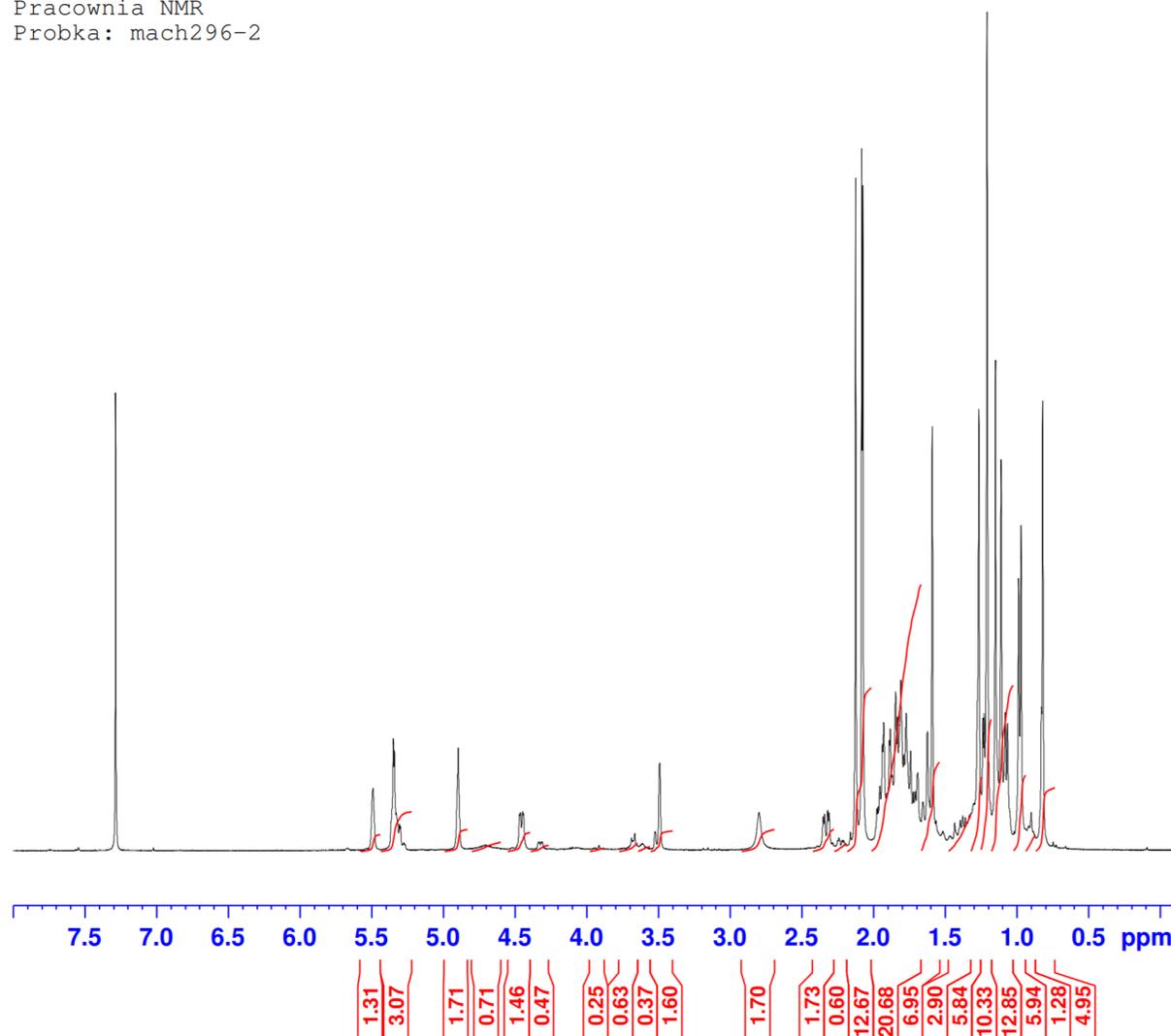
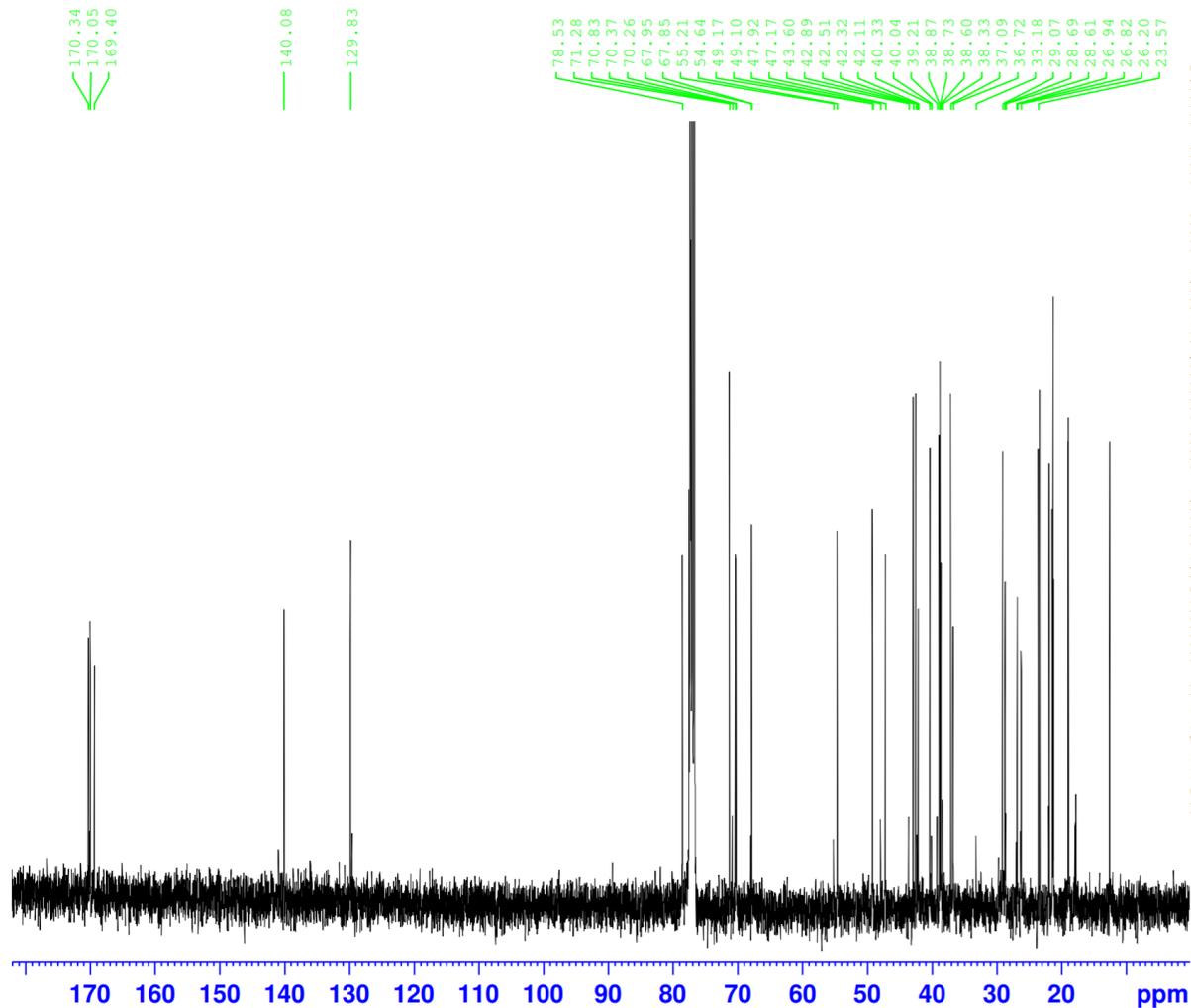


Figure S9. ¹H NMR spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2



Current Data Parameters
NAME 21-08-27-mach296-2_c13
EXPNO 49
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210828
Time 20.31 h
INSTRUM spect
PROBHD Z108618_0682 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6144
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 205.25
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SF01 100.6328883 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.20000076 W
SF02 400.1716007 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 11.30000019 W
PLW12 0.32444000 W
PLW13 0.16319001 W

F2 - Processing parameters
SI 32768
SF 100.6228270 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure S10. ^{13}C NMR spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

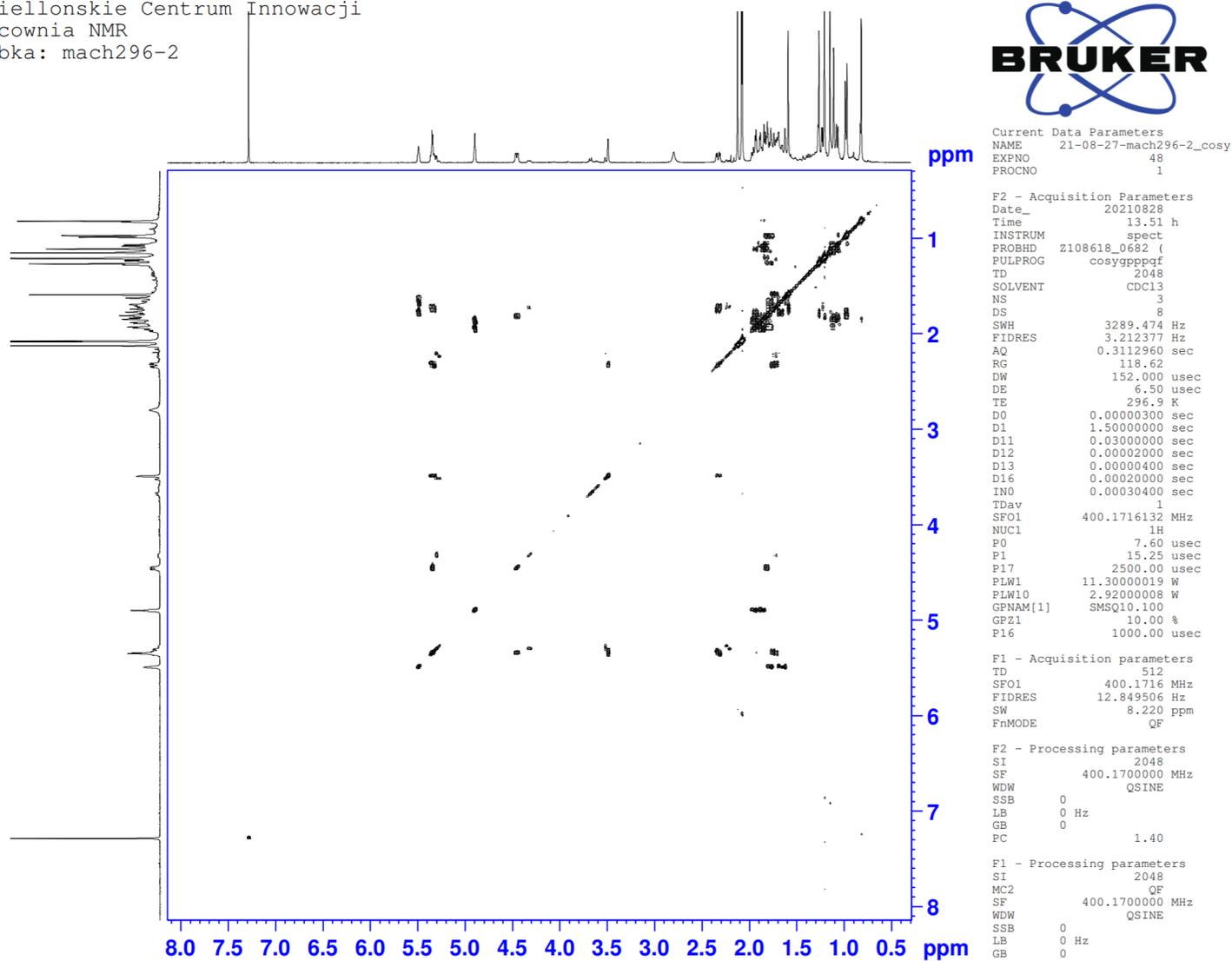


Figure S11. ^1H - ^1H COSY spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

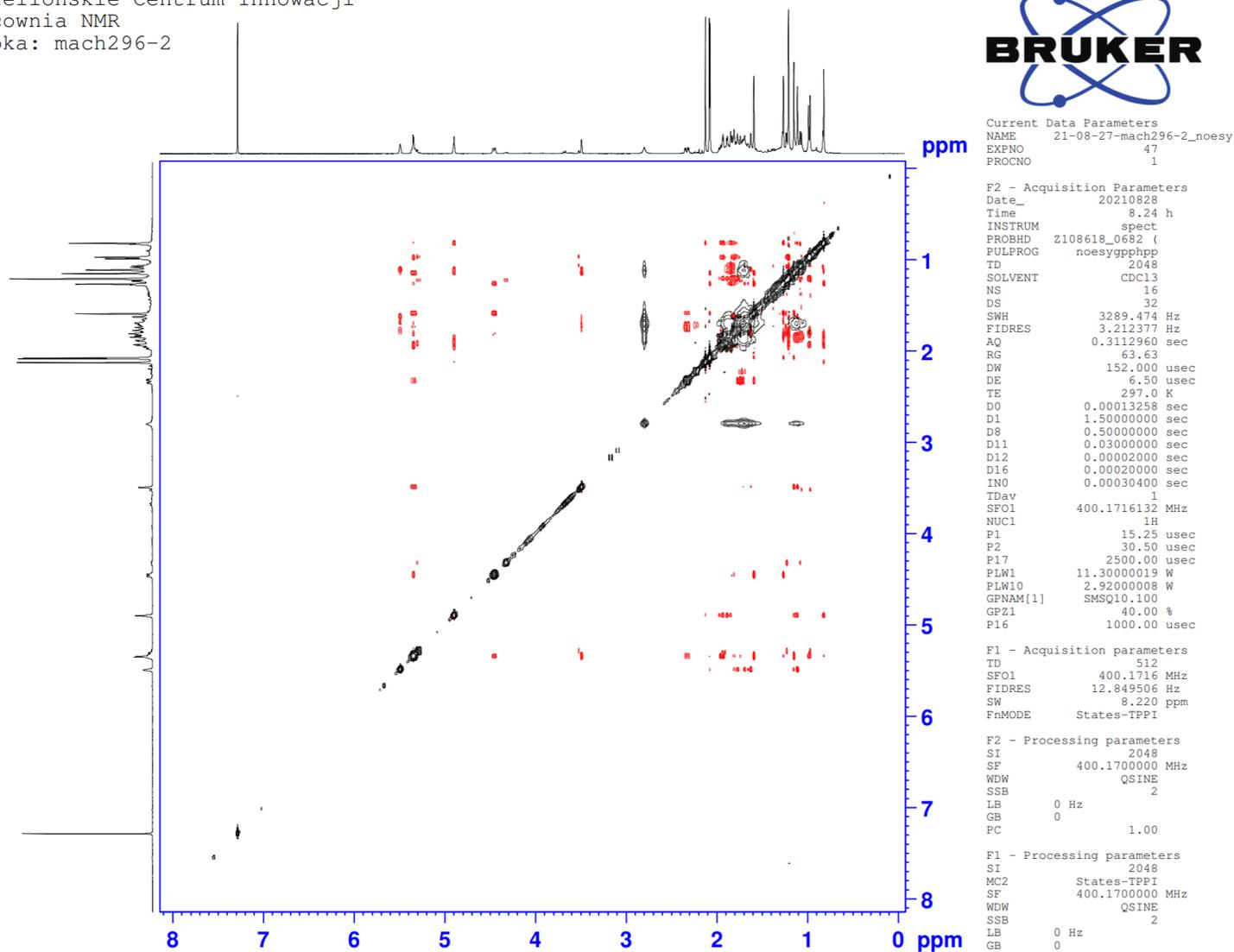


Figure S12. NOESY spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

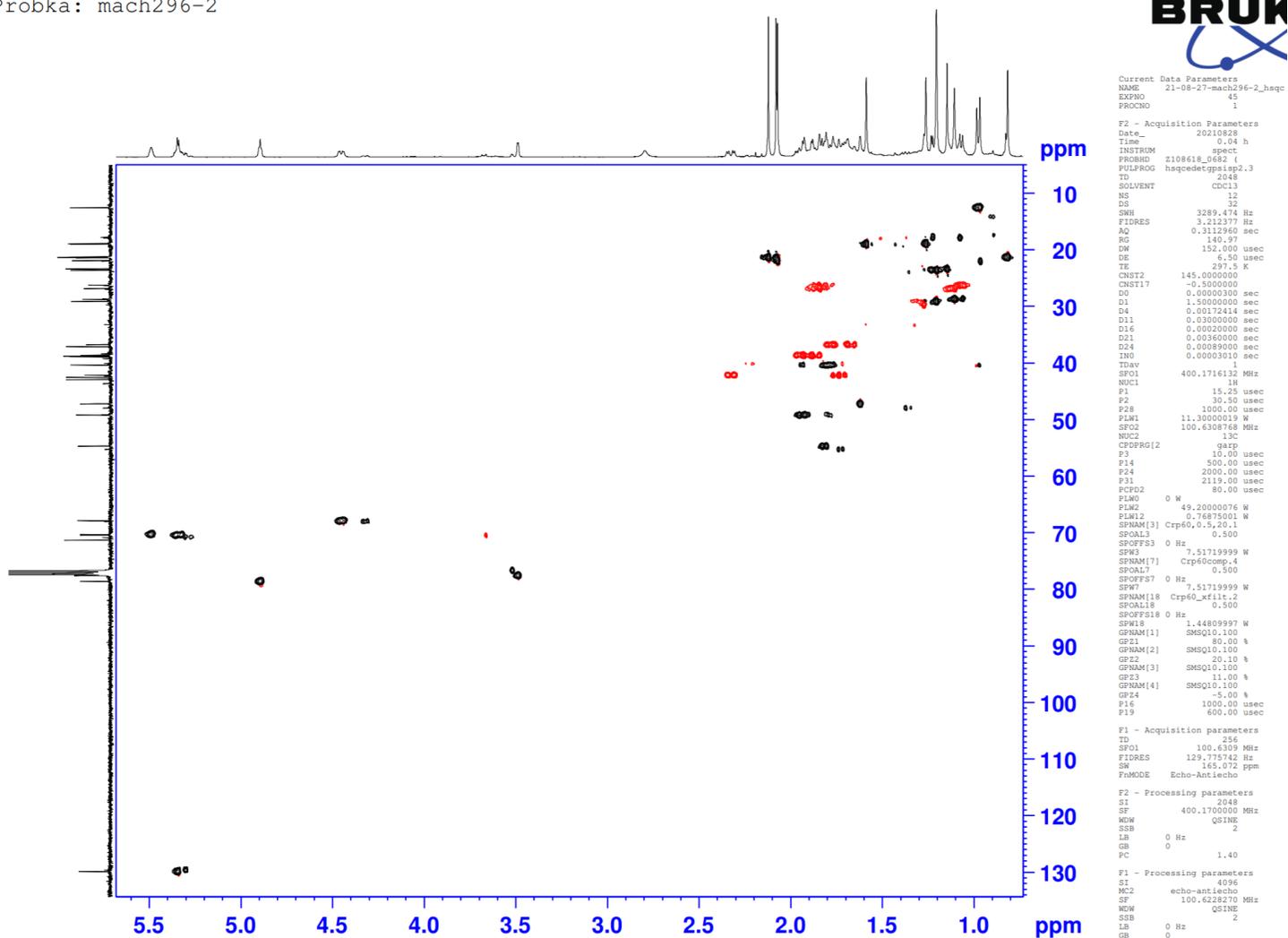
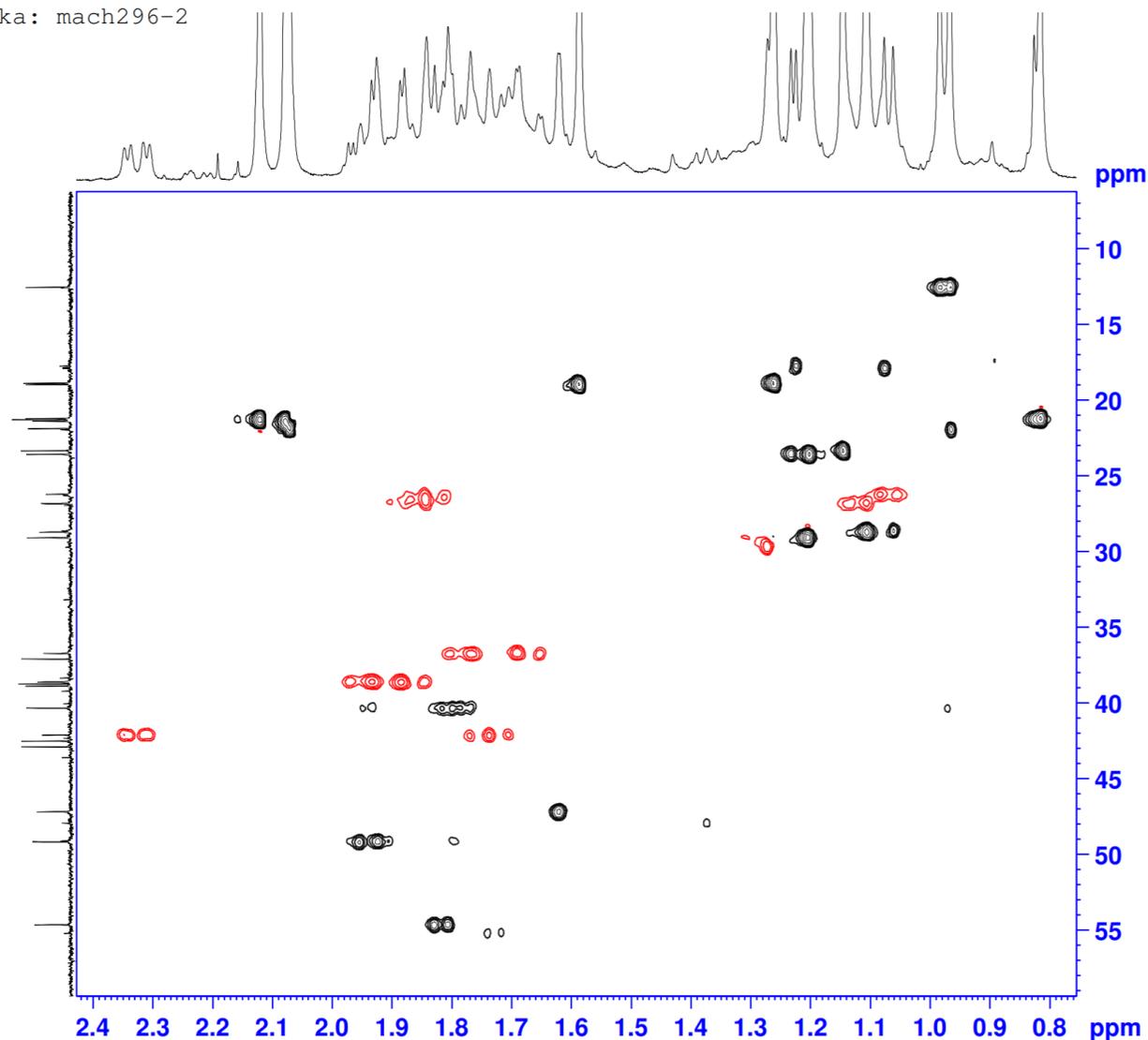


Figure S13. HSQC spectrum of compound 2.

Probka: mach296-2



Current Data Parameters
NAME 21-08-27-mach296-2_hsqc
EXPNO 45
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210828
Time 0.04 h
INSTRUM spect
PROBHD z108618_0682 f
PULPROG hsqcdeatgpsisp2.3
TD 2048
SOLVENT CDCl3
NS 12
DS 32
SWH 3289.474 Hz
FIDRES 3.212377 Hz
AQ 0.3112960 sec
RG 140.97
DW 152.000 usec
DE 6.50 usec
TE 297.5 K
CNST2 145.000000
CNST17 -0.500000
D0 0.0000000 sec
D1 1.5000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D21 0.00380000 sec
D24 0.00089000 sec
IN0 0.00003010 sec
IDAV 1
SFO1 400.1716132 MHz
NUC1 1H
P1 15.25 usec
P2 30.50 usec
P28 1000.00 usec
P1M1 11.30000019 W
SFO2 100.6308768 MHz
NUC2 13C
CPOPRG2 88FP
P3 10.00 usec
P14 500.00 usec
P24 2000.00 usec
P31 2119.00 usec
PCPD2 80.00 usec
PLM0 0 W
PLM2 49.20000076 W
PLM12 0.76875001 W
SFOAL3 Crp60_0.5_20.1
SFOAL3 0.500
SFOFF33 0 Hz
SFW3 7.51719999 W
SFOAL7 Crp60comp.4
SFOAL7 0.500
SFOFFS7 0 Hz
SFW7 7.51719999 W
SFOAL18 Crp60_kf11c.2
SFOAL18 0.500
SFOFFS18 0 Hz
SFW18 1.44809997 W
GFNAM[1] SMSQ10.100
GF21 80.00 %
GFNAM[2] SMSQ10.100
GF22 20.10 %
GFNAM[3] SMSQ10.100
GF23 11.00 %
GFNAM[4] SMSQ10.100
GF24 -5.00 %
F16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.6309 MHz
FIDRES 129.775742 Hz
SW 165.072 ppm
FhMODE Echo-Antiecho

F2 - Processing parameters
SI 2048
SF 400.1700000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 4096
MC2 echo-antiecho
SF 100.6228270 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

Figure S13a. Expansion of HSQC spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

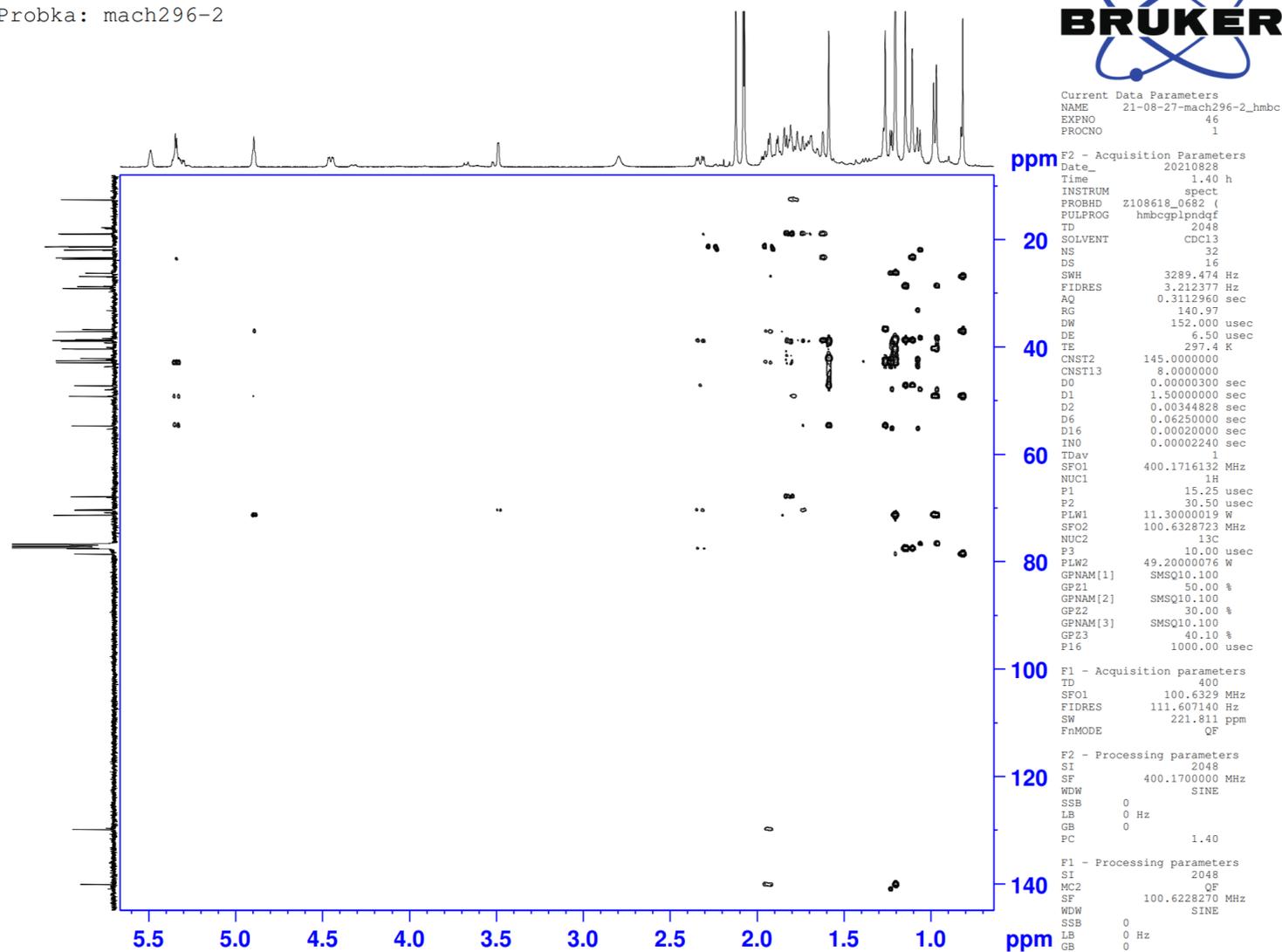


Figure S14. HMBC spectrum of compound 2.

Probka: mach296-2



Current Data Parameters
NAME 21-08-27-mach296-2_hmbc
EXPNO 46
PROCNO 1

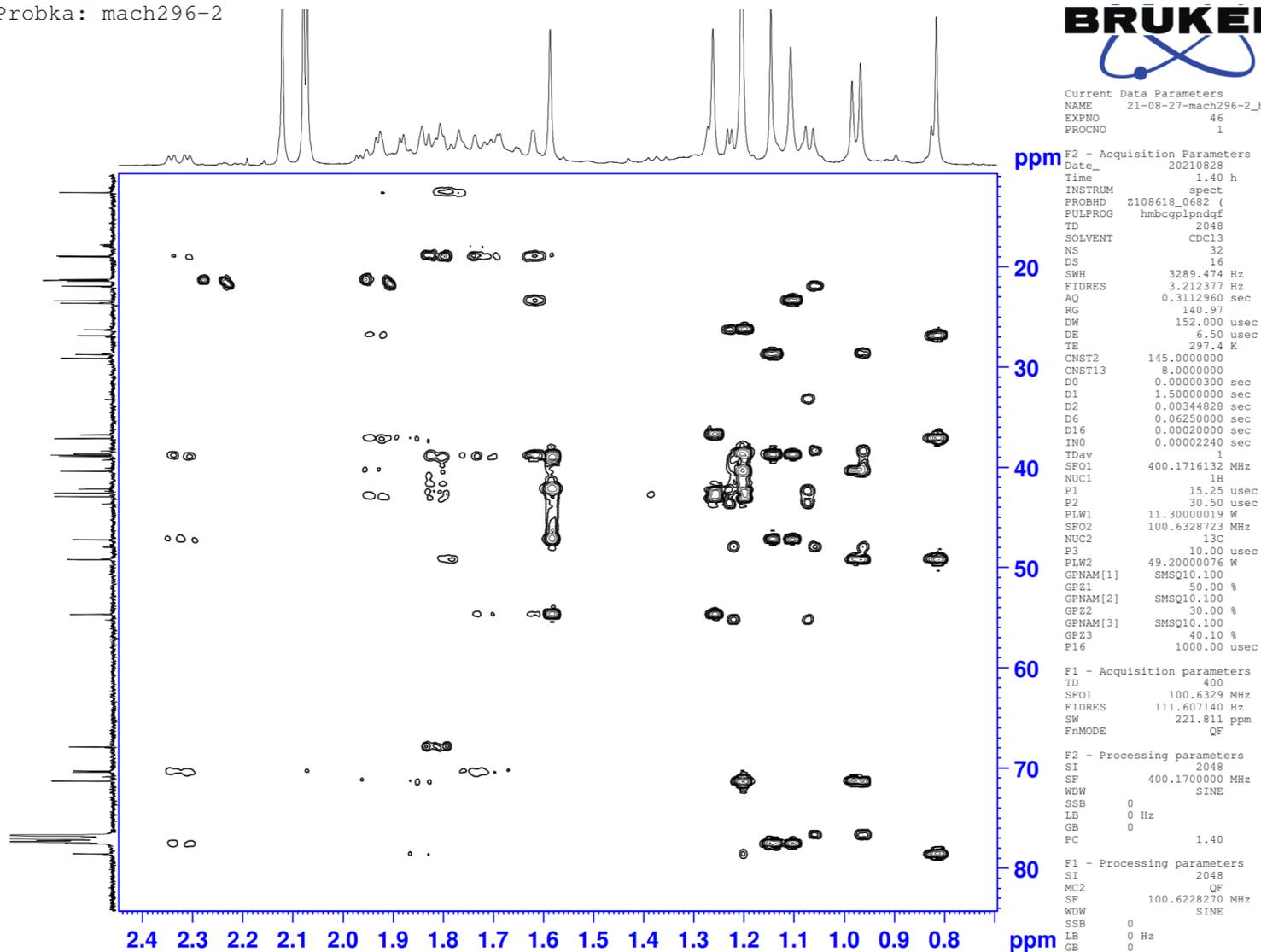


Figure S14a. Expansion of HMBC spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach117-1



Current Data Parameters
NAME 21-07-26-mach117-1
EXPNO 17
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210726
Time 12.23 h
INSTRUM spect
PROBHD Z108618_0682 (
PULPROG zg30
TD 32050
SOLVENT CDC13
NS 64
DS 0
SWH 7211.539 Hz
FIDRES 0.450018 Hz
AQ 2.2221334 sec
RG 205.25
DW 69.333 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.1732014 MHz
NUC1 1H
P1 15.25 usec
PLW1 11.30000019 W

F2 - Processing parameters
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

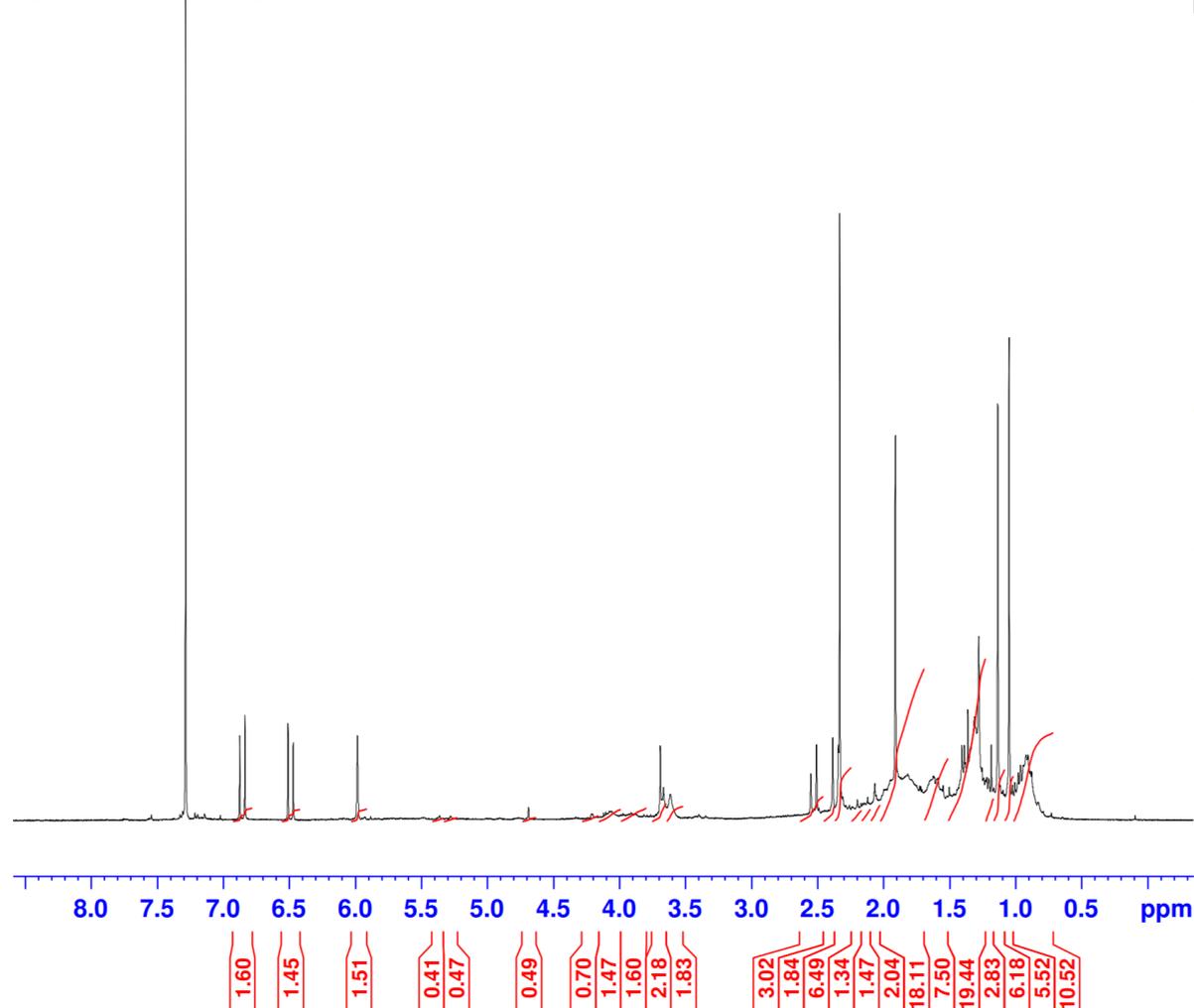


Figure S15. ^1H NMR spectrum of compound 3.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach5



Current Data Parameters
NAME 20-05-27-mach5
EXPNO 73
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200527
Time 15.43 h
INSTRUM spect
PROBHD z108618_0682 (
PULPROG zg30
TD 32050
SOLVENT CDCl3
NS 80
DS 0
SWH 6410.256 Hz
FIDRES 0.400016 Hz
AQ 2.4999001 sec
RG 205.25
DW 78.000 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1728012 MHz
NUC1 1H
P1 15.25 usec
PLW1 11.30000019 W

F2 - Processing parameters
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

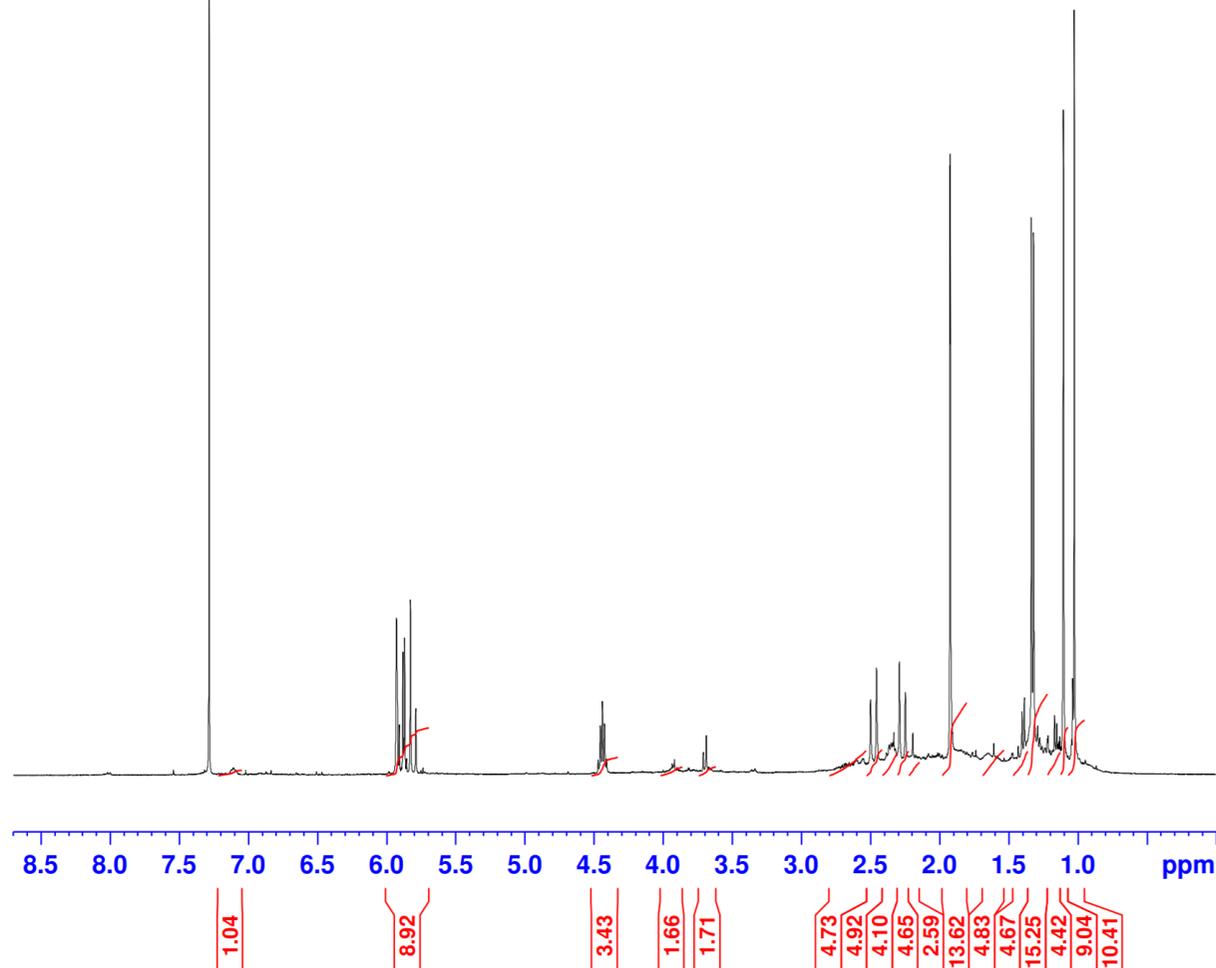


Figure S16. ^1H NMR spectrum of compound 4.

Table S1. Viability of human normal and cancer cell lines treated for 24 h with 5-100 $\mu\text{g/mL}$ of **1** or **2** (values are means of three measurements \pm SD).

Compound; dose	Cell viability [%] \pm SD							
	Prostate normal and cancer cells			Keratinocytes and melanoma cells			Colon cancer	
	PNT-2	DU145	PC3	HaCaT	A375	HTB140	HT29	Caco-2
1 ; 5 $\mu\text{g/mL}$	96.61 \pm 0.53	93.19 \pm 0.93	96.16 \pm 1.04	96.52 \pm 0.80	97.23 \pm 0.57	96.15 \pm 1.12	97.04 \pm 0.42	95.55 \pm 0.74
1 ; 10 $\mu\text{g/mL}$	96.77 \pm 0.60	83.12 \pm 1.96	90.71 \pm 0.93	94.87 \pm 1.00	96.44 \pm 0.92	93.82 \pm 0.73	95.49 \pm 0.82	88.71 \pm 0.93
1 ; 20 $\mu\text{g/mL}$	94.59 \pm 0.90	70.39 \pm 1.69	83.88 \pm 1.67	88.37 \pm 0.47	92.75 \pm 1.11	87.08 \pm 2.09	90.94 \pm 1.37	78.46 \pm 1.94
1 ; 30 $\mu\text{g/mL}$	91.05 \pm 1.07	57.25 \pm 2.20	74.81 \pm 1.17	81.25 \pm 1.77	87.25 \pm 2.17	78.92 \pm 2.08	81.48 \pm 1.89	65.89 \pm 1.21
1 ; 40 $\mu\text{g/mL}$	83.02 \pm 1.41	41.26 \pm 1.91	62.58 \pm 1.36	73.95 \pm 1.72	79.75 \pm 2.02	68.39 \pm 2.17	72.49 \pm 1.94	51.13 \pm 2.40
1 ; 50 $\mu\text{g/mL}$	70.73 \pm 2.58	27.22 \pm 2.28	45.67 \pm 1.85	65.66 \pm 1.22	70.18 \pm 1.39	59.51 \pm 1.40	64.78 \pm 1.69	35.78 \pm 1.32
1 ; 100 $\mu\text{g/mL}$	59.02 \pm 2.20	9.87 \pm 1.59	28.14 \pm 2.31	56.82 \pm 2.20	62.56 \pm 2.03	46.59 \pm 2.09	55.21 \pm 1.73	22.25 \pm 1.53
2 ; 5 $\mu\text{g/mL}$	97.49 \pm 0.79	97.30 \pm 0.27	96.56 \pm 1.35	96.84 \pm 0.60	97.28 \pm 0.33	97.48 \pm 0.79	95.76 \pm 0.69	94.66 \pm 1.42
2 ; 10 $\mu\text{g/mL}$	96.75 \pm 0.56	94.54 \pm 0.58	94.14 \pm 1.24	94.53 \pm 1.55	95.28 \pm 0.90	96.66 \pm 0.68	94.55 \pm 0.84	88.42 \pm 0.92
2 ; 20 $\mu\text{g/mL}$	96.30 \pm 1.04	90.07 \pm 0.71	87.92 \pm 1.54	90.60 \pm 0.66	91.07 \pm 1.39	96.40 \pm 0.83	90.05 \pm 0.74	81.97 \pm 1.69
2 ; 30 $\mu\text{g/mL}$	95.64 \pm 0.65	83.15 \pm 1.24	78.96 \pm 1.10	82.83 \pm 1.23	87.27 \pm 1.50	94.29 \pm 1.45	81.65 \pm 1.56	74.70 \pm 1.19
2 ; 40 $\mu\text{g/mL}$	95.37 \pm 0.75	77.13 \pm 1.63	70.32 \pm 1.60	75.68 \pm 1.76	82.63 \pm 1.36	93.72 \pm 1.11	74.77 \pm 1.13	65.80 \pm 1.25
2 ; 50 $\mu\text{g/mL}$	94.56 \pm 0.32	68.62 \pm 1.78	58.98 \pm 1.81	61.79 \pm 1.55	76.22 \pm 1.78	91.95 \pm 1.64	67.15 \pm 1.25	61.07 \pm 2.37
2 ; 100 $\mu\text{g/mL}$	93.56 \pm 0.50	57.30 \pm 1.90	47.10 \pm 2.64	54.26 \pm 1.78	67.56 \pm 1.48	89.49 \pm 1.40	56.91 \pm 1.85	49.61 \pm 1.49