

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

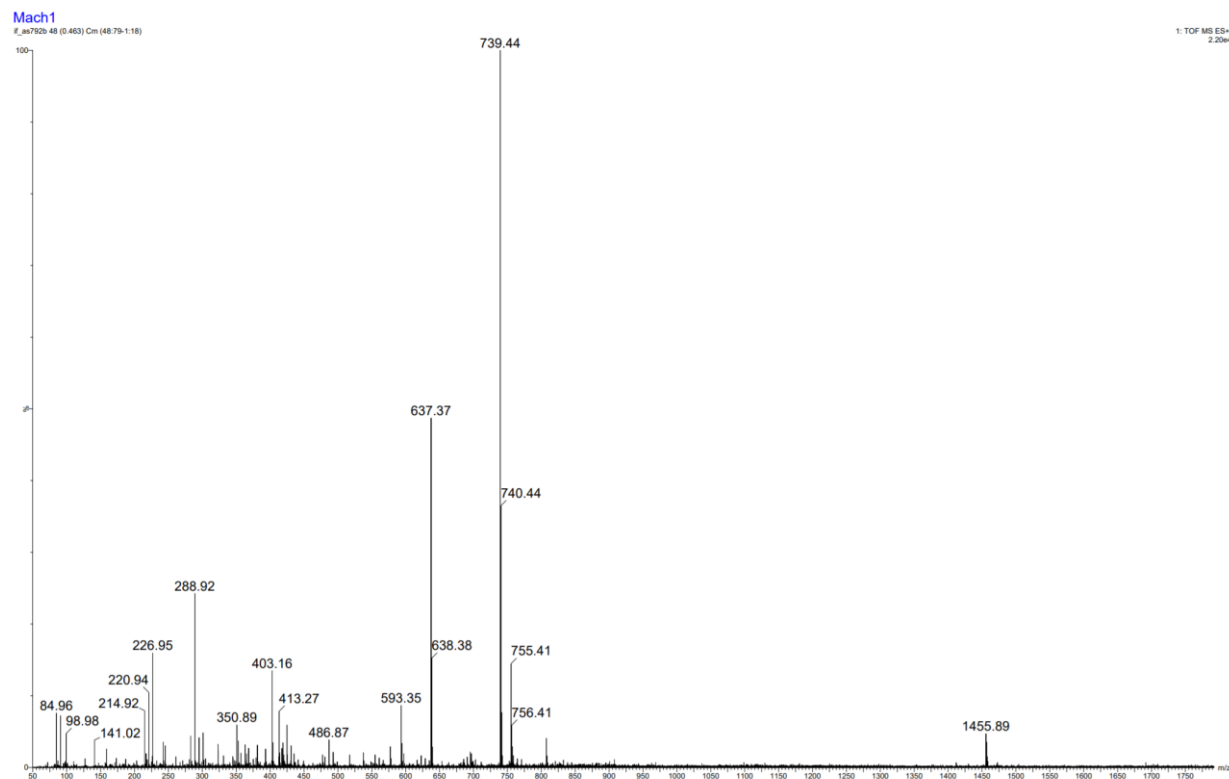


Figure S1. HR ESIMS spectrum of compound **1**.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1



Current Data Parameters
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EXPNO 37
PROCNO 1

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Time 18.17 h
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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 1.00000000 sec
TD0 1
SFO1 400.1728012 MHz
NUC1 1H
P1 15.25 usec
PLW1 11.30000019 W

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

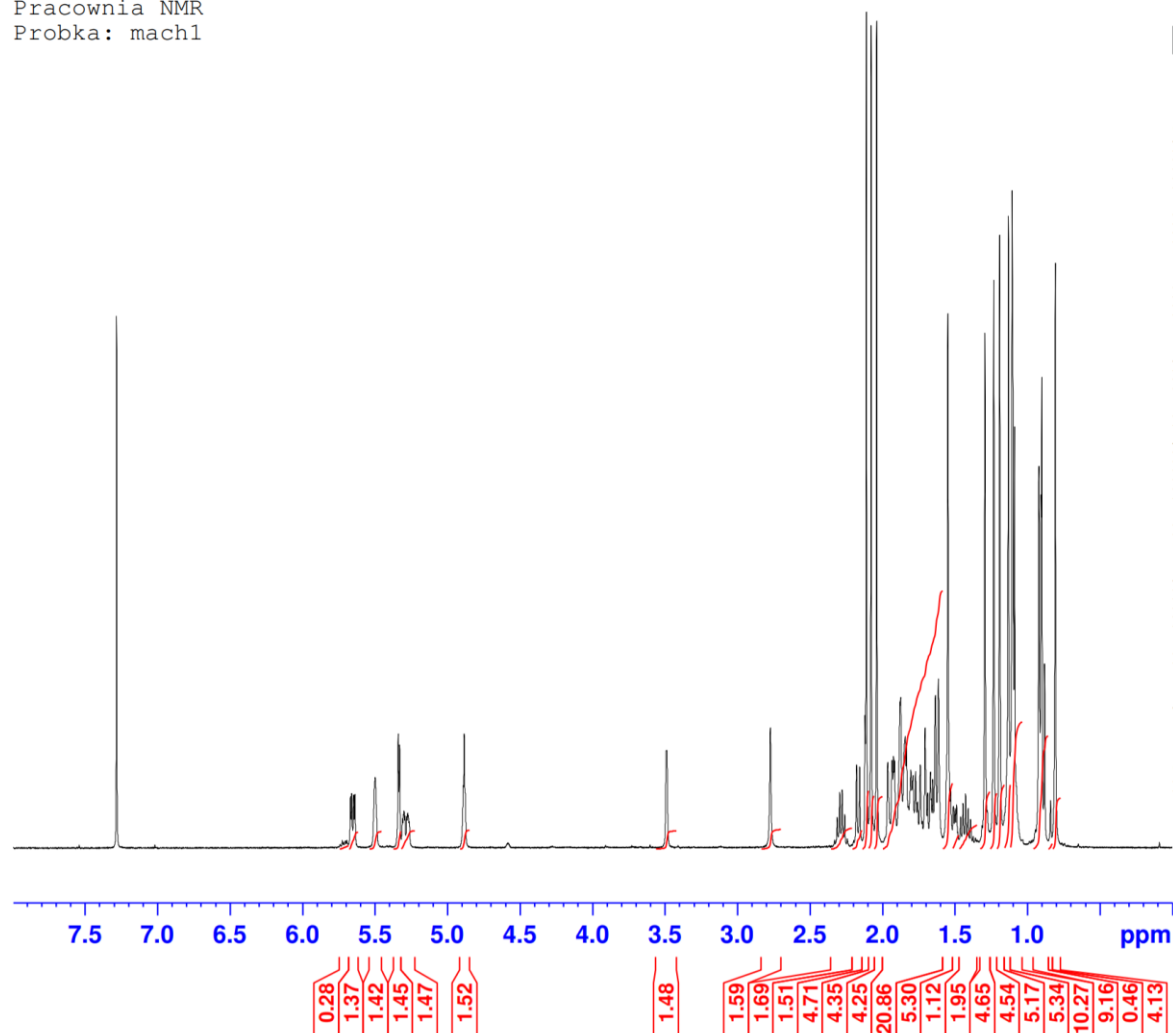


Figure S2. ^1H NMR spectrum of compound 1.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

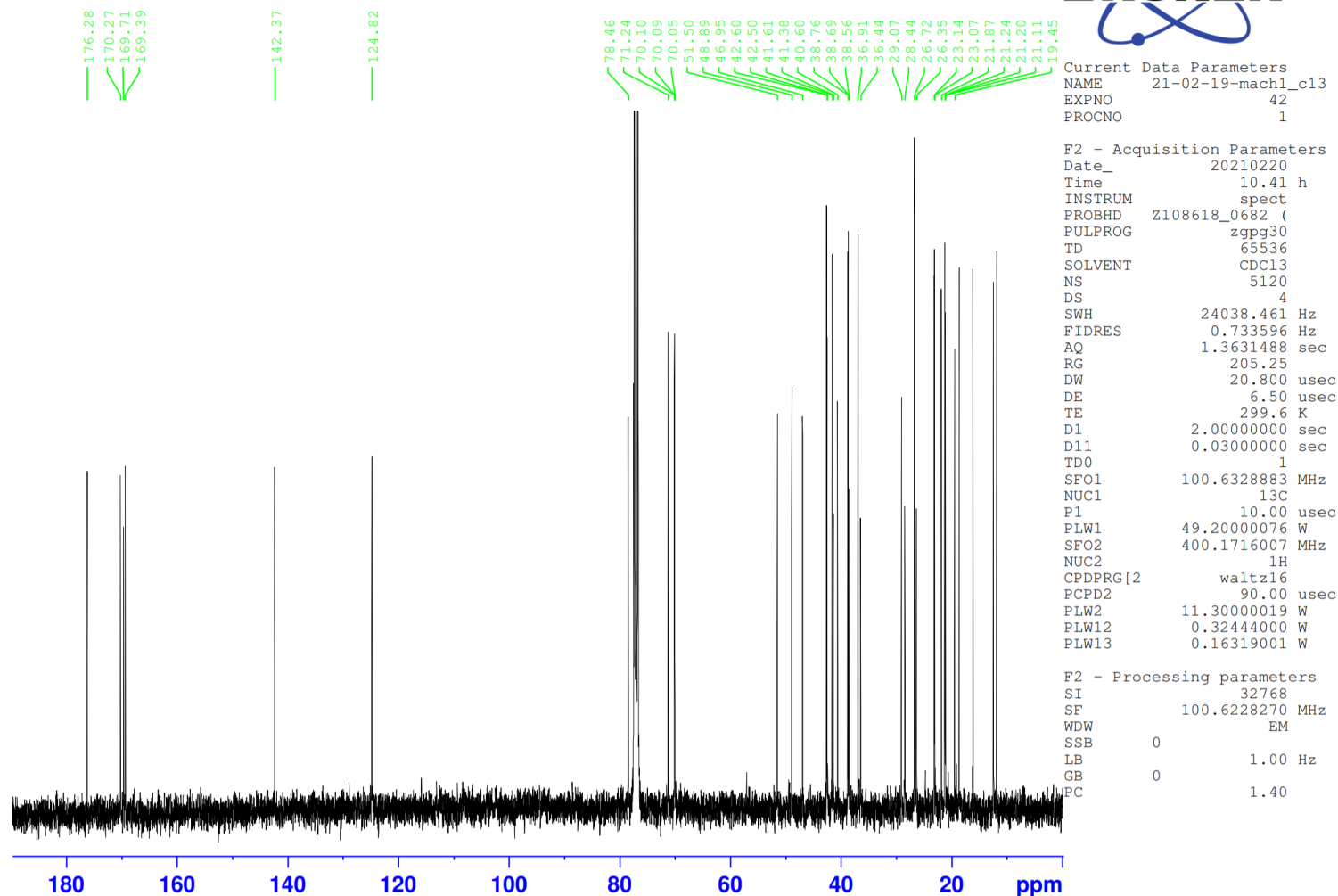


Figure S3. ^{13}C NMR spectrum of compound **1**.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

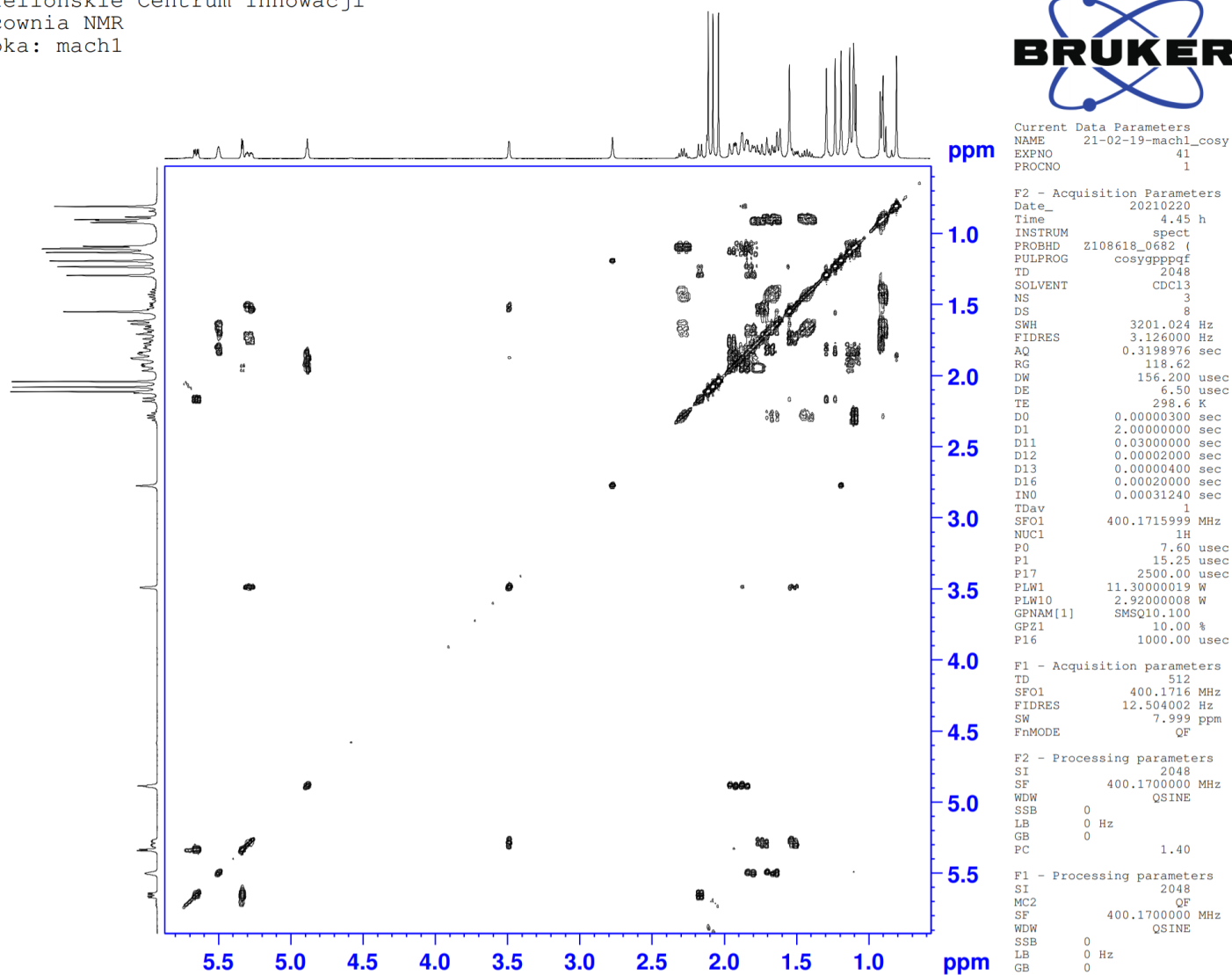


Figure S4. ^1H - ^1H COSY spectrum of compound 1.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

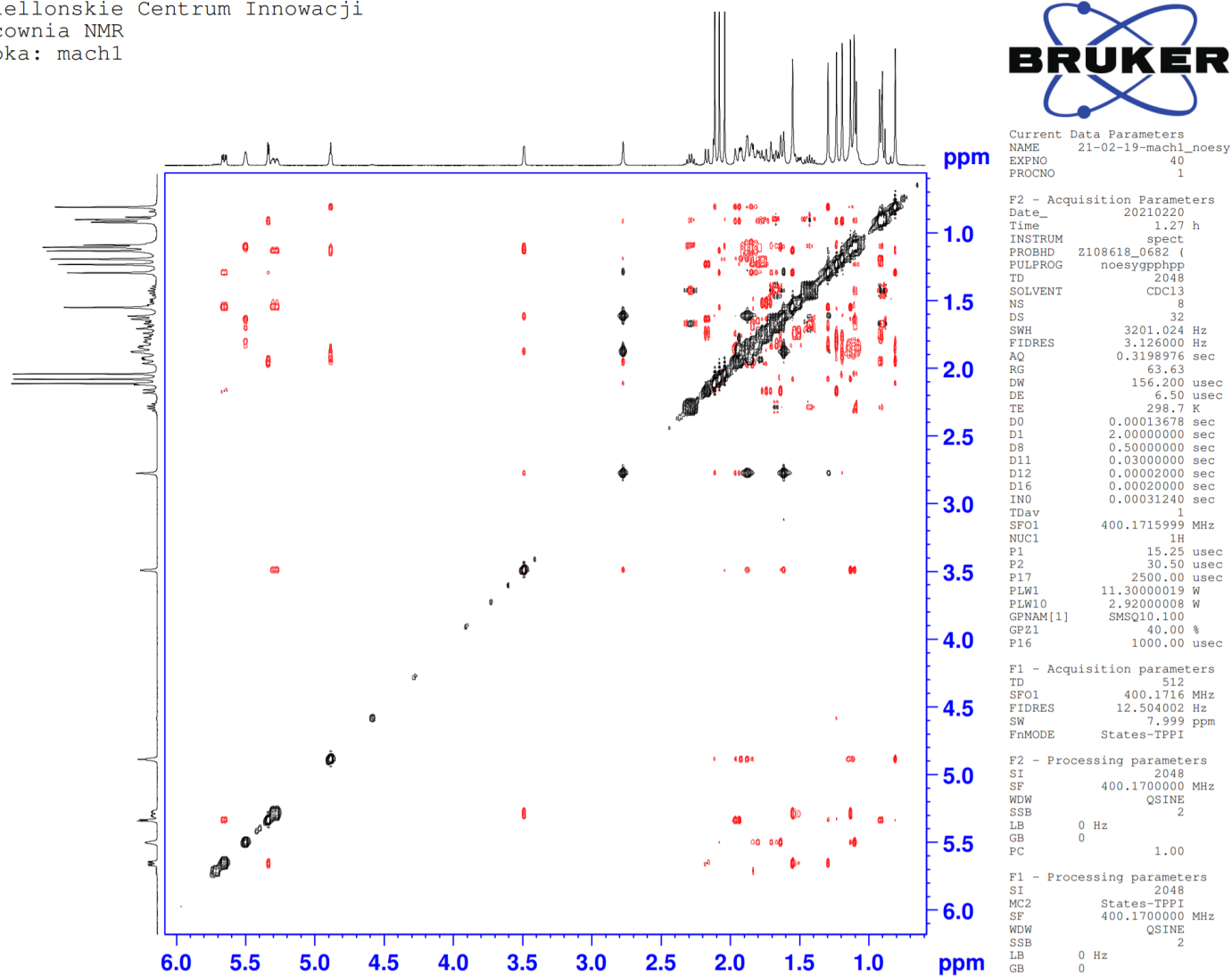


Figure S5. NOESY spectrum of compound 1.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1

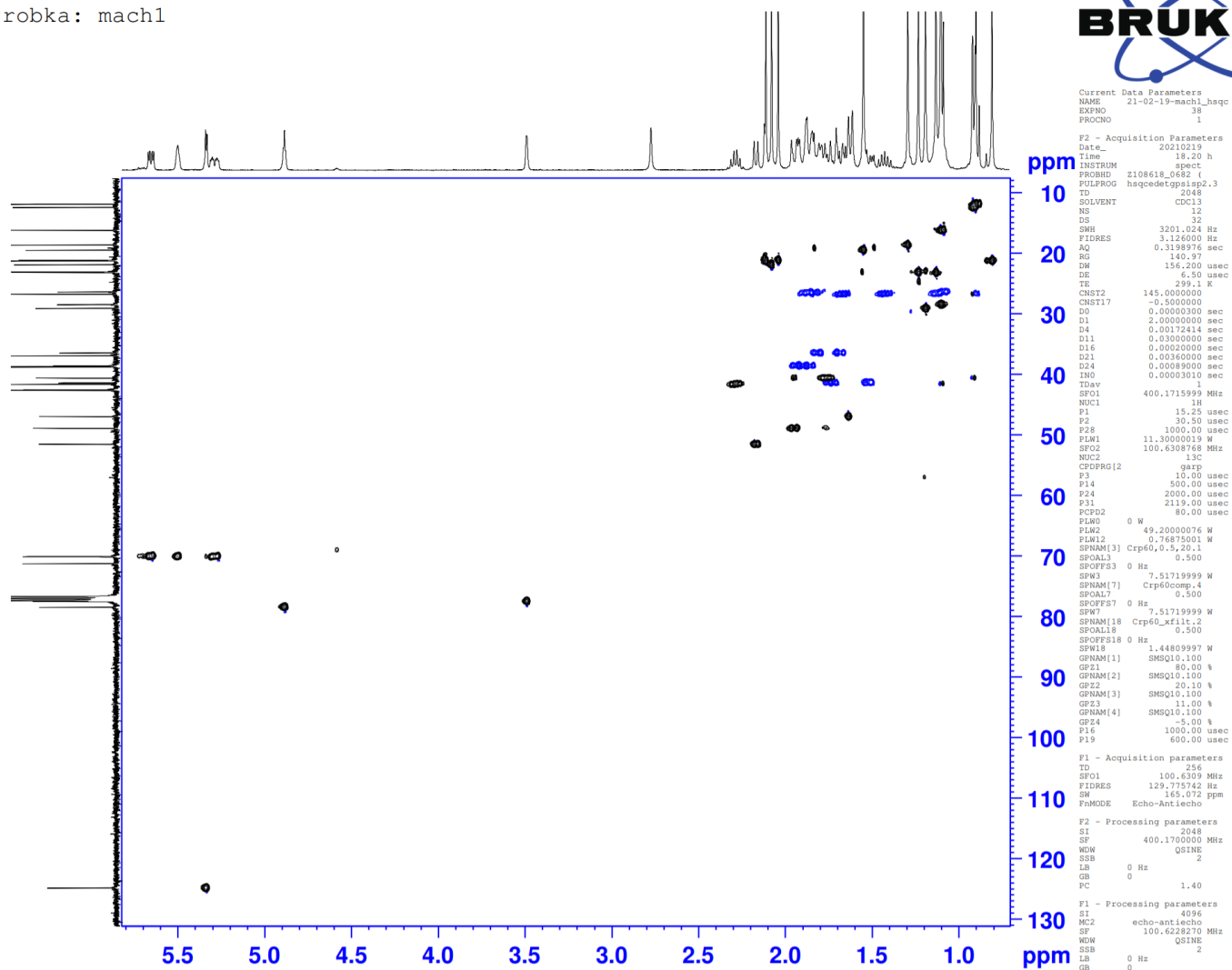


Figure S6. HSQC spectrum of compound 1.

Probka: mach1

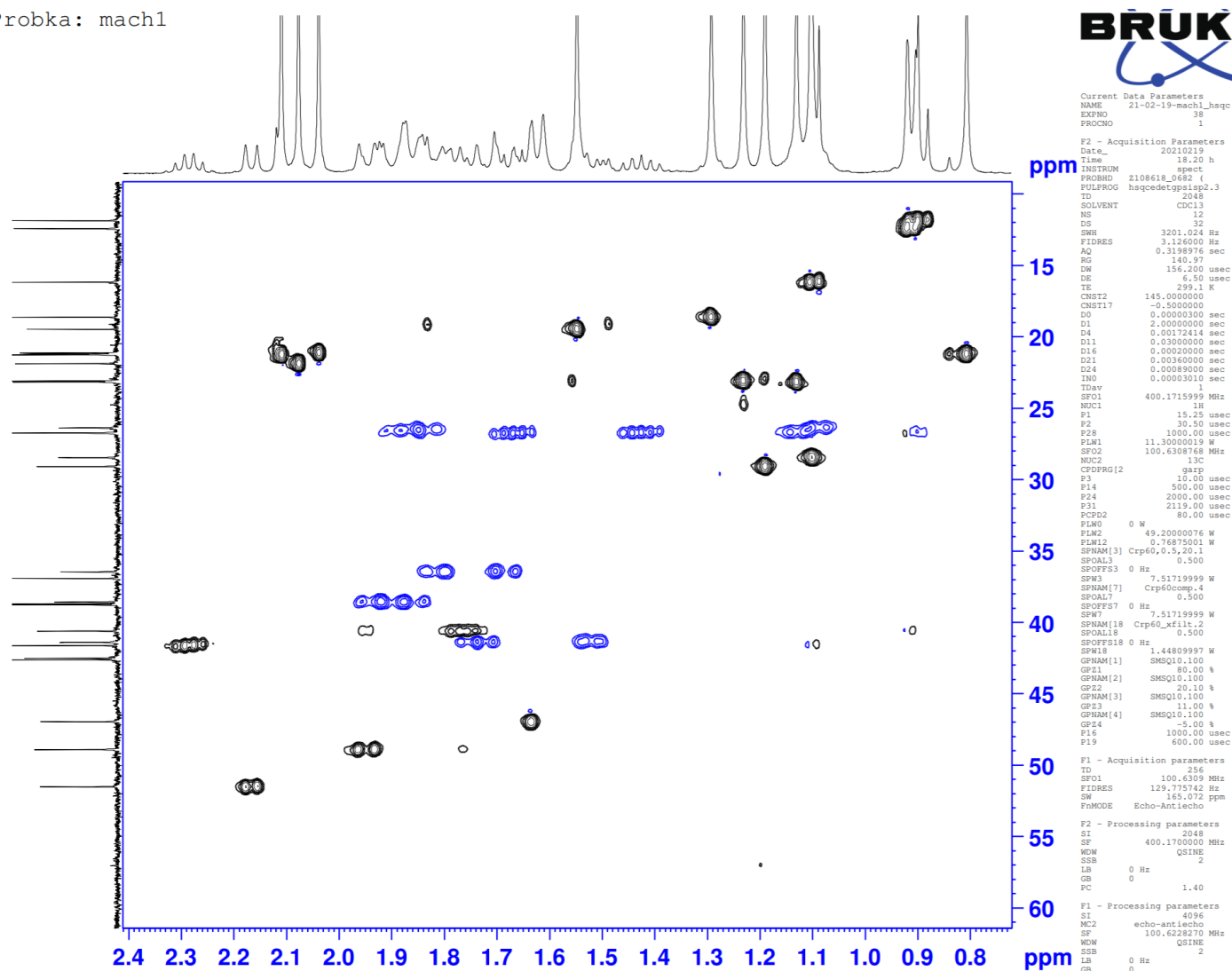


Figure S6a. Expansion of HSQC spectrum of compound **1**.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach1



Current Data Parameters
NAME 21-02-19-mach1_hmbc
EXPNO 39
PROCNO 1

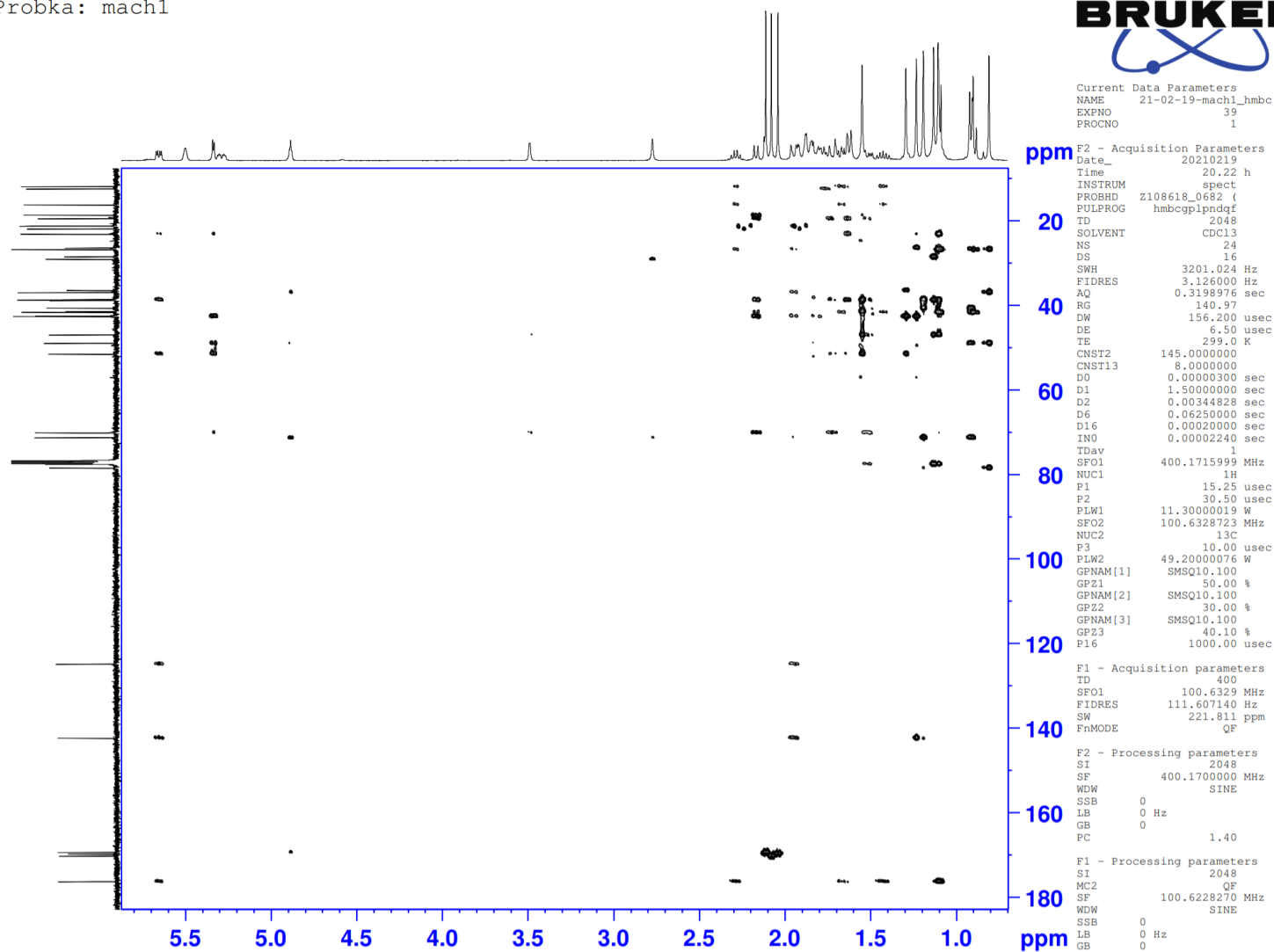


Figure S7. HMBC spectrum of compound 1.

Probka: mach1

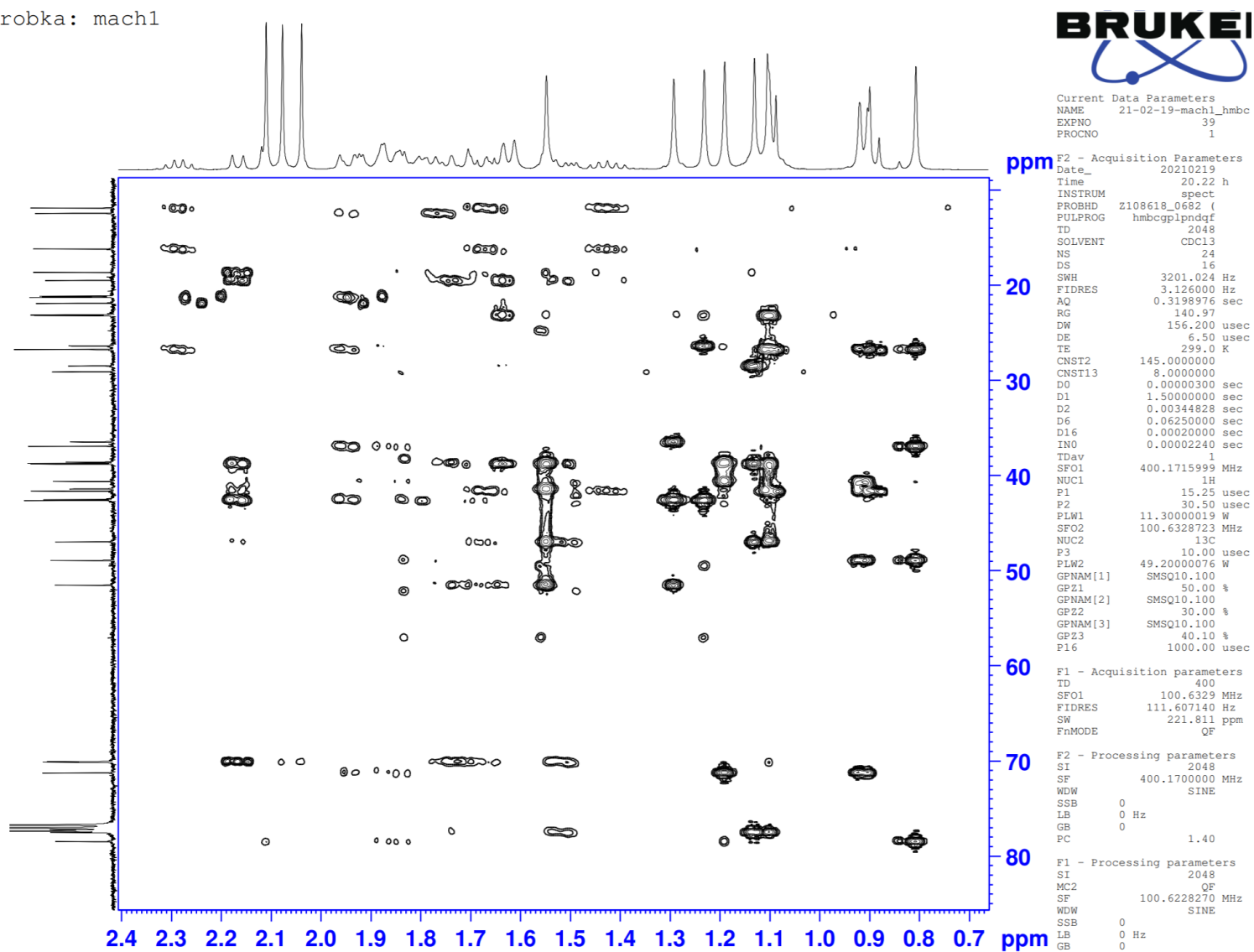


Figure S7a. Expansion of HMBC spectrum of compound 1.

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))

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7.52e4

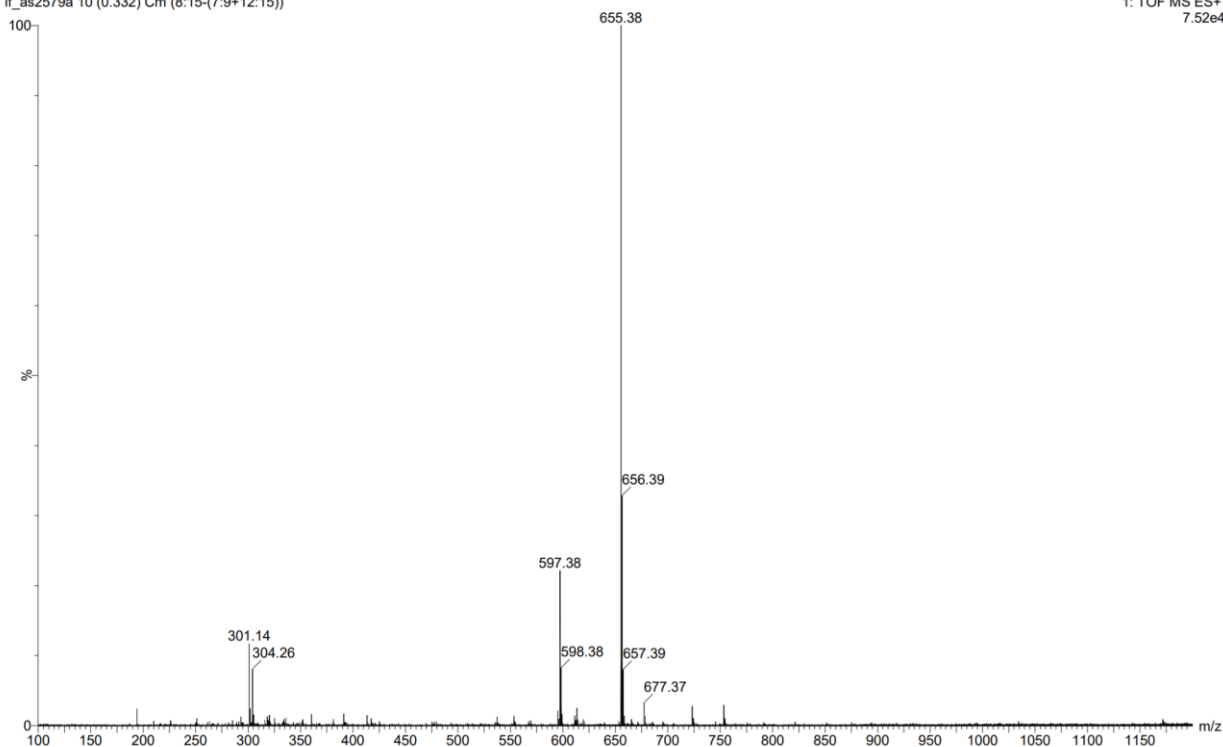


Figure S8. HR ESIMS spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2



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

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INSTRUM spect
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PULPROG zg30
TD 32050
SOLVENT CDCl3
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
SF01 400.1732014 MHz
NUC1 1H
P1 15.25 usec
PLW1 11.30000019 W

F2 - Processing parameters
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SF 400.1700000 MHz
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SSB 0
LB 0.10 Hz
GB 0
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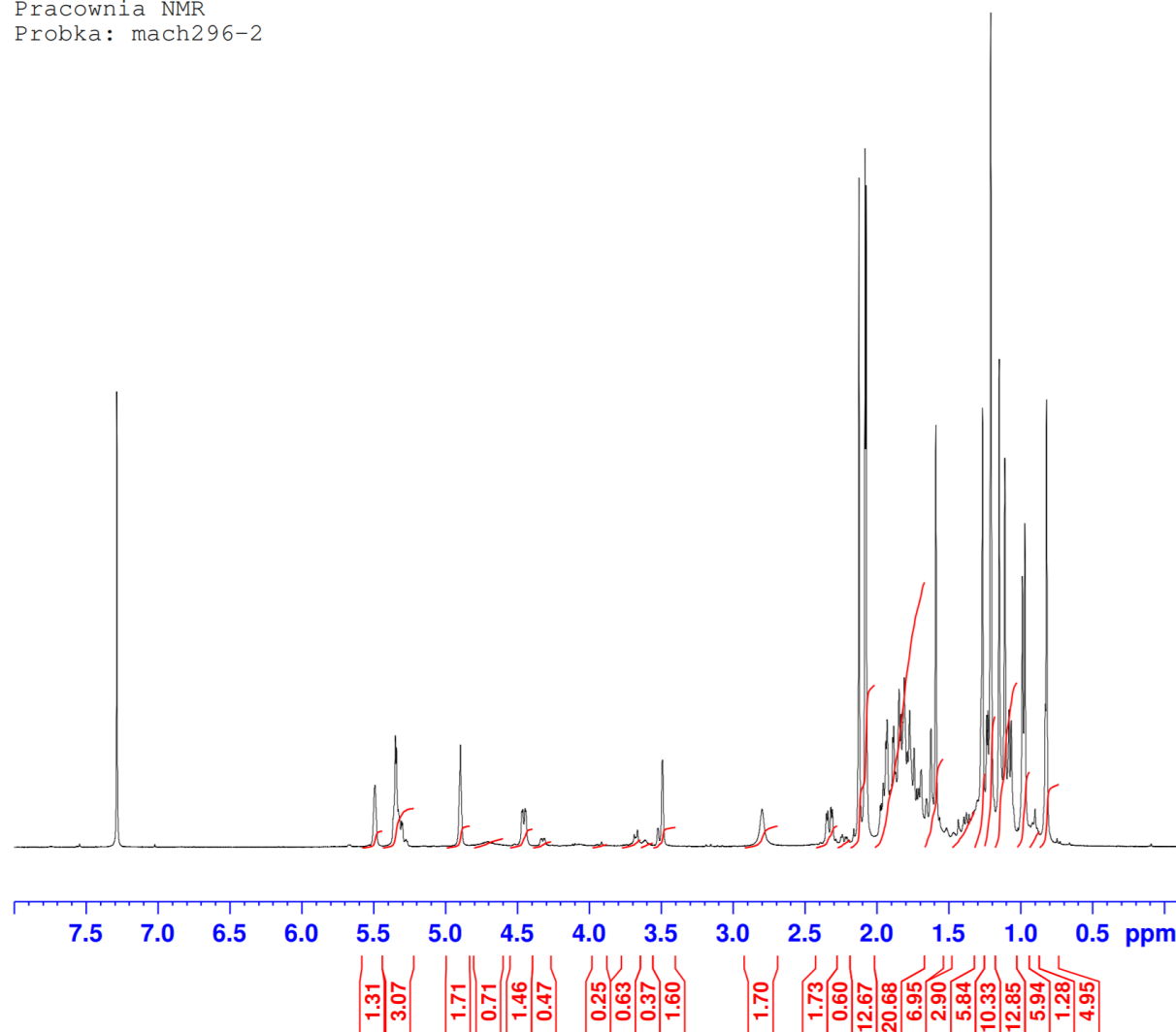


Figure S9. ^1H NMR spectrum of compound **2**.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

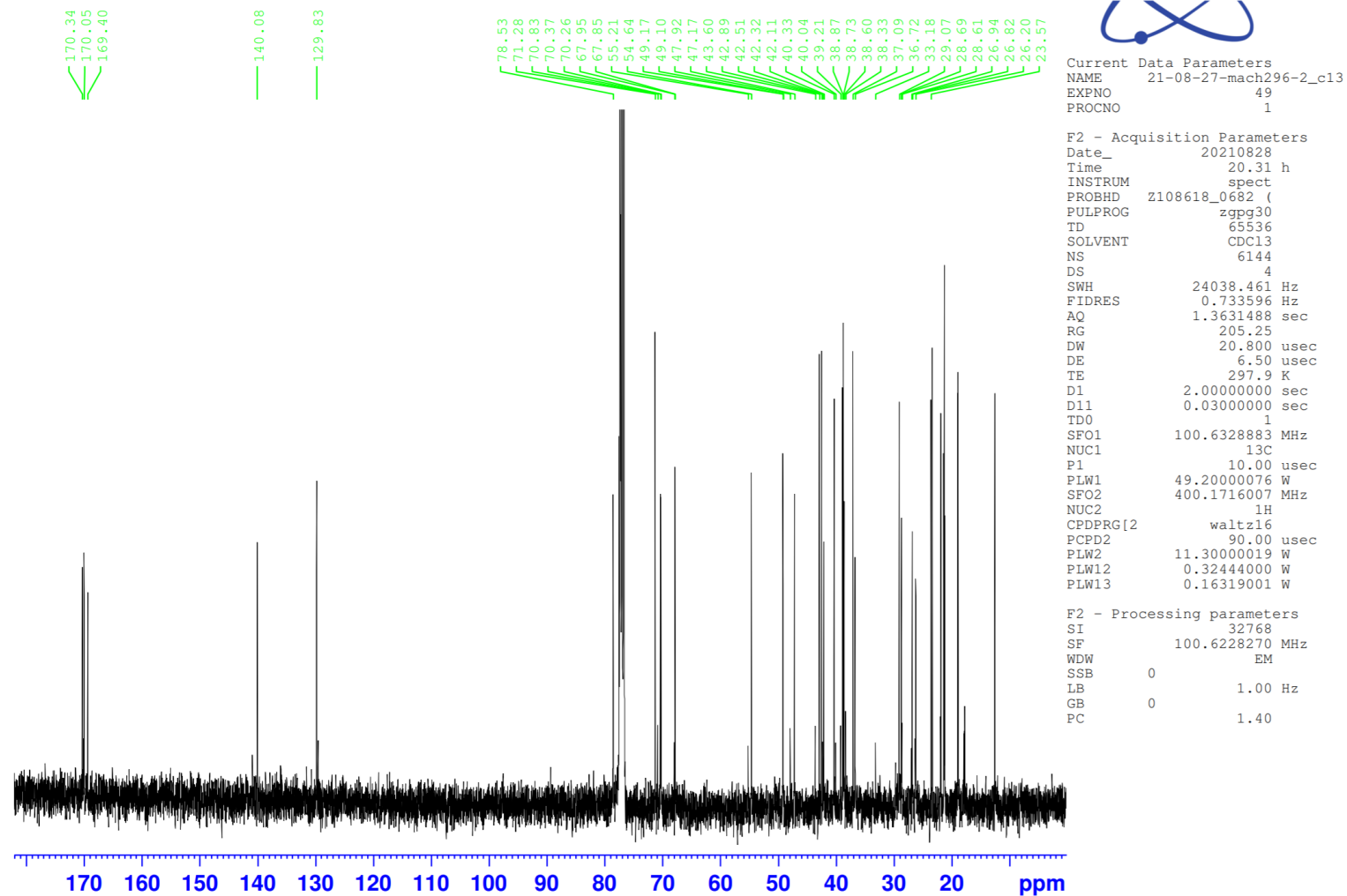


Figure S10. ^{13}C NMR spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

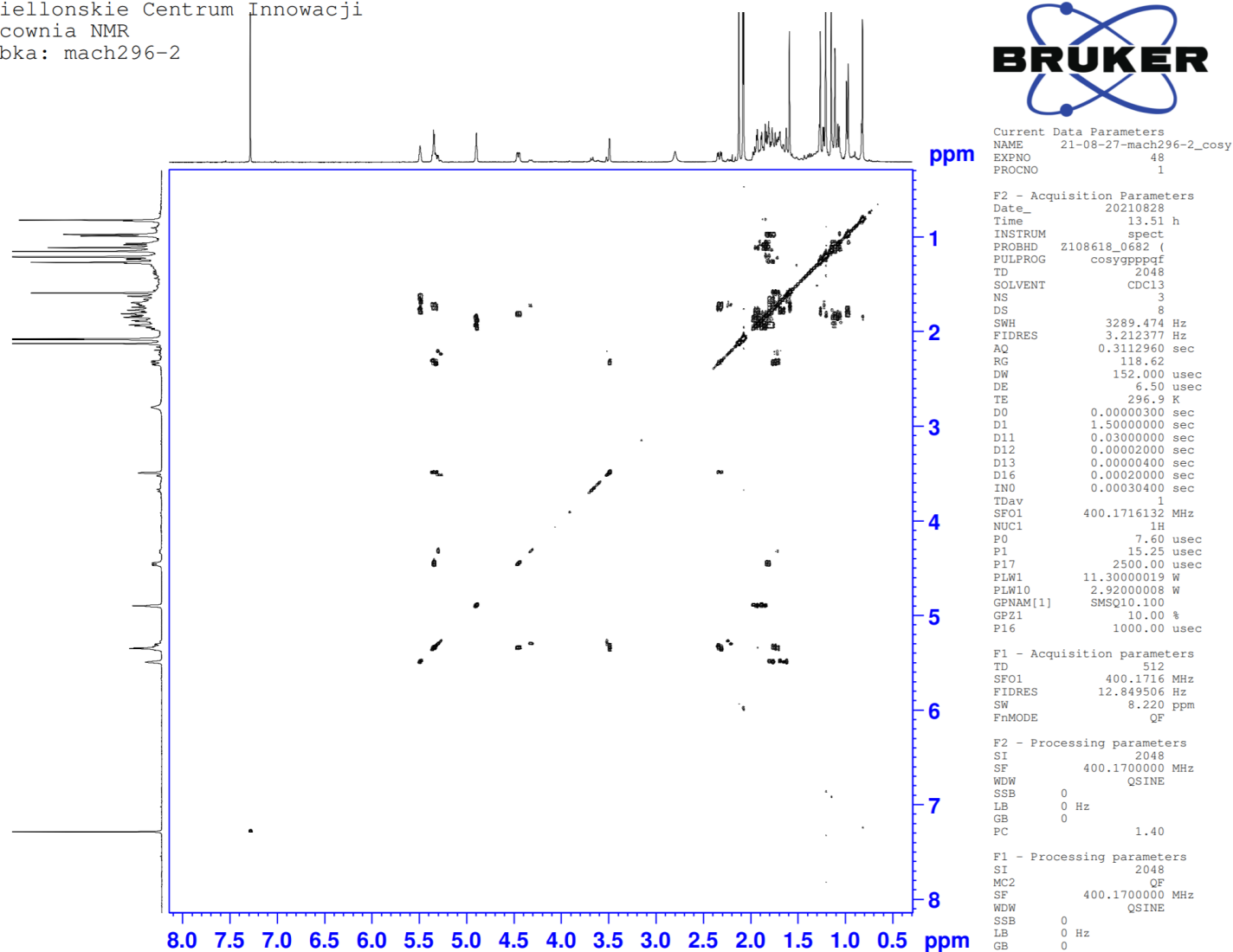


Figure S11. ^1H - ^1H COSY spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

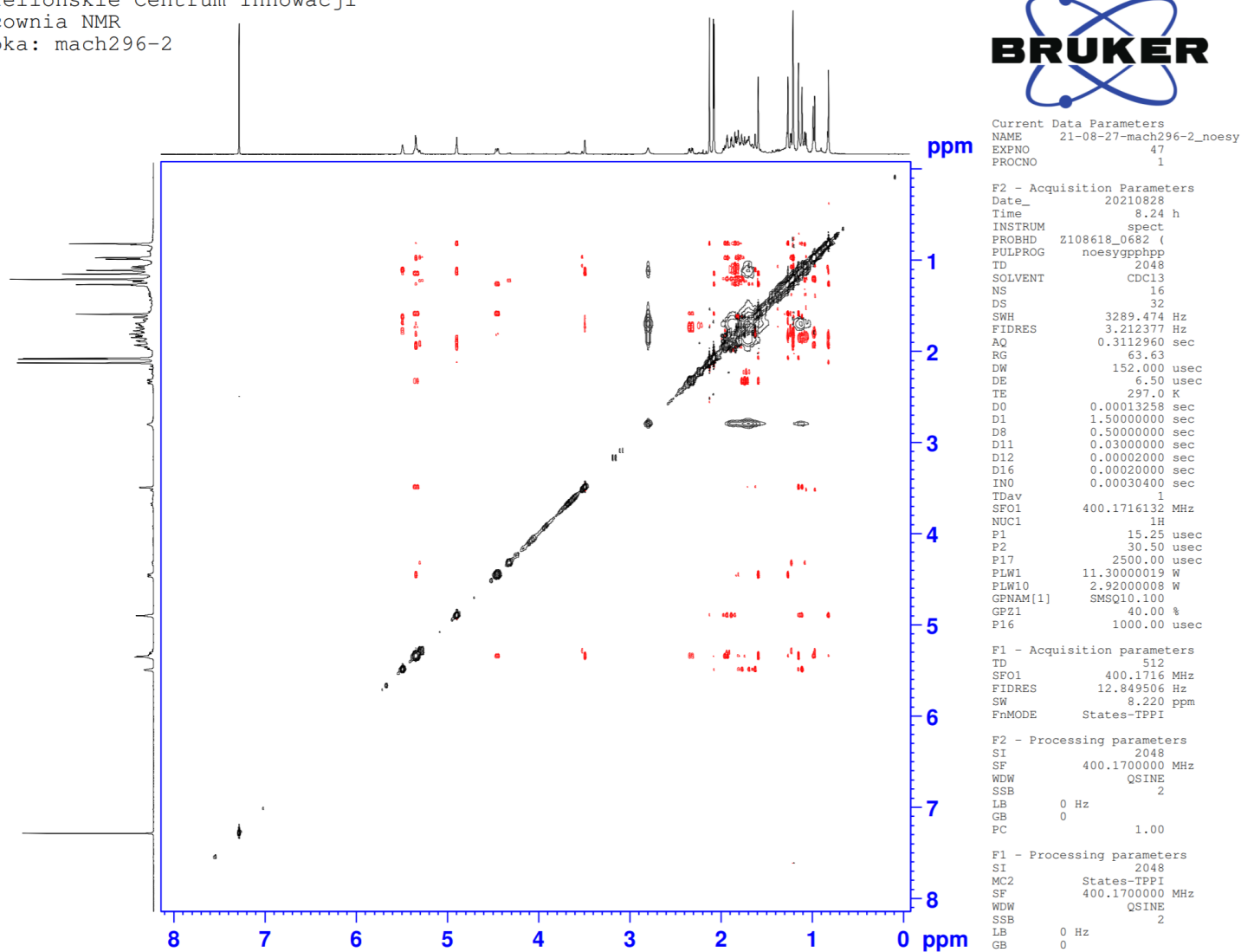


Figure S12. NOESY spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

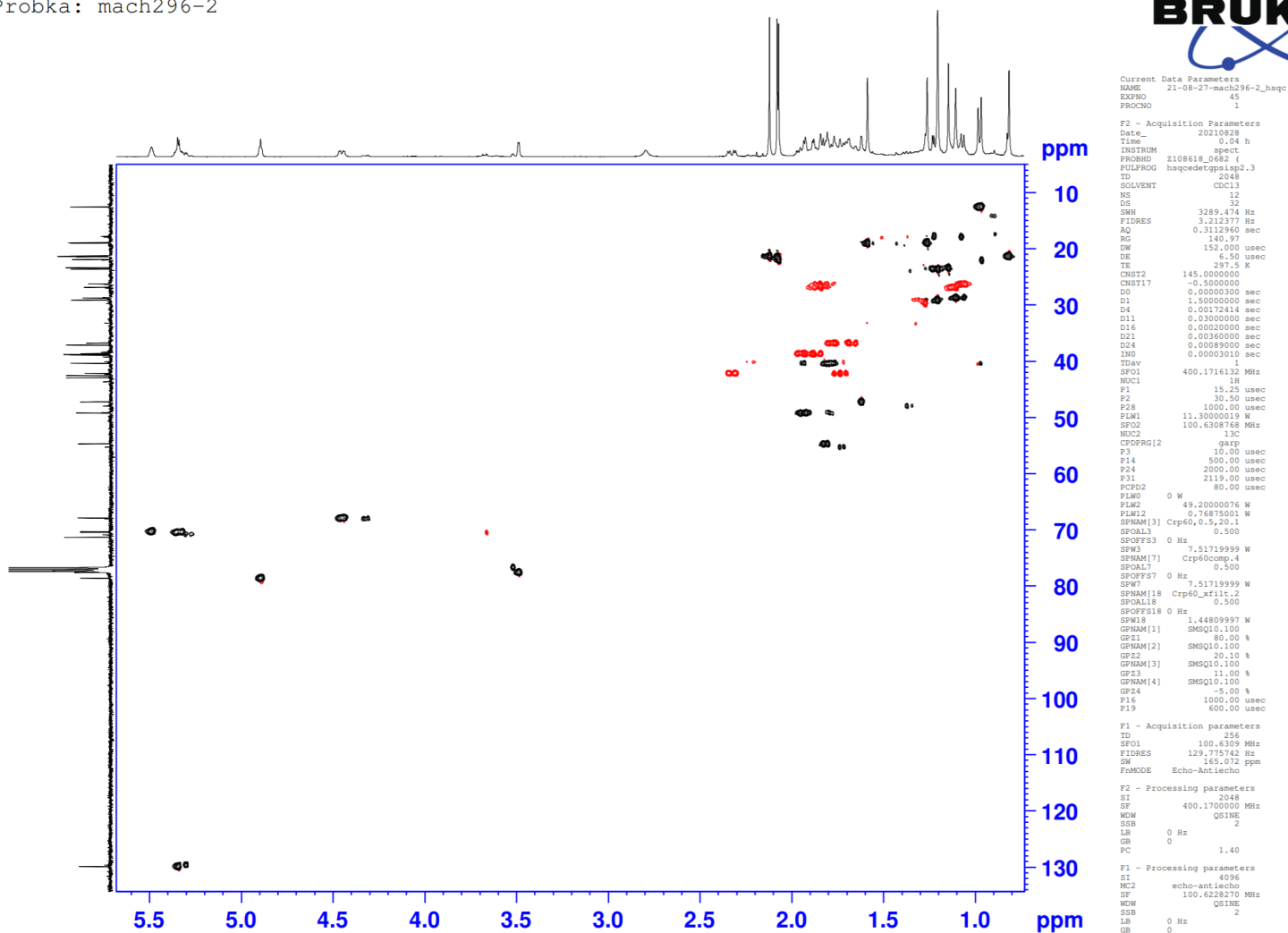


Figure S13. HSQC spectrum of compound 2.

Probka: mach296-2

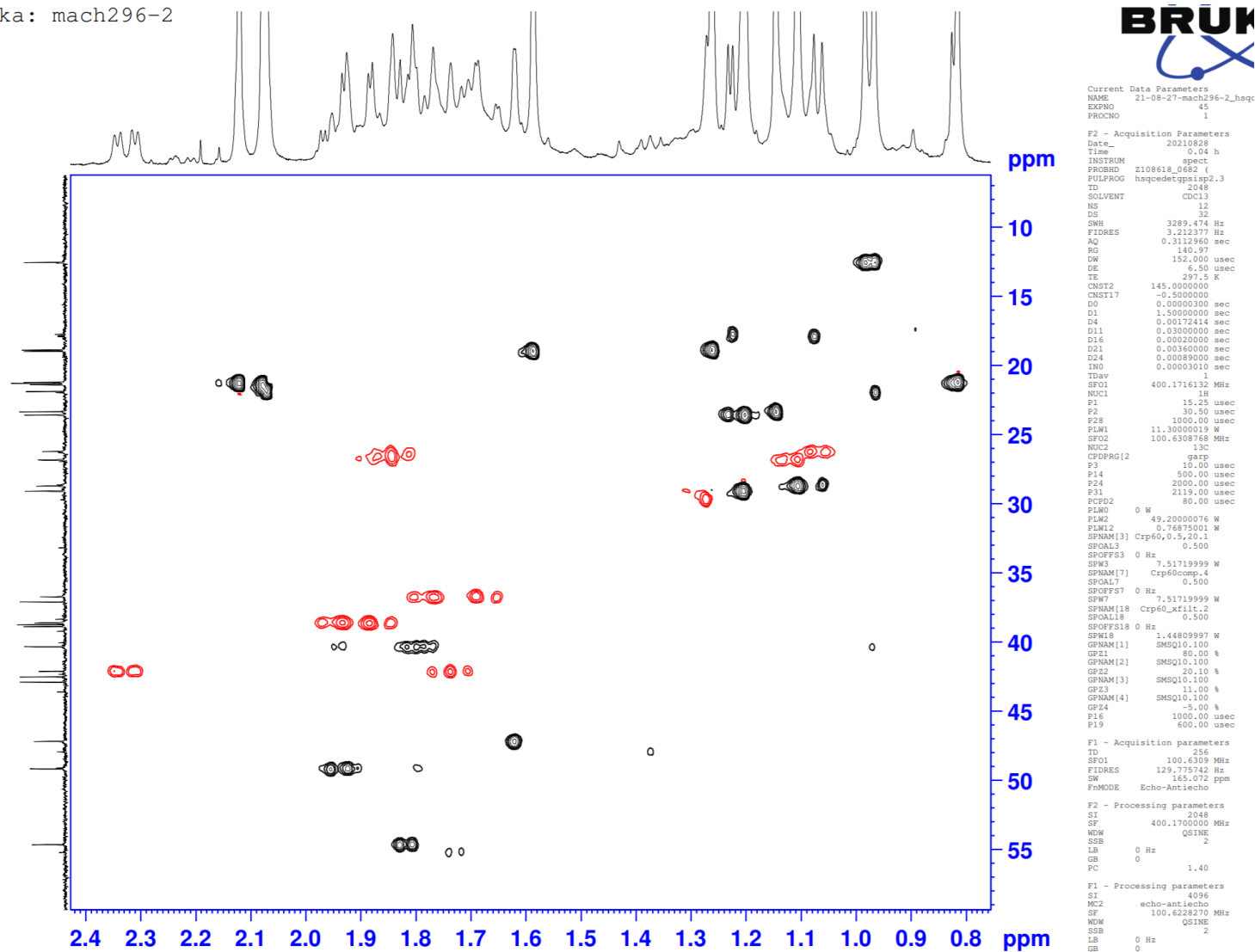


Figure S13a. Expansion of HSQC spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach296-2

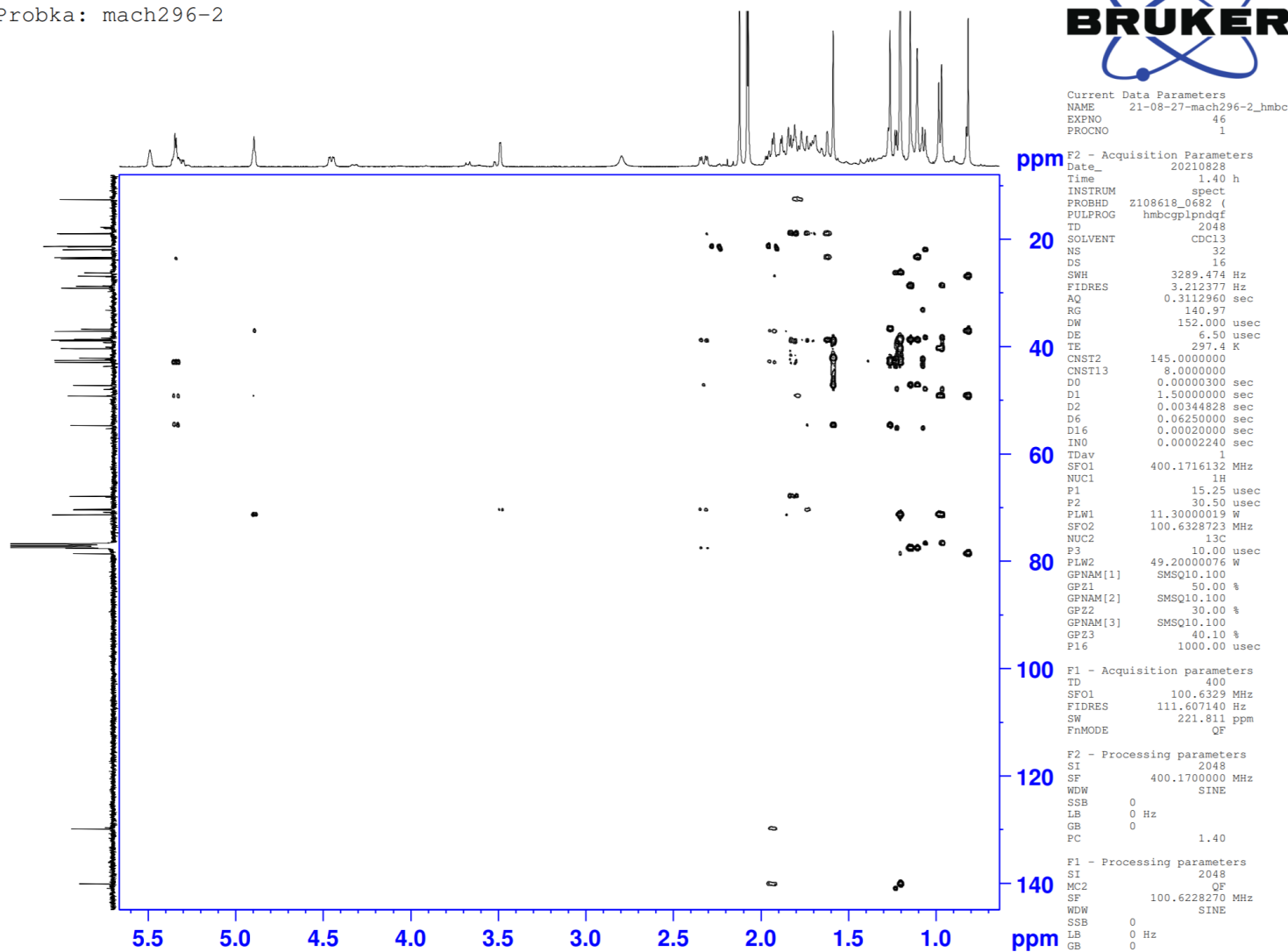


Figure S14. HMBC spectrum of compound 2.

Probka: mach296-2

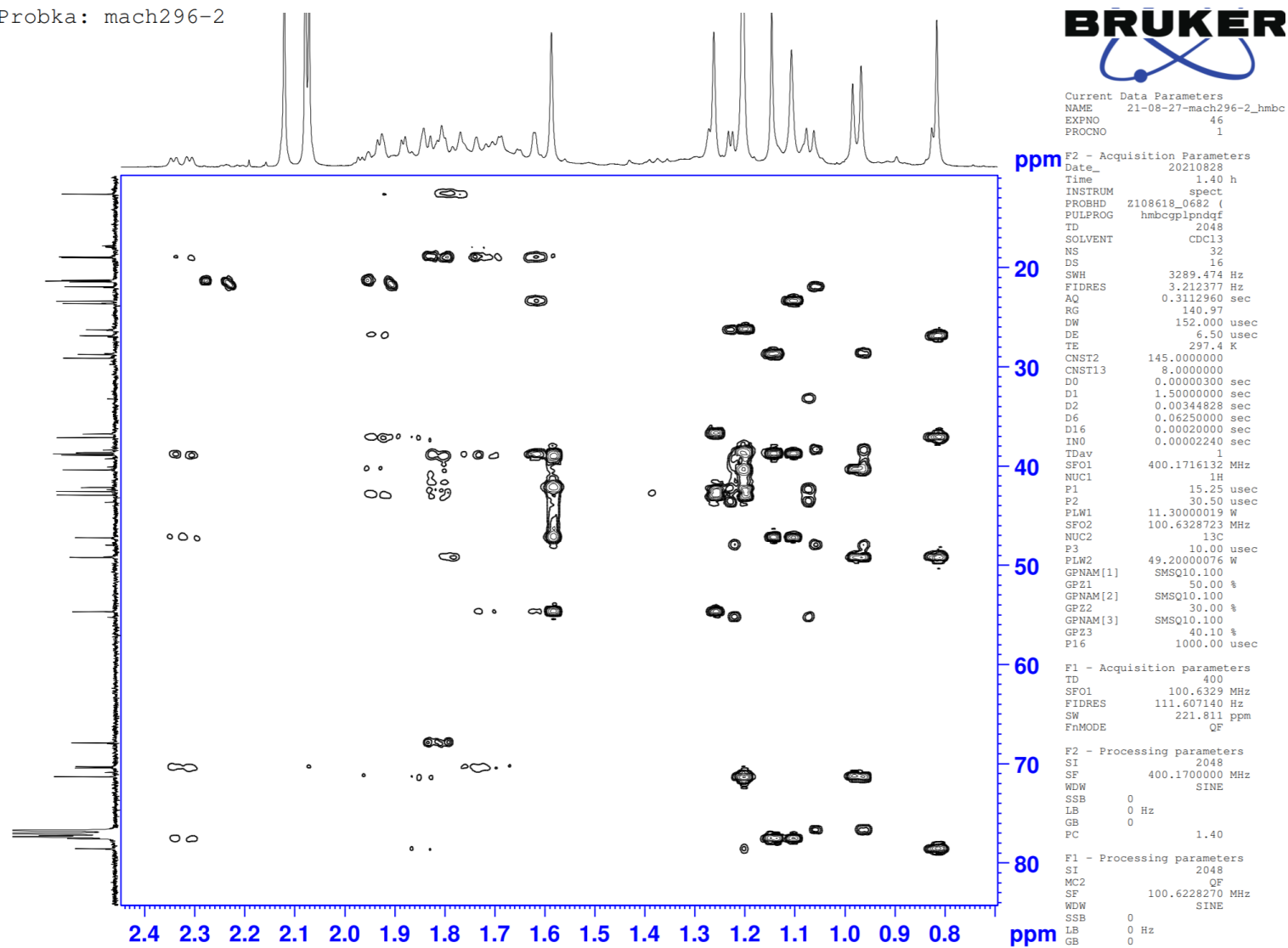


Figure S14a. Expansion of HMBC spectrum of compound 2.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach117-1



Current Data Parameters
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EXPNO 17
PROCNO 1

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INSTRUM spect
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PULPROG zg30
TD 32050
SOLVENT CDCl3
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
SF01 400.1732014 MHz
NUC1 1H
P1 15.25 usec
PLW1 11.30000019 W

F2 - Processing parameters
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SF 400.1700000 MHz
WDW EM
SSB 0
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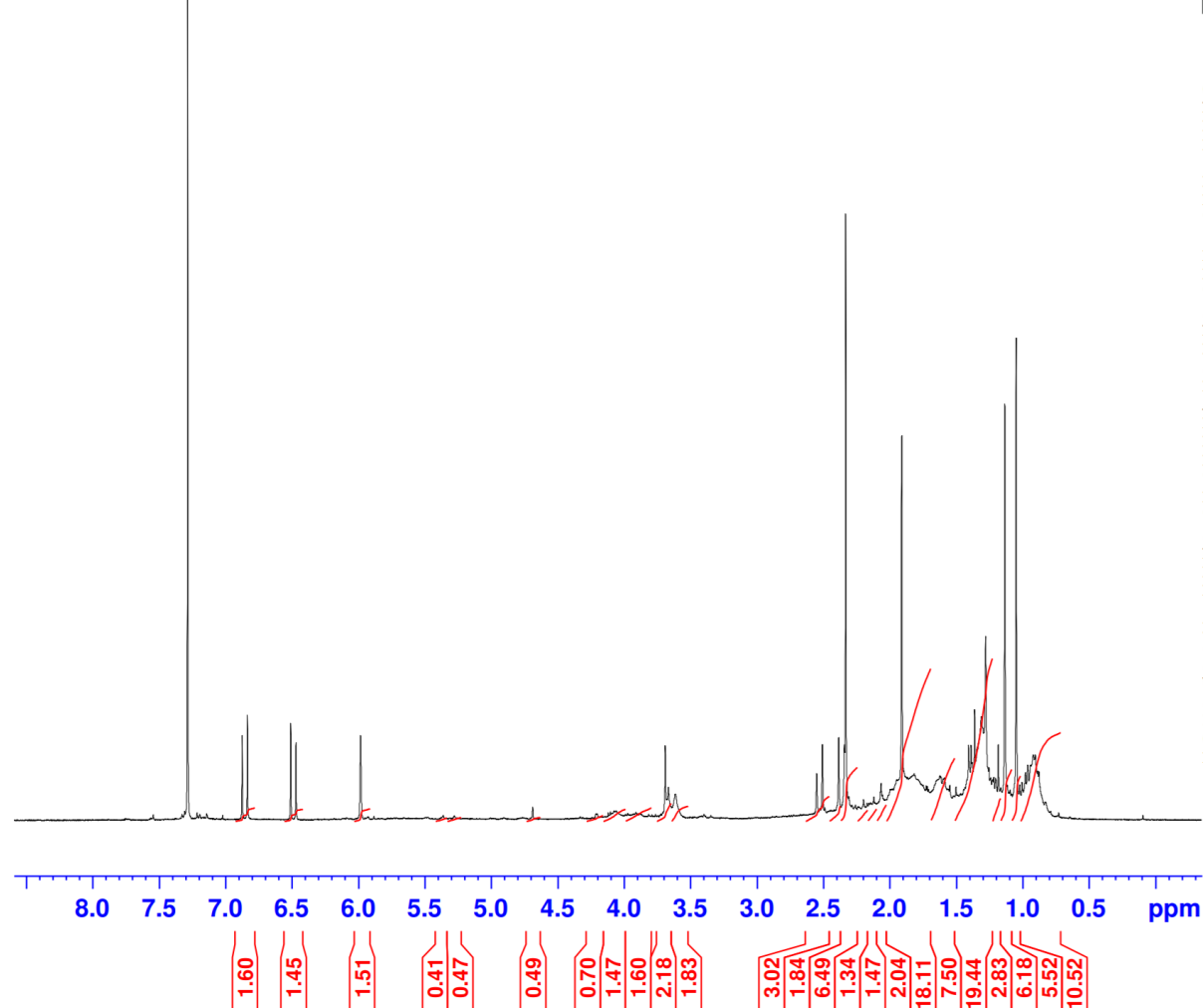


Figure S15. ^1H NMR spectrum of compound 3.

Jagiellonskie Centrum Innowacji
Pracownia NMR
Probka: mach5



Current Data Parameters
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EXPNO 73
PROCNO 1

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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
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SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

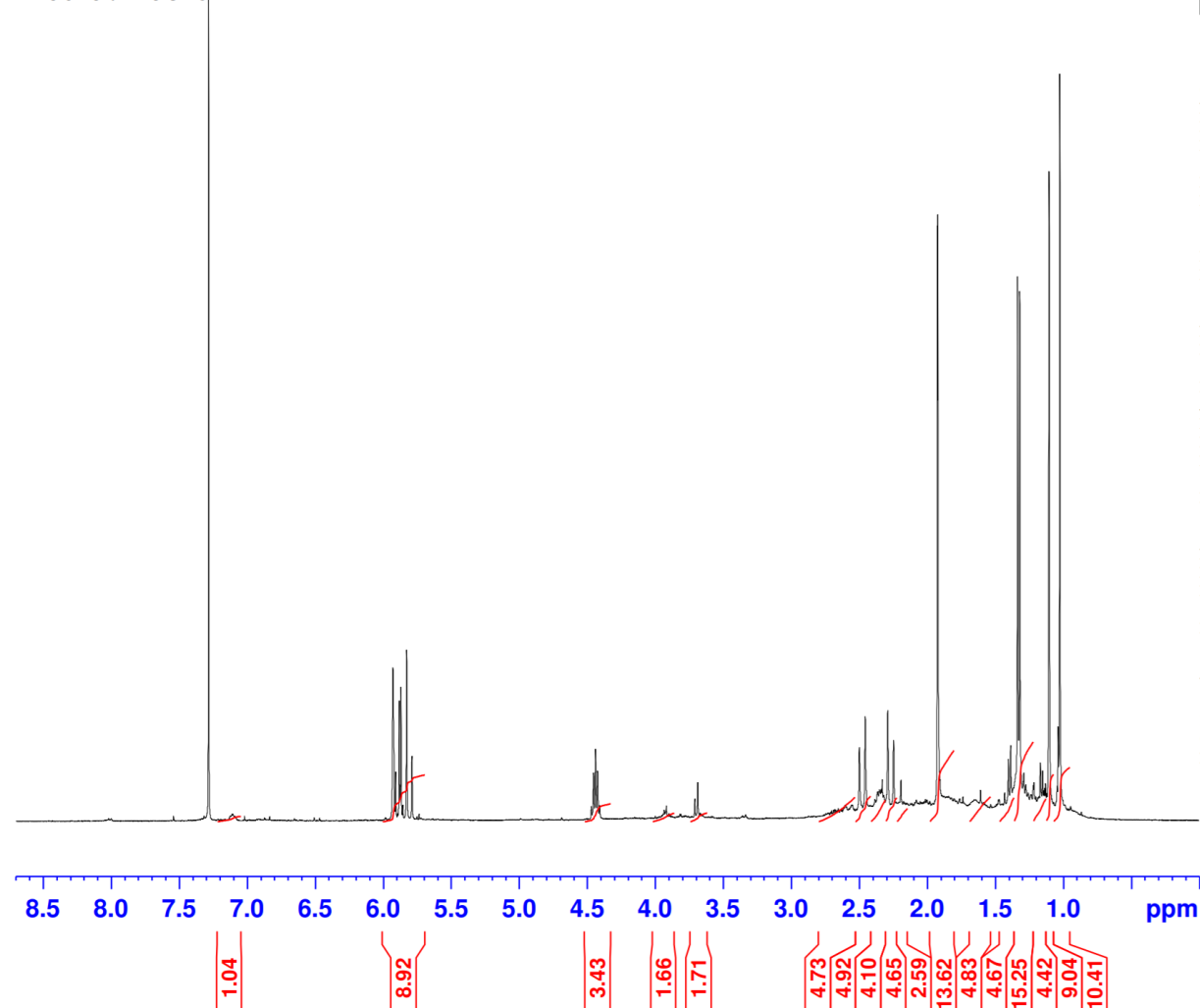


Figure S16. ^1H NMR spectrum of compound 4.

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

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