Supporting Information

Neoclerodane Diterpenoids from Reehal Fatima, *Teucrium yemense*

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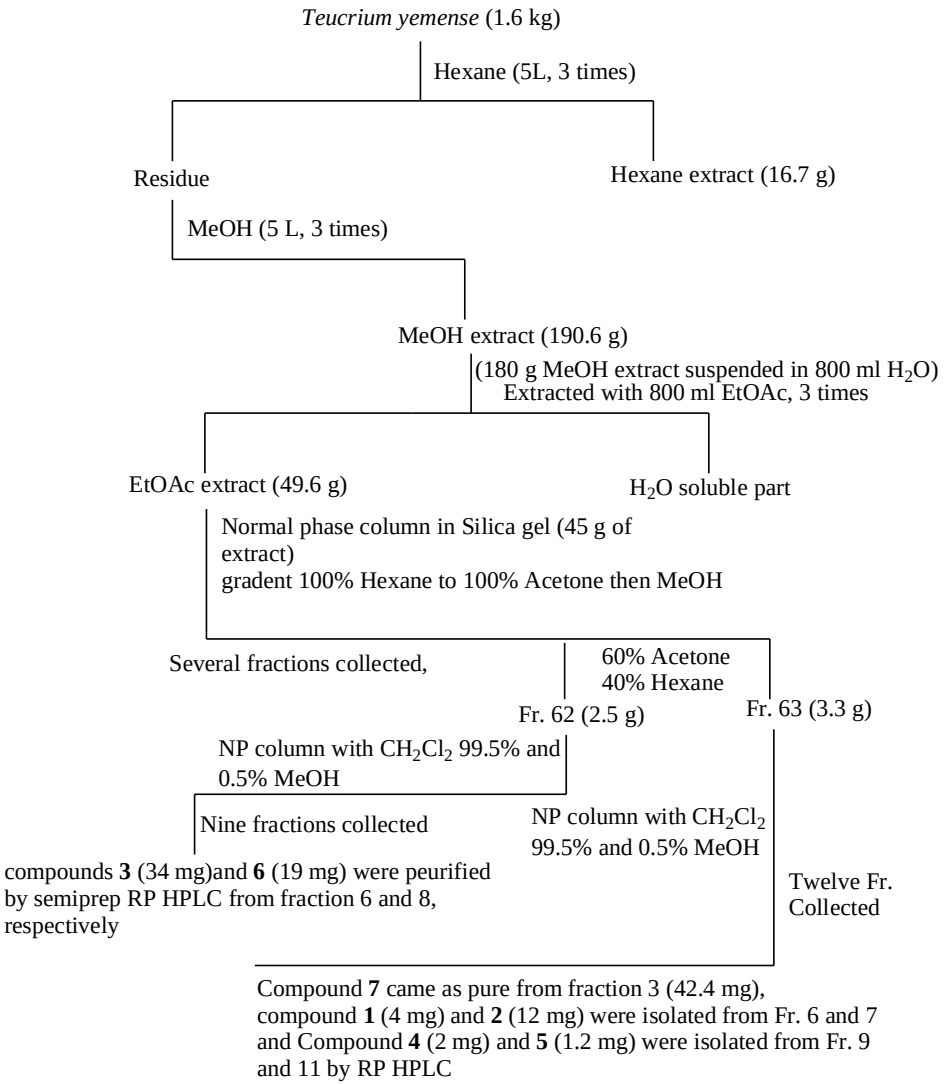
Extraction and Isolation Scheme



Compound **1**

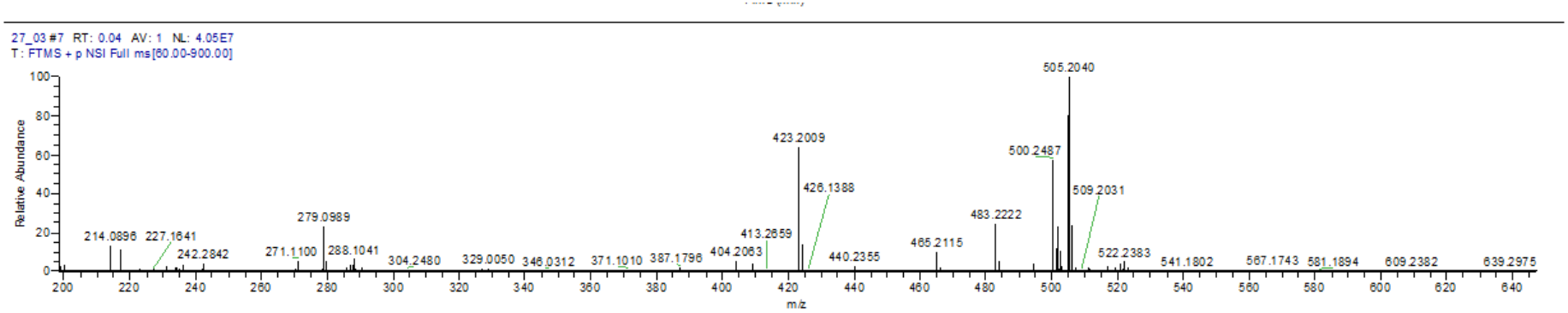


Fig S1: HRESIMS of compound **1**,

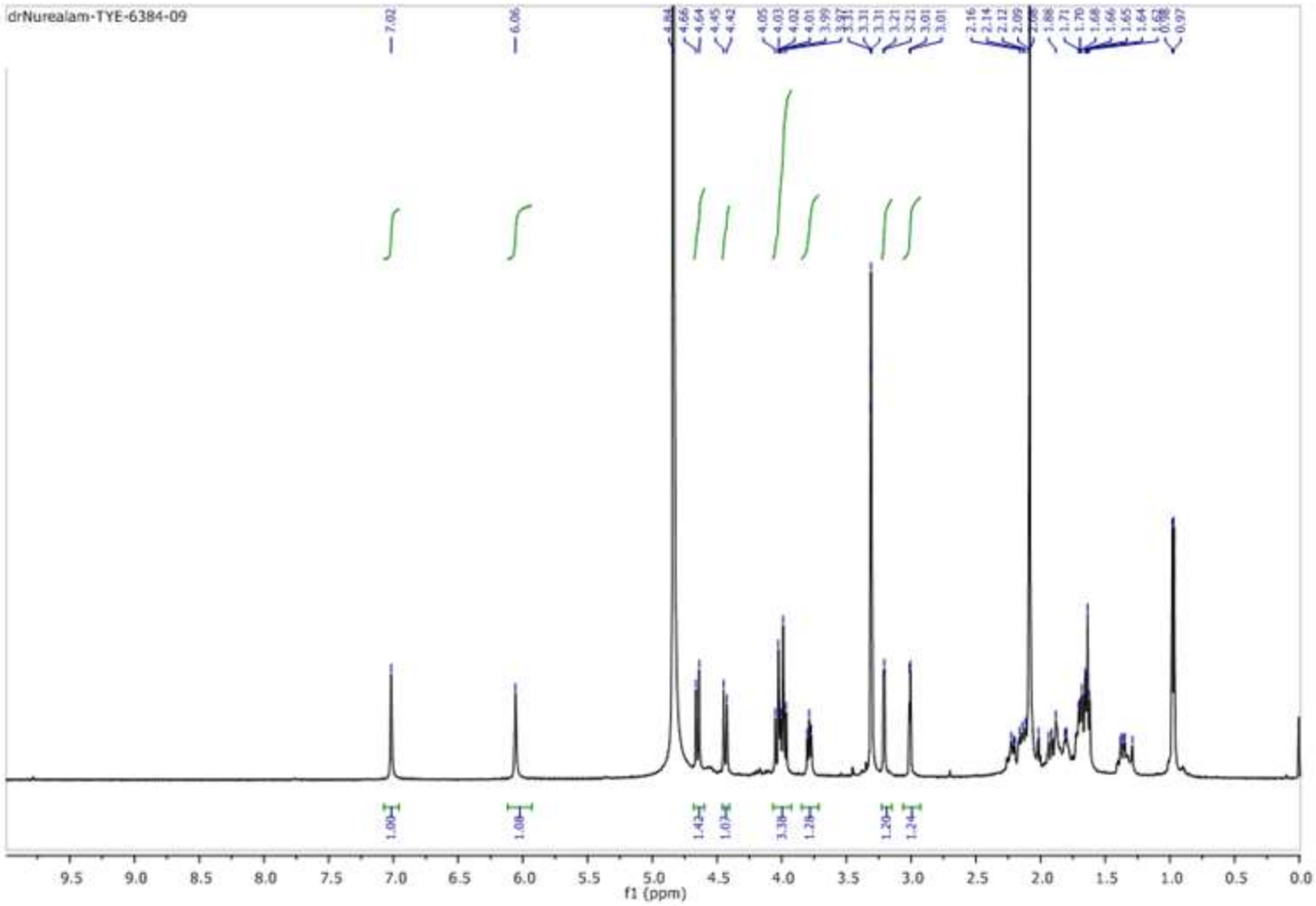


Fig S2: ^{1}H-NMR spectrum of compound **1**.

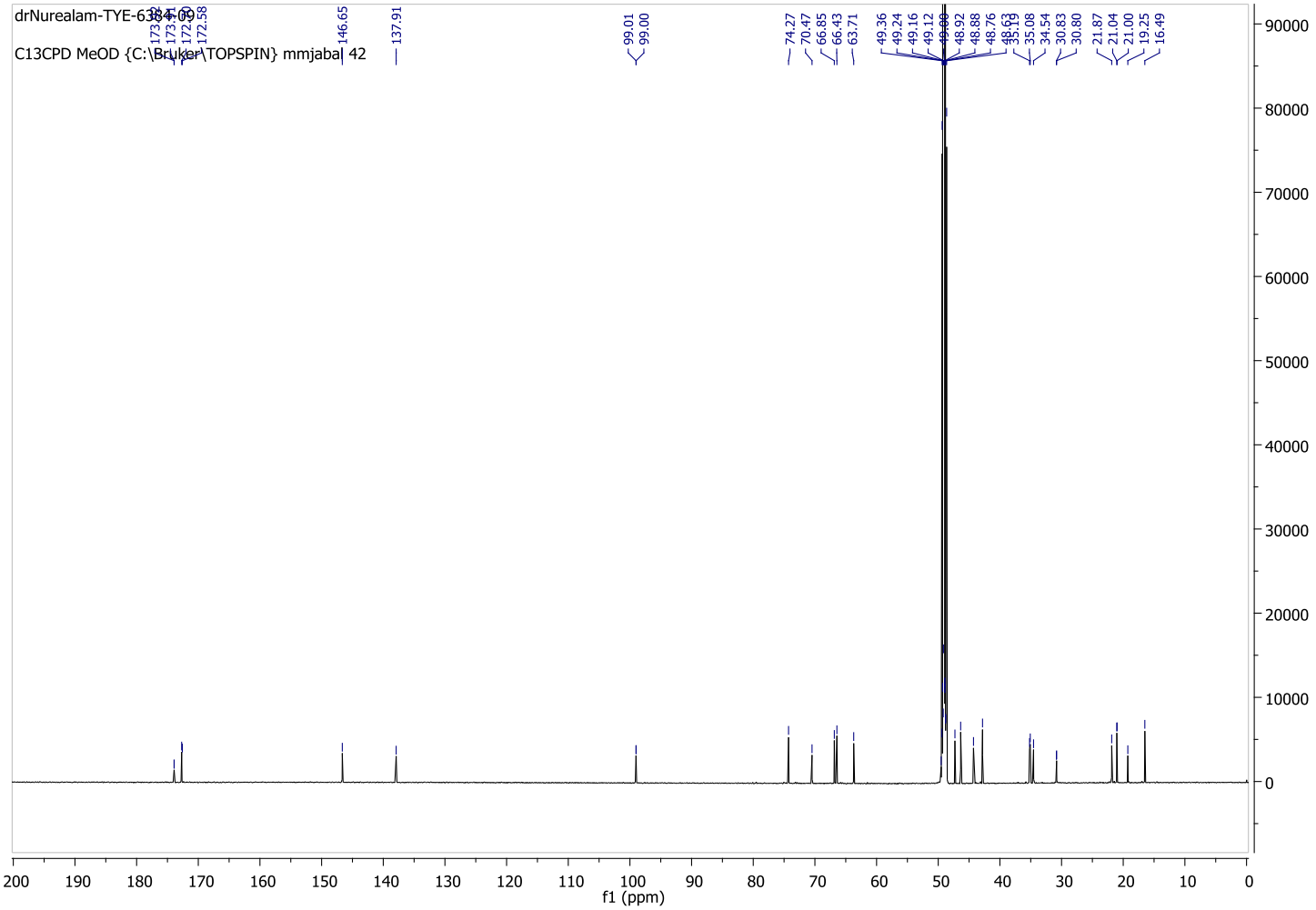


Fig S3: ^{13}C-NMR spectrum of compound **1**

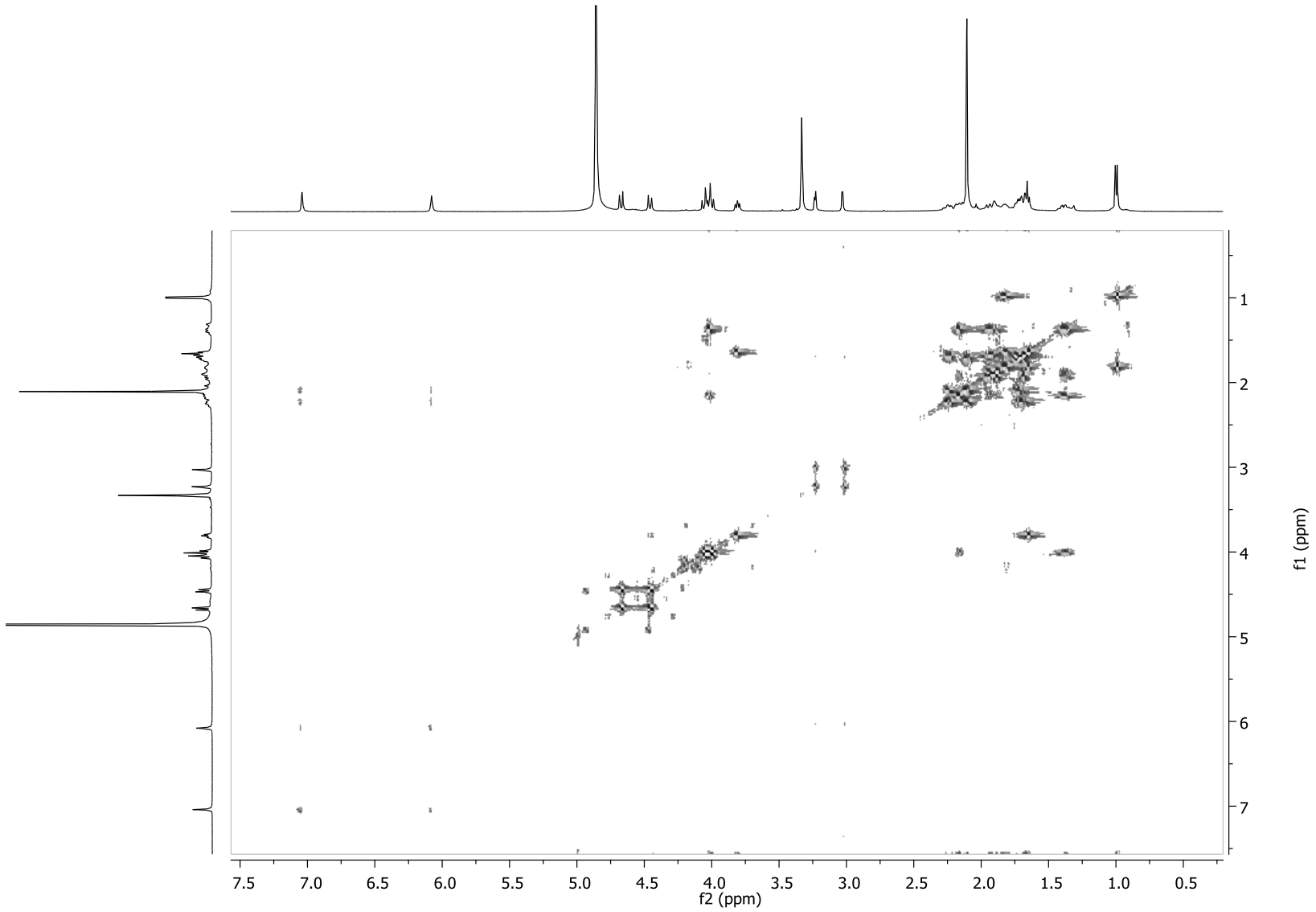


Fig S4: COSY spectrum of compound **1**

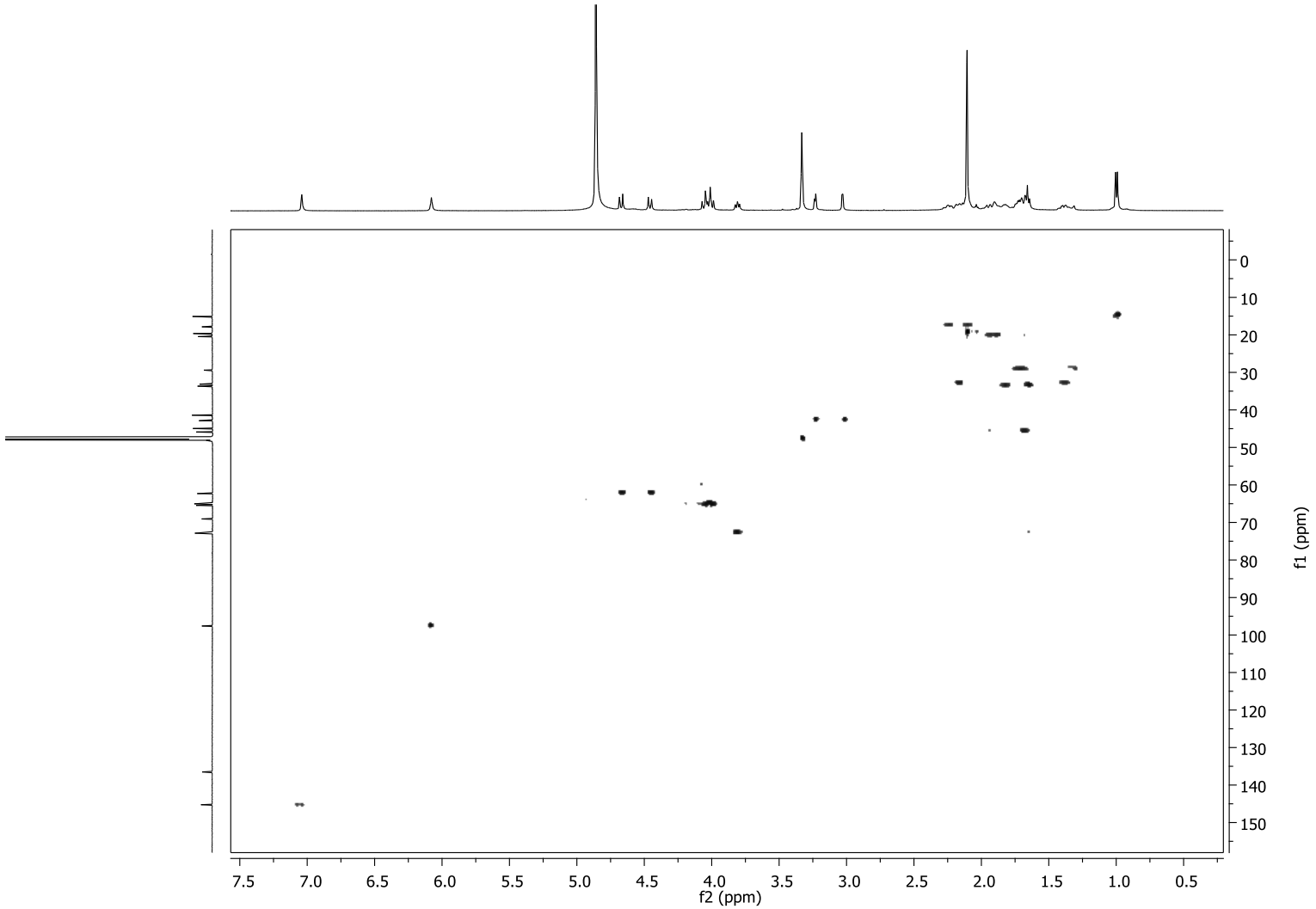


Fig S5: HSQC spectrum of compound **1**

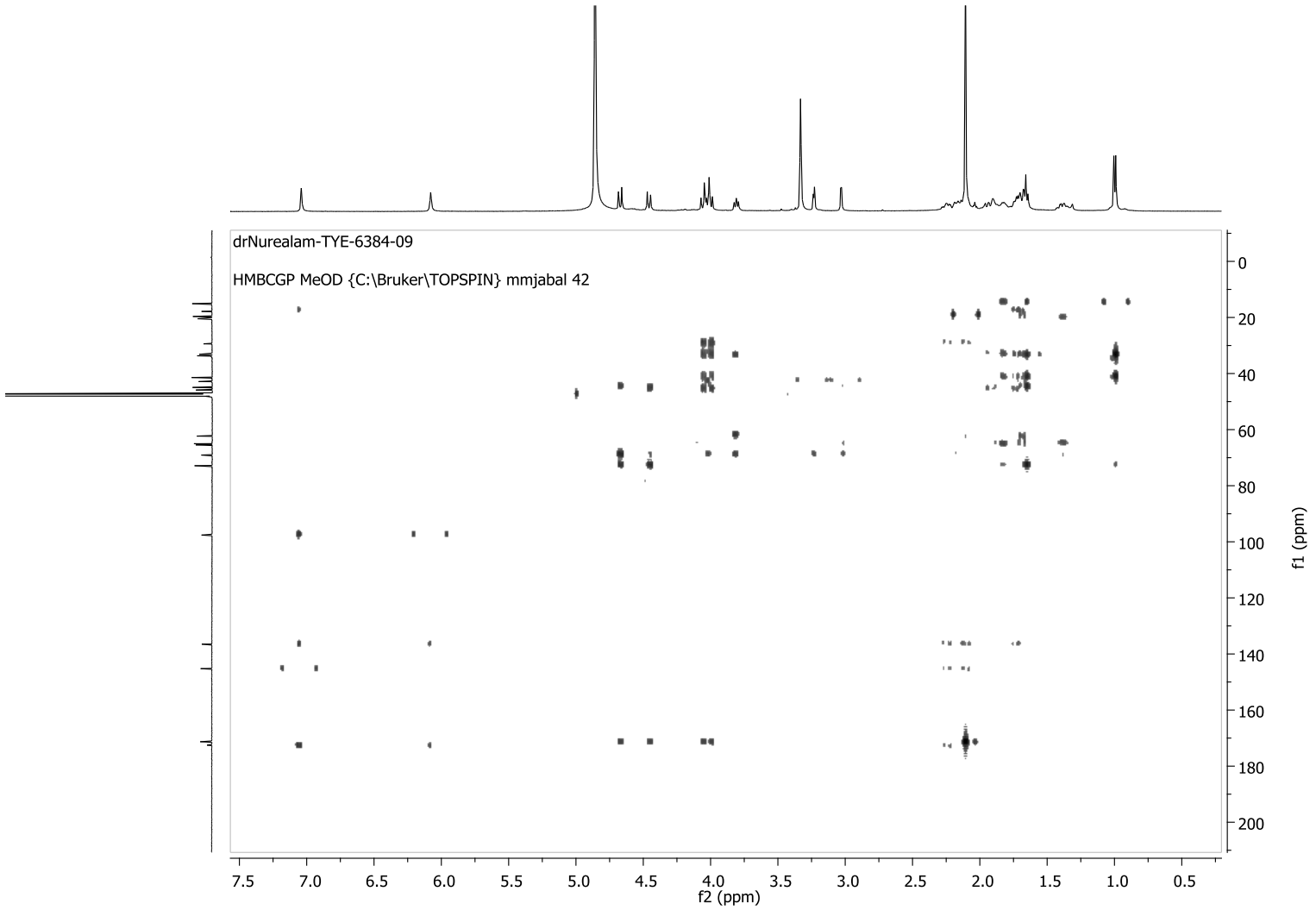


Fig S6: HMBC spectrum of compound **1**

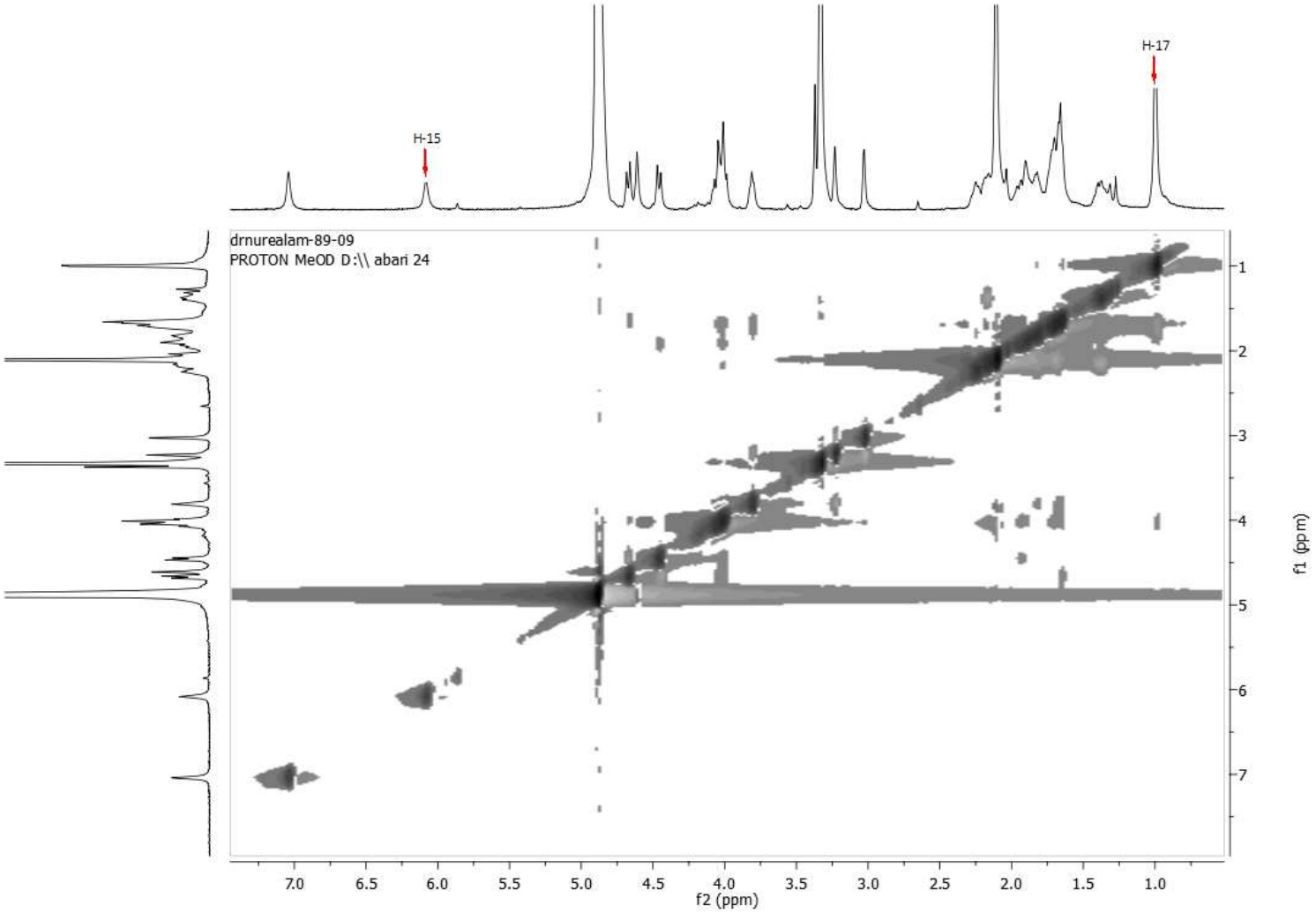


Fig S7: NOESY spectrum of compound **1,** which showed no correlation between H-15 and H-17.

Compound **2**

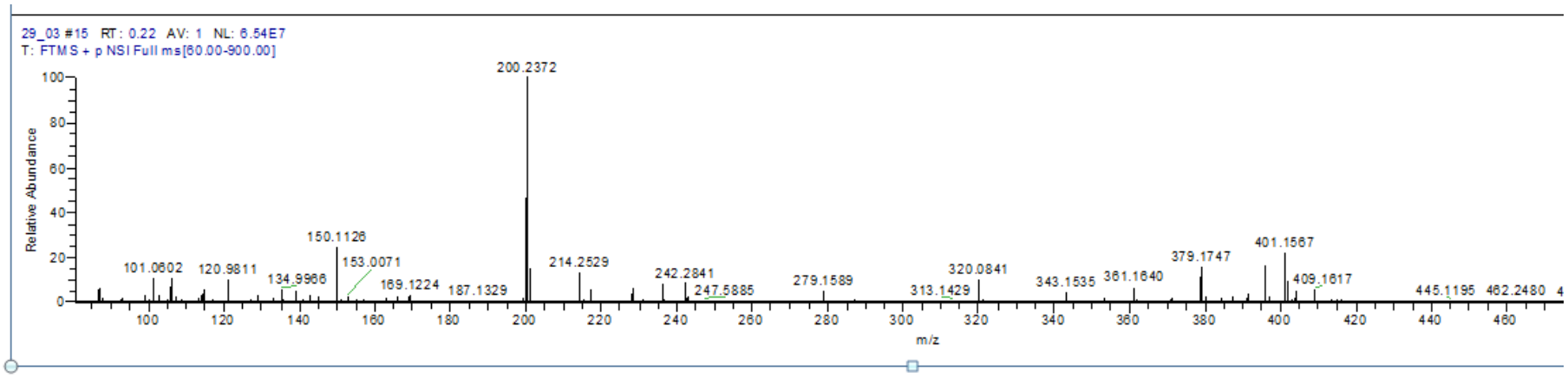


Fig S8: HRESIMS spectrum of compound **2**

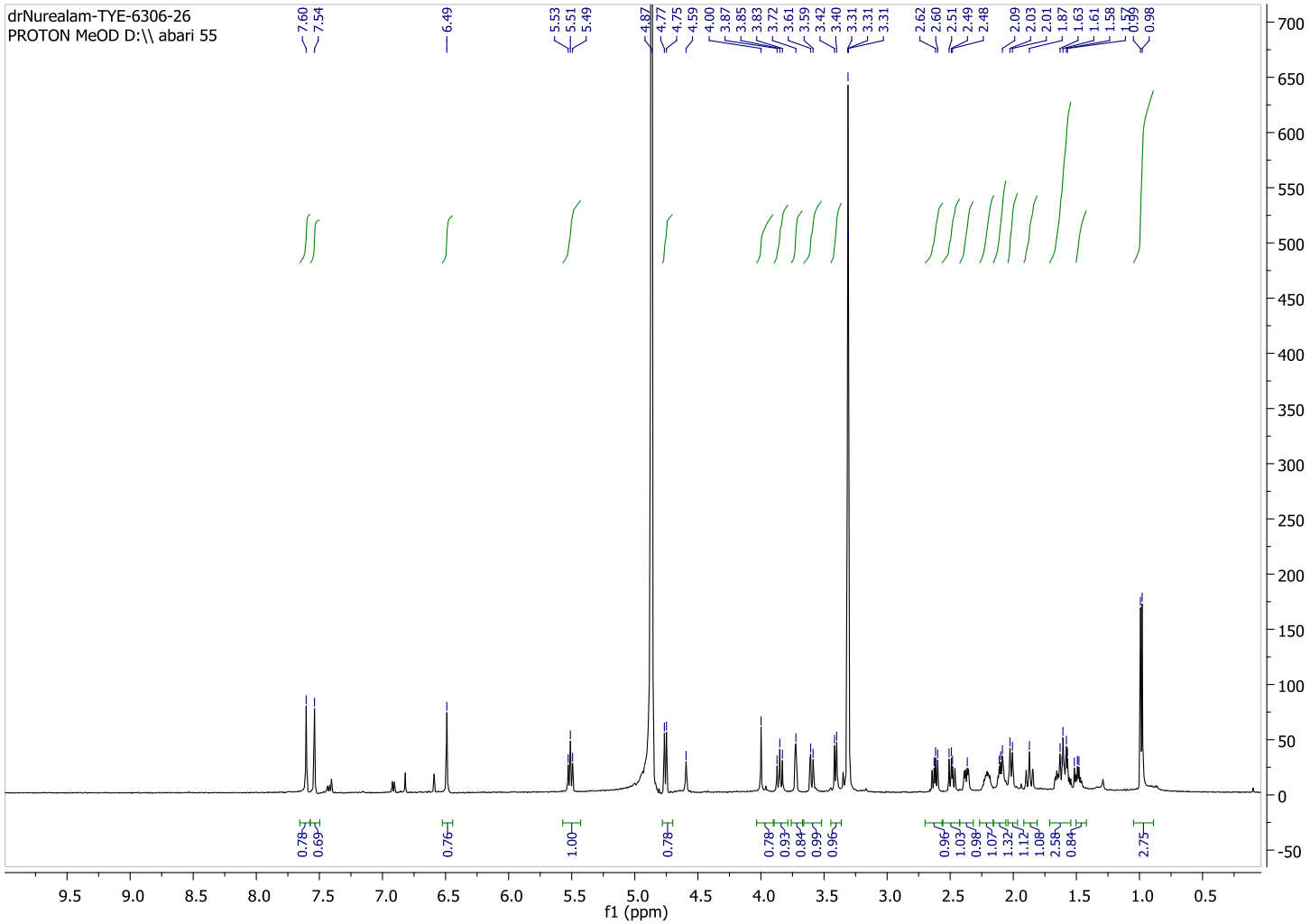


Fig S9: ^{1}H-NMR spectrum of compound **2**

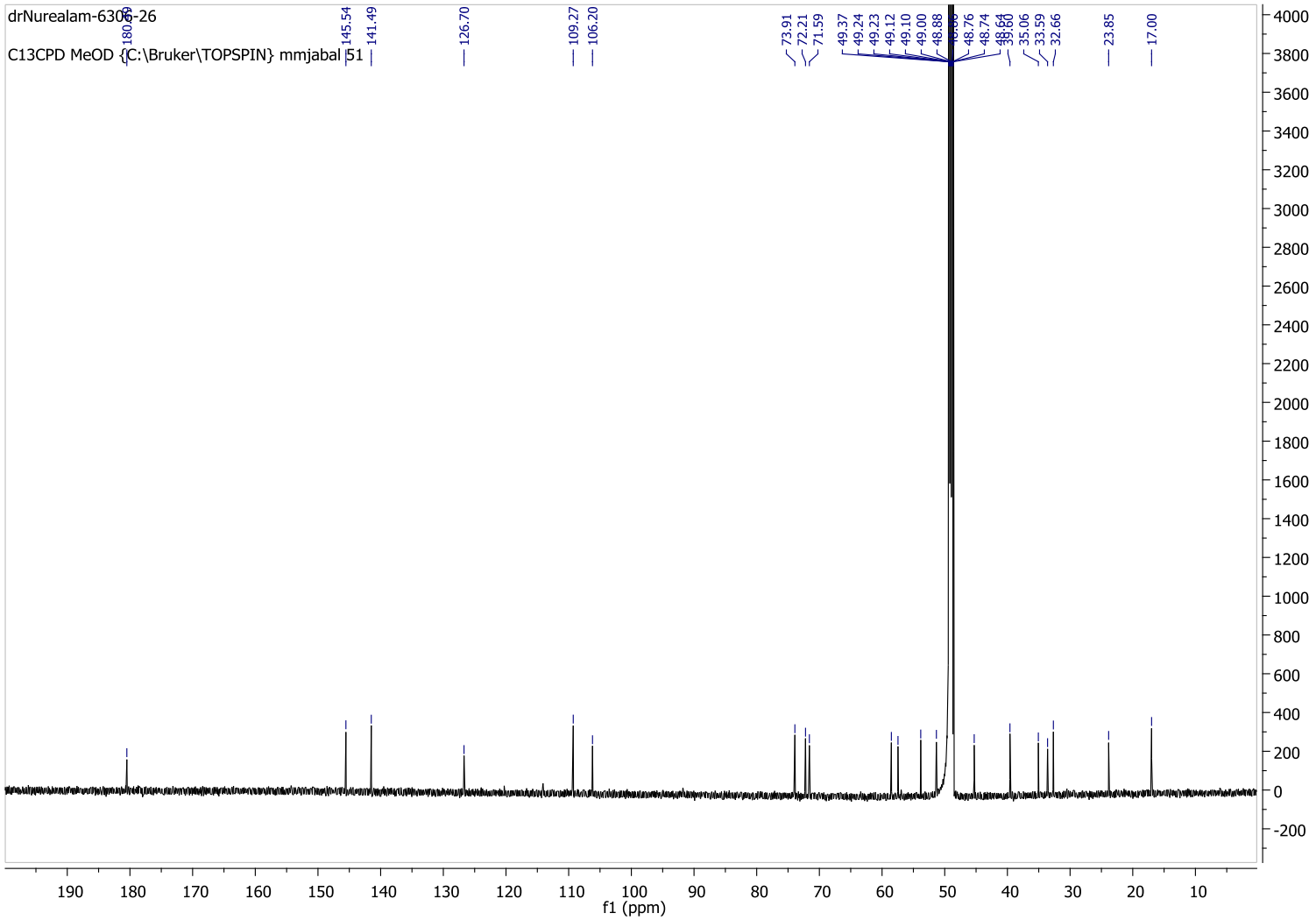


Fig S10: ^{13}C-NMR spectrum of compound **2**

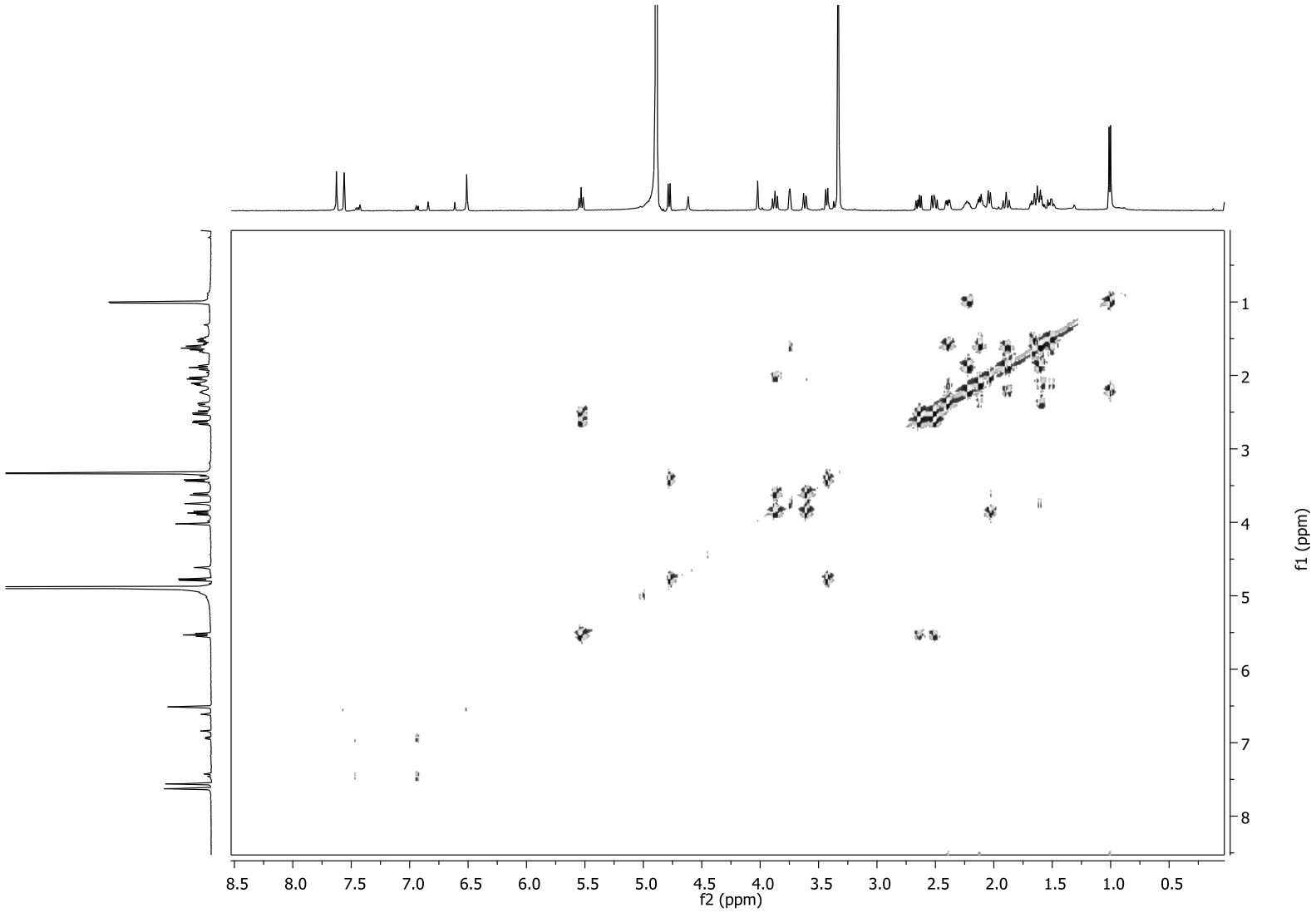


Fig S11: COSY spectrum of compound **2**

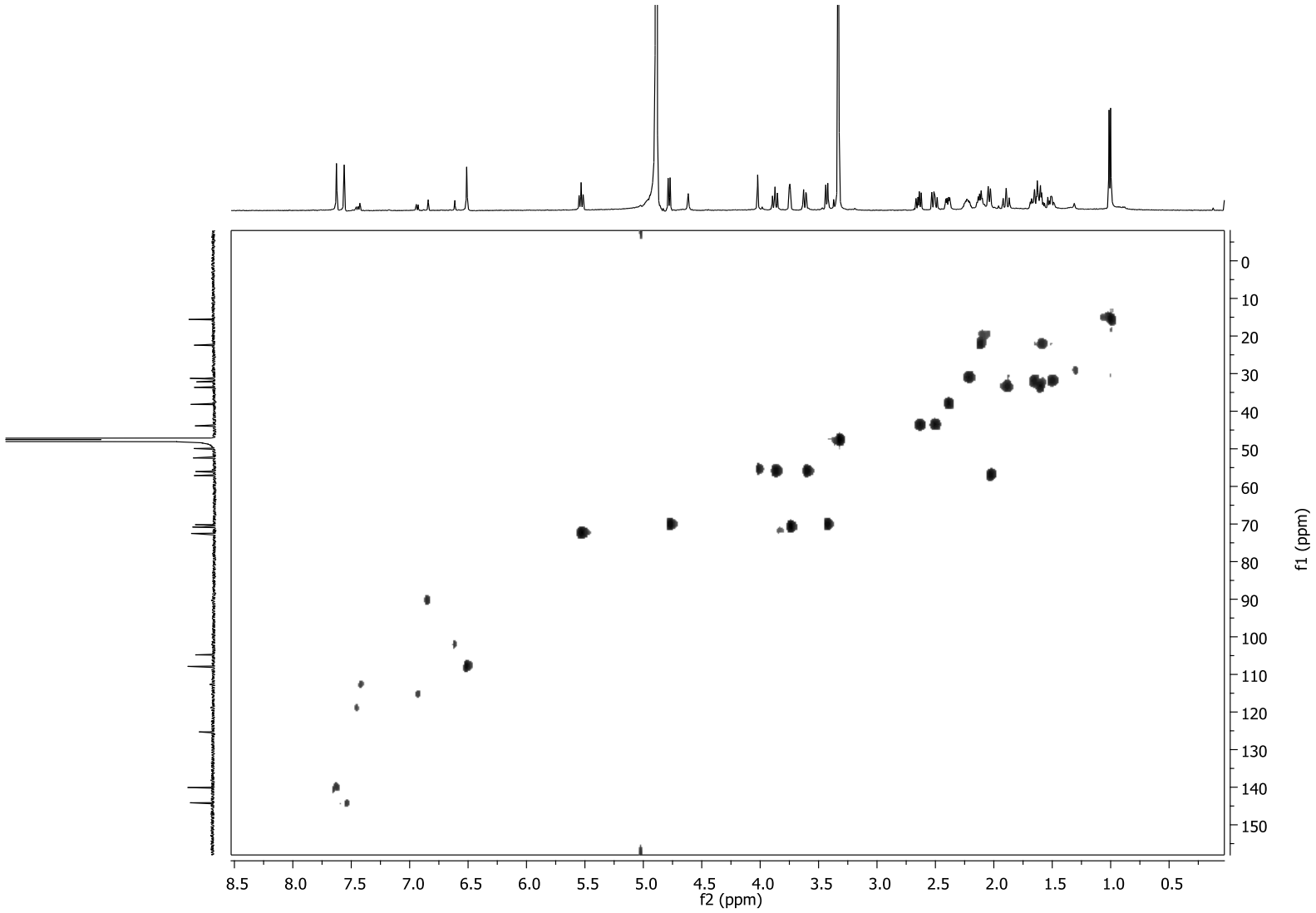


Fig S12: HSQC spectrum of compound **2**

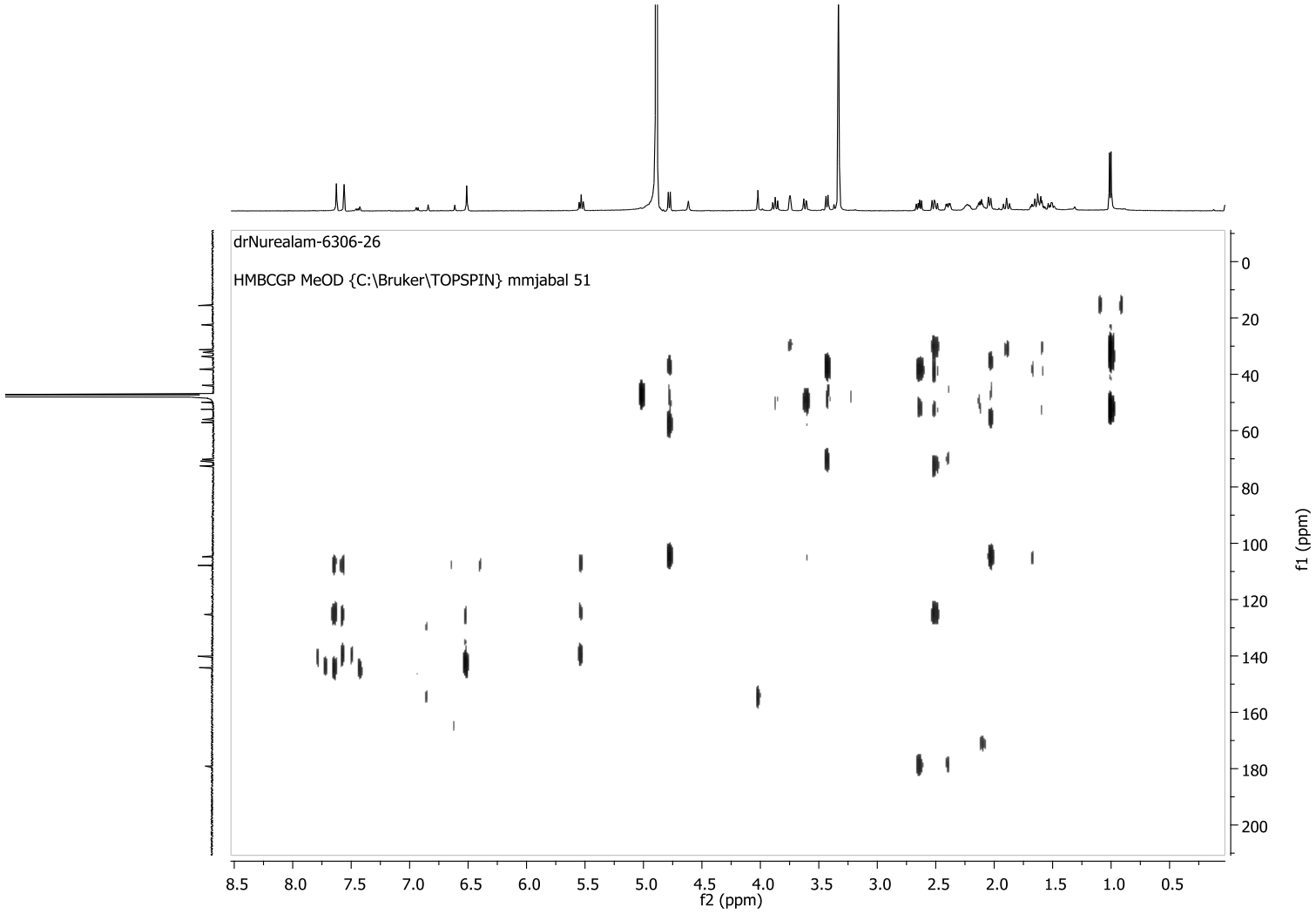


Fig S13: HMBC spectrum of compound **2**

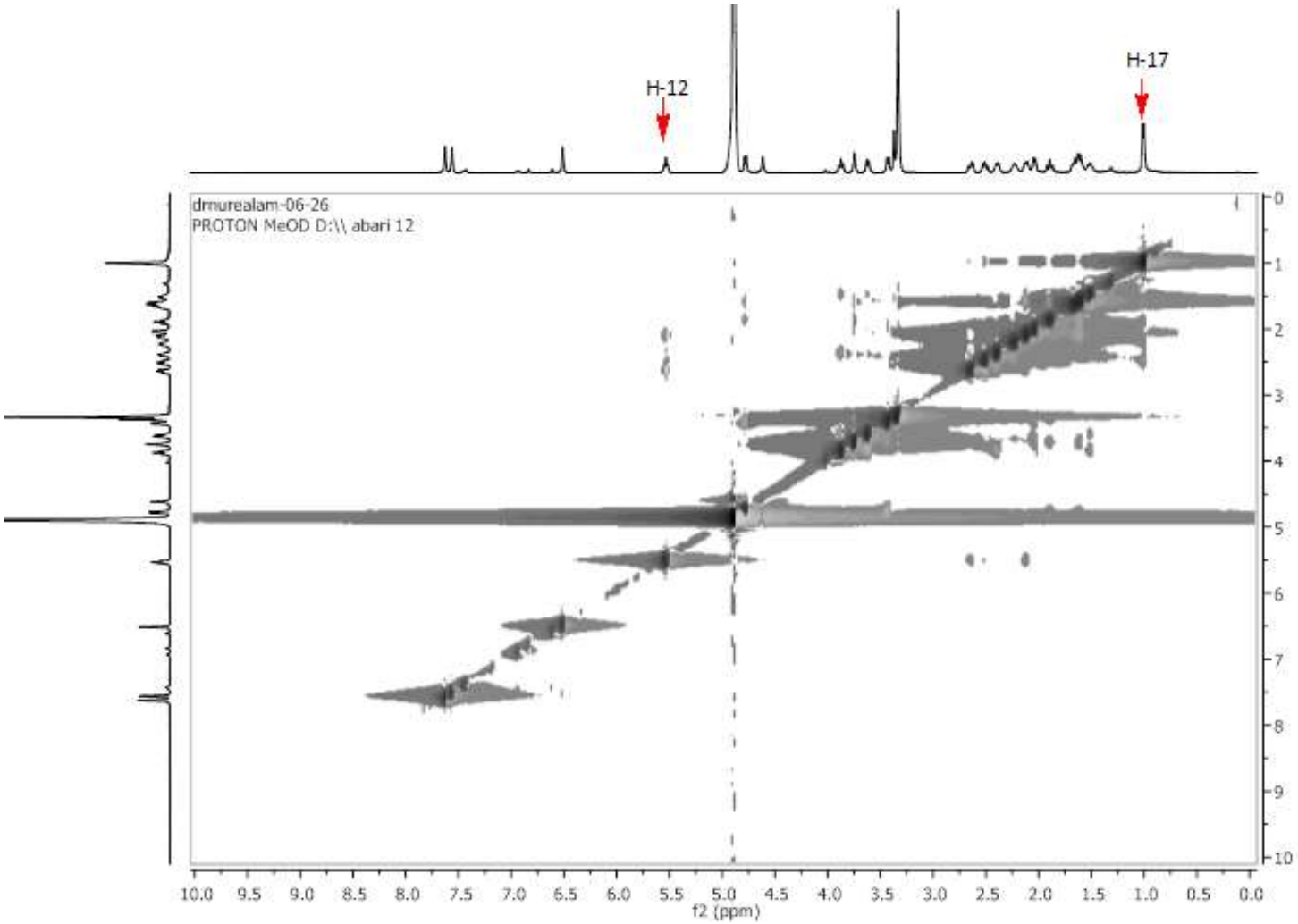


Fig S14: NOESY spectrum of compound **2,** which showed no correlation between H-12 and H-17.

Compound **3**

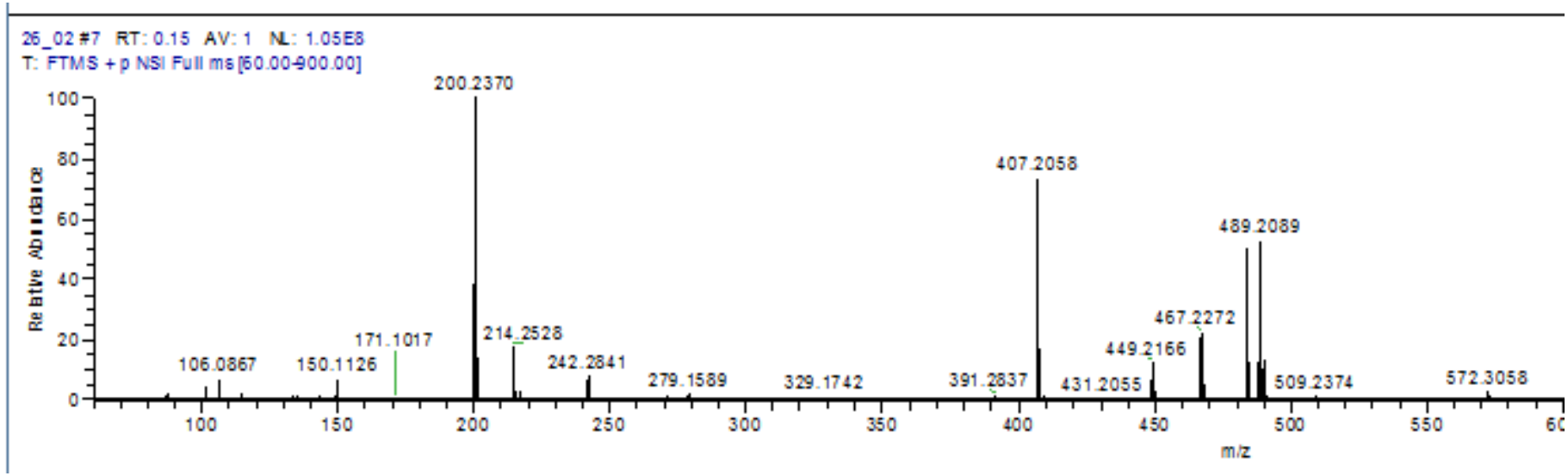


Fig S15: HRESIMS spectrum of compound **3**

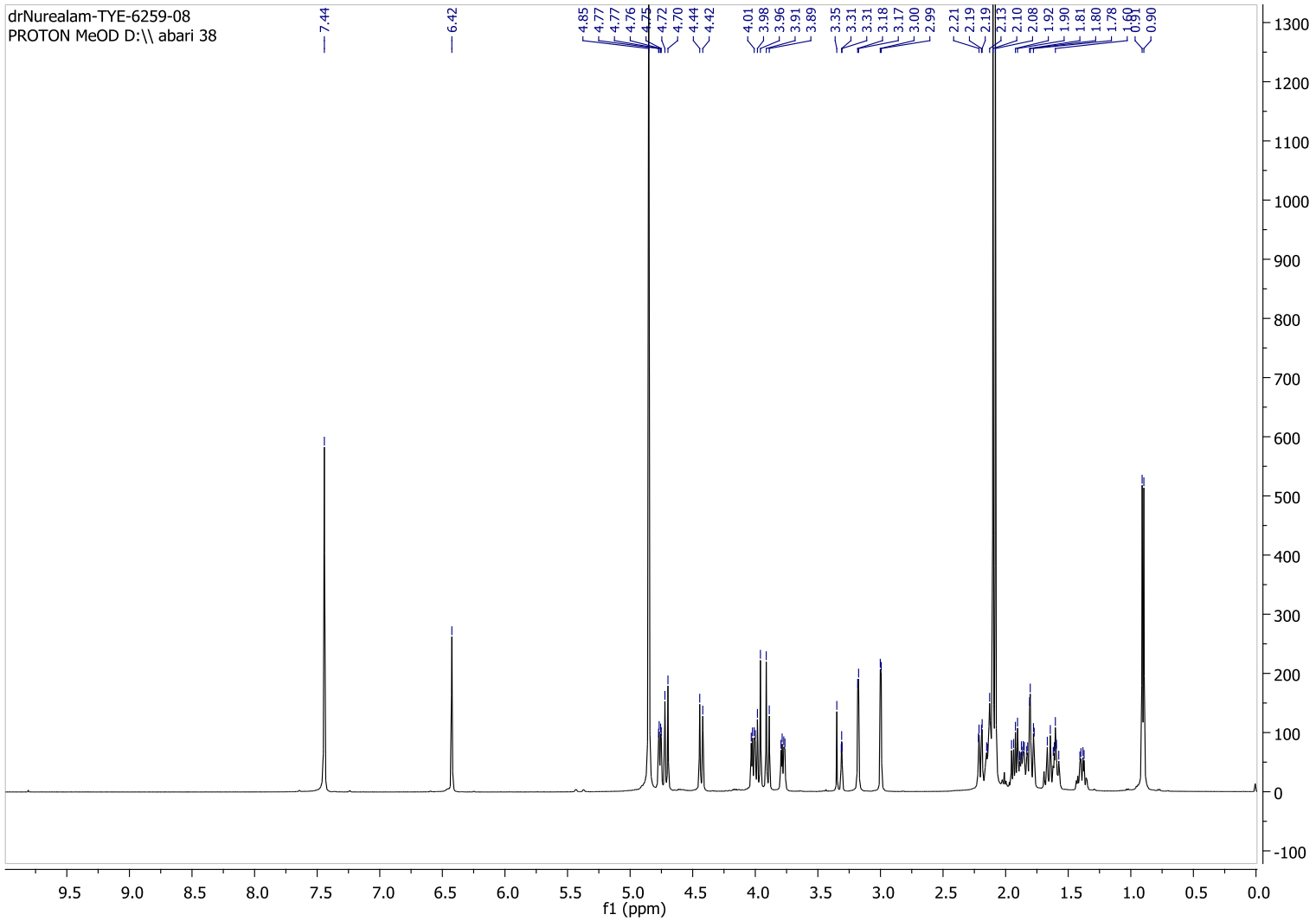


Fig S16: ^{1}H-NMR spectrum of compound **3**

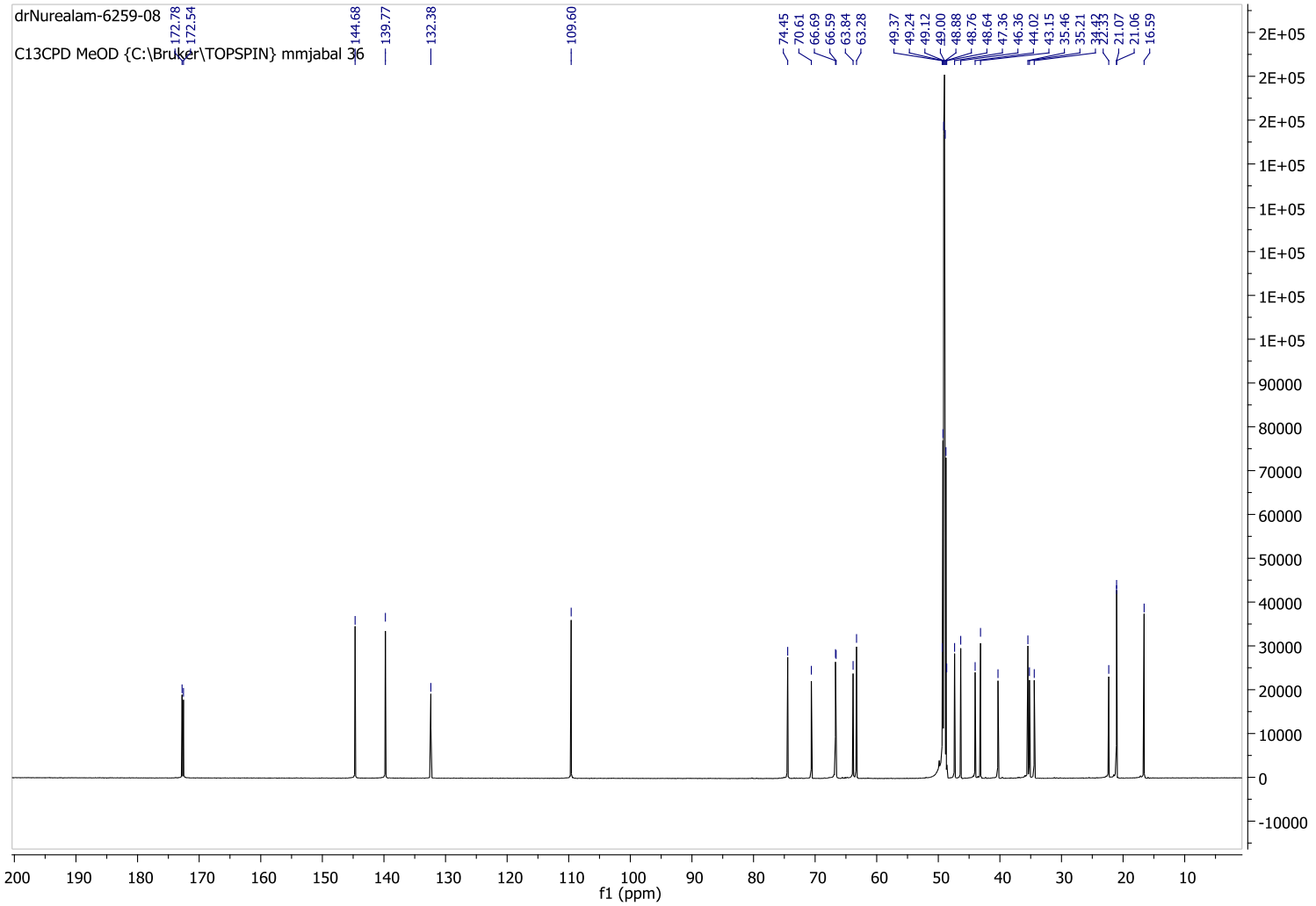


Fig S17: ^{13}C-NMR spectrum of compound **3**

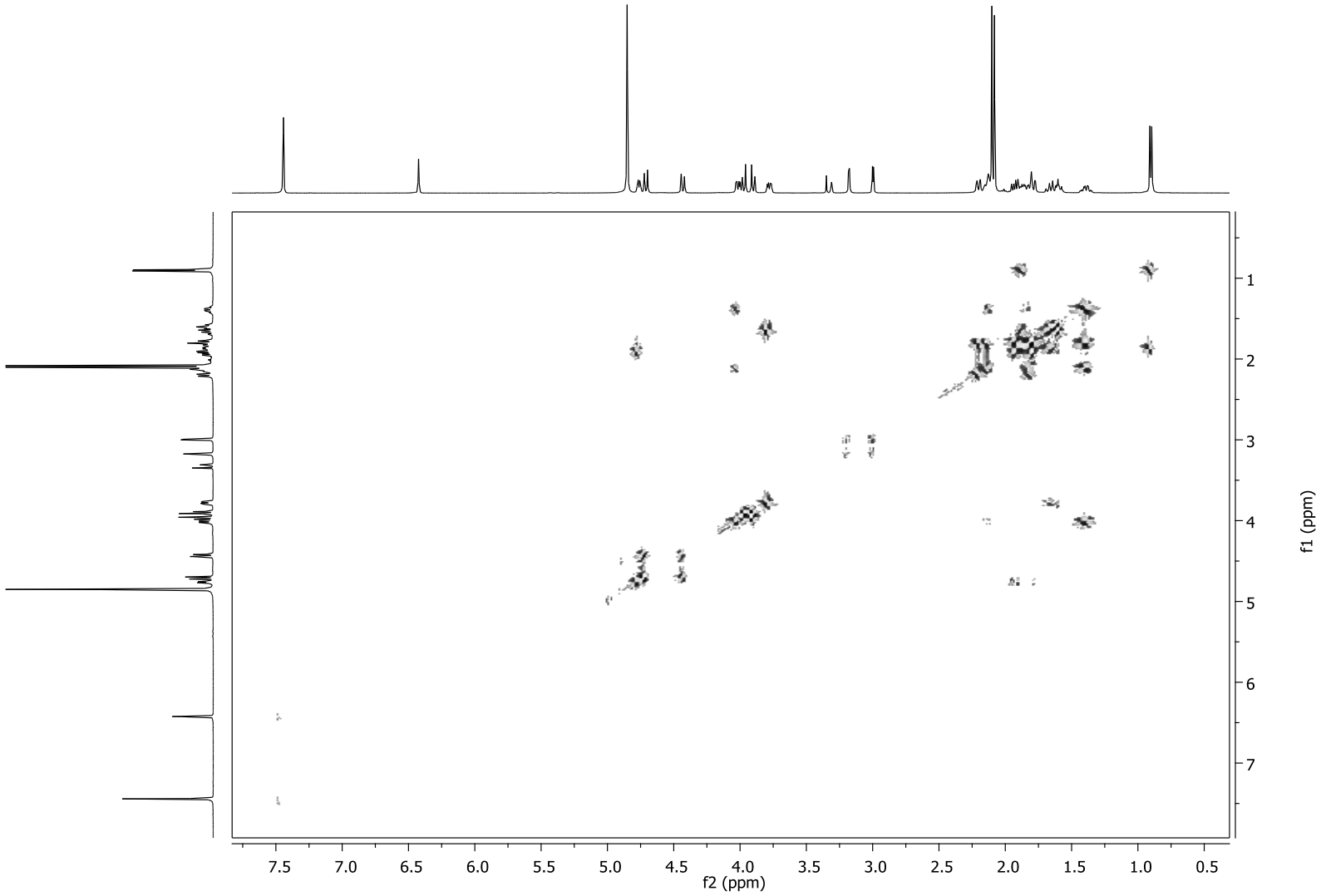


Fig S18: COSY spectrum of compound **3**

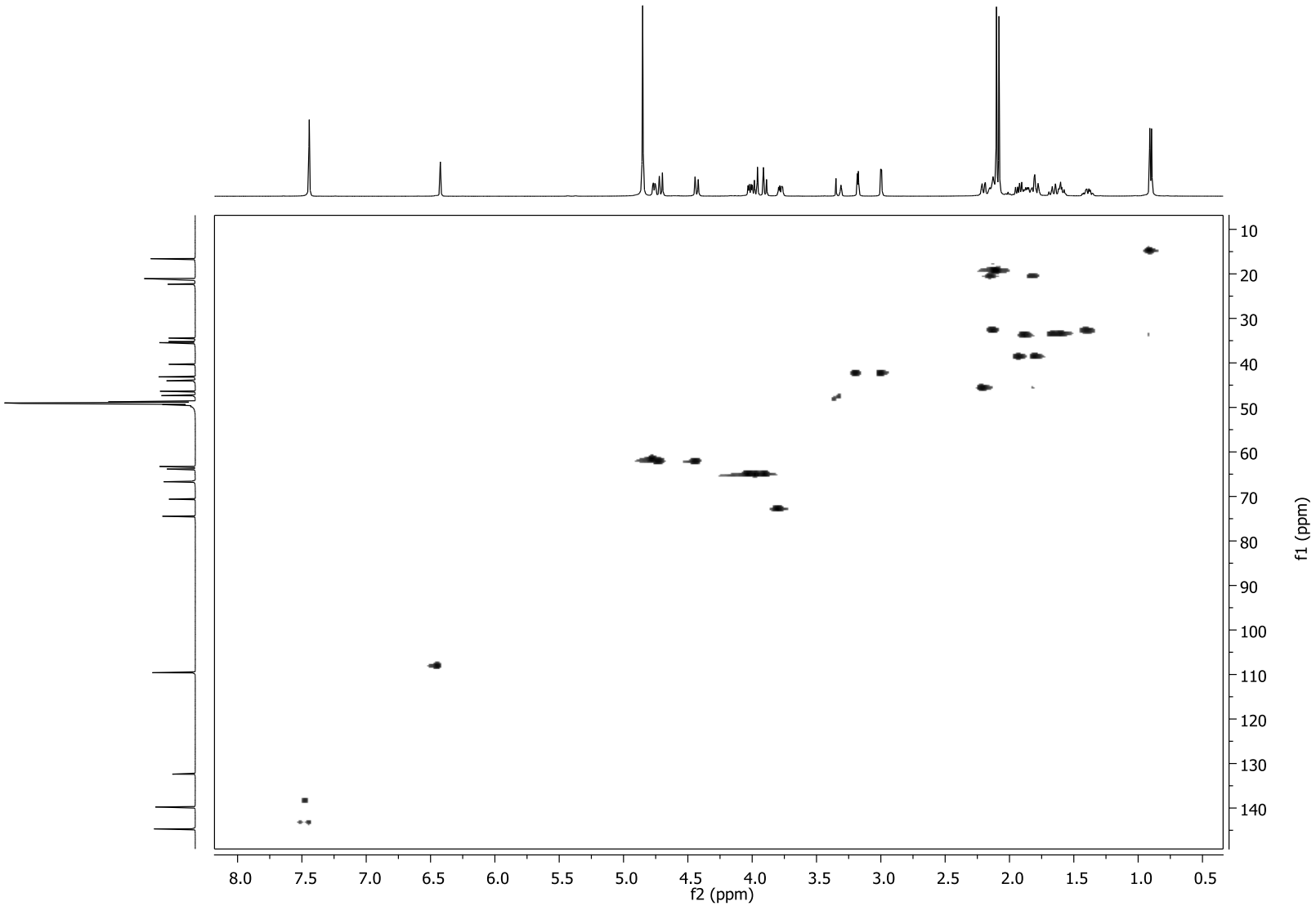


Fig S19: HSQC spectrum of compound **3**

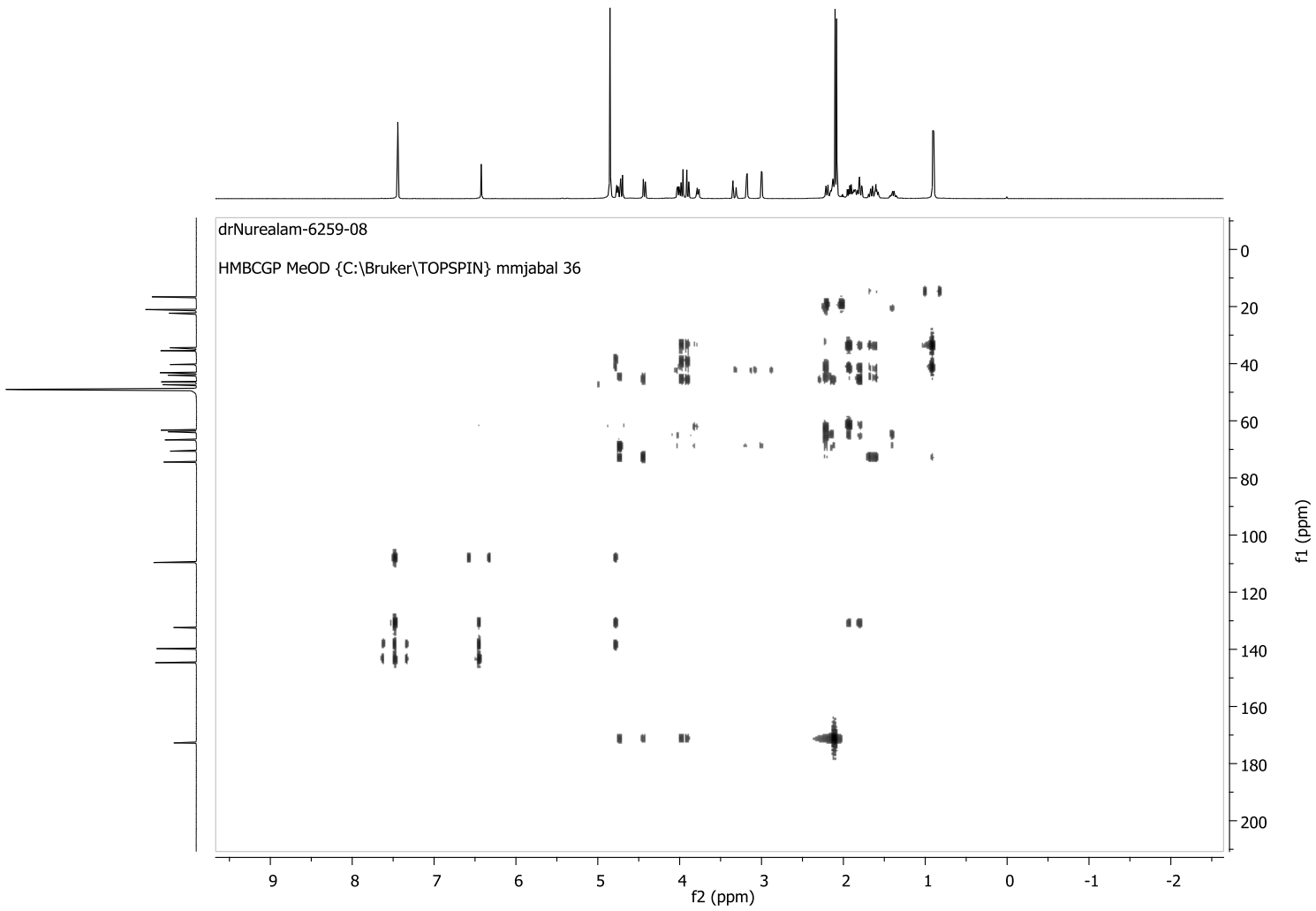


Fig S20: HMBC spectrum of compound **3**

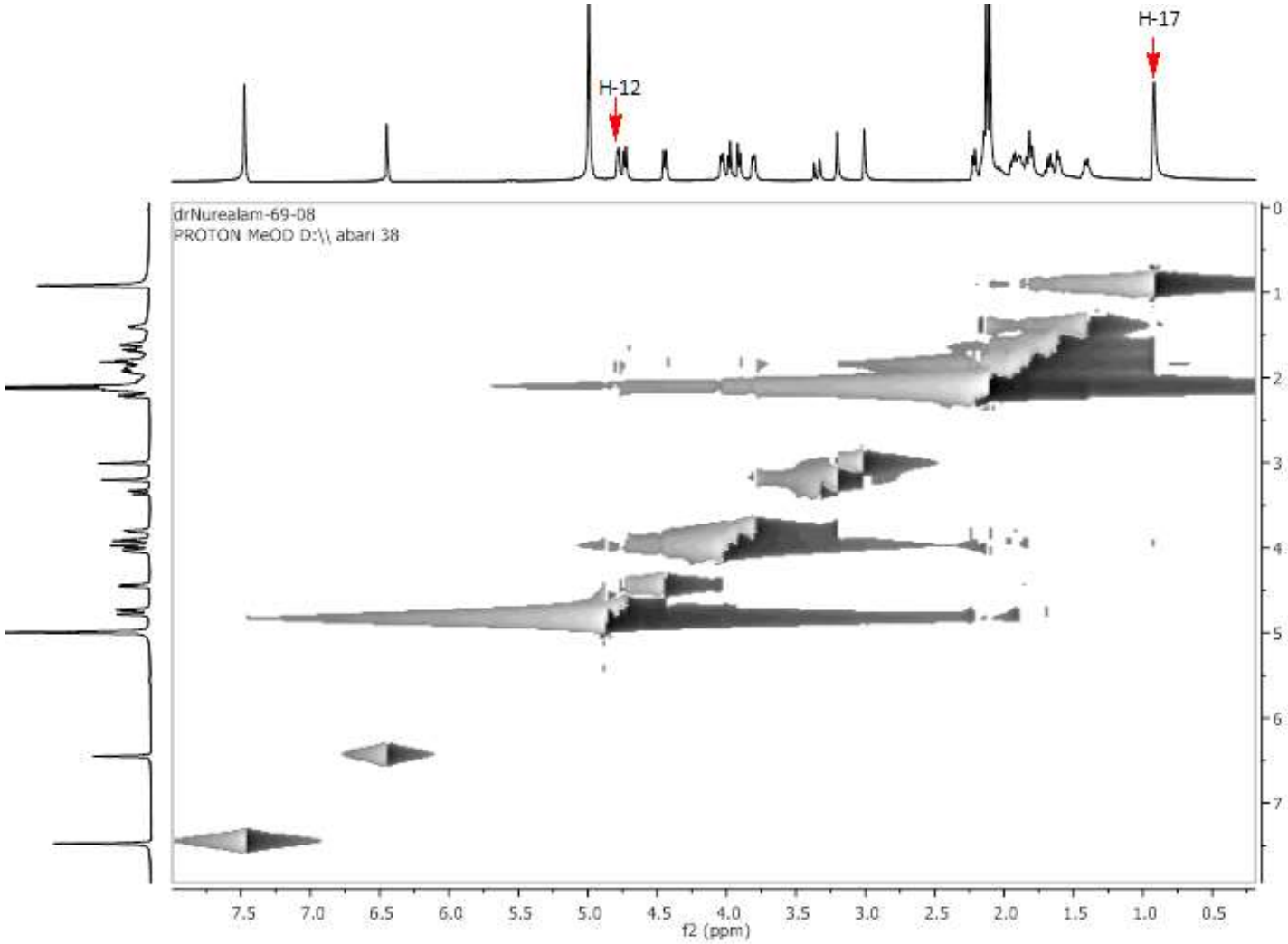


Fig S21: NOESY spectrum of compound **3,** which showed no correlation between H-12 and H-17.

Compound **4**

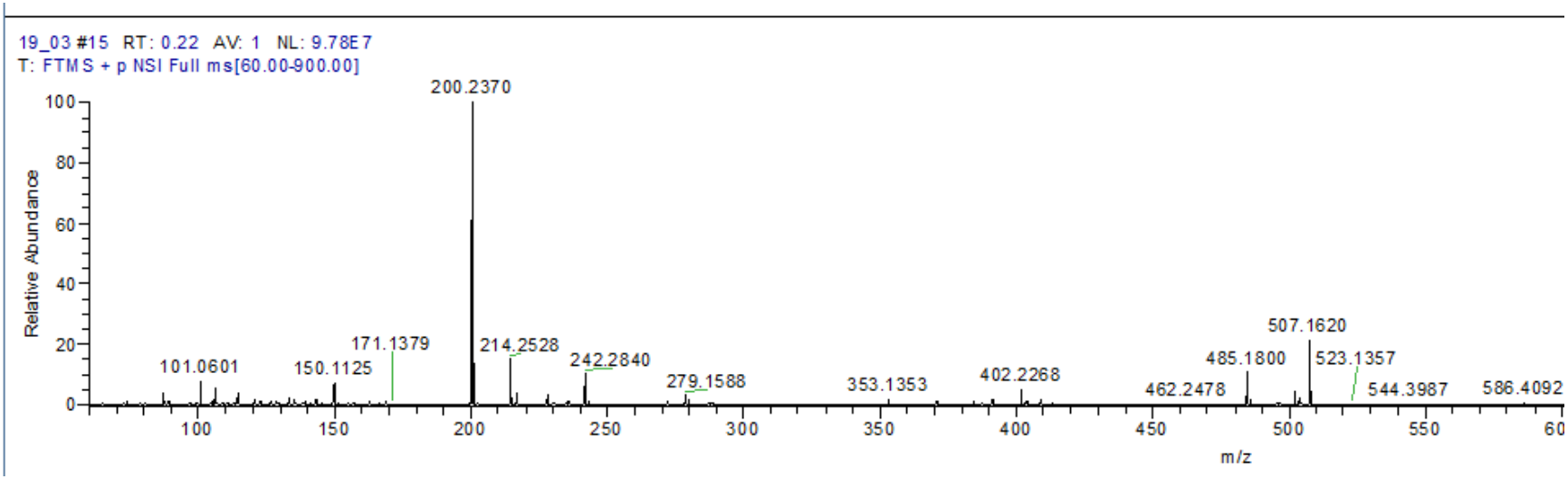


Fig S22: HRESIMS spectrum of compound **4**

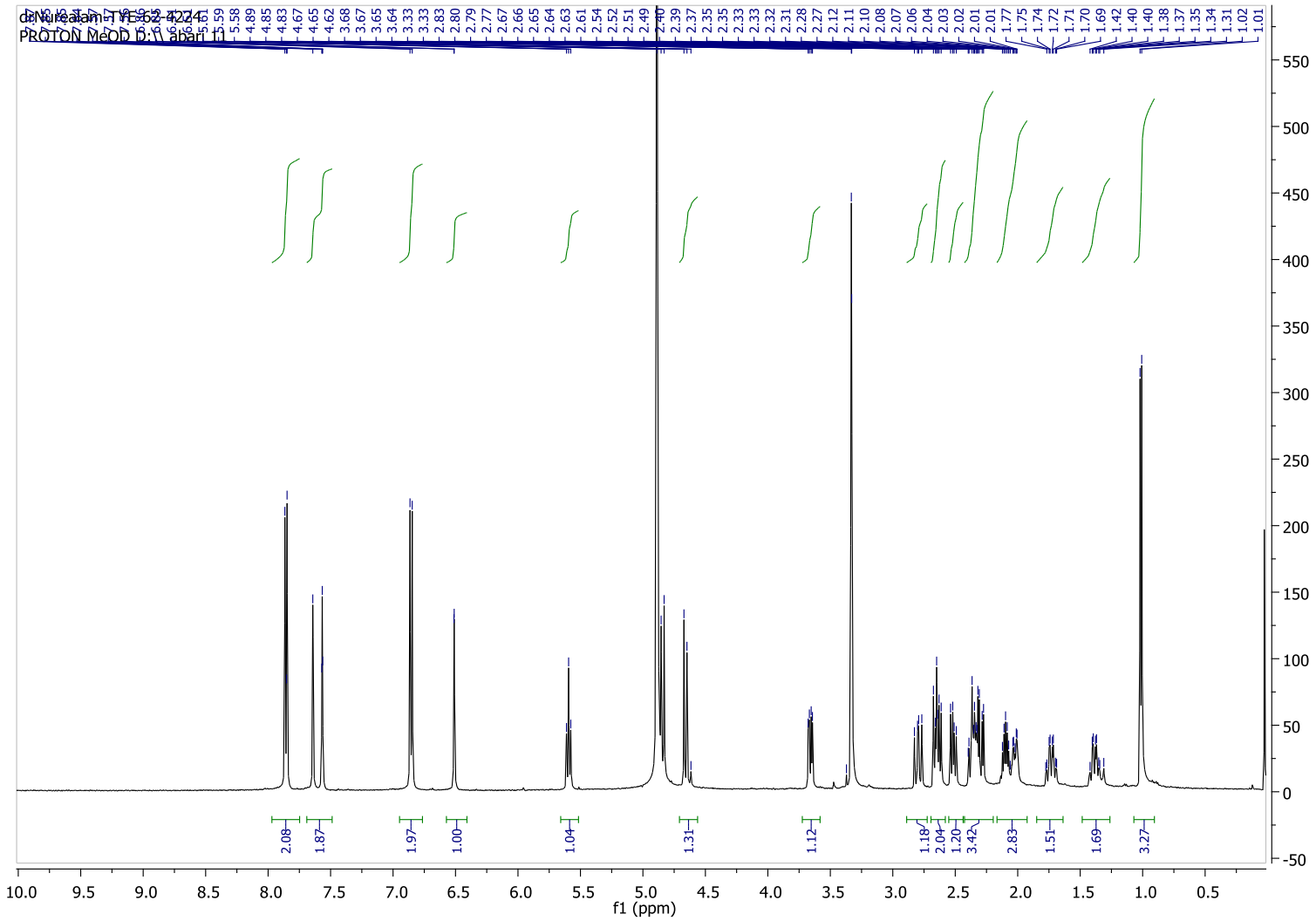


Fig S23: ^{1}H-NMR spectrum of compound **4**

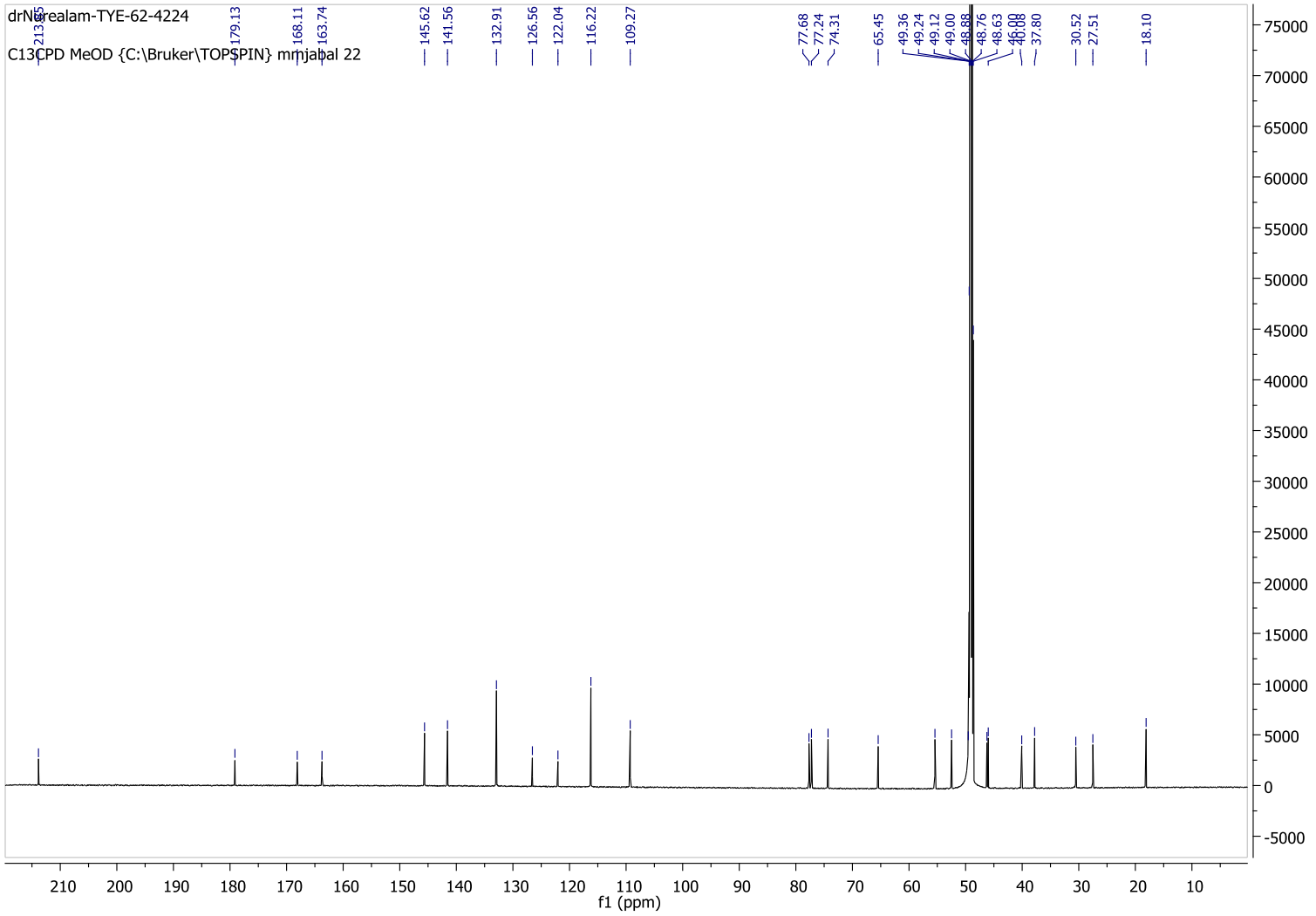


Fig S24: ^{13}C-NMR spectrum of compound **4**

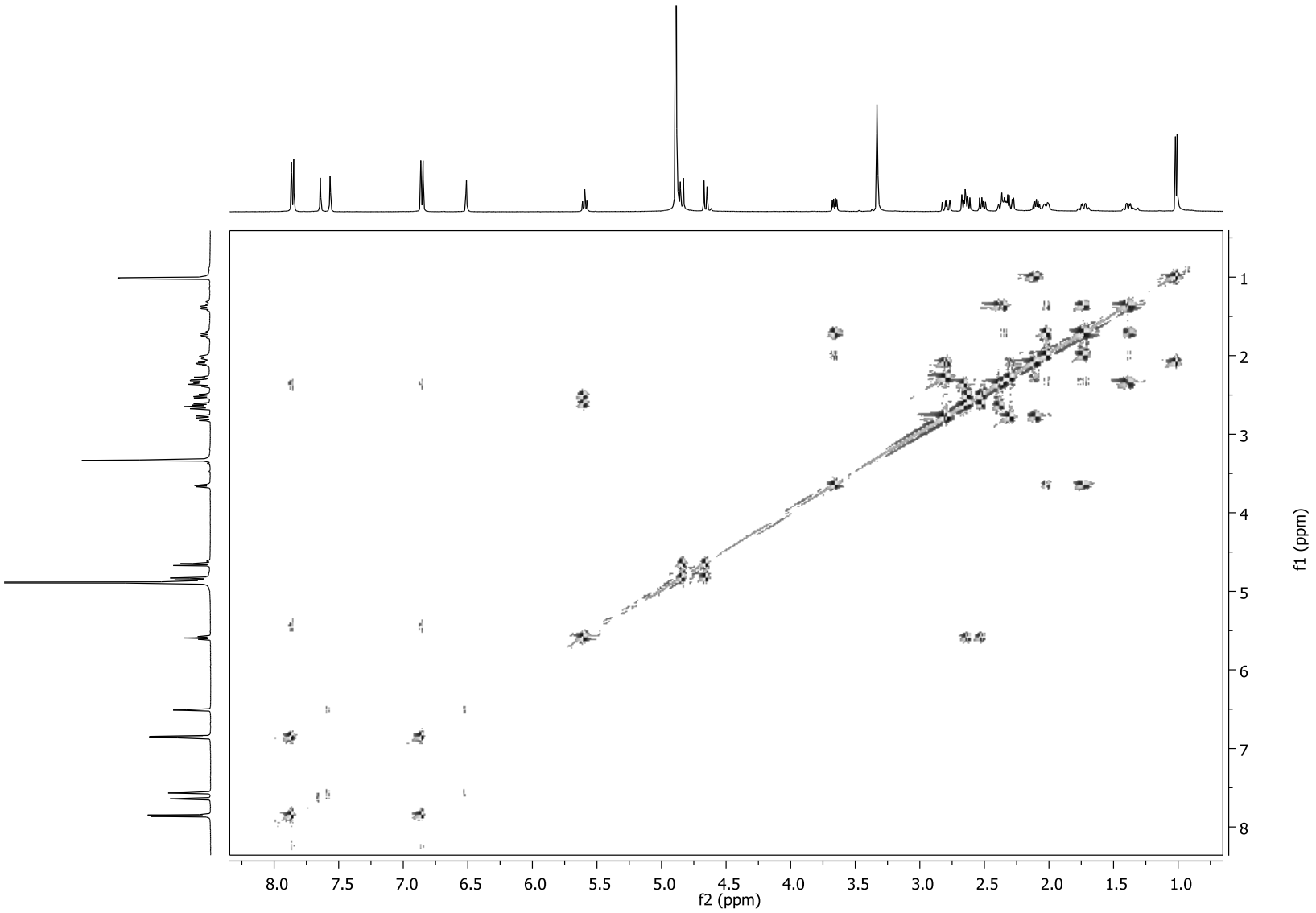


Fig S25: COSY spectrum of compound **4**

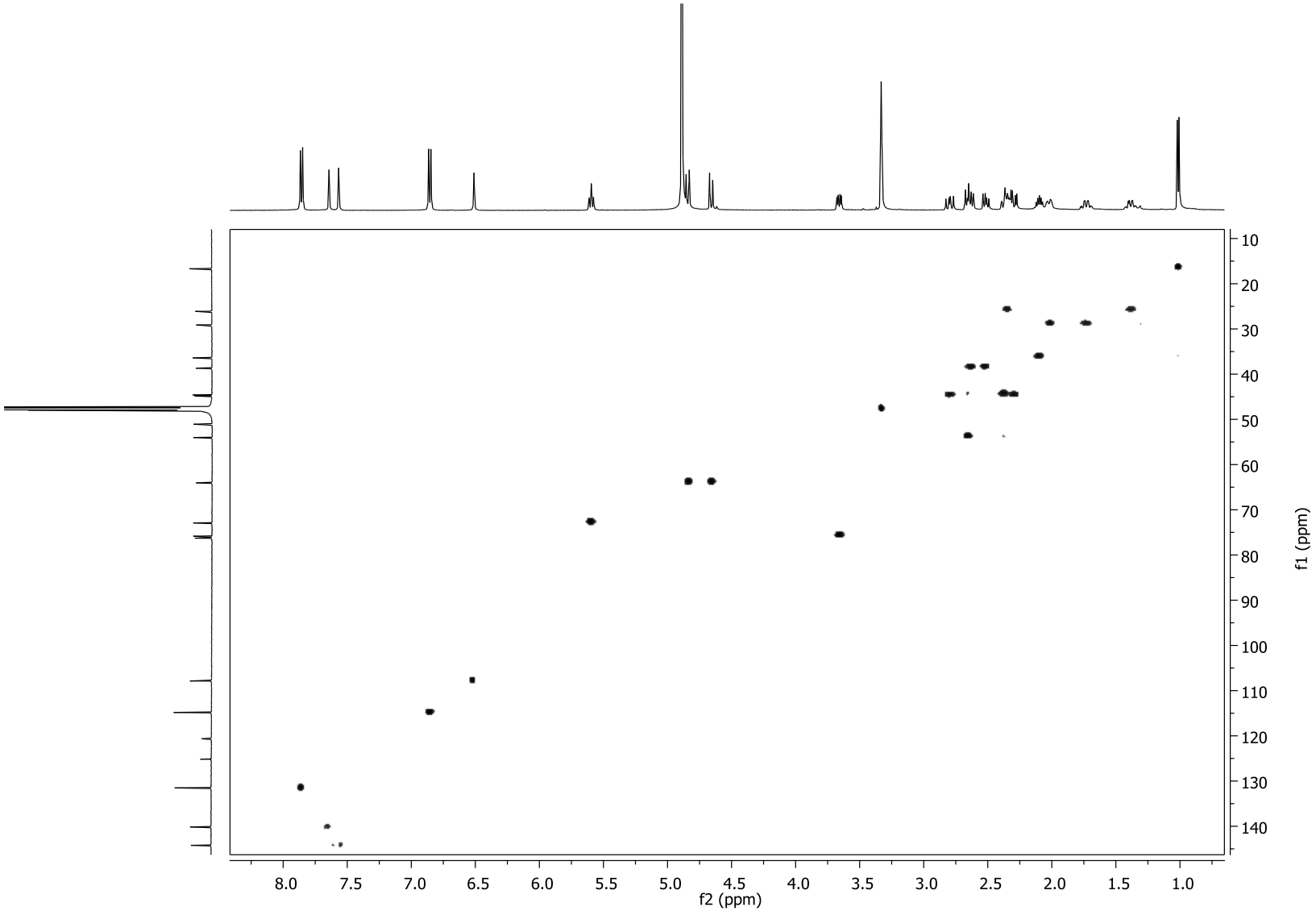


Fig S26: HSQC spectrum of compound **4**

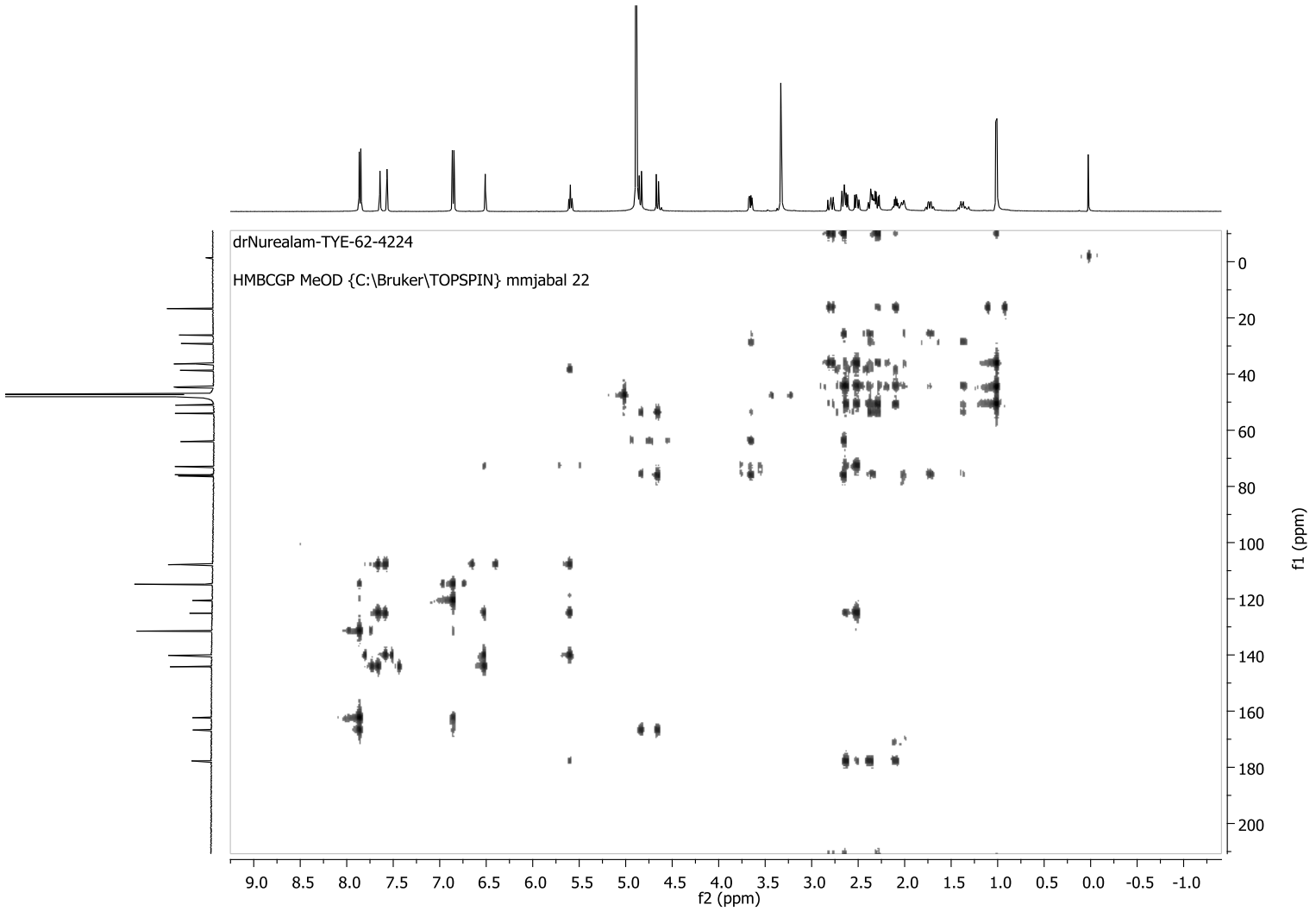


Fig S27: HMBC spectrum of compound **4**

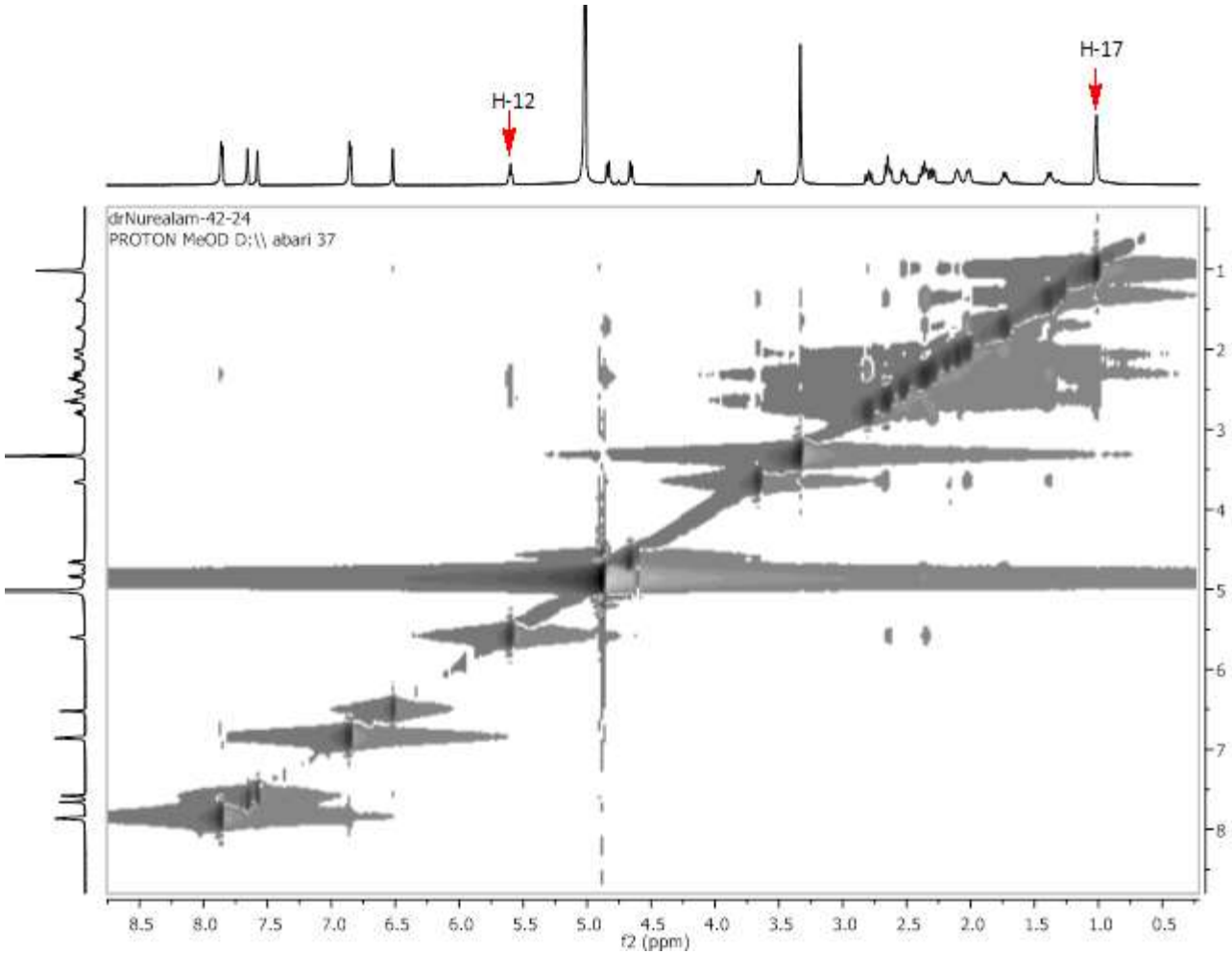


Fig S28: NOESY spectrum of compound **4,** which showed no correlation between H-12 and H-17.

Compound **5**

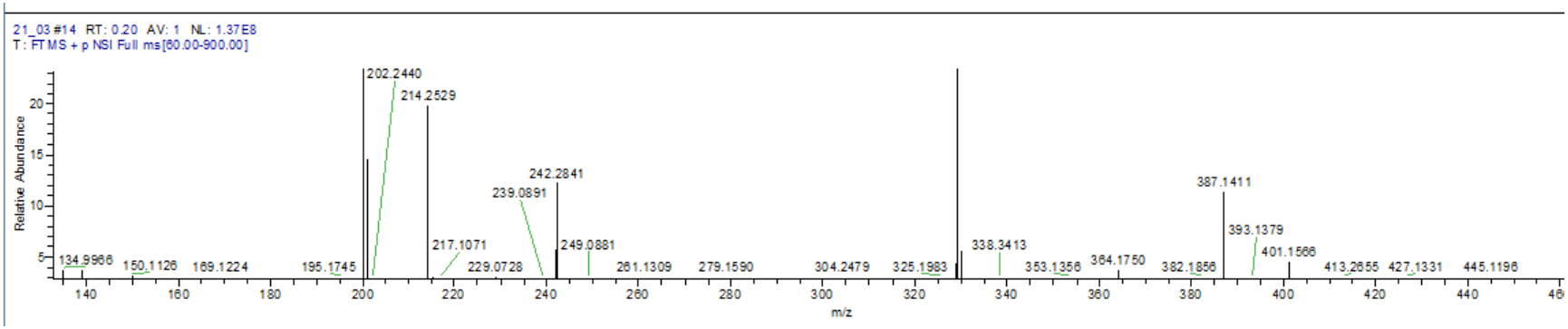


Fig S29: HRESIMS spectrum of compound **5**

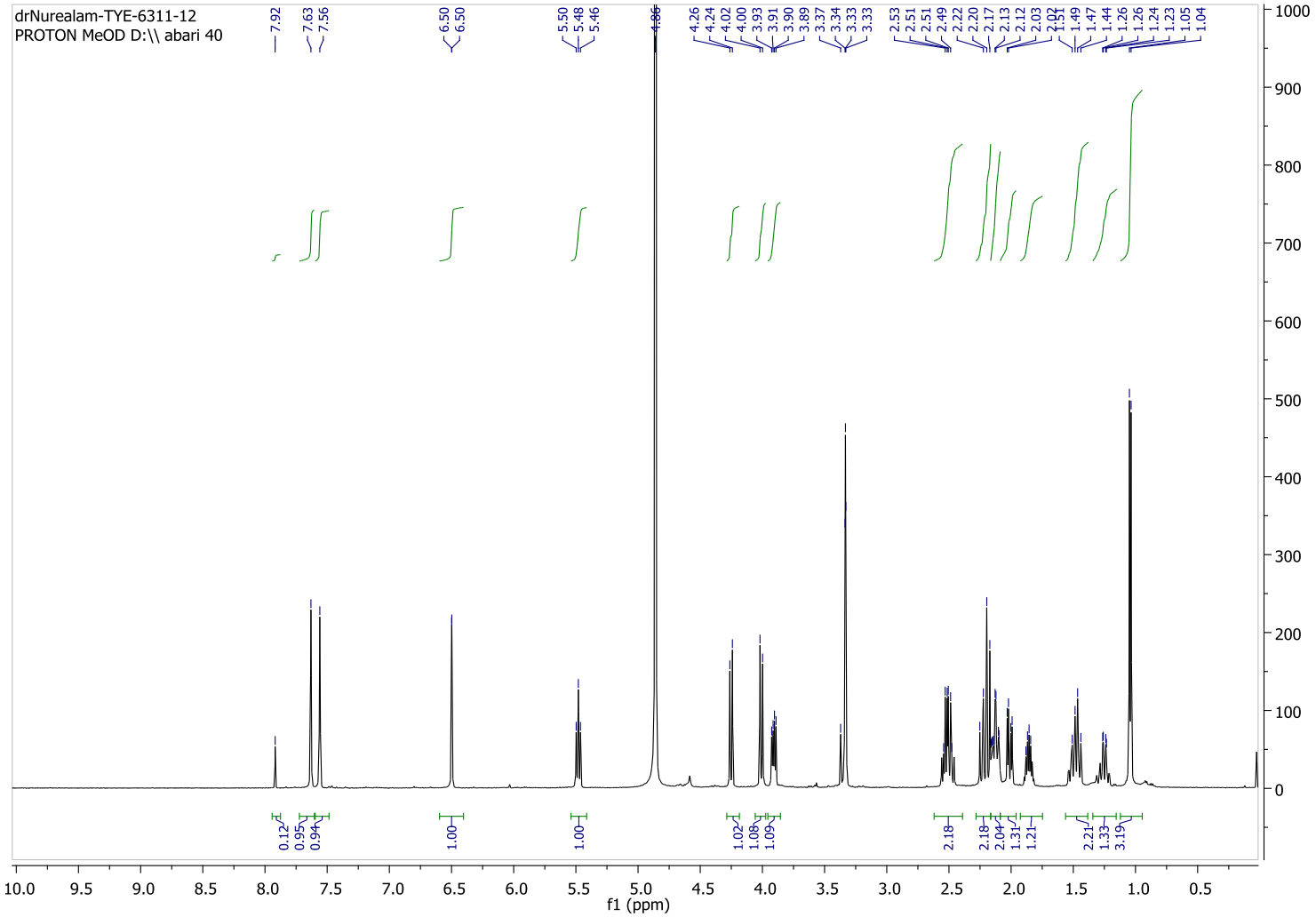


Fig S30: ^{1}H-NMR spectrum of compound **5**

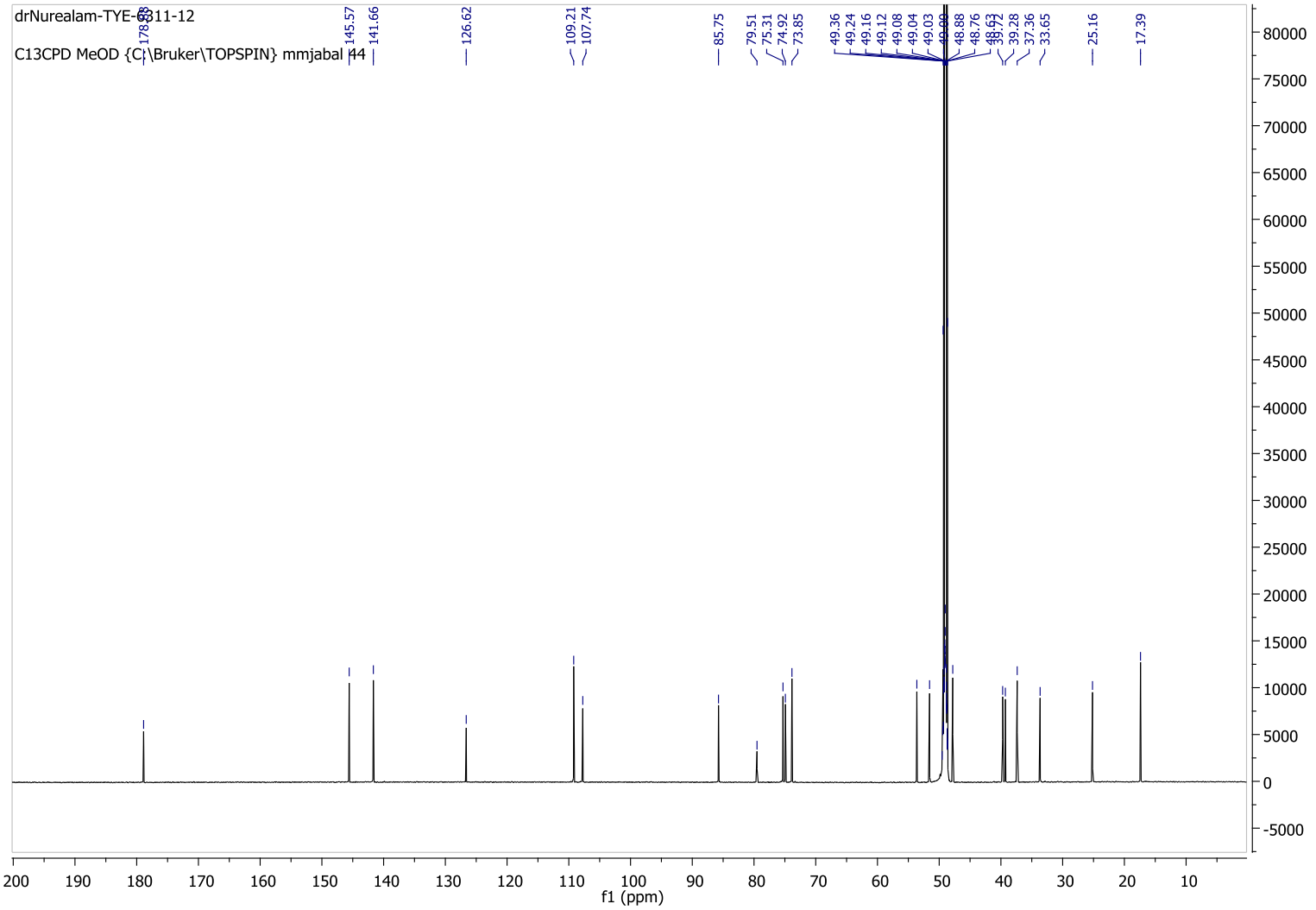


Fig S31: ^{13}C-NMR spectrum of compound **5**

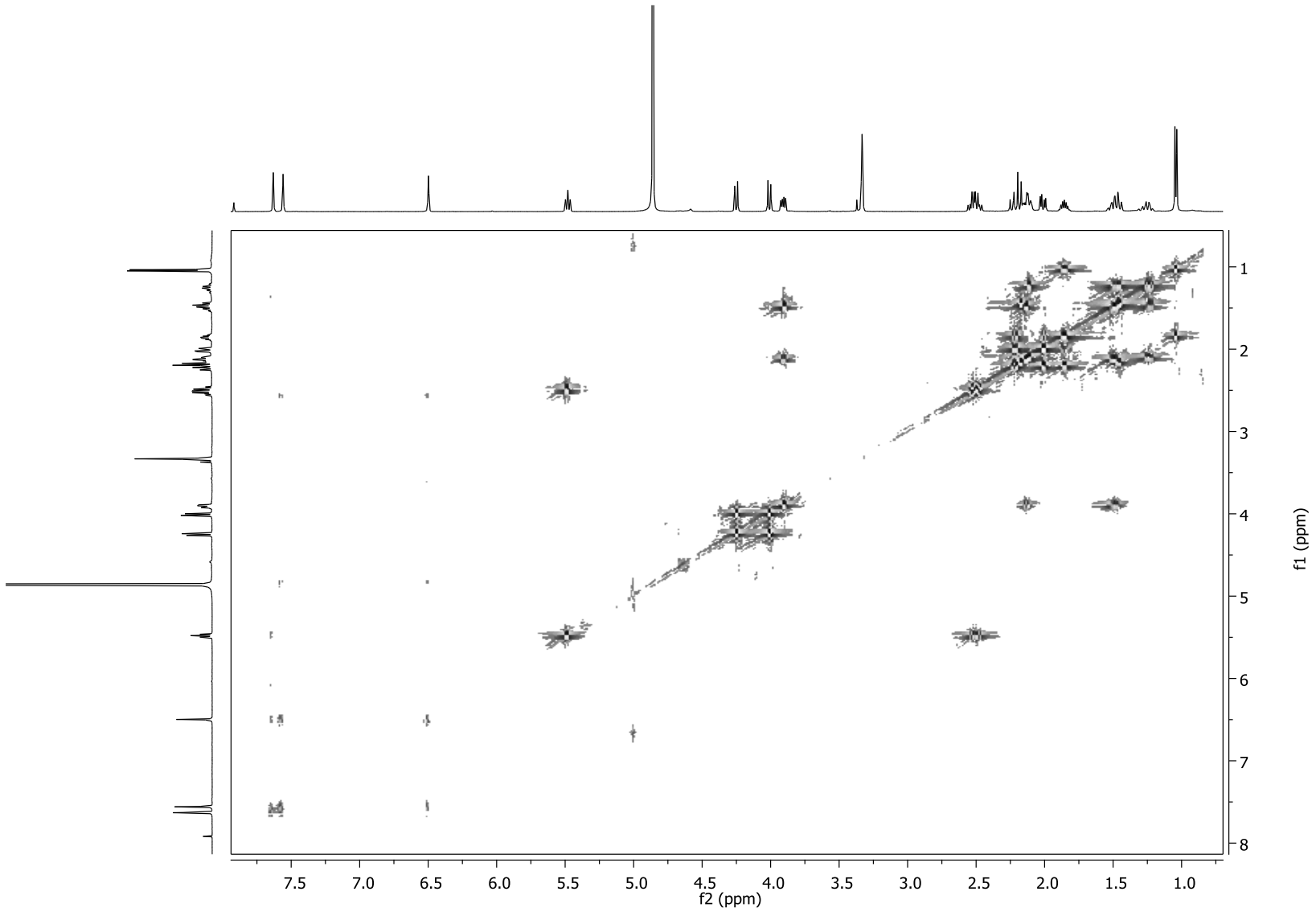
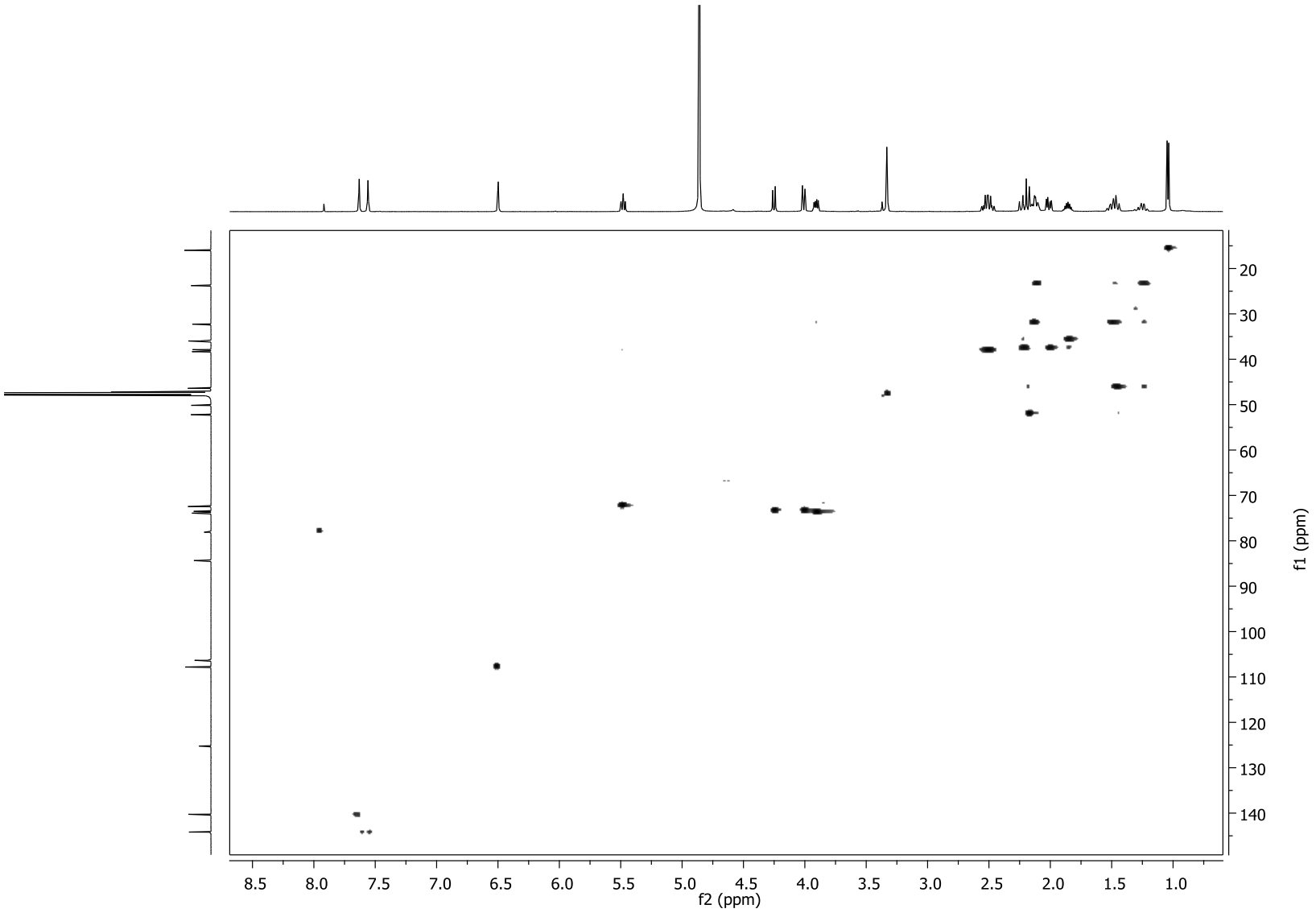


Fig S32: COSY spectrum of compound **5**



Fig

Fig S33: HSQC spectrum of compound **5**

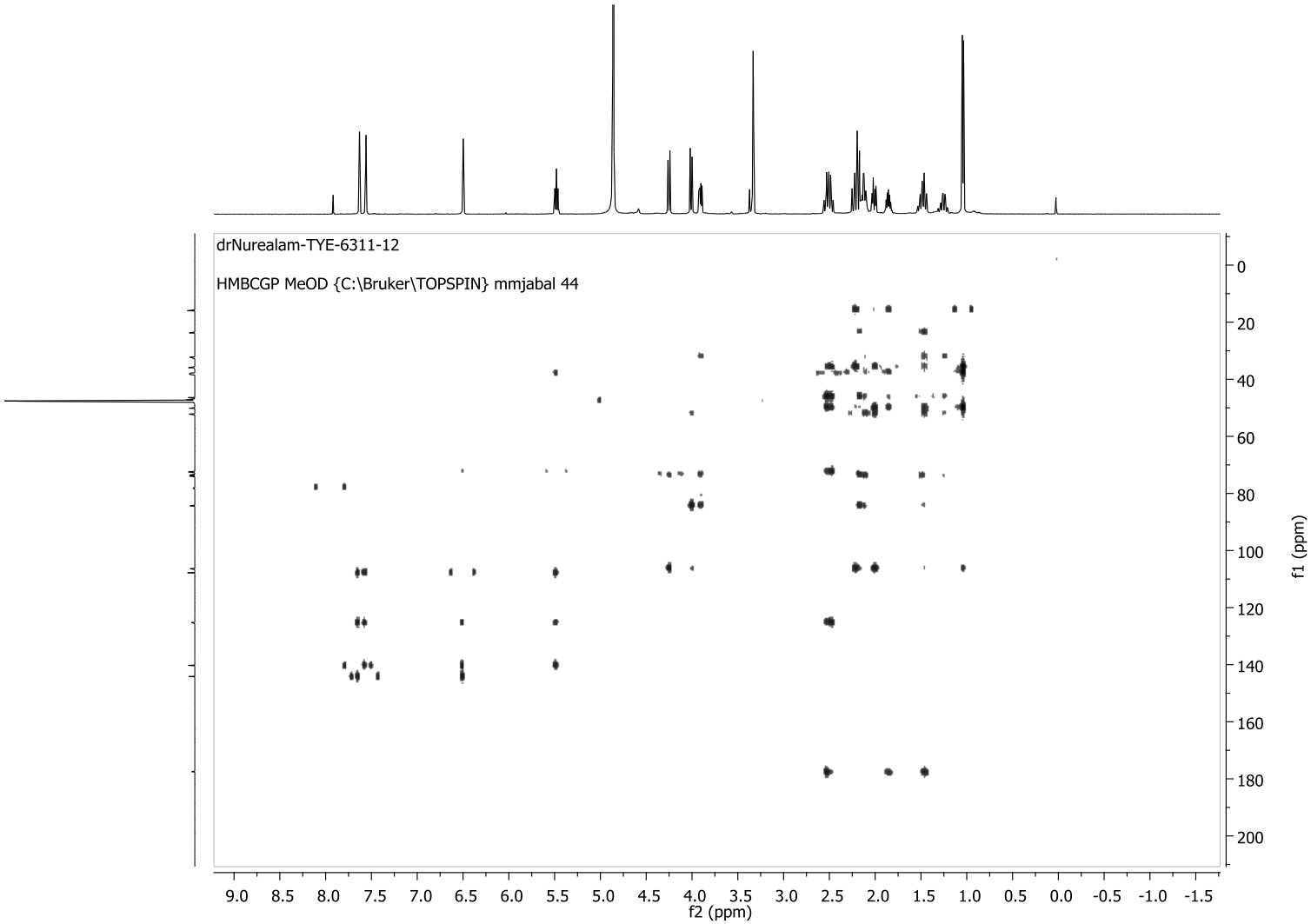


Fig S34: HMBC spectrum of compound **5**

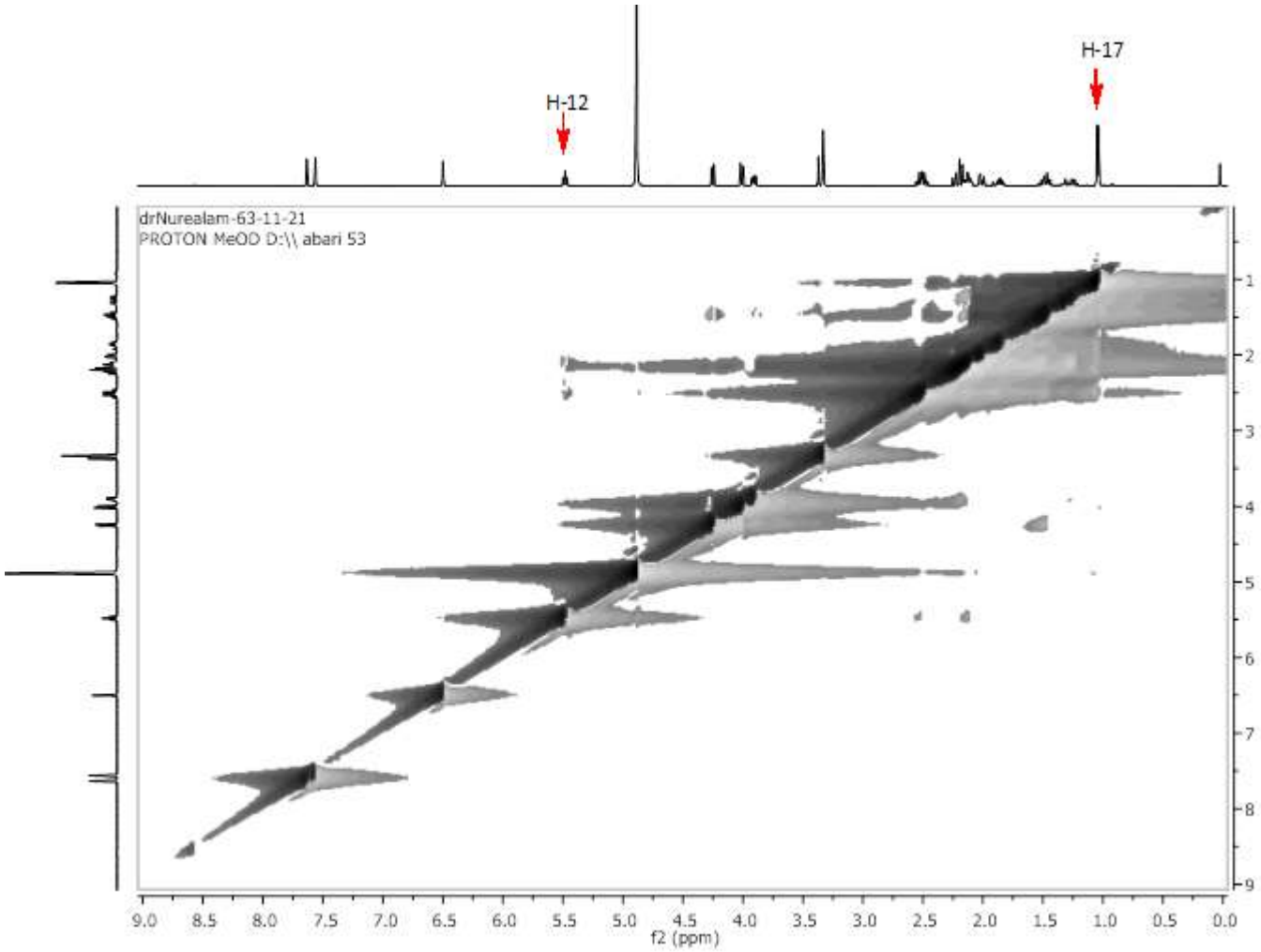


Fig S35: NOESY spectrum of compound **5,** which showed no correlation between H-12 and H-17.

*Crystal data of compound **5***

$C_{19}H_{26}O_8$	D_x = 1.361 Mg m^{-3}
M_r = 381.39	Melting point: ? K
Orthorhombic, $P2_12_12_1$	Cu $K\alpha$ radiation, λ = 1.54178 Å
a = 6.4987 (3) Å	Cell parameters from 8013 reflections
b = 6.9114 (3) Å	θ = 4.3–72.1°
c = 41.4349 (19) Å	μ = 0.89 mm^{-1}
V = 1861.05 (15) Å^3	T = 100 K
Z = 4	PLATE, colourless
F(000) = 812	0.52 × 0.36 × 0.05 mm

Data collection

Bruker APEX-II D8 venture diffractometer	3395 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus micro tube	R_{int} = 0.047
graphite	θ_{max} = 72.2°, θ_{min} = 2.1°
φ and ω scans	h = −7 6
Absorption correction: multi-scan SADABS Bruker 2014	k = −7 8
T_{min} = 0.653, T_{max} = 0.955	l = −43 51
10173 measured reflections	Standard reflections: 0
3519 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.041$	$w = 1/[\sigma^2(F_o^2) + (0.0682P)^2 + 0.6045P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.110$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.51$ e Å^{-3}
3519 reflections	$\Delta\rho_{min} = -0.44$ e Å^{-3}
265 parameters	Extinction correction: none
0 restraints	Extinction coefficient: ?
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack H D (1983), Acta Cryst. A39, 876-881
Secondary atom site location: difference Fourier map	Flack parameter: 0.00 (17)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.6120 (3)	0.7702 (3)	0.22020 (4)	0.0415 (5)
O2	0.8875 (3)	0.6138 (2)	0.31618 (3)	0.0288 (3)
O3	1.1296 (2)	0.6755 (2)	0.35223 (4)	0.0260 (3)
O4	1.1195 (2)	0.8753 (2)	0.44594 (3)	0.0208 (3)
O5	0.7805 (2)	0.98268 (18)	0.44160 (3)	0.0187 (3)
O6	0.9245 (2)	0.5640 (2)	0.46824 (3)	0.0205 (3)

O7	0.5010 (2)	0.4457 (2)	0.47144 (3)	0.0204 (3)
C1	0.7967 (4)	0.8566 (3)	0.22561 (6)	0.0365 (6)
H1A	0.8756	0.9208	0.2096	0.044*
C2	0.8528 (3)	0.8392 (3)	0.25660 (6)	0.0310 (5)
H2A	0.9748	0.8879	0.2663	0.037*
C3	0.6919 (4)	0.7322 (3)	0.27227 (5)	0.0254 (4)
C4	0.5523 (4)	0.6941 (4)	0.24915 (5)	0.0355 (5)
H4A	0.4287	0.6236	0.2525	0.043*
C5	0.6817 (3)	0.6780 (3)	0.30701 (5)	0.0233 (4)
H5A	0.5818	0.5694	0.3099	0.028*
C6	0.6294 (3)	0.8420 (3)	0.33049 (5)	0.0211 (4)
H6A	0.4889	0.8252	0.3393	0.025*
H6B	0.6372	0.9689	0.3195	0.025*
C7	0.7906 (3)	0.8302 (3)	0.35777 (4)	0.0167 (4)
C8	0.9575 (3)	0.7040 (3)	0.34295 (5)	0.0206 (4)
C9	0.8696 (3)	1.0337 (3)	0.36770 (5)	0.0199 (4)
H9A	0.7468	1.1121	0.3740	0.024*
C10	1.0146 (3)	1.0290 (3)	0.39677 (5)	0.0204 (4)
H10A	1.1382	1.1022	0.3974	0.024*
C11	0.9498 (3)	0.9014 (3)	0.42440 (4)	0.0162 (4)
C12	0.8685 (3)	0.7035 (3)	0.41450 (4)	0.0149 (4)
H12A	0.9816	0.6151	0.4074	0.018*

C13	0.7032 (3)	0.7288 (3)	0.38827 (4)	0.0143 (4)
H13A	0.5992	0.8200	0.3975	0.017*
C14	0.5903 (3)	0.5369 (3)	0.38329 (4)	0.0175 (4)
H14A	0.4924	0.5484	0.3651	0.021*
H14B	0.6902	0.4333	0.3781	0.021*
C15	0.4743 (3)	0.4871 (3)	0.41430 (4)	0.0189 (4)
H15A	0.3725	0.5899	0.4190	0.023*
H15B	0.3986	0.3641	0.4113	0.023*
C16	0.6209 (3)	0.4673 (3)	0.44264 (4)	0.0164 (4)
H16A	0.7032	0.3465	0.4395	0.020*
C17	0.7701 (3)	0.6362 (3)	0.44634 (4)	0.0152 (4)
C18	0.6785 (3)	0.8275 (3)	0.45898 (5)	0.0191 (4)
H18A	0.5283	0.8314	0.4550	0.023*
H18B	0.7030	0.8402	0.4825	0.023*
C19	0.9775 (4)	1.1418 (3)	0.34027 (5)	0.0300 (5)
H19A	1.0278	1.2668	0.3482	0.045*
H19B	0.8801	1.1633	0.3226	0.045*
H19C	1.0938	1.0647	0.3324	0.045*
O1W	0.1597 (2)	0.2271 (2)	0.47467 (3)	0.0195 (3)
H2OW	0.071 (5)	0.315 (4)	0.4718 (6)	0.025 (6)*
H1OW	0.273 (6)	0.279 (5)	0.4737 (7)	0.046 (9)*
H1O6	1.015 (5)	0.665 (5)	0.4679 (7)	0.044 (8)*

H1O7	0.568 (5)	0.402 (4)	0.4845 (7)	0.031 (7)*
H1O4	1.135 (5)	0.982 (5)	0.4545 (7)	0.045 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0699 (13)	0.0334 (9)	0.0210 (7)	−0.0133 (9)	0.0036 (8)	0.0003 (6)
O2	0.0319 (8)	0.0271 (8)	0.0272 (7)	0.0094 (6)	−0.0020 (6)	−0.0073 (6)
O3	0.0159 (7)	0.0279 (7)	0.0343 (8)	0.0036 (6)	0.0042 (5)	0.0017 (6)
O4	0.0159 (6)	0.0181 (7)	0.0283 (7)	−0.0031 (5)	−0.0048 (5)	−0.0024 (6)
O5	0.0201 (7)	0.0125 (6)	0.0235 (6)	0.0008 (5)	0.0032 (5)	−0.0002 (5)
O6	0.0156 (7)	0.0189 (7)	0.0269 (7)	−0.0026 (5)	−0.0074 (5)	0.0078 (6)
O7	0.0166 (7)	0.0231 (7)	0.0215 (7)	−0.0040 (5)	−0.0021 (5)	0.0075 (6)
C1	0.0497 (14)	0.0266 (11)	0.0333 (11)	0.0023 (10)	0.0212 (11)	0.0017 (10)
C2	0.0286 (11)	0.0278 (11)	0.0367 (12)	0.0026 (9)	0.0108 (9)	0.0021 (9)
C3	0.0328 (11)	0.0206 (9)	0.0228 (9)	−0.0024 (8)	0.0034 (8)	−0.0011 (8)
C4	0.0491 (14)	0.0349 (12)	0.0226 (10)	−0.0168 (11)	−0.0002 (10)	0.0031 (9)
C5	0.0252 (10)	0.0218 (10)	0.0230 (9)	−0.0005 (8)	−0.0004 (8)	0.0032 (8)
C6	0.0207 (9)	0.0225 (9)	0.0201 (9)	0.0036 (8)	0.0003 (7)	0.0040 (8)
C7	0.0158 (8)	0.0138 (8)	0.0203 (9)	0.0023 (7)	0.0013 (7)	0.0014 (7)
C8	0.0217 (10)	0.0164 (9)	0.0236 (9)	0.0006 (7)	0.0052 (7)	0.0008 (8)
C9	0.0217 (9)	0.0128 (8)	0.0251 (9)	−0.0005 (7)	0.0041 (7)	0.0036 (7)
C10	0.0204 (9)	0.0145 (9)	0.0264 (9)	−0.0059 (7)	0.0021 (7)	0.0016 (8)

C11	0.0131 (8)	0.0139 (8)	0.0215 (8)	−0.0008 (7)	0.0009 (7)	0.0002 (7)
C12	0.0118 (8)	0.0106 (8)	0.0224 (9)	−0.0008 (6)	−0.0001 (6)	0.0006 (7)
C13	0.0136 (8)	0.0121 (8)	0.0173 (8)	0.0011 (6)	0.0012 (7)	0.0003 (7)
C14	0.0157 (8)	0.0158 (8)	0.0209 (8)	−0.0014 (7)	−0.0025 (7)	−0.0001 (7)
C15	0.0146 (8)	0.0200 (9)	0.0221 (9)	−0.0051 (7)	−0.0022 (7)	0.0037 (7)
C16	0.0138 (8)	0.0139 (8)	0.0215 (8)	−0.0004 (7)	−0.0002 (7)	0.0026 (7)
C17	0.0127 (8)	0.0135 (8)	0.0193 (8)	−0.0004 (6)	−0.0017 (6)	0.0028 (7)
C18	0.0184 (9)	0.0157 (9)	0.0232 (9)	−0.0001 (7)	0.0024 (7)	0.0011 (7)
C19	0.0370 (12)	0.0232 (10)	0.0298 (11)	−0.0060 (9)	0.0070 (9)	0.0068 (9)
O1W	0.0153 (7)	0.0178 (7)	0.0253 (7)	−0.0043 (6)	−0.0015 (5)	0.0027 (5)

Geometric parameters (Å, °)

O1—C1	1.359 (4)	C9—C10	1.529 (3)
O1—C4	1.366 (3)	C9—C19	1.530 (3)
O2—C8	1.351 (3)	C9—H9A	1.0000
O2—C5	1.459 (3)	C10—C11	1.505 (3)
O3—C8	1.200 (3)	C10—H10A	0.9500
O4—C11	1.430 (2)	C11—C12	1.522 (2)
O4—H1O4	0.83 (4)	C12—C13	1.538 (2)
O5—C11	1.426 (2)	C12—C17	1.538 (2)
O5—C18	1.452 (2)	C12—H12A	1.0000
O6—C17	1.442 (2)	C13—C14	1.530 (2)

O6—H1O6	0.91 (4)	C13—H13A	1.0000
O7—C16	1.433 (2)	C14—C15	1.529 (3)
O7—H1O7	0.76 (3)	C14—H14A	0.9900
C1—C2	1.340 (4)	C14—H14B	0.9900
C1—H1A	0.9500	C15—C16	1.518 (2)
C2—C3	1.436 (3)	C15—H15A	0.9900
C2—H2A	0.9500	C15—H15B	0.9900
C3—C4	1.345 (3)	C16—C17	1.526 (2)
C3—C5	1.489 (3)	C16—H16A	1.0000
C4—H4A	0.9500	C17—C18	1.542 (2)
C5—C6	1.532 (3)	C18—H18A	0.9900
C5—H5A	1.0000	C18—H18B	0.9900
C6—C7	1.543 (3)	C19—H19A	0.9800
C6—H6A	0.9900	C19—H19B	0.9800
C6—H6B	0.9900	C19—H19C	0.9800
C7—C8	1.521 (3)	O1W—H2OW	0.85 (3)
C7—C13	1.552 (2)	O1W—H1OW	0.82 (4)
C7—C9	1.553 (3)		
C1—O1—C4	105.96 (19)	O4—C11—C12	108.81 (14)
C8—O2—C5	112.45 (15)	C10—C11—C12	114.71 (15)
C11—O4—H1O4	104 (2)	C11—C12—C13	109.30 (14)
C11—O5—C18	108.00 (13)	C11—C12—C17	100.64 (14)

C17—O6—H1O6	100 (2)	C13—C12—C17	110.49 (14)
C16—O7—H1O7	109 (2)	C11—C12—H12A	112.0
C2—C1—O1	111.0 (2)	C13—C12—H12A	112.0
C2—C1—H1A	124.5	C17—C12—H12A	112.0
O1—C1—H1A	124.5	C14—C13—C12	109.37 (14)
C1—C2—C3	106.3 (2)	C14—C13—C7	117.19 (15)
C1—C2—H2A	126.8	C12—C13—C7	111.78 (14)
C3—C2—H2A	126.8	C14—C13—H13A	105.9
C4—C3—C2	105.66 (19)	C12—C13—H13A	105.9
C4—C3—C5	127.5 (2)	C7—C13—H13A	105.9
C2—C3—C5	126.8 (2)	C15—C14—C13	108.59 (15)
C3—C4—O1	111.0 (2)	C15—C14—H14A	110.0
C3—C4—H4A	124.5	C13—C14—H14A	110.0
O1—C4—H4A	124.5	C15—C14—H14B	110.0
O2—C5—C3	106.72 (17)	C13—C14—H14B	110.0
O2—C5—C6	105.24 (15)	H14A—C14—H14B	108.4
C3—C5—C6	115.94 (17)	C16—C15—C14	111.14 (15)
O2—C5—H5A	109.6	C16—C15—H15A	109.4
C3—C5—H5A	109.6	C14—C15—H15A	109.4
C6—C5—H5A	109.6	C16—C15—H15B	109.4
C5—C6—C7	105.98 (16)	C14—C15—H15B	109.4
C5—C6—H6A	110.5	H15A—C15—H15B	108.0

C7—C6—H6A	110.5	O7—C16—C15	108.19 (14)
C5—C6—H6B	110.5	O7—C16—C17	109.98 (15)
C7—C6—H6B	110.5	C15—C16—C17	114.06 (15)
H6A—C6—H6B	108.7	O7—C16—H16A	108.2
C8—C7—C6	102.64 (15)	C15—C16—H16A	108.2
C8—C7—C13	109.30 (15)	C17—C16—H16A	108.2
C6—C7—C13	111.85 (15)	O6—C17—C16	103.93 (14)
C8—C7—C9	112.99 (16)	O6—C17—C12	110.81 (14)
C6—C7—C9	111.73 (15)	C16—C17—C12	114.18 (15)
C13—C7—C9	108.29 (14)	O6—C17—C18	110.59 (14)
O3—C8—O2	120.09 (18)	C16—C17—C18	116.41 (15)
O3—C8—C7	129.05 (19)	C12—C17—C18	101.11 (14)
O2—C8—C7	110.84 (17)	O5—C18—C17	106.76 (14)
C10—C9—C19	108.27 (16)	O5—C18—H18A	110.4
C10—C9—C7	113.12 (15)	C17—C18—H18A	110.4
C19—C9—C7	113.38 (16)	O5—C18—H18B	110.4
C10—C9—H9A	107.2	C17—C18—H18B	110.4
C19—C9—H9A	107.2	H18A—C18—H18B	108.6
C7—C9—H9A	107.2	C9—C19—H19A	109.5
C11—C10—C9	116.07 (15)	C9—C19—H19B	109.5
C11—C10—H10A	122.0	H19A—C19—H19B	109.5
C9—C10—H10A	122.0	C9—C19—H19C	109.5

O5—C11—O4	109.44 (15)	H19A—C19—H19C	109.5
O5—C11—C10	111.42 (15)	H19B—C19—H19C	109.5
O4—C11—C10	109.42 (15)	H2OW—O1W—H1OW	107 (3)
O5—C11—C12	102.78 (14)		
C4—O1—C1—C2	−0.7 (3)	C9—C10—C11—C12	43.7 (2)
O1—C1—C2—C3	0.3 (3)	O5—C11—C12—C13	70.74 (17)
C1—C2—C3—C4	0.1 (3)	O4—C11—C12—C13	−173.29 (14)
C1—C2—C3—C5	−179.1 (2)	C10—C11—C12—C13	−50.37 (19)
C2—C3—C4—O1	−0.5 (3)	O5—C11—C12—C17	−45.57 (16)
C5—C3—C4—O1	178.7 (2)	O4—C11—C12—C17	70.40 (16)
C1—O1—C4—C3	0.7 (3)	C10—C11—C12—C17	−166.67 (15)
C8—O2—C5—C3	128.65 (18)	C11—C12—C13—C14	−168.31 (14)
C8—O2—C5—C6	4.9 (2)	C17—C12—C13—C14	−58.46 (18)
C4—C3—C5—O2	138.4 (2)	C11—C12—C13—C7	60.22 (19)
C2—C3—C5—O2	−42.5 (3)	C17—C12—C13—C7	170.08 (15)
C4—C3—C5—C6	−104.7 (3)	C8—C7—C13—C14	−64.6 (2)
C2—C3—C5—C6	74.3 (3)	C6—C7—C13—C14	48.4 (2)
O2—C5—C6—C7	−13.7 (2)	C9—C7—C13—C14	171.95 (15)
C3—C5—C6—C7	−131.34 (18)	C8—C7—C13—C12	62.79 (19)
C5—C6—C7—C8	16.61 (19)	C6—C7—C13—C12	175.76 (14)
C5—C6—C7—C13	−100.44 (17)	C9—C7—C13—C12	−60.69 (19)
C5—C6—C7—C9	137.97 (16)	C12—C13—C14—C15	64.81 (18)

C5—O2—C8—O3	−175.15 (18)	C7—C13—C14—C15	−166.67 (15)
C5—O2—C8—C7	6.3 (2)	C13—C14—C15—C16	−60.0 (2)
C6—C7—C8—O3	167.1 (2)	C14—C15—C16—O7	172.62 (15)
C13—C7—C8—O3	−74.0 (3)	C14—C15—C16—C17	49.9 (2)
C9—C7—C8—O3	46.6 (3)	O7—C16—C17—O6	73.17 (17)
C6—C7—C8—O2	−14.4 (2)	C15—C16—C17—O6	−165.09 (15)
C13—C7—C8—O2	104.42 (17)	O7—C16—C17—C12	−165.99 (14)
C9—C7—C8—O2	−134.93 (16)	C15—C16—C17—C12	−44.3 (2)
C8—C7—C9—C10	−70.2 (2)	O7—C16—C17—C18	−48.7 (2)
C6—C7—C9—C10	174.67 (15)	C15—C16—C17—C18	73.1 (2)
C13—C7—C9—C10	51.0 (2)	C11—C12—C17—O6	−79.62 (16)
C8—C7—C9—C19	53.6 (2)	C13—C12—C17—O6	164.97 (14)
C6—C7—C9—C19	−61.6 (2)	C11—C12—C17—C16	163.45 (14)
C13—C7—C9—C19	174.82 (17)	C13—C12—C17—C16	48.03 (19)
C19—C9—C10—C11	−170.55 (17)	C11—C12—C17—C18	37.65 (15)
C7—C9—C10—C11	−44.0 (2)	C13—C12—C17—C18	−77.77 (16)
C18—O5—C11—O4	−80.17 (17)	C11—O5—C18—C17	−10.70 (19)
C18—O5—C11—C10	158.68 (15)	O6—C17—C18—O5	99.55 (17)
C18—O5—C11—C12	35.35 (17)	C16—C17—C18—O5	−142.18 (15)
C9—C10—C11—O5	−72.6 (2)	C12—C17—C18—O5	−17.87 (17)
C9—C10—C11—O4	166.27 (15)		

All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between

e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Compound **6**

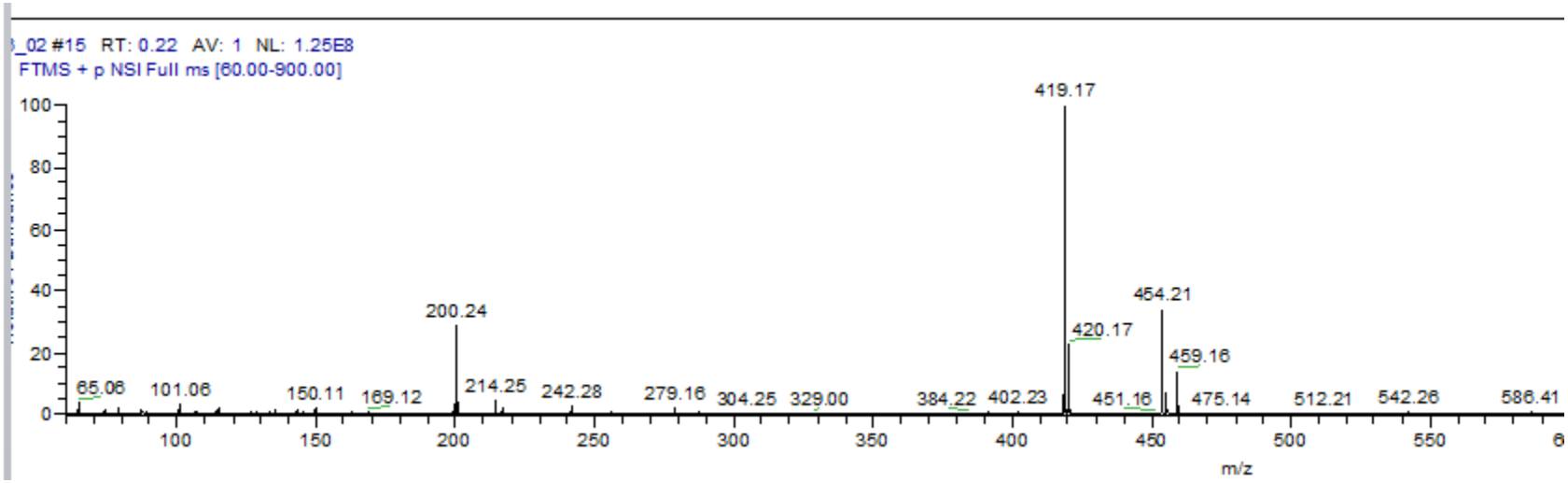


Fig S36: HRESIMS spectrum of compound **6**

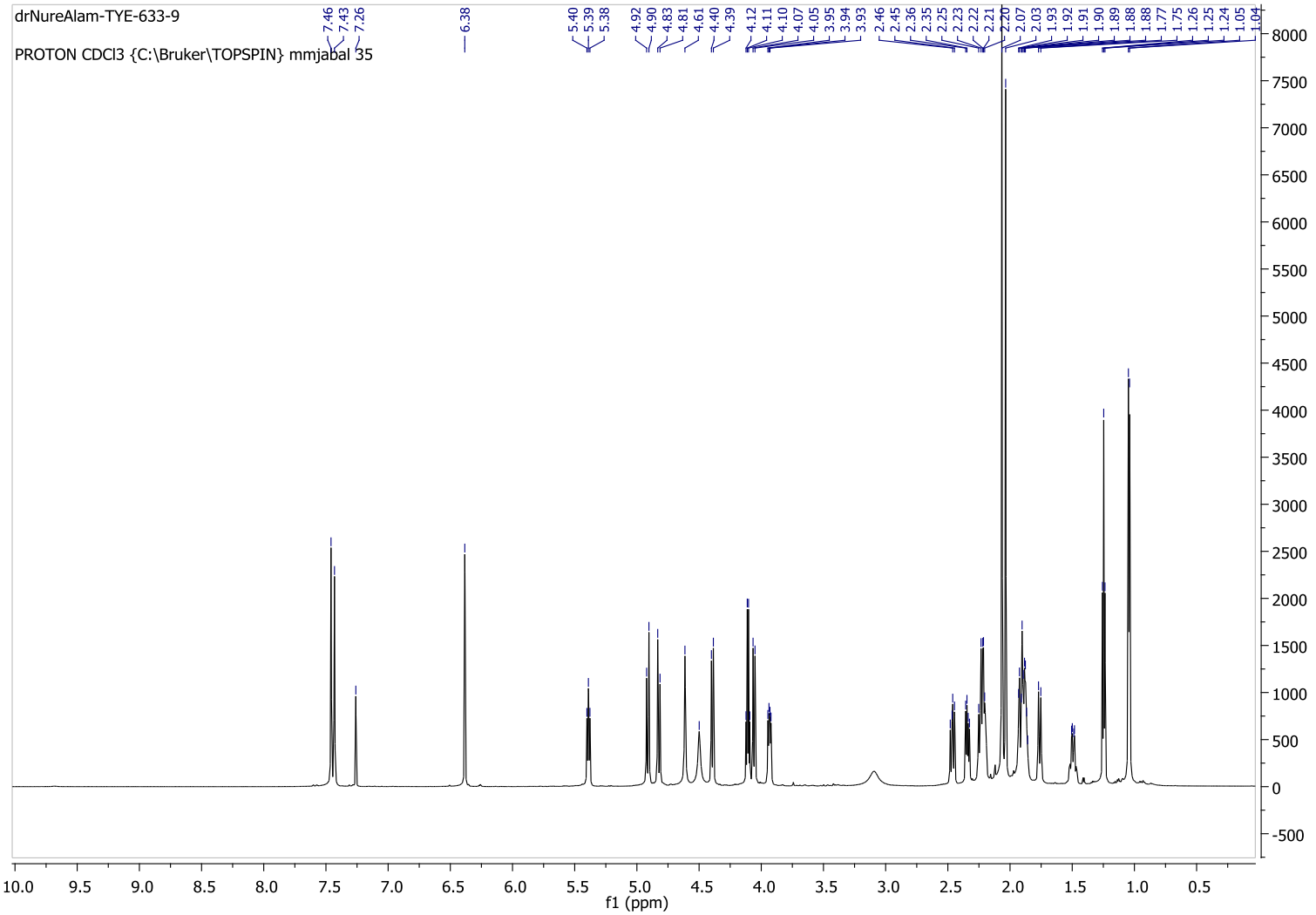


Fig S37: ^{1}H-NMR spectrum of compound **6**, having EtOAc trace with solvent $CDCl_3$

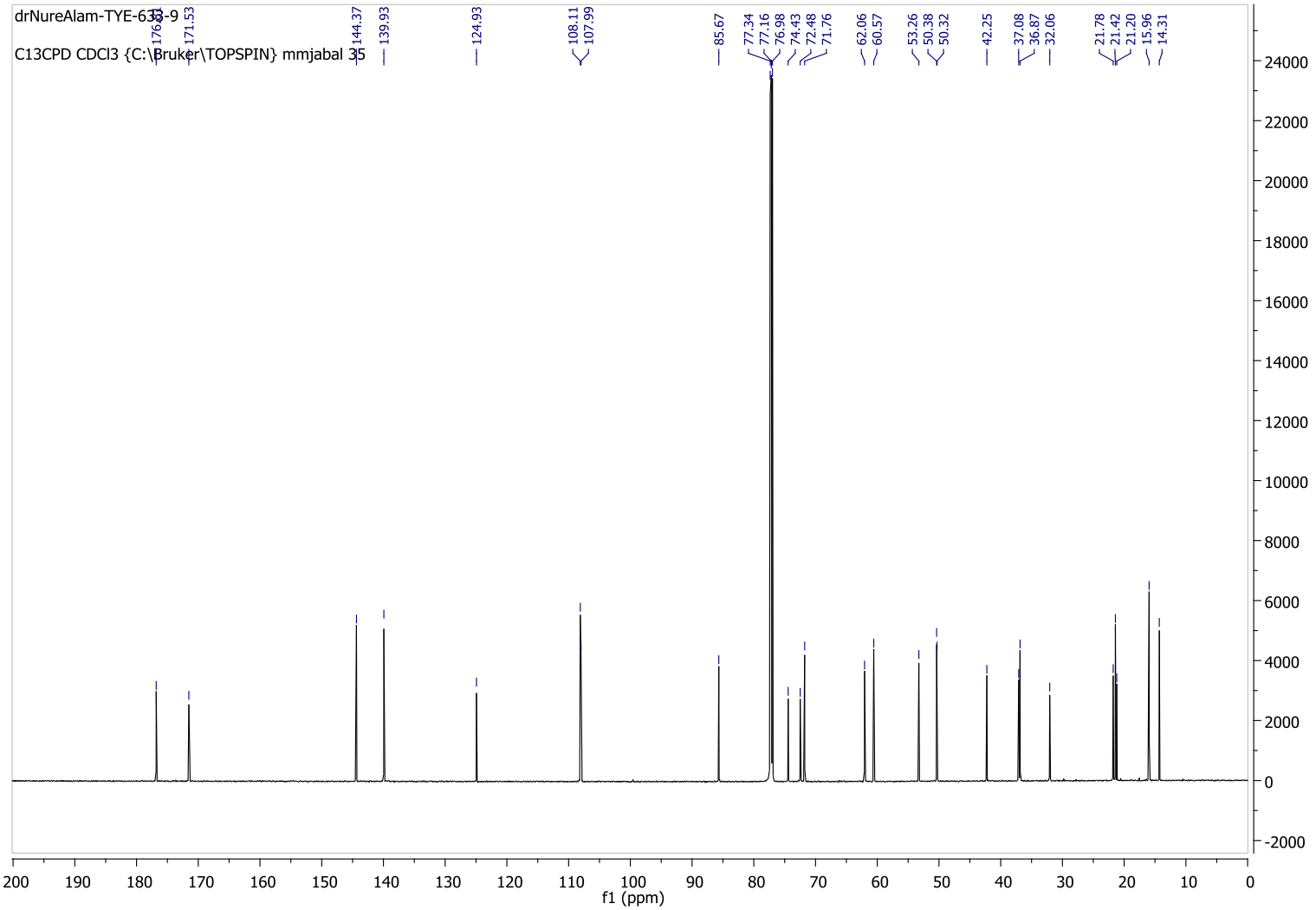


Fig S38: ^{13}C-NMR spectrum of compound **6**

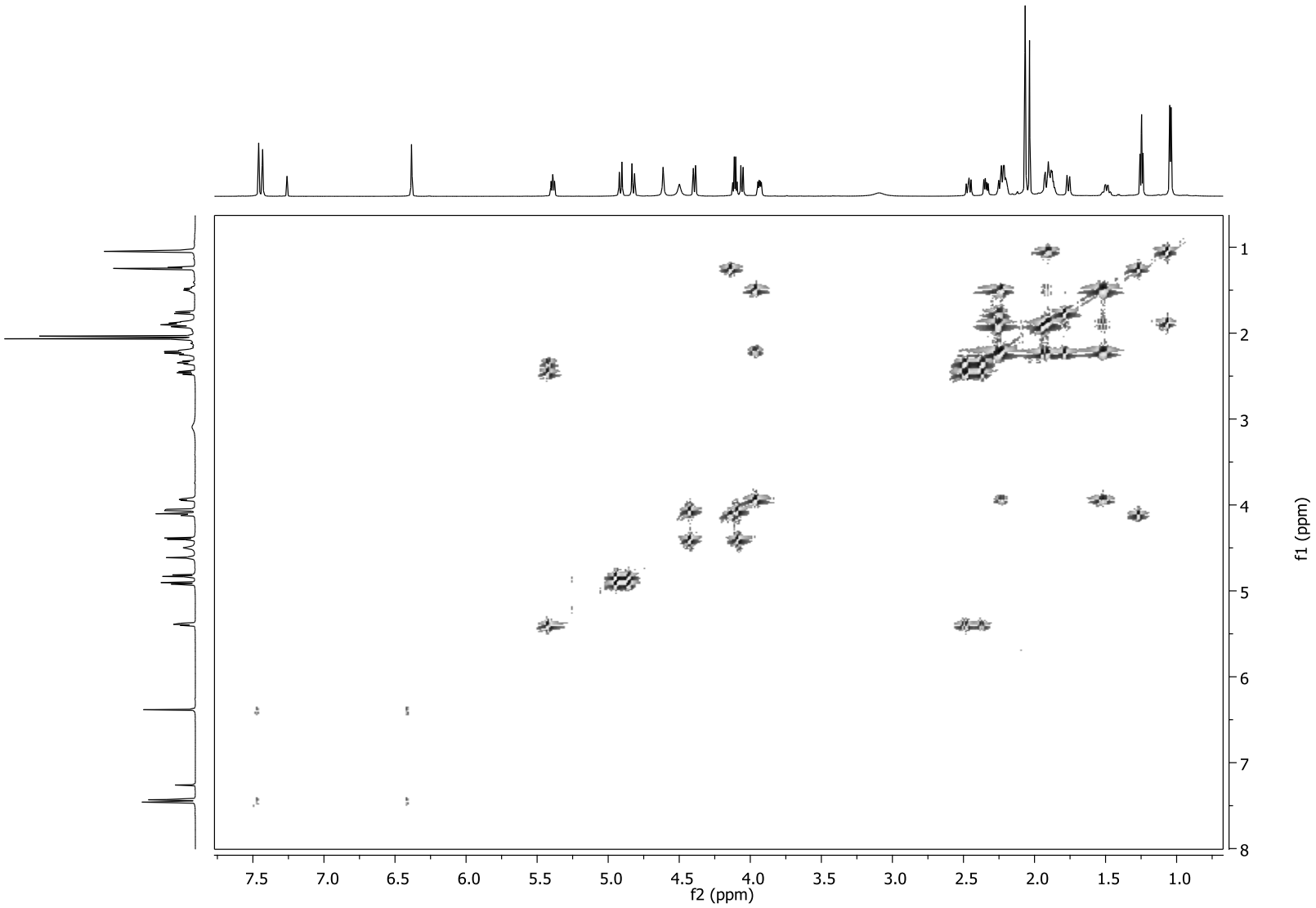


Fig S39: COSY spectrum of compound **6**

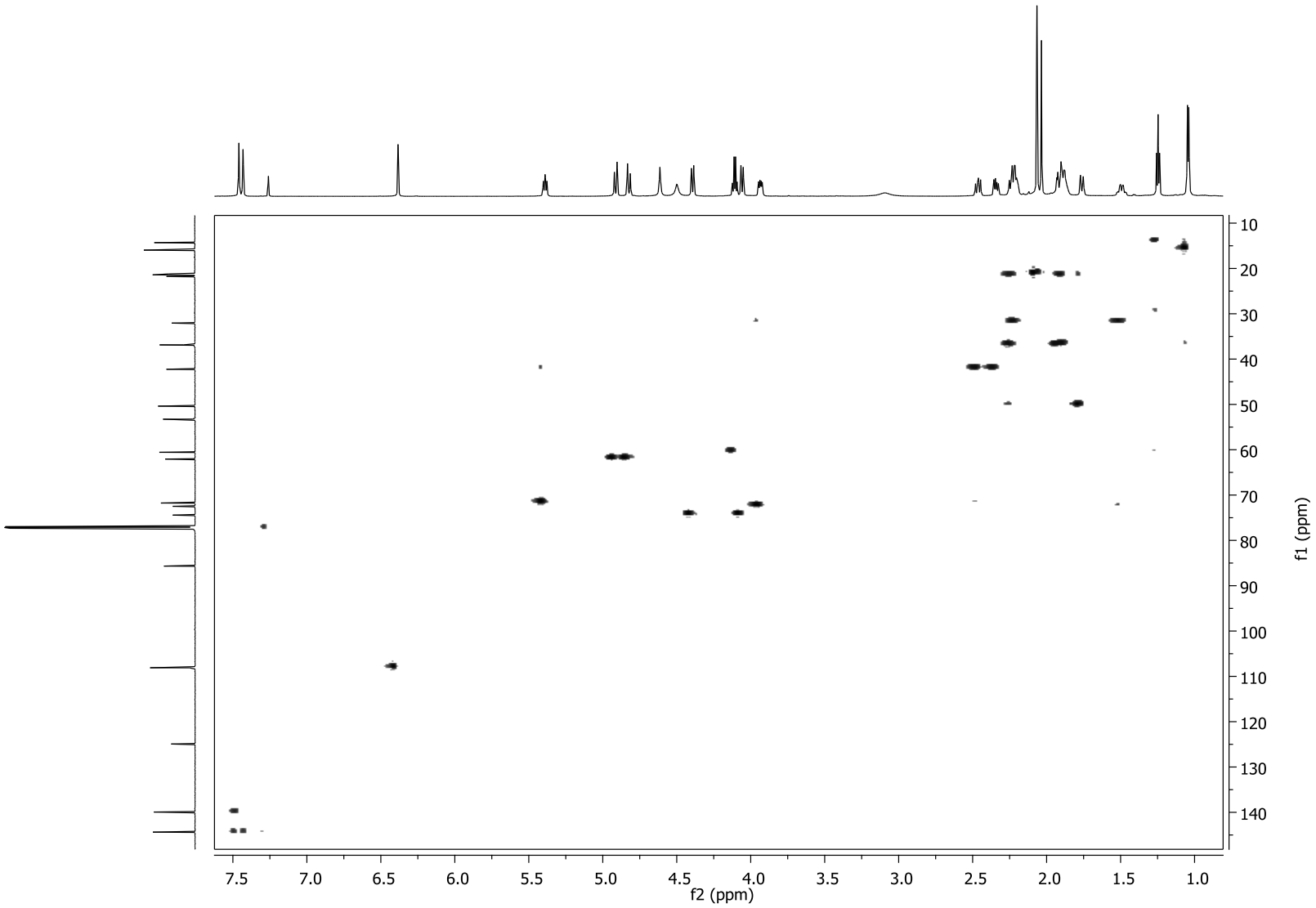


Fig S40: HSQC spectrum of compound **6**

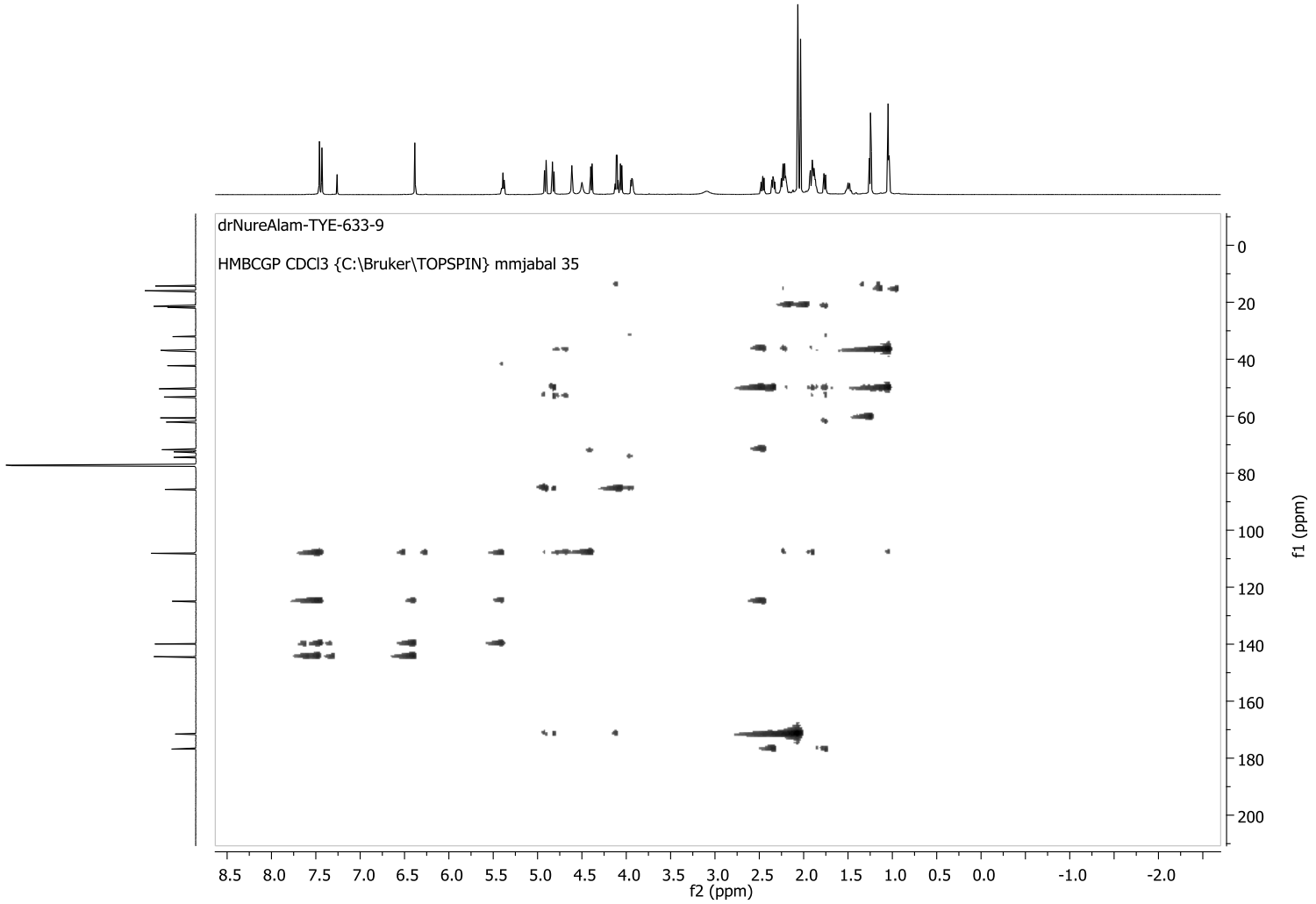


Fig S41: HMBC spectrum of compound **6**

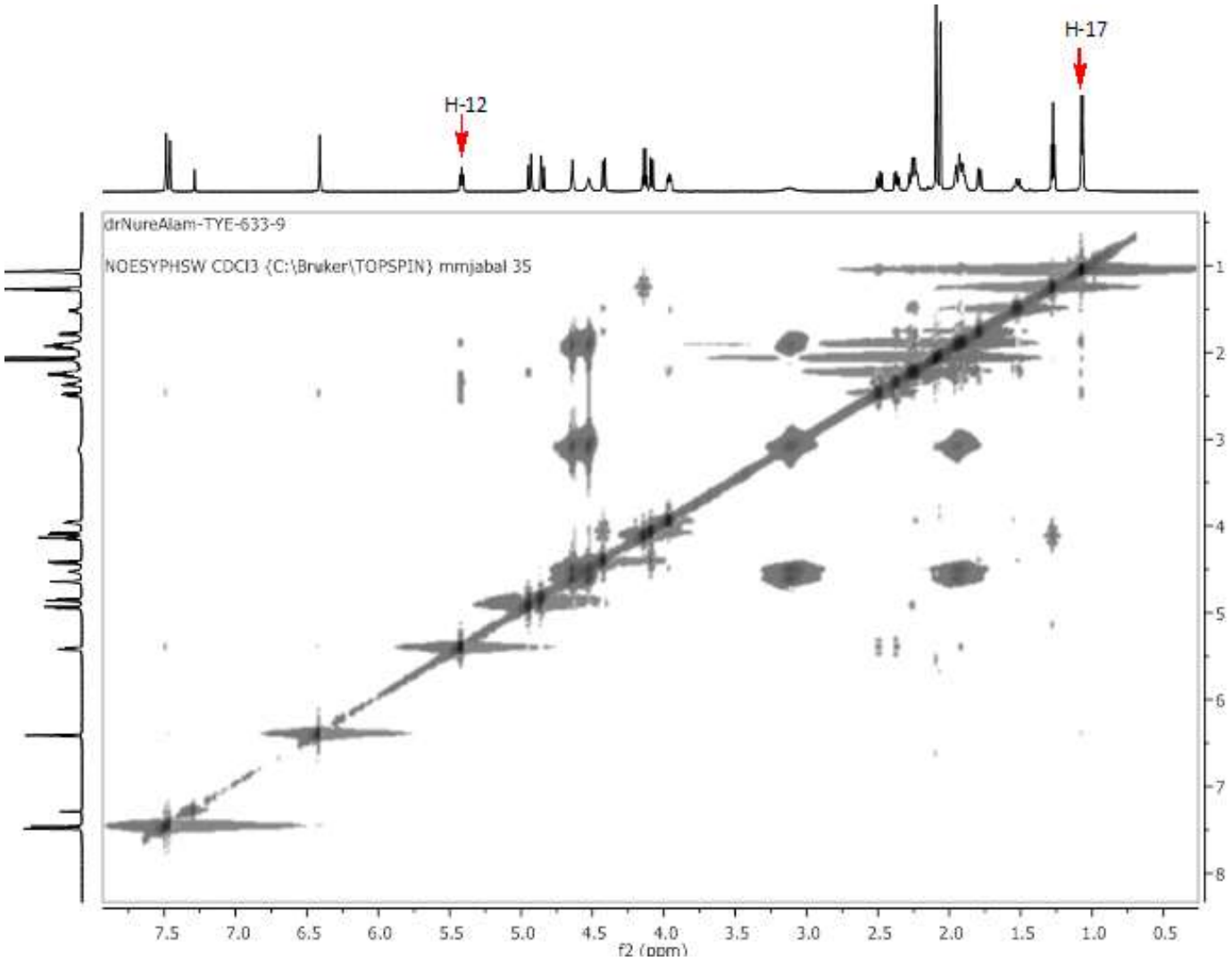


Fig S42: NOESY spectrum of compound **6,** which showed no correlation between H-12 and H-17

Compound **7**

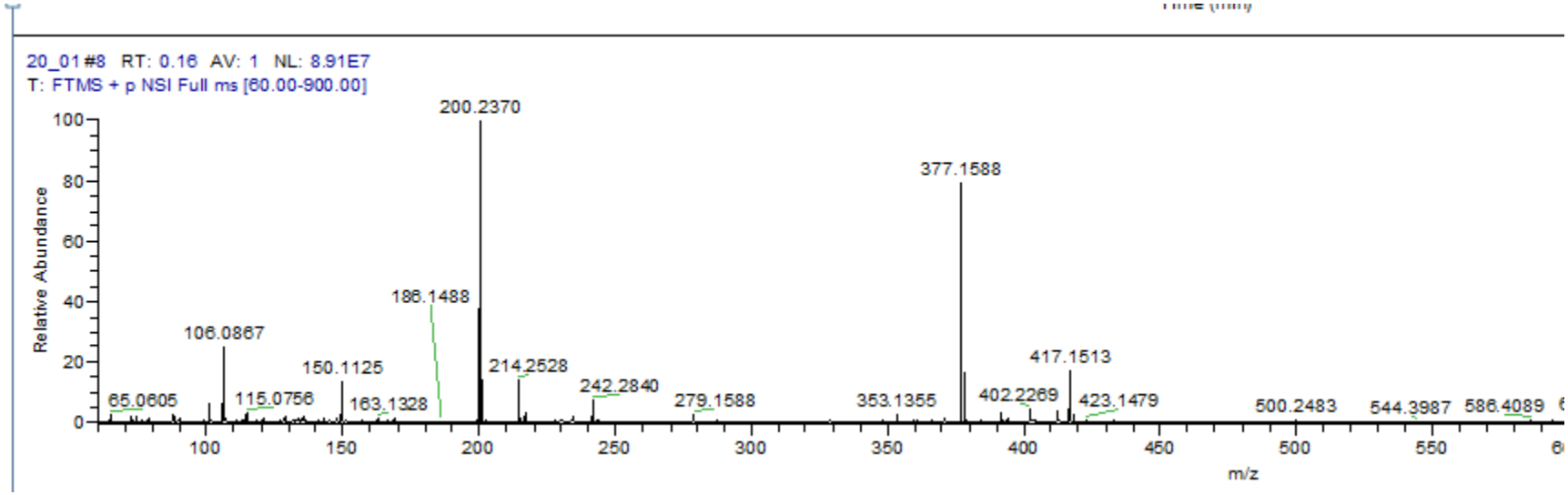


Fig S43: HRESIMS spectrum of compound **7**

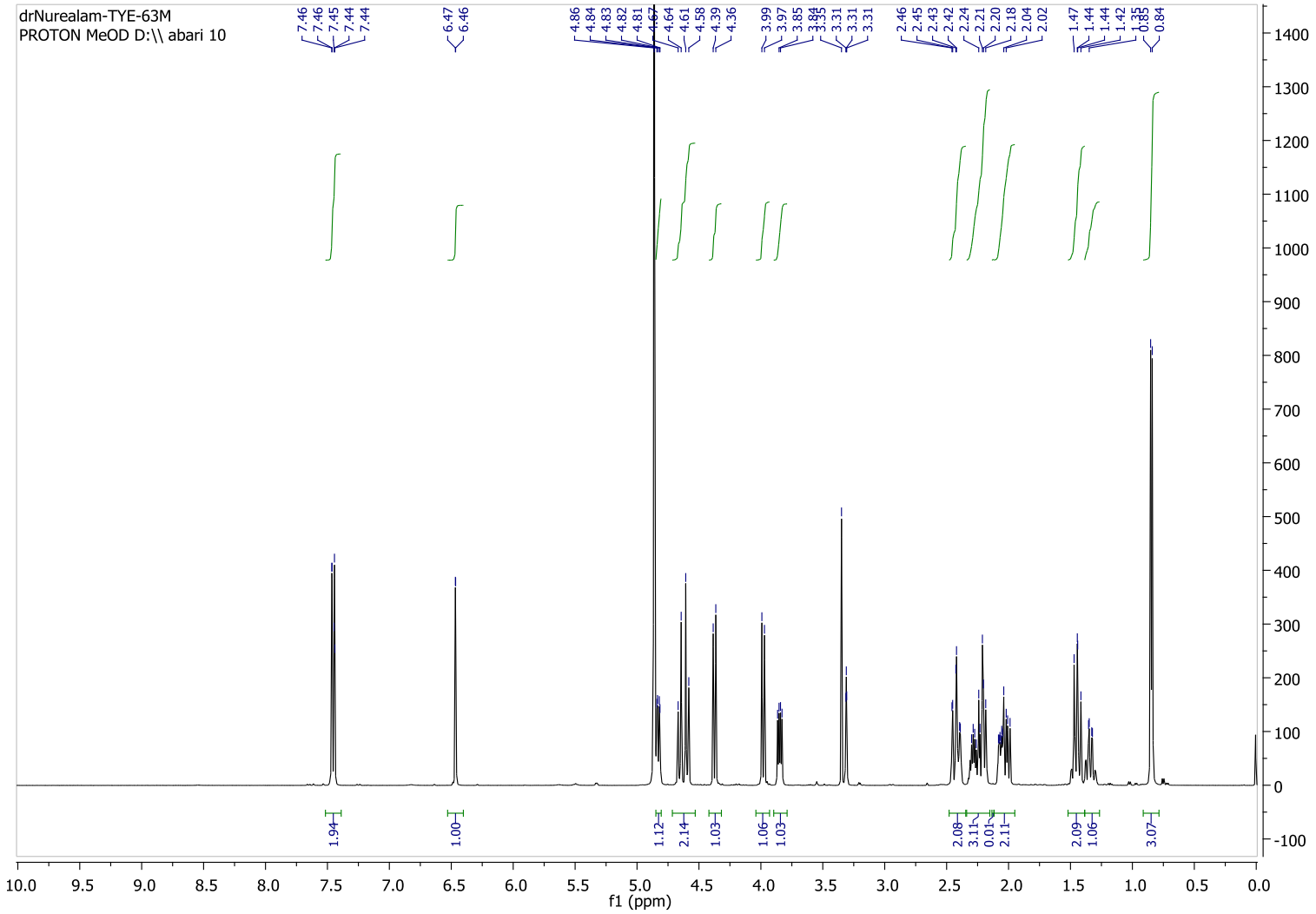


Fig S44: ^{1}H-NMR spectrum of compound **7**

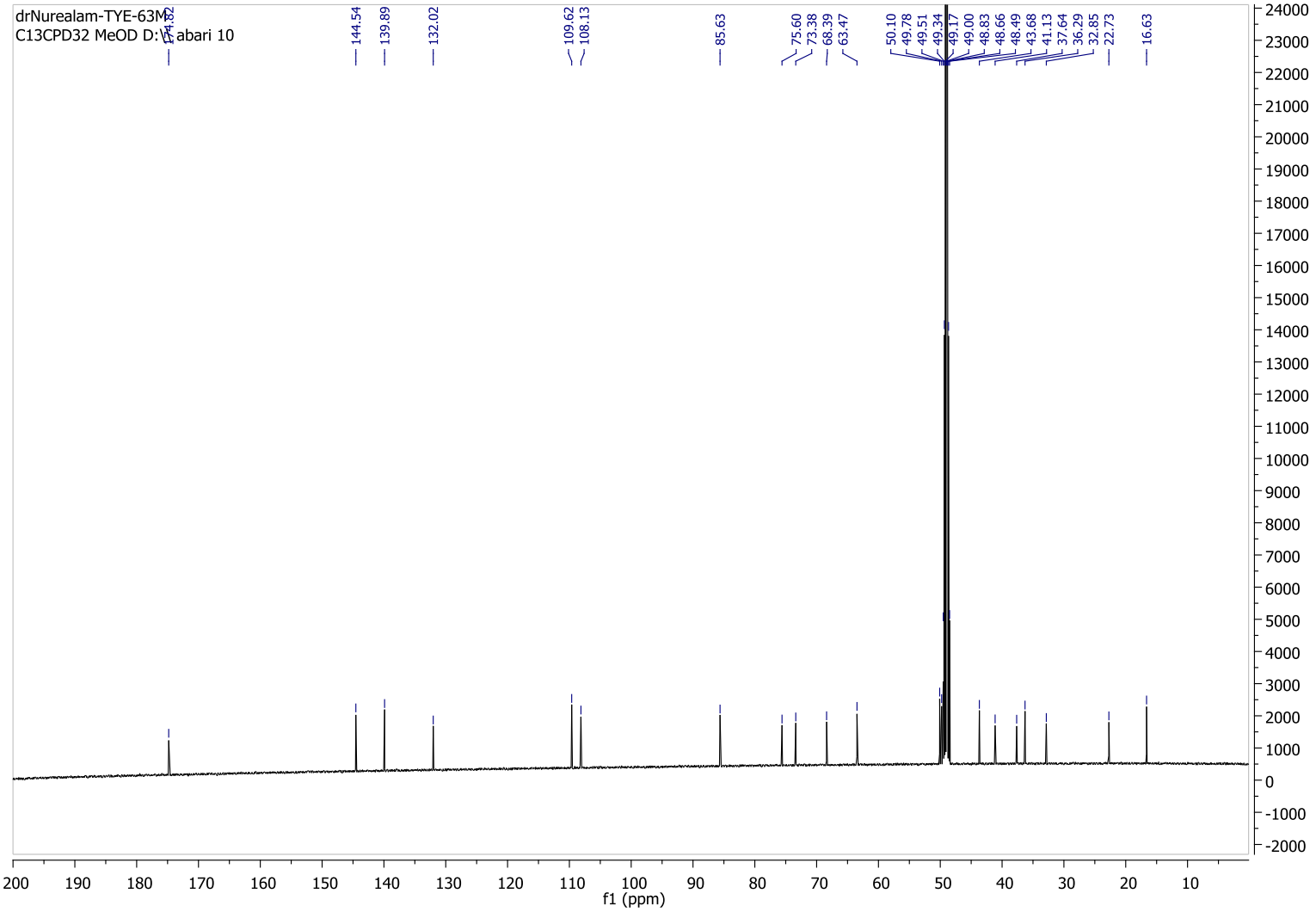


Fig S45: ^{13}C-NMR spectrum of compound **7**

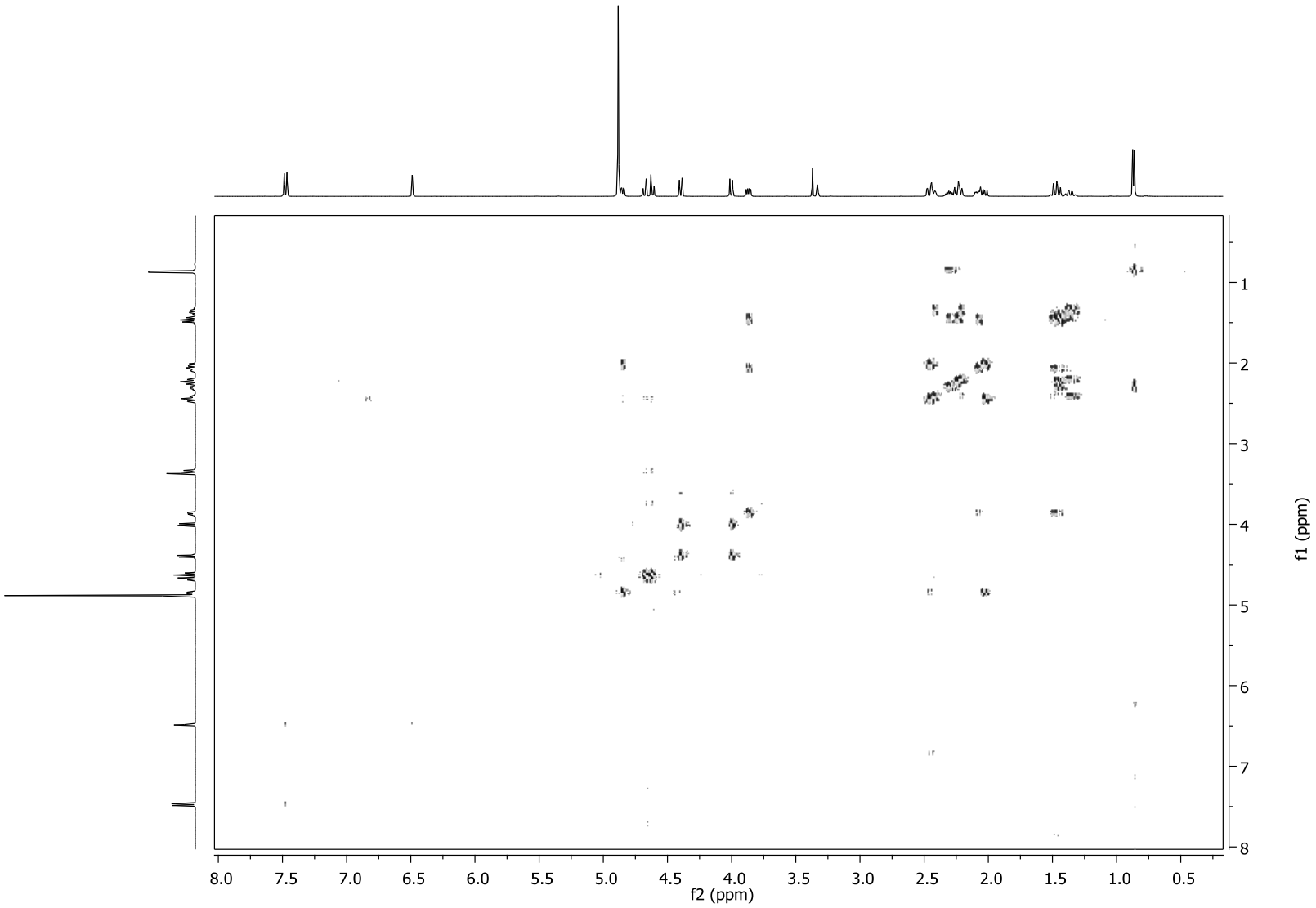


Fig S46: COSY spectrum of compound **7**

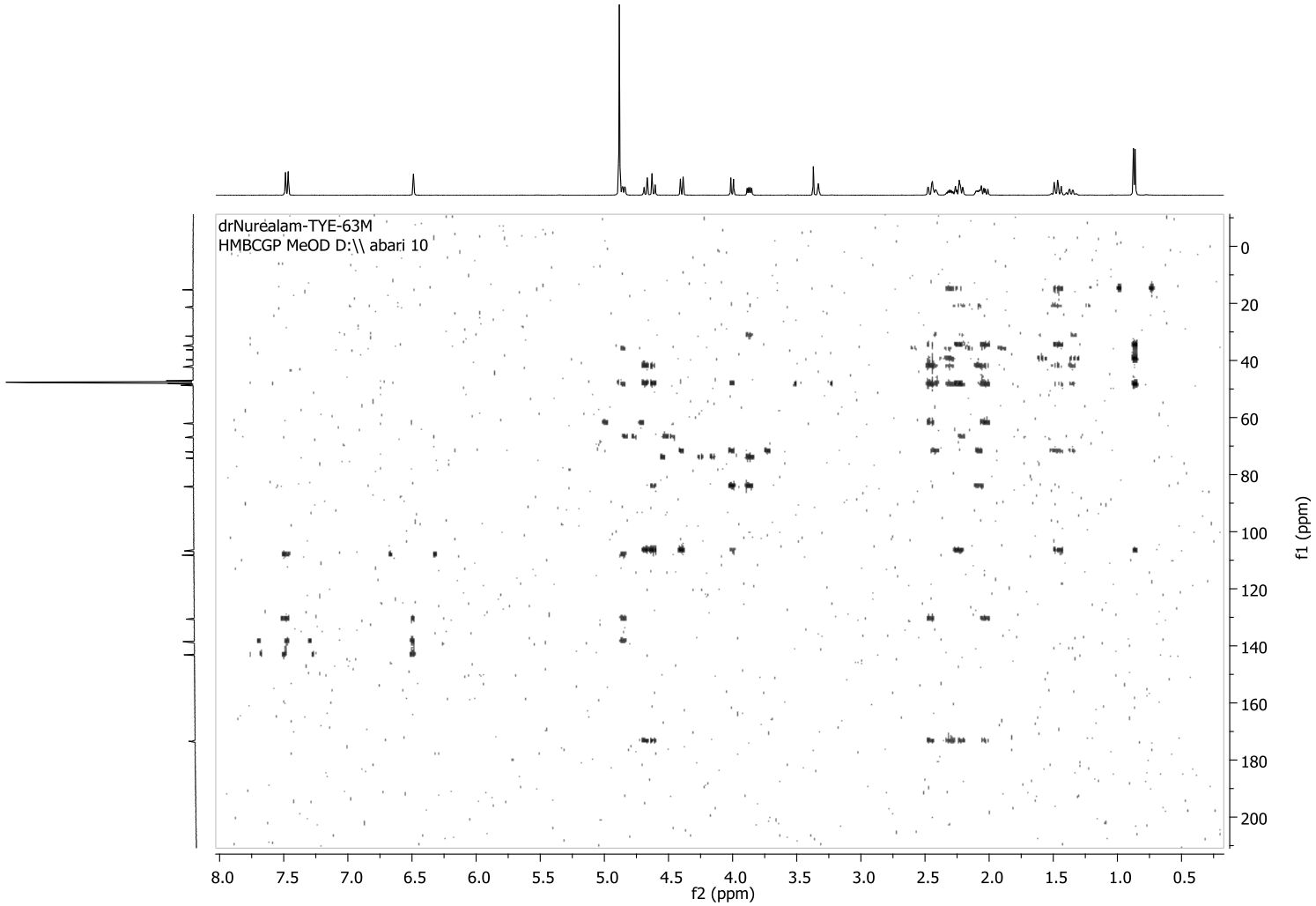


Fig S47: HMBCspectrum of compound **7**

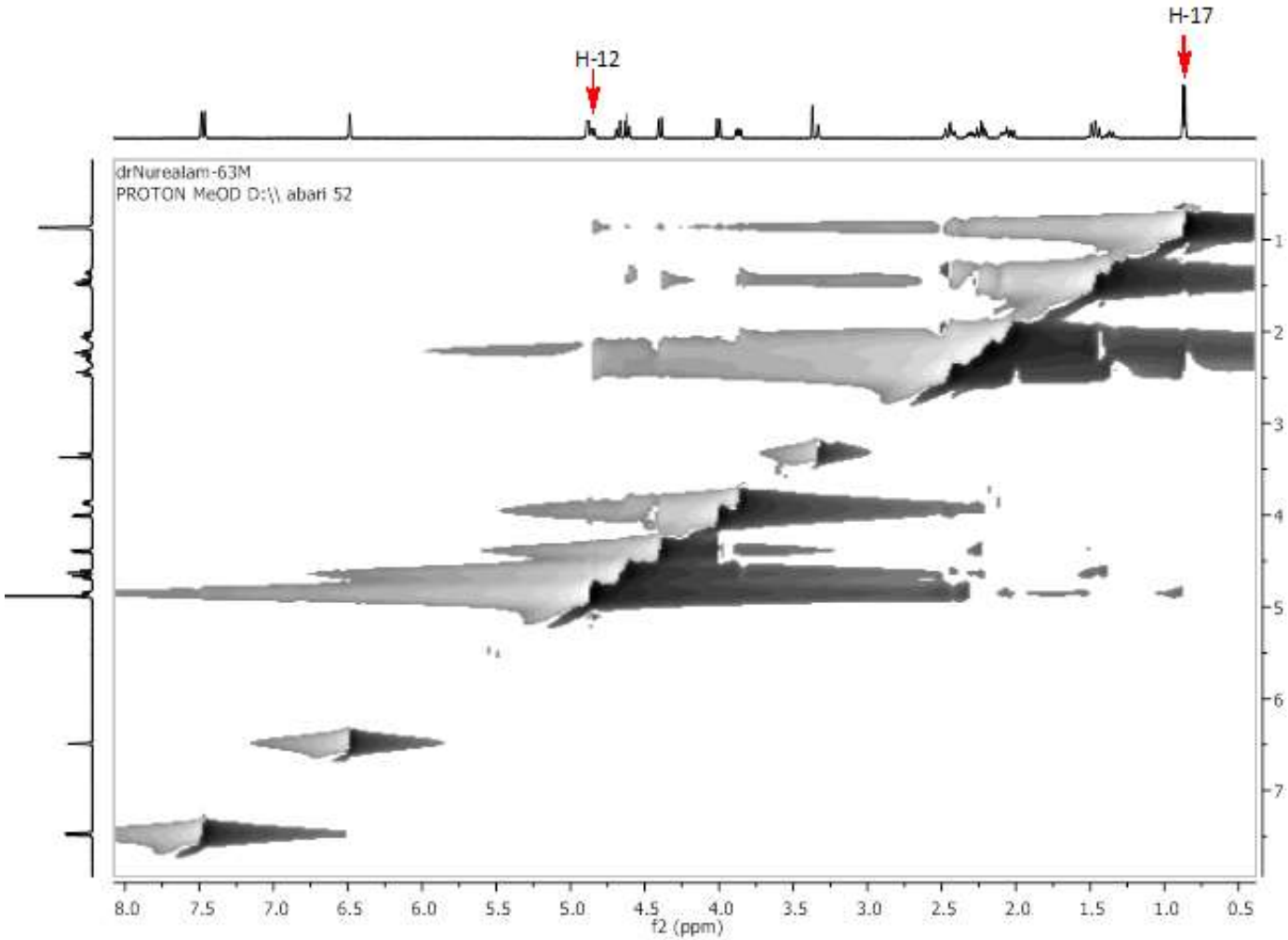


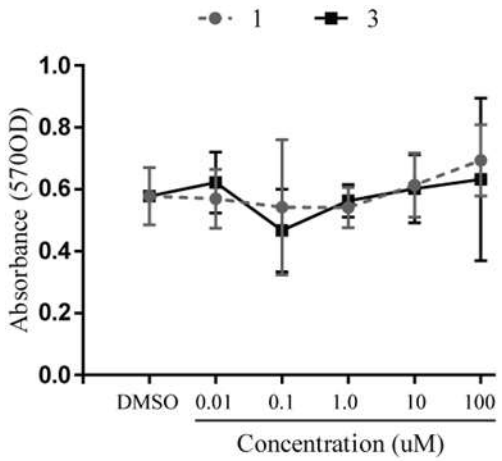
Fig S48: NOESY spectrum of compound **7,** which showed correlation between H-12 and H-17

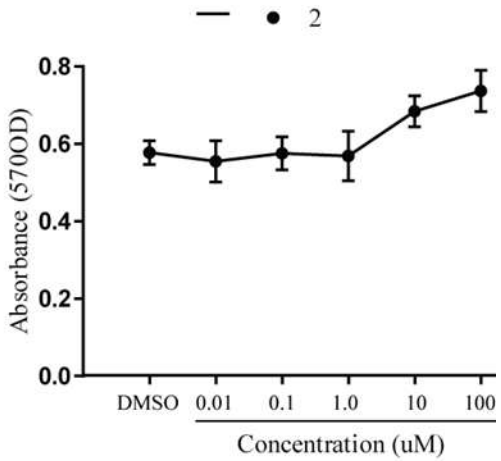
		E. coli		*S. aureus*		*P. aeruginosa*		*M. smegmatis*		*C. albicans*	
mpound	Concentration (mg mL^{-1})	% Growth	Standard error bars (triplicate) (+/-)	% Growth	Standard error bars (triplicate) (+/-)	% Growth	Standard error bars (triplicate) (+/-)	% Growth	Standard error bars (triplicate) (+/-)	% Growth	Standard error bars (triplicate) (+/-)
1	0.5	234.280	52.083	96.025	13.345	90.797	2.550	103.870	1.306	110.717	1.517
	0.25	272.940	28.948	71.568	6.647	95.271	3.362	89.977	7.639	119.210	5.823
	0.125	226.470	72.725	70.296	9.649	96.675	1.098	99.267	2.083	109.057	1.779
	0.0625	154.400	28.655	69.446	8.976	89.273	1.831	97.130	3.689	116.762	5.334
	0.03125	130.430	4.321	68.972	8.941	90.660	1.780	98.184	2.244	117.486	3.216
2	0.5	92.100	24.983	40.917	2.390	74.347	5.390	90.621	8.106	84.481	2.036
	0.25	107.990	23.578	49.415	2.019	88.977	0.984	101.870	6.337	111.953	8.286
	0.125	128.060	8.945	57.058	15.256	89.049	2.924	106.900	3.285	115.025	4.467
	0.0625	121.080	32.183	56.331	14.682	89.402	2.394	107.130	3.535	116.243	8.749
	0.03125	92.142	16.094	59.216	4.496	93.458	2.348	103.610	3.933	116.667	3.661
3	0.5	199.590	34.561	79.780	11.466	100.110	3.876	118.980	17.980	100.442	4.617
	0.25	237.690	67.271	77.301	9.317	102.160	7.194	87.060	10.445	119.262	8.672
	0.125	273.360	52.998	93.506	19.333	97.696	8.024	83.074	5.869	114.679	3.041
	0.0625	121.580	23.199	80.411	3.794	96.075	7.937	87.561	10.242	115.684	9.989
	0.03125	128.750	36.326	77.468	2.817	88.109	14.300	91.621	8.382	112.917	10.017
4	0.5	84.636	9.363	94.728	1.803	84.426	5.241	108.830	1.096	97.662	3.789
	0.25	100.290	7.009	95.343	3.049	92.757	4.096	101.230	7.325	97.579	3.270
	0.125	87.092	1.286	102.210	2.760	92.766	9.767	107.000	2.025	96.919	5.838
	0.0625	107.260	11.199	98.304	3.250	95.225	4.244	105.837	1.205	96.281	1.119
	0.03125	90.022	3.495	106.090	6.161	69.054	8.332	105.719	3.178	98.393	2.303
5	0.5	117.716	7.131	97.971	5.713	97.373	13.605	102.873	6.930	99.894	6.911
	0.25	96.082	17.325	90.816	5.450	102.246	9.960	90.682	3.957	98.237	2.693
	0.125	86.504	4.239	98.204	6.768	106.374	8.740	93.509	2.205	98.924	0.840
	0.0625	112.581	37.802	102.242	11.054	105.778	5.704	97.462	7.686	98.194	3.691
	0.03125	84.534	7.387	104.543	8.984	104.298	10.714	102.456	5.893	99.757	8.156
6	0.5	89.649	3.270	127.533	11.236	89.439	11.447	133.785	18.951	93.773	3.890
	0.25	95.974	6.352	101.295	5.488	102.588	5.289	102.078	7.883	94.003	5.478
	0.125	93.563	3.650	107.909	15.322	94.653	4.608	99.944	4.476	95.325	3.374

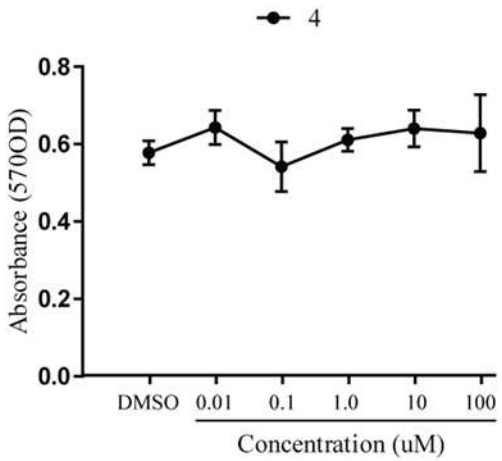
	0.0625	87.964	7.426	104.032	15.073	92.846	4.692	99.934	1.017	95.143	1.897
	0.03125	93.563	16.136	100.038	17.100	99.486	2.567	98.233	2.566	98.953	4.292
7	0.5	87.102	9.319	86.586	5.044	89.983	8.182	98.977	7.733	97.002	2.410
	0.25	93.442	3.505	90.923	6.356	100.343	2.605	95.286	3.365	99.185	2.093
	0.125	85.227	3.168	98.385	11.693	104.082	3.862	100.877	6.586	97.410	2.640
	0.0625	93.539	7.610	94.334	6.850	103.937	3.615	101.134	5.695	96.378	2.682
	0.03125	138.058	32.737	94.008	4.345	101.412	3.087	101.320	5.088	97.179	2.708

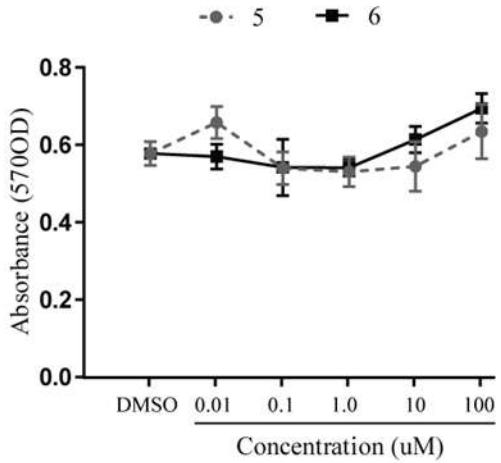
Growth = The percentage growth of a treated bacteria relative to a positive control all values have been baseline corrected based on the initial reading)
Growth = (OD600 value of treated well (24h)/ OD600 value of positive growth control (24h)) x 100

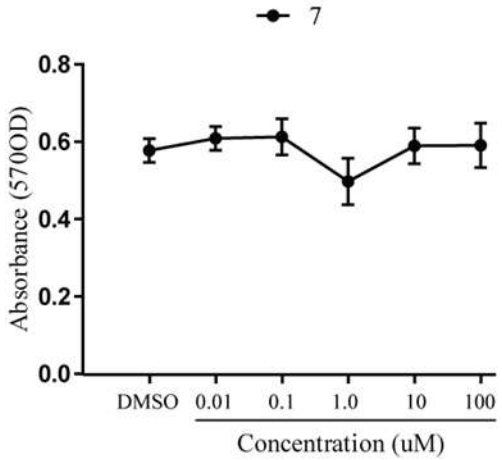
S49. Antimicrobial data of compounds **1**-**7**.


1
3
Absorbance (570OD)
1.0
0.8
0.6
0.4
0.2
0.0
DMSO
0.01
0.1
1.0
10
100
Concentration (uM)


2
Absorbance (570OD)
0.8
0.6
0.4
0.2
0.0
DMSO
0.01
0.1
1.0
10
100
Concentration (uM)


4
Absorbance (570OD)
0.8
0.6
0.4
0.2
0.0
DMSO
0.01
0.1
1.0
10
100
Concentration (uM)


5
6
Absorbance (570OD)
0.8
0.6
0.4
0.2
0.0
DMSO
0.01
0.1
1.0
10
100
Concentration (uM)

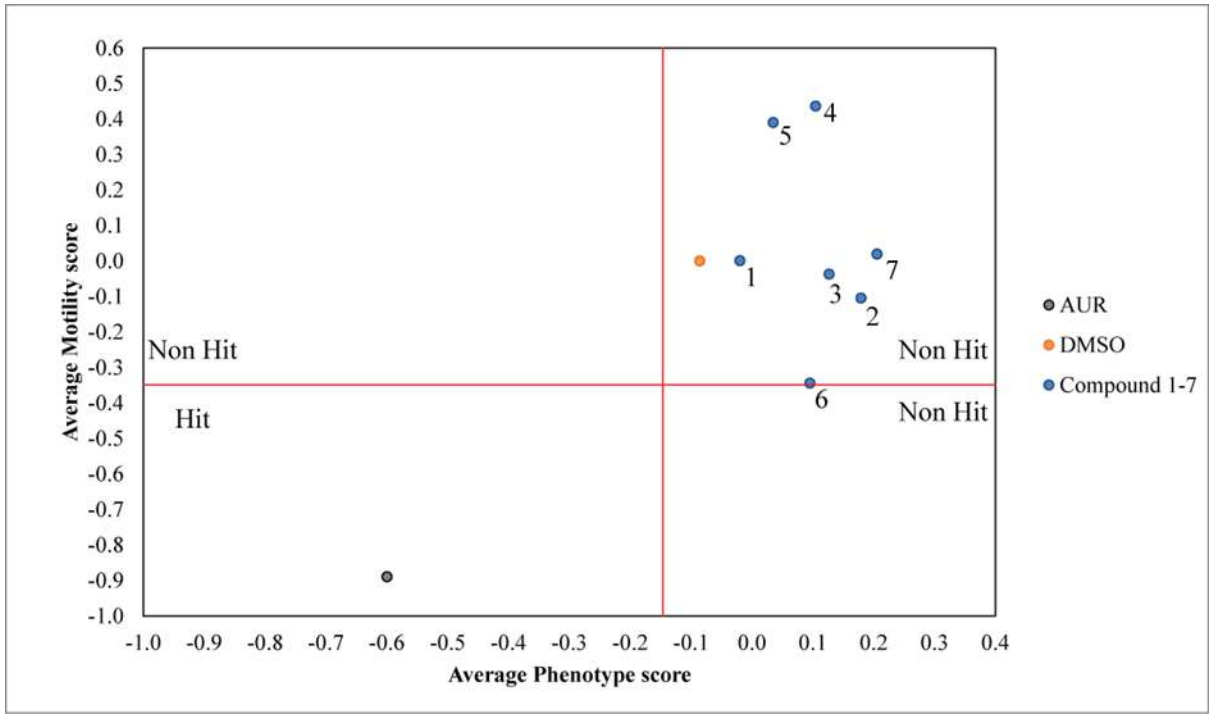

7
Absorbance (570OD)
0.8
0.6
0.4
0.2
0.0
DMSO
0.01
0.1
1.0
10
100
Concentration (uM)

S50. Compounds **1-7** show no cytotoxicity on Human Caucasian Hepatocyte Carcinoma (HepG2) cells**.** Cytotoxicity of compounds (100-0.01 uM) against HepG2 cells was deduced using the MTT assay. Each data point represents an average of three data sets (raw data available in S#), with standard error represented. All absorbance readings recorded were adjusted for background absorbance, (8 blank wells per plate). Three positive (DMSO) and negative control (Triton X-100) wells were included, (1% final concentration) and gave absorbance readings of 0.578 (SE 0.031) and 0.024 (SE 0.004) respectively. Compounds 1 and 3, as well as 5 and 6 are plotted together due to their structural similarities.

Treatment	Technical and Biological repeats												
	Conc (uM)	1a	1b	1c	2a	2b	2c	3a	3b	3c	AVE	SD	SE
1	0.001	0.704	0.597	0.552	0.541	0.586	0.552	0.676	0.611	0.381	0.578	0.093	0.031
	0.01	0.634	0.486	0.517	0.437	0.474	0.568	0.699	0.642	0.670	0.570	0.095	0.032
	0.1	0.340	0.813	0.556	0.532	0.350	0.545	0.196	0.817	0.727	0.542	0.218	0.073
	1	0.594	0.524	0.450	0.472	0.500	0.525	0.652	0.597	0.558	0.541	0.065	0.022
	10	0.517	0.793	0.644	0.518	0.639	0.451	0.687	0.649	0.623	0.613	0.103	0.034
	100	0.866	0.807	0.784	0.594	0.630	0.523	0.772	0.641	0.630	0.694	0.116	0.039
2	0.001	0.704	0.597	0.552	0.541	0.586	0.552	0.676	0.611	0.381	0.578	0.093	0.031
	0.01	0.654	0.545	0.496	0.240	0.462	0.463	0.725	0.716	0.694	0.555	0.160	0.053
	0.1	0.390	0.651	0.486	0.566	0.430	0.524	0.655	0.760	0.722	0.576	0.129	0.043
	1	0.736	0.448	0.629	0.631	0.101	0.655	0.649	0.628	0.644	0.569	0.191	0.064
	10	0.905	0.693	0.589	0.562	0.608	0.587	0.723	0.653	0.841	0.685	0.120	0.040
	100	0.811	0.992	0.978	0.541	0.593	0.654	0.751	0.670	0.641	0.737	0.161	0.054
3	0.001	0.704	0.597	0.552	0.541	0.586	0.552	0.676	0.611	0.381	0.578	0.093	0.031
	0.01	0.606	0.551	0.756	0.445	0.593	0.552	0.684	0.701	0.708	0.622	0.099	0.033
	0.1	0.318	0.578	0.486	0.485	0.434	0.471	0.305	0.390	0.739	0.467	0.133	0.044
	1	0.590	0.624	0.566	0.497	0.509	0.483	0.602	0.601	0.598	0.563	0.053	0.018
	10	0.724	0.624	0.698	0.442	0.544	0.417	0.649	0.662	0.661	0.602	0.110	0.037
	100	1.070	0.668	0.817	0.330	0.309	0.323	0.803	0.672	0.700	0.632	0.263	0.088
4	0.001	0.704	0.597	0.552	0.541	0.586	0.552	0.676	0.611	0.381	0.578	0.093	0.031
	0.01	0.574	0.689	0.499	0.492	0.561	0.586	0.872	0.751	0.762	0.643	0.132	0.044
	0.1	0.605	0.561	0.646	0.536	0.493	0.553	0.680	0.072	0.730	0.542	0.191	0.064
	1	0.663	0.542	0.646	0.527	0.471	0.554	0.680	0.697	0.720	0.611	0.088	0.029
	10	0.578	0.598	0.864	0.459	0.521	0.495	0.763	0.719	0.765	0.640	0.142	0.047
	100	0.814	0.729	0.988	0.182	0.274	0.283	0.873	0.769	0.746	0.629	0.298	0.099
5	0.001	0.704	0.597	0.552	0.541	0.586	0.552	0.676	0.611	0.381	0.578	0.093	0.031
	0.01	0.773	0.642	0.830	0.475	0.504	0.548	0.728	0.743	0.676	0.658	0.125	0.042
	0.1	0.517	0.657	0.728	0.450	0.532	0.471	0.470	0.346	0.688	0.540	0.126	0.042
	1	0.617	0.659	0.546	0.407	0.362	0.384	0.600	0.569	0.629	0.530	0.115	0.038
	10	0.650	0.708	0.572	0.310	0.302	0.280	0.665	0.753	0.661	0.545	0.192	0.064
	100	0.864	0.830	0.694	0.326	0.279	0.538	0.778	0.742	0.661	0.635	0.212	0.071
6	0.001	0.704	0.597	0.552	0.541	0.586	0.552	0.676	0.611	0.381	0.578	0.093	0.031
	0.01	0.634	0.486	0.517	0.437	0.474	0.568	0.699	0.642	0.670	0.570	0.095	0.032
	0.1	0.340	0.813	0.556	0.532	0.350	0.545	0.196	0.817	0.727	0.542	0.218	0.073
	1	0.594	0.524	0.450	0.472	0.500	0.525	0.652	0.597	0.558	0.541	0.065	0.022
	10	0.517	0.793	0.644	0.518	0.639	0.451	0.687	0.649	0.623	0.613	0.103	0.034
	100	0.866	0.807	0.784	0.594	0.630	0.523	0.772	0.641	0.630	0.694	0.116	0.039
7	0.001	0.704	0.597	0.552	0.541	0.586	0.552	0.676	0.611	0.381	0.578	0.093	0.031
	0.01	0.512	0.645	0.541	0.512	0.555	0.552	0.711	0.715	0.738	0.609	0.093	0.031
	0.1	0.716	0.583	0.600	0.410	0.425	0.528	0.693	0.786	0.775	0.613	0.141	0.047
	1	0.610	0.540	0.509	0.235	0.335	0.257	0.589	0.751	0.651	0.497	0.182	0.061
	10	0.585	0.774	0.521	0.452	0.491	0.369	0.699	0.729	0.684	0.589	0.140	0.047
	100	0.722	0.740	0.646	0.375	0.350	0.368	0.714	0.710	0.693	0.591	0.172	0.057

The above table contains both technical (a,b,c) and biological (1,2,3) replicate absorbance data for the MTT assays performed for compounds 1-7. Highlighted results, consist of the absorbance measured for the negative control, DMSO treated cells. All values have been adjusted for the background absorbance on the plate. The average (AVE) absorbance, standard deviation (SD) and standard error (SE) have also been calculated for each compound at each concentration.

S51: Absorbance data for each MTT assay performed for compounds **1**-**7**.



A Z' of 0.3 for both motility and phenotype was recorded for this assay. Schistosomula were assessed for effect on both motility and phenotype. Compounds were considered a hit if an average phenotype and motility score of -0.15 and -0.35 respectively had been achieved (Paveley *et al.*, 2012), as marked by the red hit lines. Treated schistosomula were also visually inspected to validate that no compound-induced motility or phenotypic effect had occurred. The average scores for control DMSO treated parasites (negative control) and Auranofin (AUR) treated parasites (positive control) are included for reference.

S52: Compounds **1-7** do not display anthelmintic activity against *Schistosoma mansoni* larva. Compounds were screened at a concentration of 10 μM against 24 h cultured schistosomula.

HTS Average score		
Treatment	**PHENO**	**MOT**
DMSO	-0.0857	0.0000
AUR	-0.5997	-0.8900
1	-0.0197	0.0008
2	0.1793	-0.1049
3	0.1268	-0.0370
4	0.1048	0.4366
5	0.0348	0.3898
6	0.0954	-0.3442
7	0.2054	0.0193

This table includes the scores given for DMSO treated parasites (negative control) and Auranofin (AUR) treated parasites (positive control) which are highlighted in red for reference.

S53: Average scores given for compounds 1-7, for both phenotype and motility.