Supporting Information

***Rec. Nat. Prod*. 17:6 (2023) 1046-1051**

Two New C_{21} Steroidal Glycosides from the Leaves of *Hoya parasitica*

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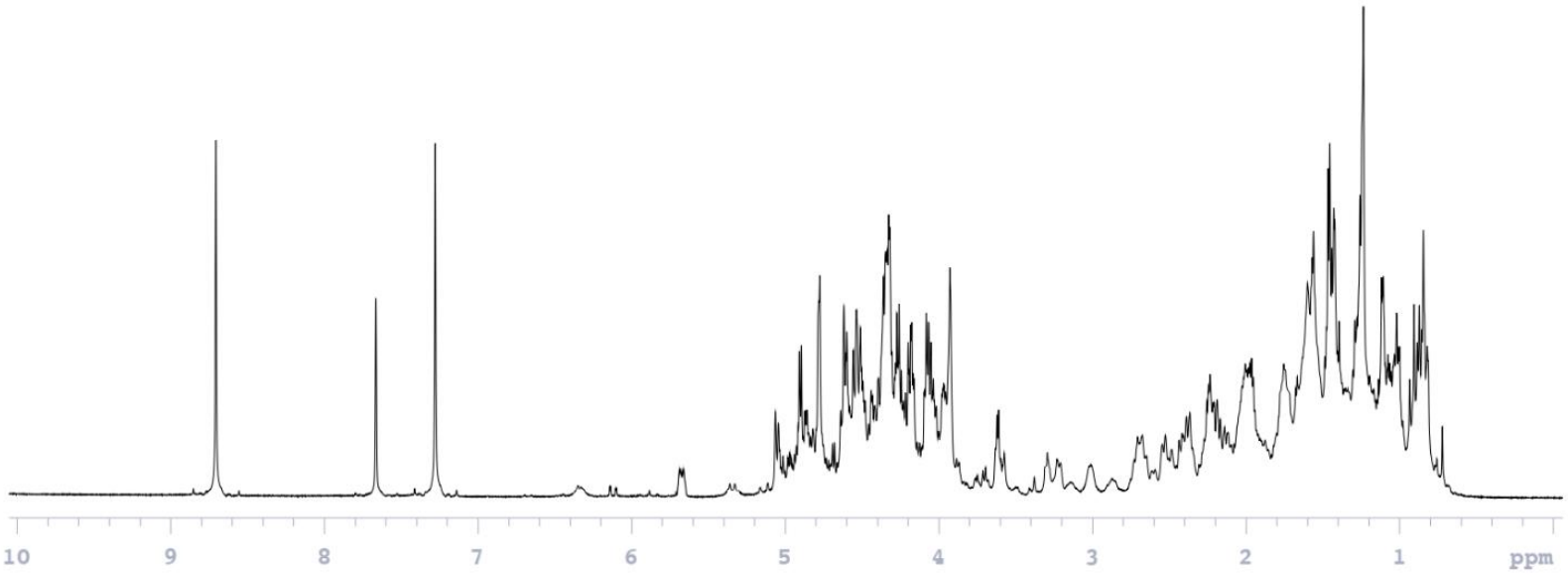


Figure S1: ^{1}H NMR spectrum of **1** in C_5D_5N at 600 MHz

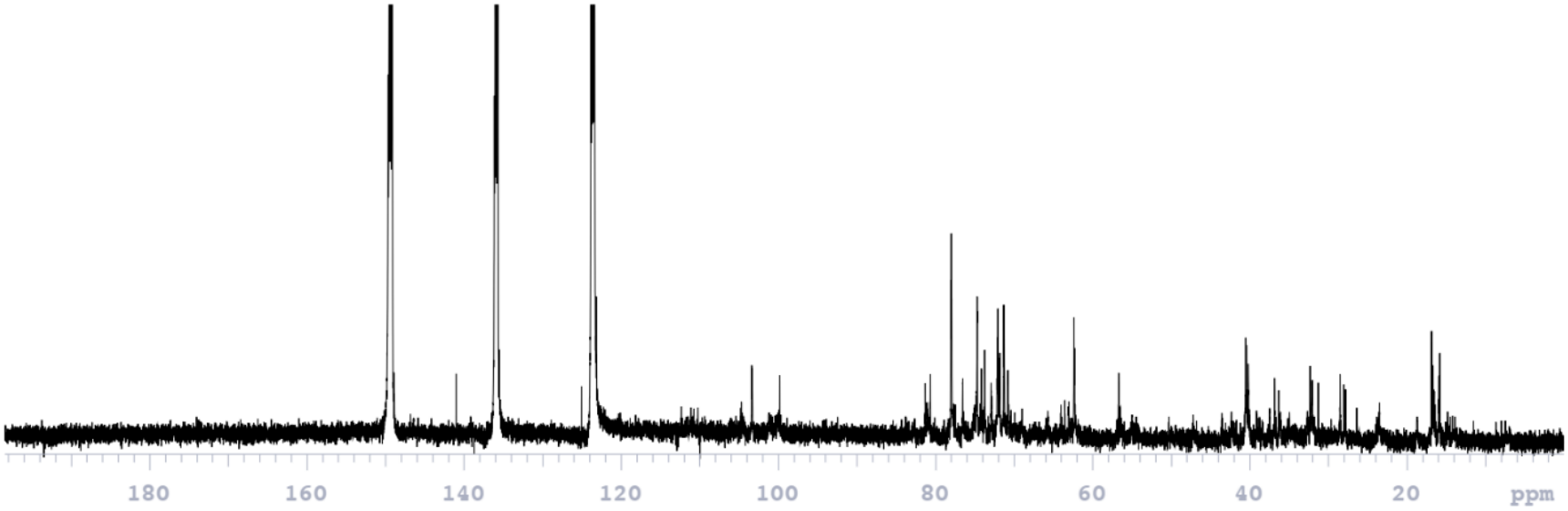


Figure S2: ^{13}C NMR spectrum of **1** in C_5D_5N at 150 MHz

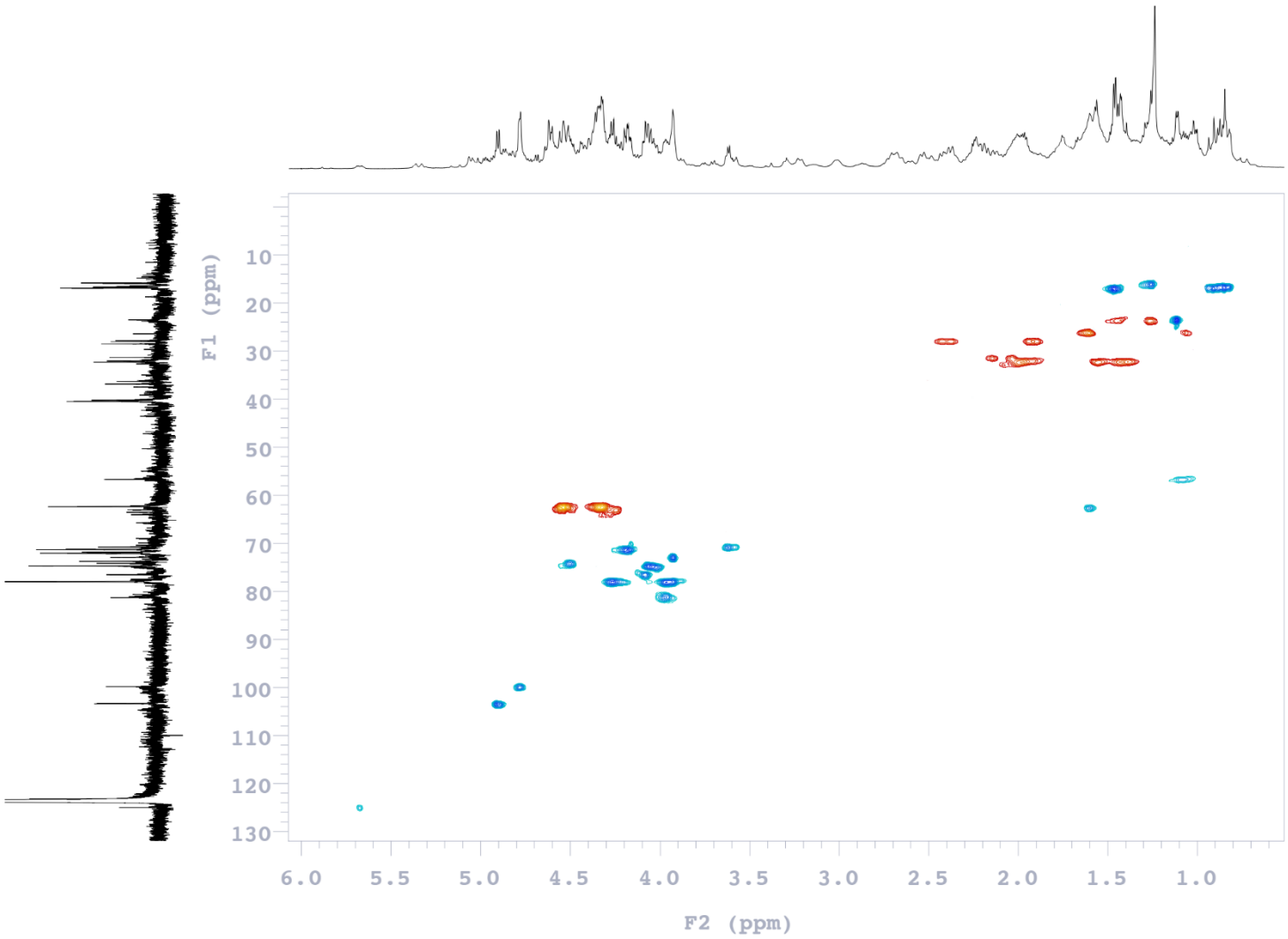


Figure S3: HSQC spectrum of **1** in C_5D_5N at 600 MHz

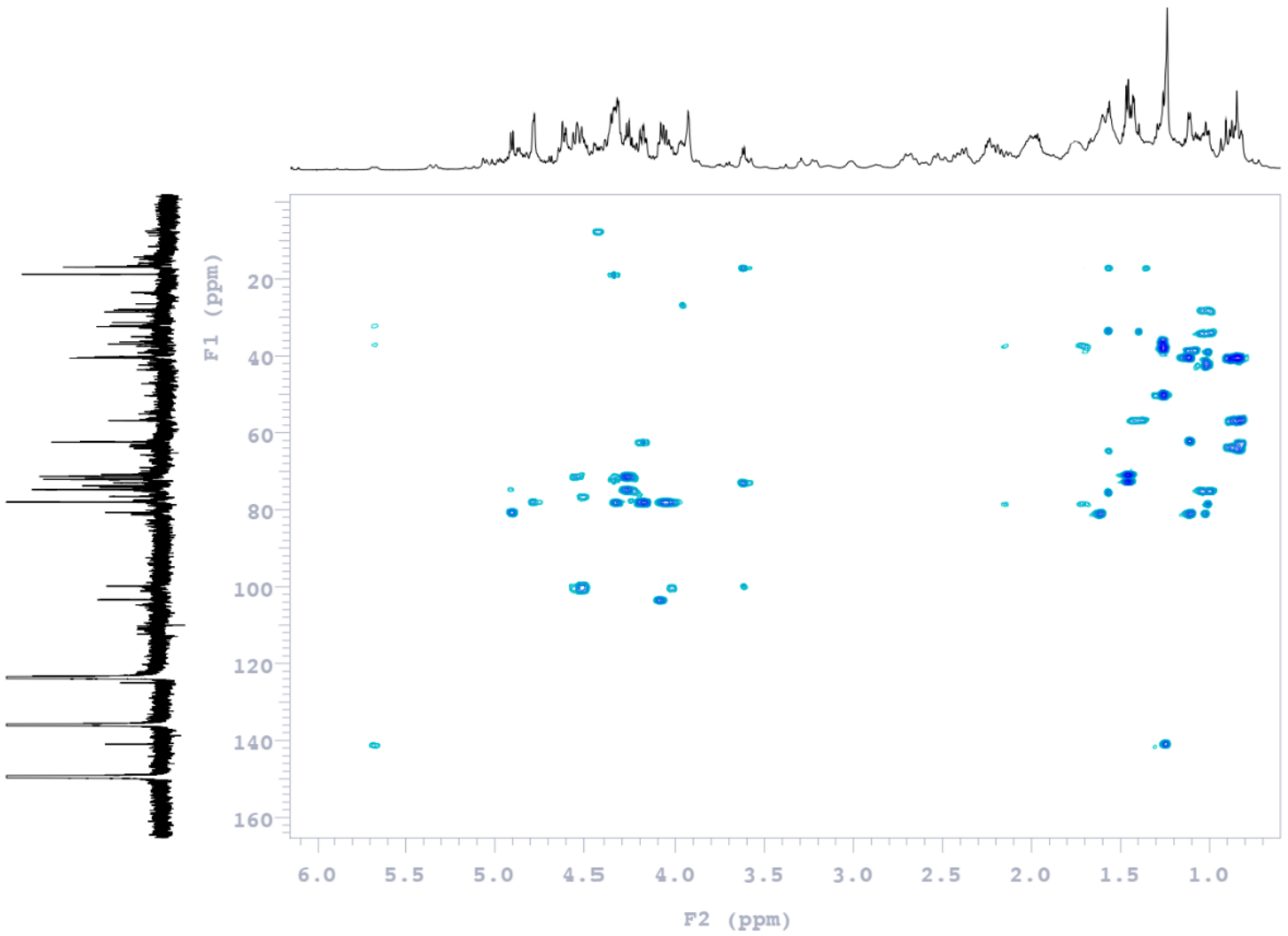


Figure S4: HMBC spectrum of **1** in C_5D_5N at 600 MHz

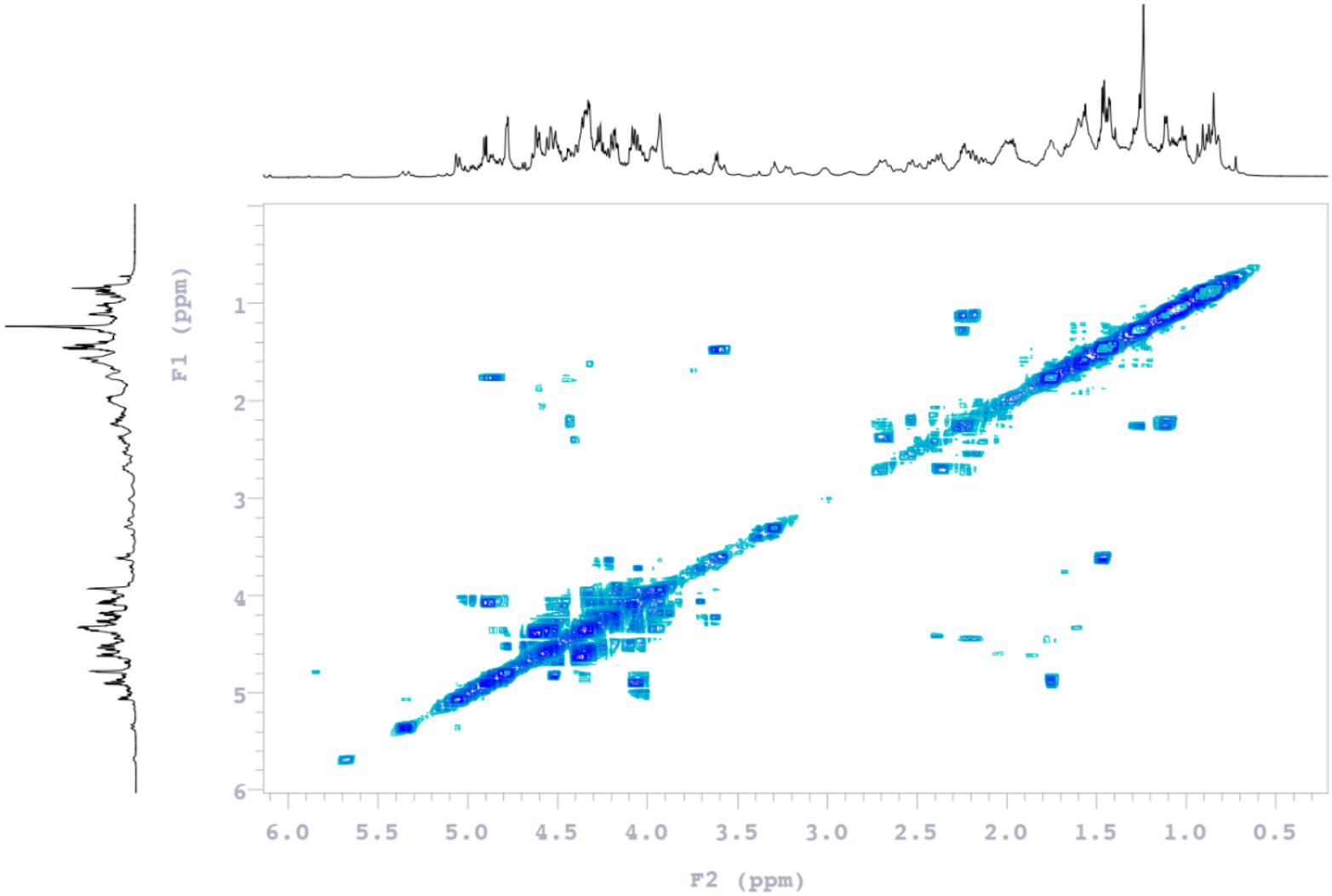


Figure S5: COSY spectrum of **1** in C_5D_5N at 600 MHz

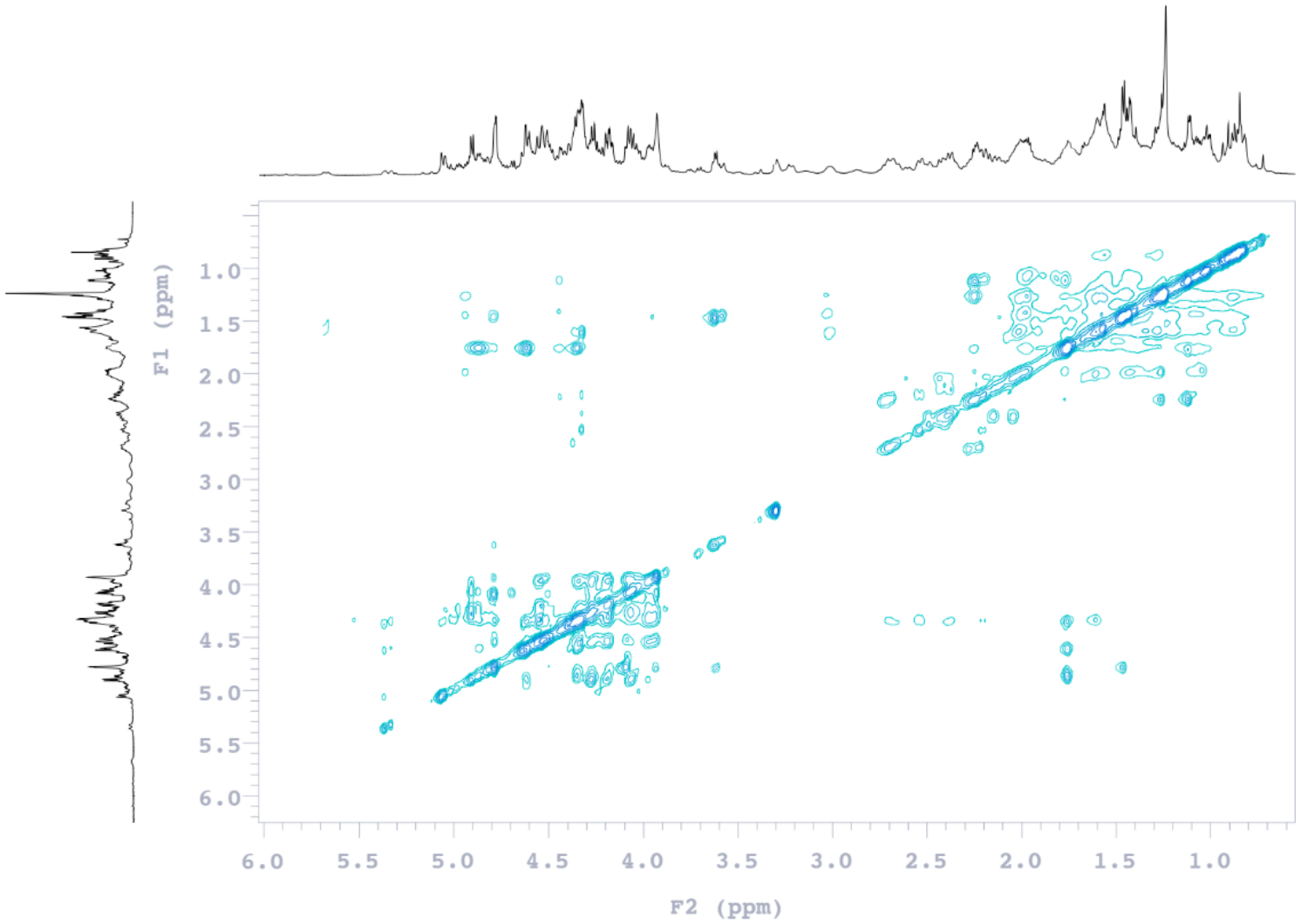


Figure S6: TOCSY spectrum of **1** in C_5D_5N at 600 MHz

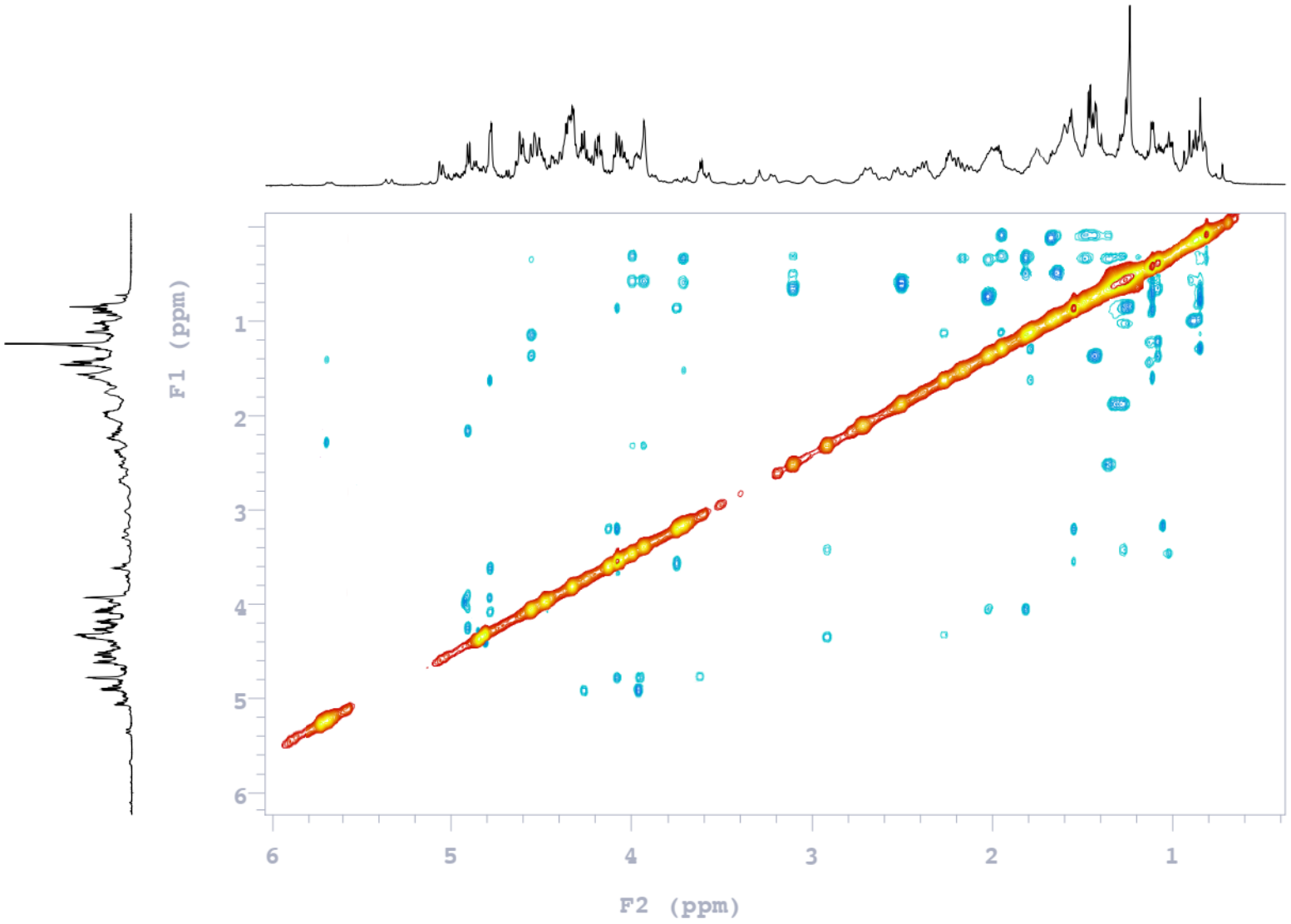
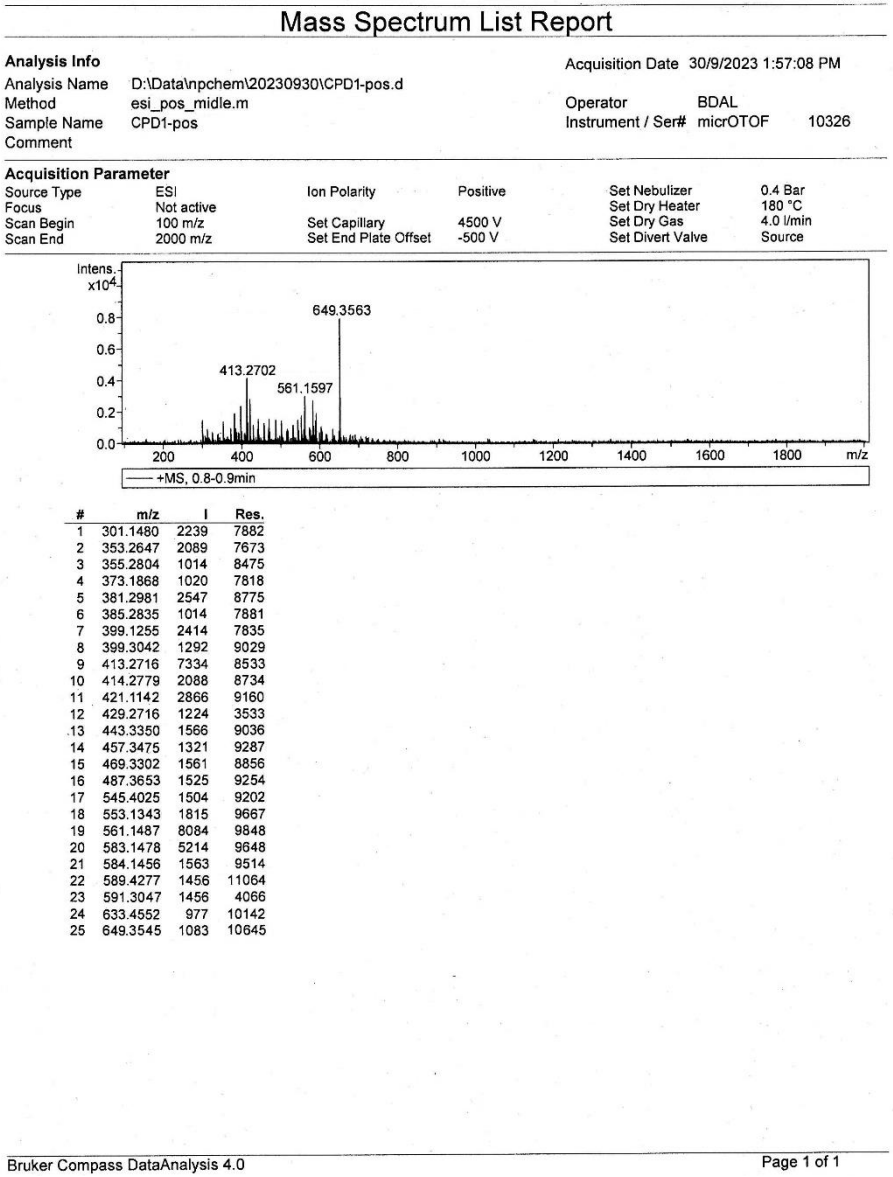


Figure S7: ROESY spectrum of **1** in C_5D_5N at 600 MHz



Mass Spectrum List Report

Analysis Info

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Sample Name	CPD1-pos	Instrument / Ser#	micrOTOF 10326
Comment			

Acquisition Parameter

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Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

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2	353.2647	2089	7673
3	355.2804	1014	8475
4	373.1868	1020	7818
5	381.2981	2547	8775
6	385.2835	1014	7881
7	399.1255	2414	7835
8	399.3042	1292	9029
9	413.2716	7334	8533
10	414.2779	2088	8734
11	421.1142	2866	9160
12	429.2716	1224	3533
13	443.3350	1566	9036
14	457.3475	1321	9287
15	469.3302	1561	8856
16	487.3653	1525	9254
17	545.4025	1504	9202
18	553.1343	1815	9667
19	561.1487	8084	9848
20	583.1478	5214	9648
21	584.1456	1563	9514
22	589.4277	1456	11064
23	591.3047	1456	4066
24	633.4552	977	10142
25	649.3545	1083	10645

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Figure S8: HR-ESI-MS (positive mode) of **1**

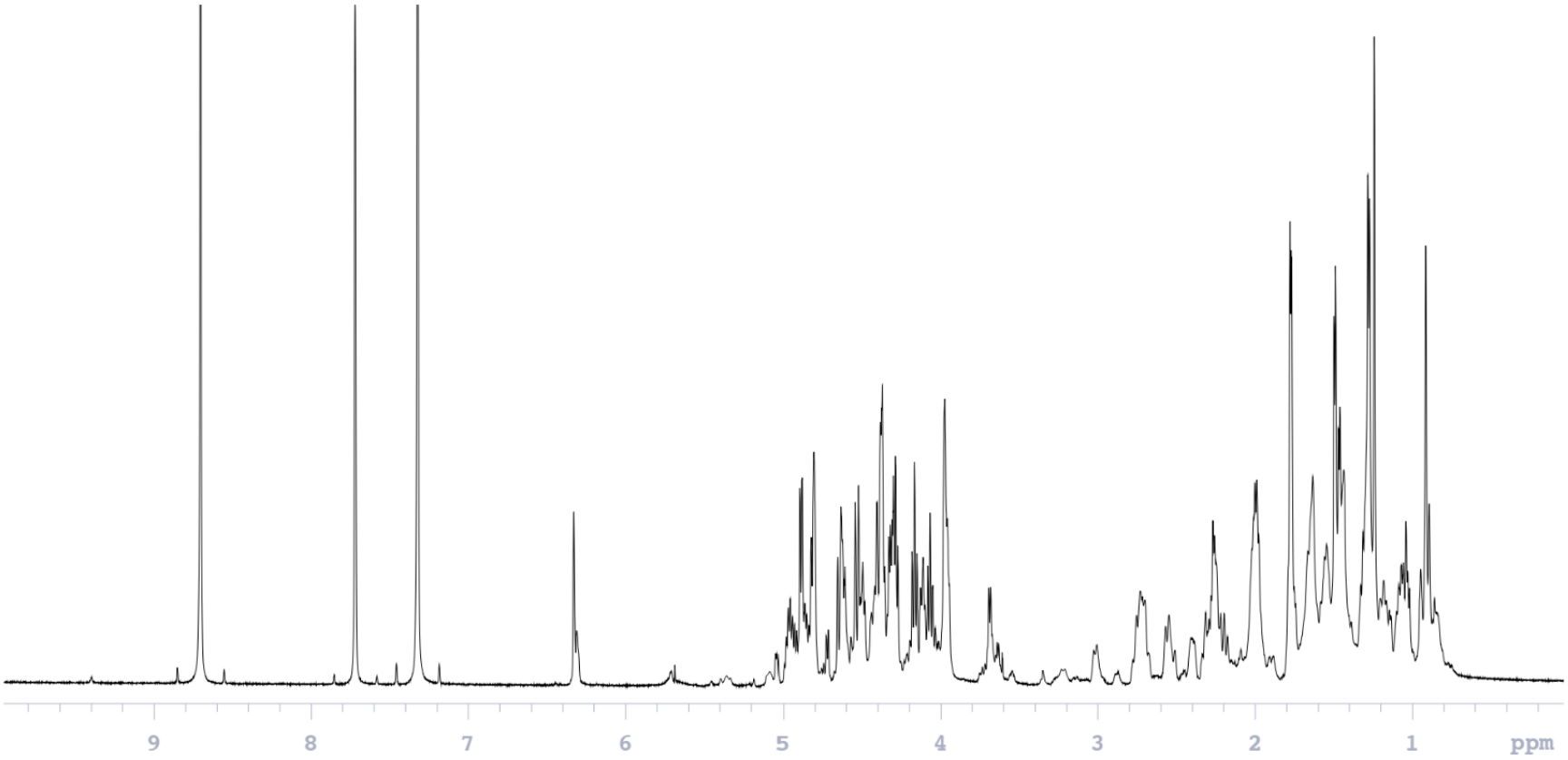

Figure S9: ^{1}H NMR spectrum of **2** in C_5D_5N at 150 MHz

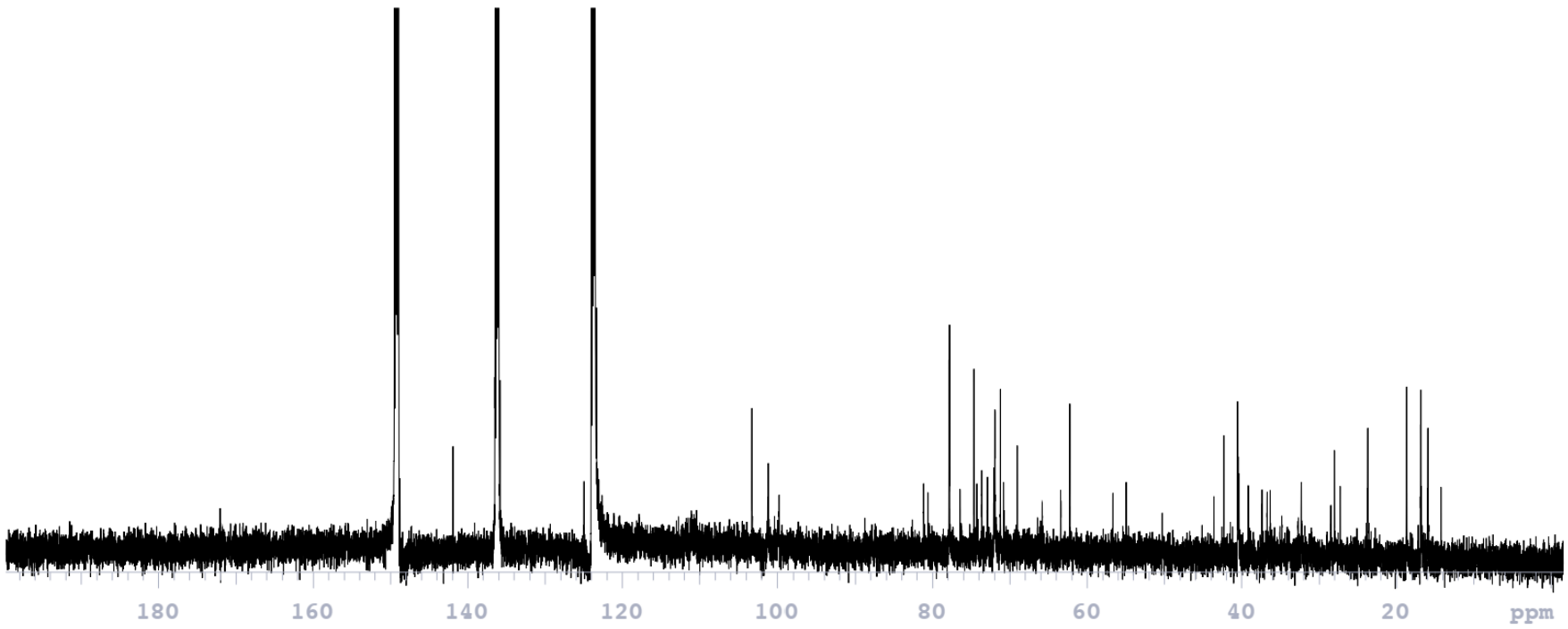

Figure S10: ^{13}C NMR spectrum of **2** in C_5D_5N at 150 MHz

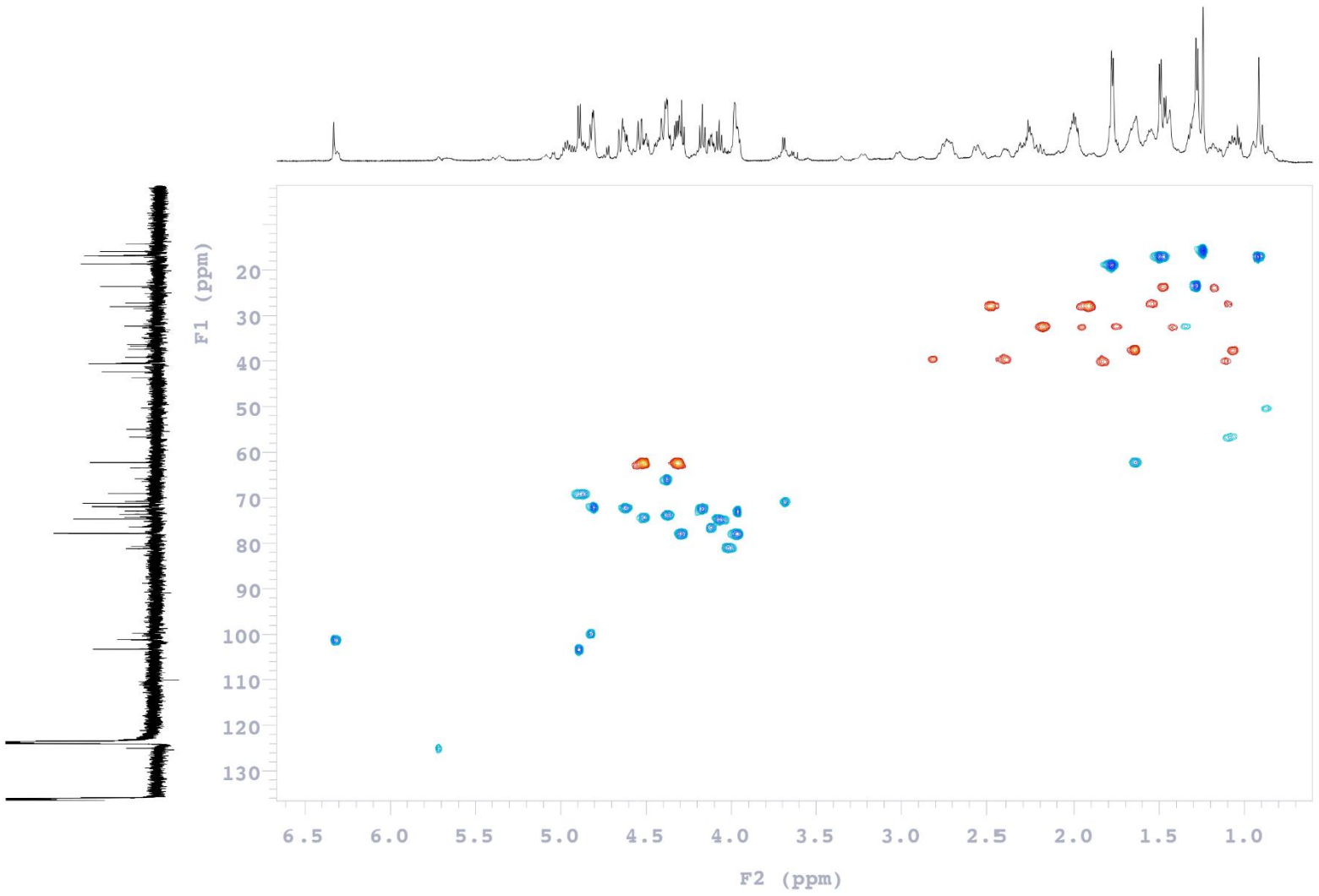

Figure S11: HSQC spectrum of **2** in C_5D_5N at 150 MHz

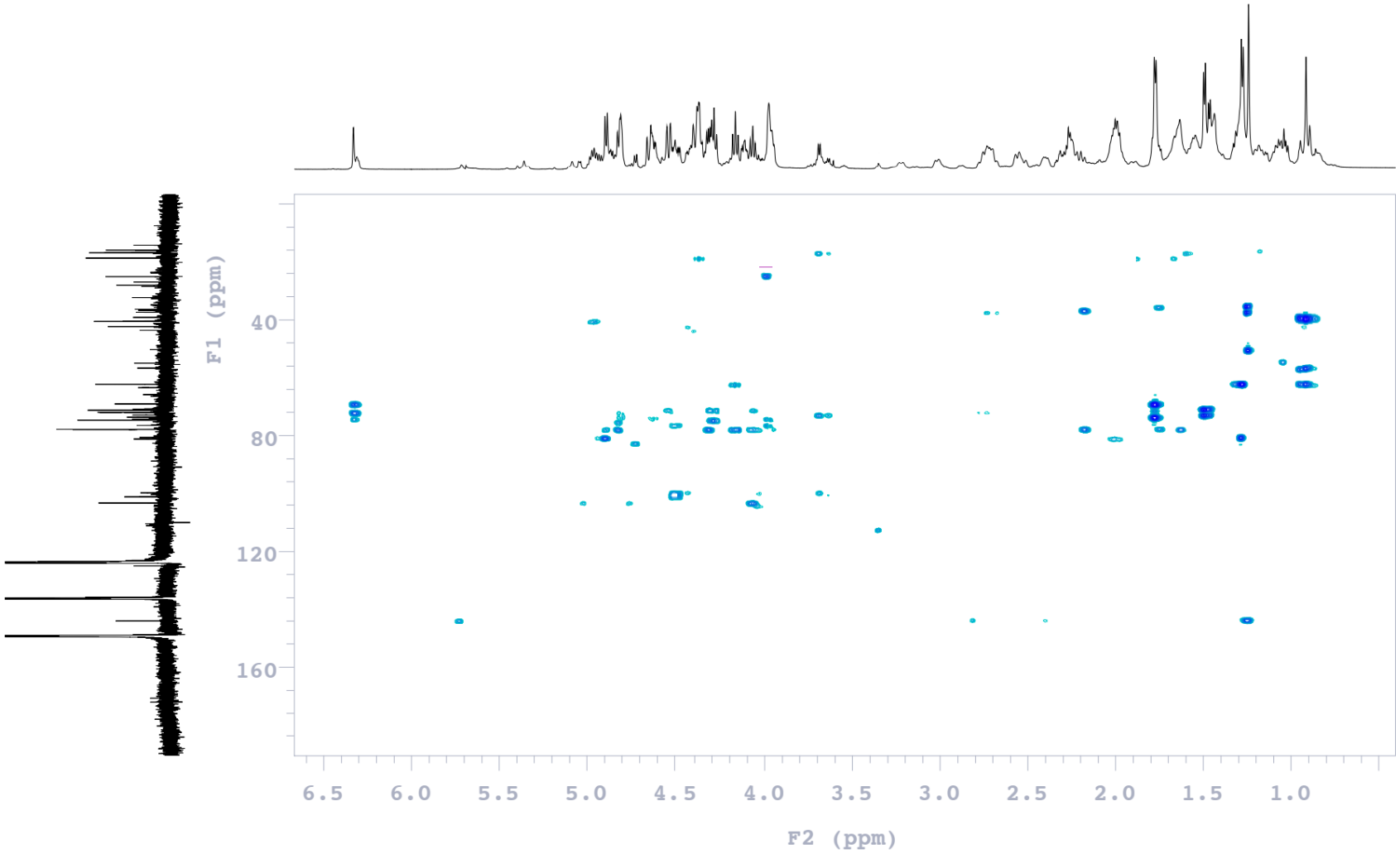

Figure S12: HMBC spectrum of **2** in C_5D_5N at 150 MHz

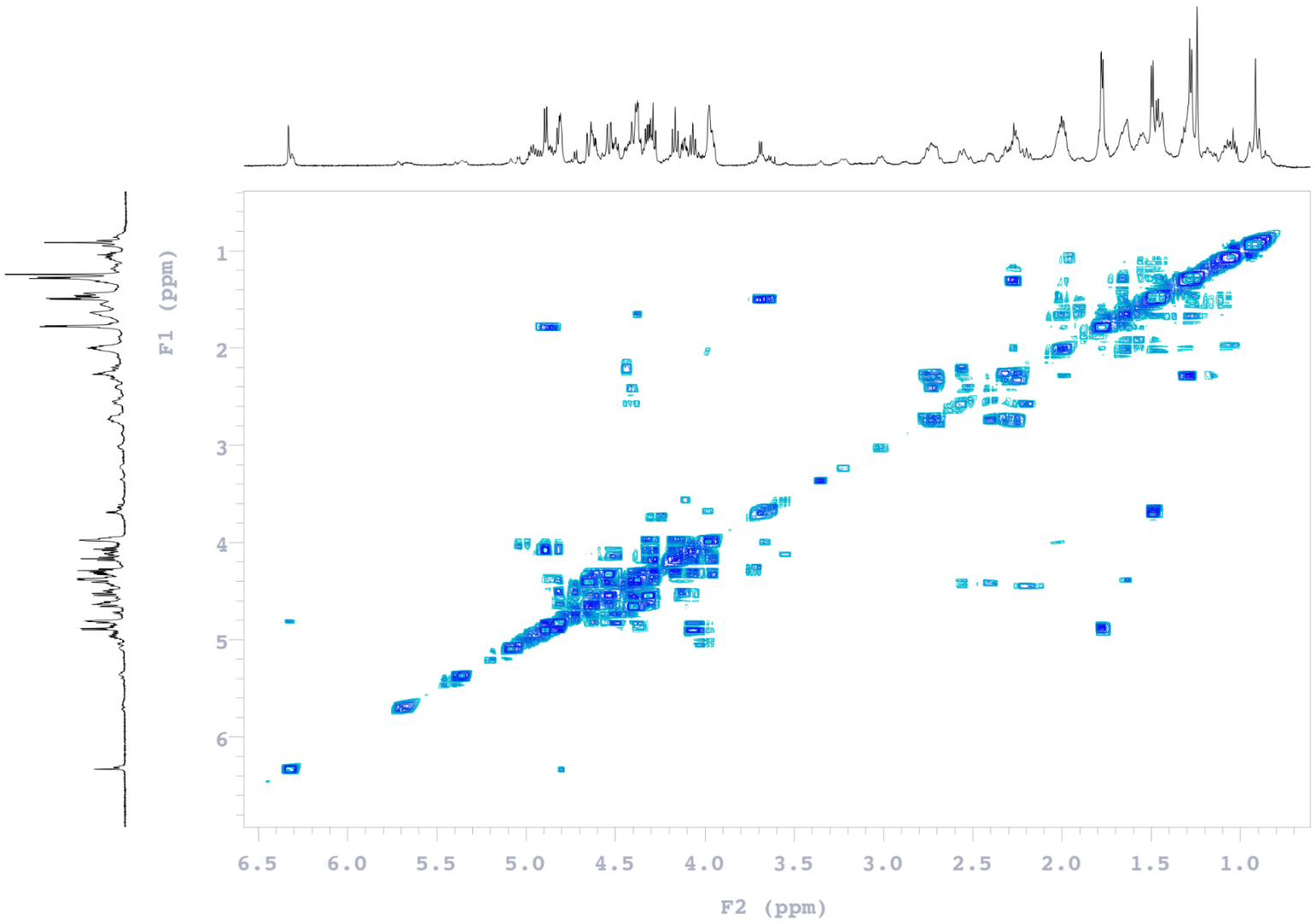

Figure S13: COSY spectrum of **2** in C_5D_5N at 600 MHz

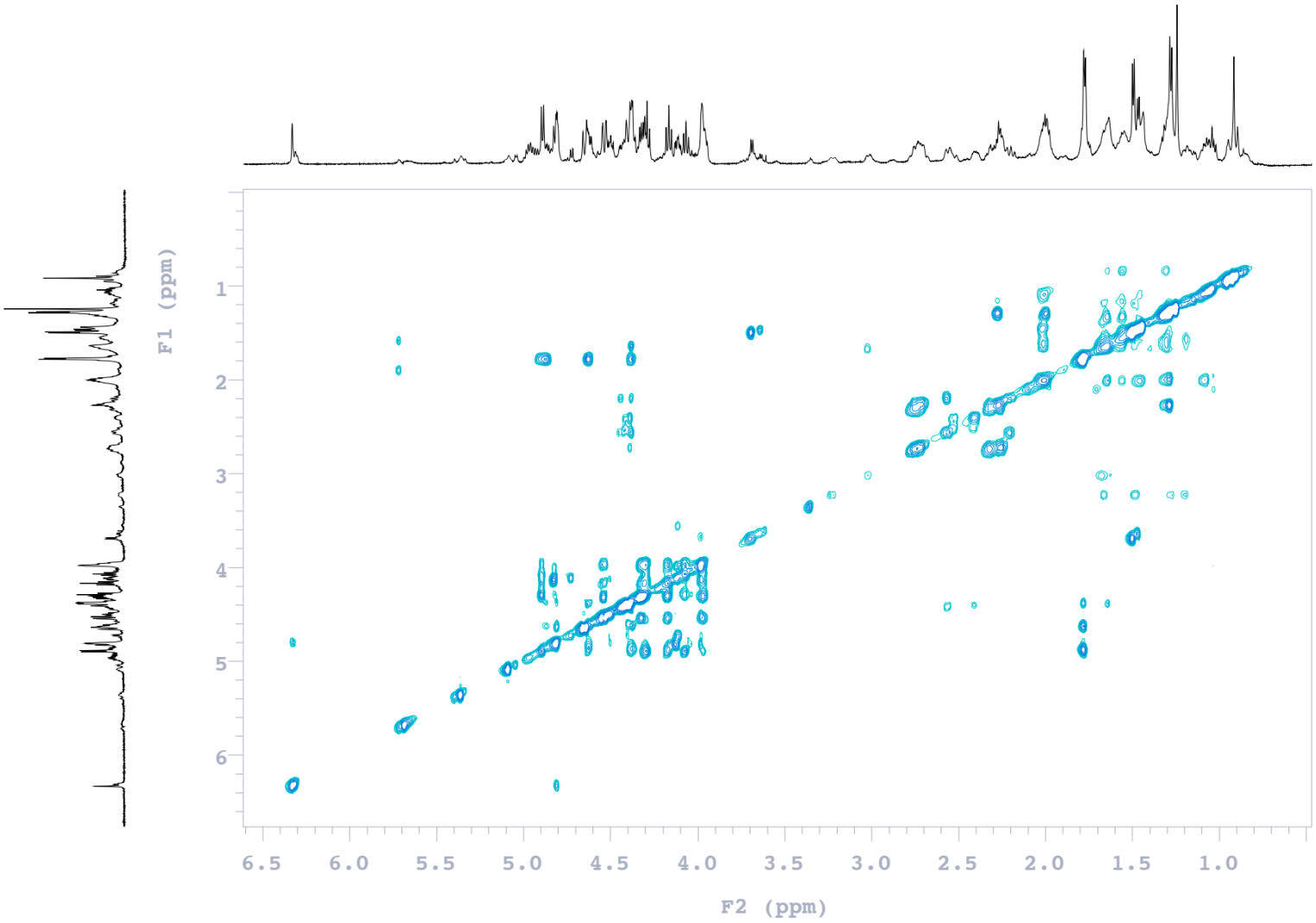

Figure S14: TOCSY spectrum of **2** in C_5D_5N at 600 MHz

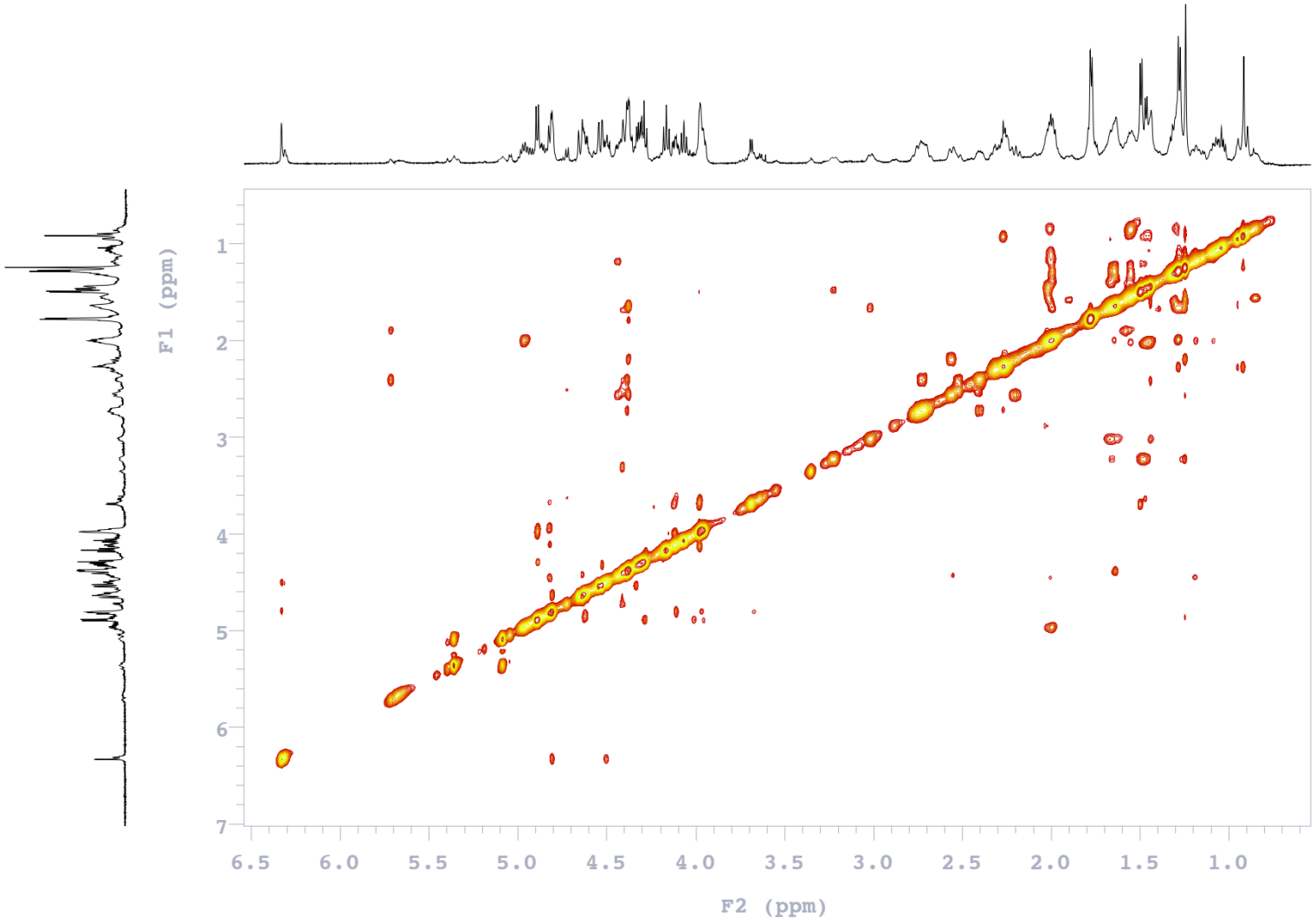

Figure S15: ROESY spectrum of **2** in C_5D_5N at 600 MHz

Mass Spectrum List Report

Analysis Info

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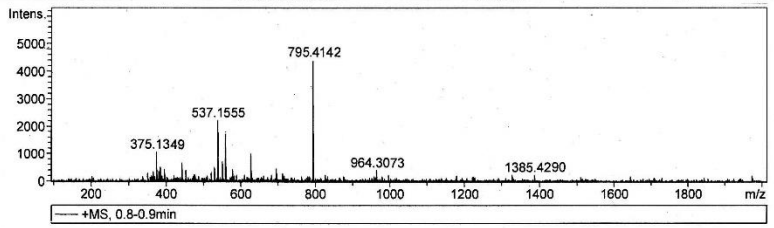
Sample Name	CPD2-pos	Instrument / Ser#	micrOTOF 10326
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



#	m/z	I	Res.
1	351.1493	310	10637
2	367.1096	375	8293
3	375.1349	1093	8451
4	384.9365	553	8265
5	397.1137	474	8579
6	452.9265	428	9242
7	529.1392	553	8513
8	537.1555	4431	9379
9	551.1229	747	9439
10	561.1514	328	9316
11	579.1745	449	4239
12	628.1365	342	11044
13	696.1128	295	5139
14	712.4179	338	4962
15	795.4142	450	10028
16	964.3073	353	46213
17	1385.4290	279	6439

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Figure S16: HR-ESI-MS (positive mode) of **2**

CAS SciFinder^{n} Task History

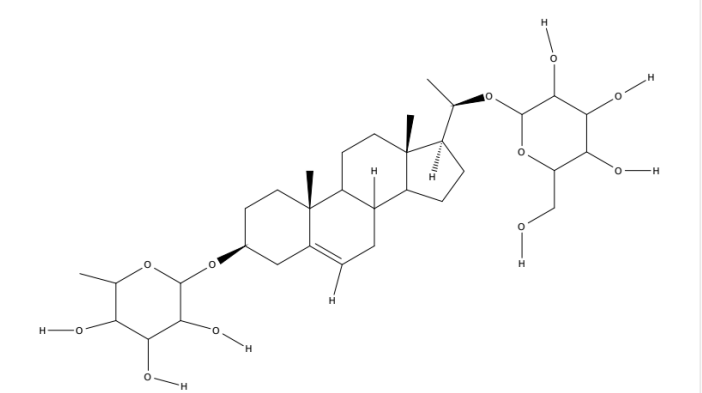
Initiating Search

September 11, 2023, 10:32AM

Substances:

Filtered By:

Stereochemistry: **Absolute Stereo Match**



Structure Match: **Substructure**

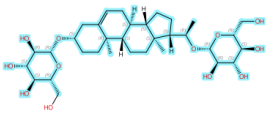
Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (6)	Substances	View Results

Figure S17a: Scifinder search for compound **1**

1

113679-33-7



Absolute stereochemistry shown

$C_{33}H_{54}O_{12}$

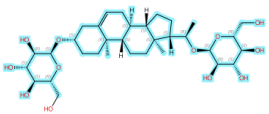
β-D-Glucopyranoside, (3β,20*R*)-pregn-5-ene-3, 20-diyl bis-

2 References | 2 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	642.78	-
Boiling Point (Predicted)	813.3±65.0 °C	Press: 760 Torr
Density (Predicted)	1.39±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.91±0.70	Most Acidic Temp: 25 °C

2

123367-47-5



Absolute stereochemistry shown

$C_{33}H_{54}O_{12}$

α-D-Glucopyranoside, (3β,20*R*)-pregn-5-ene-3, 20-diyl bis-

1 Reference | 2 Reactions | 0 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	642.78	-
Boiling Point (Predicted)	813.3±65.0 °C	Press: 760 Torr
Density (Predicted)	1.39±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.91±0.70	Most Acidic Temp: 25 °C

Figure S17b: Scifinder similarity report for compound **1**

CAS SciFinder^n

Task History

Initiating Search

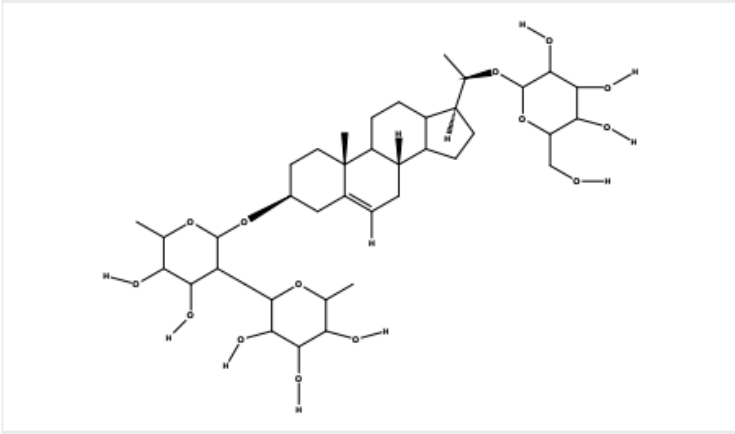
September 11, 2023, 3:25PM

Substances:

Filtered By:

Similarity: **95-98**

Number of Components: **1**



Structure Match: **Similarity**

Search Tasks

Task	Search Type	View
Exported: Returned Substance Results + Filters (22)	Substances	View Results

Figure S18a: Scifinder search for compound **2**

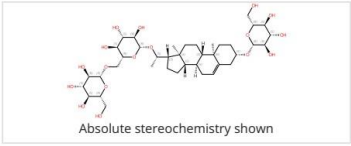
CAS SciFinder^n

Substances (22)

View in SciFinder^n

1 Similarity Score: **97**

521970-07-0



Absolute stereochemistry shown

$C_{39}H_{64}O_{17}$

(3β,20*S*)-3-(β-D-Glucopyranosyloxy)pregn-5-en-20-yl 6-*O*-β-D-glucopyranosyl-β-D-glucopyranoside

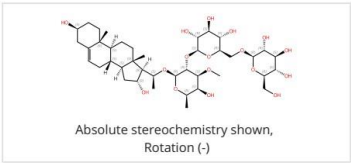
5 References | 0 Reactions | 2 Suppliers

Key Physical Properties	Value	Condition
Molecular Weight	804.92	-
Boiling Point (Predicted)	969.8±65.0 °C	Press: 760 Torr
Density (Predicted)	1.48±0.1 g/cm^3	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	12.89±0.70	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

2 Similarity Score: **96**

73532-66-8



Absolute stereochemistry shown, Rotation (-)

$C_{40}H_{66}O_{17}$

(3β,16α,20*S*)-3,16-Dihydroxypregn-5-en-20-yl *O*-β-D-glucopyranosyl-(1→6)-*O*-β-D-glucopyranosyl-(1→2)-6-deoxy-3-*O*-methyl-β-D-galactopyranoside

4 References | 2 Reactions | 0 Suppliers

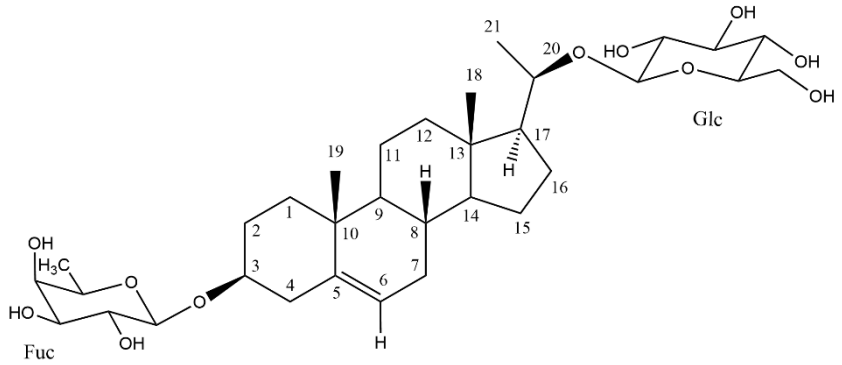
Key Physical Properties	Value	Condition
Molecular Weight	818.94	-

Figure S18b: Scifinder similarity report for compound **2**

Table S1: Comparisons of NMR data of parasiticoside A (**1**) and periseoside C

Parasiticoside A (**1**)			Periseoside C		
Position	δ_C	δ_H	**Position**	δ_C	δ_H
1	37.5	1.06 m, 1.62 m	1	37.5	0.95, 1.66
2	31.3	1.70 m, 2.14 m	2	30.2	1.70, 2.09 br d (11.2)
3	78.1	3.93 ov	3	78.1	3.91
4	39.3	2.28 m, 2.72 m	4	39.3	2.43 (br t, 12.8), 2.68 ddd (13.0, 4.5, 2.3)
5	140.9	-	5	140.9	-
6	125.0	5.67 br s	6	121.9	5.29 (m)
7	32.1	1.40 m, 1.95 m	7	32.1	1.44 (m), 1.81
8	31.8	1.30 ov	8	31.8	1.33
9	50.3	0.80 m	9	50.3	0.80
10	36.9	-	10	36.9	-
11	21.0	1.27 m, 1.45 m	11	21.0	1.32, 1.37
12	39.1	1.00 m, 1.82 m	12	39.1	1.00, 1.82
13	40.5	-	13	41.5	-
14	56.7	1.08 ov	14	56.7	0.86
15	28.0	1.91 m, 2.40 m	15	27.2	1.89 m, 2.33 m
16	26.4	1.05 m, 1.53 m	16	24.4	1.05, 1.53
17	62.4	1.60 ov	17	58.3	1.57 m
18	16.9	0.85 s	18	12.4	0.64 s
19	16.0	1.28 s	19	19.4	0.88 s
20	81.3	3.98 ov	20	81.3	3.86 m
21	23.5	1.12 d (6.0)	21	23.3	1.52 d (6.0)
Fuc-1	99.8	4.78 d (7.6)	Glc I-1	102.6	5.02 d (7.7)
2	74.2	4.52 dd (9.4, 7.6)	2	75.4	4.03 pt (7.9)
3	76.6	4.08 dd (9.4, 2.9)	3	78.3	4.27 pt (8.5)
4	72.9	3.93 br d (2.9)	4	71.7	4.23 pt (8.5)
5	70.8	3.62 br q (6.4)	5	78.6	3.95
6	17.0	1.46 d (6.4)	6	62.9	4.39 dd (11.6, 3.0), 4.54 br d (11.6)
Glc-1	103.4	4.90 d (7.6)	Glc II-1	106.2	4.93 d (7.7)

2	74.7	4.05 ov	2	75.8	3.98
3	78.0	4.26 ov	3	78.5	4.25 pt (8.5)
4	72.2	4.18 ov	4	71.8	4.21 pt (8.5)
5	78.1	3.96 m	5	78.7	3.96
6	62.4	4.33 m, 4.54 m	6	63.0	4.38 dd (11.8, 3.1), 4.53 br d (11.8)



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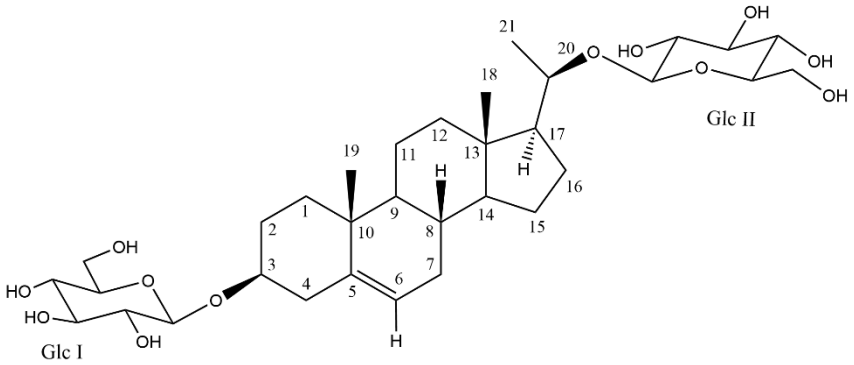


Periseoside C

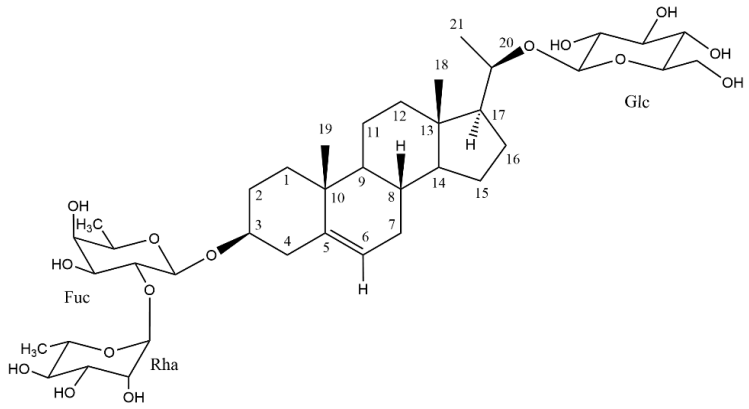
Figure S19: Structure of periseoside C which is the most similar to compound **1** according to Scifinder search.

L. Wang, Z.Q. Yin, Q.W. Zhang, X.Q. Zhang, D.M. Zhang, K. Liu, Y.L. li, X.S. Yao, and W.C. Ye (2011). Five new C_{21} steroidal glycosides from Periploca sepium, *Steroids* **76,** 238-243.

Table S2: Comparisons of NMR data of parasiticoside B (**2**) and biondianoside D

Parasiticoside B (**2**)			Biondianoside D		
Position	δ_C	δ_H	**Position**	δ_C	δ_H
1	37.4	1.08 m, 1.66 m	1	37.5	
2	32.3	1.75 m, 2.18 m	2	30.2	
3	77.9	3.97 ov	3	78.1	
4	39.2	2.40 m, 2.82 m	4	39.3	
5	140.9	-	5	140.9	5.32 br s
6	125.0	5.72 br s	6	121.9	
7	32.7	1.43 m, 1.97 m	7	32.1	
8	32.2	1.35 ov	8	31.8	
9	50.3	0.87 m	9	50.3	
10	36.3	-	10	36.9	
11	23.9	1.18 m, 1.48 m	11	21.0	
12	39.3	1.11 m, 1.83 m	12	39.0	
13	40.6	-	13	41.5	
14	56.7	1.09 ov	14	56.6	
15	28.0	1.92 m, 2.48 m	15	27.3	
16	26.8	1.09 m, 1.54 m	16	24.4	
17	62.3	1.64 ov	17	58.3	
18	16.9	0.91 s	18	12.4	0.64 s
19	15.9	1.26 s	19	19.4	0.90 s
20	81.2	4.01 ov	20	81.2	3.93 m
21	23.6	1.28 d (6.0)	21	23.6	1.62 d (6.0)
Fuc-1	99.9	4.80 d (7.6)	Glc I-1	105.3	5.03 d (7.6)
2	74.4	4.53 dd (9.4, 7.6)	2	75.5	
3	76.4	4.12 dd (9.4, 2.9)	3	78.4	
4	73.1	3.96 br d (2.9)	4	71.7	
5	70.9	3.68 br q (6.4)	5	77.3	
6	16.8	1.49 d (6.4)	6	70.1	
Glc-1	103.5	4.88 d (7.6)	Glc II-1	106.0	4.89 d (7.6)
2	74.6	4.06 ov	2	75.3	
3	77.9	4.28 ov	3	78.4	
4	72.3	4.18 ov	4	71.7	
5	78.1	3.96 m	5	78.5	

6	62.3	4.30 m, 4.52 m	6	62.8	
Rha-1	101.2	6.35 br s	Glc III-1	102.6	5.19 d (7.7)
2	72.1	4.79 br s	2	75.2	
3	72.2	4.61 dd (9.4, 3.5)	3	78.5	
4	73.8	4.35 dd (9.9, 9.4)	4	71.7	
5	69.0	4.83 dq (9.9, 5.9)	5	78.6	
6	18.7	1.78 d (5.9)	6	62.8	



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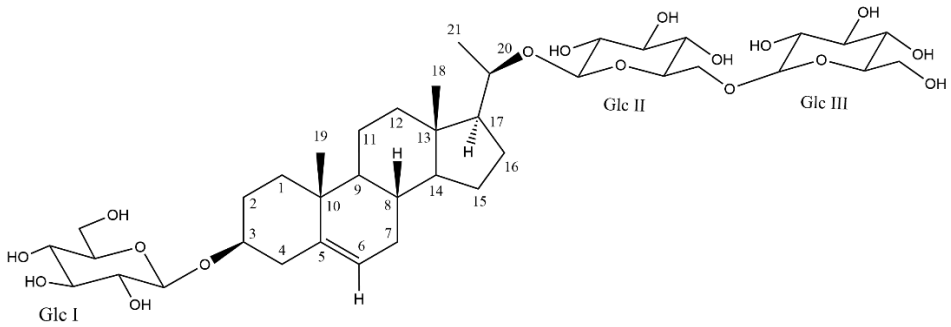

Biondianoside D

Figure S20: Structure of biondianoside D which is the most similar to compound **2** according to Scifinder search.

X.G. Tang, X.R. Zhang, S.L. Peng, X. Liao, and L.S. Ding (2003). Chemical constituents from the roots of Biondia hemsleyana, *Chem. J. Chinese Universit.* **24,** 436-441.