

The entire structure elucidation report
and the elucidation protocol from the
ACD/SE Suite tool (Advanced
Chemistry Development, Inc.
(ACD/Labs), Toronto, ON, Canada,
www.acdlabs.com) for **compound 2**

Structure Elucidation Report for compound 2

Initial Data

Composition Restrictions:

Molecular Weight = 0.000-1000.000

Double Bonds Equivalent = 0.00-100.00

Allowed Composition = C(0-100) H(0-100) O(0-20) N(0-10)

Molecular Formula = C₂₇H₃₀O₁₅

Spectral Data:

standard ¹H - 12 peaks

merged ¹H - 18 peaks

standard ¹³C - 25 peaks

merged ¹³C - 25 peaks

COSY ¹H-¹H - 26 peaks

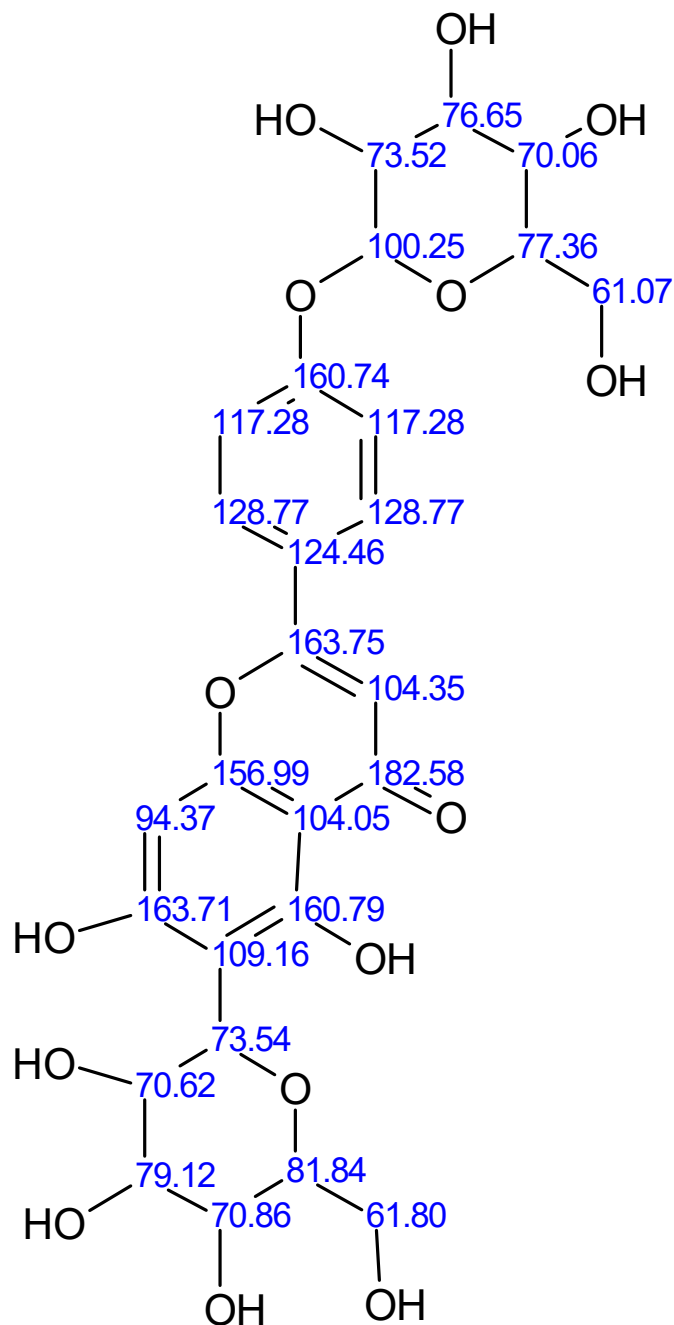
HSQC-DEPT ¹³C-¹H - 18 peaks

HMBC ¹³C-¹H - 47 peaks

Most Probable Structure

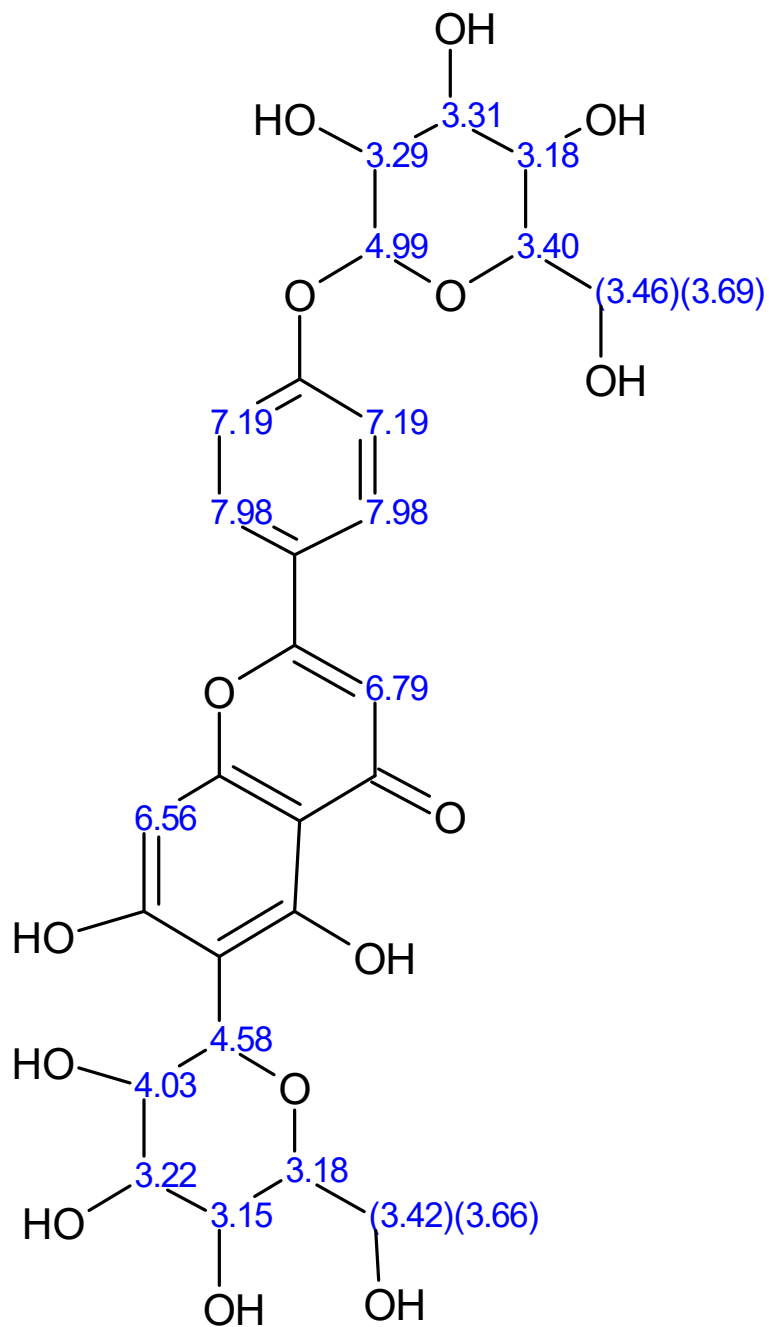
Following structure has been placed to the first position after spectra calculation

Carbon Assignment



#	N	Shift (ppm)	Atoms	XHn
1	1	61.067	1	CH2(t)
2	2	61.803	1	CH2(t)
3	3	70.060	1	CH(d)
4	4	70.621	1	CH(d)
5	5	70.857	1	CH(d)
6	6	73.520	1	CH(d)
7	7	73.539	1	CH(d)
8	8	76.654	1	CH(d)
9	9	77.363	1	CH(d)
10	10	79.122	1	CH(d)
11	11	81.839	1	CH(d)
12	12	94.370	1	CH(d)
13	13	100.246	1	CH(d)
14	19	104.055	1	C(s)
15	14	104.350	1	CH(d)
16	20	109.158	1	C(s)
17	15,16	117.278	2	CH(d)
18	21	124.462	1	C(s)
19	17,18	128.769	2	CH(d)
20	22	156.989	1	C(s)
21	23	160.736	1	C(s)
22	24	160.790	1	C(s)
23	25	163.710	1	C(s)
24	26	163.748	1	C(s)

Proton Assignment

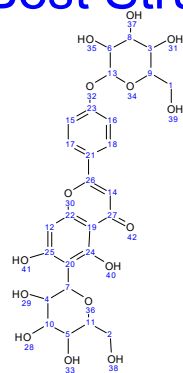


#	N	Mark	Shift (ppm)	Protons
1	5		3.155	1
2	11		3.177	1
3	3		3.178	1
4	10		3.216	1
5	6		3.286	1
6	8		3.312	1
7	9		3.400	1
8	2		3.415	1
9	1		3.465	1
10	2		3.661	1
11	1		3.691	1
12	4		4.026	1
13	7		4.583	1
14	13		4.994	1
15	12		6.556	1
16	14		6.792	1
17	15,16		7.189	1

Generated Structures

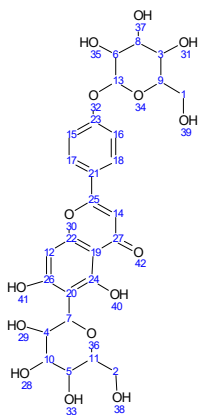
1 (ID=262)

The Best Structure



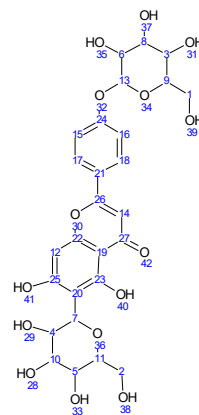
$d_N(^{13}C+^1H)$: 3.779

2 (ID=331)



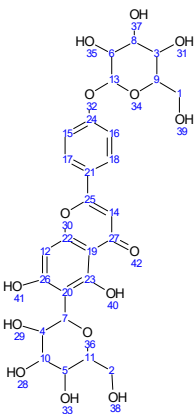
$d_N(^{13}C+^1H)$: 3.782

3 (ID=107)



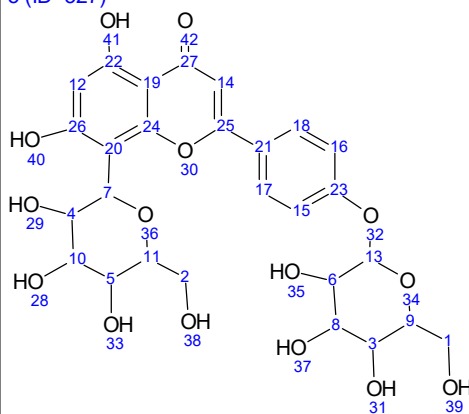
$d_N(^{13}C+^1H)$: 3.783

4 (ID=166)



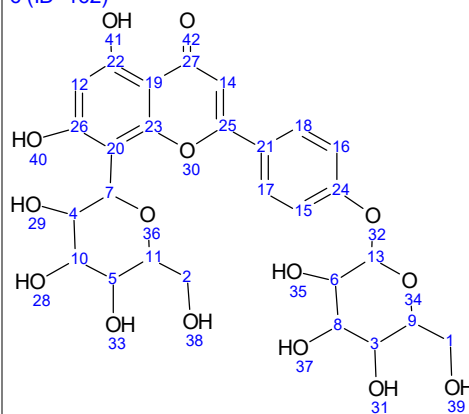
$d_N(^{13}C+^1H)$: 3.786

5 (ID=327)



$d_N(^{13}C+^1H)$: 4.339

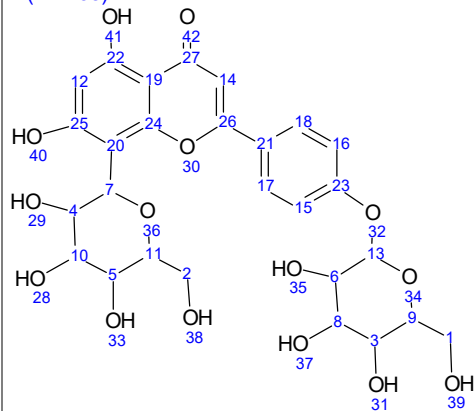
6 (ID=162)



$d_N(^{13}C+^1H)$: 4.339

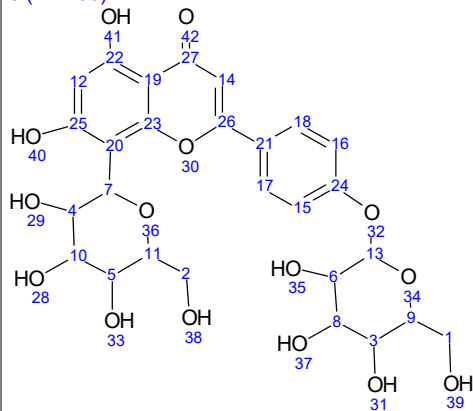
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7 (ID=258)



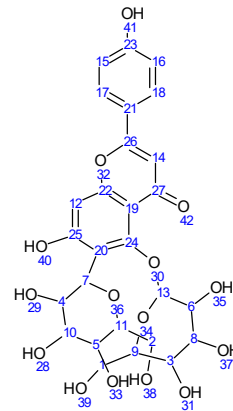
$d_N(^{13}C+^1H)$: 4.341

8 (ID=103)



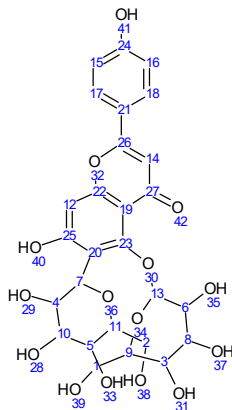
$d_N(^{13}C+^1H)$: 4.341

9 (ID=257)



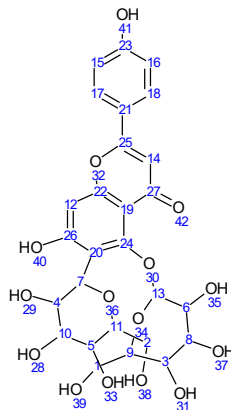
$d_N(^{13}C+^1H)$: 4.889

10 (ID=102)



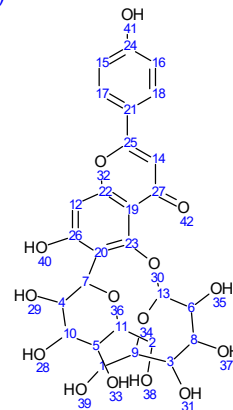
$d_N(^{13}C+^1H)$: 4.889

11 (ID=326)



$d_N(^{13}C+^1H)$: 4.892

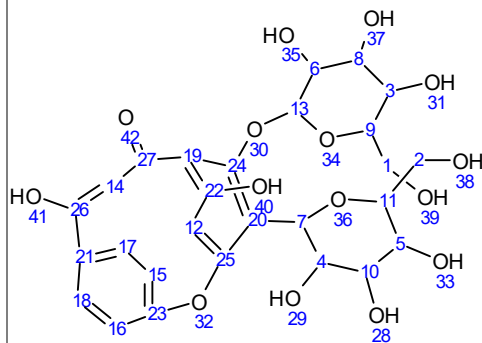
12 (ID=161)



$d_N(^{13}C+^1H)$: 4.892

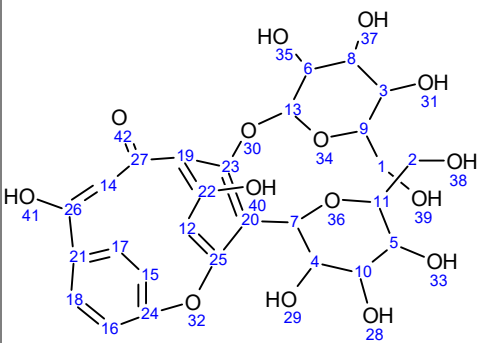
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13 (ID=255)



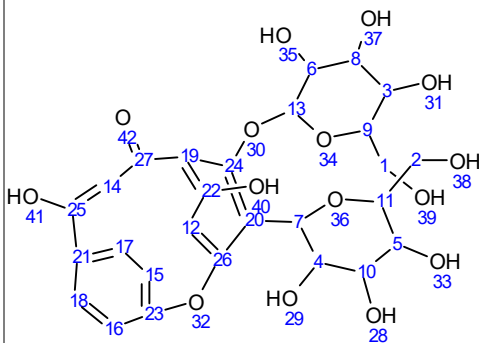
$d_N(^{13}C+^1H)$: 6.518

14 (ID=100)



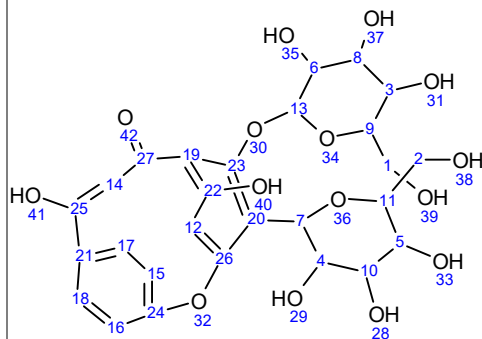
$d_N(^{13}C+^1H)$: 6.518

15 (ID=324)



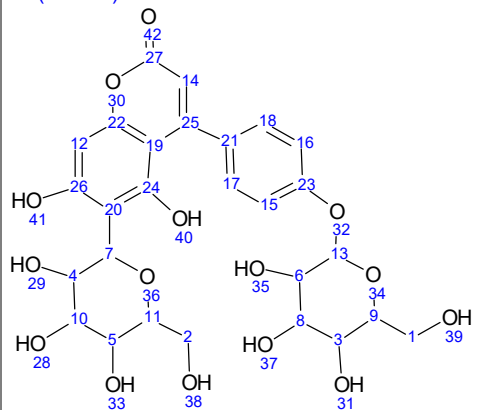
$d_N(^{13}C+^1H)$: 6.521

16 (ID=159)



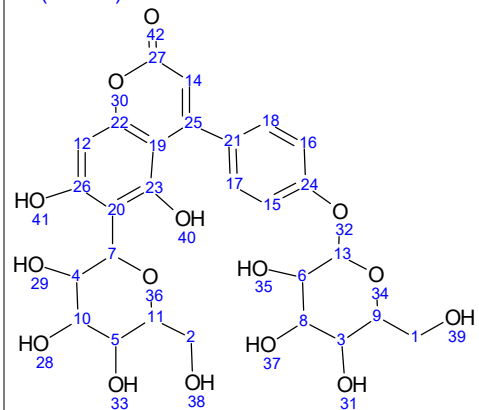
$d_N(^{13}C+^1H)$: 6.521

17 (ID=330)



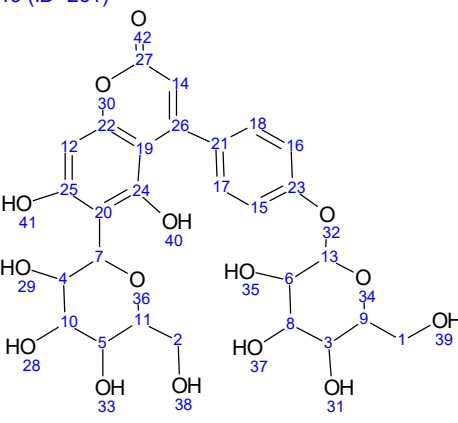
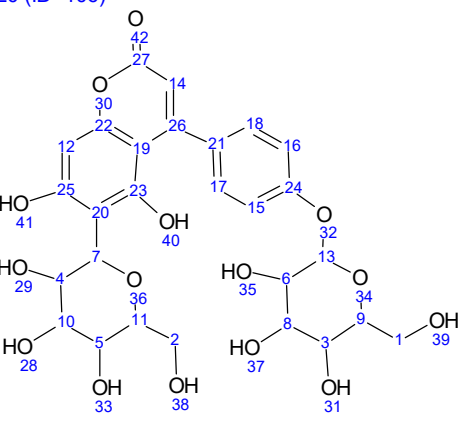
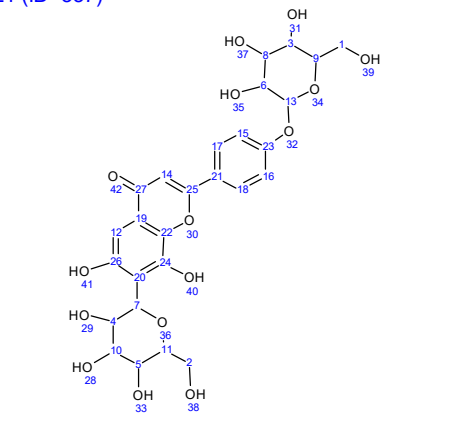
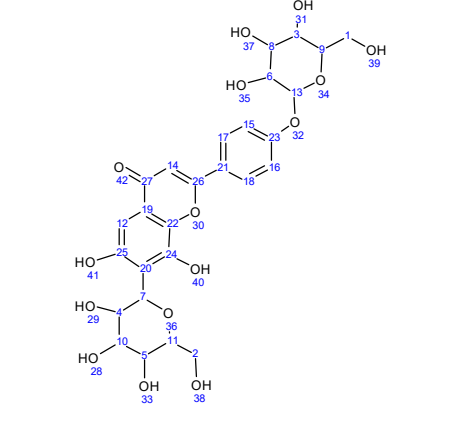
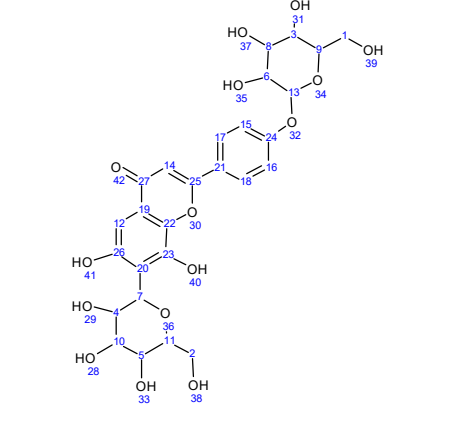
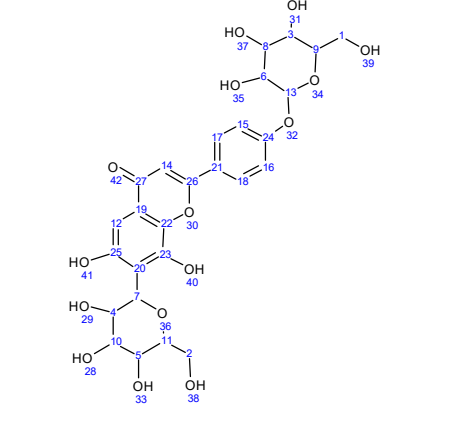
$d_N(^{13}C+^1H)$: 6.806

18 (ID=165)



$d_N(^{13}C+^1H)$: 6.806

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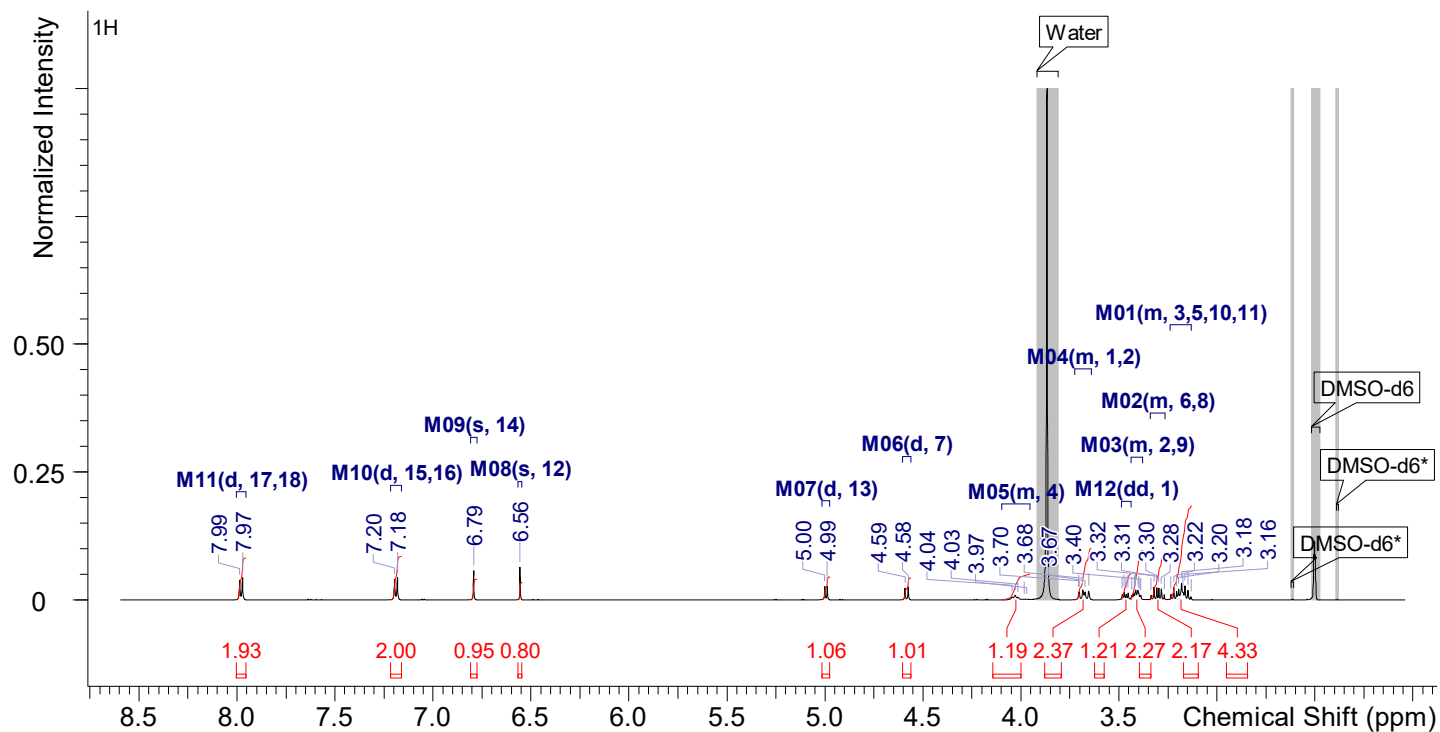
<p>19 (ID=261)</p> 	<p>20 (ID=106)</p> 	<p>21 (ID=337)</p> 
<p>$d_N(^{13}C+^1H)$: 6.806</p>	<p>$d_N(^{13}C+^1H)$: 6.806</p>	<p>$d_N(^{13}C+^1H)$: 7.212</p>
<p>22 (ID=270)</p> 	<p>23 (ID=172)</p> 	<p>24 (ID=113)</p> 
<p>$d_N(^{13}C+^1H)$: 7.212</p>	<p>$d_N(^{13}C+^1H)$: 7.212</p>	<p>$d_N(^{13}C+^1H)$: 7.212</p>

Appendix (Additional Data)

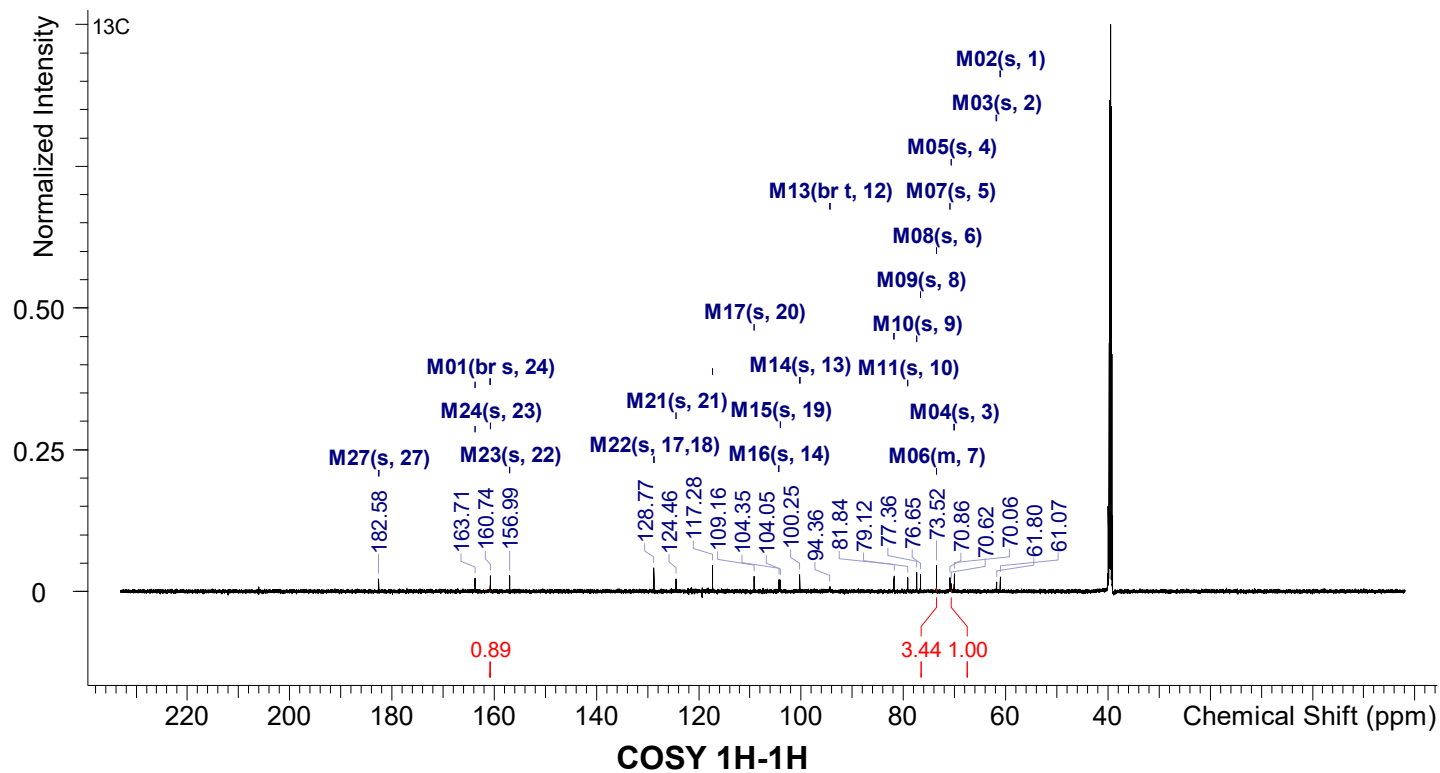
Experimental Spectra Data

standard 1H

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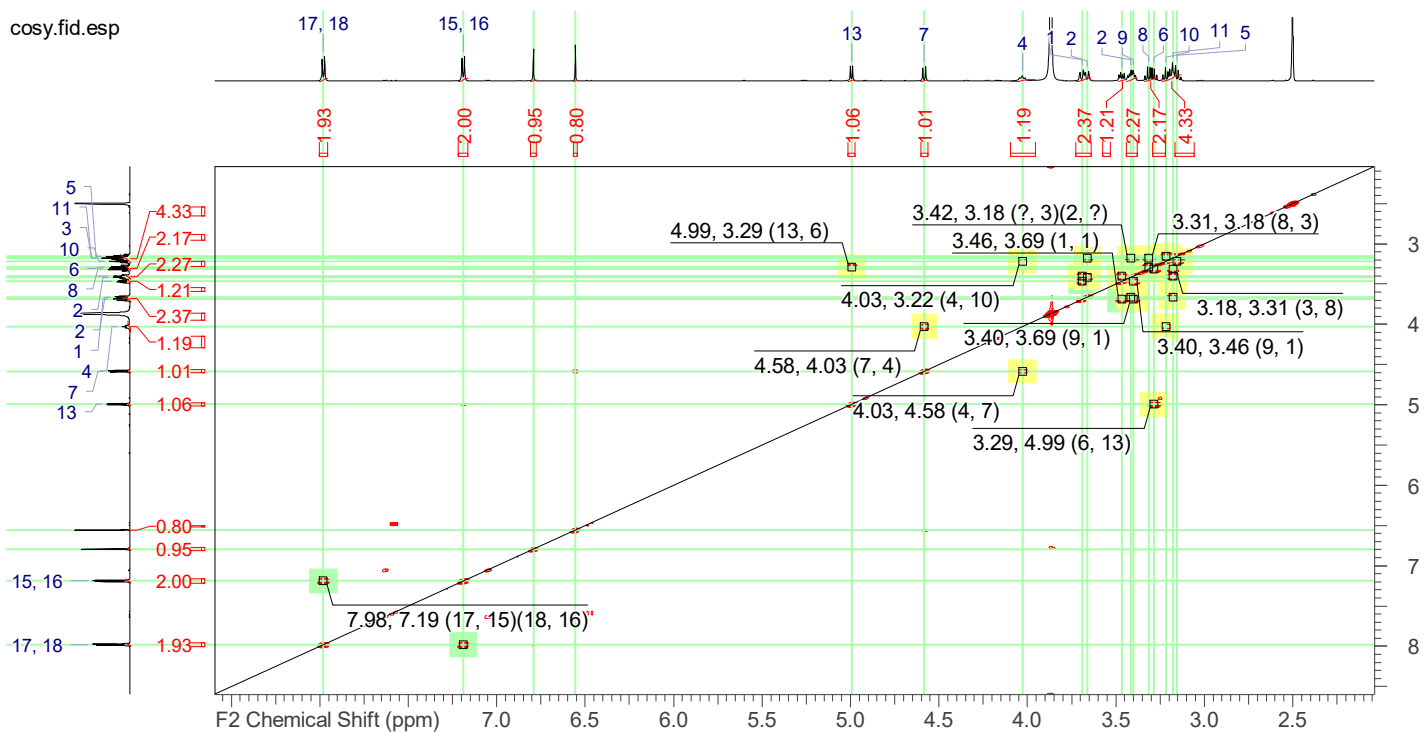


standard 13C

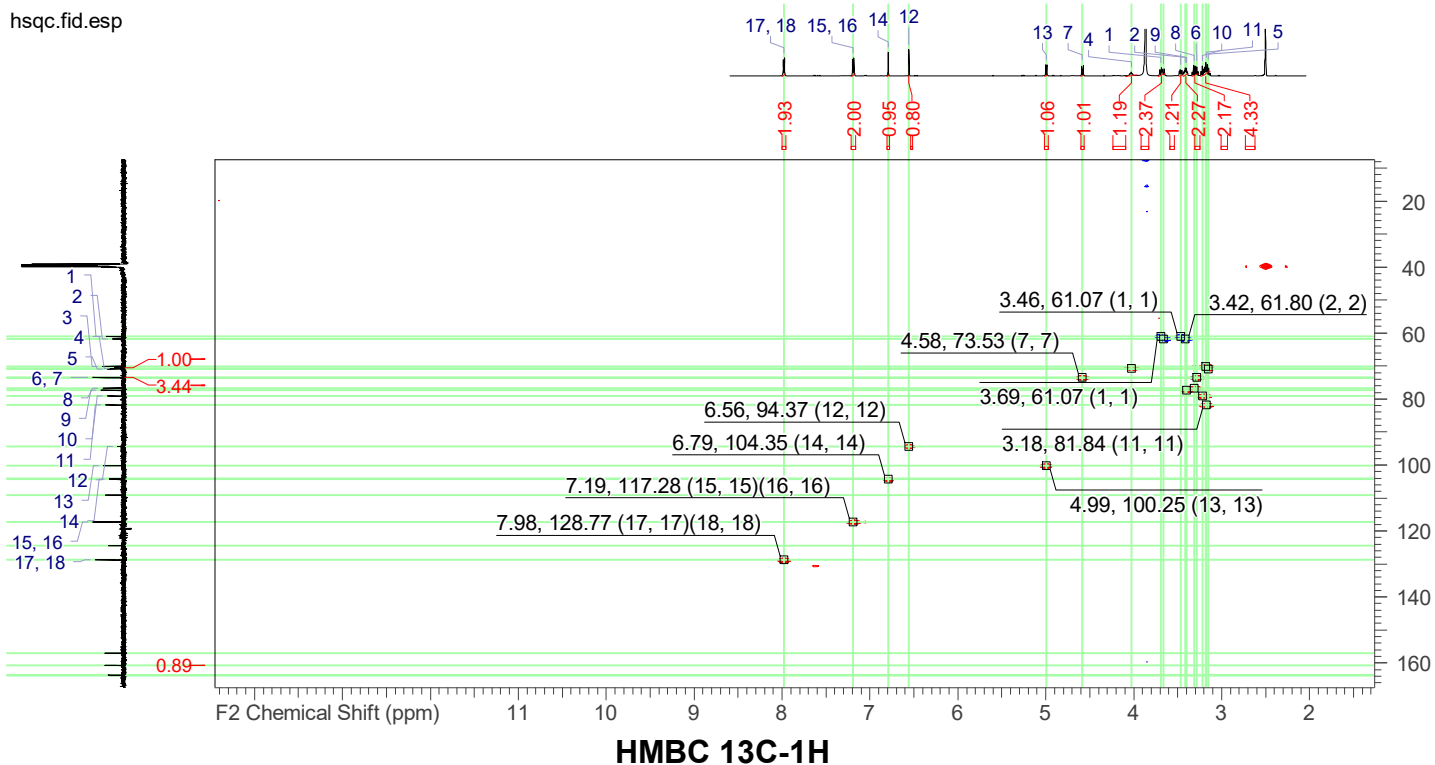


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cosy.fid.esp

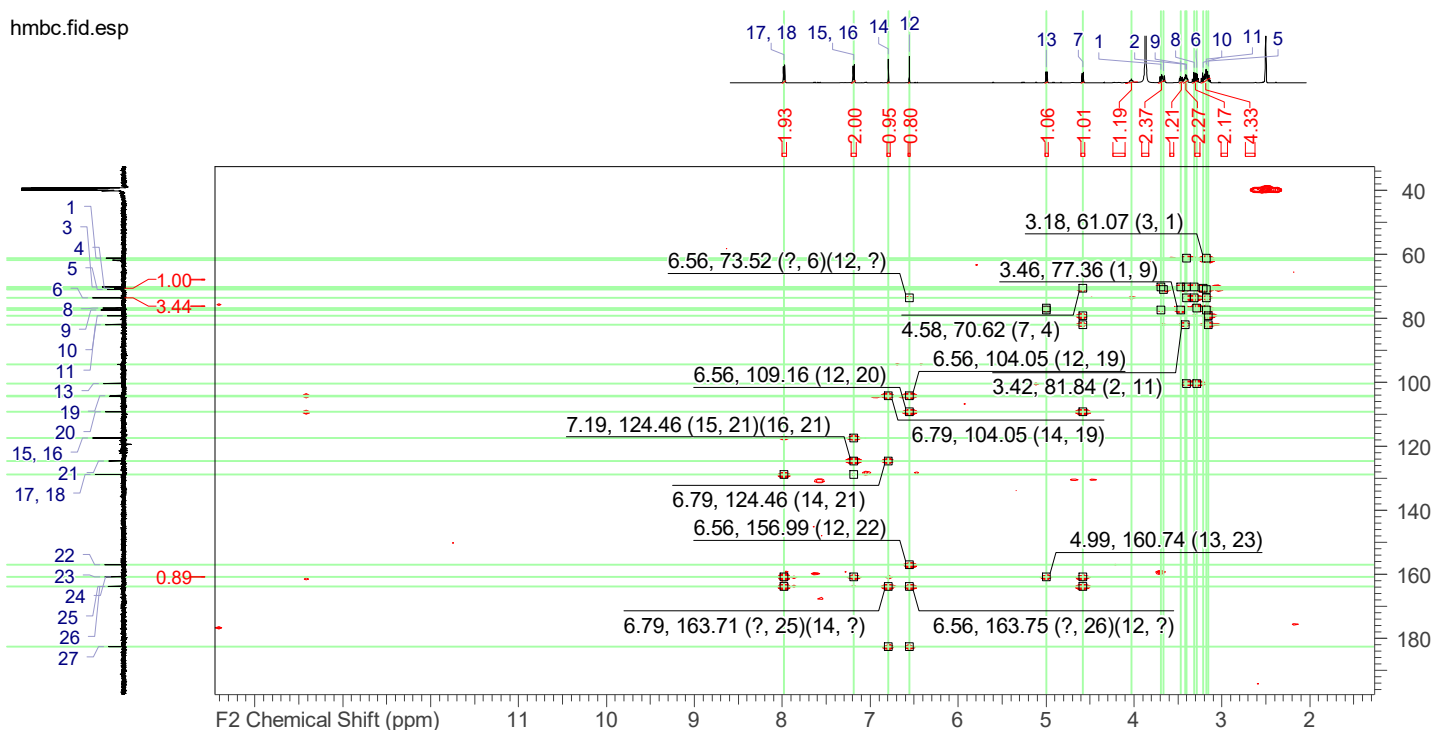


hscq.fid.esp



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hmbc.fid.esp



Elucidation Protocol

Start: Structure Generation 09/22/2023 10:24:27

Correlation Spectroscopy Based Structure Generator options:

Keep Generated Structures = Yes

Clear Generated Structures List Before Generation = Yes

Add Structures Already Existing in Generated Structures List = No

Transfer Spectra to Generated Structures = Yes

Use Assignment when Removing Duplicates = Yes

Allow Filter during Generation = Yes

Use Only 1000 First MCD(s)

Allow "Fuzzy" Generation = Yes

"Fuzzy" Generation Options were Determined Automatically

2D NMR Spectral Data Must Contain Connectivities = Real spectrum

Increase Connectivity Length when Merging Connectivities = No

Allow Bonds between Heteroatoms = No

Allow Bonds between Heteroatoms of the Same Atom Type = No

Use NMR Shifts Correlation Table = 2

Maximum bond multiplicity = 3

MCD #1 (ID = 0): (779319/0) structures have been generated and (430/0) structures stored

779319 structure(s) have been generated by Correlation Spectroscopy Based Generator and 430 structure(s) have been stored.

Generation time: 121 h 47 m 01 s (Check: 0 s, Generation: 121 h 47 m 00 s 969 ms)

No (from No) connectivities have been extended during generation

Generation has been interrupted by the user (stop button pressed)

Finish: Structure Generation 09/27/2023 12:11:30