

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](http://www.acdlabs.com)) for **compound 1**

# Structure Elucidation Report for compound 1

## 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 = C<sub>27</sub>H<sub>32</sub>O<sub>15</sub>

### Spectral Data:

standard <sup>1</sup>H - 20 peaks

merged <sup>1</sup>H - 20 peaks

standard <sup>13</sup>C - 27 peaks

merged <sup>13</sup>C - 27 peaks

COSY <sup>1</sup>H-<sup>1</sup>H - 25 peaks

HSQC-DEPT <sup>13</sup>C-<sup>1</sup>H - 20 peaks

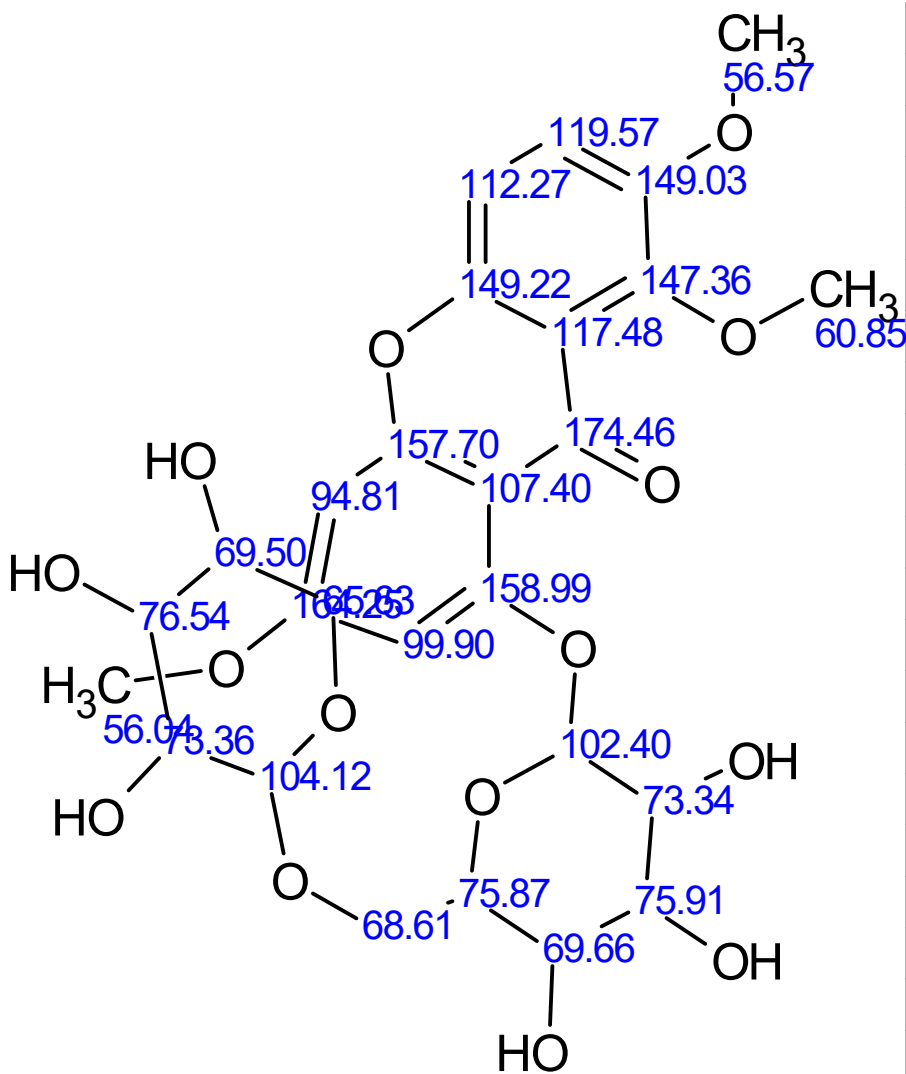
HMBC <sup>13</sup>C-<sup>1</sup>H - 49 peaks

## Most Probable Structure

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

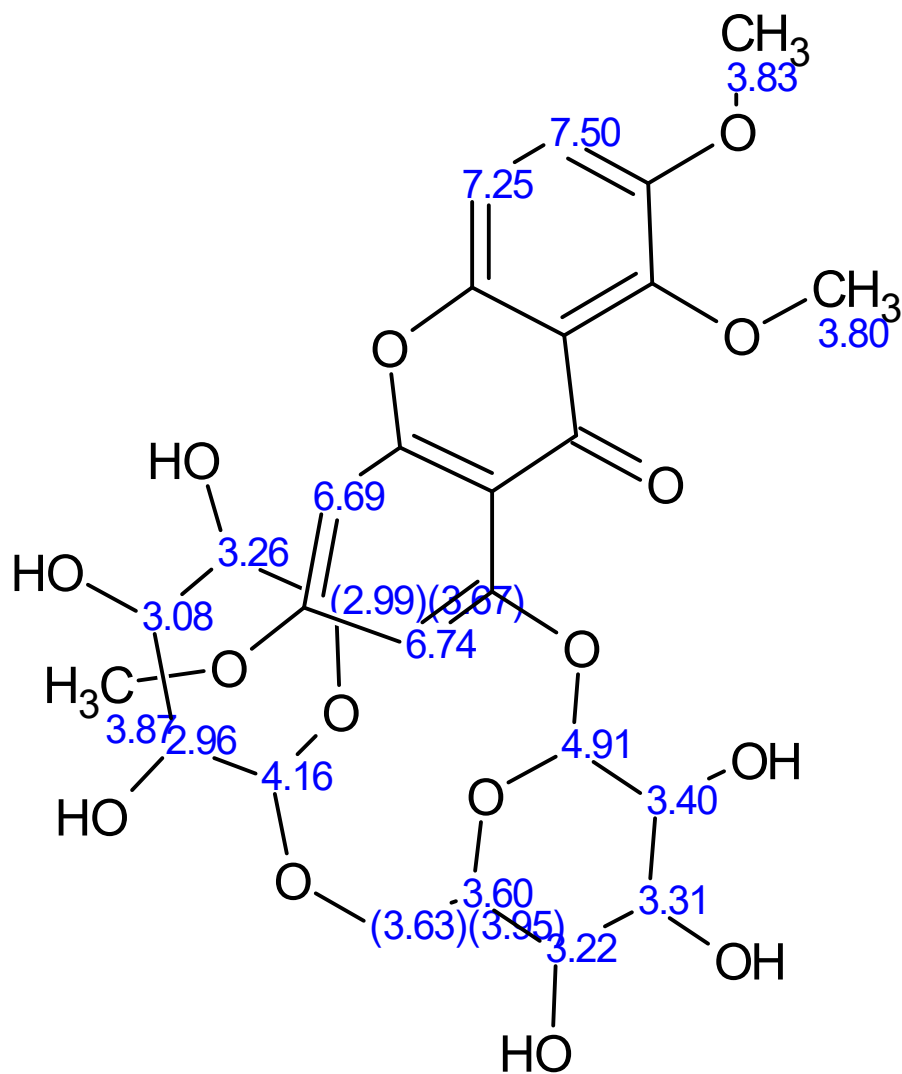
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## Carbon Assignment



#	N	Shift (ppm)	Atoms	XHn
1	1	56.035	1	CH3(q)
2	2	56.568	1	CH3(q)
3	3	60.848	1	CH3(q)
4	4	65.632	1	CH2(t)
5	5	68.609	1	CH2(t)
6	6	69.496	1	CH(d)
7	7	69.659	1	CH(d)
8	8	73.343	1	CH(d)
9	9	73.356	1	CH(d)
10	10	75.868	1	CH(d)
11	11	75.906	1	CH(d)
12	12	76.542	1	CH(d)
13	13	94.806	1	CH(d)
14	14	99.900	1	CH(d)
15	15	102.398	1	CH(d)
16	16	104.123	1	CH(d)
17	19	107.405	1	C(s)
18	17	112.269	1	CH(d)
19	20	117.476	1	C(s)
20	18	119.566	1	CH(d)
21	21	147.359	1	C(s)
22	22	149.026	1	C(s)
23	23	149.216	1	C(s)
24	24	157.699	1	C(s)
25	25	158.994	1	C(s)
26	26	164.253	1	C(s)

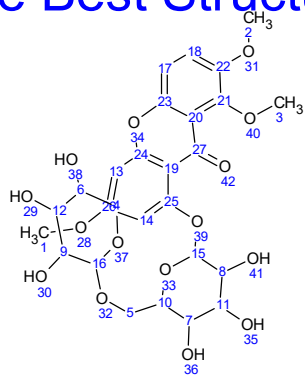
## Proton Assignment



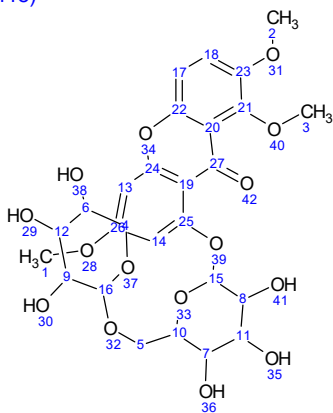
#	N	Mark	Shift (ppm)	Protons
1	9		2.959	1
2	4		2.987	1
3	12		3.077	1
4	7		3.220	1
5	6		3.256	1
6	11		3.312	1
7	8		3.404	1
8	10		3.600	1
9	5		3.627	1
10	4		3.666	1
11	3		3.795	3
12	2		3.833	3
13	1		3.869	3
14	5		3.950	1
15	16		4.161	1
16	15		4.911	1
17	13		6.694	1
18	14		6.744	1
19	17		7.247	1

## Generated Structures

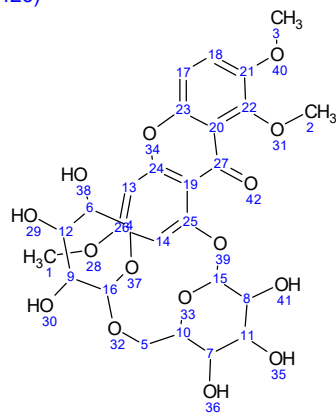
1 (ID=425)

**The Best Structure** $d_N(^{13}\text{C}+^1\text{H})$ : 5.089

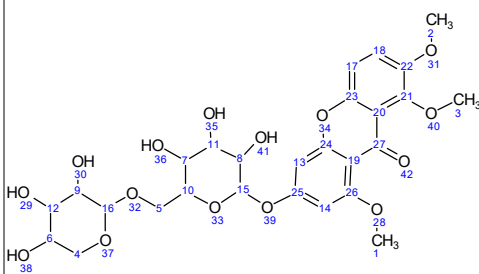
2 (ID=418)

 $d_N(^{13}\text{C}+^1\text{H})$ : 5.103

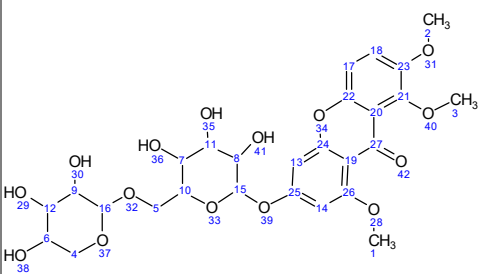
3 (ID=426)

 $d_N(^{13}\text{C}+^1\text{H})$ : 5.383

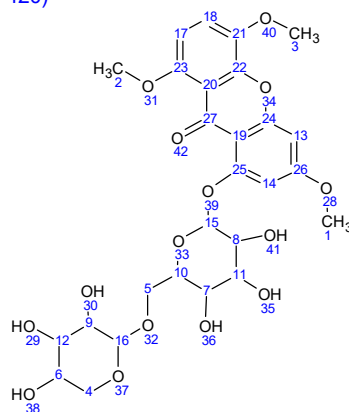
4 (ID=378)

 $d_N(^{13}\text{C}+^1\text{H})$ : 5.476

5 (ID=371)

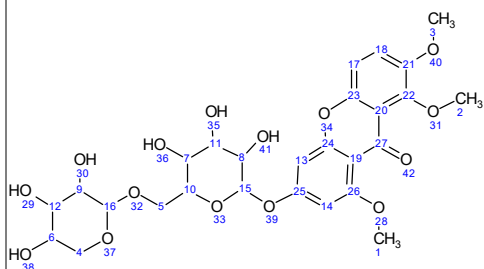
 $d_N(^{13}\text{C}+^1\text{H})$ : 5.490

6 (ID=420)

 $d_N(^{13}\text{C}+^1\text{H})$ : 5.725

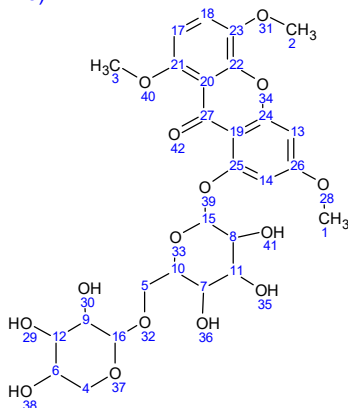
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7 (ID=379)



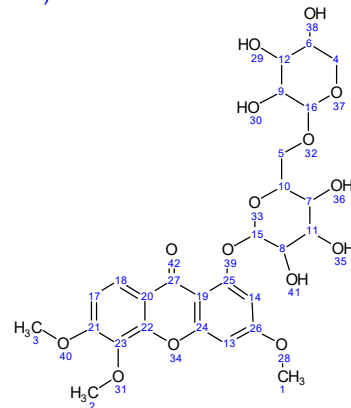
$d_N(^{13}C+^1H)$ : 5.770

8 (ID=419)



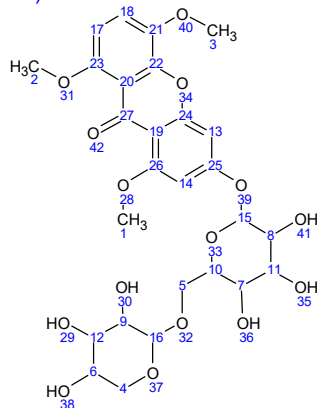
$d_N(^{13}C+^1H)$ : 5.863

9 (ID=417)



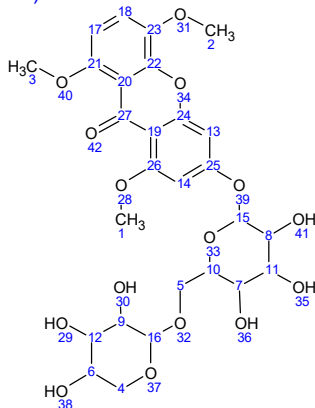
$d_N(^{13}C+^1H)$ : 5.903

10 (ID=373)



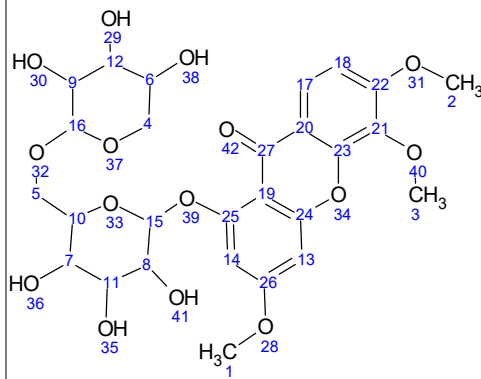
$d_N(^{13}C+^1H)$ : 6.134

11 (ID=372)



$d_N(^{13}C+^1H)$ : 6.271

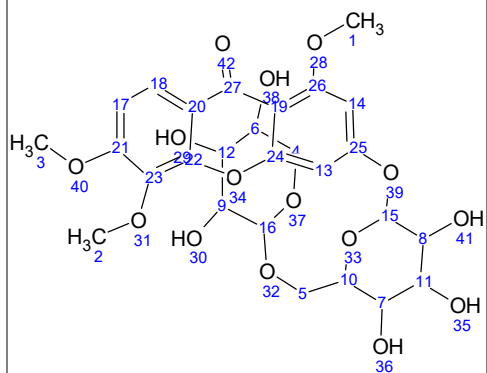
12 (ID=421)



$d_N(^{13}C+^1H)$ : 6.286

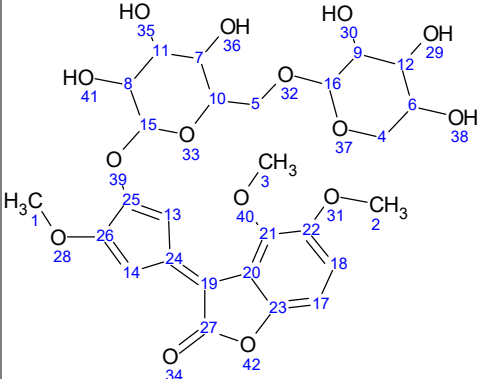
# Structure Elucidation Report for compound 1 (Page 6)

13 (ID=370)



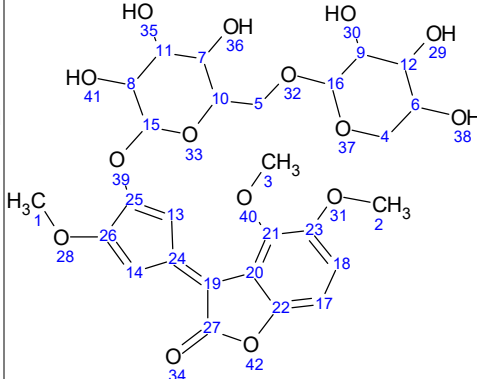
$d_N(^{13}C+^1H)$ : 6.309

14 (ID=337)



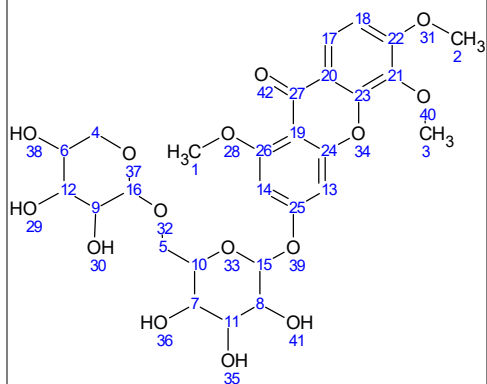
$d_N(^{13}C+^1H)$ : 6.654

15 (ID=336)



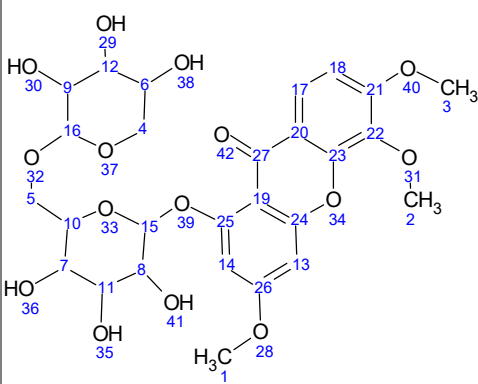
$d_N(^{13}C+^1H)$ : 6.654

16 (ID=374)



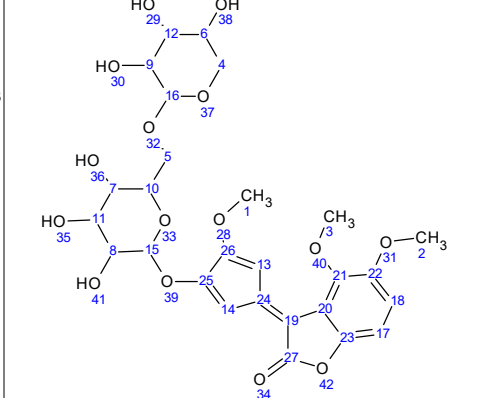
$d_N(^{13}C+^1H)$ : 6.692

17 (ID=422)



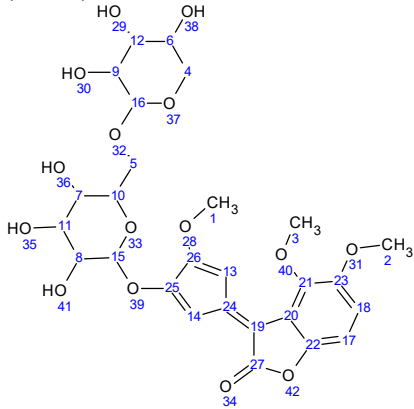
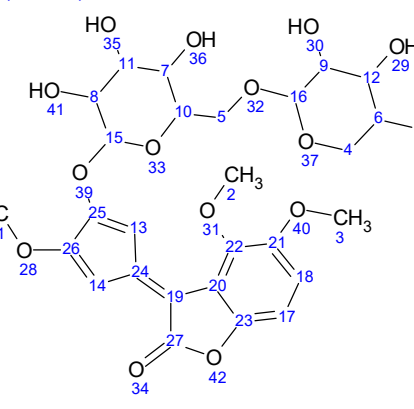
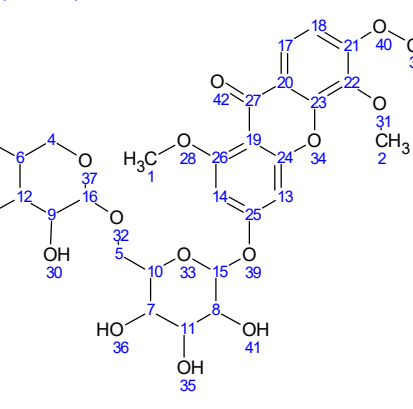
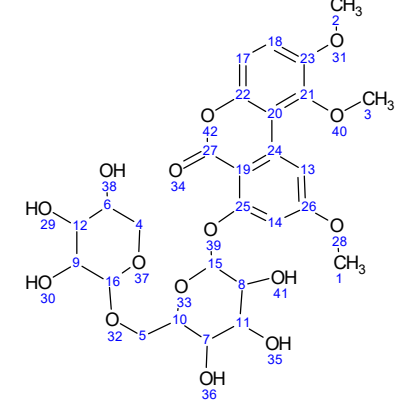
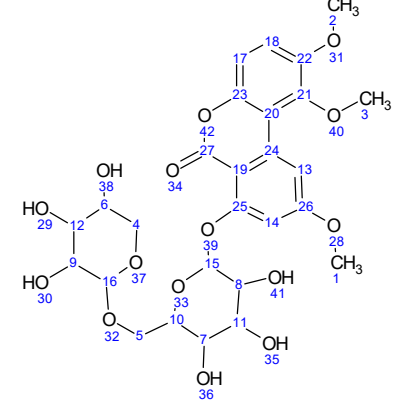
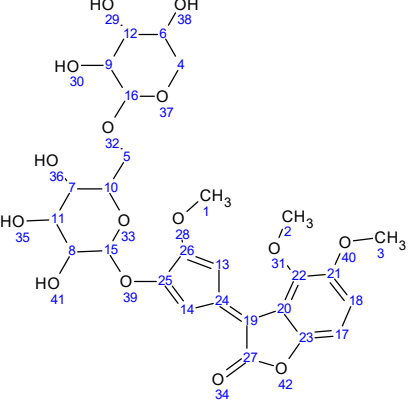
$d_N(^{13}C+^1H)$ : 6.726

18 (ID=301)



$d_N(^{13}C+^1H)$ : 6.799

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<p>19 (ID=300)</p> 	<p>20 (ID=338)</p> 	<p>21 (ID=375)</p> 
<p><math>d_N(^{13}\text{C}+^1\text{H})</math>: 6.799</p>	<p><math>d_N(^{13}\text{C}+^1\text{H})</math>: 7.095</p>	<p><math>d_N(^{13}\text{C}+^1\text{H})</math>: 7.133</p>
<p>22 (ID=393)</p> 	<p>23 (ID=394)</p> 	<p>24 (ID=302)</p> 
<p><math>d_N(^{13}\text{C}+^1\text{H})</math>: 7.192</p>	<p><math>d_N(^{13}\text{C}+^1\text{H})</math>: 7.192</p>	<p><math>d_N(^{13}\text{C}+^1\text{H})</math>: 7.236</p>

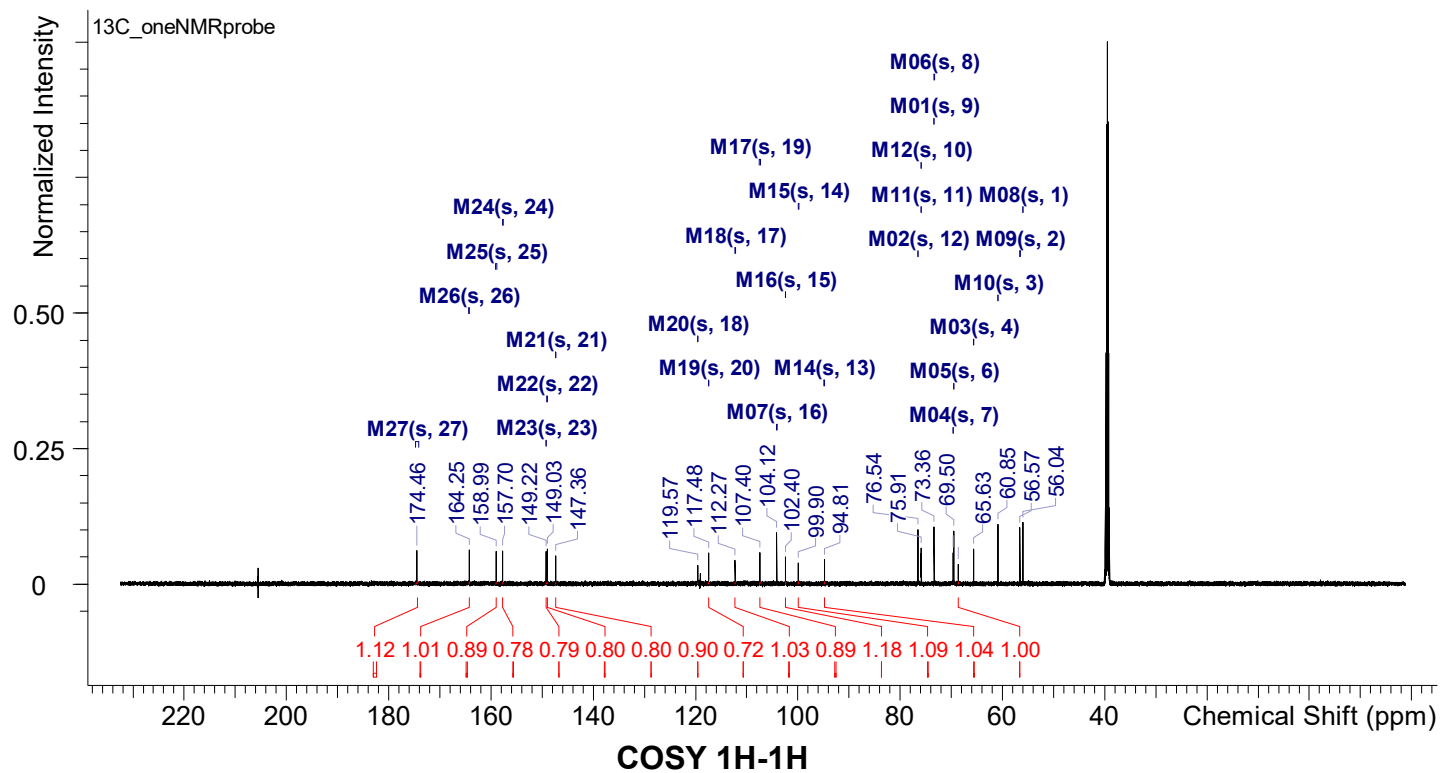
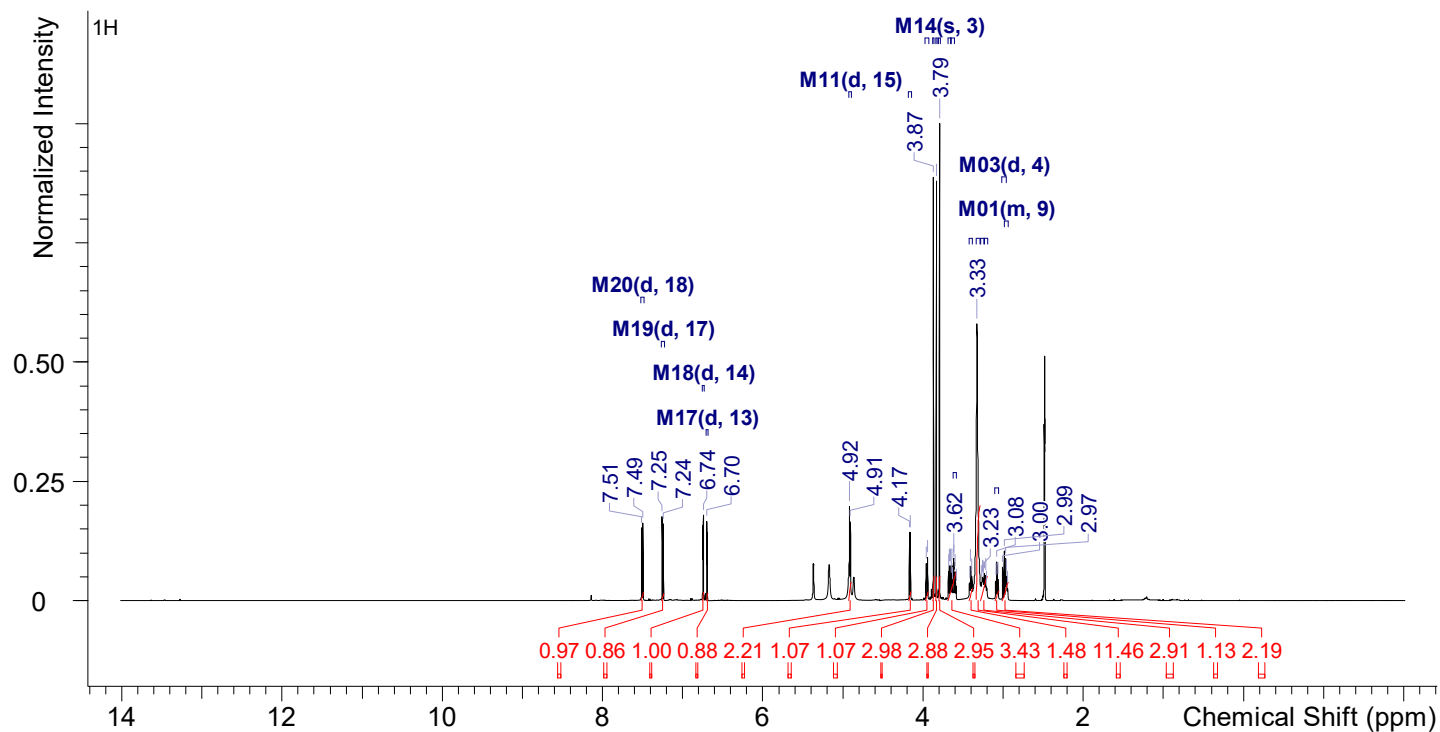
## Appendix (Additional Data)

### Experimental Spectra Data

standard 1H

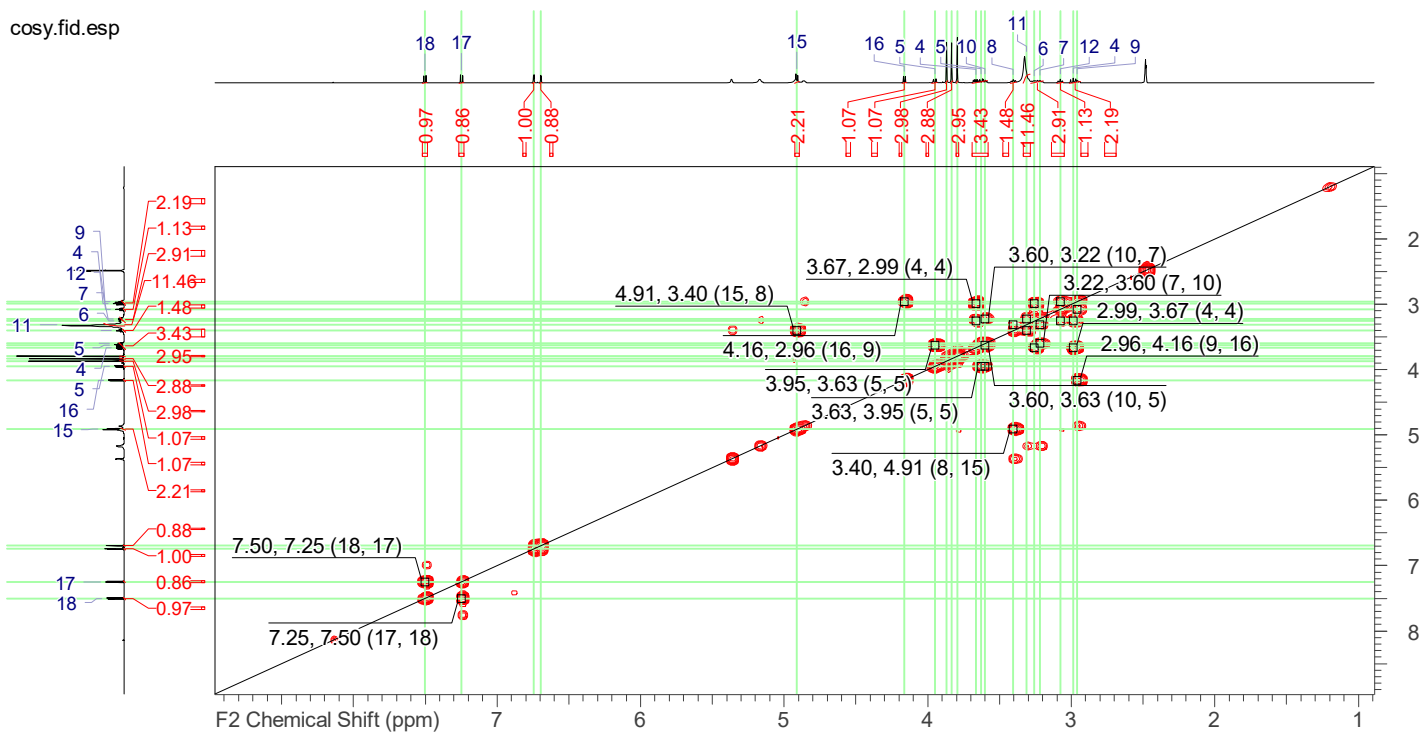


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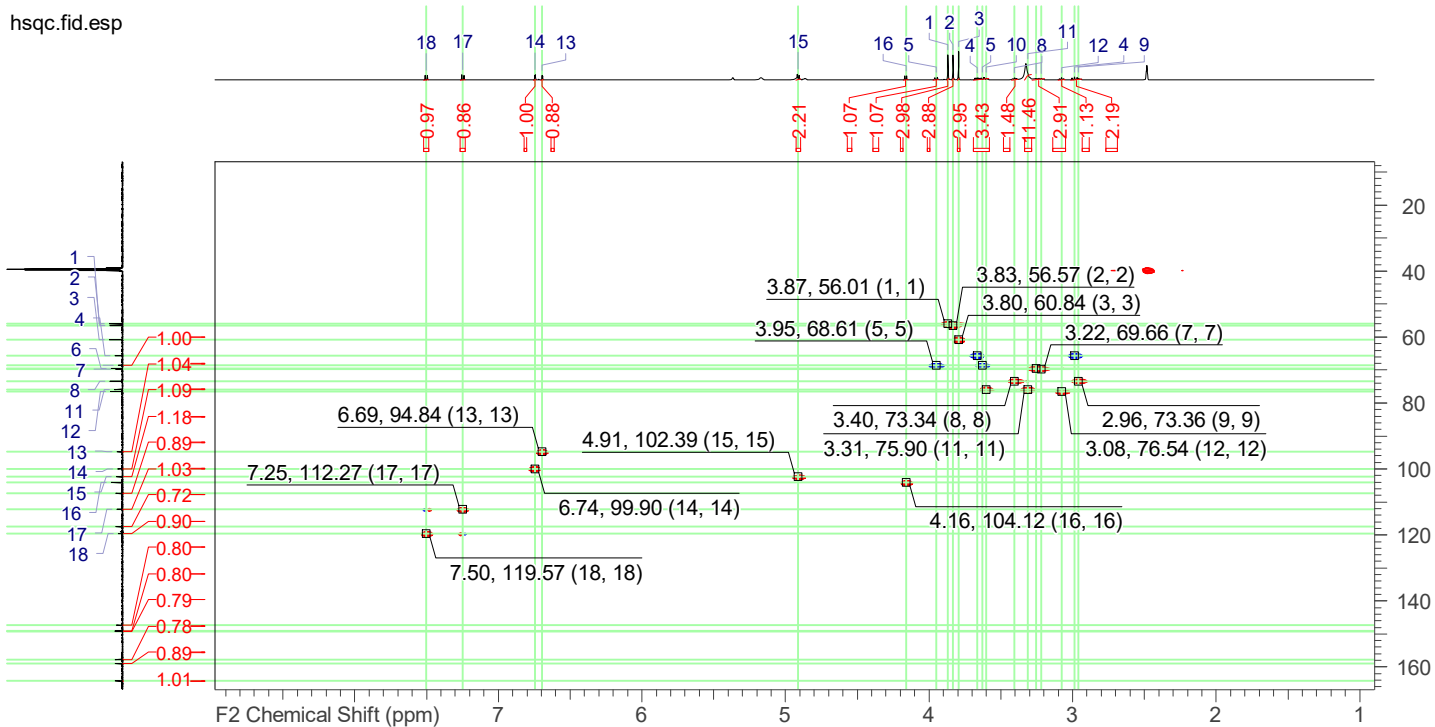


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cosy.fid.esp

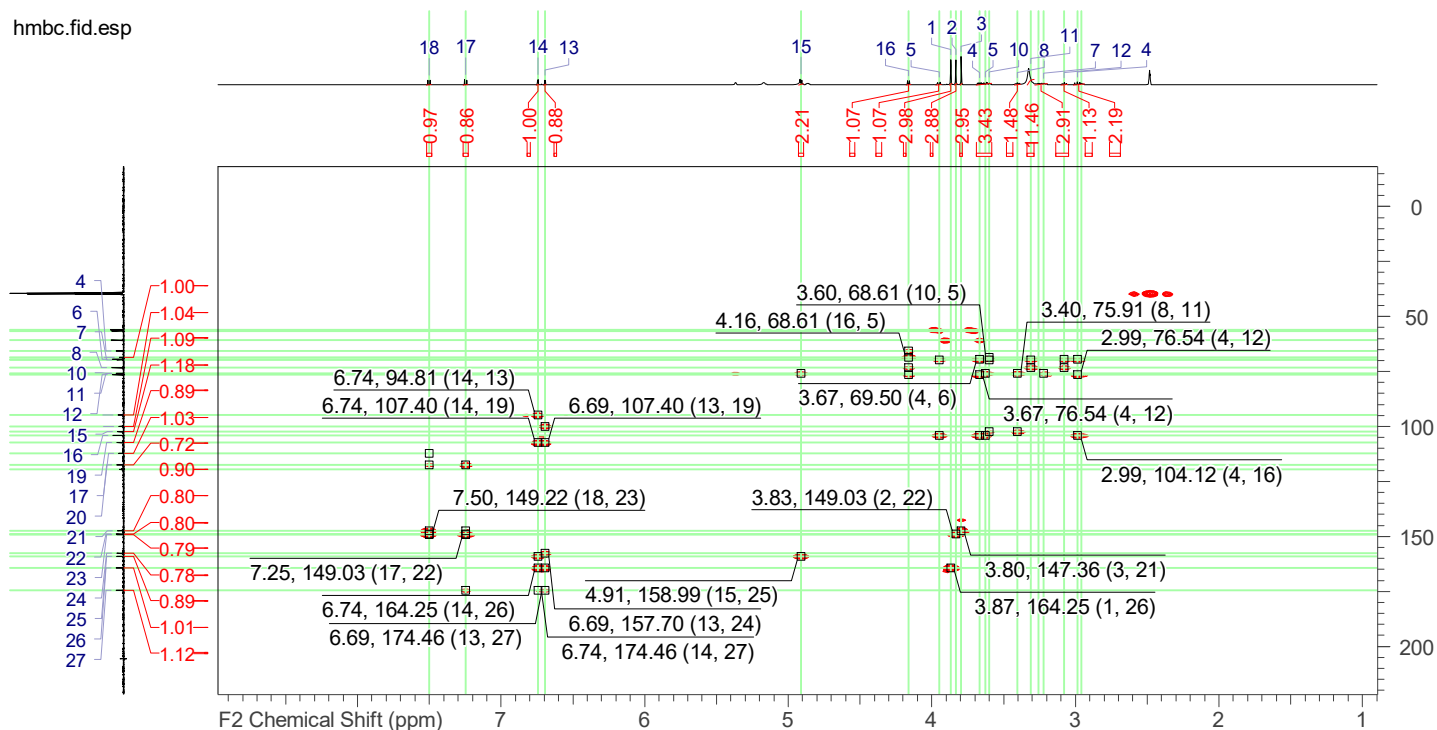


hscq.fid.esp



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hmbc.fid.esp



## Elucidation Protocol

Start: Structure Generation 07/26/2023 15:46:27

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): (197109/0) structures have been generated and (484/0) structures stored

197109 structure(s) have been generated by Correlation Spectroscopy Based Generator and 484 structure(s) have been stored.

Generation time: 2 h 09 m 15 s (Check: 5 s, Generation: 2 h 09 m 10 s 340 ms)

No (from No) connectivities have been extended during generation

Finish: Structure Generation 07/26/2023 17:55:43