

Supporting information

Hybrid flavan-flavanones from *Friesodielsia desmoides* and their inhibitory activities against nitric oxide production

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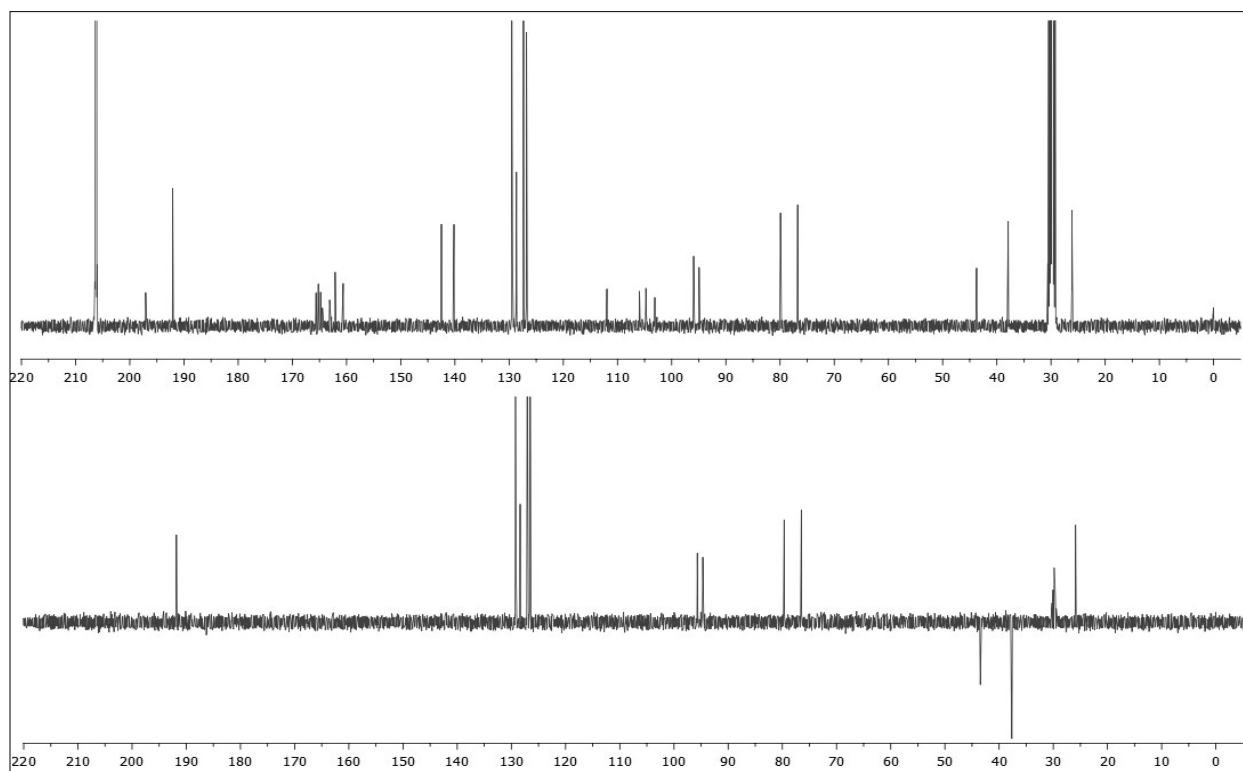
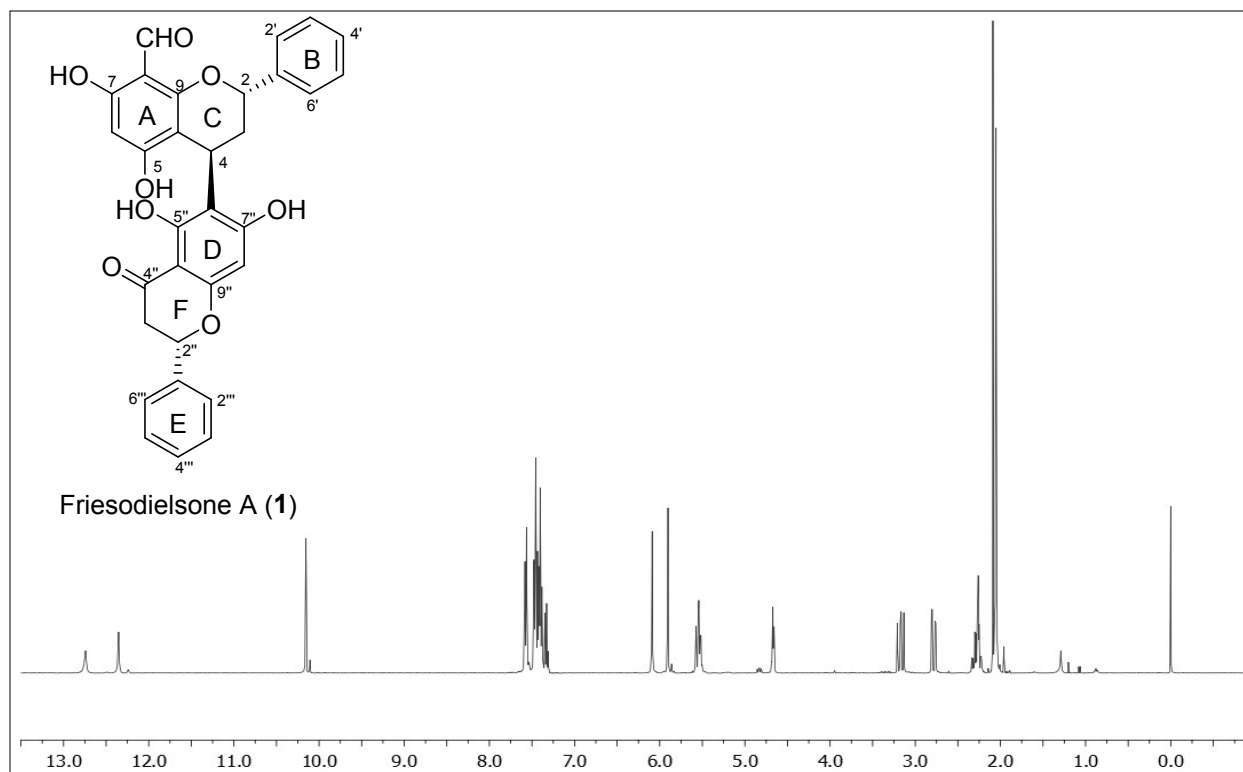
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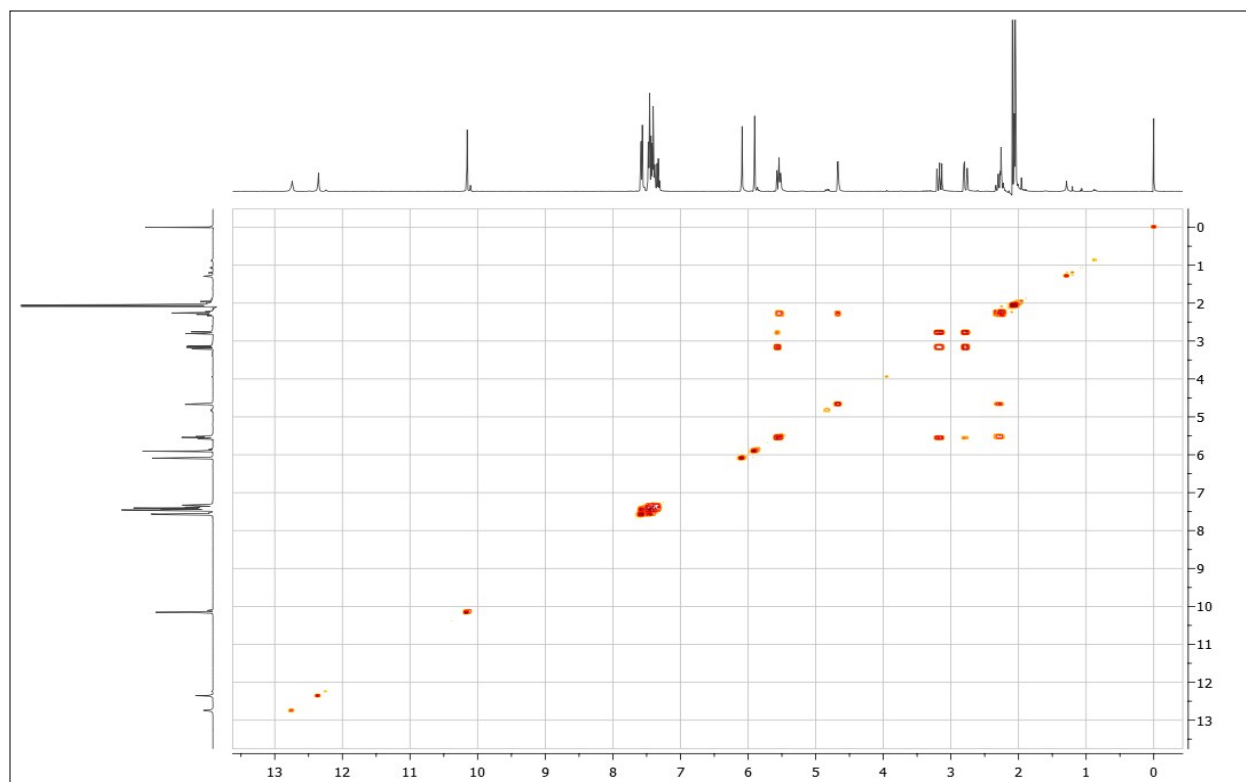
^cSchool of Chemistry, University of Wollongong, Wollongong, New South Wales, 2522 Australia

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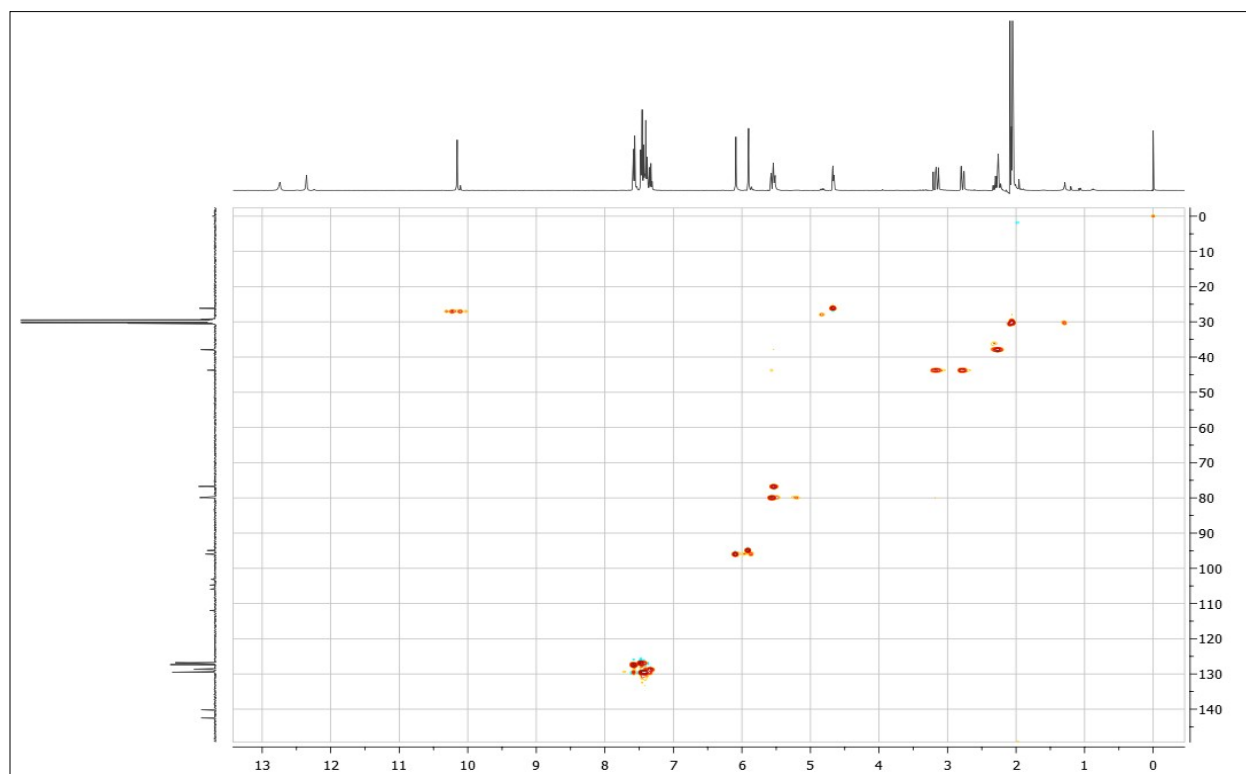
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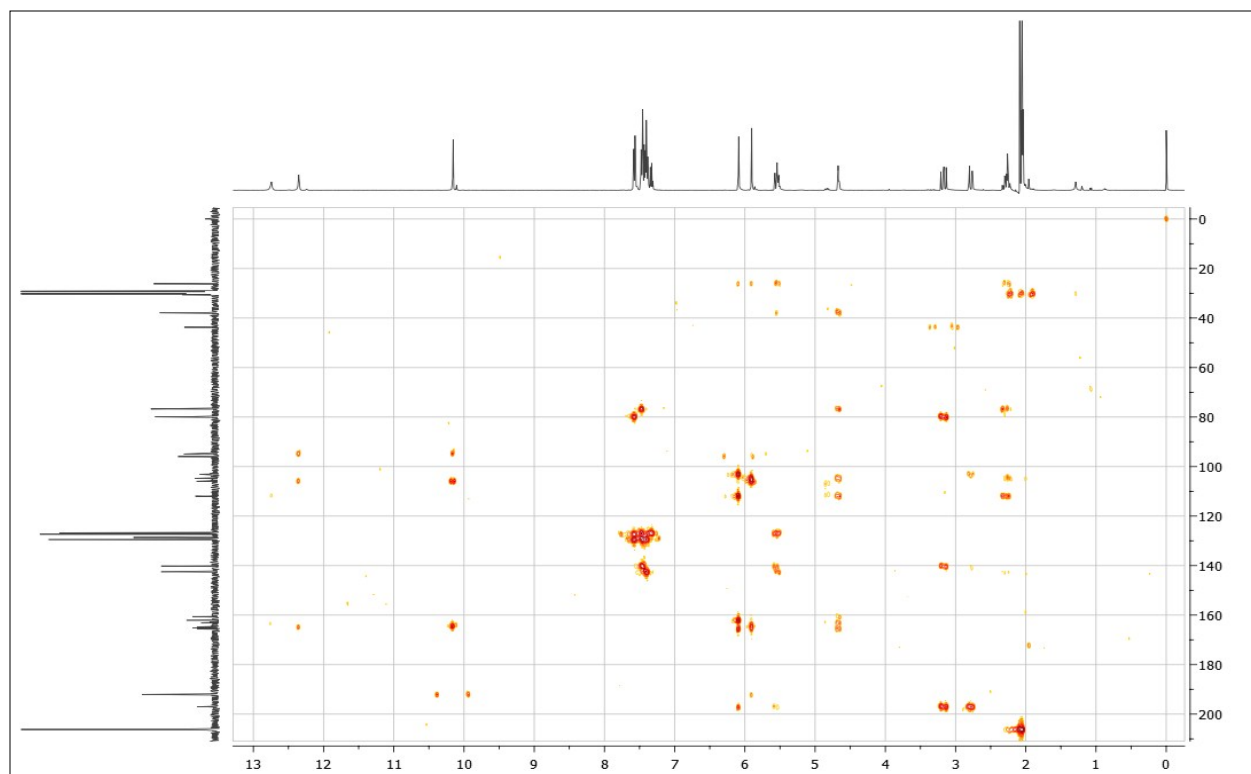




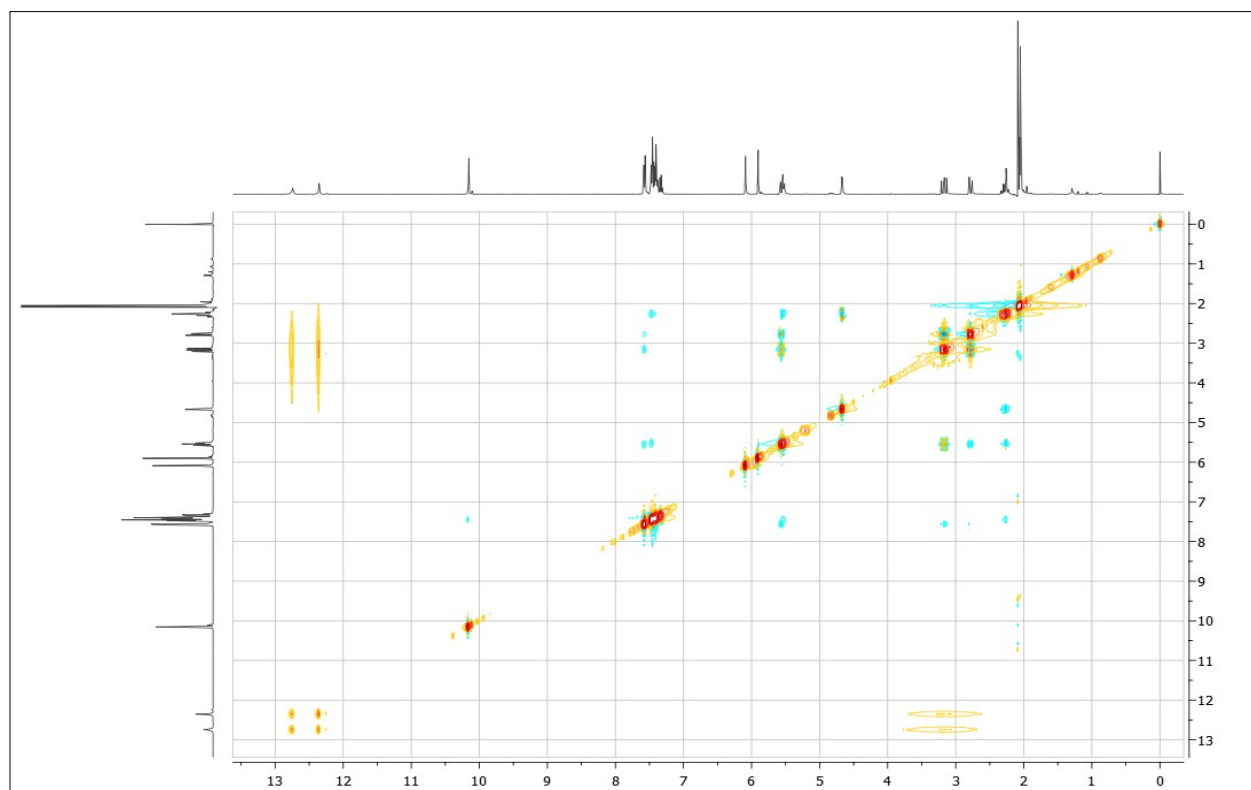
S3. COSY NMR spectrum (acetone- d_6) of compound **1**



S4. HMQC NMR spectrum (acetone- d_6) of compound **1**



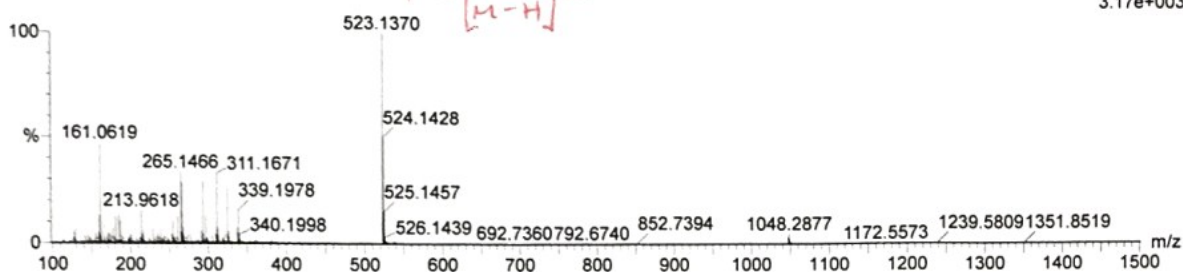
S5. HMBC NMR spectrum (acetone- d_6) of compound **1**



S6. NOESY spectrum (acetone- d_6) of compound **1**

Monoisotopic Mass, Even Electron Ions
 133 formula(e) evaluated with 3 results within limits (up to 20 closest results for each mass)
 Elements Used:
 C: 0-40 H: 0-50 N: 0-2 O: 0-10
 7EPK8B
 SP SuratL 7EPK8B 49 (0.991) Cm (43:60)

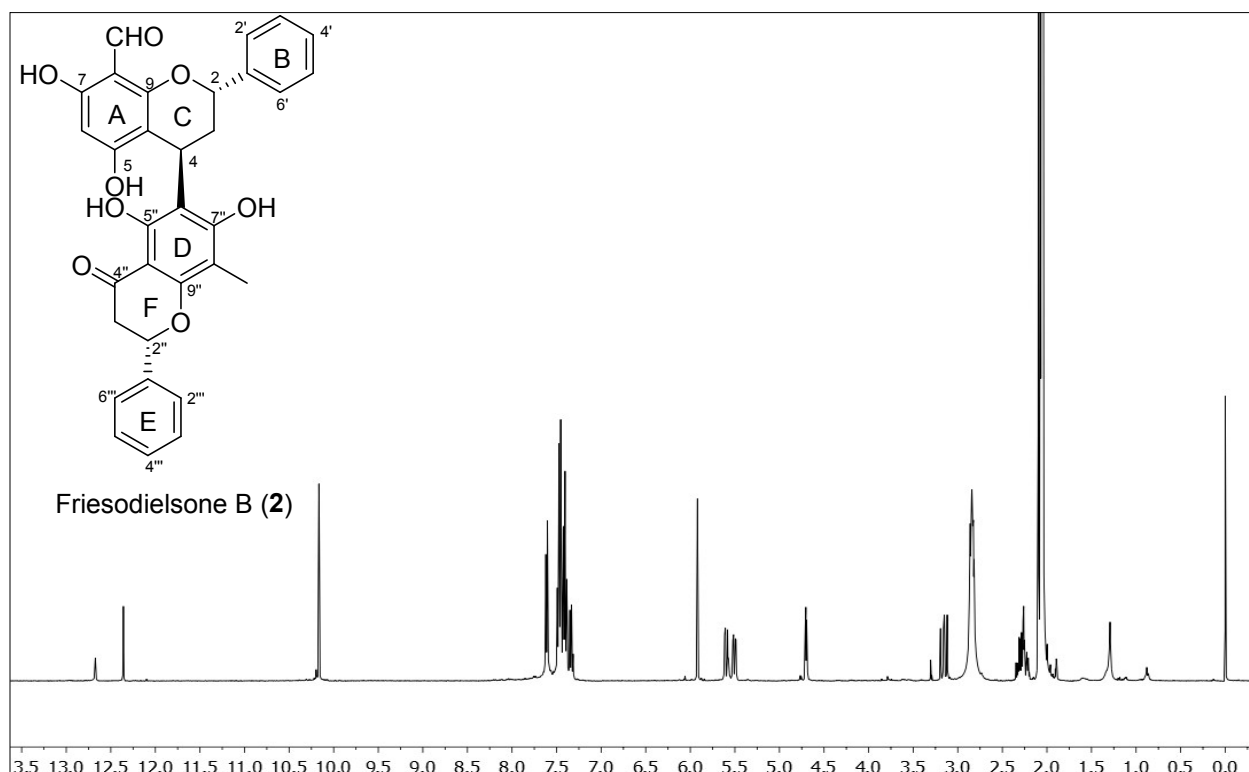
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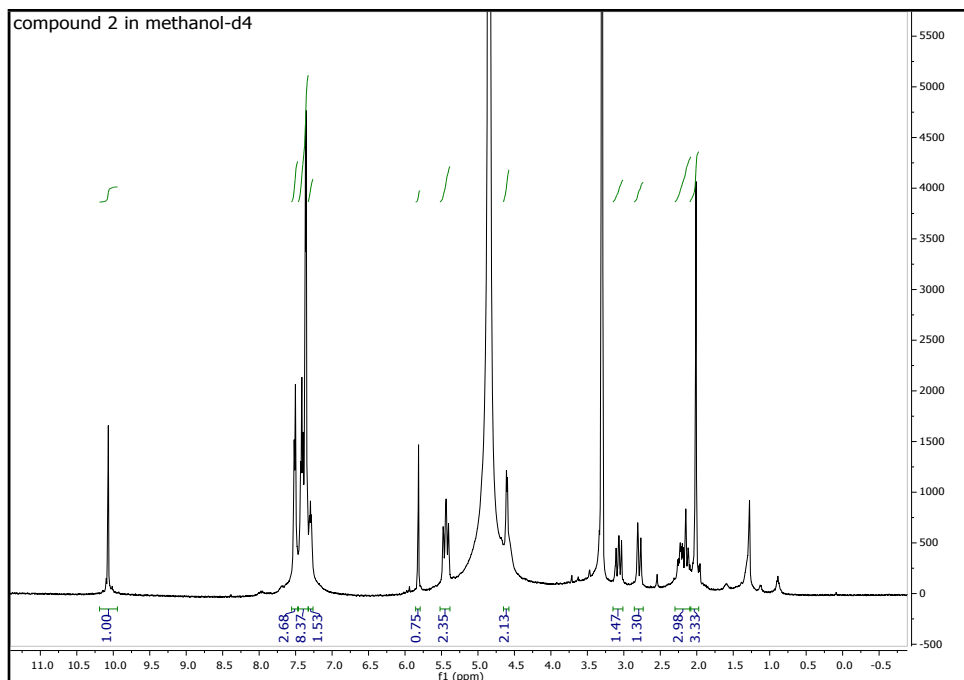
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 Maximum: 5.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
523.1370	523.1353	1.7	3.2	16.5	174.4	3.0	C26 H23 N2 O10
	523.1393	-2.3	-4.4	20.5	172.5	1.1	C31 H23 O8
	523.1334	3.6	6.9	29.5	171.8	0.5	C38 H19 O3

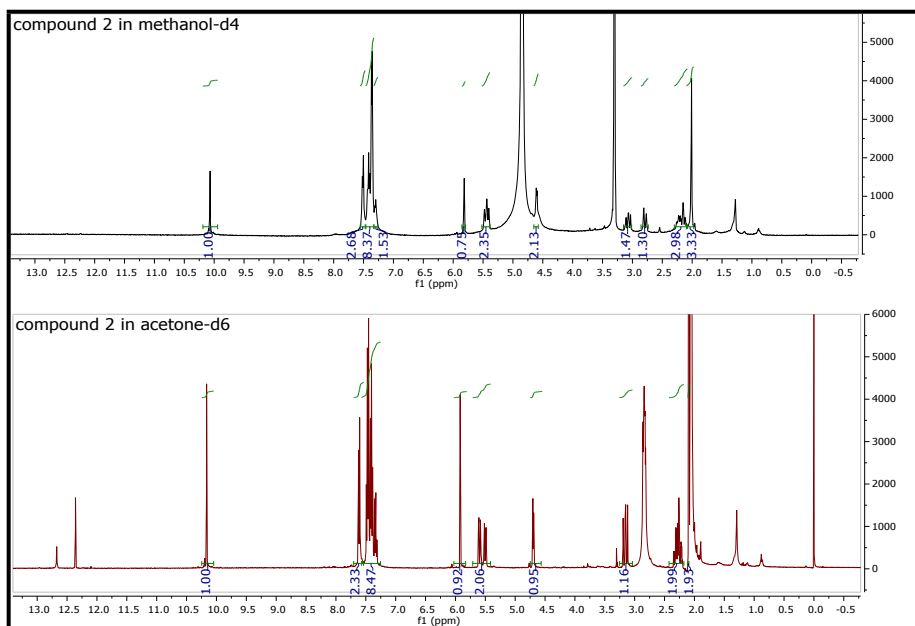
S7. HRESIMS spectrum of compound 1



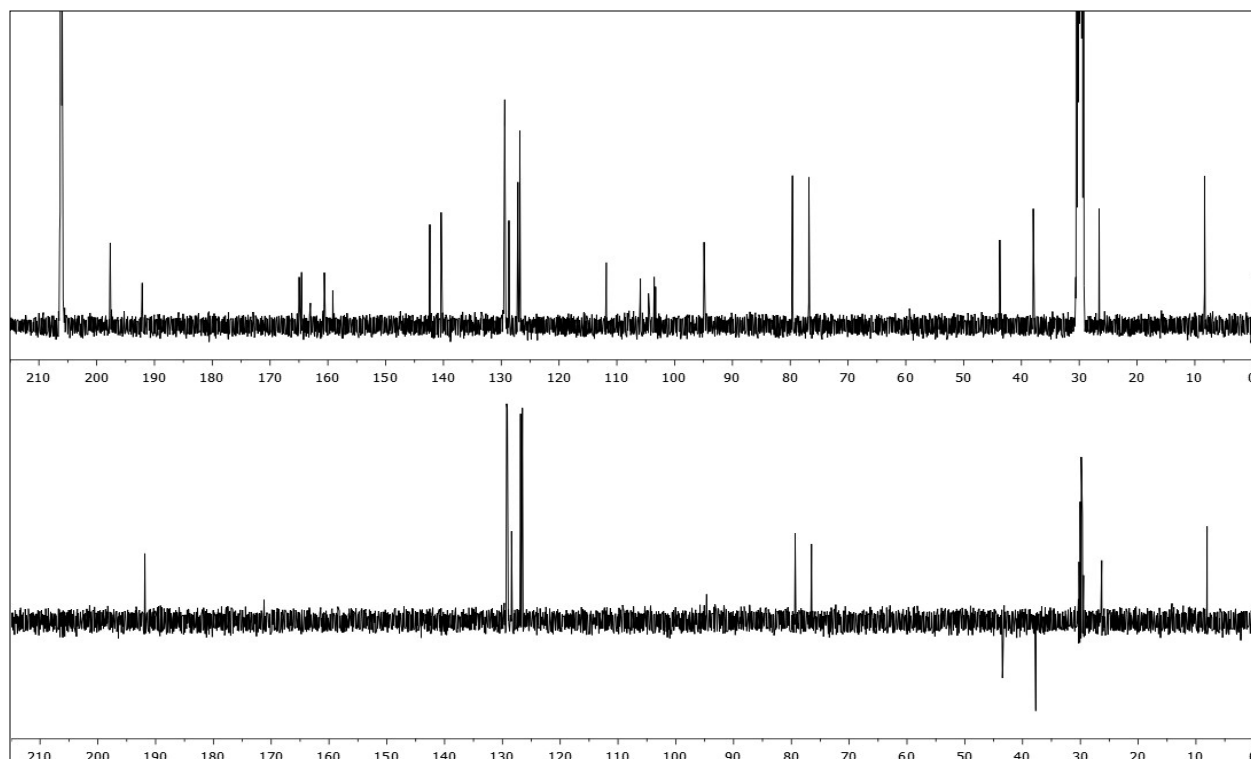
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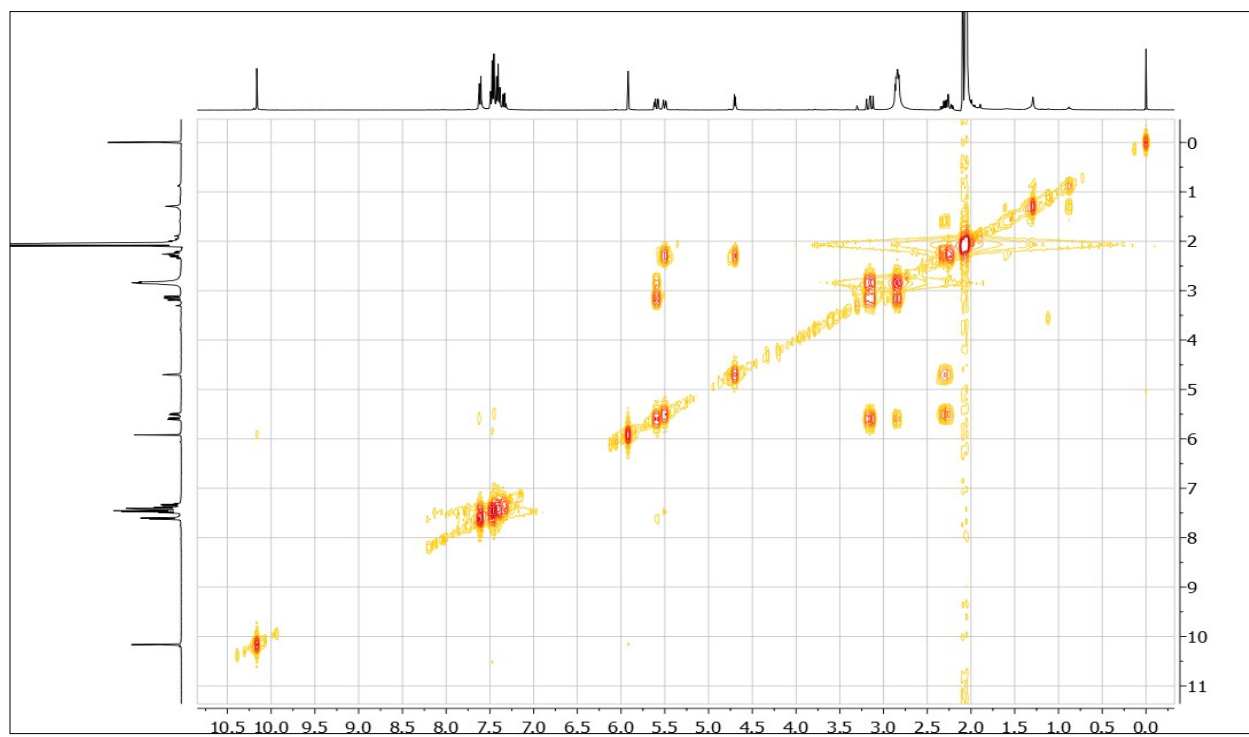
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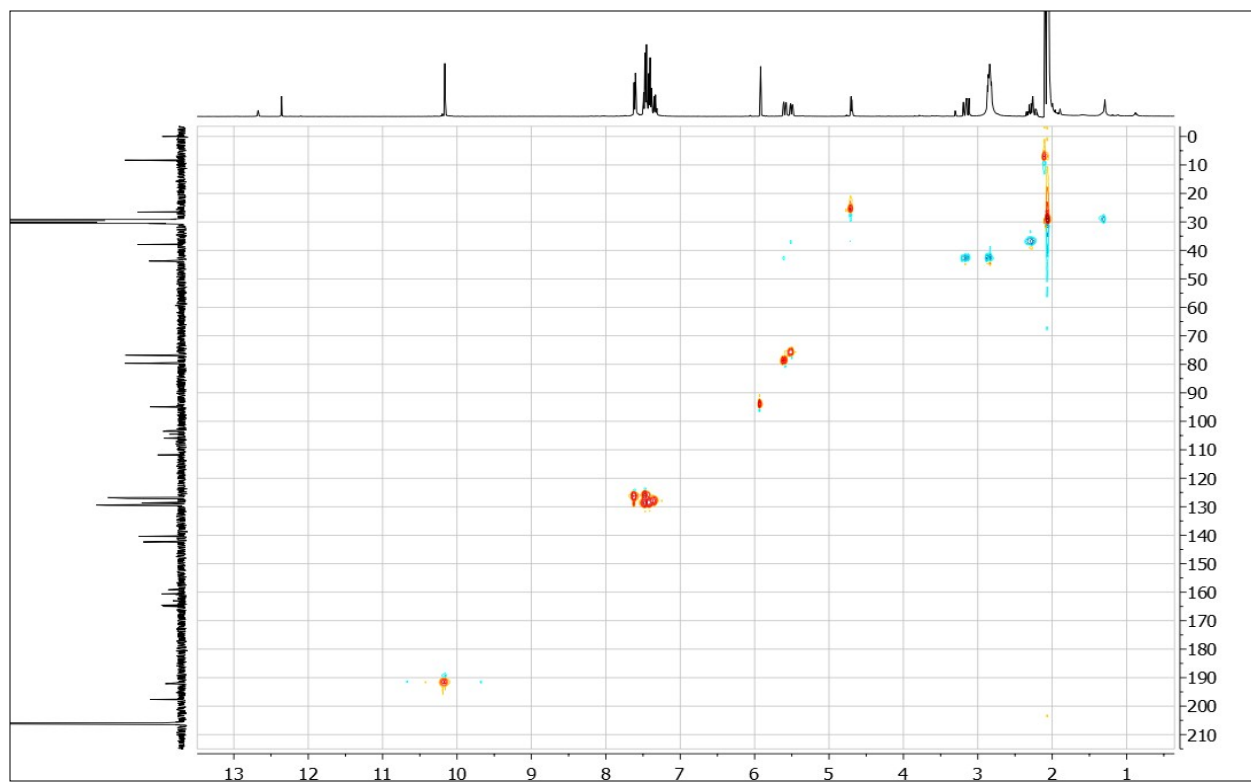
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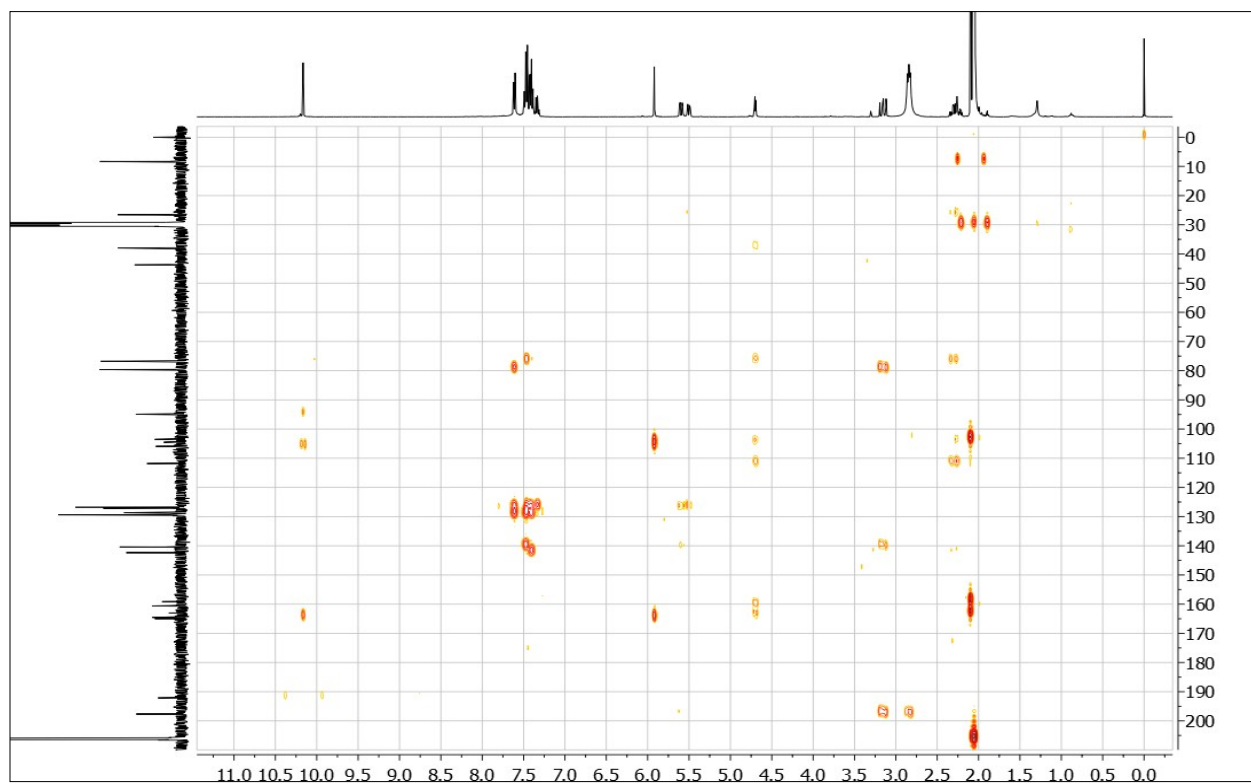
S11. ^{13}C NMR spectrum (100 MHz, acetone- d_6) of compound 2



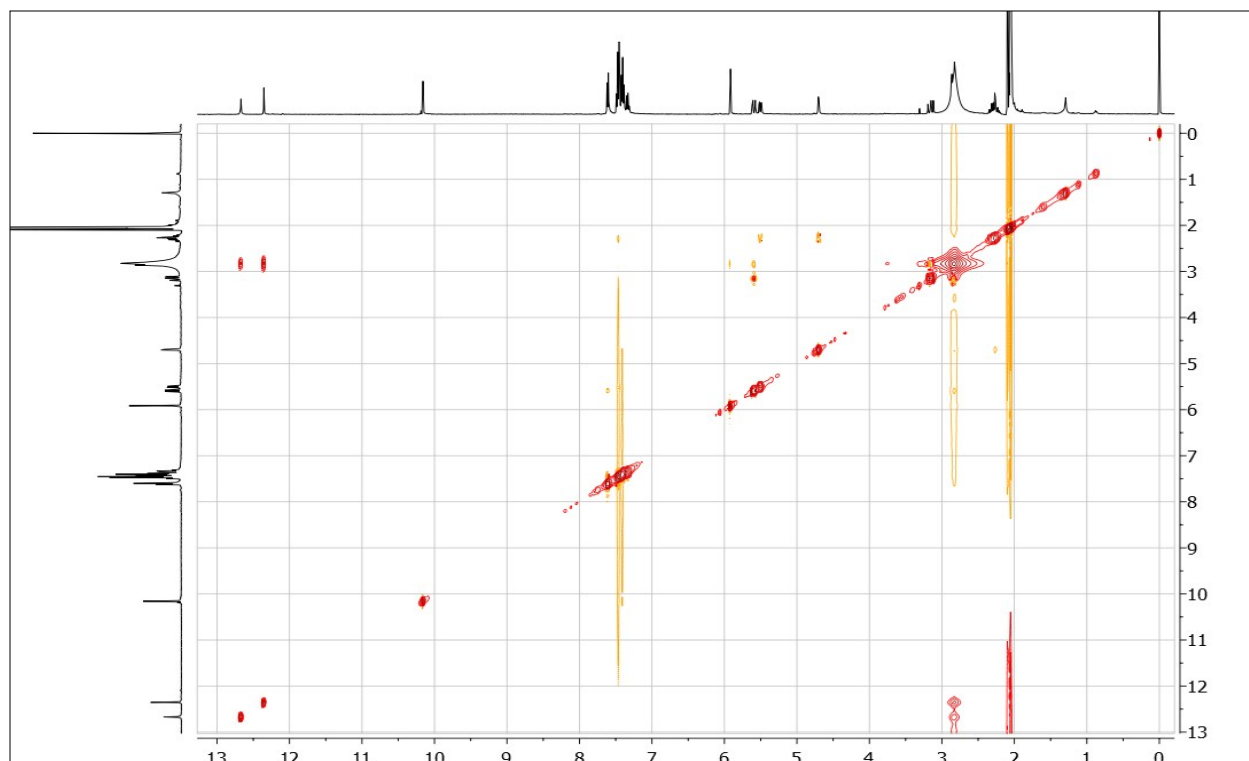
S12. COSY NMR spectrum (acetone- d_6) of compound 2



S13. HMQC NMR spectrum (acetone- d_6) of compound 2



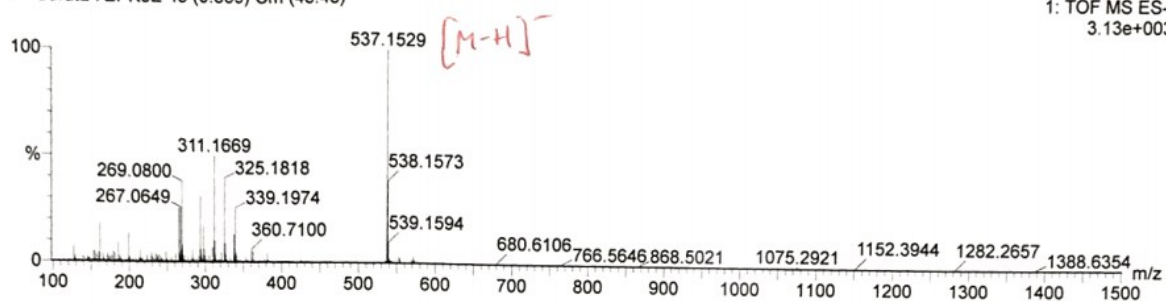
S14. HMBC NMR spectrum (acetone- d_6) of compound 2



S15. NOESY spectrum (acetone- d_6) of compound 2

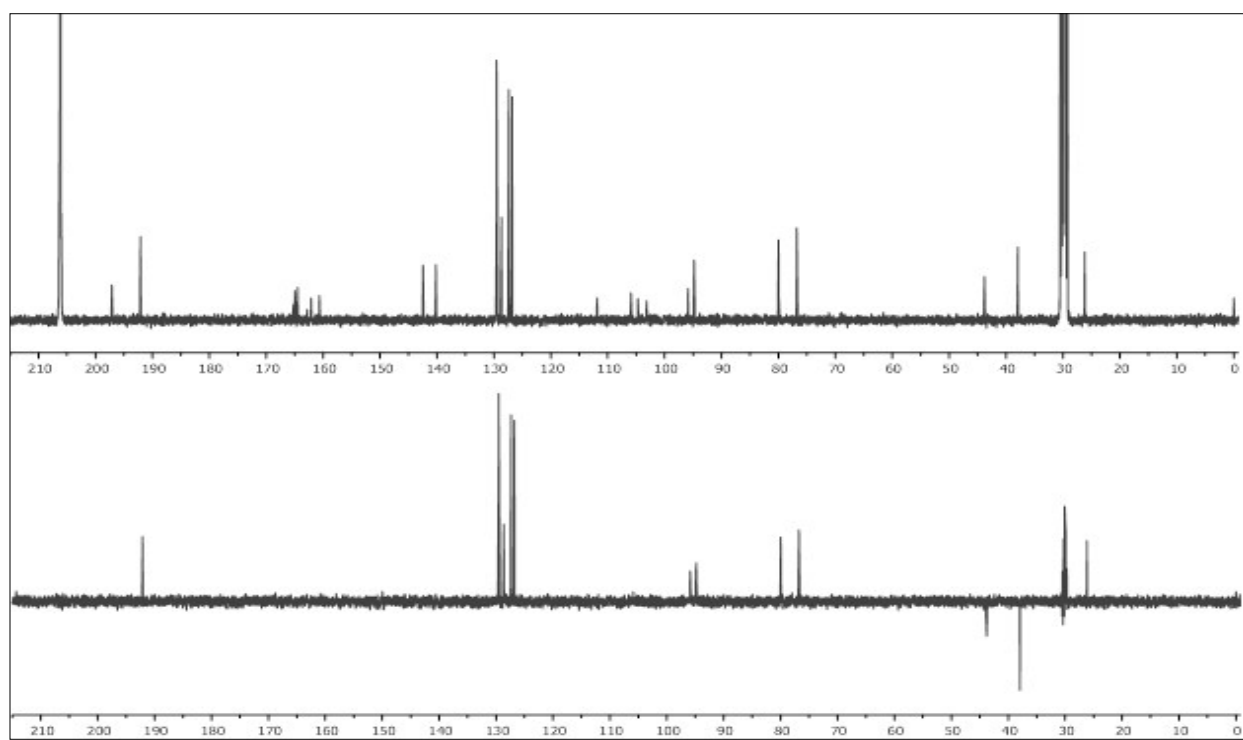
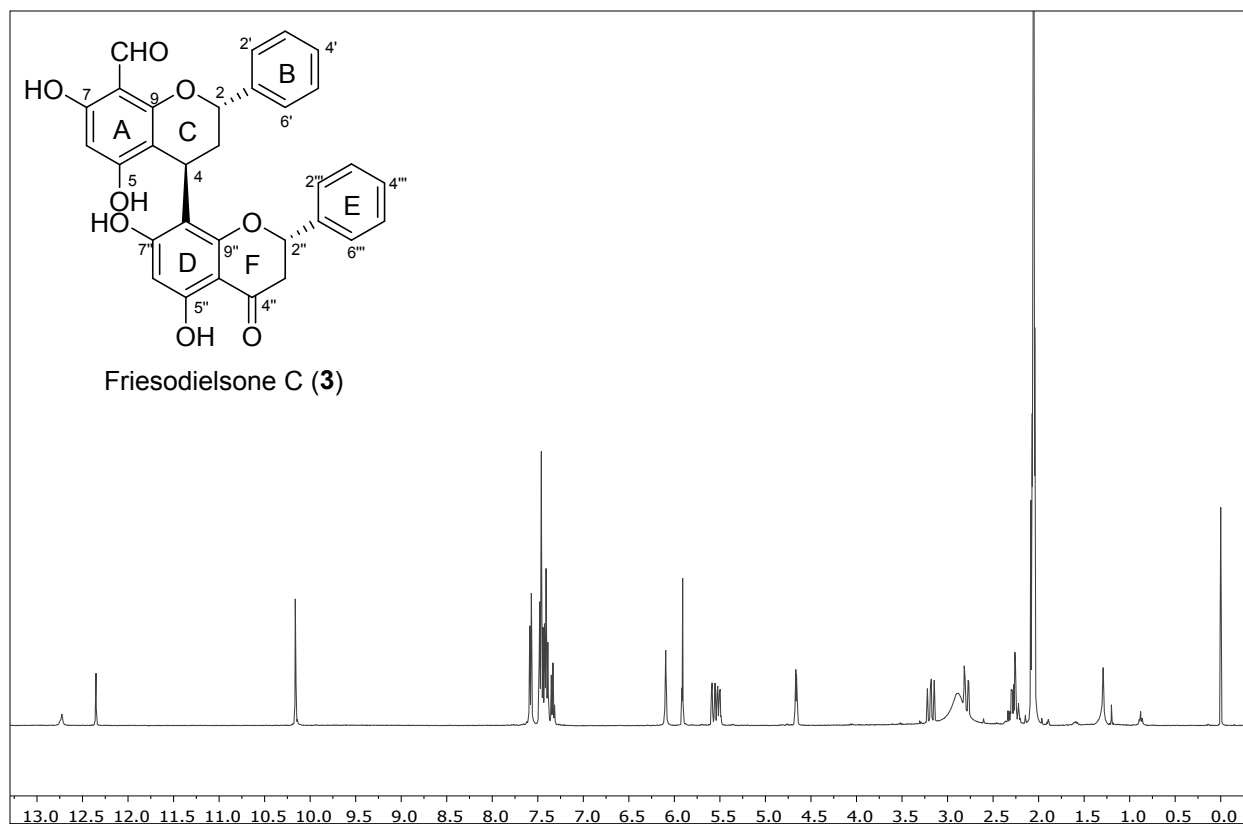
Monoisotopic Mass, Even Electron Ions
 124 formula(e) evaluated with 3 results within limits (up to 20 closest results for each mass)
 Elements Used:
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 7EPK8E
 SP SuratL 7EPK8E 43 (0.869) Cm (43:48)

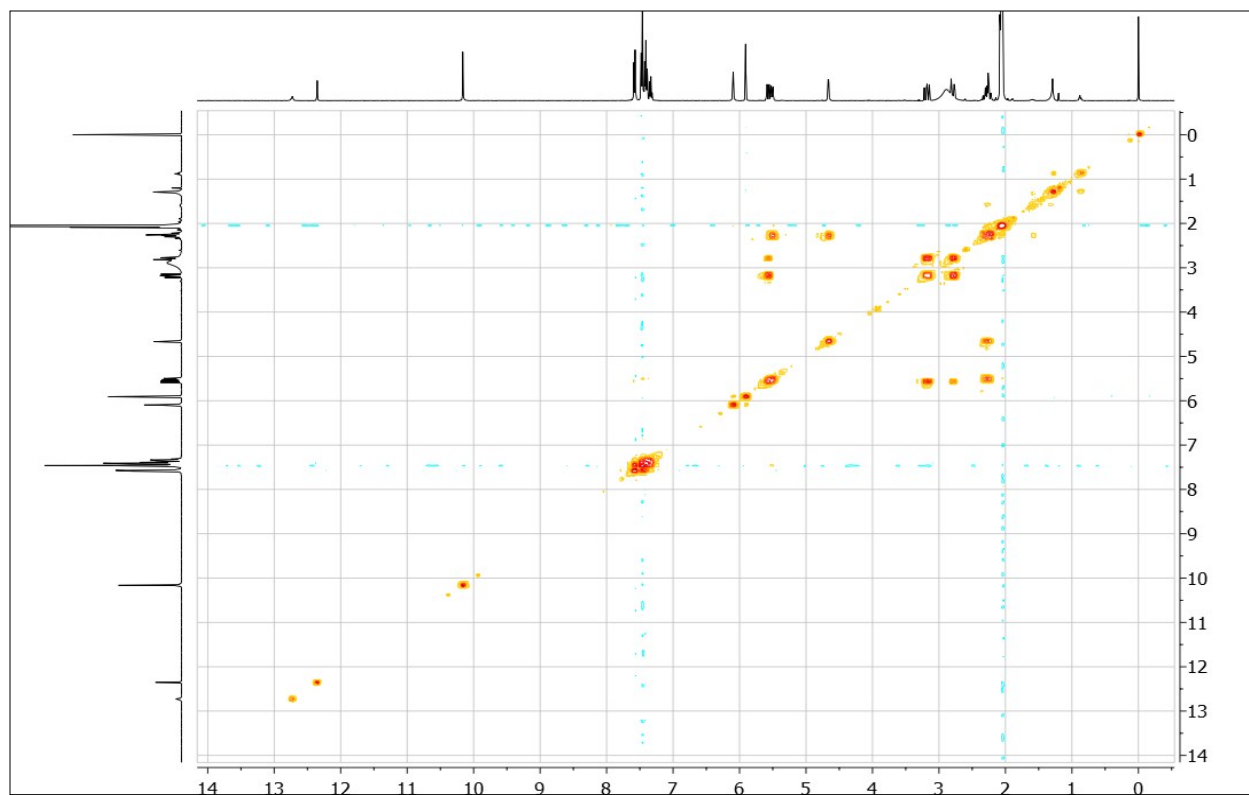
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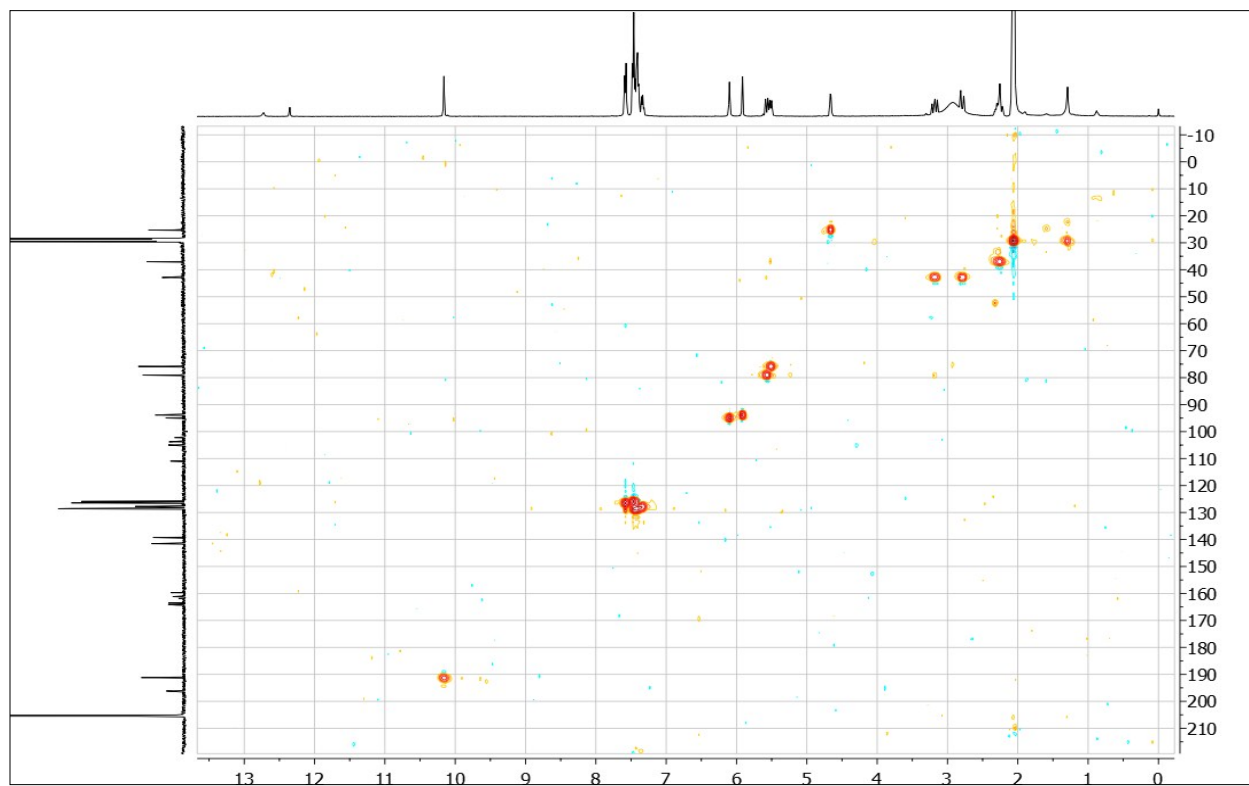
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
537.1529	537.1509	2.0	3.7	16.5	145.2	3.8	C27 H25 N2 O10
	537.1549	-2.0	-3.7	20.5	141.5	0.1	C32 H25 O8
	537.1491	3.8	7.1	29.5	144.1	2.7	C39 H21 O3

S16. HRESIMS spectrum of compound 2

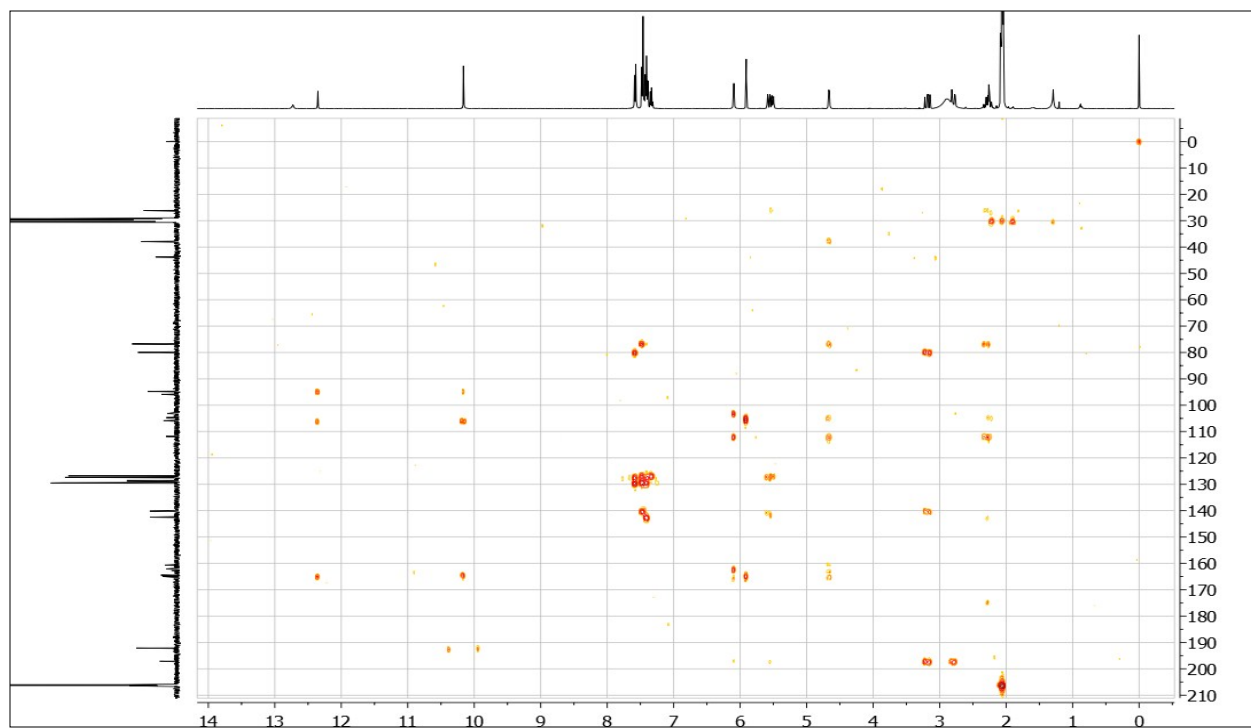




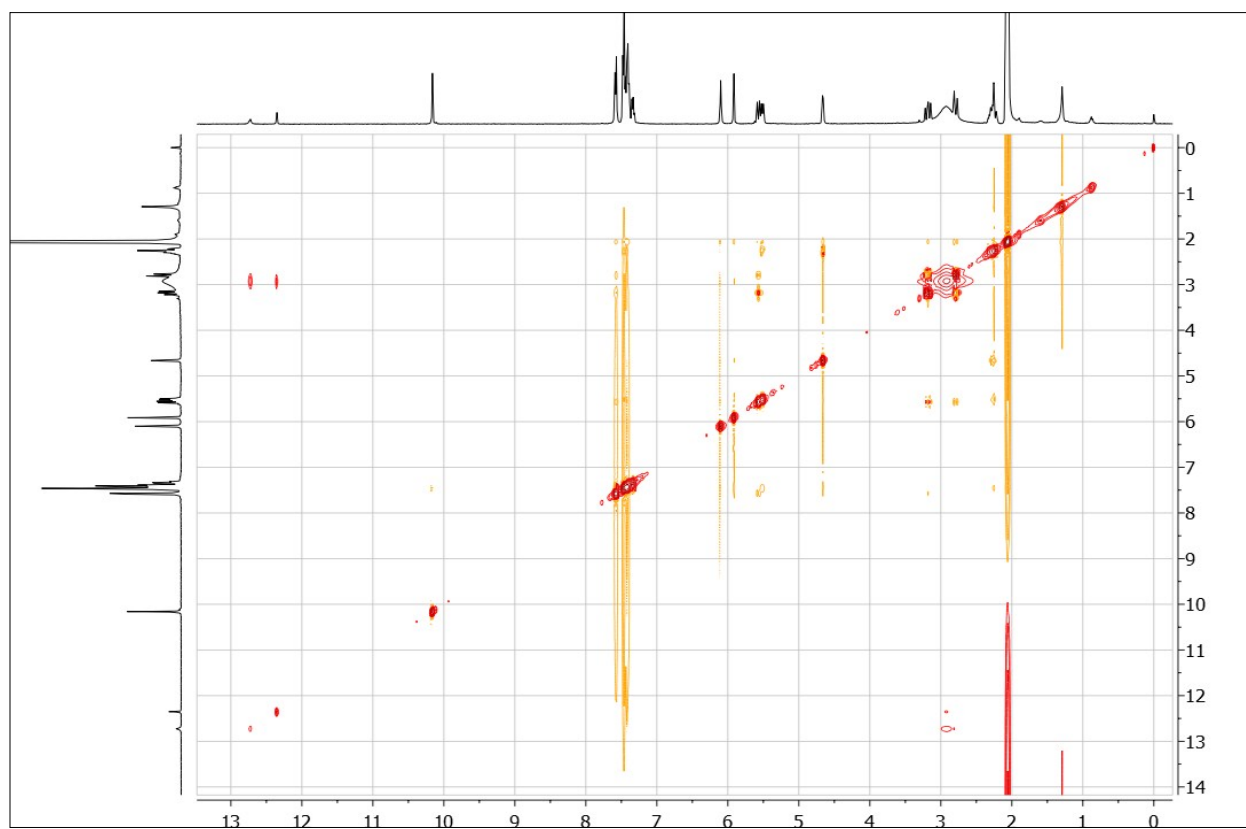
S19. COSY NMR spectrum (acetone- d_6) of compound **3**



S20. HMQC NMR spectrum (acetone- d_6) of compound **3**



S21. HMBC NMR spectrum (acetone- d_6) of compound **3**



S22. NOESY spectrum (acetone- d_6) of compound **3**

Monoisotopic Mass, Even Electron Ions
 133 formula(e) evaluated with 2 results within limits (up to 20 closest results for each mass)

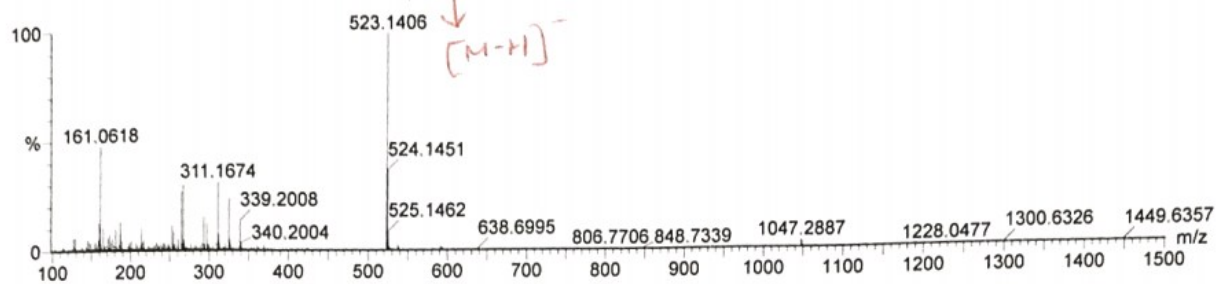
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7EPK14G

SP SuratL 7EPK14G 57 (1.147) Cm (50:71)

1: TOF MS ES-
 2.30e+003



Minimum: -1.5
 Maximum: 5.0 10.0 120.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
523.1406	523.1393	1.3	2.5	20.5	168.7	0.0	C31 H23 O8
	523.1447	-4.1	-7.8	29.5	172.9	4.2	C37 H19 N2 O2

S23. HRESIMS spectrum of compound **3**

Table S1. ^1H (400 MHz) and ^{13}C (100 MHz) spectroscopic data for friesodielsone A (**1**) in acetone- d_6 .

Position	Friesodielsone A (1)		
	δ_{C}	δ_{H} (J in Hz)	HMBC ($^1\text{H} \rightarrow ^{13}\text{C}$)
2	76.7	5.53 (dd, 3.5, 10.0)	C-3, C-4, C-1', C-2', C-6'
3	37.9	2.24-2.33 (m)	C-2, C-4, C-10, C-6
4	26.1	4.67 (dd, 2.6, 5.4)	C-2, C-3, C-9, C-10, C-5, C-6, C-7
5	162.1	-	-
6	94.9	5.90 (s)	C-7, C-8
7	164.8	-	-
8	105.9	-	-
9	160.6	-	-
10	104.7	-	-
11	192.1	10.10 (s)	C-6, C-7, C-8
1'	142.5	-	-
2',6'	126.8	7.44-7.47 (m)	C-2, C-1', C-3', C-5'
3',5'	129.4	7.40-7.42 (m)	C-1', C-2', C-4', C-6'
4'	128.6	7.30-7.34 (m)	C-2', C-3', C-5', C-6'
2''	79.9	5.57 (dd, 3.0, 13.5)	C-4'', C-1''', C-2''', C-6'''
3''	43.7	2.80 (dd, 3.0, 17.1)	C-2'', C-4'', C-10'', C-5''
		3.16 (dd, 13.5, 17.1)	C-2'', C-4'', C-10'', C-5''
4''	197.0	-	-
5''	163.1	-	-
6''	111.9	-	-
7''	165.2	-	-
8''	95.9	6.08 (s)	C-6'', C-7'', C-9''
9''	162.1	-	-
10''	103.1	-	-
1'''	140.2	-	-
2''',6'''	127.8	7.56-7.58 (m)	C-2''', C-1''', C-3''', C-5'''
3''',5'''	129.5	7.43-7.47 (m)	C-1''', C-2''', C-4''', C-6'''
4'''	129.4	7.40-7.43 (m)	C-2''', C-3''', C-5''', C-6'
7-OH	-	12.35 (s)	C-6, C-7, C-8
5''-OH	-	12.73 (s)	C-5'', C-6''

Table S2. ^1H (400 MHz) and ^{13}C (100 MHz) spectroscopic data for friesodielsone B (**2**) in acetone- d_6 .

Position	Friesodielsone B (2)		
	δ_{C}	δ_{H} (J in Hz)	HMBC ($^1\text{H} \rightarrow ^{13}\text{C}$)
2	76.7	5.52 (dd, 3.0, 10.8)	C-1', C-2', C-6'
3	37.9	2.25-2.30 (m)	C-2, C-4, C-10, C-1', C-6
4	26.5	4.70 (dd, 2.4, 5.6)	C-2, C-9, C-10, C-6, C-7
5	159.1	-	-
6	94.9	5.91 (s)	C-7, C-10
7	164.9	-	-
8	106.0	-	-
9	160.8	-	-
10	105.9	-	-
11	192.1	10.16 (s)	C-6, C-7, C-8
1'	142.3	-	-
2',6'	126.8	7.45-7.47 (m)	C-2, C-1', C-3', C-5'
3',5'	129.4	7.38-7.42 (m)	C-1', C-2', C-4', C-6'
4'	128.6	7.32-7.34 (m)	C-2', C-3', C-5', C-6'
2''	79.6	5.61 (dd, 3.0, 13.0)	C-1''', C-2''', C-6'''
3''	43.6	2.82 (dd, 3.0, 17.0)	C-2'', C-4'', C-1'''
		3.16 (dd, 13.0, 17.0)	C-2'', C-4'', C-1'''
4''	197.7	-	-
5''	160.6	-	-
6''	111.8	-	-
7''	160.6	-	-
8''	159.1	-	-
9''	164.5	-	-
10''	103.8	-	-
11''	8.32	2.09 (s)	C-8'', C-9''
1'''	140.4	-	-
2''',6'''	127.2	7.60-7.61 (m)	C-2'', C-1''', C-3''', C-5'''
3''',5'''	129.5	7.45-7.47 (m)	C-1''', C-2''', C-4''', C-6'''
4'''	129.3	7.38-7.42 (m)	C-2''', C-3''', C-5''', C-6'''
7-OH	-	12.35 (s)	C-6, C-7, C-8
5''-OH	-	12.67 (s)	C-5'', C-6'', C-10''

Table 3. ^1H (400 MHz) and ^{13}C (100 MHz) spectroscopic data for friesodielsone C (**3**) in acetone- d_6 .

Position	Friesodielsone C (3)		
	δ_{C}	δ_{H} (J in Hz)	HMBC ($^1\text{H} \rightarrow ^{13}\text{C}$)
2	76.7	5.53 (dd, 3.2, 10.7)	C-4, C-1', C-2', C-6'
3	37.9	2.25-2.32 (m)	C-2, C-4, C-8
4	26.1	4.67 (dd, 2.6, 5.5)	C-2, C-3, C-9, C-10, C-7, C-8, C-9
5	162.8	-	-
6	94.8	5.90 (s)	C-5, C-8
7	165.2	-	-
8	105.8	-	-
9	164.7	-	-
10	104.7	-	-
11	192.1	10.15(s)	C-6, C-8, C-9
1'	142.4	-	-
2',6'	126.8	7.44-7.48 (m)	C-2, C-1', C-3', C-5'
3',5'	129.4	7.39-7.42 (m)	C-1', C-2', C-4', C-6'
4'	128.6	7.33-7.35 (m)	C-2', C-3', C-5', C-6'
2''	79.9	5.59 (dd, 3.0, 13.0)	C-4'', C-1''', C-2''', C-6'''
3''	43.7	2.81 (dd, 3.0, 17.0)	C-2'', C-4'', C-1'''
		3.22 (dd, 13.0, 17.0)	C-2'', C-4'', C-1'''
4''	197.1	-	-
5''	162.0	-	-
6''	95.8	6.08 (s)	C-4'', C-5'', C-7'', C-10''
7''	162.8	-	-
8''	111.8	-	-
9''	160.6	-	-
10''	103.5	-	-
1'''	140.1	-	-
2''',6'''	129.4	7.44-7.46 (m)	C-2'', C-1''', C-3''', C-5'''
3''',5'''	129.4	7.57-7.58 (m)	C-1''', C-2''', C-4''', C-6'''
4'''	128.6	7.39-7.42 (m)	C-2''', C-3''', C-5''', C-6'''
7-OH	-	12.35 (s)	C-6, C-7, C-8
5''-OH	-	12.72 (s)	-