

Supporting Information

New isohemigossypol related conjugates and caffeoylated oleanane triterpenoids from Hibiscus syriacus roots with anti-senescence modulating activity

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1. Supplemental spectra of compounds 1–6

1.1 Compound 1

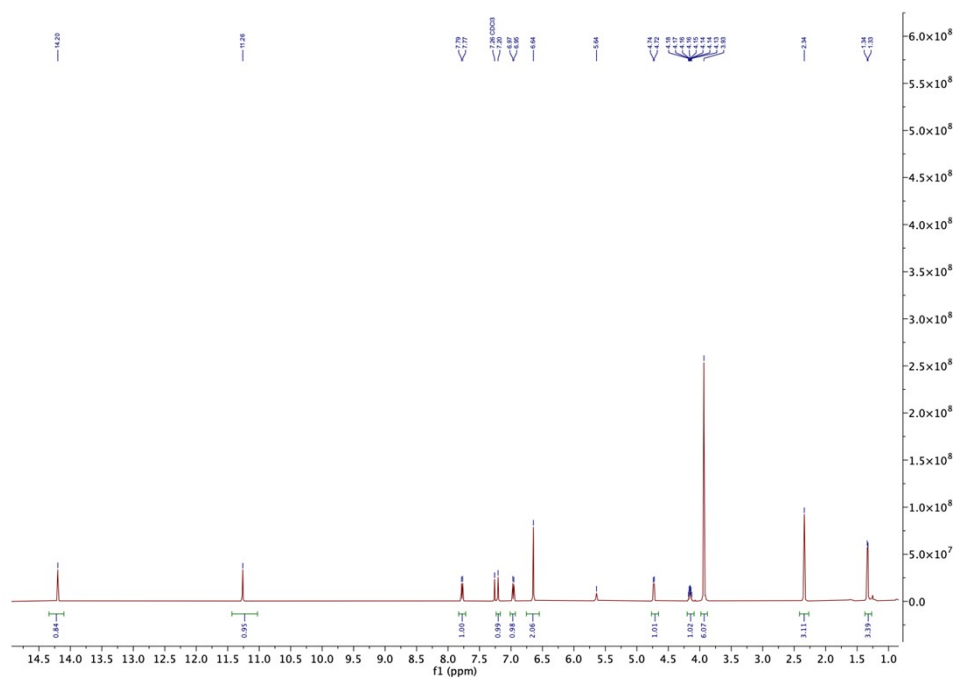


Figure S1. ¹H NMR spectrum of compound 1 (500 MHz, CDCl₃).

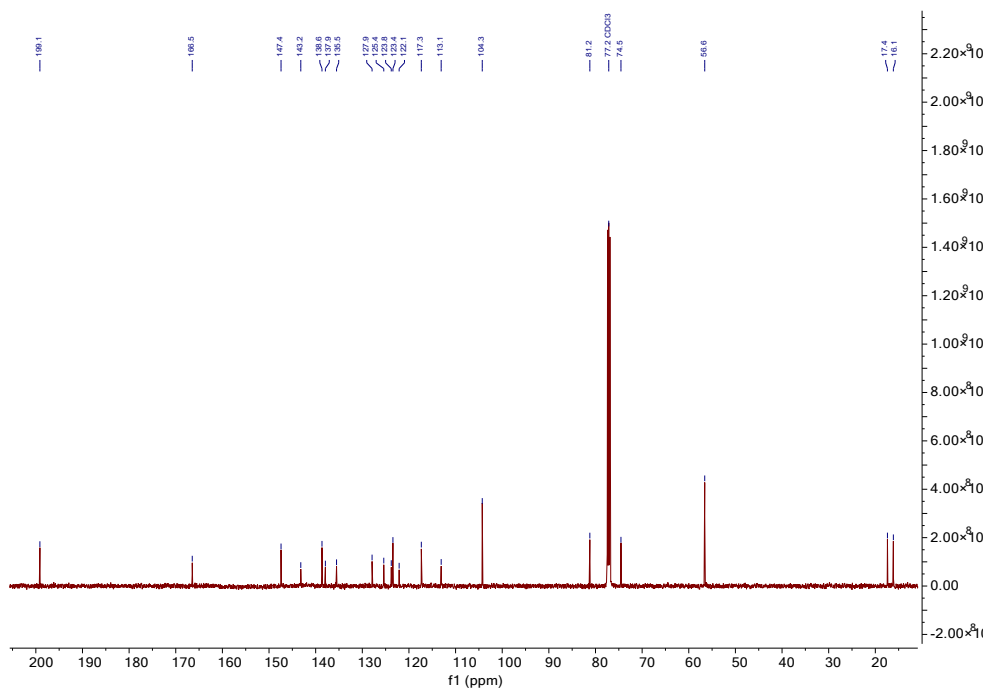


Figure S2. ¹³C NMR spectrum of compound 1 (125 MHz, CDCl₃).

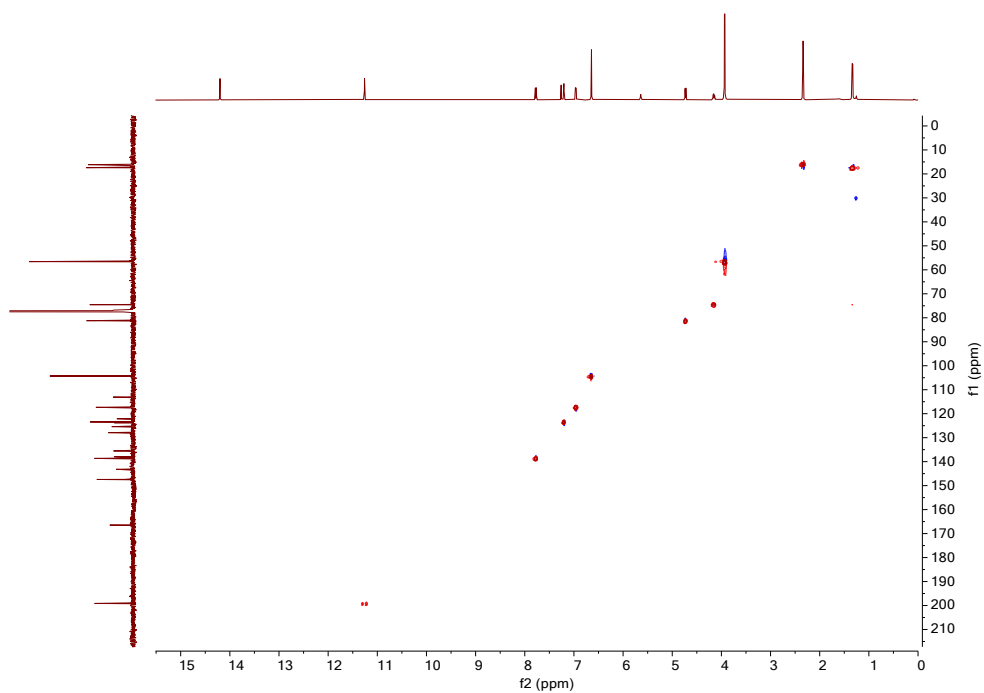


Figure S3. Edited HSQC NMR spectrum of compound **1** (500 MHz, CDCl_3).

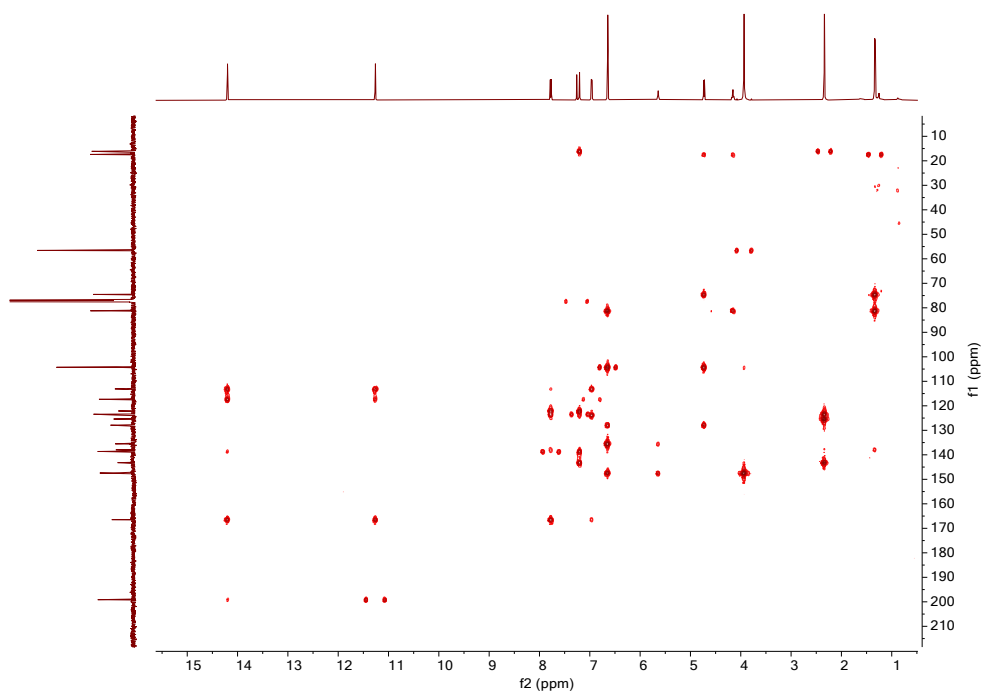


Figure S4. HMBC NMR spectrum of compound **1** (500 MHz, CDCl_3).

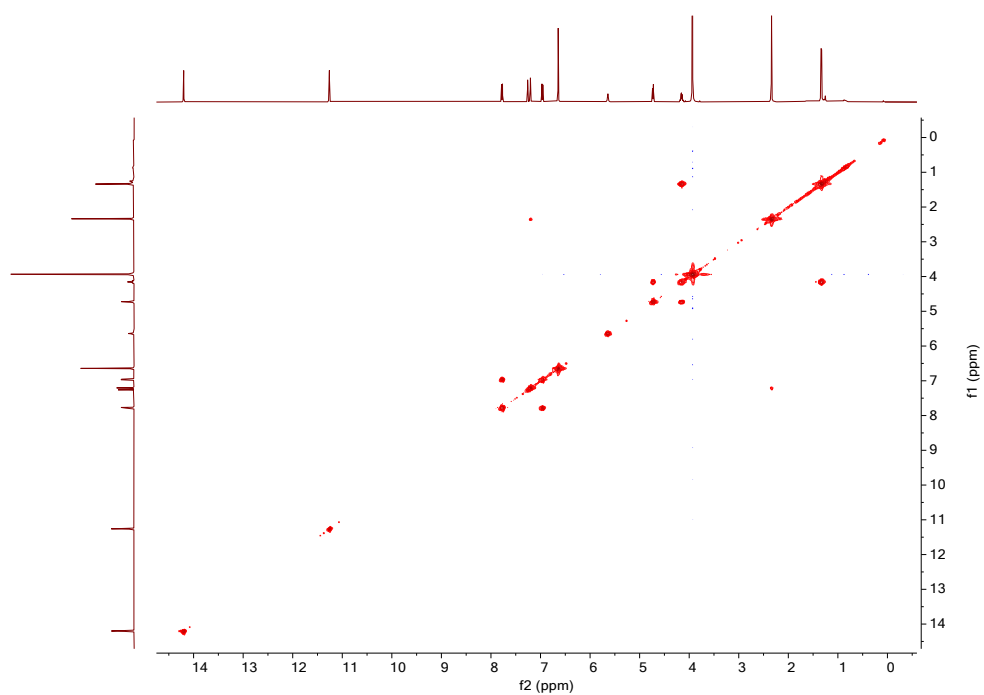


Figure S5. ¹H-¹H COSY NMR spectrum of compound **1** (500 MHz, CDCl₃).

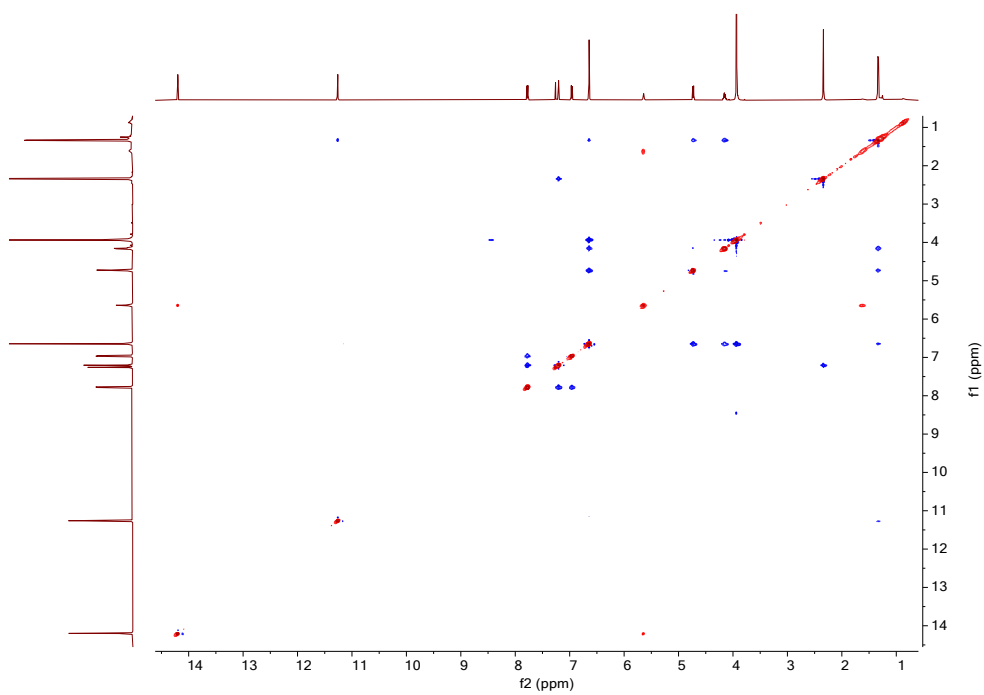


Figure S6. NOESY NMR spectrum of compound **1** (500 MHz, CDCl₃).

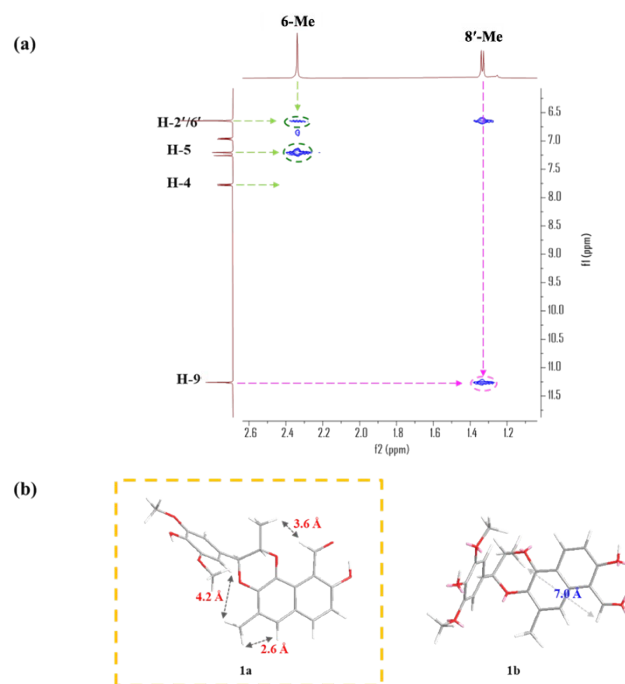


Figure S7. The key NOESY correlations to determine the position of methyl groups and dioxane ring position (a), and the possible structures depending on the dioxane ring position (b) in compound **1**.

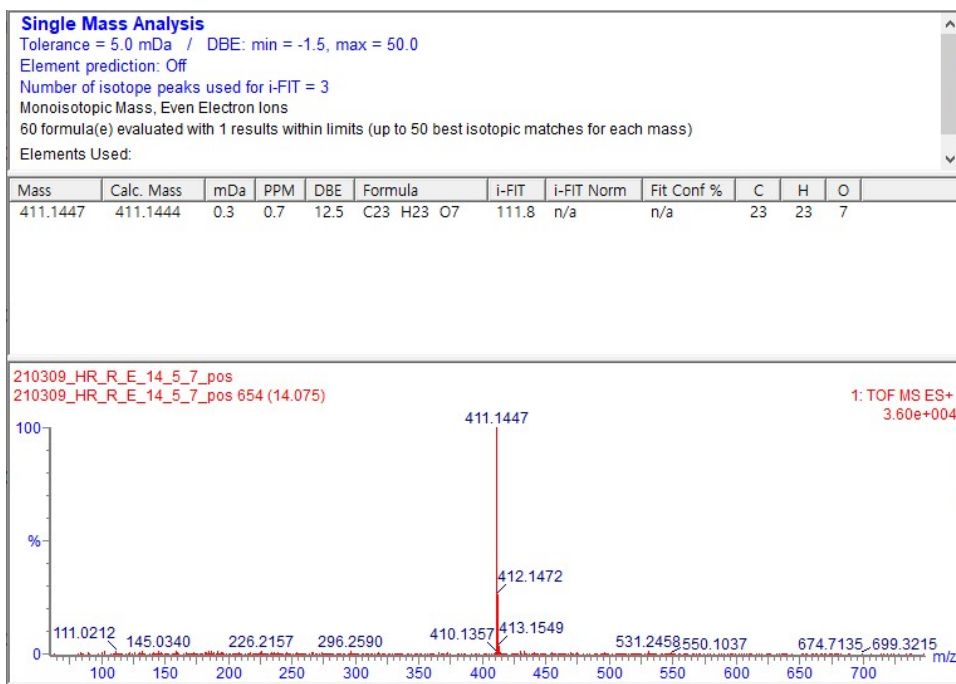


Figure S8. HRESIMS spectrum of compound 1.

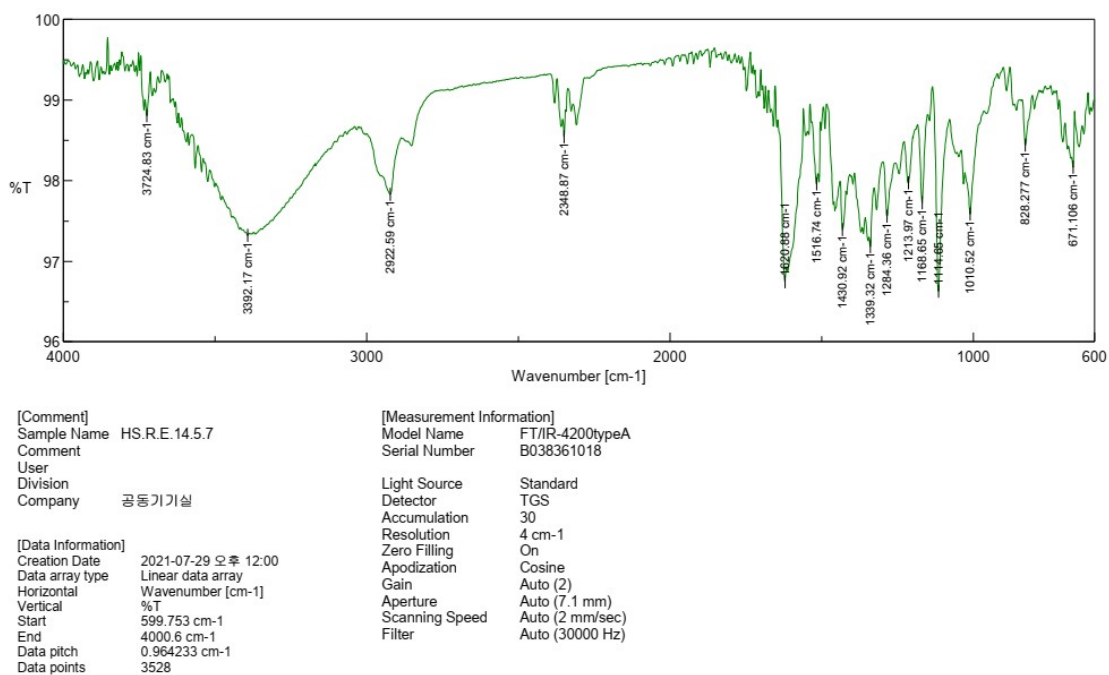


Figure S9. IR spectrum of compound 1.

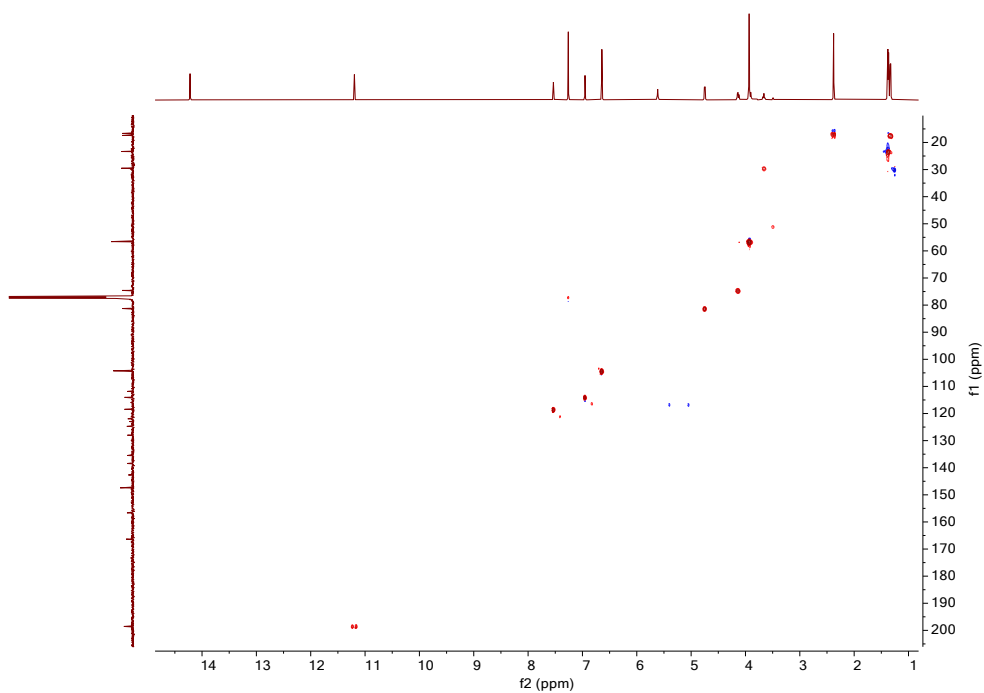


Figure S12. Edited HSQC NMR spectrum of compound **2** (500 MHz, CDCl_3).

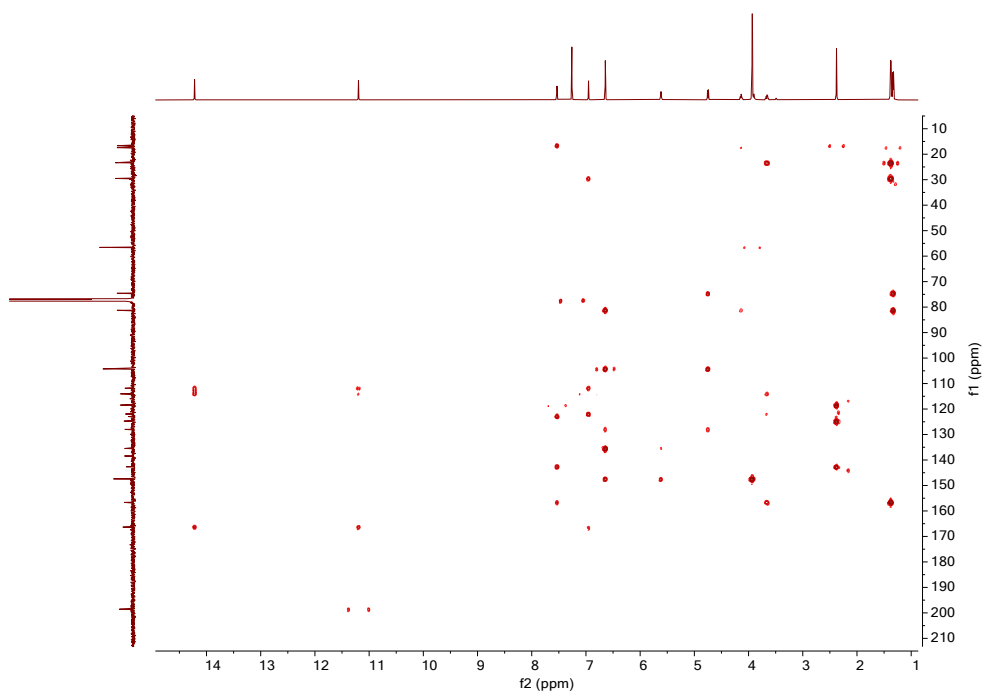


Figure S13. HMBC NMR spectrum of compound **2** (500 MHz, CDCl_3).

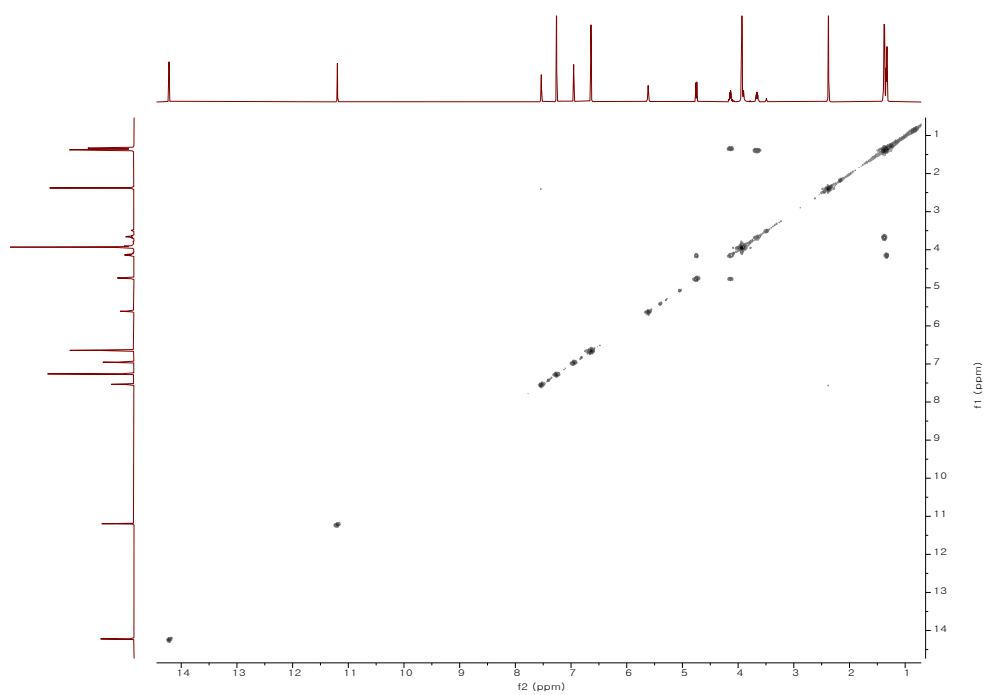


Figure S14. ¹H-¹H COSY NMR spectrum of compound **2** (500 MHz, CDCl₃).

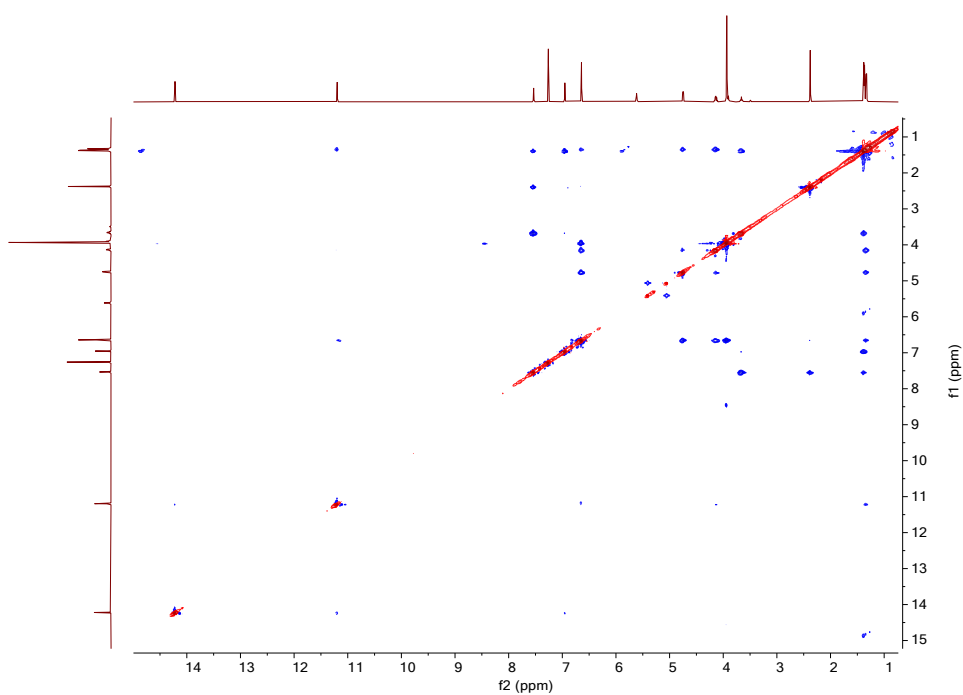


Figure S15. NOESY NMR spectrum of compound **2** (500 MHz, CDCl₃).

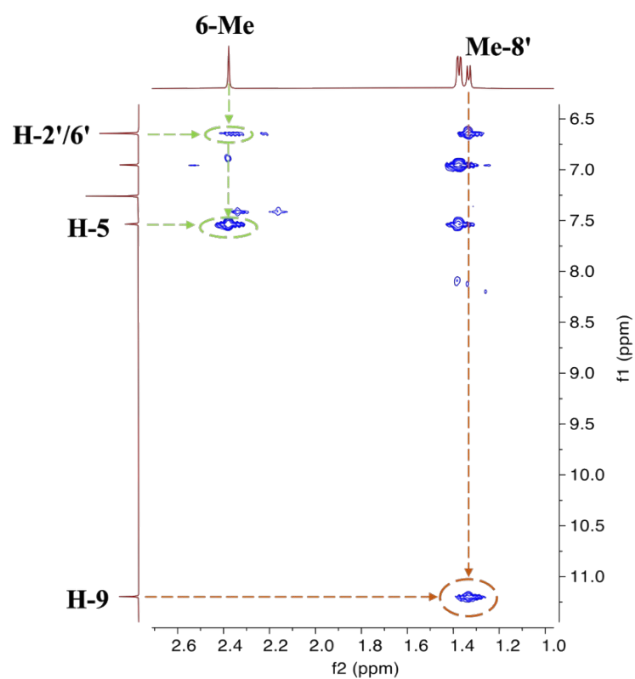


Figure S16. The key NOESY correlations to determine the position of methyl groups and dioxane ring position in compound **2**.

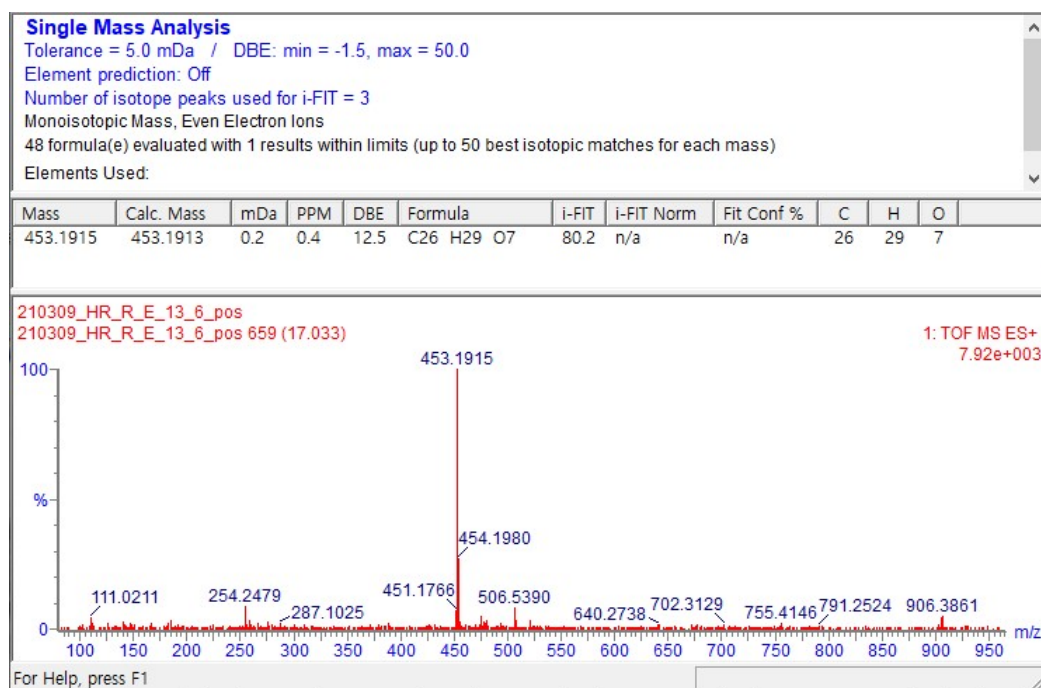
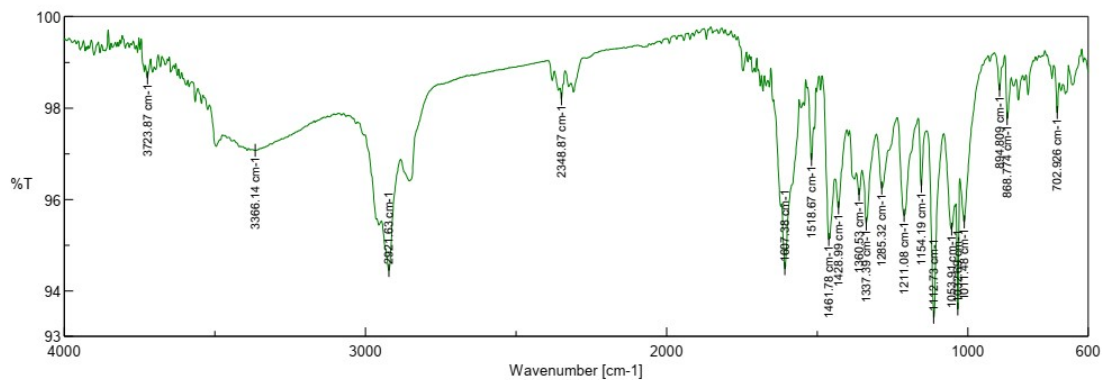


Figure S17. HRESIMS spectrum of compound **2**.



[Comment]
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 Comment
 User
 Division
 Company 공동기기실

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 Detector TGS
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 Zero Filling On
 Apodization Cosine
 Gain Auto (2)
 Aperture Auto (7.1 mm)
 Scanning Speed Auto (2 mm/sec)
 Filter Auto (30000 Hz)

[Data Information]
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 Data points 3528

Figure S18. IR spectrum of compound 2.

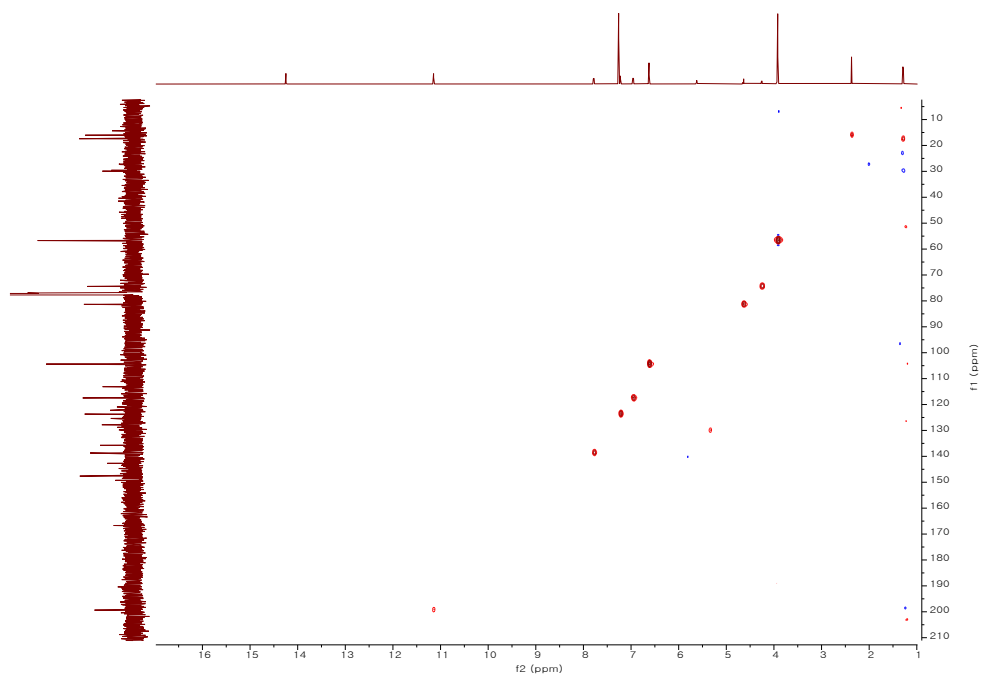


Figure S21. Edited HSQC NMR spectrum of compound **3** (600 MHz, CDCl₃).

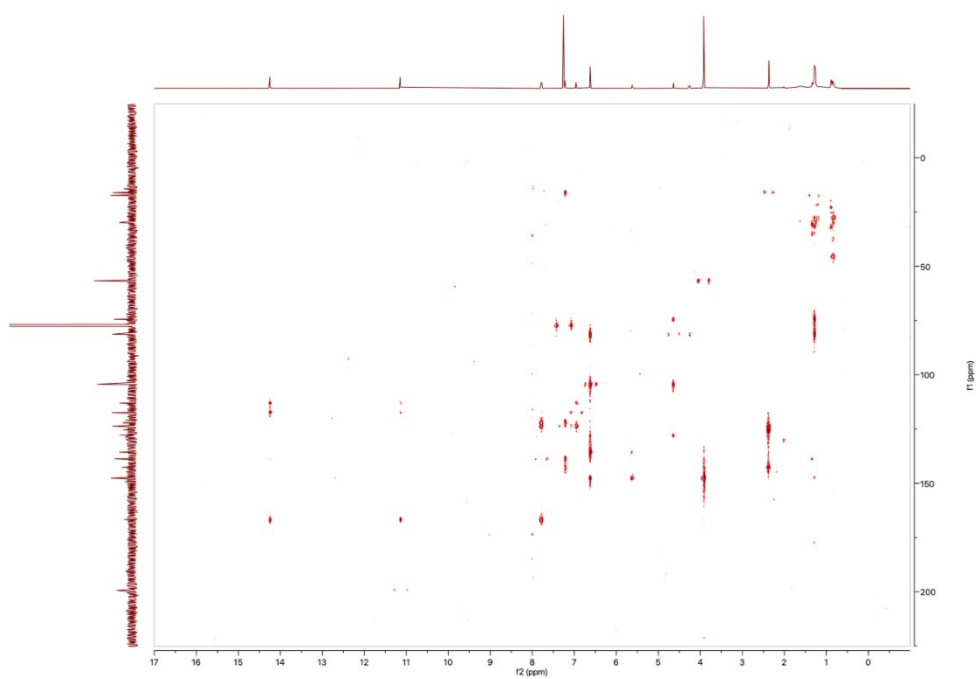


Figure S22. HMBC NMR spectrum of compound **3** (600 MHz, CDCl₃).

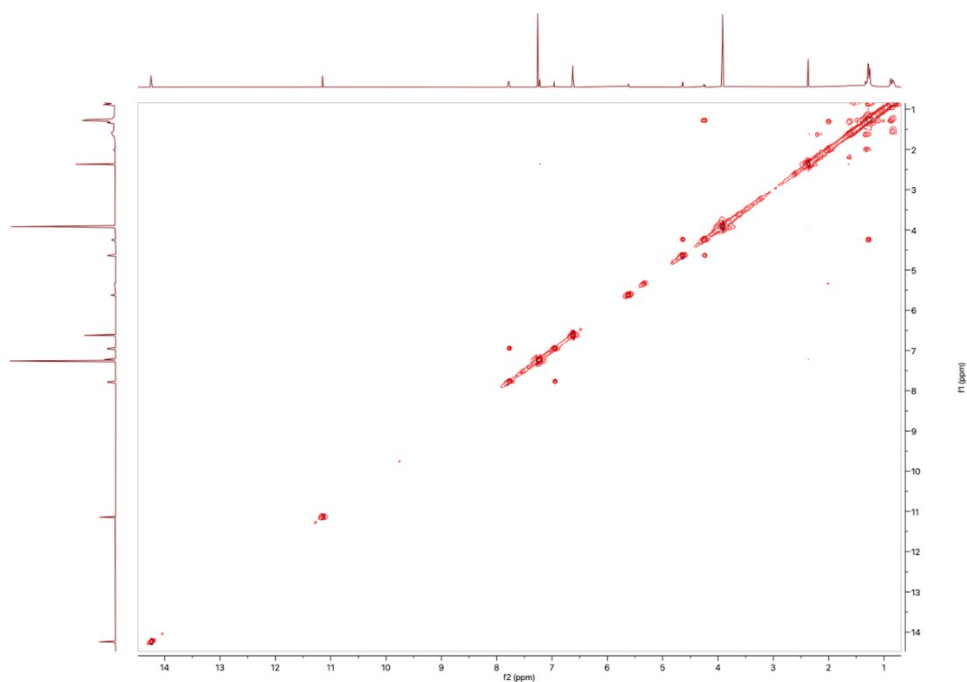


Figure S23. ^1H - ^1H COSY NMR spectrum of compound **3** (600 MHz, CDCl_3).

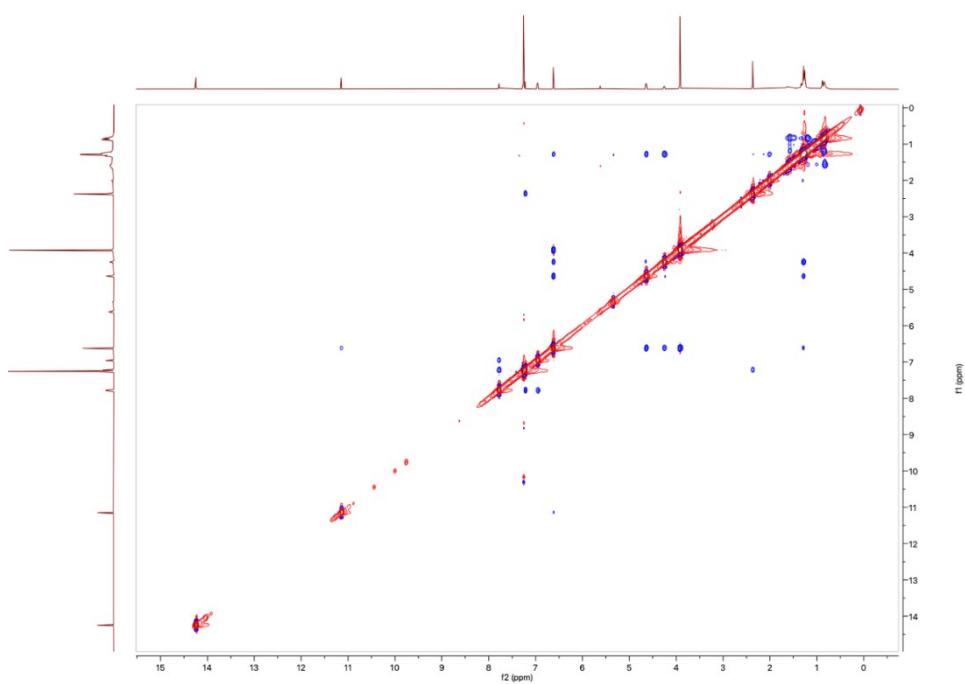


Figure S24. NOESY NMR spectrum of compound **3** (600 MHz, CDCl_3).

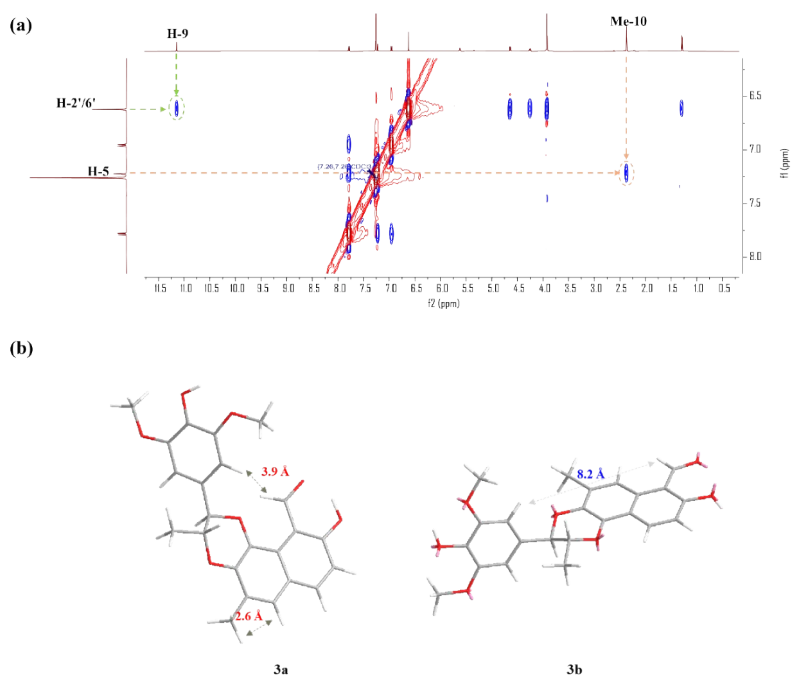


Figure S25. The key NOESY correlations to determine the position of the methyl group and dioxane ring position (a), and the possible structures of **3** depending on the dioxane ring position (b).

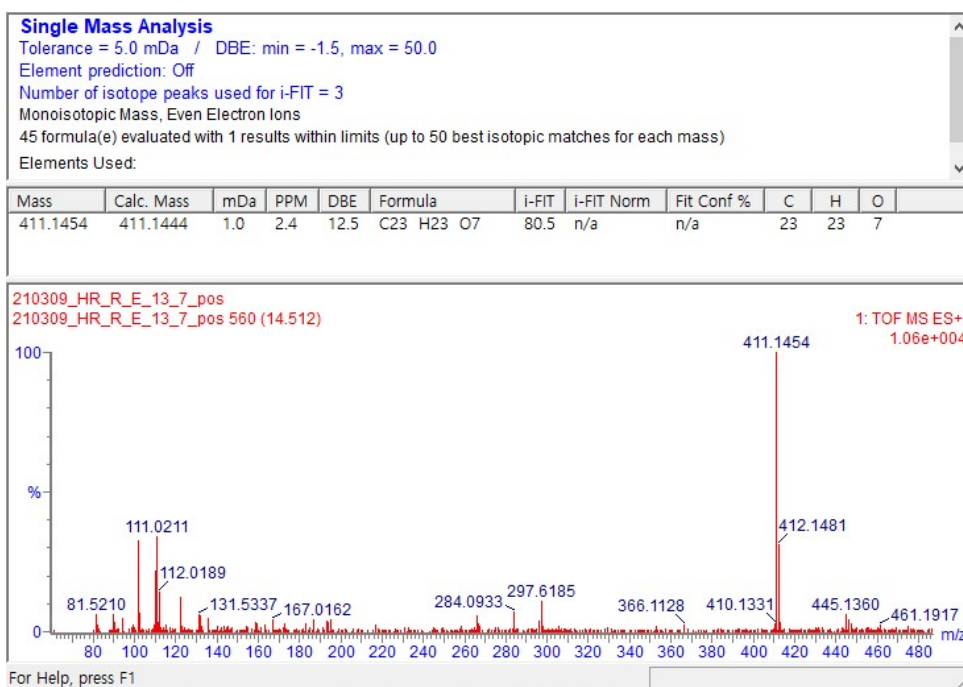
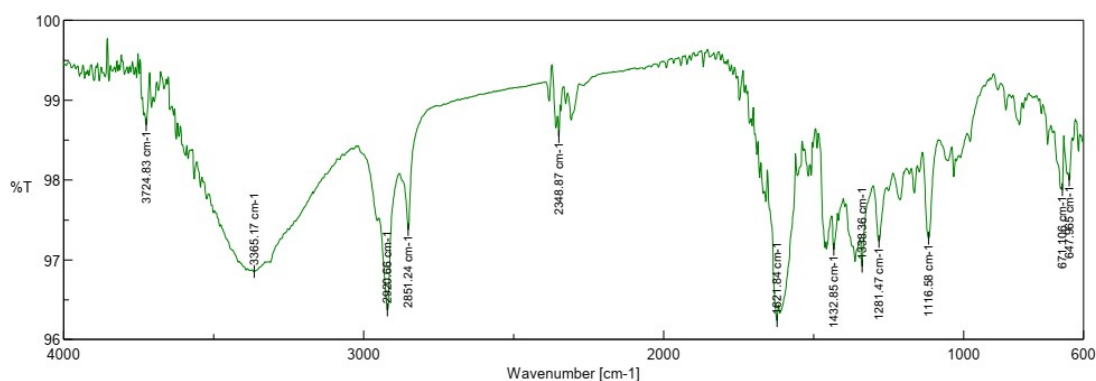


Figure S26. HRESIMS spectrum of compound **3**.



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Division		Detector	TGS
Company	공통기기실	Accumulation	30
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		Zero Filling	On
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Data array type	Linear data array	Aperture	Auto (7.1 mm)
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Vertical	%T	Filter	Auto (30000 Hz)
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End	4000.6 cm-1		
Data pitch	0.964233 cm-1		
Data points	3528		

Figure S27. IR spectrum of compound **3**.

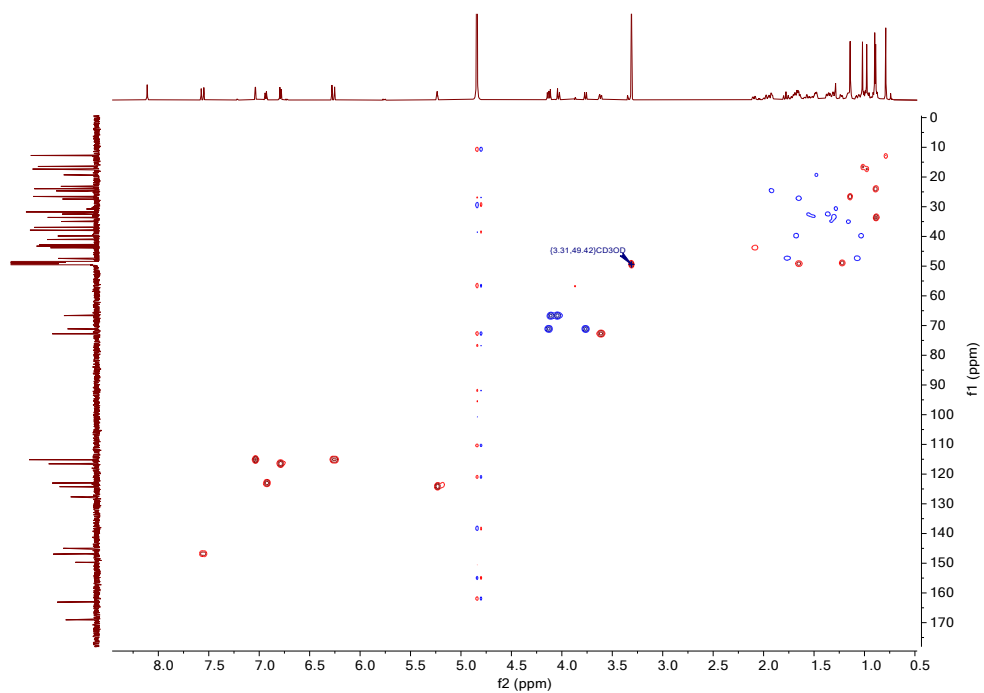


Figure S30. Edited HSQC NMR spectrum of compound **4** (600 MHz, CD₃OD).

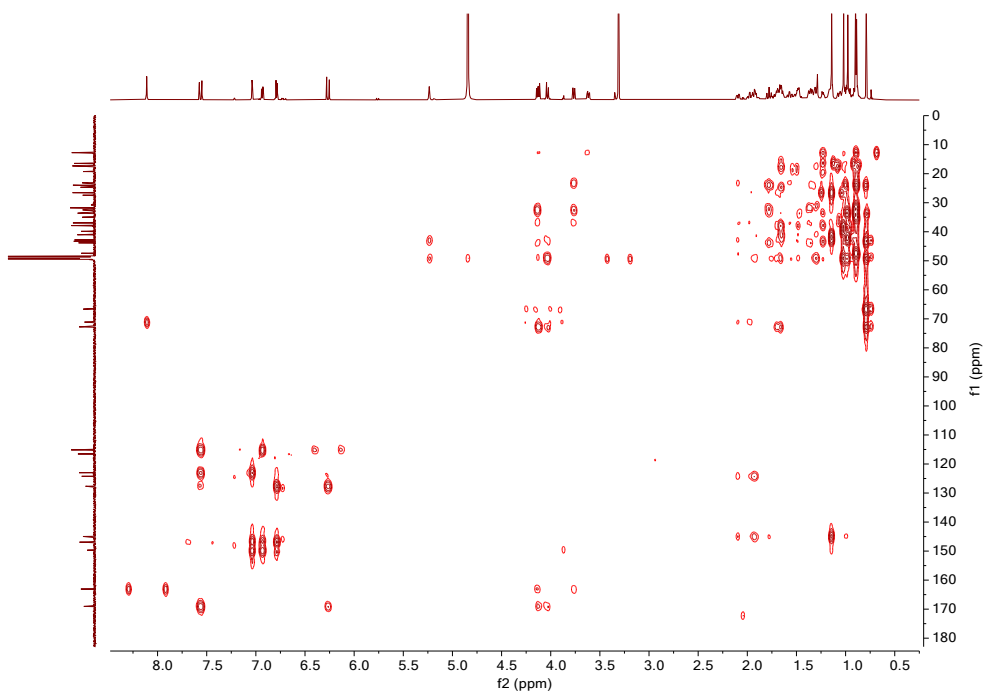


Figure S31. HMBC NMR spectrum of compound **4** (600 MHz, CD₃OD).

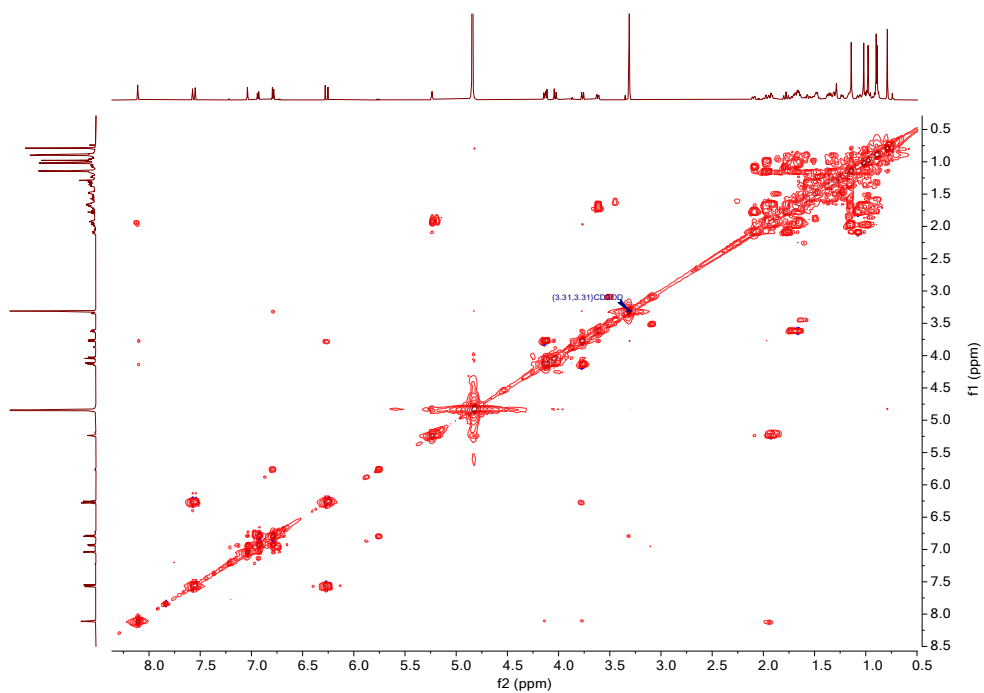


Figure S32. ¹H-¹H COSY NMR spectrum of compound **4** (600 MHz, CD₃OD).

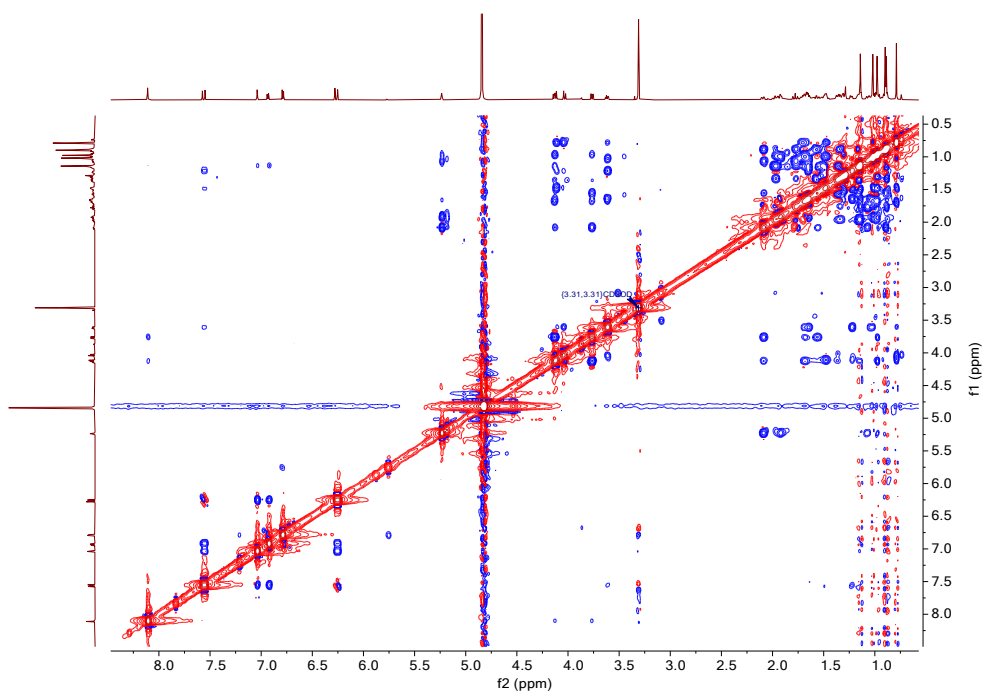


Figure S33. NOESY NMR spectrum of compound **4** (600 MHz, CD₃OD).

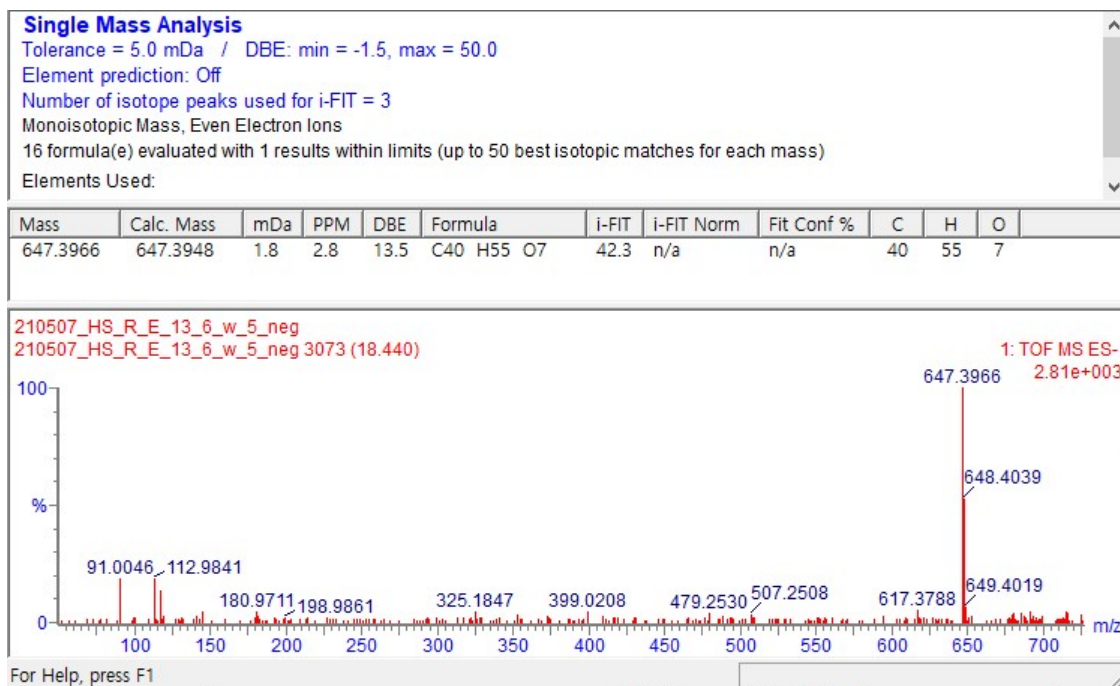


Figure S34. HRESIMS spectrum of compound 4.

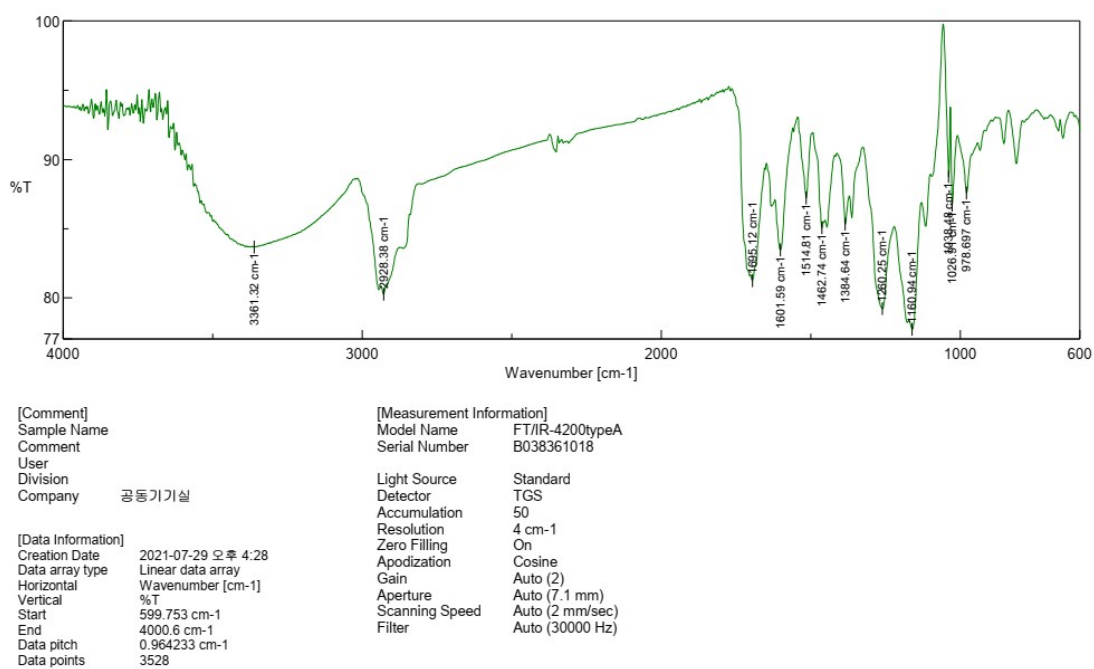


Figure S35. IR spectrum of compound 4.

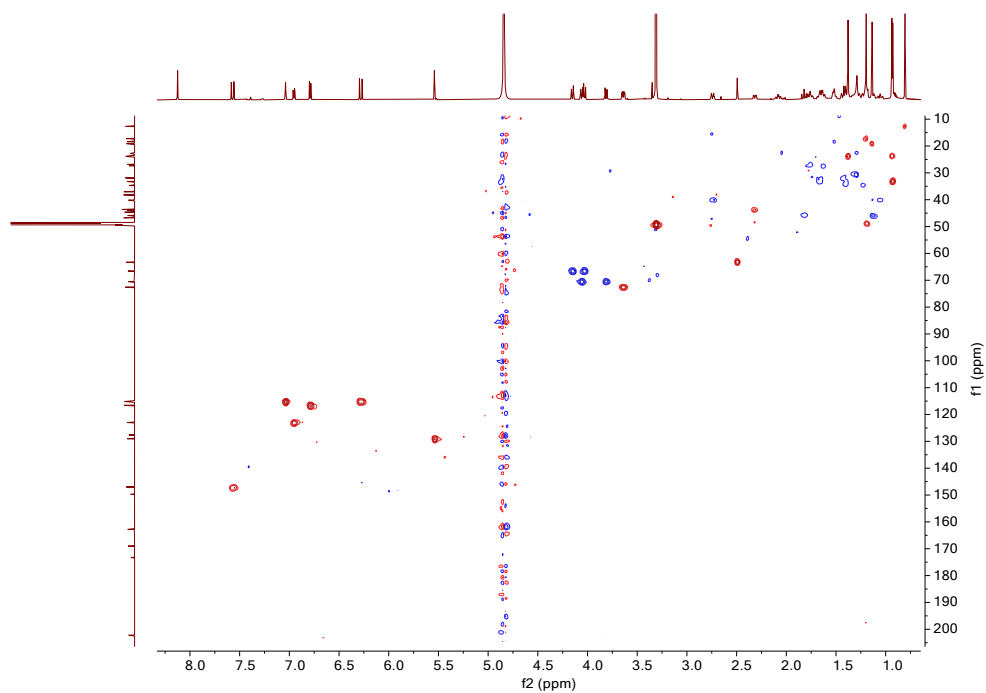


Figure S38. Edited HSQC NMR spectrum of compound **5** (600 MHz, CD₃OD).

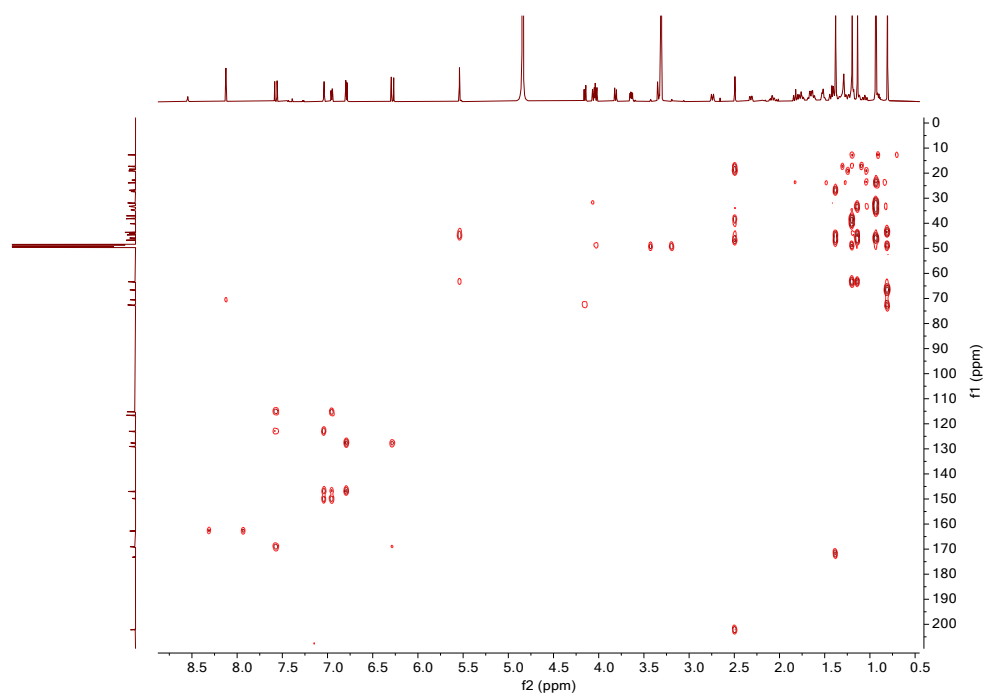


Figure S39. HMBC NMR spectrum of compound **5** (600 MHz, CD₃OD).

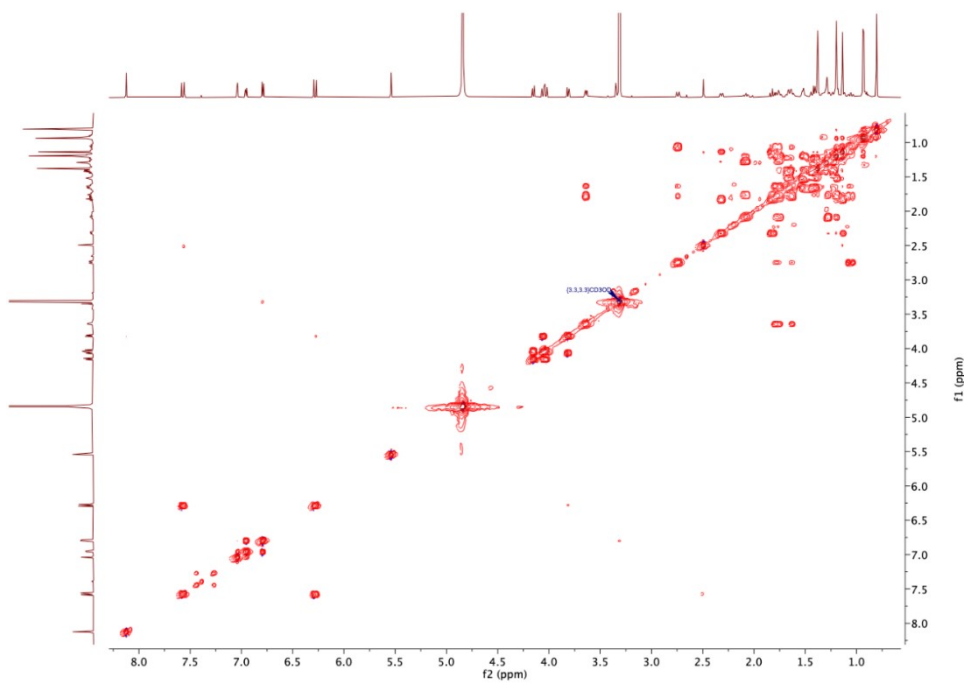


Figure S40. ^1H - ^1H COSY NMR spectrum of compound **5** (600 MHz, CD_3OD).

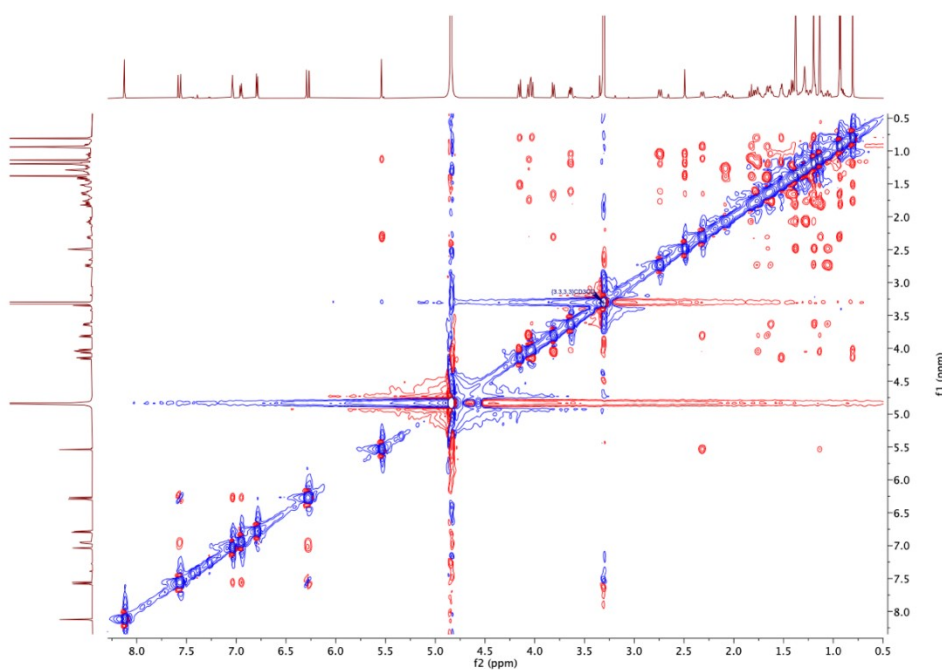


Figure S41. NOESY NMR spectrum of compound **5** (600 MHz, CD_3OD).

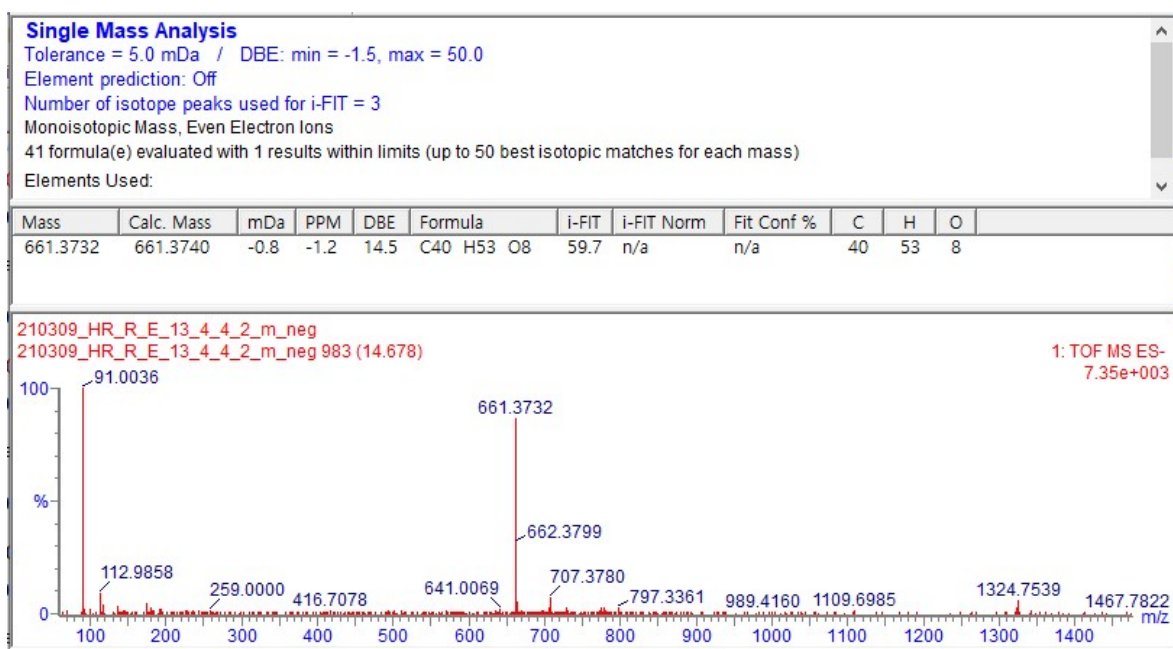


Figure S42. HRESIMS spectrum of compound 5.

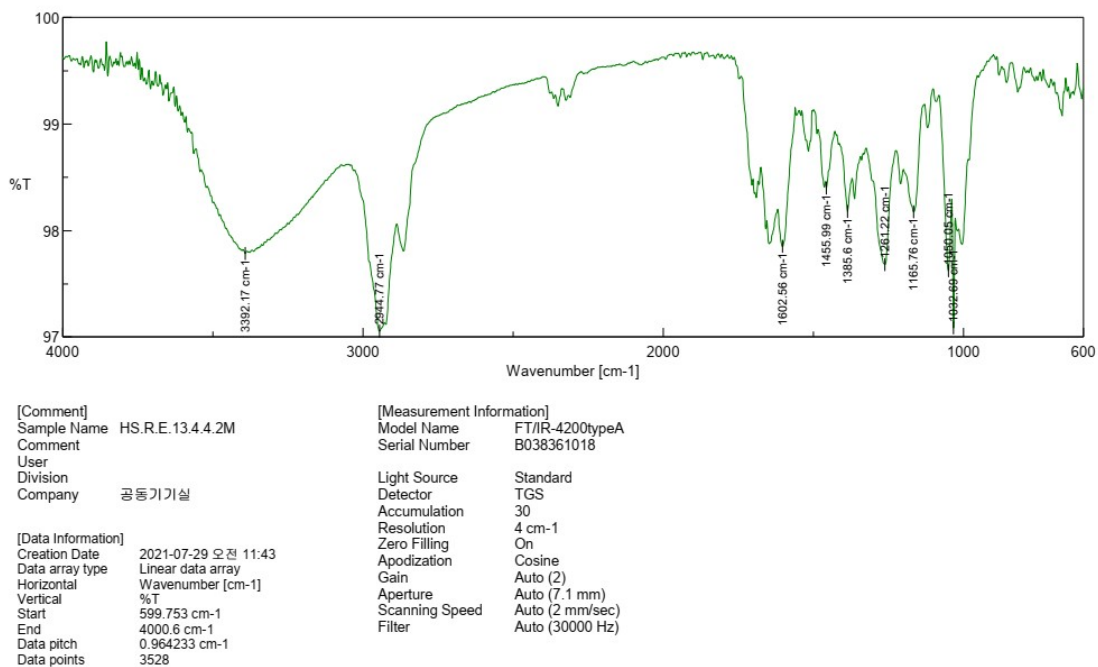


Figure S43. IR spectrum of compound 5.

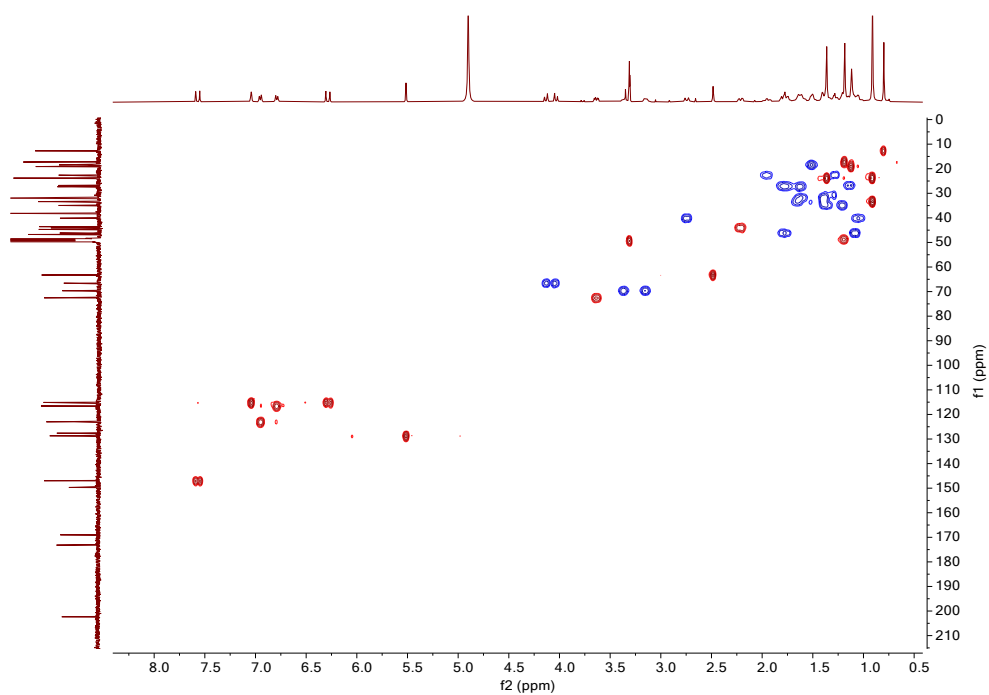


Figure S46. Edited HSQC NMR spectrum of compound **6** (400 MHz, CD₃OD).

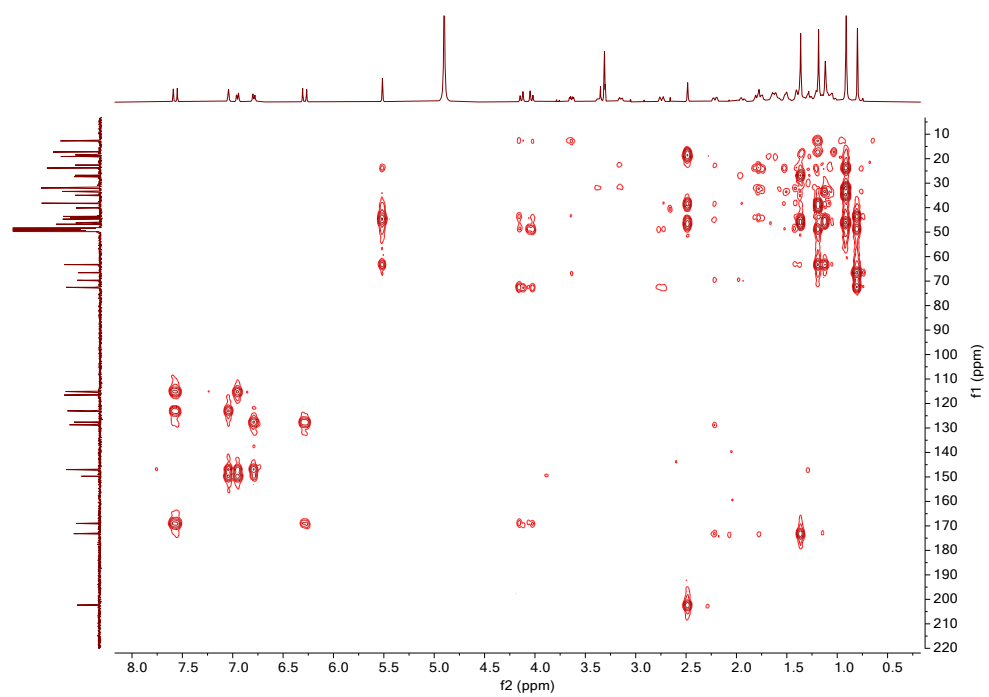


Figure S47. HMBC NMR spectrum of compound **6** (400 MHz, CD₃OD).

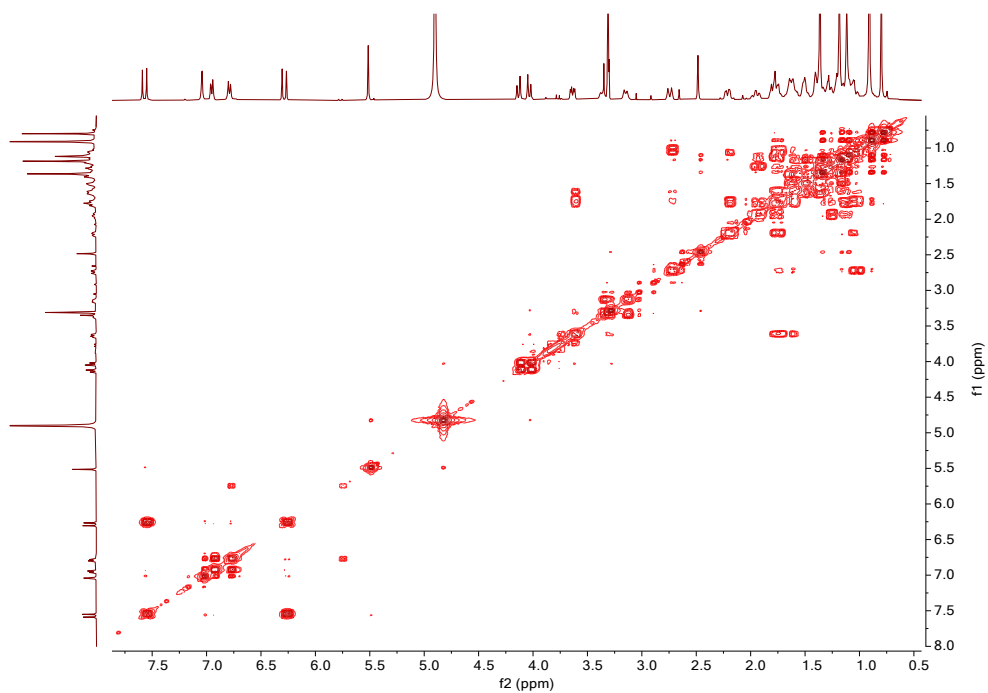


Figure S48. ¹H-¹H COSY NMR spectrum of compound **6** (400 MHz, CD₃OD).

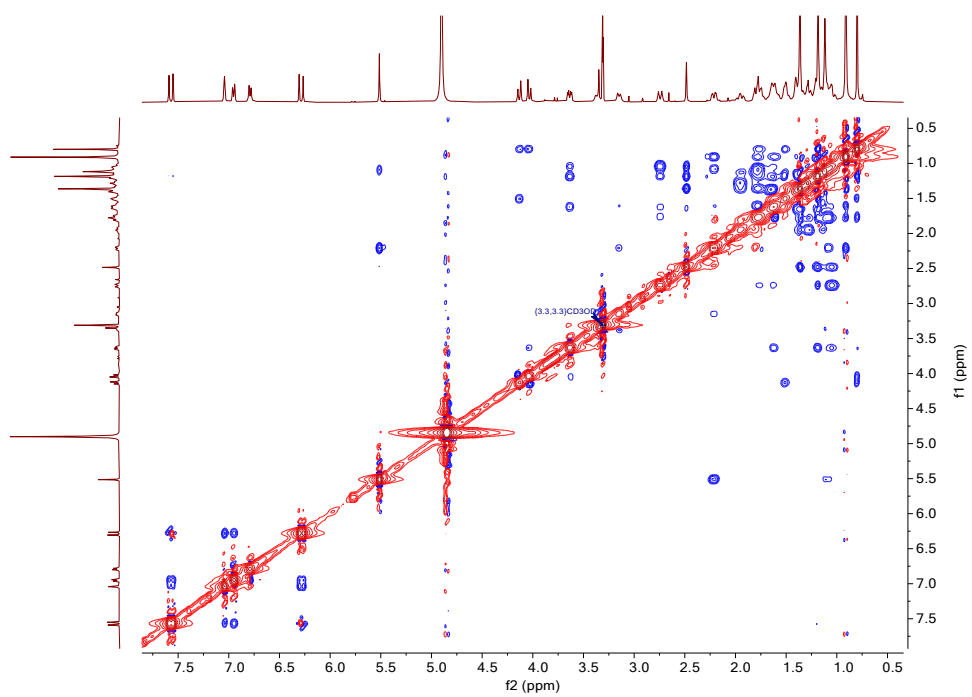


Figure S49. NOESY NMR spectrum of compound **6** (400 MHz, CD₃OD).

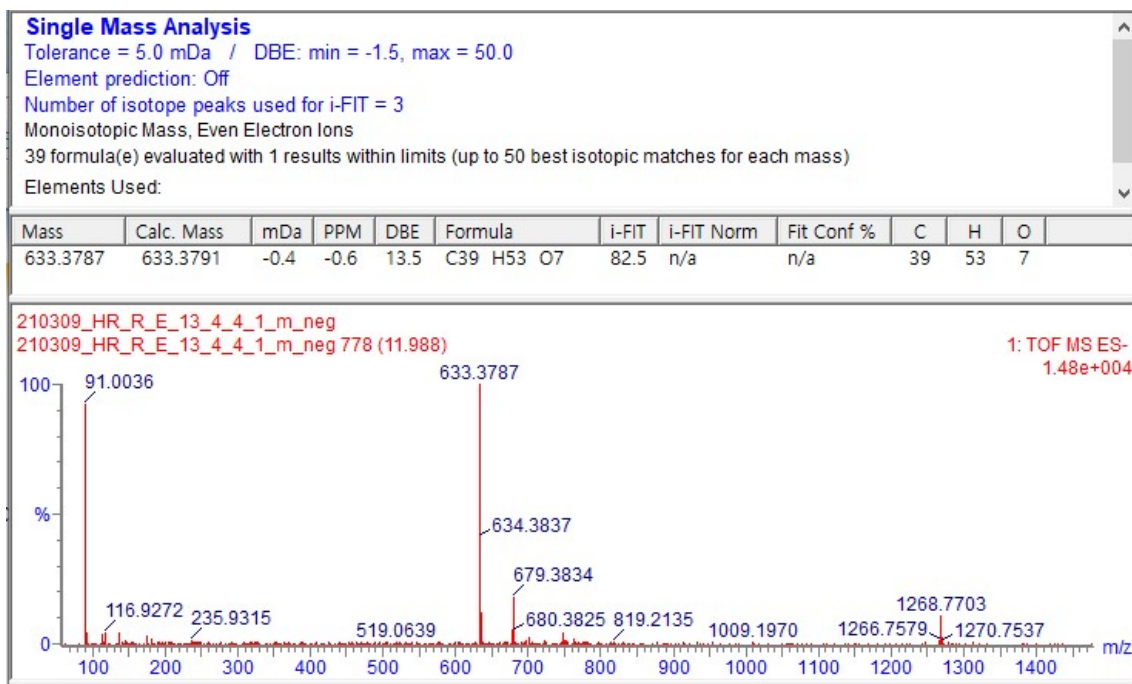
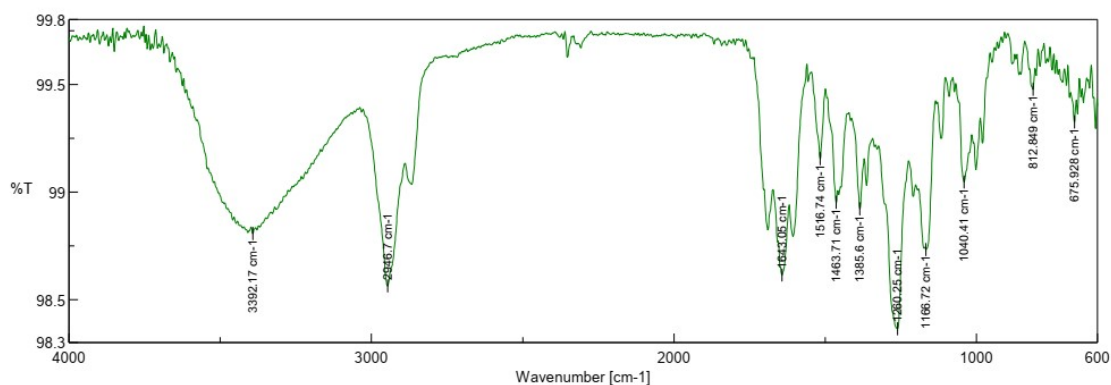


Figure S50. HRESIMS spectrum of compound 6.



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End 4000.6 cm-1	Filter Auto (30000 Hz)
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Data points 3528	

Figure S51. IR spectrum of compound 6.

2. Supplemental ECD calculation

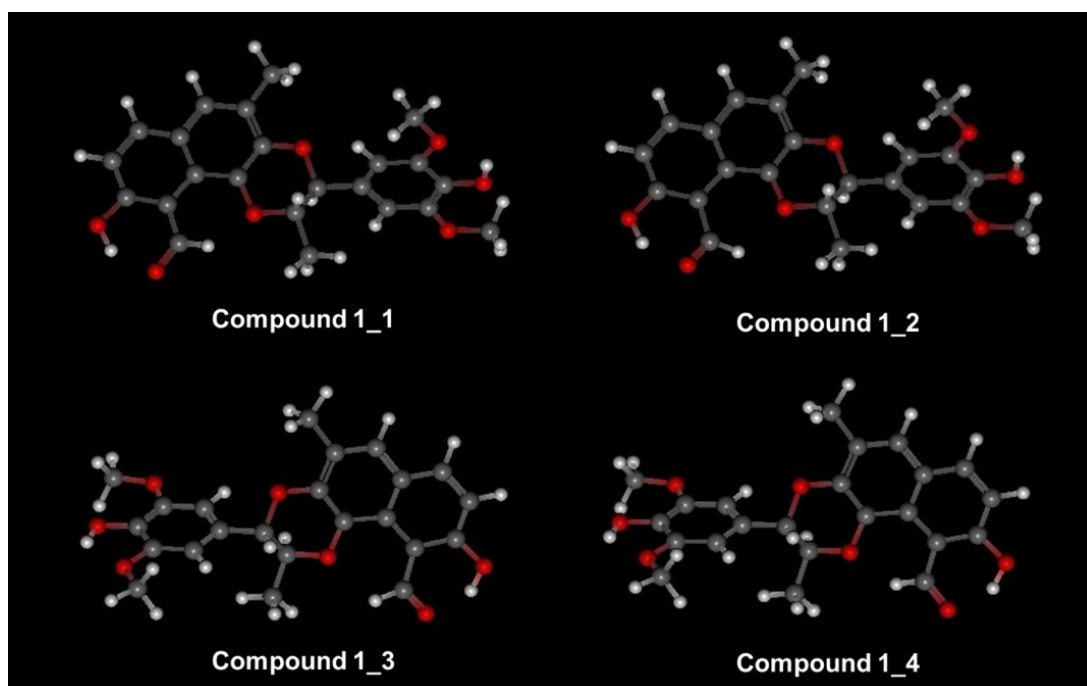


Figure S52. 3D structural models of the minimized main conformers for compound 1.

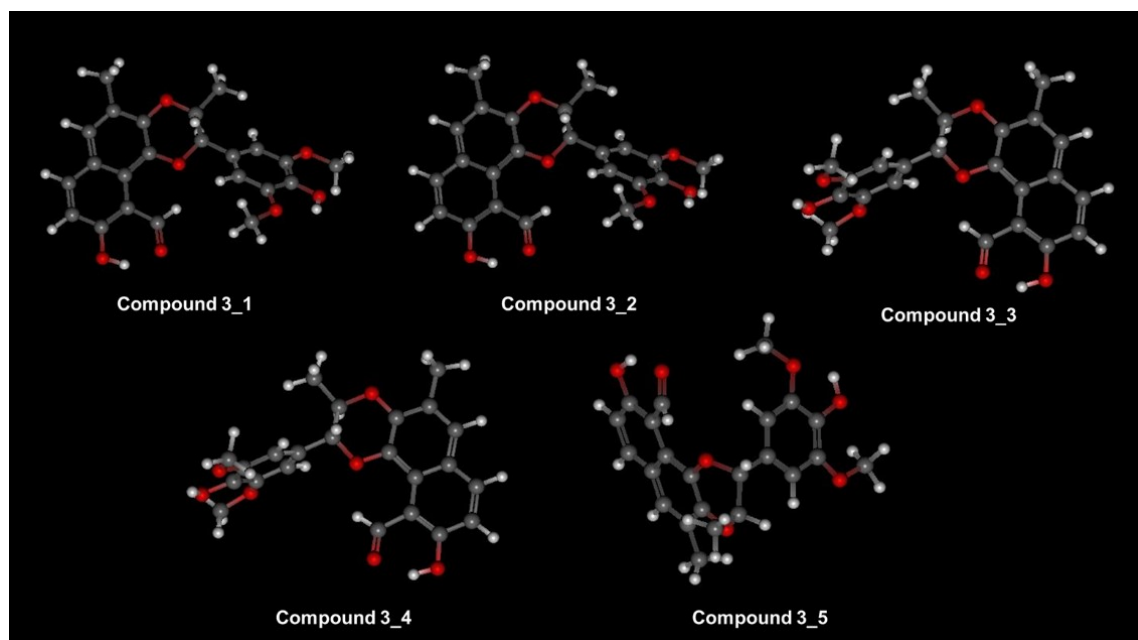


Figure S53. 3D structural models of the minimized main conformers for compound 3.

3. Supplemental biological data

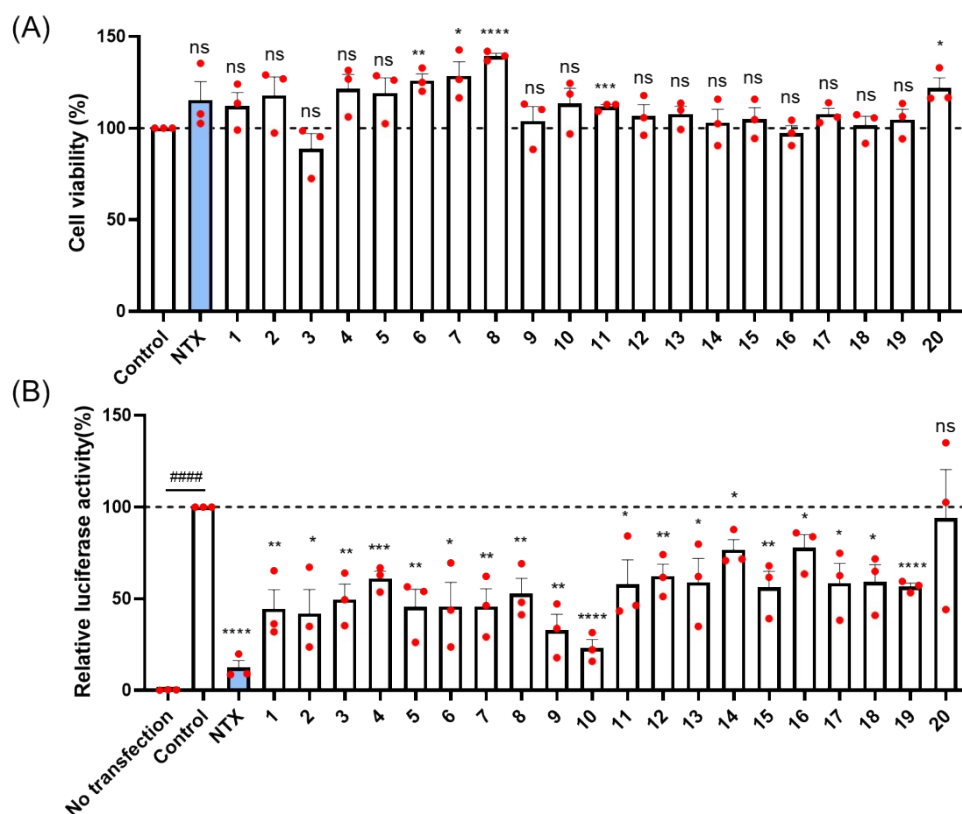


Figure S54. Effects of compounds isolated from *H. syriacus* on $p16^{INK4A}$ promoter activity.

(A) Cell viability of the isolated compounds (1–20) was determined by MTT assay. Results are expressed as relative viability (%) compared to the untreated control group (set at 100%). (B) Inhibitory effects of the compounds (10 μ M) on $p16^{INK4A}$ promoter activity. A549 cells were co-transfected with a pGL3- $p16^{INK4A}$ reporter plasmid encoding the $p16^{INK4A}$ promoter and a pSV- β -galactosidase plasmid as an internal control for 7 h. After transfection, cells were treated with each compound (10 μ M) or navitoclax (NTX, 1 μ M; positive control) for 20 h. Luciferase activity was measured using a luminescence reader and normalized to β -galactosidase activity. Data represent mean \pm SEM ($n = 3$). Statistical significance was determined using Student's *t*-test (* $p < 0.05$, ** $p < 0.01$, *** $p < 0.001$ and **** $p < 0.0001$ vs. untreated control; ##### $p < 0.0001$ vs. no-transfection control).

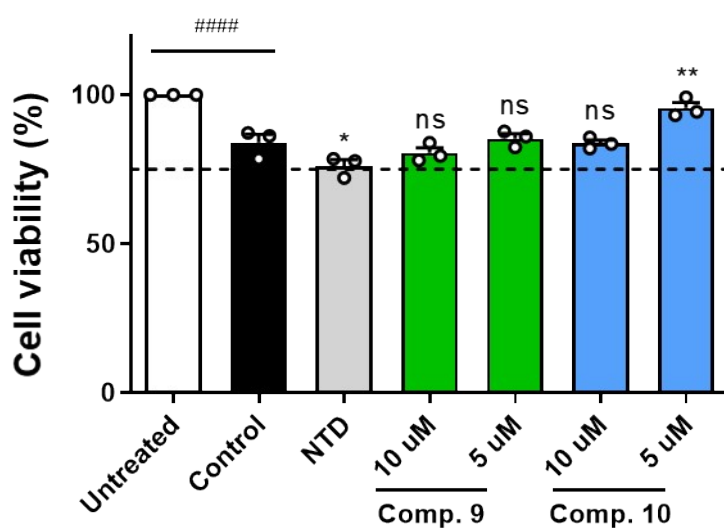


Figure S55. Cell viability of bleomycin-induced IMR-90 fibroblast treated with compounds **9** and **10**.

*IMR90 cells were exposed to bleomycin (BLM, 40 $\mu\text{g}/\text{mL}$) for 2 days and then treated with the indicated compounds or NTD (nintedanib, 5 μM ; positive control) for an additional 2 days (Control). Cell viability was quantified using the MTT assay and expressed as percentage relative to untreated cells. Data are presented as mean \pm SEM ($n = 3$). Statistical significance was determined using one-way ANOVA followed by Dunn's multiple comparisons test (#### $p < 0.0001$ vs. untreated; * $p < 0.05$ and ** $p < 0.0001$ vs. BLM-treated (control) group).*

4. Supplemental tables

Table S1. ¹H and ¹³C NMR spectroscopic data for compounds **1–3**.

pos.	1 ^a		2 ^a		3 ^b	
	δ_{H} (<i>J</i> in Hz)	δ_{C}	δ_{H} (<i>J</i> in Hz)	δ_{C}	δ_{H} (<i>J</i> in Hz)	δ_{C}
1		113.1		111.8		113.0
2		166.5		166.3		166.6
3	6.96, d (8.9)	117.3	6.95, s	114.0	6.96, d (9.1)	117.4
4	7.78, d (8.9)	138.6		156.6	7.78, d (9.1)	138.6
4a		123.8		121.9		123.7
5	7.20, s	123.4	7.53, s	118.5	7.22, s	123.6
6		125.4		124.8		125.3
7		143.2		142.7		142.6
8		137.9		138.4		138.6
8a		122.1		123.0		122.2
9	11.26, s	199.1	11.20, s	198.6	11.15, s	199.3
10			3.66, m	29.5		
11,12			1.37, d (6.8)	23.3		
1□		127.9		128.0		127.7
2□, 6□	6.64, s	104.3	6.64, s	104.2	6.62, s	104.3
3□, 5□		147.4		147.4		147.6
4□		135.5		135.5		135.7
7□	4.73 d (8.0)	81.2	4.75 d (7.9)	81.3	4.64 d (7.9)	81.3
8□	4.15 m	74.5	4.14, m	74.6	4.25, m	74.3
2-OH	14.20, s		14.22, s		14.25, s	
6-Me	2.34, s	16.1	2.38, s	16.7	2.37, s	16.0
8□-Me	1.33, d (6.2)	17.4	1.33, d (6.5)	17.4	1.29, d (6.3)	17.3
3□, 5□-OMe	3.93, s	56.6	3.93, s	56.6	3.92, s	56.6
4□-OH	5.64, s		5.62, s		5.62, s	

^aRecorded in CDCl₃ at 500 MHz for ¹H and 125MHz for ¹³C. ^bRecorded in CDCl₃ at 600 MHz for ¹H and 150MHz for ¹³C.

1 **Table S2.** ¹H and ¹³C NMR spectroscopic data for compounds **4–6**.

pos.	4^a		5^a		6^b	
	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)	δ_{C}
1	1.03, m 1.66, m	39.8	1.04, td (13.5, 3.1) 2.74, td (13.5, 3.5)	40.1	1.05 ^c 2.74, td (13.5, 3.6)	40.1
2	1.67, m	27.4	1.65 ^c 1.77 ^c	27.3	1.62 ^c 1.78 ^c	27.3
3	3.62, d (11.8, 4.5)	72.8	3.64, dd (11.9, 4.6)	72.6	3.64, dd (11.7, 4.6)	72.5
4		43.3		43.6		43.6
5	1.23, dd (8.6, 4.4)	48.0	1.19 ^c	49.0	1.18 ^c	49.0
6	1.47, m	19.3	1.52, m	18.4	1.51, m	18.4
7	1.29, m 1.47, m	33.4	1.40, m ^c 1.65, m ^c	33.4	1.39 ^c 1.64 ^c	33.4
8		41.0		46.7		46.8
9	1.64, m ^c	49.4	2.49, s	63.3	2.48, s	63.3
10		37.9		38.2		38.2
11	1.93, m ^c	24.7		202.2		202.3
12	5.24, t (3.7)	124.2	5.54, s	129.0	5.56, s	128.7
13		145.0		173.2		173.2
14		42.8		44.6		44.7
15	0.88, m 1.65, m	26.6	1.19, m ^c 1.76, m ^c	26.8	1.15 ^c 1.78 ^c	26.8
16	1.16, m 1.97, m	23.2	1.29 ^c 2.08, td (14.0, 4.7)	22.8	1.29, m 1.95, dt (13.6, 6.9)	22.6
17		37.0		37.0		38.2
18	2.10, dd (13.6, 4.6)	43.8	2.32, dd (13.6, 3.9)	44.0	2.21, dd (13.5, 4.4)	44.1
19	1.07, m 1.78, t (13.6)	47.4	1.12 ^c 1.82, t (13.5)	45.9	1.09 ^c 1.78 ^c	46.2
20		31.8		31.9		32.0
21	1.16, m 1.34, m	35.0	1.25 ^c 1.40 ^c	34.7	1.21 ^c 1.39 ^c	34.9
22	1.37, m 1.56, m	32.5	1.42 ^c 1.65 ^c	31.9	1.39 ^c 1.65 ^c	31.7
23	4.03, d (11.3) 4.14, d (11.3)	66.6	4.03, d (11.4) 4.15, d (11.4)	66.6	4.03, d (11.4) 4.13, d (11.4)	66.6
24	0.79, s	12.8	0.81, s	12.7	0.80, s	12.7
25	1.02, s	16.4	1.20, s	17.2	1.18, s	17.3
26	0.98, s	17.3	1.14, s	19.1	1.12, s	19.1
27	1.14, s	26.5	1.38, s	23.9	1.39, s	23.8
28	3.77, d (11.0) 4.12, d (11.0)	71.1	3.81, d (11.3) 4.06, d (11.3)	70.5	3.15, d (11.4) 3.36, d (11.4)	69.7
29	0.89, s	33.6	0.93, s	33.2	0.91, s	33.4
30	0.90, s	23.9	0.94, s	23.7	0.91, s	23.8
1□		127.7		127.6		127.6
2□	7.04, d (2.0)	115.1	7.04, d (2.1)	115.2	7.04, d (2.0)	115.2
3□		146.9		147.0		146.9
4□		149.7		149.8		149.7
5□	6.79, d (8.2)	116.5	6.79, d (8.2)	116.6	6.79, d (7.9)	116.6
6□	6.93, dd (8.2, 2.0)	123.0	6.95, dd (8.2, 2.1)	123.0	6.95, dd (7.9, 2.0)	123.0
7□	7.56, d (15.8)	146.9	7.57, d (15.7)	147.0	7.57, d (15.8)	147.0
8□	6.27, d (15.8)	115.1	6.28, d (15.7)	115.1	6.29, d (15.8)	115.1

	9□		169.1		169.0		169.0
	28-COH	8.11, s	163.1	8.12, s	162.8		
2	^a Recorded in methanol- <i>d</i> ₄ at 600 MHz for ¹ H and at 150 MHz for ¹³ C; ^b Recorded in methanol- <i>d</i> ₄ at 400 MHz for ¹ H and at						
3	100 MHz for ¹³ C; ^c Overlapped.						

Table S3. Calculated total energies, relative free energies (ΔG), relative population (%) and theoretical (DFT B3LYP/6-31G) averaged rotary strength values for the major compound **1** conformers.

Conf.	Gibbs free energy (298.15K)		
	G (Hartree)	ΔG (kcal/mol)	Boltzmann Distribution
Compound1_1	-1415.028394	0.000000	33.127083
Compound1_2	-1415.028393	0.000667	33.089808
Compound1_3	-1415.027419	0.399756	16.871738
Compound1_4	-1415.027423	0.398366	16.911371

Table S4. Calculated total energies, relative free energies (ΔG), relative population (%) and theoretical (DFT B3LYP/6-31G) averaged rotary strength values for the major compound **3** conformers.

Conf.	Gibbs free energy (298.15K)		
	G (Hartree)	ΔG (kcal/mol)	Boltzmann Distribution
Compound3_1	-1415.02919	0.000000	35.772830
Compound3_2	-1415.029174	0.006564	35.378728
Compound3_3	-1415.027829	0.558020	13.948307
Compound3_4	-1415.027811	0.565288	13.778268
Compound3_5	-1415.024187	2.051297	1.121868

Table S5. Optimized coordinates of the conformers of compound 1.

cartesian coordinates				cartesian coordinates			
atom	X	Y	Z	atom	X	Y	Z
c	-2.05818793	2.1200817	-0.94598065	c	-2.05336471	2.13704984	-0.89644187
c	-3.00677765	4.54818624	-1.57915068	c	-2.99886398	4.5826857	-1.46371676
c	-5.59378241	4.86666572	-1.52748914	c	-5.58470738	4.90636908	-1.38942276
c	-7.26823283	2.86467249	-0.91042309	c	-7.26111495	2.89401223	-0.81276117
c	-6.33179299	0.39529831	-0.28860594	c	-6.32786045	0.4075329	-0.25834706
c	-3.64525749	0.12060984	-0.27324748	c	-3.6422139	0.1255475	-0.26533368
c	-9.92519797	3.31950905	-0.87927663	c	-9.91648253	3.35513497	-0.75359873
c	-11.63373863	1.47578057	-0.26626639	c	-11.62641528	1.50141184	-0.17568513
c	-10.7683488	-0.99606203	0.33261788	c	-10.76420843	-0.98686269	0.35585984
c	-8.14485143	-1.58929508	0.29892899	c	-8.14272906	-1.58622014	0.29042033
c	-7.49095452	-4.2273974	0.76610494	c	-7.49340087	-4.2370107	0.68591303
h	-5.49429567	-4.78588346	0.58947936	h	-5.49982371	-4.79651327	0.48058537
o	-9.06670395	-5.87591361	1.30937155	o	-9.07023183	-5.89431658	1.19848301
o	-12.51786126	-2.70262249	0.88206765	o	-12.51504366	-2.70198336	0.87356652
o	-2.60000864	-2.14267633	0.4246449	o	-2.59858475	-2.15679881	0.36989529
c	0.00643722	-2.12440253	1.13135838	c	0.00857185	-2.15839607	1.07360709
c	1.49686723	-0.66008446	-0.89522777	c	1.49914114	-0.64959611	-0.92013961
o	0.50596867	1.85012165	-1.01347893	o	0.50981459	1.8633172	-0.98344953
c	4.30461186	-0.50376985	-0.408611	c	4.3068976	-0.50443772	-0.42909219
c	0.80581417	-4.86063634	1.47276019	c	0.80486826	-4.9029659	1.34943202
c	5.96613486	-2.09819941	-1.6919001	c	5.96879309	-2.07493116	-1.74125482
c	8.57658827	-2.07751766	-1.19765981	c	8.57889098	-2.06458968	-1.24476626
c	9.52611647	-0.40595621	0.63197549	c	9.52781048	-0.42825683	0.61678416
c	7.84245285	1.25219711	1.87983259	c	7.8439242	1.20639184	1.89485943
c	5.25532612	1.20801922	1.39003117	c	5.25713273	1.17231511	1.40252567
o	12.02357399	-0.34750926	1.23275243	o	12.02484978	-0.38213596	1.22005995
o	9.0307782	2.80233654	3.57527287	o	9.03148472	2.72365903	3.62029978
o	10.02298136	-3.76951677	-2.48195551	o	10.02609943	-3.73247333	-2.55934109
c	12.37693625	-3.00023742	-3.52018562	c	12.37839228	-2.94223353	-3.58544261
c	7.59341561	4.55651697	4.97896703	c	7.59278433	4.44739291	5.05985114
c	-1.19373718	6.63236441	-2.26840873	c	-1.18419114	6.67876476	-2.11149192
h	-6.40155674	6.71453984	-1.98789249	h	-6.39009358	6.76728984	-1.79872637
h	-10.59069064	5.22019318	-1.35682269	h	-10.5793877	5.26895107	-1.1794646
h	-13.66955301	1.8190359	-0.23005665	h	-13.66093651	1.84919415	-0.11784249
h	-11.5968483	-4.35017296	1.21905029	h	-11.59666647	-4.35989005	1.1634354
h	0.19669378	-1.08426637	2.93976092	h	0.20243229	-1.16109672	2.90568071
h	1.15272516	-1.60675438	-2.72905823	h	1.15513772	-1.55559221	-2.77454188
h	2.75797221	-4.97694806	2.18870671	h	2.75772523	-5.03871495	2.05997687
h	-0.46180849	-5.79566551	2.83907398	h	-0.46241073	-5.8681842	2.69485468
h	0.69546784	-5.89787676	-0.3350574	h	0.69083712	-5.89743523	-0.48213644
h	5.29284481	-3.41714237	-3.13228843	h	5.29608677	-3.36619344	-3.20682
h	3.96970889	2.50455149	2.34445899	h	3.97130871	2.45081236	2.3806917
h	12.23753376	0.96780458	2.51074475	h	12.23835874	0.90778524	2.52371738
h	12.93464453	-4.50422808	-4.84909574	h	12.93893363	-4.42386843	-4.93805146
h	12.18269451	-1.20050304	-4.57127868	h	12.18044303	-1.12639797	-4.6078658
h	13.84222372	-2.77616577	-2.05679991	h	13.84344854	-2.73856157	-2.11882786
h	6.62252912	5.92318801	3.72714436	h	6.62098635	5.83900628	3.83657178
h	6.17124258	3.59505176	6.17515093	h	6.17132529	3.46026039	6.23578973
h	8.93459272	5.57824468	6.19874776	h	8.93315325	5.44480417	6.30048897
h	-2.22186892	8.38049288	-2.74973639	h	-2.21010375	8.44263329	-2.536691
h	0.11923048	7.05374148	-0.69835242	h	0.14351766	7.05300608	-0.54191542
h	-0.00316852	6.09402958	-3.89792446	h	-0.00933971	6.18082298	-3.76524767

(Table S5 continued)

cartesian coordinates				cartesian coordinates			
atom	X	Y	Z	atom	X	Y	Z
c	2.06256566	2.26243745	0.73752287	c	2.06600571	2.29988815	0.61510227
c	2.99539197	4.74975449	1.11376631	c	2.99900408	4.8009335	0.88257061
c	5.57777426	5.08402746	0.98625775	c	5.58170345	5.12832968	0.74517822
c	7.26357568	3.0468661	0.53737651	c	7.26725488	3.07297777	0.38765403
c	6.34284894	0.52095607	0.17385163	c	6.34613064	0.53415542	0.13079473
c	3.66051203	0.22279493	0.23186578	c	3.66355971	0.23953221	0.20002499
c	9.91421632	3.52018547	0.41078544	c	9.91842437	3.53942791	0.24740963
c	11.63163922	1.64117946	-0.05373226	c	11.63608911	1.64189823	-0.13318074
c	10.78222575	-0.88474527	-0.39179946	c	10.78616208	-0.89551628	-0.36790471
c	8.16613547	-1.49524619	-0.250541	c	8.16934359	-1.49867405	-0.20669282
c	7.53153257	-4.17134715	-0.44185498	c	7.53388243	-4.18000451	-0.29351124
h	5.54402196	-4.72581412	-0.17240555	h	5.54512402	-4.72275143	-0.01015603
o	9.11343215	-5.85315387	-0.84833335	o	9.11634152	-5.87732835	-0.62739563
o	12.53935383	-2.62239151	-0.803778	o	12.54309361	-2.64919238	-0.70521409
o	2.6236603	-2.1049034	-0.23310475	o	2.62690386	-2.10631722	-0.16186385
c	0.0207912	-2.15152013	-0.94712442	c	0.0212811	-2.18752552	-0.86345162
c	-1.47792409	-0.53311932	0.95101329	c	-1.47157957	-0.48360522	0.96272103
o	-0.49665825	1.98052335	0.87593374	o	-0.49311675	2.02421892	0.765843
c	-4.28567096	-0.4271024	0.44542708	c	-4.28165532	-0.40315439	0.46602861
c	-0.77357189	-4.90801467	-1.06393957	c	-0.77111323	-4.94683573	-0.8482209
c	-5.23473828	1.04279482	-1.52945469	c	-5.24093982	0.96854199	-1.57345913
c	-7.82867282	1.10017075	-2.08959721	c	-7.83817984	1.00171525	-2.1208005
c	-9.49852385	-0.37389754	-0.64189803	c	-9.50053961	-0.39811031	-0.59275227
c	-8.53603111	-1.82133203	1.38384586	c	-8.52735107	-1.74461917	1.49670411
c	-5.95789337	-1.86024057	1.93261659	c	-5.94618441	-1.75945192	2.0317986
o	-12.01452263	-0.44154505	-1.15409633	o	-12.01995156	-0.48830493	-1.08556618
o	-10.3725295	-3.13042303	2.65094348	o	-10.35768336	-2.98649544	2.83832831
o	-8.56430651	2.52130423	-4.09992364	o	-8.58245762	2.32578701	-4.1928956
c	-10.71281465	4.1176407	-3.88945669	c	-10.74249477	3.91442042	-4.05892715
c	-9.69543957	-4.68855334	4.70566808	c	-9.67056311	-4.43704388	4.96698441
c	1.1702103	6.87561295	1.61813152	c	1.17362679	6.94732187	1.28883122
h	6.37322231	6.97583939	1.24634625	h	6.37778836	7.029221	0.92437894
h	10.56727156	5.46452859	0.68756132	h	10.571778	5.49346727	0.44337429
h	13.66244539	1.99802898	-0.16354207	h	13.66733239	1.99304745	-0.25292135
h	11.6295238	-4.30253573	-0.9600164	h	11.6326279	-4.33403441	-0.794293
h	-0.16994668	-1.26328579	-2.83409667	h	-0.1768323	-1.3882349	-2.78891765
h	-1.13256761	-1.33075367	2.85582575	h	-1.11723498	-1.19062064	2.90121194
h	-2.72237427	-5.0838432	-1.77752329	h	-2.72230703	-5.15750791	-1.54574436
h	0.49926742	-5.95067277	-2.3445088	h	0.49811571	-6.04795305	-2.08253041
h	-0.66498029	-5.79457964	0.8235939	h	-0.65529944	-5.74386966	1.07865835
h	-3.98923369	2.21870998	-2.67942828	h	-4.00133764	2.08597864	-2.78643688
h	-5.23403644	-2.98183271	3.50546055	h	-5.21385028	-2.80190356	3.65433705
h	-12.78820816	-1.55849903	0.0956506	h	-12.78676635	-1.54059695	0.22315654
h	-10.64227014	5.39292823	-5.5349909	h	-10.66901315	5.12484064	-5.75260498
h	-12.4952227	3.03964948	-3.91331626	h	-12.5176098	2.82431743	-4.05199803
h	-10.62929633	5.26171187	-2.13865939	h	-10.67891803	5.1263043	-2.35357883
h	-8.38612986	-6.20951614	4.11274302	h	-8.36636843	-5.98851265	4.44626107
h	-8.80807649	-3.5818931	6.24419741	h	-8.77277683	-3.25341444	6.44075034
h	-11.45893447	-5.54098212	5.40824059	h	-11.43089125	-5.24945151	5.72291237
h	2.18532337	8.67561344	1.88897775	h	2.1886526	8.7571399	1.48308238
h	-0.17966581	7.11178236	0.04084686	h	-0.17178703	7.11493912	-0.30117342
h	0.02037901	6.50038795	3.32136249	h	0.01897761	6.64749545	3.00359258

Table S6. Optimized coordinates of the conformers of compound 3.

cartesian coordinates				cartesian coordinates			
atom	X	Y	Z	atom	X	Y	Z
c	-3.91594672	3.85353959	0.4626245	c	-3.91941219	3.86577718	0.31704822
c	-6.42149224	4.81050623	0.50583752	c	-6.4288919	4.81394413	0.32432147
c	-8.35259007	3.10460362	0.11204765	c	-8.3555851	3.0801263	0.04781114
c	-7.89385025	0.49654765	-0.3128533	c	-7.88874577	0.4531906	-0.22515754
c	-5.36638267	-0.48865364	-0.39751472	c	-5.35771774	-0.5253376	-0.27211717
c	-3.39002527	1.3104344	-0.01290623	c	-3.38602271	1.30100938	-0.01200845
c	-9.98017333	-1.17075255	-0.67438296	c	-9.97059766	-1.24067733	-0.47013437
c	-9.66617849	-3.70437038	-1.09280166	c	-9.64893982	-3.79333165	-0.74101721
c	-7.19051771	-4.74168996	-1.18029879	c	-7.1695123	-4.82412797	-0.78738012
c	-5.02085968	-3.18323183	-0.85005504	c	-5.00420527	-3.24057801	-0.56631816
c	-2.57978084	-4.45904234	-0.99487554	c	-2.55893235	-4.51366597	-0.6500993
h	-0.8573601	-3.31196933	-0.78031105	h	-0.83982567	-3.3499498	-0.51096786
o	-2.34261199	-6.7658018	-1.35088707	o	-2.31457062	-6.83627693	-0.87242277
o	-7.01585294	-7.20774273	-1.58291385	o	-6.98709318	-7.30892646	-1.04537368
o	-0.92228829	0.52548059	-0.10477329	o	-0.91544473	0.52253724	-0.08055808
c	0.96265784	2.42421093	-0.48481768	c	0.95484018	2.40426338	-0.59589327
c	0.44153394	4.60034676	1.3730277	c	0.44396213	4.68482744	1.13521216
o	-2.03747185	5.56033382	0.89551638	o	-2.04559133	5.60308273	0.63224091
c	2.25176964	6.81946134	1.17314285	c	2.23993062	6.89632233	0.78104755
c	3.52978259	1.21441001	-0.18027864	c	3.53190941	1.2271235	-0.2517958
c	5.48924137	1.81766448	-1.83790538	c	5.46051853	1.72004305	-1.9804832
c	7.92531745	0.80039731	-1.54007149	c	7.90472315	0.73037746	-1.65647343
c	8.38792084	-0.86498654	0.47415807	c	8.40792757	-0.7913912	0.45874696
c	6.38023704	-1.51985444	2.11194562	c	6.43145964	-1.33597798	2.17297824
c	3.9758176	-0.48652134	1.81537807	c	4.01850971	-0.33172815	1.84796009
o	10.71929459	-1.8596069	0.88512515	o	10.74933333	-1.75131227	0.89483442
o	9.73118173	1.57199961	-3.19823994	o	9.67891151	1.38785677	-3.39616409
c	11.37633506	-0.23913477	-4.30585097	c	11.30742815	-0.49393631	-4.40622255
o	7.08819388	-3.18813035	3.95456178	o	7.17707159	-2.87169462	4.11310823
c	5.26205574	-4.08850622	5.67958793	c	5.38373309	-3.65931912	5.92565714
c	-6.86025154	7.58180877	0.98706597	c	-6.87550789	7.60739033	0.64303555
h	-10.31331916	3.76338403	0.14051331	h	-10.31892786	3.73171341	0.05241693
h	-11.88649232	-0.36768153	-0.60727223	h	-11.87977561	-0.44243406	-0.43471276
h	-11.25963056	-4.98872483	-1.36636082	h	-11.23881802	-5.09782518	-0.92509474
h	-5.14547619	-7.63476703	-1.58854672	h	-5.11502883	-7.72819637	-1.03998351
h	0.7692222	3.18963839	-2.42230107	h	0.73404703	3.05143275	-2.57342155
h	0.48125896	3.80637977	3.31042074	h	0.51154679	4.00856442	3.11625775
h	1.61085885	8.35251328	2.43280052	h	1.60812704	8.49794031	1.95730395
h	4.17994998	6.25883019	1.72663725	h	4.17832958	6.37756488	1.33992378
h	2.30304783	7.56087459	-0.77758165	h	2.26125659	7.52217989	-1.21024357
h	5.19139572	3.09690623	-3.43215248	h	5.13102136	2.88599465	-3.65349622
h	2.43392132	-1.00804136	3.07816078	h	2.50052413	-0.77048012	3.16985273
h	10.57229193	-2.98855323	2.33890489	h	10.6319787	-2.77823002	2.42497579
h	12.32277043	0.73616516	-5.8842769	h	12.21478536	0.36704561	-6.07182223
h	12.80043713	-0.93270862	-2.95304527	h	12.76365774	-1.08357333	-3.03848532
h	10.29980327	-1.86827333	-5.06039658	h	10.22186648	-2.17662509	-5.01696938
h	3.70834816	-5.08230231	4.69324551	h	3.81747486	-4.72141392	5.03473884
h	6.24492072	-5.42528829	6.93524645	h	6.39293683	-4.90604021	7.25119006
h	4.4633833	-2.53098076	6.82609788	h	4.59810021	-2.03079946	6.9784467
h	-8.89636559	8.02517181	0.96335334	h	-8.91367187	8.04086433	0.61135525
h	-6.07970648	8.16578274	2.83505855	h	-6.08071331	8.30353435	2.44553863
h	-5.91183147	8.76355424	-0.45157464	h	-5.94510876	8.70445107	-0.87252558

(Table S6 continued)

cartesian coordinates				cartesian coordinates			
atom	X	Y	Z	atom	X	Y	Z
c	4.01843493	3.75685583	-0.25746359	c	3.97740116	3.79056326	-0.38964932
c	6.54477476	4.65959587	-0.25740607	c	6.49580046	4.71471737	-0.41646486
c	8.44511353	2.87613971	-0.19991566	c	8.41088926	2.95337797	-0.25737503
c	7.93575105	0.24321451	-0.15516167	c	7.92388701	0.32139341	-0.08702038
c	5.38863904	-0.69355558	-0.13892712	c	5.38492716	-0.63607364	-0.04486961
c	3.44491258	1.18137783	-0.16261619	c	3.42555751	1.21787905	-0.17337901
c	9.99029141	-1.50035893	-0.09777391	c	9.99243608	-1.3990202	0.07202464
c	9.62544175	-4.06034443	-0.02100818	c	9.64853592	-3.95527373	0.27156026
c	7.12810245	-5.04914645	-0.00911047	c	7.15966069	-4.9644112	0.3113289
c	4.98976011	-3.41692337	-0.08352852	c	5.00846269	-3.35678084	0.13923884
c	2.52307398	-4.65223964	-0.14359782	c	2.55296449	-4.61534712	0.11551988
h	0.82562074	-3.45633602	-0.27366564	h	0.84705376	-3.44250679	-0.09079577
o	2.24172643	-6.97966501	-0.07044646	o	2.29046408	-6.93879622	0.30024023
o	6.9044328	-7.54309297	0.05951027	o	6.95621467	-7.45389871	0.49962346
o	0.96344473	0.43951004	-0.07903725	o	0.95026268	0.45874898	-0.07066125
c	-0.84145218	2.29300066	0.70135719	c	-0.87635559	2.33080544	0.60800188
c	-0.35556542	4.72746038	-0.81165521	c	-0.40192302	4.69491952	-1.01574239
o	2.17057644	5.54969209	-0.33078503	o	2.11469234	5.56119335	-0.56191941
c	-2.08973707	6.9187458	-0.15236067	c	-2.15867269	6.89899473	-0.46871956
c	-3.45814833	1.20724442	0.35678394	c	-3.4801693	1.20432068	0.297192
c	-4.15743406	0.10300595	-1.93771733	c	-4.15586196	0.00038966	-1.95381535
c	-6.60048928	-0.85869736	-2.3230895	c	-6.5855793	-1.00512425	-2.31074078
c	-8.38376934	-0.68642128	-0.36097469	c	-8.3793997	-0.77615401	-0.36398643
c	-7.65723475	0.3911637	1.97030729	c	-7.67611354	0.40261326	1.92512046
c	-5.22373466	1.33733188	2.33814407	c	-5.25597369	1.39267021	2.26455346
o	-10.78982823	-1.52774849	-0.66652643	o	-10.77420542	-1.65759409	-0.64472803
o	-7.14173132	-1.82131316	-4.64251386	o	-7.10245388	-2.06505802	-4.59275697
c	-8.36374211	-4.20716632	-4.8288256	c	-8.31501622	-4.46084939	-4.69453773
o	-9.56527637	0.40458201	3.71642168	o	-9.59180795	0.46247319	3.66183876
c	-9.12168356	1.4238961	6.13975647	c	-9.16922588	1.57862754	6.04594553
c	7.03645027	7.46285198	-0.32745442	c	6.96386627	7.51541683	-0.62125944
h	10.41979161	3.49253043	-0.19783747	h	10.38004022	3.58713094	-0.2711492
h	11.91309581	-0.73484273	-0.1101077	h	11.90878274	-0.61813133	0.03730466
h	11.19336684	-5.4029377	0.02807322	h	11.22739892	-5.27979438	0.39901101
h	5.02441501	-7.92784103	0.04053942	h	5.07976318	-7.8556494	0.48323905
h	-0.51795448	2.73221555	2.7227604	h	-0.57181329	2.86824084	2.60849101
h	-0.52477968	4.2592396	-2.84514361	h	-0.55591618	4.1305943	-3.02598352
h	-1.47842225	8.62327113	-1.18603915	h	-1.55845493	8.5583869	-1.5794886
h	-4.05968136	6.48984666	-0.67711392	h	-4.12215844	6.42725439	-0.98093517
h	-2.00985329	7.3384037	1.89161592	h	-2.09227275	7.41514245	1.55344067
h	-2.81553688	-0.07517478	-3.49542606	h	-2.80469034	-0.22406725	-3.49737069
h	-4.67808898	2.16114555	4.14880315	h	-4.7283178	2.29539789	4.04253331
h	-11.66735006	-1.24724171	0.93335729	h	-11.66135714	-1.32485294	0.93977374
h	-8.19921684	-4.78117358	-6.82407166	h	-8.11847074	-5.1192755	-6.66066283
h	-7.40791227	-5.63272552	-3.63082553	h	-7.37404078	-5.83049307	-3.42200487
h	-10.37399842	-4.0984487	-4.29281542	h	-10.33341881	-4.33614582	-4.19396361
h	-8.61106075	3.4507876	6.03445918	h	-8.68131845	3.60576052	5.86509495
h	-10.90041198	1.22299835	7.20076032	h	-10.94961032	1.39777918	7.10775511
h	-7.6050025	0.38543916	7.13966959	h	-7.64469527	0.5965284	7.08985965
h	9.08281533	7.85735992	-0.32314466	h	9.00658799	7.92832343	-0.61469533
h	6.1994073	8.33876824	-2.02962448	h	6.13872231	8.29759107	-2.37421482
h	6.17652733	8.42795231	1.31440678	h	6.07698833	8.55343611	0.96062672

(Table S6 continued)

cartesian coordinates			
atom	X	Y	Z
c	-1.55659328	-4.13874279	0.12432016
c	-2.39128148	-5.3736379	-2.10675626
c	-4.1673072	-4.13675102	-3.5610242
c	-5.15174858	-1.73657921	-2.88254637
c	-4.33204422	-0.4778084	-0.623709
c	-2.46387098	-1.76310892	0.83552859
c	-6.94835919	-0.53267349	-4.49042003
c	-7.91307859	1.81292029	-3.97333455
c	-7.14424568	3.10580843	-1.74922145
c	-5.40836842	1.98360899	-0.02696311
c	-4.91645975	3.39045339	2.28940167
h	-3.75926138	2.47537766	3.75846437
o	-5.76398131	5.53676396	2.71387602
o	-8.14649016	5.36780153	-1.35049396
o	-1.54419094	-0.66142309	2.99775131
c	0.92560737	-1.48538484	3.78657324
c	0.89703563	-4.3780121	3.92576221
o	0.22135949	-5.39056	1.50923779
c	-0.87091914	-5.385277	5.97384391
c	2.99038294	-0.29117248	2.17740314
c	4.63871203	-1.67184904	0.65146898
c	6.53003361	-0.47910205	-0.78723392
c	6.7628832	2.1594416	-0.69040113
c	5.05134311	3.56224721	0.81070309
c	3.20102093	2.36377416	2.24388251
o	8.60113668	3.39784811	-1.98701615
o	8.10414681	-1.99958435	-2.13966343
c	8.6751442	-1.37774914	-4.68766824
o	5.4763444	6.10987453	0.71031489
c	3.89748664	7.75745103	2.09518636
c	-1.32240764	-7.92292607	-2.78746453
h	-4.84851472	-5.01894275	-5.30376739
h	-7.54474646	-1.53390603	-6.20116913
h	-9.27497029	2.74892654	-5.21137971
h	-7.43127699	6.00424039	0.30851797
h	1.08414972	-0.73954028	5.7245905
h	2.82581851	-5.07542025	4.27807224
h	-0.93124384	-7.46753604	5.89214607
h	-0.18928154	-4.8197519	7.86434584
h	-2.80646807	-4.6506844	5.72798027
h	4.51177436	-3.72210754	0.48781207
h	1.90028677	3.46124009	3.40919444
h	8.37135571	5.19951265	-1.65406335
h	9.57356591	-3.07040171	-5.504533
h	6.93185555	-0.94717235	-5.7644447
h	9.97676076	0.24295145	-4.8257019
h	4.03519385	7.39539296	4.15142852
h	4.56367403	9.68768757	1.69562536
h	1.89984237	7.58063086	1.50040036
h	-2.18284787	-8.64197173	-4.5440062
h	0.74769907	-7.83234796	-3.05900455
h	-1.65720448	-9.31848712	-1.26924065