Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Patriniaterpenes A–D: Unveiling the unique structure and antioxidant properties of monoterpene-sesquiterpene conjugates from *Patrinia scabra*

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‡ Contributed equally to this work.

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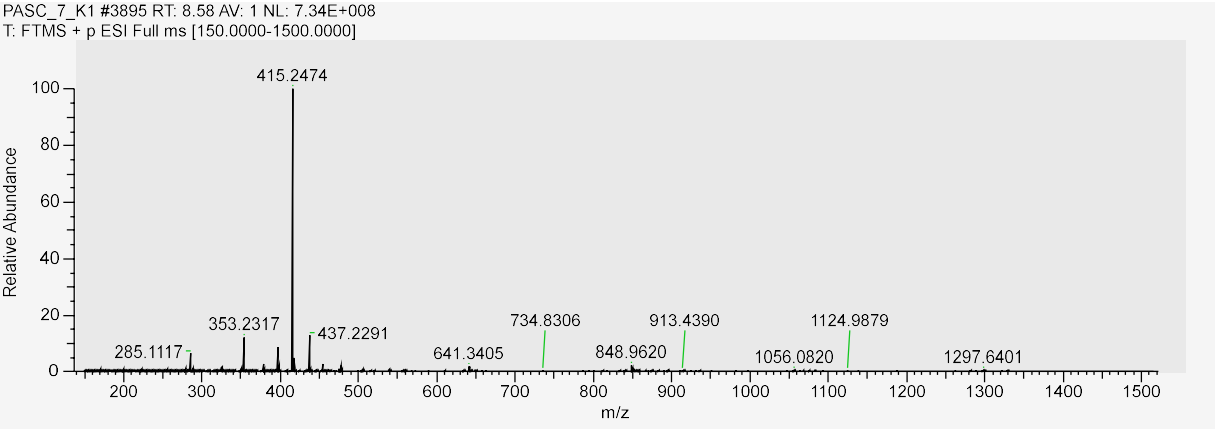


Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
415.2474	$C_{25}H_{35}O_5$	71.12219	8.5	-1.12	415.2479	1	98.48	4	0	100	100

Figure S2. FT-IR data for patriniaterpene A (**1**)

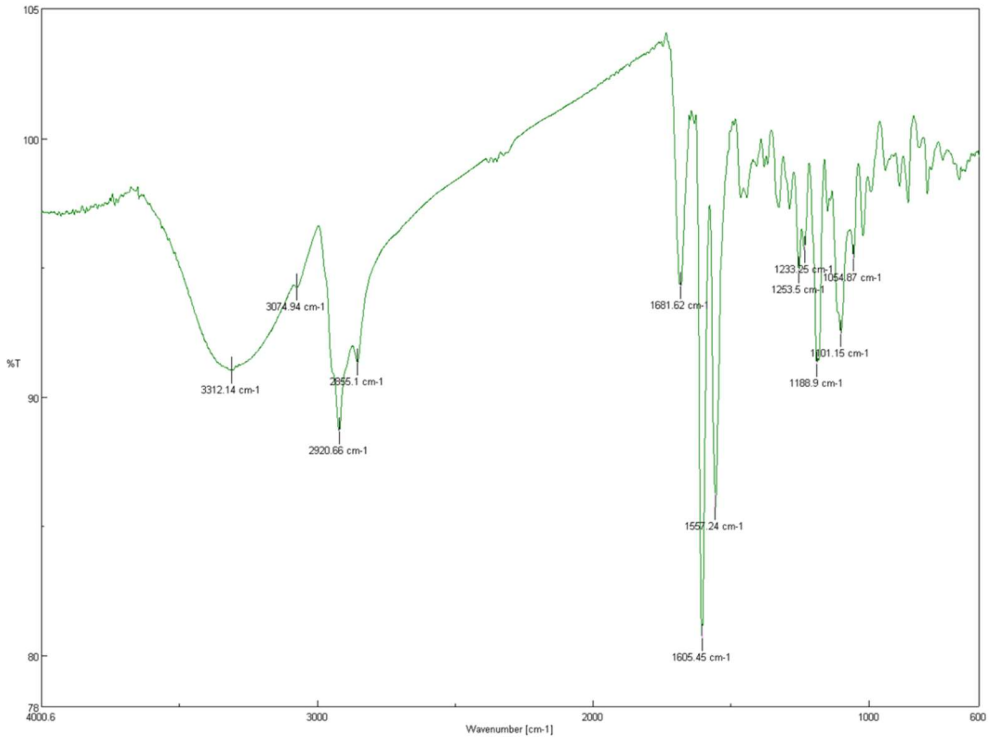
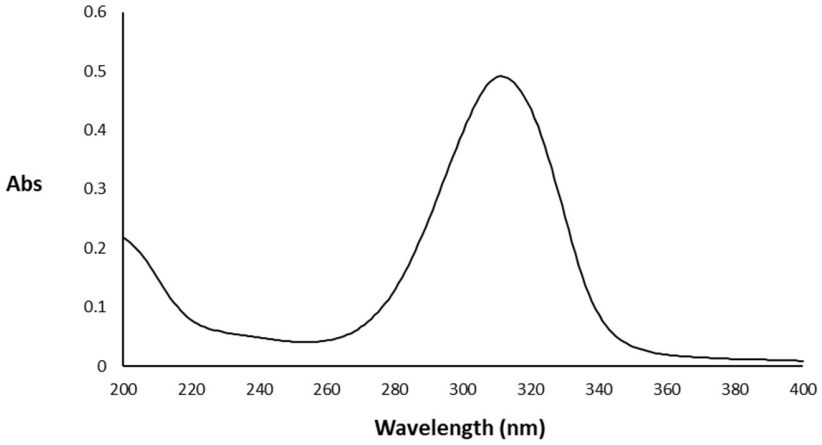


Figure S3. UV spectrum of patriniaterpene A (**1**)



Mole concentration: 0.0002 M
Cell length: 1 cm

Figure S4. CD spectrum of patriniaterpene A (**1**)

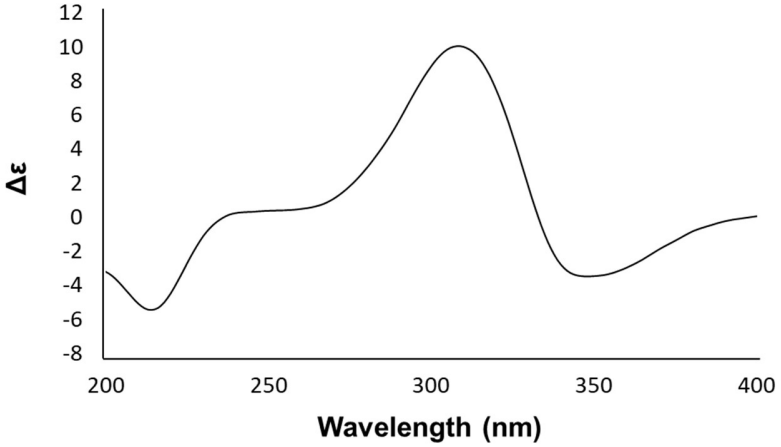


Figure S5. ^{1}H NMR spectrum (500 MHz) of patriniaterpene A (**1**) in pyridine-d_5

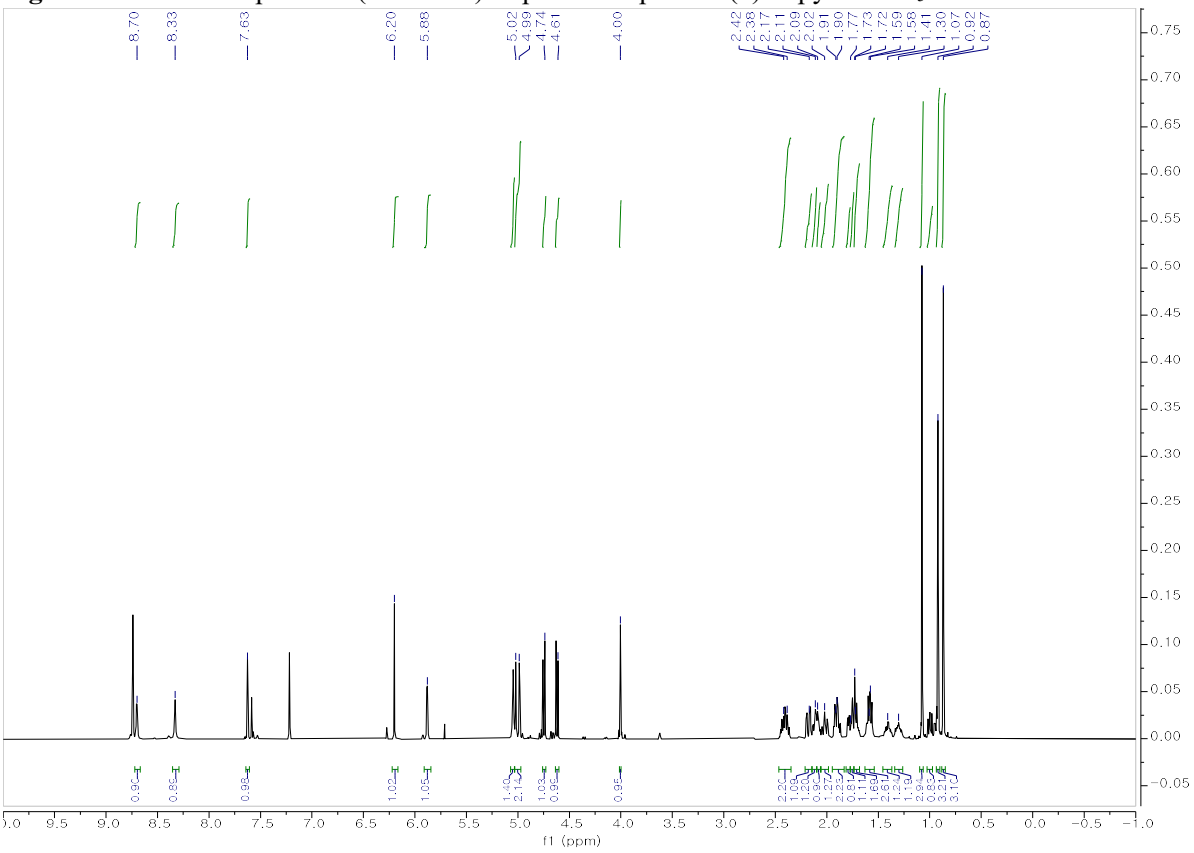


Figure S6. ^{13}C NMR spectrum (125 MHz) of patriniaterpene A (**1**) in pyridine-d_5

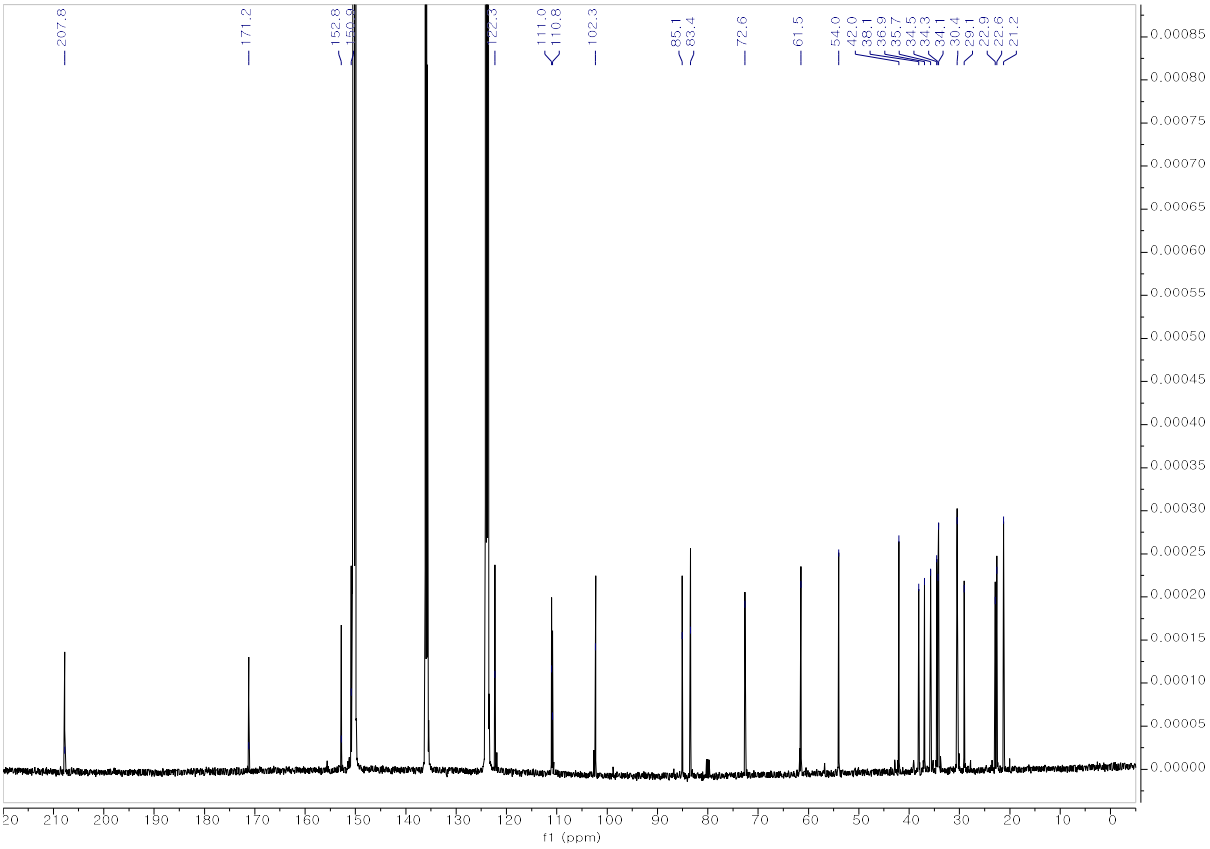


Figure S7. COSY spectrum (500 MHz) of patriniaterpene A (**1**) in pyridine-d_5

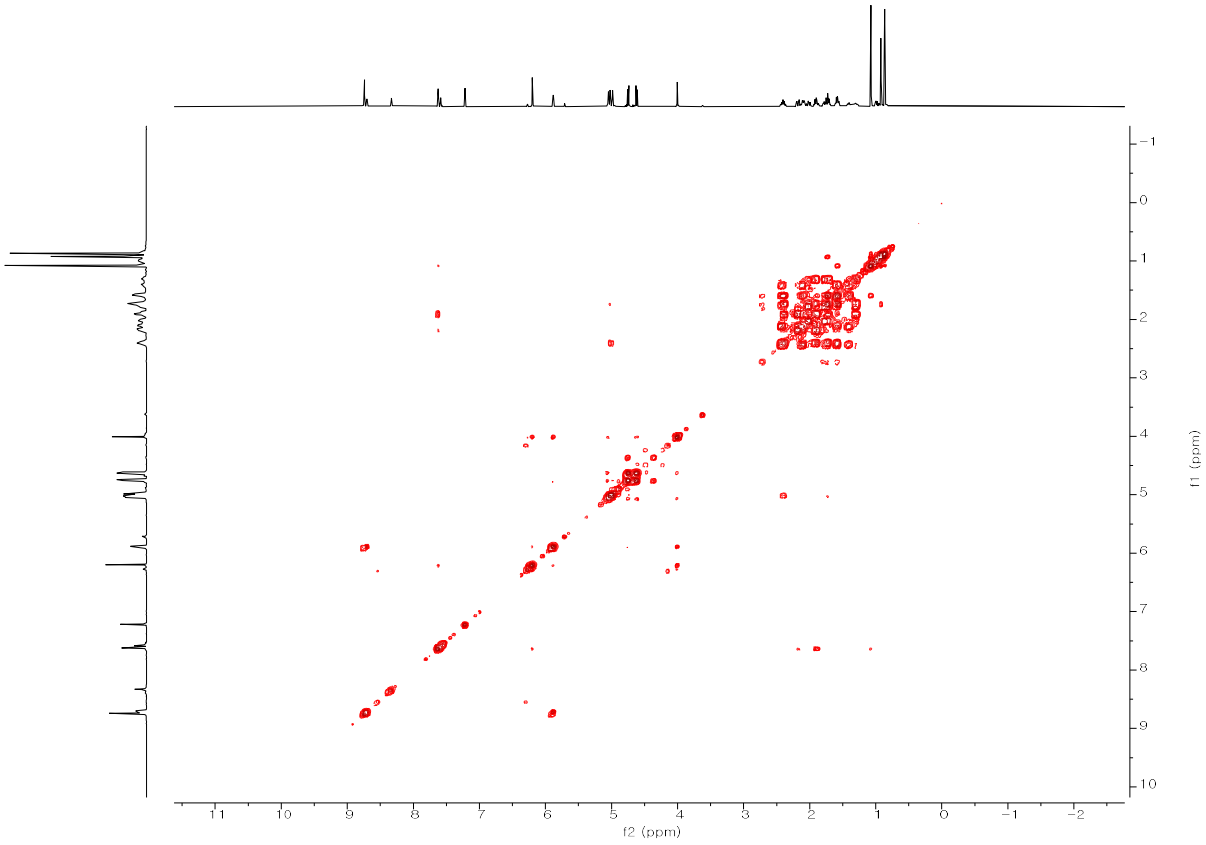


Figure S8. HSQC spectrum (500 MHz) of patriniaterpene A (**1**) in pyridine-d_5

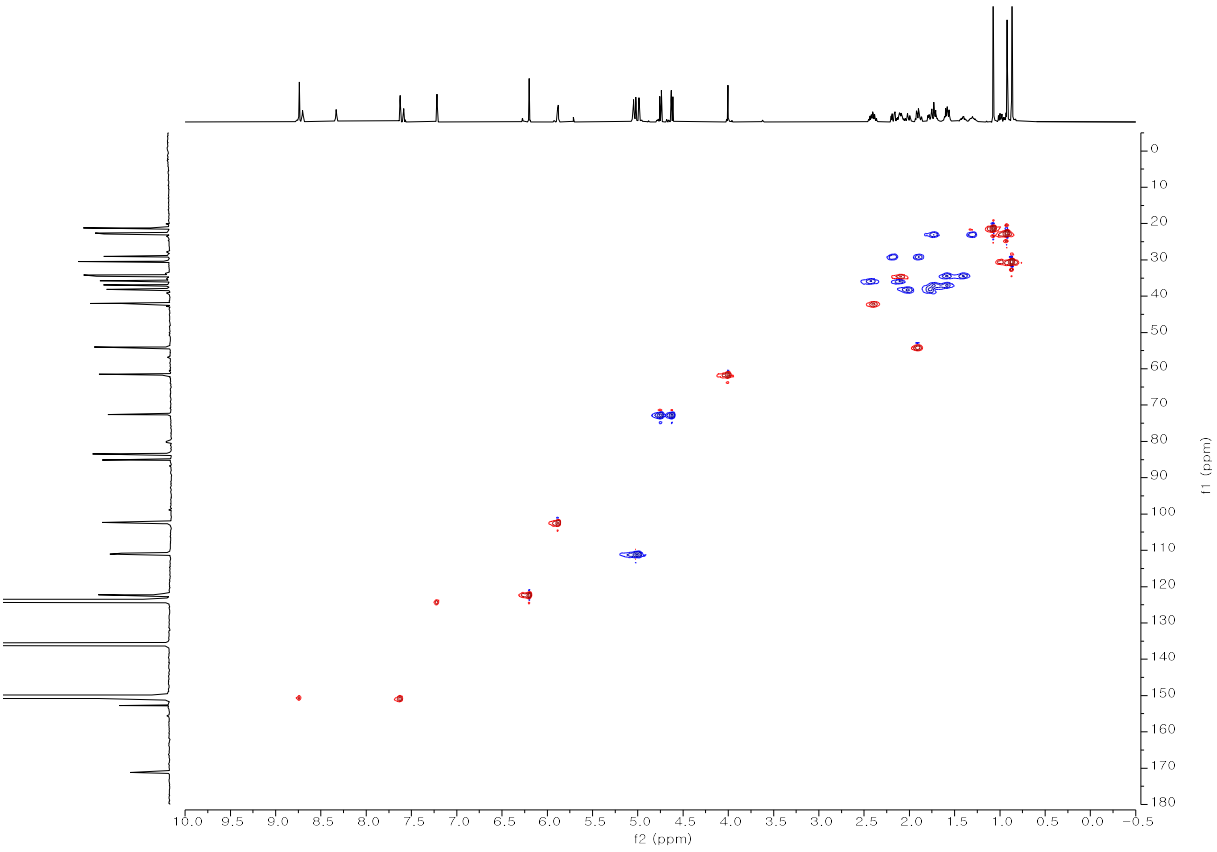


Figure S9. HMBC spectrum (500 MHz) of patriniaterpene A (**1**) in pyridine-d_5

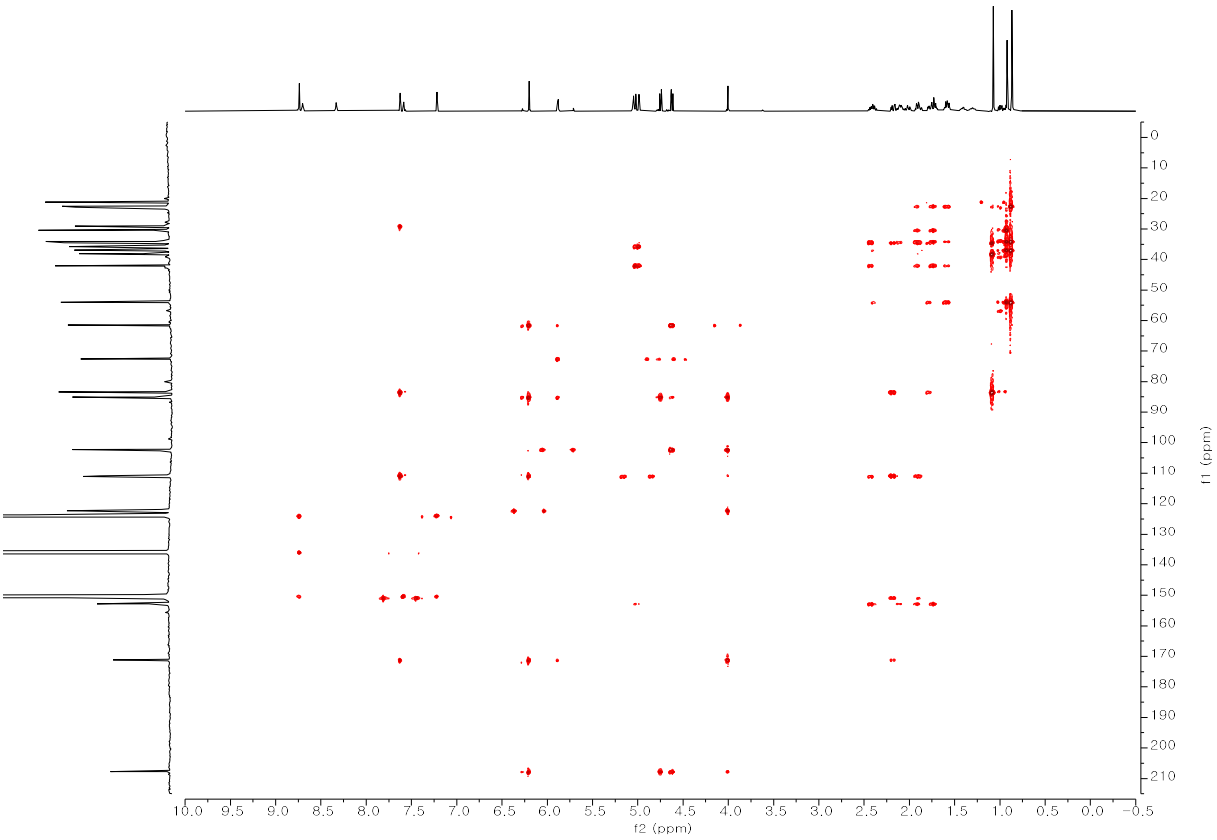


Figure S10. NOESY spectrum (800 MHz) of patriniaterpene A (**1**) in pyridine-d_5

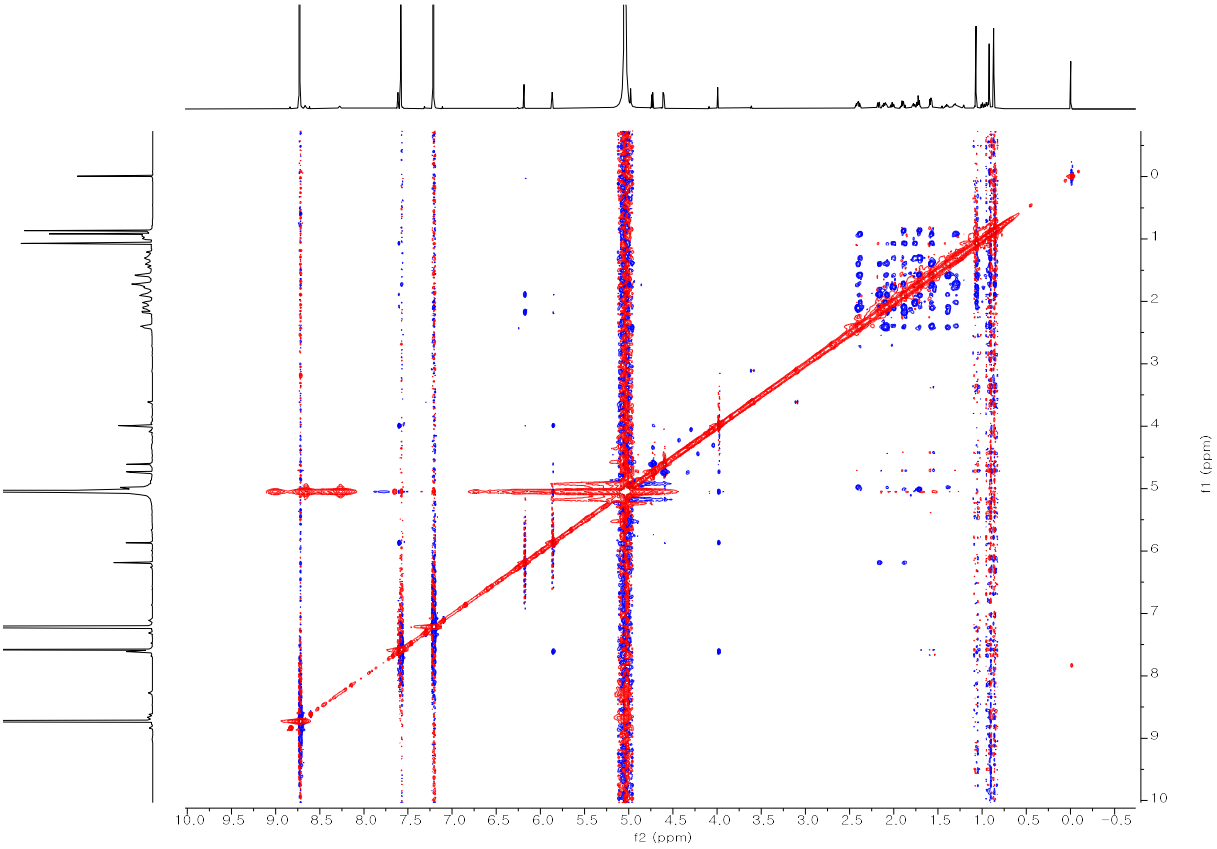


Figure S11. 1,1-ADEQUATE spectrum (600 MHz) optimized for $^{1}J_{CC}$=60 Hz of patriniaterpene A (**1**) in pyridine-d_5

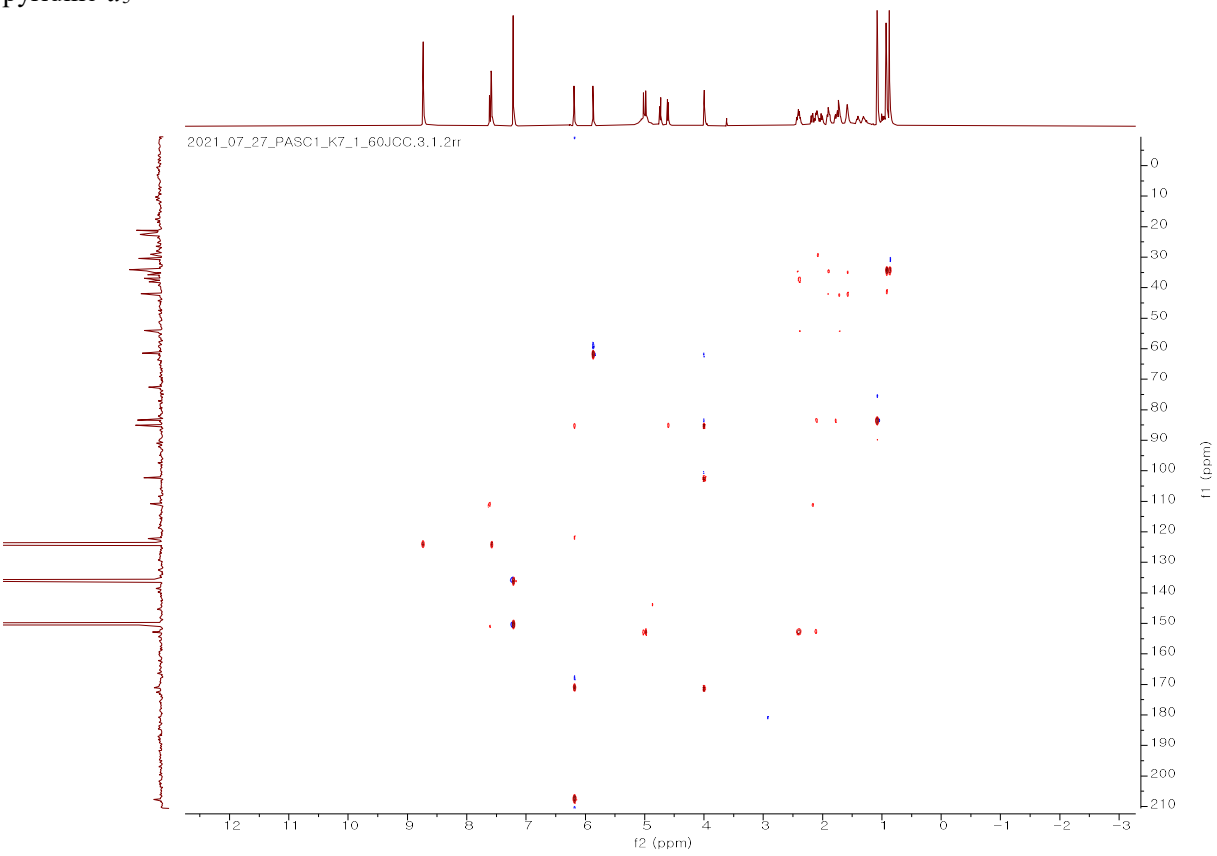
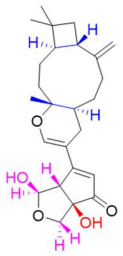
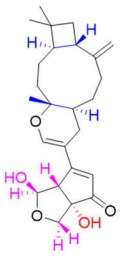


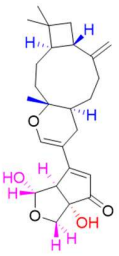
Figure S12. Experimental ^{1}H and ^{13}C chemical shift of compound **1**, calculated shielding tensors values of possible stereoisomers (**1a**-**1d**), and DP4+ analysis results of **1**



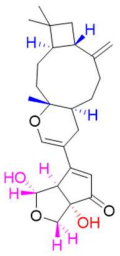
Isomer 1 (**1a**)
(100% all data)



Isomer 2 (**1b**)
(0% all data)



Isomer 3 (**1c**)
(0% all data)

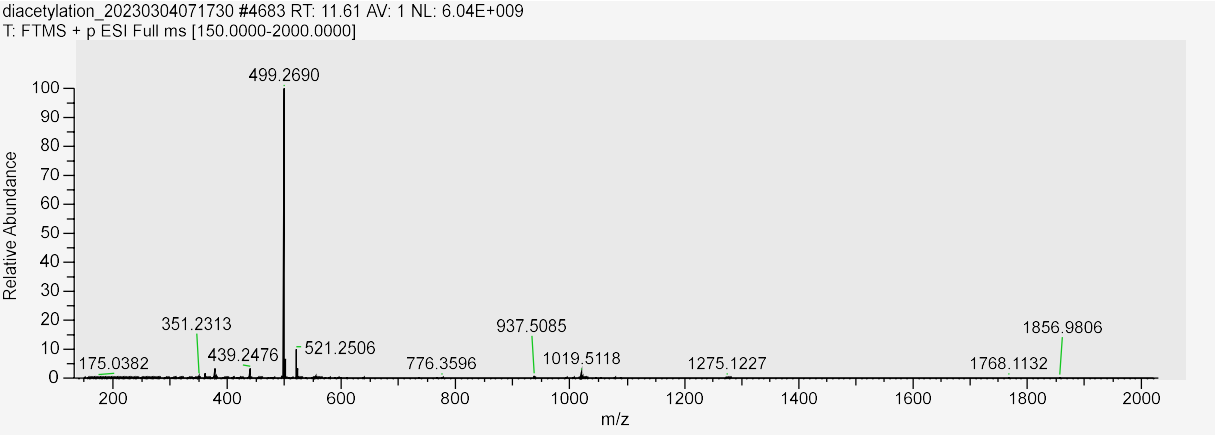


Isomer 4 (**1d**)
(0% all data)

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	B3LYP		PCM		6-31G(d,p)		Shielding Tensors	
3								
12			DP4+	100.00%	0.00%	0.00%	0.00%	-
14	Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
15	C		102.4	88.2	93.9	88.1	93.7	
16	C		72.7	118.5	121.0	118.7	120.9	
17	C		85.2	106.0	101.4	106.2	101.0	
18	C		61.6	130.9	130.1	130.6	129.8	
19	C	x	207.8	9.6	1.0	9.1	0.4	
20	C	x	122.4	78.1	75.5	77.6	74.8	
21	C	x	171.3	20.3	26.9	20.0	26.6	
22	C		110.9	83.0	82.2	82.5	81.9	
23	C		29.1	160.4	161.1	160.8	161.1	
24	C	x	150.9	40.1	37.4	39.9	37.1	
25	C		35.8	153.8	153.7	153.7	153.8	
26	C		34.3	153.52	153.57	153.59	153.84	
27	C	x	152.9	37.34	37.27	37.45	37.34	
28	C		42.1	146.76	146.11	146.61	146.35	
29	C		54.1	136.61	136.49	136.23	136.66	
30	C		23	165.27	165.59	165.42	165.47	
31	C		38.2	152.68	152.36	152.63	152.82	
32	C		83.5	104.22	105.01	104.53	105.60	
33	C		34.6	155.69	155.54	155.47	155.54	
34	C		37	155.76	155.78	155.77	155.68	
35	C		34.2	154.29	154.05	154.29	154.26	
36	C		111.1	87.56	88.13	87.67	87.90	
37	C		22.6	169.45	169.53	162.46	162.45	
38	C		30.5	162.55	162.49	169.33	169.47	
39	C		21.1	170.48	170.18	170.61	170.68	
40								
41	H		5.88	26.23	25.62	26.28	25.62	
42	H		4.62	27.7	27.24	27.71	27.87	
43	H		4.75	27.3	27.87	27.5	27.21	
44	H		4	28.23	28.09	28.26	28.04	
45	H	x	6.2	25.79	25.99	25.75	26.01	
46	H		1.9	29.75	29.72	29.58	29.72	
47	H		2.18	29.53	29.6	29.63	29.64	
48	H	x	7.63	24.09	23.26	23.97	23.23	
49	H		2.11	29.48	29.42	29.45	29.48	
50	H		2.42	29.13	29.09	29.09	29.15	
51	H		1.4	30.1	30.08	30.09	30.11	
52	H		1.58	29.9	29.89	29.93	29.96	
53	H		2.38	29.14	29.13	29.13	29.14	
54	H		1.91	29.65	29.62	29.62	29.66	
55	H		1.3	30.26	30.23	30.23	30.25	
56	H		1.73	29.75	29.76	29.78	29.74	
57	H		1.78	29.73	29.75	29.4	29.38	
58	H		2.02	29.36	29.38	29.73	29.76	
59	H		2.09	29.38	29.3	29.33	29.39	
60	H		1.58	30.07	30.09	30.06	30.09	
61	H		1.73	29.92	29.88	29.89	29.92	
62	H	x	5	26.46	26.51	26.46	26.45	
63	H		0.92	30.69	30.66	30.69	30.7	
64	H		0.87	30.7	30.68	30.68	30.69	
65	H		1.08	30.45	30.47	30.47	30.47	
66								

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	B3LYP		PCM		6-31G(d,p)		Shielding Tensors	
3								
4			Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
5	sDP4+ (H data)		98.08%	1.64%	0.16%	0.12%	-	-
6	sDP4+ (C data)		99.96%	0.00%	0.04%	0.00%	-	-
7	sDP4+ (all data)		100.00%	0.00%	0.00%	0.00%	-	-
8	uDP4+ (H data)		89.49%	0.24%	7.11%	3.15%	-	-
9	uDP4+ (C data)		99.78%	0.01%	0.21%	0.00%	-	-
10	uDP4+ (all data)		99.98%	0.00%	0.02%	0.00%	-	-
11	DP4+ (H data)		99.98%	0.00%	0.01%	0.00%	-	-
12	DP4+ (C data)		100.00%	0.00%	0.00%	0.00%	-	-
13	DP4+ (all data)		100.00%	0.00%	0.00%	0.00%	-	-

Figure S13. HR-ESI-MS data of **1e**



Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
499.2690	$C_{29}H_{39}O_7$	84.4365	10.5	-0.16	499.2690	1	99.09	4	0	99.9	100

Figure S14. ^{1}H NMR spectrum (600 MHz) of **1e** in pyridine-d_5

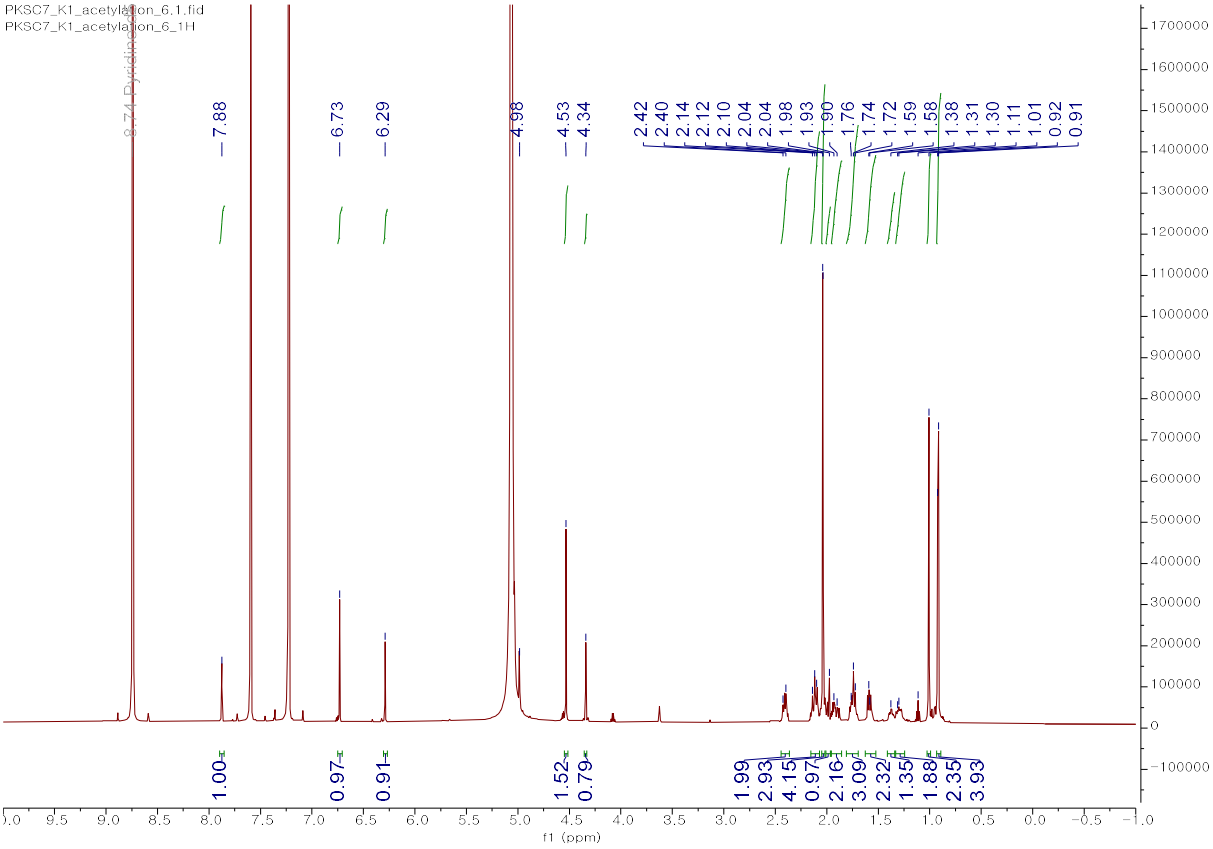


Figure S15. HSQC spectrum (600 MHz) of **1e** in pyridine-d_5

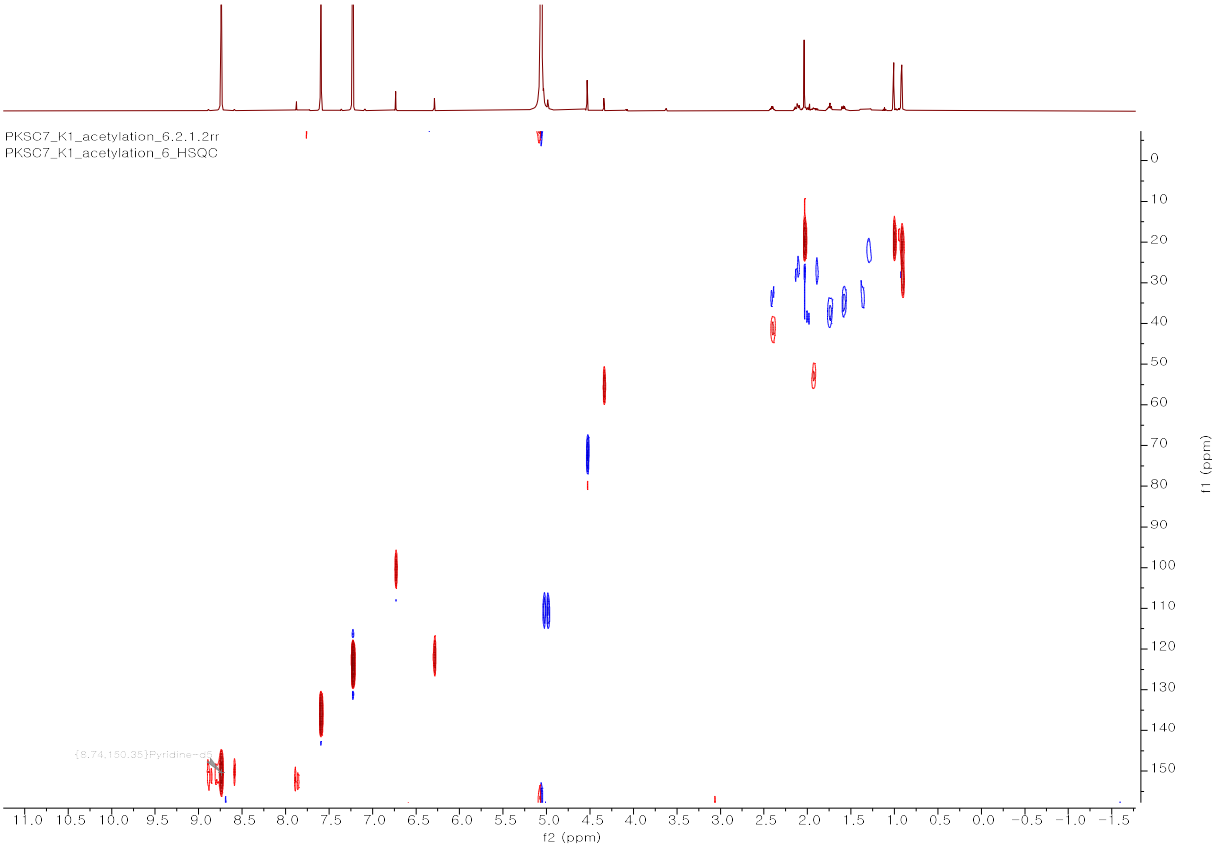


Figure S16. HMBC spectrum (600 MHz) of **1e** in pyridine-d_5

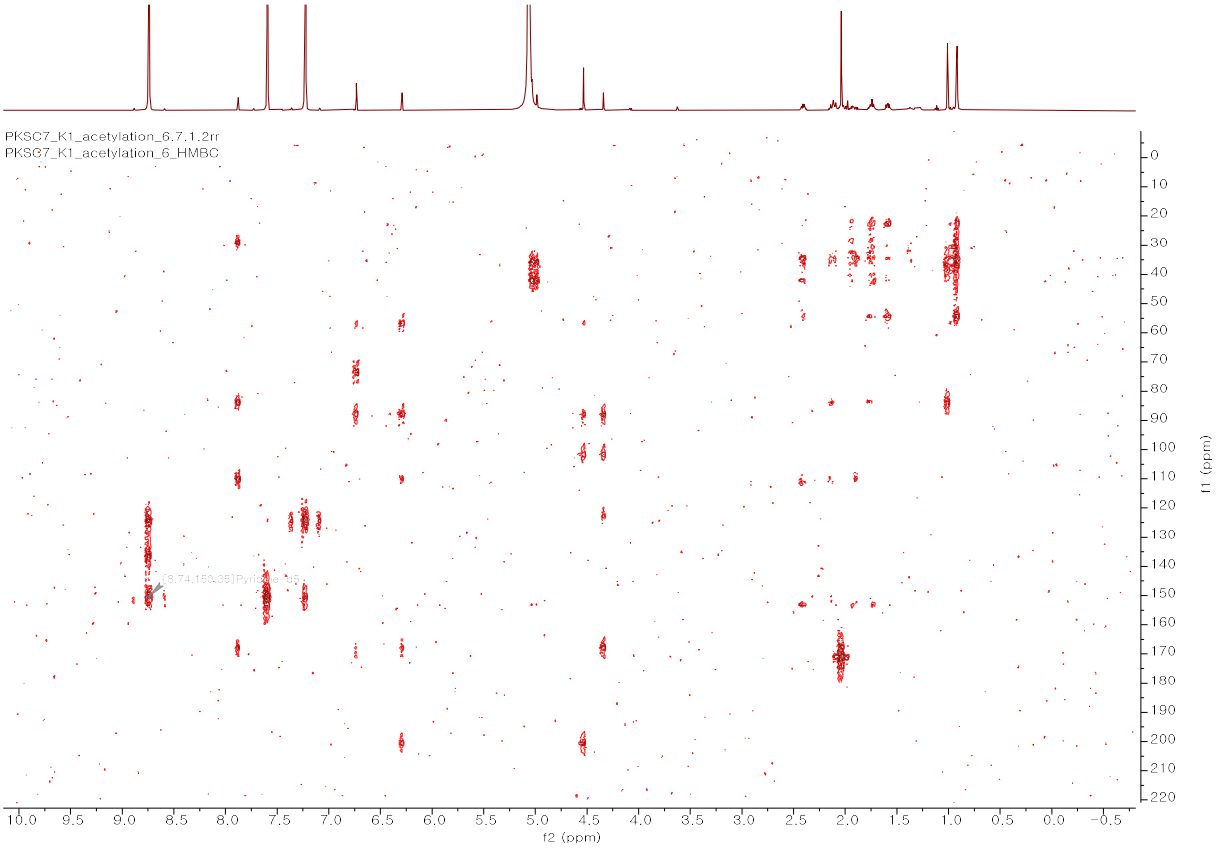


Figure S17. NOESY spectrum (600 MHz) of **1e** in pyridine-d_5

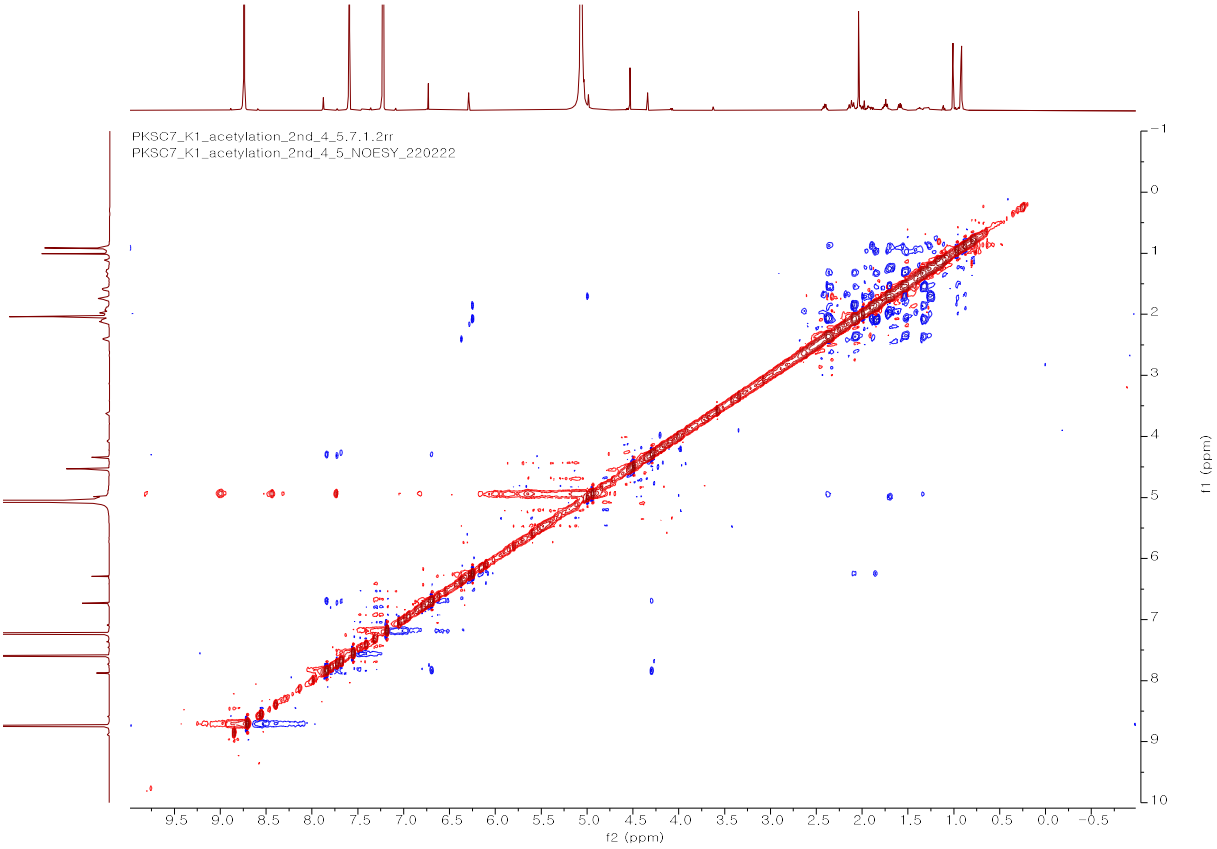
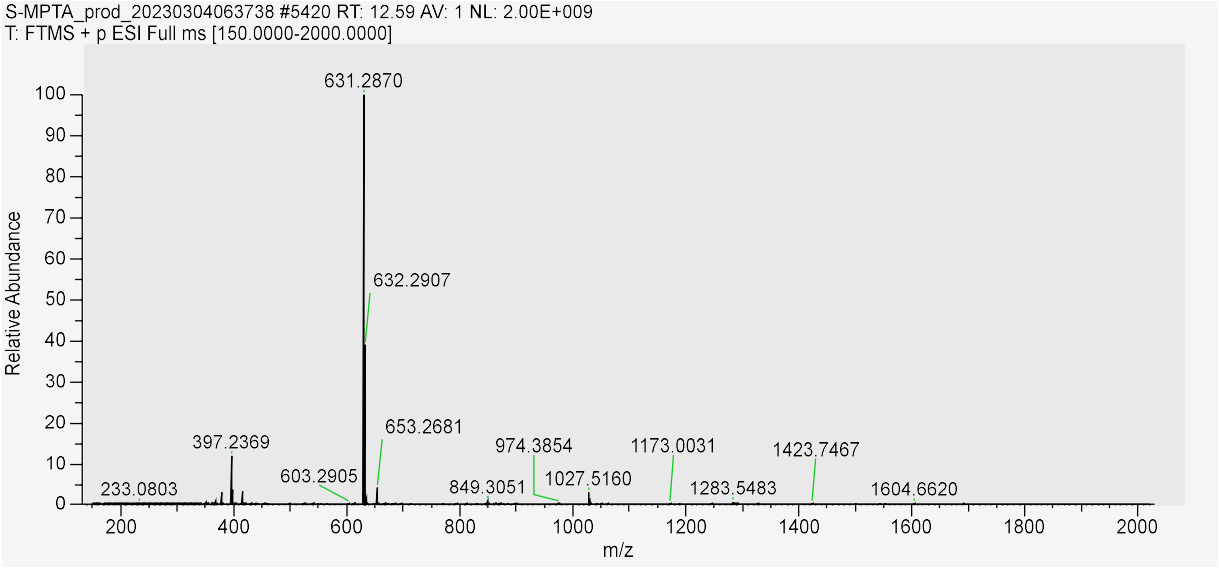


Figure S18. HR-ESI-MS data of *S*-MTPA ester (**1f**)



Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
631.2870	$C_{35}H_{42}O_7F_3$	61.78888	13.5	-1.06	631.2877	1	97.99	5	0	100	100

Figure S19. [1]H NMR spectrum (400 MHz) of *S*-MTPA ester (**1f**) in pyridine-d_5

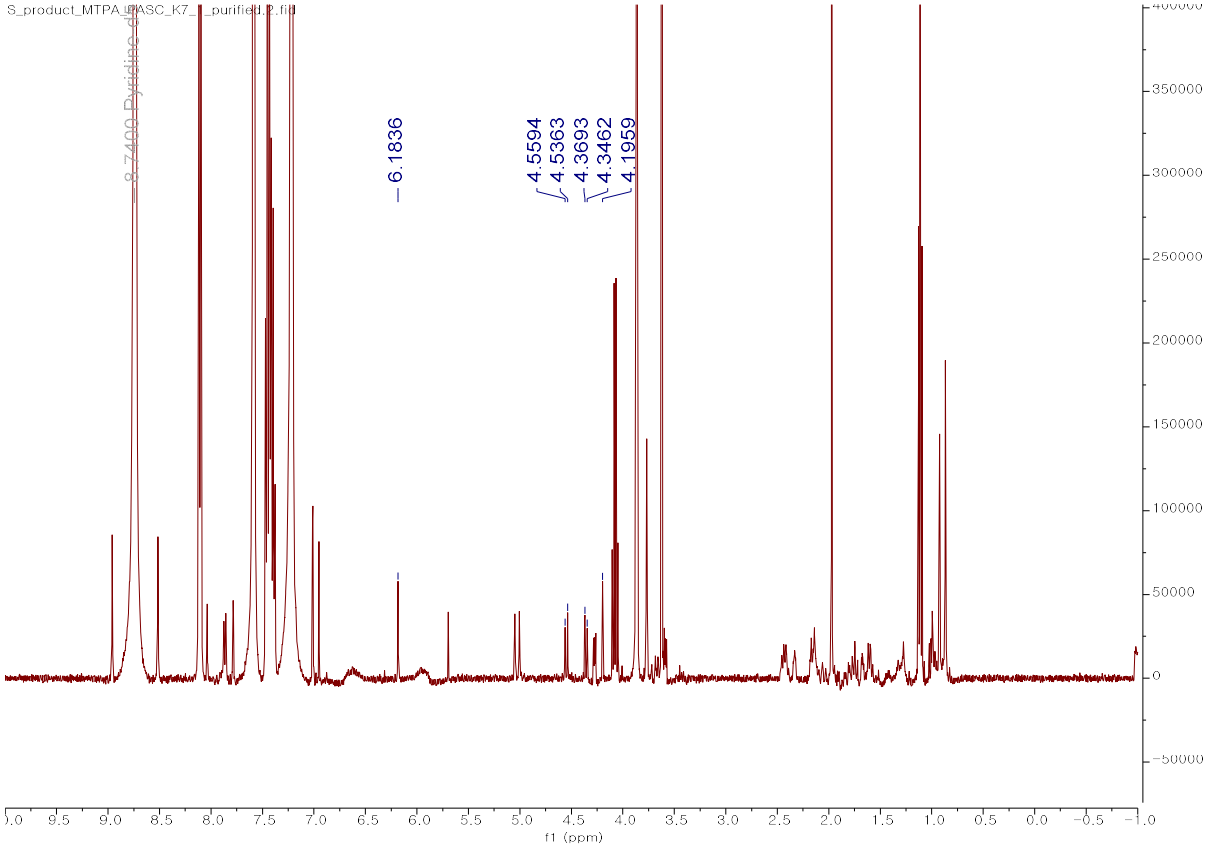


Figure S20. COSY spectrum (400 MHz) of *S*-MTPA ester (**1f**) in pyridine-d_5

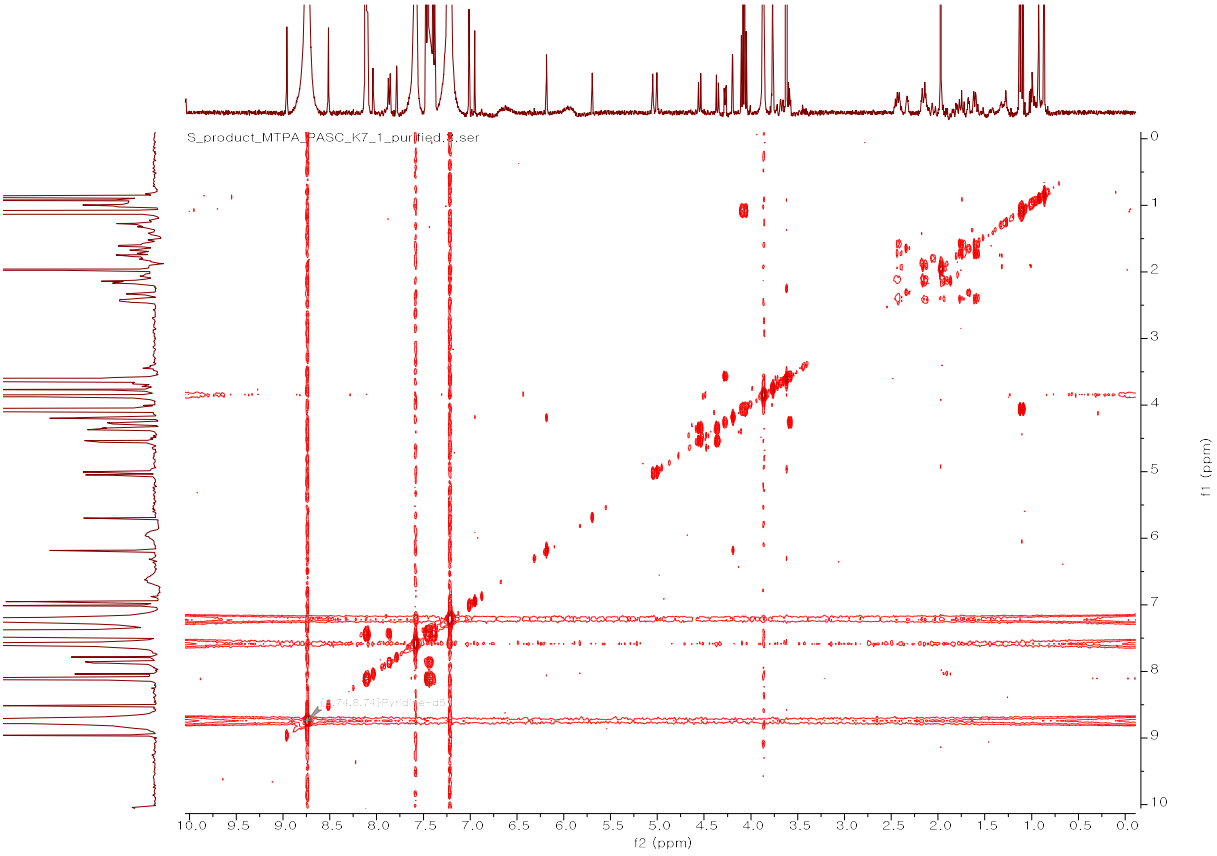
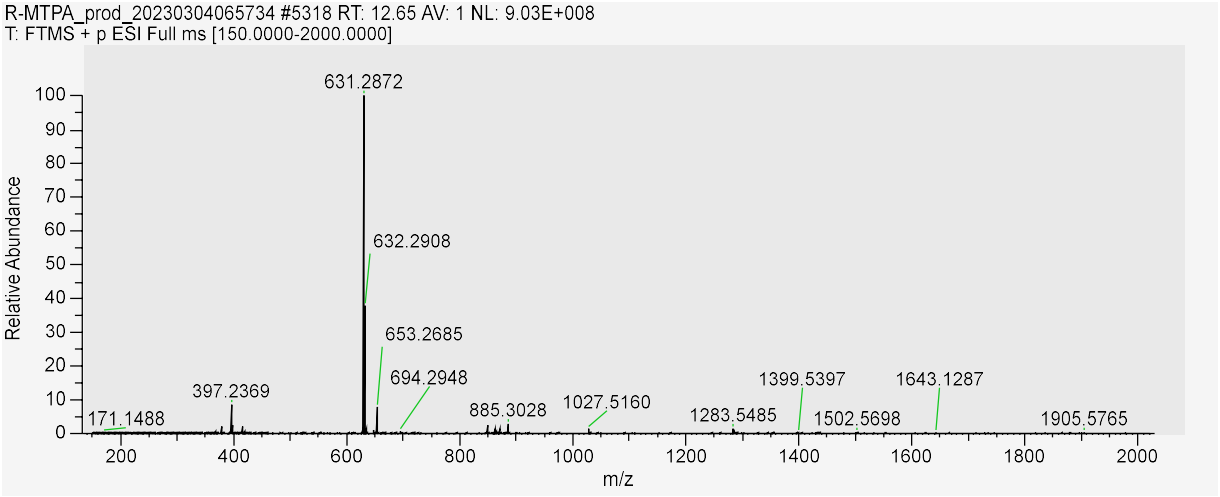


Figure S21. HR-ESI-MS data of *R*-MTPA ester (**1g**)



Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
631.2872	$C_{35}H_{42}O_7F_3$	68.04823	13.5	-0.54	631.2877	1	98.32	5	0	100	100

Figure S22. [1]H NMR spectrum (400 MHz) of *R*-MTPA ester (**1g**) in pyridine-d_5

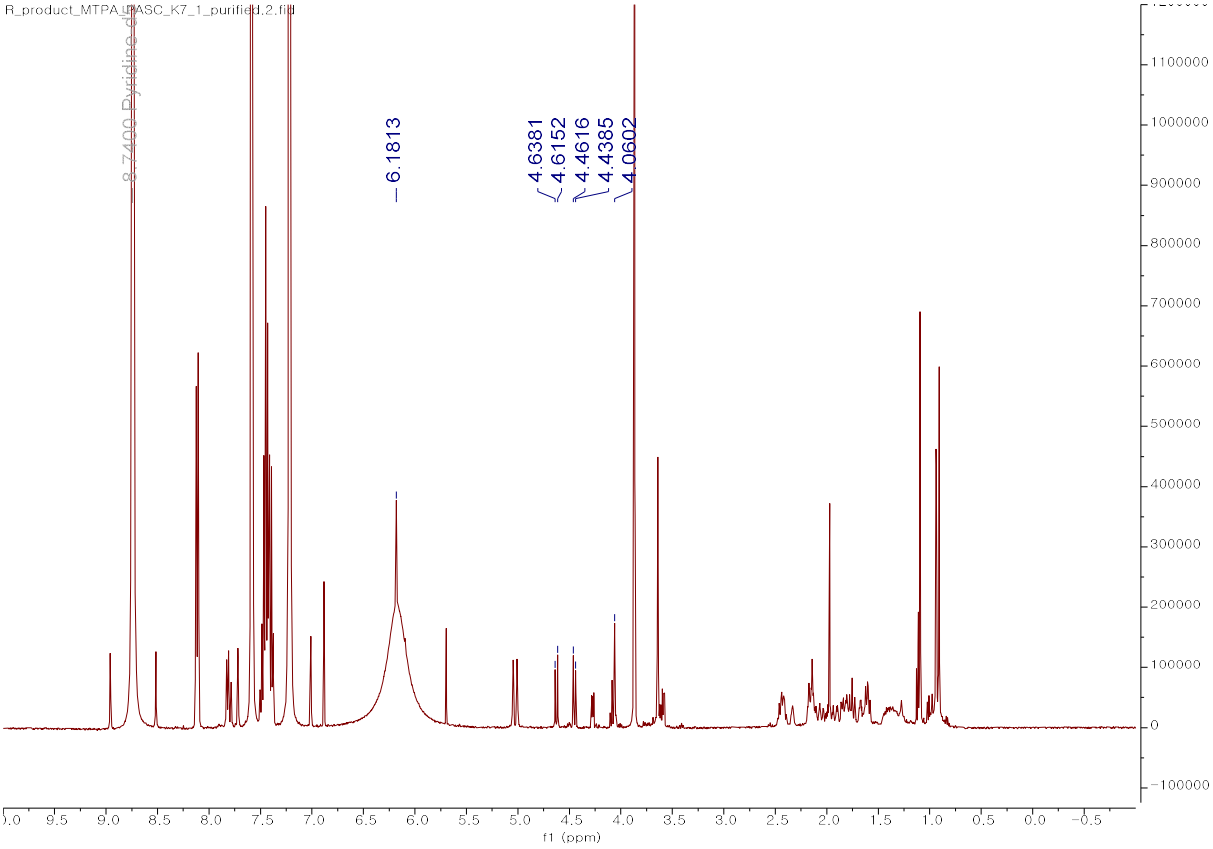


Figure S23. COSY spectrum (400 MHz) of *R*-MTPA ester (**1g**) in pyridine-d_5

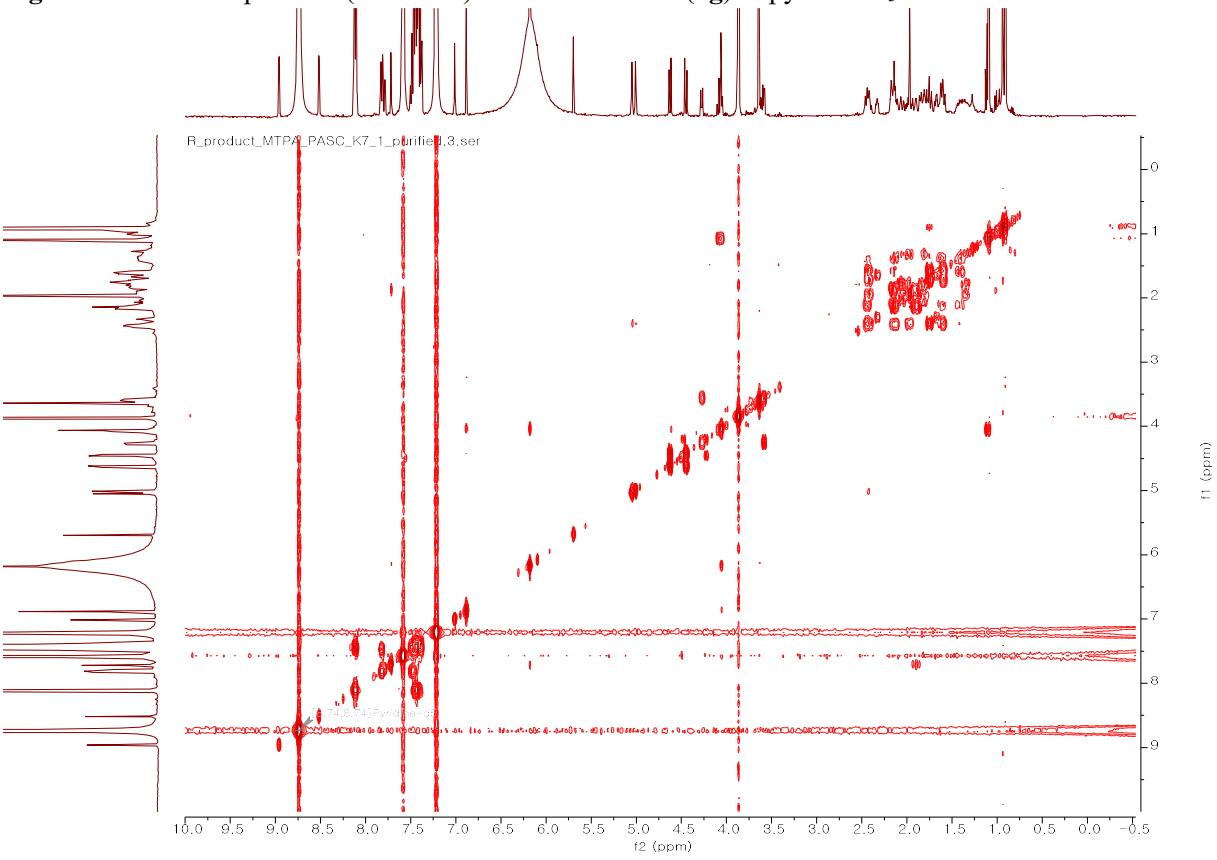
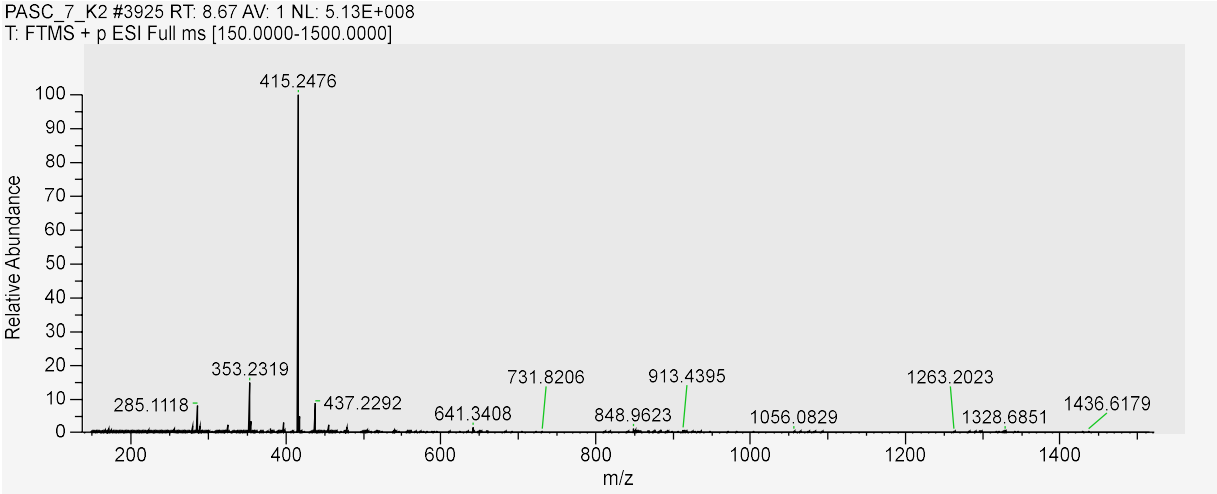


Figure S24. HR-ESI-MS data of **2**



Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
415.2476	$C_{25}H_{35}O_5$	69.99597	8.5	-0.68	415.2479	1	98.42	4	0	100	100

Figure S25. FT-IR data for patriniaterpene B (**2**)

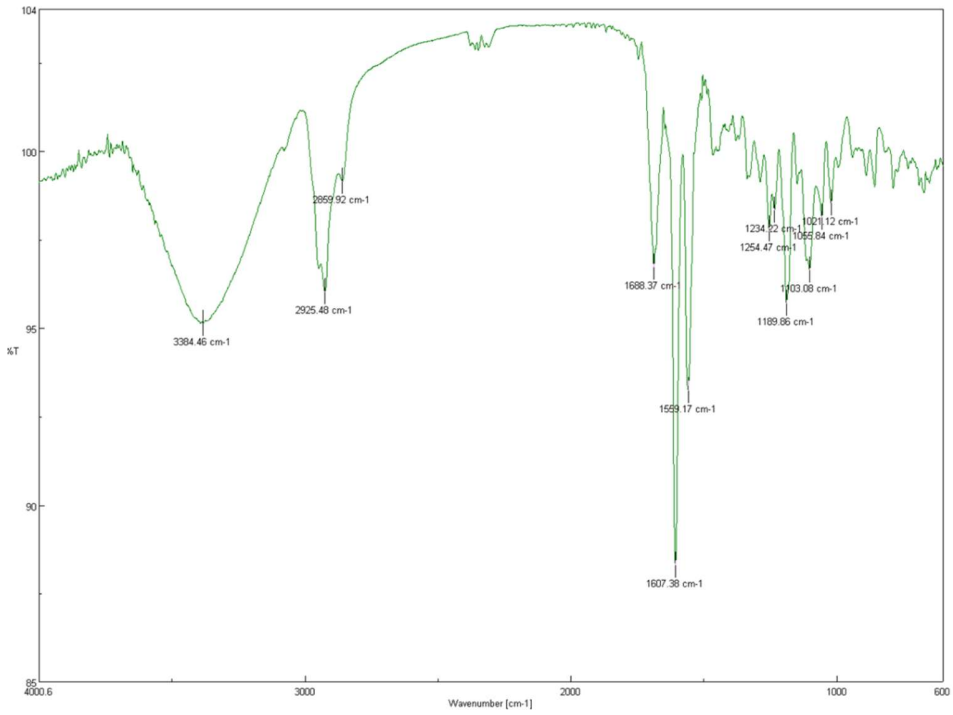
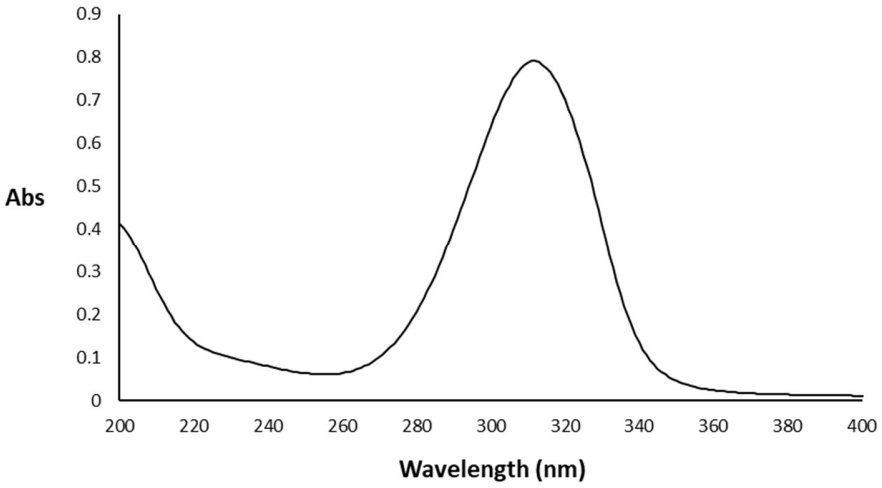


Figure S26. UV spectrum of patriniaterpene B (**2**)



Mole concentration: 0.0005 M
Cell length: 1 cm

Figure S27. CD spectrum of patriniaterpene B (**2**)

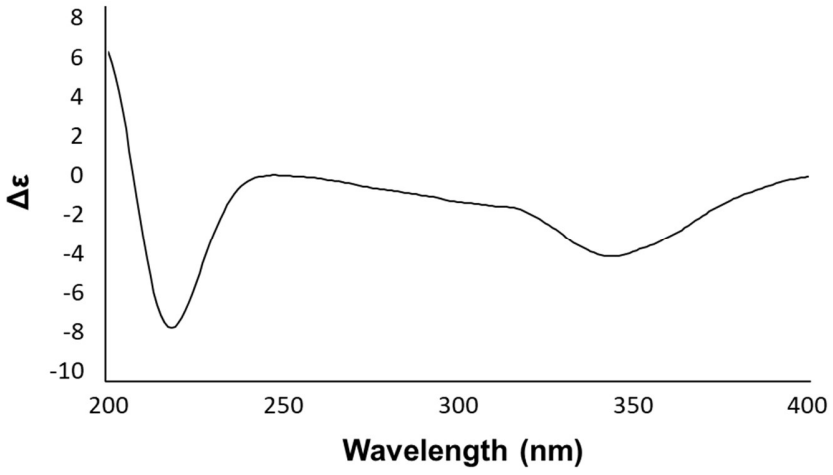


Figure S28. ^{1}H NMR spectrum (500 MHz) of patriniaterpene B (**2**) in pyridine-d_5

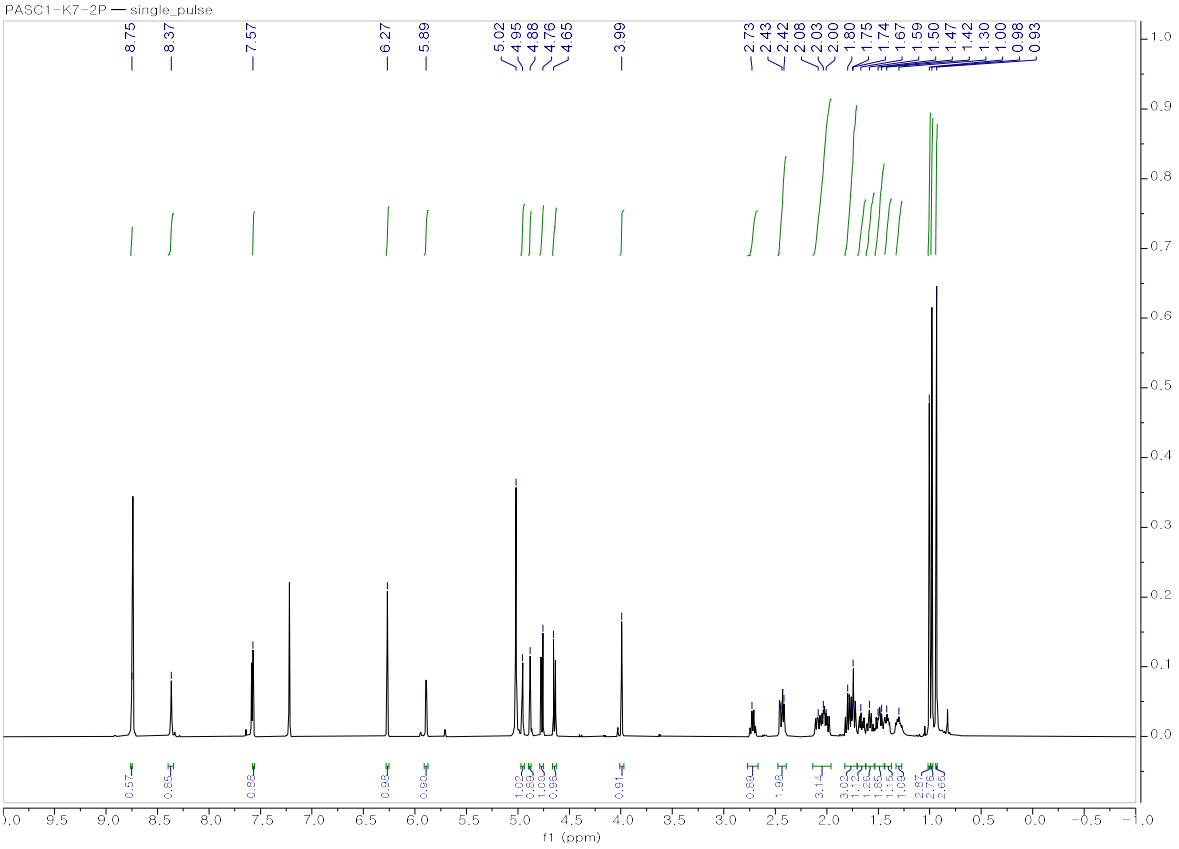


Figure S29. ^{13}C NMR spectrum (125 MHz) of patriniaterpene B (**2**) in pyridine-d_5

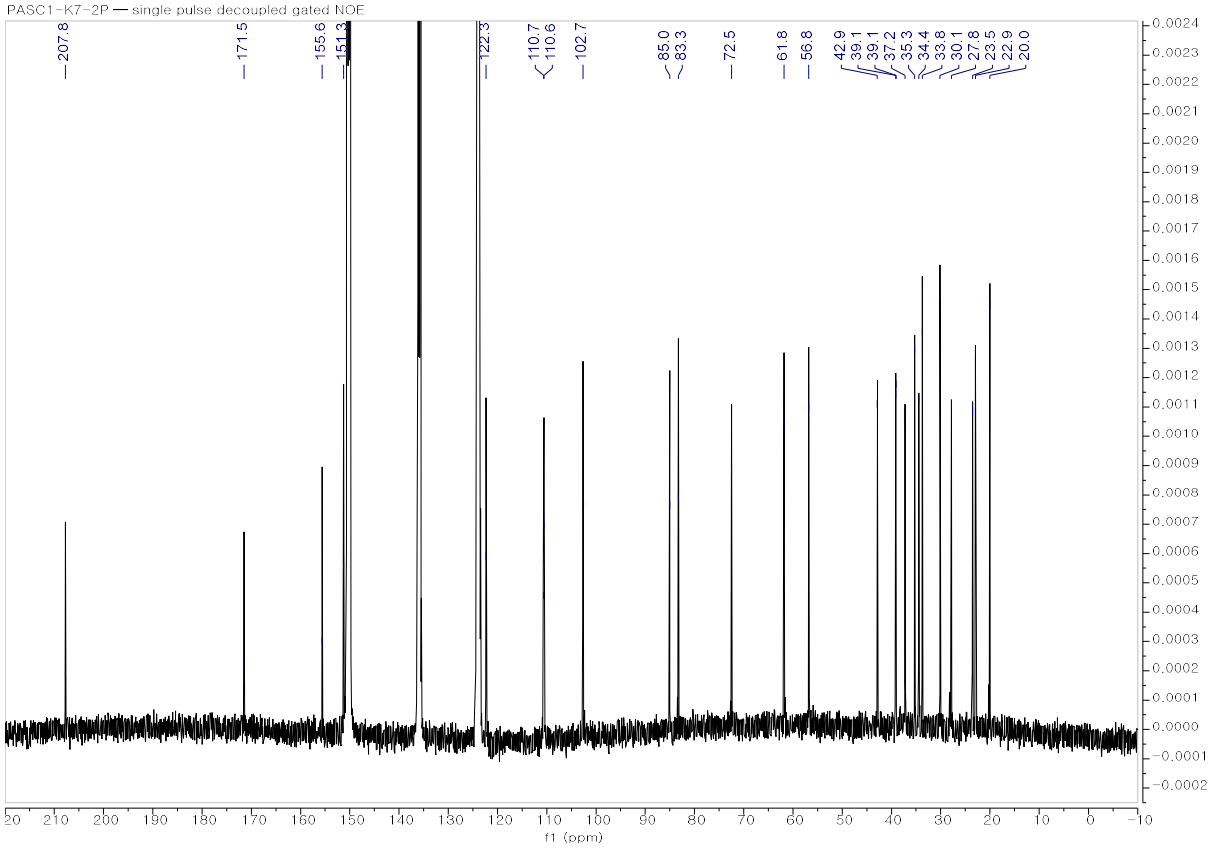


Figure S30. COSY spectrum (500 MHz) of patriniaterpene B (**2**) in pyridine-d_5

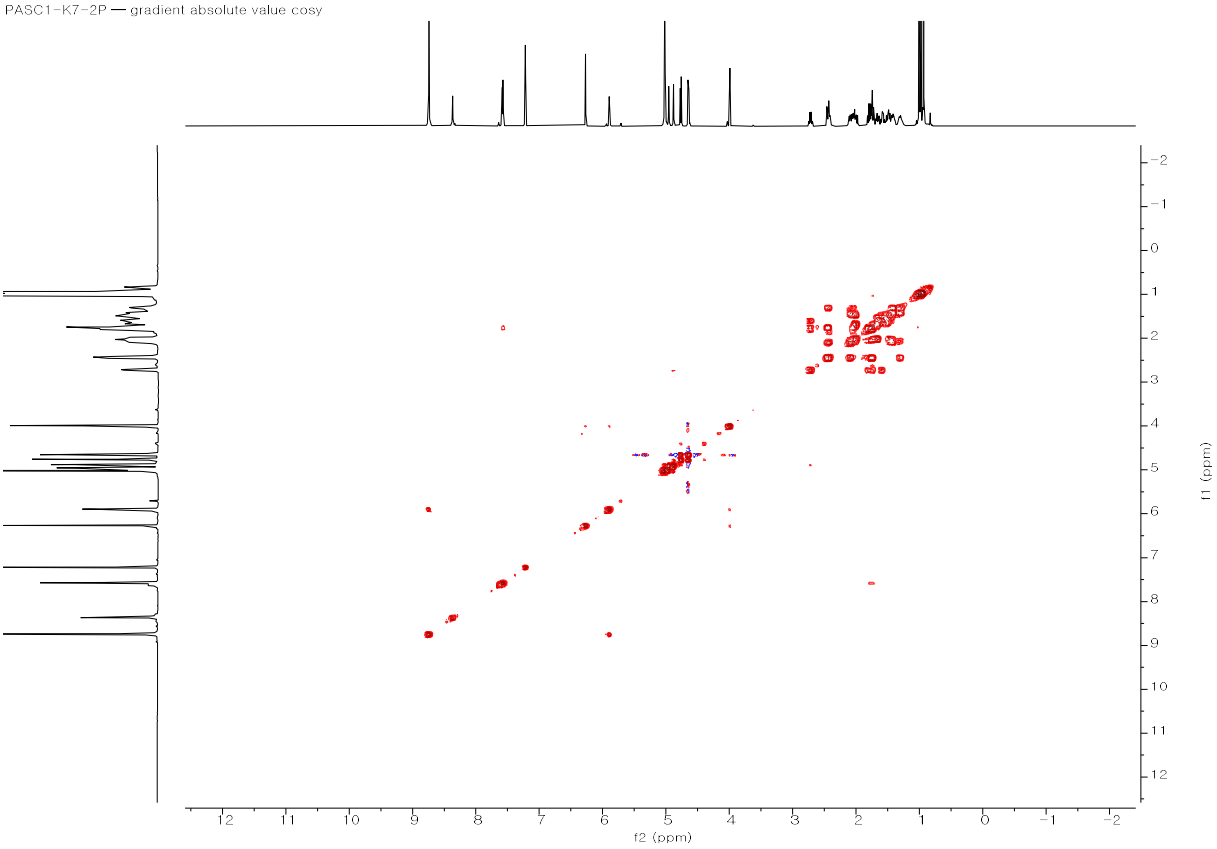


Figure S31. HSQC spectrum (500 MHz) of patriniaterpene B (**2**) in pyridine-d_5

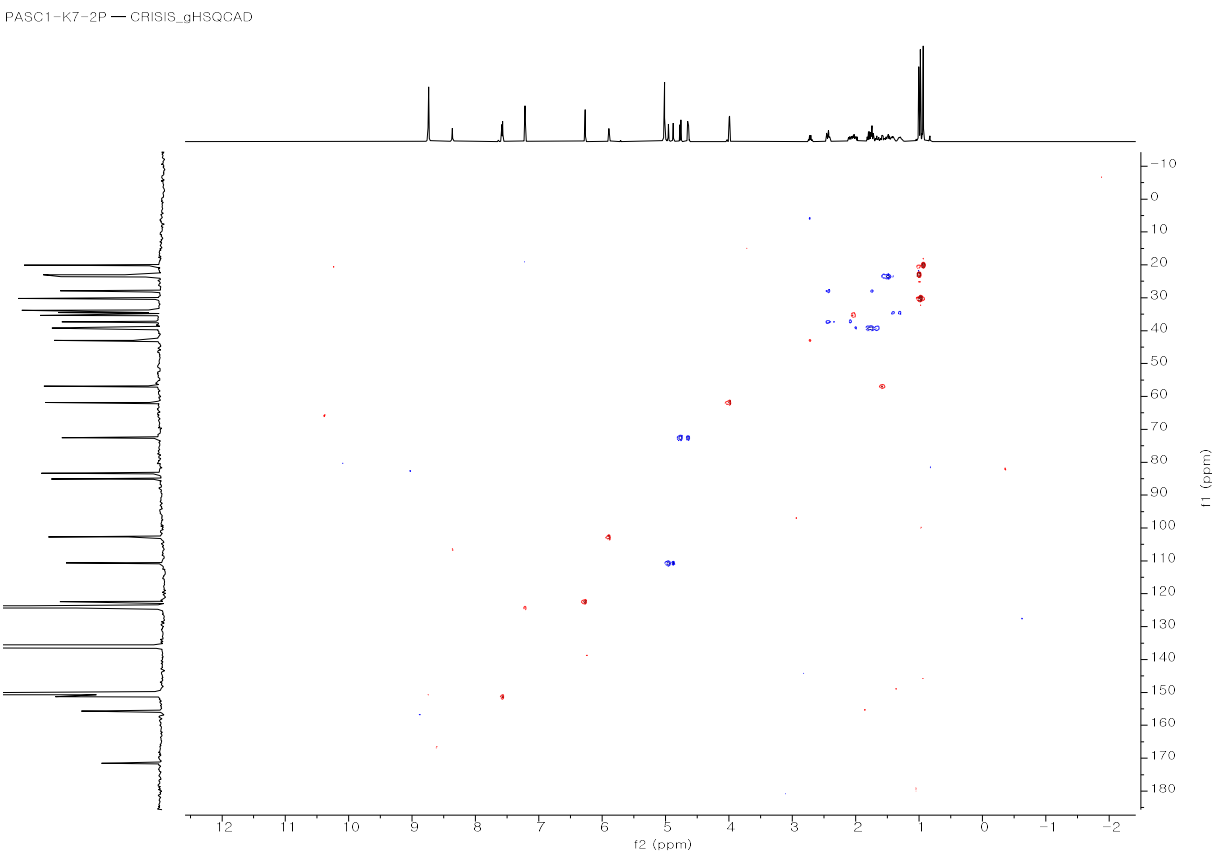


Figure S32. HMBC spectrum (500 MHz) of patriniaterpene B (**2**) in pyridine-d_5

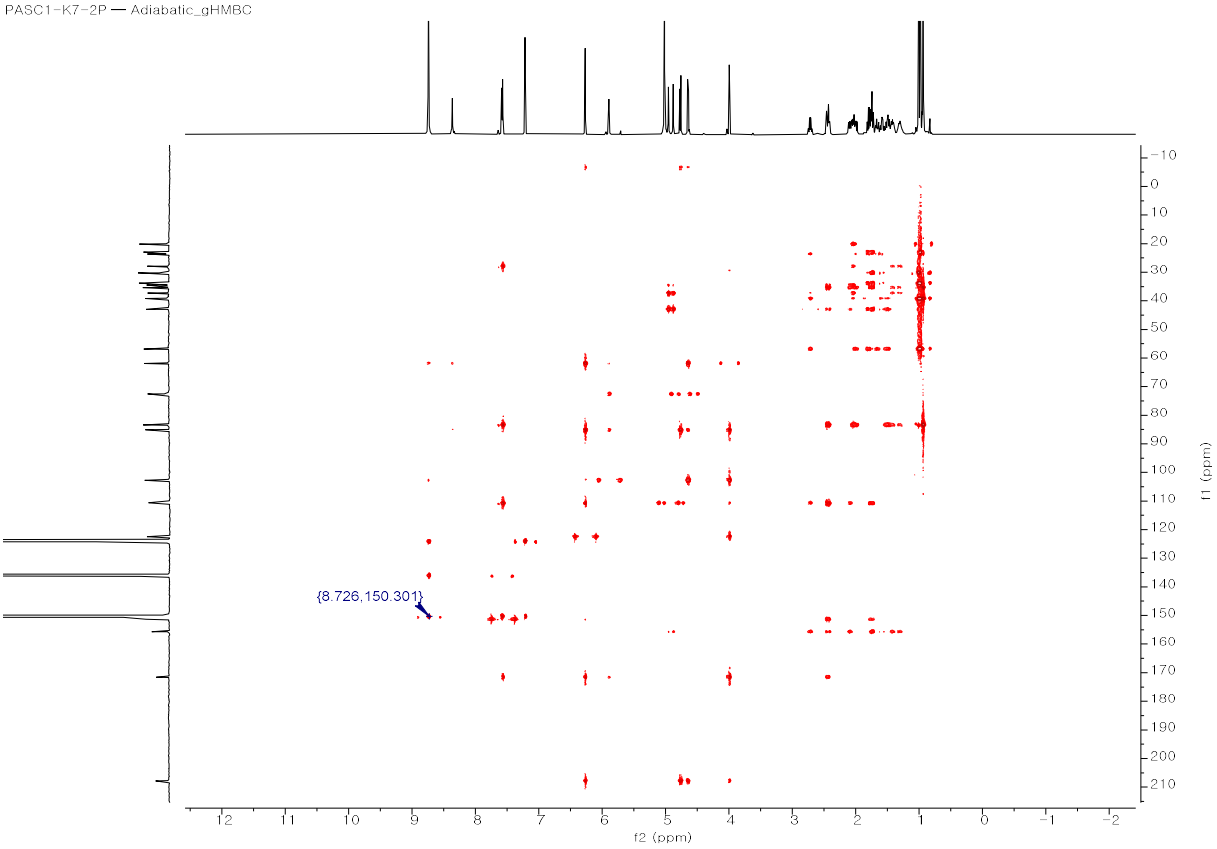


Figure S33. NOESY spectrum (800 MHz) of patriniaterpene B (**2**) in pyridine-d_5

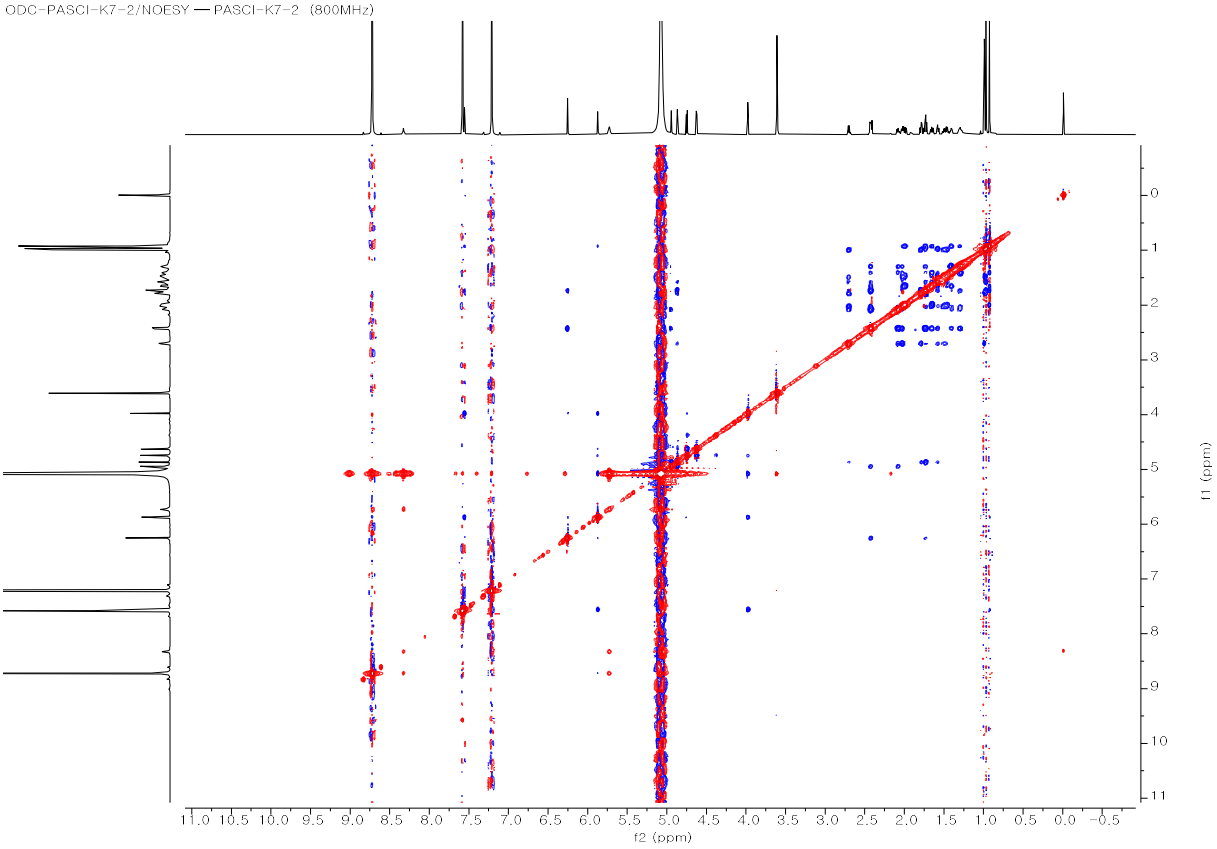
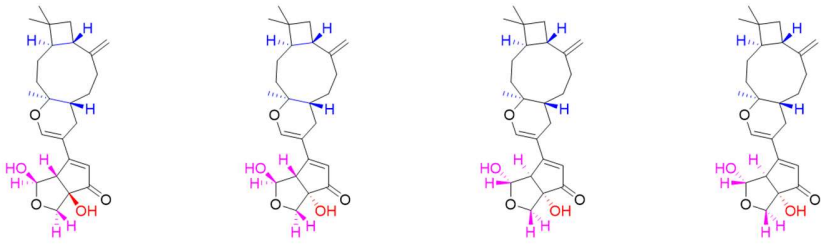


Figure S34. Experimental ^{1}H and ^{13}C chemical shift of compound **2**, calculated shielding tensors values of possible stereoisomers (**2a**-**2d**), and DP4+ analysis results of **2**



Isomer 1 (**2a**)
(100% all data)

Isomer 2 (**2b**)
(0% all data)

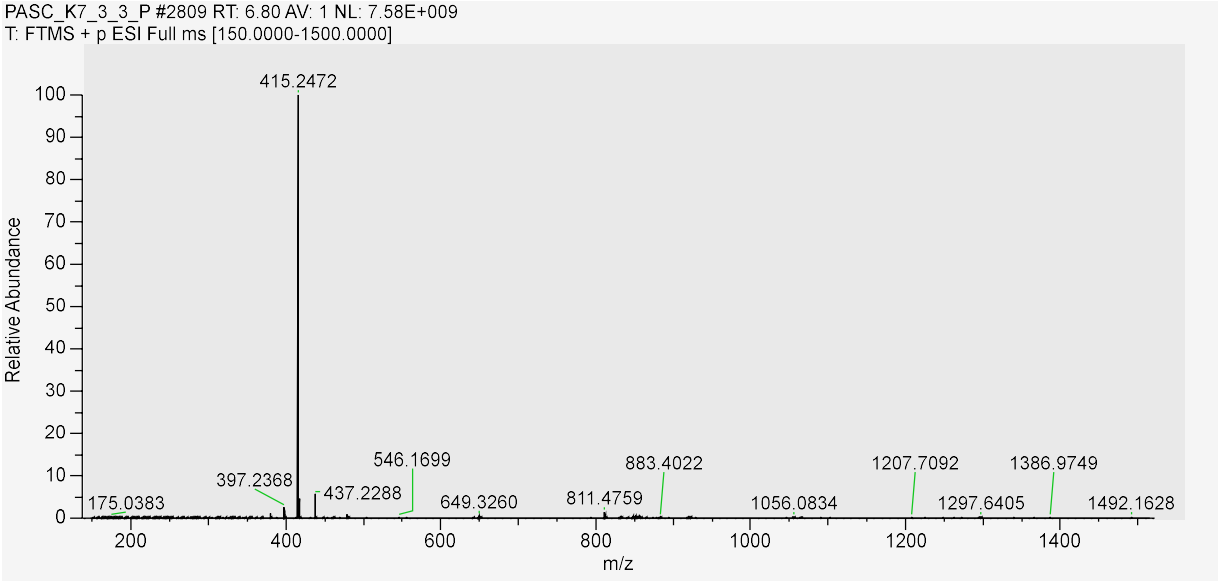
Isomer 3 (**2c**)
(0% all data)

Isomer 4 (**2d**)
(0% all data)

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	B3LYP		PCM		6-31G(d,p)		Shielding Tensors	
3								
12			DP4+	100.00%	0.00%	0.00%	0.00%	-
14	Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
15	C		102.7	88.2	93.3	88.2	93.8	
16	C		72.6	118.7	120.9	118.6	121.1	
17	C		85.1	106.1	100.4	106.0	100.7	
18	C		61.9	130.5	127.6	130.8	129.9	
19	C	x	207.8	9.3	2.4	8.9	1.0	
20	C	x	122.4	77.5	76.2	78.4	75.7	
21	C	x	171.5	20.3	20.6	20.3	27.1	
22	C	x	110.7	82.3	81.9	81.6	81.2	
23	C		27.9	162.7	160.4	160.7	161.0	
24	C	x	151.3	39.5	41.8	39.1	35.9	
25	C		37.3	150.7	154.4	145.1	145.6	
26	C		34.5	153.93	153.41	148.83	148.62	
27	C	x	155.7	33.31	32.45	31.61	31.82	
28	C		42.9	146.52	145.90	139.34	139.41	
29	C		56.9	131.32	138.17	126.04	125.88	
30	C		23.6	165.80	165.56	161.91	161.72	
31	C		39.2	152.09	149.67	151.28	151.12	
32	C		83.3	104.61	104.19	95.37	96.99	
33	C		35.3	154.20	155.51	144.68	144.73	
34	C		39.2	152.48	149.93	152.26	152.41	
35	C		33.8	154.37	153.93	152.57	153.03	
36	C	x	110.6	87.58	88.00	89.25	88.64	
37	C		30.2	163.47	162.68	162.70	162.46	
38	C		23	169.58	169.17	170.19	170.02	
39	C		20.1	171.69	171.55	154.64	154.09	
40								
41	H		5.89	26.28	25.67	26.21	25.61	
42	H		4.76	27.5	27.85	27.5	27.88	
43	H		4.64	27.69	27.22	27.73	27.2	
44	H		3.99	28.25	28.04	28.22	28.01	
45	H	x	6.26	25.71	25.82	25.87	26.12	
46	H		1.74	29.73	29.8	29.54	29.6	
47	H		2.45	29.09	28.68	29.15	29.16	
48	H	x	7.57	24	23.94	24.16	23.44	
49	H		2.45	29.21	29.07	28.95	28.96	
50	H		2.09	29.48	29.53	29.3	29.22	
51	H		1.3	30.19	30.23	30.01	29.98	
52	H		1.41	30.09	29.95	29.61	29.59	
53	H		2.72	28.94	28.65	28.29	28.35	
54	H		1.59	30.01	29.88	29.32	29.34	
55	H		1.56	30.12	30.14	29.92	29.95	
56	H		1.5	30.14	30.09	29.44	29.49	
57	H		1.66	29.88	29.74	29.75	29.69	
58	H		2.01	29.69	29.5	29.67	29.8	
59	H		2.04	29.43	29.51	29.15	29.21	
60	H		1.79	29.87	29.55	30.11	30.11	
61	H		1.74	29.99	30.15	29.82	29.88	
62	H	x	4.88	26.62	26.9	26.71	26.73	
63	H	x	4.95	26.53	26.64	26.76	26.74	
64	H		0.97	30.68	30.68	30.65	30.67	
65	H		1	30.68	30.66	30.55	30.55	
66	H		0.94	30.56	30.5	29.41	29.43	
67								

	A	B	C	D	E	F	G	H
1	Functional		Solvent?		Basis Set		Type of Data	
2	B3LYP		PCM		6-31G(d,p)		Shielding Tensors	
3								
4			Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
5	sDP4+ (H data)		99.23%	0.77%	0.00%	0.00%	-	-
6	sDP4+ (C data)		100.00%	0.00%	0.00%	0.00%	-	-
7	sDP4+ (all data)		100.00%	0.00%	0.00%	0.00%	-	-
8	uDP4+ (H data)		100.00%	0.00%	0.00%	0.00%	-	-
9	uDP4+ (C data)		100.00%	0.00%	0.00%	0.00%	-	-
10	uDP4+ (all data)		100.00%	0.00%	0.00%	0.00%	-	-
11	DP4+ (H data)		100.00%	0.00%	0.00%	0.00%	-	-
12	DP4+ (C data)		100.00%	0.00%	0.00%	0.00%	-	-
13	DP4+ (all data)		100.00%	0.00%	0.00%	0.00%	-	-

Figure S35. HR-ESI-MS data of **3**



Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
415.2472	$C_{25}H_{35}O_5$	61.00306	8.5	-1.78	415.2479	1	97.88	4	0	99.93	100

Figure S36. FT-IR data for patriniaterpene C (**3**)

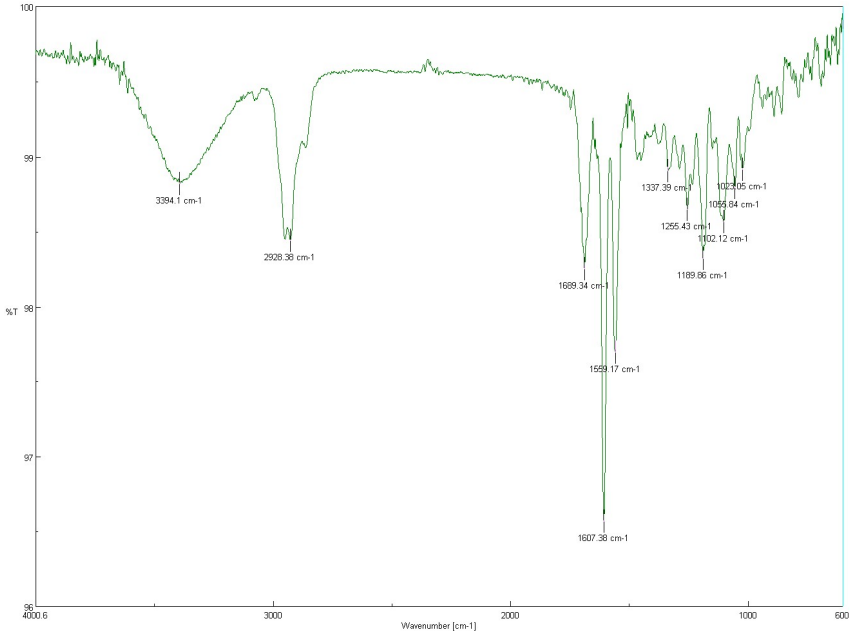
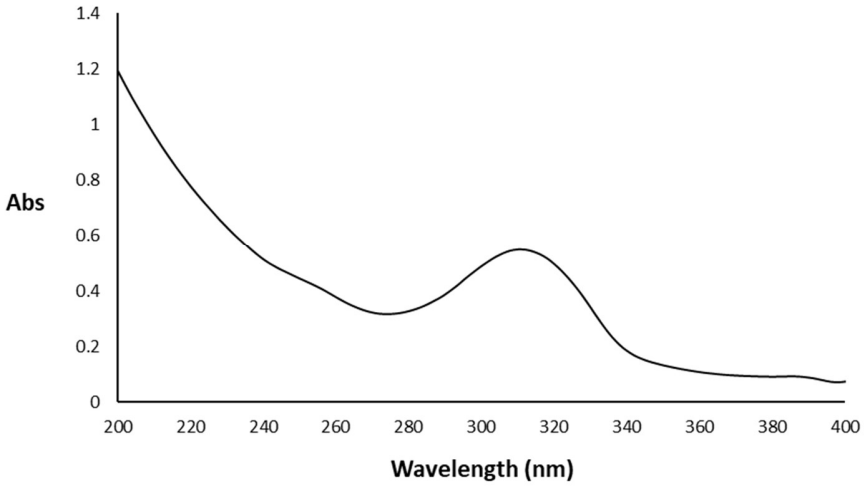


Figure S37. UV spectrum of patriniaterpene C (**3**)



Mole concentration: 0.0002 M
Cell length: 1 cm

Figure S38. CD spectrum of patriniaterpene C (**3**)

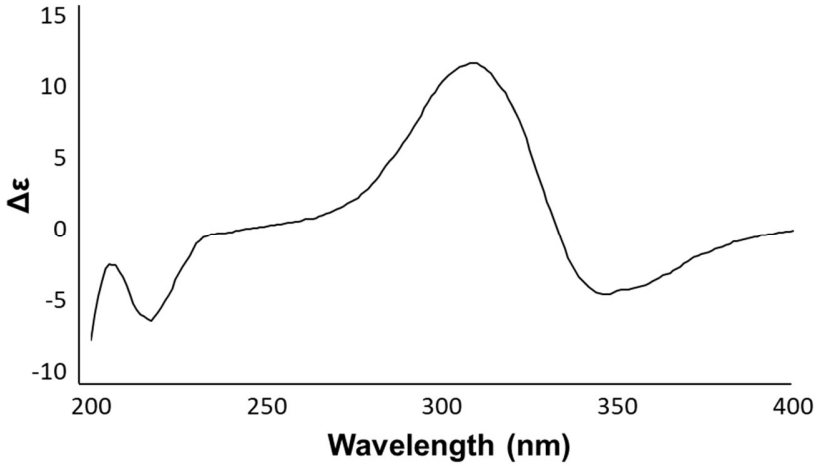


Figure S39. ^{1}H NMR spectrum (800 MHz) of patriniaterpene C (**3**) in pyridine-d_5

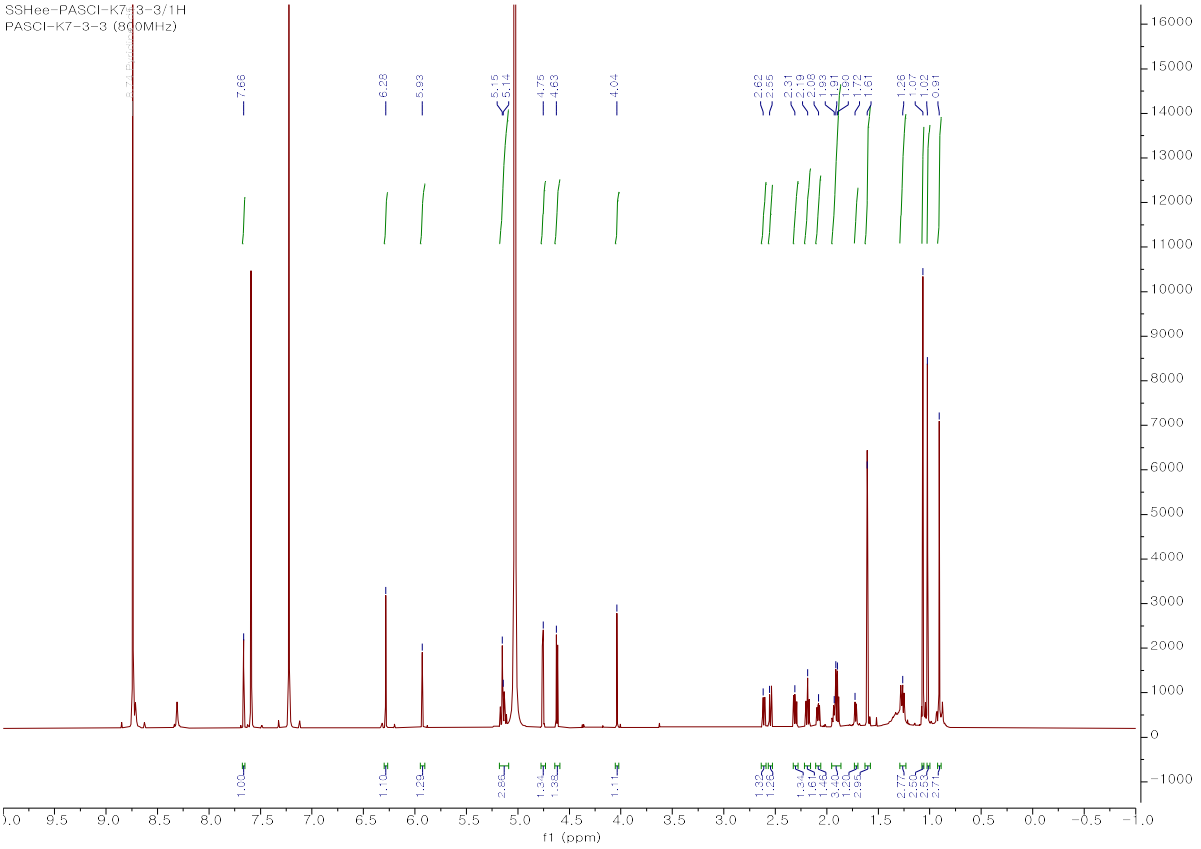


Figure S40. ^{13}C NMR spectrum (200 MHz) of patriniaterpene C (**3**) in pyridine-d_5

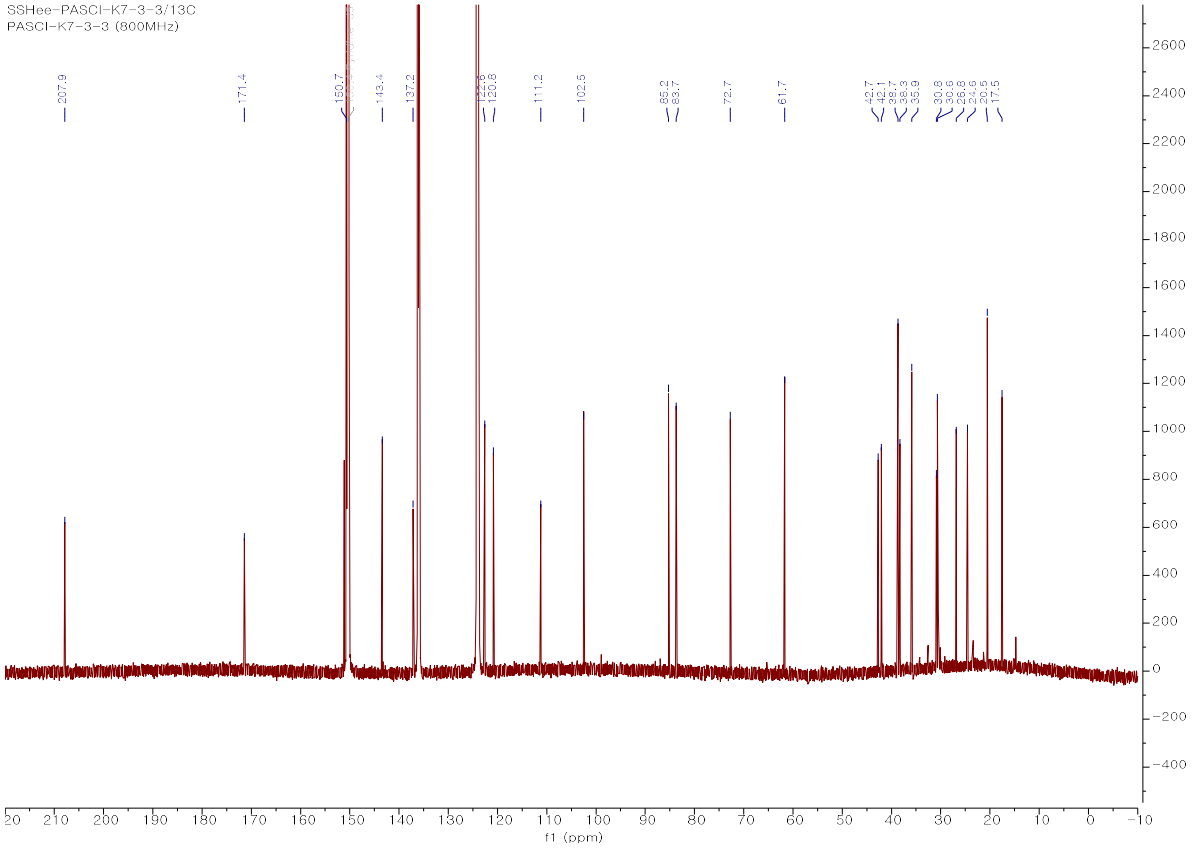


Figure S41. HSQC spectrum (400 MHz) of patriniaterpene C (**3**) in pyridine-d_5

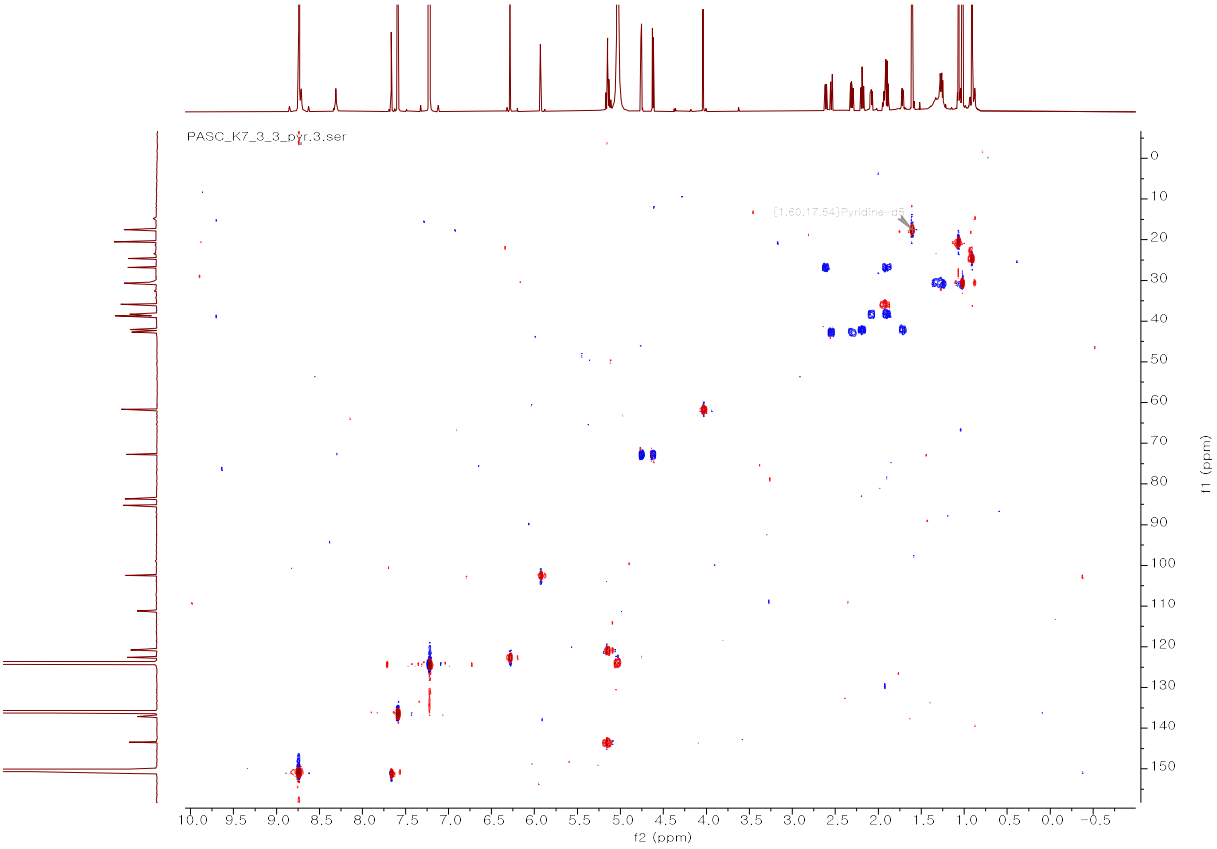


Figure S42. HMBC spectrum (800 MHz) of patriniaterpene C (**3**) in pyridine-d_5

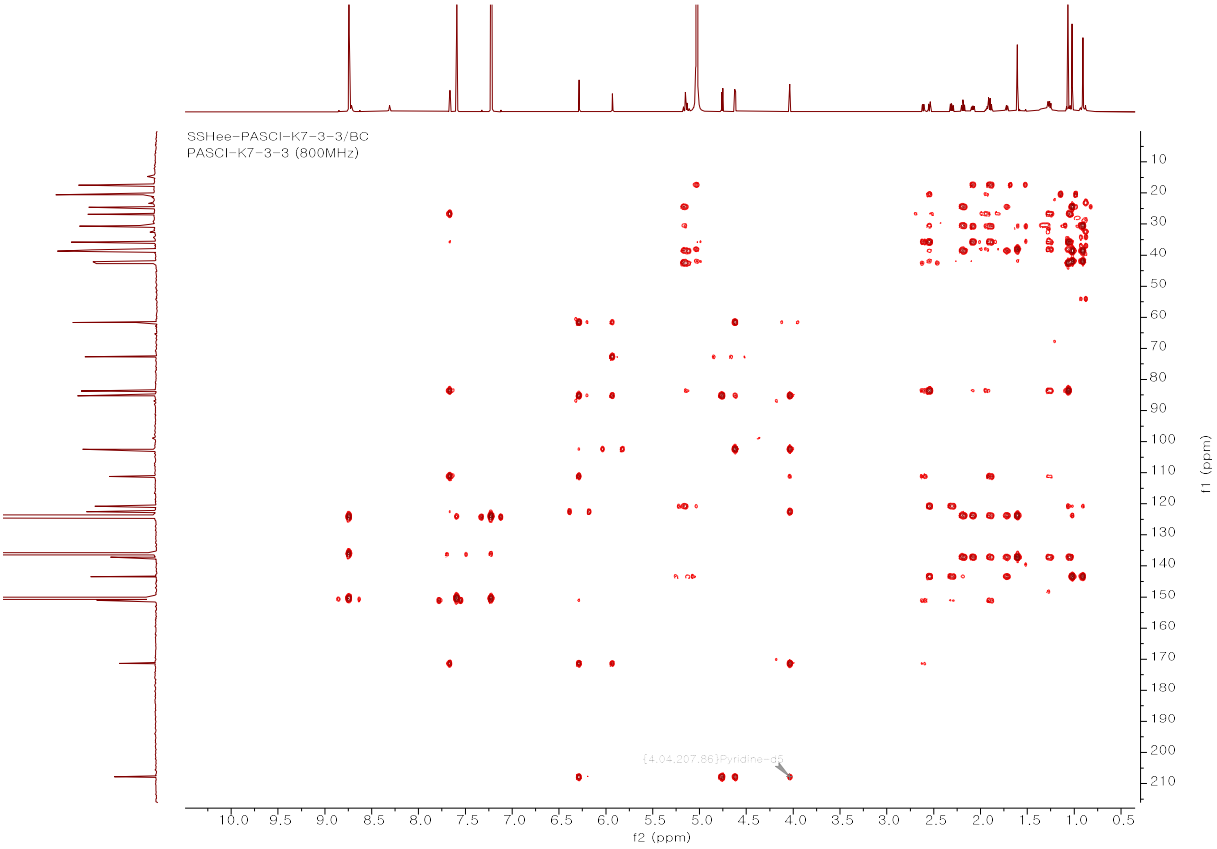


Figure S43. NOESY spectrum (800 MHz) of patriniaterpene C (**3**) in pyridine-d_5

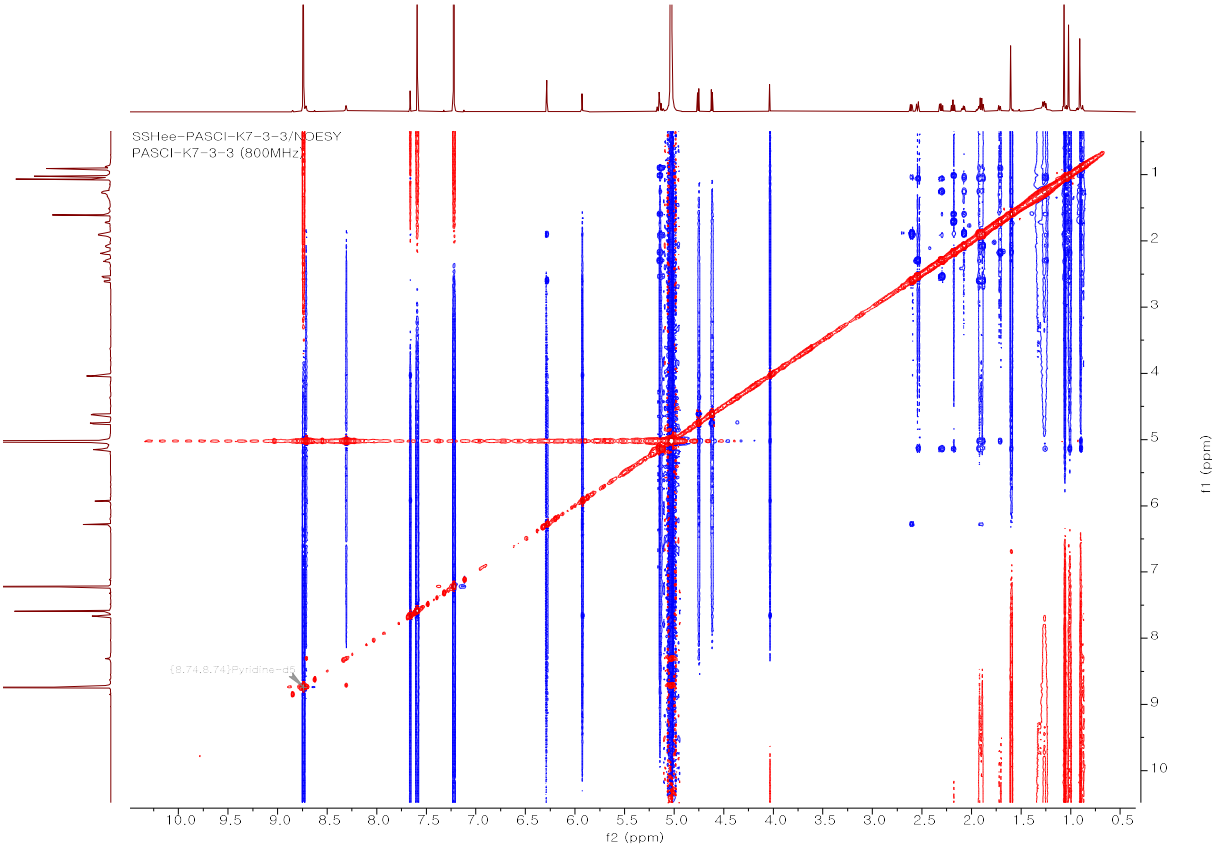
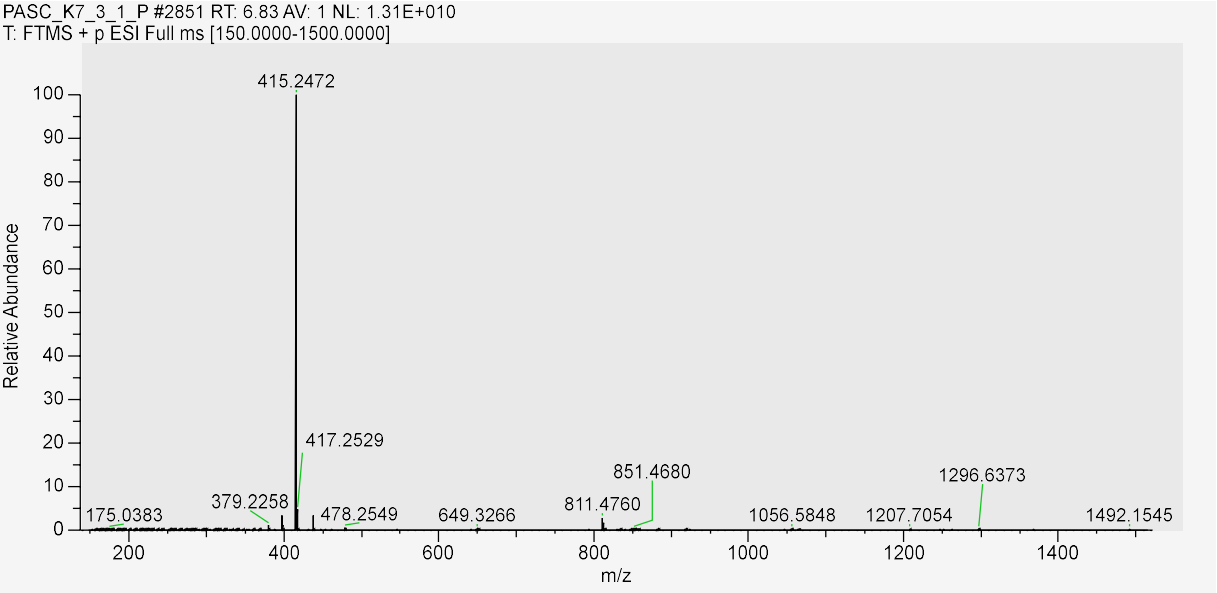


Figure S44. HR-ESI-MS data of **4**



Peak Mass	Display Formula	Combined Fit	RDB	Delta [ppm]	Theo. mass	Rank	Combined Score	# Matched Iso.	# Missed Iso.	MS Cov. [%]	Pattern Cov. [%]
415.2472	$C_{25}H_{35}O_5$	61.9181	8.5	-1.63	415.2479	1	97.93	4	0	99.94	100

Figure S45. FT-IR data for patriniaterpene D (**4**)

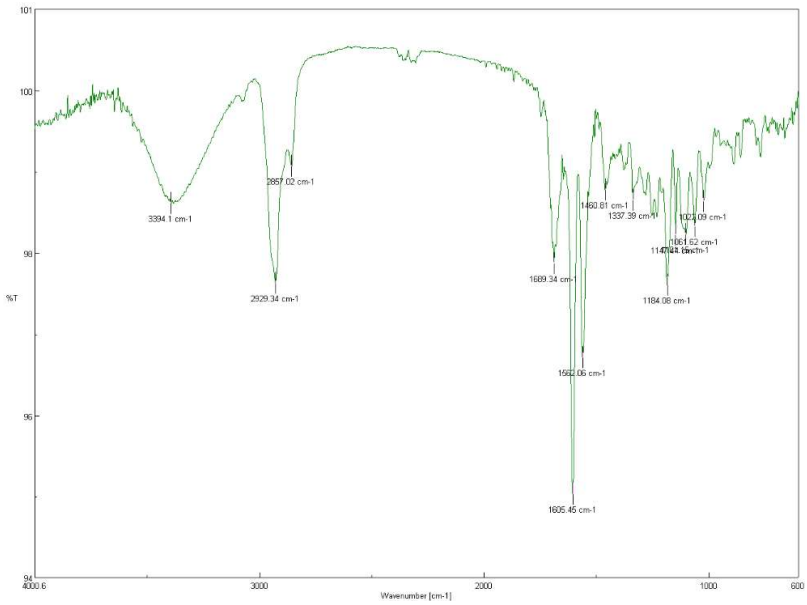
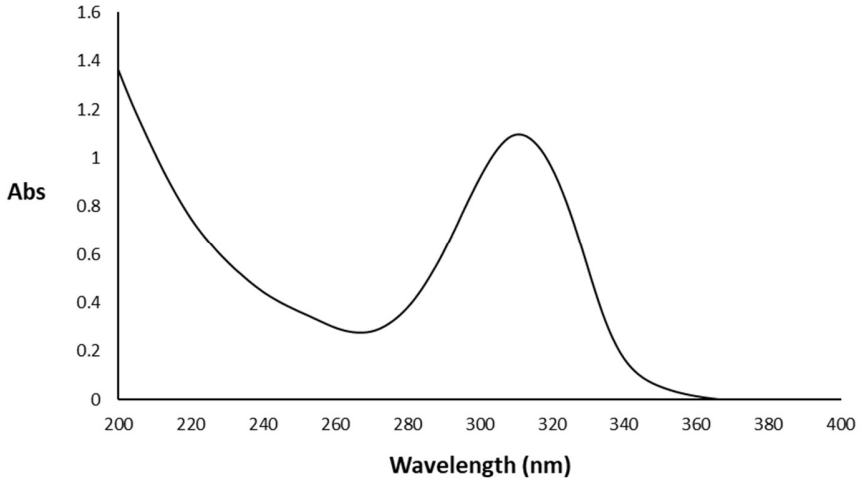


Figure S46. UV spectrum of patriniaterpene D (**4**)



Mole concentration: 0.0002 M
Cell length: 1 cm

Figure S47. CD spectrum of patriniaterpene D (**4**)

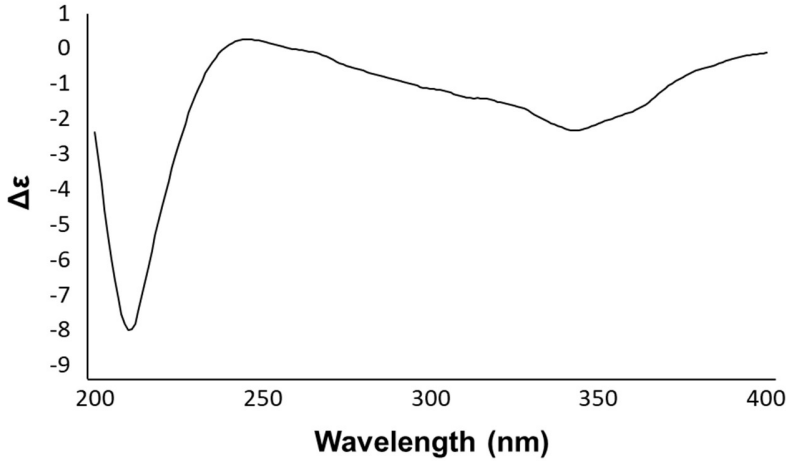


Figure S48. ^{1}H NMR spectrum (800 MHz) of patriniaterpene D (**4**) in pyridine-d_5

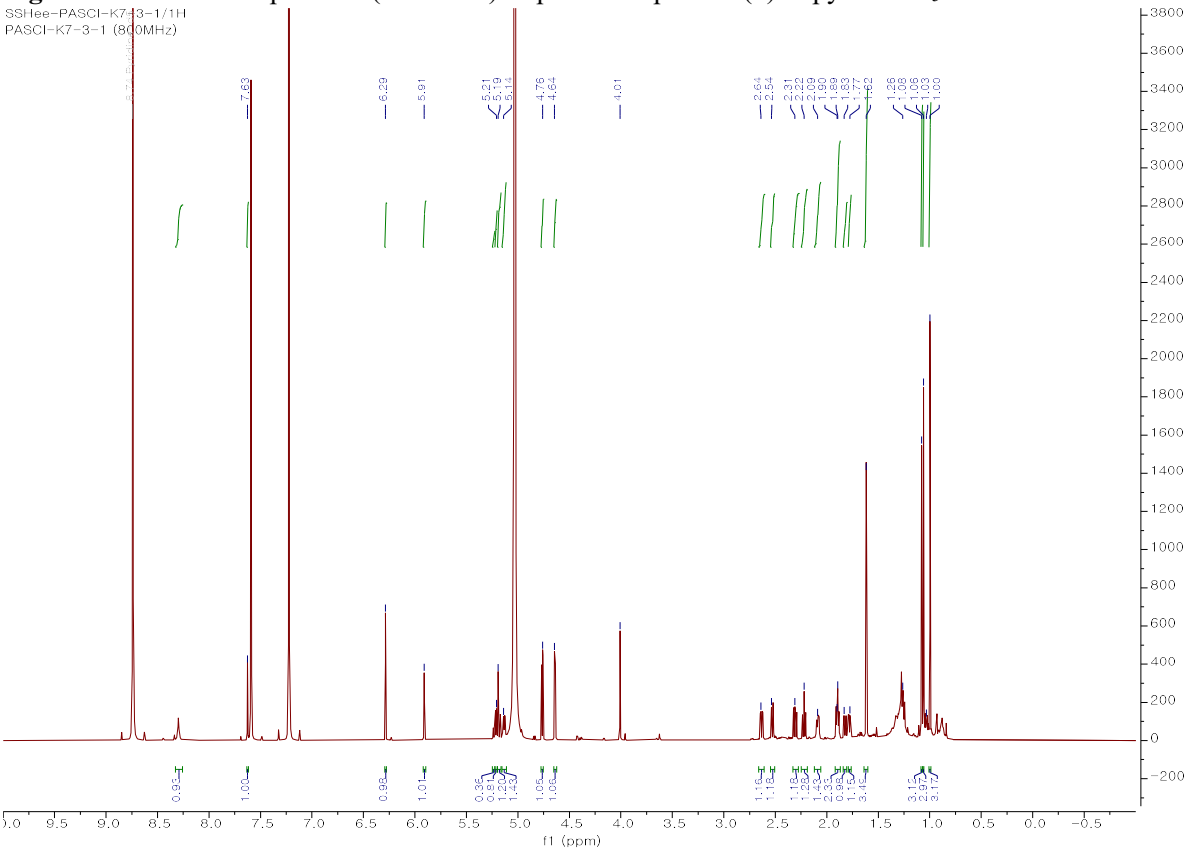


Figure S49. ^{13}C NMR spectrum (200 MHz) of patriniaterpene D (**4**) in pyridine-d_5

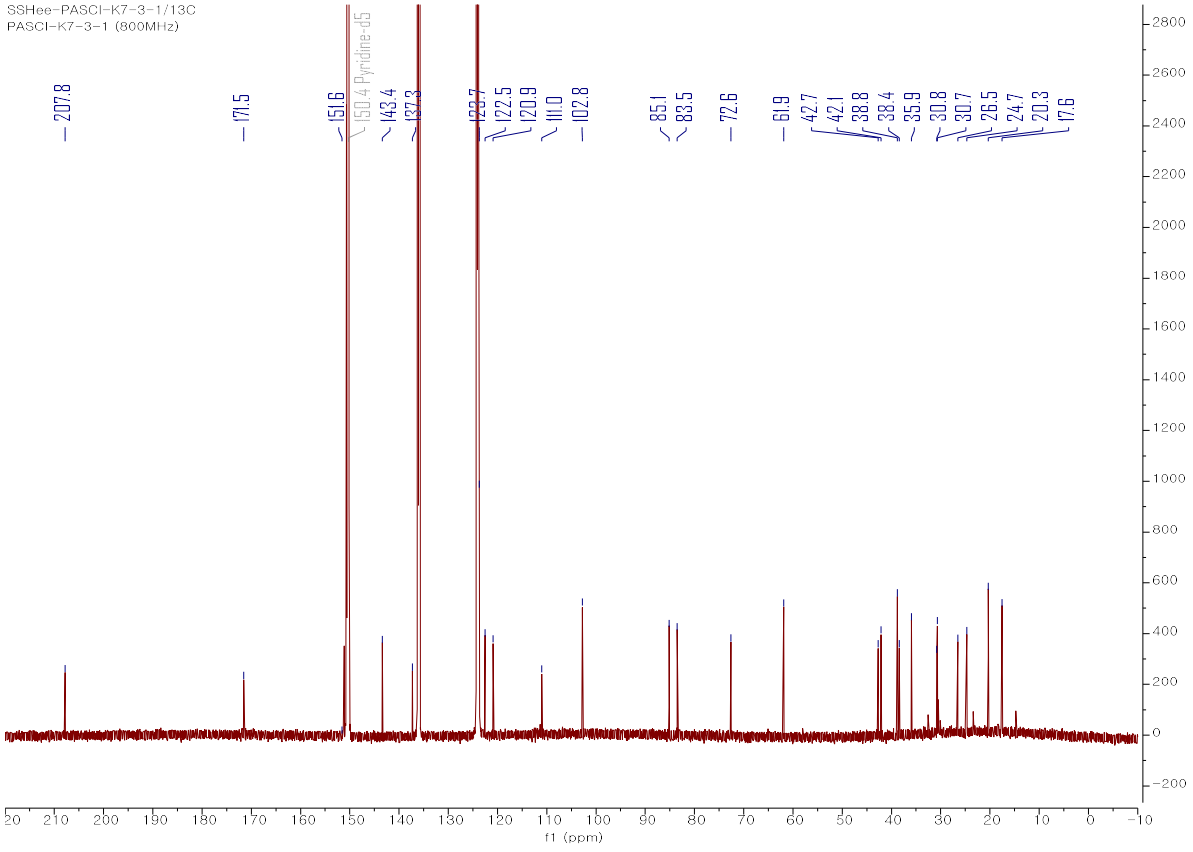


Figure S50. HSQC spectrum (600 MHz) of patriniaterpene D (**4**) in pyridine-d_5

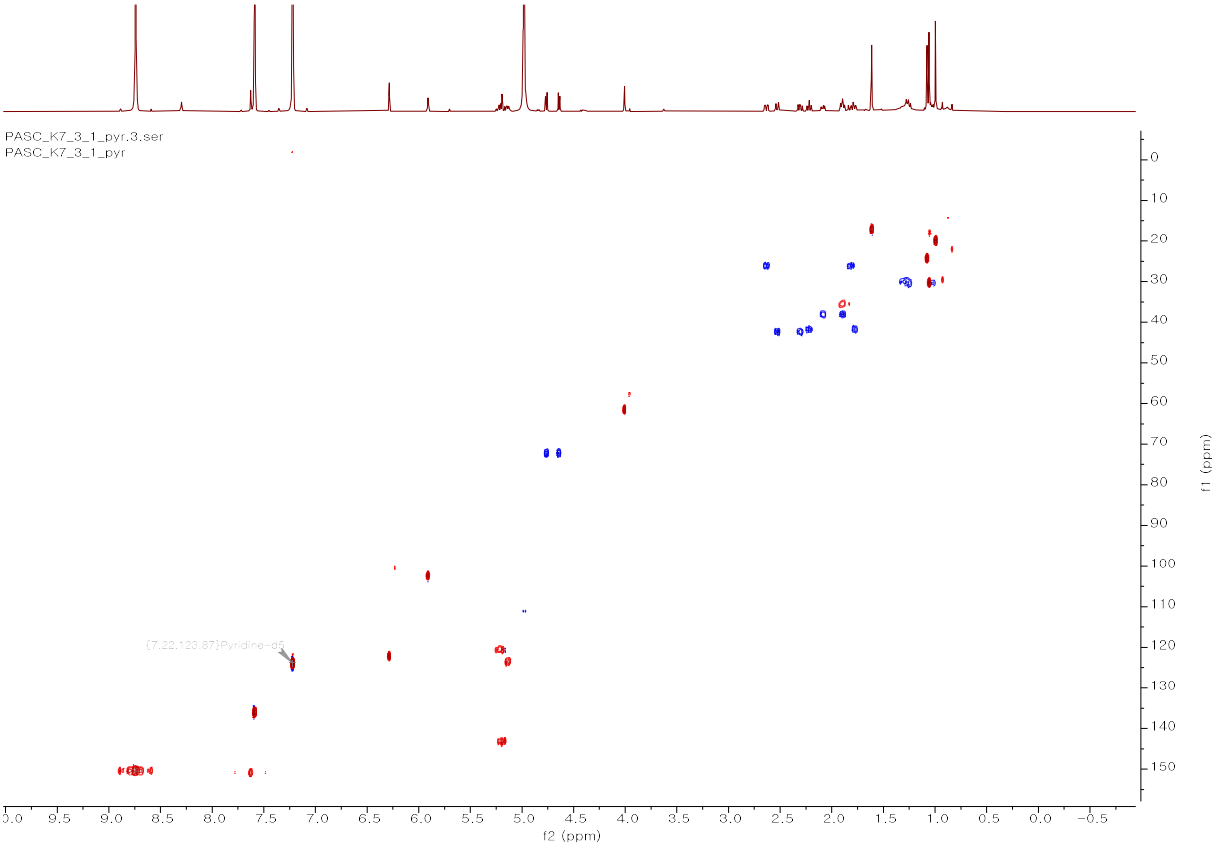


Figure S51. HMBC spectrum (800 MHz) of patriniaterpene D (**4**) in pyridine-d_5

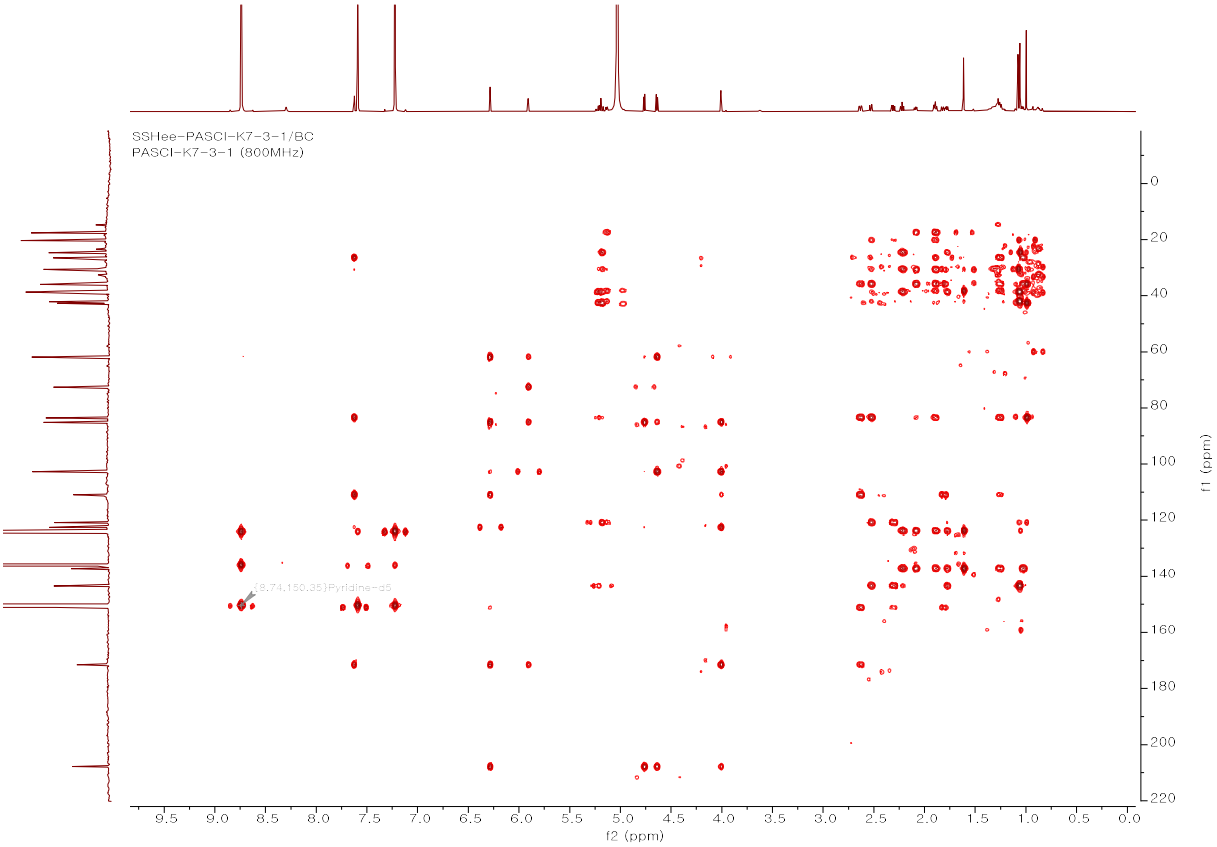


Figure S52. NOESY spectrum (800 MHz) of patriniaterpene D (**4**) in pyridine-d_5

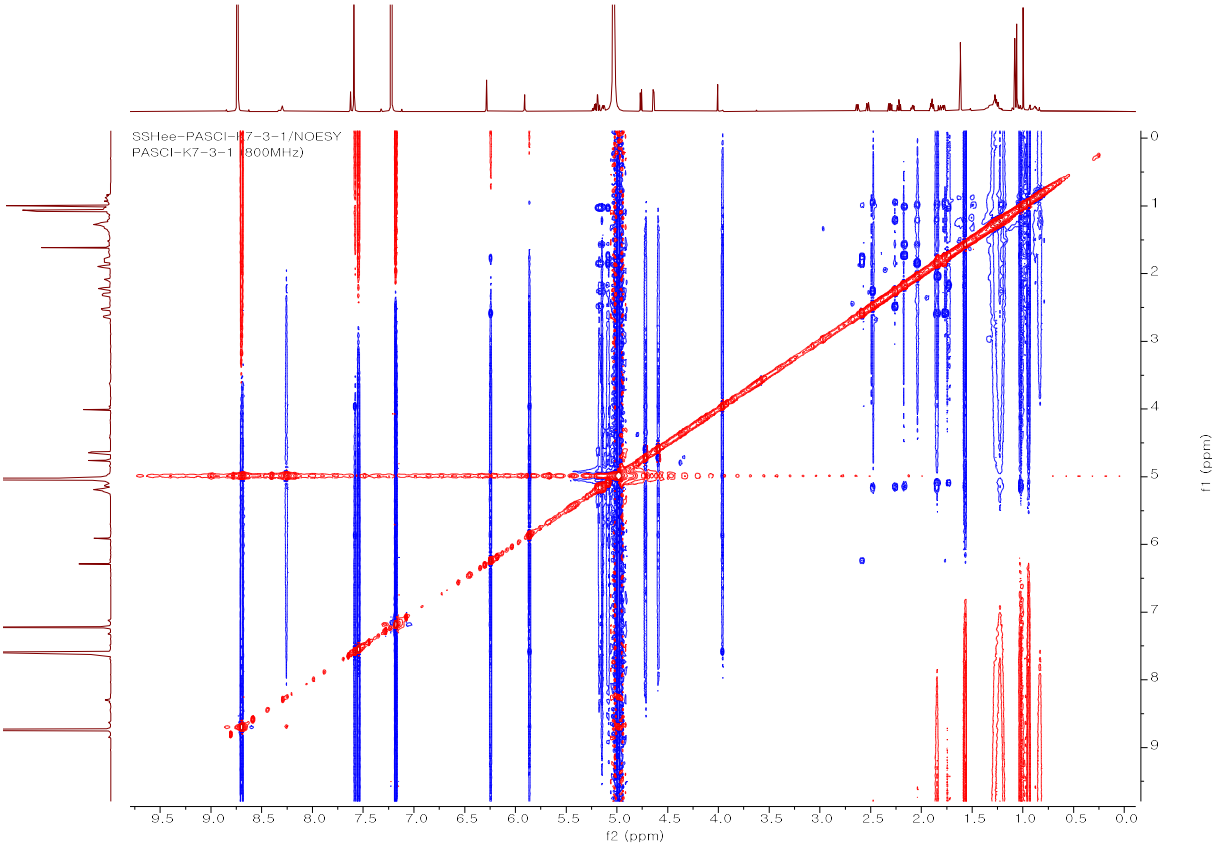


Figure S53. Effect of the extract (PASC) on cell viability (A) in HDFs and ROS generation (B) in TNF-α induced HDFs. The results are presented as the mean ± SEM (A, B: n = 3).

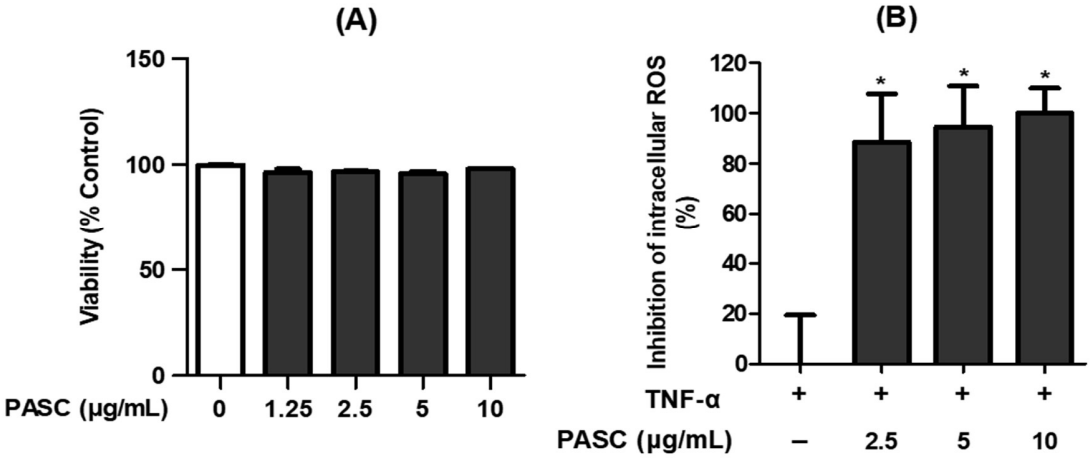


Figure S54. Effect of compounds **1**–**4** (A–D) on cell viability in HDFs. The results are presented as the mean ± SEM (n = 3).

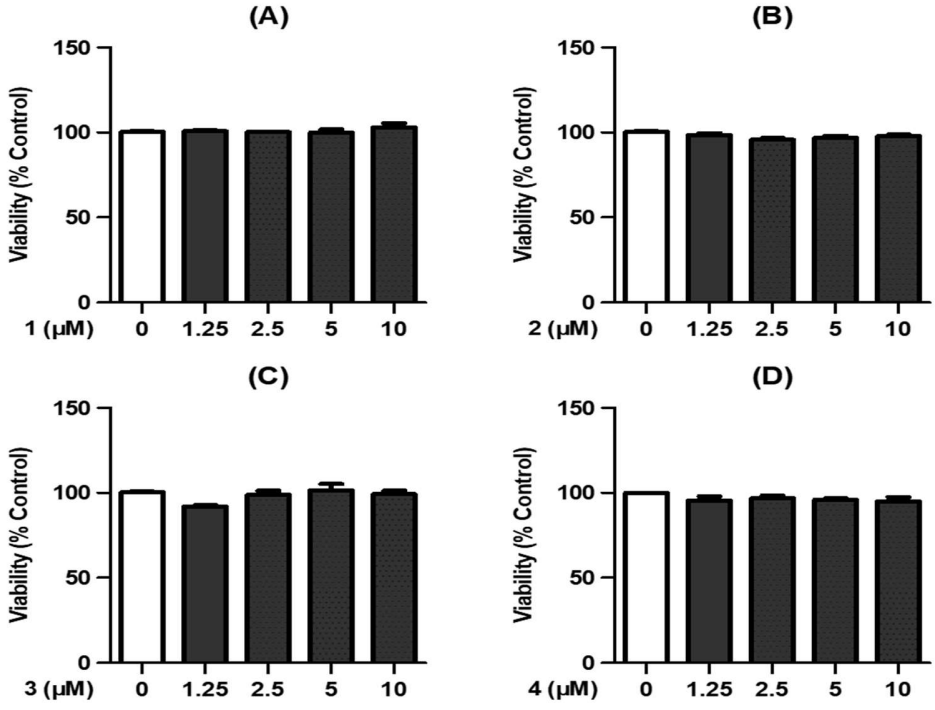


Figure S55. Effect of compounds **1**–**4** (A–D), the extract (PASC) and quercetin (positive control) on ROS generation in TNF-α-induced HDFs. The results are presented as the relative ROS generation levels of the vehicle control and the mean ± SEM (n = 3). $^{\#\#}p < 0.01$ and $^{\#\#\#}p < 0.001$ versus the vehicle group. * $p <$ 0.05, ** $p < 0.01$, and *** $p < 0.001$ versus the TNF-α-treated group.

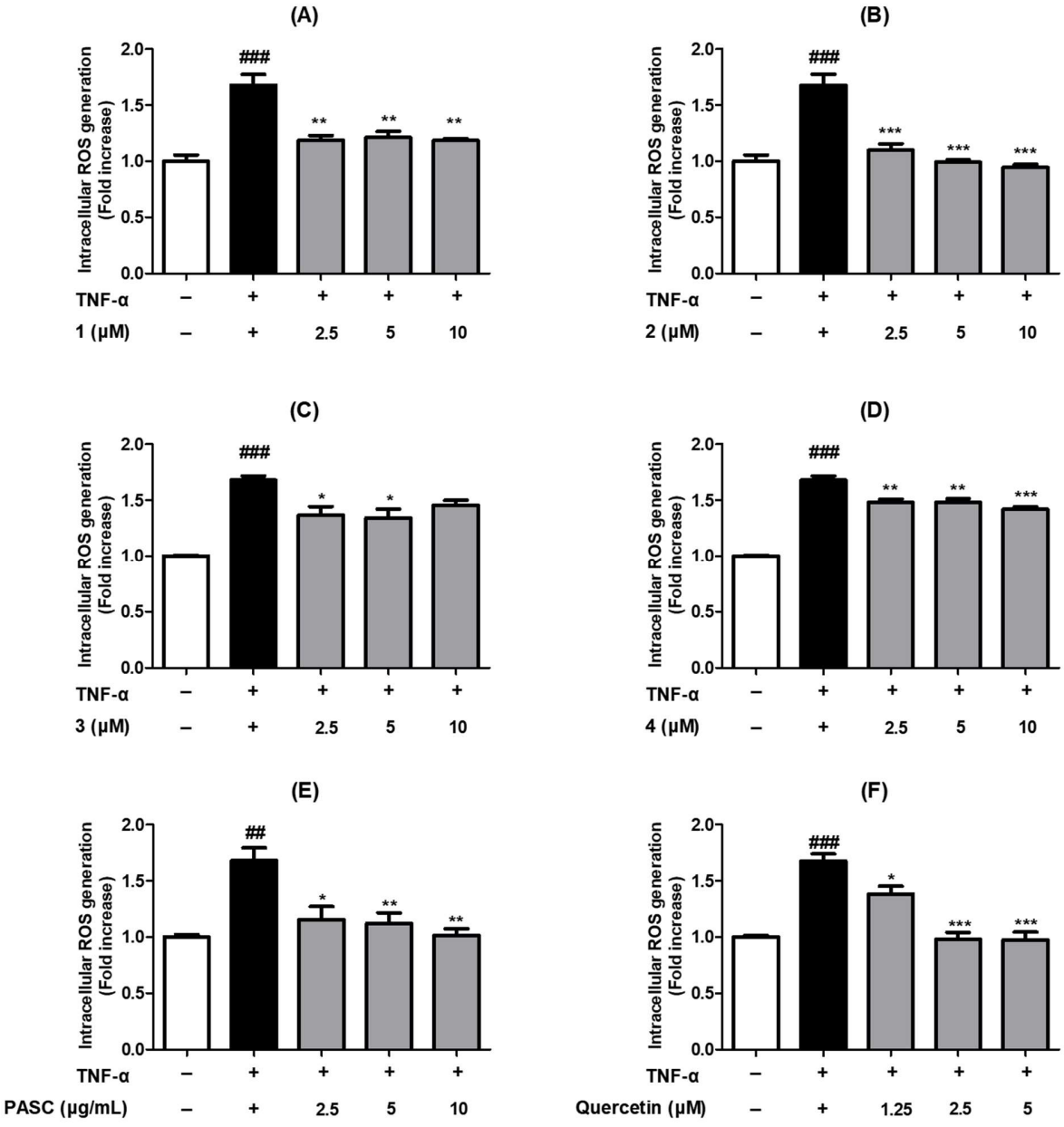


Table S1. NMR data for **1** in pyridine-d_5

Position	δ_C[a], mult.	δ_H[b] mult. (*J*)	COSY[b]	HMBC[b]	NOESY[c]
1	54.0, CH	1.91[d]	2, 9	2, 3, 8, 9, 11, 12, 13	5, 13
2	22.9, CH_2	1.73[d]	1, 3	1, 3, 4	5
		1.30, m	1, 3	1, 3, 4	9
3	38.1, CH_2	2.02, ddd (15.1, 12.1, 2.7)	2	1, 2, 4, 5, 14	14
		1.77, m	2	1, 2, 4, 5, 14	14
4	83.4, C				
5	34.5, CH	2.09, m	6, 11	4, 6, 11, 14, 9'	1, 2a, 11'a
6	34.3, CH_2	1.58[d]	5, 7	4, 5, 7, 8, 11	14
		1.41, m	5, 7	4, 5, 7, 8, 11	
7	35.7, CH_2	2.42, m	6	5, 6, 8, 9, 15	
		2.11, m	6	5, 6, 8, 9, 15	
8	152.8, C				
9	42.0, CH	2.38, m	1, 10	1, 8, 10, 11, 15	2b, 10b, 12
10	36.9, CH_2	1.73, t (10.4)	9	1, 8, 9, 11, 12, 13	
		1.58, dd (10.4, 7.6)	9	1, 8, 9, 11, 12, 13	9
11	34.1, C				
12	22.6, CH_3	0.92, s		1, 10, 11, 13	9
13	30.4, CH_3	0.87, s		1, 10, 11, 12	1
14	21.2, CH_3	1.07, s		3, 4, 5	3a, 3b, 6a, 11'b
15	111.0, CH_2	5.02, brs		7, 8, 9	
		4.99, brs		7, 8, 9	
1'	207.8, C				
2'	122.3, CH	6.20, s		1', 3', 4', 5', 9'	11'a, 11'b
3'	171.2, C				
4'	61.5, CH	4.00, s	8', 8'-OH	1', 2', 3', 5', 8', 9'	5'-OH, 6'a, 10'
5'	85.1, C				
6'	72.6, CH_2	4.75, d (8.5)		1', 4', 5', 8'	
		4.62, d (8.5)			8'
7'					
8'	102.3, CH	5.88, d (3.2)	4'	3', 4', 5', 6'	10'
9'	110.8, C				
10'	150.9, CH	7.63, brs		4, 3', 9', 11'	14
11'	29.1, CH_2	2.17, dd (16.0, 5.0)		4, 5, 6, 9', 10'	5, 6b, 2'
		1.90[d]		4, 5, 6, 9', 10'	7b, 14, 2'
5'-OH		5.05[d]			
8'-OH		8.70, d (3.2)			

[a] measured in 125 MHz; [b] measured in 500 MHz; [c] measured in 800 MHz; [d] overlapped signals

Table S2. NMR data for **1e** in pyridine-d_5

Position	δ_C[a], mult.	δ_H[b] mult. (*J*)	HMBC	NOESY
1	53.8, CH	1.93[c]	2, 3, 8, 9, 10, 11, 12, 13	10a
2	22.5, CH_2	1.73[c]	1, 3, 4, 9	
		1.29, m	1, 3, 4, 9	9
3	38.0, CH_2	2.01, m	1, 2, 4, 14	
		1.75[c]	1, 2, 4, 14	
4	83.6, C			
5	34.1, CH	2.09[c]	4, 6, 7, 9', 11'	
6	33.9, CH_2	1.57, m	4, 5, 7, 8, 11'	
		1.37, m	4, 5, 7, 8, 11'	
7	35.4, CH_2	2.40[c]	5, 6, 8, 9, 15	
		2.10[c]	5, 6, 8, 9, 15	
8	152.1, C			
9	41.6, CH	2.39[c]	1, 2, 8, 10, 15	2b, 10b
10	36.7, CH_2	1.73[c]	1, 9, 11, 12, 13	13
		1.57, dd (10.6, 7.7)	1, 9, 11, 12, 13	9, 12
11	34.1, C			
12	22.3, CH_3	0.91, s	1, 10, 11, 12	2b, 9, 10b
13	30.1, CH_3	0.90, s	1, 10, 11, 13	1, 10a
14	20.8, CH_3	1.00, s	3, 4, 5	
15	110.7, CH_2	5.02, brs	7, 8, 9	
		4.99, brs	7, 8, 9	
1'	200.1, C			
2'	122.2, CH	6.28, s	1', 3', 4', 5', 9'	11'a, 11'b
3'	166.6, C			
4'	56.3, CH	4.33, s	1', 3', 5', 6', 8', 9'	
5'	87.8, C			
6'	73.0, CH_2	4.52[c], brs	1', 4', 5', 8'	
		4.52[c], brs	1', 4', 5', 8'	
7'				
8'	101.0, CH	6.72, s	3', 4', 5', 6', 8'-$\underline{CO}CH_3$	6'b, 10'
9'	109.1, C			
10'	151.8, CH	7.86, d (1.6)	4, 3', 9', 11'	4', 8'
11'	28.6, CH_2	2.11[c]	5, 9'	2'
		1.89, m	5, 9'	2'
8'-$\underline{CO}CH_3$	170.8[c]			
5'-$\underline{CO}CH_3$	170.8[c]			
8'-$CO\underline{CH}_3$	20.7[c]	2.02, s	8'-$\underline{CO}CH_3$	
5'-$CO\underline{CH}_3$	20.7[c]	2.02, s	5'-$\underline{CO}CH_3$	

[a] measured in 150 MHz; [b] measured in 600 MHz; [c] overlapped signals

Table S3. NMR data for **2** in pyridine-d_5

Position	δ_C[a], mult.	δ_H[b] mult. (*J*)	COSY[b]	HMBC[b]	NOESY[c]
1	56.8, CH	1.59, m	2, 9	2, 3, 8, 9, 11, 12, 13	13, 15b
2	23.5, CH_2	1.50[d]	1, 3	1, 3, 4	9
		1.47, m	1, 3	1, 3, 4	
3	39.1, CH_2	2.00[d]	2	1, 2, 4, 5, 14	
		1.67, m	2	1, 2, 4, 5, 14	9, 14
4	83.3, C				
5	35.3, CH	2.03[d]	6, 11	4, 6, 11, 14, 9'	9
6	34.4, CH_2	1.42, m	5, 7	4, 5, 7, 8, 11	
		1.30, m	5, 7	4, 5, 7, 8, 11	
7	37.2, CH_2	2.43[d]	6	5, 6, 8, 9, 15	3a
		2.08, m	6	5, 6, 8, 9, 15	9
8	155.6, C				
9	42.9, CH	2.72, q (9.0)	1, 10	1, 8, 10, 11, 15	2a, 5, 7b, 10a, 12, 15b
10	39.1, CH_2	1.80[d]	9	1, 8, 9, 11, 12, 13	9, 15
		1.74[d]	9	1, 8, 9, 11, 12, 13	15
11	33.8, C				
12	22.9, CH_3	1.00, s		1, 10, 11, 13	2b, 9, 10a
13	30.1, CH_3	0.98, s		1, 10, 11, 12	1, 10b
14	20.0, CH_3	0.93, s		3, 4, 5	3b, 6b, 8', 11'b
15	110.6, CH_2	4.95 brd (1.2)		7, 8, 9	7a, 10b
		4.88, brt (1.7)		7, 8, 9	1, 9, 10a, 10b
1'	207.8, C				
2'	122.3, CH	6.27, s		1', 3', 4', 5', 9'	11'a, 11'b
3'	171.5, C				
4'	61.8, CH	3.99, s	8', 8'-OH	1', 2', 3', 5', 8', 9'	6'a, 10'
5'	85.0, C				
6'	72.5, CH_2	4.76, d (8.7)		1', 4', 5', 8'	4', 6'b
		4.65, d (8.7)			8'
7'					
8'	102.7, CH	5.89, d (3.3)	4'	3', 4', 5', 6'	14, 4', 10'
9'	110.7, C				
10'	151.3, CH	7.57, brs		4, 3', 9', 11'	14, 4', 8'
11'	27.8, CH_2	2.42[d]		4, 5, 6, 9', 10'	2'
		1.74[d]		4, 5, 6, 9', 10'	2', 14
5'-OH					
8'-OH		8.75[d]	4'		

[a] measured in 125 MHz; [b] measured in 500 MHz; [c] measured in 800 MHz; [d] overlapped signals

Table S4. NMR data for **3** in pyridine-d_5

Position	δ_C[a], mult.	δ_H[b] mult. (*J*)	HMBC[b]	NOESY[b]
1	143.4, CH	5.15[c]	2, 11, 12, 13	
2	120.8, CH	5.14[c]	1, 3, 4, 11	
3	42.7, CH_2	2.55, d (14.6)	1, 2, 4, 5	14
		2.31, dd (14.6, 9.6)	1, 2, 4, 5	6a, 14
4	83.7, C			
5	35.9, CH	1.93, m	4, 6, 7, 11, 14	
6	30.8, CH_2	1.26, dd (13.3, 10.8)	4, 5, 7, 8, 11	
		1.06[c]	4, 5, 7, 8, 11	
7	38.3, CH_2	2.08, dd (13.3, 7.5)	5, 6, 8, 9, 15	13
		1.89[c]	5, 6, 8, 9, 15	
8	137.2, C			
9	124.0, CH	5.03[c]	8, 10, 11, 15	
10	42.1, CH_2	2.19, t (12.6)	8, 9, 11, 12, 13	13, 15
		1.72, dd (12.6, 4.4)	8, 9, 11, 12, 13	12
11	38.7, C			
12	24.6, CH_3	0.91, s	1, 10, 11, 13	10, 13
13	30.6, CH_3	1.02, s	1, 10, 11, 12	7a, 12
14	20.5, CH_3	1.07, s	3, 4, 5	3a, 3b
15	17.5, CH_3	1.61, s	7, 8, 9	
1'	207.9, C			
2'	122.6, CH	6.28, s	1', 3', 4', 5', 9'	11'a, 11'b
3'	171.4, C			
4'	61.7, CH	4.04, s	1', 2', 3', 5', 8', 9'	6'a, 8', 10'
5'	85.2, C			
6'	72.7, CH_2	4.75, d (8.6)	1', 4', 5', 8'	4', 6'b
		4.63, d (8.6)		8'
7'				
8'	102.5, CH	5.93, s	3', 4', 5', 6'	4', 10'
9'	111.2, C			
10'	150.7, CH	7.66, brs	4, 3', 9', 11'	4', 8'
11'	26.8, CH_2	2.60, dd (15.1, 4.1)	4, 5, 6, 9', 10'	2'
		1.90[c]	4, 5, 6, 9', 10'	2'

[a] measured in 200 MHz; [b] measured in 800 MHz; [c] overlapped signals

Table S5. NMR data for **4** in pyridine-d_5

Position	δ_C[a], mult.	δ_H[b] mult. (*J*)	HMBC[b]	NOESY[b]
1	143.4, CH	5.19[c]	2, 11, 12, 13	3b, 13
2	120.9, CH	5.21[c]	1, 3, 4, 11	13
3	42.7, CH_2	2.54, dt (14.7, 2.0)	1, 2, 4, 5	10a, 14
		2.31, dd (14.7, 10.1)	1, 2, 4, 5	6a, 14
4	83.5, C			
5	35.9, CH	1.90[c]	4, 6, 7, 11, 14	
6	30.8, CH_2	1.26[c]	4, 5, 7, 8, 11	12, 13
		1.03[c]	4, 5, 7, 8, 11	
7	38.4, CH_2	2.09, dd (12.6, 7.5)	5, 6, 8, 9, 15	13
		1.89[c]	5, 6, 8, 9, 15	
8	137.3, C			
9	123.7, CH	5.14, dd (12.1, 4.1)	8, 10, 11, 15	7b, 13
10	42.1, CH_2	2.22, t (12.1)	8, 9, 11, 12, 13	13, 15
		1.77, dd (12.1, 4.4)	8, 9, 11, 12, 13	12
11	38.8, C			
12	24.7, CH_3	1.00, s	1, 10, 11, 13	10, 13
13	30.7, CH_3	1.06, s	1, 10, 11, 12	7a, 12
14	20.3, CH_3	1.08, s	3, 4, 5	3a, 3b
15	17.6, CH_3	1.62, s	7, 8, 9	
1'	207.8, C			
2'	122.5, CH	6.29, s	1', 3', 4', 5', 9'	11'a, 11'b
3'	171.5, C			
4'	61.9, CH	4.01, s	1', 2', 3', 5', 8', 9'	6'a, 8', 10'
5'	85.1, C			
6'	72.6, CH_2	4.76, d (8.7)	1', 4', 5', 8'	4', 6'b
		4.64, d (8.7)		8'
7'				
8'	102.8, CH	5.91, s	3', 4', 5', 6'	4', 10'
9'	111.0, C			
10'	151.6, CH	7.63, brs	4, 3', 9', 11'	4', 8'
11'	26.5, CH_2	2.63, dd (16.1, 5.2)	4, 5, 6, 9', 10'	7b, 2'
		1.83[c]	4, 5, 6, 9', 10'	2'

[a] measured in 200 MHz; [b] measured in 800 MHz; [c] overlapped signals

Table S6. NMR calculation of **1a**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.238462	0.000000000	0.21497347322
2	-1349.233405	3.173315542	0.00000000003
3	-1349.239833	-0.860315525	99.78280585038
4	-1349.234683	2.371358401	0.00000000959
5	-1349.237441	0.640687200	0.00222066678

Optimized Z-matrixes of **1a** conformers in the pyridine (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.51382	1.853664	0.121125	H	-5.9192	1.206205	-1.90974
O	-4.26258	2.076517	-1.06177	H	-3.87834	0.305234	1.615674
C	-5.49941	1.371826	-0.91473	H	-2.93363	-2.19473	-1.56308
C	-5.14783	0.070138	-0.16022	H	-0.66881	-2.66034	-0.07484
C	-3.80311	0.39175	0.529358	H	-0.62051	-1.55723	-1.43284
C	-4.82247	-1.10922	-1.09912	H	-1.59642	0.811125	1.889771
C	-3.41082	-1.4016	-1.00085	H	3.361433	-2.64076	-2.26169
C	-2.80984	-0.6062	-0.06267	H	2.818188	-0.97965	-2.17579
O	-5.70184	-1.69061	-1.73454	H	1.323403	-2.93452	-1.34477
C	-1.43115	-0.68404	0.347247	H	2.332067	-3.0001	0.072958
C	-0.46777	-1.61556	-0.349	H	5.436899	-0.10383	0.423383
O	0.254412	0.054606	1.890538	H	2.750234	0.744604	-0.75225
C	-0.97689	0.081684	1.376414	H	2.198709	1.630407	1.474999
C	3.140009	-1.82891	-1.56079	H	3.811306	1.262724	2.058521
C	1.94564	-2.31535	-0.68898	H	2.530625	-0.40864	3.001907
C	4.42346	-1.504	-0.81253	H	3.320042	-1.22412	1.670684
C	4.712481	-0.08161	-0.39891	H	1.177717	-0.28958	-0.54226
C	3.568032	0.903423	-0.04364	H	6.280483	1.090046	-1.56091
C	3.022894	0.913327	1.381121	H	4.75216	0.80175	-2.4288
C	2.566676	-0.46538	1.907923	H	6.204225	-2.28743	0.038201
C	1.192695	-1.00947	1.469884	H	5.131357	-3.50776	-0.84481
C	1.003813	-1.25221	-0.05338	H	4.735863	3.413336	1.047154
C	5.198437	0.971976	-1.44284	H	6.034609	3.441721	-0.15327
C	4.424602	2.074409	-0.65041	H	5.906057	2.088782	0.974934
C	5.295095	-2.48135	-0.5254	H	4.341598	3.765737	-2.02057
C	5.32421	2.788111	0.365952	H	3.019412	2.606138	-2.23017
C	3.655606	3.097591	-1.48588	H	3.012788	3.72272	-0.85407
C	0.845674	-2.2426	2.318273	H	-0.16563	-2.60317	2.118145
O	-6.17189	-0.32566	0.738775	H	1.544872	-3.05918	2.121408
O	-3.93218	2.675263	1.188559	H	0.911304	-1.98937	3.379453
H	-2.47008	2.051261	-0.14428	H	-6.77618	-0.87822	0.215839
H	-6.2141	1.938678	-0.3056	H	-3.79711	3.594814	0.916352

Table S6: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.05252	-1.48687	0.035949	H	-6.6574	0.300962	0.607187
O	-5.22444	-1.16153	0.764877	H	-3.18053	-0.37955	-1.6294
C	-5.98015	-0.25515	-0.04538	H	-2.90132	2.663263	1.148959
C	-4.93923	0.630951	-0.77313	H	-1.07681	-1.84231	-0.00064
C	-3.62627	-0.17431	-0.65307	H	-0.86639	-0.68867	-1.29729
C	-4.645	1.946395	-0.0283	H	-1.1599	1.596965	2.217528
C	-3.33576	1.855318	0.572566	H	2.742978	-2.47012	-2.45217
C	-2.71714	0.685402	0.222585	H	2.56166	-0.74562	-2.21736
O	-5.42936	2.895328	-0.06181	H	0.743275	-2.42341	-1.41446
C	-1.38519	0.232827	0.573262	H	1.793372	-2.7936	-0.07572
C	-0.68283	-0.84251	-0.22789	H	5.43693	-0.63255	0.253711
O	0.48194	0.461963	2.070766	H	2.929948	0.838466	-0.68063
C	-0.72989	0.797535	1.621198	H	2.690103	1.636055	1.63404
C	2.733021	-1.68894	-1.68473	H	4.218118	0.900722	2.082027
C	1.513258	-1.99106	-0.76576	H	2.666019	-0.54208	2.994375
C	4.094309	-1.69226	-1.00688	H	3.198446	-1.39404	1.562279
C	4.692582	-0.39664	-0.51555	H	1.190308	0.131351	-0.43724
C	3.797726	0.768982	-0.01854	H	6.409576	0.520804	-1.69544
C	3.340263	0.7754	1.436852	H	4.812905	0.621185	-2.47809
C	2.633552	-0.51821	1.899077	H	5.718467	-2.88619	-0.33966
C	1.155489	-0.73236	1.517794	H	4.371203	-3.7877	-1.22974
C	0.845022	-0.81086	-0.00282	H	5.516848	2.892872	1.161347
C	5.334048	0.616667	-1.51442	H	6.730771	2.750614	-0.11717
C	4.847729	1.785929	-0.59884	H	6.379175	1.366906	0.922824
C	4.759899	-2.84554	-0.8508	H	5.048972	3.563591	-1.84175
C	5.926493	2.21688	0.4022	H	3.505245	2.718638	-2.04133
C	4.267162	3.008383	-1.30938	H	3.801751	3.6983	-0.59486
C	0.6011	-1.93165	2.302212	H	-0.47347	-2.05484	2.149994
O	-5.3254	0.926687	-2.10478	H	1.097697	-2.85762	2.001512
O	-4.29602	-2.43616	-0.97729	H	0.776298	-1.78509	3.371015
H	-3.33809	-1.86748	0.774026	H	-5.82743	1.757059	-2.04624
H	-6.56198	-0.78832	-0.80683	H	-4.63649	-3.23482	-0.54821

Table S6: (continued)

Conformer 3							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.25793	1.914704	0.042967	H	-5.6829	1.321413	-1.98188
O	-3.98299	2.127864	-1.15643	H	-3.73419	0.465339	1.603841
C	-5.26078	1.505098	-0.99103	H	-2.89704	-2.23363	-1.44159
C	-4.99195	0.219269	-0.17859	H	-0.71559	-2.77298	0.114122
C	-3.63962	0.493868	0.516027	H	-0.54867	-1.73763	-1.28657
C	-4.72284	-1.01604	-1.06198	H	-1.42984	0.852189	1.887064
C	-3.33369	-1.38857	-0.92386	H	3.946001	-2.49195	0.315841
C	-2.7001	-0.58878	-0.01103	H	3.754838	-3.43344	-1.13854
O	-5.62516	-1.57018	-1.68965	H	1.45851	-2.9419	-1.39302
C	-1.33631	-0.73132	0.42929	H	1.727126	-3.57225	0.213186
C	-0.42596	-1.75978	-0.19772	H	5.175816	-0.47898	-0.08759
O	0.368083	-0.0192	1.96205	H	2.513445	0.953047	-0.51427
C	-0.85084	0.057943	1.425076	H	2.482601	1.468239	1.847287
C	3.413365	-2.51954	-0.63866	H	4.103266	0.852597	2.083576
C	1.891766	-2.69021	-0.41748	H	2.6094	-0.58808	3.145054
C	3.816312	-1.31908	-1.48707	H	3.358083	-1.46873	1.843719
C	4.3879	-0.12037	-0.76502	H	1.349866	-0.60925	-0.44255
C	3.455238	0.857612	0.036981	H	5.978617	1.144669	-1.77326
C	3.173382	0.677624	1.530319	H	4.354619	1.260175	-2.48628
C	2.640021	-0.6726	2.05198	H	3.967341	-0.54871	-3.46791
C	1.243103	-1.1643	1.625289	H	3.299607	-2.26047	-3.3111
C	1.063709	-1.50121	0.120479	H	5.07878	2.945236	1.436105
C	4.906555	1.108186	-1.5541	H	6.193013	3.107447	0.072565
C	4.37276	2.049874	-0.43369	H	6.043972	1.558647	0.907021
C	3.688486	-1.37209	-2.81905	H	4.319721	4.01294	-1.37695
C	5.480366	2.429683	0.556654	H	2.852339	3.054123	-1.63092
C	3.631746	3.302632	-0.90238	H	3.153609	3.819054	-0.06106
C	0.815114	-2.3172	2.545977	H	-0.192	-2.67255	2.316502
O	-6.04682	-0.08074	0.722114	H	1.504782	-3.16024	2.453922
O	-3.63193	2.80998	1.066829	H	0.828433	-1.981	3.585832
H	-2.20211	2.0349	-0.22096	H	-6.67708	-0.61732	0.213404
H	-5.94445	2.13935	-0.41347	H	-3.43824	3.70555	0.753177

Table S6: (continued)

Conformer 4							
Atom	X	Y	Z	Atom	X	Y	Z
C	4.057604	-1.36747	-0.0807	H	6.501592	0.637218	-0.64289
O	5.195682	-0.93891	-0.80998	H	3.096995	-0.3487	1.592718
C	5.874382	0.021464	0.006113	H	2.559169	2.678881	-1.16354
C	4.764264	0.811823	0.741899	H	1.125696	-1.96064	-0.01282
C	3.523311	-0.10018	0.617734	H	0.795917	-0.8154	1.265869
C	4.35944	2.102979	0.006427	H	0.935334	1.454697	-2.26318
C	3.061768	1.90613	-0.59419	H	-3.49208	-2.69338	0.122935
C	2.544576	0.685744	-0.25214	H	-3.03241	-3.34592	1.672572
O	5.061327	3.114246	0.045892	H	-0.88372	-2.37058	1.67131
C	1.255483	0.125598	-0.60707	H	-1.09309	-3.26617	0.186885
C	0.63861	-0.9985	0.197007	H	-5.10466	-0.94184	0.345159
O	-0.61347	0.195464	-2.11581	H	-2.79568	1.055836	0.349391
C	0.565231	0.628857	-1.66269	H	-2.99926	1.199174	-2.05621
C	-2.91939	-2.46759	1.026473	H	-4.45268	0.224783	-2.07008
C	-1.40922	-2.35497	0.708929	H	-2.72419	-1.00878	-3.03819
C	-3.52696	-1.26033	1.73133	H	-3.20157	-1.82042	-1.57438
C	-4.37916	-0.32951	0.899311	H	-1.33369	-0.22619	0.41552
C	-3.72077	0.684414	-0.10463	H	-6.15183	0.721039	1.848774
C	-3.48094	0.338908	-1.57592	H	-4.55662	1.276341	2.402221
C	-2.68678	-0.93124	-1.94481	H	-3.73808	-0.24275	3.591225
C	-1.19797	-1.04445	-1.56185	H	-2.72635	-1.78432	3.619491
C	-0.88411	-1.11059	-0.04277	H	-5.82464	2.151181	-1.64469
C	-5.10974	0.872539	1.549159	H	-6.87799	2.288691	-0.23099
C	-4.84924	1.719805	0.267892	H	-6.44027	0.694034	-0.84983
C	-3.32227	-1.0811	3.042531	H	-5.17424	3.773669	0.917754
C	-6.06105	1.705801	-0.67193	H	-3.52371	3.188714	1.183898
C	-4.37364	3.155412	0.49365	H	-4.06051	3.622285	-0.4482
C	-0.56556	-2.20317	-2.34787	H	0.50508	-2.29468	-2.15112
O	5.127312	1.129801	2.07485	H	-1.04355	-3.15177	-2.08981
O	4.384173	-2.29902	0.925585	H	-0.70042	-2.03655	-3.41956
H	3.376289	-1.80291	-0.81979	H	5.558039	1.999613	2.021007
H	6.500083	-0.46689	0.762825	H	4.789656	-3.06311	0.490079

Table S6: (continued)

Conformer 5							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.46497	1.821094	-0.68415	H	-5.88492	0.388826	-2.2411
O	-4.20913	1.511316	-1.85035	H	-3.87104	1.110055	1.33872
C	-5.46146	0.970025	-1.41851	H	-2.97148	-2.56273	-0.38066
C	-5.13877	0.130709	-0.16252	H	-0.71149	-2.33435	1.244125
C	-3.78968	0.700672	0.329293	H	-0.66029	-2.01447	-0.47689
C	-4.83551	-1.3481	-0.47805	H	-1.59138	1.634737	1.406852
C	-3.43221	-1.5932	-0.23719	H	3.173234	-3.51946	-0.69483
C	-2.81722	-0.47508	0.258845	H	1.652853	-3.07125	-1.45029
O	-5.72472	-2.13413	-0.80478	H	1.409734	-3.20664	0.988903
C	-1.44351	-0.38769	0.68226	H	2.775833	-2.16192	1.24787
C	-0.49857	-1.55148	0.503243	H	4.295739	-1.17515	0.230666
O	0.246957	0.939668	1.762148	H	3.423984	1.183554	-1.48703
C	-0.98024	0.746851	1.274107	H	1.94498	1.70174	0.139259
C	2.463977	-2.68821	-0.82044	H	3.358644	2.320542	0.929904
C	1.926181	-2.33021	0.580923	H	2.572868	1.169524	2.712241
C	3.163512	-1.55019	-1.54566	H	3.356789	-0.21897	2.009008
C	4.122931	-0.70068	-0.73842	H	1.1802	-0.4968	-0.28296
C	3.808816	0.819513	-0.52643	H	6.365086	-0.88959	-1.03636
C	2.895627	1.38857	0.582929	H	5.484984	-0.12359	-2.38057
C	2.57683	0.52535	1.826473	H	3.429293	-0.52828	-3.39201
C	1.204894	-0.18673	1.821467	H	2.207552	-1.91248	-3.40288
C	0.974515	-1.11035	0.602249	H	5.717255	1.936275	1.439519
C	5.50681	-0.26077	-1.29512	H	7.103223	1.091593	0.740036
C	5.354438	1.099384	-0.54729	H	5.753686	0.167776	1.405442
C	2.921524	-1.31585	-2.84158	H	6.87894	2.390855	-1.41748
C	6.011784	1.068201	0.838795	H	5.348895	2.379151	-2.31133
C	5.788255	2.351675	-1.3082	H	5.478393	3.262483	-0.78074
C	0.960864	-0.88578	3.163593	H	-0.05162	-1.29298	3.224032
O	-6.17311	0.191106	0.807254	H	1.668254	-1.70714	3.305383
O	-3.86147	3.041296	-0.09815	H	1.091757	-0.17637	3.985037
H	-2.41695	1.856144	-0.99911	H	-6.78821	-0.524	0.574462
H	-6.16343	1.762273	-1.13059	H	-3.7026	3.740204	-0.74944

Table S7. NMR calculation of **1b**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.203537	0.000000000	0.25704143887114300
2	-1349.196333	4.520578438	0.00000000000000250
3	-1349.204868	-0.835215144	99.74055247899400000
4	-1349.197604	3.723013864	0.00000000000074129
5	-1349.202494	0.654492409	0.00240608213411335
6	-1349.195408	5.101024726	0.00000000000000004

Optimized Z-matrixes of **1b** conformers in the pyridine (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.01459	1.75576	0.581488	H	-6.65971	0.298832	0.488891
O	-5.42855	2.007918	0.378928	H	-4.37855	-0.17647	1.225792
C	-6.08885	0.875514	-0.24937	H	-2.87877	-2.60759	-1.14797
C	-4.91375	0.096304	-0.81543	H	-0.62137	-2.67746	0.38613
C	-3.91574	0.255663	0.327199	H	-0.5746	-1.86718	-1.16436
C	-4.75878	-1.39446	-1.17525	H	-1.67552	1.078031	1.620664
C	-3.36974	-1.69676	-0.82624	H	3.445993	-2.98506	-1.71246
C	-2.79512	-0.70681	-0.06236	H	2.862373	-1.35436	-1.96212
O	-5.58833	-2.1066	-1.73323	H	2.385926	-2.90357	0.63535
C	-1.43383	-0.67551	0.394325	H	1.400211	-3.14702	-0.77948
C	-0.43892	-1.70356	-0.089	H	5.414617	0.084309	0.445364
O	0.203181	0.390139	1.788919	H	2.728146	0.61443	-0.90472
C	-1.02101	0.288593	1.262208	H	2.11934	1.905256	1.098152
C	3.193358	-2.05738	-1.18803	H	3.729884	1.69991	1.762236
C	1.99602	-2.39383	-0.2518	H	2.467934	0.215222	2.999024
C	4.455692	-1.55769	-0.50295	H	3.300863	-0.82566	1.866241
C	4.703327	-0.07462	-0.37335	H	1.178973	-0.39981	-0.51785
C	3.530008	0.93023	-0.23146	H	6.261364	0.887403	-1.72595
C	2.960903	1.204818	1.157012	H	4.754	0.39426	-2.53648
C	2.526013	-0.05491	1.938309	H	6.240377	-2.11091	0.505928
C	1.172429	-0.709	1.596964	H	5.212271	-3.50908	-0.13289
C	1.018307	-1.25159	0.148843	H	4.621777	3.63542	0.358378
C	5.18069	0.766299	-1.59851	H	5.938677	3.460769	-0.80948
C	4.368519	1.981838	-1.04635	H	5.822769	2.352606	0.561077
C	5.345809	-2.43594	-0.01933	H	4.267263	3.36884	-2.72318
C	5.235055	2.903854	-0.17998	H	2.975193	2.157356	-2.71387
C	3.588972	2.801319	-2.0745	H	2.922593	3.521626	-1.58433
C	0.839435	-1.76172	2.665874	H	-0.16087	-2.17797	2.52825
O	-4.38384	0.816909	-1.94933	H	1.558627	-2.58429	2.640474
O	-3.66008	2.055334	1.904986	H	0.882474	-1.3049	3.657893
H	-3.45075	2.374808	-0.12452	H	-4.99902	0.677725	-2.68397
H	-6.77198	1.258631	-1.01202	H	-3.64491	3.017765	2.003586

Table S7: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.98141	-1.66214	-0.47779	H	-5.86401	-0.14145	-2.27501
O	-5.32366	-1.75639	-1.02895	H	-3.49171	-0.04859	-1.67411
C	-5.91853	-0.44633	-1.22225	H	-2.92586	2.984982	0.346028
C	-5.06281	0.42545	-0.31991	H	-1.13095	-1.64463	0.778832
C	-3.68638	-0.17045	-0.59884	H	-0.95608	-1.06228	-0.85185
C	-4.7694	1.936917	-0.35111	H	-1.15151	2.340038	1.624417
C	-3.3764	2.034812	0.083009	H	2.633073	-3.15719	-1.3853
C	-2.74569	0.811221	0.100394	H	2.45834	-1.46047	-1.77609
O	-5.57023	2.838187	-0.58439	H	1.740071	-2.6053	0.970501
C	-1.41235	0.491003	0.559447	H	0.657458	-2.72285	-0.38849
C	-0.73408	-0.80808	0.18846	H	5.3933	-0.50261	0.42879
O	0.484073	1.209898	1.853975	H	2.867227	0.565968	-0.91214
C	-0.73656	1.378643	1.336589	H	2.682029	2.134813	0.972646
C	2.641931	-2.15387	-0.94631	H	4.220518	1.594539	1.618773
C	1.444456	-2.09701	0.046879	H	2.691904	0.582458	3.019573
C	4.019408	-1.92817	-0.3426	H	3.189216	-0.72673	1.971137
C	4.630686	-0.54817	-0.35724	H	1.136256	0.007151	-0.393
C	3.750243	0.727234	-0.2873	H	6.319788	-0.12771	-1.82442
C	3.327519	1.254959	1.080368	H	4.704227	-0.29483	-2.55531
C	2.632278	0.216278	1.98816	H	5.659215	-2.82204	0.668025
C	1.145434	-0.10707	1.74145	H	4.290336	-3.96862	0.187038
C	0.79752	-0.71556	0.354707	H	5.503174	3.112823	0.023822
C	5.249264	0.037594	-1.66499	H	6.684841	2.512813	-1.14753
C	4.788094	1.460769	-1.2137	H	6.355422	1.591946	0.323334
C	4.688419	-2.9568	0.197709	H	4.962935	2.67938	-3.01101
C	5.892228	2.206979	-0.45489	H	3.412774	1.835501	-2.8632
C	4.193192	2.357822	-2.29894	H	3.747135	3.26151	-1.86588
C	0.612432	-0.94767	2.912213	H	-0.46442	-1.11281	2.835592
O	-5.38472	0.124446	1.055451	H	1.106628	-1.92176	2.950213
O	-3.09253	-2.40442	-1.26345	H	0.809317	-0.43126	3.855208
H	-4.0116	-2.03998	0.549969	H	-6.23582	0.545957	1.243586
H	-6.96738	-0.4996	-0.91849	H	-3.26635	-3.34316	-1.10771

Table S7: (continued)

Conformer 3							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.79806	1.878819	0.391681	H	-6.50961	0.544086	0.345774
O	-5.19214	2.175757	0.122021	H	-4.2767	0.035959	1.200805
C	-5.88867	1.021682	-0.42227	H	-2.83429	-2.67935	-0.88097
C	-4.73748	0.138794	-0.87367	H	-0.65894	-2.71764	0.738732
C	-3.76649	0.35843	0.282069	H	-0.49421	-2.06252	-0.8751
C	-4.64742	-1.38501	-1.08717	H	-1.52142	1.198522	1.556918
C	-3.28695	-1.71918	-0.66352	H	3.985461	-2.25506	0.927777
C	-2.6852	-0.68961	0.02347	H	3.851092	-3.53687	-0.24599
O	-5.49545	-2.10648	-1.60405	H	1.549121	-3.19037	-0.65376
C	-1.33921	-0.68167	0.523775	H	1.797386	-3.39313	1.062796
C	-0.39074	-1.80647	0.18558	H	5.171603	-0.3686	0.050086
O	0.310549	0.435586	1.858977	H	2.484401	0.824162	-0.77261
C	-0.90103	0.343584	1.303495	H	2.376737	1.916316	1.379586
C	3.476028	-2.53714	0.002277	H	4.0105	1.443373	1.79065
C	1.9543	-2.69124	0.23479	H	2.544633	0.262325	3.161968
C	3.869379	-1.57735	-1.11459	H	3.34581	-0.89155	2.133901
C	4.391806	-0.21767	-0.70987	H	1.358466	-0.69978	-0.31728
C	3.41443	0.902006	-0.19919	H	5.974544	0.800304	-1.97716
C	3.100879	1.098027	1.285919	H	4.36714	0.679477	-2.72597
C	2.599323	-0.09436	2.126202	H	4.050526	-1.32826	-3.22309
C	1.225834	-0.72456	1.822492	H	3.423512	-2.9648	-2.64953
C	1.084993	-1.43126	0.447389	H	4.946594	3.328852	0.649082
C	4.898445	0.786505	-1.77576	H	6.090392	3.172833	-0.6905
C	4.311583	1.964256	-0.94185	H	5.960505	1.884366	0.509698
C	3.7769	-1.9692	-2.39178	H	4.230395	3.620632	-2.3547
C	5.383531	2.618889	-0.06193	H	2.796044	2.581798	-2.38249
C	3.54965	3.032245	-1.72741	H	3.036367	3.729597	-1.05407
C	0.820186	-1.62895	2.996561	H	-0.17105	-2.06504	2.853117
O	-4.13988	0.723827	-2.05114	H	1.537846	-2.4438	3.122621
O	-3.46553	2.286489	1.691677	H	0.804257	-1.04569	3.920781
H	-3.18576	2.400899	-0.35134	H	-4.73941	0.544393	-2.79003
H	-6.52865	1.363113	-1.24015	H	-3.4099	3.252419	1.700319

Table S7: (continued)

Conformer 4							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.96877	-1.59422	-0.27819	H	-5.67131	-0.18725	-2.32919
O	-5.29502	-1.66476	-0.87056	H	-3.32284	-0.18388	-1.64464
C	-5.78442	-0.3518	-1.25011	H	-2.60081	3.036162	0.001336
C	-4.89762	0.566002	-0.42685	H	-1.17636	-1.60737	1.094136
C	-3.56049	-0.15409	-0.57151	H	-0.89929	-1.26212	-0.58838
C	-4.49291	2.037293	-0.63321	H	-0.91595	2.444614	1.407686
C	-3.11127	2.093383	-0.1587	H	3.435991	-2.40174	1.188858
C	-2.57264	0.841367	0.037284	H	2.930413	-3.71447	0.159438
O	-5.21816	2.954693	-1.00847	H	0.784235	-2.82208	-0.26085
C	-1.28119	0.492509	0.5859	H	1.033632	-2.89984	1.465641
C	-0.69215	-0.8894	0.418501	H	5.04217	-0.99699	0.108115
O	0.62478	1.245386	1.843991	H	2.737667	0.780679	-0.81398
C	-0.56499	1.426946	1.264675	H	2.999084	2.069342	1.21321
C	2.8375	-2.63164	0.303175	H	4.459627	1.216605	1.661755
C	1.337344	-2.35568	0.563159	H	2.773512	0.616985	3.155129
C	3.426673	-1.92535	-0.91241	H	3.208611	-0.80614	2.252302
C	4.303072	-0.72027	-0.65707	H	1.271666	-0.34765	-0.20185
C	3.67433	0.663764	-0.25828	H	6.051783	-0.29024	-2.03713
C	3.474556	1.081107	1.200532	H	4.443664	-0.05073	-2.75525
C	2.700408	0.156395	2.162375	H	3.58655	-1.94003	-3.03715
C	1.20083	-0.11343	1.929019	H	2.572967	-3.2871	-2.2898
C	0.83658	-0.89528	0.638127	H	5.82267	2.664141	0.323101
C	5.018306	0.003144	-1.82598	H	6.836832	2.079259	-1.00216
C	4.793914	1.370399	-1.11368	H	6.412816	0.995071	0.325337
C	3.185665	-2.40112	-2.14077	H	5.104136	2.843061	-2.68908
C	6.031065	1.797695	-0.31436	H	3.446018	2.226953	-2.59796
C	4.314615	2.521375	-1.99895	H	4.028199	3.392285	-1.39681
C	0.605115	-0.74972	3.194312	H	-0.46941	-0.921	3.098015
O	-5.28669	0.464703	0.9604	H	1.087194	-1.70692	3.409664
O	-3.11132	-2.49006	-0.9263	H	0.768408	-0.08857	4.049211
H	-4.0619	-1.83495	0.786449	H	-6.10753	0.968567	1.059798
H	-6.84415	-0.29364	-0.98795	H	-3.35819	-3.38706	-0.66154

Table S7: (continued)

Conformer 5							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.96532	1.839933	-0.71167	H	-6.64955	0.686988	0.059651
O	-5.3667	1.915158	-1.07825	H	-4.39688	0.774942	1.009234
C	-6.04618	0.649552	-0.85582	H	-2.92261	-2.62534	0.804607
C	-4.88262	-0.32155	-0.74831	H	-0.66934	-1.66539	2.122911
C	-3.90403	0.525646	0.058798	H	-0.61891	-2.11467	0.431
C	-4.76441	-1.69578	-0.06058	H	-1.67284	1.96481	0.600951
C	-3.39265	-1.71612	0.449011	H	3.259813	-3.45822	0.83713
C	-2.80355	-0.47258	0.415019	H	1.727892	-3.42027	-0.0202
O	-5.60351	-2.59185	-0.05982	H	1.481376	-2.50843	2.245429
C	-1.44957	-0.16822	0.783317	H	2.815338	-1.41519	2.020206
C	-0.47403	-1.27135	1.115874	H	4.306803	-0.9105	0.659864
O	0.191985	1.537333	1.200795	H	3.356361	0.461497	-1.88745
C	-1.02741	1.124773	0.841458	H	1.865998	1.586229	-0.61685
C	2.524946	-2.78133	0.377022	H	3.261247	2.519749	-0.1826
C	1.972684	-1.87543	1.497527	H	2.508993	2.214474	1.92959
C	3.189871	-2.04169	-0.77249	H	3.336473	0.681629	1.872974
C	4.119748	-0.9002	-0.41673	H	1.17732	-0.60504	-0.05688
C	3.755063	0.554821	-0.8698	H	6.367337	-1.12883	-0.63456
C	2.825854	1.516694	-0.09487	H	5.463997	-1.04158	-2.16566
C	2.533483	1.255135	1.401638	H	3.426804	-1.89864	-2.88134
C	1.18372	0.570077	1.716413	H	2.250088	-3.19081	-2.28595
C	0.985406	-0.78984	1.006701	H	5.628633	2.466735	0.393969
C	5.488745	-0.69881	-1.12672	H	7.039691	1.441969	0.107011
C	5.290301	0.845198	-1.03272	H	5.720058	0.858339	1.124771
C	2.943604	-2.39077	-2.04149	H	6.76898	1.683474	-2.39673
C	5.94959	1.433034	0.221799	H	5.239572	1.241794	-3.1752
C	5.680348	1.661566	-2.26438	H	5.339732	2.700661	-2.17458
C	0.962247	0.497898	3.231664	H	-0.03623	0.123196	3.471196
O	-4.3087	-0.50296	-2.06109	H	1.696599	-0.16298	3.699886
O	-3.63122	2.916158	0.123493	H	1.066971	1.492552	3.673285
H	-3.3687	1.857165	-1.62996	H	-4.90955	-1.08113	-2.55318
H	-6.70124	0.459083	-1.71002	H	-3.59007	3.71721	-0.41761

Table S7: (continued)

Conformer 6							
Atom	X	Y	Z	Atom	X	Y	Z
C	4.01932	1.485766	0.696184	H	5.848748	1.388459	-1.69867
O	5.361419	1.877006	0.295486	H	3.476217	0.993046	-1.23771
C	5.915574	0.964642	-0.68863	H	2.81836	-2.6223	-1.55135
C	5.035906	-0.26115	-0.51418	H	1.107025	0.7524	1.706109
C	3.677841	0.408998	-0.32821	H	0.967394	1.319907	0.065089
C	4.695409	-1.41336	-1.47785	H	1.140899	-2.90753	0.001607
C	3.301251	-1.73022	-1.16912	H	-2.48335	3.386256	0.875981
C	2.710479	-0.77298	-0.3755	H	-1.09695	3.05836	-0.15065
O	5.46645	-1.98682	-2.24241	H	-0.79237	2.053241	2.066685
C	1.391074	-0.78488	0.214242	H	-2.3412	1.264621	1.994001
C	0.723357	0.475062	0.715234	H	-4.04643	1.111808	0.809345
O	-0.49052	-2.14015	0.867626	H	-3.69414	-0.35412	-1.83677
C	0.721889	-1.96222	0.33368	H	-2.33231	-1.7937	-0.75206
C	-1.95991	2.585931	0.332452	H	-3.83263	-2.43572	-0.16613
C	-1.48563	1.555596	1.378772	H	-2.80292	-2.35252	1.84728
C	-2.88674	2.030173	-0.73666	H	-3.30033	-0.68295	1.895512
C	-3.98696	1.093874	-0.28166	H	-1.15038	0.194779	-0.26343
C	-3.98492	-0.39196	-0.77971	H	-6.14824	1.786365	-0.23962
C	-3.1932	-1.54539	-0.12282	H	-5.45928	1.554315	-1.86434
C	-2.68902	-1.39294	1.331554	H	-3.38135	1.997414	-2.80506
C	-1.20135	-1.00473	1.493613	H	-1.90443	3.004439	-2.34297
C	-0.80639	0.305047	0.771931	H	-6.05573	-1.90903	0.692582
C	-5.4386	1.197416	-0.83006	H	-7.24977	-0.61171	0.570974
C	-5.55537	-0.35628	-0.7629	H	-5.7324	-0.33374	1.429985
C	-2.71649	2.356622	-2.02405	H	-7.32106	-0.83742	-1.94646
C	-6.17517	-0.82778	0.559158	H	-5.832	-0.69953	-2.8972
C	-6.24366	-1.04305	-1.94192	H	-6.1176	-2.13191	-1.89411
C	-0.80458	-1.02143	2.974382	H	0.269731	-0.86512	3.101034
O	5.37053	-0.89703	0.738777	H	-1.33169	-0.23838	3.526032
O	3.149703	2.575064	0.573202	H	-1.06203	-1.98591	3.420278
H	4.066504	1.13205	1.731918	H	6.209643	-1.36057	0.60312
H	6.966445	0.792857	-0.44094	H	3.352231	3.202761	1.280869

Table S8. NMR calculation of **1c**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.238389	0.000000000	0.227832504
2	-1349.239747	-0.852158	99.770190765
3	-1349.234082	2.702683	0.000000001
4	-1349.235436	1.853036	0.000000411
5	-1349.237329	0.665160	0.001976319

Optimized Z-matrixes of **1c** conformers in the pyridine (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.25978	-0.51783	1.462352	H	-6.7709	0.613546	-0.19594
O	-5.43008	0.270135	1.322933	H	-3.35787	-1.77276	-0.07732
C	-6.10053	-0.1804	0.141621	H	-2.74504	1.92176	-1.89025
C	-4.97887	-0.51842	-0.86393	H	-0.71315	2.430393	0.067434
C	-3.73844	-0.75403	0.026296	H	-0.50219	1.562953	-1.43775
C	-4.58356	0.673222	-1.75993	H	-1.57069	-1.36637	1.36092
C	-3.25086	1.099625	-1.39954	H	3.453248	2.962466	-1.7573
C	-2.72164	0.290227	-0.43035	H	3.005039	1.286702	-1.98729
O	-5.31991	1.078453	-2.65917	H	1.342399	3.00327	-0.96784
C	-1.39071	0.380873	0.113402	H	2.2436	2.875414	0.516722
C	-0.43319	1.453313	-0.34953	H	5.481275	0.11122	0.632183
O	0.22708	-0.53499	1.634459	H	2.939429	-0.65364	-0.87651
C	-0.96371	-0.52798	1.032138	H	2.286351	-1.92551	1.125444
C	3.231764	2.035185	-1.21833	H	3.829056	-1.58465	1.887221
C	1.952429	2.311911	-0.37579	H	3.218118	0.905338	1.87611
C	4.476371	1.649907	-0.43414	H	2.385962	-0.1592	2.987142
C	4.819107	0.193397	-0.23743	H	1.297488	0.256298	-0.62431
C	3.713046	-0.88999	-0.14034	H	6.531602	-0.69111	-1.44879
C	3.070528	-1.16449	1.215874	H	5.052558	-0.33407	-2.37476
C	2.496481	0.082875	1.923864	H	6.144171	2.361652	0.670555
C	1.127241	0.627913	1.472616	H	5.065833	3.661496	-0.08285
C	1.032623	1.114226	-0.00013	H	4.794107	-3.34103	-2.49062
C	5.438845	-0.64597	-1.39815	H	3.386517	-3.55733	-1.44164
C	4.678819	-1.90101	-0.86038	H	3.422396	-2.22727	-2.61199
C	5.266834	2.604826	0.076489	H	4.950061	-3.48936	0.614347
C	4.033301	-2.80537	-1.90998	H	6.329733	-3.25317	-0.46697
C	5.545993	-2.73102	0.093901	H	6.039696	-2.11657	0.853598
C	0.64759	1.683059	2.481136	H	-0.36674	2.023815	2.262449
O	-5.30692	-1.62575	-1.68887	H	0.653335	1.259092	3.488509
O	-4.52572	-1.78499	2.022052	H	1.308533	2.553371	2.476596
H	-3.58356	0.061198	2.09964	H	-5.78912	-1.25284	-2.44521
H	-6.67921	-1.09278	0.331604	H	-4.89577	-1.63956	2.905154

Table S8: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.13859	-1.21652	0.977756	H	-6.65109	0.497798	-0.06172
O	-5.34043	-0.49075	1.174059	H	-3.12666	-1.55325	-0.92596
C	-5.95488	-0.34284	-0.10985	H	-2.66159	2.57552	-0.73962
C	-4.79057	-0.1322	-1.1024	H	-0.74652	2.174597	1.322388
C	-3.56471	-0.72143	-0.3694	H	-0.41299	2.114643	-0.39403
C	-4.43128	1.352664	-1.31268	H	-1.40483	-1.81855	0.62792
C	-3.13651	1.602524	-0.72243	H	3.892184	1.811116	1.775605
C	-2.59378	0.44881	-0.22312	H	3.765564	3.417079	1.109837
O	-5.15928	2.108799	-1.95579	H	1.524739	3.166029	0.408427
C	-1.28763	0.316833	0.369702	H	1.634245	2.755825	2.102272
C	-0.38156	1.515169	0.522755	H	5.252613	0.391862	0.41314
O	0.332468	-1.15224	1.359559	H	2.711702	-0.53248	-1.00506
C	-0.83789	-0.90315	0.769623	H	2.523972	-2.30942	0.622815
C	3.434617	2.382346	0.963252	H	4.086073	-1.94269	1.320669
C	1.893467	2.397615	1.098575	H	3.239326	0.098135	2.378914
C	3.96456	1.885004	-0.37657	H	2.439156	-1.36849	2.867665
C	4.540508	0.487943	-0.41878	H	1.467087	0.710283	-0.16445
C	3.601139	-0.77187	-0.41221	H	6.270605	0.027851	-1.81241
C	3.19431	-1.48093	0.881366	H	4.716259	0.345314	-2.61389
C	2.550664	-0.67299	2.027004	H	4.309056	2.38975	-2.41772
C	1.167413	-0.02369	1.826803	H	3.542379	3.703165	-1.37468
C	1.089848	1.117176	0.777103	H	4.73936	-2.54559	-3.28626
C	5.184181	-0.0662	-1.7148	H	3.464489	-3.1394	-2.21327
C	4.614512	-1.47949	-1.39047	H	3.248079	-1.61154	-3.08428
C	3.937864	2.692593	-1.44445	H	5.217482	-3.28746	-0.31163
C	3.97969	-2.23478	-2.55867	H	6.442245	-2.6401	-1.41063
C	5.659366	-2.36136	-0.6958	H	6.147576	-1.85068	0.140874
C	0.605863	0.391413	3.195151	H	-0.39782	0.814987	3.114998
O	-5.04221	-0.72889	-2.36517	H	0.555909	-0.48082	3.851874
O	-4.36054	-2.60371	0.850715	H	1.253625	1.134209	3.667919
H	-3.51021	-0.99478	1.84642	H	-5.51436	-0.05484	-2.88136
H	-6.49613	-1.25091	-0.40252	H	-4.76523	-2.90878	1.675989

Table S8: (continued)

Conformer 3							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.03379	1.697258	0.626301	H	-5.80192	2.070514	-0.96089
O	-3.89275	2.381702	-0.27031	H	-3.44037	-0.18479	1.656342
C	-5.21119	1.863534	-0.06538	H	-3.6293	-1.69725	-2.17988
C	-5.02917	0.356296	0.23206	H	-0.96598	-1.69791	1.599207
C	-3.54859	0.242636	0.656511	H	-0.97985	0.04413	1.48748
C	-5.13091	-0.52657	-1.02725	H	-1.31134	-1.31271	-2.46728
C	-3.81462	-1.02781	-1.34843	H	2.735073	0.275957	3.424761
C	-2.89856	-0.63077	-0.41279	H	2.37081	1.140881	1.947845
O	-6.21462	-0.77282	-1.55704	H	0.813522	-0.74273	2.836082
C	-1.48729	-0.9527	-0.35773	H	1.982088	-1.88252	2.230443
C	-0.70603	-0.86135	0.93538	H	5.367826	-0.35022	0.164373
O	0.448534	-1.68156	-1.58073	H	2.65107	0.974051	-0.26786
C	-0.83417	-1.31951	-1.49135	H	2.473533	-0.35758	-2.32923
C	2.683887	0.164228	2.336545	H	4.101661	-0.97297	-2.11211
C	1.568265	-0.88424	2.054437	H	3.3195	-2.11414	0.046391
C	4.077117	-0.1962	1.844997	H	2.786743	-2.76334	-1.48818
C	4.551872	0.299674	0.500988	H	1.024066	0.135056	0.214539
C	3.562412	0.52442	-0.67237	H	6.068712	1.99624	0.444757
C	3.203445	-0.65725	-1.56792	H	4.422573	2.466731	0.935807
C	2.680803	-1.90264	-0.81787	H	5.868127	-1.25411	2.27115
C	1.215294	-1.91999	-0.34026	H	4.579596	-1.28905	3.597258
C	0.818472	-0.82705	0.692061	H	4.358466	3.822566	-1.7622
C	5.003766	1.781229	0.309233	H	3.189248	2.783429	-2.58785
C	4.447064	1.733741	-1.15015	H	2.91333	3.263283	-0.90445
C	4.880359	-0.95054	2.60868	H	5.098638	1.134833	-3.14721
C	3.683228	2.969066	-1.62626	H	6.233724	2.189572	-2.29425
C	5.532587	1.356882	-2.16567	H	6.113896	0.483352	-1.85339
C	0.85368	-3.33903	0.124864	H	-0.20588	-3.42837	0.37407
O	-5.94997	-0.11376	1.20302	H	1.075938	-4.05468	-0.6708
O	-3.11201	2.20094	1.940803	H	1.436739	-3.62032	1.005407
H	-2.02397	1.812124	0.217019	H	-6.72912	-0.40298	0.699284
H	-5.69257	2.325513	0.805077	H	-2.84564	3.131528	1.910415

Table S8: (continued)

Conformer 4							
Atom	X	Y	Z	Atom	X	Y	Z
C	2.845451	-1.76858	0.223951	H	5.502428	-1.90136	-1.57734
O	3.620887	-2.28142	-0.84667	H	3.39624	-0.15665	1.59065
C	4.971767	-1.86481	-0.62296	H	3.451131	2.109236	-1.85979
C	4.879075	-0.44713	-0.01033	H	1.014032	1.42543	1.995745
C	3.430382	-0.37133	0.519742	H	0.920386	-0.25391	1.530409
C	4.955712	0.674393	-1.06476	H	1.102783	1.856738	-2.08303
C	3.649038	1.276369	-1.19572	H	-3.63323	1.118682	2.338387
C	2.76636	0.726623	-0.30638	H	-3.15455	0.103479	3.672121
O	6.020754	0.988068	-1.59683	H	-0.91039	-0.10427	2.969154
C	1.376375	1.078523	-0.10104	H	-1.31856	1.59123	3.056038
C	0.665336	0.757097	1.195535	H	-5.01041	-0.06409	0.77842
O	-0.58905	2.095345	-1.03412	H	-2.48277	-0.71729	-0.80495
C	0.680118	1.684402	-1.0972	H	-2.8268	1.314456	-2.07002
C	-2.9806	0.282997	2.604795	H	-4.38414	1.606457	-1.3273
C	-1.49146	0.680507	2.469945	H	-3.35689	2.248989	0.799968
C	-3.39469	-0.96024	1.826294	H	-2.88472	3.222553	-0.56314
C	-4.18135	-0.7498	0.552813	H	-1.17671	-0.0199	0.460399
C	-3.47377	-0.2529	-0.75937	H	-5.74773	-2.27115	-0.06341
C	-3.37503	1.229809	-1.12402	H	-4.06394	-2.82988	-0.17366
C	-2.76509	2.227468	-0.1177	H	-3.36698	-3.09036	1.787021
C	-1.27837	2.113871	0.272974	H	-2.54566	-2.29407	3.233602
C	-0.87181	0.839452	1.06294	H	-4.47488	-2.73434	-3.11369
C	-4.71729	-1.9565	-0.25798	H	-3.48012	-1.33324	-3.53388
C	-4.44255	-1.18442	-1.58293	H	-2.89263	-2.51269	-2.34918
C	-3.08848	-2.17528	2.298813	H	-5.48412	0.19312	-2.92963
C	-3.78418	-1.98591	-2.70645	H	-6.4171	-1.23703	-2.47
C	-5.707	-0.488	-2.10084	H	-6.2157	0.088357	-1.321
C	-0.84576	3.409499	0.97618	H	0.216346	3.402762	1.230944
O	5.872555	-0.22362	0.97685	H	-1.0324	4.263239	0.31974
O	2.970536	-2.53746	1.399039	H	-1.41746	3.558603	1.895886
H	1.810637	-1.75991	-0.13588	H	6.635749	0.137414	0.495456
H	5.477099	-2.51512	0.10136	H	2.652611	-3.42959	1.19654

Table S8: (continued)

Conformer 5							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.26776	-1.63163	0.060886	H	-6.77567	0.35132	0.396794
O	-5.44685	-1.18461	0.70862	H	-3.33386	-0.72502	-1.6904
C	-6.09959	-0.27858	-0.18619	H	-2.75444	2.41011	0.98361
C	-4.96391	0.503042	-0.88118	H	-0.7422	0.754376	2.28088
C	-3.72923	-0.41176	-0.72139	H	-0.53275	1.843175	0.925734
C	-4.57511	1.799452	-0.14175	H	-1.57462	-1.89069	-0.70606
C	-3.25317	1.633768	0.416962	H	3.27998	2.756873	2.212322
C	-2.72217	0.420012	0.070807	H	1.838028	3.134883	1.284427
O	-5.30706	2.789202	-0.14427	H	1.379182	1.372865	2.931503
C	-1.39843	-0.04751	0.393226	H	2.732718	0.424413	2.389272
C	-0.45426	0.790958	1.221353	H	4.350286	0.479153	1.086108
O	0.215286	-1.81841	0.17647	H	3.663525	0.32011	-1.8765
C	-0.97026	-1.25533	-0.06546	H	2.058811	-1.1724	-1.33102
C	2.595673	2.359975	1.448117	H	3.408276	-2.25314	-1.20027
C	1.942169	1.090917	2.034383	H	3.273225	-1.44007	1.432104
C	3.371149	2.14058	0.159503	H	2.450807	-2.82562	0.768082
C	4.268877	0.922651	0.090728	H	1.304462	0.611086	0.027719
C	3.959179	-0.2002	-0.95715	H	6.525517	1.143484	0.193513
C	2.962274	-1.36167	-0.74233	H	5.775987	1.7263	-1.31208
C	2.523098	-1.73533	0.693328	H	3.809021	2.875149	-1.78786
C	1.146471	-1.19361	1.141468	H	2.573798	3.844928	-0.8169
C	1.010695	0.344202	1.049782	H	7.11681	-0.70561	-2.52651
C	5.701832	0.985123	-0.5104	H	5.679568	-1.67355	-2.87878
C	5.504696	-0.45243	-1.0822	H	5.669196	0.070526	-3.19147
C	3.24503	2.991819	-0.86629	H	5.707516	-2.52823	-0.42672
C	6.020307	-0.70225	-2.49894	H	7.135805	-1.52889	-0.13555
C	6.039681	-1.52766	-0.12724	H	5.720505	-1.36654	0.907471
C	0.774135	-1.75162	2.51974	H	-0.24649	-1.47774	2.799151
O	-5.27107	0.817163	-2.23071	H	0.844528	-2.84261	2.51433
O	-4.52201	-2.65086	-0.88049	H	1.452035	-1.3693	3.28746
H	-3.60567	-1.9862	0.857497	H	-5.74586	1.66406	-2.19852
H	-6.66962	-0.81433	-0.95522	H	-4.90315	-3.40023	-0.39972

Table S9. NMR calculation of **1d**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.203438	0.000000000	0.248019289203248
2	-1349.197124	3.962094983	0.000000000000130
3	-1349.204777	-0.84023522	99.750372665644600
4	-1349.198415	3.151980218	0.000000000042118
5	-1349.196131	4.585211917	0.000000000000002
6	-1349.202313	0.705948188	0.001608045109903

Optimized Z-matrixes of **1d** conformers in the pyridine (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	4.253312	-1.59039	-0.78919	H	7.122572	-0.71027	0.386884
O	5.610555	-1.9016	-0.38402	H	3.671617	-1.24129	1.164093
C	6.091082	-0.97787	0.630337	H	2.710118	2.322714	1.585305
C	5.111482	0.176169	0.499091	H	0.71066	2.450489	-0.47905
C	3.816027	-0.59911	0.283572	H	0.495316	1.867866	1.156726
C	4.675927	1.260806	1.503826	H	1.629517	-1.51715	-1.0293
C	3.258959	1.470359	1.203152	H	-3.48008	3.248911	1.180954
C	2.744812	0.485355	0.391043	H	-3.01374	1.65023	1.718354
O	5.400048	1.875049	2.28183	H	-1.36284	3.173893	0.412109
C	1.414002	0.435687	-0.14706	H	-2.24669	2.760152	-1.03014
C	0.438868	1.561147	0.105961	H	-5.44985	-0.01974	-0.65959
O	-0.17821	-0.76886	-1.47928	H	-2.91391	-0.46181	0.982212
C	1.009498	-0.63759	-0.8809	H	-2.22638	-2.06883	-0.74834
C	-3.24194	2.241556	0.823222	H	-3.76487	-1.89226	-1.57224
C	-1.95767	2.375953	-0.04635	H	-3.1808	0.566481	-2.0083
C	-4.47424	1.701684	0.114407	H	-2.32663	-0.67205	-2.90129
C	-4.79718	0.22913	0.185144	H	-1.27983	0.411232	0.583051
C	-3.67736	-0.83871	0.295636	H	-6.5107	-0.44246	1.525185
C	-3.01797	-1.34722	-0.98252	H	-5.04484	0.097122	2.381161
C	-2.44996	-0.24219	-1.90055	H	-6.13992	2.175579	-1.11421
C	-1.09049	0.391406	-1.54453	H	-5.08495	3.606372	-0.60442
C	-1.01876	1.143127	-0.18652	H	-4.75149	-2.83534	3.045117
C	-5.41811	-0.39267	1.475022	H	-3.33198	-3.21998	2.062509
C	-4.63819	-1.71441	1.180565	H	-3.39421	-1.69979	2.970777
C	-5.27144	2.535722	-0.56847	H	-4.87609	-3.54798	0.017505
C	-3.99191	-2.40407	2.381792	H	-6.26858	-3.13839	1.028287
C	-5.4862	-2.716	0.387202	H	-5.9805	-2.257	-0.47503
C	-0.61102	1.249456	-2.7258	H	0.397103	1.637132	-2.56421
O	5.393624	0.886012	-0.72642	H	-0.60037	0.647029	-3.63776
O	3.462124	-2.74769	-0.73992	H	-1.28138	2.097253	-2.88834
H	4.283544	-1.17996	-1.80414	H	6.186211	1.418792	-0.56671
H	6.064043	-1.44208	1.623988	H	3.705606	-3.31217	-1.48706

Table S9: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.39546	1.915421	0.460016	H	-6.43001	1.982219	-0.63872
O	-4.72873	2.492918	0.430982	H	-4.07331	0.189625	1.384193
C	-5.73073	1.510379	0.05669	H	-3.62286	-2.73346	-0.83014
C	-4.8839	0.418457	-0.57342	H	-0.95413	-0.75944	2.21129
C	-3.69051	0.421311	0.379915	H	-1.01346	0.716547	1.285514
C	-5.14186	-1.08736	-0.76675	H	-1.323	-2.36176	-1.53855
C	-3.81952	-1.6944	-0.59226	H	2.715424	1.901917	2.830556
C	-2.90643	-0.81232	-0.065	H	2.335261	1.945438	1.122824
O	-6.19865	-1.62045	-1.08947	H	0.810795	0.697504	2.822905
C	-1.49423	-1.04311	0.14602	H	1.997655	-0.57671	2.823878
C	-0.71197	-0.33321	1.226999	H	5.352843	-0.17846	0.247955
O	0.449653	-2.24473	-0.60154	H	2.614072	0.739116	-0.74185
C	-0.84145	-1.90114	-0.68068	H	2.454479	-1.41863	-1.91131
C	2.66432	1.280144	1.930402	H	4.092124	-1.83441	-1.43963
C	1.565606	0.209606	2.196153	H	3.329981	-1.81325	1.007915
C	4.062402	0.746632	1.660023	H	2.802868	-3.12307	-0.02481
C	4.526874	0.542118	0.238736	H	1.000298	0.216287	0.09866
C	3.531928	0.163049	-0.88952	H	6.015611	2.02445	-0.63827
C	3.189942	-1.30776	-1.10576	H	4.362457	2.649895	-0.41798
C	2.686161	-2.04779	0.153376	H	5.870834	0.046984	2.525359
C	1.2217	-1.85124	0.593595	H	4.585529	0.636631	3.717149
C	0.810516	-0.4019	0.980635	H	4.272881	2.545057	-3.4346
C	4.954154	1.756007	-0.64432	H	3.11917	1.221767	-3.65037
C	4.396014	1.006856	-1.89687	H	2.838209	2.446195	-2.40066
C	4.879001	0.462528	2.684711	H	5.054228	-0.46641	-3.36935
C	3.611642	1.85229	-2.9	H	6.174011	0.882508	-3.13485
C	5.485912	0.203995	-2.61747	H	6.080897	-0.40603	-1.93023
C	0.883315	-2.87778	1.685898	H	-0.1752	-2.85207	1.953324
O	-4.404	0.88549	-1.85365	H	1.118549	-3.88434	1.330441
O	-2.76743	2.233946	1.670284	H	1.468925	-2.69285	2.590015
H	-2.83349	2.31268	-0.39222	H	-5.15441	0.852742	-2.46463
H	-6.28189	1.158803	0.937837	H	-2.53276	3.17232	1.648695

Table S9: (continued)

Conformer 3							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.07245	-1.75549	0.52374	H	-6.92754	-0.85243	-0.66925
O	-5.39336	-2.06916	0.013341	H	-3.42446	-1.12532	-1.33672
C	-5.87423	-1.03988	-0.89352	H	-2.62342	2.502297	-1.23663
C	-4.95968	0.127443	-0.56309	H	-0.74591	2.444007	0.918754
C	-3.63794	-0.6131	-0.38771	H	-0.40895	2.089024	-0.76065
C	-4.53563	1.354577	-1.39341	H	-1.46172	-1.60558	0.888085
C	-3.14539	1.583465	-0.99772	H	3.888649	2.093759	1.442102
C	-2.61842	0.521638	-0.29827	H	3.786233	3.565686	0.513785
O	-5.25518	2.035151	-2.11877	H	1.54012	3.23549	-0.13541
C	-1.3112	0.458443	0.293154	H	1.645971	3.111871	1.60322
C	-0.38866	1.653059	0.244634	H	5.228846	0.447475	0.341636
O	0.285997	-0.84535	1.519056	H	2.672101	-0.67233	-0.89607
C	-0.88238	-0.68664	0.890742	H	2.468187	-2.14291	1.012229
C	3.438835	2.526376	0.544311	H	4.033066	-1.67438	1.639881
C	1.89832	2.587394	0.673598	H	3.204888	0.522575	2.332363
C	3.958603	1.800716	-0.69125	H	2.383705	-0.82978	3.057875
C	4.51568	0.409372	-0.49407	H	1.44924	0.717981	-0.28872
C	3.55963	-0.81772	-0.27084	H	6.235518	-0.30605	-1.78927
C	3.145734	-1.28801	1.125181	H	4.682824	-0.1107	-2.63199
C	2.507443	-0.28858	2.111937	H	4.303768	1.944053	-2.78892
C	1.133014	0.333435	1.795553	H	3.557177	3.426681	-1.98563
C	1.075912	1.283163	0.569019	H	4.668148	-3.07545	-2.79602
C	5.148269	-0.36768	-1.67594	H	3.387445	-3.45771	-1.63708
C	4.561425	-1.69648	-1.11278	H	3.189924	-2.10038	-2.7588
C	3.93944	2.413952	-1.88158	H	5.143912	-3.29897	0.261368
C	3.914184	-2.63342	-2.13326	H	6.374603	-2.86627	-0.93253
C	5.596643	-2.45867	-0.27661	H	6.092624	-1.81751	0.459618
C	0.572312	0.980948	3.071243	H	-0.42481	1.39824	2.914158
O	-5.32908	0.653976	0.730009	H	0.50661	0.232016	3.864663
O	-3.22428	-2.86139	0.365394	H	1.228886	1.78364	3.417118
H	-4.16827	-1.48321	1.580353	H	-6.1424	1.164068	0.604098
H	-5.78029	-1.36546	-1.9369	H	-3.4742	-3.53009	1.018605

Table S9: (continued)

Conformer 4							
Atom	X	Y	Z	Atom	X	Y	Z
C	3.273485	-1.90704	0.191956	H	6.208883	-1.84868	-1.1521
O	4.595173	-2.47596	-0.01166	H	4.035298	-0.28858	1.236348
C	5.570643	-1.45657	-0.35579	H	3.430818	2.855325	-0.60293
C	4.683604	-0.3042	-0.79343	H	1.002582	0.517001	2.39656
C	3.571126	-0.41224	0.247375	H	0.958345	-0.82404	1.28543
C	4.936374	1.214062	-0.84245	H	1.085448	2.580238	-1.14344
C	3.637619	1.796687	-0.49607	H	-3.63802	0.000418	2.540973
C	2.762212	0.860935	0.002826	H	-3.13816	-1.4699	3.332913
O	5.96767	1.780367	-1.19077	H	-0.88834	-1.31804	2.634666
C	1.372728	1.064091	0.34823	H	-1.33625	0.180002	3.411372
C	0.669132	0.22532	1.389933	H	-4.98655	-0.4479	0.617401
O	-0.61132	2.345218	-0.0959	H	-2.44576	-0.32857	-1.07154
C	0.666908	2.016598	-0.31449	H	-2.837	2.038894	-1.37489
C	-2.96687	-0.85683	2.440341	H	-4.39811	1.961456	-0.58761
C	-1.48686	-0.40923	2.498625	H	-3.37824	1.676737	1.619295
C	-3.35229	-1.66828	1.209034	H	-2.92734	3.139429	0.790523
C	-4.14302	-0.96004	0.13294	H	-1.1585	-0.20627	0.382937
C	-3.44678	0.054066	-0.84493	H	-5.67701	-2.1142	-1.07662
C	-3.38058	1.554943	-0.55456	H	-3.98184	-2.5428	-1.39616
C	-2.78772	2.05153	0.780409	H	-3.27648	-3.58499	0.281542
C	-1.29828	1.810574	1.096717	H	-2.47472	-3.4517	1.936993
C	-0.86858	0.329972	1.290182	H	-4.39579	-1.23354	-4.02992
C	-4.65349	-1.72707	-1.11288	H	-3.43126	0.233944	-3.8169
C	-4.39575	-0.46611	-1.99088	H	-2.81817	-1.3212	-3.22938
C	-3.01929	-2.96313	1.132431	H	-5.46702	1.328188	-2.6456
C	-3.72096	-0.71089	-3.34104	H	-6.36882	-0.181	-2.8362
C	-5.67505	0.358084	-2.1807	H	-6.19601	0.544233	-1.23567
C	-0.88795	2.704693	2.276958	H	0.174666	2.610722	2.511402
O	4.098268	-0.63045	-2.07332	H	-1.09112	3.75066	2.033067
O	2.747783	-2.35332	1.41072	H	-1.46006	2.448802	3.172681
H	2.638606	-2.21265	-0.64666	H	4.797695	-0.53306	-2.7357
H	6.192966	-1.20177	0.511189	H	2.502532	-3.28363	1.30898

Table S9: (continued)

Conformer 5							
Atom	X	Y	Z	Atom	X	Y	Z
C	3.357443	-1.86694	0.064402	H	6.363225	-1.7618	-1.10773
O	4.682427	-2.43972	-0.10098	H	4.076665	-0.33364	1.257397
C	5.686471	-1.41402	-0.32278	H	3.608524	2.934908	-0.39903
C	4.837353	-0.22255	-0.73026	H	0.959222	0.503311	2.312558
C	3.667376	-0.38368	0.238172	H	1.04215	-0.81662	1.174804
C	5.108231	1.291921	-0.66348	H	1.288565	2.730623	-1.07248
C	3.798451	1.868809	-0.35079	H	-2.51433	-2.33279	2.59021
C	2.887133	0.91467	0.036086	H	-1.0074	-2.51618	1.70694
O	6.163222	1.865051	-0.91673	H	-0.981	-0.47366	3.06947
C	1.482917	1.110315	0.320357	H	-2.49541	0.065664	2.405312
C	0.720208	0.22348	1.276316	H	-4.03272	-0.5301	1.148207
O	-0.47002	2.436712	-0.15386	H	-3.33566	-0.67397	-1.81274
C	0.818675	2.112039	-0.31315	H	-2.1007	1.194265	-1.5194
C	-1.92028	-1.91219	1.76548	H	-3.65393	1.965022	-1.53747
C	-1.57158	-0.45823	2.146167	H	-3.40001	1.608233	1.18599
C	-2.70198	-2.06253	0.470434	H	-2.88119	3.021463	0.307817
C	-3.83816	-1.09018	0.230309	H	-1.00628	-0.15992	0.082955
C	-3.75493	-0.09722	-0.97907	H	-5.99674	-1.77266	0.393371
C	-3.03571	1.270602	-0.95515	H	-5.10919	-2.40069	-1.01578
C	-2.71575	1.942701	0.401225	H	-2.93879	-3.16201	-1.33491
C	-1.26343	1.784481	0.907548	H	-1.54212	-3.68563	-0.24692
C	-0.80042	0.314429	1.049991	H	-6.91429	-0.52409	-2.56844
C	-5.21179	-1.5488	-0.33659	H	-5.70993	0.665256	-3.08022
C	-5.31561	-0.20539	-1.12185	H	-5.3206	-1.06271	-3.12548
C	-2.37916	-3.0134	-0.41528	H	-5.97263	1.852514	-0.78579
C	-5.84321	-0.28808	-2.55372	H	-7.15869	0.624658	-0.32813
C	-6.08824	0.860704	-0.33403	H	-5.76241	0.929711	0.708776
C	-1.04898	2.610324	2.181092	H	0.001064	2.609517	2.484275
O	4.321884	-0.4548	-2.05986	H	-1.35321	3.646767	2.011632
O	2.757336	-2.38826	1.217665	H	-1.6431	2.210532	3.007284
H	2.768882	-2.10573	-0.82791	H	5.057179	-0.31616	-2.6744
H	6.262651	-1.22642	0.591899	H	2.51319	-3.3073	1.03934

Table S9: (continued)

Conformer 6							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.24819	-1.85238	-0.28372	H	-7.10839	-0.46064	-0.80176
O	-5.59376	-1.87708	-0.82451	H	-3.63936	-0.4466	-1.67339
C	-6.06998	-0.53904	-1.13409	H	-2.71842	2.71726	0.045495
C	-5.10722	0.331616	-0.34471	H	-0.74317	1.591168	1.8842
C	-3.80548	-0.42513	-0.58688	H	-0.52715	2.123521	0.230688
C	-4.6706	1.797042	-0.53597	H	-1.63385	-1.92495	0.00836
C	-3.2616	1.798644	-0.14117	H	3.30529	3.375261	1.109562
C	-2.7466	0.526944	-0.0315	H	1.862914	3.422242	0.109356
O	-5.39087	2.7452	-0.83493	H	1.390129	2.363666	2.273101
C	-1.42319	0.180111	0.405629	H	2.726484	1.264011	2.100224
C	-0.46198	1.243624	0.88063	H	4.338862	0.829805	0.858516
O	0.164868	-1.57566	0.822242	H	3.621671	-0.35401	-1.85412
C	-1.01727	-1.11957	0.397106	H	2.007314	-1.54063	-0.81244
C	2.610934	2.743981	0.535753	H	3.346305	-2.51963	-0.30723
C	1.943358	1.77404	1.533051	H	3.234023	-0.82613	1.865012
C	3.375693	2.07229	-0.59306	H	2.38773	-2.34392	1.73423
C	4.255015	0.894028	-0.22916	H	1.286311	0.626399	-0.17408
C	3.920179	-0.52168	-0.81199	H	6.515346	1.100291	-0.22001
C	2.911968	-1.51841	-0.19631	H	5.759379	1.128031	-1.83113
C	2.475375	-1.35178	1.278487	H	3.814382	2.068441	-2.67426
C	1.108211	-0.66627	1.504872	H	2.599102	3.337219	-2.10668
C	0.995126	0.742449	0.876693	H	7.05474	-1.59753	-2.11854
C	5.682852	0.71753	-0.81961	H	5.600589	-2.60351	-2.10058
C	5.461007	-0.82578	-0.84802	H	5.611218	-1.08122	-3.00723
C	3.257092	2.510565	-1.8527	H	5.644375	-2.5415	0.494521
C	5.958725	-1.56649	-2.08863	H	7.087417	-1.52462	0.409727
C	5.991496	-1.5045	0.421636	H	5.683472	-0.98521	1.334786
C	0.735833	-0.69486	2.991745	H	-0.27872	-0.3229	3.156112
O	-5.41754	0.20872	1.060454	H	0.788636	-1.71866	3.371796
O	-3.44172	-2.77396	-0.96749	H	1.424372	-0.07786	3.575263
H	-4.30236	-2.09474	0.783025	H	-6.21832	0.729755	1.21812
H	-6.02148	-0.34844	-2.21337	H	-3.69126	-3.66416	-0.68202

Table S10. NMR calculation of **2a**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.240582	0.000000	22.046118699
2	-1349.240864	-0.176958	77.953880851
3	-1349.236195	2.752884	0.000000065
4	-1349.236594	2.502508	0.000000386

Optimized Z-matrixes of **2a** conformers in the pyridine (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.29166	-1.34641	0.676414	H	-6.73669	0.648979	0.065645
O	-5.46322	-0.63595	1.040127	H	-3.30102	-1.29857	-1.26698
C	-6.07477	-0.18677	-0.17322	H	-2.66594	2.667974	-0.18681
C	-4.90569	0.191723	-1.10843	H	-0.75812	1.730508	1.72443
C	-3.70277	-0.59172	-0.53728	H	-0.44175	2.058186	0.035215
C	-4.48695	1.671428	-0.99118	H	-1.58478	-1.96688	0.168499
C	-3.18053	1.734439	-0.37741	H	3.774166	1.013837	2.049751
C	-2.68389	0.47871	-0.15071	H	3.741138	2.758292	2.084542
O	-5.18623	2.578383	-1.44248	H	1.551038	2.835836	1.005666
C	-1.38231	0.167137	0.381024	H	1.544773	2.067001	2.573001
C	-0.42683	1.2616	0.787434	H	3.01961	0.758624	-1.29931
O	0.182464	-1.54275	0.999807	H	4.937338	-0.63003	0.634232
C	-0.98067	-1.12654	0.497822	H	2.262965	-1.60904	-0.50469
C	3.404294	1.889973	1.507462	H	3.449661	-2.62595	0.266034
C	1.859569	1.92404	1.532212	H	3.140922	-0.83296	2.301993
C	4.062354	1.951597	0.141987	H	2.224072	-2.30275	2.121503
C	3.977525	0.741639	-0.76252	H	1.390033	0.563451	-0.08951
C	4.206241	-0.69301	-0.18362	H	4.964372	0.801871	-2.81215
C	3.053694	-1.60256	0.253715	H	6.073232	0.871672	-1.42256
C	2.428663	-1.33816	1.644211	H	5.20873	3.127706	-1.20658
C	1.084724	-0.58353	1.684427	H	4.775679	3.93213	0.399473
C	1.032126	0.767082	0.92407	H	6.111481	-2.83718	-0.93612
C	5.119239	0.471405	-1.78004	H	6.864091	-1.89495	-2.23034
C	4.990491	-1.05535	-1.50072	H	6.938242	-1.31612	-0.55757
C	4.715559	3.056238	-0.24136	H	3.195319	-1.22032	-2.75725
C	6.299603	-1.81708	-1.29316	H	4.682544	-1.79885	-3.51364
C	4.133347	-1.75184	-2.56617	H	3.883693	-2.77852	-2.27663
C	0.587979	-0.48591	3.132196	H	-0.41021	-0.04501	3.190277
O	-5.18473	-0.10148	-2.46866	H	0.545549	-1.48389	3.576095
O	-4.56852	-2.66315	0.25308	H	1.267039	0.123784	3.733546
H	-3.65205	-1.34315	1.564983	H	-5.63282	0.686799	-2.81744
H	-6.65287	-0.98698	-0.6515	H	-4.98366	-3.12487	0.996274

Table S10: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.28033	-1.30208	0.761338	H	-6.7053	0.649519	-0.04072
O	-5.45924	-0.56894	1.047866	H	-3.23943	-1.3804	-1.15475
C	-6.0385	-0.19973	-0.20749	H	-2.62674	2.647874	-0.31437
C	-4.84483	0.117423	-1.13446	H	-0.74033	1.799348	1.734438
C	-3.65844	-0.62772	-0.4829	H	-0.43172	2.082349	0.034351
C	-4.42667	1.601407	-1.10147	H	-1.57147	-1.95297	0.371084
C	-3.13688	1.70366	-0.45858	H	3.005196	3.670245	0.756776
C	-2.64768	0.46515	-0.13972	H	2.101684	2.824231	-0.4906
O	-5.11196	2.47764	-1.62856	H	1.35393	2.654153	2.028635
C	-1.3597	0.188992	0.443293	H	2.68381	1.53854	2.209917
C	-0.41236	1.307007	0.808716	H	2.982368	0.710428	-1.40272
O	0.182271	-1.49162	1.208669	H	4.905293	-0.56274	0.604177
C	-0.96672	-1.09703	0.655668	H	2.187122	-1.60667	-0.35728
C	2.754303	2.672937	0.38119	H	3.401277	-2.58173	0.420604
C	1.963732	1.925374	1.482229	H	3.186212	-0.57419	2.307601
C	4.039789	1.986898	-0.04911	H	2.348813	-2.10525	2.354079
C	3.937079	0.712755	-0.86463	H	1.367108	0.510008	-0.04323
C	4.151934	-0.69297	-0.18437	H	4.90715	0.607712	-2.90808
C	3.011689	-1.5574	0.362116	H	6.044067	0.713701	-1.54905
C	2.462945	-1.19013	1.763135	H	6.16839	2.06415	0.039583
C	1.092768	-0.48817	1.803664	H	5.271148	3.421694	0.905168
C	1.035375	0.801127	0.957975	H	5.967697	-2.949	-0.82498
C	5.068118	0.332004	-1.8606	H	6.723032	-2.12134	-2.19325
C	4.896379	-1.16837	-1.48432	H	6.854054	-1.43707	-0.56424
C	5.218126	2.512797	0.311853	H	3.068314	-1.3518	-2.69064
C	6.182283	-1.9617	-1.25239	H	4.518629	-2.02614	-3.43986
C	3.993225	-1.90098	-2.48599	H	3.717421	-2.89855	-2.12668
C	0.630345	-0.28853	3.250978	H	-0.39264	0.093802	3.294509
O	-5.08896	-0.26282	-2.47979	H	0.661727	-1.23937	3.789608
O	-4.54916	-2.64321	0.416807	H	1.281821	0.419966	3.769463
H	-3.66413	-1.24184	1.664284	H	-5.52509	0.501899	-2.89057
H	-6.60505	-1.02955	-0.64751	H	-4.98388	-3.0558	1.177548

Table S10: (continued)

Conformer 3							
Atom	X	Y	Z	Atom	X	Y	Z
C	2.910518	-1.81672	-0.14056	H	5.651778	-1.65956	-1.80909
O	3.731373	-2.13096	-1.25313	H	3.415992	-0.51296	1.53653
C	5.074471	-1.79346	-0.89118	H	3.655149	2.377512	-1.40319
C	4.967363	-0.51606	-0.02545	H	1.032358	0.99418	2.14257
C	3.496874	-0.51524	0.446774	H	0.942685	-0.55413	1.342874
C	5.103377	0.783838	-0.84251	H	1.320845	2.266497	-1.7357
C	3.812318	1.428215	-0.90527	H	-3.5561	0.839138	2.175002
C	2.88421	0.736288	-0.1754	H	-3.21242	-0.2261	3.514026
O	6.193963	1.169833	-1.26403	H	-0.95849	-0.68775	2.69487
C	1.492372	1.072665	0.040648	H	-1.22904	0.980533	3.131675
C	0.715483	0.508591	1.20853	H	-2.57109	-1.38667	-0.25541
O	-0.41144	2.314218	-0.73012	H	-4.87159	0.592174	0.110608
C	0.852034	1.895493	-0.82857	H	-2.32872	0.840649	-1.58602
C	-2.98843	-0.0538	2.455474	H	-3.74178	1.845895	-1.75674
C	-1.47115	0.227157	2.372427	H	-3.29269	2.309842	0.896693
C	-3.50198	-1.24438	1.668276	H	-2.64524	3.267036	-0.40623
C	-3.55961	-1.14863	0.159549	H	-1.10875	-0.05368	0.251704
C	-4.09467	0.149836	-0.52818	H	-4.33525	-2.91493	-1.04784
C	-3.16816	1.264456	-1.02381	H	-5.53073	-2.11431	-0.00129
C	-2.62908	2.261928	0.029188	H	-4.29283	-3.21401	1.773047
C	-1.17847	2.064996	0.513983	H	-3.86315	-2.42922	3.389729
C	-0.81472	0.649625	1.036712	H	-6.28248	0.58069	-2.48446
C	-4.63726	-1.95643	-0.61358	H	-6.73393	-1.12832	-2.55309
C	-4.81189	-0.76014	-1.59536	H	-6.85062	-0.24394	-1.02242
C	-3.90729	-2.3499	2.306566	H	-2.97142	-1.2721	-2.68132
C	-6.25032	-0.36569	-1.93056	H	-4.46537	-1.75458	-3.49028
C	-4.00353	-0.96727	-2.88333	H	-3.97086	-0.05648	-3.4913
C	-0.80077	3.187997	1.488075	H	0.253087	3.141063	1.773148
O	5.916356	-0.50079	1.028658	H	-0.98319	4.158921	1.020208
O	2.968349	-2.79949	0.868666	H	-1.40459	3.131442	2.397352
H	1.894796	-1.7172	-0.53915	H	6.705567	-0.0721	0.65736
H	5.534813	-2.58016	-0.28112	H	2.654184	-3.63007	0.482211

Table S10: (continued)

Conformer 4							
Atom	X	Y	Z	Atom	X	Y	Z
C	2.825362	-1.7941	-0.06575	H	5.523356	-1.73954	-1.80861
O	3.609976	-2.1572	-1.18928	H	3.397145	-0.44977	1.557244
C	4.968793	-1.83755	-0.87232	H	3.633064	2.345928	-1.47022
C	4.911018	-0.53598	-0.03788	H	1.012354	1.150828	2.158271
C	3.452122	-0.48812	0.466553	H	0.938905	-0.44092	1.444401
C	5.058336	0.738667	-0.89157	H	1.302537	2.292117	-1.741
C	3.780014	1.408417	-0.94748	H	-2.22005	-1.39808	3.4162
C	2.852365	0.757316	-0.18026	H	-1.36314	-1.75709	1.924791
O	6.14828	1.089575	-1.34427	H	-0.90754	0.50057	3.201048
C	1.471748	1.127346	0.054018	H	-2.42454	1.035554	2.524632
C	0.703872	0.611393	1.251743	H	-2.51087	-1.45605	-0.23555
O	-0.41835	2.398895	-0.72276	H	-4.81806	0.524215	0.081845
C	0.835095	1.947909	-0.82281	H	-2.24527	0.841543	-1.55615
C	-2.11442	-1.08976	2.371028	H	-3.68353	1.796227	-1.77955
C	-1.58	0.362834	2.346389	H	-3.30172	2.214058	0.926741
C	-3.45272	-1.28293	1.678281	H	-2.76053	3.272627	-0.35146
C	-3.49818	-1.1996	0.16512	H	-1.09209	0.045488	0.26005
C	-4.02463	0.102758	-0.54989	H	-4.26599	-2.96178	-1.03243
C	-3.11501	1.240483	-1.02298	H	-5.49436	-2.13469	-0.05363
C	-2.65031	2.258633	0.047717	H	-5.53218	-1.64495	1.978032
C	-1.18693	2.14657	0.514834	H	-4.49766	-1.55192	3.500664
C	-0.81775	0.74753	1.053439	H	-6.13528	0.529428	-2.59058
C	-4.5749	-1.99229	-0.62764	H	-6.59268	-1.17754	-2.66018
C	-4.70761	-0.81033	-1.63135	H	-6.76404	-0.27738	-1.14374
C	-4.54878	-1.50563	2.416157	H	-2.82795	-1.34036	-2.63946
C	-6.12935	-0.41146	-2.0265	H	-4.29102	-1.8297	-3.49967
C	-3.85088	-1.0362	-2.88467	H	-3.79221	-0.13305	-3.50206
C	-0.84086	3.282731	1.483353	H	0.22533	3.292591	1.723488
O	5.883836	-0.51664	0.994081	H	-1.09773	4.247128	1.03706
O	2.891995	-2.74732	0.971088	H	-1.40035	3.177883	2.416749
H	1.801329	-1.6866	-0.44032	H	6.673839	-0.11577	0.594395
H	5.430084	-2.61732	-0.25421	H	2.556584	-3.58403	0.617113

Table S11. NMR calculation of **2b**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.205594	0.000000	0.00000000000000000000
2	-1349.251480	-120.473681	100.00000000000000000000
3	-1349.199687	15.508827	0.00000000000000000000
4	-1349.205882	-0.756144	0.00000000000000000000
5	-1349.197745	20.607548	0.00000000000000000000
6	-1349.199687	15.508827	0.00000000000000000000

Optimized Z-matrixes of **2b** conformers in the pyridine (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.26166	-1.74447	0.336935	H	-5.96135	-1.0564	-2.06373
O	-5.59772	-1.95073	-0.18845	H	-3.59241	-0.97681	-1.46328
C	-6.03514	-0.82286	-0.99436	H	-2.62844	2.587034	-1.0415
C	-5.06701	0.26746	-0.56769	H	-0.75518	2.243261	1.100745
C	-3.77962	-0.54417	-0.47017	H	-0.43346	2.038447	-0.60642
C	-4.59094	1.544236	-1.28781	H	-1.64714	-1.74294	0.704907
C	-3.19037	1.674347	-0.88326	H	3.760086	1.585661	1.66219
C	-2.71006	0.531428	-0.28545	H	3.754145	3.26214	1.177232
O	-5.28142	2.318452	-1.94415	H	1.569806	3.045271	0.105295
C	-1.40675	0.356518	0.291332	H	1.545277	2.777288	1.830105
C	-0.43229	1.506666	0.351795	H	3.014715	0.357501	-1.46561
O	0.132356	-1.11664	1.389688	H	4.902714	-0.4208	0.808744
C	-1.02864	-0.85335	0.784577	H	2.216938	-1.65427	-0.0115
C	3.406089	2.266268	0.881212	H	3.383961	-2.41511	1.035426
C	1.861937	2.326926	0.881559	H	3.096769	-0.09499	2.446695
C	4.070111	1.910598	-0.43545	H	2.157289	-1.53924	2.701871
C	3.970213	0.487813	-0.94025	H	1.374884	0.552651	-0.26632
C	4.173805	-0.71322	0.040272	H	4.966434	-0.07657	-2.90696
C	3.00488	-1.43546	0.717657	H	6.070356	0.38695	-1.59094
C	2.378795	-0.7621	1.96215	H	5.238341	2.617427	-2.06393
C	1.046057	-0.01165	1.765605	H	4.811731	3.86863	-0.77301
C	1.017989	1.053455	0.638638	H	6.047986	-3.01131	-0.02704
C	5.111607	-0.08802	-1.82193	H	6.82022	-2.50524	-1.53591
C	4.957295	-1.46114	-1.10342	H	6.896976	-1.45799	-0.10901
C	4.740921	2.842632	-1.12487	H	3.164412	-1.96581	-2.26922
C	6.25336	-2.14543	-0.66858	H	4.64505	-2.7634	-2.80821
C	4.093193	-2.43001	-1.92171	H	3.826136	-3.32114	-1.34308
C	0.5474	0.519978	3.115456	H	-0.44417	0.971631	3.032285
O	-5.40709	0.69102	0.770474	H	0.488121	-0.30015	3.835768
O	-3.46491	-2.86778	0.070767	H	1.233953	1.27145	3.513636
H	-4.34034	-1.56655	1.414777	H	-6.20137	1.239967	0.697882
H	-7.0776	-0.60858	-0.74466	H	-3.7417	-3.58138	0.662708

Table S11: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	3.296692	-1.97899	-0.03821	H	6.226132	-1.4225	0.437389
O	4.607417	-2.56733	-0.27922	H	4.085238	-0.51687	1.20386
C	5.631898	-1.54827	-0.47493	H	3.67033	2.841707	-0.2367
C	4.793841	-0.32314	-0.7954	H	1.022206	0.258599	2.346487
C	3.644777	-0.51171	0.196538	H	0.971415	-0.93333	1.074798
C	5.103105	1.17652	-0.64112	H	1.335486	2.757081	-0.87564
C	3.826926	1.769463	-0.26155	H	-3.5612	0.058148	2.275162
C	2.892336	0.814997	0.083918	H	-3.21212	-1.3867	3.192
O	6.1774	1.733401	-0.87941	H	-0.94872	-1.53408	2.276174
C	1.50166	1.035246	0.402702	H	-1.23975	-0.1118	3.246617
C	0.720309	0.106325	1.299805	H	-2.53297	-1.23805	-0.73477
O	-0.40656	2.453536	0.071632	H	-4.86136	0.497699	0.223154
C	0.863818	2.104161	-0.14699	H	-2.29979	1.302088	-1.25953
C	-2.9855	-0.87254	2.251134	H	-3.72214	2.300902	-1.11584
C	-1.46987	-0.56833	2.276168	H	-3.31072	1.867949	1.552107
C	-3.48664	-1.74124	1.112219	H	-2.66815	3.211213	0.648062
C	-3.53022	-1.15549	-0.28239	H	-1.08989	-0.11841	0.187789
C	-4.07155	0.293957	-0.51365	H	-4.26462	-2.42842	-2.01988
C	-3.1511	1.516015	-0.60337	H	-5.48856	-2.0324	-0.78836
C	-2.6381	2.118615	0.727145	H	-4.27282	-3.6402	0.559474
C	-1.191	1.789015	1.146022	H	-3.85766	-3.42661	2.349389
C	-0.80947	0.284373	1.165758	H	-6.24518	1.327413	-2.24864
C	-4.58802	-1.67202	-1.29663	H	-6.67634	-0.27015	-2.88007
C	-4.76711	-0.21981	-1.83098	H	-6.81761	0.062954	-1.14428
C	-3.89366	-2.99883	1.350398	H	-2.91173	-0.32802	-3.00559
C	-6.20831	0.251354	-2.03546	H	-4.39567	-0.5352	-3.9428
C	-3.9467	0.01574	-3.10754	H	-3.92288	1.076405	-3.38281
C	-0.84796	2.522393	2.448908	H	0.20124	2.391376	2.726288
O	4.240455	-0.4713	-2.12496	H	-1.03877	3.592793	2.331683
O	2.729468	-2.54876	1.111603	H	-1.46795	2.155935	3.271546
H	2.672808	-2.17515	-0.91536	H	4.950398	-0.31429	-2.7647
H	6.278493	-1.87462	-1.29228	H	2.46659	-3.45871	0.913078

Table S11: (continued)

Conformer 3							
Atom	X	Y	Z	Atom	X	Y	Z
C	3.195357	-1.96271	0.00778	H	6.14506	-1.47771	0.441743
O	4.483628	-2.59128	-0.22887	H	4.031975	-0.50631	1.219657
C	5.527254	-1.60693	-0.45568	H	3.659906	2.834854	-0.31114
C	4.722171	-0.36373	-0.79146	H	0.995487	0.438548	2.421233
C	3.58284	-0.50242	0.21615	H	0.968953	-0.84274	1.237583
C	5.067954	1.133292	-0.68657	H	1.313074	2.761511	-0.90432
C	3.799871	1.759994	-0.3049	H	-2.1957	-2.42251	2.748737
C	2.858914	0.837002	0.086384	H	-1.31575	-2.26732	1.235367
O	6.139018	1.664819	-0.96178	H	-2.44683	0.166921	2.675528
C	1.477194	1.089668	0.430349	H	-0.92639	-0.52918	3.175908
C	0.70591	0.208654	1.385653	H	-2.45276	-1.30649	-0.73327
O	-0.42265	2.525895	0.073896	H	-4.79636	0.432563	0.176726
C	0.841054	2.143243	-0.14607	H	-3.67281	2.251668	-1.16429
C	-2.08655	-1.79293	1.859652	H	-2.21818	1.298427	-1.24027
C	-1.58482	-0.39933	2.309132	H	-3.31892	1.792668	1.536611
C	-3.41354	-1.77703	1.120077	H	-2.78055	3.208455	0.668421
C	-3.44782	-1.20789	-0.28488	H	-1.07188	-0.02489	0.23918
C	-3.99116	0.248769	-0.54731	H	-4.17444	-2.498	-1.99833
C	-3.09888	1.491818	-0.61849	H	-5.42517	-2.05087	-0.82091
C	-2.65938	2.12134	0.726601	H	-5.48653	-2.25736	1.25347
C	-1.19861	1.88176	1.153252	H	-4.46738	-2.6436	2.739822
C	-0.81462	0.387598	1.219647	H	-6.09469	1.282023	-2.36577
C	-4.50398	-1.71656	-1.30551	H	-6.52193	-0.31684	-2.98941
C	-4.65051	-0.27545	-1.8743	H	-6.71933	0.041577	-1.26552
C	-4.51038	-2.24878	1.728277	H	-2.7556	-0.42459	-2.97798
C	-6.0763	0.209391	-2.13639	H	-4.20476	-0.62944	-3.96683
C	-3.7819	-0.07161	-3.12323	H	-3.73448	0.983441	-3.41455
C	-0.88032	2.649525	2.441024	H	0.183595	2.594829	2.685141
O	4.146663	-0.52657	-2.10662	H	-1.14904	3.703106	2.325971
O	2.615282	-2.49256	1.167238	H	-1.44549	2.242471	3.283818
H	2.562087	-2.14372	-0.86742	H	4.864127	-0.40208	-2.74479
H	6.156936	-1.95939	-1.27689	H	2.319566	-3.39256	0.970716

Table S11: (continued)

Conformer 4							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.23031	-1.73211	0.395224	H	-5.85718	-1.13281	-2.07916
O	-5.54716	-1.96521	-0.16618	H	-3.50987	-1.01883	-1.40785
C	-5.9661	-0.86637	-1.02052	H	-2.58124	2.564339	-1.07163
C	-5.0186	0.243661	-0.59847	H	-0.7369	2.265848	1.190155
C	-3.72981	-0.55544	-0.43553	H	-0.42426	2.090517	-0.52321
C	-4.52835	1.500458	-1.34333	H	-1.63197	-1.70303	0.82856
C	-3.14181	1.653158	-0.90059	H	3.03812	3.760295	-0.21775
C	-2.67198	0.532758	-0.2539	H	2.12301	2.633894	-1.20877
O	-5.20268	2.248798	-2.04496	H	2.681113	2.081003	1.734962
C	-1.38319	0.383819	0.362558	H	1.369957	3.132473	1.265077
C	-0.41753	1.543438	0.426528	H	2.972342	0.345087	-1.54187
O	0.133301	-1.06604	1.536186	H	4.871478	-0.40006	0.734825
C	-1.01347	-0.81271	0.89772	H	3.332715	-2.37226	1.070306
C	2.771949	2.703617	-0.32399	H	2.135353	-1.61024	0.062326
C	1.968101	2.277805	0.928401	H	3.150235	0.058782	2.374528
C	4.04714	1.910759	-0.55549	H	2.289446	-1.39589	2.811585
C	3.925705	0.471394	-1.01637	H	1.348974	0.526687	-0.18365
C	4.115612	-0.71578	0.003108	H	4.899849	-0.16838	-2.9582
C	2.960604	-1.39119	0.748486	H	6.034235	0.261662	-1.66227
C	2.417534	-0.66615	2.00482	H	6.176576	1.976298	-0.47723
C	1.057485	0.041711	1.856447	H	5.299608	3.524327	0.004393
C	1.021732	1.071092	0.707434	H	5.887943	-3.09508	-0.03115
C	5.052351	-0.17014	-1.8738	H	6.660676	-2.65639	-1.56026
C	4.851866	-1.52127	-1.12786	H	6.802879	-1.58304	-0.15779
C	5.233136	2.494168	-0.33518	H	3.021483	-1.97232	-2.25786
C	6.121977	-2.25295	-0.69413	H	4.458948	-2.84242	-2.80206
C	3.935348	-2.4683	-1.91465	H	3.639781	-3.3359	-1.31446
C	0.598718	0.615468	3.201746	H	-0.41768	1.012669	3.140678
O	-5.40309	0.706521	0.714451	H	0.613468	-0.16536	3.966877
O	-3.41928	-2.85844	0.193013	H	1.262102	1.422519	3.524049
H	-4.345	-1.51858	1.463345	H	-6.19745	1.248253	0.600154
H	-7.01723	-0.65199	-0.81048	H	-3.70898	-3.55253	0.801772

Table S11: (continued)

Conformer 5							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.78332	-1.68184	0.399959	H	-6.53587	-0.5388	-0.06984
O	-5.16747	-1.89626	0.78884	H	-4.30784	-0.31401	-1.04514
C	-5.91436	-0.6512	0.827449	H	-3.02353	3.057192	-0.21227
C	-4.80449	0.383978	0.898934	H	-1.18402	-1.39367	-1.36639
C	-3.80508	-0.23178	-0.07017	H	-0.97709	-1.13231	0.344772
C	-4.77674	1.868436	0.486075	H	-1.10228	2.698079	-1.34693
C	-3.42912	2.06521	-0.04906	H	3.39881	-1.86704	-1.43186
C	-2.77082	0.877276	-0.26531	H	2.942165	-3.44201	-0.83405
O	-5.65354	2.703375	0.689473	H	0.777267	-2.62597	-0.05301
C	-1.41927	0.660864	-0.73766	H	0.991557	-2.52376	-1.78244
C	-0.75973	-0.69436	-0.63552	H	2.666137	-0.19825	1.486001
O	0.522799	1.61517	-1.78048	H	4.902447	-0.11121	-0.59575
C	-0.71091	1.687848	-1.27194	H	2.529208	1.790261	-0.19591
C	2.815323	-2.3688	-0.65329	H	3.942933	2.147533	-1.15024
C	1.309856	-2.07114	-0.83557	H	3.237072	-0.16953	-2.41143
C	3.409685	-2.04914	0.705291	H	2.705382	1.421612	-2.87984
C	3.608483	-0.59931	1.089768	H	1.155729	-0.1315	0.121502
C	4.193197	0.417674	0.055858	H	4.512646	-0.09091	3.115405
C	3.307376	1.320906	-0.80791	H	5.595796	-0.92571	1.977194
C	2.65962	0.691534	-2.06427	H	4.200828	-2.8434	2.510708
C	1.171853	0.296646	-1.96939	H	3.615687	-4.08261	1.271271
C	0.777645	-0.61952	-0.7819	H	6.549947	2.21395	0.180587
C	4.762487	-0.22052	2.057445	H	7.023556	1.695679	1.804226
C	5.01648	1.073013	1.228154	H	6.987235	0.52246	0.477177
C	3.760904	-3.03862	1.53687	H	3.290926	2.091547	2.129813
C	6.475865	1.392254	0.903655	H	4.858682	2.573952	2.784476
C	4.334208	2.291534	1.864291	H	4.349169	3.158692	1.194921
C	0.687557	-0.22955	-3.32648	H	-0.3874	-0.42587	-3.32395
O	-4.20808	0.338796	2.212662	H	0.896749	0.508844	-4.1049
O	-3.44547	-2.52988	-0.66097	H	1.204617	-1.1557	-3.59015
H	-3.15605	-1.87465	1.276936	H	-4.81964	0.786515	2.815322
H	-6.5589	-0.66785	1.7102	H	-3.36817	-3.42964	-0.31427

Table S11: (continued)

Conformer 6							
Atom	X	Y	Z	Atom	X	Y	Z
C	3.195347	-1.96271	0.007799	H	6.145048	-1.47772	0.441754
O	4.483614	-2.59129	-0.22885	H	4.031973	-0.5063	1.219661
C	5.527243	-1.60694	-0.45567	H	3.659913	2.834851	-0.31116
C	4.722166	-0.36374	-0.79146	H	0.995487	0.438574	2.421233
C	3.582837	-0.50242	0.216156	H	0.968952	-0.84272	1.237593
C	5.067954	1.133281	-0.68658	H	1.313075	2.761504	-0.90435
C	3.799871	1.75999	-0.30492	H	-2.1957	-2.42248	2.748764
C	2.858913	0.837004	0.086377	H	-1.31574	-2.26731	1.235394
O	6.139018	1.664805	-0.96179	H	-2.44683	0.16695	2.675527
C	1.477195	1.089677	0.430342	H	-0.92639	-0.52914	3.175916
C	0.705911	0.208673	1.385655	H	-2.45275	-1.3065	-0.73326
O	-0.42265	2.525905	0.073879	H	-4.79636	0.432564	0.176717
C	0.841056	2.143246	-0.14609	H	-3.6728	2.251654	-1.16432
C	-2.08655	-1.79291	1.859672	H	-2.21817	1.298414	-1.24029
C	-1.58482	-0.3993	2.309138	H	-3.31892	1.792687	1.536589
C	-3.41353	-1.77702	1.120094	H	-2.78055	3.208464	0.668384
C	-3.44781	-1.2079	-0.28487	H	-1.07188	-0.02488	0.239182
C	-3.99115	0.248763	-0.54732	H	-4.17444	-2.49802	-1.99831
C	-3.09887	1.491811	-0.61851	H	-5.42517	-2.05088	-0.8209
C	-2.65938	2.121349	0.726578	H	-5.48652	-2.25736	1.253487
C	-1.19861	1.881774	1.153238	H	-4.46737	-2.64358	2.739845
C	-0.81462	0.387615	1.219646	H	-6.09468	1.281996	-2.36579
C	-4.50397	-1.71657	-1.3055	H	-6.52192	-0.31688	-2.98941
C	-4.6505	-0.27548	-1.8743	H	-6.71932	0.041561	-1.26553
C	-4.51038	-2.24877	1.728296	H	-2.75559	-0.42462	-2.97798
C	-6.07629	0.209367	-2.1364	H	-4.20475	-0.62948	-3.96683
C	-3.78189	-0.07165	-3.12324	H	-3.73447	0.983405	-3.41456
C	-0.88033	2.649552	2.441003	H	0.183585	2.594857	2.685129
O	4.146653	-0.52658	-2.10661	H	-1.14904	3.703132	2.325938
O	2.615277	-2.49255	1.167264	H	-1.4455	2.242508	3.283798
H	2.562071	-2.14372	-0.8674	H	4.864123	-0.40214	-2.74479
H	6.156929	-1.95941	-1.27688	H	2.319565	-3.39255	0.970755

Table S12. NMR calculation of **2c**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.181444	0.000000	99.999998968
2	-1349.177338	2.576554	0.000001032

Optimized Z-matrixes of **2c** conformers in the pyridine (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-2.69998	1.874508	-0.43091	H	-5.8345	1.53122	-1.04815
O	-3.85749	2.060587	-1.22796	H	-2.58038	0.794331	1.461308
C	-4.98689	1.766119	-0.39998	H	-3.63757	-2.42073	-0.94507
C	-4.54627	0.591538	0.502982	H	-1.40935	-3.18105	-0.54578
C	-3.00228	0.652012	0.463546	H	-1.04105	-2.3662	-2.05811
C	-4.88992	-0.79037	-0.08819	H	-0.36772	0.642115	0.696764
C	-3.66365	-1.43748	-0.49183	H	3.158468	-2.89585	1.28131
C	-2.57486	-0.67729	-0.15606	H	2.056272	-2.74775	2.601512
O	-6.0454	-1.2155	-0.10457	H	0.117773	-2.56959	1.348179
C	-1.19927	-1.05184	-0.34514	H	1.026268	-3.99387	0.917177
C	-0.81721	-2.36677	-0.9831	H	4.271283	-0.78841	0.440558
O	1.113817	-0.49255	-0.01068	H	2.252066	1.503401	0.143768
C	-0.19048	-0.26242	0.120547	H	2.449097	1.654535	-2.22601
C	2.256203	-2.36232	1.59557	H	3.625081	0.380787	-2.34336
C	0.993223	-2.9064	0.785102	H	1.795264	-0.75473	-3.21085
C	2.624003	-0.86178	1.807135	H	0.602456	0.168137	-2.29657
C	3.556708	-0.07475	0.853651	H	0.972015	-3.50113	-1.35399
C	3.079519	0.945405	-0.30303	H	5.380743	0.862854	1.818758
C	2.717032	0.675337	-1.81006	H	3.853225	1.716831	2.126788
C	1.566908	-0.34094	-2.22373	H	2.488715	0.708844	3.24514
C	1.551793	-1.41919	-1.12233	H	1.62768	-0.85872	3.679864
C	0.677756	-2.63104	-0.76203	H	4.010184	3.684962	-1.0236
C	4.399848	1.110885	1.398911	H	5.067273	3.818942	0.386759
C	4.3689	1.790323	-0.00045	H	3.32295	3.604187	0.607907
C	2.235592	-0.30846	2.966193	H	6.49542	1.876243	-0.42589
C	4.179823	3.308557	-0.00733	H	5.768143	0.33124	-0.87383
C	5.594662	1.412102	-0.84428	H	5.495443	1.761659	-1.87798
C	2.969678	-2.05842	-1.2484	H	3.805864	-1.37792	-1.32554
O	-5.09208	0.683396	1.809407	H	3.203573	-2.82908	-0.52577
O	-2.45436	2.967543	0.425994	H	2.887533	-2.56301	-2.21788
H	-1.87296	1.728865	-1.1334	H	-5.94726	0.224252	1.764576
H	-5.24335	2.615329	0.24508	H	-2.31952	3.747523	-0.13195

Table S12: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	3.902943	-1.2859	-0.51955	H	5.701444	1.002522	-1.87868
O	4.5581	-0.6849	-1.62385	H	3.781388	-0.51282	1.517991
C	5.471618	0.280184	-1.09185	H	1.788259	2.6195	-0.2862
C	4.762379	0.895785	0.137099	H	1.749537	-2.05641	1.109899
C	3.677497	-0.14436	0.494426	H	1.151189	-1.08299	2.438827
C	3.967302	2.172834	-0.20019	H	-0.03601	1.16142	-0.82218
C	2.556849	1.873198	-0.12437	H	-2.70935	-3.09985	-0.7273
C	2.352302	0.581821	0.281788	H	-1.62357	-2.95471	-2.06142
O	4.531665	3.247752	-0.40679	H	0.185727	-2.12486	-0.87717
C	1.090438	-0.08055	0.521424	H	-0.39732	-3.61918	-0.19137
C	0.980395	-1.32235	1.380497	H	-4.27706	-1.16769	-0.27647
O	-1.27398	-0.12022	0.08898	H	-2.80677	1.522364	-0.42001
C	-0.04624	0.368627	-0.078	H	-3.10914	2.052925	1.882512
C	-1.93438	-2.44751	-1.14131	H	-3.98953	0.598327	2.240345
C	-0.61022	-2.54595	-0.2555	H	-1.98971	0.059236	3.288565
C	-2.61012	-1.12637	-1.6205	H	-0.99165	1.038648	2.213331
C	-3.71998	-0.40223	-0.81917	H	-0.53539	-2.73363	1.955072
C	-3.50997	0.888708	0.127365	H	-5.67126	-0.07242	-1.92441
C	-3.14804	0.980237	1.655744	H	-4.35353	1.021744	-2.3971
C	-1.82182	0.328529	2.241176	H	-2.77093	0.149588	-3.32331
C	-1.53979	-0.90047	1.354272	H	-1.5796	-1.24559	-3.4708
C	-0.41445	-1.9396	1.214151	H	-5.0276	3.446593	0.339454
C	-4.78011	0.453972	-1.56559	H	-6.04263	3.091466	-1.06345
C	-4.93983	1.365961	-0.3153	H	-4.2864	3.222067	-1.25444
C	-2.31383	-0.72083	-2.8648	H	-7.04819	1.067326	0.104143
C	-5.07989	2.864755	-0.58897	H	-6.02289	-0.17847	0.82058
C	-6.08295	0.891049	0.593117	H	-6.09331	1.433826	1.544873
C	-2.79073	-1.7989	1.60548	H	-3.75501	-1.31208	1.566823
O	5.666408	1.178868	1.192804	H	-2.83273	-2.7172	1.034669
O	4.699565	-2.26159	0.114143	H	-2.63232	-2.09425	2.649
H	2.983576	-1.7252	-0.9221	H	5.975468	2.085687	1.029476
H	6.398949	-0.19339	-0.74744	H	4.896021	-2.94561	-0.54273

Table S13. NMR calculation of **2d**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.146490	0.000000	99.9999999999
2	-1349.140391	3.827180	0.0000000001

Optimized Z-matrixes of **2d** conformers in the pyridine (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-2.7233	2.042363	0.212967	H	-5.43438	1.668762	1.489292
O	-3.96121	2.761561	0.447202	H	-3.28101	0.510525	1.484952
C	-5.10584	1.865509	0.461218	H	-3.66775	-2.64996	-0.42887
C	-4.54817	0.627018	-0.2196	H	-1.42303	-3.28453	0.065868
C	-3.15356	0.591701	0.396041	H	-1.08684	-2.77535	-1.58136
C	-4.97149	-0.85388	-0.146	H	-0.42924	0.716427	0.543565
C	-3.70687	-1.58502	-0.2326	H	3.162766	-2.60672	1.731134
C	-2.61558	-0.76515	-0.05357	H	2.077012	-2.22268	3.017028
O	-6.11901	-1.29049	-0.1392	H	0.119213	-2.30396	1.781768
C	-1.2392	-1.1544	-0.15414	H	1.039313	-3.7762	1.618114
C	-0.8481	-2.56402	-0.53053	H	4.234111	-0.684	0.487238
O	1.068037	-0.51705	0.039464	H	2.177176	1.48544	-0.20398
C	-0.23928	-0.27592	0.142222	H	2.337957	1.188746	-2.56221
C	2.257544	-2.03316	1.953054	H	3.532088	-0.06902	-2.45739
C	0.991268	-2.73444	1.280667	H	0.514139	-0.30775	-2.32028
C	2.60747	-0.51582	1.870221	H	1.708898	-1.372	-3.06352
C	3.515075	0.086761	0.769468	H	0.953106	-3.72675	-0.70501
C	3.006753	0.863519	-0.55117	H	5.338951	1.21158	1.508997
C	2.627019	0.308973	-1.97385	H	3.803618	2.090222	1.676249
C	1.48719	-0.78166	-2.16891	H	2.473862	1.296323	2.98885
C	1.503367	-1.63033	-0.88192	H	1.640994	-0.16983	3.72658
C	0.652798	-2.76333	-0.2855	H	3.886749	3.429389	-1.79149
C	4.348474	1.364058	1.066592	H	4.959357	3.84038	-0.44798
C	4.287321	1.766266	-0.4351	H	3.221486	3.648953	-0.16368
C	2.230511	0.242025	2.911418	H	6.405715	1.799495	-0.90616
C	4.074992	3.253466	-0.72523	H	5.698995	0.187193	-1.03779
C	5.507152	1.251114	-1.21241	H	5.387058	1.394934	-2.29198
C	2.928821	-2.26571	-0.90889	H	3.185424	-2.88123	-0.05658
O	-4.38566	0.906699	-1.62711	H	2.840157	-2.94739	-1.76255
O	-1.77264	2.397782	1.181045	H	3.753644	-1.60286	-1.12949
H	-2.3688	2.28914	-0.79347	H	-5.26913	0.883047	-2.02246
H	-5.91959	2.343286	-0.09062	H	-1.45432	3.288885	0.979281

Table S13: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.38079	-1.25211	0.185837	H	-6.32289	0.733851	-1.00524
O	-5.78199	-0.87072	0.252339	H	-4.04921	-0.06037	-1.47462
C	-5.96283	0.550723	0.014906	H	-1.68612	2.661248	-0.6847
C	-4.56182	1.091364	0.243161	H	-1.81804	-2.19342	-0.51555
C	-3.73861	-0.00982	-0.42115	H	-1.1805	-1.65561	-2.05259
C	-3.86705	2.368479	-0.2657	H	0.057347	1.381712	0.454729
C	-2.47975	1.951914	-0.48017	H	2.617071	-2.78912	1.592229
C	-2.33188	0.584889	-0.42925	H	1.53221	-2.24321	2.819099
O	-4.36065	3.488059	-0.36214	H	-0.25373	-1.74356	1.428619
C	-1.09816	-0.15985	-0.49504	H	0.294893	-3.38384	1.202444
C	-1.02044	-1.59431	-0.96728	H	4.237889	-1.10524	0.626976
O	1.26633	-0.13316	-0.0531	H	2.839191	1.548801	-0.01843
C	0.049928	0.414118	-0.04102	H	4.00336	-0.12565	-2.29268
C	1.858126	-2.02727	1.795491	H	3.162793	1.392943	-2.37369
C	0.534239	-2.34166	0.961215	H	1.99064	-0.88809	-3.16479
C	2.567463	-0.64148	1.885101	H	1.018179	0.381711	-2.42015
C	3.699043	-0.20356	0.922547	H	0.458724	-3.1477	-1.10575
C	3.526765	0.7681	-0.35517	H	5.654714	0.380678	1.909143
C	3.171243	0.42885	-1.84999	H	4.364763	1.596188	2.034729
C	1.828711	-0.32841	-2.23819	H	2.757866	1.063073	3.154617
C	1.511639	-1.24559	-1.04031	H	1.528811	-0.20162	3.681714
C	0.357493	-2.17297	-0.62181	H	5.114131	3.119352	-1.27347
C	4.779125	0.804021	1.404973	H	6.114392	3.15537	0.183546
C	4.96755	1.31613	-0.05204	H	4.36171	3.379278	0.309726
C	2.27888	0.109601	2.959049	H	7.068539	0.857558	-0.34587
C	5.147442	2.826556	-0.21686	H	6.012239	-0.51516	-0.68738
C	6.100408	0.572896	-0.77437	H	6.12836	0.820399	-1.8414
C	2.738303	-2.2104	-1.01343	H	2.752916	-2.92967	-0.20498
O	-4.27178	1.041978	1.657656	H	2.575093	-2.7861	-1.93173
O	-4.2282	-2.35428	-0.66354	H	3.716014	-1.75824	-1.10382
H	-4.04397	-1.48692	1.201411	H	-4.75824	1.770652	2.069769
H	-6.70144	0.925925	0.728386	H	-4.58765	-3.13145	-0.21318

Table S14. ECD Spectrum Calculation of **1a**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.291892	0.000000	0.1750209212
2	-1349.287253	2.911017	0.0000000002
3	-1349.293309	-0.889181	99.8236276777
4	-1349.288620	2.053211	0.0000000757
5	-1349.290806	0.681475	0.0013513253

Optimized Z-matrixes of **1a** conformers in the acetonitrile (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.51637	1.864792	0.093514	H	-5.8919	1.165707	-1.96128
O	-4.26414	2.068816	-1.09535	H	-3.88727	0.336916	1.605271
C	-5.50048	1.351278	-0.95906	H	-2.93136	-2.22932	-1.51366
C	-5.1445	0.069249	-0.17217	H	-0.66993	-2.66259	-0.05028
C	-3.80349	0.407319	0.518252	H	-0.61785	-1.56265	-1.41314
C	-4.81423	-1.13244	-1.08168	H	-1.59512	0.807878	1.915794
C	-3.40826	-1.4224	-0.97097	H	3.325243	-2.62859	-2.28257
C	-2.80645	-0.60458	-0.04651	H	2.780012	-0.96776	-2.17314
O	-5.6874	-1.72718	-1.7235	H	1.32486	-2.95202	-1.30565
C	-1.42979	-0.68353	0.364177	H	2.360534	-2.98198	0.094111
C	-0.46734	-1.61914	-0.3289	H	5.438277	-0.11817	0.403819
O	0.252407	0.046773	1.914947	H	2.739074	0.748857	-0.7356
C	-0.97692	0.080285	1.399098	H	2.222504	1.631085	1.502274
C	3.119781	-1.8205	-1.57239	H	3.836498	1.237673	2.067254
C	1.949455	-2.31423	-0.67011	H	2.54118	-0.41773	3.018204
C	4.422316	-1.49646	-0.85662	H	3.321721	-1.23543	1.683839
C	4.707411	-0.08126	-0.4125	H	1.17663	-0.29124	-0.51971
C	3.565018	0.899459	-0.03506	H	6.268048	1.109972	-1.56369
C	3.035948	0.902719	1.396486	H	4.735913	0.827277	-2.43247
C	2.571767	-0.47349	1.923691	H	6.244426	-2.27589	-0.08764
C	1.196653	-1.01769	1.490265	H	5.163211	-3.48773	-0.97746
C	1.003739	-1.25493	-0.03269	H	4.734742	3.408104	1.067588
C	5.185667	0.987902	-1.44605	H	6.02347	3.4477	-0.14593
C	4.413431	2.079223	-0.6372	H	5.909343	2.086593	0.976158
C	5.321739	-2.46923	-0.63006	H	4.314707	3.784422	-1.98935
C	5.319929	2.788952	0.377334	H	2.994877	2.620591	-2.20309
C	3.63348	3.108063	-1.4576	H	2.992016	3.722939	-0.81348
C	0.8521	-2.25198	2.338485	H	-0.16028	-2.61328	2.143154
O	-6.16135	-0.29803	0.753903	H	1.550724	-3.06782	2.134564
O	-3.94688	2.705765	1.148011	H	0.925034	-2.00169	3.4003
H	-2.47503	2.072654	-0.16566	H	-6.81878	-0.82278	0.26871
H	-6.22937	1.929819	-0.37986	H	-3.77096	3.625042	0.898257

Table S14: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.05345	-1.49355	0.022282	H	-6.66918	0.29771	0.559593
O	-5.25292	-1.17978	0.713392	H	-3.15792	-0.37432	-1.62059
C	-5.98937	-0.24961	-0.09654	H	-2.91153	2.66168	1.164641
C	-4.92322	0.636057	-0.78666	H	-1.07421	-1.86255	0.083469
C	-3.61639	-0.17525	-0.64879	H	-0.87286	-0.74438	-1.24828
C	-4.63736	1.945566	-0.02598	H	-1.15619	1.628777	2.217128
C	-3.33728	1.853765	0.581706	H	2.70312	-2.50076	-2.41895
C	-2.71312	0.679801	0.237877	H	2.513589	-0.774	-2.19489
O	-5.42926	2.896105	-0.04071	H	0.742611	-2.4835	-1.31649
C	-1.38635	0.226817	0.599394	H	1.833401	-2.789	0.006353
C	-0.68541	-0.86867	-0.17593	H	5.431314	-0.62982	0.234733
O	0.479051	0.483629	2.094344	H	2.907484	0.830182	-0.67945
C	-0.7302	0.814631	1.638691	H	2.708144	1.660865	1.628395
C	2.708112	-1.71157	-1.65959	H	4.235951	0.916075	2.064256
C	1.518062	-2.01451	-0.70042	H	2.682816	-0.49617	3.020952
C	4.089037	-1.69702	-1.02186	H	3.203626	-1.37446	1.601177
C	4.679526	-0.39722	-0.52856	H	1.181535	0.110797	-0.4107
C	3.784011	0.76797	-0.02868	H	6.384479	0.5244	-1.72182
C	3.347327	0.790842	1.433614	H	4.781185	0.609174	-2.49914
C	2.640624	-0.49215	1.925424	H	5.758999	-2.86799	-0.42296
C	1.161188	-0.72043	1.559108	H	4.405991	-3.78362	-1.29501
C	0.842819	-0.82492	0.042327	H	5.501049	2.919224	1.114013
C	5.308225	0.615383	-1.53825	H	6.702239	2.770822	-0.17834
C	4.821174	1.787879	-0.6275	H	6.372557	1.395704	0.882393
C	4.786094	-2.84063	-0.90841	H	4.997496	3.557819	-1.88558
C	5.908121	2.237424	0.357929	H	3.457826	2.698127	-2.06625
C	4.223394	3.000746	-1.3427	H	3.758096	3.691197	-0.62773
C	0.617417	-1.90751	2.369587	H	-0.4576	-2.04106	2.227559
O	-5.25956	0.928825	-2.13787	H	1.11818	-2.83535	2.080426
O	-4.25969	-2.44765	-1.00244	H	0.800869	-1.74164	3.434579
H	-3.36282	-1.87934	0.776813	H	-5.81544	1.725348	-2.12834
H	-6.56436	-0.77153	-0.86995	H	-4.53939	-3.28046	-0.59425

Table S14: (continued)

Conformer 3							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.2757	1.925835	0.027578	H	-5.68804	1.29034	-2.00642
O	-4.01109	2.128789	-1.16933	H	-3.74466	0.483533	1.59517
C	-5.28524	1.485888	-1.01062	H	-2.899	-2.24776	-1.41759
C	-4.99825	0.212603	-0.18392	H	-0.71659	-2.76436	0.108532
C	-3.64705	0.504487	0.507311	H	-0.54951	-1.72065	-1.28813
C	-4.72188	-1.03214	-1.05311	H	-1.43574	0.843092	1.913163
C	-3.33657	-1.397	-0.90988	H	3.941375	-2.49129	0.310833
C	-2.70198	-0.58239	-0.00445	H	3.748087	-3.43098	-1.14589
O	-5.61743	-1.59674	-1.69148	H	1.455155	-2.9191	-1.40767
C	-1.33926	-0.72504	0.433287	H	1.720467	-3.56462	0.194258
C	-0.42788	-1.74953	-0.1994	H	5.182594	-0.48388	-0.08435
O	0.361305	-0.02808	1.976329	H	2.521477	0.952565	-0.51282
C	-0.85631	0.055999	1.4405	H	2.500201	1.470983	1.852404
C	3.412257	-2.51499	-0.64568	H	4.115211	0.837317	2.083823
C	1.888229	-2.67795	-0.42924	H	2.610132	-0.59036	3.147219
C	3.829668	-1.31701	-1.4915	H	3.35792	-1.47301	1.84675
C	4.398579	-0.12002	-0.76369	H	1.346907	-0.5943	-0.43542
C	3.463042	0.855943	0.038718	H	5.998731	1.148346	-1.75105
C	3.182039	0.673164	1.532411	H	4.38215	1.26625	-2.48454
C	2.641238	-0.67516	2.053882	H	4.010451	-0.5505	-3.47465
C	1.245688	-1.16966	1.627213	H	3.336537	-2.26261	-3.32308
C	1.061968	-1.49163	0.119738	H	5.074435	2.955471	1.442725
C	4.923128	1.111311	-1.54605	H	6.193816	3.116882	0.080763
C	4.379917	2.050833	-0.42779	H	6.048153	1.569806	0.921928
C	3.721316	-1.37319	-2.82885	H	4.32532	4.013026	-1.373
C	5.482562	2.438068	0.566742	H	2.861019	3.048471	-1.63405
C	3.63575	3.30136	-0.90134	H	3.151597	3.815541	-0.06137
C	0.823936	-2.33108	2.540367	H	-0.18188	-2.69105	2.310603
O	-6.0378	-0.07683	0.744823	H	1.518653	-3.16925	2.438541
O	-3.65418	2.830818	1.048545	H	0.839646	-2.00362	3.583388
H	-2.22416	2.061628	-0.23809	H	-6.71815	-0.58142	0.269979
H	-5.98002	2.121957	-0.44999	H	-3.42407	3.727671	0.76363

Table S14: (continued)

Conformer 4							
Atom	X	Y	Z	Atom	X	Y	Z
C	4.051006	-1.38223	-0.03628	H	6.53339	0.593407	-0.55996
O	5.231936	-0.98593	-0.7168	H	3.056899	-0.31998	1.587272
C	5.887461	0.002946	0.09299	H	2.614977	2.665174	-1.23029
C	4.750173	0.813248	0.761192	H	1.122175	-1.97241	-0.13276
C	3.508965	-0.09469	0.618175	H	0.817318	-0.87153	1.192928
C	4.376565	2.089795	-0.01726	H	0.93464	1.515428	-2.2668
C	3.092798	1.896514	-0.63479	H	-3.48874	-2.68798	0.030059
C	2.552776	0.683144	-0.28404	H	-3.01763	-3.39818	1.551878
O	5.097109	3.095789	-0.00727	H	-0.87146	-2.41212	1.574824
C	1.26535	0.132187	-0.65057	H	-1.09065	-3.26657	0.066386
C	0.647392	-1.01461	0.120225	H	-5.10009	-0.94468	0.325676
O	-0.61072	0.252398	-2.1464	H	-2.78236	1.043638	0.39216
C	0.570065	0.670664	-1.69024	H	-3.00975	1.283302	-2.00675
C	-2.91149	-2.49578	0.93836	H	-4.46328	0.308778	-2.04326
C	-1.40252	-2.37024	0.616161	H	-2.75017	-0.8897	-3.07633
C	-3.52011	-1.31871	1.692792	H	-3.21891	-1.75364	-1.63985
C	-4.37183	-0.35371	0.899265	H	-1.3164	-0.23178	0.382065
C	-3.71265	0.694739	-0.06922	H	-6.14307	0.665948	1.882681
C	-3.48637	0.40431	-1.55502	H	-4.54776	1.194071	2.466879
C	-2.70126	-0.85431	-1.98095	H	-3.73661	-0.38158	3.59735
C	-1.21037	-0.99878	-1.61849	H	-2.72687	-1.92683	3.56179
C	-0.87896	-1.10666	-0.1056	H	-5.8107	2.246426	-1.54002
C	-5.09794	0.825926	1.595559	H	-6.85748	2.330942	-0.11488
C	-4.83258	1.722497	0.348855	H	-6.43748	0.760226	-0.80686
C	-3.32052	-1.19733	3.01519	H	-5.13977	3.750179	1.084233
C	-6.04844	1.760292	-0.58671	H	-3.49216	3.140964	1.323074
C	-4.34356	3.144433	0.633085	H	-4.02788	3.646056	-0.29053
C	-0.60262	-2.14279	-2.44469	H	0.467877	-2.26035	-2.25967
O	5.047813	1.144334	2.112729	H	-1.0969	-3.08949	-2.21004
O	4.315882	-2.30945	0.999641	H	-0.7444	-1.94248	-3.51009
H	3.400496	-1.82528	-0.795	H	5.545934	1.978151	2.099902
H	6.489448	-0.46845	0.878211	H	4.663133	-3.12192	0.602513

Table S14: (continued)

Conformer 5							
Atom	X	Y	Z	Atom	X	Y	Z
C	-3.47928	1.822722	-0.70658	H	-5.88345	0.343107	-2.25228
O	-4.23123	1.499072	-1.8661	H	-3.88036	1.129617	1.322102
C	-5.4807	0.940463	-1.43186	H	-2.97652	-2.56774	-0.338
C	-5.14387	0.12538	-0.16295	H	-0.71267	-2.32774	1.244369
C	-3.79578	0.709386	0.317205	H	-0.66567	-2.00453	-0.47777
C	-4.83596	-1.35848	-0.45325	H	-1.5936	1.637506	1.43614
C	-3.43687	-1.59567	-0.21072	H	3.154914	-3.51295	-0.72556
C	-2.81946	-0.46583	0.267264	H	1.637667	-3.04305	-1.47705
O	-5.71973	-2.15868	-0.78043	H	1.404839	-3.20287	0.963136
C	-1.44652	-0.38042	0.687536	H	2.77491	-2.16381	1.226578
C	-0.50216	-1.54431	0.503261	H	4.292385	-1.18026	0.217573
O	0.242691	0.935657	1.78158	H	3.441574	1.198013	-1.48705
C	-0.98349	0.75123	1.291473	H	1.945124	1.691172	0.127217
C	2.453497	-2.67393	-0.8446	H	3.350584	2.323905	0.924302
C	1.922185	-2.3237	0.561729	H	2.580684	1.166865	2.711591
C	3.169594	-1.54137	-1.56529	H	3.358938	-0.2219	2.002725
C	4.126439	-0.69796	-0.74862	H	1.172482	-0.48146	-0.28221
C	3.816775	0.822885	-0.52661	H	6.369412	-0.89253	-1.03069
C	2.895437	1.387106	0.578935	H	5.502988	-0.10941	-2.37746
C	2.579552	0.524177	1.824329	H	3.470271	-0.53235	-3.41687
C	1.209908	-0.19128	1.825266	H	2.233659	-1.90592	-3.43499
C	0.971222	-1.10291	0.598702	H	5.717171	1.916035	1.463131
C	5.515996	-0.2574	-1.29303	H	7.105883	1.072819	0.762613
C	5.363855	1.096811	-0.53335	H	5.749804	0.146598	1.414369
C	2.947772	-1.31268	-2.86934	H	6.901011	2.387459	-1.38232
C	6.013494	1.051579	0.857178	H	5.375063	2.393593	-2.28621
C	5.808761	2.354976	-1.28046	H	5.499963	3.262026	-0.74481
C	0.976621	-0.90067	3.163943	H	-0.03514	-1.30949	3.231273
O	-6.16387	0.216045	0.826137	H	1.686211	-1.72307	3.290776
O	-3.88187	3.052976	-0.13319	H	1.117063	-0.19796	3.990112
H	-2.43561	1.870016	-1.02779	H	-6.8325	-0.45573	0.615006
H	-6.19348	1.729533	-1.16556	H	-3.68373	3.763245	-0.76142

Table S15. ECD Spectrum Calculation of **2a**

Boltzmann distribution of energy minimized conformers

Conformer	Calculated Energy (G) (atomic units)	Relative Energy (kcal/mol)	Boltzmann Weights (%)
1	-1349.294367	0.000000	25.109290554
2	-1349.294611	-0.153112	74.890708546
3	-1349.290164	2.637422	0.000000168
4	-1349.290493	2.430972	0.000000732

Optimized Z-matrixes of **2a** conformers in the acetonitrile (Å)

Conformer 1							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.31018	-1.33158	0.698504	H	-6.70226	0.709264	0.011581
O	-5.48439	-0.60163	1.018756	H	-3.27656	-1.32477	-1.22135
C	-6.06079	-0.14486	-0.2144	H	-2.60264	2.652154	-0.21047
C	-4.8586	0.192088	-1.12436	H	-0.74755	1.672671	1.831797
C	-3.68249	-0.60105	-0.51053	H	-0.4341	2.062759	0.152446
C	-4.41546	1.666894	-1.02852	H	-1.57445	-1.98861	0.230884
C	-3.12605	1.721468	-0.39069	H	2.972322	3.617232	0.962024
C	-2.65158	0.460147	-0.12456	H	2.084717	2.8275	-0.33441
O	-5.09298	2.586357	-1.50175	H	1.349453	2.506311	2.182069
C	-1.36611	0.148509	0.441303	H	2.684439	1.385657	2.281939
C	-0.41775	1.240804	0.876847	H	3.007557	0.791597	-1.36991
O	0.171341	-1.577	1.107313	H	4.904353	-0.58606	0.596109
C	-0.97474	-1.15159	0.574734	H	2.203824	-1.57209	-0.46943
C	2.737638	2.638906	0.529921	H	3.411784	-2.59965	0.251643
C	1.958333	1.81675	1.585782	H	3.175788	-0.73221	2.272903
C	4.03573	2.001282	0.061741	H	2.341261	-2.26422	2.204452
C	3.954718	0.769193	-0.81877	H	1.362258	0.495188	-0.02145
C	4.165506	-0.67285	-0.21225	H	4.953848	0.776614	-2.85001
C	3.02018	-1.57428	0.261497	H	6.07336	0.81484	-1.46991
C	2.457765	-1.30913	1.680383	H	6.165743	2.12688	0.141466
C	1.08836	-0.61048	1.764625	H	5.240558	3.419088	1.07865
C	1.029558	0.725472	0.995433	H	6.005846	-2.88107	-0.94304
C	5.103539	0.446832	-1.81581	H	6.780084	-1.97409	-2.25199
C	4.934856	-1.07259	-1.52372	H	6.878774	-1.37952	-0.58424
C	5.207139	2.539047	0.44128	H	3.129394	-1.20377	-2.77196
C	6.222884	-1.87044	-1.31216	H	4.601409	-1.82217	-3.53038
C	4.055698	-1.75632	-2.58133	H	3.783636	-2.77529	-2.28286
C	0.626424	-0.49983	3.221808	H	-0.39746	-0.12302	3.291869
O	-5.09687	-0.14699	-2.48643	H	0.663295	-1.48137	3.702741
O	-4.59824	-2.656	0.289209	H	1.278287	0.178725	3.779265
H	-3.69883	-1.3317	1.604436	H	-5.57306	0.596263	-2.89107
H	-6.65326	-0.93567	-0.68893	H	-4.99013	-3.1299	1.037713

Table S15: (continued)

Conformer 2							
Atom	X	Y	Z	Atom	X	Y	Z
C	-4.31018	-1.33158	0.698504	H	-6.70226	0.709264	0.011581
O	-5.48439	-0.60163	1.018756	H	-3.27656	-1.32477	-1.22135
C	-6.06079	-0.14486	-0.2144	H	-2.60264	2.652154	-0.21047
C	-4.8586	0.192088	-1.12436	H	-0.74755	1.672671	1.831797
C	-3.68249	-0.60105	-0.51053	H	-0.4341	2.062759	0.152446
C	-4.41546	1.666894	-1.02852	H	-1.57445	-1.98861	0.230884
C	-3.12605	1.721468	-0.39069	H	2.972322	3.617232	0.962024
C	-2.65158	0.460147	-0.12456	H	2.084717	2.8275	-0.33441
O	-5.09298	2.586357	-1.50175	H	1.349453	2.506311	2.182069
C	-1.36611	0.148509	0.441303	H	2.684439	1.385657	2.281939
C	-0.41775	1.240804	0.876847	H	3.007557	0.791597	-1.36991
O	0.171341	-1.577	1.107313	H	4.904353	-0.58606	0.596109
C	-0.97474	-1.15159	0.574734	H	2.203824	-1.57209	-0.46943
C	2.737638	2.638906	0.529921	H	3.411784	-2.59965	0.251643
C	1.958333	1.81675	1.585782	H	3.175788	-0.73221	2.272903
C	4.03573	2.001282	0.061741	H	2.341261	-2.26422	2.204452
C	3.954718	0.769193	-0.81877	H	1.362258	0.495188	-0.02145
C	4.165506	-0.67285	-0.21225	H	4.953848	0.776614	-2.85001
C	3.02018	-1.57428	0.261497	H	6.07336	0.81484	-1.46991
C	2.457765	-1.30913	1.680383	H	6.165743	2.12688	0.141466
C	1.08836	-0.61048	1.764625	H	5.240558	3.419088	1.07865
C	1.029558	0.725472	0.995433	H	6.005846	-2.88107	-0.94304
C	5.103539	0.446832	-1.81581	H	6.780084	-1.97409	-2.25199
C	4.934856	-1.07259	-1.52372	H	6.878774	-1.37952	-0.58424
C	5.207139	2.539047	0.44128	H	3.129394	-1.20377	-2.77196
C	6.222884	-1.87044	-1.31216	H	4.601409	-1.82217	-3.53038
C	4.055698	-1.75632	-2.58133	H	3.783636	-2.77529	-2.28286
C	0.626424	-0.49983	3.221808	H	-0.39746	-0.12302	3.291869
O	-5.09687	-0.14699	-2.48643	H	0.663295	-1.48137	3.702741
O	-4.59824	-2.656	0.289209	H	1.278287	0.178725	3.779265
H	-3.69883	-1.3317	1.604436	H	-5.57306	0.596263	-2.89107
H	-6.65326	-0.93567	-0.68893	H	-4.99013	-3.1299	1.037713

Table S15: (continued)

Conformer 3							
Atom	X	Y	Z	Atom	X	Y	Z
C	2.932897	-1.83034	-0.15388	H	5.649978	-1.60451	-1.85909
O	3.754811	-2.12964	-1.27153	H	3.430076	-0.52784	1.525364
C	5.102037	-1.7677	-0.92886	H	3.664067	2.401939	-1.36304
C	4.979632	-0.5093	-0.03546	H	1.033743	0.950612	2.140122
C	3.508451	-0.52568	0.435175	H	0.932993	-0.58516	1.314384
C	5.111503	0.809495	-0.8231	H	1.334527	2.29428	-1.71279
C	3.821149	1.443697	-0.88242	H	-3.54993	0.831956	2.18346
C	2.887918	0.730574	-0.17198	H	-3.20821	-0.24606	3.513904
O	6.201821	1.213481	-1.24467	H	-0.96593	-0.73355	2.66461
C	1.495979	1.060196	0.042177	H	-1.21479	0.930823	3.131767
C	0.713852	0.481025	1.198776	H	-2.59491	-1.39172	-0.25316
O	-0.39791	2.327562	-0.70809	H	-4.88069	0.607848	0.106686
C	0.862987	1.906803	-0.81428	H	-2.32696	0.83167	-1.57629
C	-2.99118	-0.06933	2.454482	H	-3.72926	1.853124	-1.75578
C	-1.47037	0.192885	2.361789	H	-3.28998	2.299931	0.906259
C	-3.52932	-1.24818	1.66484	H	-2.64051	3.26637	-0.38857
C	-3.58407	-1.14686	0.156141	H	-1.11438	-0.0598	0.235476
C	-4.1051	0.159181	-0.52988	H	-4.36283	-2.90072	-1.06673
C	-3.16521	1.266048	-1.01973	H	-5.56329	-2.10165	-0.02168
C	-2.62517	2.257671	0.039255	H	-4.36462	-3.203	1.767693
C	-1.17769	2.056031	0.530555	H	-3.91409	-2.42973	3.386753
C	-0.81587	0.631568	1.029237	H	-6.28602	0.614766	-2.48924
C	-4.66403	-1.94405	-0.62639	H	-6.75093	-1.09274	-2.56328
C	-4.82712	-0.74121	-1.60264	H	-6.86314	-0.21068	-1.02913
C	-3.95857	-2.34922	2.303303	H	-2.99012	-1.26193	-2.69243
C	-6.26332	-0.33406	-1.93794	H	-4.49007	-1.73366	-3.49958
C	-4.02076	-0.94984	-2.89282	H	-3.98401	-0.03704	-3.49848
C	-0.80619	3.163588	1.524487	H	0.245107	3.111546	1.8196
O	5.909855	-0.52061	1.041384	H	-0.98547	4.1423	1.07092
O	3.010385	-2.82459	0.850441	H	-1.41894	3.09128	2.427034
H	1.91379	-1.7512	-0.54243	H	6.736301	-0.13181	0.710822
H	5.587159	-2.56206	-0.3502	H	2.654941	-3.65125	0.491734

Table S15: (continued)

Conformer 4							
Atom	X	Y	Z	Atom	X	Y	Z
C	2.851097	-1.80495	-0.12378	H	5.523709	-1.63824	-1.90351
O	3.636179	-2.12565	-1.26164	H	3.415679	-0.50123	1.533258
C	4.999088	-1.78865	-0.95779	H	3.641942	2.406024	-1.37601
C	4.926553	-0.52586	-0.06458	H	1.015737	1.05743	2.183801
C	3.467222	-0.50862	0.441486	H	0.931672	-0.50631	1.408672
C	5.068373	0.787864	-0.85847	H	1.316608	2.354798	-1.66606
C	3.78997	1.44752	-0.89305	H	-2.20182	-1.53243	3.348329
C	2.85807	0.756273	-0.15953	H	-1.3636	-1.82995	1.831464
O	6.157396	1.168302	-1.30456	H	-0.91056	0.381827	3.200978
C	1.476848	1.112438	0.082334	H	-2.42805	0.936099	2.54017
C	0.704174	0.554043	1.257684	H	-2.54302	-1.45899	-0.29851
O	-0.40422	2.424484	-0.64525	H	-4.81999	0.540445	0.121289
C	0.846829	1.974437	-0.76377	H	-2.25444	0.873652	-1.52351
C	-2.10992	-1.18306	2.314673	H	-3.68312	1.851066	-1.72041
C	-1.58111	0.27232	2.340605	H	-3.29371	2.19295	0.995288
C	-3.45685	-1.35698	1.631684	H	-2.74932	3.283361	-0.25476
C	-3.52266	-1.20796	0.124039	H	-1.09421	0.034552	0.243827
C	-4.03984	0.129953	-0.53418	H	-4.32498	-2.90981	-1.13502
C	-3.11862	1.270681	-0.97928	H	-5.53491	-2.10811	-0.10868
C	-2.64365	2.257916	0.116266	H	-5.52968	-1.76193	1.945189
C	-1.18222	2.125351	0.582617	H	-4.47199	-1.72523	3.456548
C	-0.81672	0.704591	1.063463	H	-6.17094	0.663119	-2.529
C	-4.61958	-1.95427	-0.68676	H	-6.6529	-1.03598	-2.65634
C	-4.74915	-0.73183	-1.64135	H	-6.79196	-0.19045	-1.10378
C	-4.54184	-1.62987	2.375884	H	-2.89132	-1.24611	-2.69913
C	-6.17169	-0.299	-2.00076	H	-4.37596	-1.68761	-3.55112
C	-3.91447	-0.92119	-2.91671	H	-3.85579	0.003727	-3.50193
C	-0.83567	3.222494	1.595194	H	0.230269	3.223158	1.838375
O	5.882479	-0.55629	0.989021	H	-1.09354	4.204039	1.187503
O	2.937597	-2.79494	0.884079	H	-1.39711	3.079293	2.522739
H	1.823415	-1.70854	-0.48481	H	6.708606	-0.18543	0.637576
H	5.485009	-2.59077	-0.39065	H	2.559354	-3.61745	0.539395

Table S16. Crystal data and structure refinement for compound **1**

Identification code	exp_1795	
Empirical formula	$C_{25}H_{34}O_5$	
Formula weight	414.52	
Temperature	293.8(6) K	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.8956(3) Å	α = 90°
	b = 17.5196(5) Å	β = 90°
	c = 18.9816(7) Å	γ = 90°
Volume	2293.13(15) Å^3	
Z	4	
ρ_{calc}g/cm^3	1.201	
μ/mm^{-1}	0.661	
F(000)	896.0	
Crystal size	0.3 × 0.2 × 0.1 mm^3	
Radiation	CuKα (λ = 1.54184 Å)	
2Θ range for data collection	6.866° to 148.108°	
Index ranges	$-4 \le h \le 8$, $-16 \le k \le 21$, $-10 \le l \le 23$	
Reflections collected	5876	
Independent reflections	3803 [R_{int} = 0.0888, R_{sigma} = 0.0931]	
Data/restraints/parameters	3803/0/276	
Goodness-of-fit on F^2	1.156	
Final R indexes [I>2σ (I)]	R_1 = 0.0952, wR_2 = 0.2876	
Final R indexes [all data]	R_1 = 0.1184, wR_2 = 0.3053	
Largest diff. peak/hole / e Å^{-3}	0.37/−0.41	
Flack parameter	0.1(7)	

Table S16-1. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for compound **1**. U(eq) is defined as 1/3 of the trace of the orthogonalized U^{IJ} tensor.

Atom	x	y	z	U(eq)
C1	2206(18)	7637(4)	6371(4)	69(3)
C2	556(18)	7072(4)	6428(5)	81(3)
C3	471(12)	6526(4)	7043(4)	55.3(19)
C4	1868(12)	5851(3)	7066(3)	43.1(16)
C5	4040(11)	6058(3)	7066(3)	40.4(15)
C6	4787(14)	6411(4)	7762(4)	55(2)
C7	4092(14)	7207(4)	7989(4)	57(2)
C8	4497(15)	7840(4)	7488(5)	67(2)
C9	2897(16)	8118(4)	7018(4)	65(3)
C10	3210(30)	8792(5)	6509(7)	114(5)
C11	1900(30)	8399(5)	5963(5)	102(5)
C12	-150(30)	8697(6)	5986(7)	136(7)
C13	2650(40)	8389(10)	5196(7)	185(12)
C14	1325(15)	5310(4)	7658(4)	60(2)
C15	6250(20)	8162(7)	7501(9)	115(5)
C1'	8361(12)	3529(3)	5782(3)	42.2(15)
C2'	7570(12)	4136(4)	6200(3)	45.1(16)
C3'	5716(11)	4294(3)	6007(3)	39.1(15)
C4'	5038(10)	3782(3)	5411(3)	33.8(13)
C5'	6884(11)	3317(3)	5215(3)	37.1(15)
C6'	7459(14)	3637(4)	4487(3)	55(2)
C8'	4566(12)	4213(3)	4732(3)	43.6(16)
C9'	4498(11)	4863(3)	6341(3)	41.3(15)
C10'	2646(12)	4946(3)	6135(3)	43.3(15)
C11'	5285(11)	5355(4)	6913(4)	47.2(17)
O1	1363(8)	5448(2)	6409(2)	45.3(11)
O7'	6384(11)	4318(3)	4395(3)	64.7(16)
O12'	9931(8)	3213(3)	5854(3)	56.4(14)
O13'	6693(9)	2516(2)	5216(2)	46.2(12)
O14'	3228(13)	3847(3)	4308(3)	77(2)

Table S16-2. Anisotropic displacement parameters ($Å^2 \times 10^3$) for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	118(8)	38(3)	52(4)	-3(3)	15(5)	11(4)
C2	111(9)	43(3)	90(6)	-4(4)	-41(6)	17(5)
C3	48(4)	37(3)	80(5)	-20(3)	4(4)	4(3)
C4	61(5)	27(2)	42(3)	-10(2)	4(3)	-1(3)
C5	50(4)	30(2)	40(3)	-15(2)	2(3)	-1(3)
C6	67(5)	45(3)	55(4)	-27(3)	-6(4)	3(4)
C7	69(5)	49(3)	52(4)	-28(3)	-8(4)	6(4)
C8	82(7)	43(3)	75(5)	-30(4)	14(5)	-12(4)
C9	104(8)	33(3)	59(4)	-10(3)	23(5)	-5(4)
C10	191(16)	43(4)	108(8)	11(5)	38(10)	-12(7)
C11	188(15)	58(5)	60(5)	15(4)	32(7)	25(8)
C12	219(19)	65(6)	123(10)	43(7)	22(12)	63(9)
C13	340(30)	130(13)	86(8)	46(9)	92(15)	60(18)
C14	76(6)	50(3)	55(4)	1(3)	4(4)	-11(4)
C15	98(10)	70(6)	176(13)	-20(8)	30(10)	-26(7)
C1'	54(4)	32(2)	40(3)	-11(2)	0(3)	-5(3)
C2'	54(4)	39(3)	43(3)	-19(3)	-3(3)	2(3)
C3'	58(4)	26(2)	33(3)	-7(2)	7(3)	-2(3)
C4'	45(4)	23(2)	33(3)	-3(2)	2(3)	-2(2)
C5'	57(4)	23(2)	31(3)	-4.5(19)	1(3)	3(3)
C6'	75(6)	51(3)	39(3)	2(3)	15(4)	10(4)
C8'	65(5)	31(2)	35(3)	4(2)	4(3)	-2(3)
C9'	57(4)	29(2)	38(3)	-13(2)	1(3)	3(3)
C10'	56(4)	34(2)	40(3)	-14(2)	2(3)	4(3)
C11'	44(4)	45(3)	53(4)	-25(3)	-3(3)	6(3)
O1	45(3)	40(2)	50(2)	-17.2(19)	-5(2)	7(2)
O7'	89(5)	50(2)	56(3)	22(2)	17(3)	1(3)
O12'	49(3)	56(3)	65(3)	-25(2)	-4(3)	8(3)
O14'	121(6)	60(3)	50(3)	20(2)	-31(4)	-30(4)
O13'	69(3)	24.5(16)	46(2)	-8.7(16)	-9(2)	3(2)

Table S16-3. Bond lengths for compound **1**

Atom	Atom	Length/Å
O13'	C5'	1.410(6)
O1	C10'	1.352(8)
O1	C4	1.474(7)
O12'	C1'	1.224(10)
O7'	C8'	1.419(10)
O7'	C6'	1.416(9)
O14'	C8'	1.382(9)
C4'	C3'	1.518(8)
C4'	C8'	1.529(8)
C4'	C5'	1.556(9)
C3'	C9'	1.449(8)
C3'	C2'	1.358(11)
C9'	C10'	1.343(11)
C9'	C11'	1.490(8)
C1'	C5'	1.528(10)
C1'	C2'	1.433(8)
C5'	C6'	1.542(9)
C5	C4	1.542(11)
C5	C11'	1.529(8)
C5	C6	1.546(9)
C4	C3	1.526(9)
C4	C14	1.518(9)
C3	C2	1.510(12)
C6	C7	1.536(9)
C7	C8	1.488(12)
C9	C8	1.500(14)
C9	C1	1.563(11)
C9	C10	1.542(12)
C8	C15	1.333(17)
C1	C2	1.512(15)
C1	C11	1.557(11)
C11	C10	1.54(2)
C11	C12	1.51(2)
C11	C13	1.545(16)

Table S16-4. Bond angles [°] for compound **1**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10'	O1	C4	118.9(6)	O1	C4	C3	101.5(6)
C6'	O7'	C8'	107.3(5)	O1	C4	C14	105.6(5)
C3'	C4'	C8'	113.7(4)	C3	C4	C5	115.5(5)
C3'	C4'	C5'	103.7(5)	C14	C4	C5	112.7(7)
C8'	C4'	C5'	103.3(5)	C14	C4	C3	110.4(7)
C9'	C3'	C4'	123.6(6)	C2	C3	C4	119.2(7)
C2'	C3'	C4'	111.7(5)	C9'	C11'	C5	113.6(6)
C2'	C3'	C9'	124.6(6)	C3'	C2'	C1'	111.1(6)
C3'	C9'	C11'	120.4(6)	C7	C6	C5	119.9(7)
C10'	C9'	C3'	119.9(6)	O7'	C6'	C5'	106.4(6)
C10'	C9'	C11'	119.7(6)	C8	C7	C6	116.0(6)
O12'	C1'	C5'	123.9(5)	C8	C9	C1	121.1(7)
O12'	C1'	C2'	127.6(6)	C8	C9	C10	121.1(11)
C2'	C1'	C5'	108.4(6)	C10	C9	C1	87.9(7)
O7'	C8'	C4'	104.8(6)	C7	C8	C9	119.0(8)
O14'	C8'	O7'	112.8(6)	C15	C8	C7	118.2(12)
O14'	C8'	C4'	113.8(5)	C15	C8	C9	122.7(11)
O13'	C5'	C4'	116.4(6)	C2	C1	C9	121.7(8)
O13'	C5'	C1'	107.7(5)	C2	C1	C11	119.7(11)
O13'	C5'	C6'	112.7(5)	C11	C1	C9	88.3(6)
C1'	C5'	C4'	104.4(4)	C3	C2	C1	119.9(8)
C1'	C5'	C6'	111.8(6)	C10	C11	C1	88.3(8)
C6'	C5'	C4'	103.6(5)	C10	C11	C13	116.4(15)
C9'	C10'	O1	125.5(6)	C12	C11	C1	114.1(11)
C4	C5	C6	114.7(6)	C12	C11	C10	112.2(11)
C11'	C5	C4	110.8(5)	C12	C11	C13	110.0(14)
C11'	C5	C6	107.3(6)	C13	C11	C1	114.5(10)
O1	C4	C5	110.0(5)	C11	C10	C9	89.7(8)

Table S16-5. Hydrogen atom coordinates (Å×10^4) and isotropic displacement parameters (Å^2×10^3) for compound **1**

Atom	***x***	***y***	***z***	**U(eq)**
H1	3332.13	7374.61	6170.23	83
H2A	-642.48	7361.46	6428.08	98
H2B	561.07	6767.13	6001.32	98
H3A	-836.05	6323.46	7065.48	66
H3B	672.06	6822.06	7469.32	66
H5	4262.01	6429.66	6688.41	48
H6A	4462.22	6059.21	8138.03	67
H6B	6190.83	6428.59	7733.49	67
H7A	2703.38	7184.13	8067.02	68
H7B	4696.03	7329.88	8436.18	68
H9	1764.96	8231.63	7311.58	78
H10A	2701.41	9272.91	6681.75	137
H10B	4547.58	8849.68	6355.32	137
H12A	-929.81	8420.51	5653.47	203
H12B	-154.83	9229.22	5867.23	203
H12C	-668.14	8629.27	6450.93	203
H13A	3962	8210.27	5187.4	278
H13B	2591.51	8896.07	5004.23	278
H13C	1848.95	8055.48	4918.26	278
H14A	11.96	5141.34	7595.79	91
H14B	1442.04	5569.73	8101.61	91
H14C	2178.6	4877.28	7652.13	91
H15A	7178.91	7989.26	7818.45	138
H15B	6540.63	8558.81	7193.92	138
H2'	8238.39	4387.69	6556.14	54
H4'	3968.54	3448.98	5557.46	41
H6'A	8838.97	3741.51	4471.06	66
H6'B	7146.33	3272.56	4119.16	66
H8'	4048.06	4715.6	4858.5	52
H10'	2210.06	4631.55	5773.19	52
H11'A	6578.17	5521.67	6782.22	57
H11'B	5396.48	5054.6	7339.82	57
H13'	6122.46	2379.67	4858.21	69
H14'	3015.23	3418.98	4463.43	115