

Supporting Information

Chemical Constituents of *Aerides odorata* and Their Anti-Neuroinflammatory Effects on LPS-Activated BV2 Microglial Cells

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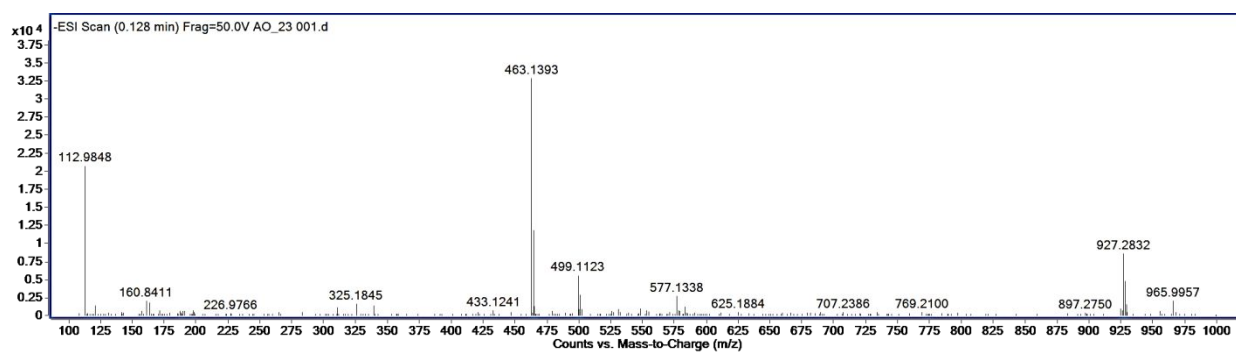


Figure S1. HR-ESI-MS spectrum of compound **1**

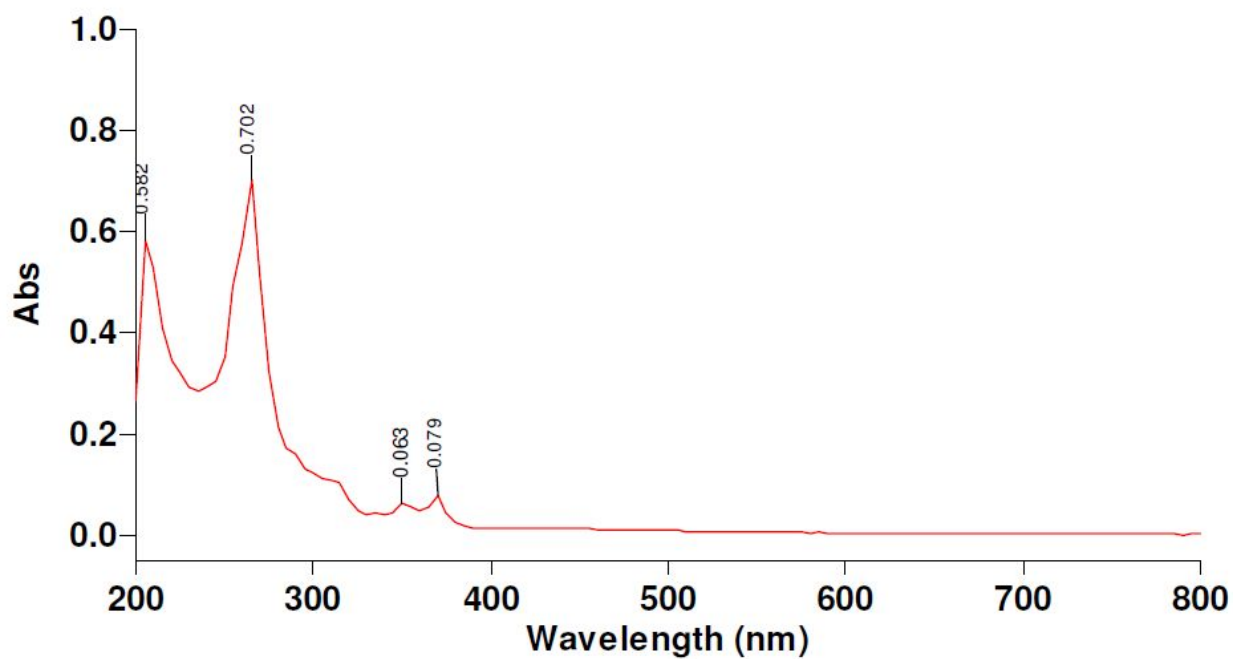


Figure S2. UV spectrum of compound **1** (0.0625 mg in 3ml of methanol)

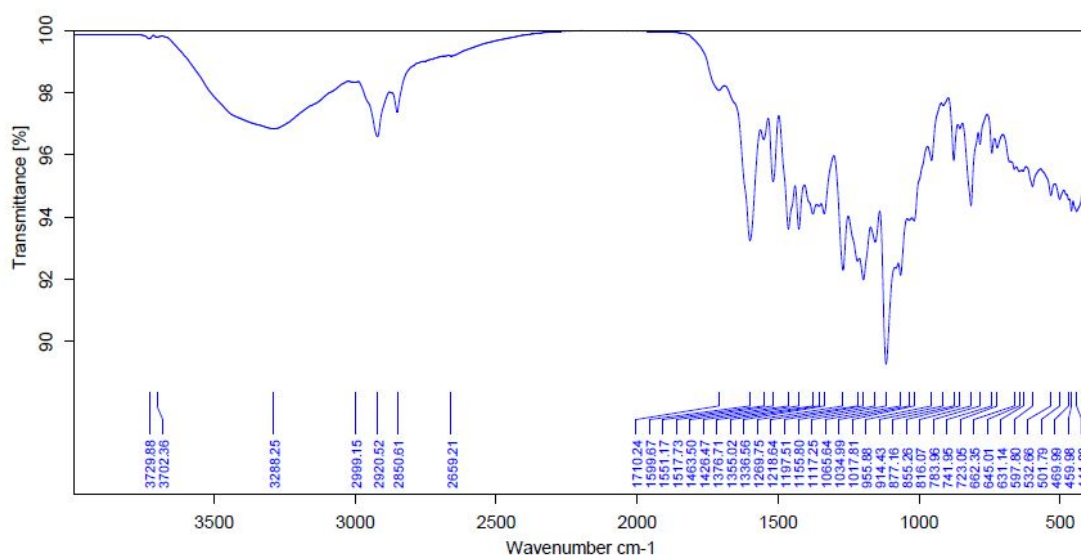


Figure S3. FT-IR spectrum of compound **1**

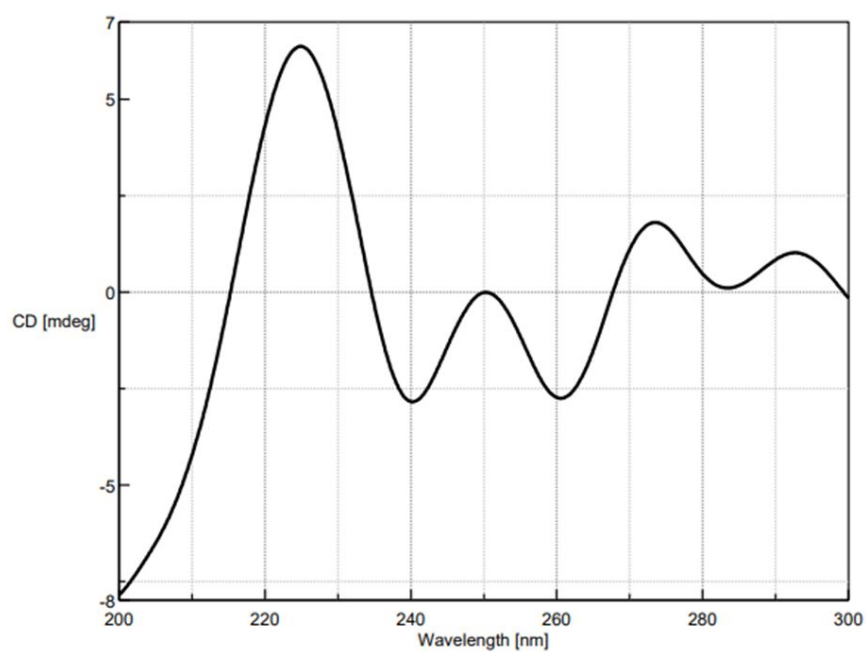


Figure S4. CD spectrum of compound **1**

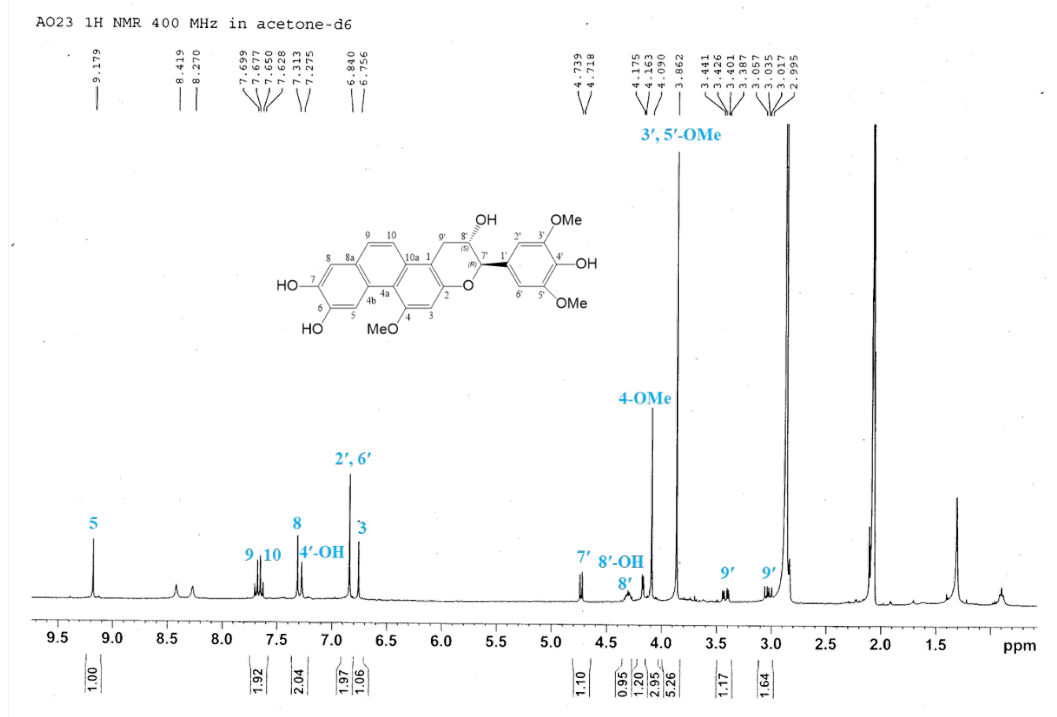


Figure S5. ^1H NMR (acetone- d_6 , 400 MHz) spectrum of compound 1

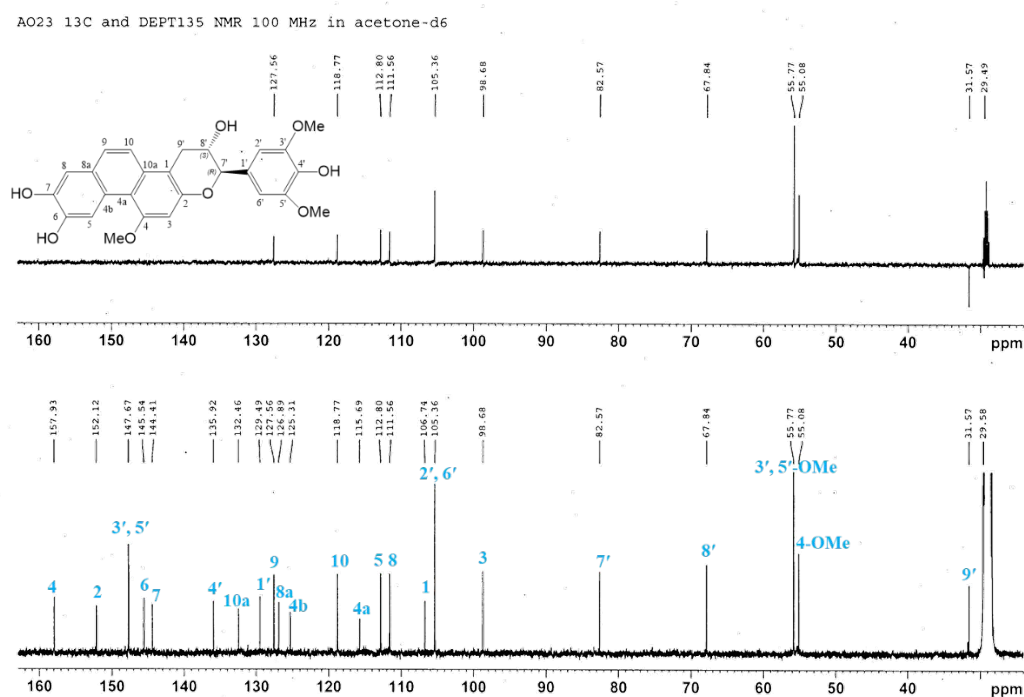


Figure S6. ^{13}C NMR and DEPT (acetone- d_6 , 100 MHz) spectrum of compound 1

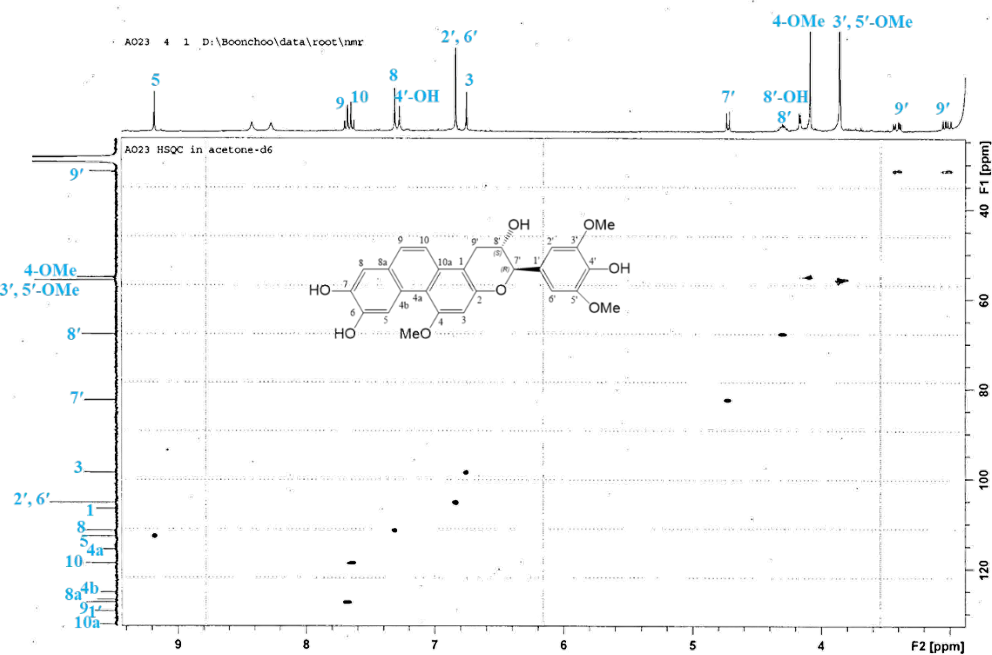


Figure S7. HSQC (acetone- d_6 , 400/100 MHz) spectrum of compound **1**

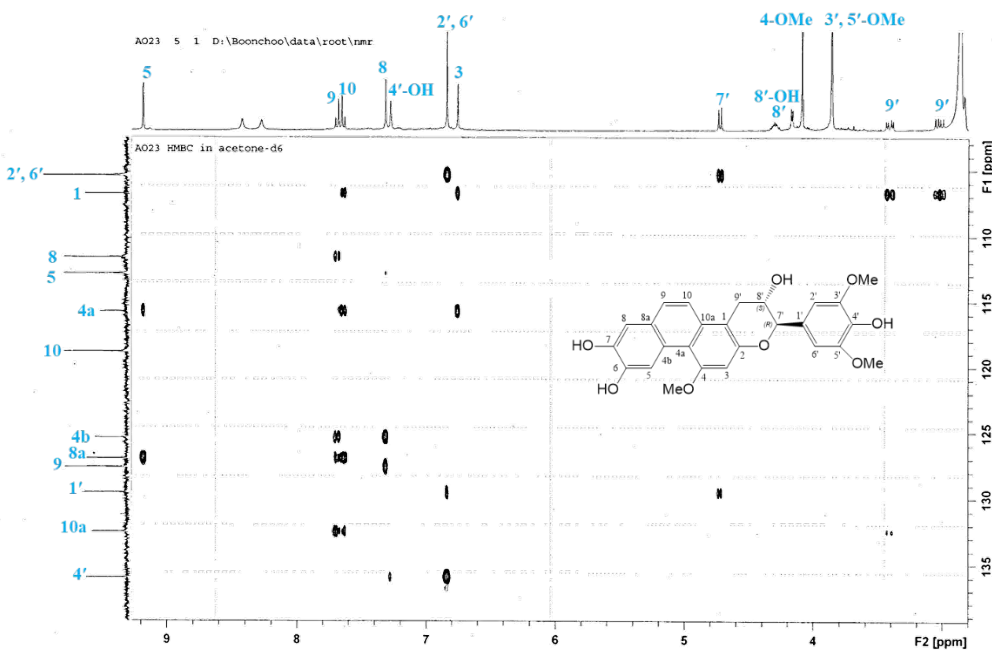


Figure S8. HMBC (acetone- d_6 , 400/100 MHz) spectrum 1 of compound **1**

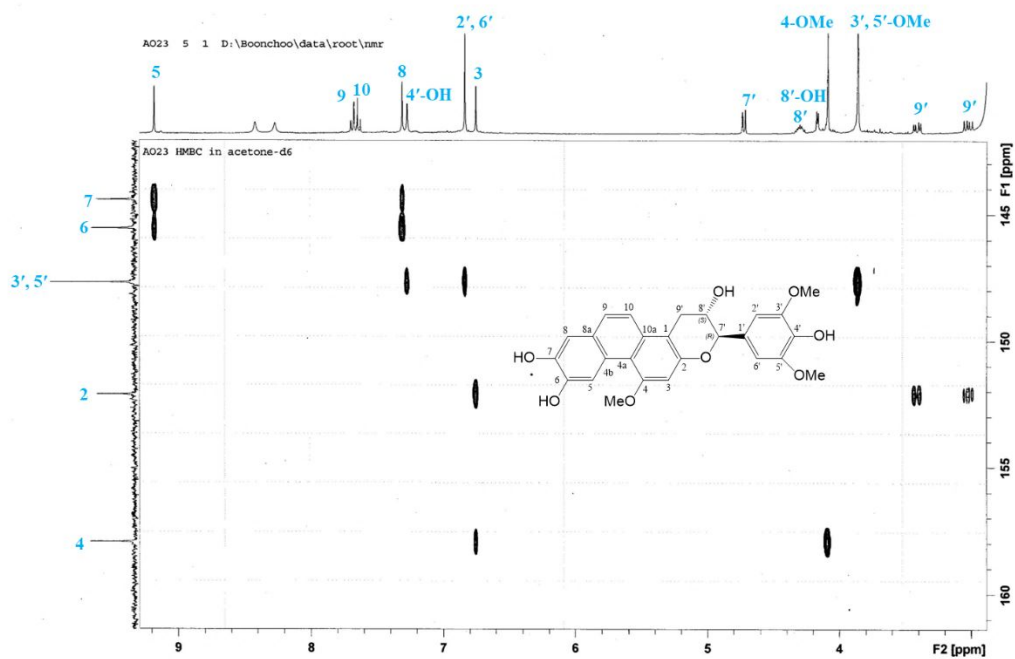


Figure S9. HMBC (acetone- d_6 , 400/100 MHz) spectrum 2 of compound 1

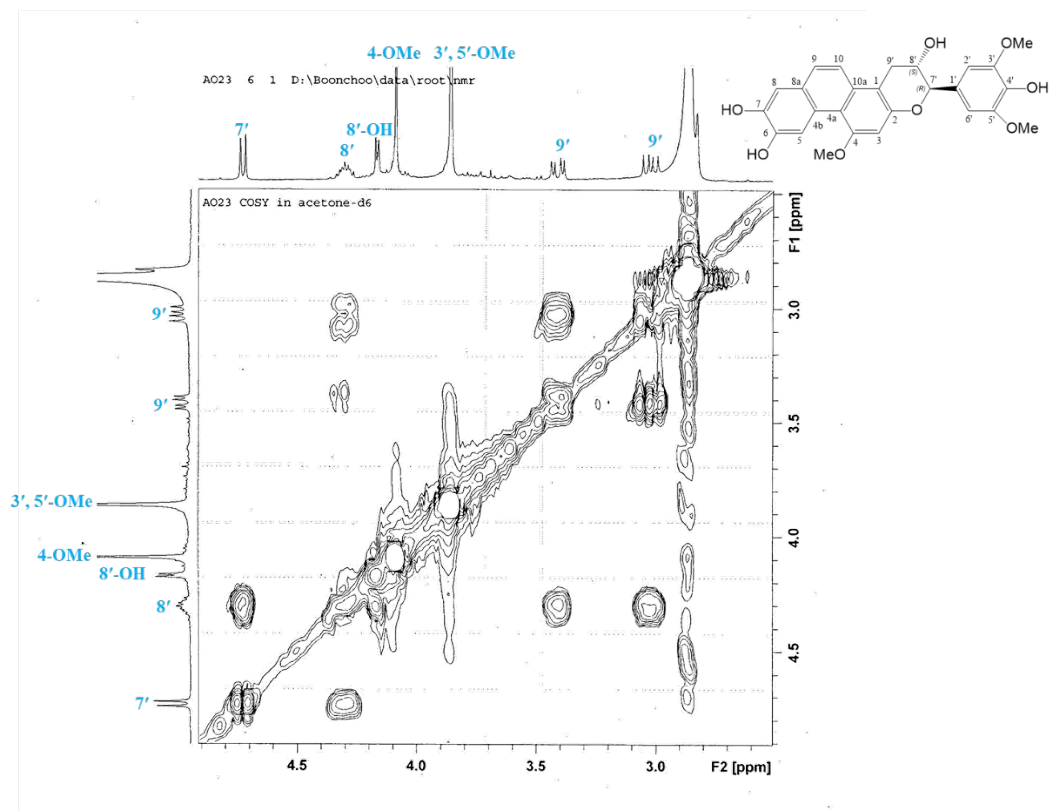


Figure S10. COSY (acetone- d_6 , 400 MHz) spectrum of compound 1

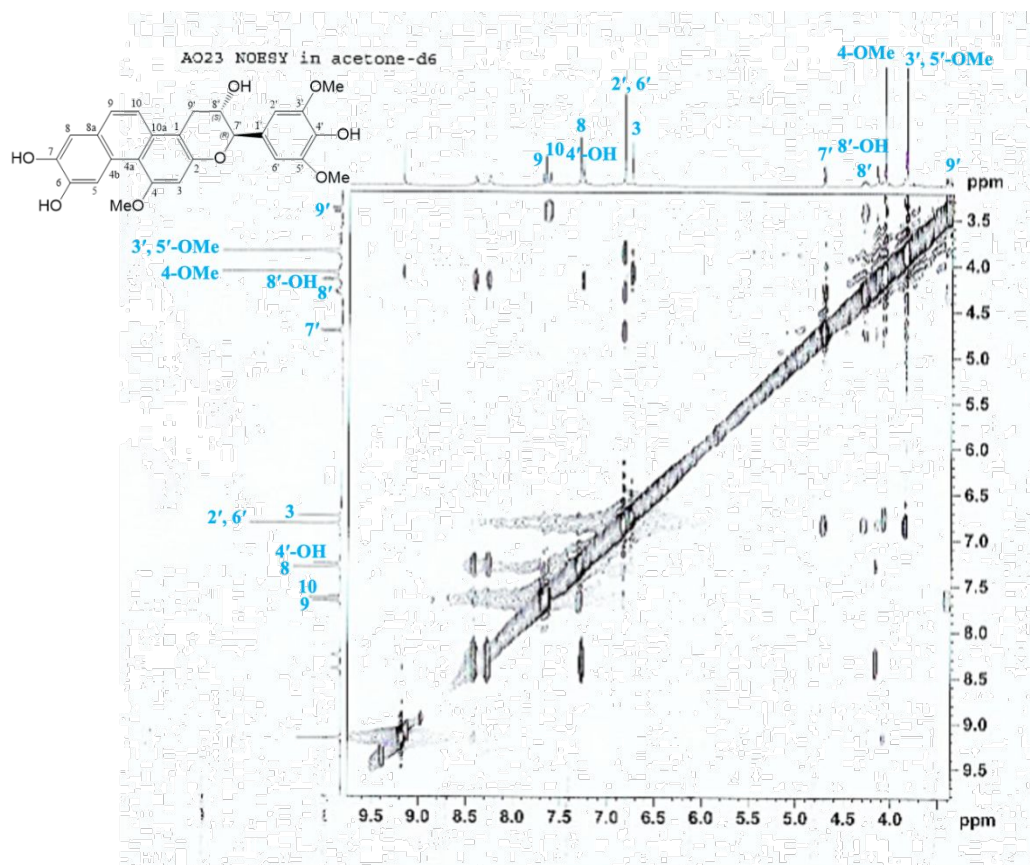


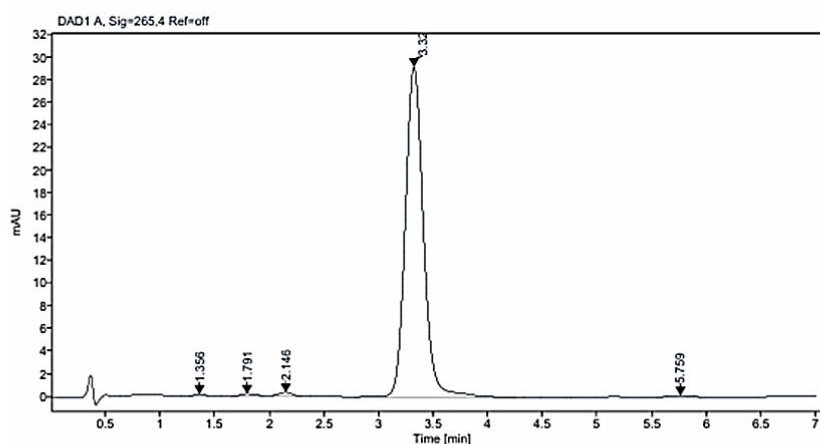
Figure S11. NOESY (acetone-*d*₆, 400 MHz) spectrum of compound 1

Area Percent Report

Compound1_0.05mg/mL_40%MeOH_formic



Data file: C:\Users\Public\Documents\ChemStation\1\Data\Monsin\Purity180526 2026-05-18 13-24-21\005-P1-C1-Compound1_0.05mg_mL_40%MeOH_fo.D
Sample name: Compound1_0.05mg/mL_40%MeOH_formic
Description:
Sample amount: 0.000 **Sample type:** Sample
Instrument: LC1290_DAD **Location:** P1-C1
Injection date: 2026-05-18 14:03:05+07:00 **Injection:** 1 of 1
Acq. method: Purity_phenan.M **Injection volume:** 1.000
Analysis method: Purity_phenan.M **Acq. operator:** SYSTEM
Last changed: 2026-05-18 14:04:01+07:00



Signal: DAD1 A, Sig=265,4 Ref=off		
RT [min]	Area	Area%
1.356	1.1066	0.3218
1.791	1.9053	0.5541
2.146	2.8693	0.8344
3.320	335.7447	97.6392
5.759	2.2369	0.6505
Sum	343.8628	

Figure S12. HPLC chromatogram of compound 1

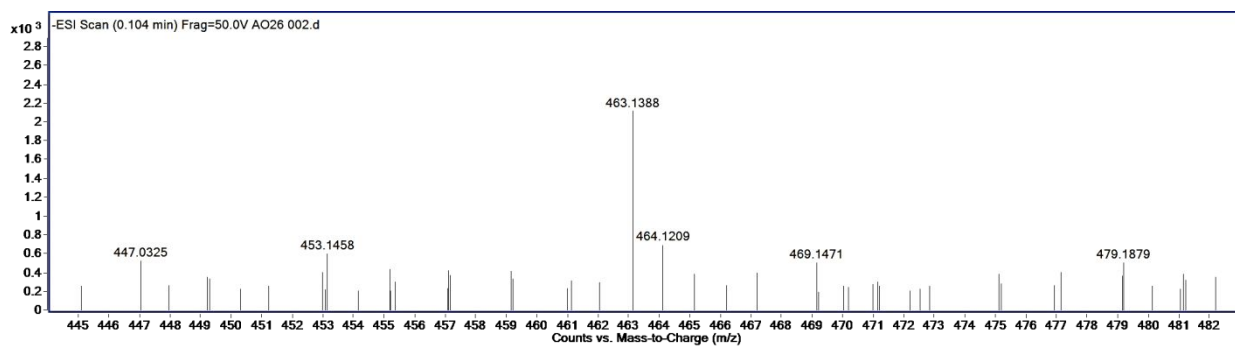


Figure S13. HR-ESI-MS spectrum of compound **2**

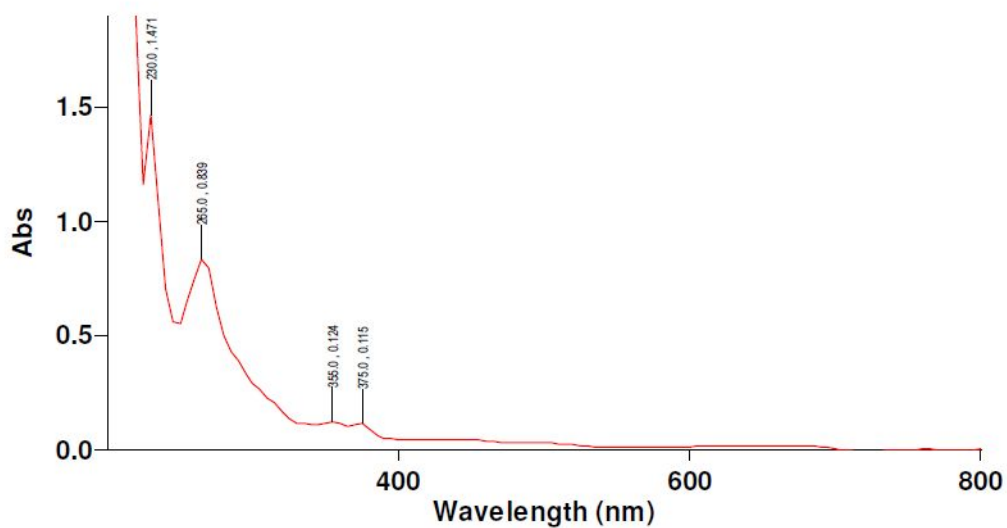


Figure S14. UV spectrum of compound **2** (0.125 mg in 3 ml of methanol)

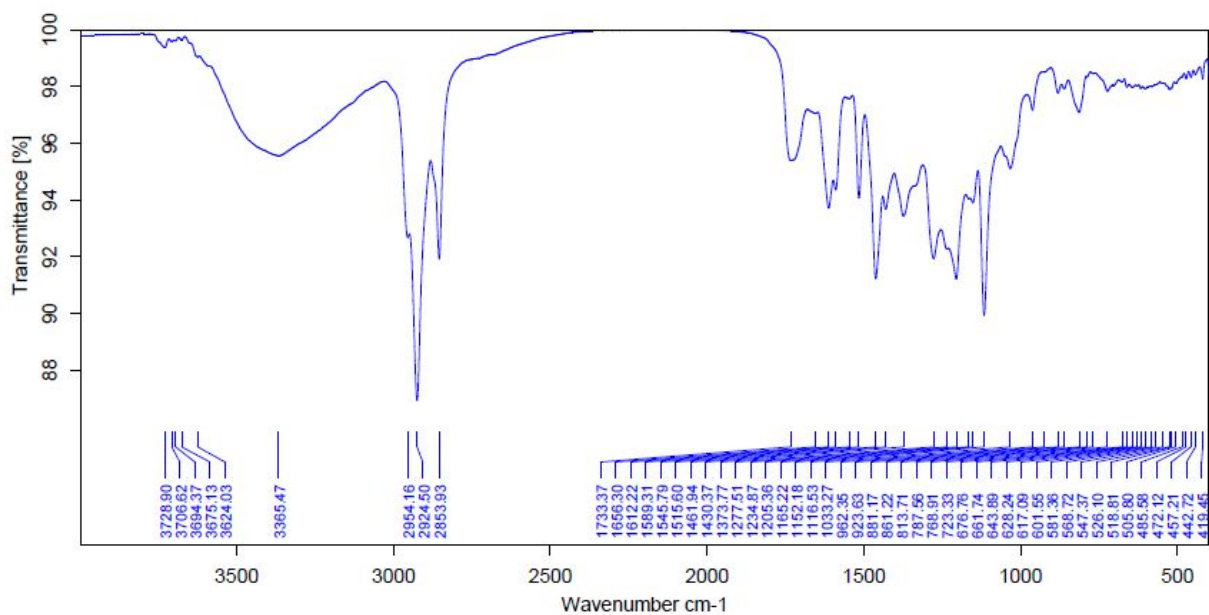


Figure S15. FT-IR spectrum of compound 2

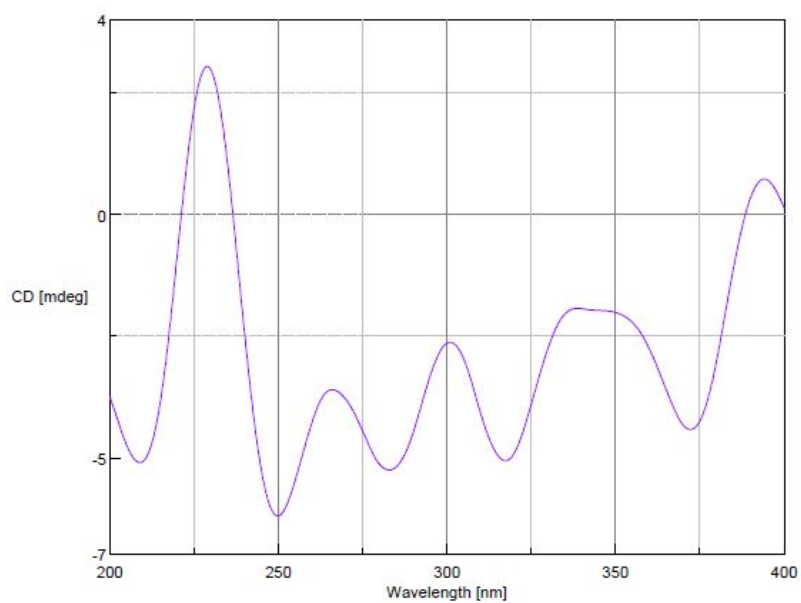


Figure S16. CD spectrum of compound 2

C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1 0
C	4	B4	3	A3	2	D2 0
C	5	B5	4	A4	3	D3 0
C	3	B6	2	A5	1	D4 0
C	4	B7	3	A6	2	D5 0
C	8	B8	4	A7	3	D6 0
C	7	B9	3	A8	2	D7 0
C	9	B10	8	A9	4	D8 0
H	11	B11	9	A10	8	D9 0
C	11	B12	9	A11	8	D10 0
C	13	B13	11	A12	9	D11 0
C	14	B14	13	A13	11	D12 0
H	7	B15	3	A14	2	D13 0
H	6	B16	5	A15	4	D14 0
H	10	B17	7	A16	3	D15 0
H	15	B18	14	A17	13	D16 0
O	1	B19	2	A18	3	D17 0
C	20	B20	1	A19	2	D18 0
H	21	B21	20	A20	1	D19 0
C	2	B22	1	A21	20	D20 0
H	23	B23	2	A22	1	D21 0
C	21	B24	20	A23	1	D22 0
H	25	B25	21	A24	20	D23 0
H	25	B26	21	A25	20	D24 0
O	25	B27	21	A26	20	D25 0
H	28	B28	25	A27	21	D26 0
C	23	B29	2	A28	1	D27 0
C	30	B30	23	A29	2	D28 0
C	30	B31	23	A30	2	D29 0
C	31	B32	30	A31	23	D30 0
H	31	B33	30	A32	23	D31 0
C	32	B34	30	A33	23	D32 0
H	32	B35	30	A34	23	D33 0
C	33	B36	31	A35	30	D34 0
O	33	B37	31	A36	30	D35 0
O	35	B38	32	A37	30	D36 0
O	37	B39	33	A38	31	D37 0
H	40	B40	37	A39	33	D38 0
C	38	B41	33	A40	31	D39 0
H	42	B42	38	A41	33	D40 0
H	42	B43	38	A42	33	D41 0
H	42	B44	38	A43	33	D42 0
C	39	B45	35	A44	32	D43 0
H	46	B46	39	A45	35	D44 0
H	46	B47	39	A46	35	D45 0
H	46	B48	39	A47	35	D46 0
O	14	B49	13	A48	11	D47 0
H	50	B50	14	A49	13	D48 0
O	13	B51	11	A50	9	D49 0
H	52	B52	13	A51	11	D50 0
O	5	B53	4	A52	3	D51 0
C	54	B54	5	A53	4	D52 0
H	55	B55	54	A54	5	D53 0
H	55	B56	54	A55	5	D54 0
H	55	B57	54	A56	5	D55 0

B1	1.37542395	A1	120.16056618	D1	-1.68326996
B2	1.40864322	A2	120.08276924	D2	1.31347947
B3	1.43796292	A3	116.75389548	D3	-0.38151929
B4	1.43934672	A4	122.30429067	D4	177.92911525
B5	1.39243896	A5	119.73012988	D5	-179.14491628
B6	1.43251663	A6	118.50573845	D6	-1.09274682
B7	1.46202669	A7	118.69201018	D7	179.92141031
B8	1.43303366	A8	121.05165997	D8	-179.93708695
B9	1.35799400	A9	120.59547628	D9	179.89842637
B10	1.41553603	A10	118.97910966	D10	-0.19187852
B11	1.08672598	A11	120.95476702	D11	-0.00985419
B12	1.37461872	A12	119.21358033	D12	0.12519241
B13	1.41414664	A13	120.73697973	D13	0.07787432
B14	1.37997814	A14	118.48368822	D14	179.87386808
B15	1.08339776	A15	121.97449781	D15	179.80773056
B16	1.08023547	A16	120.44085248	D16	-179.89591962
B17	1.08640117	A17	117.37162889	D17	-178.25455740
B18	1.07624349	A18	114.36824762	D18	-6.48828114
B19	1.36361944	A19	107.26656185	D19	-107.05613843
B20	1.45911436	A20	106.72089772	D20	-1.16034012
B21	1.09523484	A21	108.81830502	D21	-107.86394629
B22	1.51321688	A22	110.10678623	D22	134.21144696
B23	1.09884165	A23	109.83503661	D23	-172.70533396
B24	1.51085860	A24	107.69354334	D24	-56.09957371
B25	1.10076341	A25	108.73614799	D25	66.03712940
B26	1.09994893	A26	108.79682435	D26	-178.36954924
B27	1.42029552	A27	107.65366576	D27	128.99613210
B28	0.96614543	A28	116.45365766	D28	142.27240945
B29	1.51566678	A29	120.13963227	D29	-40.49133686
B30	1.39411269	A30	120.53027179	D30	178.57649235
B31	1.39649055	A31	120.72105022	D31	-1.85298262
B32	1.39850205	A32	121.06885282	D32	-178.67239968
B33	1.08501900	A33	120.63908469	D33	2.44021362
B34	1.39468783	A34	120.88360240	D34	0.36793810
B35	1.08438181	A35	120.15677837	D35	176.66077965
B36	1.40569105	A36	116.50452957	D36	-176.21000994
B37	1.36862364	A37	116.61734852	D37	170.88744648
B38	1.36912534	A38	120.37275565	D38	94.02849333
B39	1.38623677	A39	109.96947714	D39	136.01038763
B40	0.96803038	A40	118.30514336	D40	-156.39603197
B41	1.43318583	A41	106.07389380	D41	84.47259125
B42	1.09146794	A42	111.56233233	D42	-38.14288898
B43	1.09214307	A43	110.91161630	D43	-135.14340095
B44	1.09534244	A44	118.27846642	D44	-84.28377386
B45	1.43301073	A45	111.54956063	D45	156.64238328
B46	1.09225471	A46	106.08474917	D46	38.39093143
B47	1.09146809	A47	110.94769482	D47	-179.84218906
B48	1.09547425	A48	119.55787184	D48	0.14200130
B49	1.36538767	A49	107.55874189	D49	-179.93410443
B50	0.97020386	A50	125.79560184	D50	0.37339485
B51	1.36946095	A51	110.29738078	D51	179.53091280
B52	0.96691081	A52	117.25949487	D52	-179.79393639
B53	1.36181057	A53	119.33984423	D53	61.14189461
B54	1.42451526	A54	111.31985332	D54	-61.26173452
B55	1.09528626	A55	111.31518441	D55	179.94134885
B56	1.09527843	A56	105.63522799		
B57	1.08971940				

Figure S17. z-matrix coordinates of the optimized structures SS2 of compound **2**

RR2

C

C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	0
C	4	B4	3	A3	2	D2	0
C	5	B5	4	A4	3	D3	0
C	3	B6	2	A5	1	D4	0
C	4	B7	3	A6	2	D5	0
C	8	B8	4	A7	3	D6	0
C	7	B9	3	A8	2	D7	0
C	9	B10	8	A9	4	D8	0
H	11	B11	9	A10	8	D9	0
C	11	B12	9	A11	8	D10	0
C	13	B13	11	A12	9	D11	0
C	14	B14	13	A13	11	D12	0
H	7	B15	3	A14	2	D13	0
H	6	B16	5	A15	4	D14	0
H	10	B17	7	A16	3	D15	0
H	15	B18	14	A17	13	D16	0
O	1	B19	2	A18	3	D17	0
C	20	B20	1	A19	2	D18	0
H	21	B21	20	A20	1	D19	0
C	2	B22	1	A21	20	D20	0
H	23	B23	2	A22	1	D21	0
C	21	B24	20	A23	1	D22	0
H	25	B25	21	A24	20	D23	0
H	25	B26	21	A25	20	D24	0
O	25	B27	21	A26	20	D25	0
H	28	B28	25	A27	21	D26	0
C	23	B29	2	A28	1	D27	0
C	30	B30	23	A29	2	D28	0
C	30	B31	23	A30	2	D29	0
C	31	B32	30	A31	23	D30	0
H	31	B33	30	A32	23	D31	0
C	32	B34	30	A33	23	D32	0
H	32	B35	30	A34	23	D33	0
C	33	B36	31	A35	30	D34	0
O	33	B37	31	A36	30	D35	0
O	35	B38	32	A37	30	D36	0
O	37	B39	33	A38	31	D37	0
H	40	B40	37	A39	33	D38	0
C	38	B41	33	A40	31	D39	0
H	42	B42	38	A41	33	D40	0
H	42	B43	38	A42	33	D41	0
H	42	B44	38	A43	33	D42	0
C	39	B45	35	A44	32	D43	0
H	46	B46	39	A45	35	D44	0
H	46	B47	39	A46	35	D45	0
H	46	B48	39	A47	35	D46	0
O	14	B49	13	A48	11	D47	0
H	50	B50	14	A49	13	D48	0
O	13	B51	11	A50	9	D49	0
H	52	B52	13	A51	11	D50	0
O	5	B53	4	A52	3	D51	0
C	54	B54	5	A53	4	D52	0
H	55	B55	54	A54	5	D53	0
H	55	B56	54	A55	5	D54	0
H	55	B57	54	A56	5	D55	0

RR2

B1	1.37542395	A1	120.16056618	D1	1.68326996
B2	1.40864322	A2	120.08276924	D2	-1.31347947
B3	1.43796292	A3	116.75389548	D3	0.38156327
B4	1.43934672	A4	122.30430803	D4	-
B5	1.39243903	A5	119.73012988	D5	177.92911525
B6	1.43251663	A6	118.50573845	D6	179.14491628
B7	1.46202669	A7	118.69201018	D7	-
B8	1.43303366	A8	121.05164146	D8	179.92136635
B9	1.35799389	A9	120.59547628	D9	-
B10	1.41553603	A10	118.97910966	D10	179.89842637
B11	1.08672598	A11	120.95476702	D11	0.19187852
B12	1.37461872	A12	119.21358033	D12	0.00985419
B13	1.41414664	A13	120.73697973	D13	-0.12519241
B14	1.37997814	A14	118.48368822	D14	-0.07787432
B15	1.08339776	A15	121.97451006	D15	-
B16	1.08023417	A16	120.44085031	D16	179.87383370
B17	1.08640205	A17	117.37162889	D17	-
B18	1.07624349	A18	114.36822970	D18	179.89591962
B19	1.36361941	A19	107.26657536	D19	178.25451570
B20	1.45911436	A20	106.72086858	D20	6.48831071
B21	1.09523566	A21	108.81830502	D21	107.05608798
B22	1.51321688	A22	110.10678623	D22	1.16029842
B23	1.09884165	A23	109.83503661	D23	107.86394629
B24	1.51085860	A24	107.69352755	D24	-
B25	1.10076267	A25	108.73608312	D25	134.21148861
B26	1.09994930	A26	108.79678985	D26	172.70530079
B27	1.42029598	A27	107.65361789	D27	56.09960458
B28	0.96614494	A28	116.45365766	D28	-66.03713922
B29	1.51566678	A29	120.13960289	D29	178.36949711
B30	1.39411329	A30	120.53027179	D30	-
B31	1.39649055	A31	120.72098410	D31	128.99613210
B32	1.39850237	A32	121.06887912	D32	-
B33	1.08501854	A33	120.63906622	D33	142.27239264
B34	1.39468841	A34	120.88360240	D34	40.49133686
B35	1.08438181	A35	120.15681467	D35	-
B36	1.40569105	A36	116.50447847	D36	178.57647658
B37	1.36862300	A37	116.61726941	D37	1.85304829
B38	1.36912519	A38	120.37275824	D38	178.67236707
B39	1.38623594	A39	109.96955749	D39	-2.44021362
B40	0.96803015	A40	118.30513501	D40	-0.36797045
B41	1.43318696	A41	106.07387505	D41	-
B42	1.09146877	A42	111.56237135	D42	176.66076550
B43	1.09214262	A43	110.91155812	D43	176.21001355
B44	1.09534315	A44	118.27842877	D44	-
B45	1.43301212	A45	111.54951180	D45	170.88745661
B46	1.09225486	A46	106.08473806	D46	-94.02847817
B47	1.09146715	A47	110.94765654	D47	-
B48	1.09547296	A48	119.55787184	D48	136.01043878
B49	1.36538767	A49	107.55874189	D49	156.39603027
B50	0.97020386	A50	125.79560184	D50	-84.47250656

RR2

B51 1.36946095	A51 110.29738078	D51 179.53091280
B52 0.96691081	A52 117.25949487	D52 179.79393639
B53 1.36181057	A53 119.33984423	D53 -61.14189461
B54 1.42451526	A54 111.31985332	D54 61.26176622
B55 1.09528626	A55 111.31519014	D55 179.94134885
B56 1.09527925	A56 105.63522799	
B57 1.08971940		

Figure S18. z-matrix coordinates of the optimized structures *RR2* of compound **2**

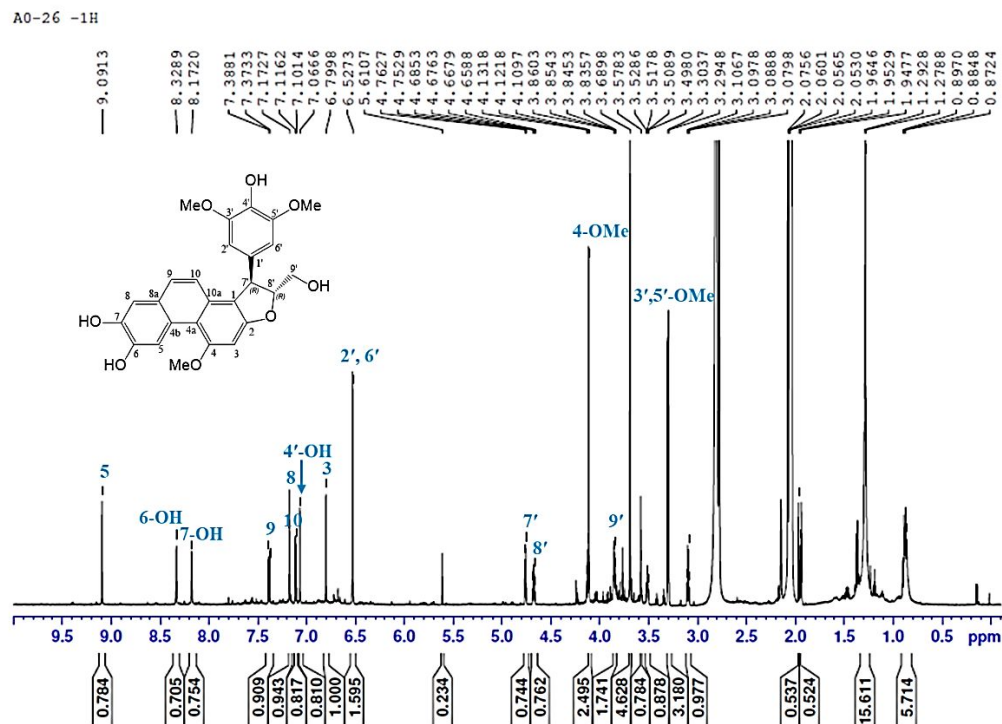
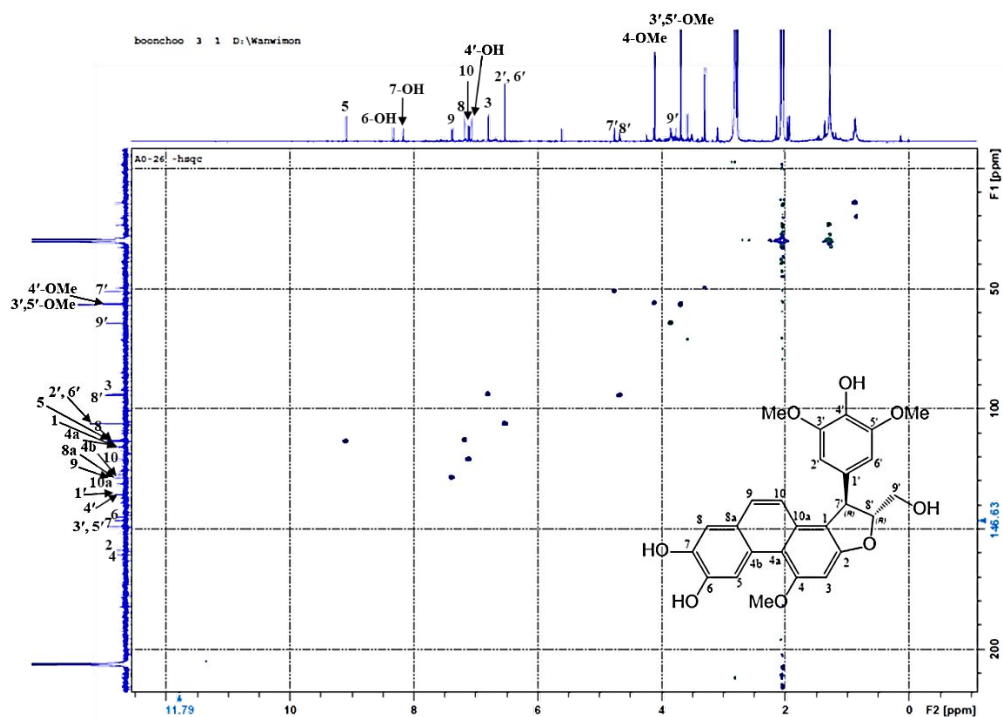
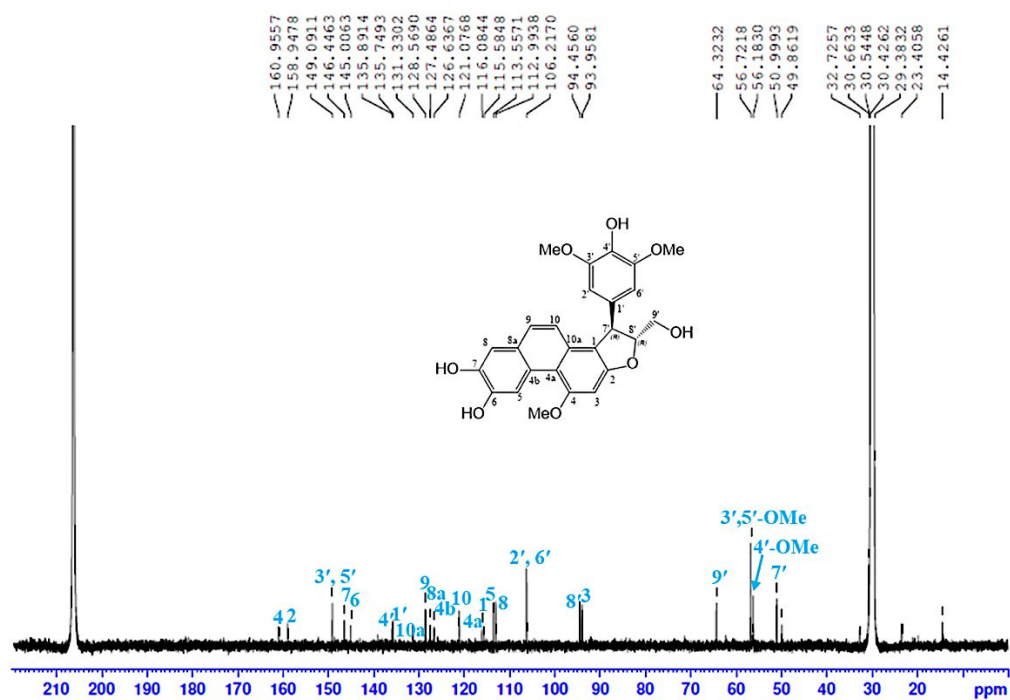


Figure S19. ^1H NMR (acetone- d_6 , 600 MHz) spectrum of compound **2**



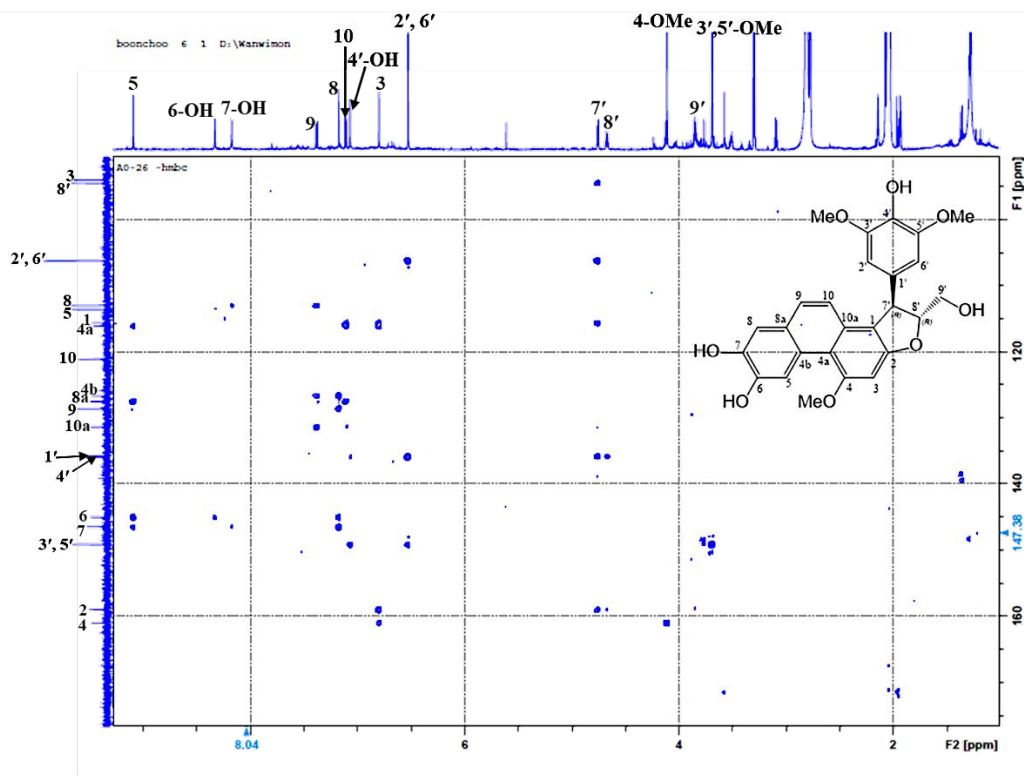


Figure S22. HMBC (acetone- d_6 , 600/150 MHz) spectrum 1 of compound 2

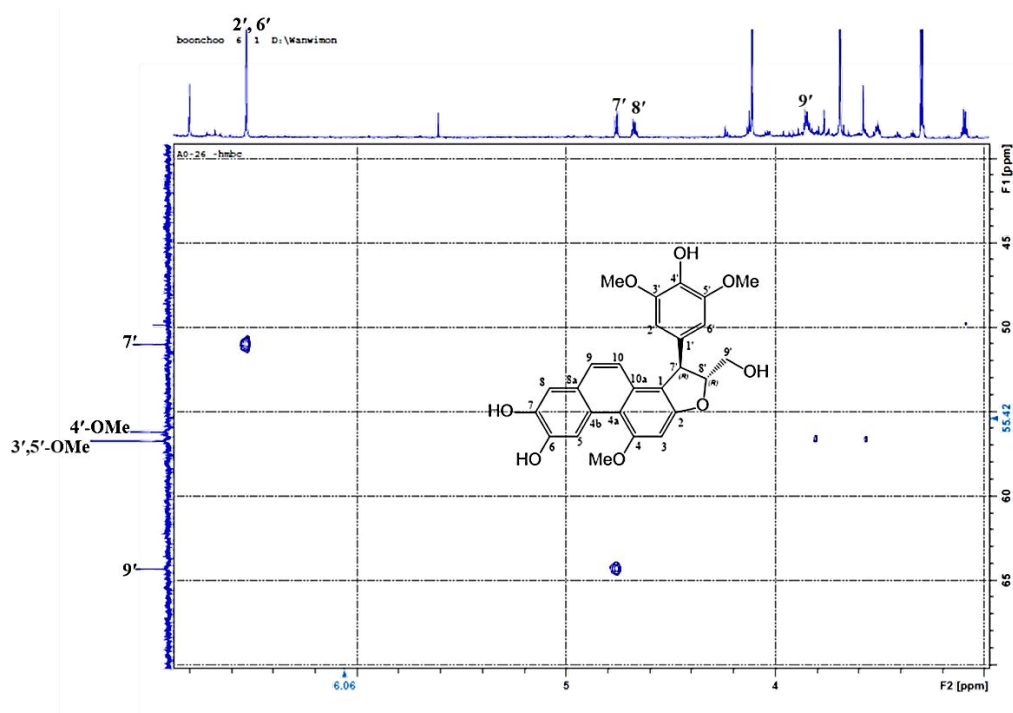


Figure S23. HMBC (acetone- d_6 , 600/150 MHz) spectrum 2 of compound 2

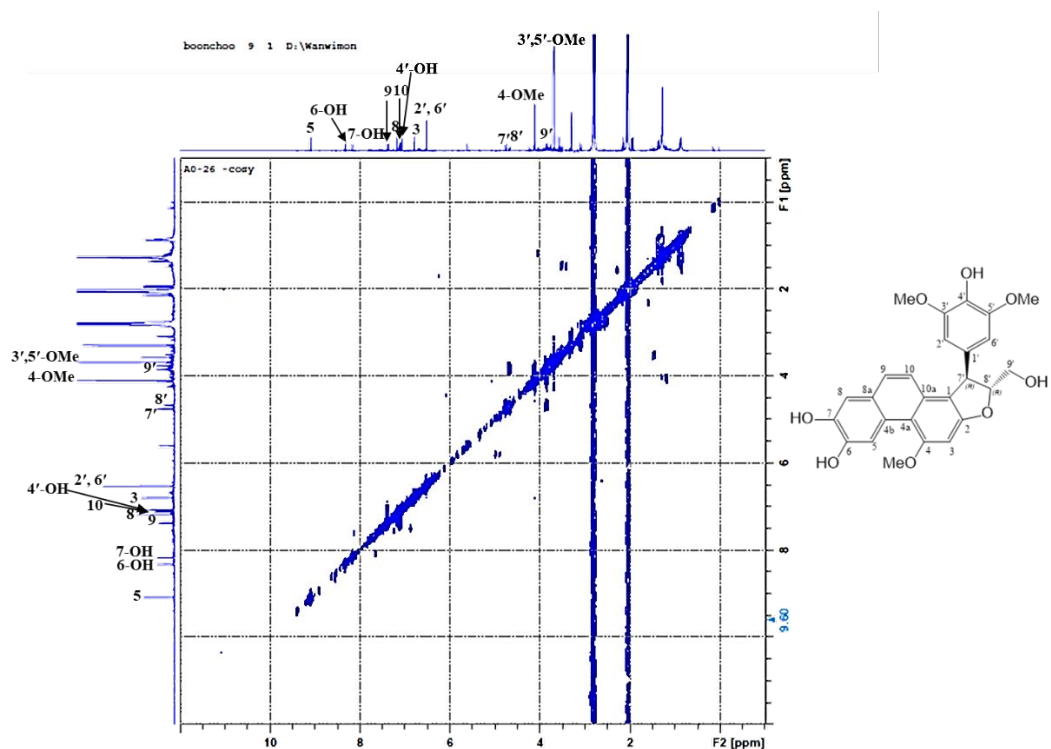


Figure S24. COSY (acetone- d_6 , 600 MHz) spectrum of compound **2**

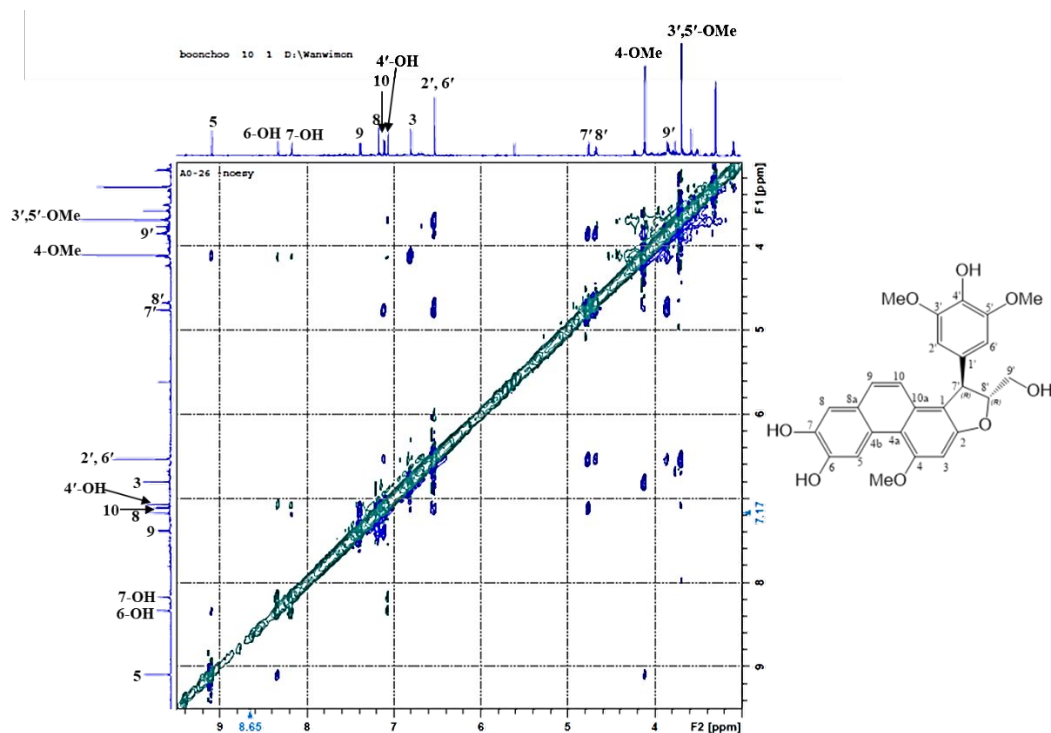


Figure S25. NOESY (acetone- d_6 , 600 MHz) spectrum of compound **2**.

Area Percent Report

Compound2_0.5mg/mL_40%MeOH_formic



Data file: C:\Users\Public\Documents\ChemStation\1\Data\Monsin\Purity180526 2026-05-18 13-24-21\007-P1-B2-Compound2_0.5mg_mL_40%MeOH_for.D

Sample name: Compound2_0.5mg/mL_40%MeOH_formic

Description:

Sample amount: 0.000 **Sample type:** Sample

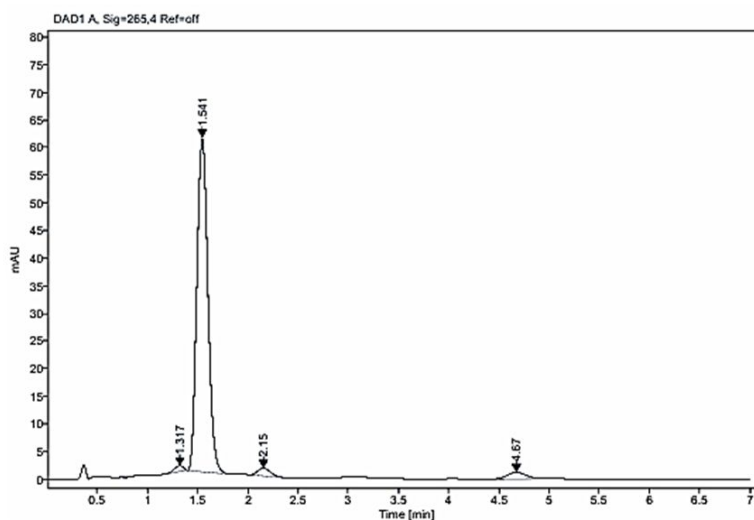
Instrument: LC1290_DAD **Location:** P1-B2

Injection date: 2026-05-18 14:19:02+07:00 **Injection:** 1 of 1

Acq. method: Purity_phenan.M **Injection volume:** 1.000

Analysis method: Purity_phenan.M **Acq. operator:** SYSTEM

Last changed: 2026-05-18 14:04:01+07:00



Signal: DAD1 A, Sig=265,4 Ref=off

RT [min]	Area	Area%
1.317	6.6626	1.3435
1.541	461.1832	92.9972
2.150	12.5886	2.5385
4.670	15.4765	3.1208
Sum	495.9109	

Figure S26. HPLC chromatogram of compound **2**

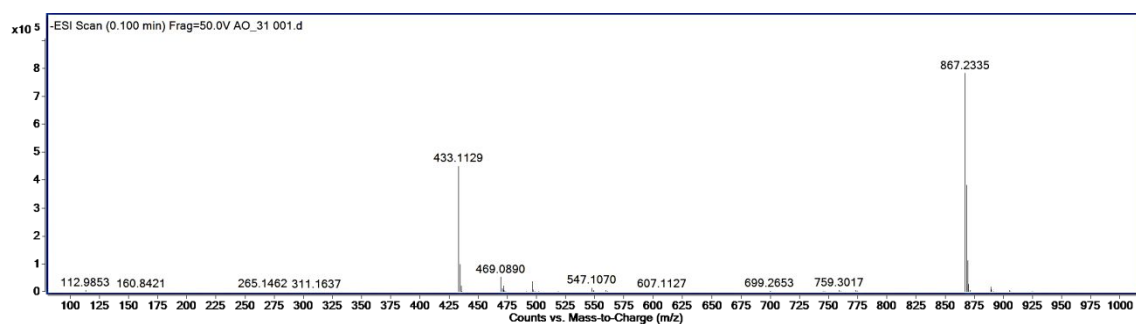


Figure S27. HR-ESI-MS spectrum of compound **3**

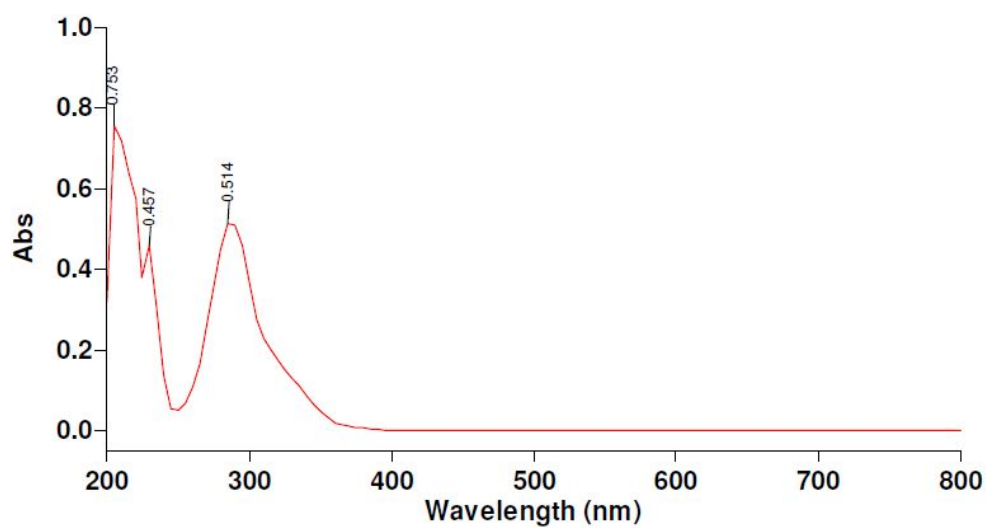


Figure S28. UV spectrum of compound **3** (0.0625 mg per 3 ml of methanol)

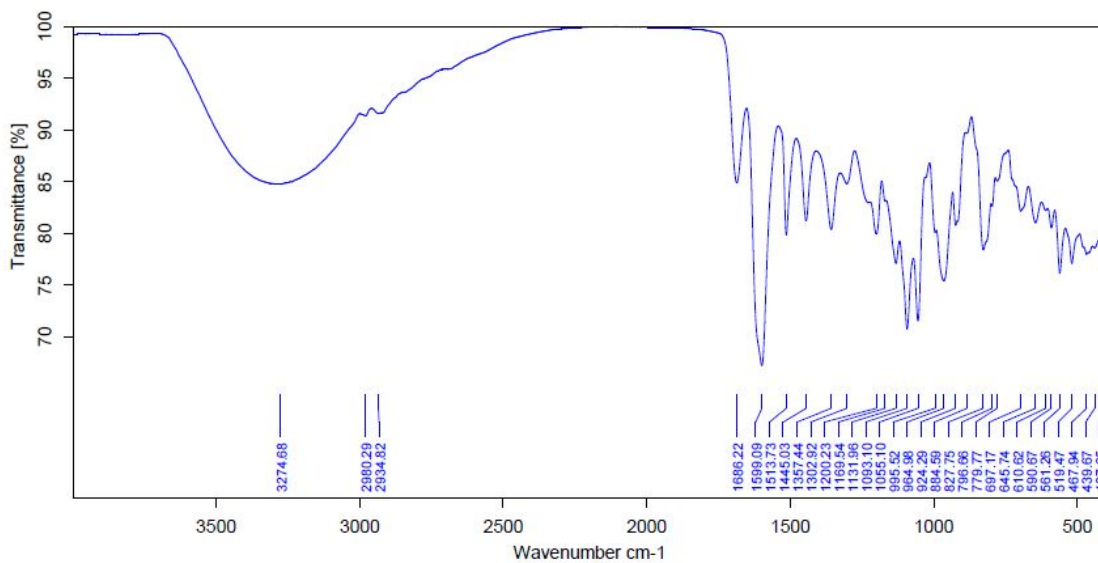


Figure S29. FT-IR spectrum of compound **3**.

AO31 1H NMR 400 MHz in methanol-d₄

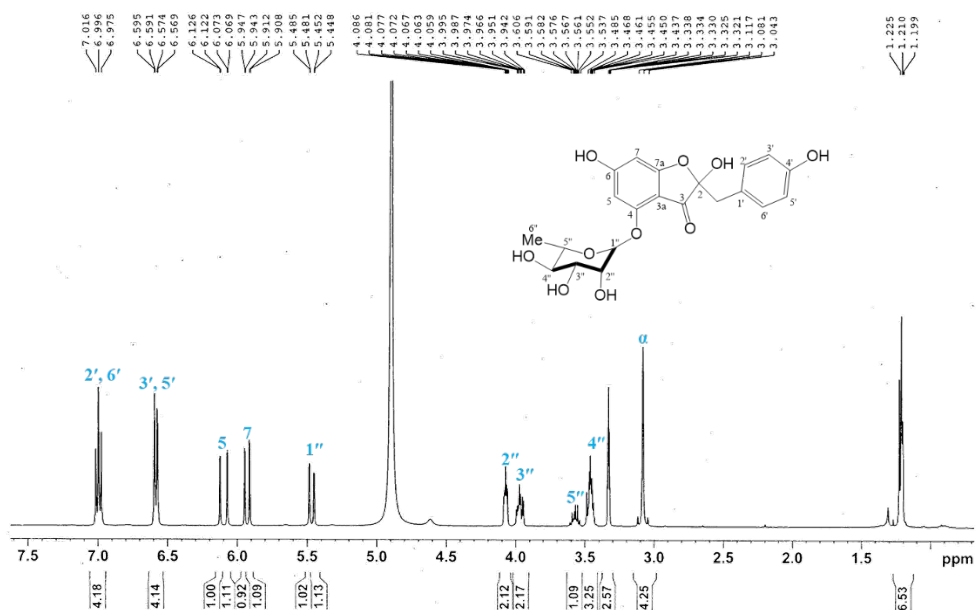


Figure S30. ¹H NMR (methanol-*d*₄, 400 MHz) spectrum of compound **3**

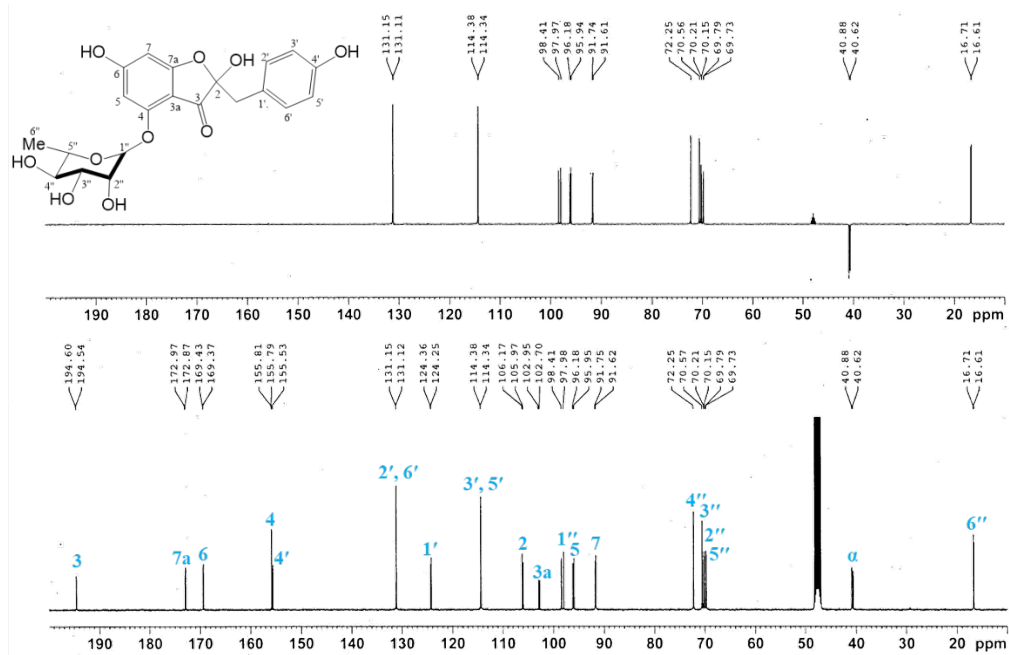


Figure S31. ^{13}C NMR and DEPT (methanol- d_4 , 100 MHz) spectrum of compound 3

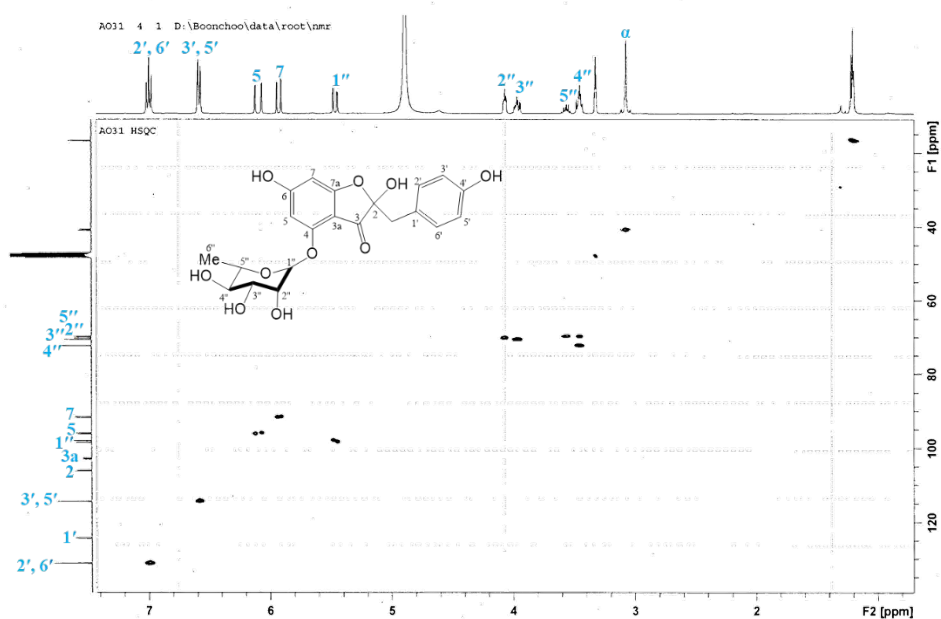


Figure S32. HSQC (methanol- d_4 , 400/100 MHz) spectrum of compound 3.

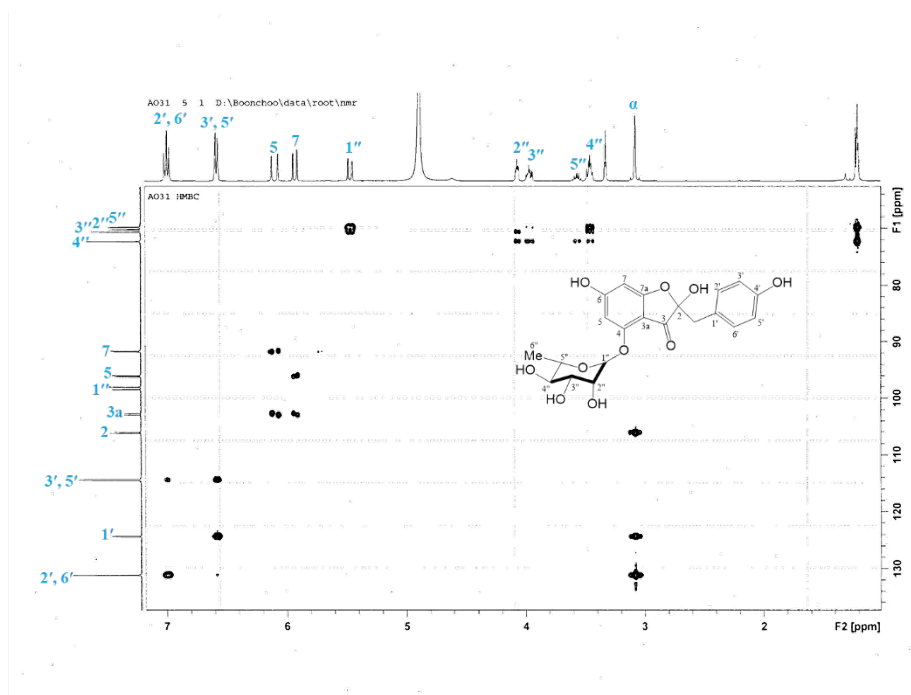


Figure S33. HMBC (methanol- d_4 , 400/100 MHz) spectrum 1 of compound **3**.

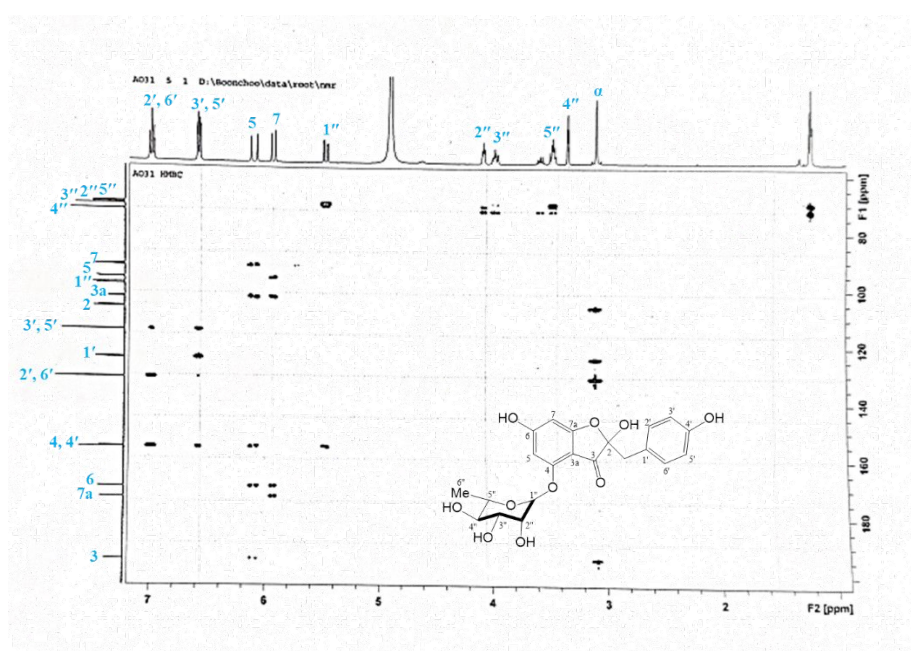


Figure S34. HMBC (methanol- d_4 , 400/100 MHz) spectrum 2 of compound **3**.

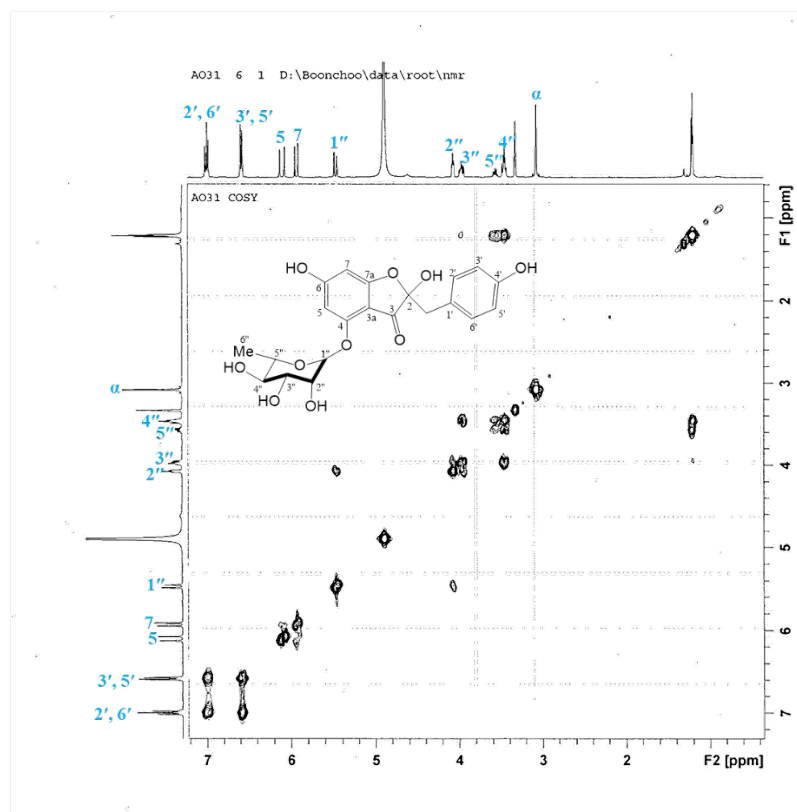


Figure S35. COSY (methanol- d_4 , 400 MHz) spectrum of compound 3.

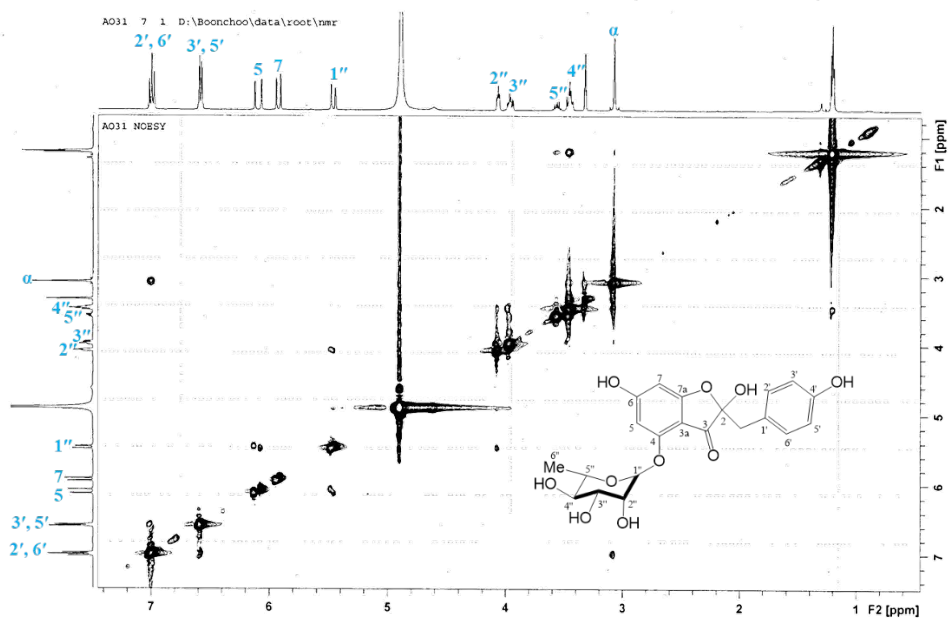


Figure S36. NOESY (methanol- d_4 , 400 MHz) spectrum of compound 3.

Area Percent Report

Compound3_0.05mg/mL_25%MeOH_formic



Data file: C:\Users\Public\Documents\ChemStation\1\Data\Monsin\Purity180526 2026-05-18 14-53-01\001-P1-C3-Compound3_0.05mg_mL_25%MeOH_fo.D

Sample name: Compound3_0.05mg/mL_25%MeOH_formic

Description:

Sample amount: 0.000 **Sample type:** Sample

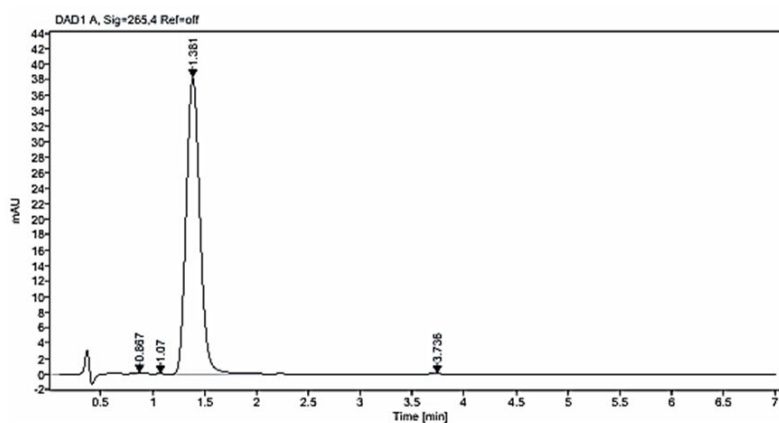
Instrument: LC1290_DAD **Location:** P1-C3

Injection date: 2026-05-18 14:53:56+07:00 **Injection:** 1 of 1

Acq. method: Purity_Phenolic.M **Injection volume:** 1.000

Analysis method: Purity_Phenolic.M **Acq. operator:** SYSTEM

Last changed: 2026-05-18 15:02:57+07:00



Signal: DAD1 A, Sig=265,4 Ref=off

RT [min]	Area	Area%
0.867	0.5403	0.1536
1.070	0.1684	0.0479
1.381	349.6864	99.4044
3.736	1.3864	0.3941
Sum	351.7815	

Figure S37. HPLC chromatogram of compound **3**

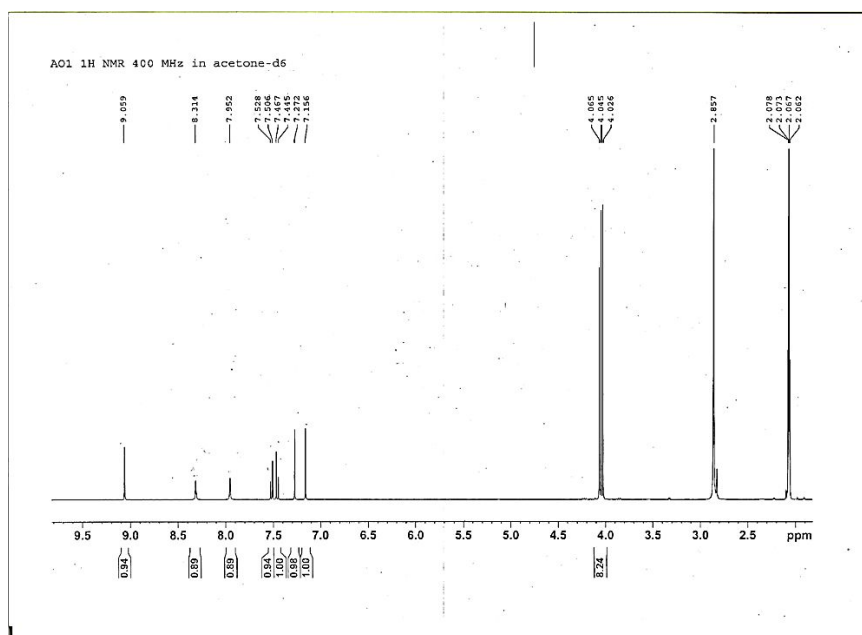


Figure S38. ^1H NMR (acetone- d_6 , 600 MHz) spectrum of compound **4**

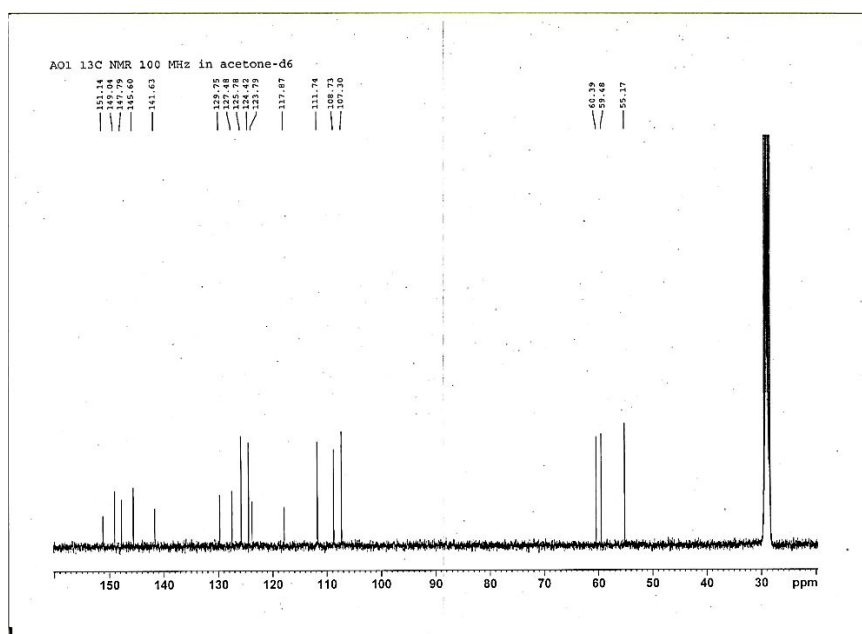
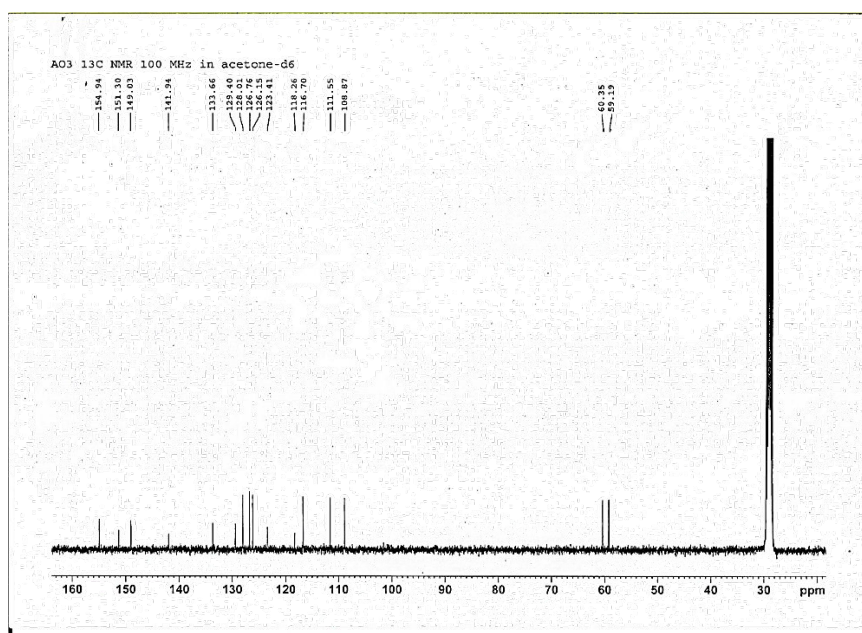
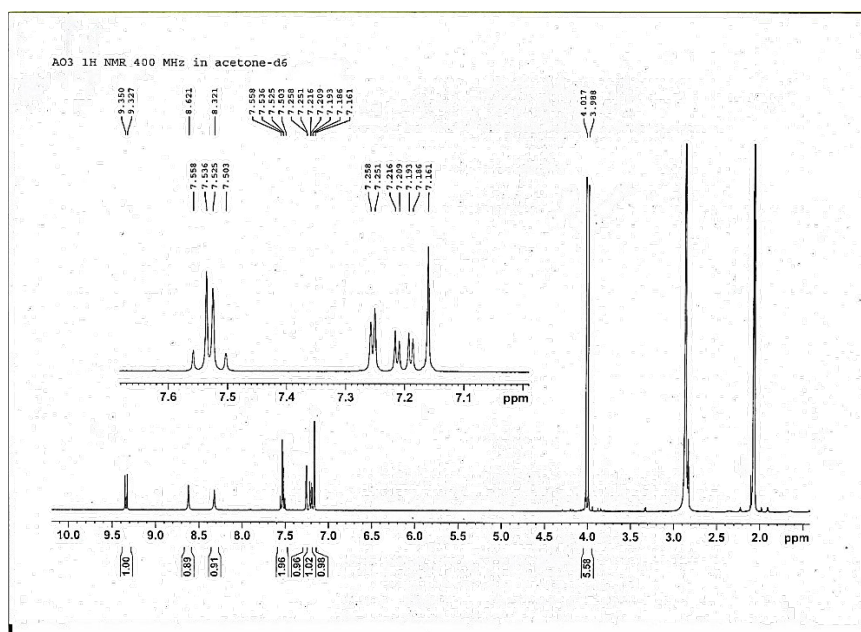


Figure S39. ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of compound **4**



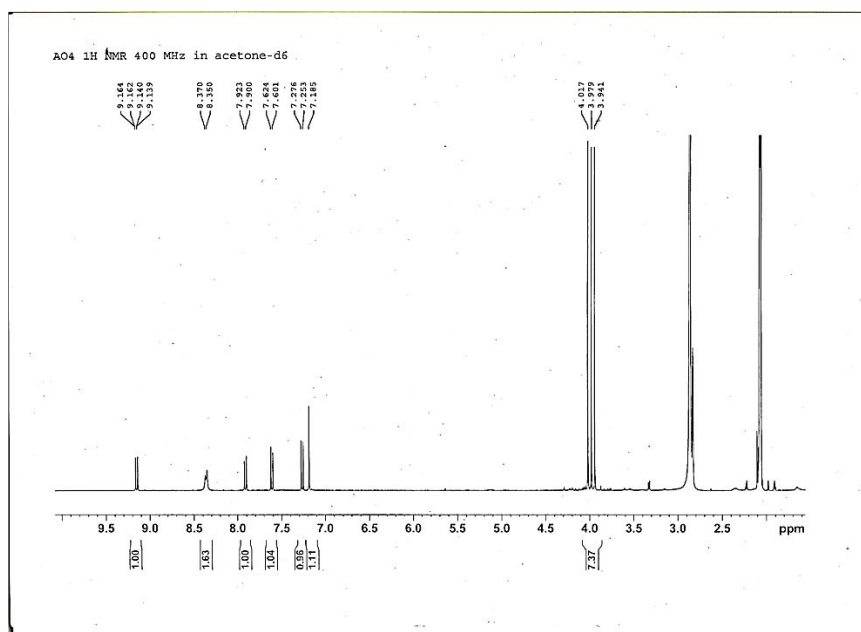


Figure S44. ¹H NMR (acetone- *d*₆, 600 MHz) spectrum of compound **7**

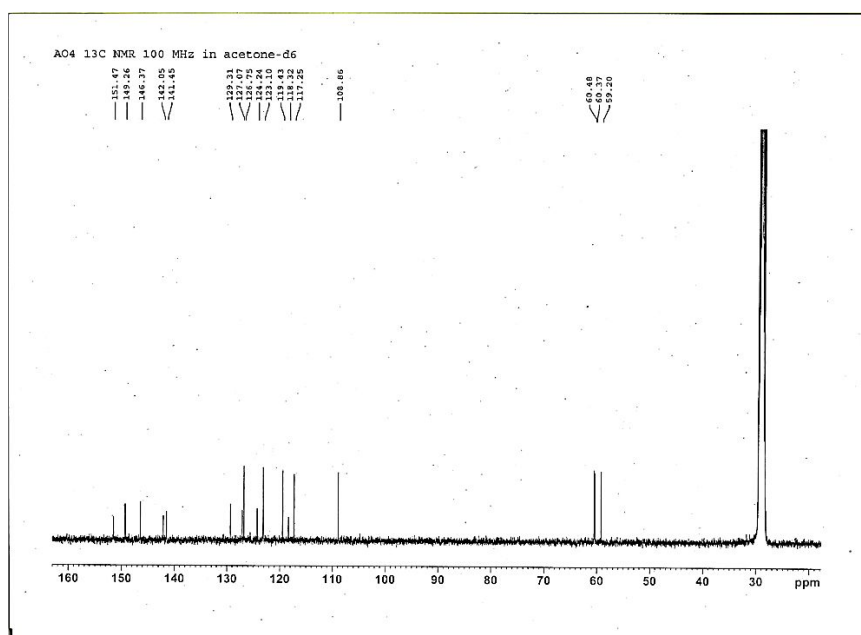


Figure S45. ¹³C NMR (acetone- *d*₆, 150 MHz) spectrum of compound **7**

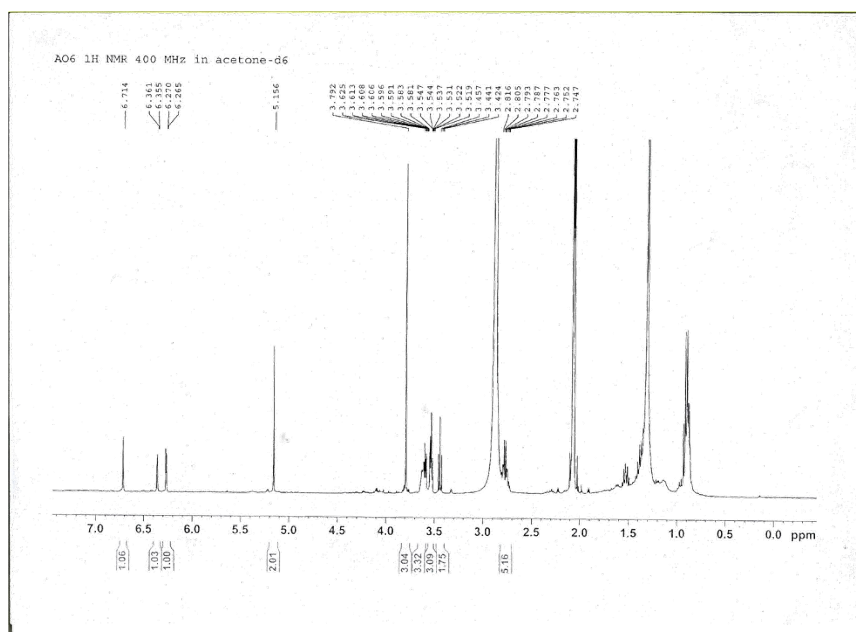


Figure S46. ^1H NMR (acetone- d_6 , 600 MHz) spectrum of compound **8**

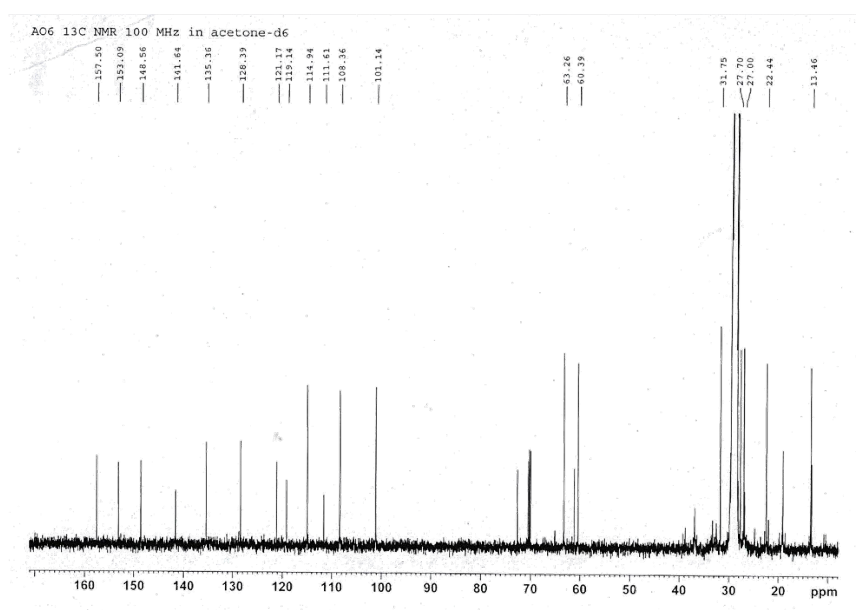


Figure S47. ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of compound **8**

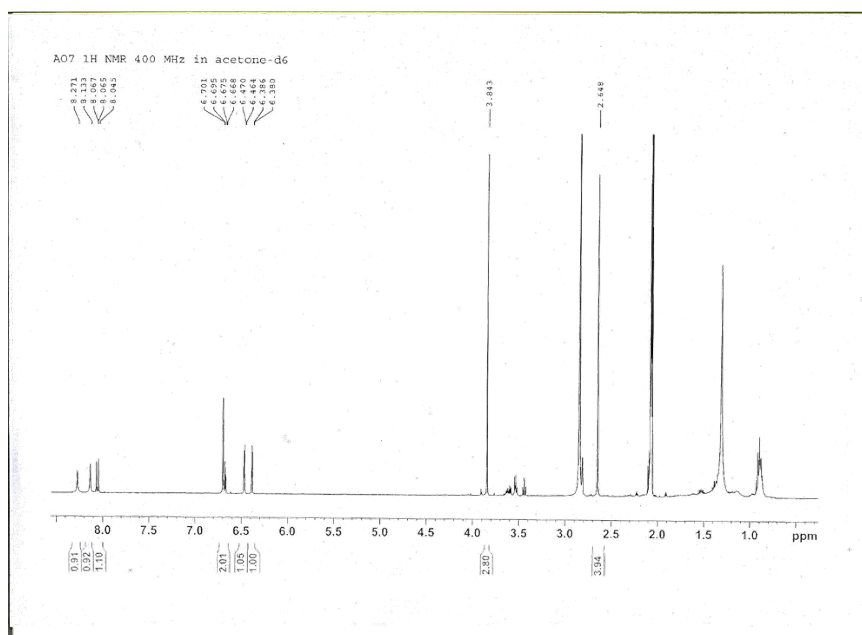


Figure S48. ¹H NMR (acetone- *d*₆, 600 MHz) spectrum of compound **9**

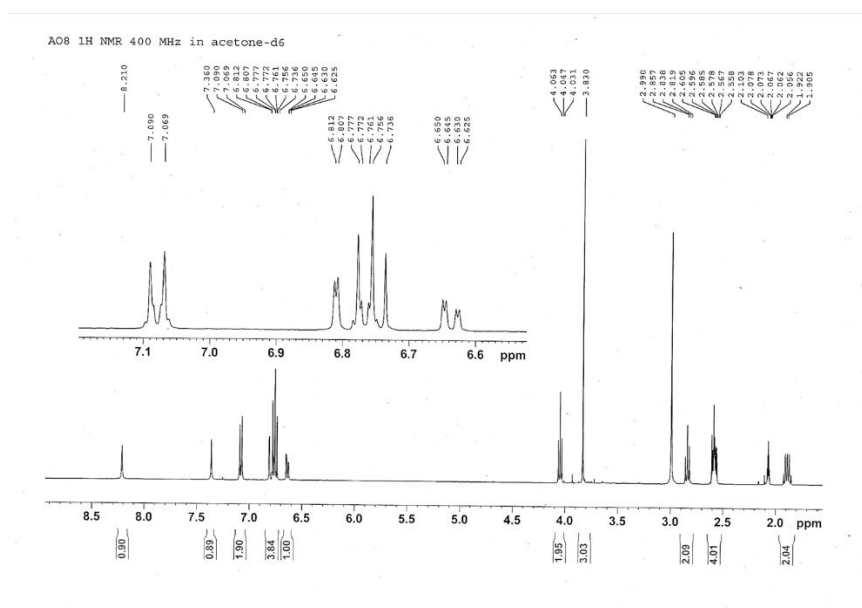
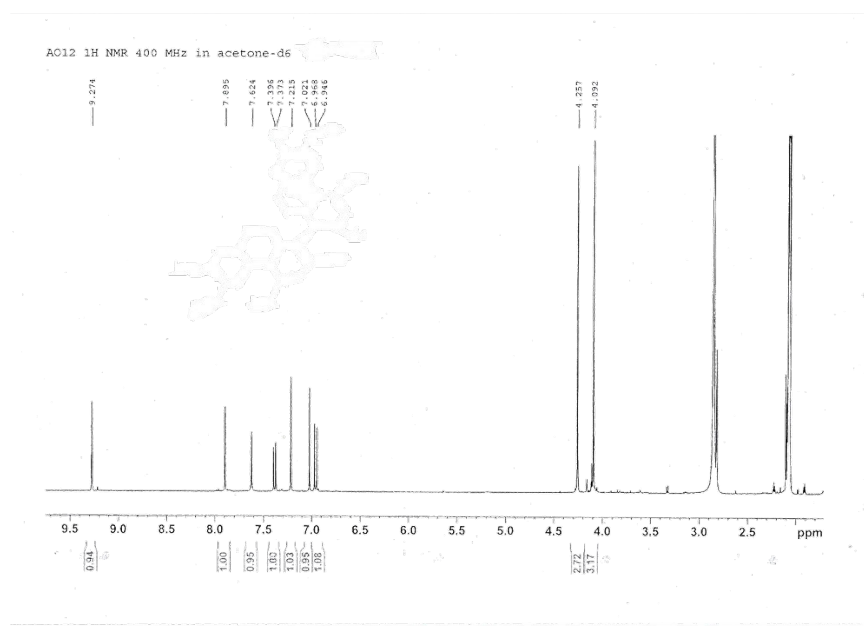
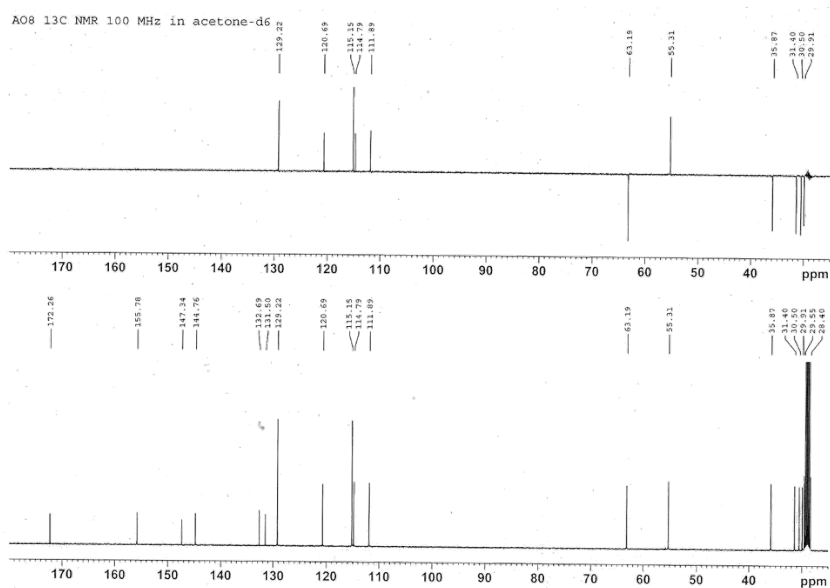


Figure S49. ¹H NMR (acetone- *d*₆, 600 MHz) spectrum of compound **10**



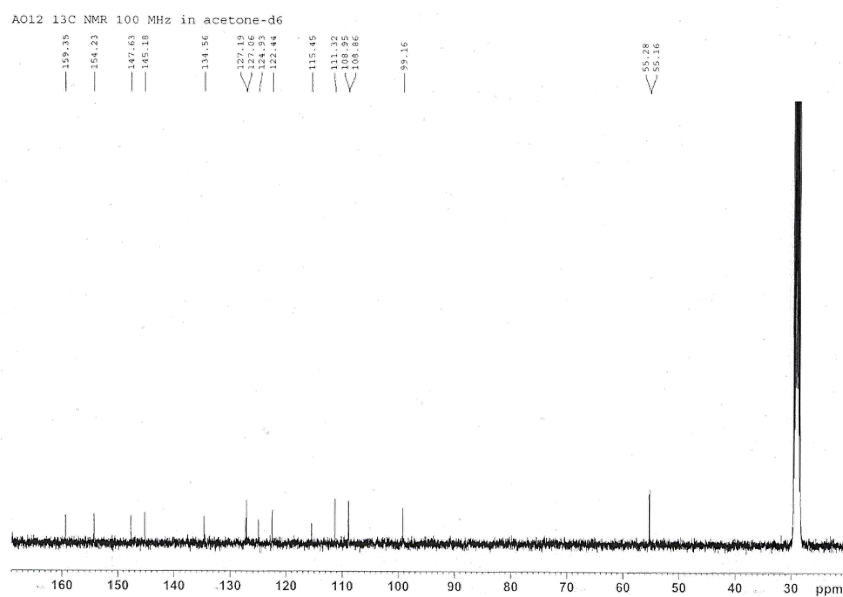


Figure S52. ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of compound **13**

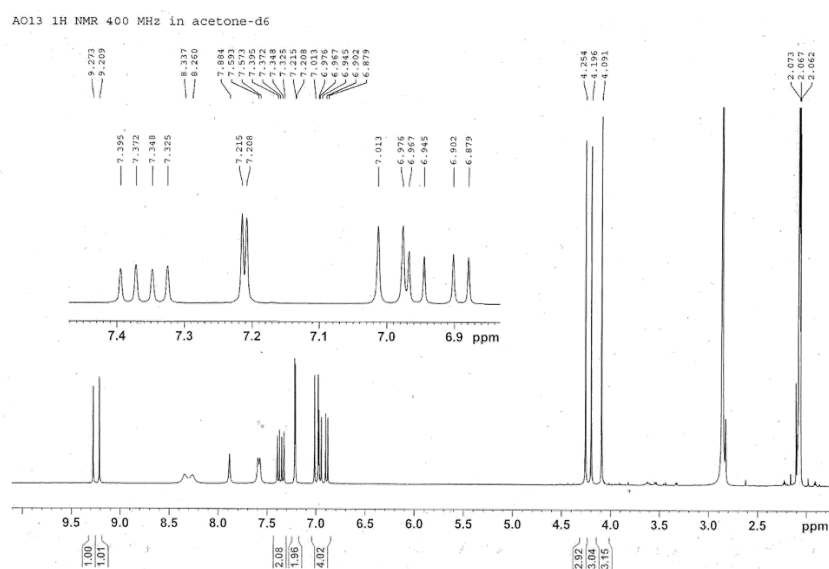


Figure S53. ^1H NMR (acetone- d_6 , 600 MHz) spectrum of compound **14**

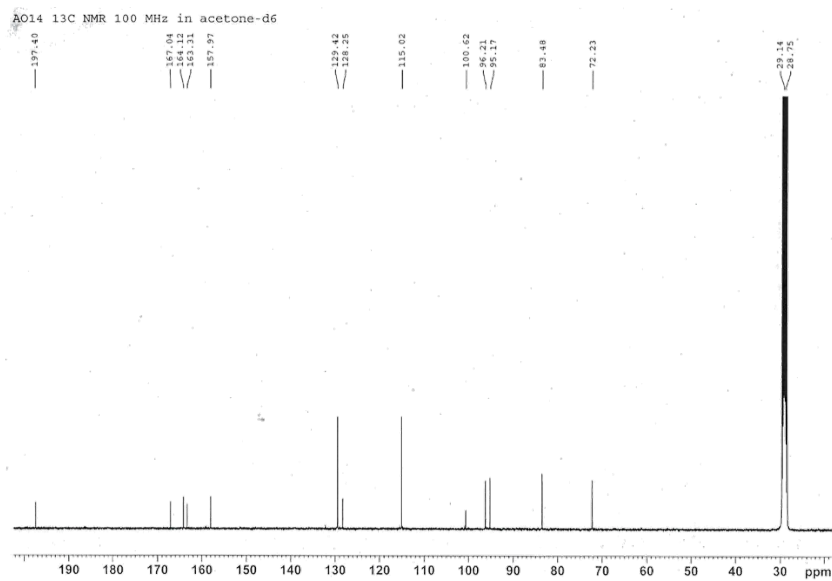


Figure S56. ¹³C NMR (acetone- *d*₆, 150 MHz) spectrum of compound **15**

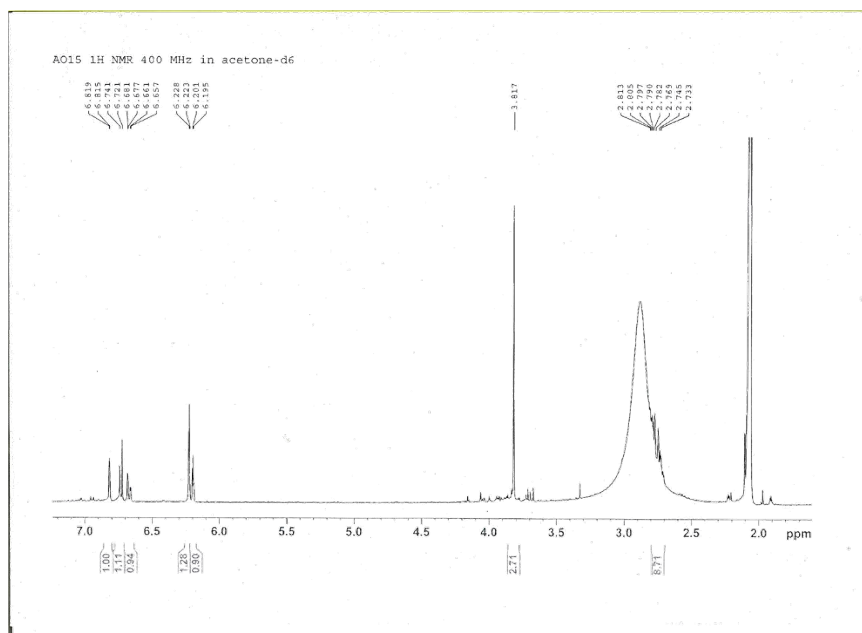


Figure S57. ¹H NMR (acetone- *d*₆, 600 MHz) spectrum of compound **16**

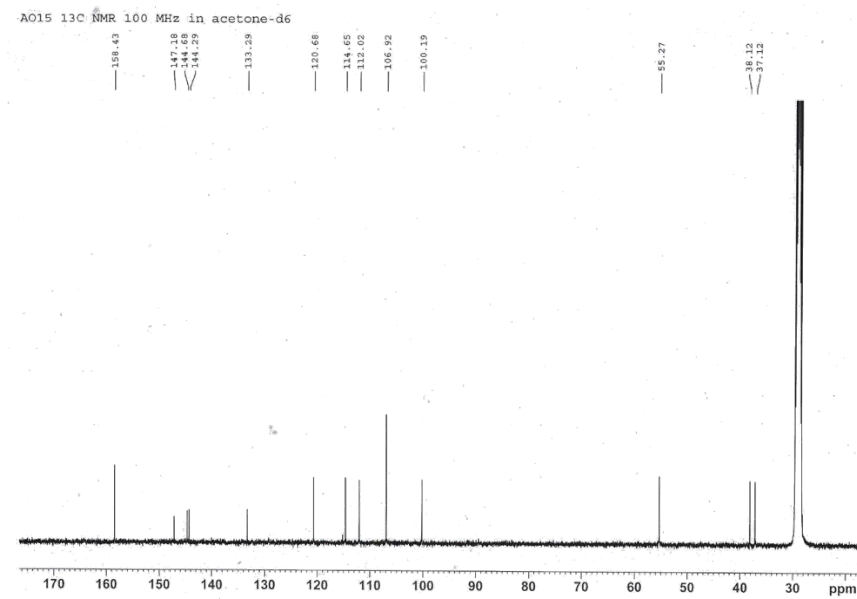


Figure S58. ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of compound **16**

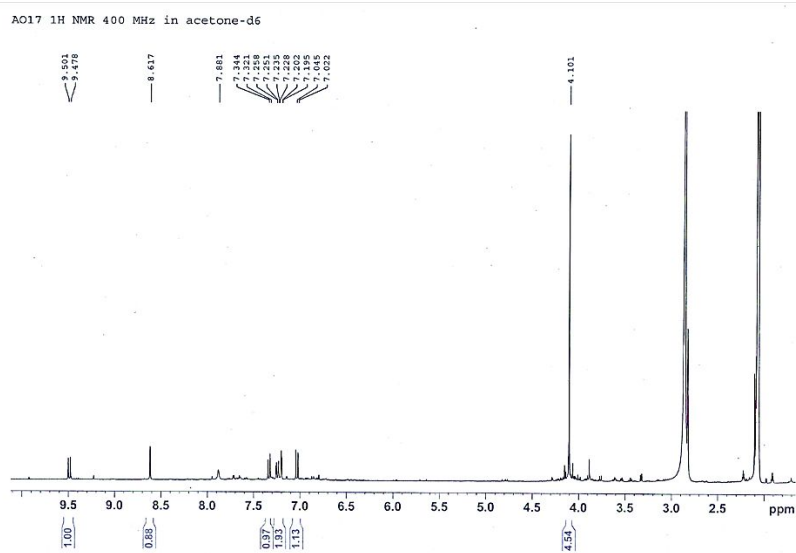


Figure S59. ^1H NMR (acetone- d_6 , 600 MHz) spectrum of compound **17**

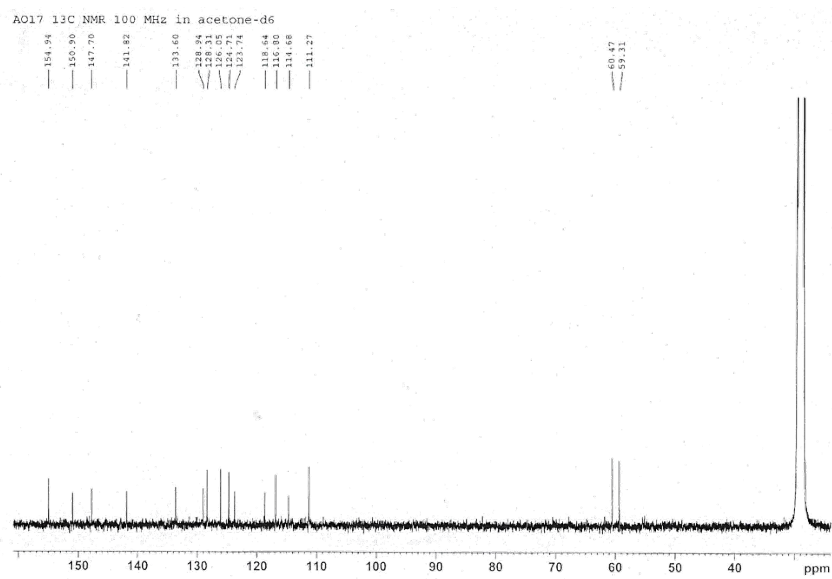


Figure S60. ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of compound **17**

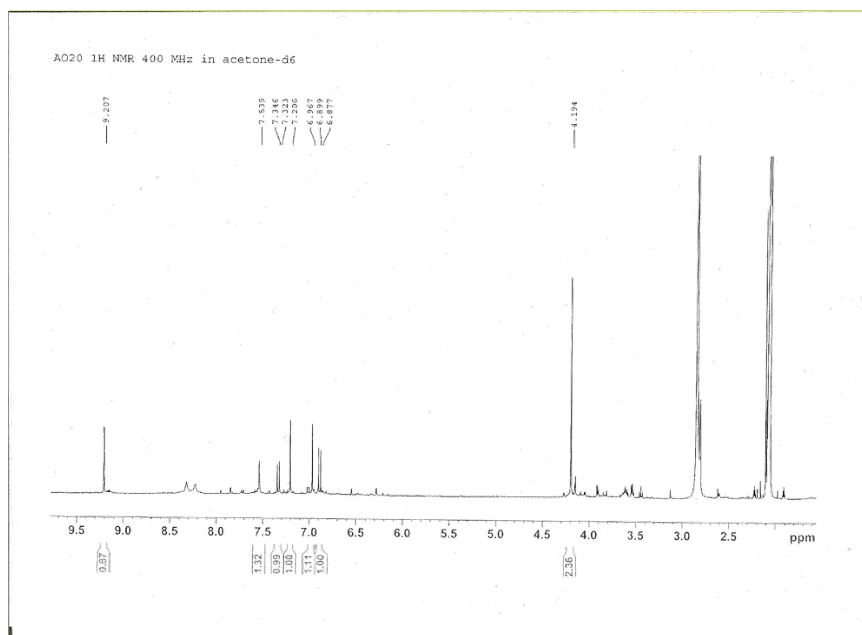


Figure S61. ^1H NMR (acetone- d_6 , 600 MHz) spectrum of compound **18**

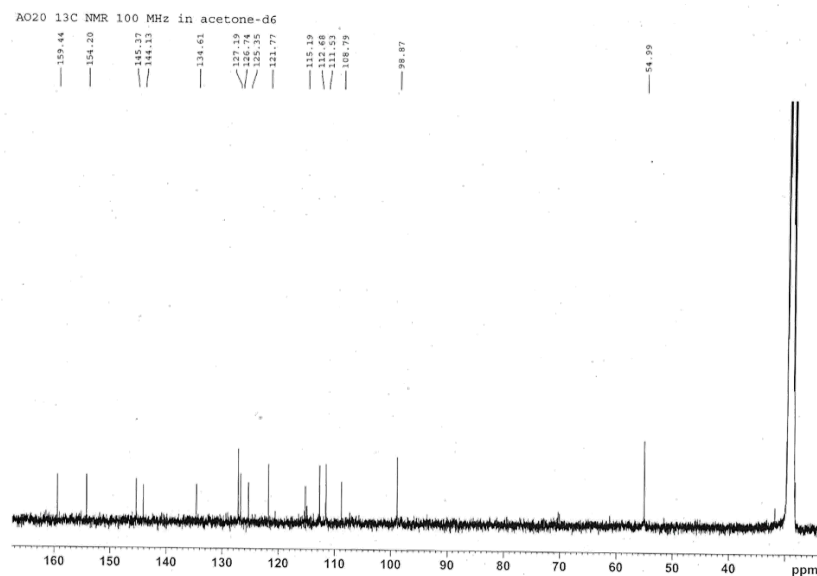


Figure S62. ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of compound **18**

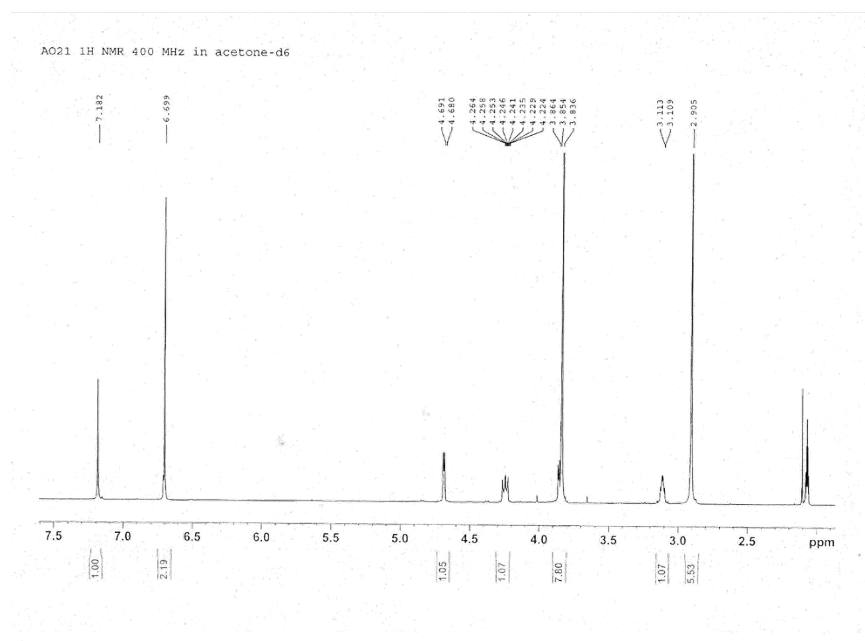


Figure S63. ^1H NMR (acetone- d_6 , 600 MHz) spectrum of compound **19**

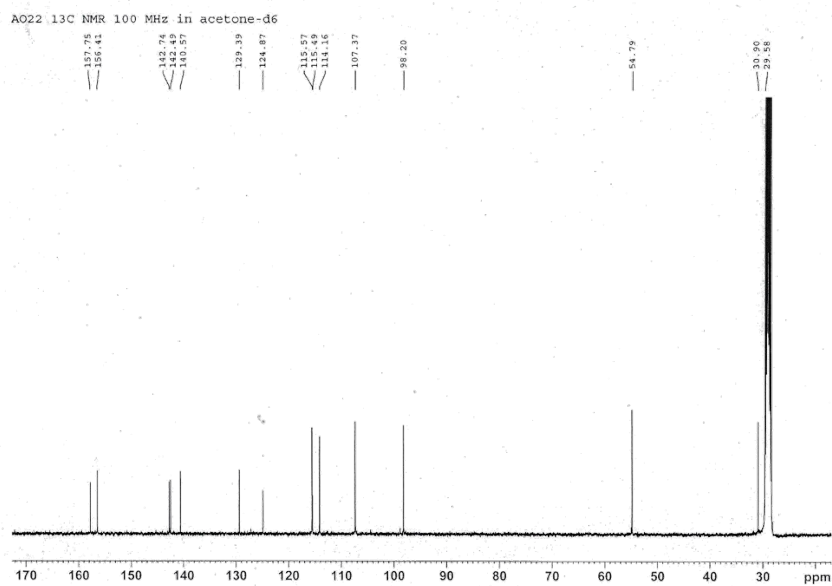


Figure S66. ^{13}C NMR (acetone- d_6 , 150 MHz) spectrum of compound **20**

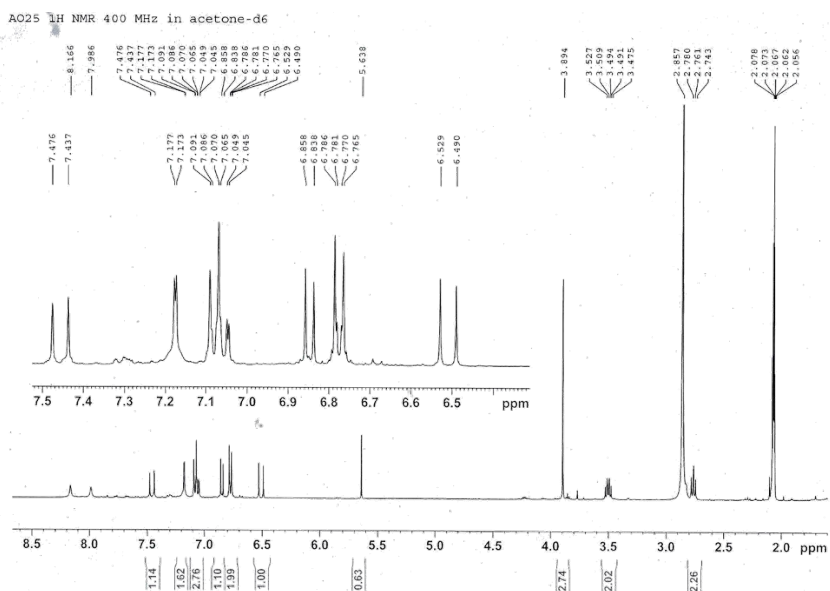


Figure S67. ^1H NMR (acetone- d_6 , 600 MHz) spectrum of compound **21**

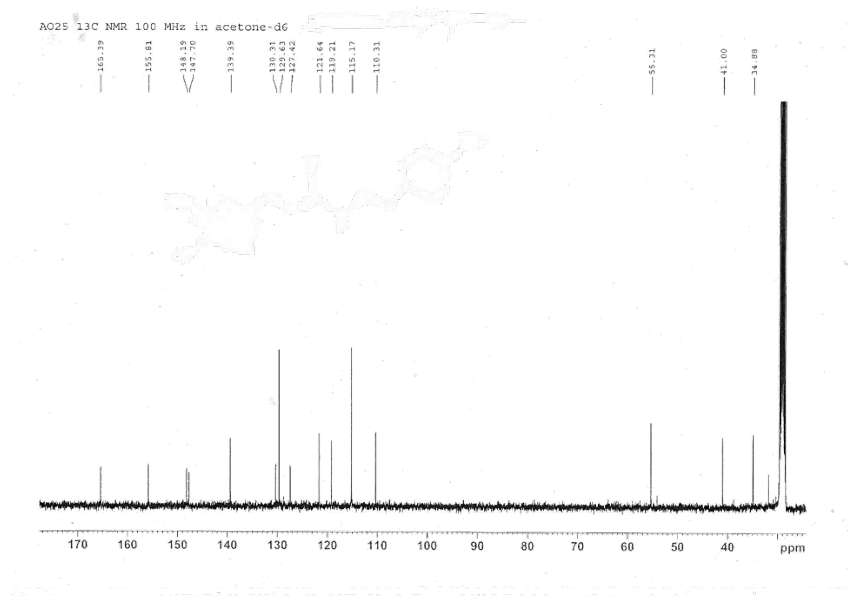


Figure S68. ¹³C NMR (acetone-*d*₆, 150 MHz) spectrum of compound **21**

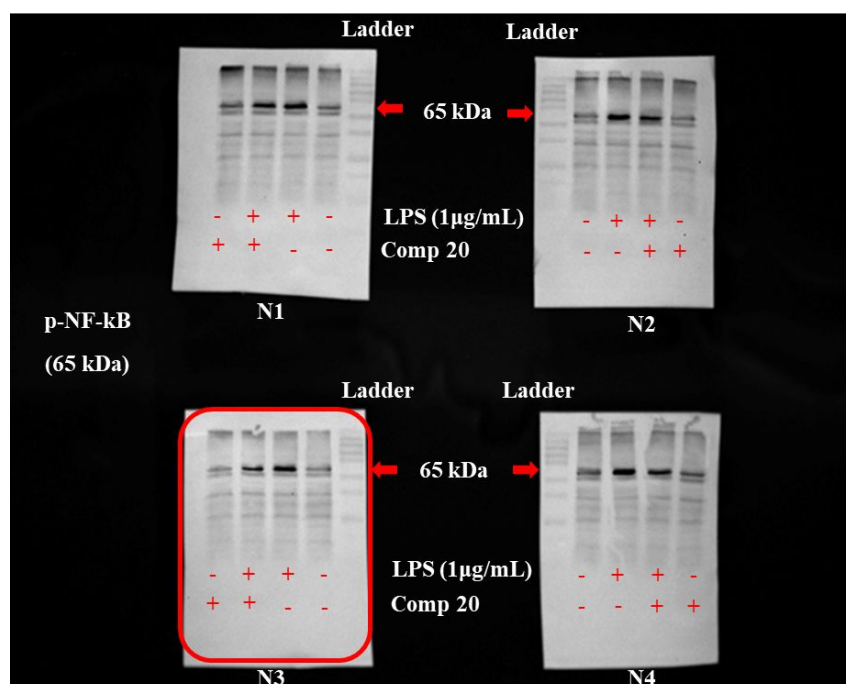


Figure S69. The whole western blots of p-NFκB (n=4)

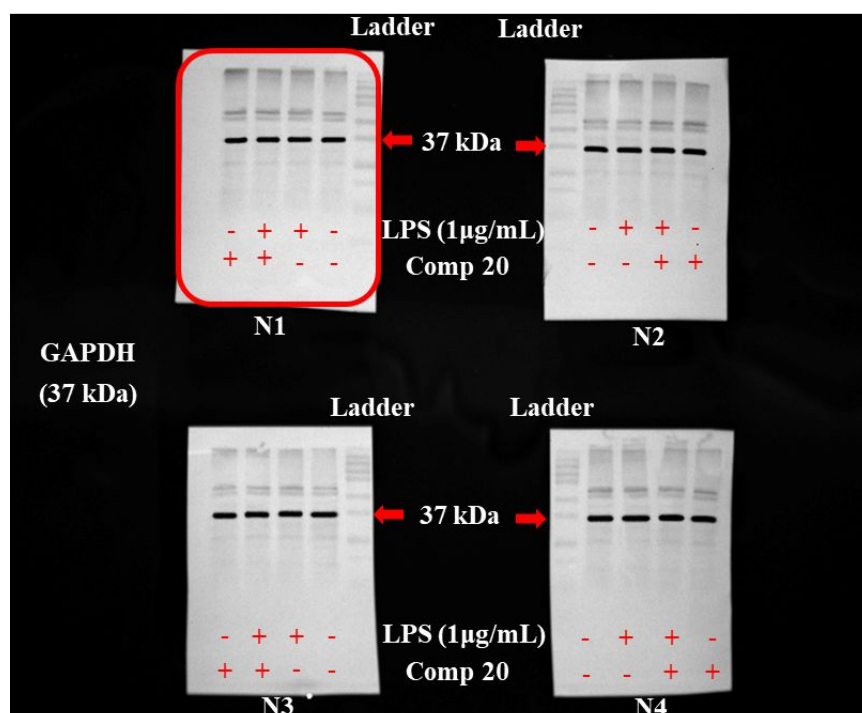


Figure S70. The whole western blots of GAPDH (n=4)

* Red boxes = Representative bands presented in the main figures of the manuscript.

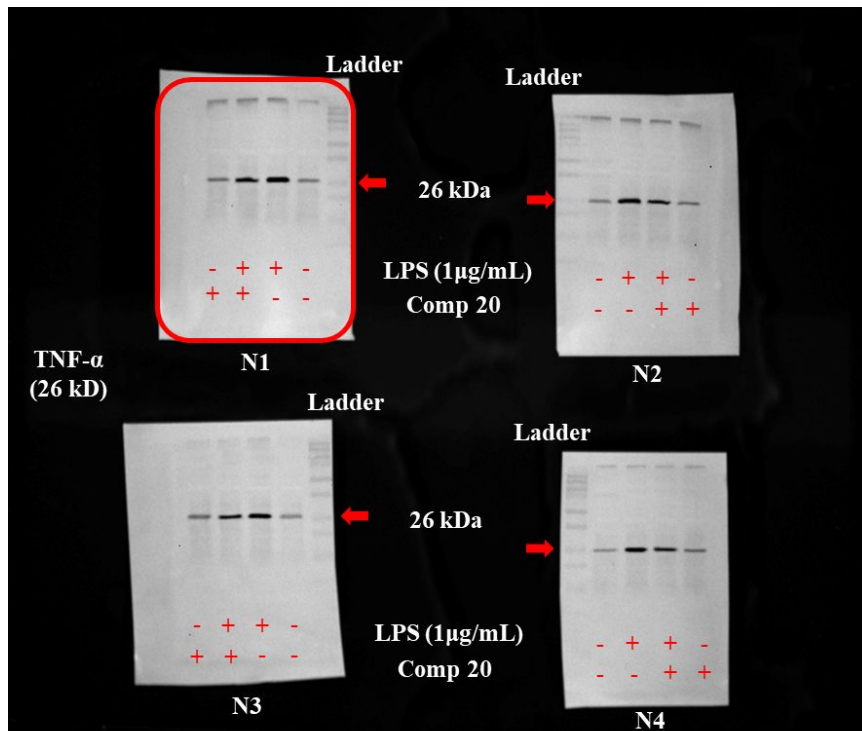


Figure S71. The whole western blots of TNF-α (n=4)

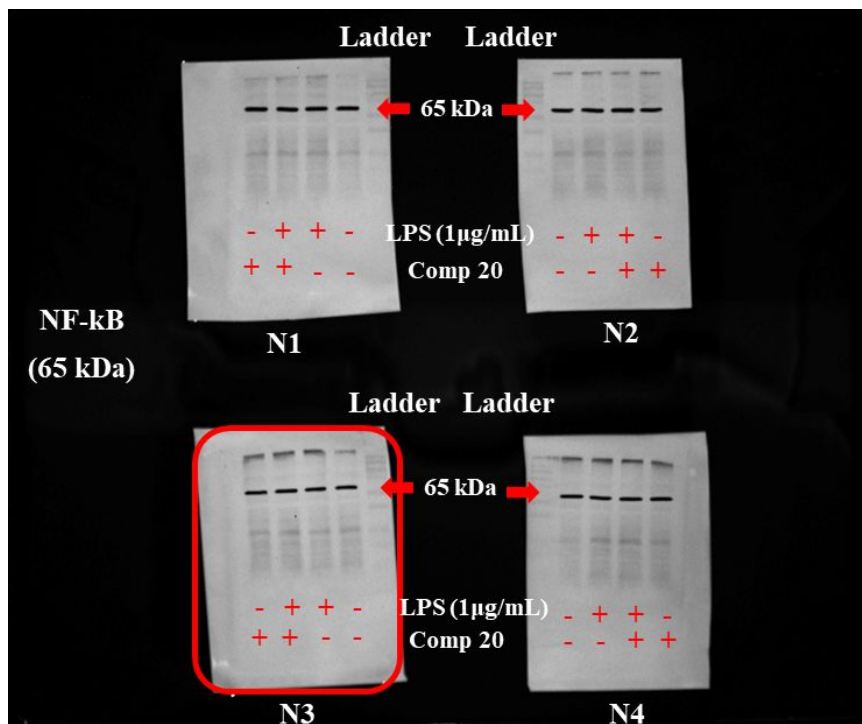


Figure S72. The whole western blots of NF-κB (n=4)

* Red boxes = Representative bands presented in the main figures of the manuscript.