Supporting Information

Prioritization before dereplication, an effective strategy to target new metabolites in whole extract: Ghosalin from *Murraya paniculata* root

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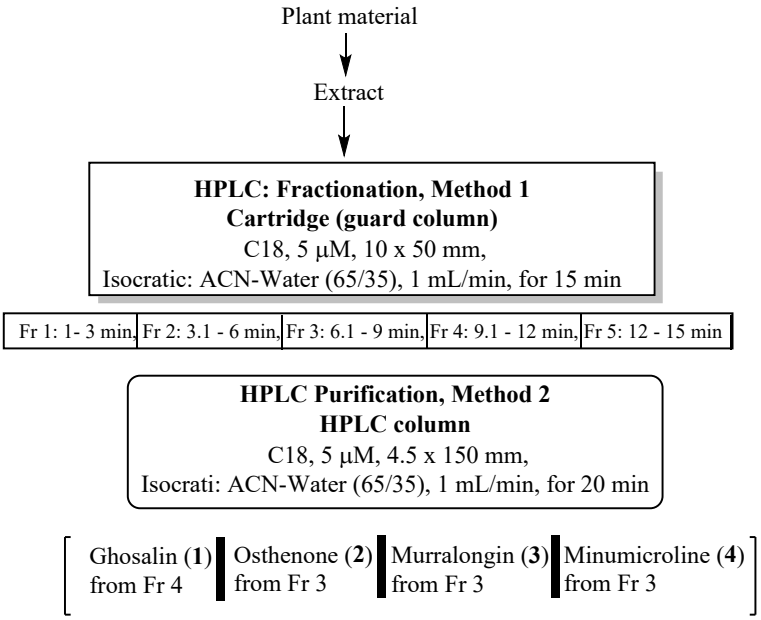
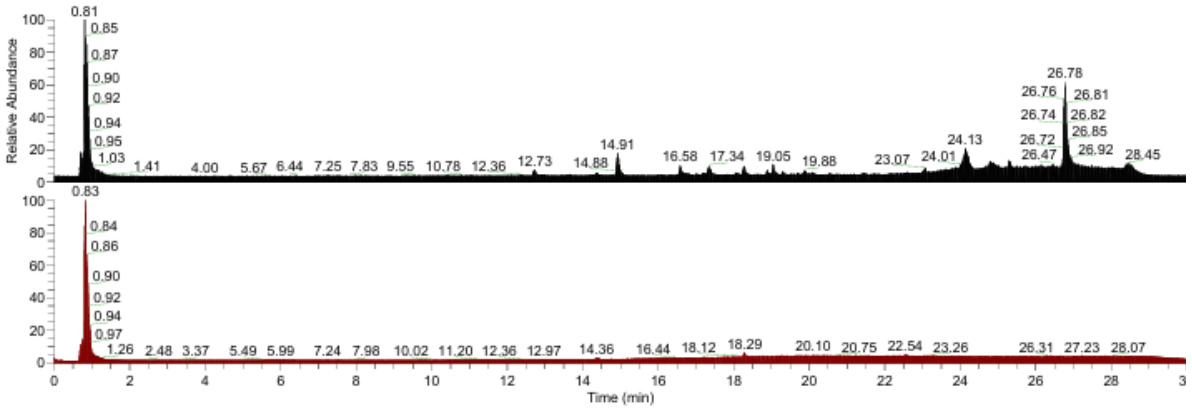
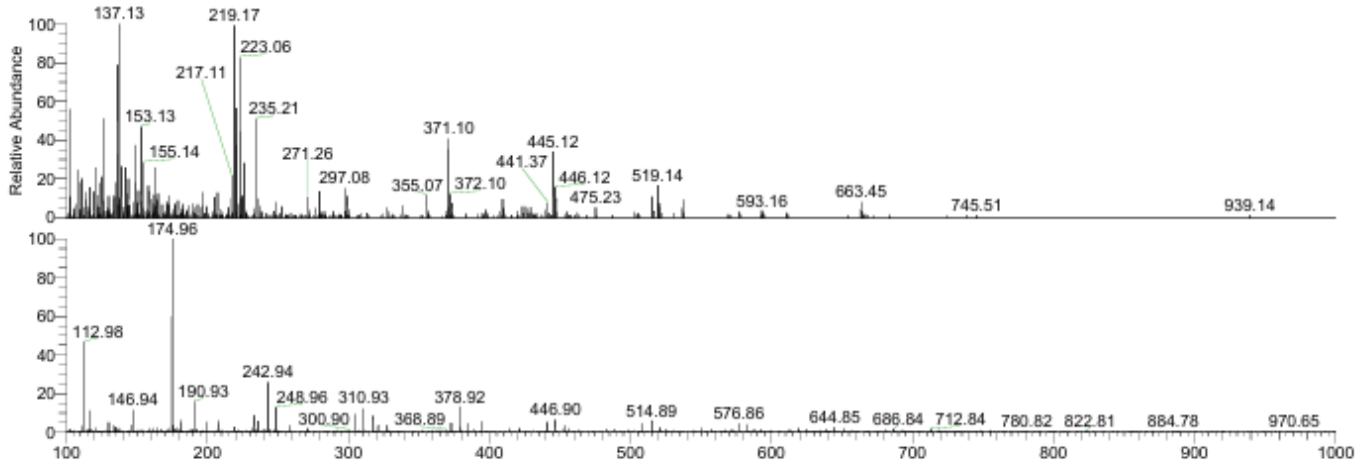
S.1. Flow chart of isolation scheme

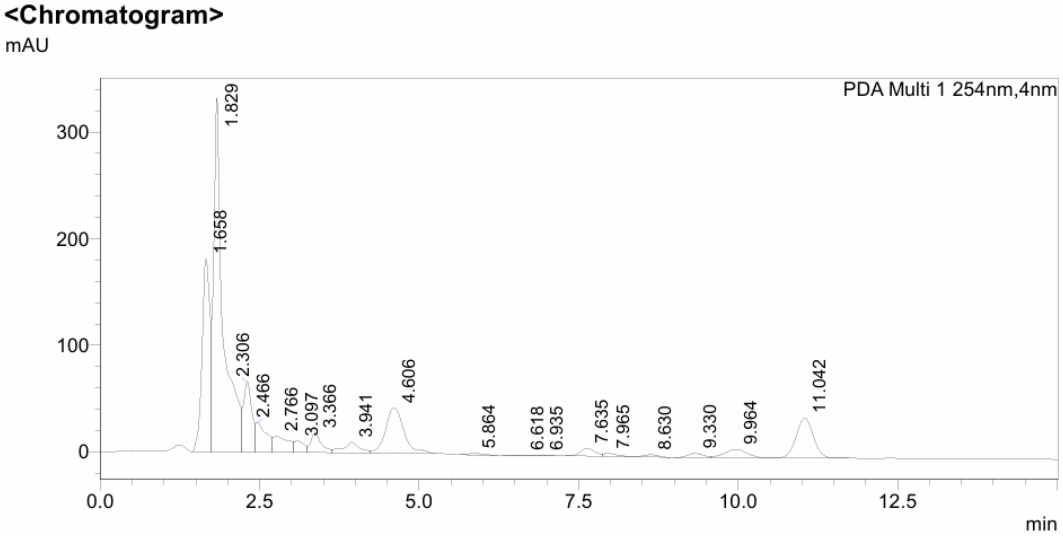


S.2. TIC of LC-HRMS of crude

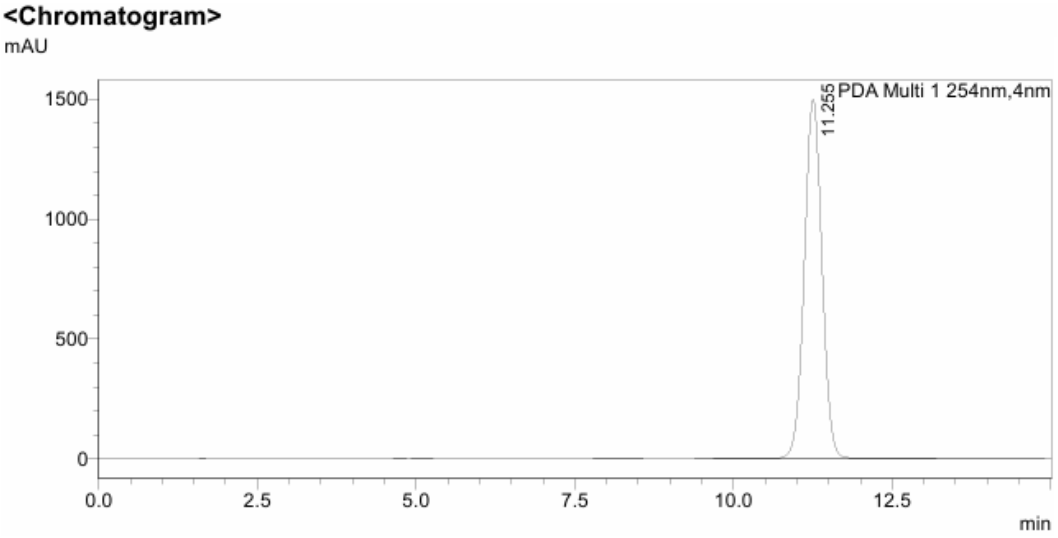




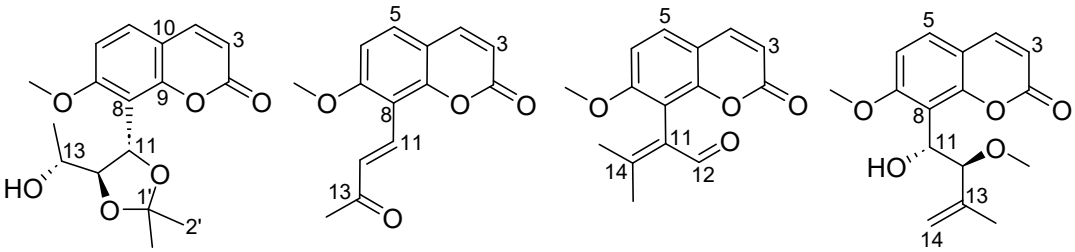
S.3. HPLCs of crude on cartridge column for fractionation.



S.4. HPLCs of Ghosalin (1).



S.5. Chemical structures of compounds isolated from *M. paniculata*



S.6. Data NMR

Ghosalin (1)**:** Rectangular crystals, SC-XRD analysis HRESIMS m/z 321.1331 $[M+H]^+$ calcd for $C_{17}H_{20}O_6$+H^+ ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53(d, 1H, J=10), 7.33(d, 1H, J=10), 6.80(d, 1H, J=5), 6.17(d,

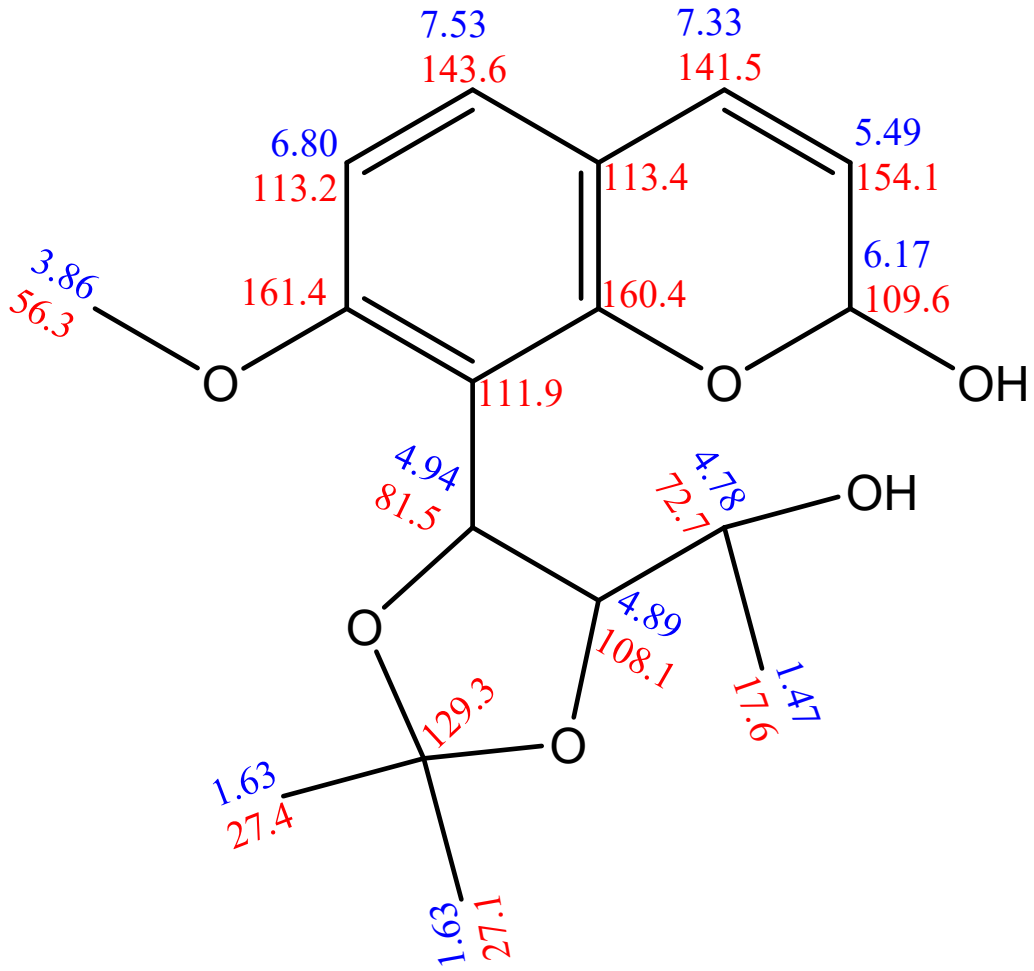
1H, J=10), 5.49(d, 1H, J=5), 4.94(d, 1H, J=10), 4.89(s, 1H), 4.78(s, 1H), 3.86(s, 3H), 1.63(d, 6H, J=20), 1.47(s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.4, 160.4, 154.1, 143.6, 141.5, 129.3, 113.4, 113.2, 111.9, 109.6, 108.1, 81.6, 72.7, 56.3, 27.4, 27.1, 17.6.
Osthenone (2). Transparent needles. HRESIMS *m/z* 245.0793 $[M+H]^+$ (calcd for $C_{14}H_{12}O_4+H^+$, 245.0803)
Murranlongin (3): 20 mg, White powder, HRMESIMS *m/z* 259.0948 $[M+H]^+$ (calcd for $C_{15}H_{14}O_4+H^+$, 259.0965). ^{1}H NMR (500 MHz, MeOD) δ 10.13 (s, 1H), 7.81 (d, 1H, J=10), 7.53 (d, 1H, J=10), 6.99 (d, 1H, J=10), 6.12 (d, 1H, J=10), 3.76 (s, 3H), 2.36 (s, 3H), 1.70 (s, 3H). ^{13}C NMR (126 MHz, MeOD) δ 189.9, 161.9, 161.3, 160.4, 152.5, 144.8, 129.4, 129.1, 113.1, 112.8, 112, 108, 55.5, 23.7, 18.4.
Minumicrolin (4) 35 mg, White particles, HRMESIMS *m/z* 299.0891 $[M+Na]^+$ (calcd for $C_{15}H_{16}O_5$ $+Na^+$, 299.0890). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77(d, 1H, J=10), 7.54(d, 1H, J=10), 7.03(d, 1H, J=5), 6.39(d, 1H, J=10), 5.56(t, 1H, J=5), 5.11(d, 2H, J=10), 4.66(d, 1H, J=10), 4.11(s, 3H), 2.03(s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 161, 160.8, 153.8, 145.6, 144.3, 129, 117, 114.3, 113.9, 113.7, 108.5, 78.9, 69, 56.9, 18.5.

S.7. DNP search for compounds in *M. paniculata*

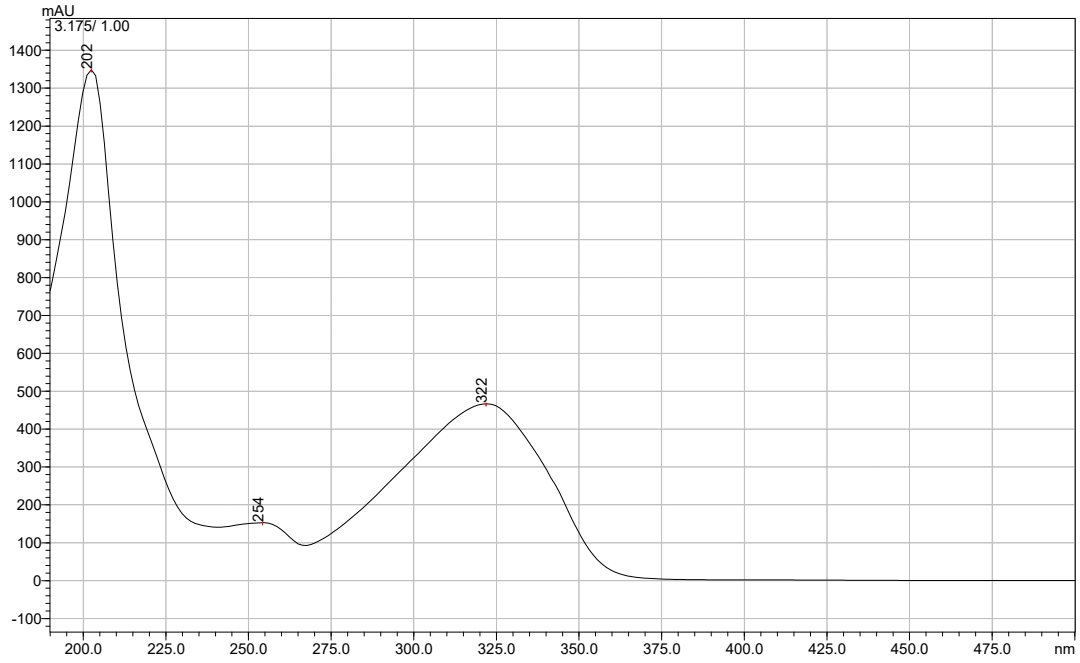
S.8. DNP search for aromatic compounds in *M. paniculata*

S.9. DNP search for coumarin compounds in *M. paniculata*

Spectral information of compound 1



S.10. UV Spectra of compound 1



S.11. X-ray data of compound 1

Table 2 Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for ov_SK-IIA_auto. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*Z*	U(eq)
O001	7709(3)	5231(3)	4139(2)	62.8(6)
O002	6225(3)	6132(3)	1716(2)	65.3(7)
O003	8365(3)	6785(3)	888(2)	76.1(8)
O004	3711(3)	9865(3)	2777(3)	83.5(9)
O005	9715(4)	3131(4)	4682(3)	98.0(10)
C006	6391(4)	6375(4)	4394(3)	57.4(8)
C007	6244(4)	7521(4)	2135(3)	56.6(8)
C008	7969(4)	7554(4)	1943(3)	58.4(8)
C009	5695(4)	7538(4)	3440(3)	56.8(8)
C00A	4366(4)	8727(5)	3723(4)	66.8(9)
C00B	8114(4)	9136(4)	1684(4)	66.9(9)
C00C	8538(5)	4010(5)	5003(4)	73.0(10)
C00D	5798(4)	6311(5)	5591(3)	65.8(9)
C00E	6580(5)	5019(6)	6477(3)	78.4(12)
C00F	7495(5)	5728(5)	875(3)	70.0(10)
C00G	3783(5)	8705(6)	4914(4)	81.5(12)
C00H	7869(5)	3939(6)	6220(4)	79.6(12)
C00I	4484(5)	7504(6)	5811(4)	83.0(13)
O00J	8678(6)	9682(6)	2608(5)	143.5(17)
C00K	2310(5)	11057(6)	2986(6)	100.8(16)
C00L	8509(7)	4124(6)	1317(6)	110.1(18)
C00M	6798(7)	5922(8)	-409(4)	120(2)
C00N	7609(9)	10036(7)	440(5)	127(2)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for ov_SK-IIA_auto. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+…]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O001	55.6(13)	75.8(16)	54.3(13)	-6.7(11)	10.1(10)	-17.3(11)
O002	66.7(15)	82.5(16)	60.2(13)	-23.7(12)	21.3(11)	-36.9(12)
O003	81.8(17)	88.4(18)	75.3(17)	-31.4(14)	36.2(13)	-43.3(14)
O004	61.5(16)	76.8(18)	103(2)	-19.3(16)	13.2(14)	-4.7(13)
O005	71.7(19)	104(2)	94(2)	6.4(18)	13.7(16)	0.5(17)
C006	48.2(17)	76(2)	56.4(18)	-22.5(16)	13.4(14)	-25.8(16)
C007	50.8(18)	65(2)	56.4(18)	-12.5(15)	7.7(13)	-19.9(15)
C008	52.7(18)	69(2)	56.3(18)	-10.9(15)	10.4(14)	-22.2(15)
C009	47.7(17)	70(2)	58.3(18)	-18.4(16)	11.4(14)	-22.1(15)
C00A	56(2)	72(2)	80(2)	-29(2)	14.2(17)	-22.9(17)
C00B	60(2)	69(2)	76(2)	-9.6(18)	5.8(16)	-24.5(17)
C00C	64(2)	90(3)	66(2)	-3(2)	-0.6(17)	-28(2)
C00D	62(2)	95(3)	53.1(19)	-23.6(18)	13.6(15)	-37.2(19)
C00E	82(3)	125(4)	47.5(19)	-16(2)	9.9(17)	-58(3)
C00F	83(3)	79(2)	62(2)	-26.1(18)	30.1(18)	-38(2)
C00G	68(2)	93(3)	91(3)	-43(3)	29(2)	-23(2)
C00H	72(3)	110(3)	61(2)	2(2)	0.5(18)	-40(2)
C00I	78(3)	123(4)	67(2)	-44(3)	28(2)	-46(3)
O00J	141(4)	138(4)	175(4)	-61(3)	20(3)	-60(3)
C00K	56(2)	82(3)	160(5)	-29(3)	18(3)	-10(2)
C00L	129(4)	76(3)	126(4)	-24(3)	62(3)	-27(3)
C00M	140(5)	193(6)	65(3)	-40(3)	31(3)	-97(5)
C00N	187(6)	108(4)	96(4)	25(3)	-27(4)	-78(4)

Table 4 Bond Lengths for ov_SK-IIA_auto.		
Atom	**Atom**	**Length/Å**
O001	C006	1.369(4)
O001	C00C	1.382(5)
O002	C007	1.426(4)
O002	C00F	1.435(4)
O003	C008	1.427(4)
O003	C00F	1.408(4)
O004	C00A	1.358(5)
O004	C00K	1.423(5)
O005	C00C	1.191(5)
C006	C009	1.383(5)
C006	C00D	1.408(5)
C007	C008	1.530(4)
C007	C009	1.506(4)
C008	C00B	1.493(5)
C009	C00A	1.408(5)
C00A	C00G	1.397(6)
C00B	O00J	1.347(6)
C00B	C00N	1.485(6)

Table 4 Bond Lengths for ov_SK-IIA_auto.		
Atom	**Atom**	**Length/Å**
C00C	C00H	1.454(6)
C00D	C00E	1.423(6)
C00D	C00I	1.380(6)
C00E	C00H	1.322(6)
C00F	C00L	1.493(7)
C00F	C00M	1.499(6)
C00G	C00I	1.365(7)

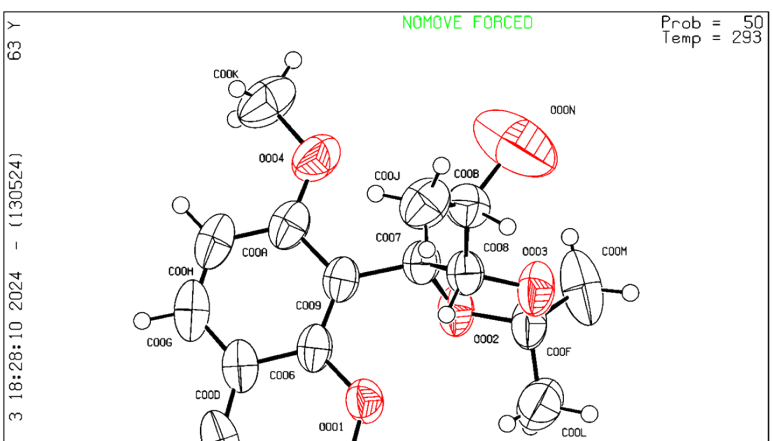
Table 5 Bond Angles for ov_SK-IIA_auto.			
Atom	**Atom**	**Atom**	**Angle/˚**
C006	O001	C00C	123.8(3)
C007	O002	C00F	108.4(2)
C00F	O003	C008	109.5(2)
C00A	O004	C00K	118.6(4)
O001	C006	C009	117.4(3)
O001	C006	C00D	119.3(3)
C009	C006	C00D	123.3(3)
O002	C007	C008	103.6(3)
O002	C007	C009	110.1(3)
C009	C007	C008	115.9(3)
O003	C008	C007	101.5(3)
O003	C008	C00B	110.7(3)
C00B	C008	C007	113.5(3)
C006	C009	C007	122.8(3)
C006	C009	C00A	116.8(3)
C00A	C009	C007	120.3(3)
O004	C00A	C009	115.9(3)
O004	C00A	C00G	123.3(4)
C00G	C00A	C009	120.8(4)
O00J	C00B	C008	117.7(4)
O00J	C00B	C00N	123.4(4)
C00N	C00B	C008	118.9(4)
O001	C00C	C00H	115.8(4)
O005	C00C	O001	117.3(4)
O005	C00C	C00H	126.9(4)
C006	C00D	C00E	117.8(4)
C00I	C00D	C006	117.3(4)
C00I	C00D	C00E	124.9(4)
C00H	C00E	C00D	121.9(4)
O002	C00F	C00L	108.1(3)
O002	C00F	C00M	109.7(4)
O003	C00F	O002	106.5(3)
O003	C00F	C00L	111.8(4)
O003	C00F	C00M	107.7(3)

Table 5 Bond Angles for ov_SK-IIA_auto.			
Atom	**Atom**	**Atom**	**Angle/˚**
C00L	C00F	C00M	112.8(4)
C00I	C00G	C00A	119.9(4)
C00E	C00H	C00C	121.2(4)
C00G	C00I	C00D	121.9(4)

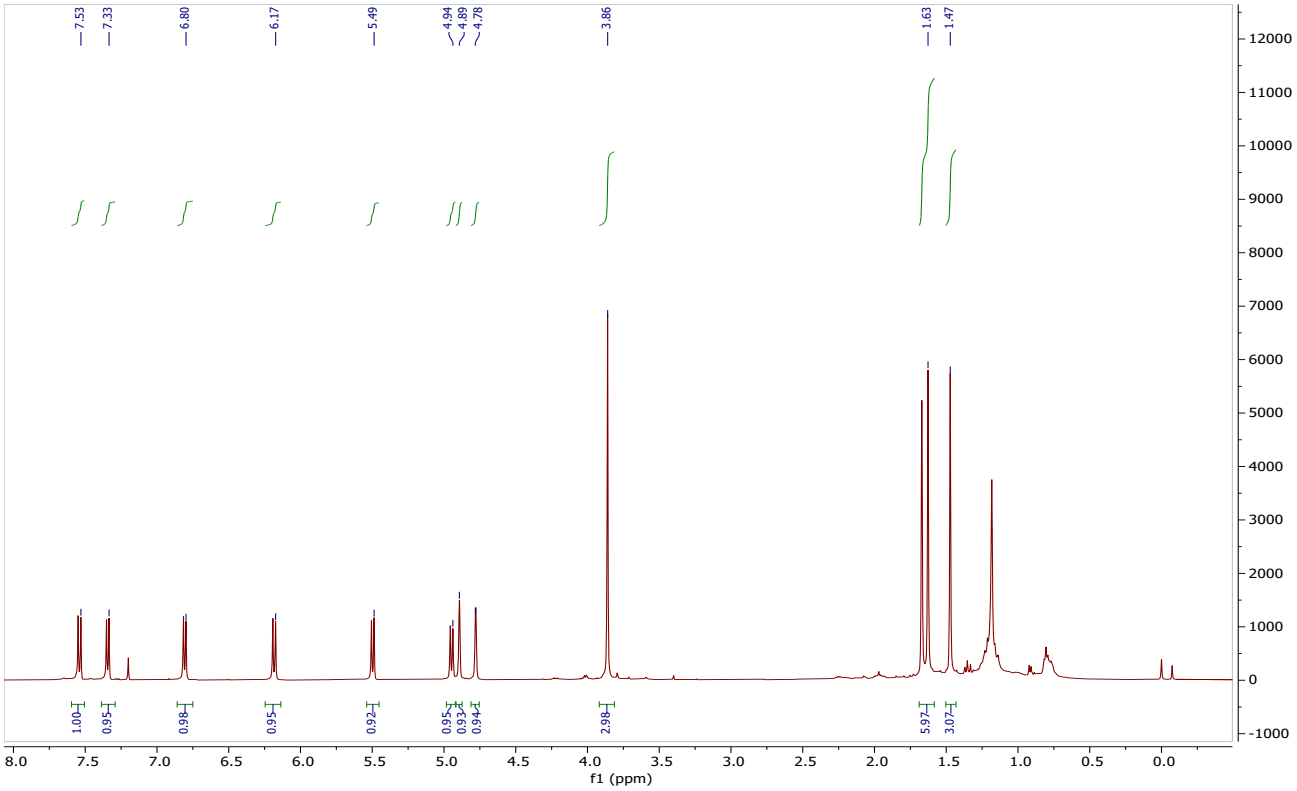
Table 6 Torsion Angles for ov_SK-IIA_auto.				
A	**B**	**C**	**D**	**Angle/˚**
O001	C006	C009	C007	5.0(5)
O001	C006	C009	C00A	-178.4(3)
O001	C006	C00D	C00E	-1.8(5)
O001	C006	C00D	C00I	178.9(3)
O001	C00C	C00H	C00E	-2.4(6)
O002	C007	C008	O003	31.5(3)
O002	C007	C008	C00B	150.3(3)
O002	C007	C009	C006	54.2(4)
O002	C007	C009	C00A	-122.2(3)
O003	C008	C00B	O00J	-143.2(4)
O003	C008	C00B	C00N	37.8(5)
O004	C00A	C00G	C00I	178.6(4)
O005	C00C	C00H	C00E	177.6(4)
C006	O001	C00C	O005	-176.2(3)
C006	O001	C00C	C00H	3.8(5)
C006	C009	C00A	O004	179.3(3)
C006	C009	C00A	C00G	-0.7(5)
C006	C00D	C00E	C00H	3.1(6)
C006	C00D	C00I	C00G	-0.3(6)
C007	O002	C00F	O003	5.7(4)
C007	O002	C00F	C00L	126.0(4)
C007	O002	C00F	C00M	-110.6(4)
C007	C008	C00B	O00J	103.4(4)
C007	C008	C00B	C00N	-75.6(5)
C007	C009	C00A	O004	-4.0(5)
C007	C009	C00A	C00G	175.9(3)
C008	O003	C00F	O002	16.0(4)
C008	O003	C00F	C00L	-101.8(4)
C008	O003	C00F	C00M	133.7(4)
C008	C007	C009	C006	-63.0(4)
C008	C007	C009	C00A	120.6(4)
C009	C006	C00D	C00E	177.3(3)
C009	C006	C00D	C00I	-2.0(5)
C009	C007	C008	O003	152.3(3)
C009	C007	C008	C00B	-89.0(4)
C009	C00A	C00G	C00I	-1.4(6)
C00A	C00G	C00I	C00D	1.9(6)

Table 6 Torsion Angles for ov_SK-IIA_auto.				
A	**B**	**C**	**D**	**Angle/°**
C00C	O001	C006	C009	179.1(3)
C00C	O001	C006	C00D	-1.7(5)
C00D	C006	C009	C007	-174.2(3)
C00D	C006	C009	C00A	2.4(5)
C00D	C00E	C00H	C00C	-0.9(6)
C00E	C00D	C00I	C00G	-179.5(4)
C00F	O002	C007	C008	-23.2(4)
C00F	O002	C007	C009	-147.8(3)
C00F	O003	C008	C007	-29.3(4)
C00F	O003	C008	C00B	-150.1(3)
C00I	C00D	C00E	C00H	-177.6(4)
C00K	O004	C00A	C009	176.5(3)
C00K	O004	C00A	C00G	-3.4(6)

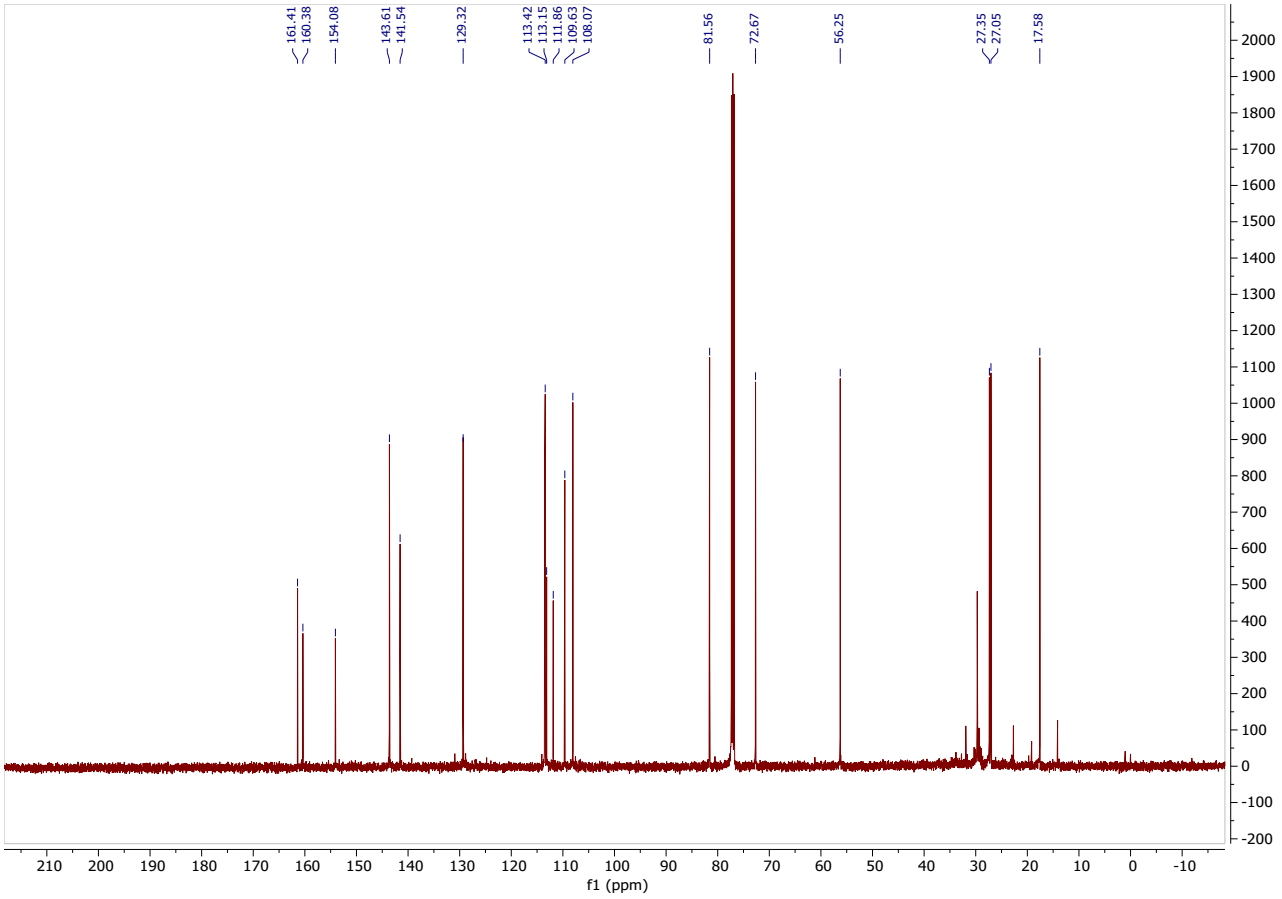
Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for ov_SK-IIA_auto.				
Atom	***x***	***y***	***z***	**U(eq)**
H007	5512.29	8389.57	1599.04	68
H008	8665.1	6969.03	2656.48	70
H00B	9207.92	8725.6	1410.64	80
H00E	6172.58	4932.38	7261.01	94
H00G	2918.51	9508.39	5094.55	98
H00H	8356.19	3119.6	6827.69	96
H00I	4064.34	7489.26	6593.06	100
H00A	1929.06	11725.77	2224.83	151
H00C	2564.05	11630.32	3580.83	151
H00D	1492.73	10618.21	3293.96	151
H00F	8989.17	4079.33	2114.91	165
H00K	9336.79	3811.69	745.09	165
H00L	7852.6	3451.62	1376.13	165
H00M	6175.85	5228.87	-440.1	180
H00N	7650.05	5705.03	-974.9	180
H00O	6120.25	6957.55	-632.86	180
H00P	8267.87	9522.69	-167.81	190
H00Q	7726.52	11038.71	422.08	190
H00R	6505.61	10127.61	261.87	190
H00J	8840(70)	10680(40)	2610(50)	121(19)



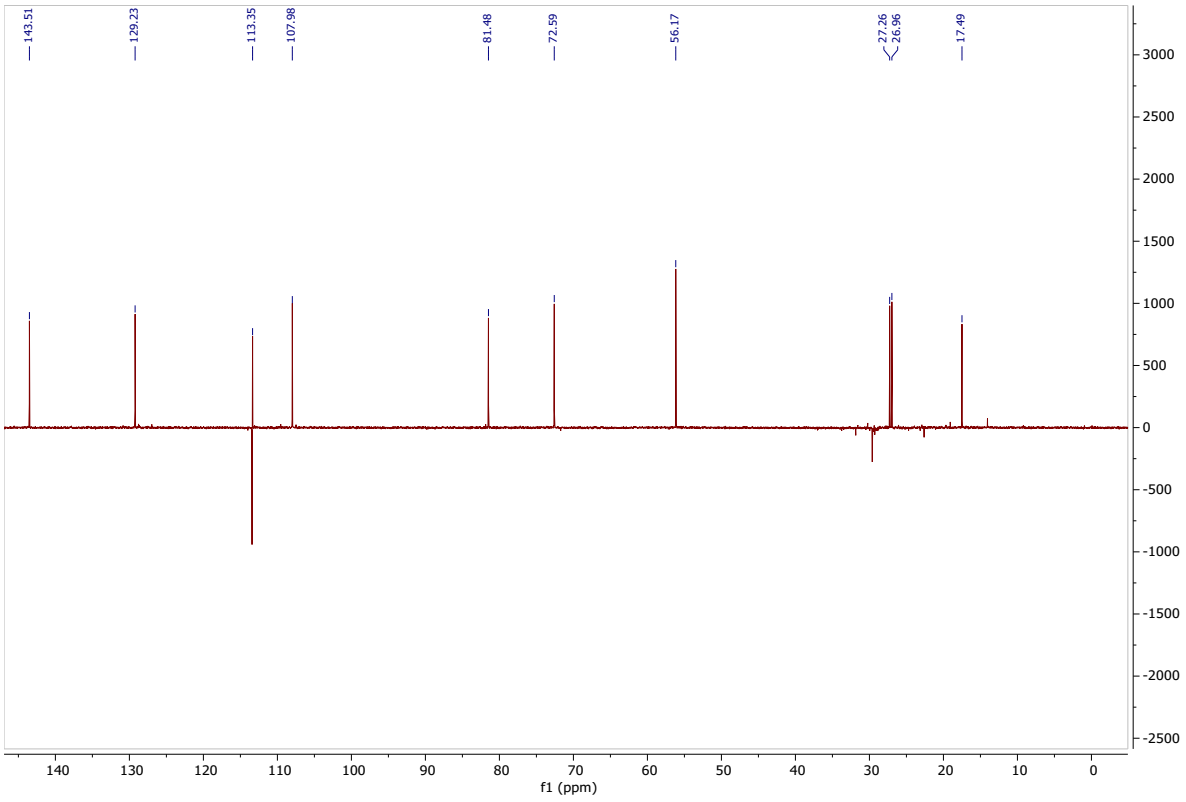
S.12. ^{1}H NMR spectrum of compound 1 in $CDCl_3$



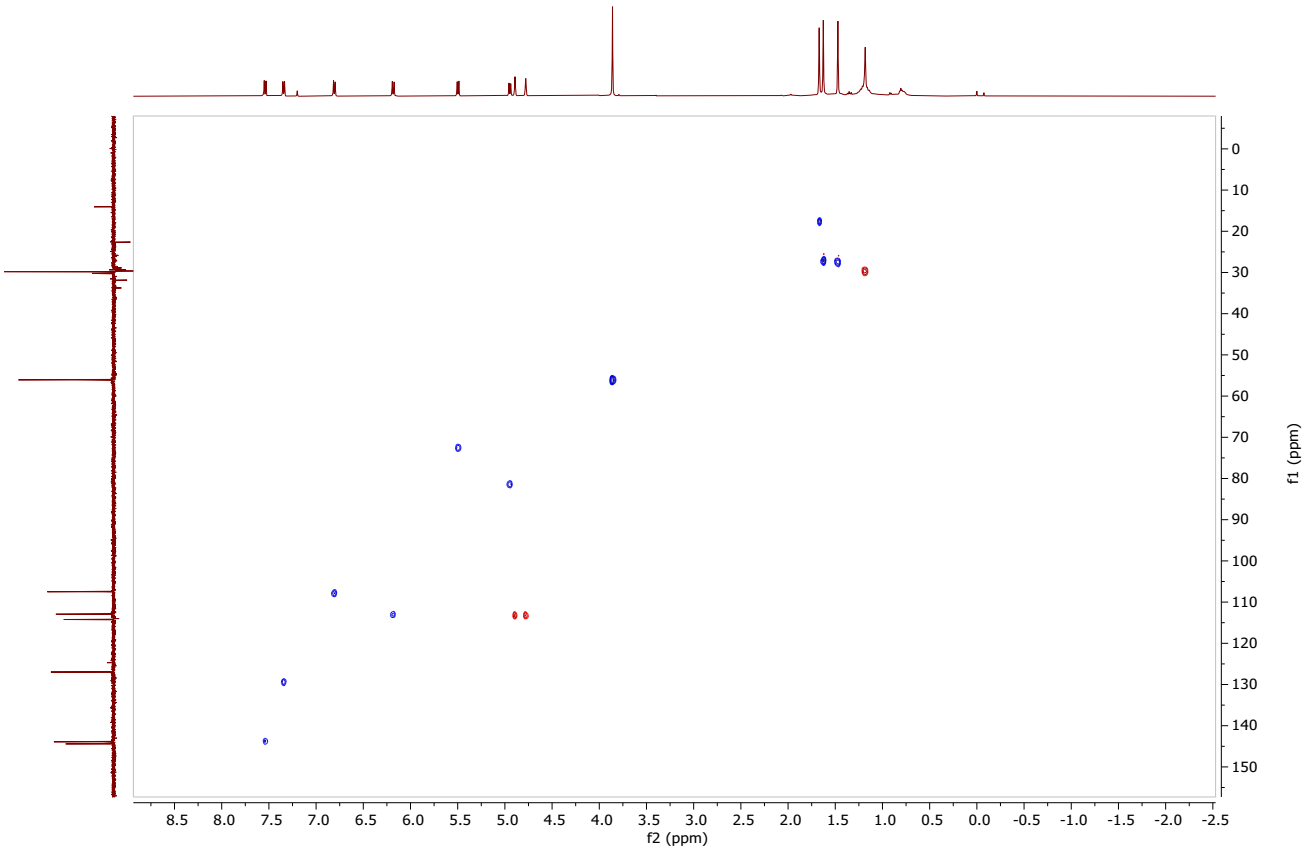
S.13. ^{13}C NMR spectrum of compound 1 in $CDCl_3$



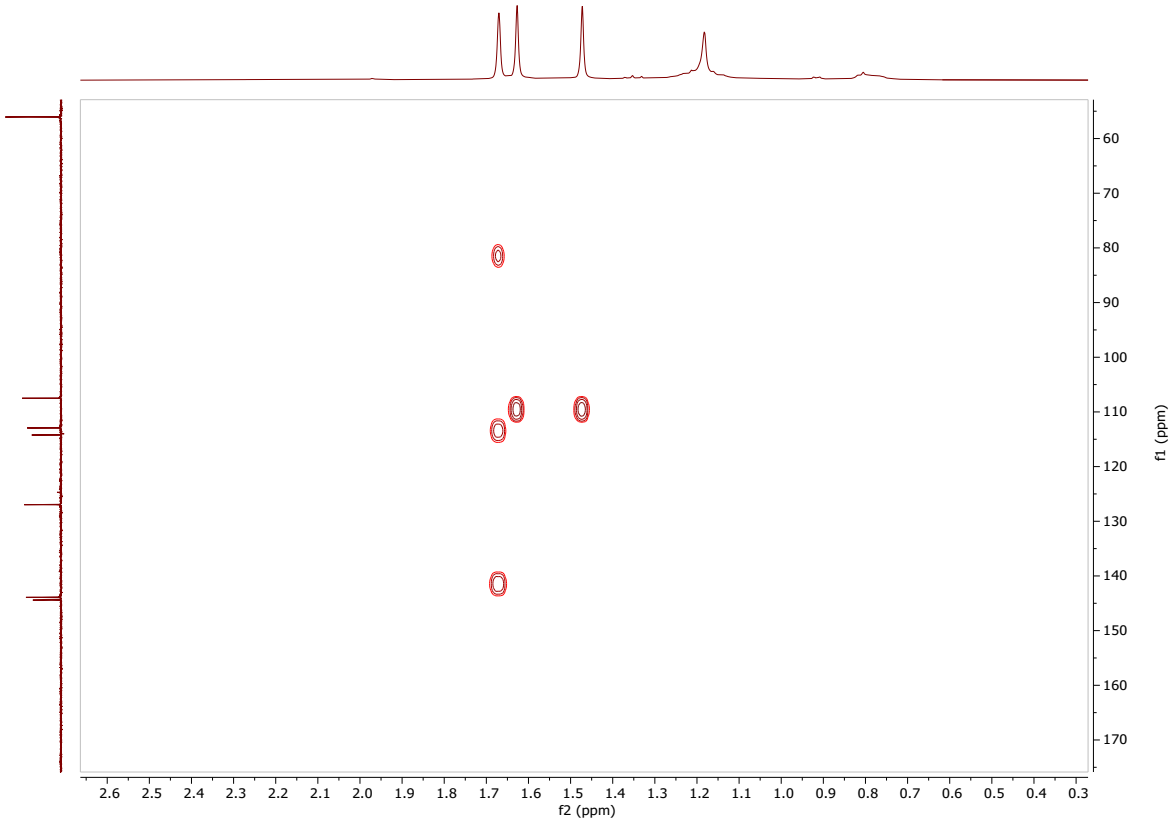
S.14. DEPT-135 NMR spectrum of compound 1 in $CDCl_3$



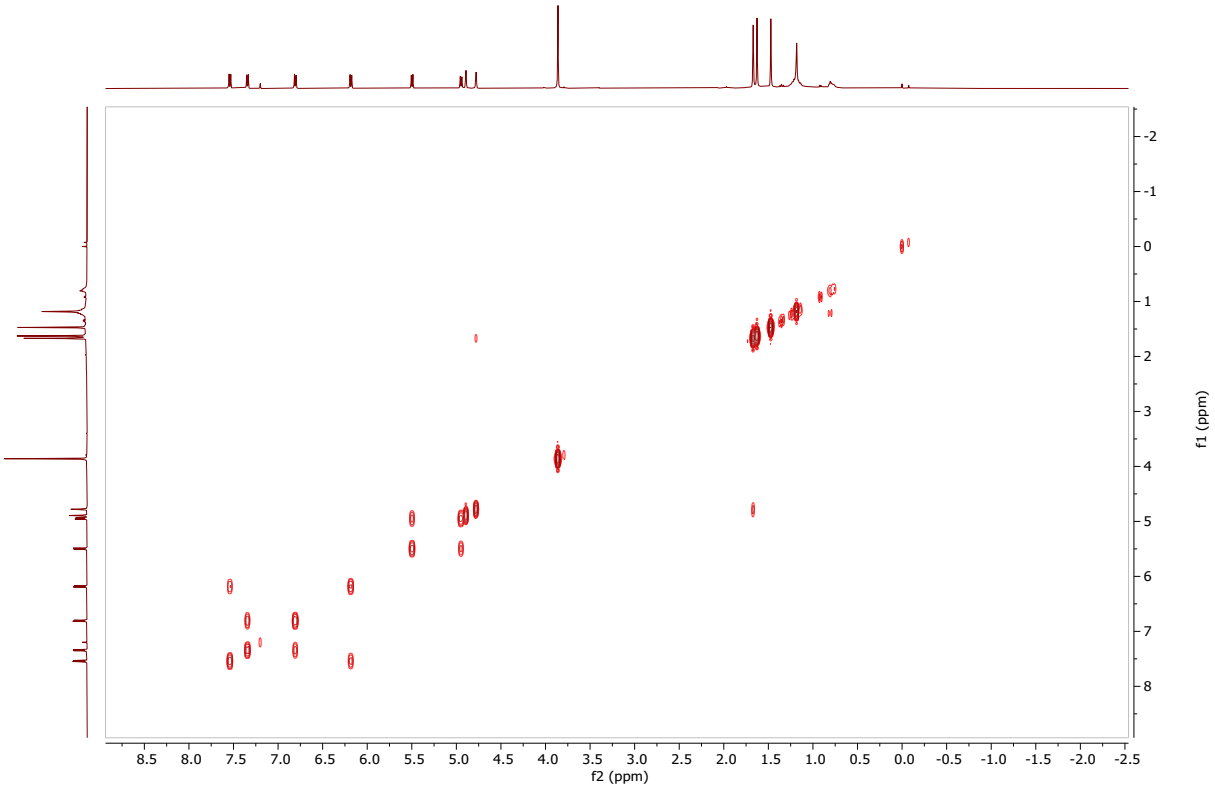
S.15. HSQC spectrum of compound 1 in $CDCl_3$



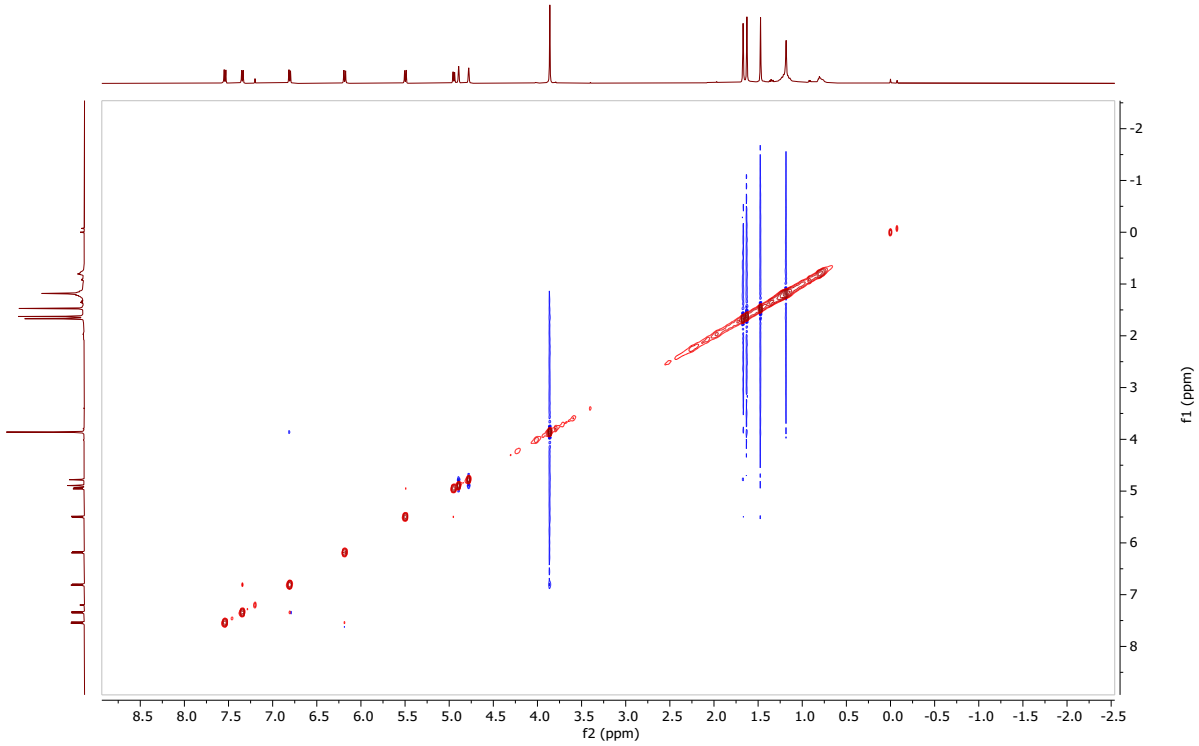
S.16. HMBC spectrum of compound 1 in $CDCl_3$



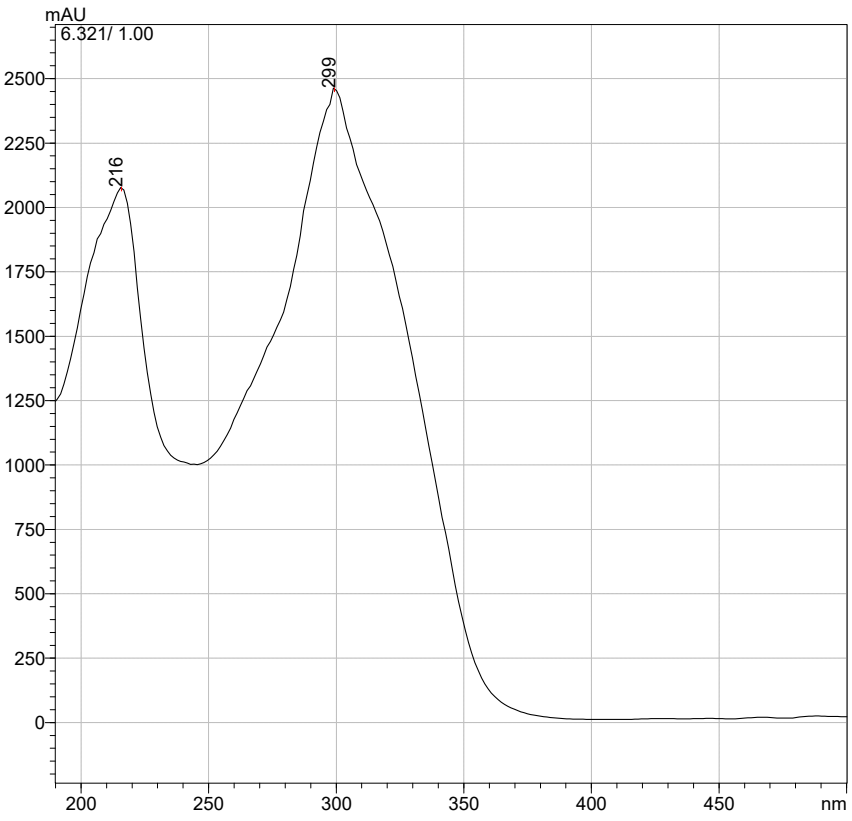
S.17: ^{1}H-^{1}H COSY NMR spectrum of compound 1 in $CDCl_3$

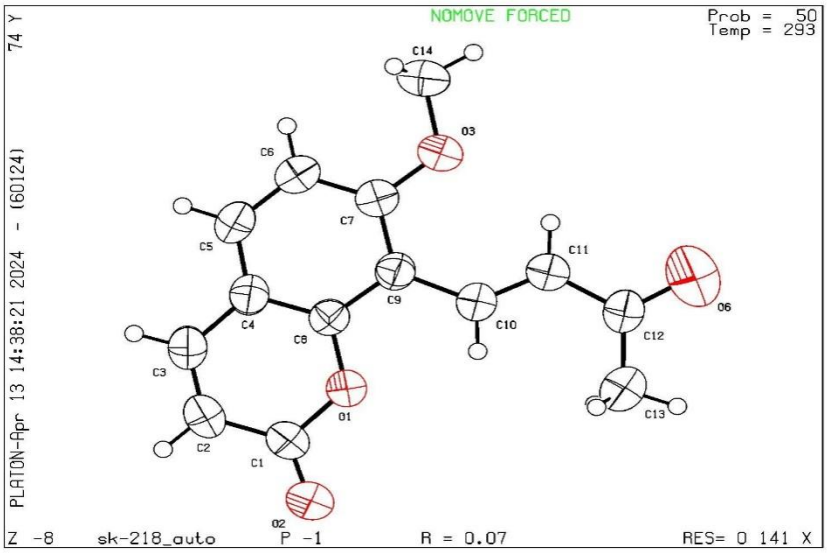


S.18. NOESY spectrum of compound 1 in $CDCl_3$



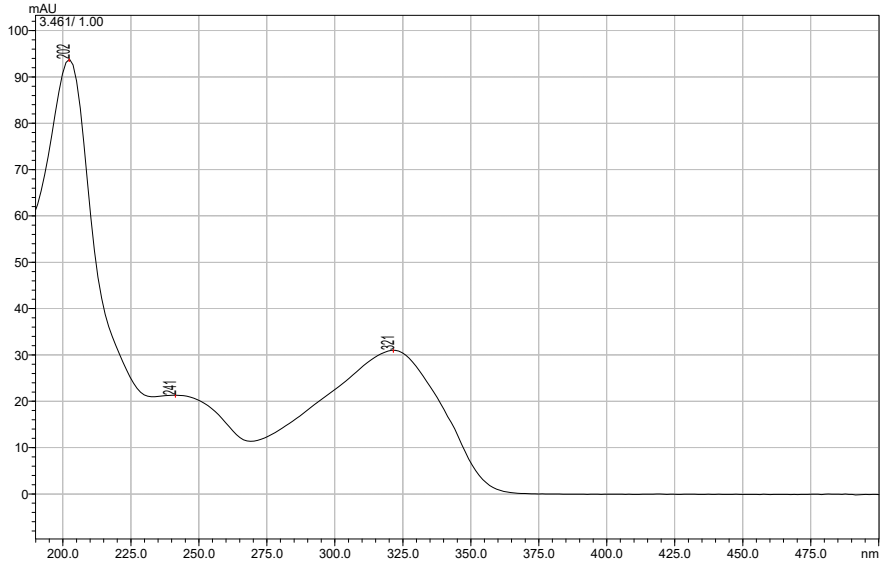
S.19. UV Spectra of compound 2

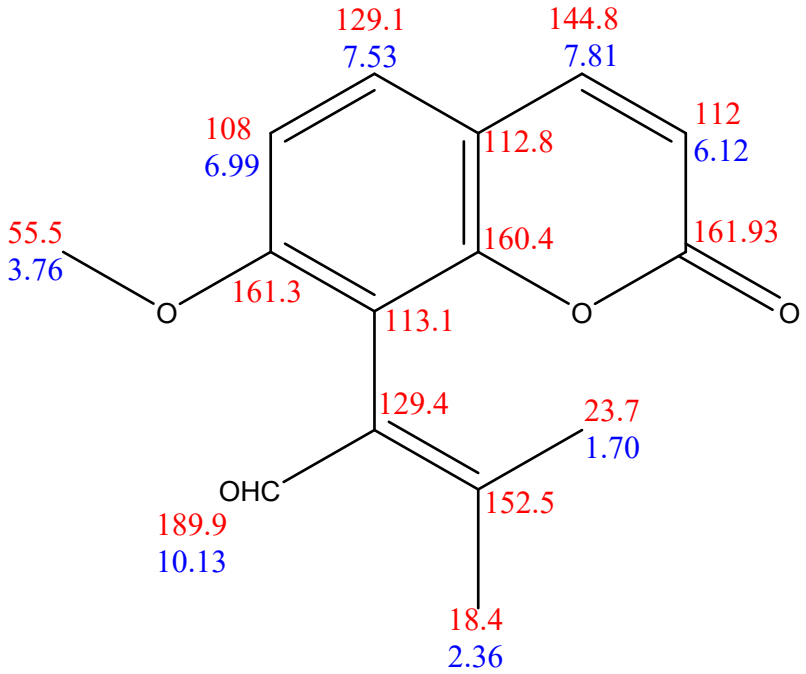




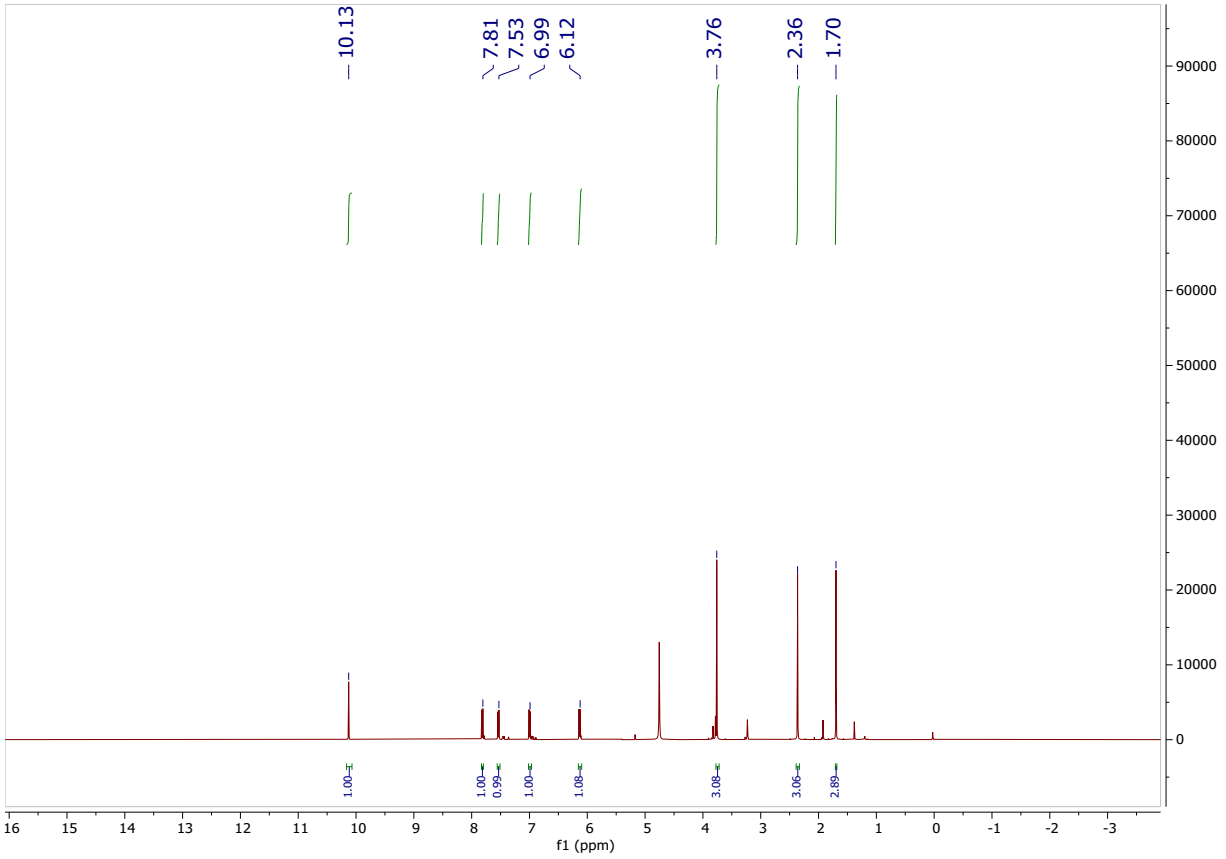
Spectral information of compound 3

S.20. UV Spectra of compound 3

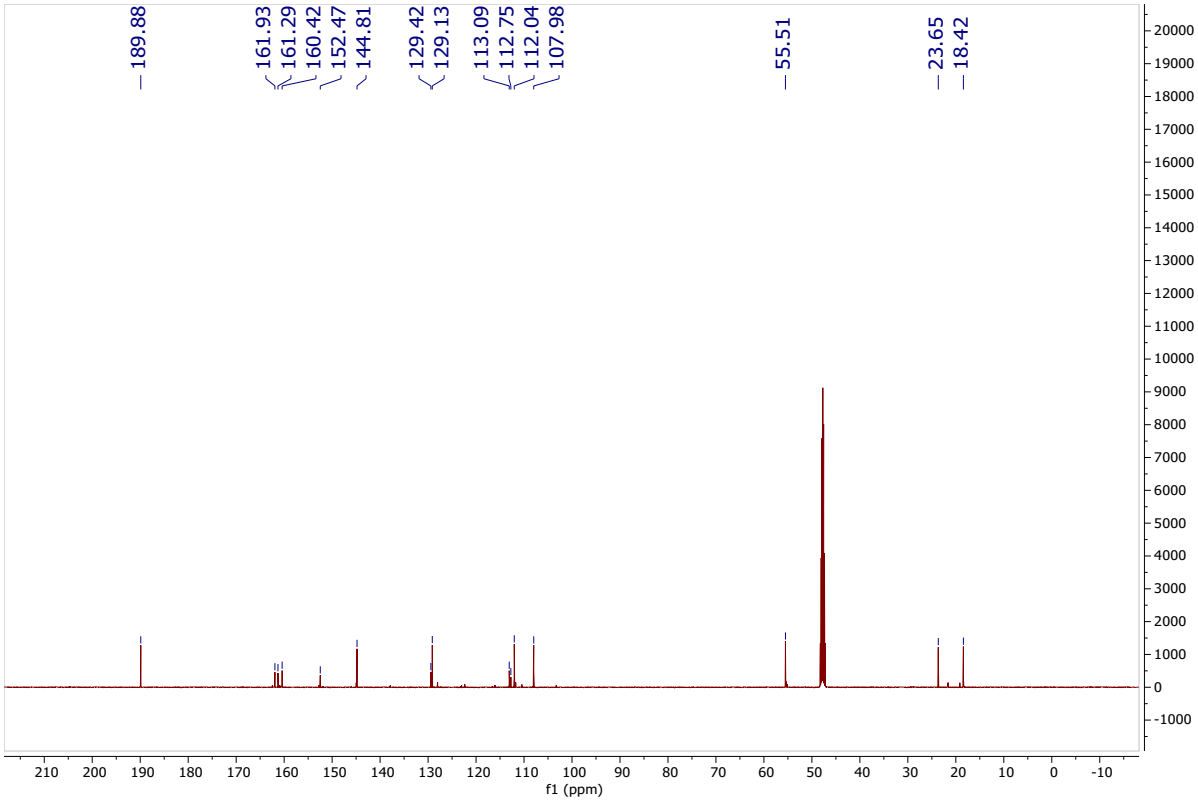




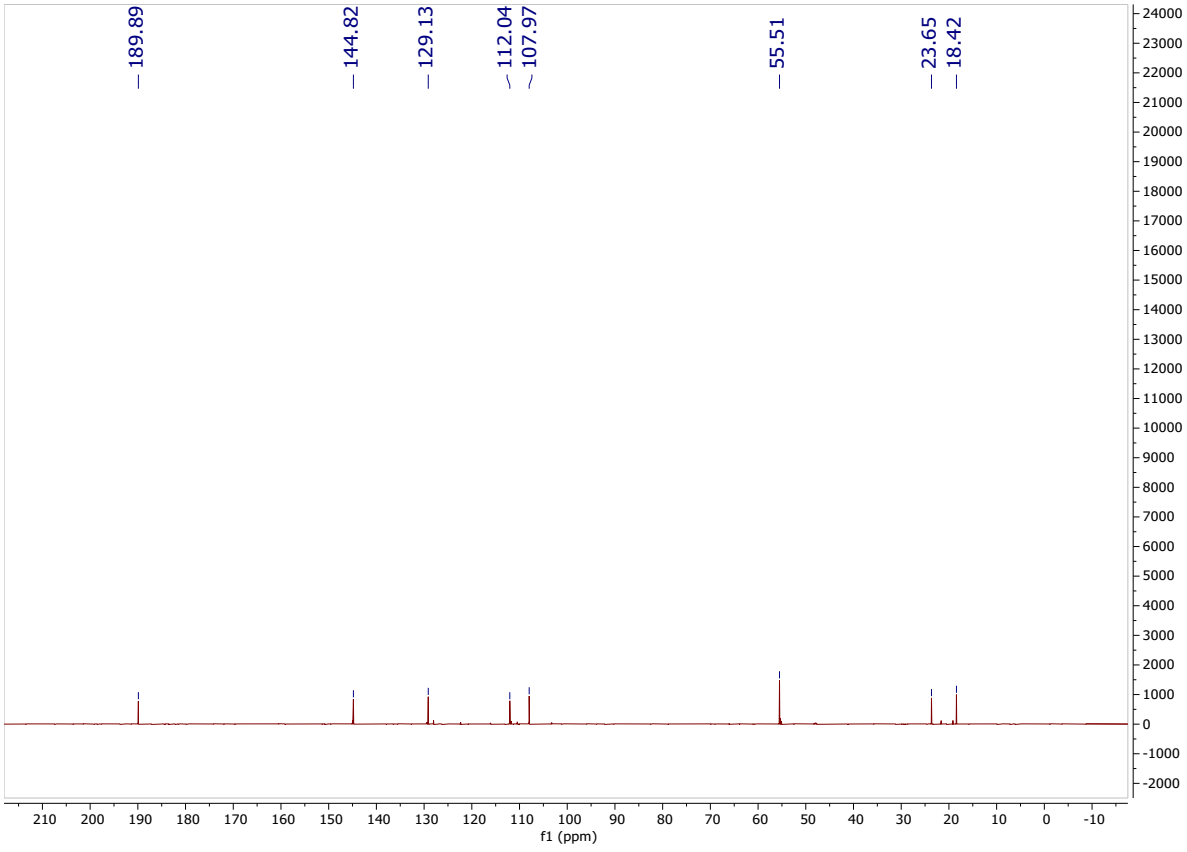
S.21. ^{1}H NMR spectrum of compound 3 in CD_3OD



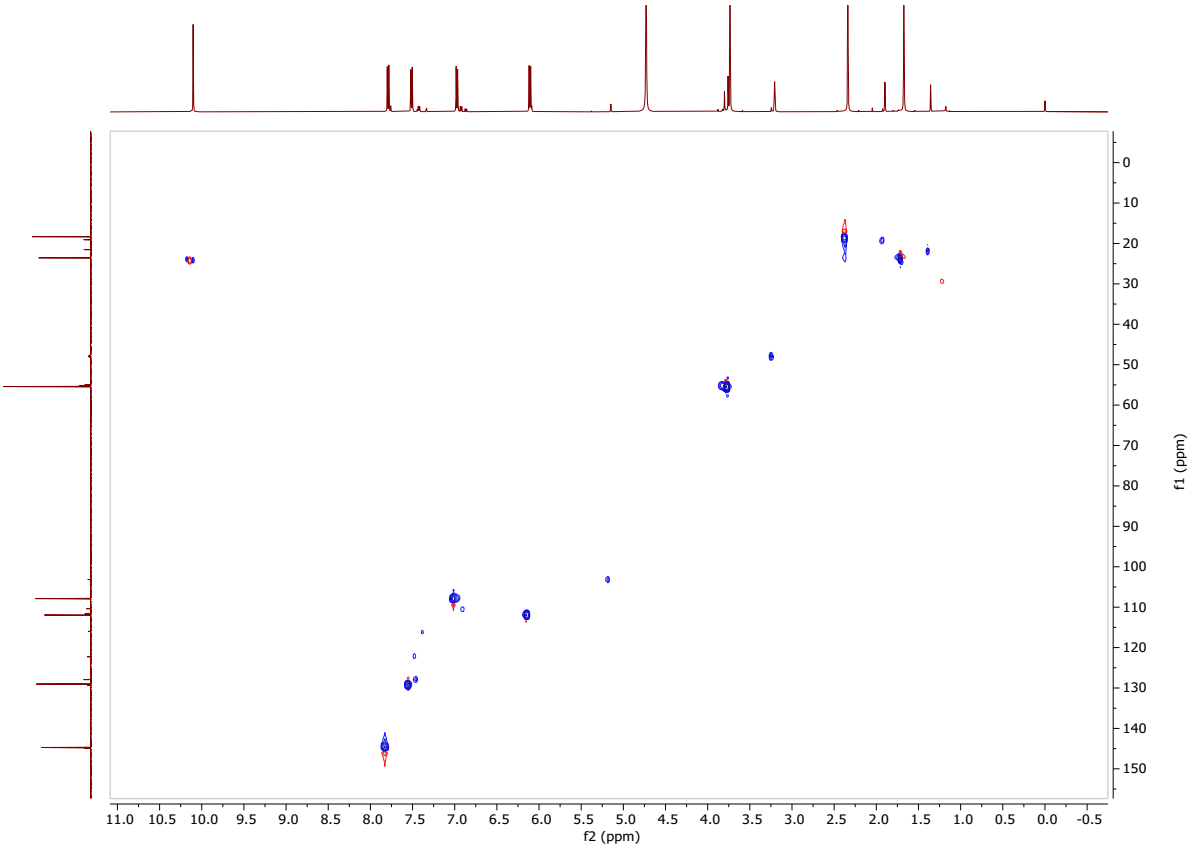
S.22. ^{13}C NMR spectrum of compound 3 in CD_3OD



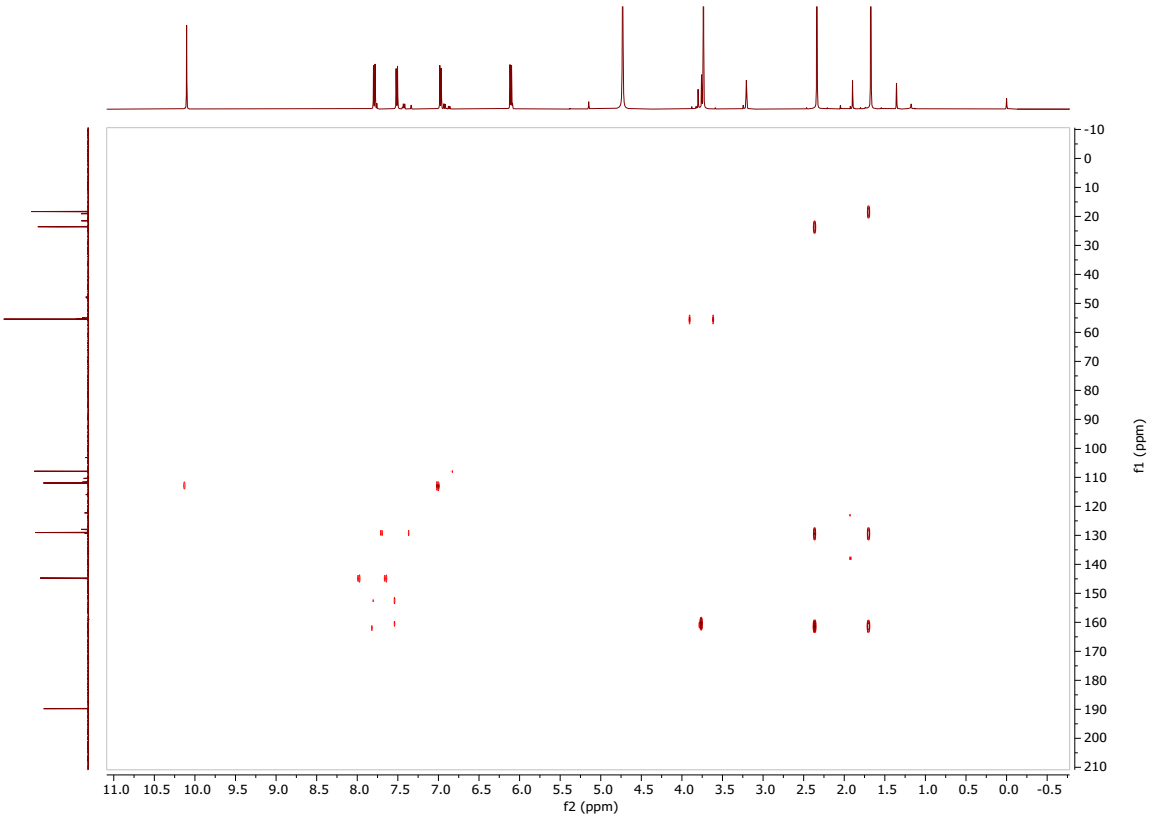
S.23. DEPT-135 NMR spectrum of compound 3 in CD_3OD



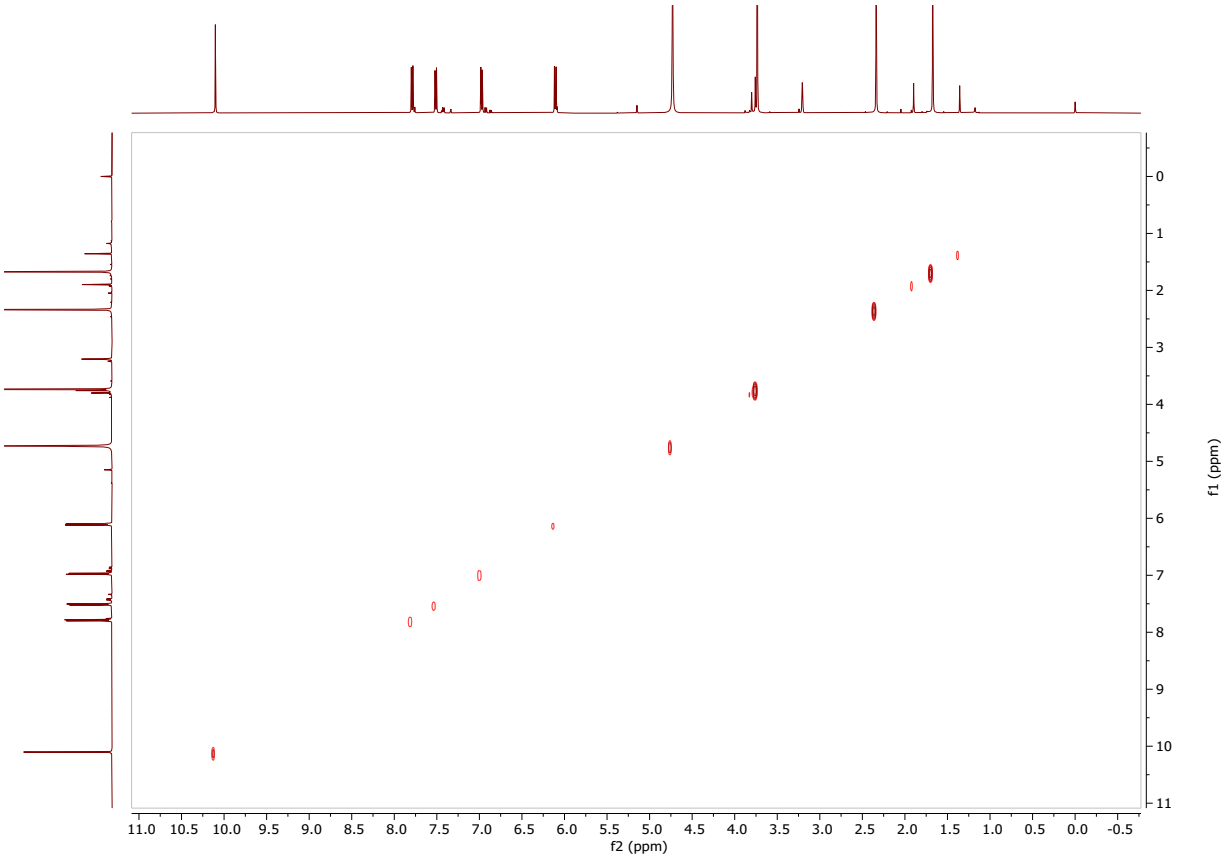
S.24. HSQC spectrum of compound 3 in CD_3OD



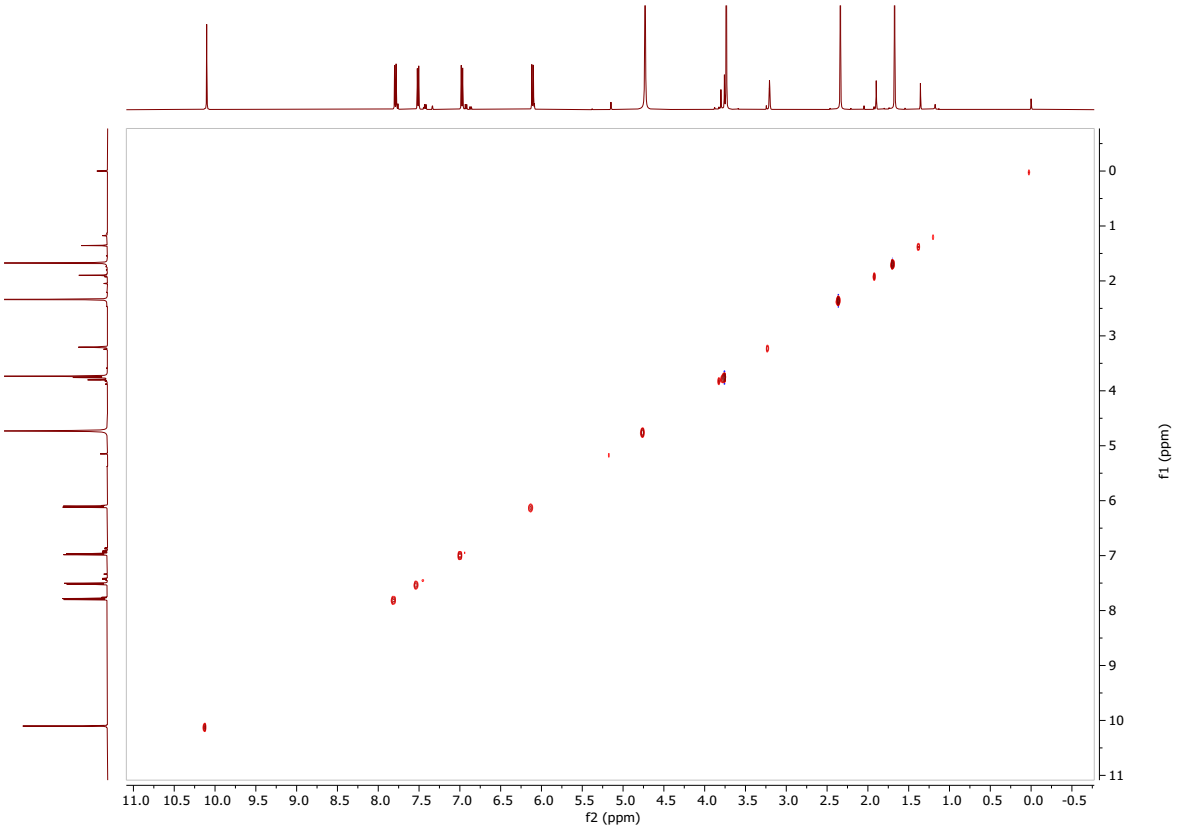
S.25. HMBC spectrum of compound 3 in CD_3OD



S.26. ^{1}H-^{1}H COSY NMR spectrum of compound 3 in CD_3OD

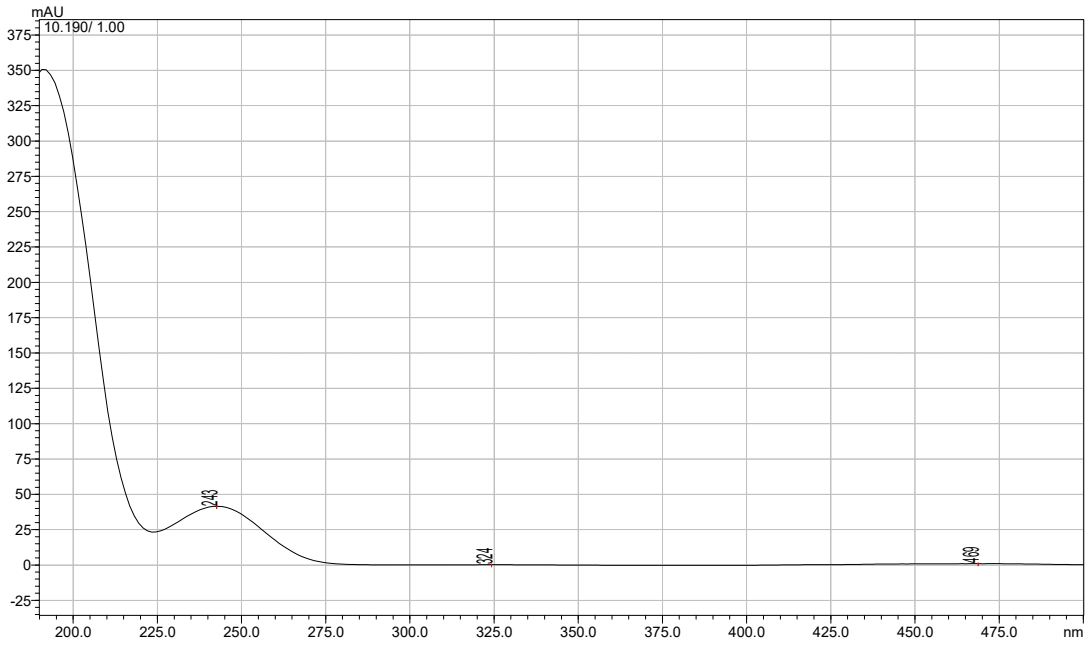


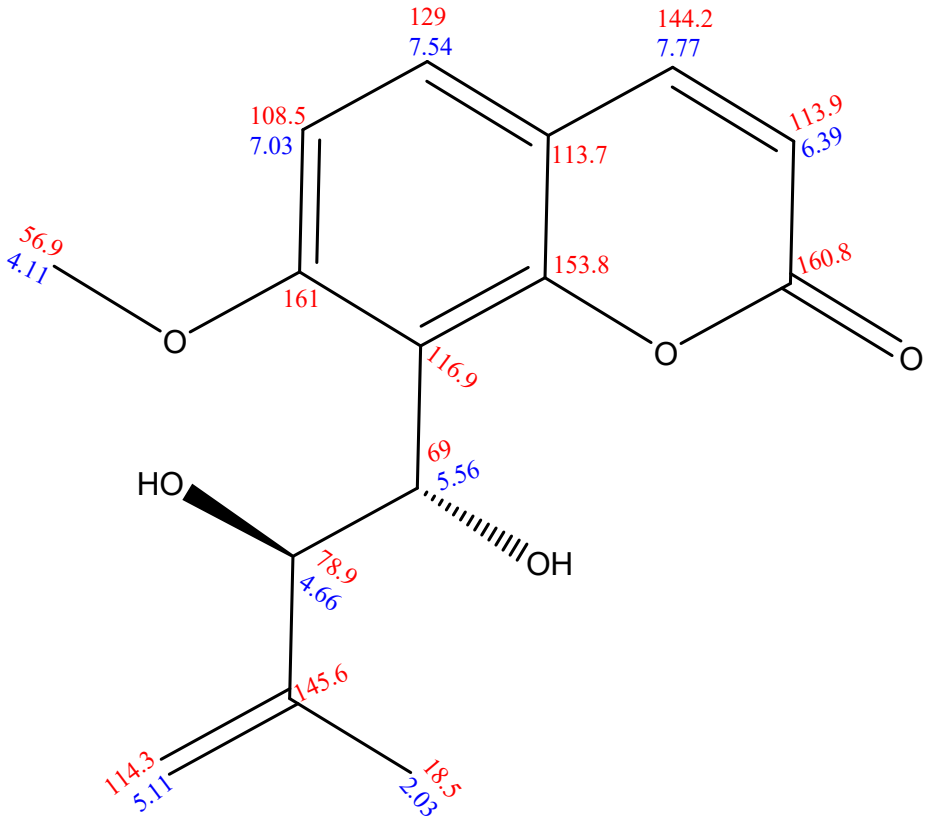
S.27. NOESY spectrum of compound 3 in CD_3OD



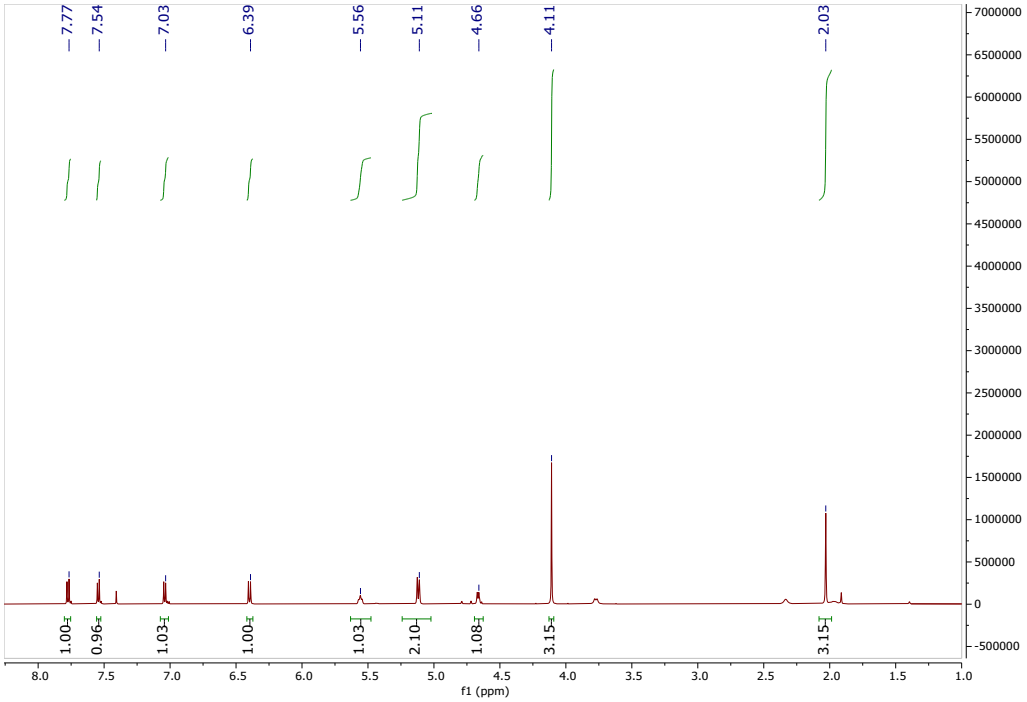
Spectral information of compound 4

S.28. UV Spectra of compound 4

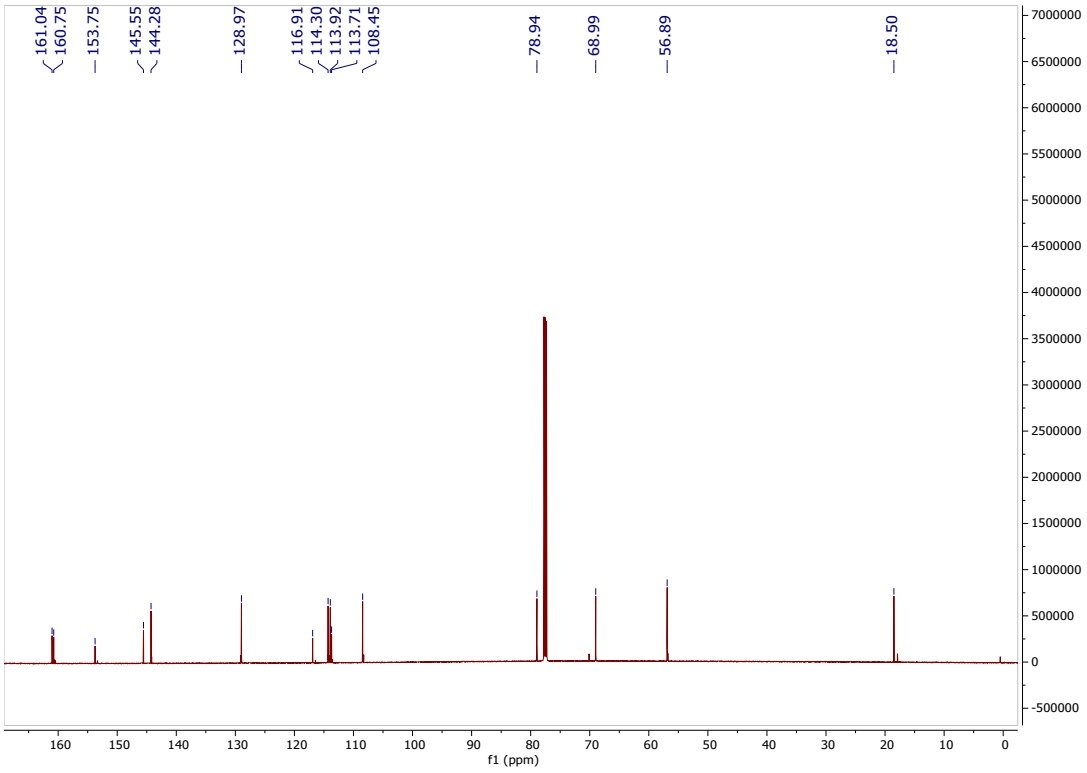




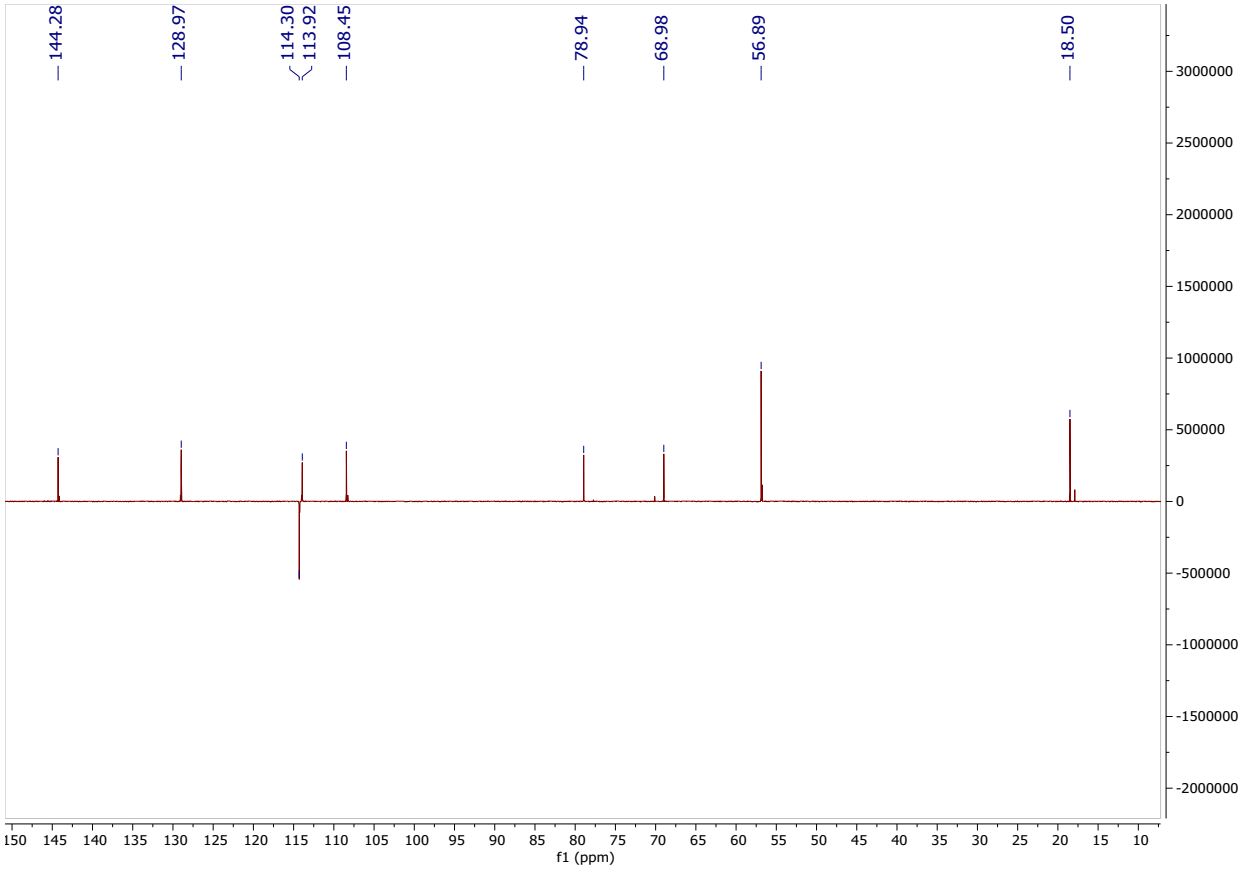
S.29. ^{1}H NMR spectrum of compound 4 in $CDCl_3$



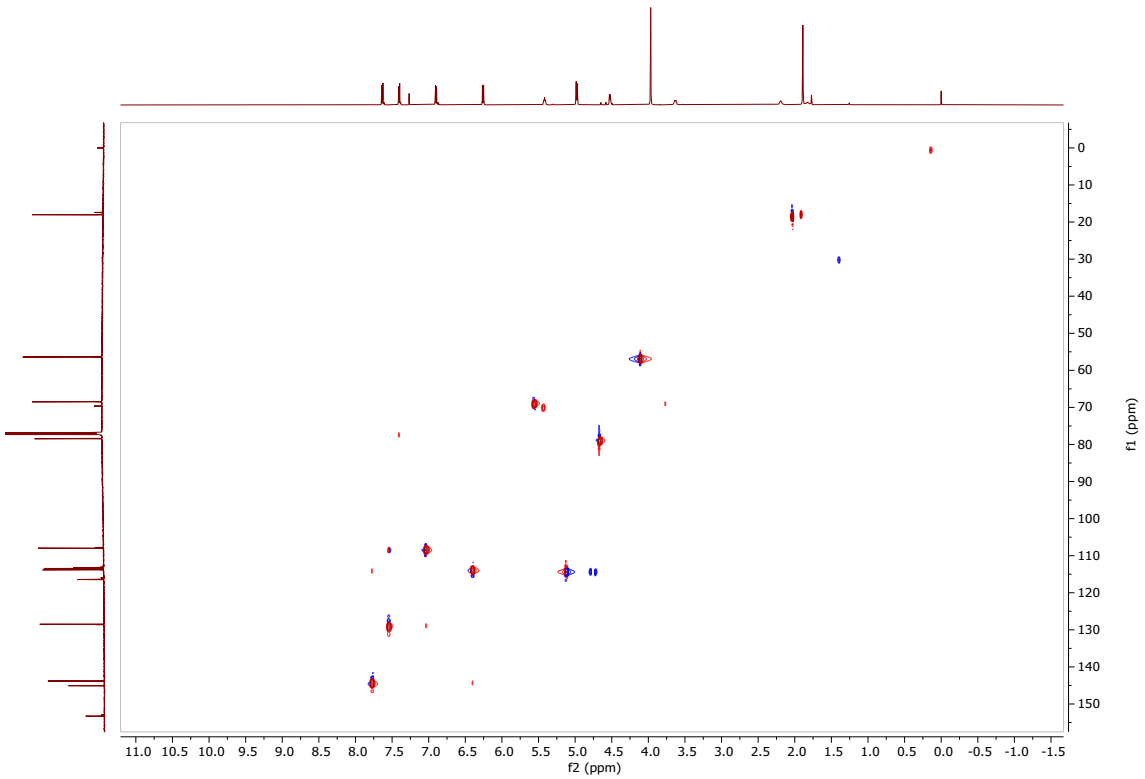
S.30. ^{13}C NMR spectrum of compound 4 in $CDCl_3$



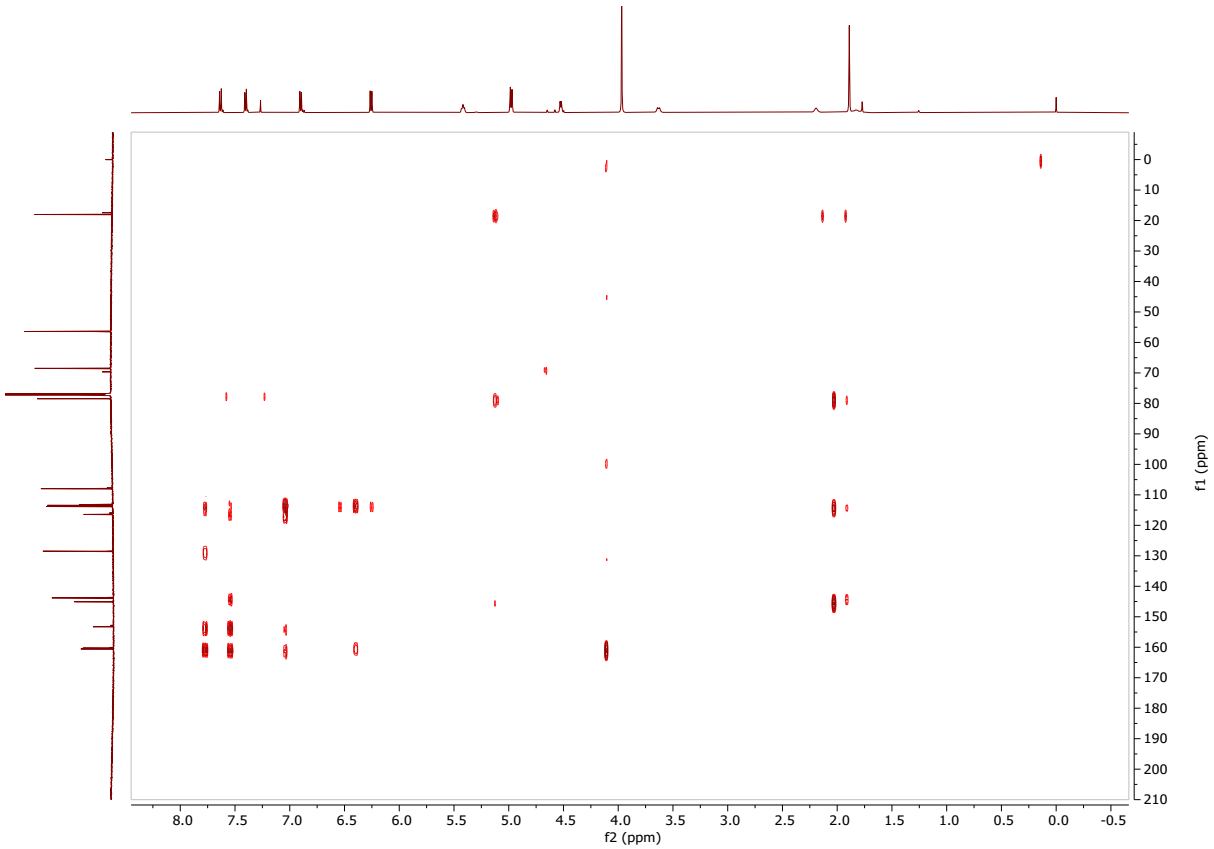
S.31. DEPT-135 NMR spectrum of compound 4 in $CDCl_3$



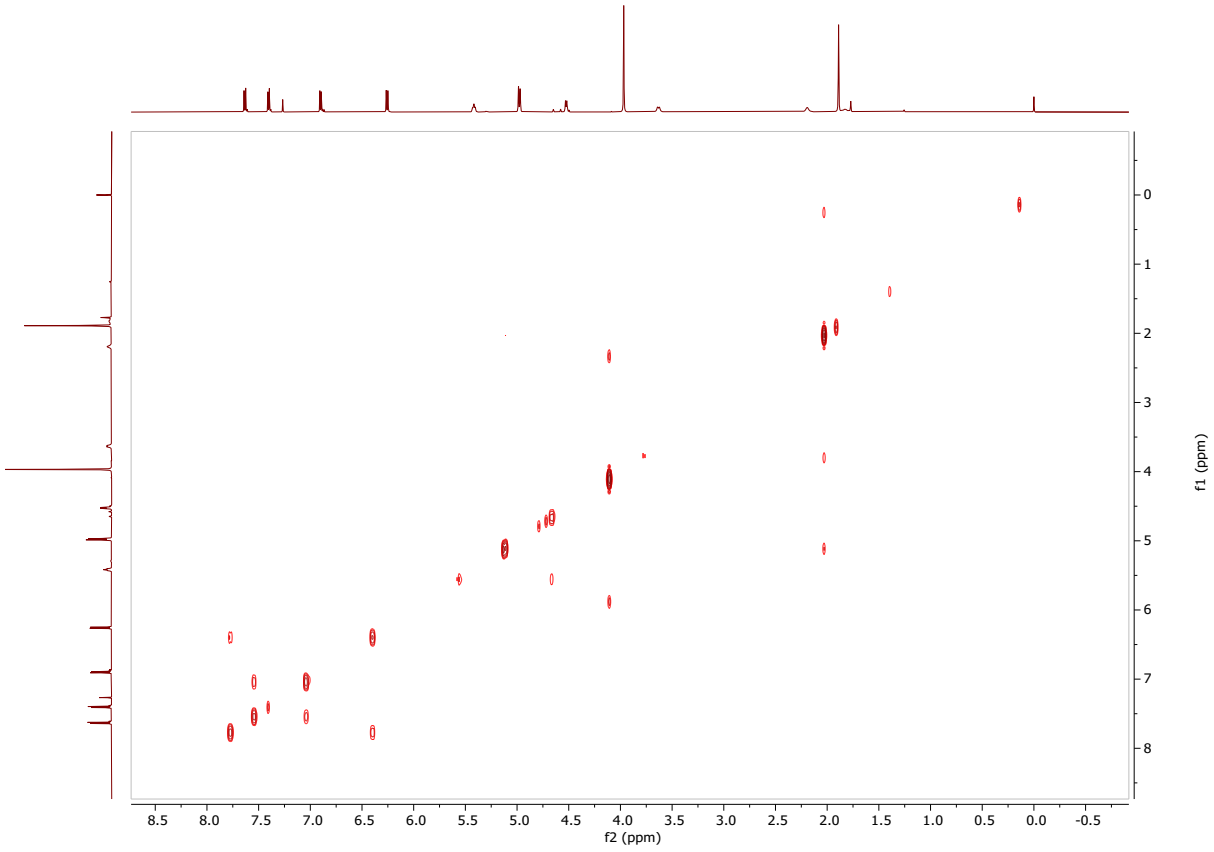
S.32. HSQC spectrum of compound 4 in $CDCl_3$



S.33. HMBC spectrum of compound 4 in $CDCl_3$



S.34. ^{1}H-^{1}H COSY NMR spectrum of compound 4 in $CDCl_3$



S 35. Calculation for DoU

· a compound which contains elements other than carbon and hydrogen:

$$DoU = \frac{2C + 2 + N - X - H}{2}$$

C is the number of carbons

N is the number of nitrogens

X is the number of halogens (F, Cl, Br, I)

H is the number of hydrogens