Electronic Supplementary Infomation

Catalyst-controlled regiodivergent Friedel-Crafts reactions of 1-naphthols with 2,3-dioxopyrrolidines: synthesis of polycyclic 2-pyrrolidinones

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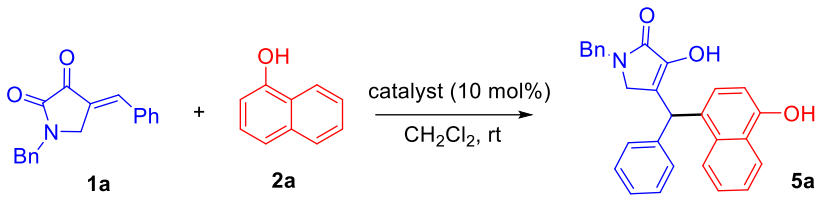
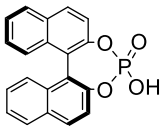
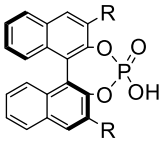
1. Catalyst Screening for *para*-Selective Friedel-Crafts Reaction[a]

Table S1





CPA-1



CPA-2, R = Ph
CPA-3, R = $SiPh_3$
CPA-4, R = 3,5-bis(trifluoromethyl)phenyl
CPA-5, R = 2,4,6-triisopropylphenyl
CPA-6, R = 2-naphthalenyl
CPA-7, R = 9-anthracenyl

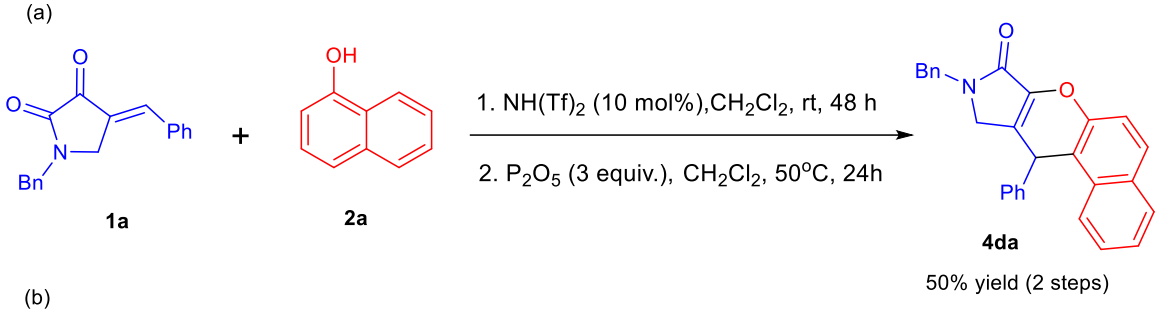
Entry	Cat.	Time (h)	Yield (%)[b]	ee (%)[c]
1	**CPA-1**	48	64	7
2	**CPA-2**	24	52	4
3	**CPA-3**	48	trace	-
4	**CPA-4**	48	56	1
5	**CPA-5**	48	32	0
6	**CPA-6**	48	38	5
7	**CPA-7**	48	42	3

[a] Unless otherwise noted, the reaction was carried out by using 0.1 mmol of 1a, 0.15 mmol of 2a, 10 mol % of catalyst in 1.0 mL of CH_2Cl_2 at rt (25 ˚C) for 24-48h [b]Isolated yield. [c]Determinated by chiral HPLC analysis.

2. Further Substrate Scope Examination

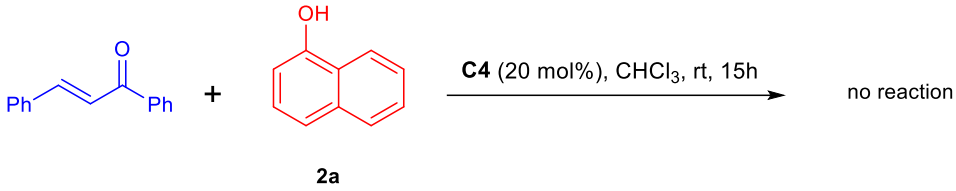
Scheme S1

(a)



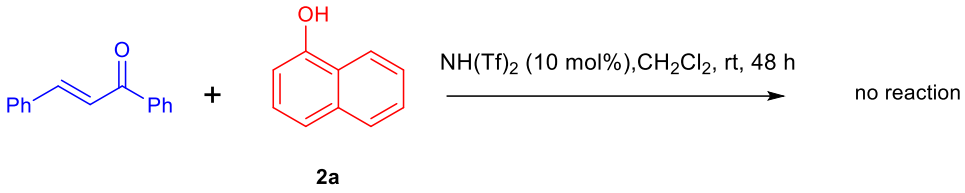
50% yield (2 steps)

(b)



no reaction

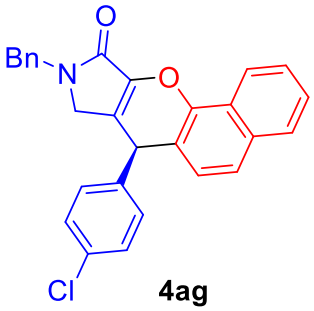
(c)



no reaction

3. X-Ray Crystallographic Analysis Data

CCDC 222256393 (4ag)



4ag

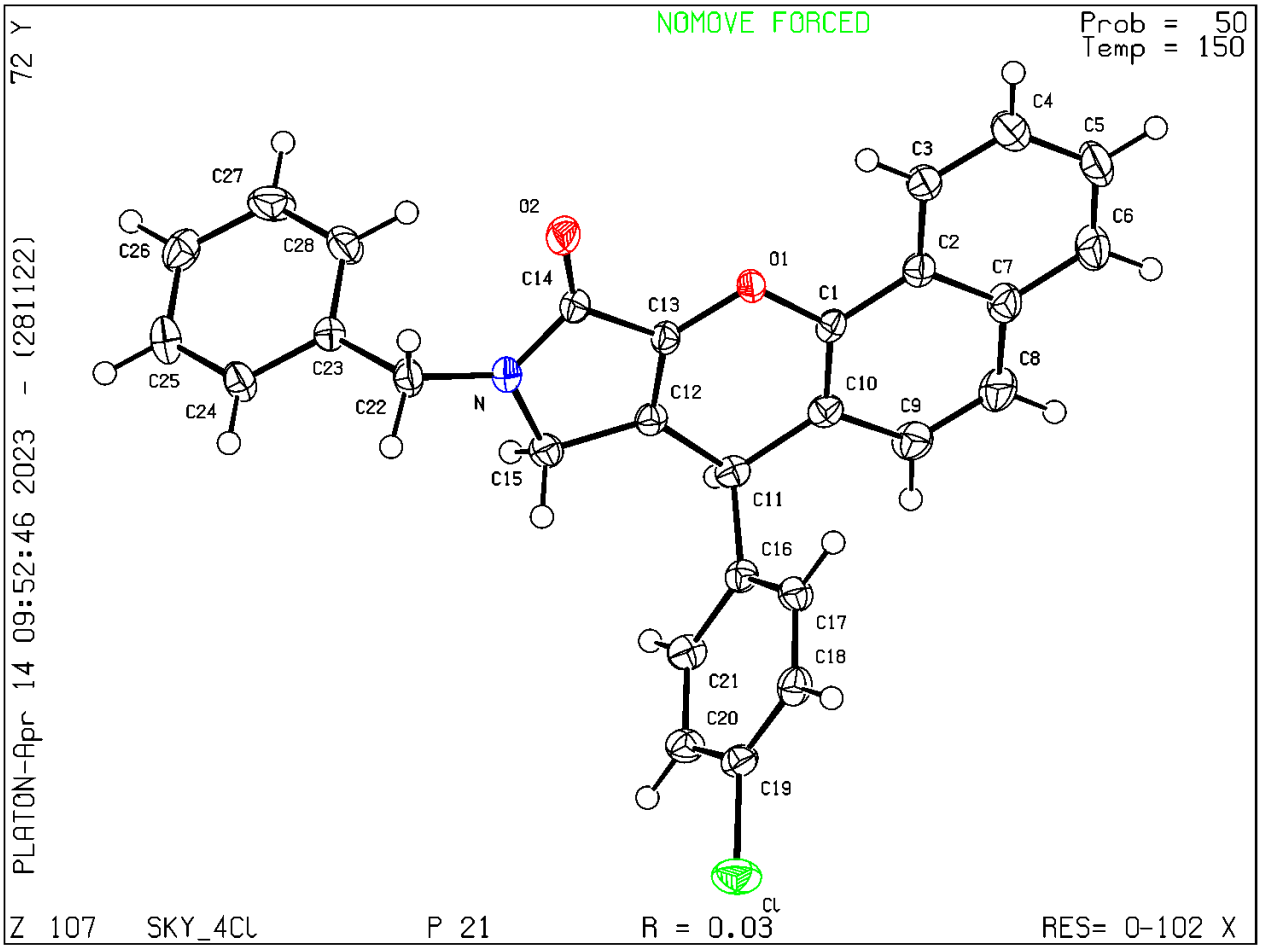


Figure S1. ORTEP drawing of **4ag** showing thermal ellipsoids at the 50% probability level

The crystal was obtained by liquid/liquid diffusion using a mixture of CH_2Cl_2 and Hexanes as solvents.

Table 1. Crystal data and structure refinement for **4ag**.

Identification code	**4ag**	
Empirical formula	C28 H20 Cl N O2	
Formula weight	437.90	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 10.6868(7) Å	a= 90°.
	b = 9.8097(5) Å	b= 110.720(2)°.
	c = 11.0347(7) Å	g = 90°.
Volume	1081.99(11) $Å^3$	
Z	2	
Density (calculated)	1.344 Mg/m^3	
Absorption coefficient	0.203 mm^{-1}	
F(000)	456	
Crystal size	0.250 x 0.240 x 0.160 mm^3	
Theta range for data collection	2.865 to 27.911°.	
Index ranges	-14<=h<=14, -12<=k<=12, -14<=l<=14	
Reflections collected	29069	
Independent reflections	5155 [R(int) = 0.0593]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6932	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5155 / 1 / 289	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0284, wR2 = 0.0693	
R indices (all data)	R1 = 0.0371, wR2 = 0.0721	
Absolute structure (Flack) parameter	-0.007(17)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.190 and -0.227 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4ag**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl	4503(1)	3259(1)	4041(1)	38(1)
O(1)	1610(1)	10741(1)	4568(1)	21(1)
O(2)	3659(1)	11647(1)	6998(1)	29(1)
N	3526(2)	9431(2)	7651(1)	23(1)
C(1)	683(2)	10069(2)	3525(2)	19(1)
C(2)	86(2)	10923(2)	2430(2)	21(1)
C(3)	434(2)	12311(2)	2410(2)	24(1)
C(4)	-170(2)	13095(2)	1329(2)	31(1)
C(5)	-1143(2)	12524(2)	224(2)	35(1)
C(6)	-1491(2)	11187(2)	224(2)	36(1)
C(7)	-897(2)	10342(2)	1322(2)	28(1)
C(8)	-1243(2)	8955(2)	1360(2)	35(1)
C(9)	-636(2)	8182(2)	2425(2)	30(1)
C(10)	358(2)	8715(2)	3550(2)	21(1)
C(11)	990(2)	7788(2)	4706(2)	20(1)
C(12)	1911(2)	8638(2)	5781(2)	19(1)
C(13)	2160(2)	9939(2)	5639(2)	19(1)
C(14)	3191(2)	10499(2)	6810(2)	22(1)
C(15)	2794(2)	8192(2)	7107(2)	23(1)
C(16)	1784(2)	6606(2)	4434(2)	20(1)
C(17)	2530(2)	6778(2)	3636(2)	23(1)
C(18)	3364(2)	5755(2)	3505(2)	26(1)
C(19)	3447(2)	4549(2)	4180(2)	24(1)
C(20)	2722(2)	4340(2)	4981(2)	26(1)
C(21)	1890(2)	5384(2)	5098(2)	25(1)
C(22)	4605(2)	9490(2)	8894(2)	24(1)
C(23)	4149(2)	9713(2)	10029(2)	21(1)
C(24)	4710(2)	8967(2)	11158(2)	27(1)
C(25)	4330(2)	9205(2)	12220(2)	31(1)
C(26)	3388(2)	10197(2)	12158(2)	31(1)
C(27)	2813(2)	10930(2)	11025(2)	37(1)
C(28)	3190(2)	10689(2)	9970(2)	32(1)

Table 3. Bond lengths [Å] and angles [°] for **4ag**.

Cl-C(19)	1.7373(19)
O(1)-C(13)	1.367(2)
O(1)-C(1)	1.391(2)
O(2)-C(14)	1.220(2)
N-C(14)	1.361(2)
N-C(15)	1.455(3)
N-C(22)	1.448(2)
C(1)-C(10)	1.377(2)
C(1)-C(2)	1.422(3)
C(2)-C(3)	1.414(3)
C(2)-C(7)	1.419(3)
C(3)-C(4)	1.374(3)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.409(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.363(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.419(3)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.415(3)
C(8)-C(9)	1.355(3)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.418(3)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.517(3)
C(11)-C(12)	1.498(2)
C(11)-C(16)	1.528(2)
C(11)-H(11A)	1.0000
C(12)-C(13)	1.325(2)
C(12)-C(15)	1.499(2)
C(13)-C(14)	1.476(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(21)	1.388(3)
C(16)-C(17)	1.391(2)
C(17)-C(18)	1.383(3)

C(17)-H(17A)	0.9500
C(18)-C(19)	1.384(3)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.382(3)
C(20)-C(21)	1.392(3)
C(20)-H(20A)	0.9500
C(21)-H(21A)	0.9500
C(22)-C(23)	1.511(2)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.385(3)
C(23)-C(28)	1.387(3)
C(24)-C(25)	1.389(3)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.384(3)
C(25)-H(25A)	0.9500
C(26)-C(27)	1.383(3)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.381(3)
C(27)-H(27A)	0.9500
C(28)-H(28A)	0.9500
C(13)-O(1)-C(1)	113.94(13)
C(14)-N-C(15)	112.89(15)
C(14)-N-C(22)	122.99(17)
C(15)-N-C(22)	123.76(15)
C(10)-C(1)-O(1)	123.46(16)
C(10)-C(1)-C(2)	123.05(16)
O(1)-C(1)-C(2)	113.48(15)
C(3)-C(2)-C(1)	122.63(17)
C(3)-C(2)-C(7)	119.48(18)
C(1)-C(2)-C(7)	117.90(17)
C(4)-C(3)-C(2)	120.49(19)
C(4)-C(3)-H(3A)	119.8
C(2)-C(3)-H(3A)	119.8
C(3)-C(4)-C(5)	120.3(2)
C(3)-C(4)-H(4A)	119.8
C(5)-C(4)-H(4A)	119.8
C(6)-C(5)-C(4)	120.0(2)

C(6)-C(5)-H(5A)	120.0
C(4)-C(5)-H(5A)	120.0
C(5)-C(6)-C(7)	121.5(2)
C(5)-C(6)-H(6A)	119.3
C(7)-C(6)-H(6A)	119.3
C(8)-C(7)-C(6)	122.98(19)
C(8)-C(7)-C(2)	118.85(18)
C(6)-C(7)-C(2)	118.18(19)
C(9)-C(8)-C(7)	120.91(19)
C(9)-C(8)-H(8A)	119.5
C(7)-C(8)-H(8A)	119.5
C(8)-C(9)-C(10)	122.3(2)
C(8)-C(9)-H(9A)	118.9
C(10)-C(9)-H(9A)	118.9
C(1)-C(10)-C(9)	117.03(17)
C(1)-C(10)-C(11)	123.73(16)
C(9)-C(10)-C(11)	119.23(17)
C(12)-C(11)-C(10)	107.73(14)
C(12)-C(11)-C(16)	108.80(14)
C(10)-C(11)-C(16)	113.73(14)
C(12)-C(11)-H(11A)	108.8
C(10)-C(11)-H(11A)	108.8
C(16)-C(11)-H(11A)	108.8
C(13)-C(12)-C(11)	123.09(16)
C(13)-C(12)-C(15)	108.26(16)
C(11)-C(12)-C(15)	128.38(15)
C(12)-C(13)-O(1)	127.87(16)
C(12)-C(13)-C(14)	111.97(16)
O(1)-C(13)-C(14)	120.14(15)
O(2)-C(14)-N	127.02(18)
O(2)-C(14)-C(13)	128.79(16)
N-C(14)-C(13)	104.19(15)
N-C(15)-C(12)	102.68(15)
N-C(15)-H(15A)	111.2
C(12)-C(15)-H(15A)	111.2
N-C(15)-H(15B)	111.2
C(12)-C(15)-H(15B)	111.2
H(15A)-C(15)-H(15B)	109.1

C(21)-C(16)-C(17)	118.75(16)
C(21)-C(16)-C(11)	119.88(16)
C(17)-C(16)-C(11)	120.99(15)
C(18)-C(17)-C(16)	120.84(17)
C(18)-C(17)-H(17A)	119.6
C(16)-C(17)-H(17A)	119.6
C(19)-C(18)-C(17)	119.03(17)
C(19)-C(18)-H(18A)	120.5
C(17)-C(18)-H(18A)	120.5
C(18)-C(19)-C(20)	121.78(17)
C(18)-C(19)-Cl	119.70(14)
C(20)-C(19)-Cl	118.52(15)
C(19)-C(20)-C(21)	118.16(17)
C(19)-C(20)-H(20A)	120.9
C(21)-C(20)-H(20A)	120.9
C(16)-C(21)-C(20)	121.44(17)
C(16)-C(21)-H(21A)	119.3
C(20)-C(21)-H(21A)	119.3
N-C(22)-C(23)	114.13(15)
N-C(22)-H(22A)	108.7
C(23)-C(22)-H(22A)	108.7
N-C(22)-H(22B)	108.7
C(23)-C(22)-H(22B)	108.7
H(22A)-C(22)-H(22B)	107.6
C(24)-C(23)-C(28)	118.98(17)
C(24)-C(23)-C(22)	120.33(16)
C(28)-C(23)-C(22)	120.68(16)
C(23)-C(24)-C(25)	120.46(18)
C(23)-C(24)-H(24A)	119.8
C(25)-C(24)-H(24A)	119.8
C(24)-C(25)-C(26)	120.09(19)
C(24)-C(25)-H(25A)	120.0
C(26)-C(25)-H(25A)	120.0
C(25)-C(26)-C(27)	119.55(18)
C(25)-C(26)-H(26A)	120.2
C(27)-C(26)-H(26A)	120.2
C(28)-C(27)-C(26)	120.23(19)
C(28)-C(27)-H(27A)	119.9

C(26)-C(27)-H(27A)	119.9
C(23)-C(28)-C(27)	120.67(19)
C(23)-C(28)-H(28A)	119.7
C(27)-C(28)-H(28A)	119.7

Symmetry transformations used to generate equivalent atoms:

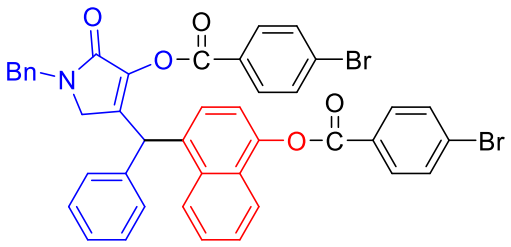
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4ag**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl	41(1)	31(1)	47(1)	0(1)	22(1)	12(1)
O(1)	25(1)	18(1)	16(1)	1(1)	3(1)	-2(1)
O(2)	36(1)	24(1)	22(1)	-2(1)	4(1)	-7(1)
N	28(1)	24(1)	17(1)	1(1)	6(1)	1(1)
C(1)	16(1)	23(1)	17(1)	-4(1)	5(1)	-1(1)
C(2)	18(1)	27(1)	20(1)	-2(1)	8(1)	4(1)
C(3)	24(1)	26(1)	23(1)	1(1)	9(1)	2(1)
C(4)	32(1)	32(1)	30(1)	8(1)	13(1)	7(1)
C(5)	34(1)	44(1)	24(1)	10(1)	6(1)	12(1)
C(6)	32(1)	44(1)	24(1)	0(1)	0(1)	6(1)
C(7)	22(1)	34(1)	23(1)	-3(1)	3(1)	3(1)
C(8)	28(1)	37(1)	29(1)	-9(1)	-2(1)	-4(1)
C(9)	26(1)	26(1)	33(1)	-6(1)	4(1)	-5(1)
C(10)	18(1)	23(1)	24(1)	-3(1)	9(1)	0(1)
C(11)	21(1)	19(1)	23(1)	-1(1)	10(1)	-3(1)
C(12)	21(1)	21(1)	19(1)	0(1)	10(1)	0(1)
C(13)	21(1)	22(1)	15(1)	0(1)	7(1)	1(1)
C(14)	25(1)	24(1)	17(1)	0(1)	8(1)	2(1)
C(15)	28(1)	21(1)	22(1)	2(1)	11(1)	0(1)
C(16)	19(1)	18(1)	20(1)	-2(1)	6(1)	-4(1)
C(17)	28(1)	21(1)	23(1)	3(1)	12(1)	0(1)
C(18)	26(1)	31(1)	22(1)	-1(1)	12(1)	0(1)
C(19)	22(1)	22(1)	26(1)	-6(1)	6(1)	0(1)
C(20)	30(1)	19(1)	29(1)	0(1)	12(1)	-3(1)
C(21)	28(1)	22(1)	28(1)	0(1)	16(1)	-3(1)
C(22)	22(1)	32(1)	17(1)	2(1)	4(1)	5(1)
C(23)	22(1)	22(1)	19(1)	0(1)	6(1)	1(1)
C(24)	25(1)	32(1)	22(1)	6(1)	6(1)	6(1)
C(25)	29(1)	42(1)	19(1)	6(1)	6(1)	-1(1)
C(26)	38(1)	34(1)	25(1)	-5(1)	18(1)	-6(1)
C(27)	50(1)	29(1)	42(1)	6(1)	28(1)	15(1)
C(28)	41(1)	30(1)	25(1)	10(1)	15(1)	12(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4ag**.

	x	y	z	U(eq)
H(3A)	1091	12705	3150	29
H(4A)	69	14028	1326	37
H(5A)	-1556	13071	-521	42
H(6A)	-2146	10812	-528	43
H(8A)	-1910	8559	629	42
H(9A)	-885	7251	2417	36
H(11A)	269	7409	4989	24
H(15A)	2259	7873	7624	28
H(15B)	3408	7454	7061	28
H(17A)	2465	7608	3175	28
H(18A)	3872	5878	2960	31
H(20A)	2789	3508	5439	31
H(21A)	1384	5258	5645	30
H(22A)	5219	10238	8875	29
H(22B)	5116	8627	9030	29
H(24A)	5358	8287	11206	32
H(25A)	4717	8687	12989	37
H(26A)	3139	10374	12888	37
H(27A)	2156	11602	10973	45
H(28A)	2789	11196	9195	38

CCDC 2227147 (7)



7

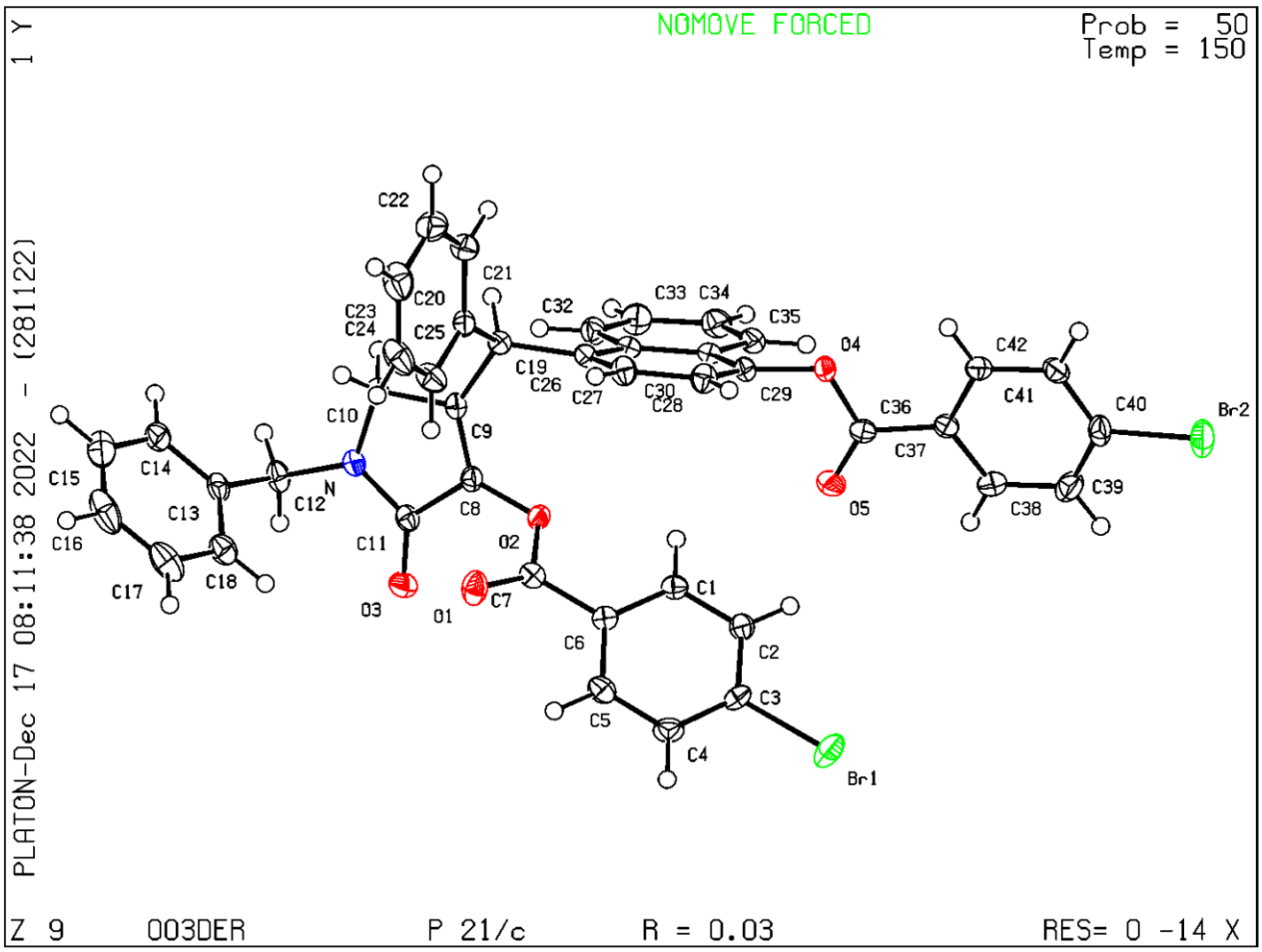


Figure S2. ORTEP drawing of **7** showing thermal ellipsoids at the 50% probability level

The crystal was obtained by liquid/liquid diffusion using a mixture of $CHCl_3$ and Hexanes as solvents.

Table 1. Crystal data and structure refinement for **7**.

Identification code	003DER	
Empirical formula	C42 H29 Br2 N O5	
Formula weight	787.48	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 22.2390(6) Å	a= 90°.
	b = 9.4028(3) Å	b= 91.6868(13)°.
	c = 16.3805(6) Å	g = 90°.
Volume	3423.82(19) $Å^3$	
Z	4	
Density (calculated)	1.528 Mg/m^3	
Absorption coefficient	2.416 mm^{-1}	
F(000)	1592	
Crystal size	0.420 x 0.290 x 0.180 mm^3	
Theta range for data collection	2.626 to 27.913°.	
Index ranges	-29<=h<=29, -12<=k<=12, -21<=l<=21	
Reflections collected	70351	
Independent reflections	8177 [R(int) = 0.0605]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.5887	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8177 / 0 / 451	
Goodness-of-fit on F^2	1.004	
Final R indices [I>2sigma(I)]	R1 = 0.0343, wR2 = 0.0792	
R indices (all data)	R1 = 0.0477, wR2 = 0.0855	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.267 and -0.840 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	5002(1)	2748(1)	4776(1)	33(1)
Br(2)	7514(1)	9301(1)	3728(1)	36(1)
O(1)	2036(1)	4619(2)	4336(1)	29(1)
O(2)	2416(1)	5676(2)	3230(1)	20(1)
O(3)	1418(1)	3778(2)	2704(1)	26(1)
O(4)	4475(1)	9313(2)	3214(1)	21(1)
O(5)	4643(1)	7022(2)	2887(1)	26(1)
N	889(1)	5871(2)	2530(1)	21(1)
C(1)	3572(1)	4947(2)	3713(1)	19(1)
C(2)	4149(1)	4478(2)	3920(1)	21(1)
C(3)	4215(1)	3356(2)	4461(1)	20(1)
C(4)	3728(1)	2679(2)	4795(1)	25(1)
C(5)	3155(1)	3167(2)	4596(1)	25(1)
C(6)	3077(1)	4304(2)	4060(1)	18(1)
C(7)	2456(1)	4842(2)	3909(1)	19(1)
C(8)	1841(1)	6118(2)	3016(1)	18(1)
C(9)	1632(1)	7441(2)	2988(1)	18(1)
C(10)	989(1)	7373(2)	2676(1)	21(1)
C(11)	1376(1)	5067(2)	2737(1)	20(1)
C(12)	305(1)	5293(3)	2289(1)	24(1)
C(13)	-126(1)	5213(2)	2985(1)	21(1)
C(14)	-658(1)	5983(3)	2961(2)	28(1)
C(15)	-1062(1)	5848(3)	3589(2)	39(1)
C(16)	-934(1)	4951(3)	4239(2)	42(1)
C(17)	-398(1)	4193(3)	4272(2)	36(1)
C(18)	6(1)	4327(3)	3650(1)	26(1)
C(19)	1907(1)	8860(2)	3207(1)	18(1)
C(20)	1635(1)	9457(2)	3984(1)	20(1)
C(21)	1553(1)	10921(2)	4039(1)	25(1)
C(22)	1296(1)	11516(3)	4718(2)	32(1)
C(23)	1120(1)	10640(3)	5356(2)	35(1)
C(24)	1211(1)	9185(3)	5311(2)	34(1)
C(25)	1465(1)	8596(3)	4619(1)	28(1)

C(26)	2594(1)	8868(2)	3216(1)	19(1)
C(27)	2932(1)	8993(2)	3929(1)	23(1)
C(28)	3566(1)	9079(2)	3924(1)	24(1)
C(29)	3850(1)	9067(2)	3202(1)	20(1)
C(30)	3530(1)	8946(2)	2444(1)	19(1)
C(31)	2892(1)	8828(2)	2454(1)	19(1)
C(32)	2573(1)	8711(2)	1688(1)	22(1)
C(33)	2868(1)	8752(3)	971(1)	28(1)
C(34)	3497(1)	8902(3)	965(1)	27(1)
C(35)	3821(1)	8984(2)	1685(1)	22(1)
C(36)	4836(1)	8180(2)	3060(1)	19(1)
C(37)	5484(1)	8550(2)	3145(1)	18(1)
C(38)	5901(1)	7505(2)	2956(1)	25(1)
C(39)	6511(1)	7736(3)	3093(2)	29(1)
C(40)	6694(1)	9026(3)	3418(1)	25(1)
C(41)	6290(1)	10106(2)	3576(1)	23(1)
C(42)	5680(1)	9861(2)	3435(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for **7**.

Br(1)-C(3)	1.900(2)
Br(2)-C(40)	1.894(2)
O(1)-C(7)	1.203(3)
O(2)-C(7)	1.361(2)
O(2)-C(8)	1.382(2)
O(3)-C(11)	1.217(3)
O(4)-C(36)	1.362(3)
O(4)-C(29)	1.408(2)
O(5)-C(36)	1.202(3)
N-C(11)	1.356(3)
N-C(10)	1.449(3)
N-C(12)	1.451(3)
C(1)-C(6)	1.392(3)
C(1)-C(2)	1.389(3)
C(1)-H(1A)	0.9500
C(2)-C(3)	1.383(3)
C(2)-H(2A)	0.9500
C(3)-C(4)	1.382(3)
C(4)-C(5)	1.385(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.391(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.485(3)
C(8)-C(9)	1.328(3)
C(8)-C(11)	1.492(3)
C(9)-C(10)	1.505(3)
C(9)-C(19)	1.507(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(12)-C(13)	1.513(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.386(3)
C(13)-C(18)	1.396(3)
C(14)-C(15)	1.393(4)
C(14)-H(14A)	0.9500

C(15)-C(16)	1.381(4)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.389(4)
C(16)-H(16A)	0.9500
C(17)-C(18)	1.385(3)
C(17)-H(17A)	0.9500
C(18)-H(18A)	0.9500
C(19)-C(26)	1.528(3)
C(19)-C(20)	1.533(3)
C(19)-H(19A)	1.0000
C(20)-C(25)	1.379(3)
C(20)-C(21)	1.392(3)
C(21)-C(22)	1.384(3)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.394(4)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.385(4)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.396(3)
C(24)-H(24A)	0.9500
C(25)-H(25A)	0.9500
C(26)-C(27)	1.374(3)
C(26)-C(31)	1.431(3)
C(27)-C(28)	1.413(3)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.357(3)
C(28)-H(28A)	0.9500
C(29)-C(30)	1.418(3)
C(30)-C(35)	1.419(3)
C(30)-C(31)	1.424(3)
C(31)-C(32)	1.428(3)
C(32)-C(33)	1.363(3)
C(32)-H(32A)	0.9500
C(33)-C(34)	1.407(3)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.366(3)
C(34)-H(34A)	0.9500
C(35)-H(35A)	0.9500

C(36)-C(37)	1.484(3)
C(37)-C(42)	1.387(3)
C(37)-C(38)	1.393(3)
C(38)-C(39)	1.386(3)
C(38)-H(38A)	0.9500
C(39)-C(40)	1.382(4)
C(39)-H(39A)	0.9500
C(40)-C(41)	1.386(3)
C(41)-C(42)	1.387(3)
C(41)-H(41A)	0.9500
C(42)-H(42A)	0.9500

C(7)-O(2)-C(8)	114.76(15)
C(36)-O(4)-C(29)	117.14(16)
C(11)-N-C(10)	112.63(17)
C(11)-N-C(12)	124.11(19)
C(10)-N-C(12)	122.80(18)
C(6)-C(1)-C(2)	119.89(19)
C(6)-C(1)-H(1A)	120.1
C(2)-C(1)-H(1A)	120.1
C(3)-C(2)-C(1)	118.53(19)
C(3)-C(2)-H(2A)	120.7
C(1)-C(2)-H(2A)	120.7
C(4)-C(3)-C(2)	122.42(19)
C(4)-C(3)-Br(1)	118.72(16)
C(2)-C(3)-Br(1)	118.85(16)
C(3)-C(4)-C(5)	118.7(2)
C(3)-C(4)-H(4A)	120.6
C(5)-C(4)-H(4A)	120.6
C(4)-C(5)-C(6)	119.9(2)
C(4)-C(5)-H(5A)	120.0
C(6)-C(5)-H(5A)	120.0
C(1)-C(6)-C(5)	120.48(19)
C(1)-C(6)-C(7)	121.81(19)
C(5)-C(6)-C(7)	117.64(18)
O(1)-C(7)-O(2)	122.85(19)
O(1)-C(7)-C(6)	125.38(19)
O(2)-C(7)-C(6)	111.73(17)

C(9)-C(8)-O(2)	127.71(19)
C(9)-C(8)-C(11)	111.78(18)
O(2)-C(8)-C(11)	120.44(18)
C(8)-C(9)-C(10)	107.47(18)
C(8)-C(9)-C(19)	132.95(18)
C(10)-C(9)-C(19)	119.57(18)
N-C(10)-C(9)	103.71(17)
N-C(10)-H(10A)	111.0
C(9)-C(10)-H(10A)	111.0
N-C(10)-H(10B)	111.0
C(9)-C(10)-H(10B)	111.0
H(10A)-C(10)-H(10B)	109.0
O(3)-C(11)-N	127.3(2)
O(3)-C(11)-C(8)	128.3(2)
N-C(11)-C(8)	104.36(18)
N-C(12)-C(13)	113.31(18)
N-C(12)-H(12A)	108.9
C(13)-C(12)-H(12A)	108.9
N-C(12)-H(12B)	108.9
C(13)-C(12)-H(12B)	108.9
H(12A)-C(12)-H(12B)	107.7
C(14)-C(13)-C(18)	119.7(2)
C(14)-C(13)-C(12)	120.7(2)
C(18)-C(13)-C(12)	119.6(2)
C(13)-C(14)-C(15)	120.0(2)
C(13)-C(14)-H(14A)	120.0
C(15)-C(14)-H(14A)	120.0
C(16)-C(15)-C(14)	120.2(2)
C(16)-C(15)-H(15A)	119.9
C(14)-C(15)-H(15A)	119.9
C(15)-C(16)-C(17)	120.1(2)
C(15)-C(16)-H(16A)	120.0
C(17)-C(16)-H(16A)	120.0
C(16)-C(17)-C(18)	120.0(3)
C(16)-C(17)-H(17A)	120.0
C(18)-C(17)-H(17A)	120.0
C(17)-C(18)-C(13)	120.1(2)
C(17)-C(18)-H(18A)	119.9

C(13)-C(18)-H(18A)	119.9
C(9)-C(19)-C(26)	113.98(17)
C(9)-C(19)-C(20)	110.78(16)
C(26)-C(19)-C(20)	114.12(17)
C(9)-C(19)-H(19A)	105.7
C(26)-C(19)-H(19A)	105.7
C(20)-C(19)-H(19A)	105.7
C(25)-C(20)-C(21)	119.5(2)
C(25)-C(20)-C(19)	122.4(2)
C(21)-C(20)-C(19)	118.15(19)
C(22)-C(21)-C(20)	120.6(2)
C(22)-C(21)-H(21A)	119.7
C(20)-C(21)-H(21A)	119.7
C(21)-C(22)-C(23)	119.6(2)
C(21)-C(22)-H(22A)	120.2
C(23)-C(22)-H(22A)	120.2
C(24)-C(23)-C(22)	120.0(2)
C(24)-C(23)-H(23A)	120.0
C(22)-C(23)-H(23A)	120.0
C(23)-C(24)-C(25)	119.8(2)
C(23)-C(24)-H(24A)	120.1
C(25)-C(24)-H(24A)	120.1
C(20)-C(25)-C(24)	120.4(2)
C(20)-C(25)-H(25A)	119.8
C(24)-C(25)-H(25A)	119.8
C(27)-C(26)-C(31)	119.16(18)
C(27)-C(26)-C(19)	122.05(18)
C(31)-C(26)-C(19)	118.69(18)
C(26)-C(27)-C(28)	121.43(19)
C(26)-C(27)-H(27A)	119.3
C(28)-C(27)-H(27A)	119.3
C(29)-C(28)-C(27)	119.6(2)
C(29)-C(28)-H(28A)	120.2
C(27)-C(28)-H(28A)	120.2
C(28)-C(29)-O(4)	118.12(19)
C(28)-C(29)-C(30)	121.96(19)
O(4)-C(29)-C(30)	119.67(18)
C(29)-C(30)-C(35)	122.39(19)

C(29)-C(30)-C(31)	118.08(18)
C(35)-C(30)-C(31)	119.50(19)
C(30)-C(31)-C(32)	117.75(19)
C(30)-C(31)-C(26)	119.71(19)
C(32)-C(31)-C(26)	122.51(18)
C(33)-C(32)-C(31)	121.1(2)
C(33)-C(32)-H(32A)	119.5
C(31)-C(32)-H(32A)	119.5
C(32)-C(33)-C(34)	120.8(2)
C(32)-C(33)-H(33A)	119.6
C(34)-C(33)-H(33A)	119.6
C(35)-C(34)-C(33)	120.0(2)
C(35)-C(34)-H(34A)	120.0
C(33)-C(34)-H(34A)	120.0
C(34)-C(35)-C(30)	120.8(2)
C(34)-C(35)-H(35A)	119.6
C(30)-C(35)-H(35A)	119.6
O(5)-C(36)-O(4)	122.92(19)
O(5)-C(36)-C(37)	125.08(19)
O(4)-C(36)-C(37)	112.00(17)
C(42)-C(37)-C(38)	119.9(2)
C(42)-C(37)-C(36)	122.42(19)
C(38)-C(37)-C(36)	117.67(19)
C(39)-C(38)-C(37)	120.6(2)
C(39)-C(38)-H(38A)	119.7
C(37)-C(38)-H(38A)	119.7
C(40)-C(39)-C(38)	118.5(2)
C(40)-C(39)-H(39A)	120.8
C(38)-C(39)-H(39A)	120.8
C(39)-C(40)-C(41)	121.9(2)
C(39)-C(40)-Br(2)	119.59(17)
C(41)-C(40)-Br(2)	118.37(18)
C(42)-C(41)-C(40)	119.0(2)
C(42)-C(41)-H(41A)	120.5
C(40)-C(41)-H(41A)	120.5
C(41)-C(42)-C(37)	120.1(2)
C(41)-C(42)-H(42A)	120.0
C(37)-C(42)-H(42A)	120.0

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

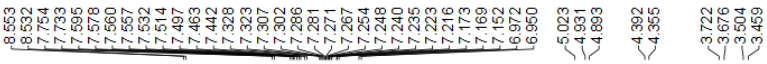
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	25(1)	44(1)	30(1)	8(1)	2(1)	14(1)
Br(2)	17(1)	54(1)	38(1)	15(1)	1(1)	-3(1)
O(1)	21(1)	43(1)	23(1)	7(1)	5(1)	1(1)
O(2)	15(1)	22(1)	21(1)	5(1)	1(1)	2(1)
O(3)	27(1)	18(1)	35(1)	-1(1)	5(1)	-1(1)
O(4)	14(1)	18(1)	31(1)	-2(1)	1(1)	-2(1)
O(5)	27(1)	18(1)	31(1)	-2(1)	-2(1)	-3(1)
N	16(1)	21(1)	27(1)	2(1)	-1(1)	-3(1)
C(1)	22(1)	19(1)	16(1)	1(1)	1(1)	1(1)
C(2)	20(1)	22(1)	20(1)	1(1)	4(1)	0(1)
C(3)	21(1)	21(1)	19(1)	-1(1)	1(1)	8(1)
C(4)	30(1)	23(1)	23(1)	8(1)	2(1)	3(1)
C(5)	26(1)	25(1)	24(1)	6(1)	5(1)	-2(1)
C(6)	20(1)	19(1)	16(1)	0(1)	1(1)	1(1)
C(7)	22(1)	20(1)	16(1)	-1(1)	0(1)	-2(1)
C(8)	15(1)	22(1)	18(1)	2(1)	2(1)	-1(1)
C(9)	15(1)	22(1)	18(1)	0(1)	2(1)	-2(1)
C(10)	15(1)	20(1)	27(1)	2(1)	0(1)	0(1)
C(11)	18(1)	21(1)	19(1)	0(1)	4(1)	-2(1)
C(12)	18(1)	31(1)	22(1)	0(1)	-2(1)	-7(1)
C(13)	17(1)	22(1)	24(1)	-5(1)	-1(1)	-6(1)
C(14)	21(1)	21(1)	42(1)	-6(1)	-1(1)	-4(1)
C(15)	26(1)	29(1)	62(2)	-23(1)	10(1)	-4(1)
C(16)	41(2)	45(2)	43(2)	-23(1)	22(1)	-21(1)
C(17)	44(2)	42(2)	23(1)	-5(1)	4(1)	-21(1)
C(18)	26(1)	27(1)	25(1)	-2(1)	-2(1)	-7(1)
C(19)	17(1)	18(1)	19(1)	1(1)	1(1)	0(1)
C(20)	15(1)	21(1)	22(1)	-2(1)	2(1)	-1(1)
C(21)	26(1)	22(1)	28(1)	0(1)	0(1)	-1(1)
C(22)	31(1)	25(1)	39(1)	-9(1)	2(1)	3(1)
C(23)	32(1)	40(2)	35(1)	-13(1)	12(1)	-5(1)
C(24)	37(1)	36(1)	28(1)	-5(1)	13(1)	-13(1)

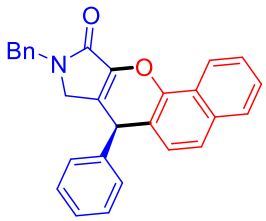
C(25)	33(1)	25(1)	27(1)	-1(1)	7(1)	-6(1)
C(26)	18(1)	16(1)	24(1)	1(1)	3(1)	-2(1)
C(27)	22(1)	27(1)	20(1)	-2(1)	4(1)	-1(1)
C(28)	22(1)	26(1)	22(1)	-4(1)	-2(1)	-1(1)
C(29)	15(1)	17(1)	27(1)	-1(1)	0(1)	-2(1)
C(30)	19(1)	13(1)	24(1)	1(1)	1(1)	-1(1)
C(31)	19(1)	14(1)	22(1)	2(1)	1(1)	-1(1)
C(32)	20(1)	24(1)	23(1)	1(1)	-2(1)	-2(1)
C(33)	29(1)	35(1)	21(1)	6(1)	-1(1)	1(1)
C(34)	30(1)	28(1)	23(1)	5(1)	6(1)	0(1)
C(35)	22(1)	21(1)	25(1)	3(1)	4(1)	-1(1)
C(36)	22(1)	18(1)	16(1)	2(1)	1(1)	0(1)
C(37)	20(1)	19(1)	17(1)	4(1)	2(1)	0(1)
C(38)	27(1)	19(1)	30(1)	0(1)	1(1)	3(1)
C(39)	23(1)	32(1)	33(1)	2(1)	4(1)	8(1)
C(40)	16(1)	36(1)	23(1)	10(1)	2(1)	-2(1)
C(41)	24(1)	21(1)	25(1)	5(1)	-1(1)	-5(1)
C(42)	23(1)	18(1)	24(1)	2(1)	2(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7**.

	x	y	z	U(eq)
H(1A)	3516	5705	3335	23
H(2A)	4491	4919	3695	25
H(4A)	3786	1895	5155	30
H(5A)	2814	2725	4825	30
H(10A)	712	7743	3087	25
H(10B)	933	7927	2165	25
H(12A)	361	4327	2064	29
H(12B)	125	5893	1850	29
H(14A)	-746	6603	2516	34
H(15A)	-1427	6375	3571	47
H(16A)	-1213	4852	4663	51
H(17A)	-309	3582	4722	44
H(18A)	375	3816	3676	31
H(19A)	1777	9523	2758	22
H(21A)	1675	11518	3606	30
H(22A)	1239	12516	4750	38
H(23A)	939	11042	5820	42
H(24A)	1100	8590	5751	40
H(25A)	1520	7597	4585	33
H(27A)	2735	9022	4435	27
H(28A)	3792	9144	4424	28
H(32A)	2148	8604	1678	27
H(33A)	2646	8678	468	34
H(34A)	3696	8947	461	32
H(35A)	4247	9068	1677	27
H(38A)	5766	6627	2730	30
H(39A)	6796	7024	2967	35
H(41A)	6427	10999	3778	28
H(42A)	5397	10592	3538	26

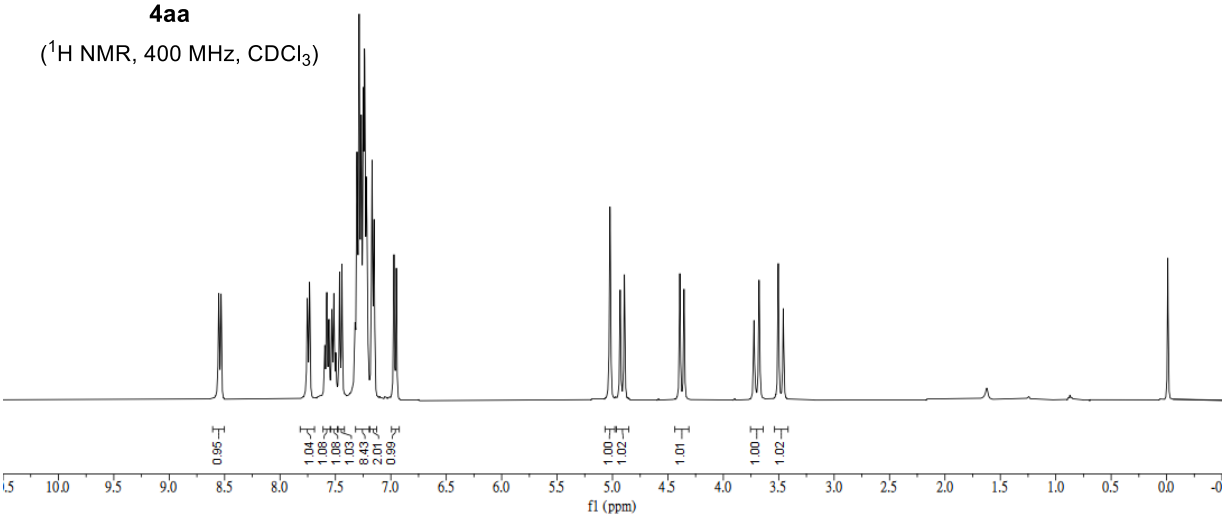
4. Copies of NMR Spectra of Products 4, 5 and 7

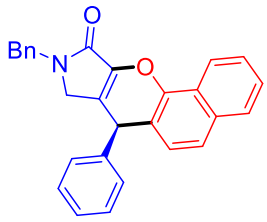




4aa

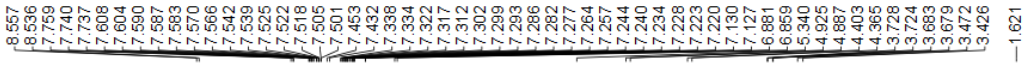
(^{1}H NMR, 400 MHz, $CDCl_3$)

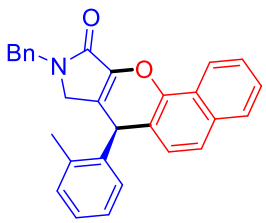




4aa

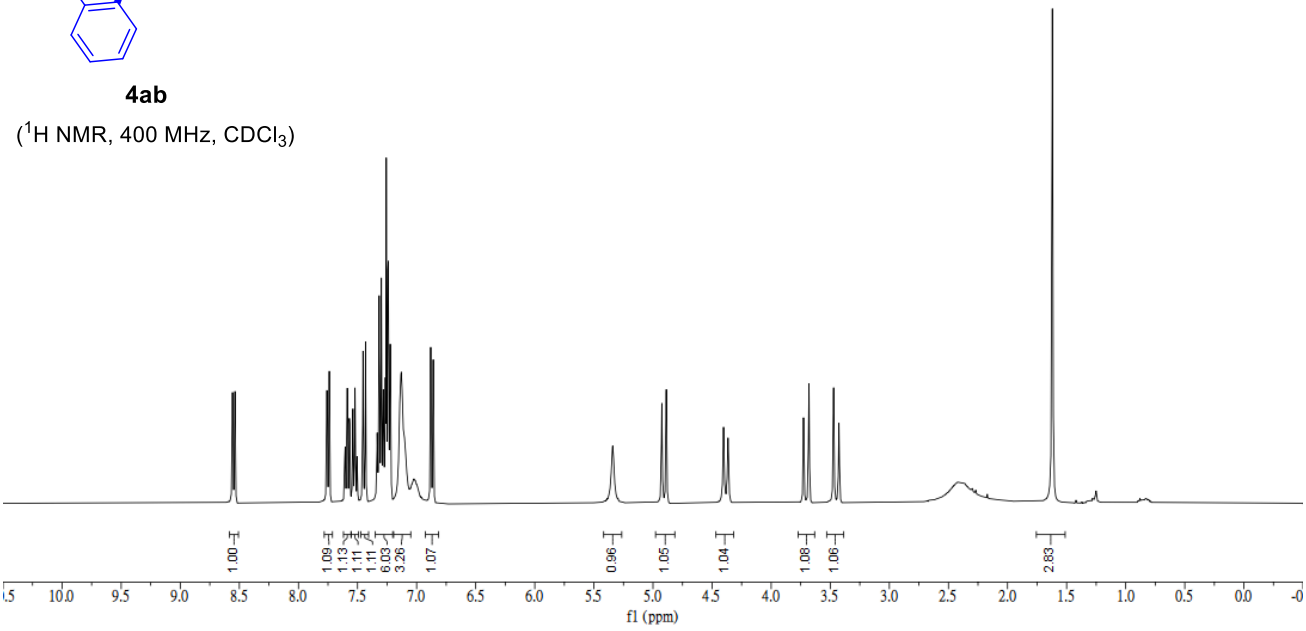
(^{13}C NMR, 100 MHz, $CDCl_3$)

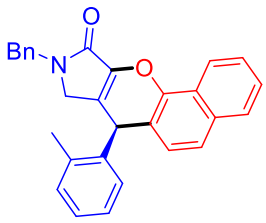




4ab

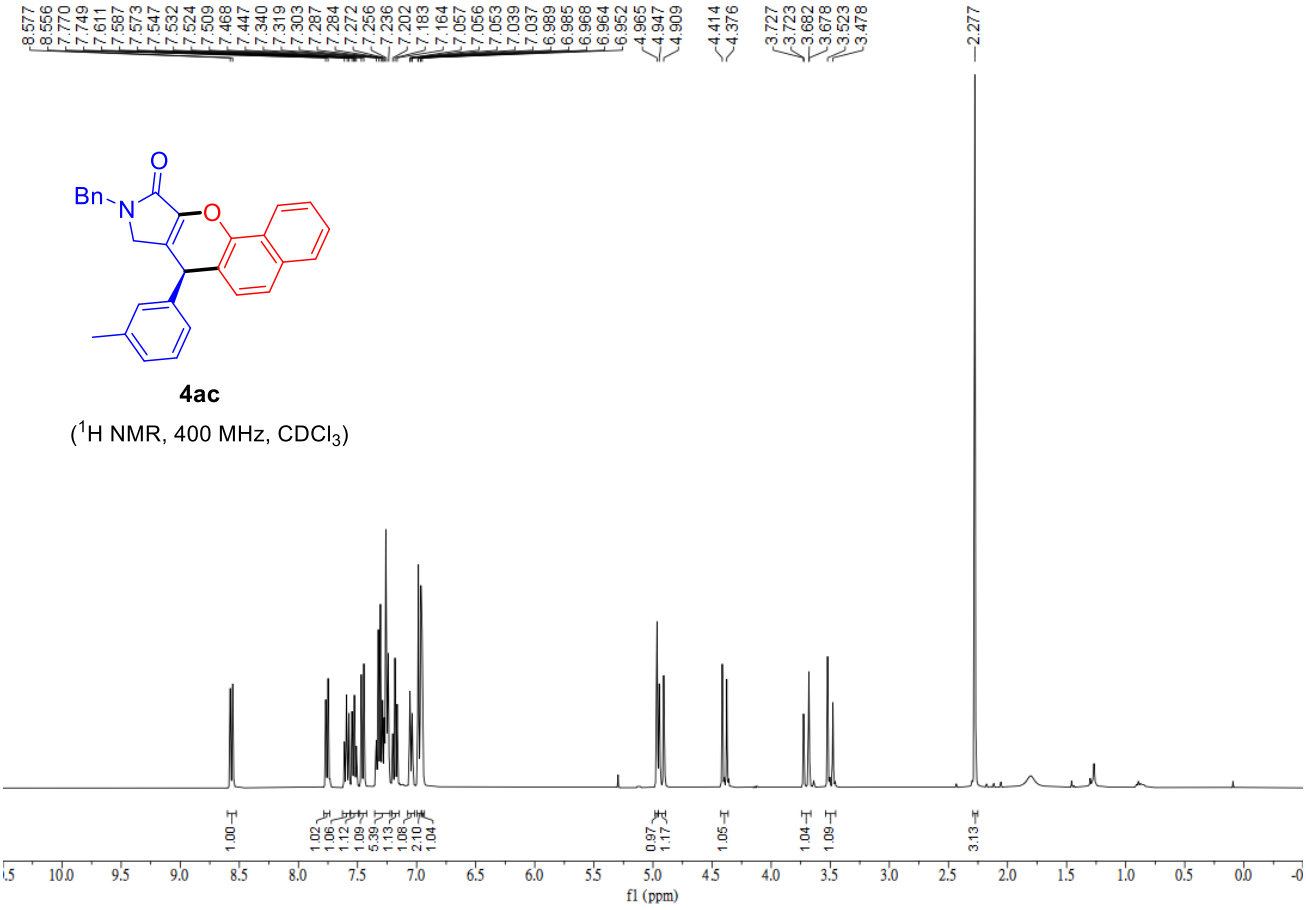
(^{1}H NMR, 400 MHz, $CDCl_3$)





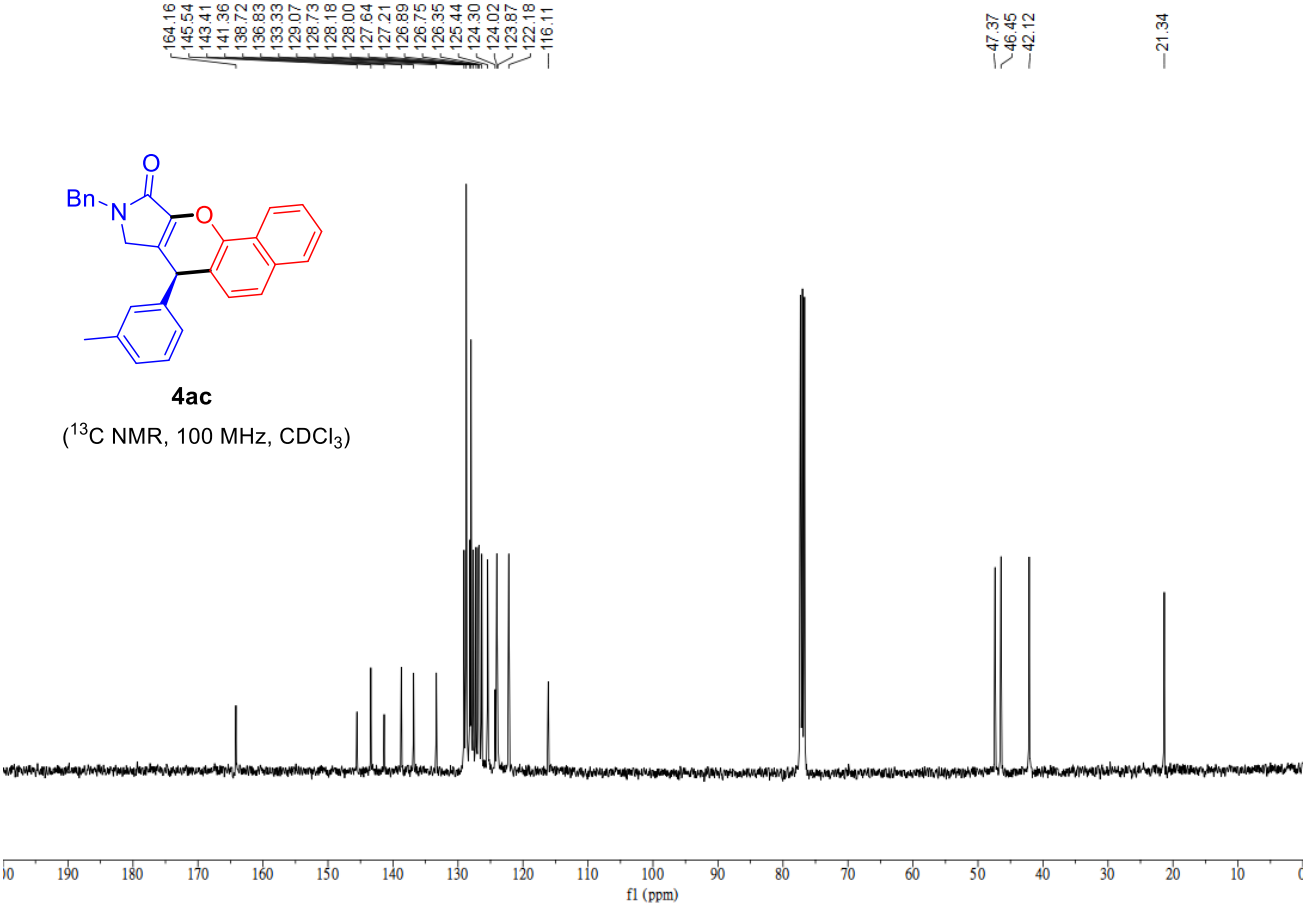
4ab

(^{13}C NMR, 100 MHz, $CDCl_3$)



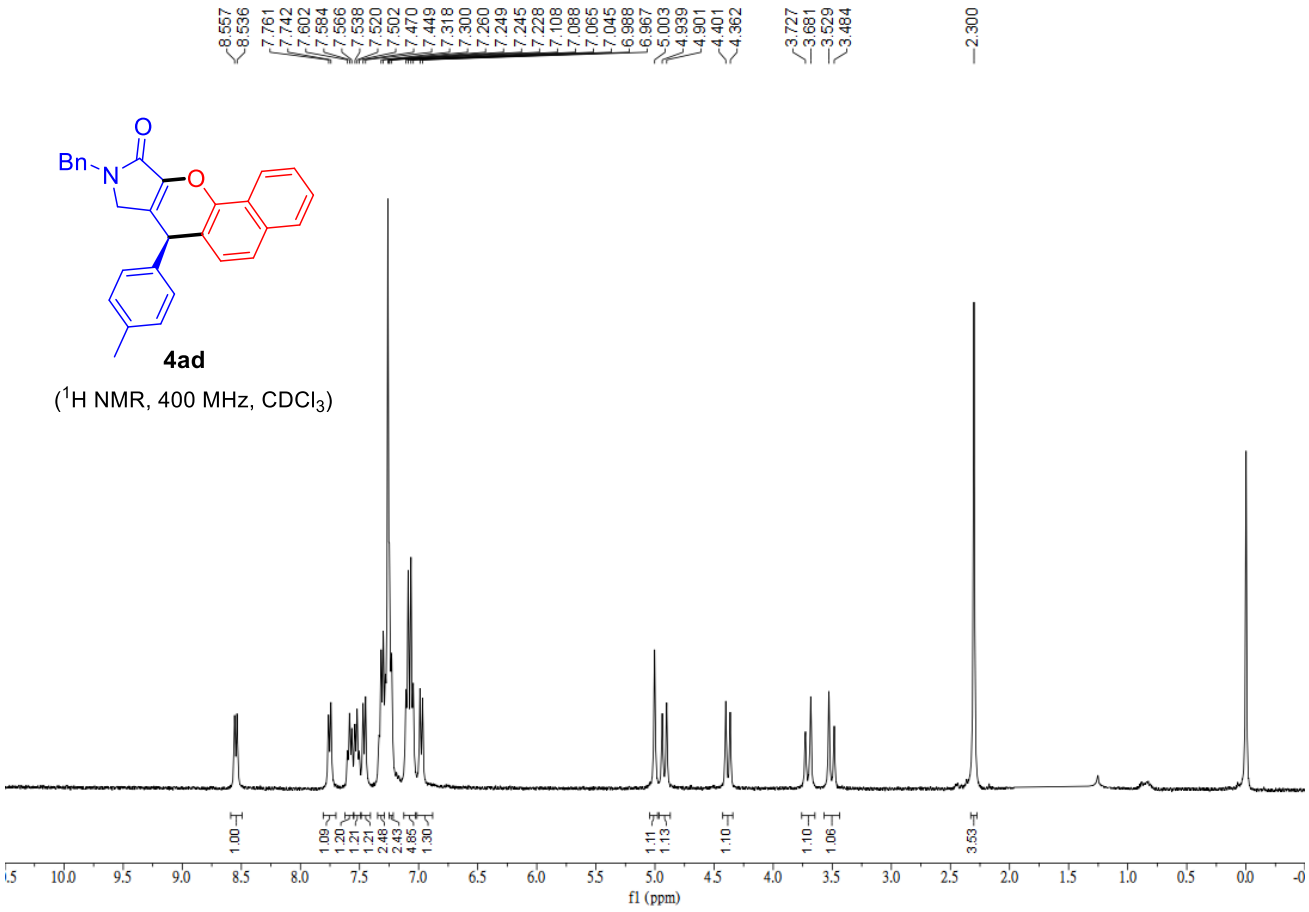
4ac

(^{1}H NMR, 400 MHz, $CDCl_3$)



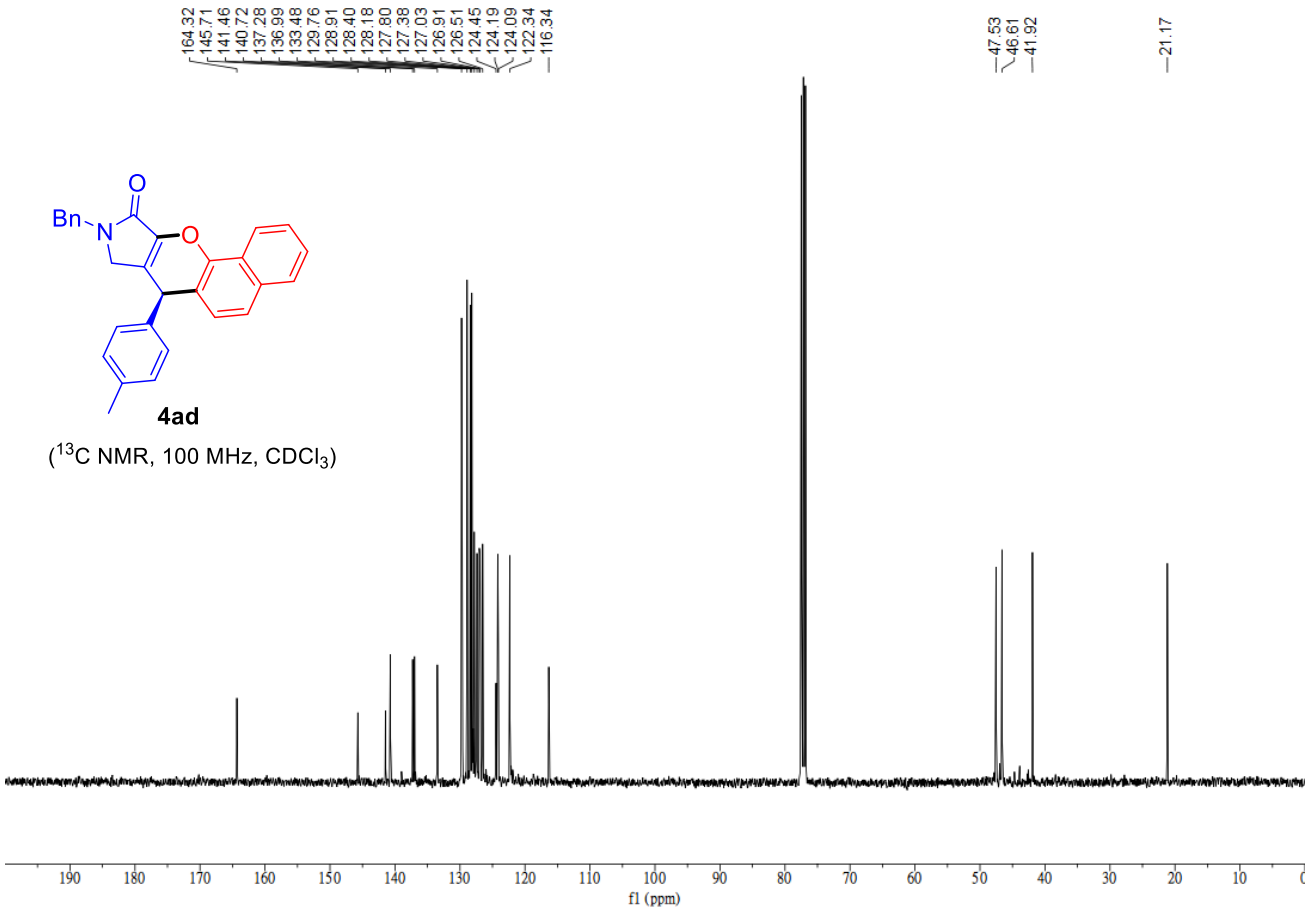
4ac

(^{13}C NMR, 100 MHz, $CDCl_3$)



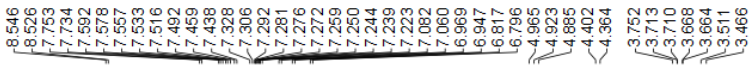
4ad

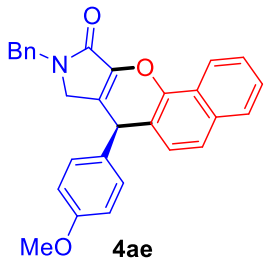
(^{1}H NMR, 400 MHz, $CDCl_3$)



4ad

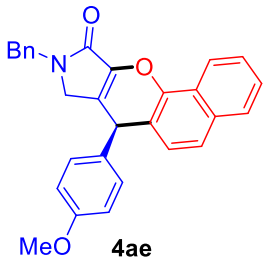
(^{13}C NMR, 100 MHz, $CDCl_3$)





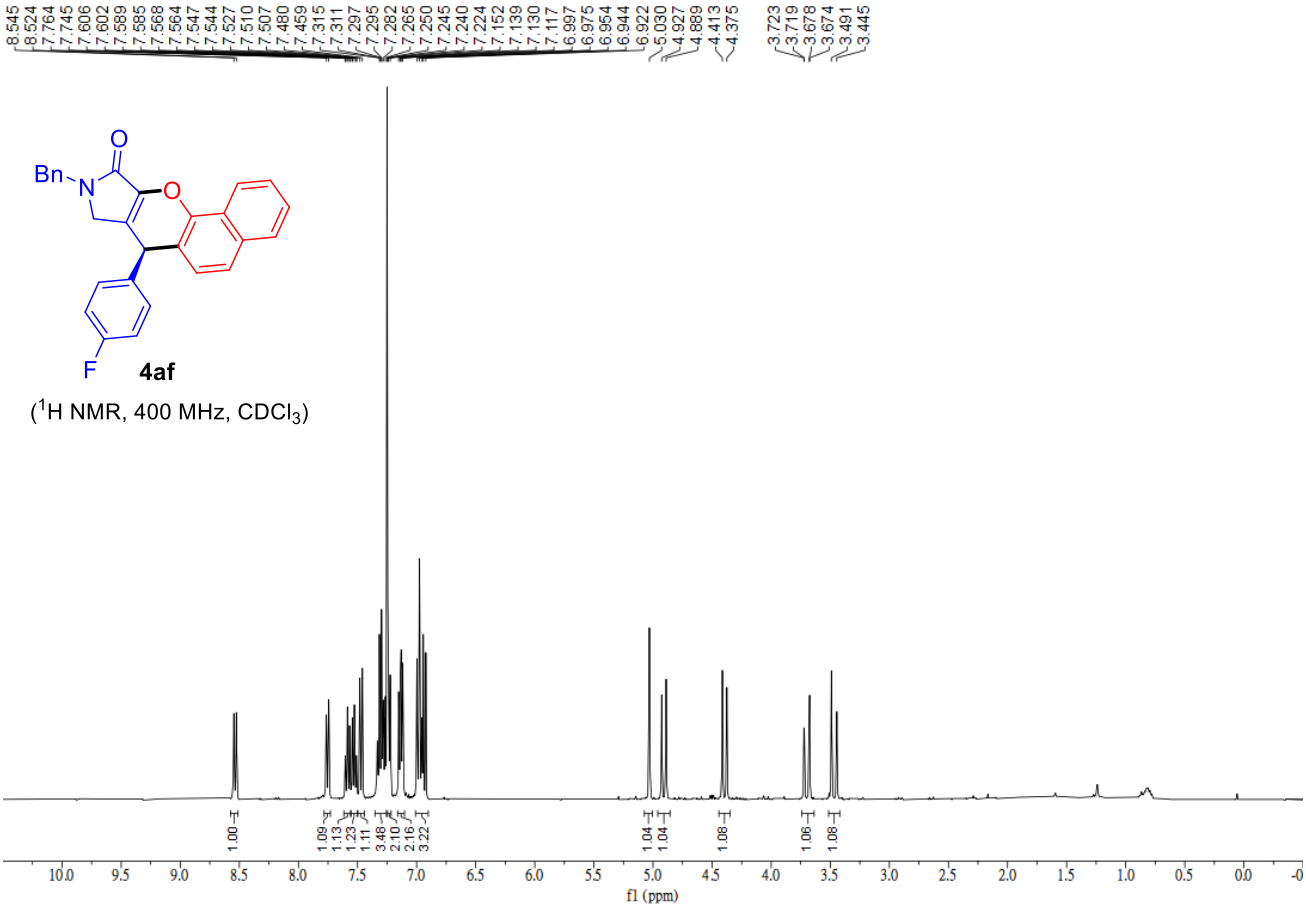
4ae

(^{1}H NMR, 400 MHz, $CDCl_3$)

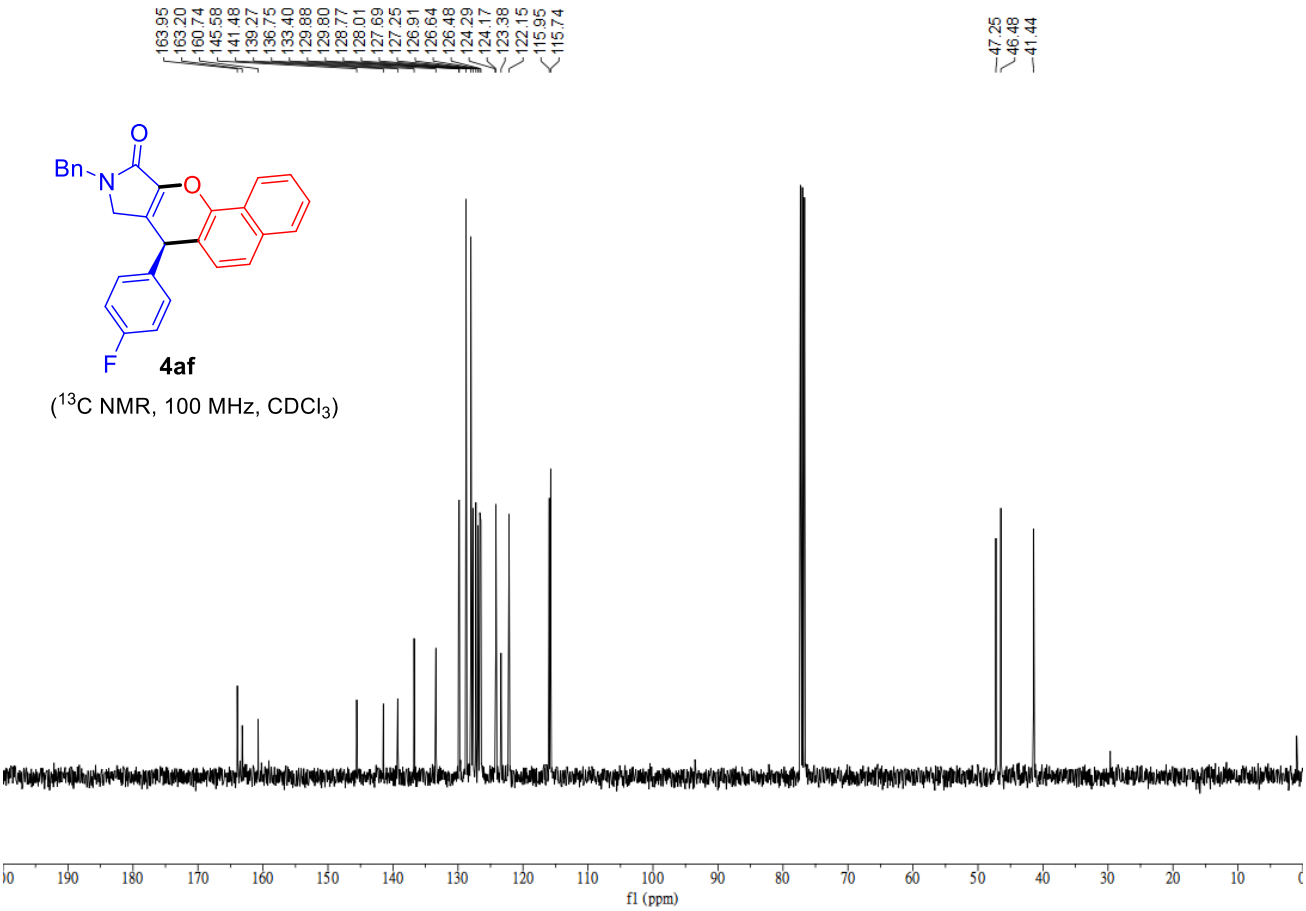


4ae

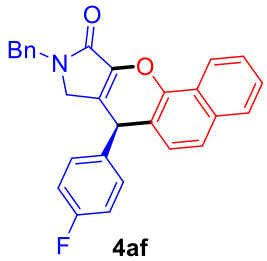
(^{13}C NMR, 100 MHz, $CDCl_3$)



(^{1}H NMR, 400 MHz, $CDCl_3$)

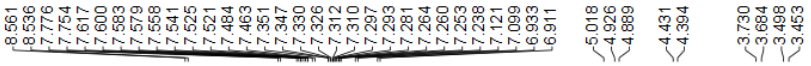


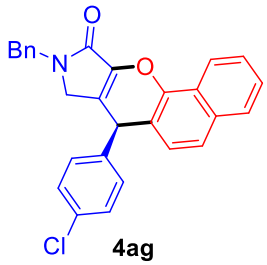
(^{13}C NMR, 100 MHz, $CDCl_3$)



4af

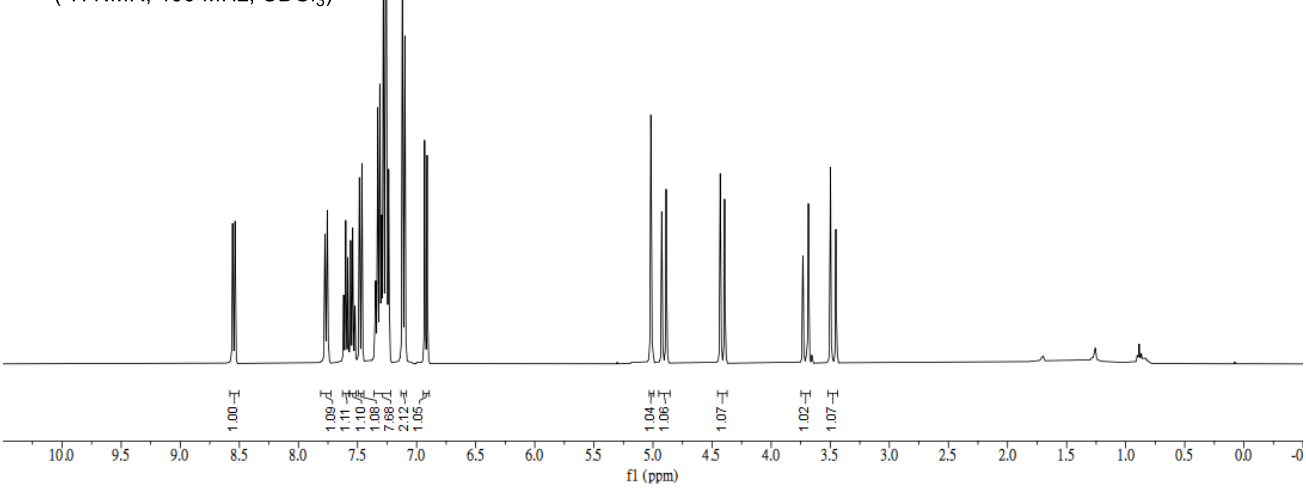
(^{19}F NMR, 376 MHz, $CDCl_3$)

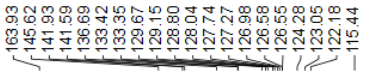


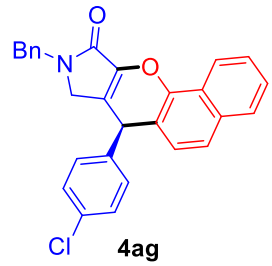


4ag

(^{1}H NMR, 400 MHz, $CDCl_3$)

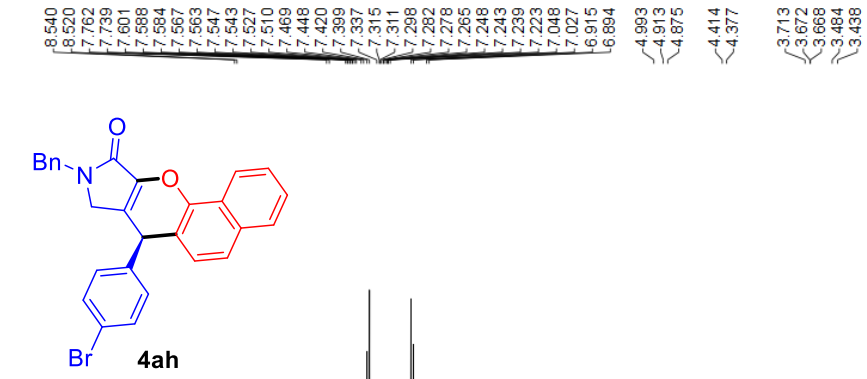






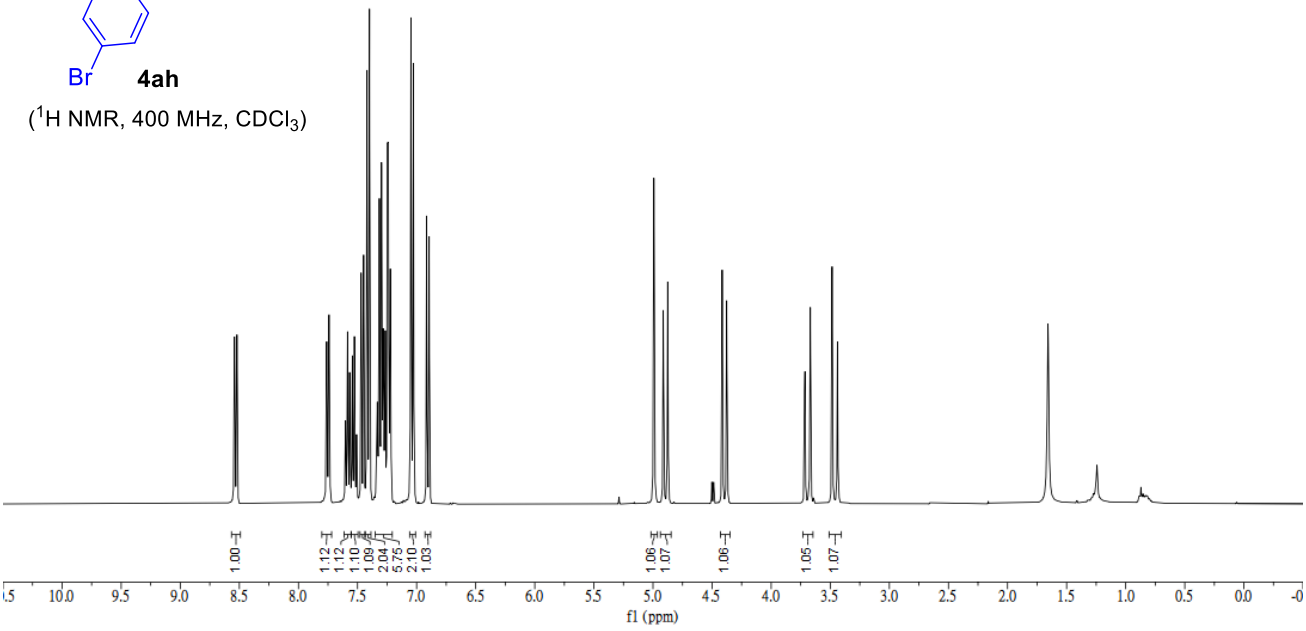
4ag

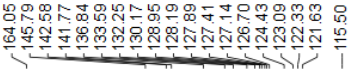
(^{13}C NMR, 100 MHz, $CDCl_3$)

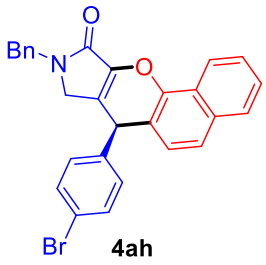


4ah

(^{1}H NMR, 400 MHz, $CDCl_3$)







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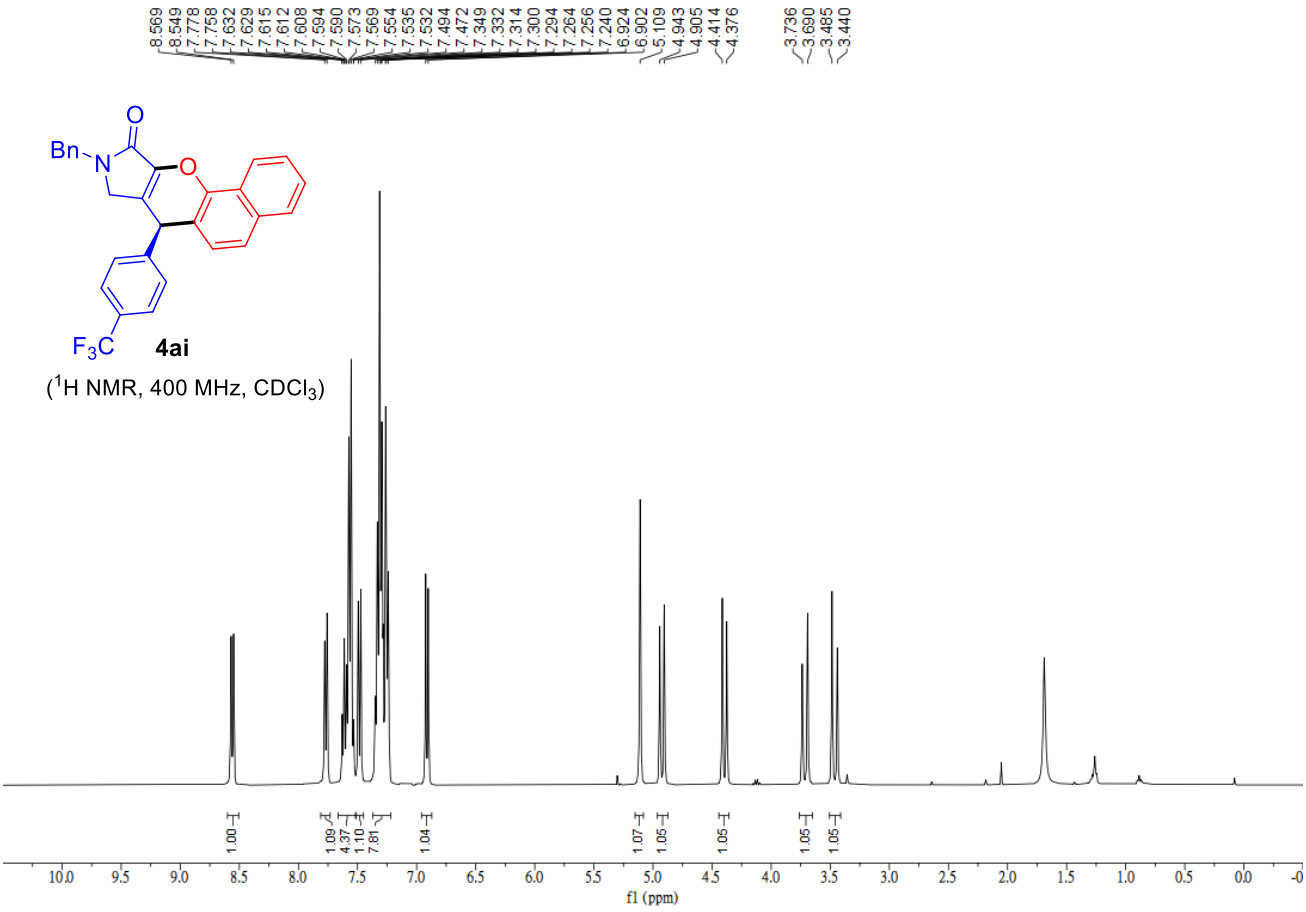
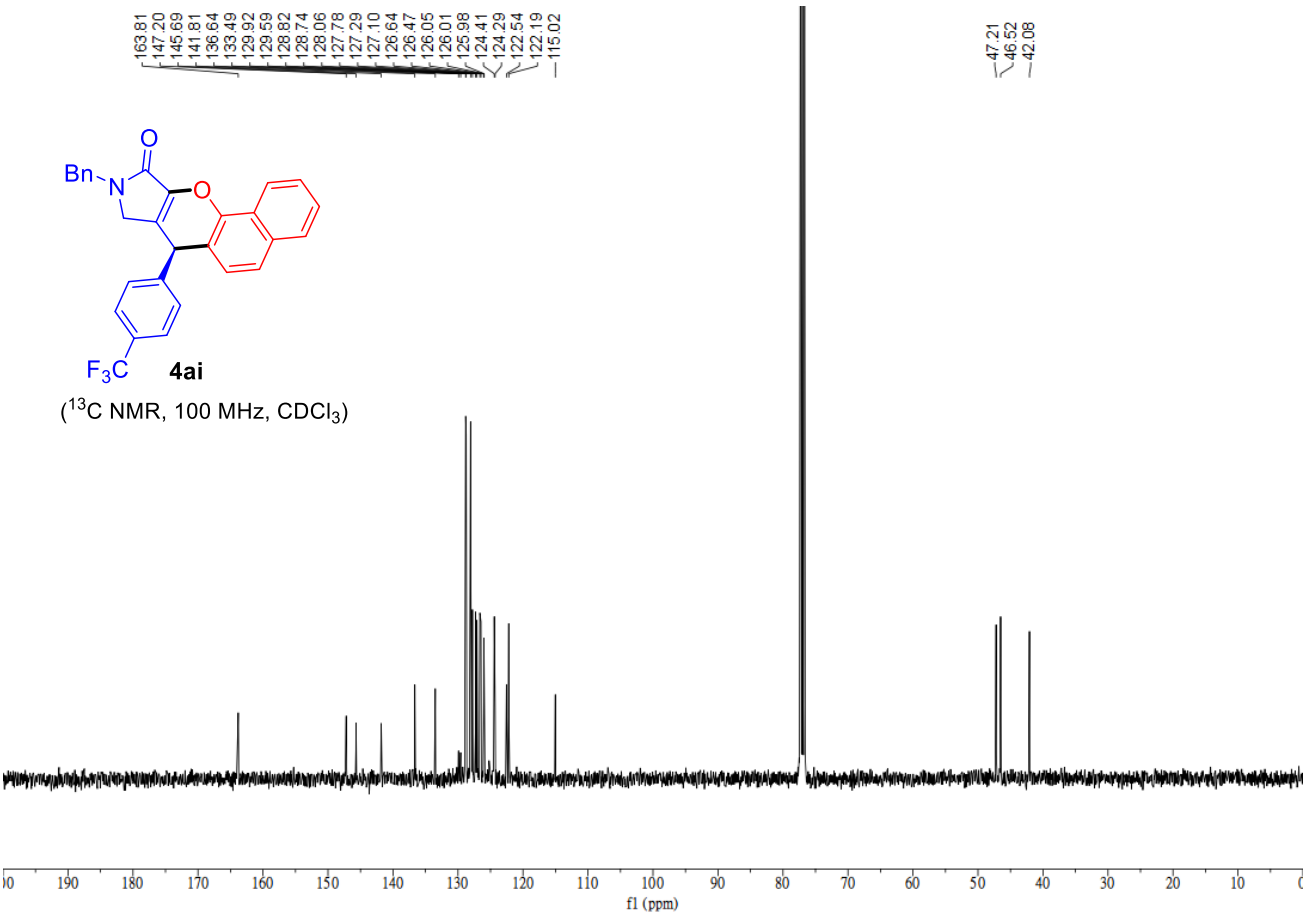
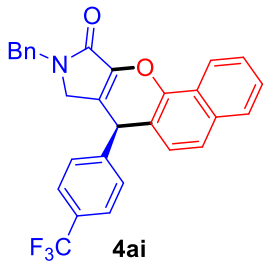
(^{13}C NMR, 100 MHz, $CDCl_3$)



(^{1}H NMR, 400 MHz, $CDCl_3$)

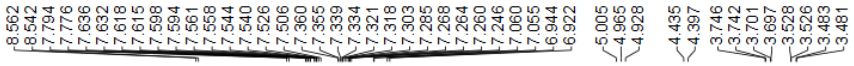


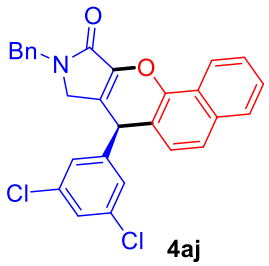
(^{13}C NMR, 100 MHz, $CDCl_3$)



4ai

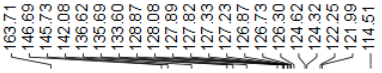
(^{19}F NMR, 376 MHz, $CDCl_3$)

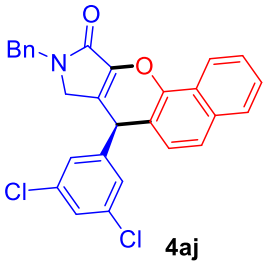




4aj

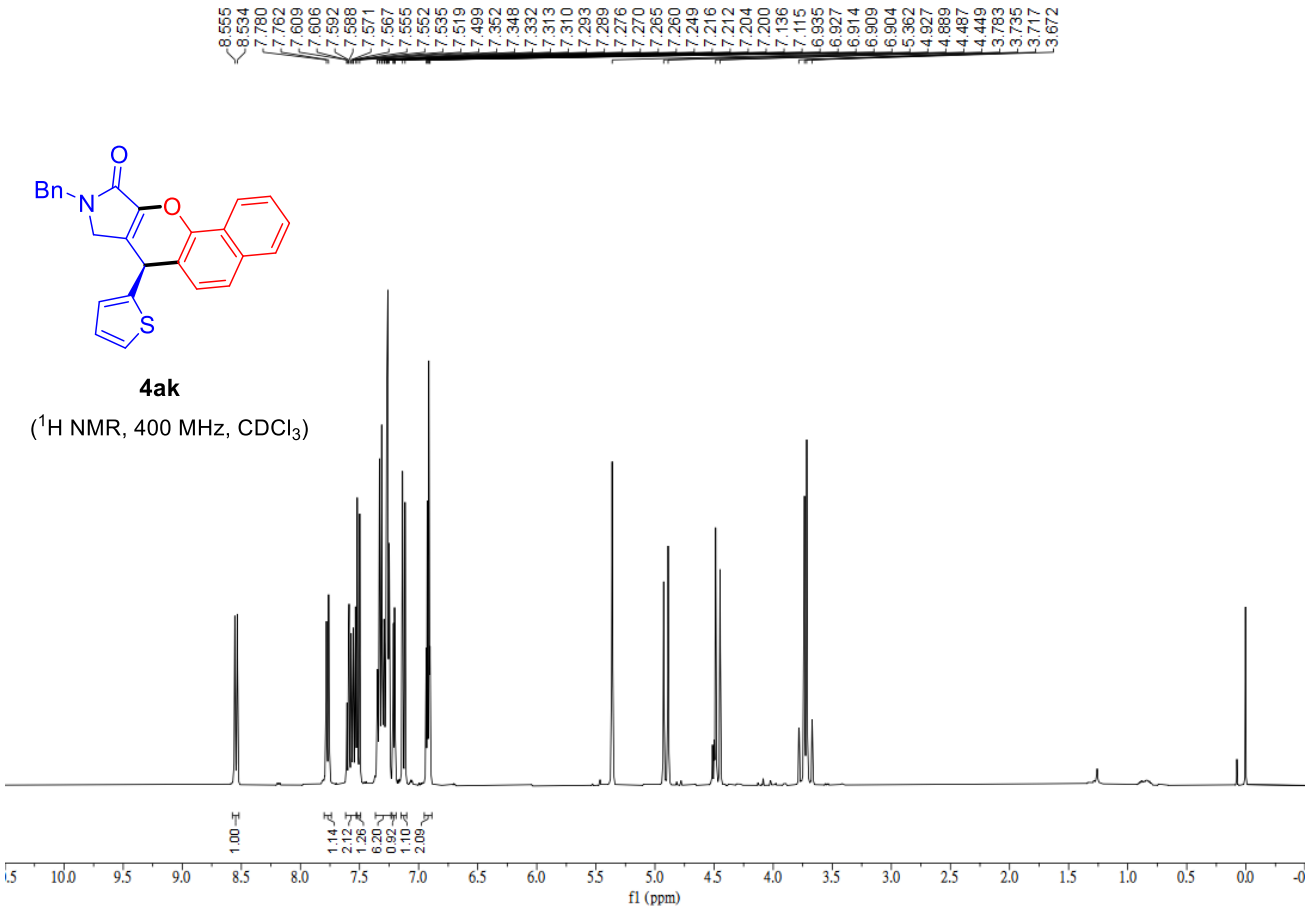
(^{1}H NMR, 400 MHz, $CDCl_3$)





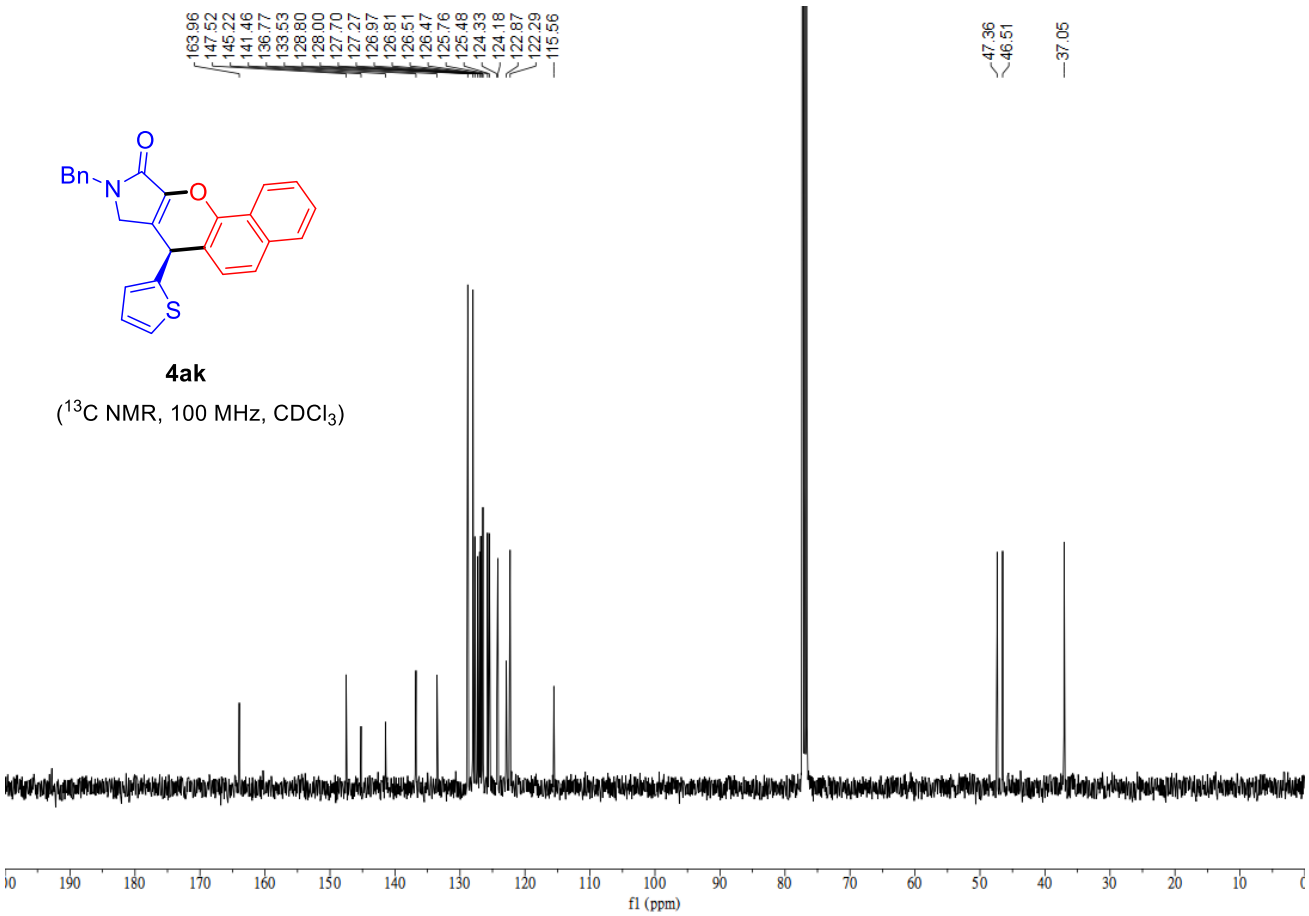
4aj

(^{13}C NMR, 100 MHz, $CDCl_3$)



4ak

(^{1}H NMR, 400 MHz, $CDCl_3$)



4ak

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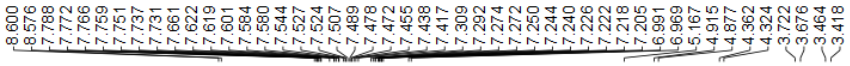
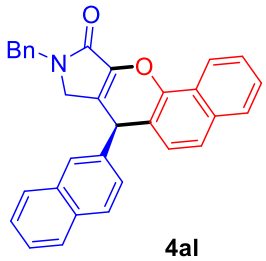
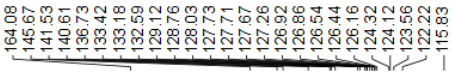
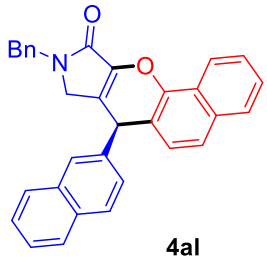




4al

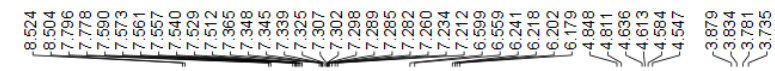
(^{1}H NMR, 400 MHz, $CDCl_3$)

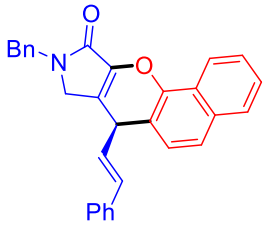




4al

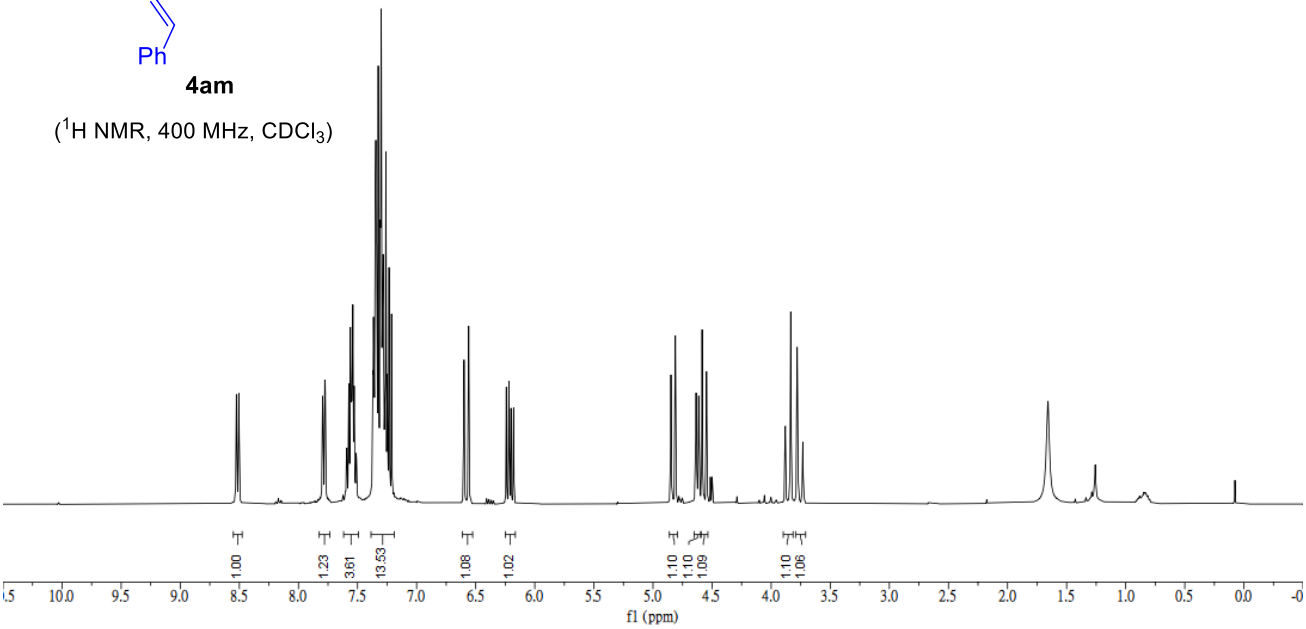
(^{13}C NMR, 100 MHz, $CDCl_3$)

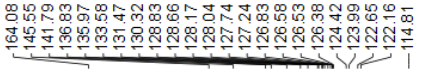


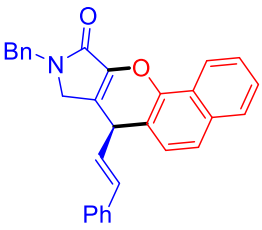


4am

(^{1}H NMR, 400 MHz, $CDCl_3$)

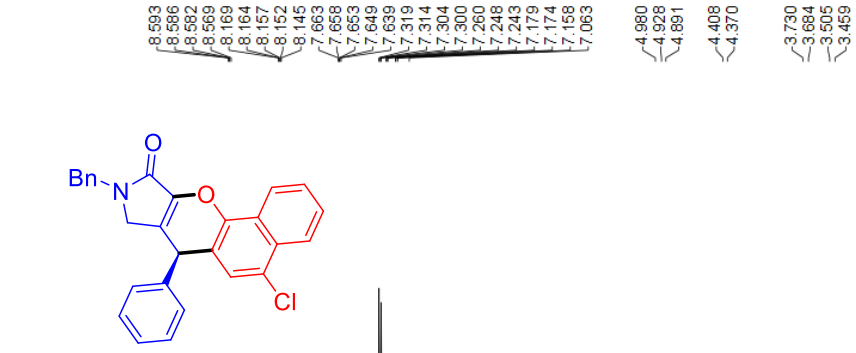






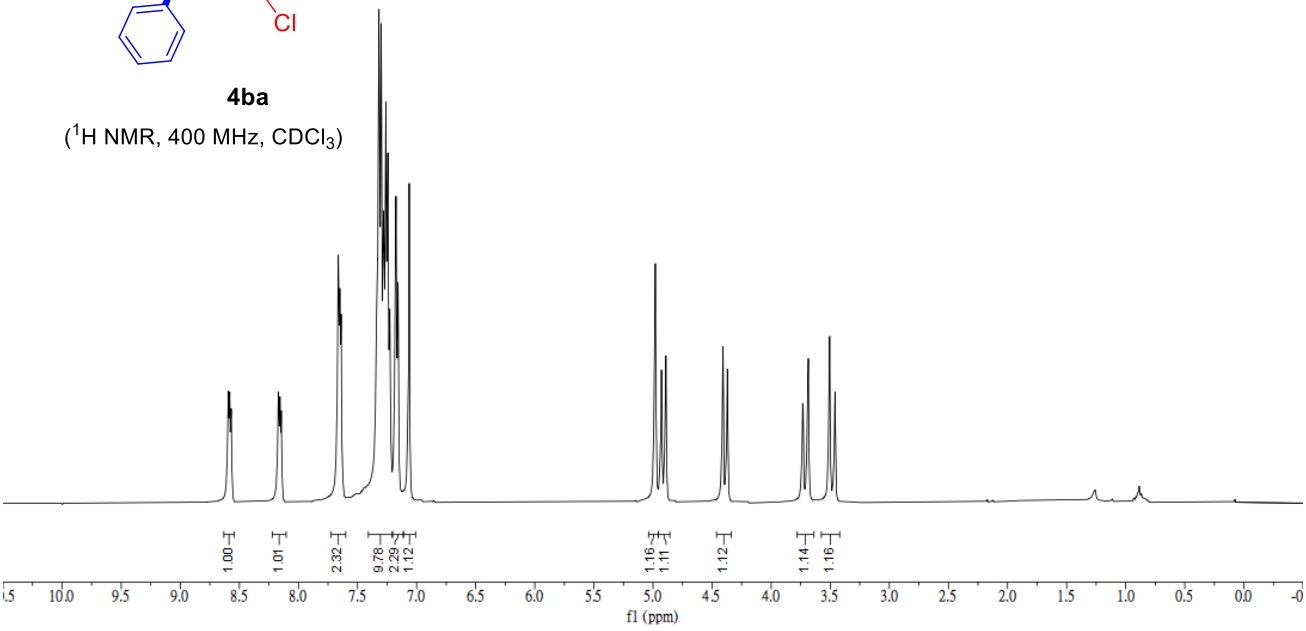
4am

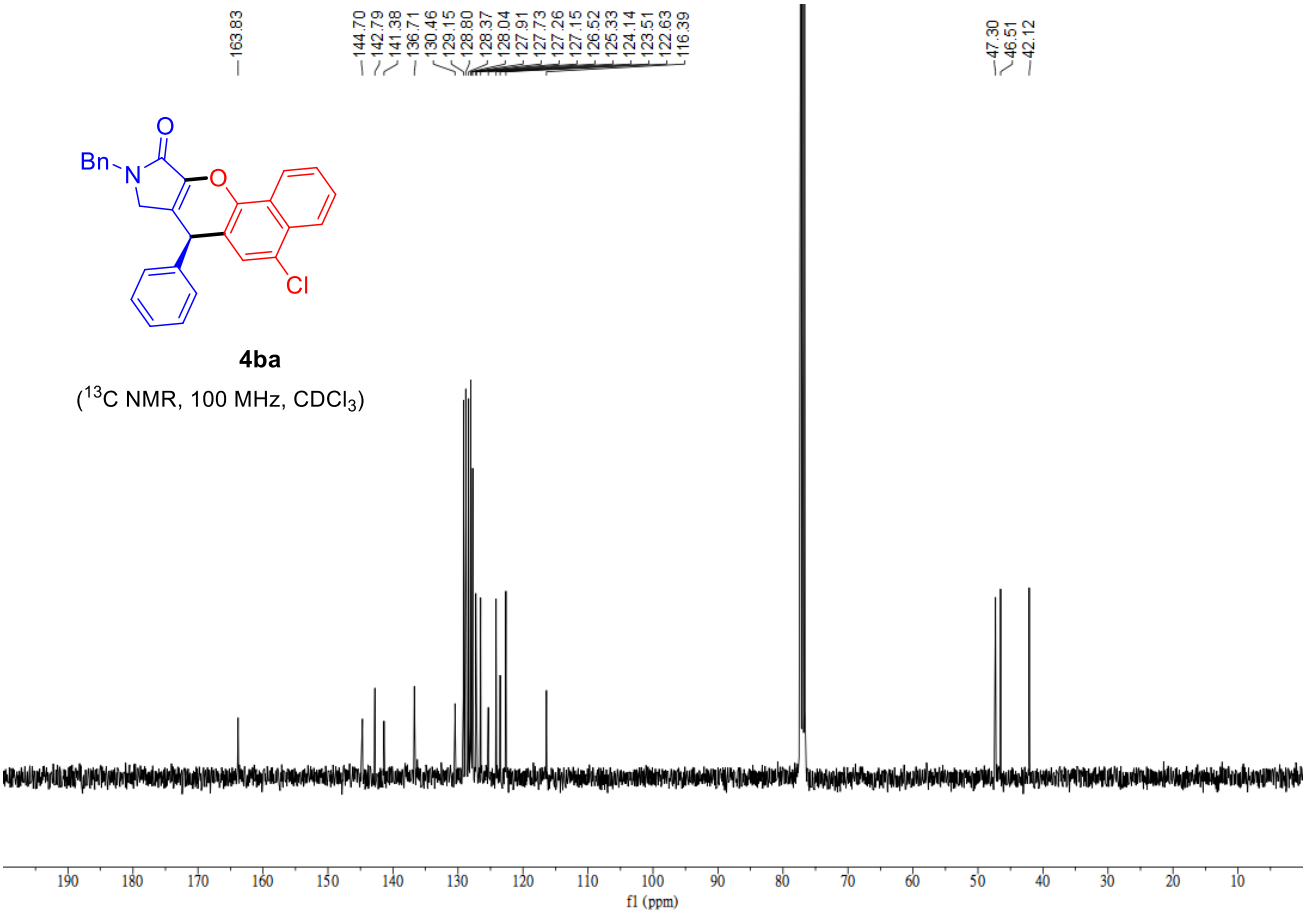
(^{13}C NMR, 100 MHz, $CDCl_3$)



4ba

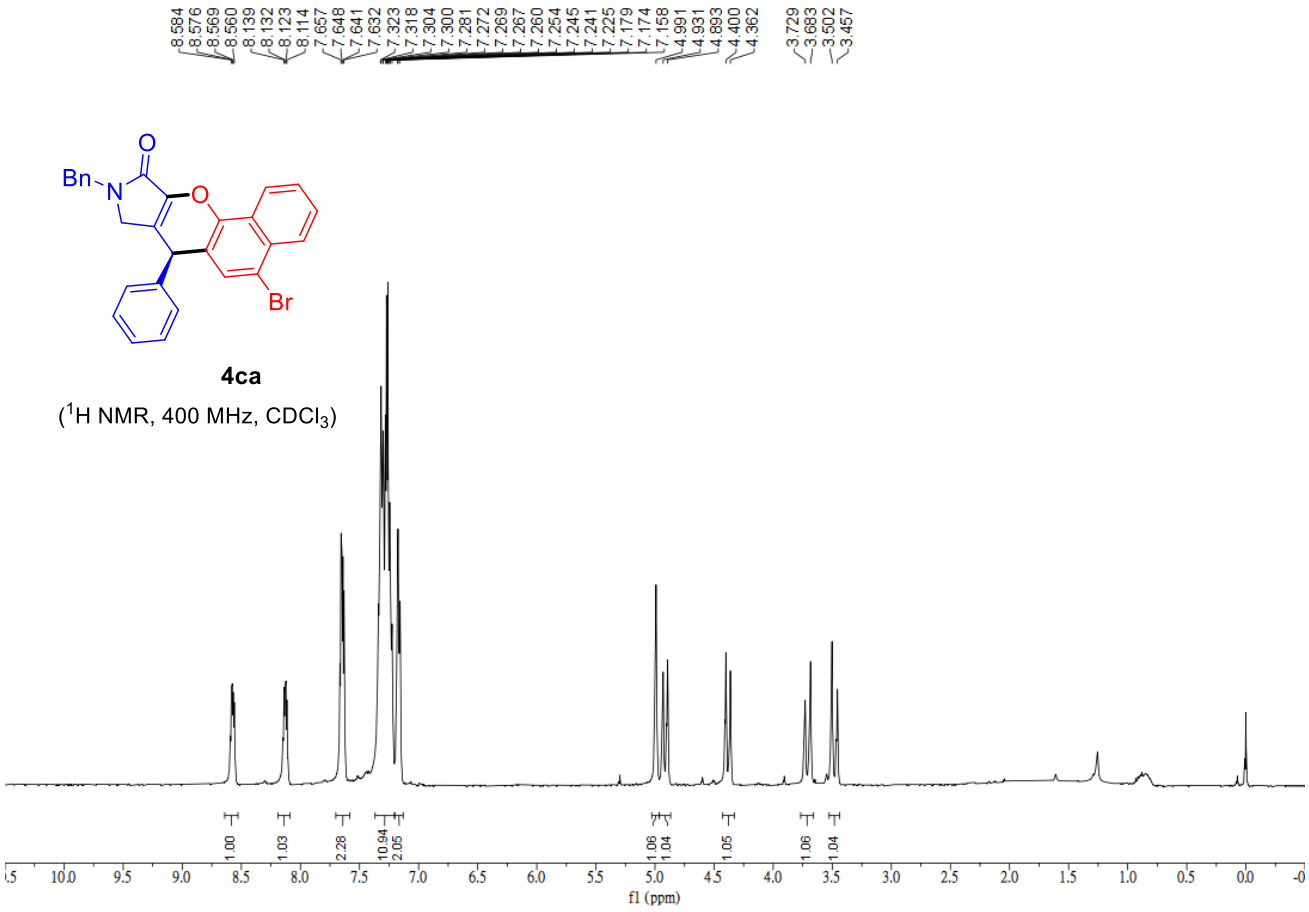
(^{1}H NMR, 400 MHz, $CDCl_3$)





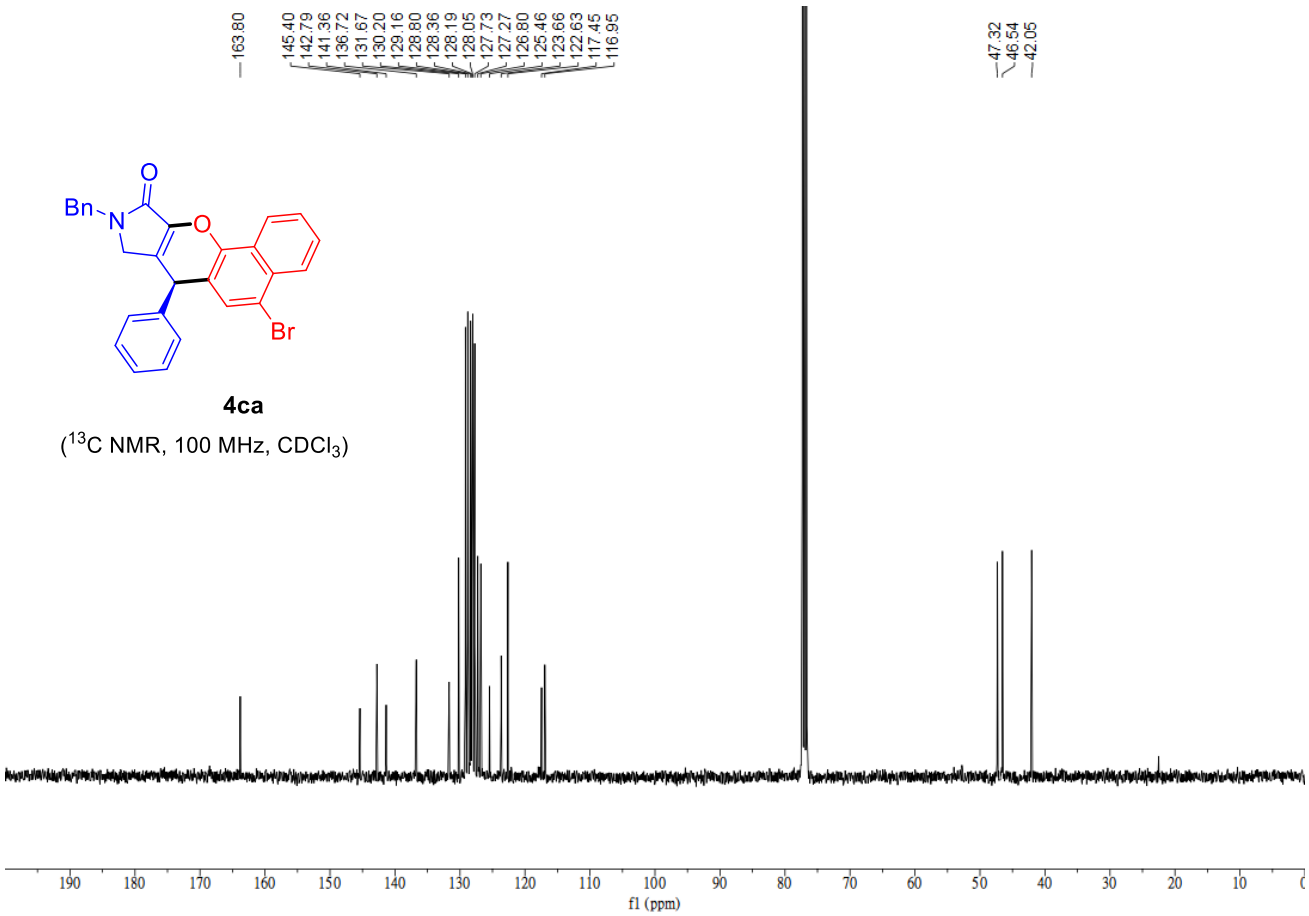
4ba

(^{13}C NMR, 100 MHz, $CDCl_3$)



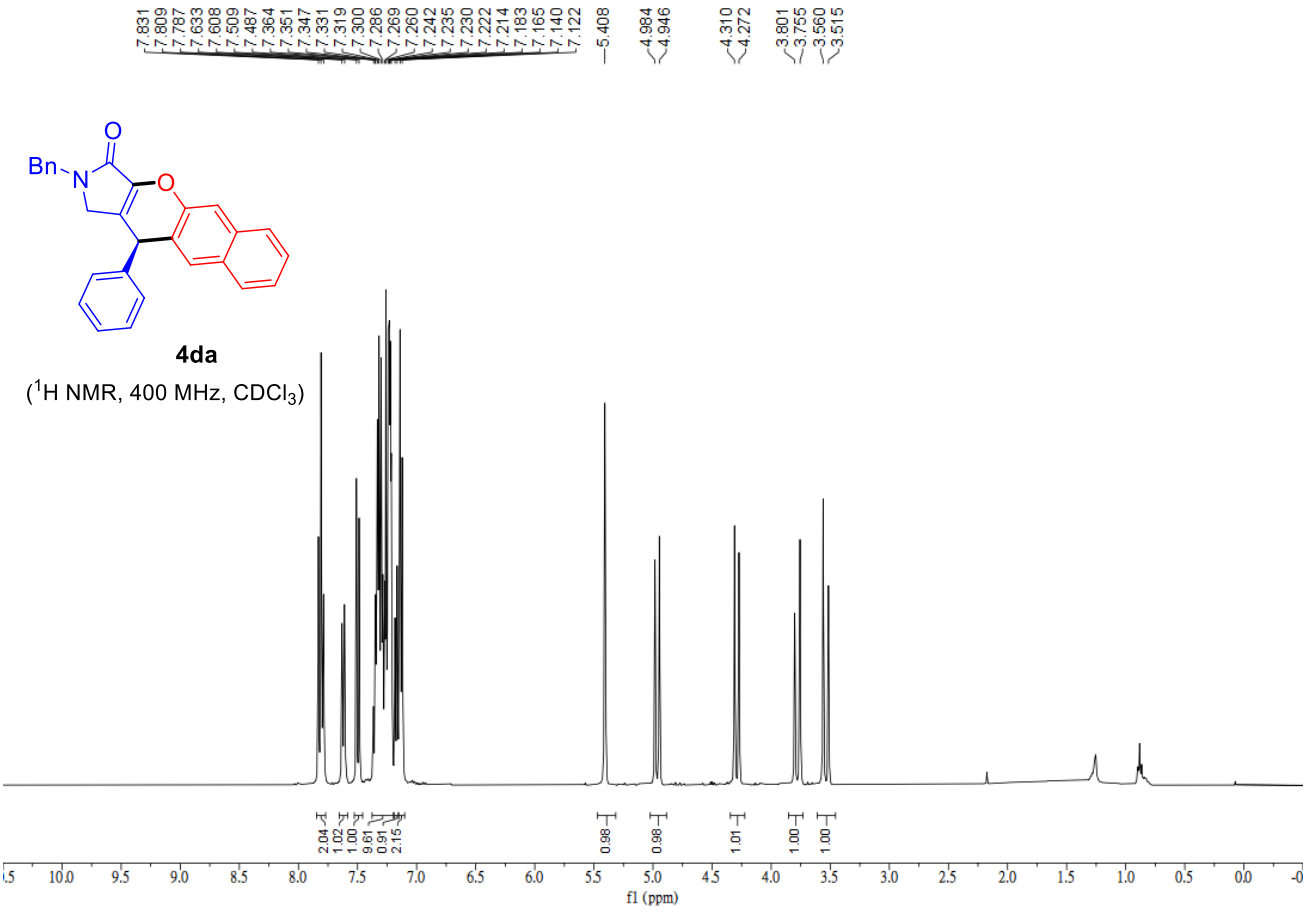
4ca

(^{1}H NMR, 400 MHz, $CDCl_3$)



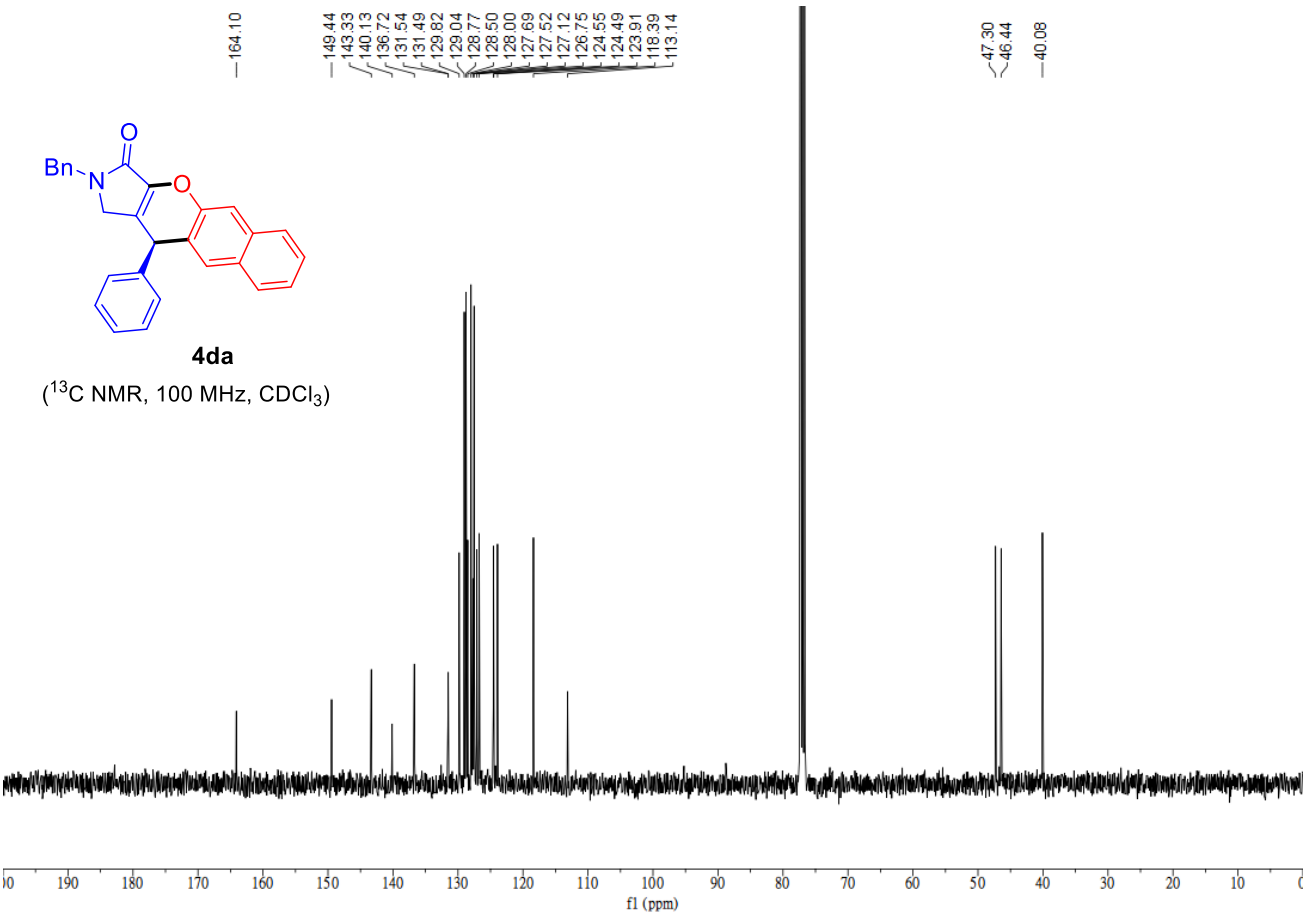
4ca

(^{13}C NMR, 100 MHz, $CDCl_3$)



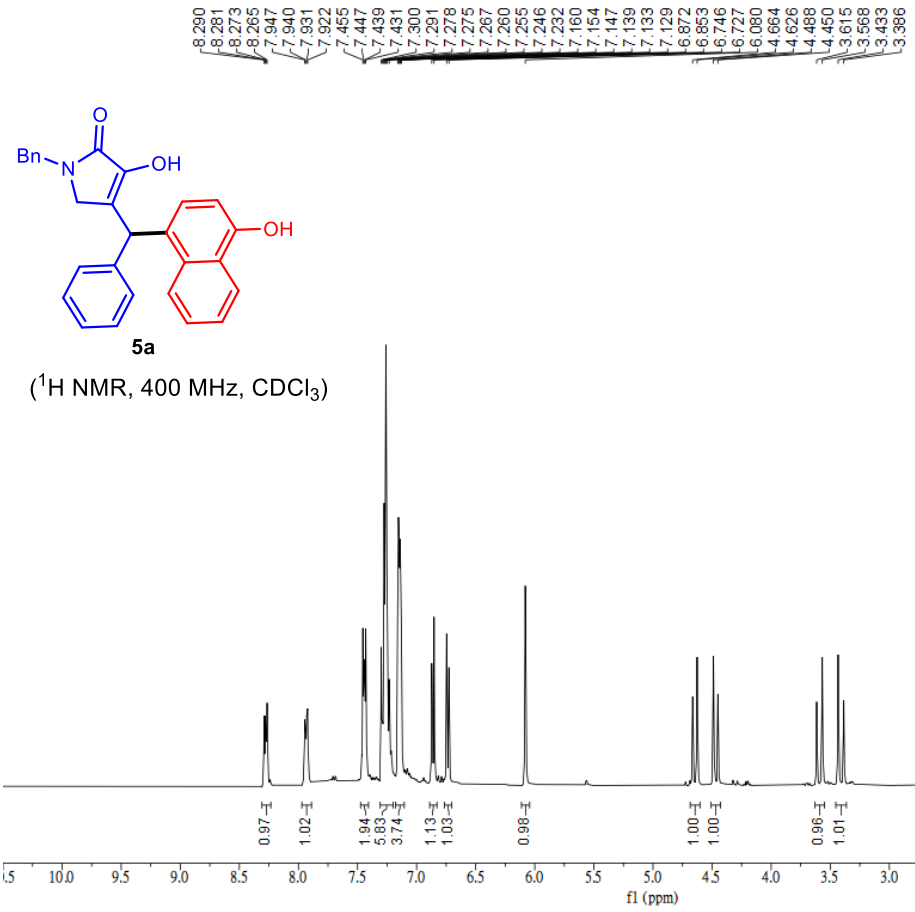
4da

(^{1}H NMR, 400 MHz, $CDCl_3$)



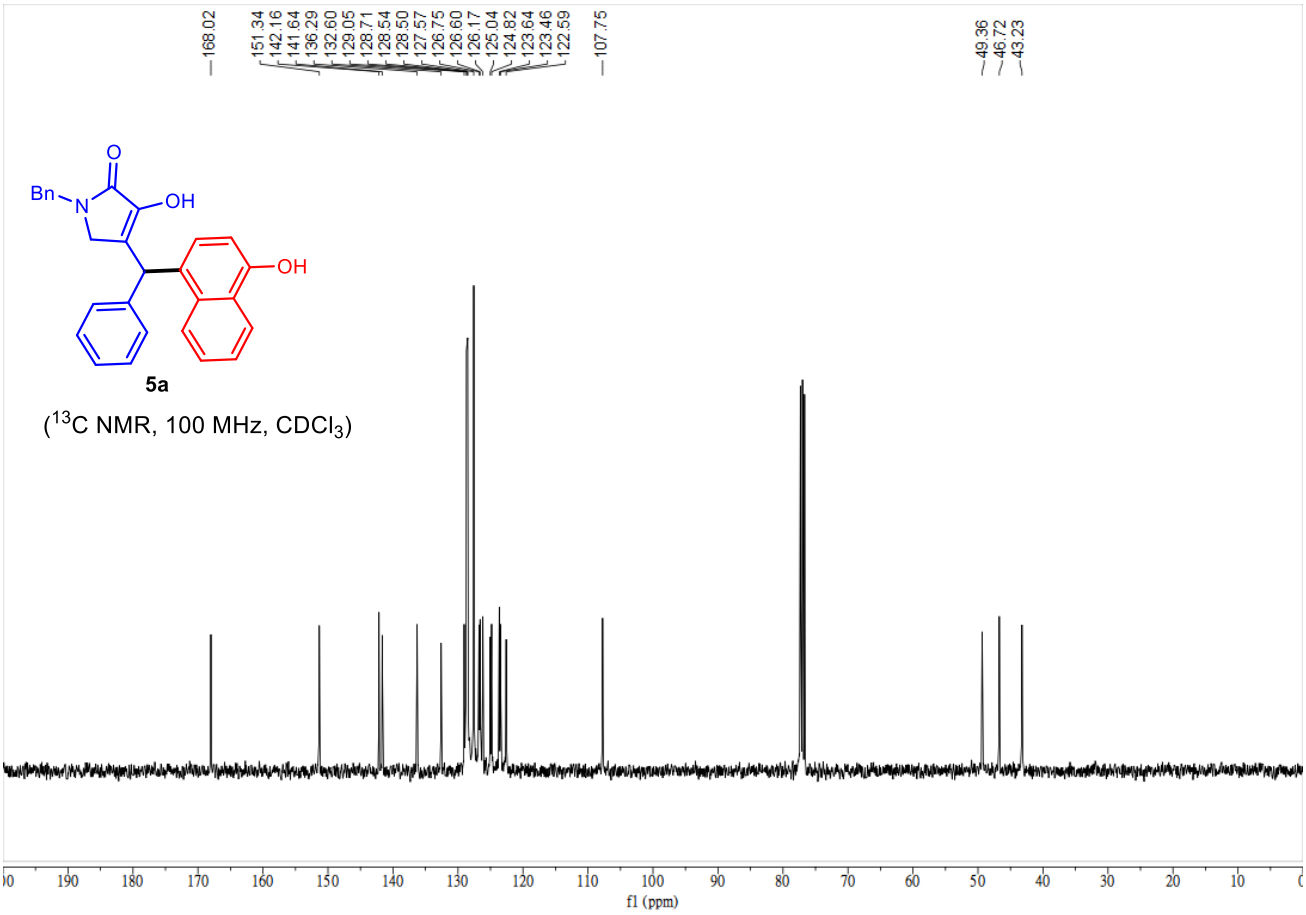
4da

(^{13}C NMR, 100 MHz, $CDCl_3$)



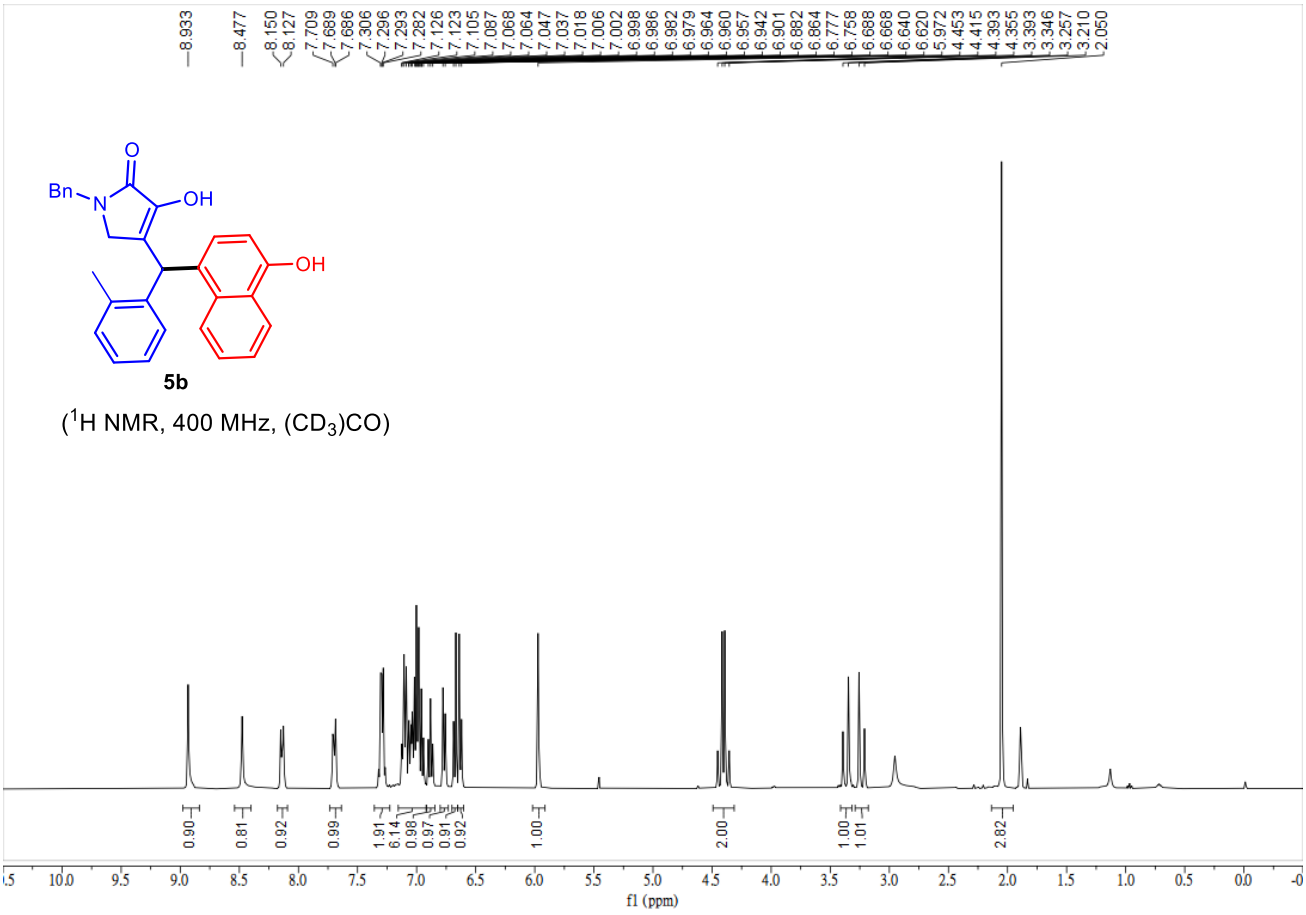
5a

(^{1}H NMR, 400 MHz, $CDCl_3$)



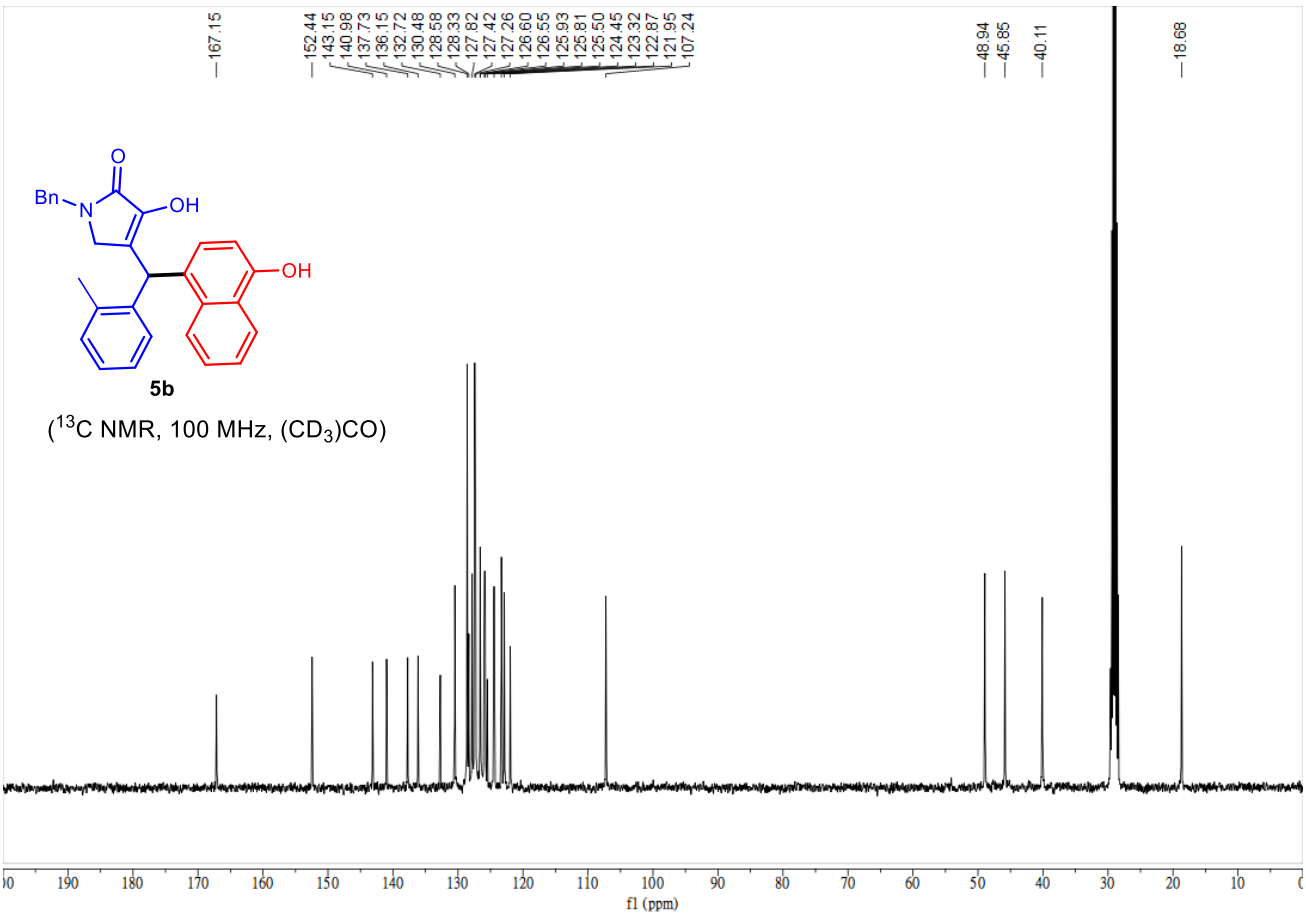
5a

(^{13}C NMR, 100 MHz, $CDCl_3$)



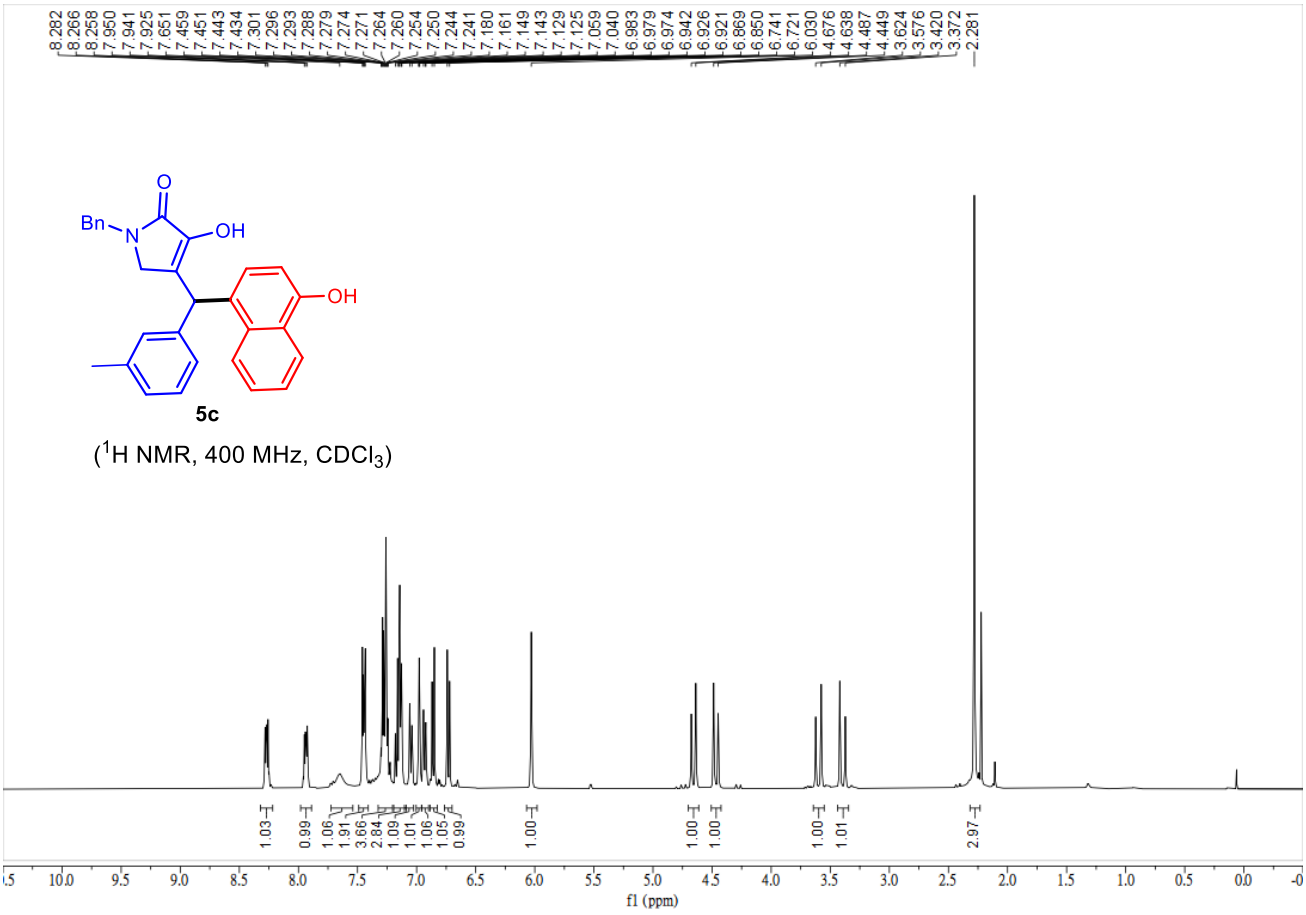
5b

(^{1}H NMR, 400 MHz, $(CD_3)CO$)



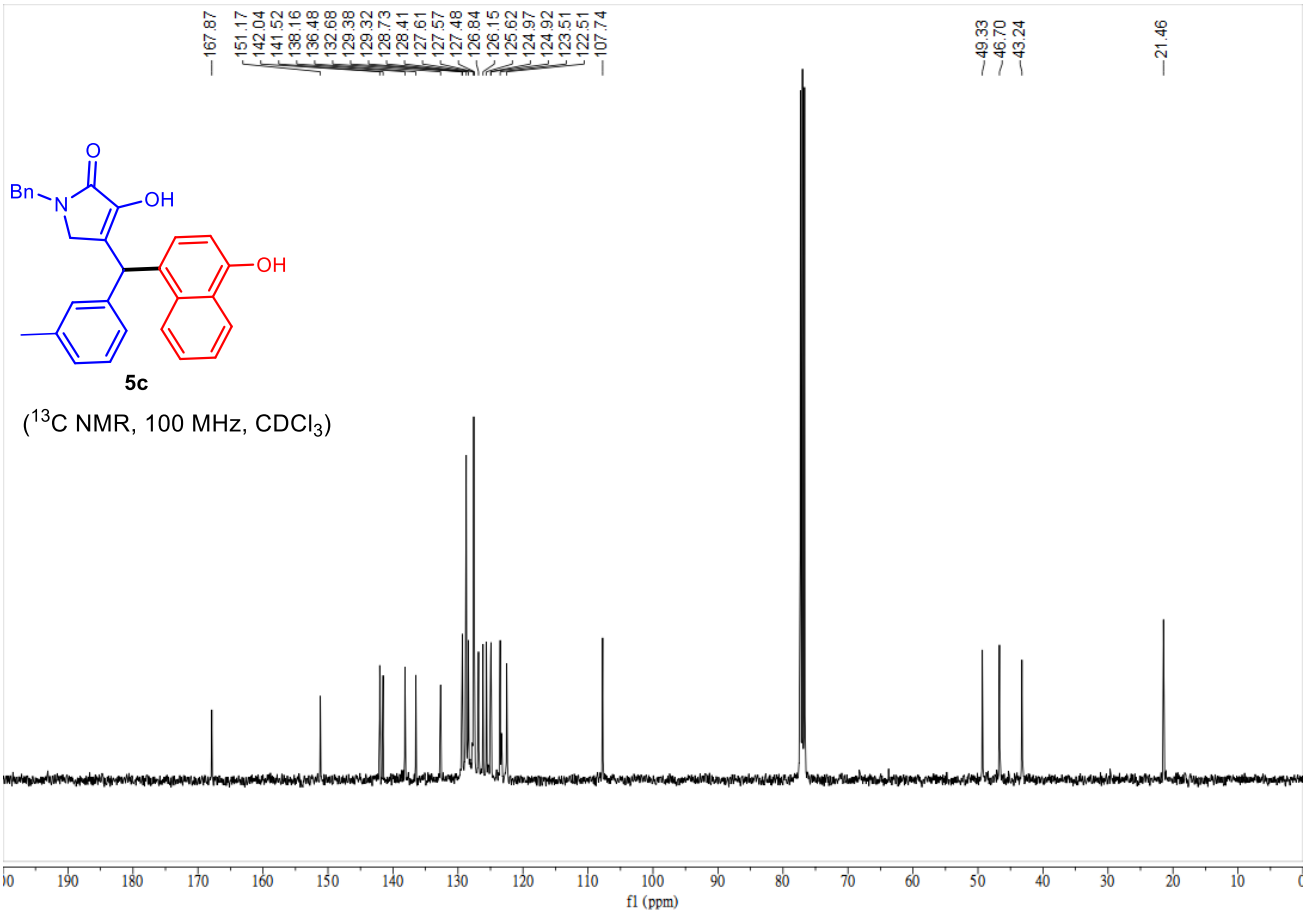
5b

(^{13}C NMR, 100 MHz, $(CD_3)CO$)



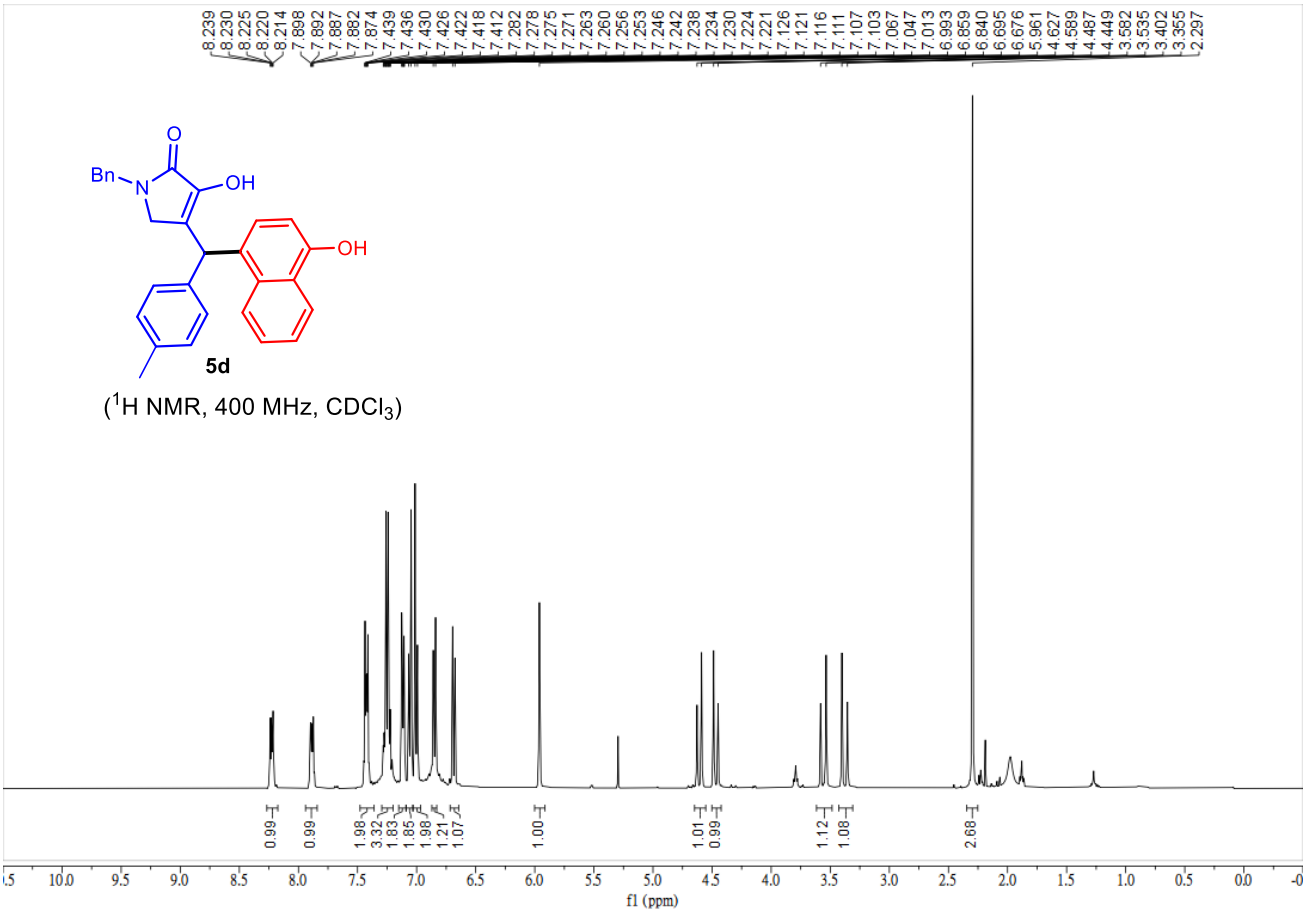
5c

(^{1}H NMR, 400 MHz, $CDCl_3$)

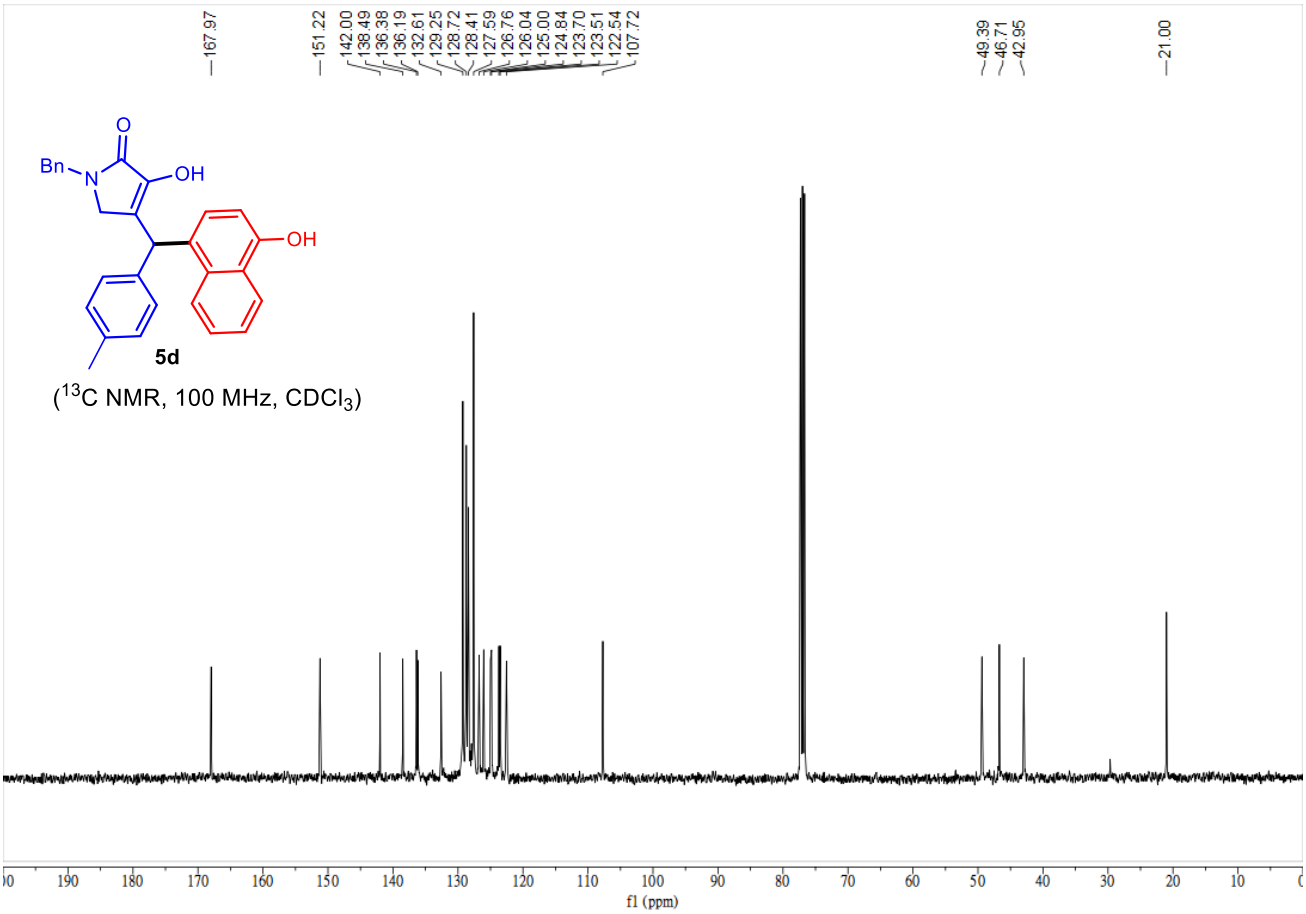


5c

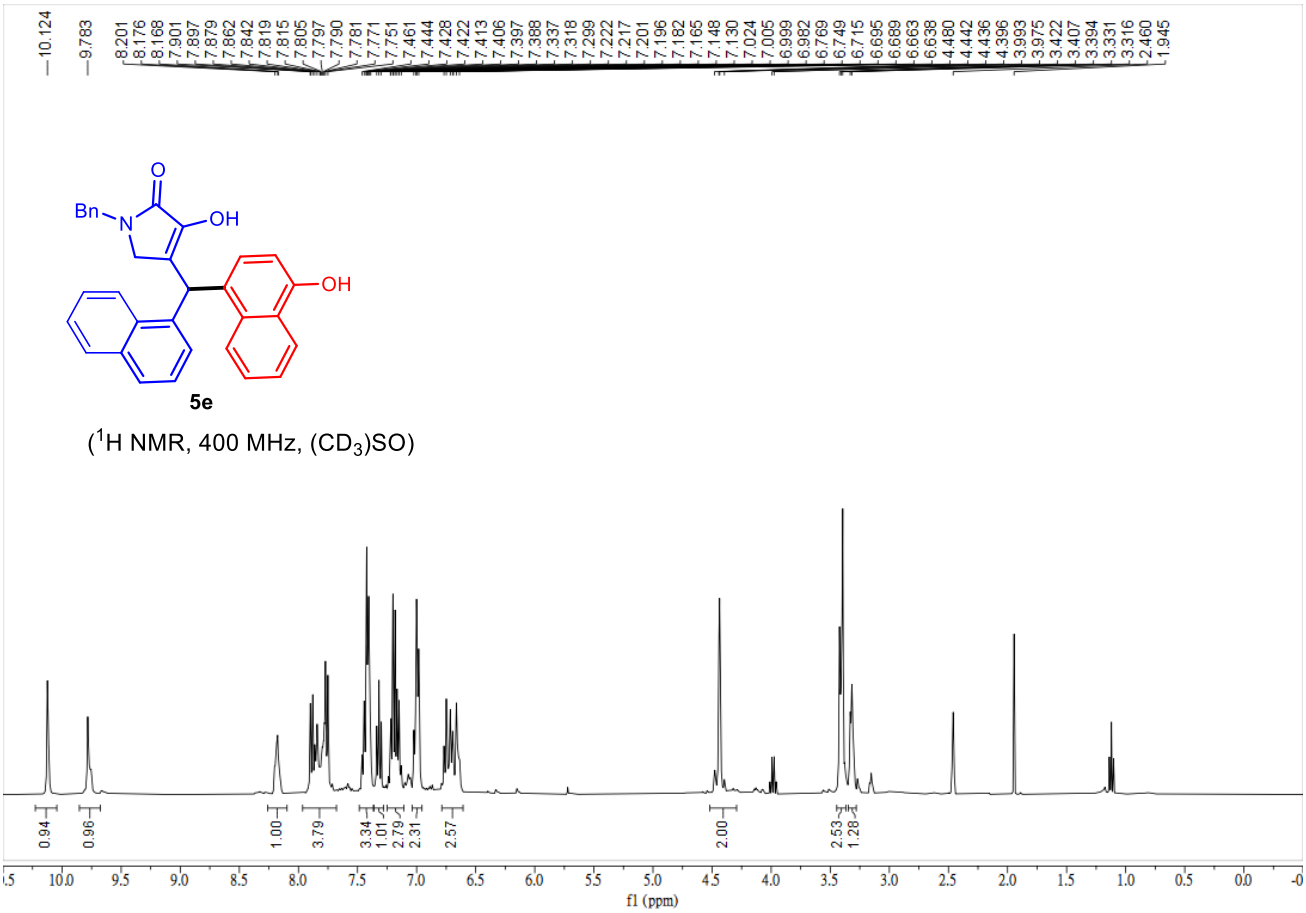
(^{13}C NMR, 100 MHz, $CDCl_3$)



(^{1}H NMR, 400 MHz, $CDCl_3$)

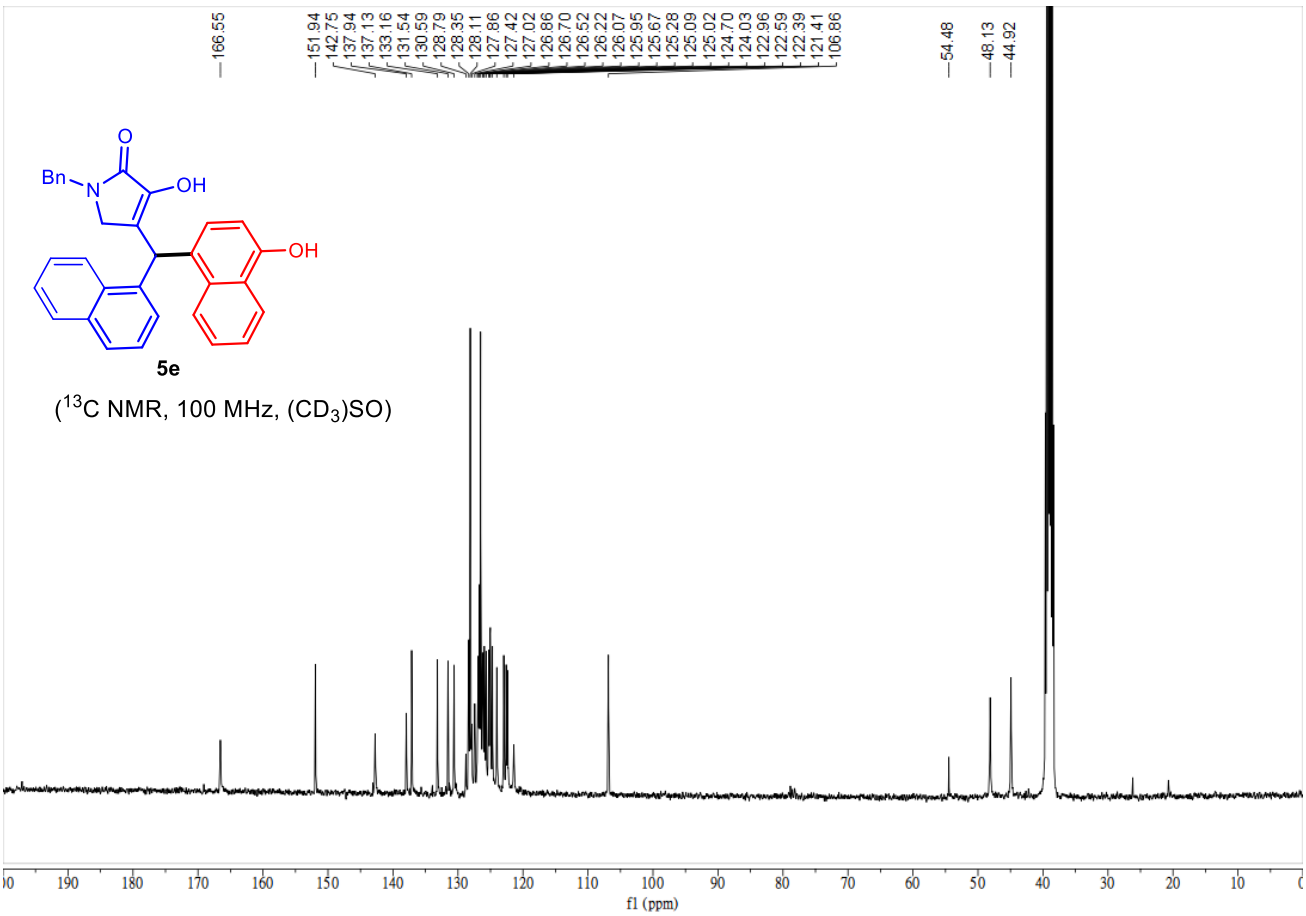


(^{13}C NMR, 100 MHz, $CDCl_3$)



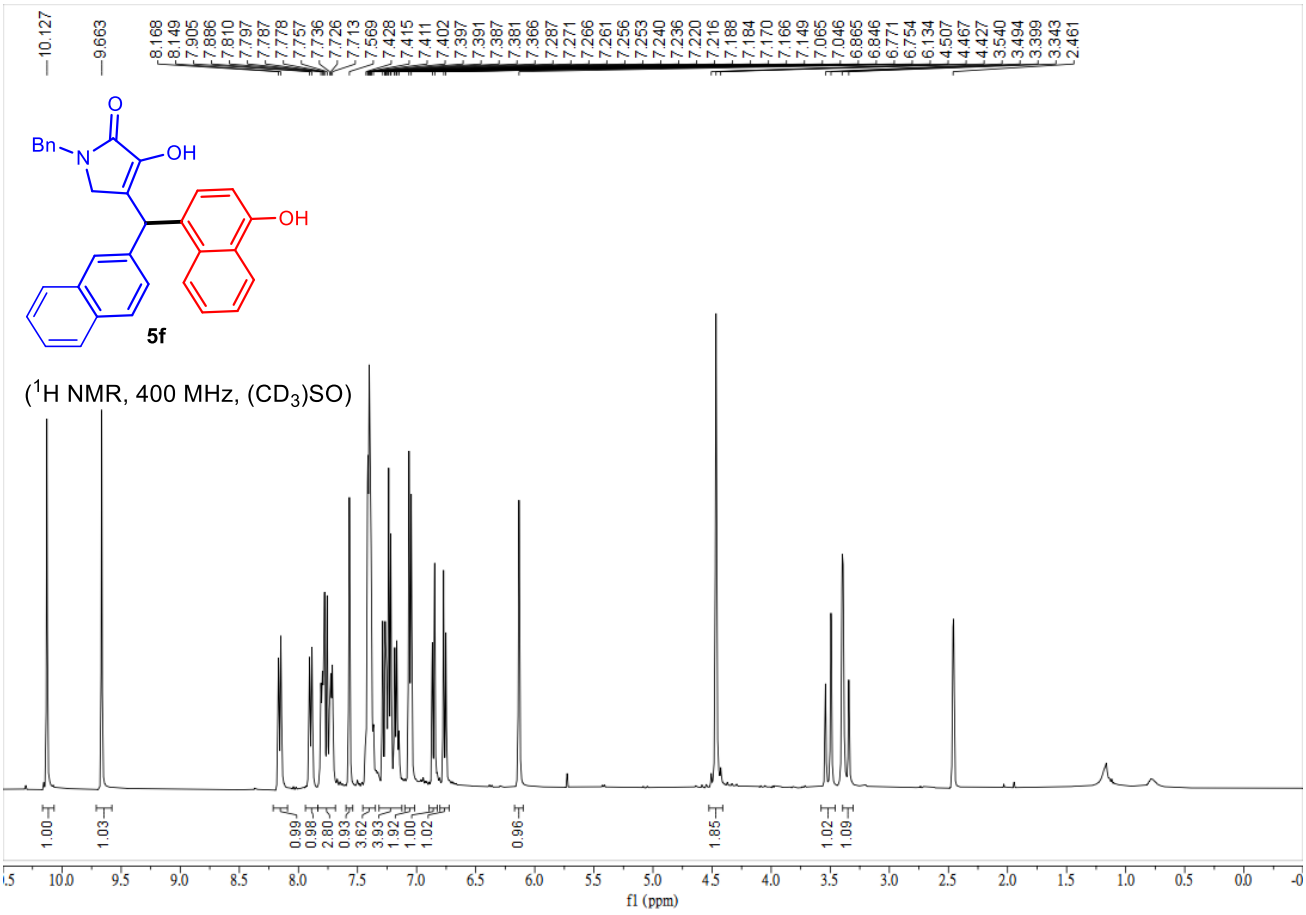
5e

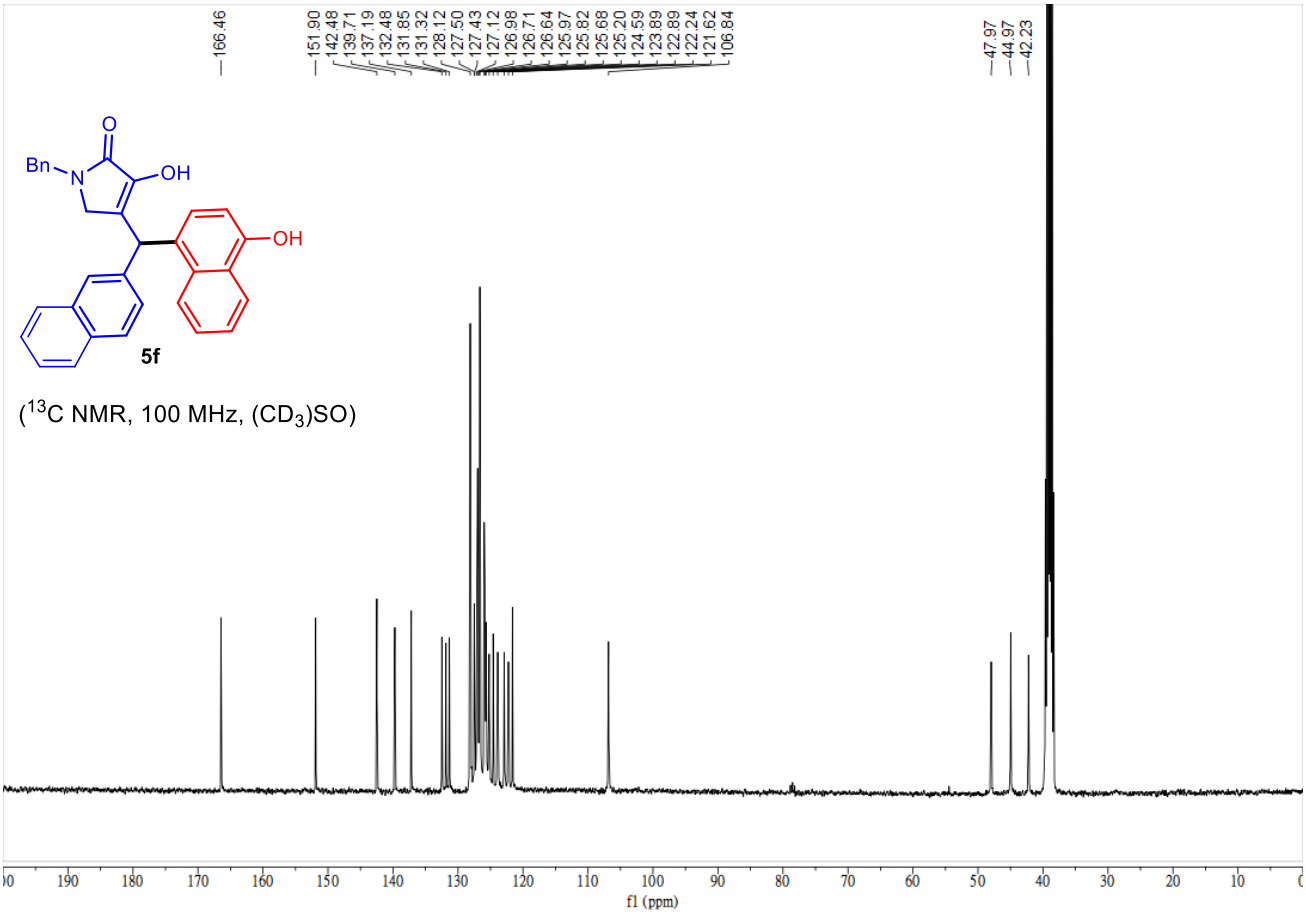
(^{1}H NMR, 400 MHz, $(CD_3)SO$)

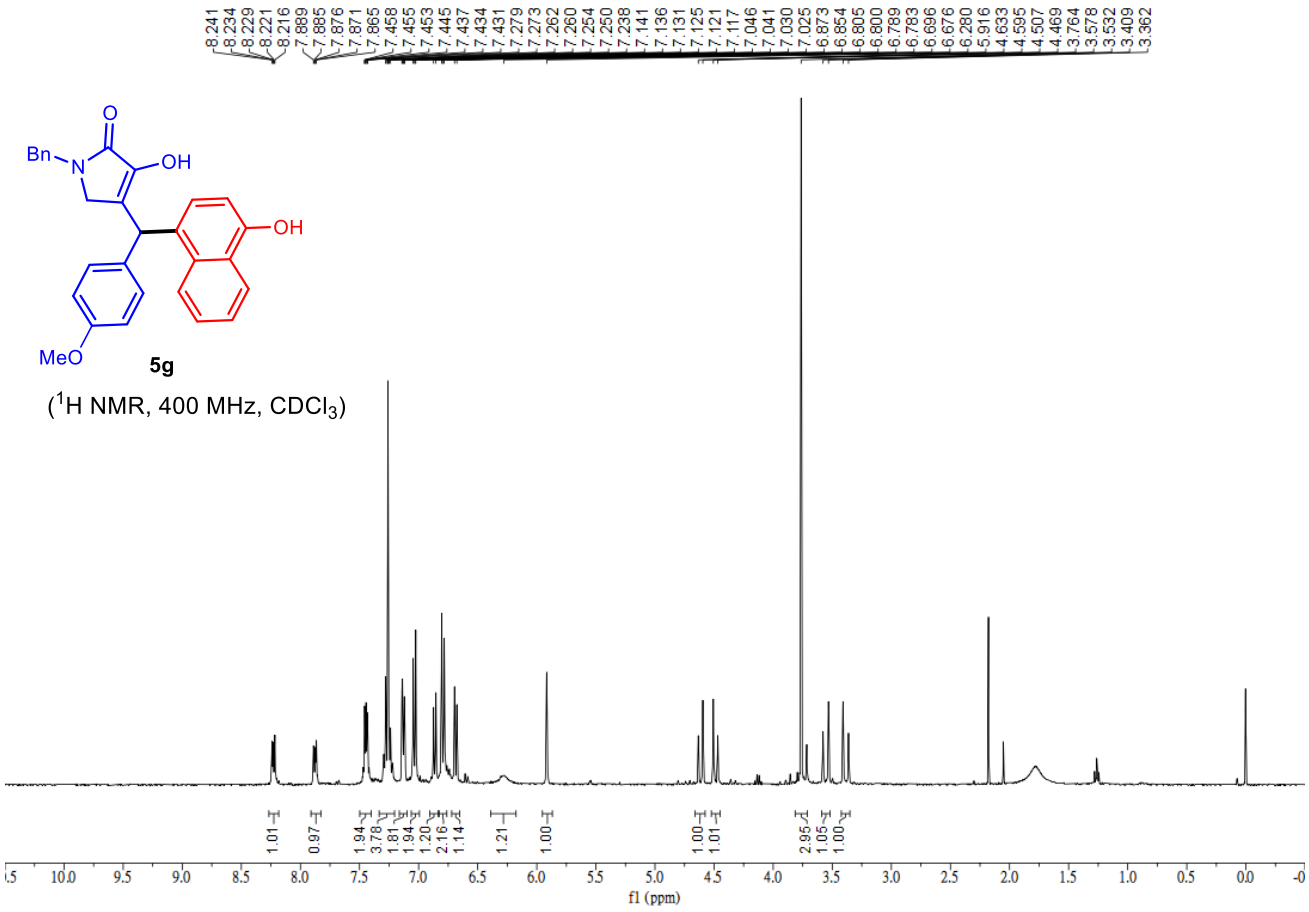


5e

(^{13}C NMR, 100 MHz, $(CD_3)SO$)

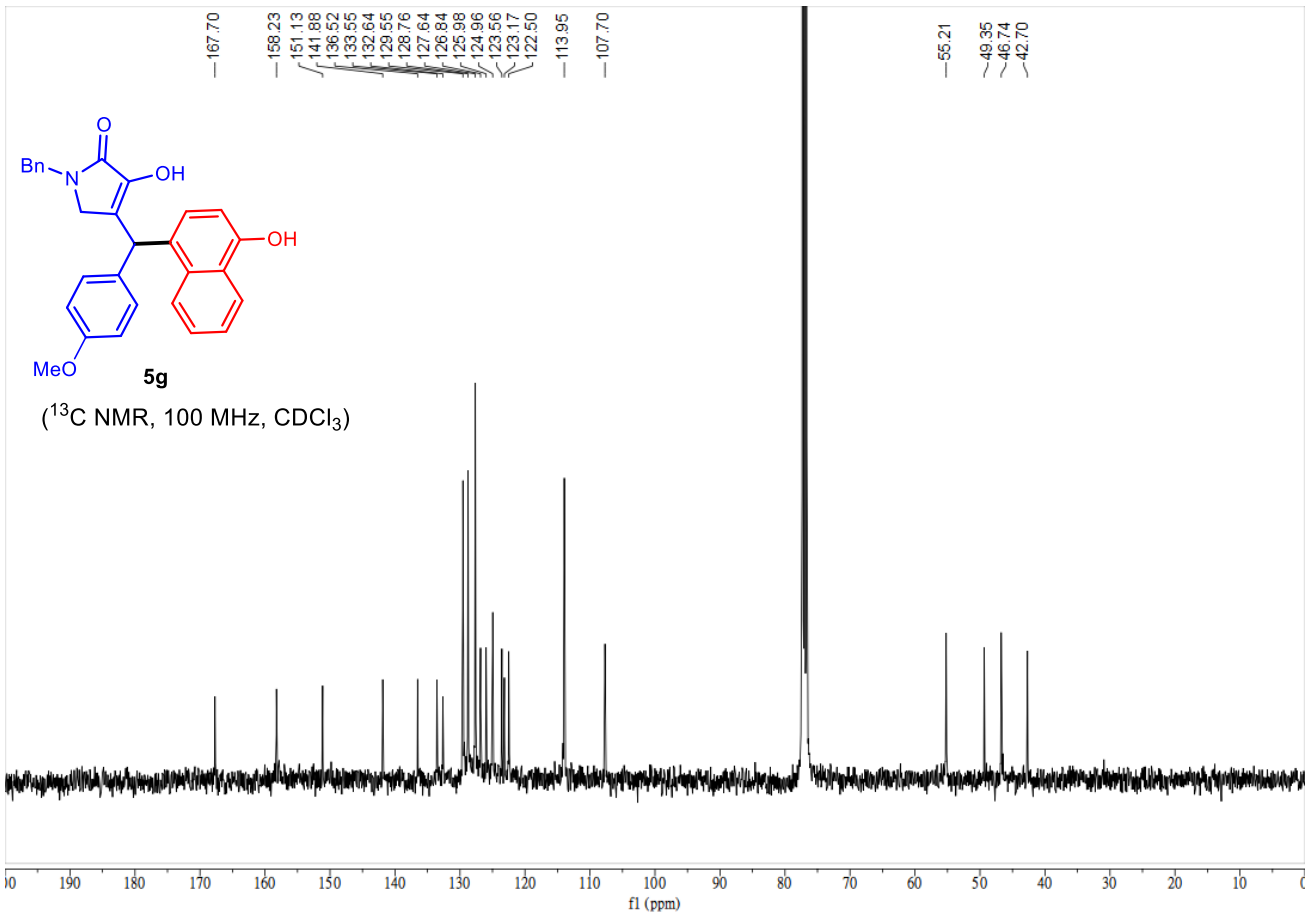

10.127
9.663
8.168
8.149
7.905
7.886
7.810
7.797
7.787
7.778
7.757
7.736
7.726
7.713
7.569
7.428
7.415
7.411
7.402
7.397
7.391
7.387
7.381
7.366
7.287
7.271
7.266
7.261
7.256
7.253
7.240
7.236
7.220
7.216
7.188
7.184
7.170
7.166
7.149
7.065
7.046
6.865
6.846
6.771
6.754
6.134
4.507
4.467
4.427
3.540
3.494
3.399
3.343
2.461
Bn
N
O
OH
OH
5f
(1H NMR, 400 MHz, (CD3)SO)
1.00
1.03
0.99
0.98
2.80
0.93
3.62
3.93
1.92
1.00
1.02
0.96
1.85
1.02
1.09
f1 (ppm)


166.46
151.90
142.48
139.71
137.19
132.48
131.85
131.32
128.12
127.50
127.43
127.12
126.98
126.71
126.64
125.97
125.82
125.68
125.20
124.59
123.89
122.89
122.24
121.62
106.84
47.97
44.97
42.23
Bn
N
O
OH
OH
5f
(13C NMR, 100 MHz, (CD3)SO)
f1 (ppm)



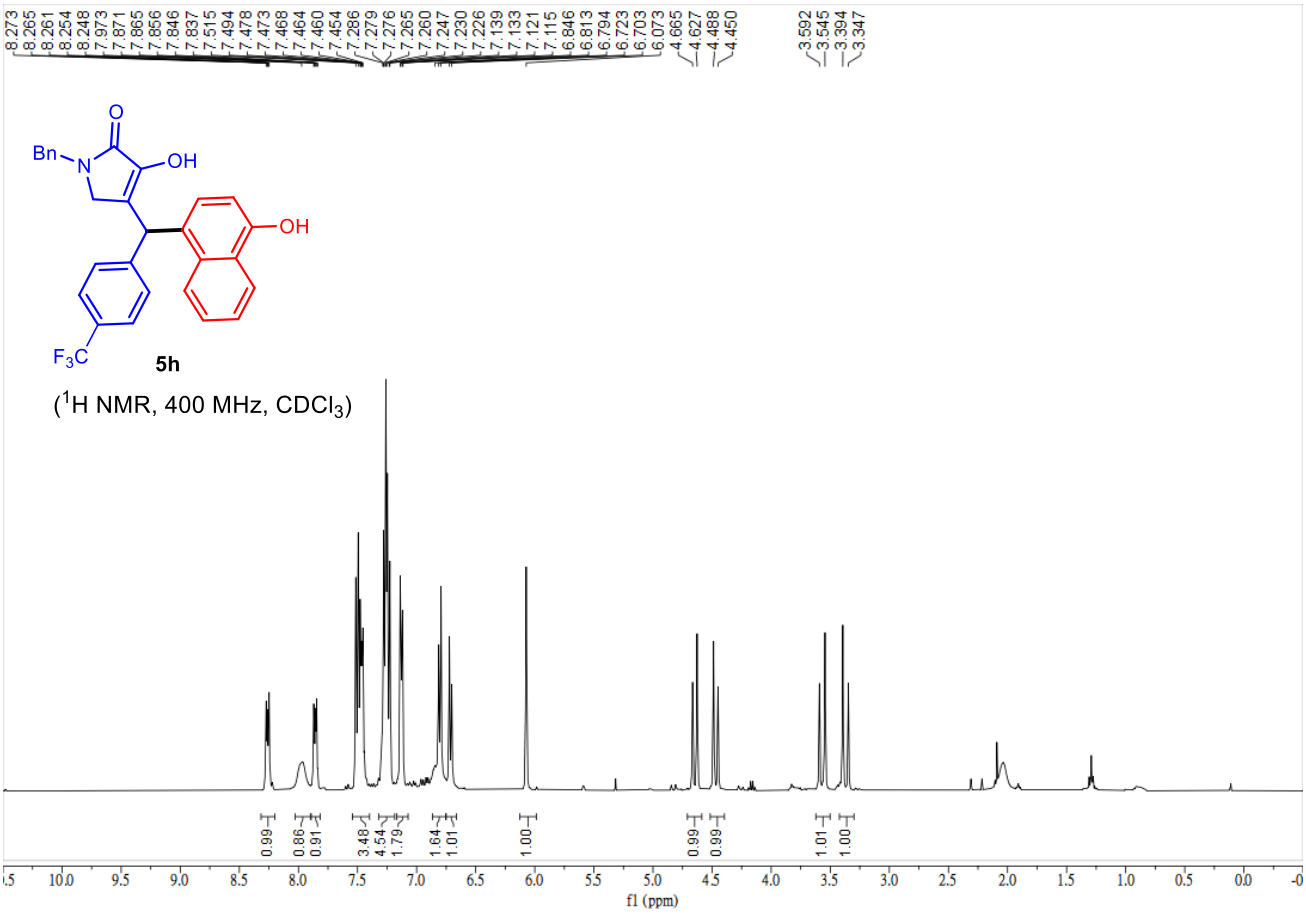
5g

(^{1}H NMR, 400 MHz, $CDCl_3$)



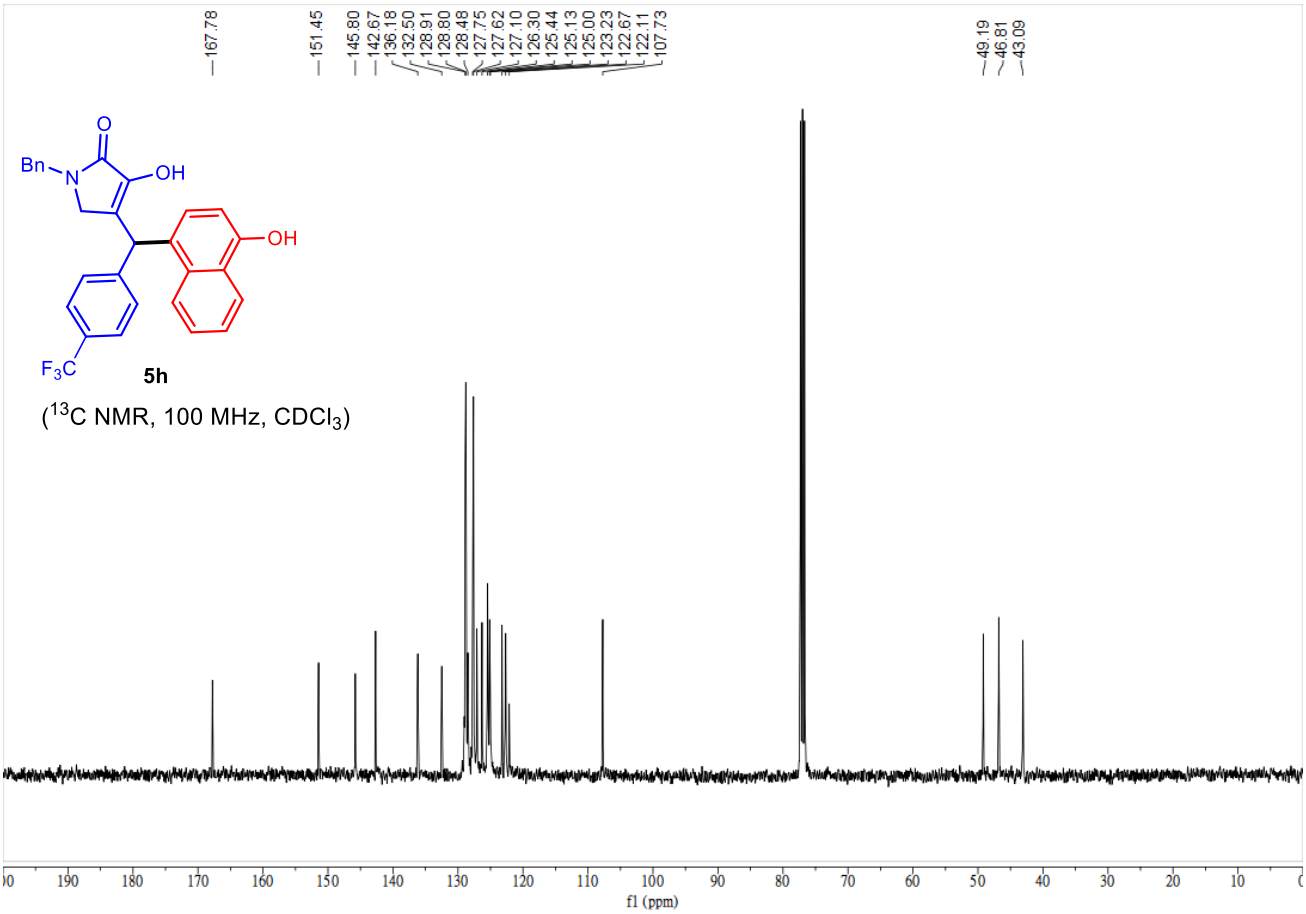
5g

(^{13}C NMR, 100 MHz, $CDCl_3$)



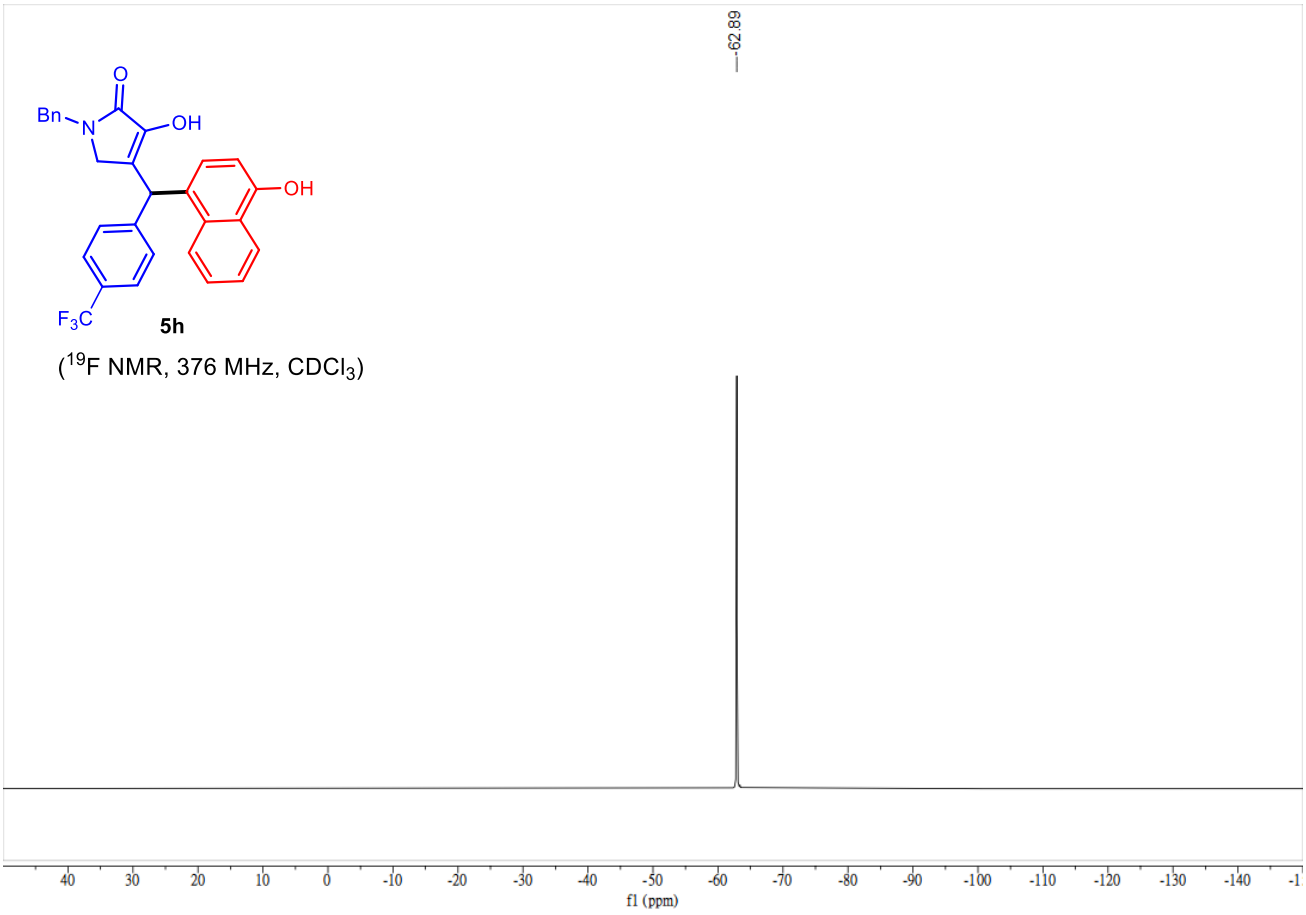
5h

(^{1}H NMR, 400 MHz, $CDCl_3$)



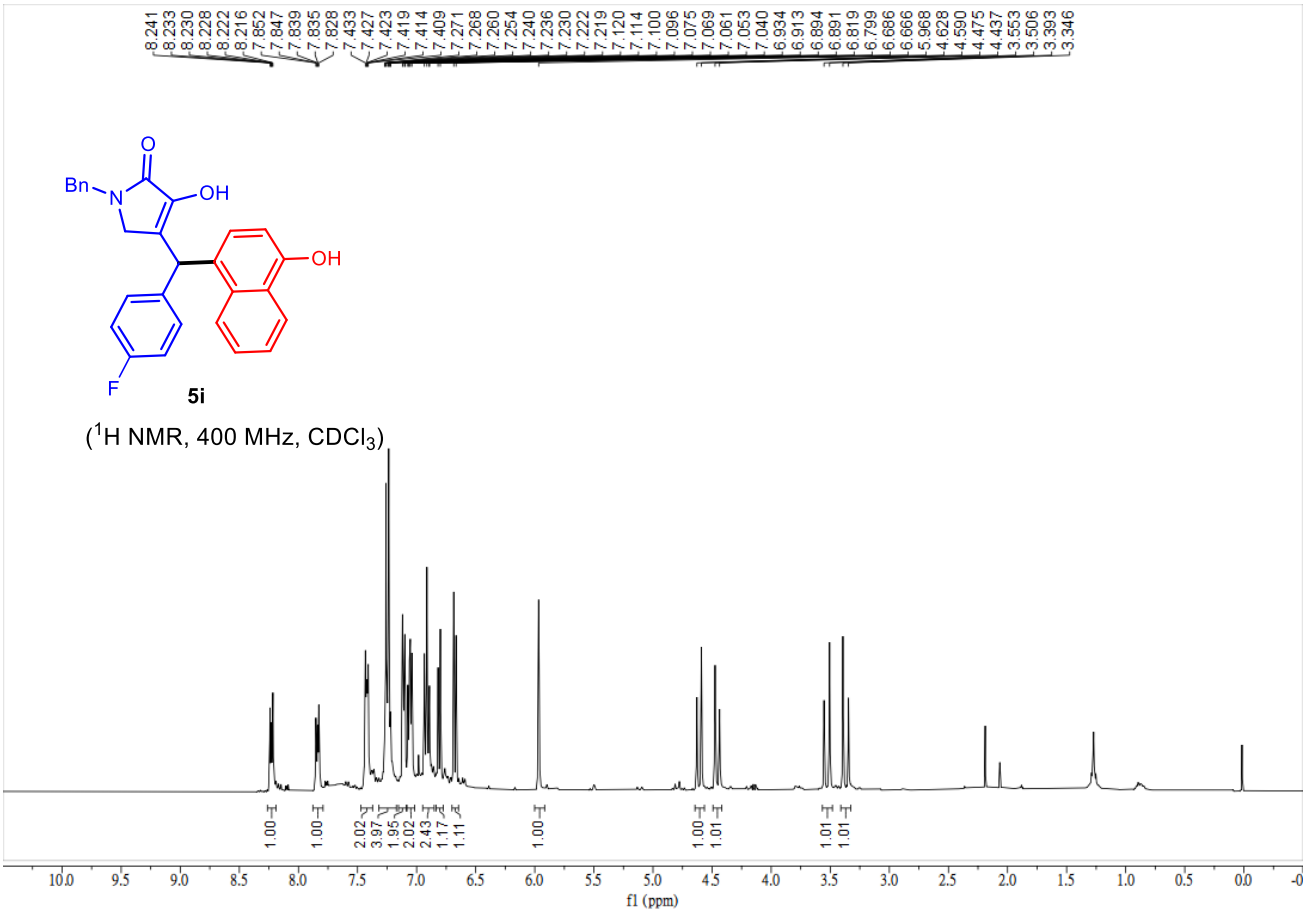
5h

(^{13}C NMR, 100 MHz, $CDCl_3$)



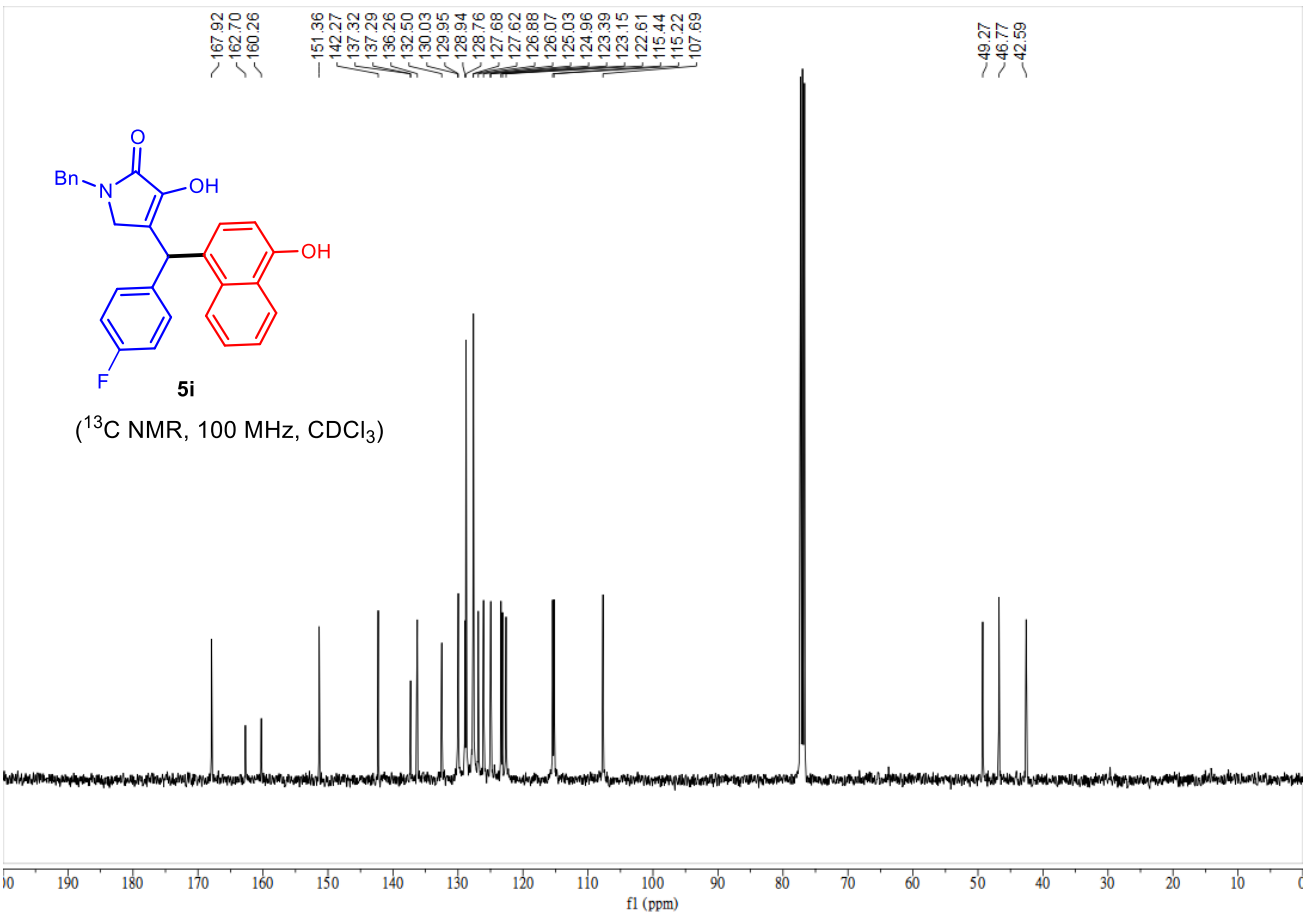
5h

(^{19}F NMR, 376 MHz, $CDCl_3$)



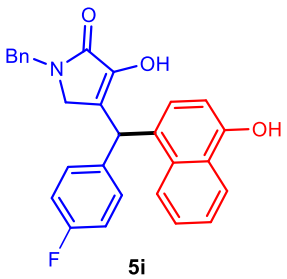
5i

(^{1}H NMR, 400 MHz, $CDCl_3$)



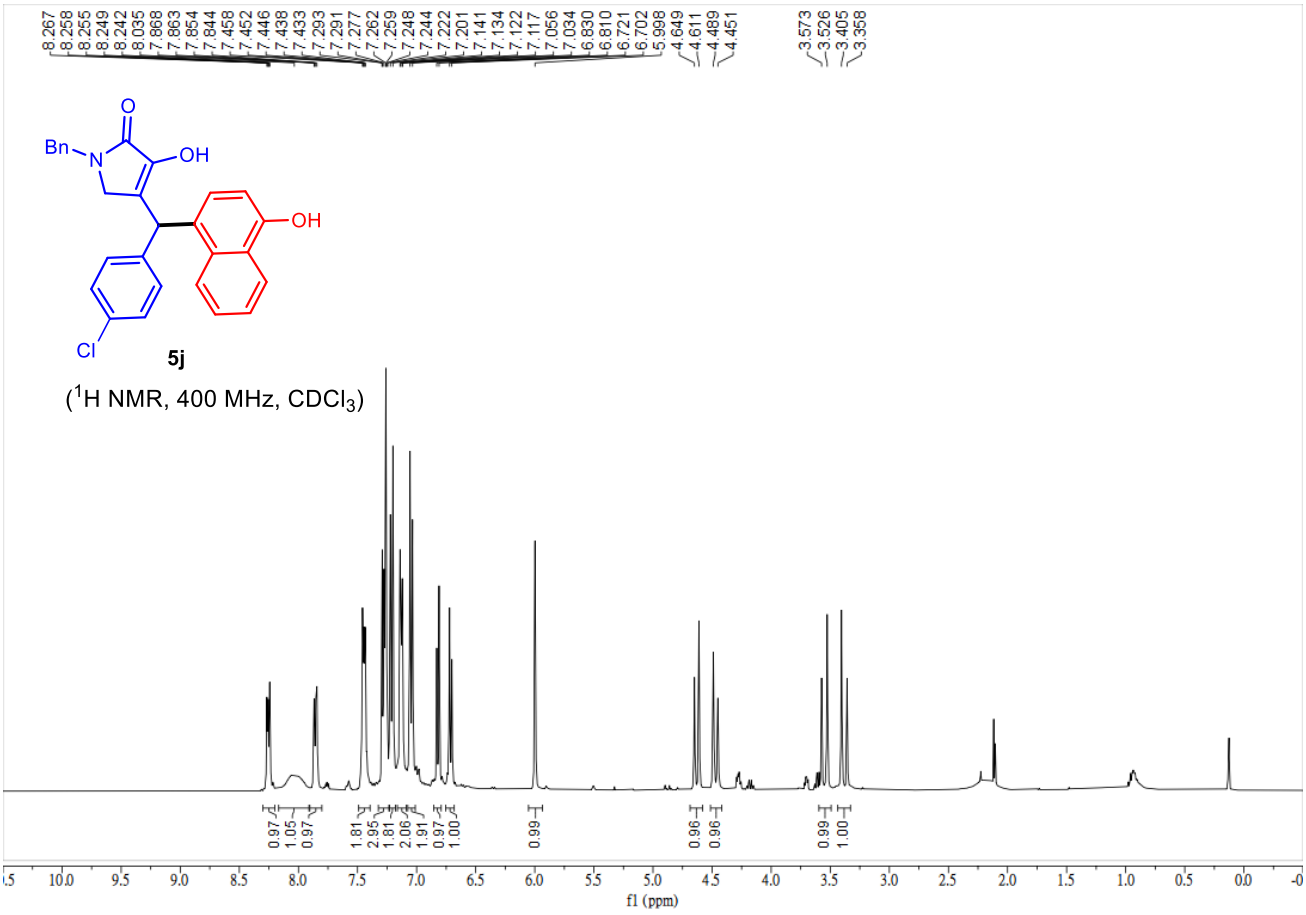
5i

(^{13}C NMR, 100 MHz, $CDCl_3$)



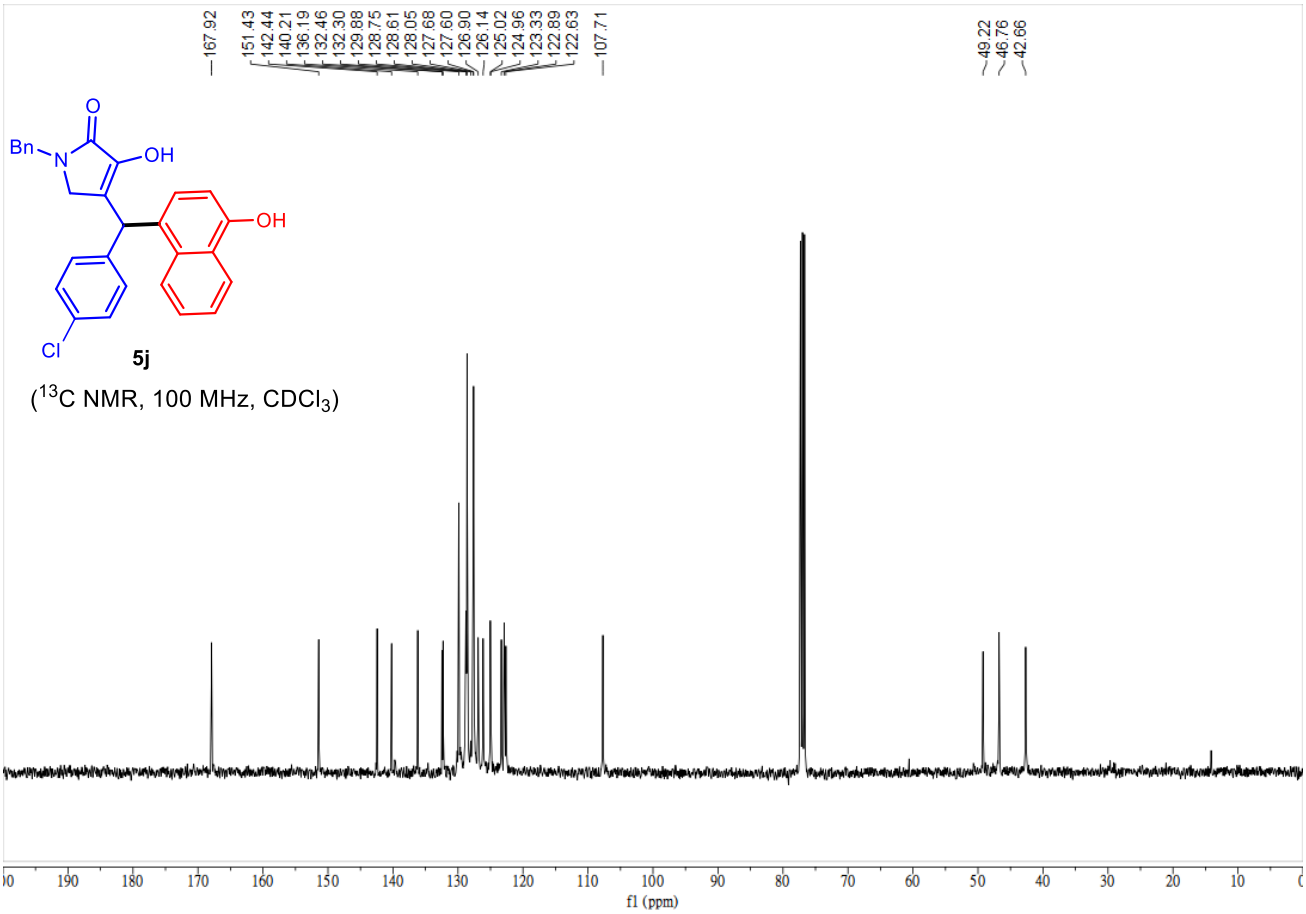
5i

(^{19}F NMR, 376 MHz, $CDCl_3$)



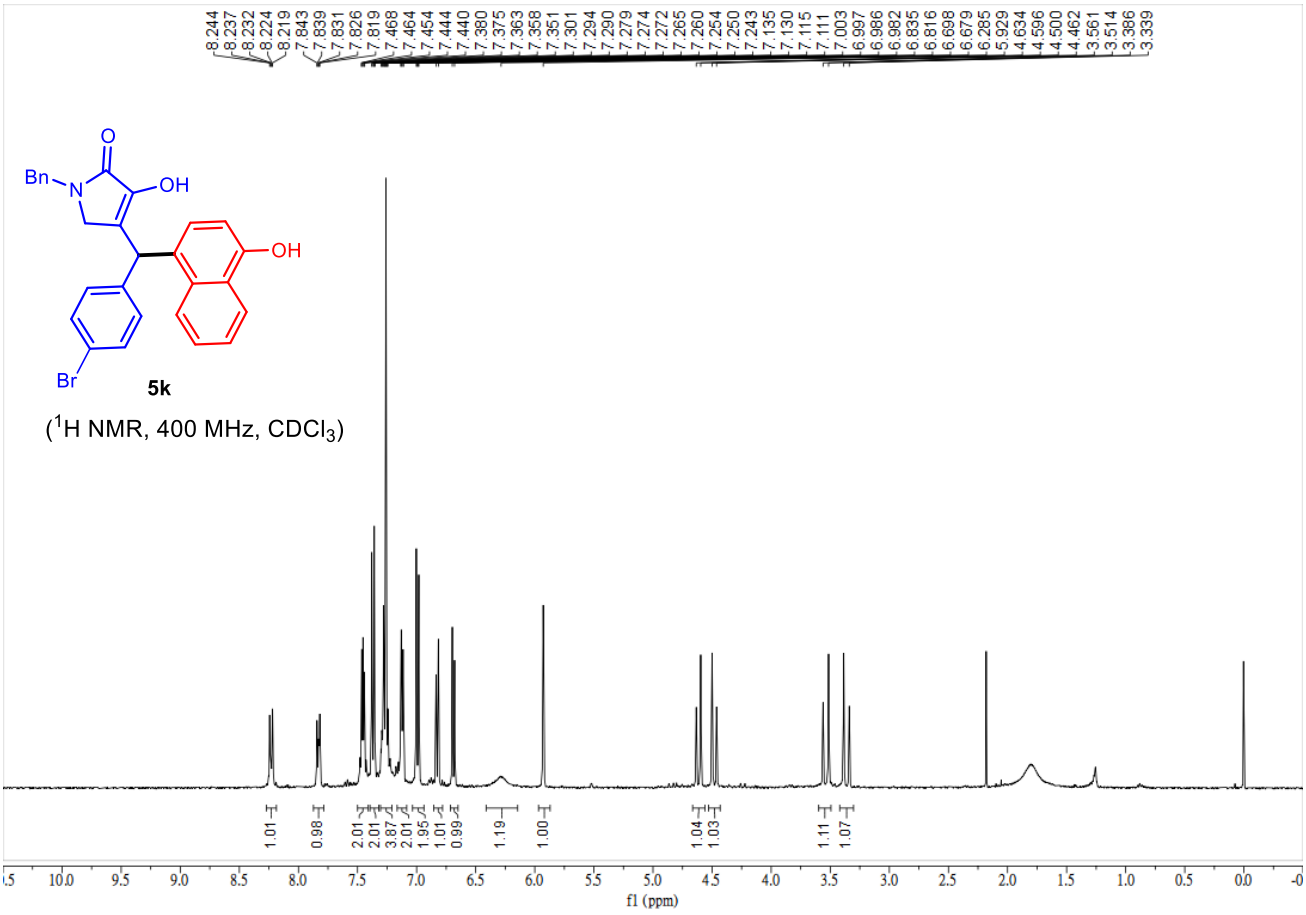
5j

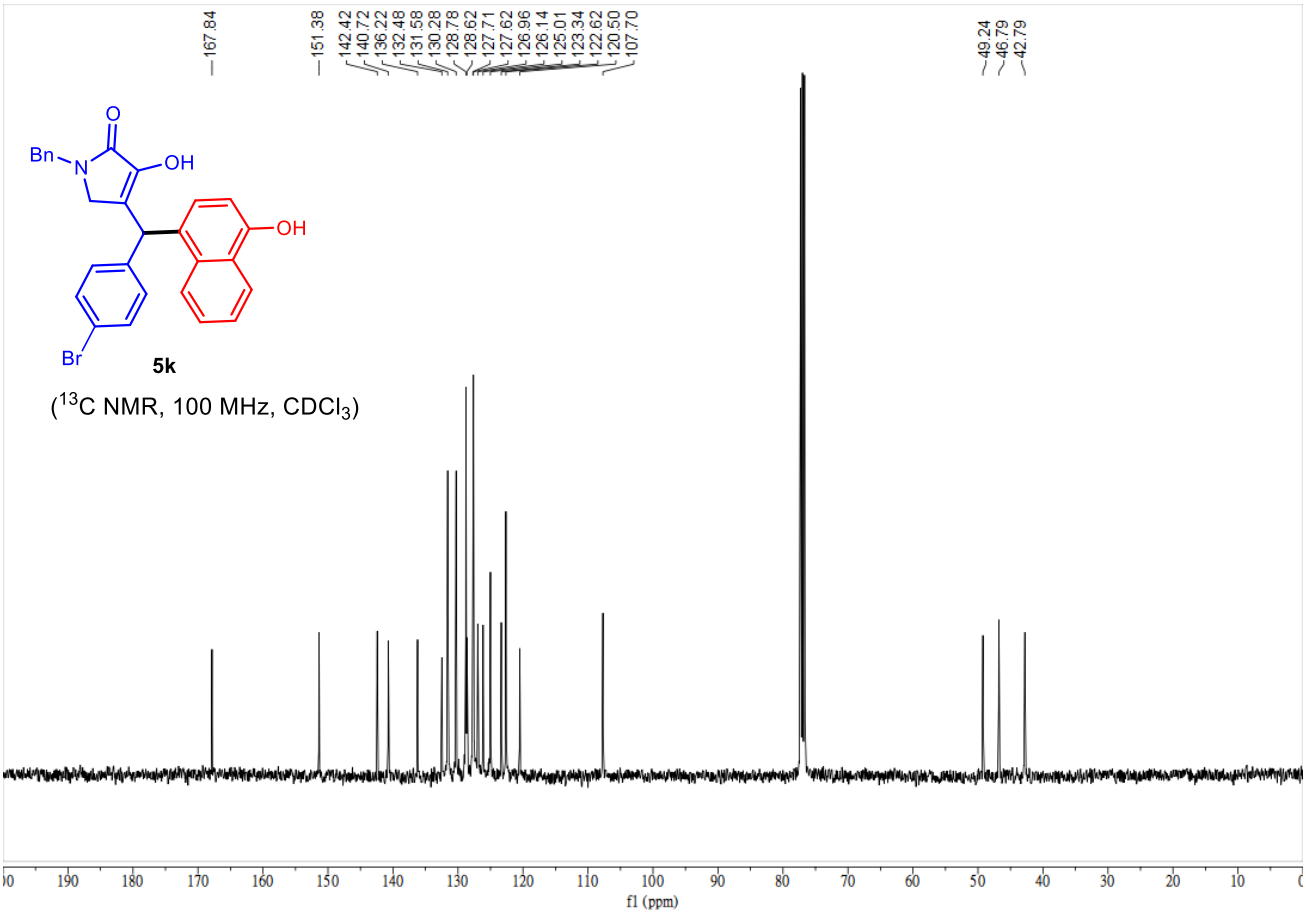
(^{1}H NMR, 400 MHz, $CDCl_3$)

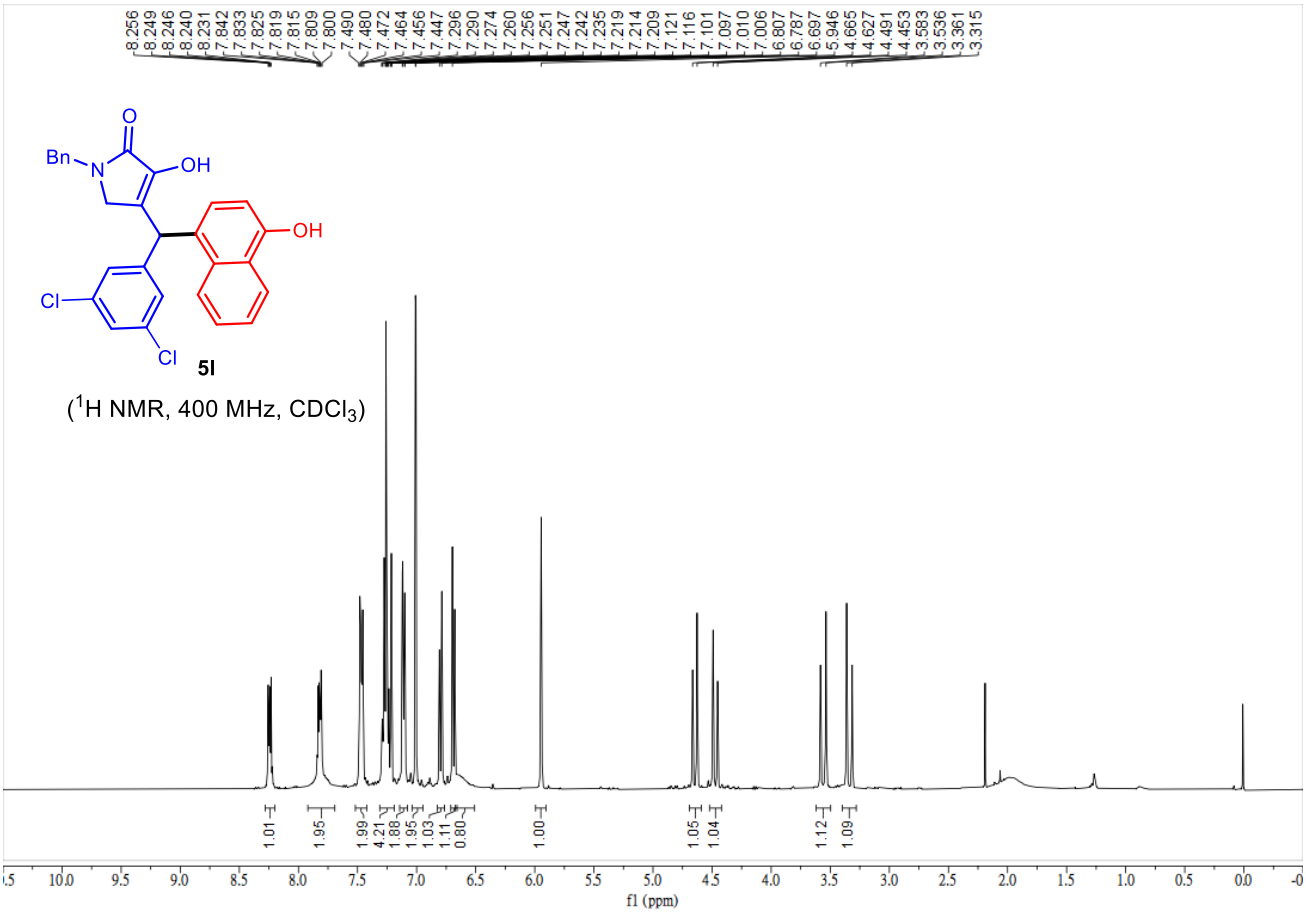


5j

(^{13}C NMR, 100 MHz, $CDCl_3$)

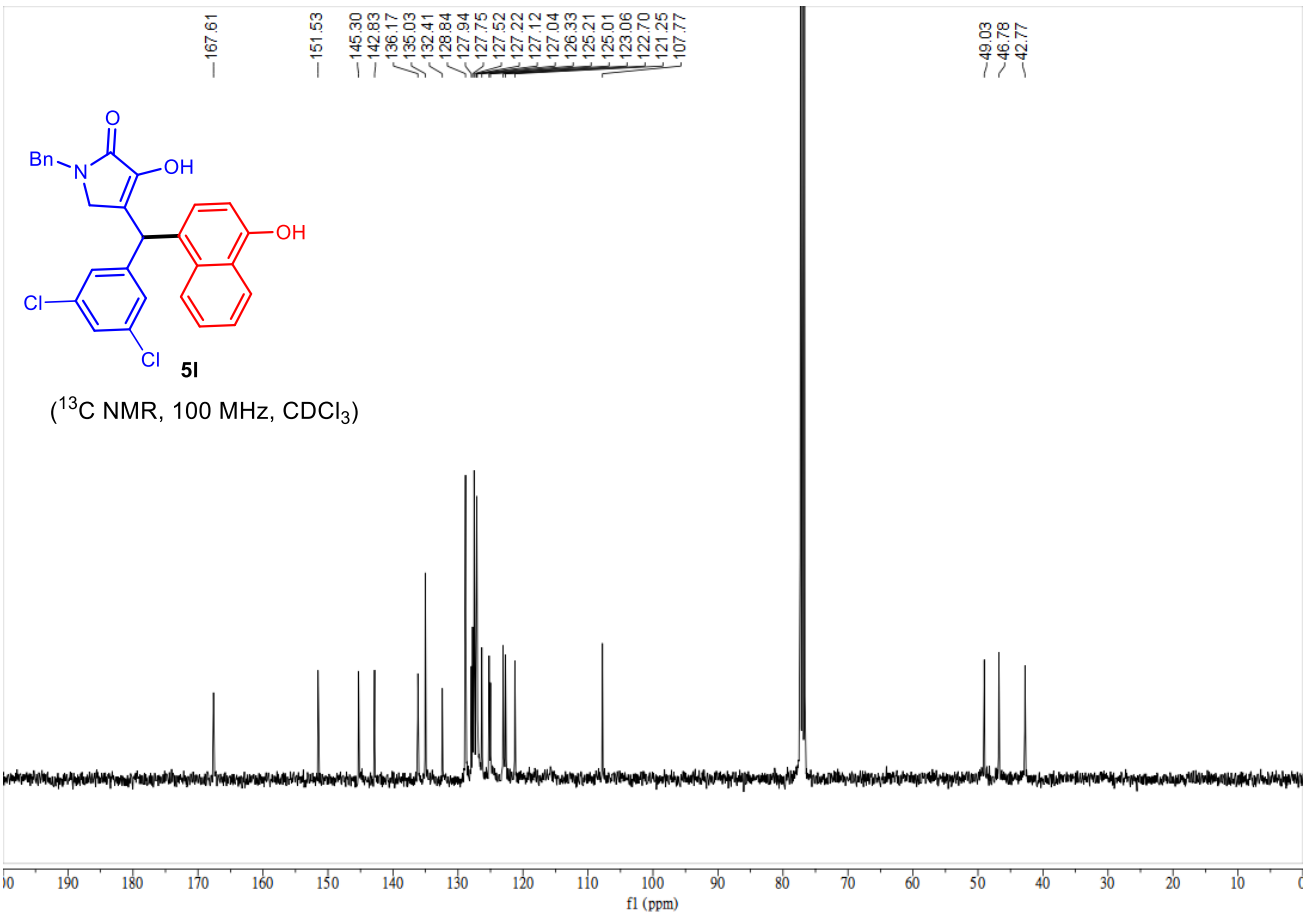

8.244
8.237
8.232
8.224
8.219
7.843
7.839
7.831
7.826
7.819
7.468
7.464
7.454
7.444
7.440
7.380
7.375
7.363
7.358
7.351
7.301
7.294
7.290
7.279
7.274
7.272
7.265
7.260
7.254
7.250
7.243
7.135
7.130
7.115
7.111
7.003
6.997
6.986
6.982
6.835
6.816
6.698
6.679
6.285
5.929
4.634
4.596
4.500
4.462
3.561
3.514
3.386
3.339
Bn
N
O
OH
OH
Br
5k
(1H NMR, 400 MHz, CDCl3)
1.01
0.98
2.01
2.01
3.87
2.01
1.95
1.01
0.99
1.19
1.00
1.04
1.03
1.11
1.07
f1 (ppm)


167.84
151.38
142.42
140.72
136.22
132.48
131.58
130.28
128.78
128.62
127.71
127.62
126.96
126.14
125.01
123.34
122.62
120.50
107.70
49.24
46.79
42.79
Bn
N
O
OH
OH
Br
5k
(13C NMR, 100 MHz, CDCl3)
f1 (ppm)



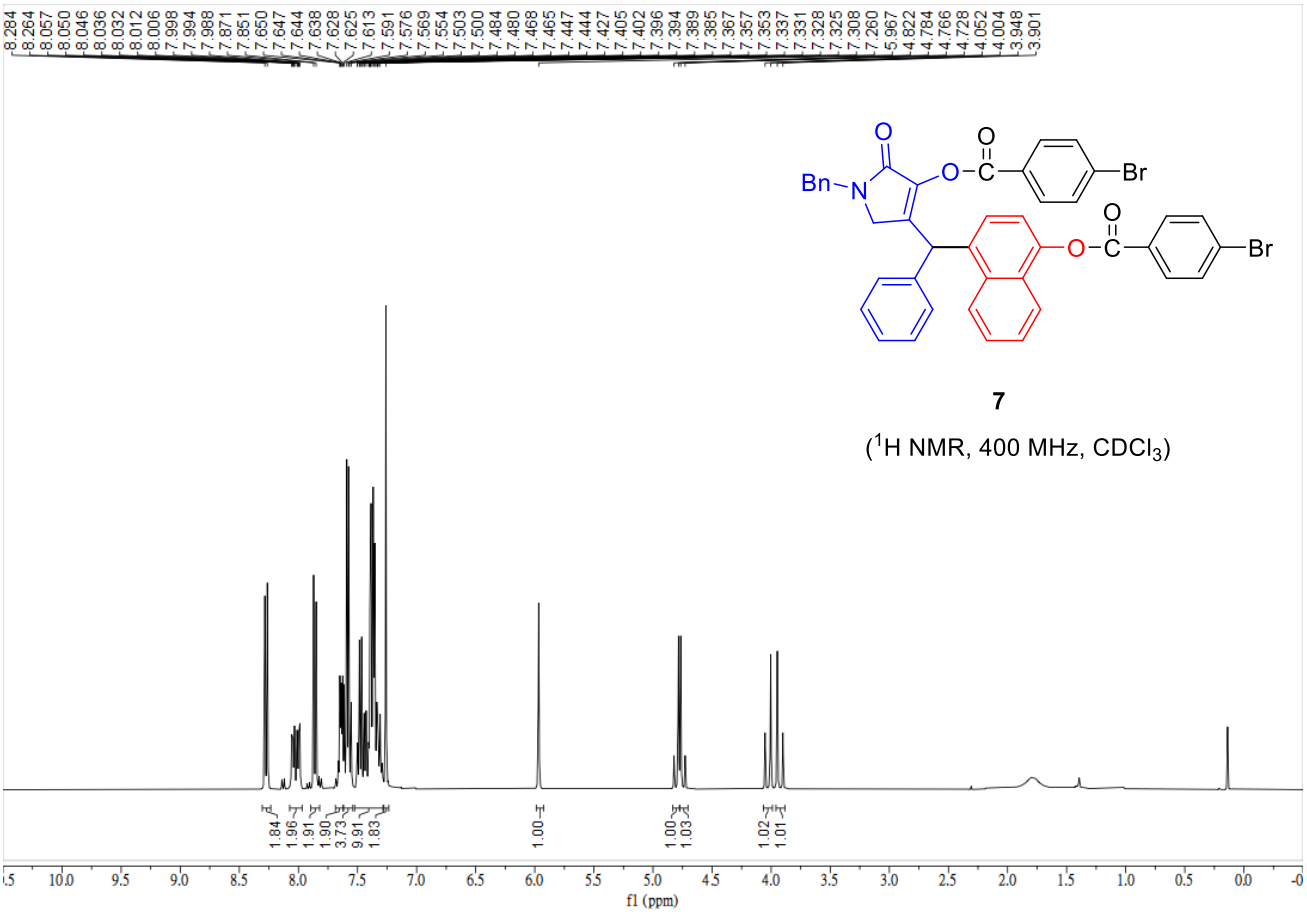
5l

(^{1}H NMR, 400 MHz, $CDCl_3$)



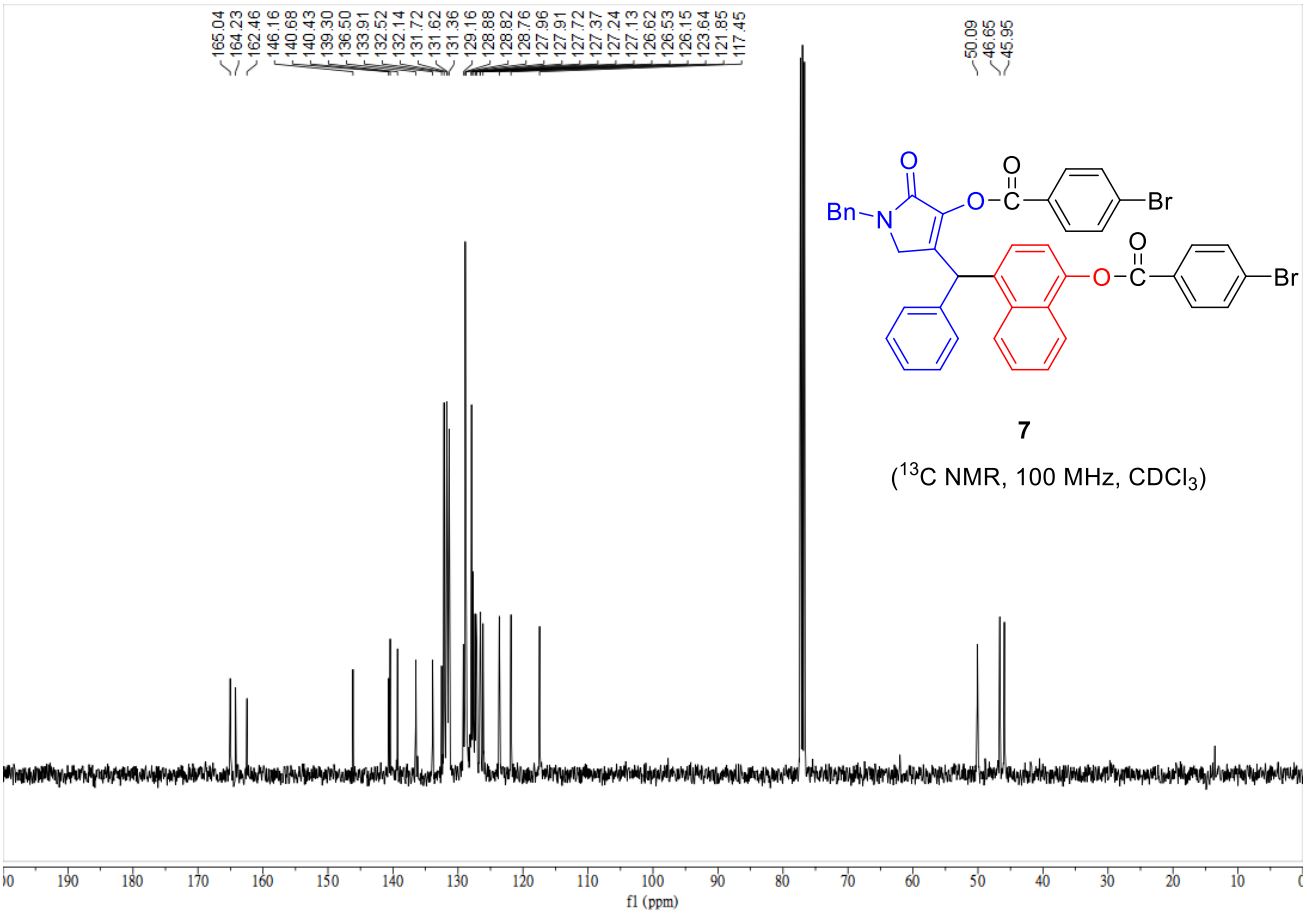
5l

(^{13}C NMR, 100 MHz, $CDCl_3$)



7

(^{1}H NMR, 400 MHz, $CDCl_3$)

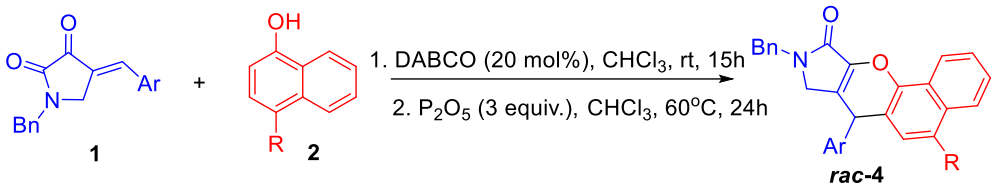


7

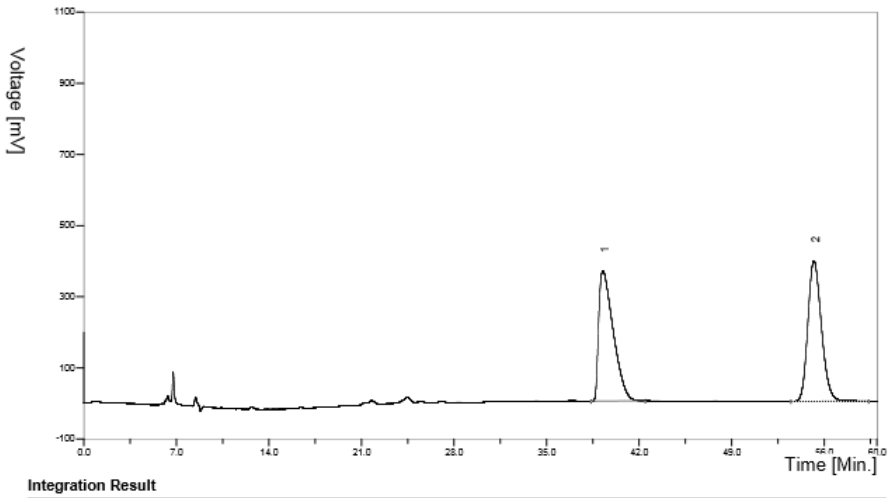
(^{13}C NMR, 100 MHz, $CDCl_3$)

5. Copies of HPLC Spectra of Products 4

We prepared ***rac*-4** using DABCO as the catalyst.



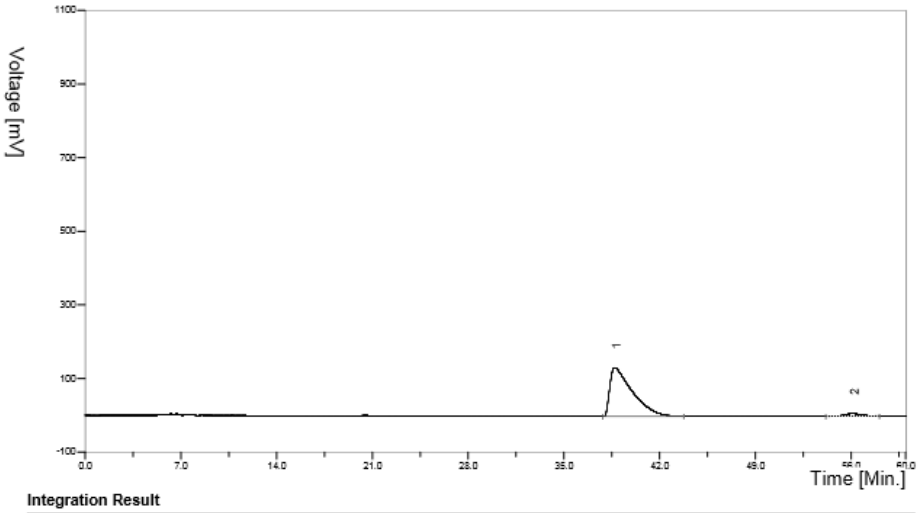
rac-4aa



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	39.27	27953.90	49.7787
2	55.23	28202.46	50.2213
Total		56156.37	100

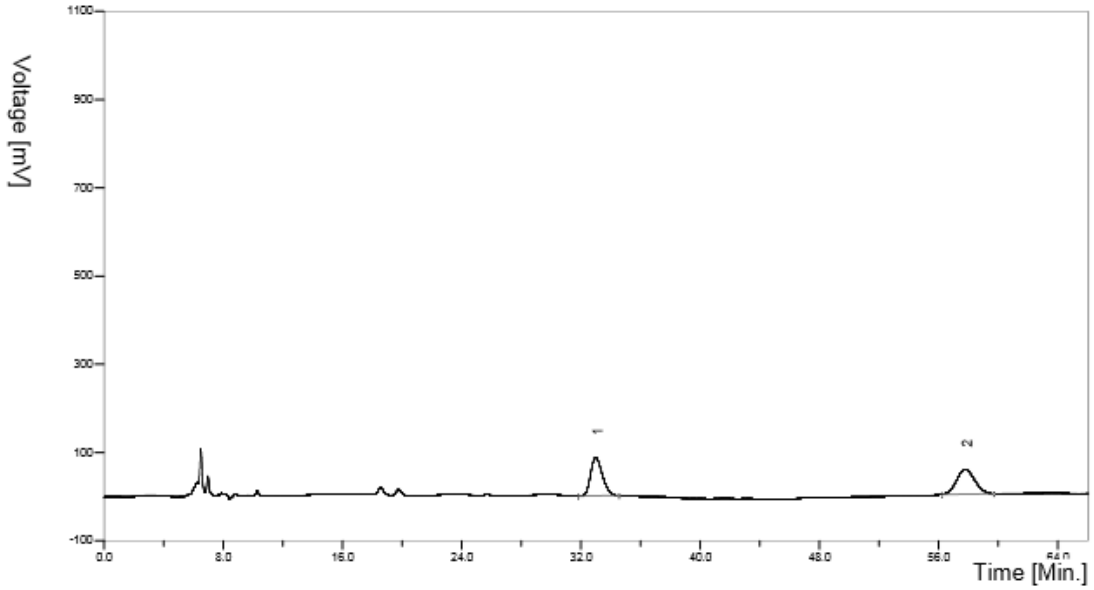
4aa



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	38.73	14992.94	96.4023
2	56.13	559.53	3.5977
Total		15552.47	100

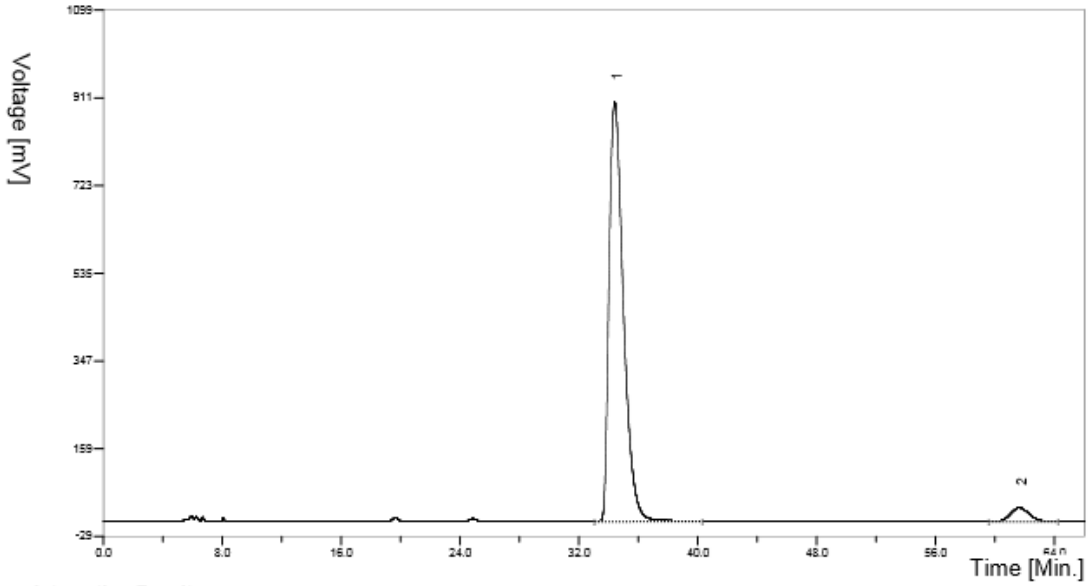
***rac*-4ab**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	32.99	4775.32	50.1420
2	57.77	4748.27	49.8580
Total		9523.58	100

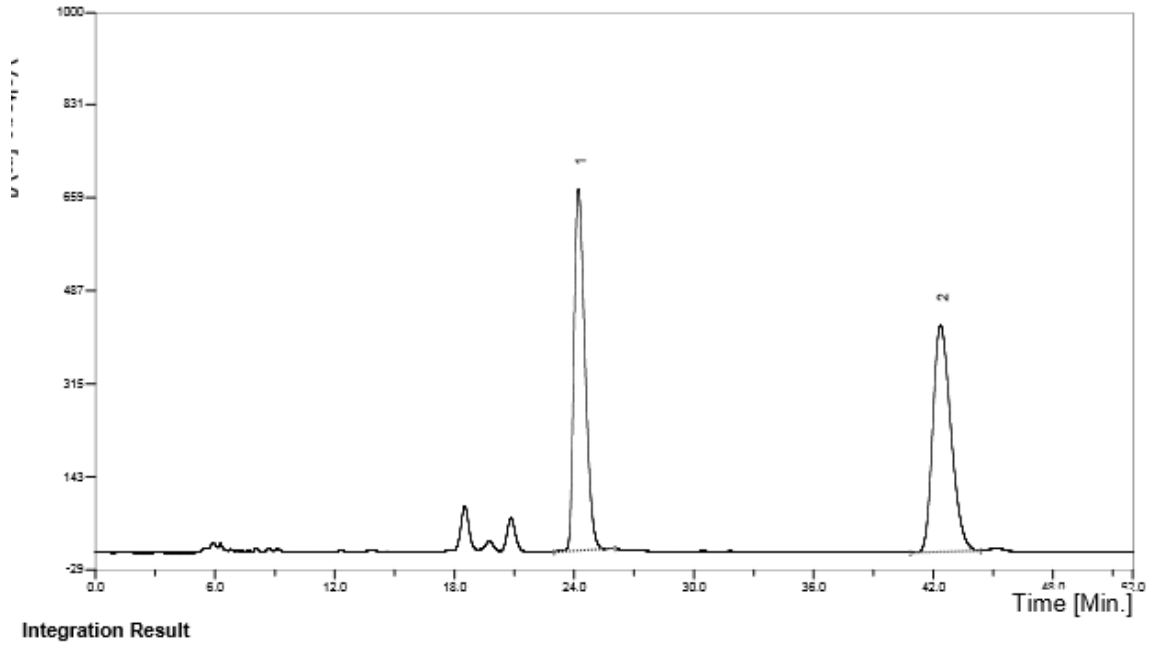
4ab



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	34.42	60314.03	95.8127
2	61.64	2635.87	4.1873
Total		62949.90	100

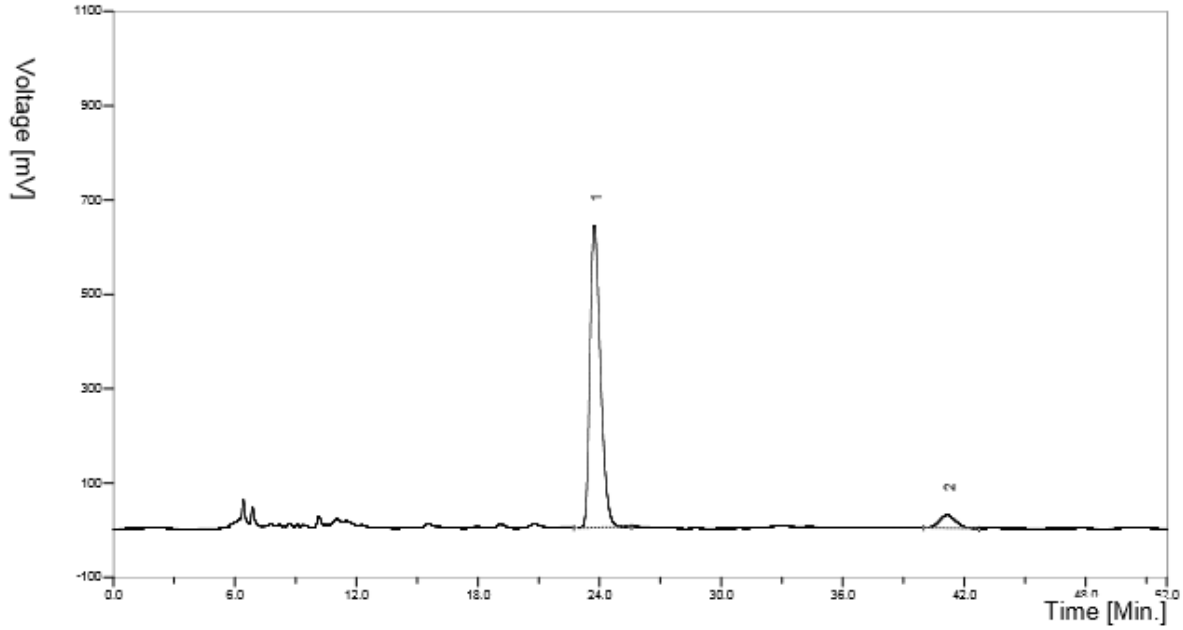
***rac*-4ac**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	24.21	25489.83	49.1948
2	42.36	26324.26	50.8052
Total		51814.09	100

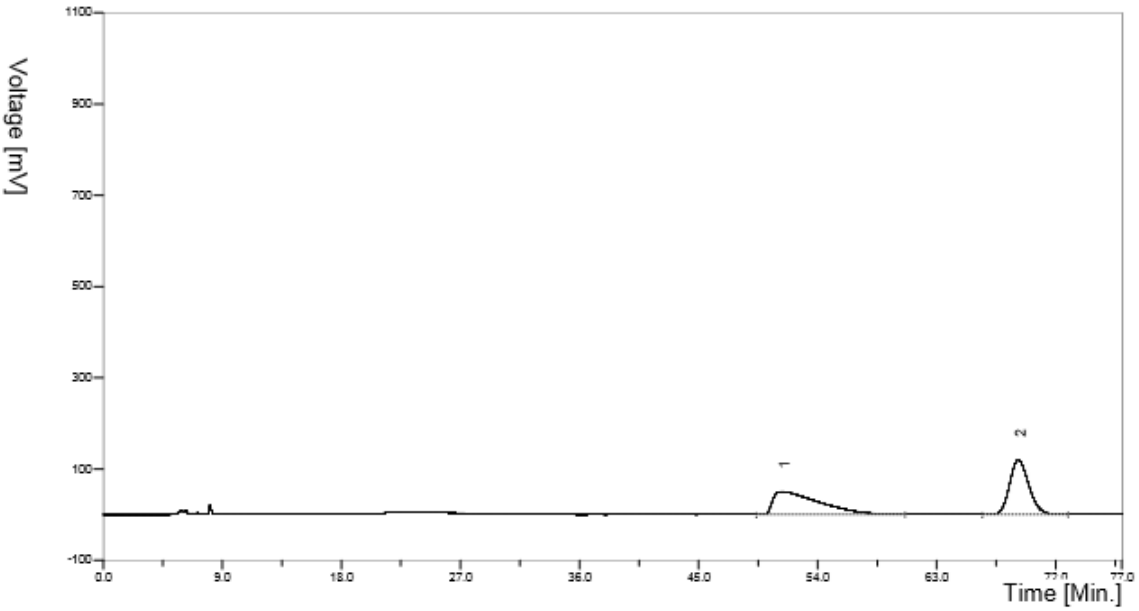
4ac



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	23.74	22837.63	93.7546
2	41.16	1521.32	6.2454
Total		24358.95	100

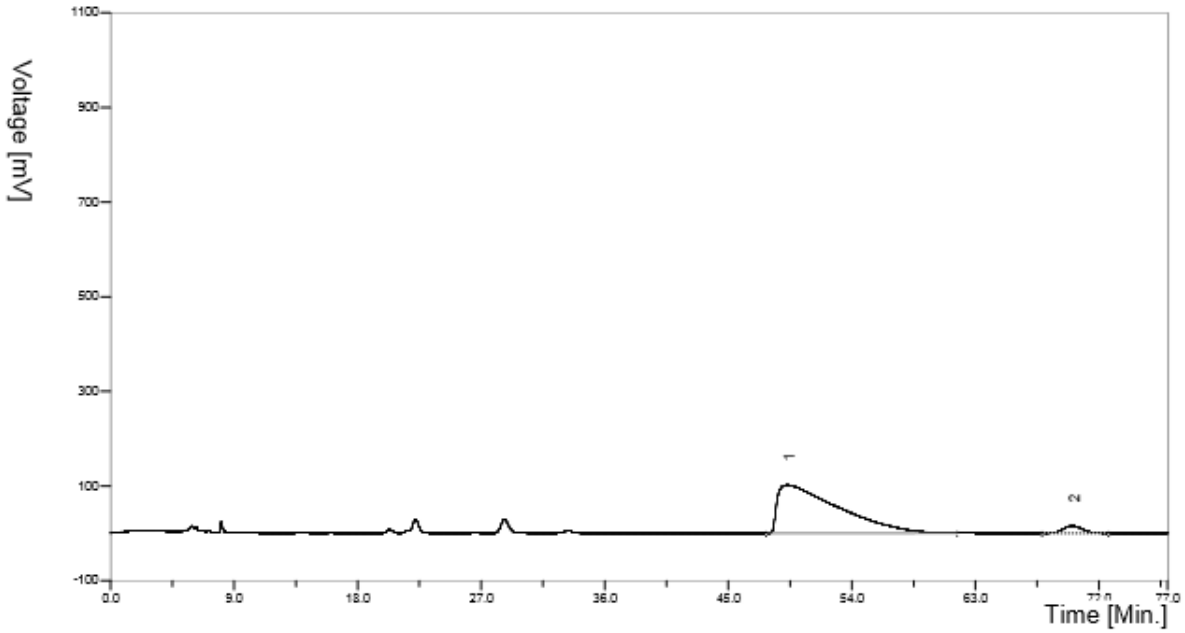
***rac*-4ad**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	51.33	12127.50	50.2790
2	69.17	11992.92	49.7210
Total		24120.43	100

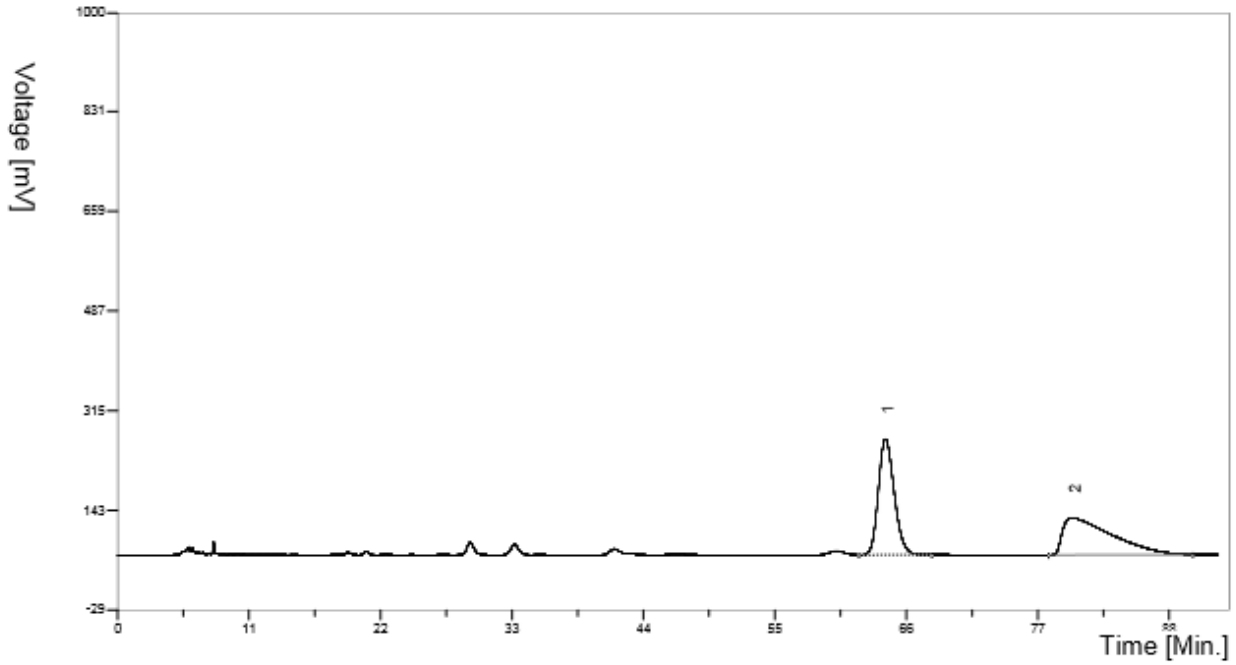
4ad



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	49.27	31754.29	95.2831
2	70.05	1571.95	4.7169
Total		33326.23	100

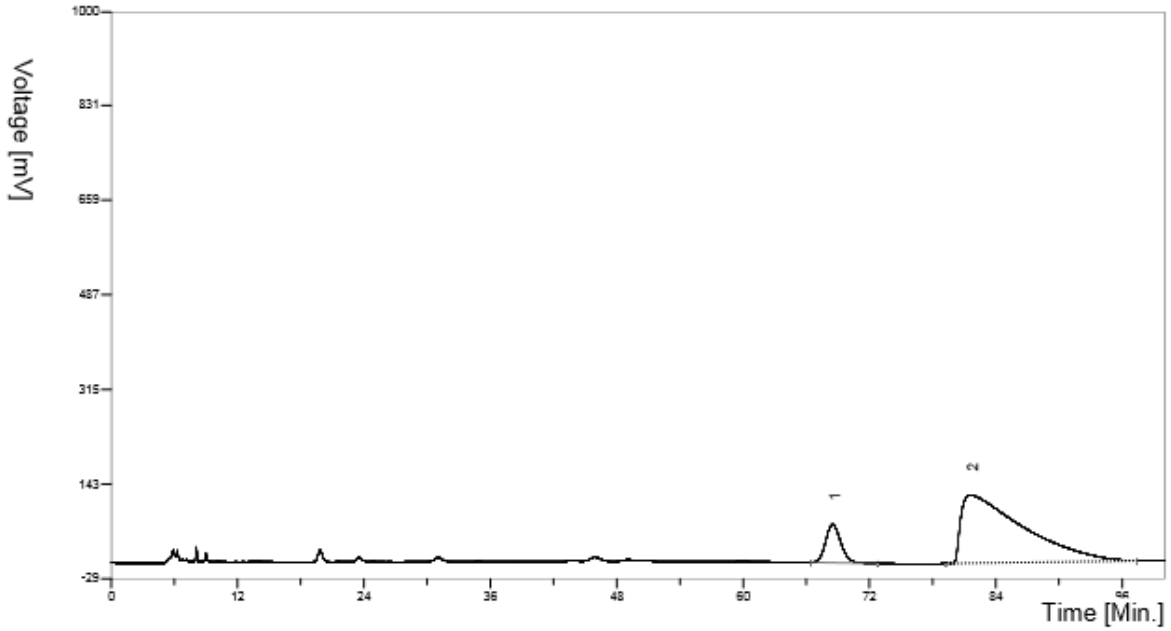
***rac*-4ae**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	64.26	18384.00	50.1461
2	79.91	18276.86	49.8539
Total		36660.85	100

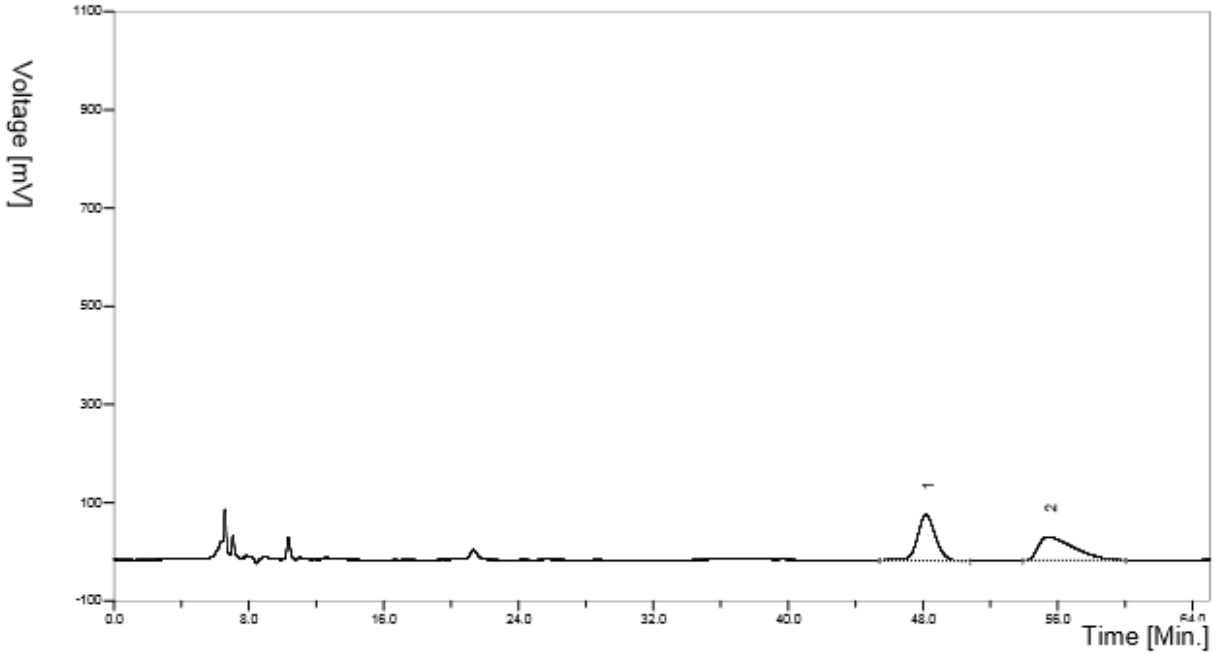
4ae



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	68.51	6913.46	11.9581
2	81.63	50900.60	88.0419
Total		57814.06	100

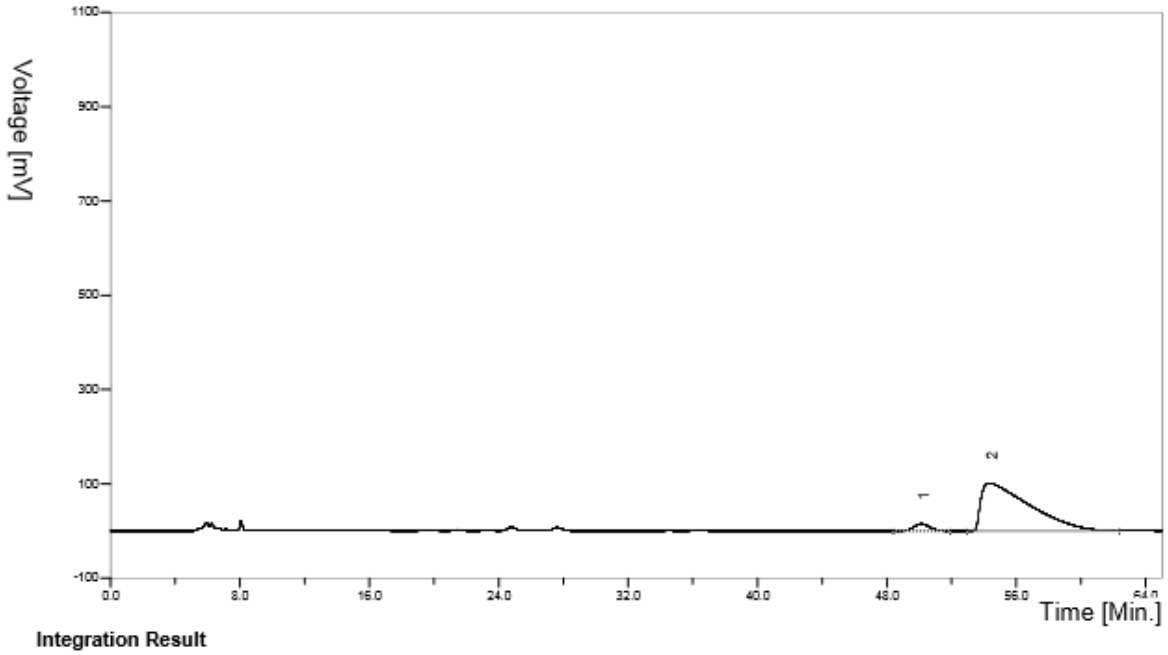
***rac*-4af**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	48.19	6953.72	49.6631
2	55.45	7048.07	50.3369
Total		14001.78	100

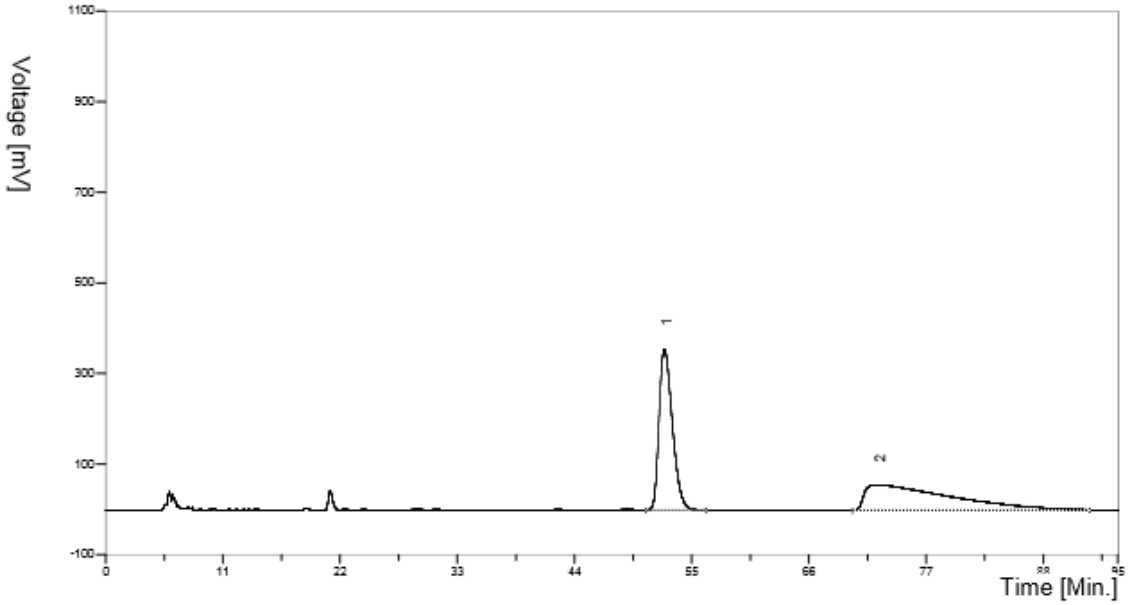
4af



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	50.14	1092.79	4.9062
2	54.36	21181.03	95.0938
Total		22273.82	100

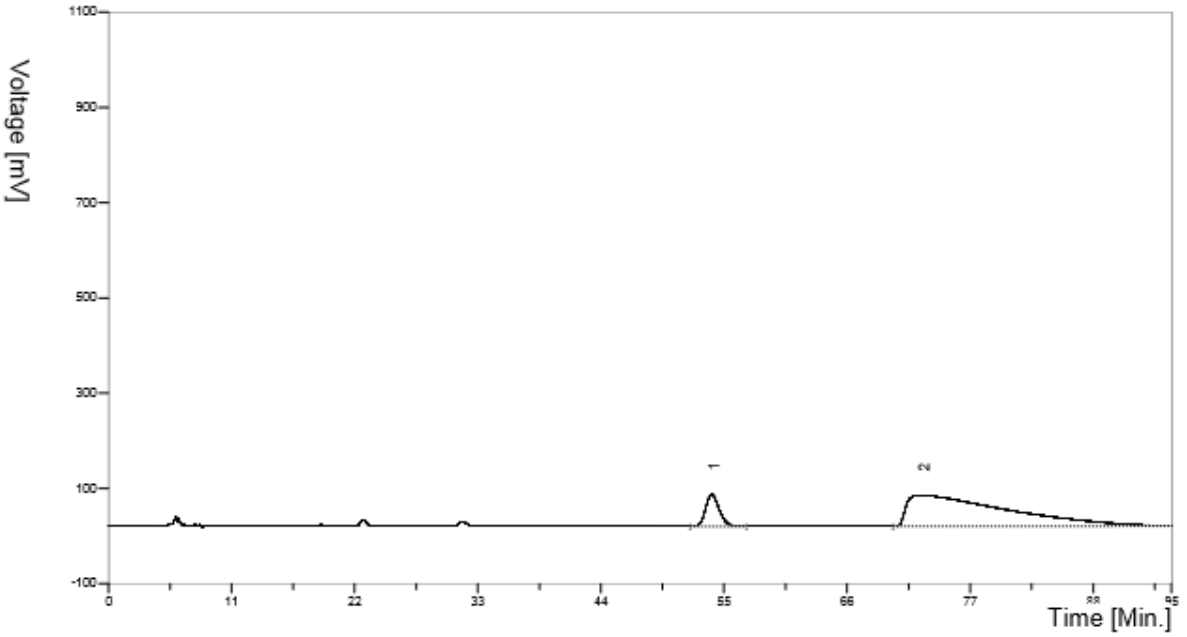
***rac*-4ag**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	52.44	30826.42	49.8659
2	72.48	30992.20	50.1341
Total		61818.62	100

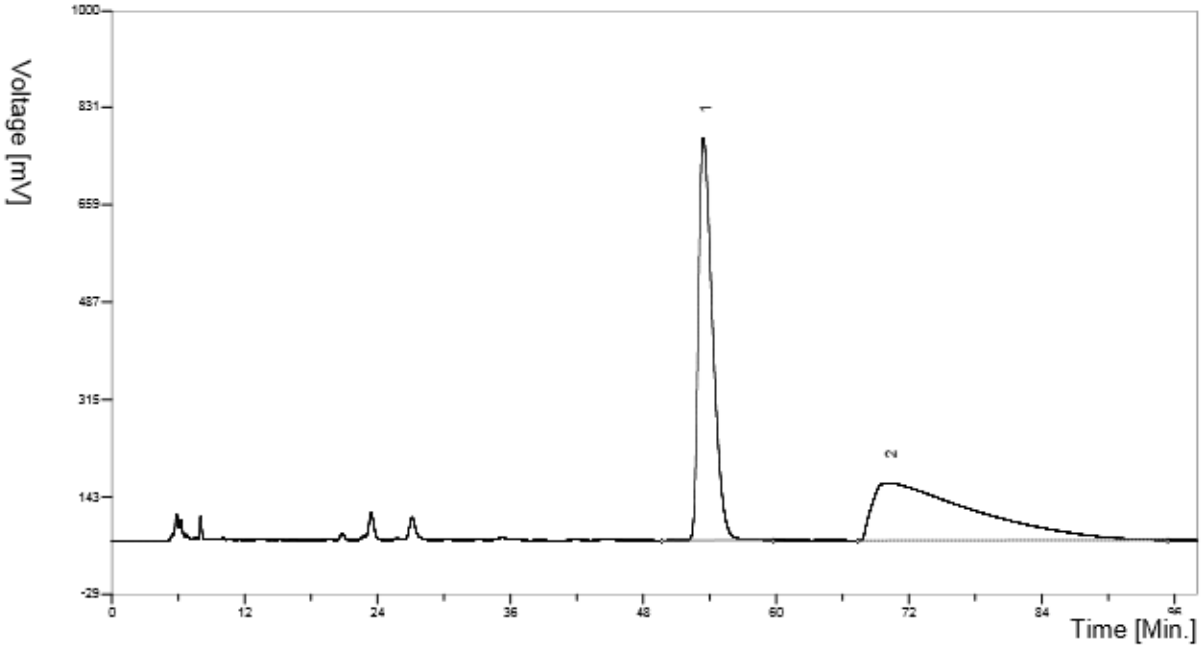
4ag



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	53.91	5643.47	12.2185
2	72.70	40544.32	87.7815
Total		46187.78	100

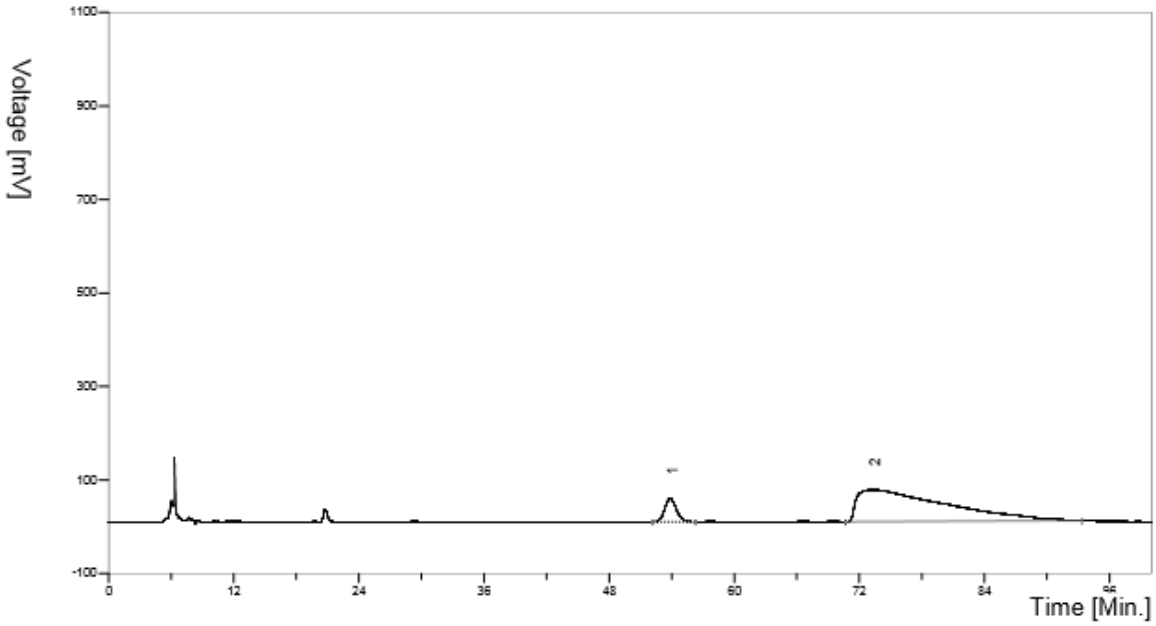
***rac*-4ah**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	53.44	63358.99	49.4051
2	70.17	64884.95	50.5949
Total		128243.94	100

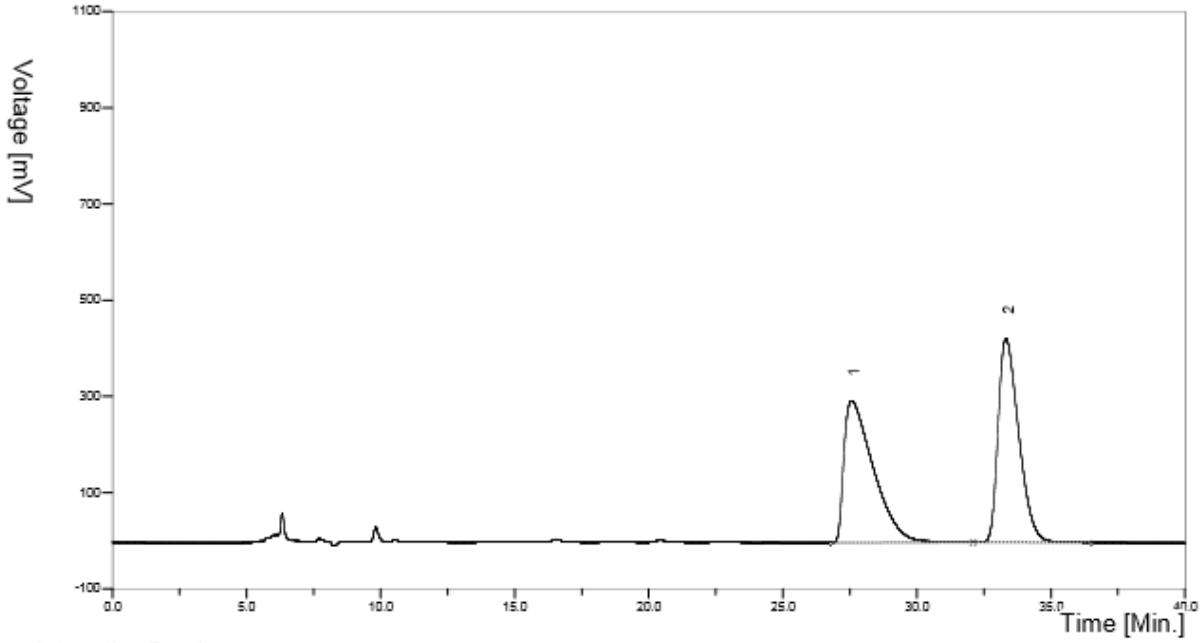
4ah



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	53.86	3845.08	8.6652
2	73.30	40528.54	91.3348
Total		44373.61	100

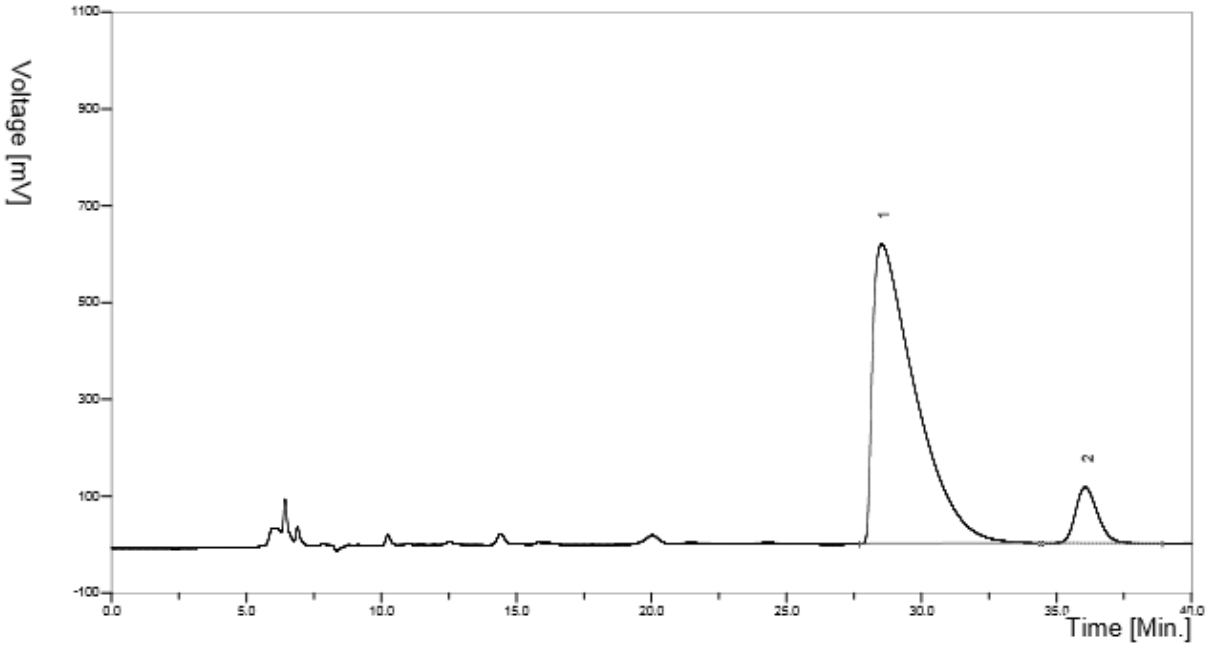
***rac*-4ai**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	27.57	22558.64	49.9327
2	33.32	22619.47	50.0673
Total		45178.11	100

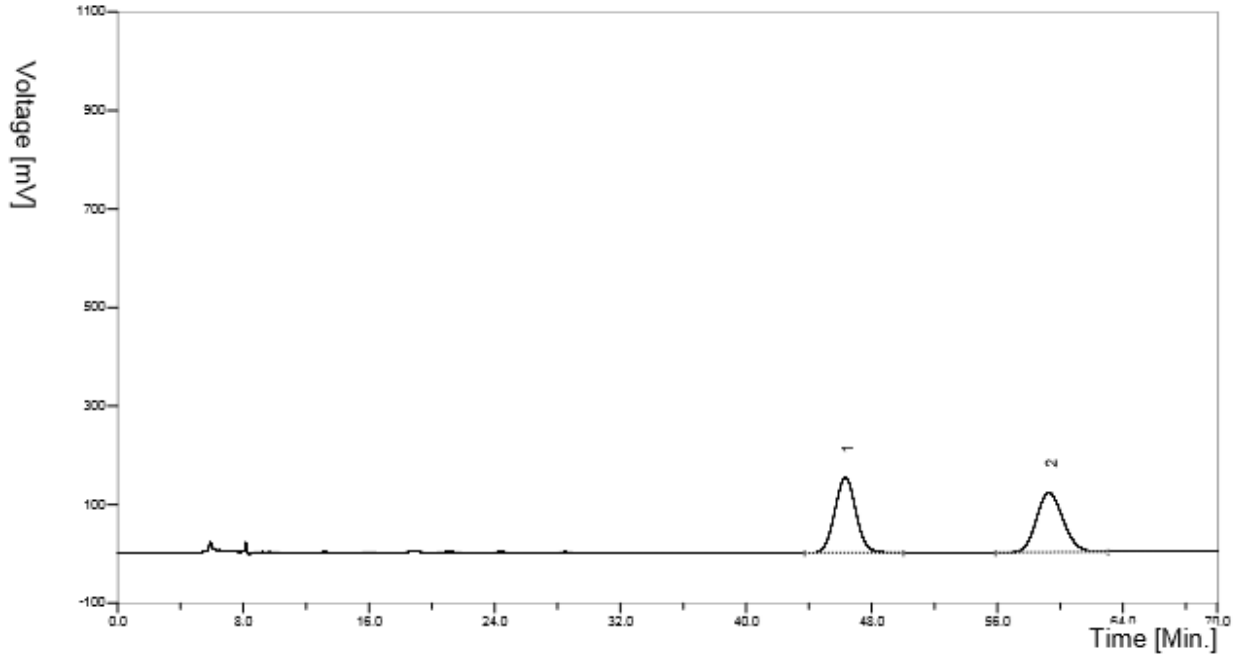
4ai



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	28.53	67738.87	91.1539
2	36.06	6573.81	8.8461
Total		74312.68	100

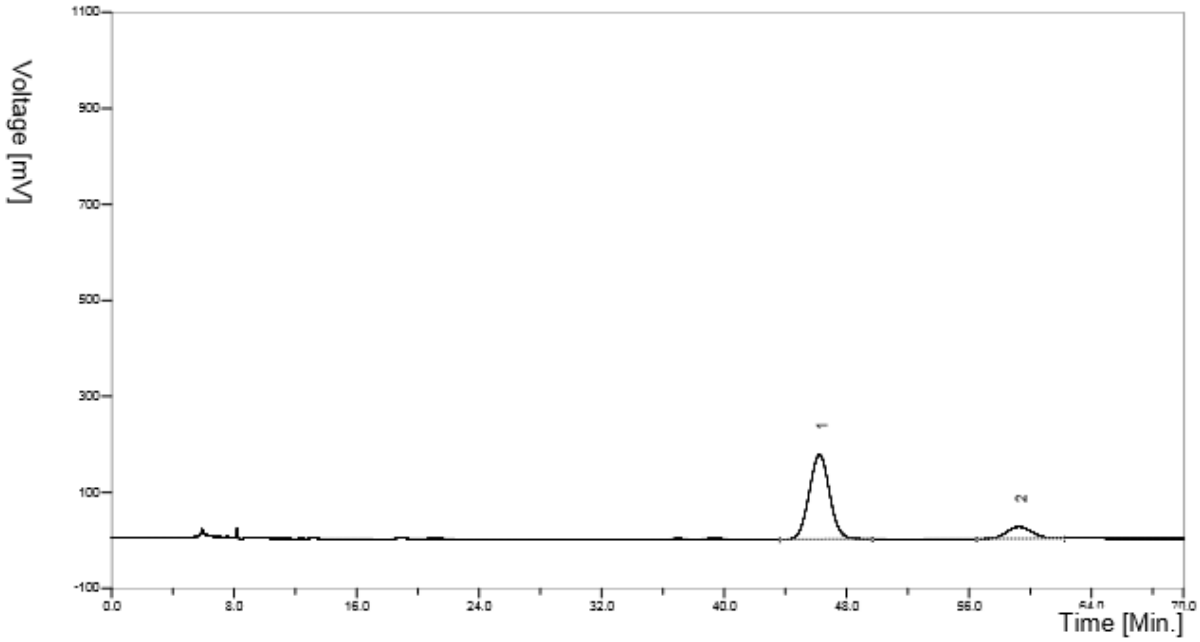
***rac*-4aj**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	46.33	14272.29	49.9313
2	59.29	14311.55	50.0687
Total		28583.84	100

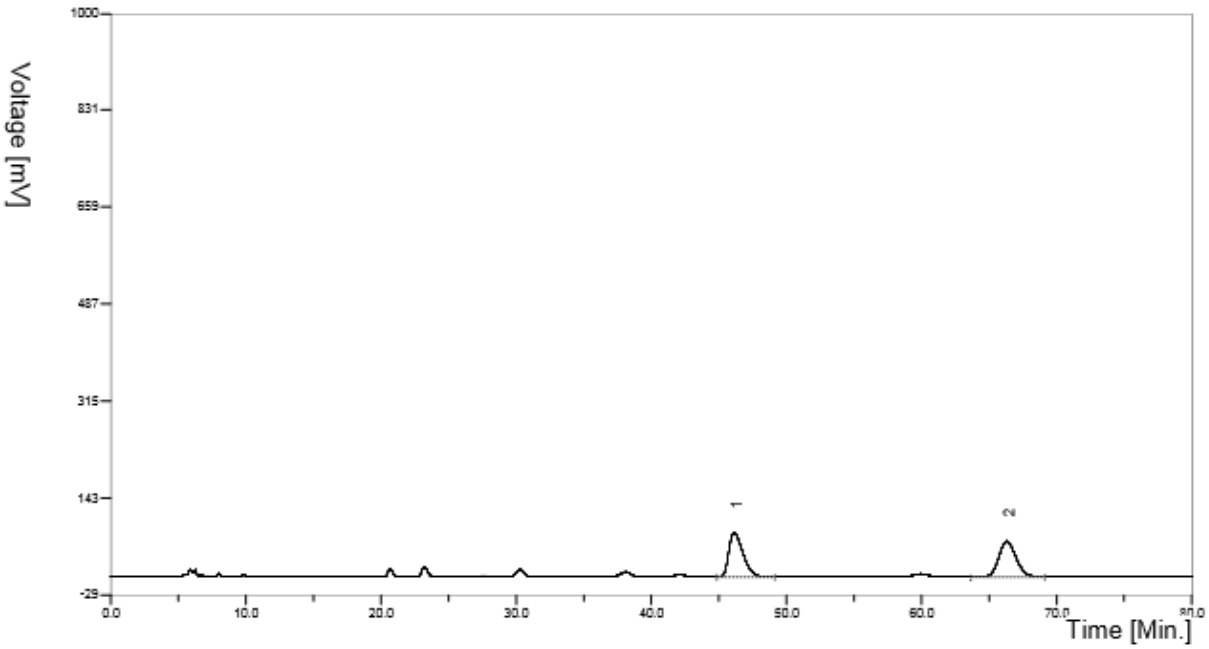
4aj



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	46.24	16308.41	85.1498
2	59.26	2844.19	14.8502
Total		19152.60	100

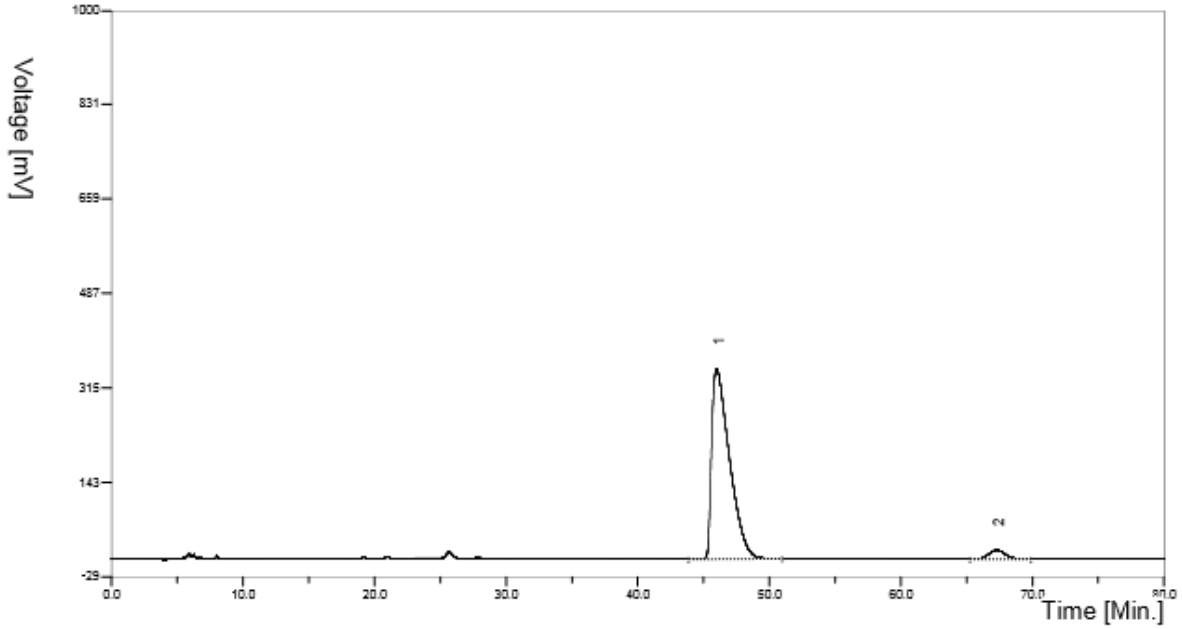
***rac*-4ak**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	46.14	5683.08	50.0897
2	66.31	5662.73	49.9103
Total		11345.81	100

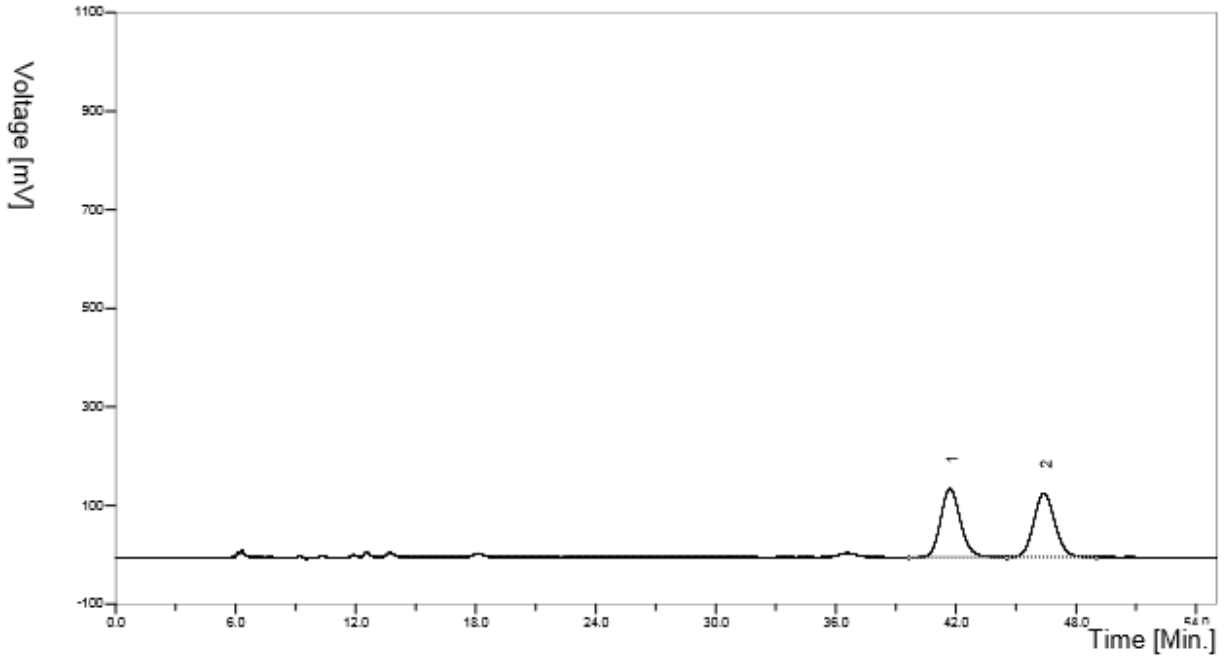
4ak



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	46.00	32743.81	95.6217
2	67.27	1499.28	4.3783
Total		34243.08	100

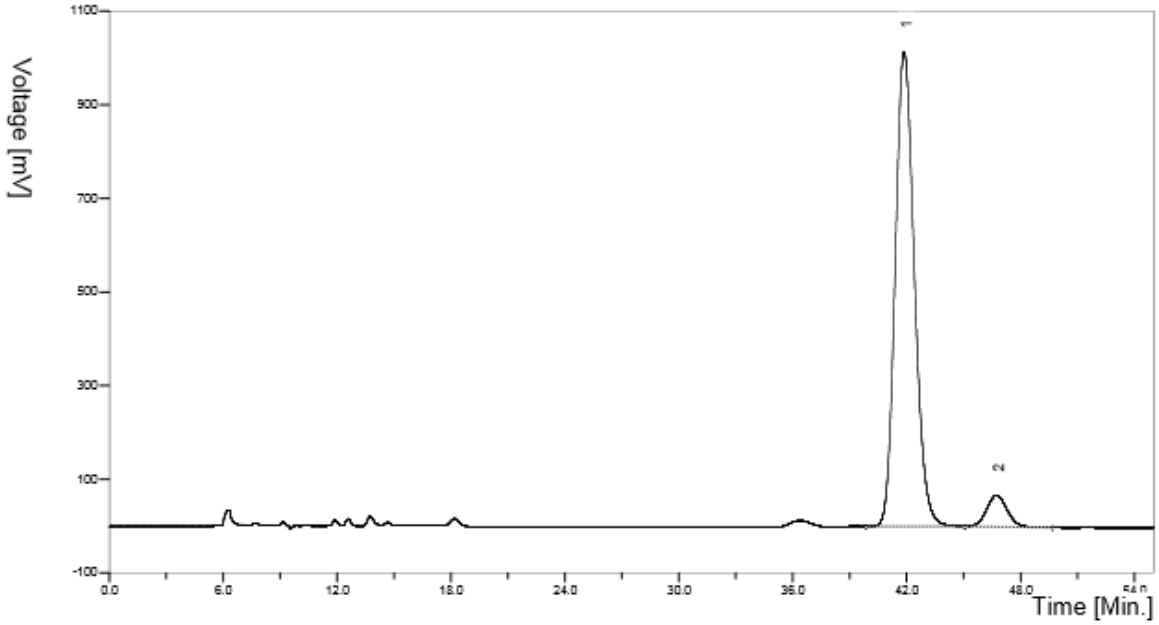
***rac*-4al**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	41.70	9545.17	50.1581
2	46.39	9484.97	49.8419
Total		19030.14	100

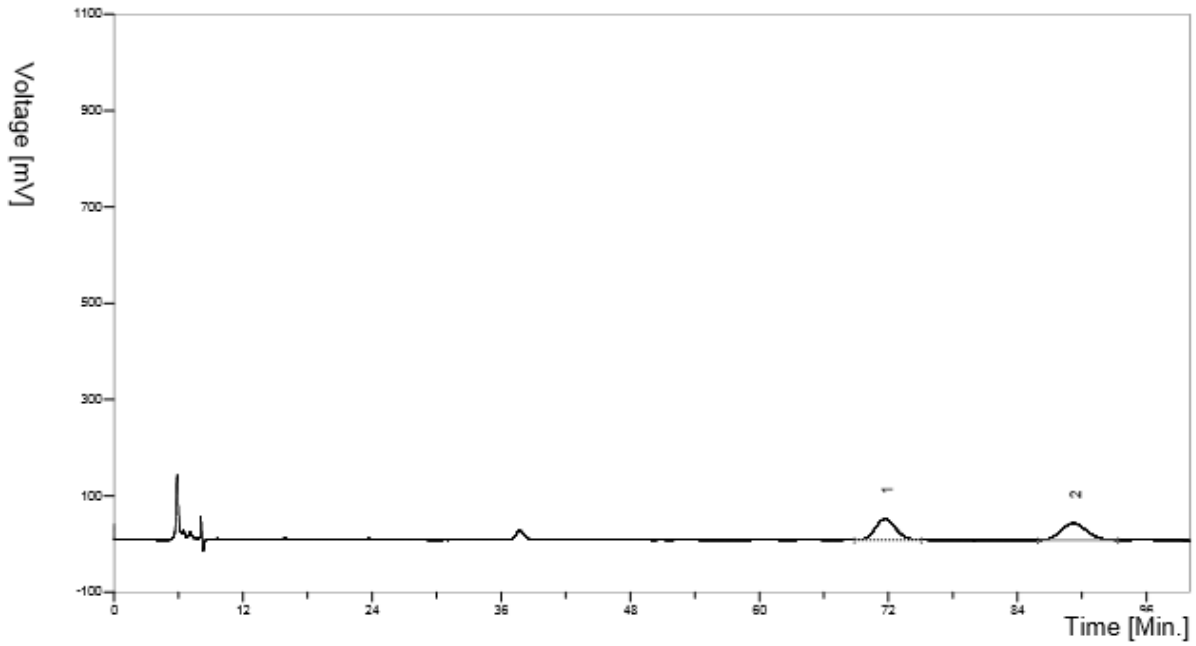
4al



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	41.86	70816.56	93.3656
2	46.74	5032.13	6.6344
Total		75848.69	100

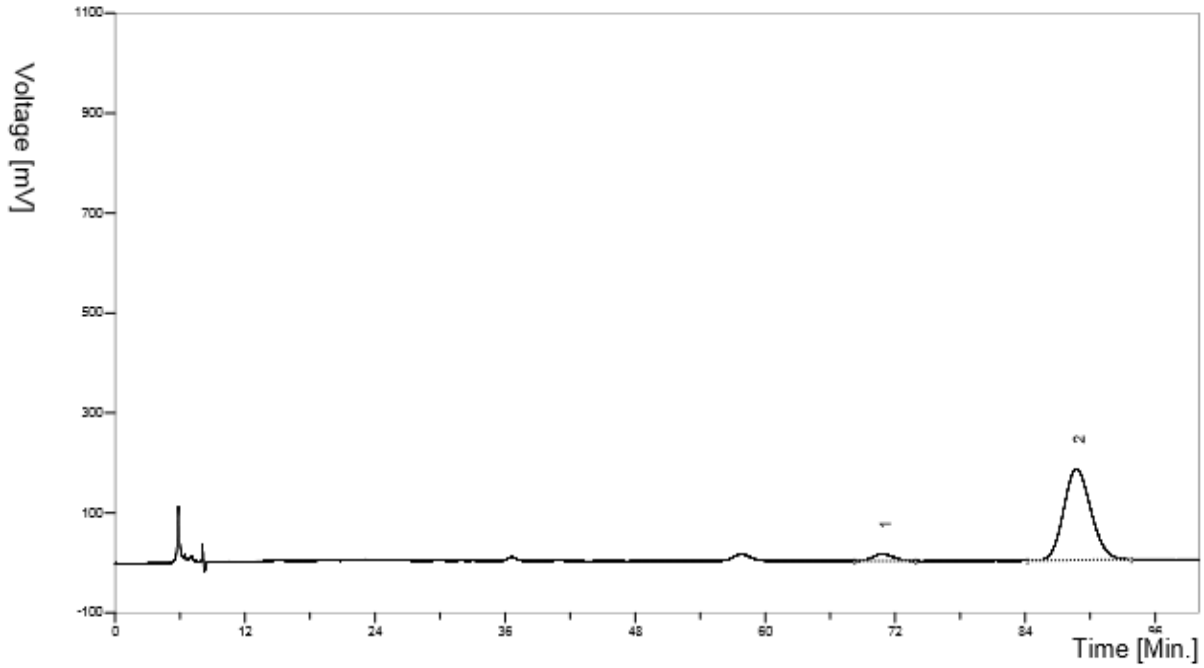
***rac*-4am**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	71.69	5724.98	49.6028
2	89.19	5816.67	50.3972
Total		11541.65	100

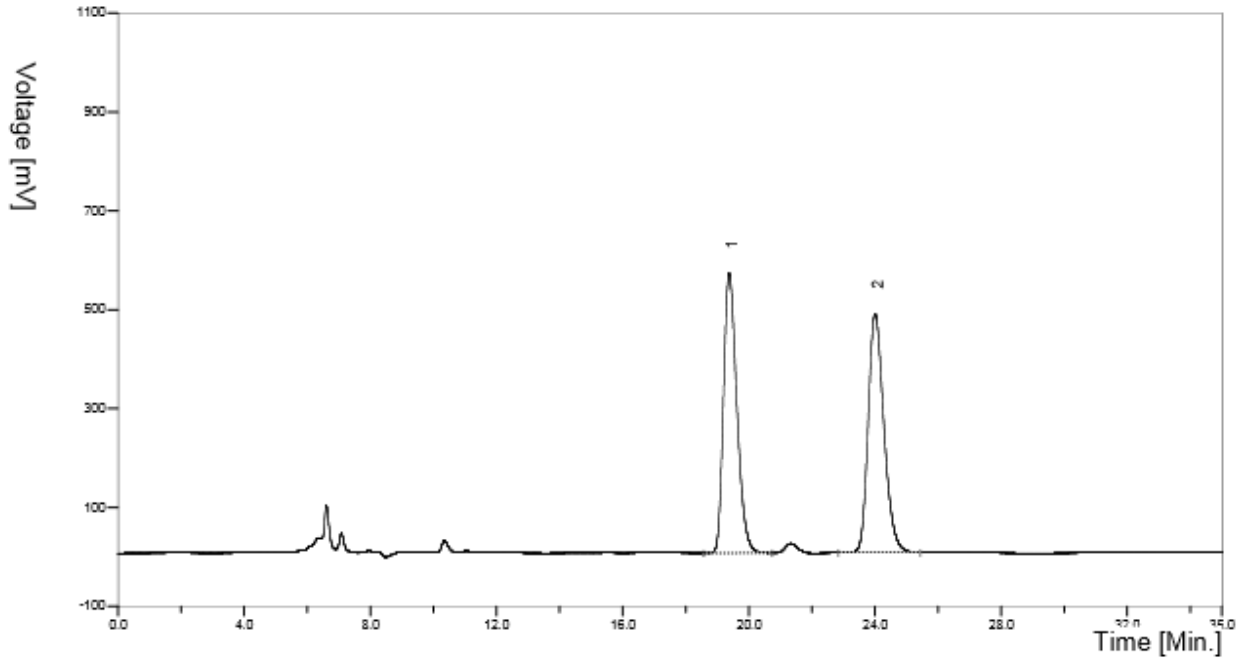
4am



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	70.87	1888.01	5.5920
2	88.74	31874.76	94.4080
Total		33762.77	100

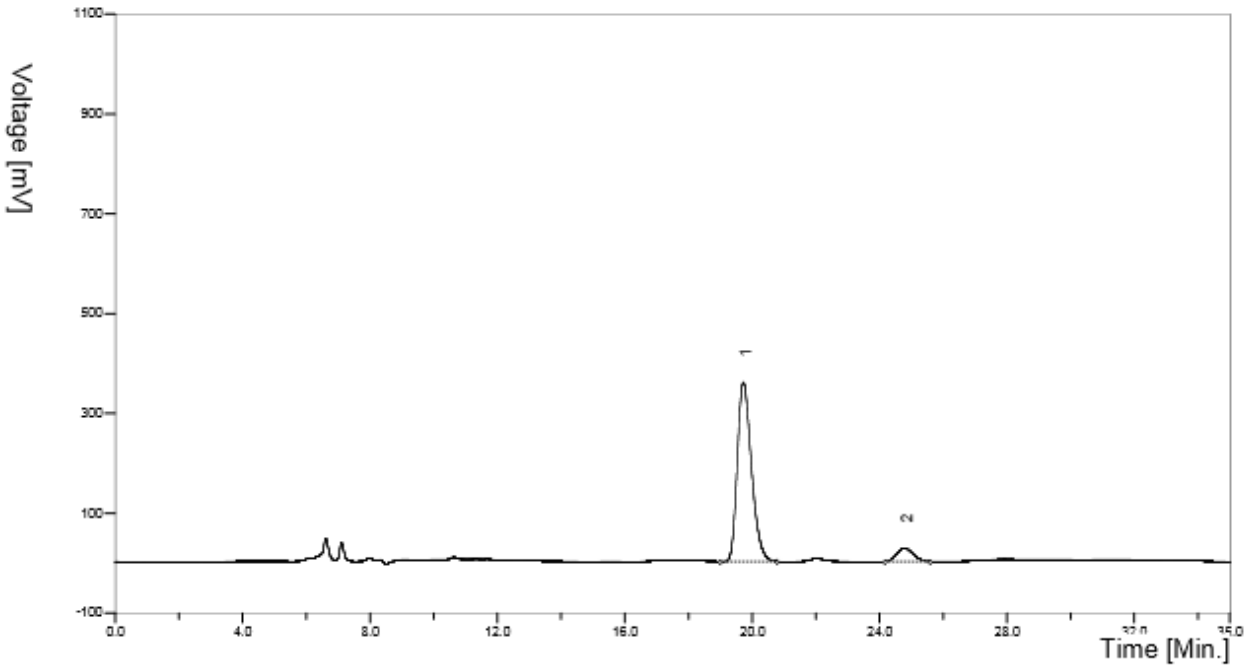
***rac*-4ba**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	19.38	16605.52	49.8354
2	24.01	16715.22	50.1646
Total		33320.75	100

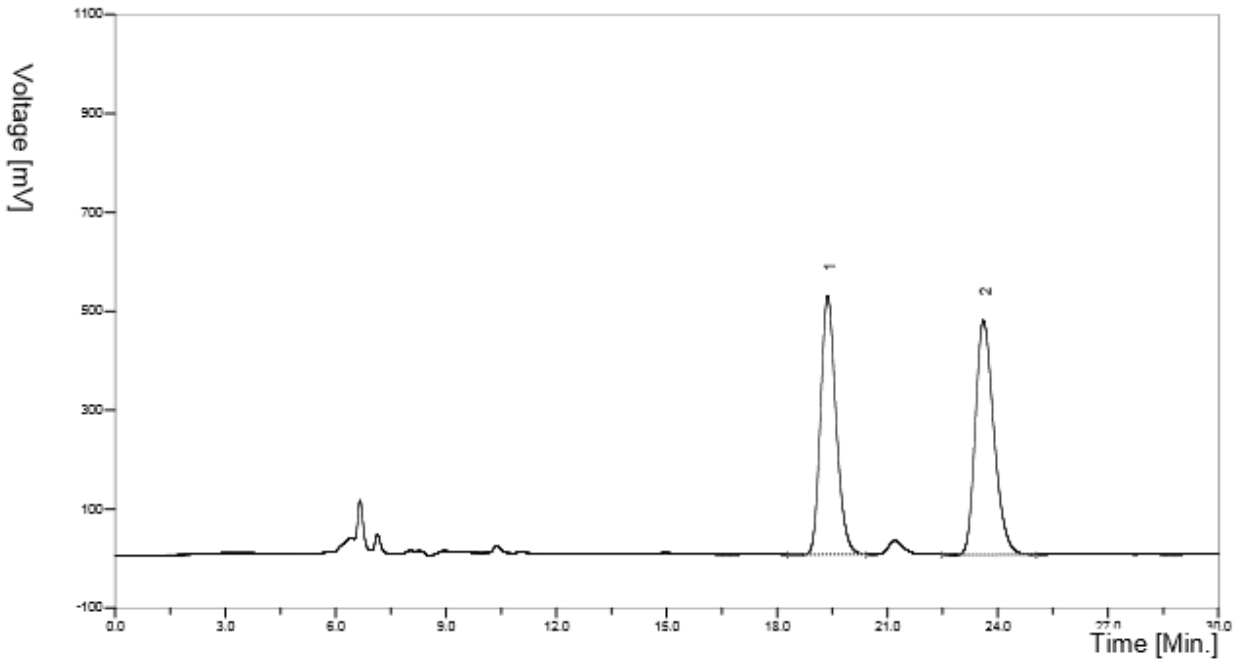
4ba



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	19.72	11096.31	91.9156
2	24.78	975.97	8.0844
Total		12072.27	100

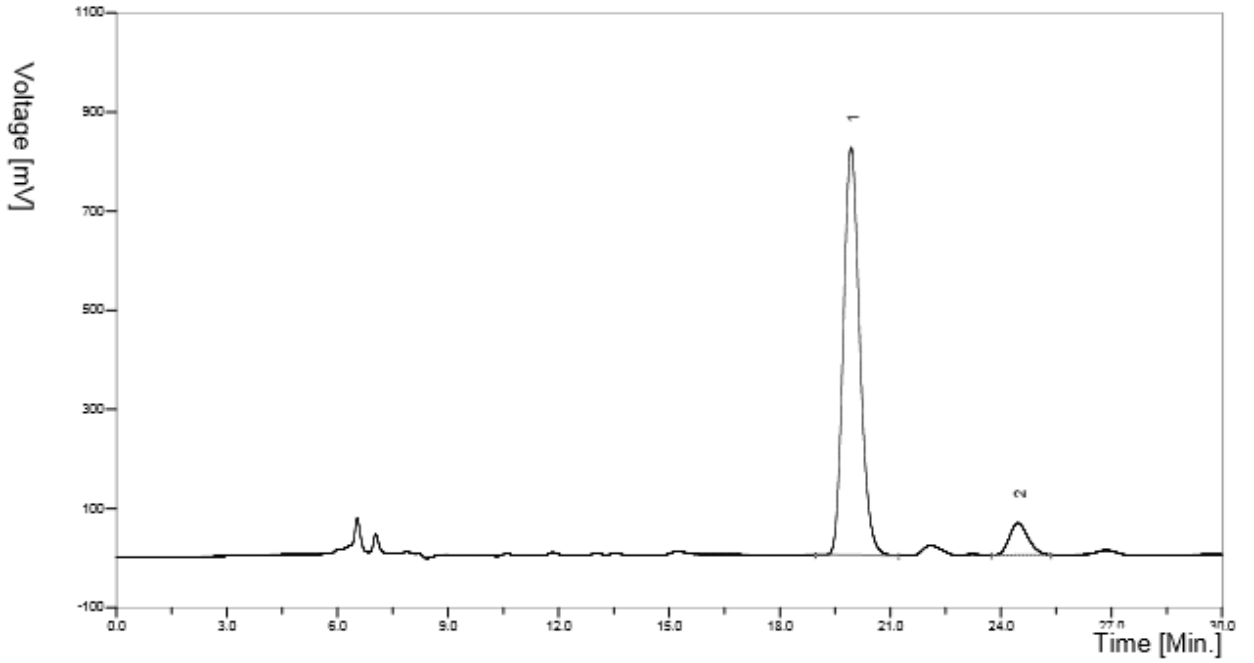
***rac*-4ca**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	19.38	15241.09	48.0323
2	23.61	16489.83	51.9677
Total		31730.91	100

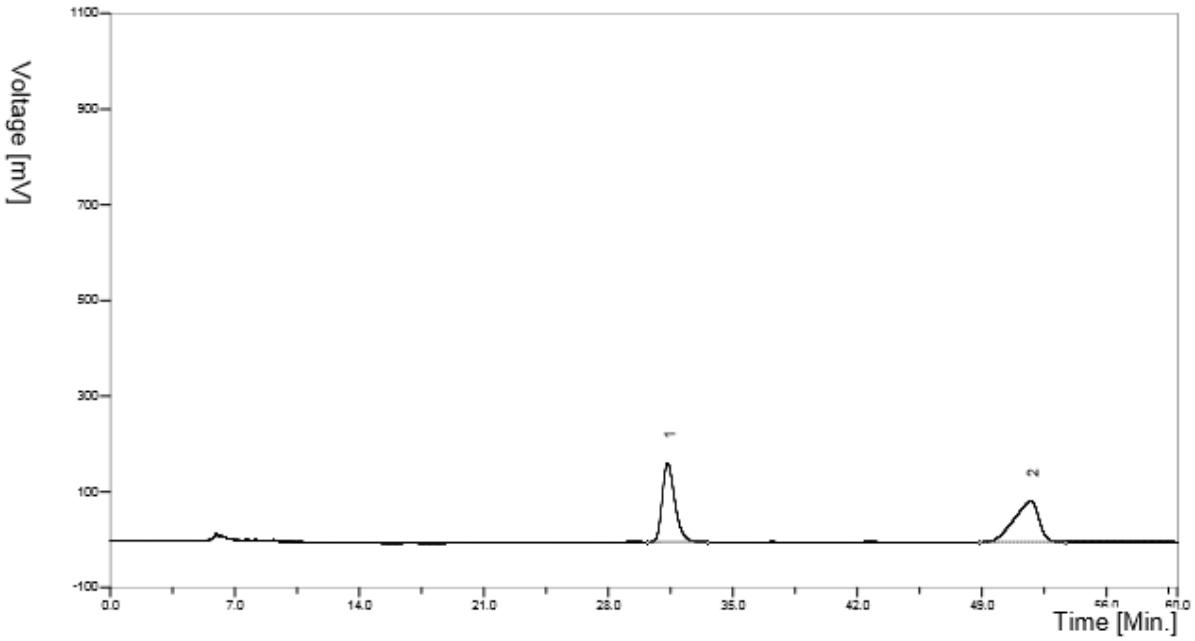
4ca



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	19.94	25406.41	91.6627
2	24.46	2310.88	8.3373
Total		27717.29	100

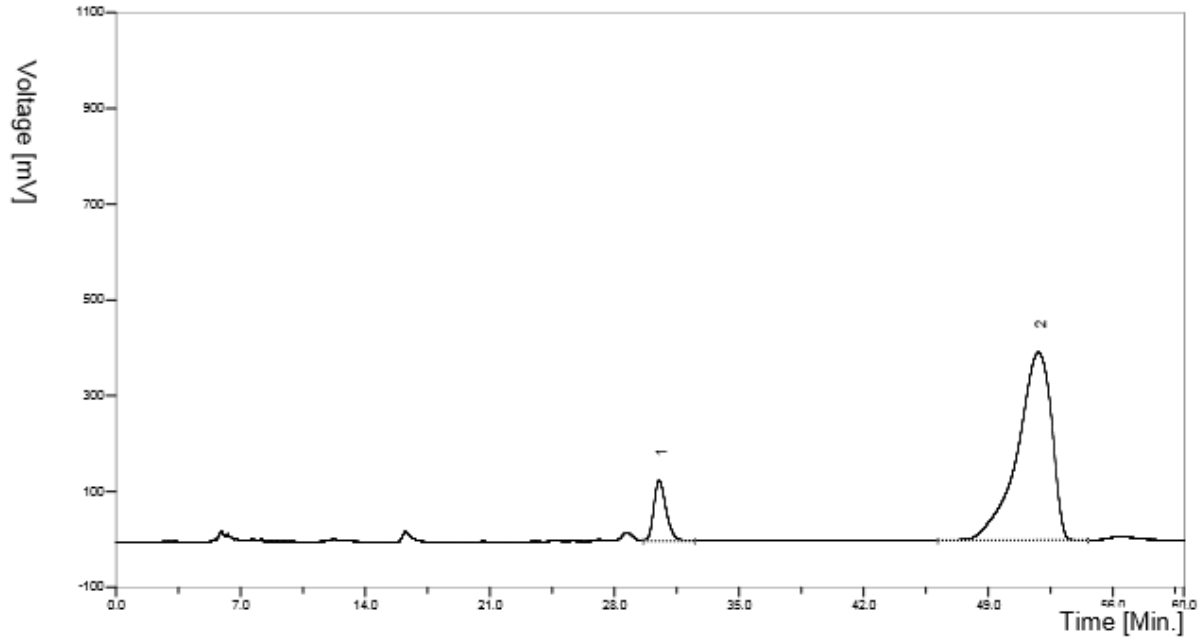
***rac*-4da**



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	31.34	8154.60	49.6678
2	51.74	8263.68	50.3322
Total		16418.27	100

4da



Integration Result

#	Ret. Time(min)	Area(mv.sec)	Area Percentage(%)
1	30.52	6014.52	10.3069
2	51.82	52339.61	89.6931
Total		58354.12	100

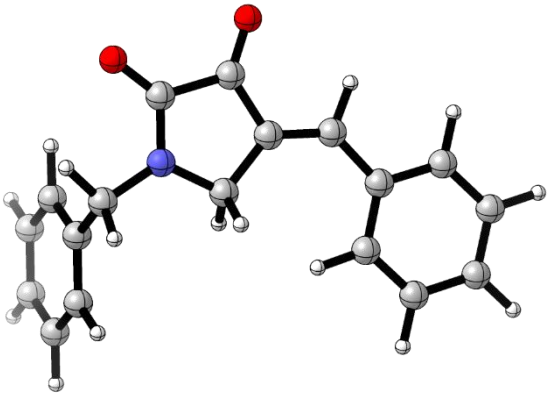
6. Computational Methods

All calculations were performed using the Becke's three parameter functional varied by Lee-Yang-Parr correlation functional (B3LYP)[1-3] with the split-valence 6-31G(d,p)[4-5] basis set of the density functional theory (DFT) implemented within the IEFPCM model (in CH_2Cl_2) in the Gaussian 16 (Revision 1.1).[6] Single point energy calculations for the optimized geometry were performed using M06-2X functional[7] with 6-311G(d,p) basis set for all the atoms using an IEFPCM solvation model (in CH_2Cl_2). Computed structures are illustrated with CYLView.[8] Energy profile are illustrated with mechaSVG.[9]

1. A. D. Becke, *J. Chem. Phys.* **1992**, *96*, 2155.
2. A. D. Becke, *J. Chem. Phys*. **1993**, *98*, 5648.
3. C. Lee, W. Yang, R. G. Parr, *J. Chem. Phys*. **1980**, *72*, 5639.
4. K. Raghavachari, J. S. Binkley, R. Seeger, J. A. Pople, *J. Chem. Phys.* **1980**, *72*, 650.
5. J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev*. **2005**, *105*, 2999.
6. Gaussian 16, Revision 1.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.
7. Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06 Functionals and 12 Other Functionals (Theoretical Chemistry Accounts DOI 10.1007/S00214-007-0310-x). *Theor. Chem. Acc*. **2008**, *120*, 215.
8. CYLview20; C. Y. Legault, Université de Sherbrooke, 2020 (http://www.cylview.org)
9. R. A. Angnes, mechaSVG, GitHub repository, 2020, doi: 10.5281/zenodo.3970267.

7. Cartesian Coordinates of All Reported Structures

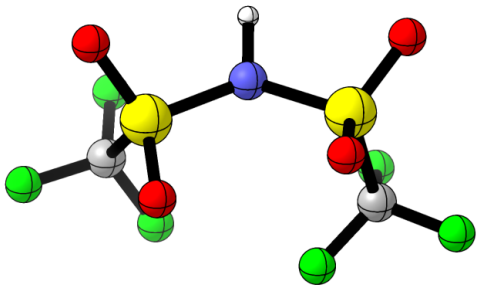
1a



E(B3LYP, 6-31G(d,p), IEFPCM(DCM)) =-900.179814921 Hartree
E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))=-900.009216 Hartree

C	-0.03593	0.27640	-0.69488
C	-1.01648	1.21623	-0.03602
C	-0.32313	2.48854	0.22172
C	1.11763	2.32260	-0.28533
H	0.14949	-0.62603	-0.09794
H	-0.36500	-0.04453	-1.69238
N	1.19248	1.06765	-0.80432
C	2.41398	0.51552	-1.38027
H	2.17591	0.08251	-2.35800
H	3.08003	1.36796	-1.53818
C	3.07490	-0.52448	-0.49295
C	3.62031	-0.14815	0.74345
C	3.15107	-1.86377	-0.88930

$NH(TF)_2$

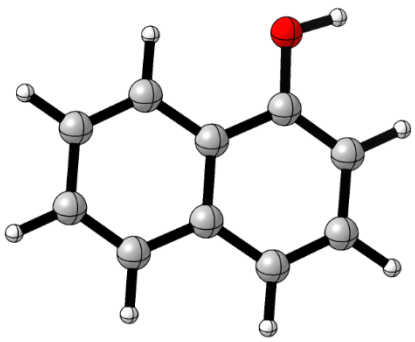


E(B3LYP, 6-31G(d,p) IEFPCM(DCM)) =-1827.70902024 Hartree
E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -1827.664740 Hartree

N	-0.00564	0.76805	-0.71103
H	-0.11903	1.07007	-1.67929
S	1.62351	0.86027	-0.20481
S	-1.42108	0.87208	0.23519
C	1.99983	-0.94976	0.13262
C	-2.20301	-0.79228	-0.16343
F	1.18887	-1.39339	1.08814
F	3.26404	-1.02926	0.53038
F	1.82332	-1.65033	-0.98046
F	-3.39439	-0.82718	0.42178
F	-1.43441	-1.76954	0.30265
F	-2.33532	-0.90347	-1.48177
O	-2.27906	1.88431	-0.36294

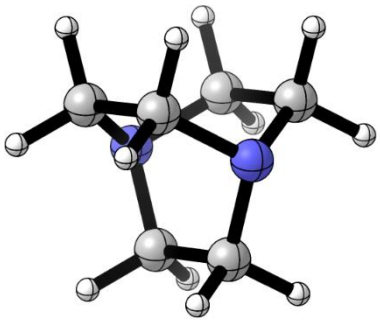
C	4.22898	-1.09550	1.56514
H	3.56960	0.89182	1.05472
C	3.76353	-2.81457	-0.06801
H	2.73390	-2.16459	-1.84705
C	4.30211	-2.43228	1.16081
H	4.65084	-0.79177	2.51871
H	3.81727	-3.85072	-0.38893
H	4.77843	-3.16929	1.80052
O	2.01368	3.15822	-0.22697
O	-0.75458	3.50794	0.73655
C	-2.31568	1.05433	0.30733
H	-2.75988	1.93514	0.77109
C	-3.21660	-0.08003	0.16511
C	-2.85000	-1.32516	-0.39029
C	-4.54432	0.08254	0.61572
C	-3.77759	-2.35753	-0.48825
H	-1.84166	-1.49480	-0.74538
C	-5.47001	-0.95121	0.51589
H	-4.84132	1.03447	1.04644
C	-5.08877	-2.17601	-0.03729
H	-3.47801	-3.30853	-0.91746
H	-6.48590	-0.80358	0.86855
H	-5.80773	-2.98560	-0.11667
O	-1.05070	0.86115	1.63953
O	1.74728	1.56395	1.05890
O	2.34870	1.24644	-1.40689

2a



E(B3LYP, 6-31G(d,p), IEFPCM(DCM))
=-461.131539038 Hartree

DABCO

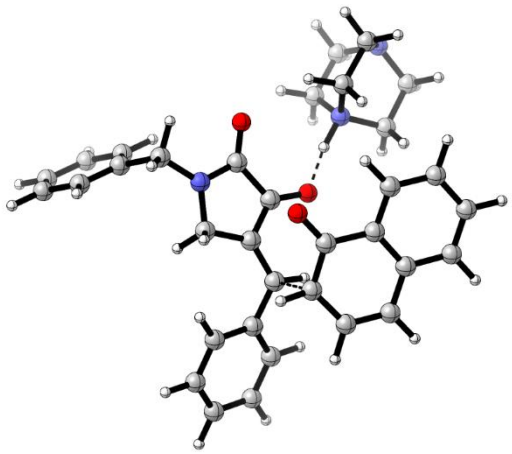


E(B3LYP, 6-31G(d,p), IEFPCM(DCM))
=-345.348596 Hartree

E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -461.040876 Hartree

C	2.74356	0.29337	0.00000
C	1.77836	1.27572	0.00000
C	0.39517	0.94561	0.00000
C	0.02695	-0.43949	0.00000
C	1.04202	-1.43235	0.00000
C	2.37226	-1.07331	0.00000
H	-0.33002	2.98958	0.00001
H	3.79533	0.56403	0.00000
H	2.06160	2.32489	0.00000
C	-0.61893	1.94274	0.00000
C	-1.36311	-0.77276	0.00000
H	0.75151	-2.47687	0.00001
H	3.14183	-1.83943	0.00000
C	-2.32695	0.21604	-0.00001
C	-1.94588	1.57884	0.00000
H	-3.38001	-0.05306	-0.00002
H	-2.72089	2.33952	0.00000
O	-1.66432	-2.10484	-0.00001
H	-2.62538	-2.21644	0.00009

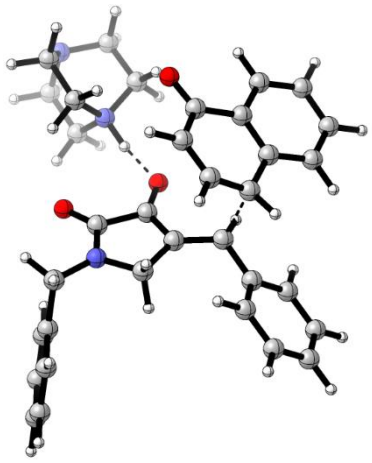
***o*-A-Ts**



E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -345.246921 Hartree

C	-0.78116	-0.98891	-0.97023
C	0.78148	-0.98852	-0.97037
H	-1.18071	-1.97151	-0.69666
H	-1.18106	-0.73467	-1.95789
H	1.18158	-1.97112	-0.69757
H	1.18108	-0.73338	-1.95792
C	-0.78148	-0.34573	1.34133
H	-1.18109	0.38248	2.05546
H	-1.18154	-1.32816	1.61478
C	0.78109	-0.34620	1.34143
H	1.18105	0.38126	2.05614
H	1.18052	-1.32907	1.61424
C	0.78132	1.33474	-0.37073
H	1.18061	2.06243	0.34412
H	1.18156	1.58995	-1.35798
C	-0.78125	1.33458	-0.37145
H	-1.18136	2.06270	0.34252
H	-1.18063	1.58900	-1.35924
N	-1.29177	0.00000	-0.00018
N	1.29177	0.00004	0.00020

***p*-A-Ts**



E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-1706.65099544 Hartree Frequency -300.74 E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -1706.324161 Hartree Thermal correction to Gibbs Free Energy= -6.9 kcal/mol				E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-1706.6480349 Hartree Frequency -325.42 E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -1706.321389 Hartree Thermal correction to Gibbs Free Energy= -5.1 kcal/mol			
C	1.06979	-3.00296	0.35942	C	-1.22337	1.31819	2.61641
C	1.96221	-3.76961	-0.47120	C	-0.15165	2.13867	2.41770
C	3.23516	-3.35773	-0.73072	C	-0.08885	3.05673	1.31802
C	3.77574	-2.18249	-0.09252	C	-1.35632	3.41096	0.68482
C	2.97412	-1.44577	0.82247	C	-2.50163	2.60483	0.90097
C	1.58966	-1.87564	1.12129	C	-2.43352	1.44312	1.81836
C	3.52422	-0.34059	1.49502	C	-3.71383	2.92601	0.26747
C	4.82946	0.06445	1.25482	C	-3.80670	4.02663	-0.57280
C	5.61999	-0.64552	0.33051	C	-2.67380	4.82703	-0.79322
C	5.10204	-1.75046	-0.32634	C	-1.46808	4.52276	-0.17525
H	1.58282	-4.67562	-0.93639	H	0.72939	2.02904	3.04676
H	3.87803	-3.92580	-1.39797	H	0.64269	3.85499	1.38914
H	2.89125	0.17568	2.20998	H	-4.57609	2.29789	0.46608
H	5.24648	0.91689	1.78409	H	-4.74914	4.27254	-1.05312
H	6.64388	-0.33451	0.14179	H	-2.74200	5.69453	-1.44386
H	5.71999	-2.30671	-1.02701	H	-0.59599	5.14848	-0.34587
O	0.87745	-1.26434	1.94818	O	-3.38503	0.63855	1.92228
H	0.23704	-3.51938	0.82611	H	-1.22458	0.55802	3.39197
H	1.23541	2.10612	-0.48028	H	-2.12147	-1.27865	-0.64512
N	1.74012	3.07992	-0.40267	N	-3.00244	-1.91817	-0.56445
C	0.83690	4.13489	-0.97152	C	-2.86750	-3.03149	-1.55915

H	0.63176	3.85484	-2.00719	H	-2.78150	-2.57114	-2.54608
H	-0.09312	4.07920	-0.40560	H	-1.92965	-3.53780	-1.32912
C	2.03507	3.38038	1.03853	C	-3.10746	-2.47739	0.82799
H	1.07826	3.35368	1.55985	H	-2.18851	-3.03673	1.00352
H	2.65715	2.56429	1.41105	H	-3.14520	-1.62125	1.50520
C	3.01882	3.02254	-1.18341	C	-4.21821	-1.09148	-0.86498
H	3.62317	2.21998	-0.75556	H	-4.24752	-0.30249	-0.11095
H	2.76133	2.74920	-2.20872	H	-4.06939	-0.63942	-1.84799
C	1.56876	5.50316	-0.85254	C	-4.12436	-3.93957	-1.42780
H	0.99296	6.19386	-0.23045	H	-3.83898	-4.95049	-1.12346
H	1.68904	5.96370	-1.83709	H	-4.64545	-4.01628	-2.38638
C	2.75116	4.76073	1.09903	C	-4.39067	-3.35583	0.88504
H	3.74446	4.66187	1.54561	H	-5.09817	-2.95750	1.61776
H	2.18010	5.46312	1.71235	H	-4.14442	-4.37902	1.18317
C	3.69993	4.42027	-1.08076	C	-5.45474	-2.03642	-0.81446
H	4.69625	4.32949	-0.63940	H	-6.18681	-1.66780	-0.09055
H	3.81530	4.86547	-2.07280	H	-5.94682	-2.08389	-1.79015
N	2.90133	5.33479	-0.24896	N	-5.06050	-3.40140	-0.42687
C	-2.10192	-1.02404	0.63279	C	2.13838	-0.08556	0.84766
C	-0.89158	-0.97811	-0.26489	C	1.01921	0.59243	0.09568
C	-0.31595	0.29589	-0.18291	C	0.05222	-0.35919	-0.23998
C	-1.18745	1.14121	0.72052	C	0.55814	-1.70950	0.23912
H	-3.02893	-1.29427	0.10967	H	3.11732	0.02636	0.36186
H	-1.96669	-1.72250	1.47023	H	2.24430	0.28239	1.88015
N	-2.19529	0.33924	1.15165	N	1.74156	-1.48956	0.87137
C	-3.23767	0.77286	2.06737	C	2.55826	-2.54346	1.45220
H	-3.30090	0.06280	2.90002	H	2.85476	-2.24870	2.46547
H	-2.90080	1.73316	2.46939	H	1.90410	-3.41675	1.53280
C	-4.59886	0.92318	1.40946	C	3.79027	-2.88043	0.62930
C	-5.69100	0.15846	1.83151	C	5.07583	-2.69514	1.14773
C	-4.77846	1.84489	0.36766	C	3.64931	-3.38871	-0.67045
C	-6.94285	0.31005	1.22848	C	6.20405	-3.01214	0.38592
H	-5.56283	-0.55900	2.63833	H	5.19647	-2.30240	2.15443
C	-6.02490	1.99598	-0.23757	C	4.77281	-3.70288	-1.43321
H	-3.93470	2.44543	0.03829	H	2.65278	-3.53909	-1.07694
C	-7.11189	1.22811	0.19204	C	6.05462	-3.51523	-0.90643
H	-7.78172	-0.29119	1.56704	H	7.19619	-2.86265	0.80202
H	-6.15139	2.71481	-1.04210	H	4.65040	-4.09754	-2.43777

H	-8.08316	1.34672	-0.27923	H	6.92956	-3.76098	-1.50105
O	-1.03038	2.33613	1.00556	O	0.00765	-2.80742	0.08742
O	0.72328	0.73883	-0.76558	O	-1.04896	-0.23647	-0.86819
C	-0.27604	-2.02402	-0.98852	C	0.90489	1.98242	-0.20519
H	0.51375	-1.65685	-1.63903	H	0.11098	2.16025	-0.92556
C	-1.00237	-3.18964	-1.55061	C	2.09098	2.84952	-0.43742
C	-2.01522	-3.88205	-0.86138	C	3.19648	2.90238	0.43191
C	-0.66744	-3.63086	-2.84374	C	2.11250	3.67063	-1.57941
C	-2.67636	-4.95862	-1.45107	C	4.28514	3.72874	0.15793
H	-2.27805	-3.59527	0.15096	H	3.19838	2.31392	1.34337
C	-1.32994	-4.70572	-3.43539	C	3.20283	4.49567	-1.85564
H	0.11765	-3.11541	-3.39003	H	1.26720	3.64946	-2.26158
C	-2.34085	-5.37388	-2.74202	C	4.29647	4.52681	-0.98889
H	-3.45392	-5.47753	-0.89788	H	5.12576	3.75316	0.84547
H	-1.05576	-5.02084	-4.43812	H	3.19672	5.11380	-2.74880
H	-2.85815	-6.21202	-3.19928	H	5.14604	5.16914	-1.20034

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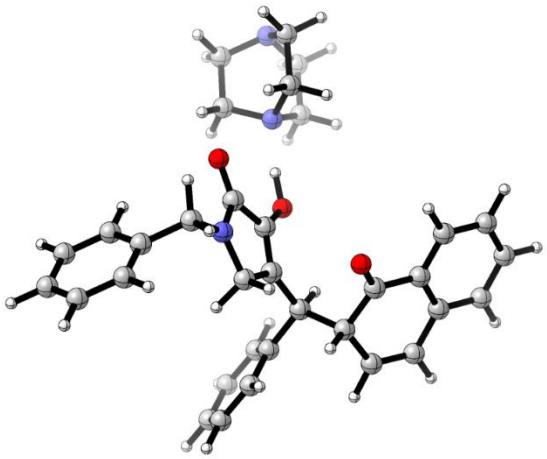

E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-1706.67037356 Hartree
E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -1706.350299 Hartree
Thermal correction to Gibbs Free Energy= -23.3 kcal/mol

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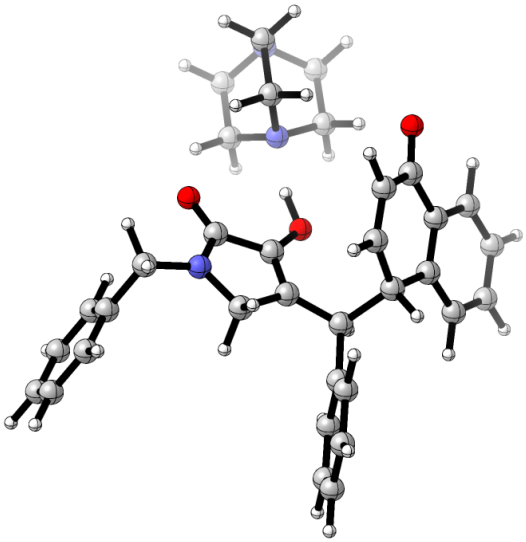

E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-1706.66451837 Hartree
E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -1706.348063 Hartree

Thermal correction to Gibbs Free Energy= -21.9 kcal/mol

C	0.86105	-3.05387	0.46501	C	-1.77189	1.35426	2.52757
C	1.61288	-4.10445	-0.30379	C	-0.57181	1.86041	2.20633
C	2.95264	-4.18112	-0.30999	C	-0.30737	2.68587	0.98274
C	3.78666	-3.27697	0.47747	C	-1.57016	3.09520	0.25010
C	3.18107	-2.35464	1.36400	C	-2.82407	2.54536	0.57335
C	1.70467	-2.32076	1.50568	C	-2.95536	1.56152	1.68048
C	3.97334	-1.50274	2.14458	C	-3.97273	2.93908	-0.13003
C	5.36036	-1.54151	2.04379	C	-3.88850	3.87906	-1.14916
C	5.96541	-2.45250	1.16875	C	-2.64482	4.43492	-1.47144
C	5.18776	-3.31413	0.39868	C	-1.50100	4.04551	-0.77823
H	1.02491	-4.78748	-0.90881	H	0.28201	1.65686	2.84891
H	3.45732	-4.93241	-0.91197	H	0.18028	3.61090	1.31729
H	3.47656	-0.81610	2.82186	H	-4.92198	2.49557	0.15121
H	5.97079	-0.87248	2.64220	H	-4.78013	4.18501	-1.68780
H	7.04803	-2.49163	1.09155	H	-2.56870	5.17691	-2.26091
H	5.66362	-4.02470	-0.27144	H	-0.54134	4.48640	-1.03518
O	1.16048	-1.70534	2.41851	O	-4.01276	0.96230	1.90213
H	0.03317	-3.51541	1.01636	H	-1.91517	0.73795	3.41018
H	0.97139	1.96869	-0.63996	H	-1.85653	-1.09839	-0.46327
N	1.49464	3.52128	-0.74102	N	-3.11963	-2.10740	-0.42740
C	0.44939	4.35968	-1.38002	C	-2.89512	-3.26800	-1.32464
H	0.24345	3.93686	-2.36895	H	-2.74630	-2.87991	-2.33779
H	-0.45562	4.26068	-0.77732	H	-1.96578	-3.74561	-1.00832
C	1.78390	4.05345	0.61444	C	-3.31220	-2.59299	0.96386
H	0.86814	3.95670	1.20102	H	-2.38460	-3.08496	1.26590
H	2.54416	3.40944	1.06856	H	-3.46066	-1.71523	1.60008
C	2.73042	3.58336	-1.55813	C	-4.34605	-1.38853	-0.85619
H	3.47913	2.93917	-1.08639	H	-4.47982	-0.53214	-0.18945
H	2.50448	3.16372	-2.54357	H	-4.17595	-1.00770	-1.86842
C	0.95135	5.83377	-1.47718	C	-4.12249	-4.22808	-1.25091
H	0.29033	6.51247	-0.92787	H	-3.82563	-5.22079	-0.89584
H	0.98208	6.17465	-2.51763	H	-4.58557	-4.35579	-2.23536

C	2.27356	5.53048	0.50034	C	-4.53985	-3.55460	1.01230
H	3.27904	5.64849	0.91838	H	-5.30935	-3.17811	1.69462
H	1.60892	6.20933	1.04509	H	-4.24810	-4.55084	1.36170
C	3.21655	5.06459	-1.65560	C	-5.56404	-2.36453	-0.80123
H	4.22377	5.17681	-1.24057	H	-6.33744	-1.98886	-0.12298
H	3.24997	5.40055	-2.69741	H	-6.02118	-2.48275	-1.78957
N	2.30861	5.95658	-0.91178	N	-5.14197	-3.69579	-0.32736
C	-1.68548	-0.97384	1.02430	C	2.14591	-0.16194	0.82343
C	-0.48711	-0.85870	0.11759	C	0.90984	0.49112	0.25488
C	-0.15498	0.44640	-0.01031	C	-0.01402	-0.46434	0.00274
C	-1.11096	1.28284	0.78213	C	0.53479	-1.80214	0.38804
H	-2.55389	-1.42685	0.52740	H	3.02853	-0.01790	0.18529
H	-1.45914	-1.56267	1.92273	H	2.41042	0.21617	1.82192
N	-1.96950	0.40905	1.38397	N	1.78360	-1.56878	0.89340
C	-3.06416	0.81652	2.24792	C	2.69231	-2.62390	1.31410
H	-3.02981	0.22856	3.17226	H	3.15550	-2.33624	2.26456
H	-2.86475	1.86066	2.50756	H	2.06508	-3.50119	1.49765
C	-4.43396	0.68666	1.60289	C	3.76694	-2.95069	0.29045
C	-5.40550	-0.16269	2.14185	C	5.11829	-2.71677	0.56447
C	-4.74391	1.42865	0.45367	C	3.41080	-3.49642	-0.95195
C	-6.66649	-0.27086	1.54852	C	6.10080	-3.02213	-0.38168
H	-5.17576	-0.74208	3.03286	H	5.40539	-2.29586	1.52503
C	-5.99958	1.32067	-0.14168	C	4.38859	-3.79964	-1.89793
H	-3.99482	2.09416	0.03308	H	2.36269	-3.68500	-1.16804
C	-6.96544	0.46966	0.40487	C	5.73758	-3.56302	-1.61503
H	-7.41079	-0.93480	1.97876	H	7.14638	-2.83523	-0.15438
H	-6.22794	1.90248	-1.03011	H	4.10044	-4.22476	-2.85510
H	-7.94400	0.38675	-0.05894	H	6.49891	-3.80109	-2.35209
O	-1.13731	2.51439	0.88129	O	-0.00951	-2.90536	0.27884
O	0.84726	0.95362	-0.72952	O	-1.22467	-0.28270	-0.52079
C	0.22204	-2.00456	-0.54997	C	0.74415	1.97399	-0.00571
H	1.06067	-1.56534	-1.09914	H	0.29354	2.05653	-0.99955
C	-0.67779	-2.69634	-1.57644	C	2.08205	2.70328	-0.06576
C	-1.71160	-3.56795	-1.20231	C	2.75854	3.12877	1.08756
C	-0.49627	-2.42939	-2.94027	C	2.68292	2.93964	-1.31036
C	-2.53899	-4.15196	-2.16325	C	3.99443	3.77189	0.99891
H	-1.87561	-3.80415	-0.15451	H	2.32053	2.96490	2.06852
C	-1.32248	-3.01039	-3.90358	C	3.91854	3.58258	-1.40349

H	0.29864	-1.75542	-3.24827	H	2.17519	2.61736	-2.21583
C	-2.34840	-3.87487	-3.51827	C	4.57939	4.00160	-0.24767
H	-3.33246	-4.82483	-1.85102	H	4.49840	4.09469	1.90530
H	-1.16172	-2.78868	-4.95474	H	4.36121	3.75905	-2.37950
H	-2.99161	-4.32994	-4.26555	H	5.53910	4.50482	-0.31718

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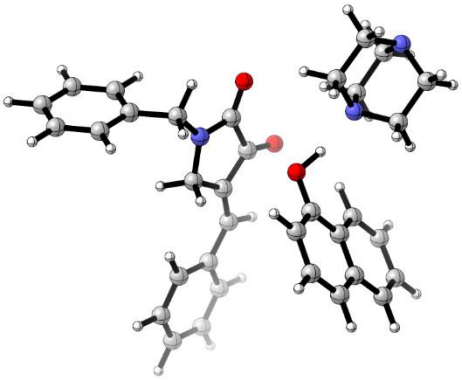

E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-1706.6713599 Hartree
E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -1706.348589 Hartree
Thermal correction to Gibbs Free Energy= -22.2 kcal/mol

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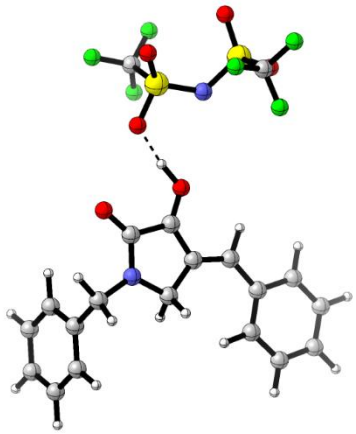


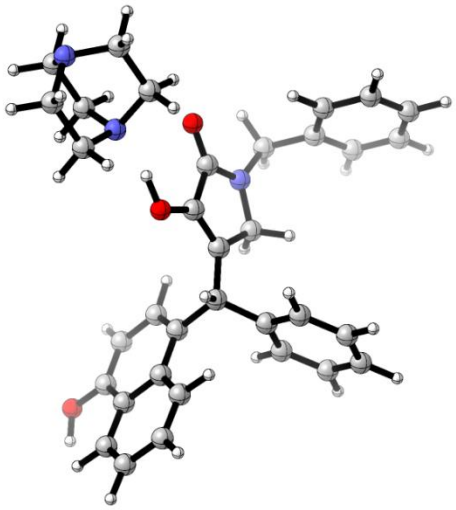
E(B3LYP, 6-31G(d,p), IEFPCM(DCM)) = -3188.967078 Hartree
E(M062X, 6-311G(d,p), IEFPCM(DCM), (SP))= -3188.739101 Hartree
Thermal correction to Gibbs Free Energy= -15.2 kcal/mol

C	1.55738	-3.20406	1.79250	C	2.51401	-0.99411	-1.22202
C	1.98789	-4.54702	1.87961	C	1.25740	-0.28144	-0.76561
C	2.82833	-5.08199	0.92873	C	1.42858	1.13486	-1.03864
C	3.24818	-4.29329	-0.17631	C	2.82036	1.32429	-1.63923
C	2.79389	-2.93686	-0.29234	H	3.01212	-1.53652	-0.40668
C	1.95860	-2.39643	0.74221	H	2.32543	-1.71441	-2.03166
C	3.16407	-2.18197	-1.43776	N	3.36880	0.08085	-1.72464
C	3.98288	-2.72295	-2.40595	C	4.72601	-0.15521	-2.20609

C	4.46558	-4.04751	-2.27469	H	4.70230	-0.98278	-2.92577
C	4.09944	-4.81315	-1.19030	H	5.01216	0.75472	-2.74179
H	1.66137	-5.15323	2.72011	C	5.70917	-0.45476	-1.08882
H	3.17297	-6.10941	1.00485	C	6.04890	0.54961	-0.17050
H	2.76614	-1.18061	-1.55883	C	6.28266	-1.72285	-0.95352
H	4.25032	-2.13635	-3.28004	C	6.94512	0.28445	0.86318
H	5.11485	-4.46268	-3.04019	H	5.61172	1.53970	-0.27590
H	4.45286	-5.83686	-1.09632	C	7.18323	-1.98912	0.08113
O	1.51851	-1.11101	0.69319	H	6.03115	-2.50598	-1.66607
H	0.92163	-2.77450	2.56043	C	7.51433	-0.98608	0.99163
H	2.27512	-0.44231	0.54342	H	7.20557	1.07110	1.56611
N	3.37502	0.81473	0.62932	H	7.62436	-2.97803	0.17298
C	3.39272	1.68535	-0.57546	H	8.21554	-1.18992	1.79629
H	3.76331	1.08625	-1.41293	O	3.32377	2.39081	-1.96455
H	2.36150	1.96881	-0.79781	O	0.65943	2.07162	-0.81962
C	2.87668	1.60689	1.78513	C	0.15118	-0.76619	-0.13301
H	1.85791	1.92398	1.54802	H	-0.57503	-0.01140	0.15521
H	2.83123	0.93938	2.65164	C	-0.04672	-2.09655	0.43742
C	4.75683	0.35752	0.91736	C	0.60701	-3.25773	-0.02405
H	4.72065	-0.28537	1.80266	C	-0.90913	-2.21423	1.54694
H	5.09091	-0.25610	0.07536	C	0.41300	-4.48203	0.60859
C	4.30679	2.92238	-0.30948	H	1.24370	-3.21317	-0.90017
H	3.73523	3.85415	-0.37429	C	-1.08615	-3.43639	2.18987
H	5.11701	2.98106	-1.04424	H	-1.43341	-1.33351	1.90448
C	3.82532	2.81954	2.03676	C	-0.42640	-4.57487	1.72248
H	4.28119	2.76688	3.03133	H	0.91706	-5.36766	0.23202
H	3.27781	3.76585	1.97452	H	-1.74444	-3.50157	3.05146
C	5.68192	1.59565	1.13996	H	-0.56963	-5.53099	2.21801
H	6.15195	1.56326	2.12868	C	-4.73772	-0.80908	0.77444
H	6.48385	1.62695	0.39478	C	-3.76196	-1.35246	-0.03362
N	4.90775	2.84550	1.03557	C	-3.03431	-0.54483	-0.94930
C	-1.82190	-1.12226	-0.24325	C	-3.35079	0.85018	-1.02061
C	-0.98421	-1.13619	-1.49765	C	-4.34946	1.38698	-0.16794
C	-0.18840	0.10127	-1.52082	C	-5.03043	0.57376	0.71197
C	-0.59330	0.91480	-0.28443	H	-1.79508	-2.13757	-1.74610
H	-2.89502	-1.22377	-0.44559	H	-5.28993	-1.44553	1.46132
H	-1.52989	-1.91867	0.45504	H	-3.54089	-2.41569	0.01189
N	-1.54330	0.18558	0.35566	C	-2.00907	-1.07449	-1.78345

C	-2.13704	0.58807	1.62275	C	-2.65018	1.66778	-1.96425
H	-1.88421	-0.15541	2.38858	H	-4.56825	2.44725	-0.22975
H	-1.64682	1.52779	1.89304	H	-5.79809	0.99242	1.35694
C	-3.64300	0.76446	1.54861	C	-1.72795	1.10256	-2.83177
C	-4.49134	0.01559	2.37066	C	-1.42518	-0.26935	-2.74060
C	-4.20428	1.69342	0.66062	H	-1.21764	1.72872	-3.55693
C	-5.87645	0.19225	2.31396	H	-0.68735	-0.68740	-3.42128
H	-4.06640	-0.70815	3.06171	O	-2.95304	2.98565	-1.96123
C	-5.58589	1.86829	0.59903	H	-2.30775	3.47998	-2.50250
H	-3.55333	2.28140	0.01904	N	0.97389	4.73123	-1.59903
C	-6.42631	1.11792	1.42703	H	0.99886	3.71084	-1.35288
H	-6.52245	-0.39553	2.95954	S	2.02380	5.78359	-0.71164
H	-6.00795	2.59247	-0.09163	S	0.41510	5.09997	-3.12675
H	-7.50244	1.25584	1.37968	O	0.49798	6.53415	-3.33166
O	-0.15176	2.01336	0.04329	O	-0.82160	4.34331	-3.33495
O	0.63171	0.47165	-2.34608	O	3.36956	5.80066	-1.26483
C	-0.89519	-2.03686	-2.50224	O	1.30404	7.00736	-0.40204
H	-0.19635	-1.75182	-3.28839	C	1.64281	4.29062	-4.30067
C	-1.57646	-3.30590	-2.71959	C	2.07795	4.76026	0.87385
C	-2.45491	-3.90751	-1.79320	F	2.87596	4.66904	-4.00756
C	-1.33845	-3.97396	-3.93943	F	1.52993	2.96341	-4.20703
C	-3.07061	-5.12085	-2.08482	F	1.32826	4.67375	-5.53848
H	-2.65244	-3.43820	-0.83790	F	2.78760	3.64927	0.69316
C	-1.95713	-5.18581	-4.22983	F	2.66960	5.52587	1.78845
H	-0.66027	-3.52666	-4.66059	F	0.84760	4.45093	1.26901
C	-2.82741	-5.76336	-3.30243	C	2.51401	-0.99411	-1.22202
H	-3.74134	-5.56979	-1.35872	C	1.25740	-0.28144	-0.76561
H	-1.76018	-5.68050	-5.17586	C	1.42858	1.13486	-1.03864
H	-3.31091	-6.70988	-3.52411	C	2.82036	1.32429	-1.63923

5a-DABCO

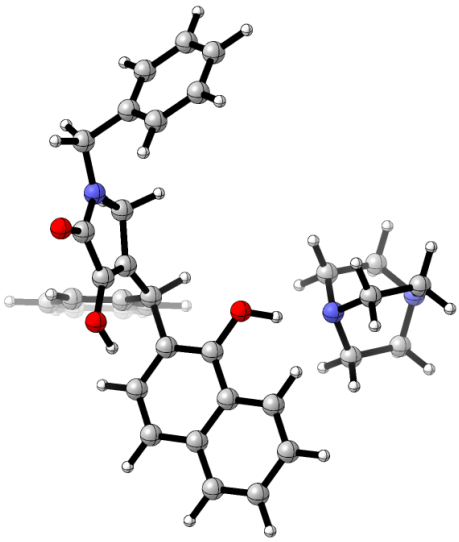


E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-1706.679493 Hartree
E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -1706.363018 Hartree

Thermal correction to Gibbs Free Energy= -22.2 kcal/mol

C	-3.31816	-1.36402	2.62735	C	-1.09931	-2.01906	0.24779
C	-2.43158	-0.66583	1.78139	C	-1.43481	-3.05527	-0.66622
C	-2.64878	-0.53185	0.42513	C	-2.65162	-3.09036	-1.30969
C	-3.80442	-1.16987	-0.14145	C	-3.63572	-2.10464	-1.03573
C	-4.69851	-1.91634	0.70264	C	-3.33672	-1.06658	-0.09492
C	-4.43868	-1.96936	2.10841	C	-2.03777	-1.02155	0.51441
C	-5.80309	-2.59103	0.11863	C	-4.34587	-0.11935	0.22539
C	-6.05350	-2.52106	-1.23286	C	-5.58133	-0.16979	-0.38298
C	-5.19642	-1.76812	-2.06363	C	-5.86601	-1.17377	-1.34022
C	-4.10553	-1.11727	-1.53156	C	-4.91654	-2.12066	-1.65267
H	-1.54177	-0.22989	2.22195	H	-0.70245	-3.83199	-0.86227
H	-6.45498	-3.20647	0.73459	H	-2.87675	-3.88304	-2.01716
H	-6.90096	-3.04925	-1.65913	H	-4.13586	0.63199	0.97800

o-A-IM-3-DABCO



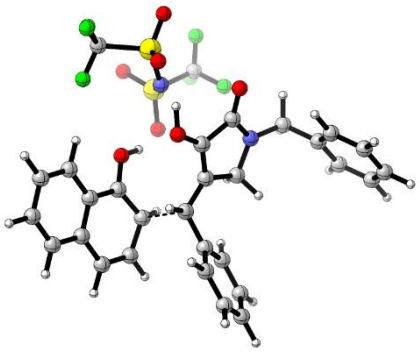
E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-1706.67912764 Hartree
E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -1706.362509 Hartree

Thermal correction to Gibbs Free Energy= -31.3 kcal/mol

H	-5.39469	-1.70679	-3.12958	H	-6.34535	0.55641	-0.12160
H	-3.46563	-0.54275	-2.18983	H	-6.84084	-1.20117	-1.81804
O	-5.26398	-2.63216	2.97601	H	-5.13608	-2.90335	-2.37399
H	-3.13262	-1.42906	3.69410	O	-1.72233	-0.02899	1.38266
C	-0.00956	1.79203	0.95163	H	-0.42416	-1.14490	-1.74376
C	-0.33914	0.54024	0.17406	H	-1.85904	0.89953	0.97428
C	0.76061	-0.24464	0.11978	C	2.57092	-0.68744	0.85129
C	1.88177	0.41664	0.85857	C	1.27364	-1.10525	0.19263
H	-0.09188	2.69703	0.33456	C	1.24214	-0.56077	-1.04130
H	-0.66176	1.94018	1.82554	C	2.47756	0.24481	-1.29276
N	1.36770	1.57711	1.37027	H	2.38748	-0.09737	1.76076
C	2.17140	2.55961	2.07932	H	3.18660	-1.55026	1.13934
H	1.60527	2.92223	2.94535	N	3.23931	0.11008	-0.16332
H	3.04479	2.01510	2.45043	C	4.52671	0.76146	0.02357
C	2.61105	3.73179	1.21853	H	5.22568	0.04041	0.46160
C	2.12067	5.02086	1.44736	H	4.88400	1.01260	-0.97911
C	3.52147	3.52757	0.17125	C	4.45943	2.01162	0.88405
C	2.52898	6.09137	0.64778	C	3.87382	3.18104	0.37625
H	1.41656	5.19045	2.25871	C	4.96875	2.02022	2.18677
C	3.92856	4.59359	-0.62823	C	3.79991	4.33303	1.15848
H	3.90746	2.52731	-0.00549	H	3.48404	3.17978	-0.63824
C	3.43309	5.87921	-0.39208	C	4.89490	3.17343	2.97318
H	2.13940	7.08743	0.83769	H	5.43127	1.12148	2.58762
H	4.63681	4.42416	-1.43438	C	4.30977	4.33147	2.46073
H	3.75262	6.70958	-1.01508	H	3.35206	5.23489	0.75109
O	3.04320	0.02049	0.98751	H	5.29586	3.16559	3.98261
O	0.87650	-1.41874	-0.49786	H	4.25471	5.22982	3.06857
C	-1.67379	0.24385	-0.47271	O	2.75812	0.89513	-2.29730
H	-1.43634	-0.41557	-1.31747	O	0.32283	-0.59473	-2.03395
C	-2.27252	1.53045	-1.05884	C	0.26979	-1.95885	0.93676
C	-3.21729	2.29566	-0.36499	H	0.09379	-1.44788	1.89084
C	-1.82501	1.99184	-2.30520	C	0.81346	-3.34912	1.28230
C	-3.70278	3.48958	-0.90275	C	1.69921	-4.03634	0.44214
H	-3.58355	1.94734	0.59601	C	0.39699	-3.97220	2.46721
C	-2.31050	3.18177	-2.84637	C	2.15419	-5.31475	0.77525
H	-1.08554	1.41145	-2.85203	H	2.04027	-3.56486	-0.47550
C	-3.25282	3.93685	-2.14496	C	0.84905	-5.24825	2.80293
H	-4.43825	4.06761	-0.35008	H	-0.28919	-3.45107	3.13022

H	-1.95398	3.51866	-3.81577	C	1.73061	-5.92518	1.95639
H	-3.63412	4.86308	-2.56487	H	2.84149	-5.83079	0.11094
H	1.79798	-1.84459	-0.41645	H	0.51673	-5.71212	3.72724
H	-6.11819	-2.78698	2.55468	H	2.08636	-6.91744	2.21759

_o_-B-Ts



E(B3LYP, 6-31G(d,p), IEFPCM(DCM)) =-3189.014643 Hartree

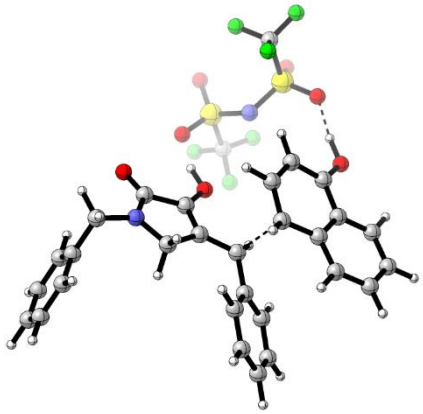
Frequency -329.86

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3188.737606 Hartree

Thermal correction to Gibbs Free

Energy= -14.2 kcal/mol

_p_-B-Ts



E(B3LYP, 6-31G(d,p), IEFPCM(DCM)) =-3189.020982 Hartree

Frequency -325.16

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3188.735544 Hartree

Thermal correction to Gibbs

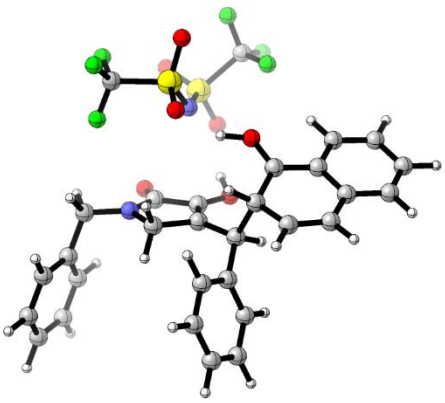
Free Energy= -12.9 kcal/mol

C	2.27309	-0.43568	0.48530	C	-3.45650	-0.54992	-1.15485
C	1.42394	0.59952	-0.22870	C	-2.25072	0.04536	-0.45599
C	0.60930	-0.06477	-1.11321	C	-1.33743	-0.95917	-0.25762
C	0.96240	-1.52912	-1.13080	C	-1.87945	-2.26211	-0.76749
H	3.34794	-0.25122	0.36524	H	-4.37619	-0.44793	-0.56344
H	2.05459	-0.47563	1.56335	H	-3.64776	-0.09513	-2.13877
N	1.89604	-1.68785	-0.14680	N	-3.09677	-1.95100	-1.31800
C	2.56663	-2.95505	0.11343	C	-4.00066	-2.95965	-1.85660

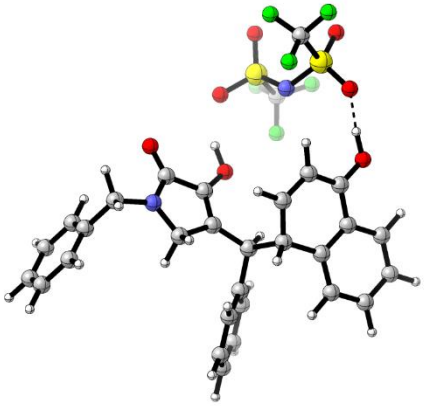
H	2.58554	-3.12663	1.19492	H	-4.39343	-2.60620	-2.81719
H	1.92999	-3.72141	-0.33625	H	-3.37775	-3.83806	-2.04824
C	3.97035	-3.01934	-0.46050	C	-5.14226	-3.30920	-0.91870
C	4.15734	-3.03384	-1.85065	C	-4.87880	-3.99045	0.27868
C	5.09059	-3.06288	0.37519	C	-6.46046	-2.95714	-1.22448
C	5.44148	-3.08822	-2.38862	C	-5.91762	-4.30880	1.15098
H	3.28858	-3.00955	-2.50308	H	-3.85690	-4.27393	0.51620
C	6.37874	-3.11991	-0.16290	C	-7.50320	-3.27803	-0.35177
H	4.95505	-3.06107	1.45436	H	-6.67540	-2.43641	-2.15495
C	6.55593	-3.13105	-1.54579	C	-7.23265	-3.95286	0.83794
H	5.57425	-3.10439	-3.46652	H	-5.70313	-4.84087	2.07313
H	7.23986	-3.15711	0.49819	H	-8.52319	-3.00200	-0.60310
H	7.55597	-3.17735	-1.96698	H	-8.04138	-4.20513	1.51745
O	0.53977	-2.36879	-1.90964	O	-1.34635	-3.35830	-0.69494
O	-0.27374	0.44604	-1.93814	O	-0.16628	-0.82190	0.30739
C	1.53794	2.03215	-0.10483	C	-2.05114	1.38646	0.02755
H	1.03455	2.55032	-0.91785	H	-1.24000	1.43474	0.75019
C	2.87107	2.63414	0.19841	C	-3.20044	2.25314	0.37331
C	3.64332	2.27196	1.31538	C	-4.31456	2.42850	-0.46860
C	3.38251	3.59761	-0.68472	C	-3.18826	2.92056	1.61051
C	4.89408	2.84656	1.53094	C	-5.38536	3.22696	-0.07520
H	3.25846	1.55652	2.03538	H	-4.33763	1.95779	-1.44600
C	4.63954	4.16366	-0.47525	C	-4.26758	3.70679	2.01067
H	2.79465	3.89426	-1.54848	H	-2.33097	2.80660	2.26718
C	5.39928	3.79039	0.63337	C	-5.36931	3.86282	1.16955
H	5.47490	2.55775	2.40162	H	-6.23502	3.35283	-0.73940
H	5.02187	4.89862	-1.17700	H	-4.24358	4.20104	2.97692
H	6.37594	4.23373	0.80116	H	-6.20855	4.47917	1.47685
C	-2.73233	5.84654	-1.18590	C	-1.11548	5.97425	0.15771
C	-1.59365	6.04809	-0.42017	C	-1.49725	4.83425	-0.53248
C	-0.97005	4.96976	0.23537	C	-0.60390	3.75691	-0.69625
C	-1.54084	3.67138	0.09582	C	0.70745	3.88077	-0.15436
C	-2.70758	3.48387	-0.67790	C	1.07440	5.04293	0.55996
C	-3.29169	4.56260	-1.31775	C	0.17123	6.07780	0.71620
H	0.57262	6.15818	1.21625	H	-1.82926	2.59267	-2.05955
H	-3.19931	6.68985	-1.68602	H	-1.81743	6.79574	0.26561
H	-1.17223	7.04381	-0.31724	H	-2.49338	4.76569	-0.95679
C	0.20134	5.14984	1.06025	C	-0.98649	2.52921	-1.37694

C	-0.92662	2.57021	0.79367	C	1.67454	2.83736	-0.40640
H	-3.12541	2.48811	-0.76629	H	2.07764	5.10963	0.96447
H	-4.18135	4.41801	-1.92171	H	0.45760	6.97327	1.25836
C	0.37353	2.72431	1.38724	C	1.34395	1.74471	-1.24196
C	0.81762	4.09099	1.63599	C	0.06471	1.62491	-1.72491
H	0.63969	1.97574	2.12974	H	2.09470	0.99407	-1.45363
H	1.70175	4.23353	2.24632	H	-0.17836	0.76578	-2.34204
O	-1.56781	1.44315	0.78864	O	2.85233	2.96615	0.14969
H	-1.21465	0.68098	1.35299	H	3.48991	2.21862	-0.09119
N	-1.92188	-1.40255	0.00089	N	3.27652	-0.80527	0.09560
H	-0.90124	-0.26302	-2.25441	H	0.40278	-1.65061	0.34414
S	-2.93246	-1.84888	-1.19045	S	3.04800	-2.21017	0.88575
S	-2.09003	-1.64563	1.57135	S	4.74500	-0.24735	-0.28271
O	-3.45153	-1.71010	2.10372	O	5.86867	-0.62892	0.56623
O	-1.12674	-0.68293	2.19837	O	4.56273	1.19834	-0.60133
O	-2.37456	-1.21300	-2.40396	O	1.66440	-2.64884	0.58430
O	-3.31435	-3.25783	-1.21638	O	4.11699	-3.19978	0.80440
C	-1.32872	-3.31111	1.96452	C	5.08179	-0.96505	-1.97946
C	-4.54024	-0.90264	-0.91247	C	2.95807	-1.67418	2.67794
F	-1.34730	-3.49573	3.28769	F	5.09637	-2.29471	-1.92355
F	-2.02440	-4.27393	1.36952	F	4.12282	-0.57253	-2.83018
F	-0.05862	-3.35621	1.54147	F	6.26117	-0.52383	-2.42080
F	-4.28486	0.31662	-0.40923	F	1.90447	-0.86587	2.85438
F	-5.15219	-0.75968	-2.09170	F	2.81326	-2.75154	3.45223
F	-5.34035	-1.55763	-0.07997	F	4.06868	-1.02420	3.02616

***o*-B-IM2**



***p*-B-IM2**



E(B3LYP, 6-31G(d,p), IEFPCM(DCM)) =-3189.0222232 Hartree

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3188.750177 Hartree

Thermal correction to Gibbs Free Energy= -22.1 kcal/mol

C	2.26249	-0.39396	0.51533	C	-3.21115	-0.62634	-1.06426
C	1.42224	0.64659	-0.19790	C	-2.13060	0.06914	-0.26651
C	0.65701	0.00716	-1.11135	C	-1.30436	-0.87190	0.23370
C	0.98006	-1.45425	-1.12686	C	-1.75090	-2.23192	-0.18423
H	3.33758	-0.21245	0.40239	H	-4.21218	-0.45336	-0.64882
H	2.04682	-0.44016	1.59267	H	-3.23870	-0.30976	-2.11714
N	1.88684	-1.64398	-0.12811	N	-2.85072	-2.03602	-0.96972
C	2.53988	-2.91793	0.14253	C	-3.64121	-3.11647	-1.54282
H	2.52774	-3.09791	1.22229	H	-3.82567	-2.90007	-2.60081
H	1.91324	-3.67871	-0.32993	H	-3.00848	-4.00700	-1.48856
C	3.96074	-2.99546	-0.38808	C	-4.95714	-3.35675	-0.82286
C	4.19672	-2.98059	-1.77096	C	-4.96047	-3.81907	0.50152
C	5.05071	-3.08499	0.48407	C	-6.17917	-3.12438	-1.46244
C	5.49728	-3.05204	-2.26768	C	-6.16319	-4.04258	1.16996
H	3.35358	-2.91778	-2.45366	H	-4.01475	-4.00720	1.00270
C	6.35556	-3.15917	-0.01172	C	-7.38651	-3.35006	-0.79510
H	4.87862	-3.10119	1.55748	H	-6.18770	-2.76828	-2.48966
C	6.58109	-3.14168	-1.38830	C	-7.38053	-3.80843	0.52247
H	5.66680	-3.04321	-3.34048	H	-6.15261	-4.40391	2.19415
H	7.19204	-3.22962	0.67752	H	-8.32789	-3.16638	-1.30474
H	7.59386	-3.19969	-1.77609	H	-8.31715	-3.98474	1.04310
O	0.53900	-2.28931	-1.91431	O	-1.22343	-3.30037	0.12518
O	-0.22255	0.52999	-1.97328	O	-0.22967	-0.68116	1.00994
C	1.54059	2.12923	0.00521	C	-1.98313	1.55301	-0.03538
H	1.16199	2.61865	-0.89540	H	-1.30412	1.65182	0.81595
C	2.98839	2.57070	0.19499	C	-3.30074	2.22105	0.33487
C	3.70421	2.31565	1.37461	C	-4.32819	2.41684	-0.60084

E(B3LYP, 6-31G(d,p), IEFPCM(DCM)) =-3189.033659 Hartree

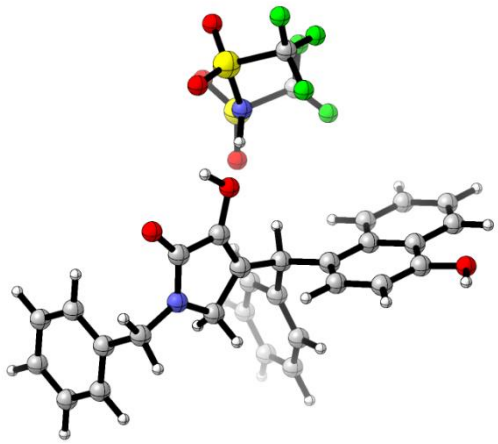
E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3188.755709 Hartree

Thermal correction to Gibbs Free Energy= -25.6 kcal/mol

C	3.64024	3.22418	-0.85812	C	-3.51868	2.62036	1.66004
C	5.03844	2.70531	1.49514	C	-5.53889	2.99733	-0.22016
H	3.22266	1.81852	2.21249	H	-4.18999	2.12303	-1.63807
C	4.97693	3.61009	-0.74072	C	-4.73000	3.19886	2.04390
H	3.09967	3.42918	-1.77794	H	-2.73420	2.47542	2.39763
C	5.67992	3.35281	0.43670	C	-5.74383	3.39050	1.10447
H	5.57542	2.50284	2.41681	H	-6.32116	3.14198	-0.95921
H	5.46496	4.11423	-1.56933	H	-4.87755	3.50218	3.07604
H	6.71817	3.65551	0.53124	H	-6.68527	3.84342	1.39987
C	-2.81050	5.88532	-0.97090	C	-0.99697	5.91760	0.01866
C	-1.61471	6.08725	-0.28956	C	-1.50988	4.73183	-0.50462
C	-0.92977	5.00577	0.28177	C	-0.67290	3.63872	-0.74922
C	-1.49461	3.70267	0.15423	C	0.71167	3.78177	-0.47413
C	-2.72064	3.51556	-0.52607	C	1.21959	4.98100	0.06993
C	-3.36621	4.59975	-1.09269	C	0.36639	6.04233	0.31915
H	0.64452	6.20397	1.20384	H	-1.96465	2.50116	-2.02697
H	-3.32429	6.73438	-1.41074	H	-1.66540	6.75511	0.19199
H	-1.20318	7.08671	-0.19317	H	-2.56730	4.65820	-0.72850
C	0.30087	5.18924	1.03000	C	-1.22058	2.32333	-1.24195
C	-0.81660	2.60144	0.77006	C	1.61199	2.70886	-0.82701
H	-3.13279	2.51739	-0.60973	H	2.28157	5.06230	0.26887
H	-4.29822	4.45943	-1.62881	H	0.75280	6.96827	0.73090
C	0.59538	2.72314	1.22141	C	1.14900	1.57345	-1.57066
C	0.99617	4.14071	1.49953	C	-0.17539	1.41470	-1.78631
H	0.76709	2.08212	2.09164	H	1.87435	0.85248	-1.92725
H	1.92099	4.28807	2.04257	H	-0.51528	0.54215	-2.33308
O	-1.46560	1.49382	0.85459	O	2.85540	2.82981	-0.48799
H	-1.06401	0.70754	1.34030	H	3.43913	2.04873	-0.77308
N	-2.02156	-1.32907	-0.03924	N	3.29850	-0.77954	0.11106
H	-0.81795	-0.18547	-2.28769	H	0.29383	-1.50703	1.09386
S	-3.04891	-1.77766	-1.20690	S	3.24405	-1.88653	1.30405
S	-2.13511	-1.62717	1.52691	S	4.64871	-0.38413	-0.66582
O	-3.48465	-1.66168	2.10339	O	5.93003	-0.57417	0.01546
O	-1.12453	-0.72771	2.15950	O	4.39977	0.94561	-1.29827
O	-2.52243	-1.17111	-2.44359	O	1.88567	-2.45909	1.32032
O	-3.43068	-3.19362	-1.21041	O	4.38295	-2.80400	1.39527
C	-1.43523	-3.33789	1.84109	C	4.66989	-1.52049	-2.15313
C	-4.65474	-0.83931	-0.89430	C	3.32233	-0.81782	2.83789

F	-1.33060	-3.51861	3.16072	F	4.68901	-2.79020	-1.74656
F	-2.25218	-4.25680	1.33086	F	3.57912	-1.31060	-2.89546
F	-0.22854	-3.45870	1.28518	F	5.75667	-1.26968	-2.88439
F	-4.39709	0.36815	-0.37419	F	2.25748	-0.01470	2.88948
F	-5.28667	-0.68478	-2.06054	F	3.33396	-1.60491	3.91598
F	-5.43802	-1.51576	-0.05788	F	4.43324	-0.07646	2.81995

5a-NH(TF)$_2$

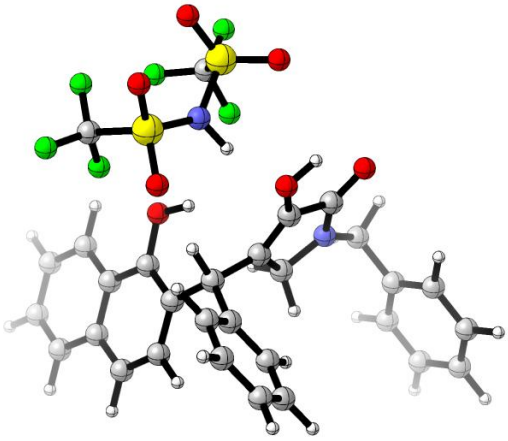


E(RB3LYP, 6-31G(d,p), IEFPCM(DCM)) =-3189.04006557 Hartree

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3188.761168 Hartree

Thermal correction to Gibbs Free Energy= -29.0 kcal/mol

***o*-A-IM-3-NH(TF)$_2$**



E(RB3LYP, 6-31G(d,p),IEFPCM(DCM)) =-3189.040359 Hartree

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3188.750258 Hartree

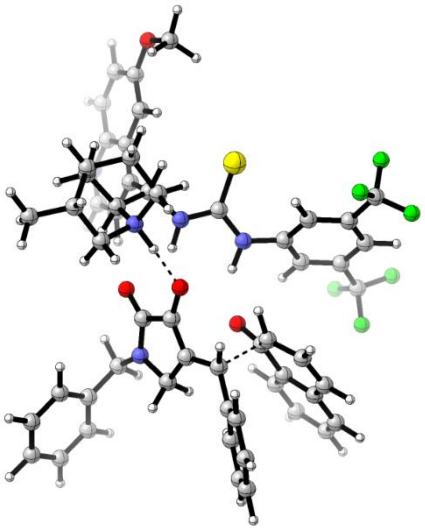
Thermal correction to Gibbs Free Energy= -22.2 kcal/mol

C	3.26256	0.50190	0.85610	C	2.51001	0.12933	-0.57696
C	1.75951	0.42106	0.66933	C	1.32108	0.25531	0.35972
C	1.34929	-0.69790	1.28589	C	0.94073	1.54447	0.33448
C	2.48047	-1.42016	1.90949	C	1.80003	2.34741	-0.56837
H	3.79135	0.46846	-0.10420	H	3.41249	-0.21637	-0.05756
H	3.57215	1.42405	1.36623	H	2.31724	-0.57380	-1.39662
N	3.58701	-0.66834	1.66588	N	2.70133	1.47989	-1.09655
C	4.94142	-1.05798	2.03798	C	3.76019	1.85776	-2.02601
H	5.44394	-0.19752	2.49187	H	3.75182	1.16222	-2.87167
H	4.82920	-1.82505	2.80953	H	3.48560	2.84702	-2.40308
C	5.76128	-1.59034	0.87531	C	5.13776	1.89355	-1.38805
C	5.40540	-2.79879	0.25831	C	5.43543	2.85412	-0.41027
C	6.87624	-0.89033	0.40298	C	6.12521	0.97577	-1.76083
C	6.15110	-3.29376	-0.81042	C	6.69652	2.89254	0.18247
H	4.54334	-3.35069	0.62354	H	4.67472	3.57392	-0.11965
C	7.62685	-1.38599	-0.66690	C	7.39113	1.01405	-1.16947
H	7.16192	0.04594	0.87585	H	5.90543	0.22922	-2.51989
C	7.26488	-2.58768	-1.27600	C	7.67833	1.97148	-0.19631
H	5.86752	-4.23208	-1.27811	H	6.91639	3.64306	0.93607
H	8.49065	-0.83218	-1.02283	H	8.14888	0.29613	-1.46920
H	7.84649	-2.97475	-2.10741	H	8.66132	2.00333	0.26415
O	2.38144	-2.49210	2.51451	O	1.67134	3.55978	-0.75567
O	0.10398	-1.23145	1.41256	O	-0.06201	2.18094	0.99379
C	0.92428	1.42438	-0.09929	C	0.72659	-0.87744	1.18275
H	0.13984	0.83281	-0.58527	H	-0.34763	-0.66297	1.26342
C	1.74591	2.06493	-1.22814	C	1.23986	-0.86494	2.62603
C	2.43620	3.26985	-1.04836	C	2.60349	-0.76505	2.93701
C	1.84714	1.40873	-2.46355	C	0.31770	-0.95029	3.67714
C	3.21260	3.80593	-2.07837	C	3.03289	-0.75717	4.26488
H	2.35687	3.79724	-0.10262	H	3.34118	-0.69269	2.14419
C	2.62016	1.94461	-3.49455	C	0.74527	-0.94196	5.00630
H	1.31109	0.47605	-2.61786	H	-0.74376	-1.01108	3.45407

C	3.30747	3.14572	-3.30454	C	2.10505	-0.84653	5.30486
H	3.73939	4.74299	-1.92218	H	4.09341	-0.67884	4.48529
H	2.68232	1.42551	-4.44666	H	0.01351	-1.00427	5.80636
H	3.90752	3.56516	-4.10663	H	2.43956	-0.83688	6.33785
C	-2.56512	3.66804	-1.43773	C	0.28730	-6.19222	-2.69280
C	-1.45780	2.97307	-0.99967	C	0.94952	-6.02071	-1.49795
C	-0.92317	3.16984	0.30484	C	0.92908	-4.76904	-0.82388
C	-1.58008	4.12775	1.14876	C	0.20286	-3.68586	-1.41281
C	-2.71527	4.83235	0.67116	C	-0.46996	-3.88906	-2.64788
C	-3.20161	4.60852	-0.59800	C	-0.42827	-5.11597	-3.27292
H	-2.94946	3.49074	-2.43780	H	2.15442	-5.37685	0.85756
H	-0.98503	2.26654	-1.67103	H	0.31197	-7.15447	-3.19567
C	0.21881	2.44845	0.79926	H	1.50032	-6.84330	-1.04974
C	-1.07695	4.35209	2.46808	C	1.60233	-4.55714	0.40731
H	-3.19389	5.55035	1.32722	C	0.17856	-2.42843	-0.73591
H	-4.07167	5.15224	-0.95331	H	-1.01582	-3.06335	-3.08951
C	0.01603	3.64965	2.92309	H	-0.94560	-5.26133	-4.21653
C	0.64853	2.70388	2.08491	C	0.83805	-2.23650	0.47401
H	0.39257	3.81545	3.92898	C	1.55147	-3.33103	1.02828
H	1.49226	2.15508	2.48943	H	2.06170	-3.19047	1.97410
O	-1.73744	5.27691	3.22375	O	-0.54147	-1.44318	-1.35675
H	-1.31286	5.34246	4.09062	H	-0.38329	-0.58779	-0.93278
H	0.21242	-2.07304	1.90010	H	-0.00948	3.12029	0.72160
N	-2.03118	-1.94802	-0.26574	N	-2.79825	1.59940	0.53012
H	-1.18866	-1.53679	0.18471	H	-1.82315	1.68498	0.87427
S	-2.03413	-1.79850	-1.95582	S	-3.82325	0.71261	1.55359
S	-2.75760	-3.14931	0.68788	S	-3.20293	2.75222	-0.64292
C	-3.56851	-0.75386	-2.24211	C	-4.27459	-0.75103	0.46317
C	-3.95109	-2.10527	1.69904	C	-2.57704	1.88090	-2.18760
F	-4.63835	-1.42644	-1.82726	F	-5.02412	-0.32767	-0.55012
F	-3.65505	-0.51708	-3.54654	F	-4.95646	-1.61249	1.20898
F	-3.45872	0.38893	-1.57571	F	-3.16469	-1.31818	0.00414
F	-4.55149	-2.90953	2.56947	F	-2.73717	2.69949	-3.21825
F	-4.85063	-1.54743	0.89639	F	-3.25954	0.75842	-2.37859
F	-3.26453	-1.16488	2.33989	F	-1.27989	1.59848	-2.02829
O	-1.73984	-3.61693	1.62336	O	-2.32520	3.89825	-0.44254
O	-3.54577	-4.04325	-0.14280	O	-4.64734	2.85937	-0.75238
O	-2.26361	-3.07220	-2.61540	O	-5.05364	1.43036	1.83641

O	-0.87782	-0.95768	-2.24518	O	-2.93749	0.21470	2.59888

TS-1



E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-3736.69331923 Hartree

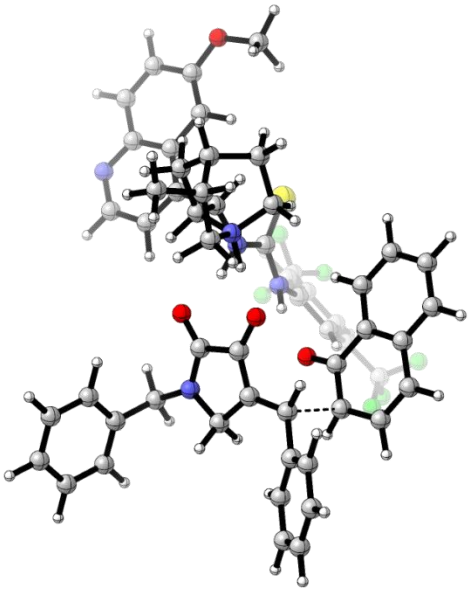
Frequency -326.49

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3736.216449 Hartree

Thermal correction to Gibbs Free Energy= 2.37 kcal/mol

C	-3.41913	-1.75064	0.92858
N	-2.48433	-1.59707	2.11343
C	-2.40564	-2.91432	2.84200
C	-4.80955	-2.19071	1.46549
C	-3.75615	-3.22916	3.53346
C	-4.79220	-2.20704	3.00733
C	-2.93182	-0.51728	3.06123
C	-4.38553	-0.80592	3.50596
C	-3.47824	-0.46215	0.06883
H	-2.95518	-2.53624	0.33401
C	-4.20846	-0.76834	-1.24564
C	-3.61434	-1.60882	-2.16928
C	-4.28748	-1.93281	-3.36600

TS-2



E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-3736.69391771 Hartree

Frequency -320.52

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3736.213632 Hartree

Thermal correction to Gibbs Free Energy= 4.14 kcal/mol

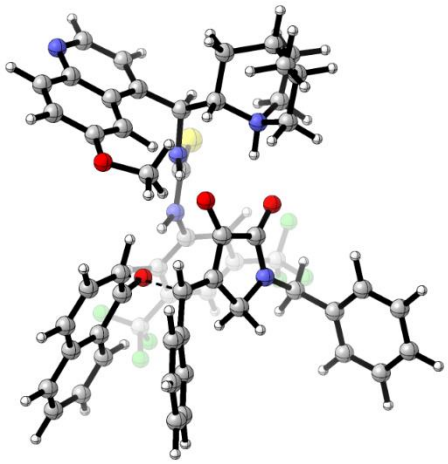
C	1.96372	-2.82816	-0.62803
N	0.82333	-2.76425	-1.62551
C	0.23415	-4.14791	-1.78671
C	2.96916	-3.90075	-1.13934
C	1.21496	-5.06677	-2.55079
C	2.58383	-4.34806	-2.56454
C	1.26911	-2.24447	-2.96395
C	2.46091	-3.09795	-3.45972
C	2.63430	-1.45064	-0.37606
H	1.48448	-3.14196	0.30047
C	3.61756	-1.60706	0.79744
C	3.10970	-1.77288	2.07295
C	3.98268	-1.97858	3.16192

N	-5.49109	-1.48962	-3.67750	N	5.29629	-2.03934	3.05065
C	-6.09933	-0.65329	-2.79106	C	5.82788	-1.86855	1.80831
C	-5.50238	-0.23819	-1.55229	C	5.03907	-1.63302	0.63190
C	-7.39702	-0.17287	-3.12639	C	7.24563	-1.92885	1.68756
C	-8.07339	0.67936	-2.29631	C	7.86201	-1.75817	0.47786
C	-7.47699	1.10946	-1.07863	C	7.08529	-1.50329	-0.68643
C	-6.22268	0.65932	-0.71212	C	5.70671	-1.44354	-0.61208
N	-2.13871	0.07989	-0.14547	N	1.62293	-0.42645	-0.11765
C	-1.81675	1.39506	-0.02434	C	1.86896	0.90608	-0.23611
N	-0.50019	1.67206	-0.23420	N	0.79774	1.68558	0.14723
C	0.11032	2.95186	-0.24730	C	0.81198	3.06373	0.44070
C	0.97406	3.24975	-1.30581	C	-0.33177	3.81806	0.14784
C	1.65138	4.46954	-1.33444	C	-0.38350	5.17048	0.48677
C	1.46840	5.40904	-0.32196	C	0.69196	5.79734	1.11177
C	0.61076	5.10128	0.73506	C	1.82158	5.03484	1.41466
C	-0.05828	3.87875	0.78738	C	1.88798	3.68053	1.09624
O	-8.23716	1.97430	-0.35371	O	7.81288	-1.32747	-1.82254
C	-7.70090	2.49038	0.86168	C	7.11876	-1.02904	-3.03055
C	2.63012	4.74256	-2.44432	C	-1.59705	5.97328	0.10327
F	2.79556	6.06748	-2.65801	F	-1.75667	7.05964	0.89303
F	2.23375	4.19059	-3.61306	F	-2.73258	5.24416	0.18620
F	3.85431	4.23437	-2.16851	F	-1.51835	6.42618	-1.17133
C	0.37168	6.11940	1.81699	C	2.95422	5.67105	2.17470
F	1.44445	6.92221	2.00080	F	3.10034	6.97838	1.85923
F	0.09388	5.53856	3.00612	F	4.13569	5.06260	1.93689
F	-0.67430	6.92846	1.52452	F	2.74947	5.61742	3.51460
H	-1.57414	-2.83452	3.54451	H	-0.72295	-4.01695	-2.29231
H	-2.14110	-3.66318	2.09138	H	0.02976	-4.51212	-0.77677
H	-5.06805	-3.17463	1.06677	H	2.98352	-4.75353	-0.45626
H	-5.58586	-1.50254	1.11967	H	3.98313	-3.49592	-1.14782
H	-3.64246	-3.04942	4.60933	H	0.87606	-5.14738	-3.59080
H	-5.78770	-2.46182	3.38323	H	3.35461	-5.01636	-2.95986
H	-2.82684	0.44192	2.55297	H	1.51239	-1.18869	-2.84763
H	-2.22681	-0.53210	3.89453	H	0.40150	-2.31004	-3.62223
H	-4.45894	-0.75144	4.59580	H	2.29948	-3.38783	-4.50178
H	-4.01893	0.31224	0.60953	H	3.18059	-1.13351	-1.26362
H	-2.63270	-2.03368	-1.98416	H	2.03939	-1.74983	2.25284
H	-3.80876	-2.59471	-4.08601	H	3.56964	-2.10785	4.16106

H	-7.82672	-0.50513	-4.06552	H	7.81753	-2.11167	2.59116
H	-9.06048	1.05439	-2.54569	H	8.94151	-1.79834	0.37706
H	-5.76466	1.02581	0.19520	H	5.13147	-1.20741	-1.49514
H	-1.42378	-0.59933	-0.40147	H	0.84465	-0.72914	0.48045
H	0.16361	0.91303	-0.44307	H	-0.14313	1.30170	-0.00867
H	1.12036	2.52149	-2.09407	H	-1.17956	3.33320	-0.32172
H	1.98866	6.35817	-0.35084	H	0.65022	6.84941	1.36386
H	-0.70146	3.64316	1.62300	H	2.76857	3.10882	1.35224
H	-8.45721	3.16721	1.25956	H	7.88553	-0.91677	-3.79723
H	-6.77140	3.04298	0.68464	H	6.54968	-0.09653	-2.94344
H	-7.51318	1.68893	1.58644	H	6.43988	-1.84341	-3.31211
H	-5.06453	-0.05006	3.09881	H	3.38922	-2.51870	-3.42876
C	-4.16161	-4.69497	3.34901	C	1.24426	-6.48053	-1.96178
H	-5.09412	-4.90813	3.88057	H	1.90698	-7.12803	-2.54396
H	-4.30692	-4.94967	2.29401	H	1.59321	-6.48328	-0.92380
H	-3.39098	-5.36385	3.74614	H	0.24492	-6.92774	-1.97456
S	-2.98048	2.58546	0.34986	S	3.31840	1.51950	-0.85961
H	-1.47263	-1.39072	1.79131	H	-0.00869	-2.18580	-1.26359
C	2.98023	0.67690	1.21152	C	-4.18649	1.03611	-1.44410
C	4.08860	1.36948	1.83495	C	-5.01545	1.17956	-2.61617
C	5.21342	1.68222	1.14167	C	-4.48181	1.18364	-3.86670
C	5.31628	1.39846	-0.27167	C	-3.05327	1.15062	-4.05977
C	4.20777	0.83565	-0.96467	C	-2.18012	1.13562	-2.93361
C	2.95043	0.57598	-0.24280	C	-2.74204	1.15913	-1.56953
C	4.29756	0.59255	-2.34778	C	-0.78897	1.17560	-3.14529
C	5.46477	0.87141	-3.04234	C	-0.25817	1.20093	-4.42530
C	6.56484	1.42416	-2.36224	C	-1.11765	1.19267	-5.53921
C	6.48870	1.68752	-1.00279	C	-2.49016	1.17080	-5.35626
H	4.02360	1.59456	2.89633	H	-6.09177	1.23293	-2.48294
H	6.05460	2.16352	1.63257	H	-5.11965	1.24551	-4.74416
H	3.42911	0.17981	-2.85082	H	-0.13448	1.18956	-2.28315
H	5.52964	0.67001	-4.10740	H	0.81789	1.23576	-4.56748
H	7.47739	1.65179	-2.90585	H	-0.70455	1.21573	-6.54370
H	7.33849	2.12275	-0.48348	H	-3.15571	1.18089	-6.21562
O	1.90588	0.23074	-0.85537	O	-2.02605	1.24069	-0.53347
H	1.99579	0.80151	1.65469	H	-4.58466	1.38895	-0.49741
C	2.62141	-2.88089	-0.22105	C	-3.68099	-0.93536	1.66367
C	2.21869	-2.01900	0.95018	C	-3.47187	-1.17796	0.19128

C	0.83584	-1.87024	0.95151	C	-2.12813	-1.50499	-0.03210
C	0.30093	-2.63451	-0.23187	C	-1.44460	-1.52139	1.31520
H	3.21026	-2.33448	-0.96973	H	-3.95628	0.10482	1.88889
H	3.19382	-3.77177	0.06672	H	-4.44172	-1.58646	2.11324
N	1.34335	-3.26359	-0.82172	N	-2.36833	-1.21183	2.24735
C	1.24409	-4.02297	-2.05821	C	-2.09364	-1.11459	3.67595
H	0.18512	-4.00524	-2.33388	H	-1.00514	-1.07863	3.77220
H	1.79918	-3.50514	-2.85027	H	-2.49705	-0.16601	4.04609
C	1.74279	-5.45165	-1.93174	C	-2.66243	-2.27329	4.47574
C	1.23035	-6.30112	-0.94112	C	-2.15842	-3.56894	4.29099
C	2.70431	-5.94959	-2.81706	C	-3.68894	-2.07127	5.40382
C	1.67016	-7.62021	-0.84099	C	-2.67363	-4.63934	5.01999
H	0.48537	-5.92333	-0.24593	H	-1.35676	-3.73156	3.57535
C	3.14362	-7.27269	-2.72218	C	-4.20553	-3.14263	6.13775
H	3.11197	-5.29894	-3.58665	H	-4.08440	-1.07032	5.55716
C	2.62824	-8.11068	-1.73324	C	-3.69986	-4.42840	5.94615
H	1.26445	-8.26757	-0.06888	H	-2.27289	-5.63775	4.87060
H	3.89092	-7.64412	-3.41726	H	-5.00191	-2.97083	6.85593
H	2.97030	-9.13841	-1.65538	H	-4.09969	-5.26232	6.51539
O	-0.88463	-2.65076	-0.60987	O	-0.24048	-1.76915	1.52867
O	0.08416	-1.18791	1.72620	O	-1.53315	-1.78220	-1.11701
C	3.06290	-1.27453	1.82937	C	-4.38147	-0.97487	-0.87394
H	2.53871	-1.01212	2.74553	H	-4.00474	-1.37616	-1.81172
C	4.47922	-1.64565	2.09059	C	-5.85466	-1.11671	-0.73246
C	5.40034	-1.97001	1.07981	C	-6.58698	-0.58412	0.34360
C	4.92208	-1.68961	3.42438	C	-6.55779	-1.82372	-1.72376
C	6.70542	-2.34705	1.39523	C	-7.96619	-0.76923	0.43178
H	5.10999	-1.90193	0.03807	H	-6.08658	-0.00061	1.10863
C	6.22500	-2.06994	3.74208	C	-7.93622	-2.01377	-1.63387
H	4.22879	-1.43338	4.22126	H	-6.01162	-2.23357	-2.56867
C	7.12281	-2.40426	2.72646	C	-8.64698	-1.48855	-0.55321
H	7.39972	-2.59081	0.59643	H	-8.51089	-0.34624	1.27079
H	6.53831	-2.10436	4.78148	H	-8.45445	-2.57033	-2.40932
H	8.13936	-2.69936	2.96895	H	-9.72085	-1.63233	-0.48151

TS-3



E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-3736.69612287 Hartree

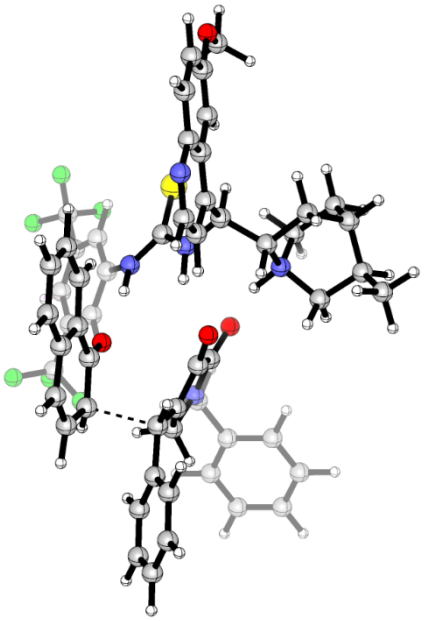
Frequency -303.69

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3736.21945 Hartree

Thermal correction to Gibbs Free Energy= 0.00 kcal/mol

C	4.07846	-1.23022	0.55259
N	3.17009	-2.13732	1.36702
C	3.45686	-1.91787	2.83251
C	5.53248	-1.73488	0.72836
C	4.93592	-2.27292	3.14610
C	5.57996	-2.80060	1.84130
C	3.33772	-3.59663	1.02553
C	4.78367	-4.03077	1.36209
C	3.63360	-1.15402	-0.92721
H	3.95211	-0.25949	1.02671
C	4.52103	-0.24087	-1.78241

TS-4



E(B3LYP, 6-31G(d,p), IEFPCM($CHCl_3$)) =-3736.69963781 Hartree

Frequency -313.59

E(M062X, 6-311G(d,p), IEFPCM($CHCl_3$), (SP))= -3736.21945 Hartree

Thermal correction to Gibbs Free Energy= 0.49 kcal/mol

C	-2.53204	-1.31333	2.16571
N	-1.55243	-0.57472	3.05726
C	-0.98145	-1.55007	4.05744
C	-3.72685	-1.76997	3.04383
C	-2.10576	-2.09035	4.98147
C	-3.43804	-1.44973	4.52371
C	-2.17497	0.59419	3.77617
C	-3.32448	0.08010	4.67503
C	-2.96504	-0.47918	0.93433
H	-1.95411	-2.16600	1.81087
C	-3.79368	-1.38250	0.01368

C	5.15767	-0.82191	-2.86269	C	-3.21256	-2.51275	-0.52952
C	5.96985	-0.04959	-3.72122	C	-3.97896	-3.38643	-1.33027
N	6.17340	1.24269	-3.56353	N	-5.25718	-3.20319	-1.60156
C	5.55906	1.85164	-2.50918	C	-5.85221	-2.08453	-1.09976
C	4.71412	1.16545	-1.57041	C	-5.16638	-1.11603	-0.29133
C	5.78213	3.24752	-2.34888	C	-7.22712	-1.87674	-1.40424
C	5.22907	3.93948	-1.30492	C	-7.89273	-0.76867	-0.95359
C	4.41043	3.26259	-0.36196	C	-7.20932	0.20558	-0.17441
C	4.13869	1.91271	-0.50287	C	-5.87702	0.03583	0.15315
N	2.21622	-0.82774	-1.03903	N	-1.81237	0.09071	0.24435
C	1.32033	-1.57471	-1.73766	C	-1.64180	1.41275	-0.02833
N	0.06367	-1.04842	-1.74068	N	-0.52375	1.65295	-0.77787
C	-1.12563	-1.72207	-2.09815	C	0.18569	2.84662	-1.02605
C	-2.05949	-1.05906	-2.89950	C	1.55378	2.69400	-1.31417
C	-3.28569	-1.66232	-3.18499	C	2.34934	3.80641	-1.56780
C	-3.59431	-2.92762	-2.68822	C	1.81140	5.09405	-1.55399
C	-2.65573	-3.58083	-1.88763	C	0.45036	5.23635	-1.29416
C	-1.43054	-2.98807	-1.58682	C	-0.36861	4.13374	-1.03859
O	3.93914	4.04562	0.64830	O	-7.97123	1.27189	0.19010
C	3.48334	3.40041	1.84054	C	-7.35983	2.31024	0.95219
C	-4.29769	-0.90061	-3.99608	C	3.80064	3.60256	-1.90572
F	-4.94399	0.02798	-3.23916	F	4.33131	2.54029	-1.24358
F	-5.24870	-1.70482	-4.51647	F	4.55146	4.68101	-1.59341
F	-3.72632	-0.22948	-5.01879	F	3.98762	3.36128	-3.22356
C	-2.98926	-4.90200	-1.25141	C	-0.15110	6.61498	-1.22951
F	-3.33053	-4.74766	0.05642	F	-0.14527	7.10517	0.03441
F	-1.94178	-5.75452	-1.27359	F	-1.43684	6.62847	-1.64490
F	-4.02786	-5.51694	-1.85539	F	0.52922	7.50068	-1.99227
H	2.74545	-2.53898	3.37892	H	-0.20456	-1.01193	4.60290
H	3.21581	-0.87183	3.03241	H	-0.50165	-2.33678	3.47142
H	6.18786	-0.89009	0.95138	H	-3.90625	-2.83681	2.89508
H	5.89724	-2.17498	-0.20507	H	-4.64305	-1.25425	2.73921
H	4.93927	-3.10157	3.86337	H	-1.91037	-1.73214	5.99881
H	6.61860	-3.08462	2.03447	H	-4.25689	-1.82279	5.14606
H	3.08242	-3.71702	-0.02838	H	-2.50384	1.30657	3.01770
H	2.58516	-4.12878	1.60913	H	-1.36945	1.06268	4.34415
H	4.77694	-4.80190	2.13800	H	-3.13373	0.34362	5.71946
H	3.73534	-2.15126	-1.36110	H	-3.56523	0.36542	1.26639

H	5.02728	-1.87902	-3.06964	H	-2.16397	-2.73862	-0.35880
H	6.46243	-0.52654	-4.56692	H	-3.50973	-4.27254	-1.75340
H	6.41657	3.73888	-3.07891	H	-7.72522	-2.62589	-2.01063
H	5.40638	5.00074	-1.16595	H	-8.93910	-0.59929	-1.18517
H	3.45406	1.44293	0.18851	H	-5.35837	0.80302	0.71120
H	1.85687	-0.12961	-0.37702	H	-1.03143	-0.56379	0.10343
H	-0.08820	-0.06755	-1.45826	H	-0.02030	0.82465	-1.13293
H	-1.82790	-0.07047	-3.27543	H	1.97880	1.69750	-1.34321
H	-4.54294	-3.39493	-2.91827	H	2.43366	5.95880	-1.74589
H	-0.71876	-3.49024	-0.94469	H	-1.42272	4.26839	-0.84947
H	3.21760	4.20388	2.52882	H	-8.13695	3.05619	1.11949
H	4.28741	2.79591	2.27892	H	-6.52526	2.76636	0.40809
H	2.61705	2.75706	1.66276	H	-7.00010	1.93609	1.91818
H	5.25792	-4.46467	0.47744	H	-4.26643	0.55664	4.38847
C	5.68950	-1.10138	3.78659	C	-2.12756	-3.62250	5.02457
H	6.72367	-1.38163	4.00977	H	-2.91481	-3.97984	5.69570
H	5.71235	-0.22006	3.13706	H	-2.30121	-4.05978	4.03595
H	5.21385	-0.80443	4.72679	H	-1.17305	-4.01231	5.39268
S	1.72983	-3.01151	-2.55963	S	-2.72787	2.60741	0.51997
H	2.15312	-1.89246	1.24191	H	-0.72330	-0.22569	2.50352
C	-0.14857	3.24456	-0.17459	C	2.46128	-2.10417	-2.74248
C	-0.07623	4.68445	-0.16110	C	2.54512	-3.20999	-3.66448
C	-1.10070	5.45147	-0.62101	C	1.44542	-3.69163	-4.30260
C	-2.27075	4.84299	-1.20978	C	0.16872	-3.03656	-4.16651
C	-2.33855	3.42817	-1.35422	C	0.04672	-1.87389	-3.35045
C	-1.20311	2.59325	-0.92682	C	1.22748	-1.34472	-2.64563
C	-3.46620	2.84080	-1.95617	C	-1.18627	-1.19541	-3.30322
C	-4.52239	3.62234	-2.39920	C	-2.28609	-1.65886	-4.00789
C	-4.46142	5.02050	-2.26029	C	-2.17637	-2.82253	-4.78965
C	-3.35349	5.61866	-1.67883	C	-0.96818	-3.49600	-4.86794
H	0.81079	5.15140	0.25977	H	3.50981	-3.68668	-3.80909
H	-1.05084	6.53571	-0.57405	H	1.51636	-4.55258	-4.96159
H	-3.49296	1.76270	-2.06263	H	-1.26247	-0.29168	-2.71037
H	-5.38894	3.15484	-2.85717	H	-3.23085	-1.12714	-3.95435
H	-5.28391	5.63595	-2.61388	H	-3.03790	-3.18748	-5.34136
H	-3.30787	6.69996	-1.57817	H	-0.87747	-4.38478	-5.48710
O	-1.17723	1.35671	-1.16346	O	1.18521	-0.28854	-1.95430
H	0.78018	2.68386	-0.12550	H	3.36329	-1.52621	-2.56572

C	-2.02815	0.41230	1.92749	C	3.59874	-0.88975	0.48750
C	-0.76762	1.23299	1.78689	C	2.50889	-1.85780	0.10355
C	0.30947	0.37119	1.57560	C	1.30150	-1.44761	0.69203
C	-0.21853	-1.04128	1.65679	C	1.61695	-0.22014	1.52807
H	-2.56588	0.59279	2.86673	H	4.43846	-1.35775	1.01691
H	-2.73092	0.56969	1.09979	H	4.00948	-0.34977	-0.37802
N	-1.54674	-0.96984	1.88133	N	2.92453	0.06312	1.37041
C	-2.42820	-2.12389	2.00942	C	3.60160	1.20571	1.97323
H	-3.24737	-2.02938	1.28873	H	4.05665	1.80341	1.17669
H	-1.83454	-2.99439	1.71950	H	2.81517	1.80762	2.43701
C	-2.98491	-2.29854	3.41124	C	4.65041	0.81172	2.99726
C	-4.36226	-2.24334	3.64710	C	5.99428	1.15081	2.80978
C	-2.12051	-2.52999	4.49092	C	4.28284	0.10969	4.15413
C	-4.87150	-2.41816	4.93677	C	6.95652	0.79931	3.76035
H	-5.04152	-2.06543	2.81726	H	6.28983	1.69525	1.91652
C	-2.62538	-2.70132	5.77875	C	5.24099	-0.24542	5.10210
H	-1.04904	-2.57931	4.31537	H	3.24000	-0.15435	4.30936
C	-4.00415	-2.64608	6.00508	C	6.58201	0.09950	4.90742
H	-5.94362	-2.37328	5.10429	H	7.99618	1.07022	3.60154
H	-1.94551	-2.88231	6.60629	H	4.94317	-0.78749	5.99498
H	-4.39747	-2.78112	7.00827	H	7.32819	-0.17587	5.64680
O	0.45380	-2.08735	1.54292	O	0.81443	0.41942	2.23811
O	1.53465	0.61214	1.31908	O	0.13462	-1.93586	0.64246
C	-0.62299	2.65058	1.80071	C	2.59754	-2.94203	-0.80099
H	0.38330	2.94906	2.08000	H	1.67281	-3.51336	-0.84378
C	-1.64854	3.57528	2.33693	C	3.80955	-3.79078	-0.94595
C	-3.02943	3.42369	2.11570	C	5.11617	-3.27695	-1.03121
C	-1.22449	4.66007	3.12619	C	3.64482	-5.18629	-0.99482
C	-3.94671	4.30508	2.68535	C	6.21419	-4.12915	-1.14199
H	-3.39290	2.63129	1.47262	H	5.28278	-2.20538	-1.03658
C	-2.14032	5.54014	3.69989	C	4.74273	-6.03939	-1.09991
H	-0.16156	4.80367	3.30074	H	2.64282	-5.60256	-0.94131
C	-3.50824	5.36311	3.48476	C	6.03409	-5.51408	-1.17189
H	-5.00760	4.16789	2.49828	H	7.21340	-3.70892	-1.20938
H	-1.78559	6.36349	4.31293	H	4.58820	-7.11407	-1.12811
H	-4.22560	6.04694	3.92858	H	6.89112	-6.17535	-1.25694