Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Unprecedented Access of Functionalized Pyrrolo[2,1-a]isoquinolines from the Domino Reaction of Isoquinolinium Ylides and Electrophilic Benzannulated Heterocycles

Sheba Ann Babu,[a,b] Rajalekshmi A. R.,[a] Nitha P. R.,[a,b] Vishnu K. Omanakuttan,[a,b] Rahul P.,[a,b] Sunil Varughese[a,b*] and Jubi John[a,b*]

[a]Chemical Sciences and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology (CSIR-NIIST), Thiruvananthapuram 695019, India.
[b]Academy of Scientific and Innovative Research (AcSIR), Ghaziabad-201002, India.

* E-mail: s.varughese@niist.res.in, jubijohn@niist.res.in

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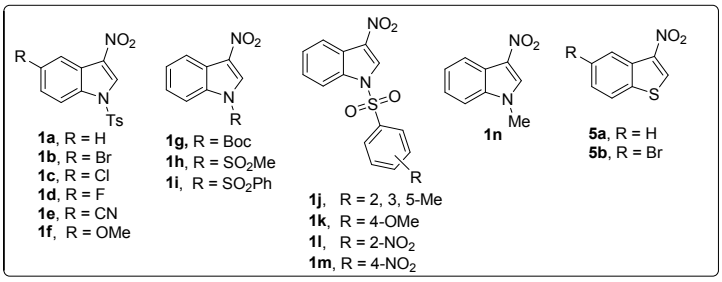
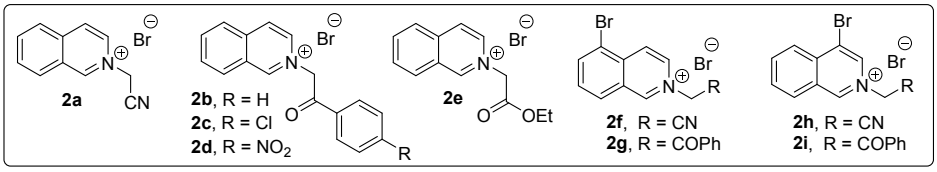
1.Procedure for the synthesis of electrophilic benzannulated heterocycles (1 and 5) isoquinolinium salts (2a-2i):

- 3-Nitroindoles (**1a**-**1n**) and 3-nitrobenzothiophenes (**5a**-**5b**) were prepared by following a literature report;E. T. Pelkey and G. W. Gribble, *Synthesis*, 1999, 1117



- All isoquinolinium salts (**2a**-**2i**) were prepared by following a previously reported procedure (S. Mahmoud, T. Aboul-Fadl, M. Sheha, H. Farag and A. M. I. Mouhamed, *Arch. Pharm. Pharm. Med. Chem*., 2003, 573).

  To isoquinoline dissolved in acetone at 0 °C, α-halocarbonyl compound was added and the mixture was stirred at room temperature for a period of time. After the completion of the reaction, the precipitate formed was filtered and washed with diethyl ether to get the pure product.

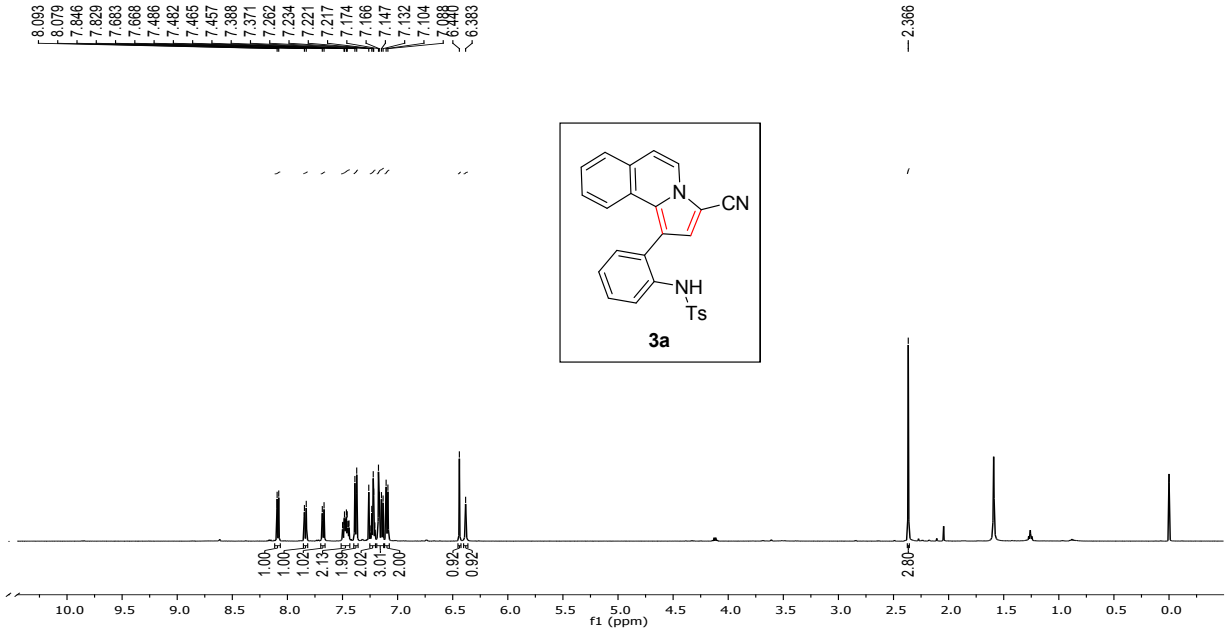


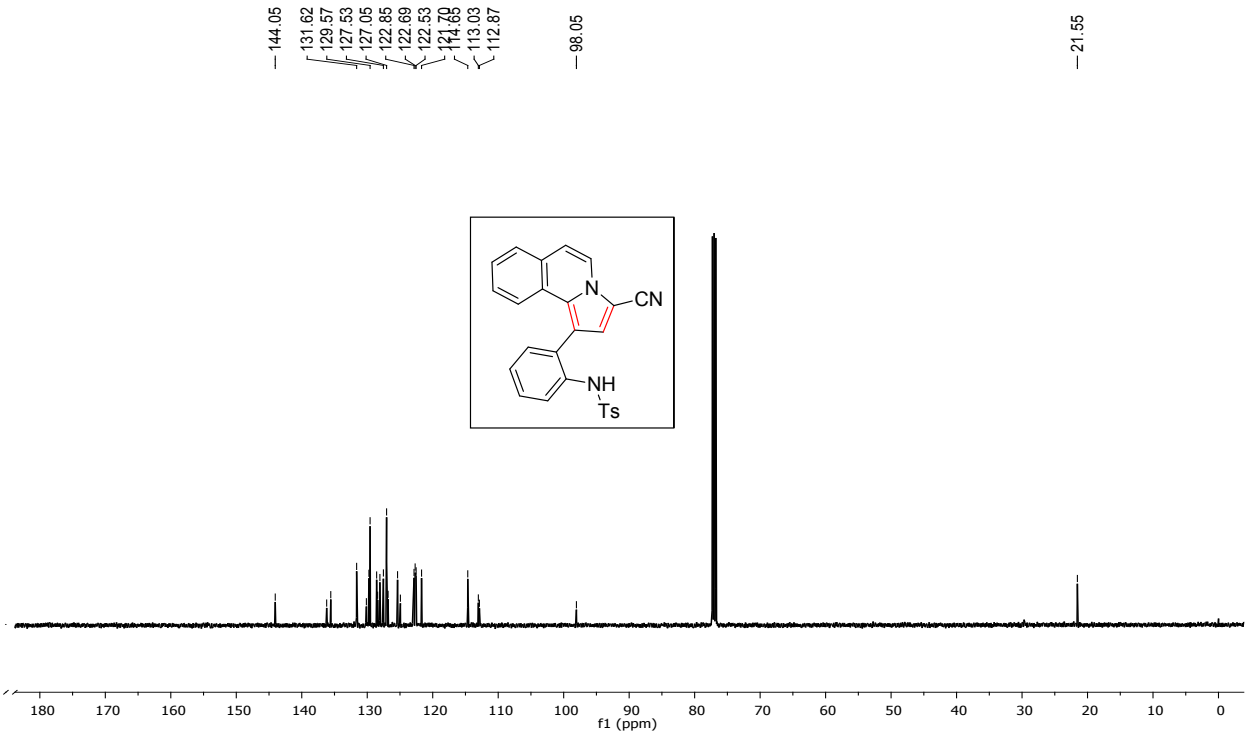
2. Procedure for scale up of 3a

A mixture of 3-nitro-*N*-tosyl indole 1a (1.0 g, 3.16 mmol), 2-(cyanomethyl)isoquinolin-2-ium-bromide 2a (1.18 mg, 4.74 mmol) and KOH (708 mg, 12.64 mmol) was weighed into a dry reaction tube. Dry DMF (18.0 mL) was added and allowed to stir at room temperature for 12 h. After completion of the reaction as indicated from the TLC, water was added and the aqueous layer extracted thrice with ethyl acetate. The organic layer was dried over anhydrous Na_2SO_4 and the solvent was removed under vacuum. The residue was then purified by activated neutral alumina column chromatography (20% ethyl acetate in hexane) to afford 3a (994 mg, 72%).

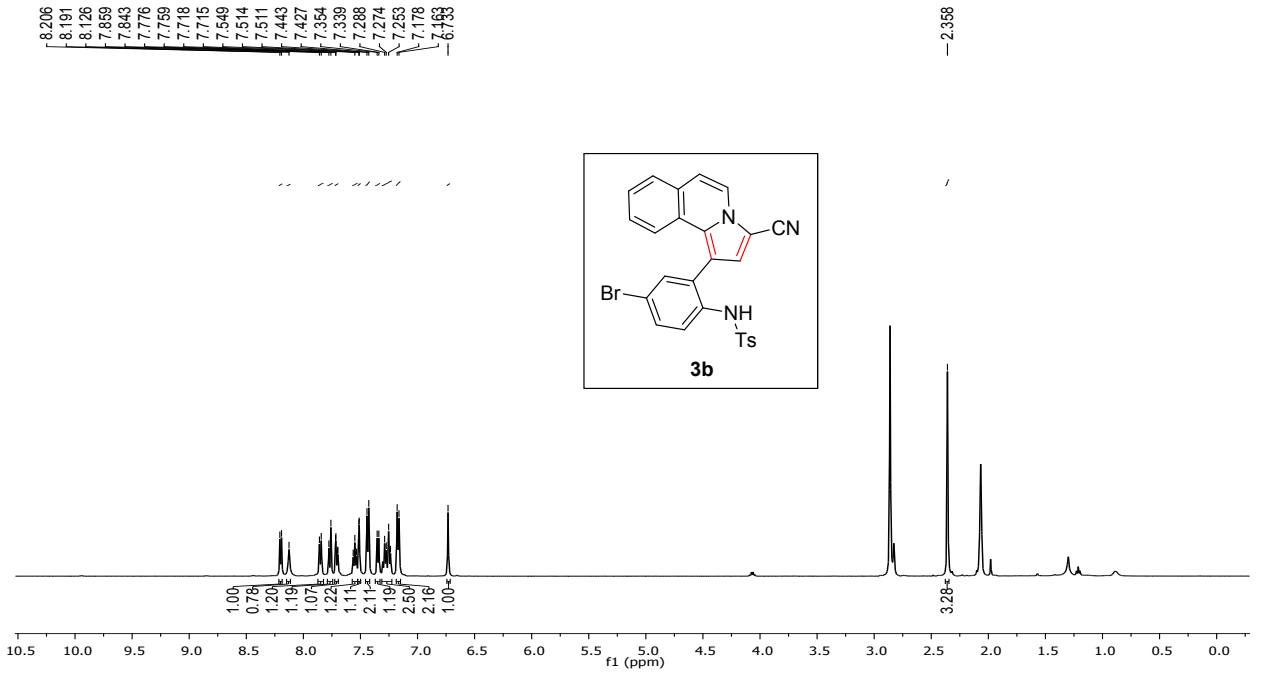
3. ^{1}H NMR &^{13}C NMR Spectra

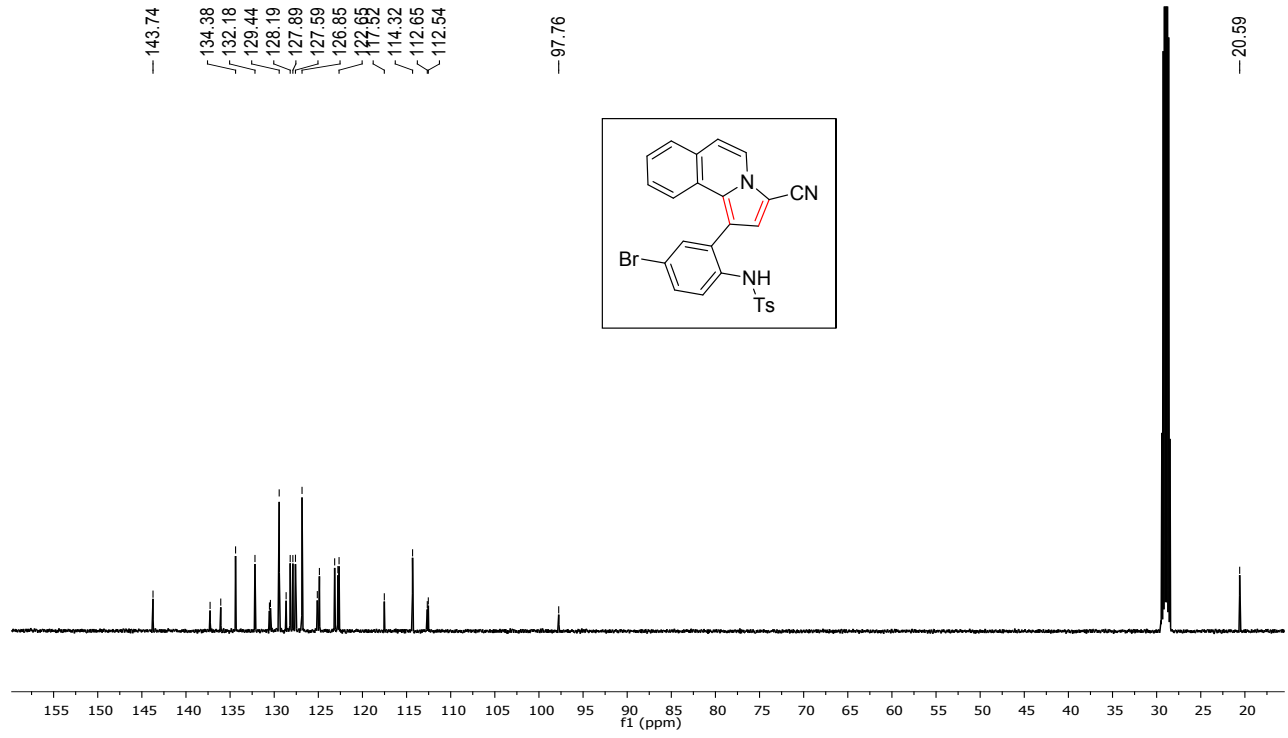
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **3a**



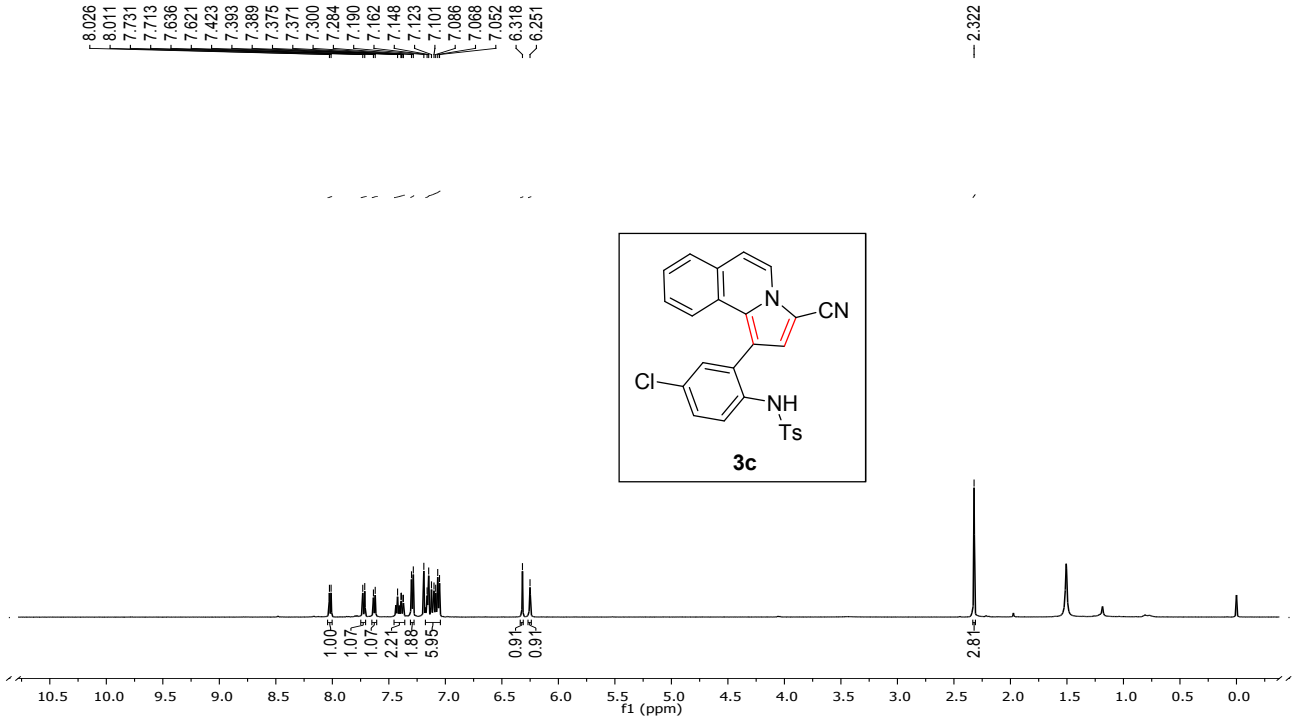


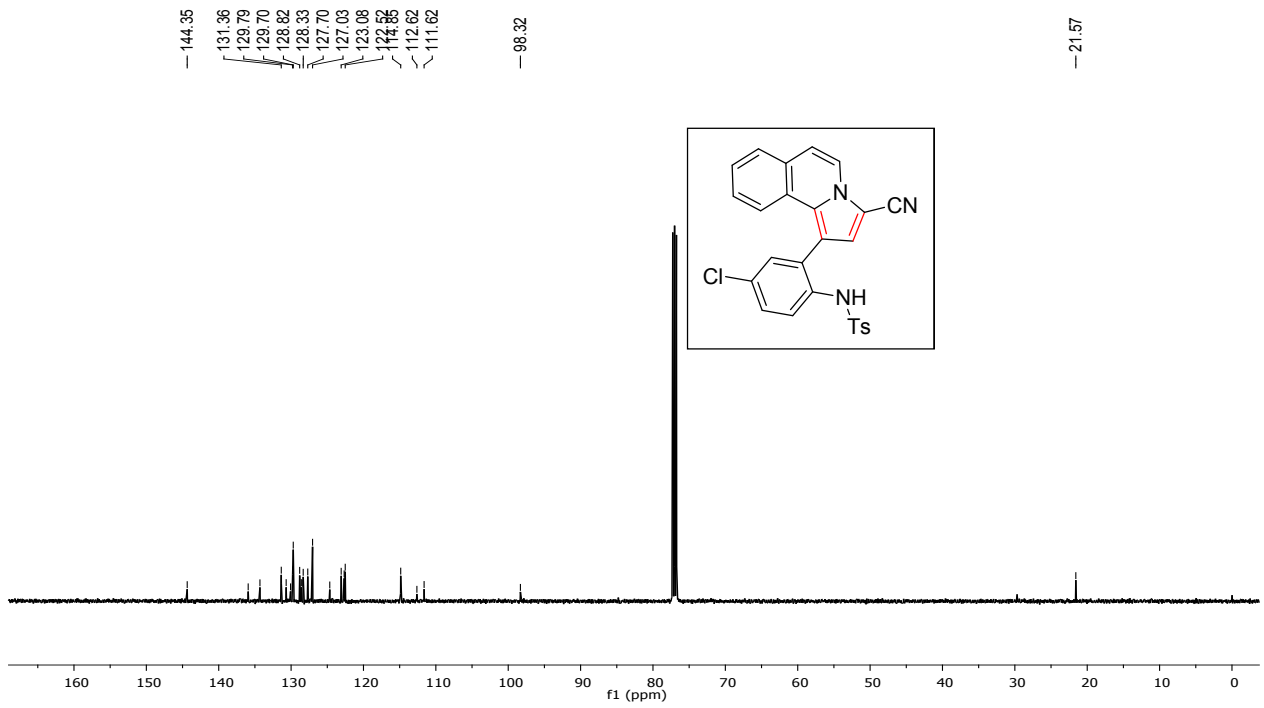
^{1}H NMR (500 MHz, $(CD_3)_2CO$) &^{13}C{^{1}H} (125 MHz, $(CD_3)_2CO$) Spectra of **3b**



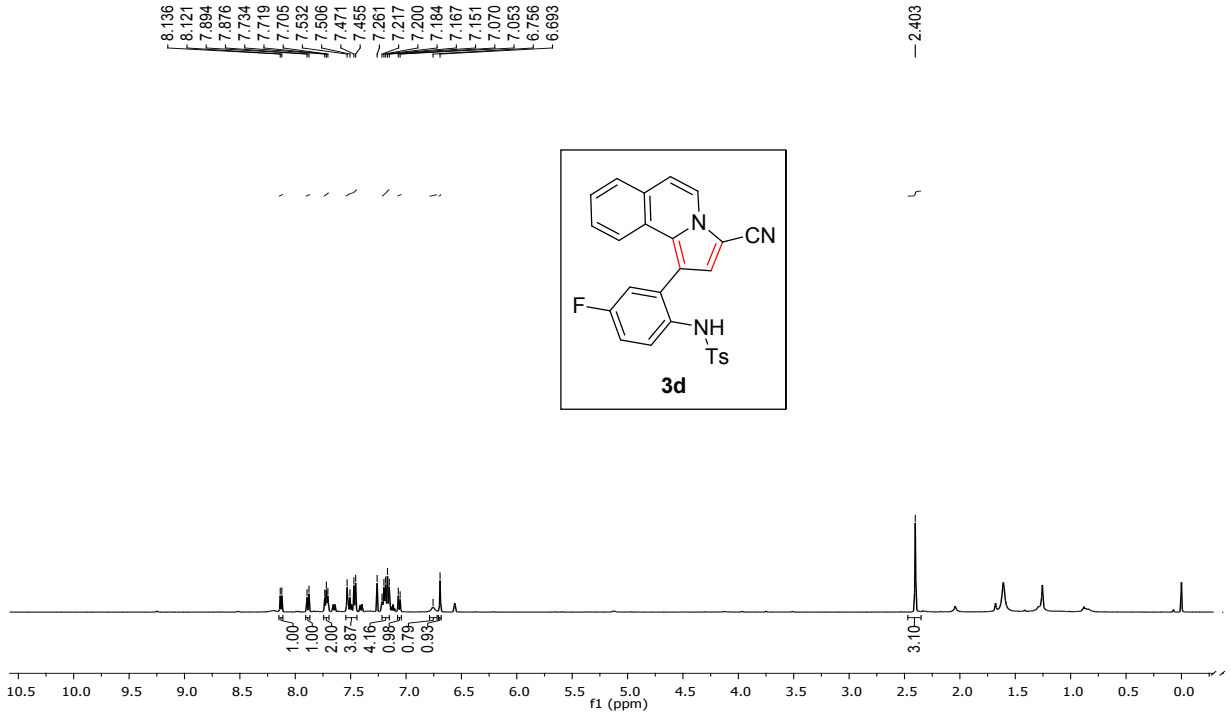


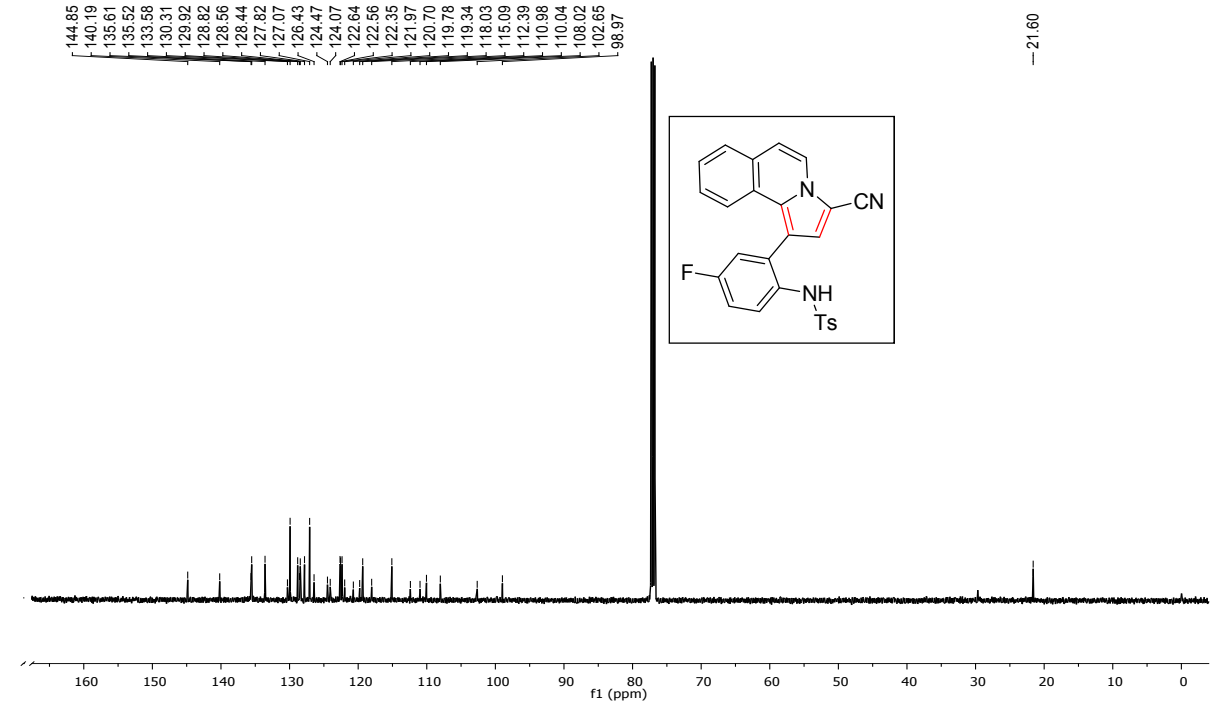
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$)Spectra of **3c**



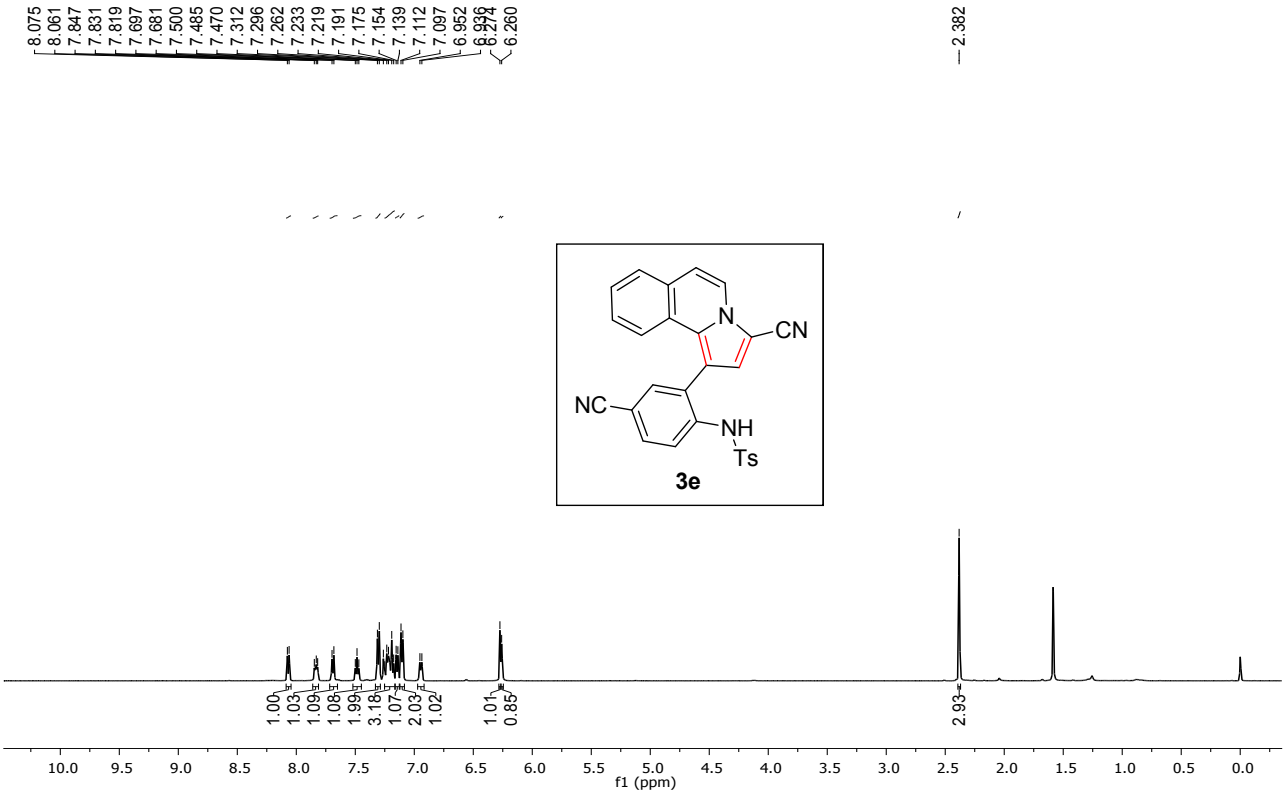


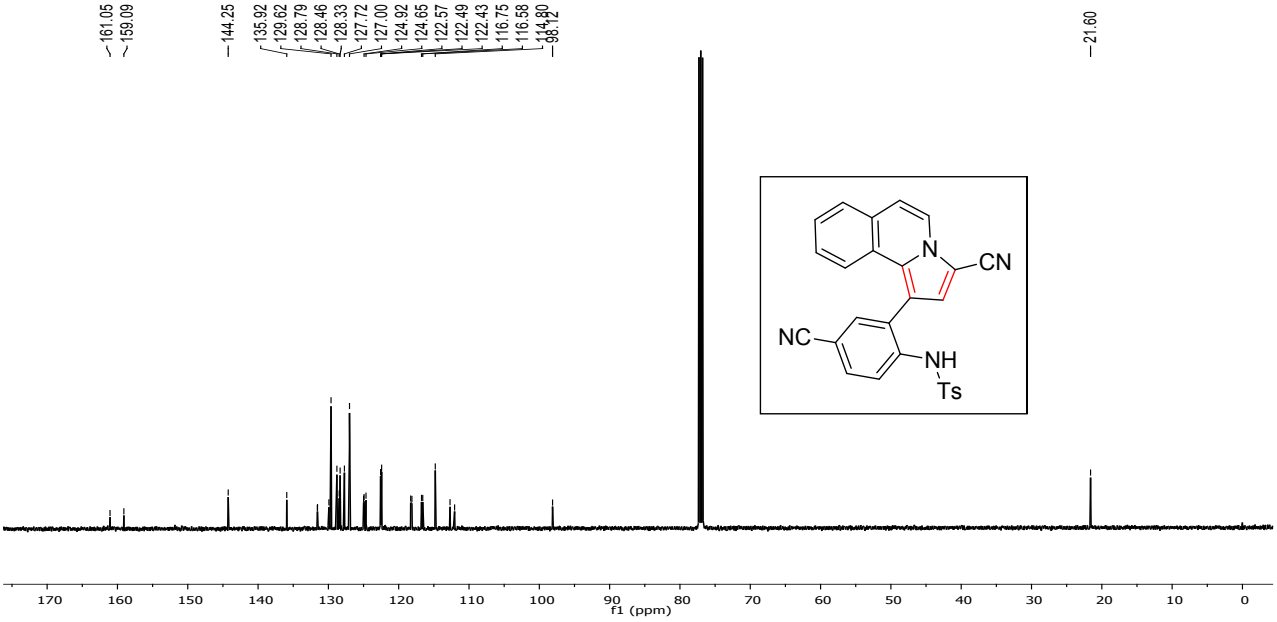
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **3d**



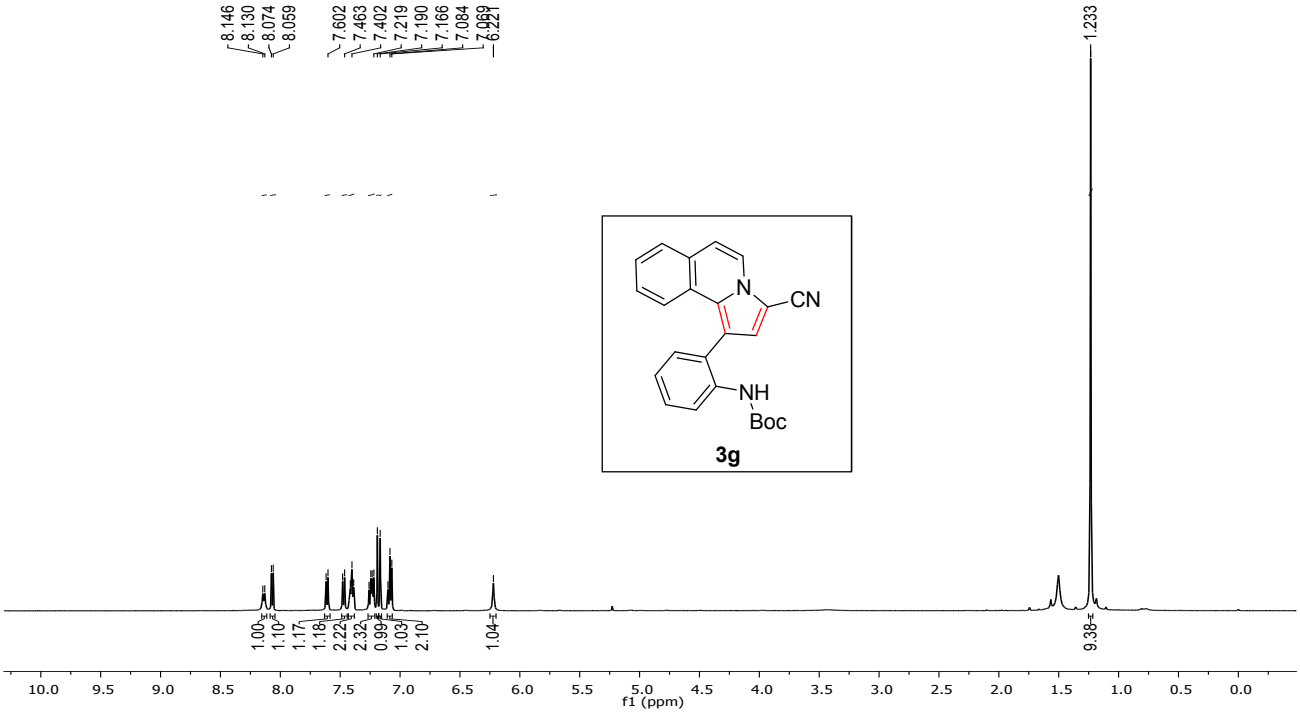


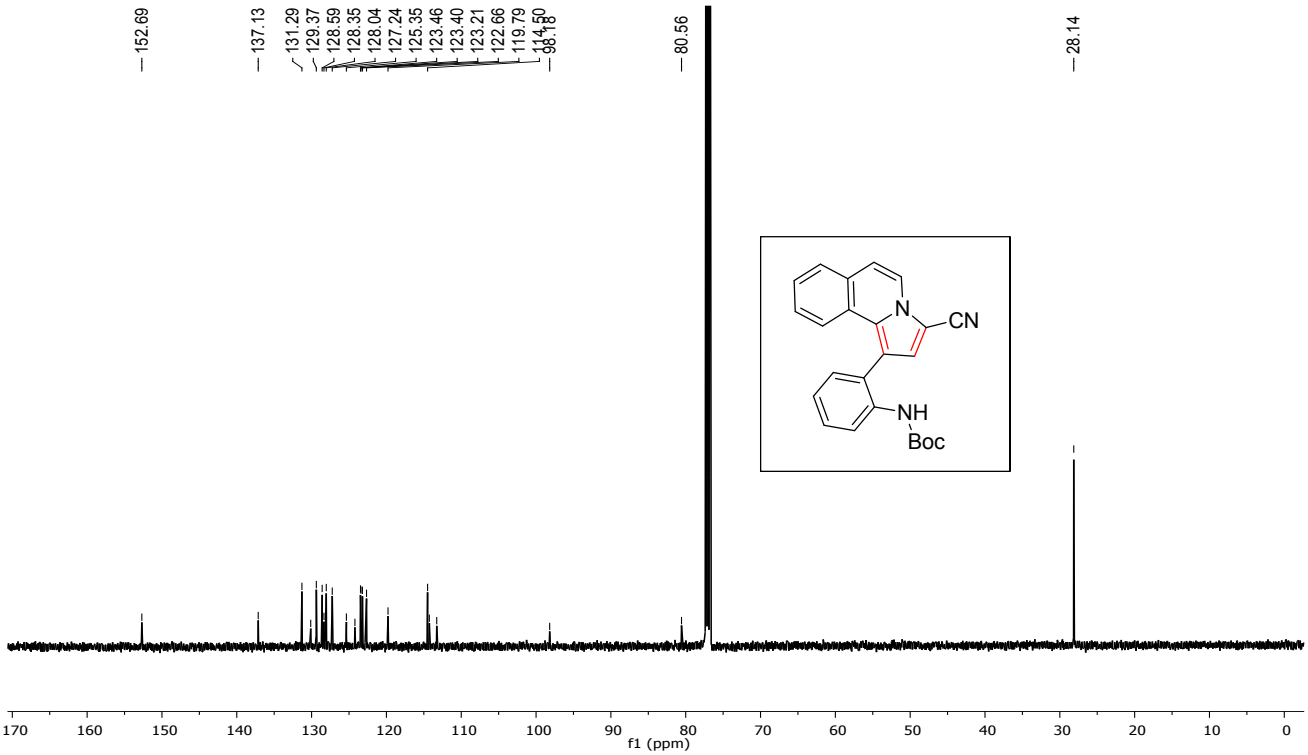
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **3e**





^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **3g**





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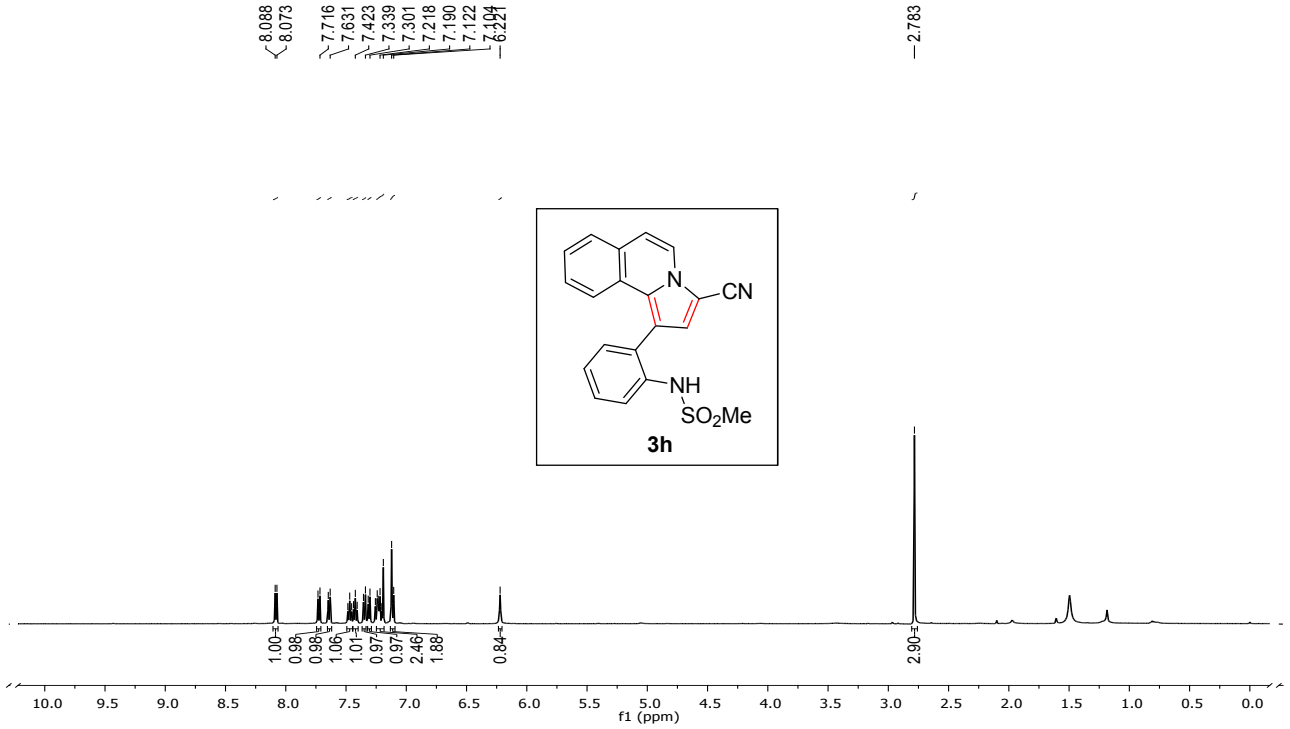
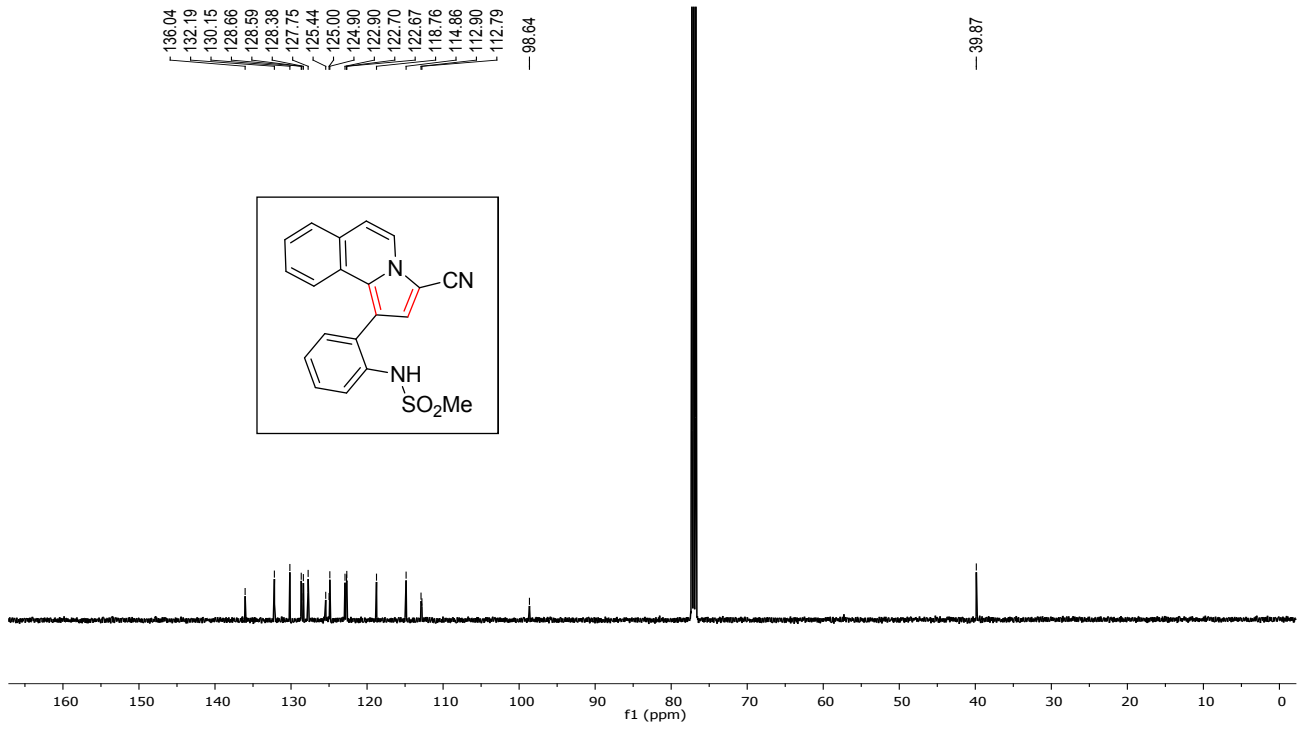
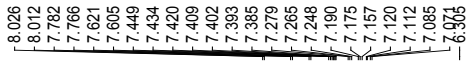
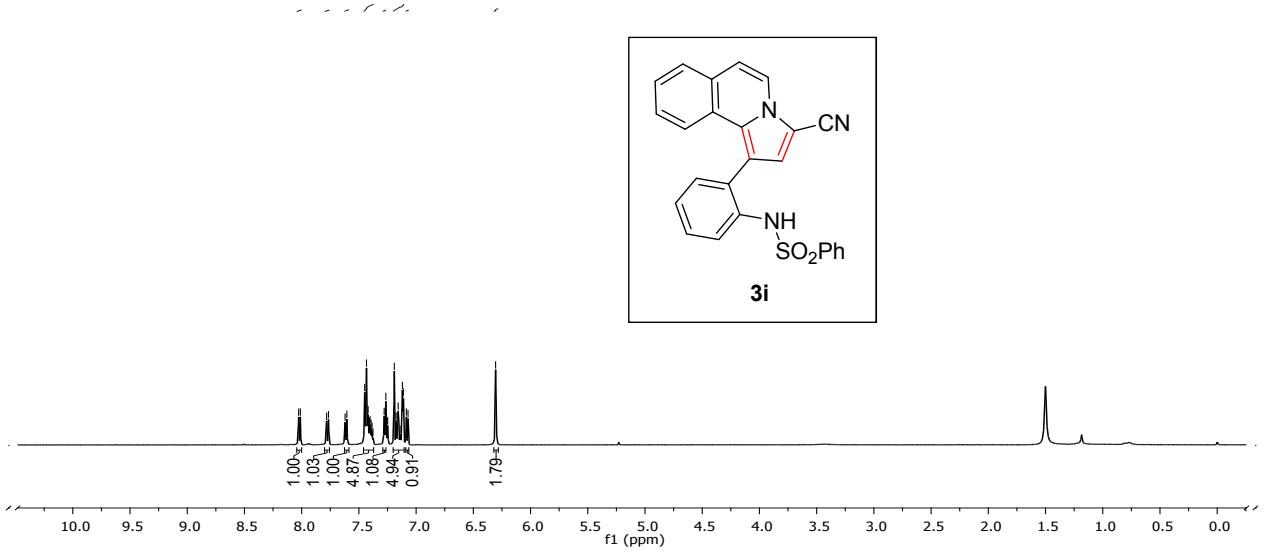
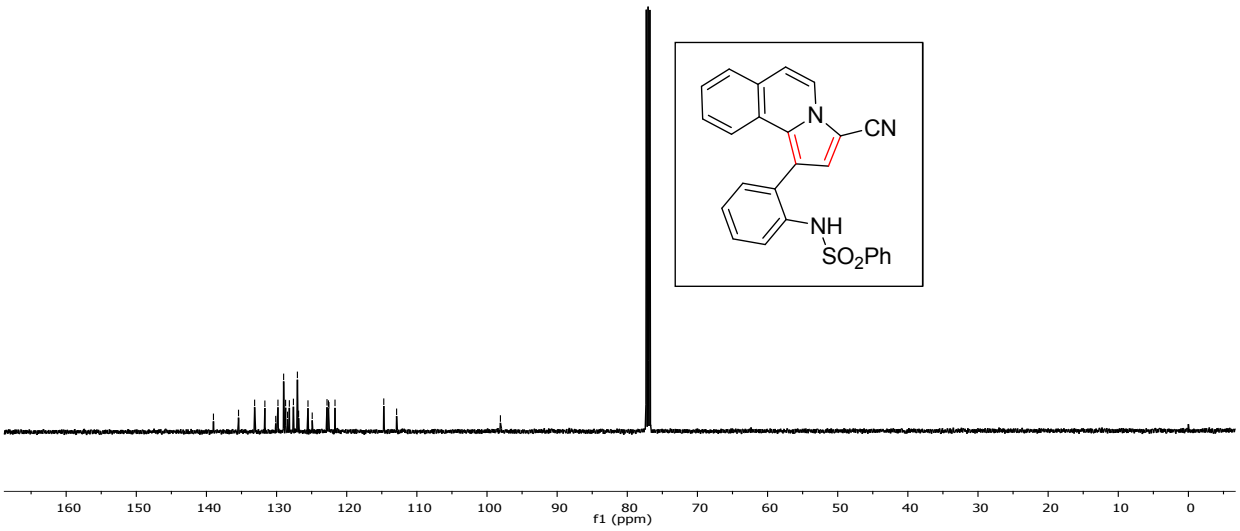




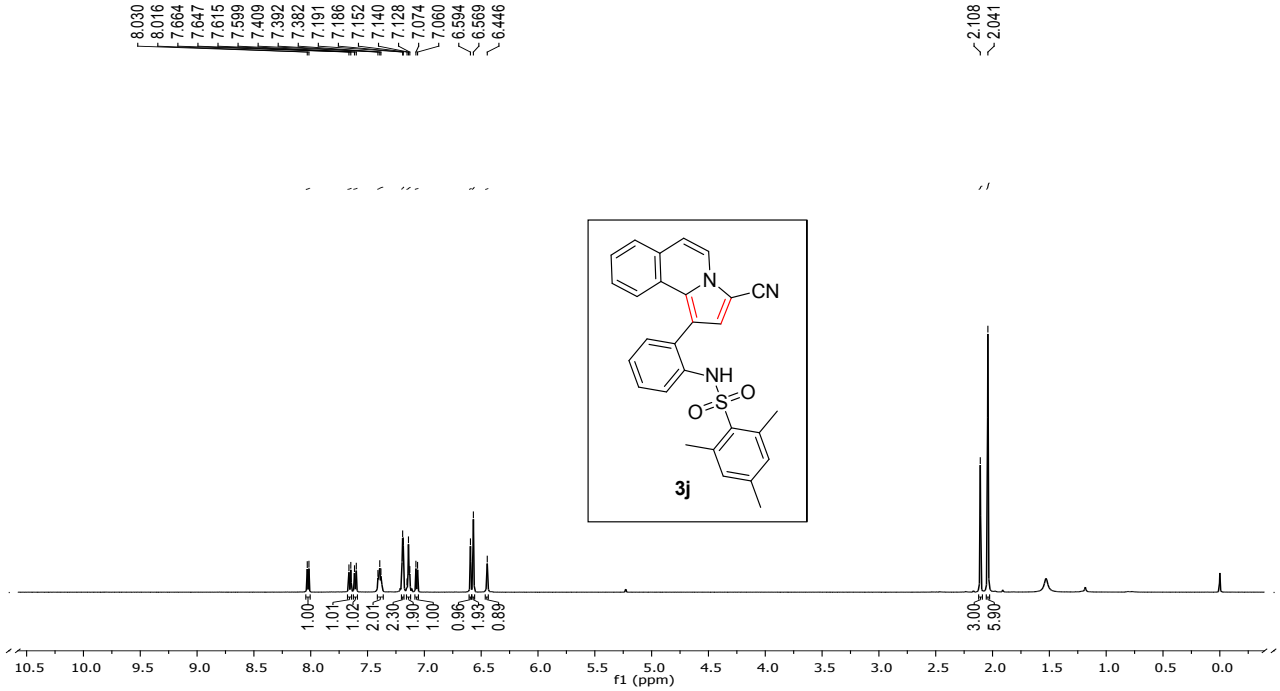
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **3i**

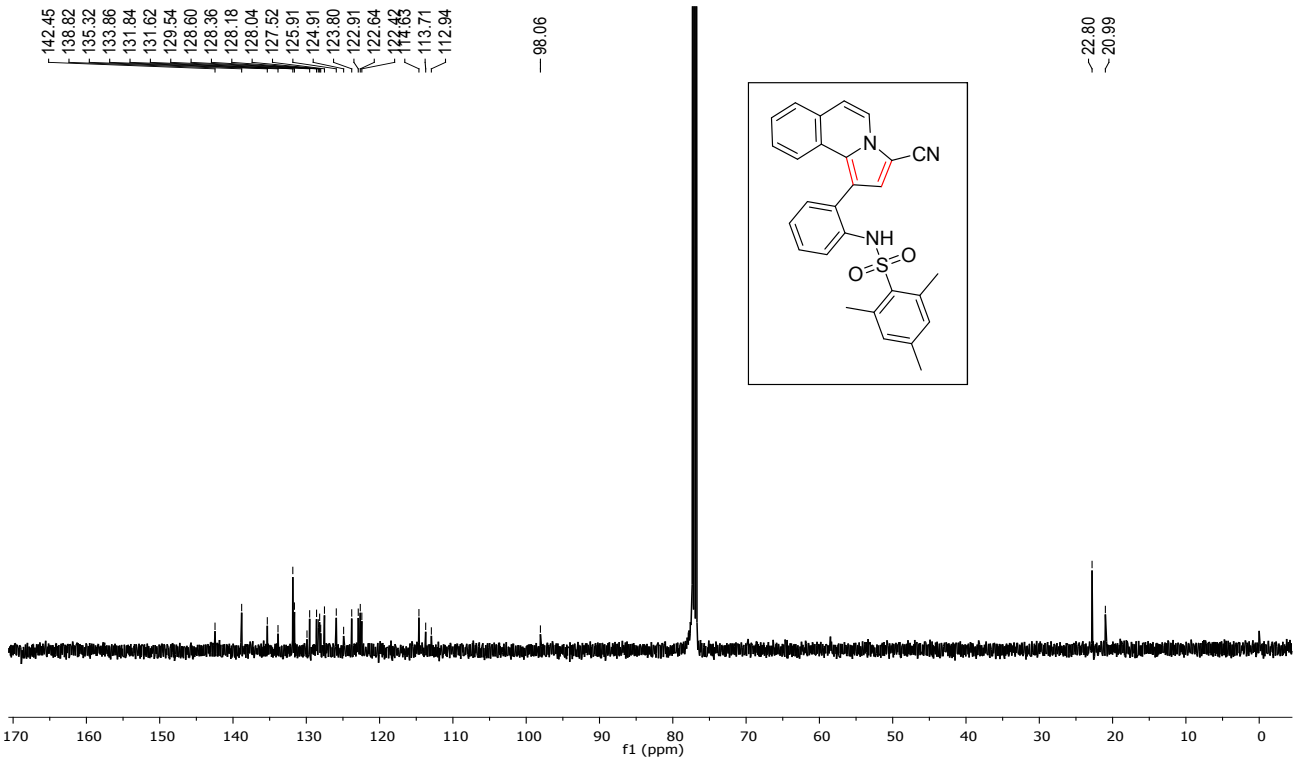




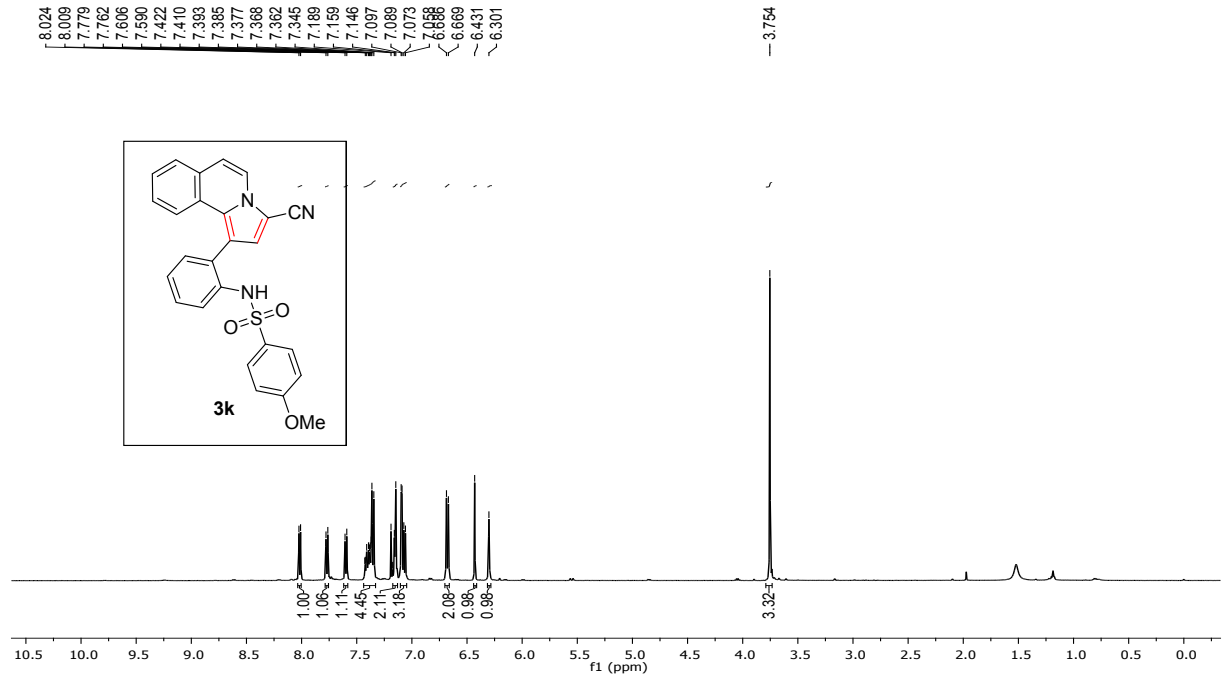


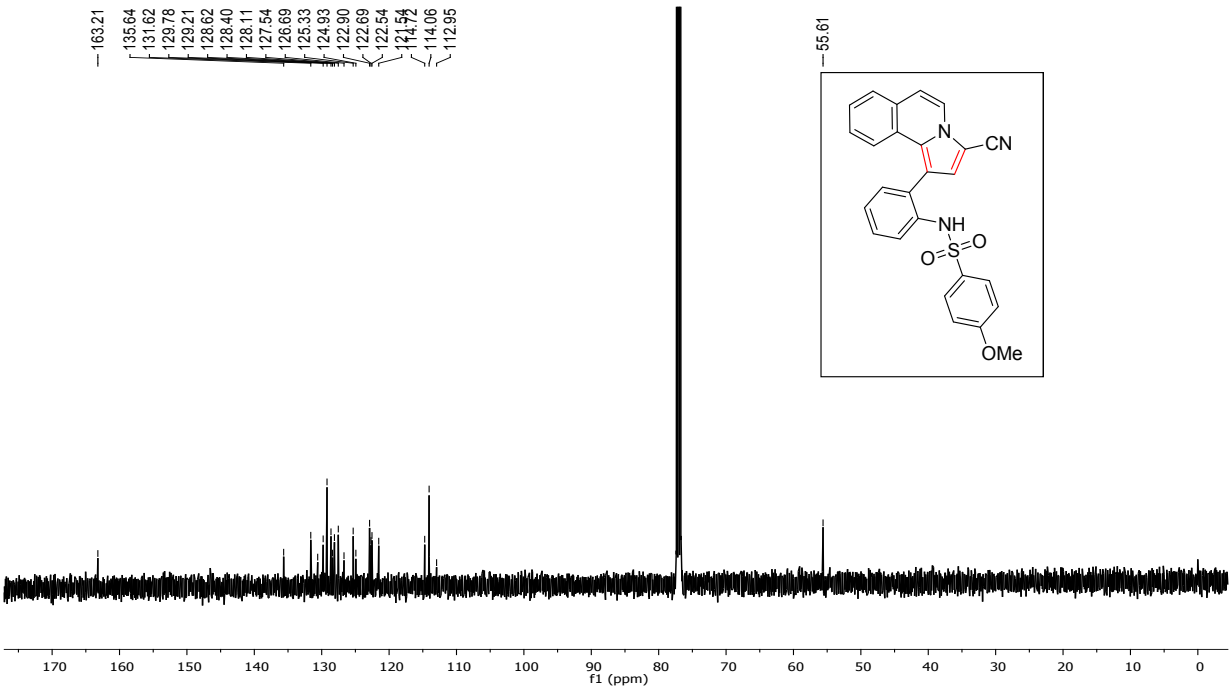
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **3j**





^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$)Spectra of **3k**





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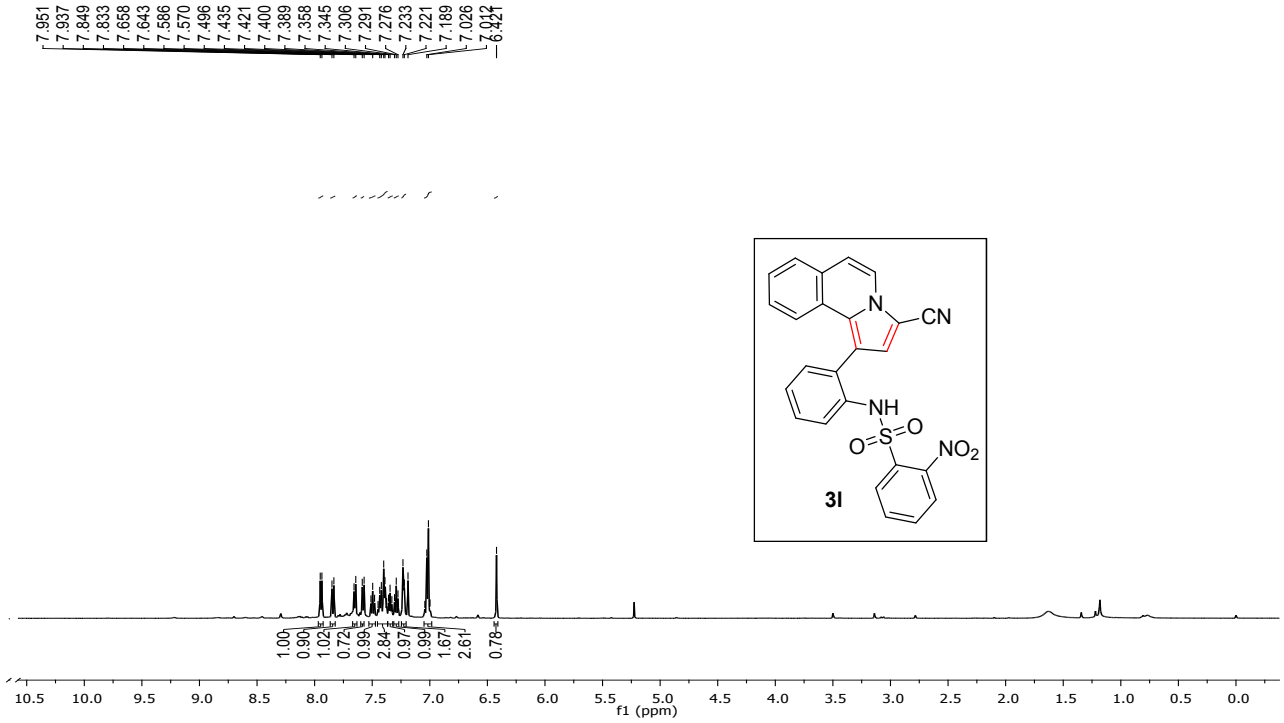
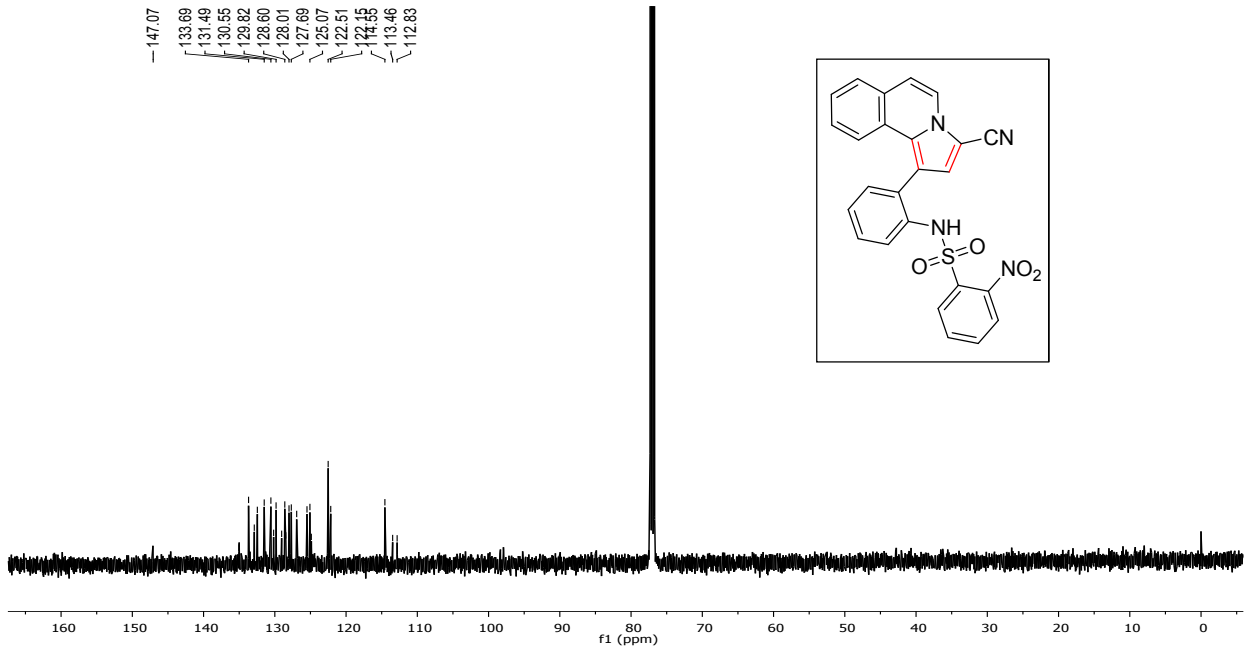
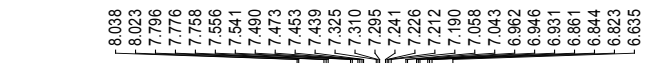
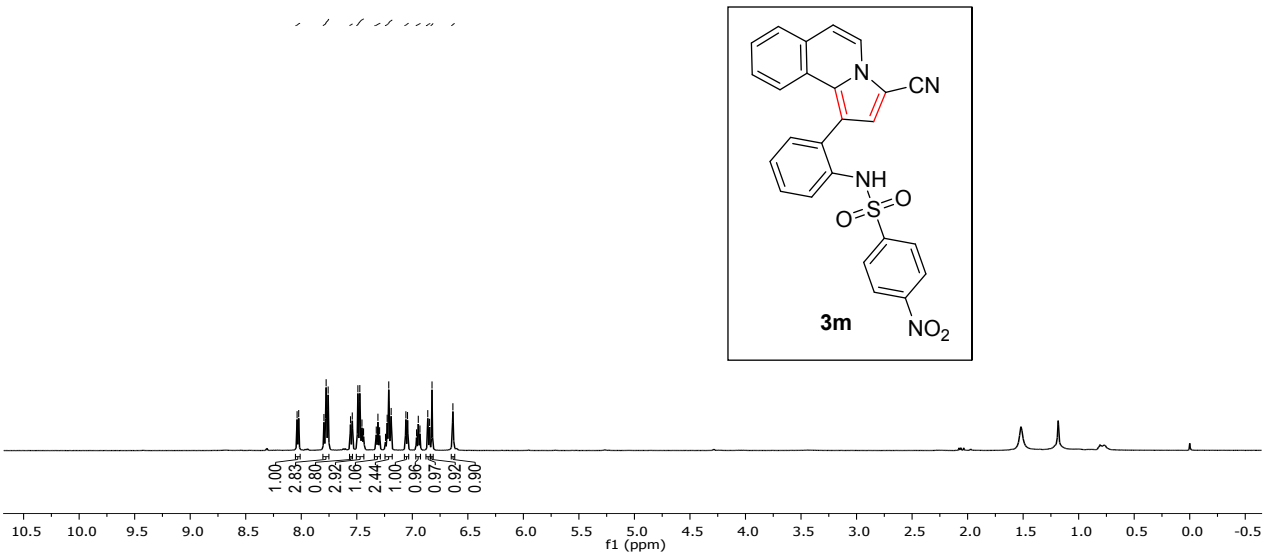
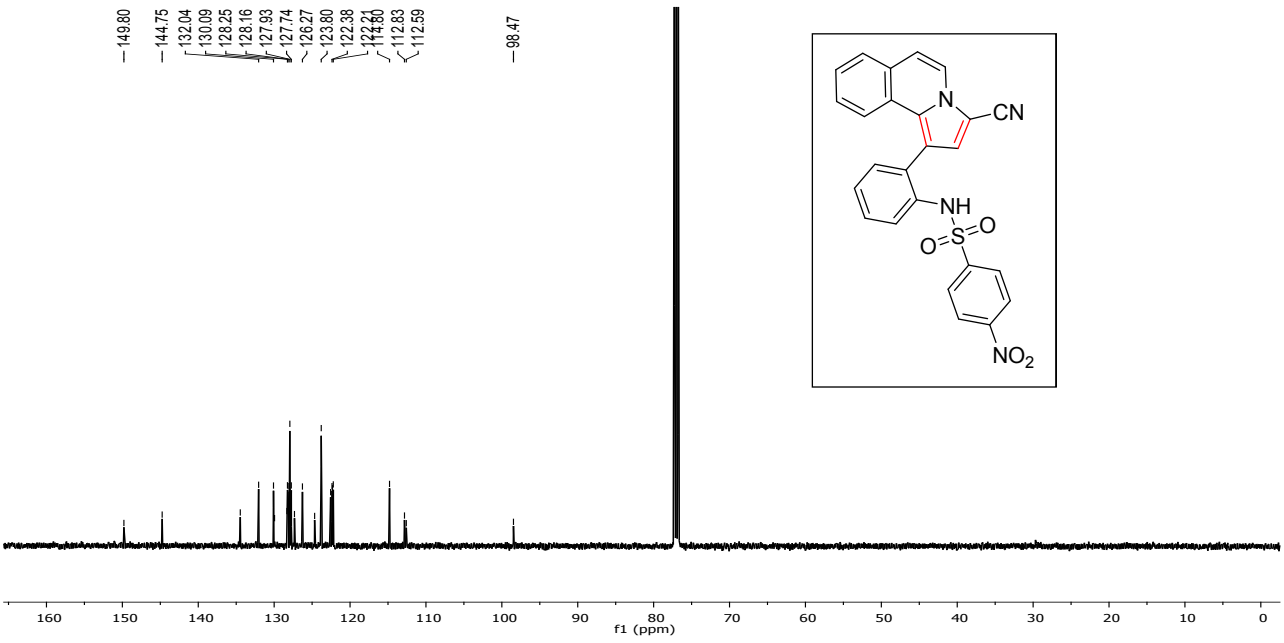




^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **3m**







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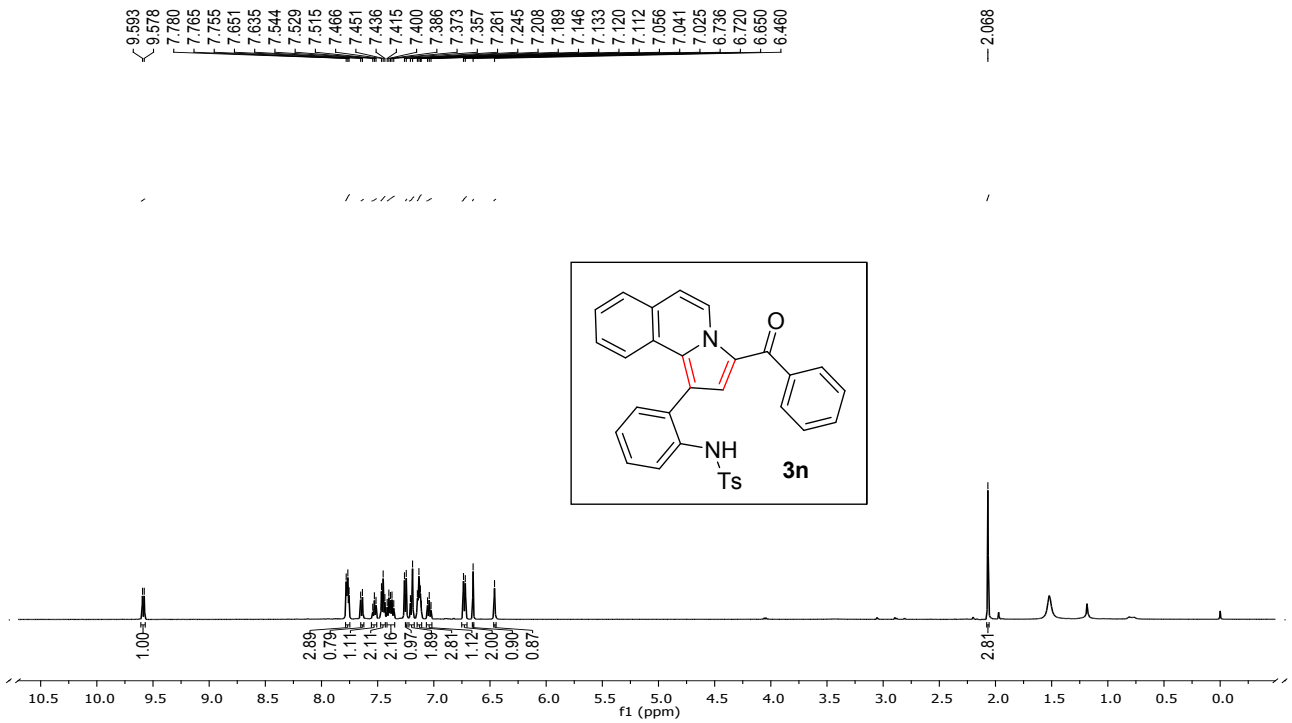

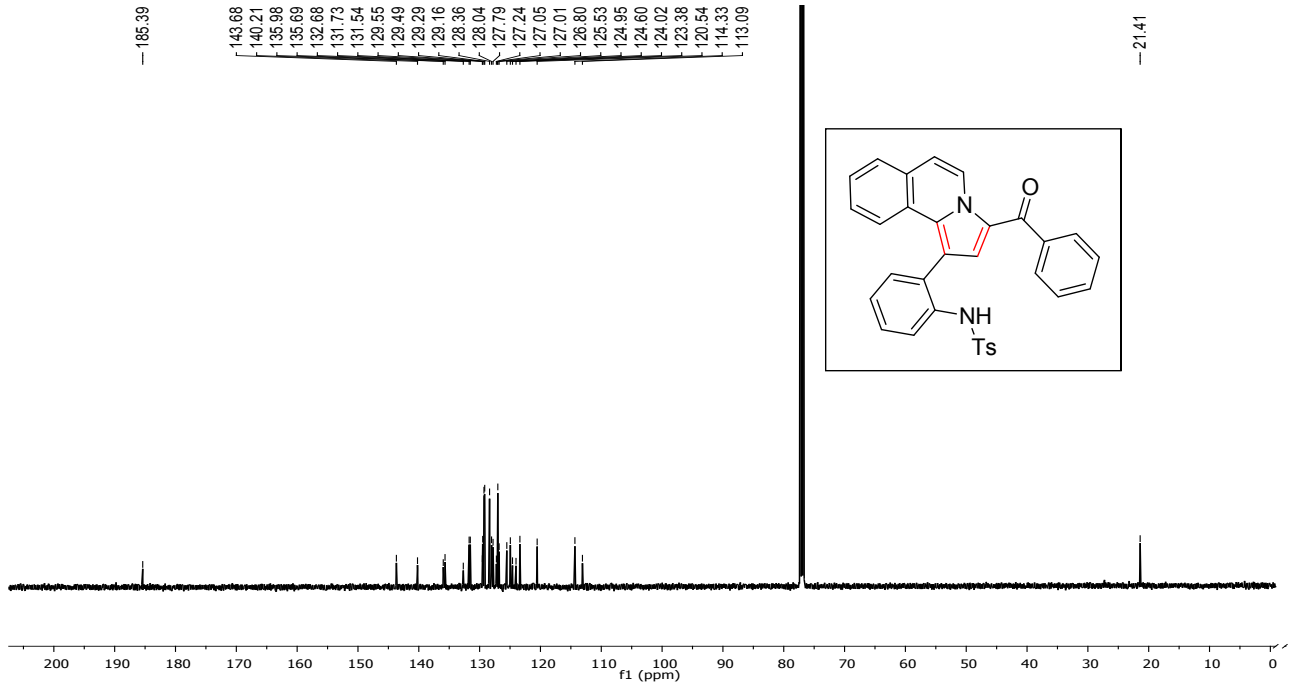

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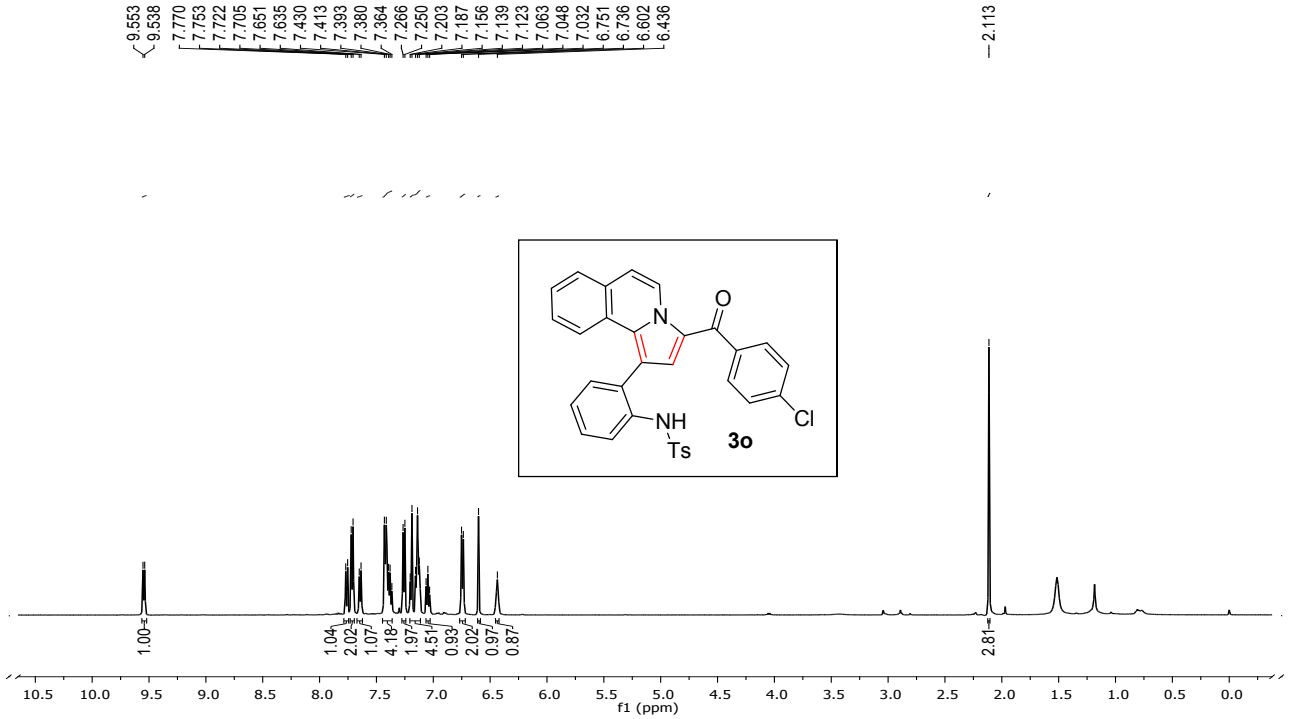

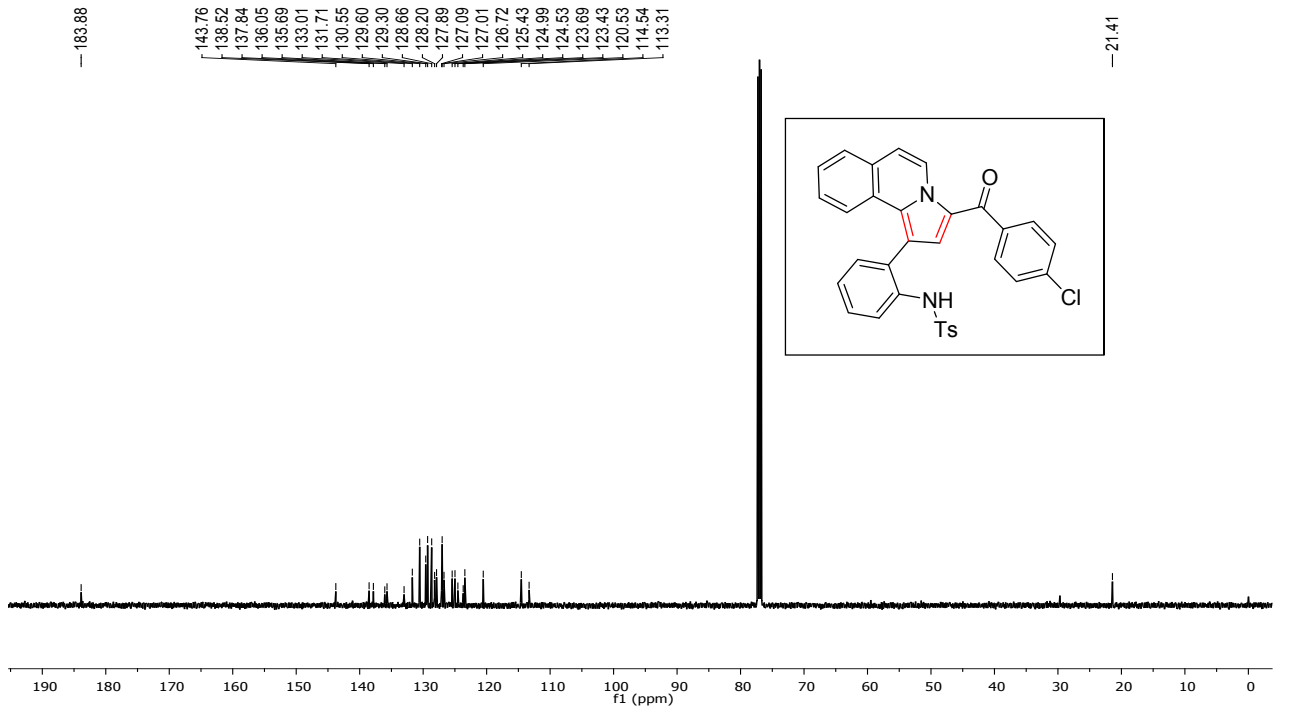

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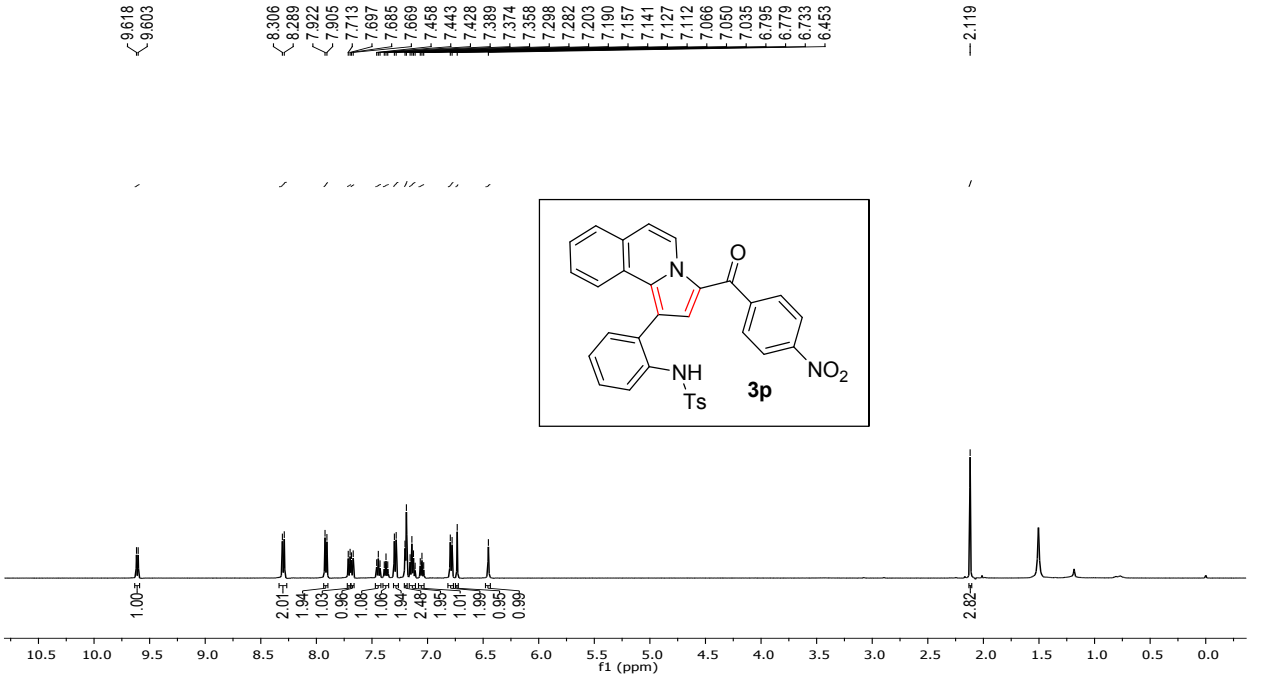

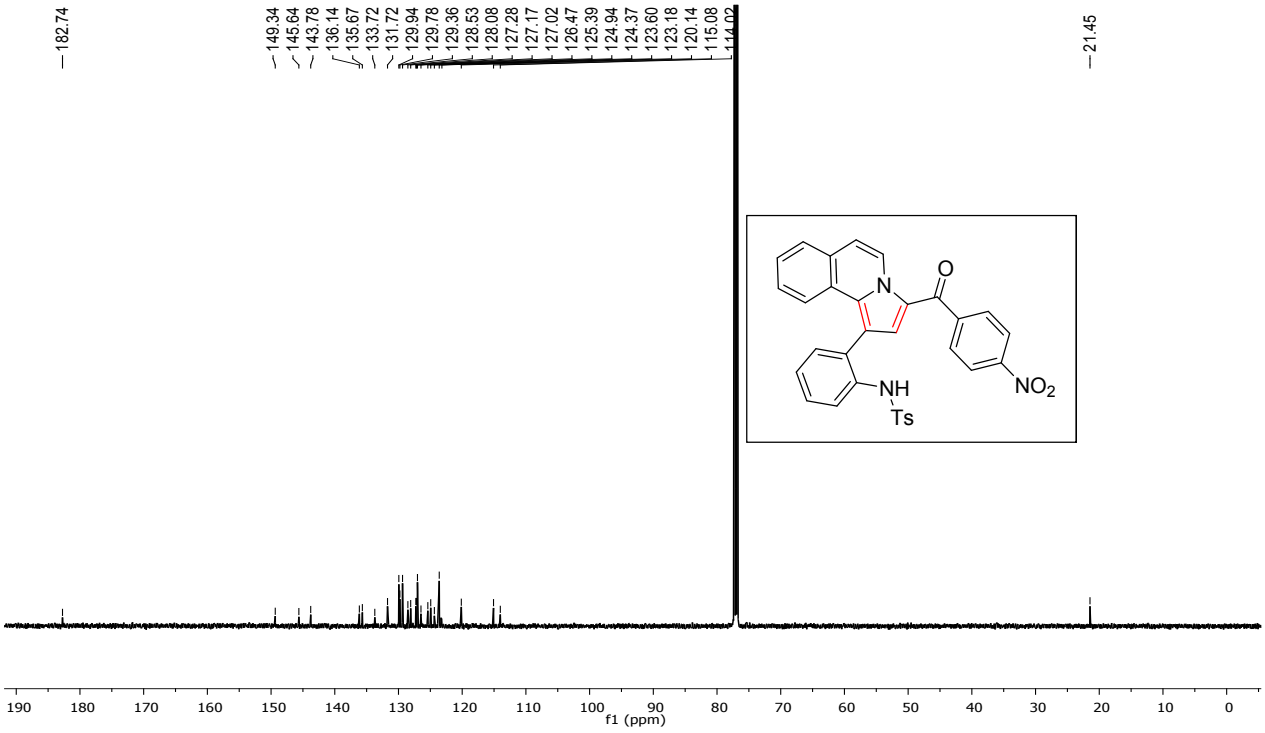

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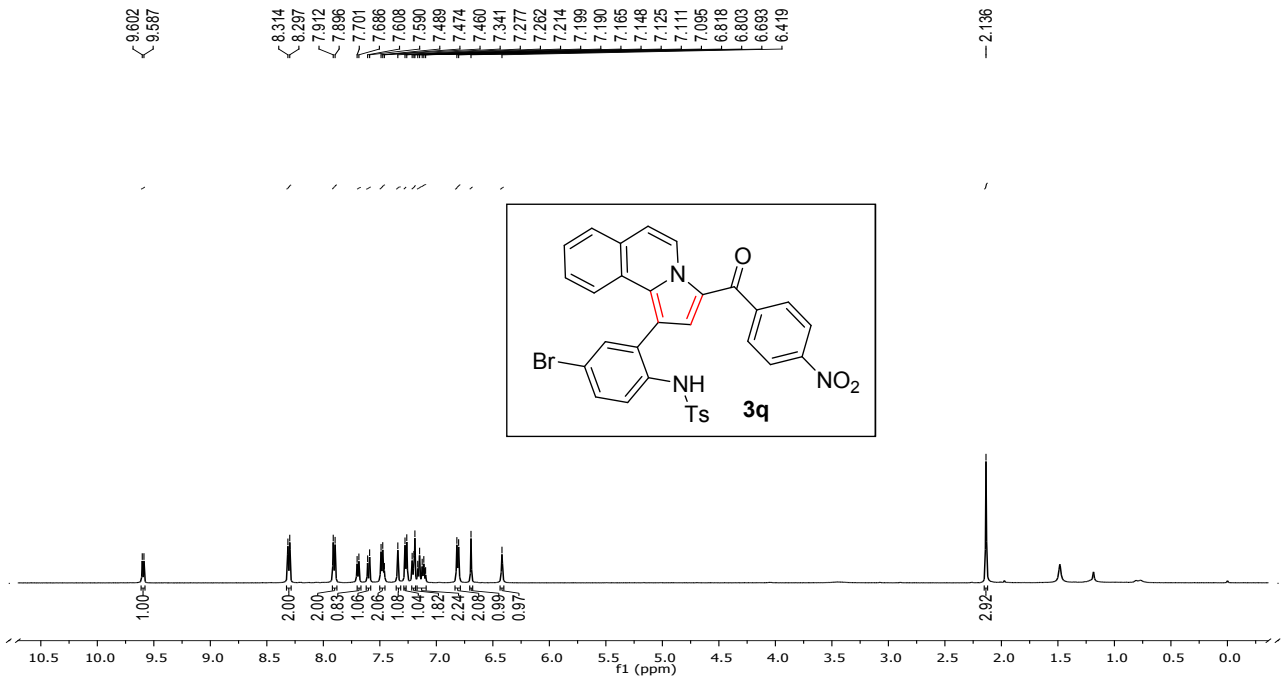

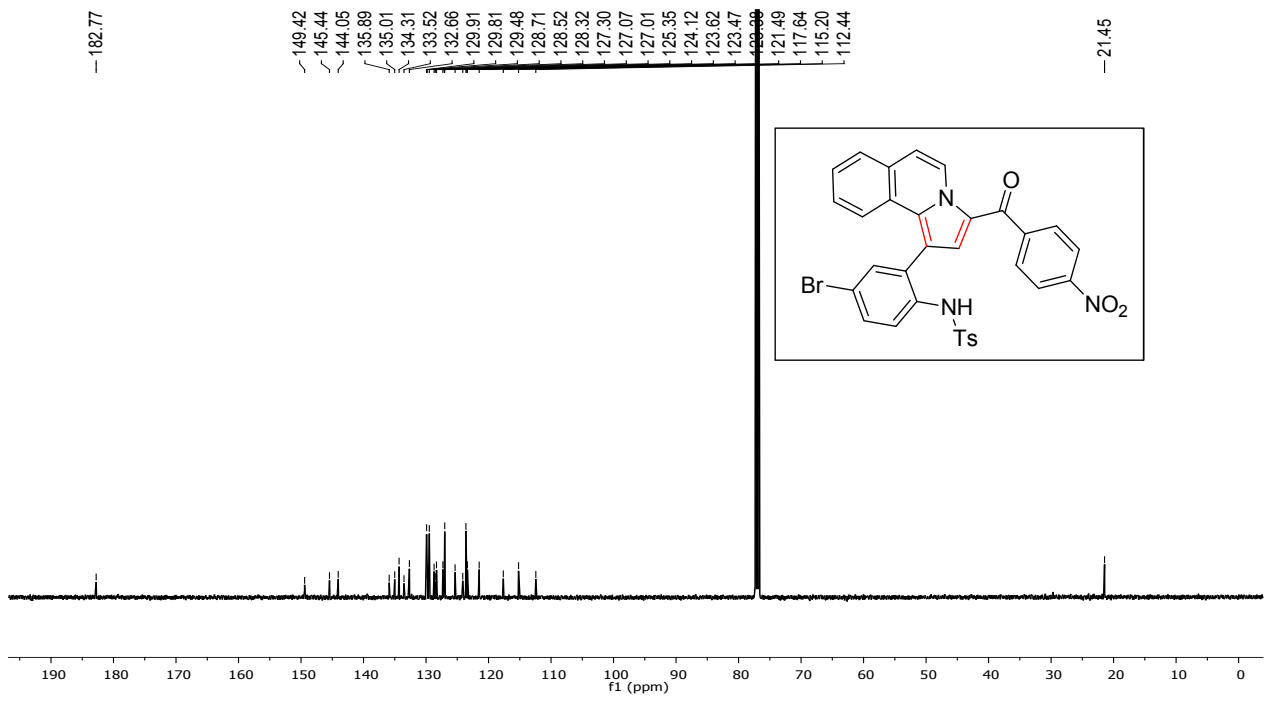

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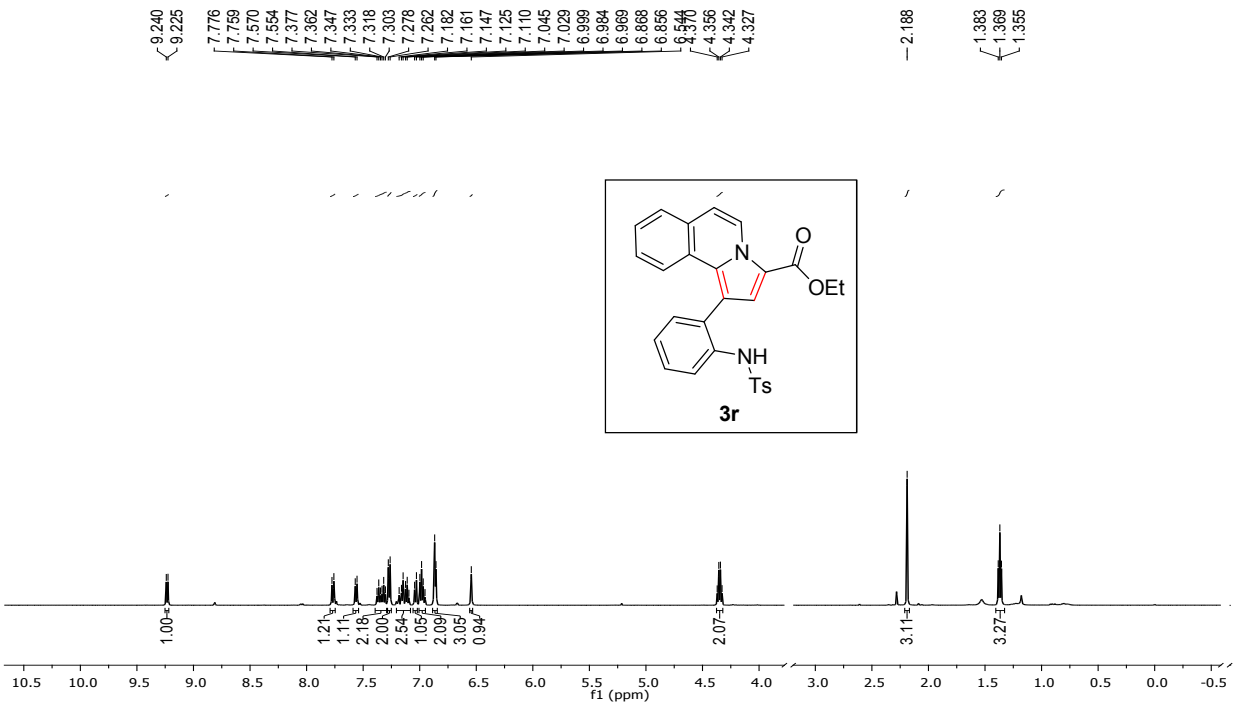

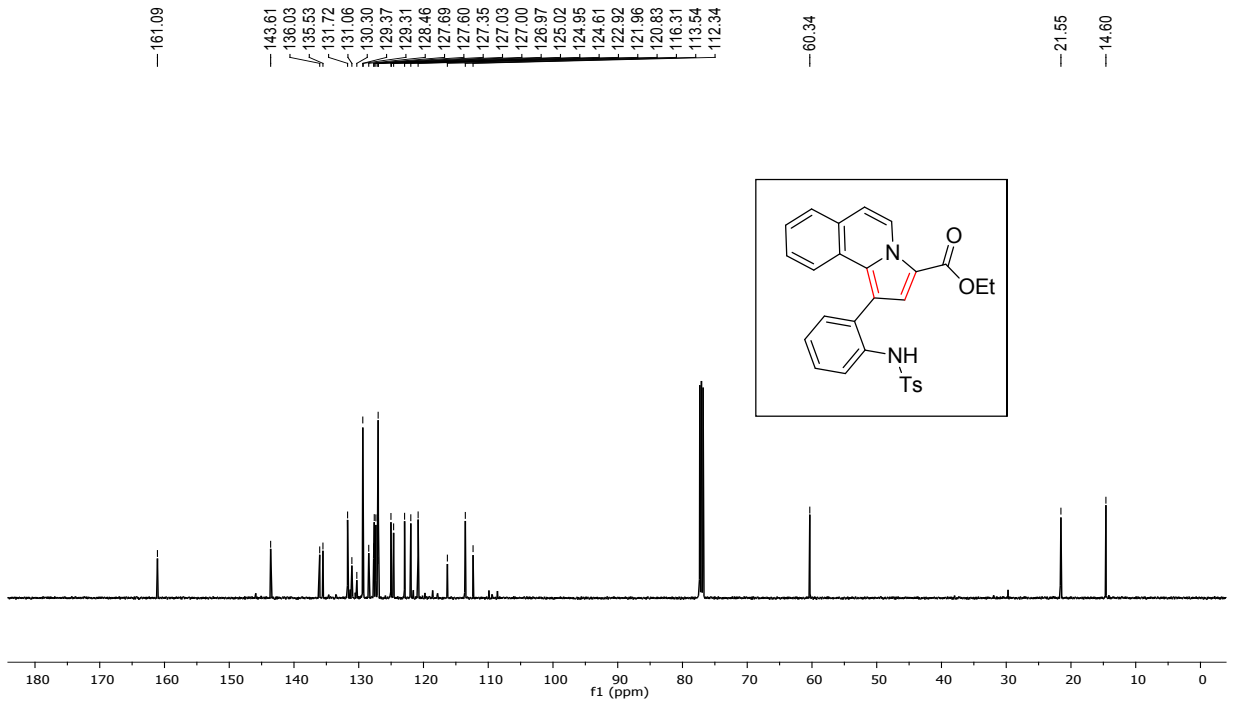

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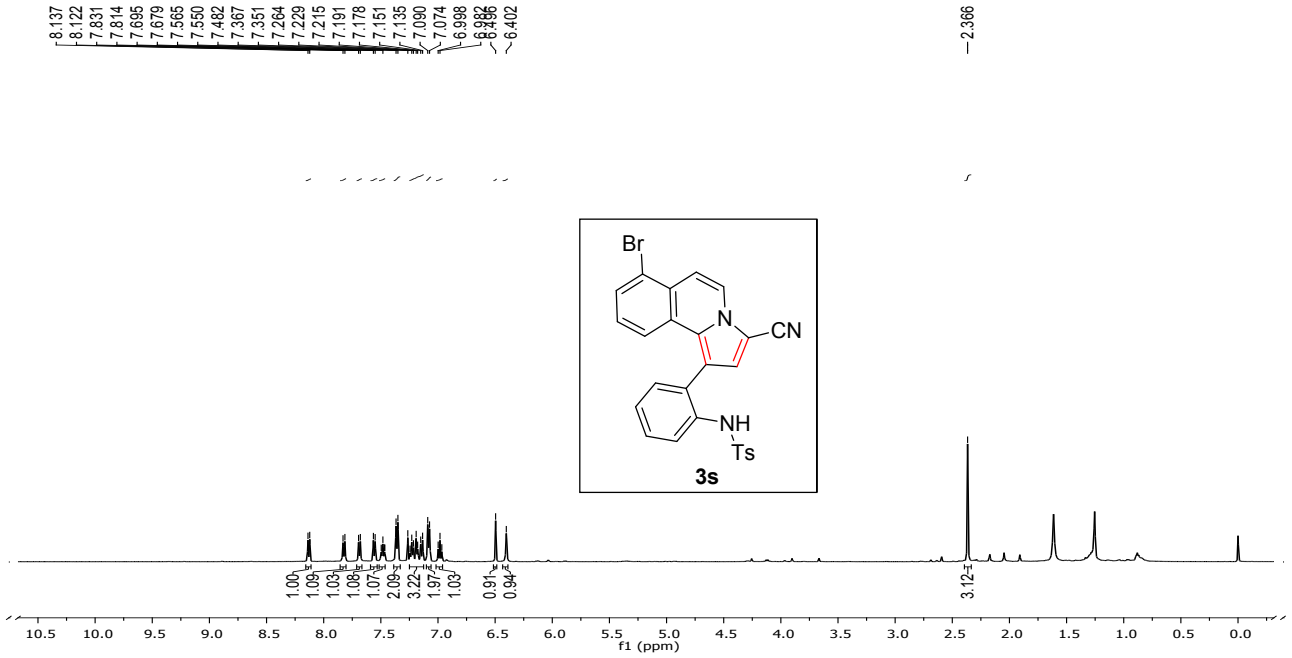

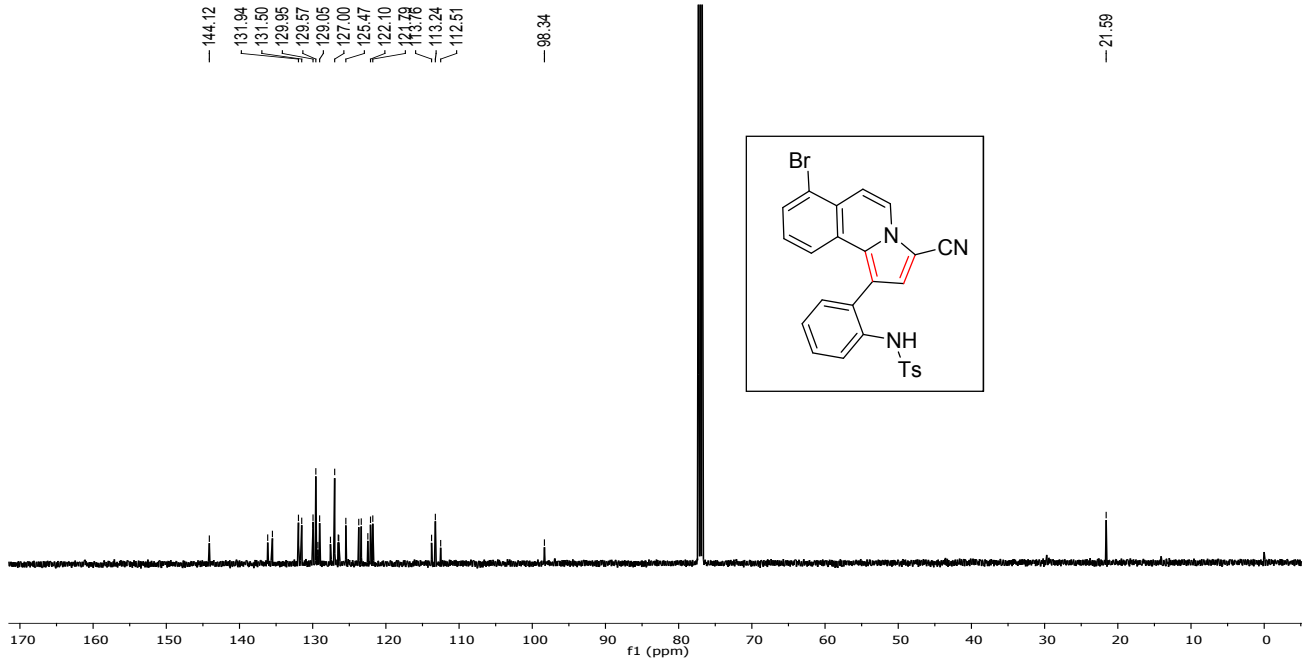

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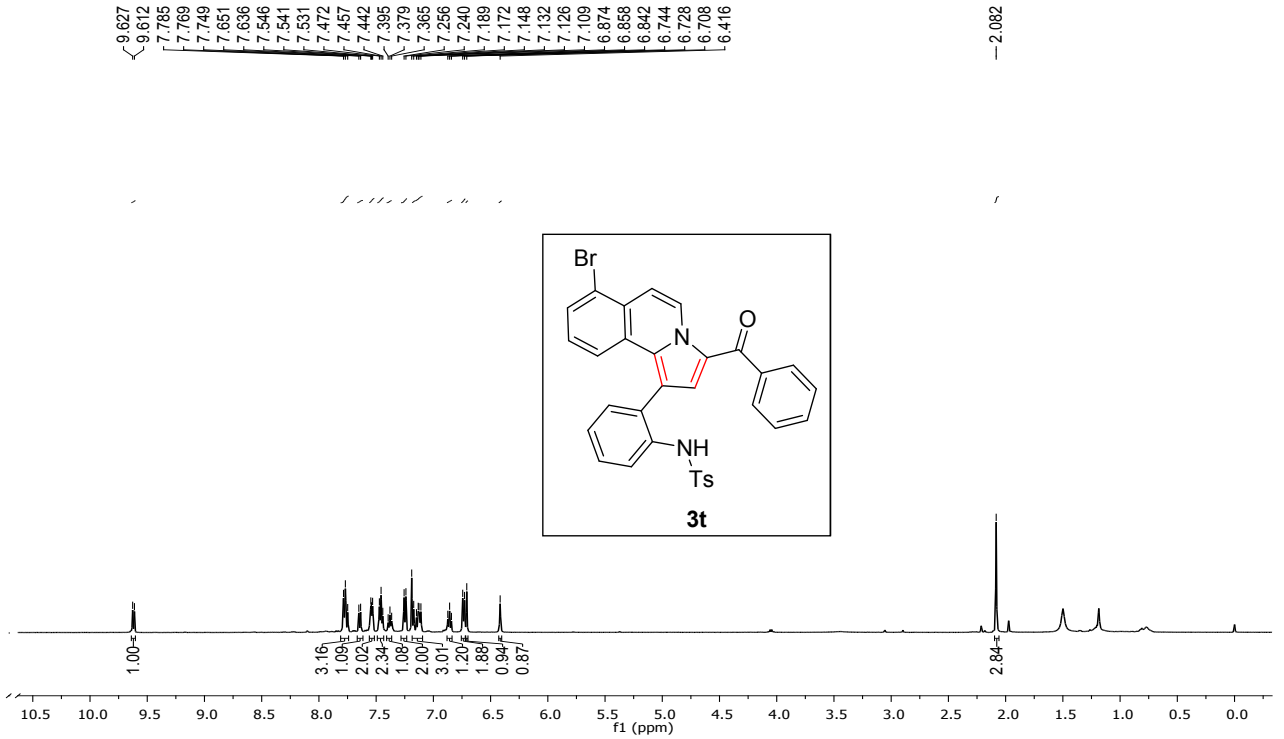

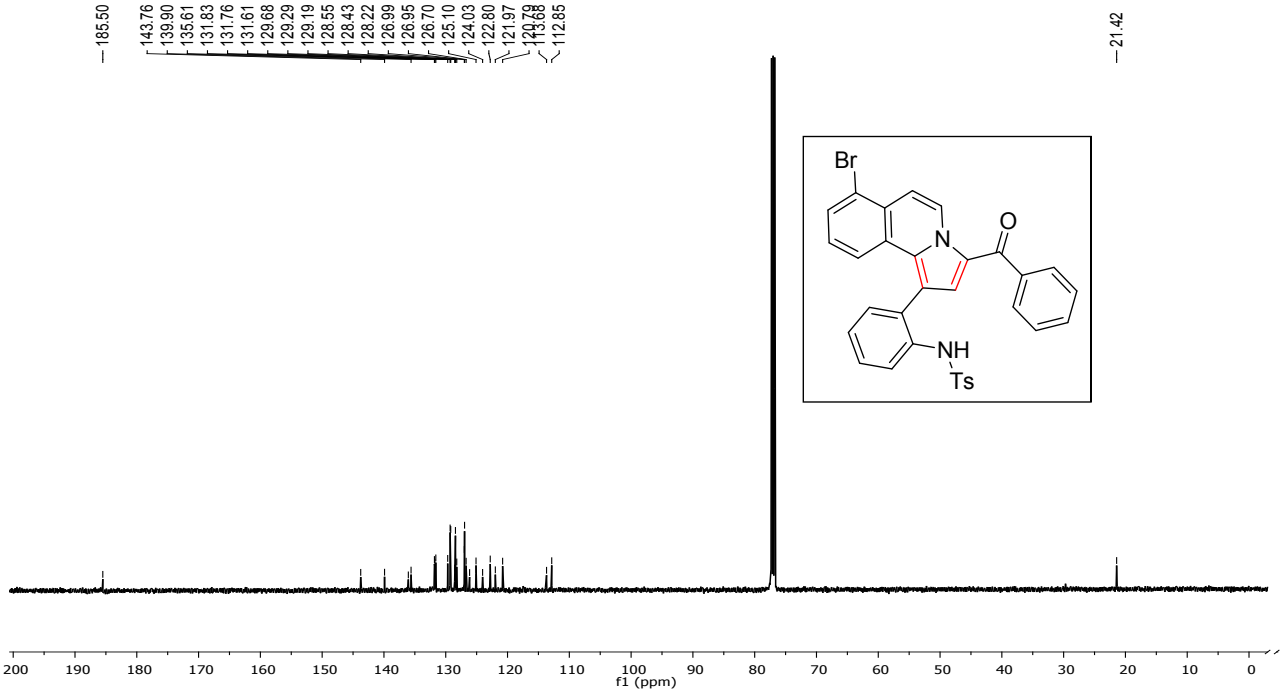

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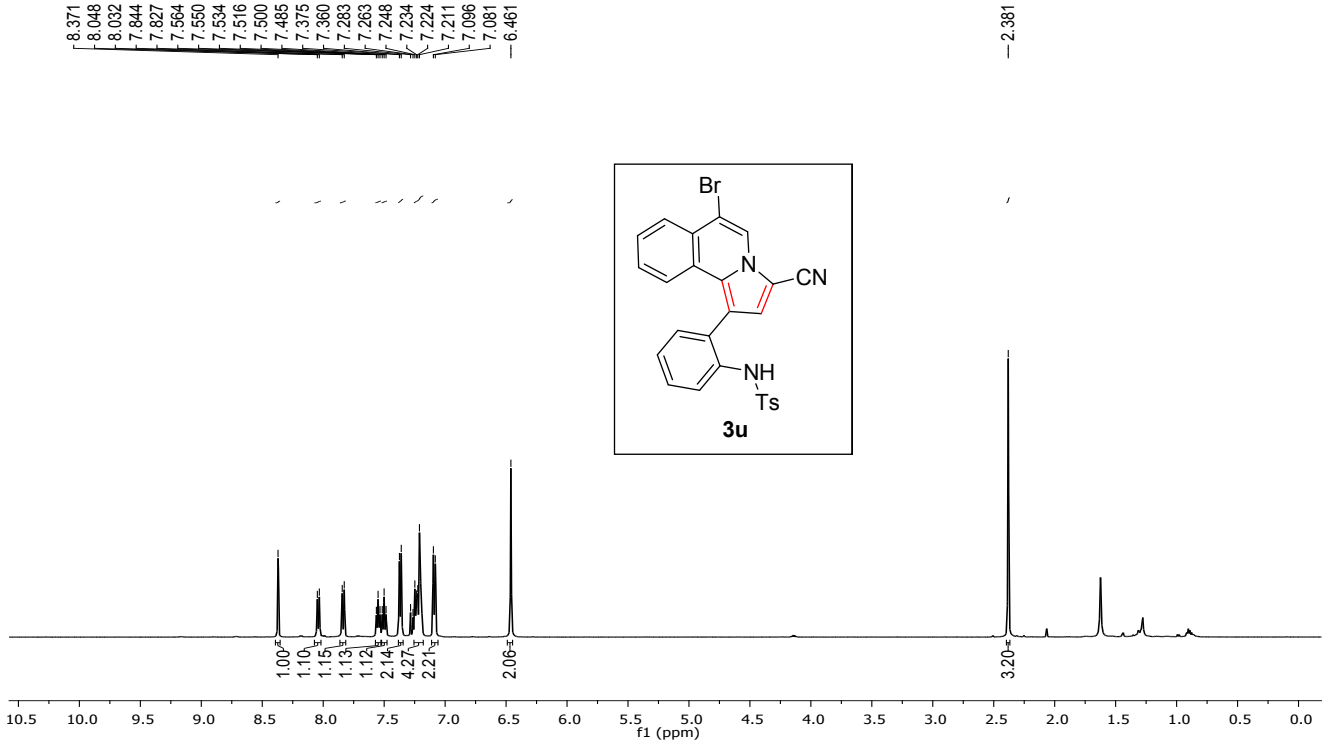

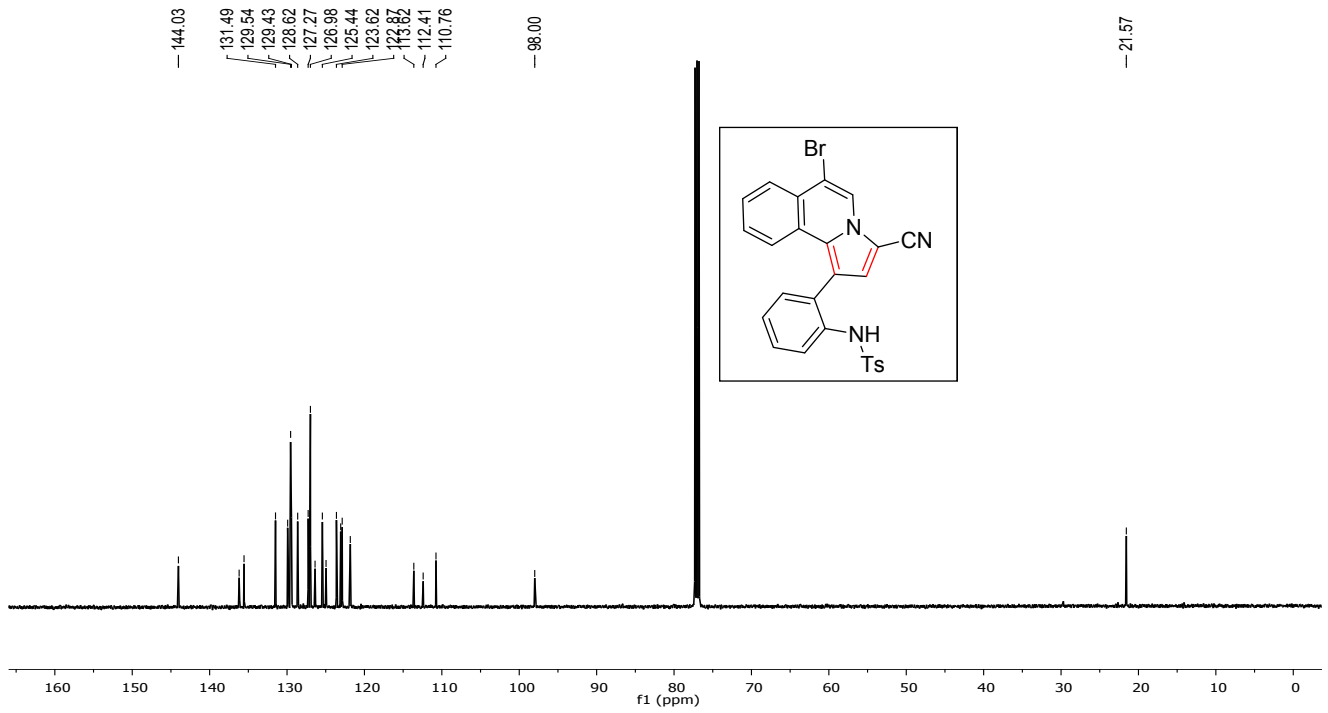

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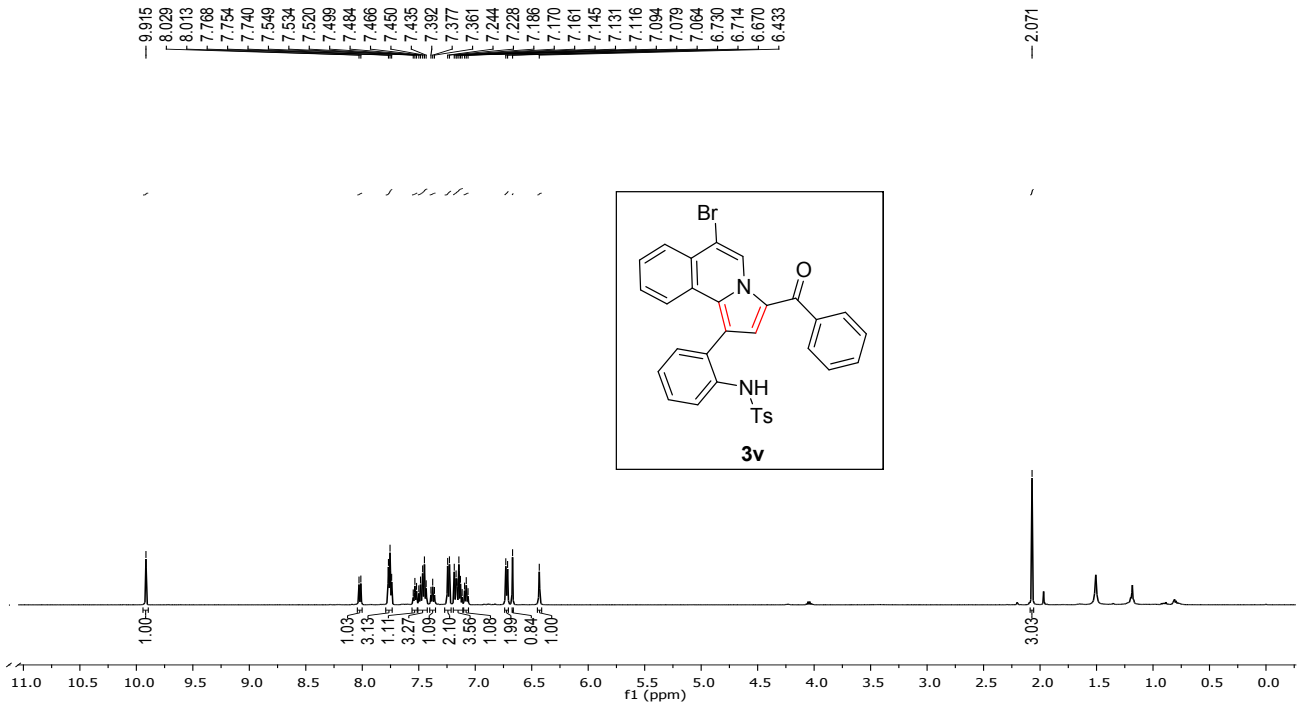

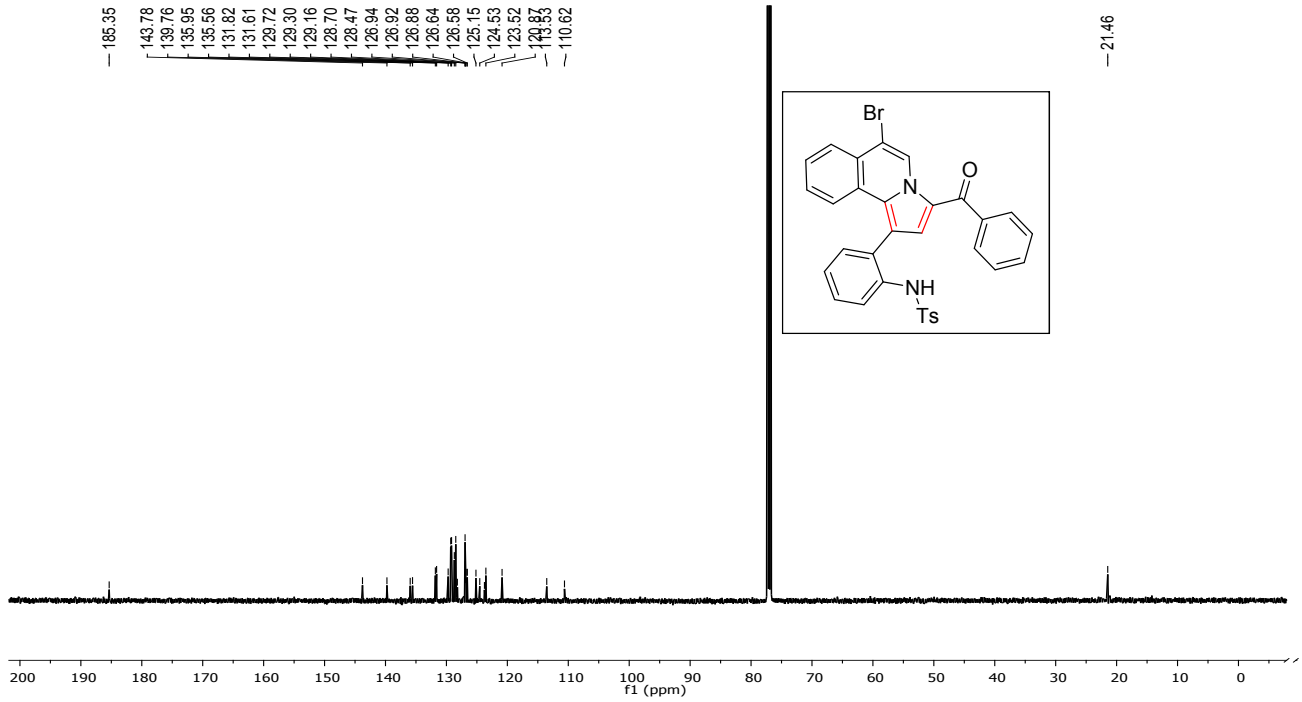

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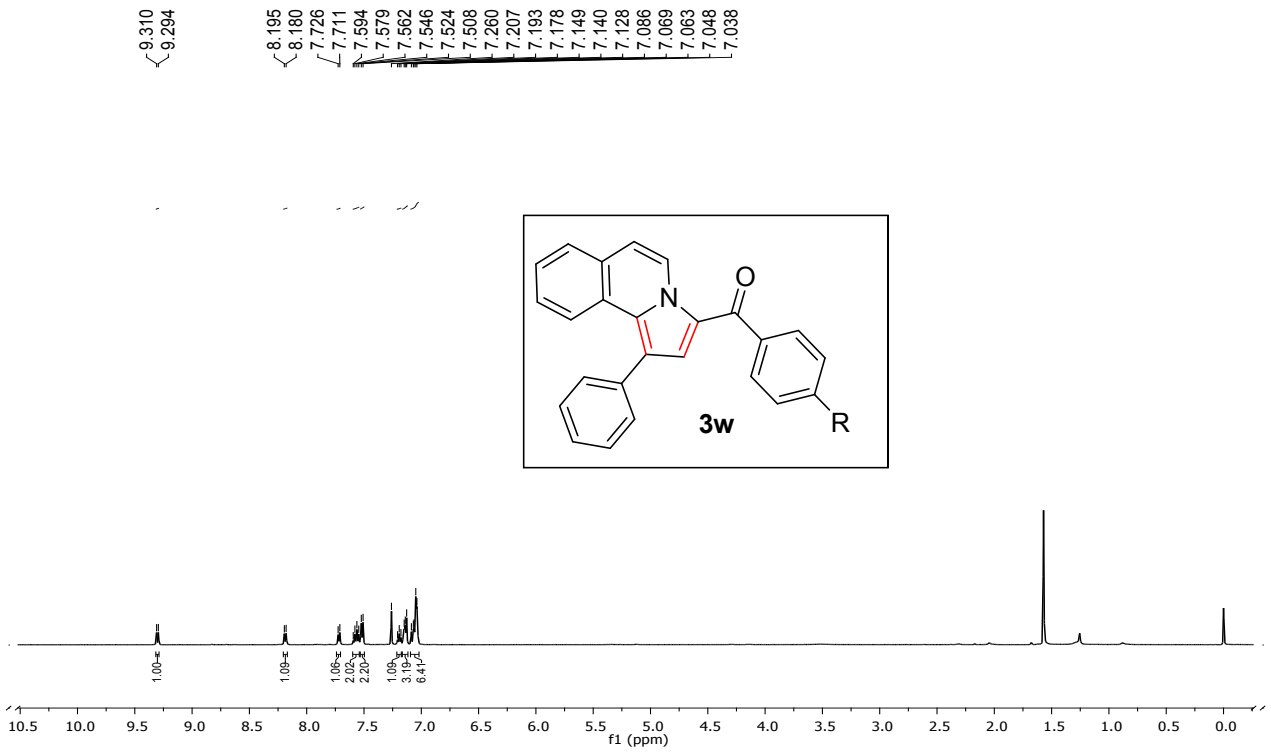
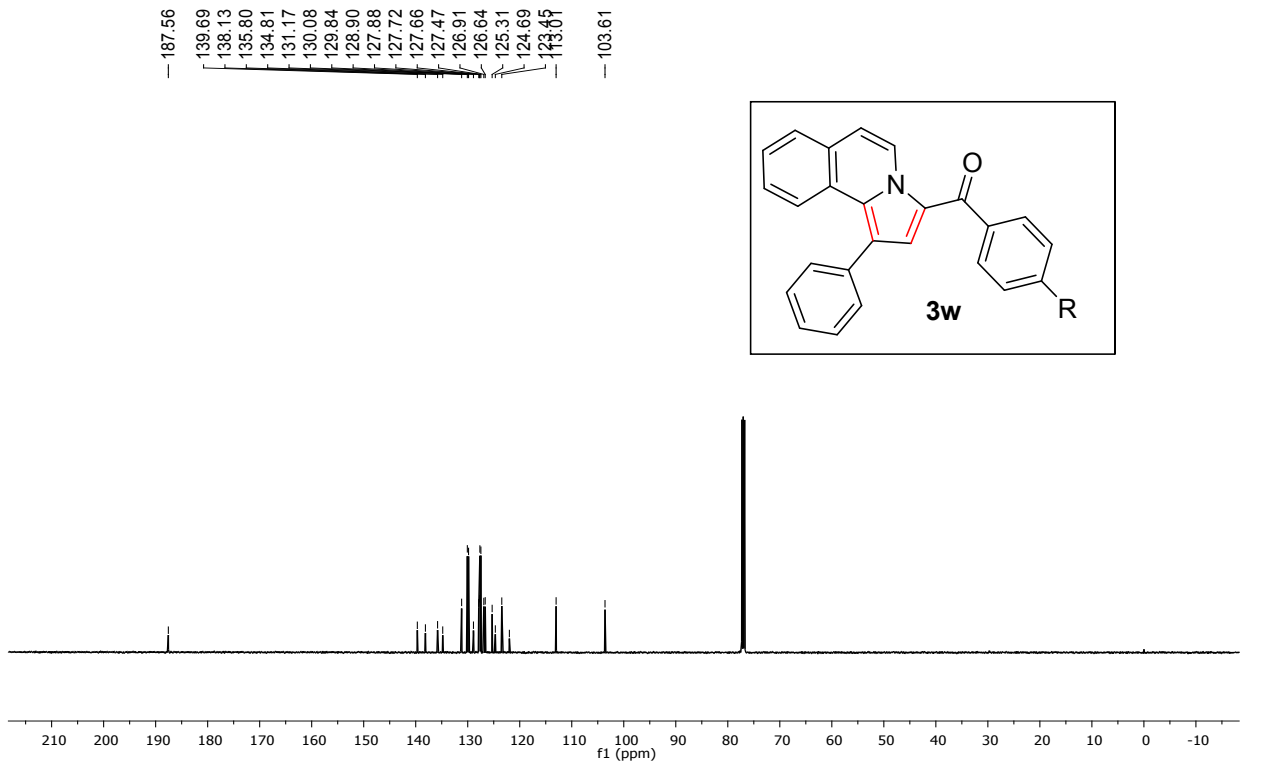
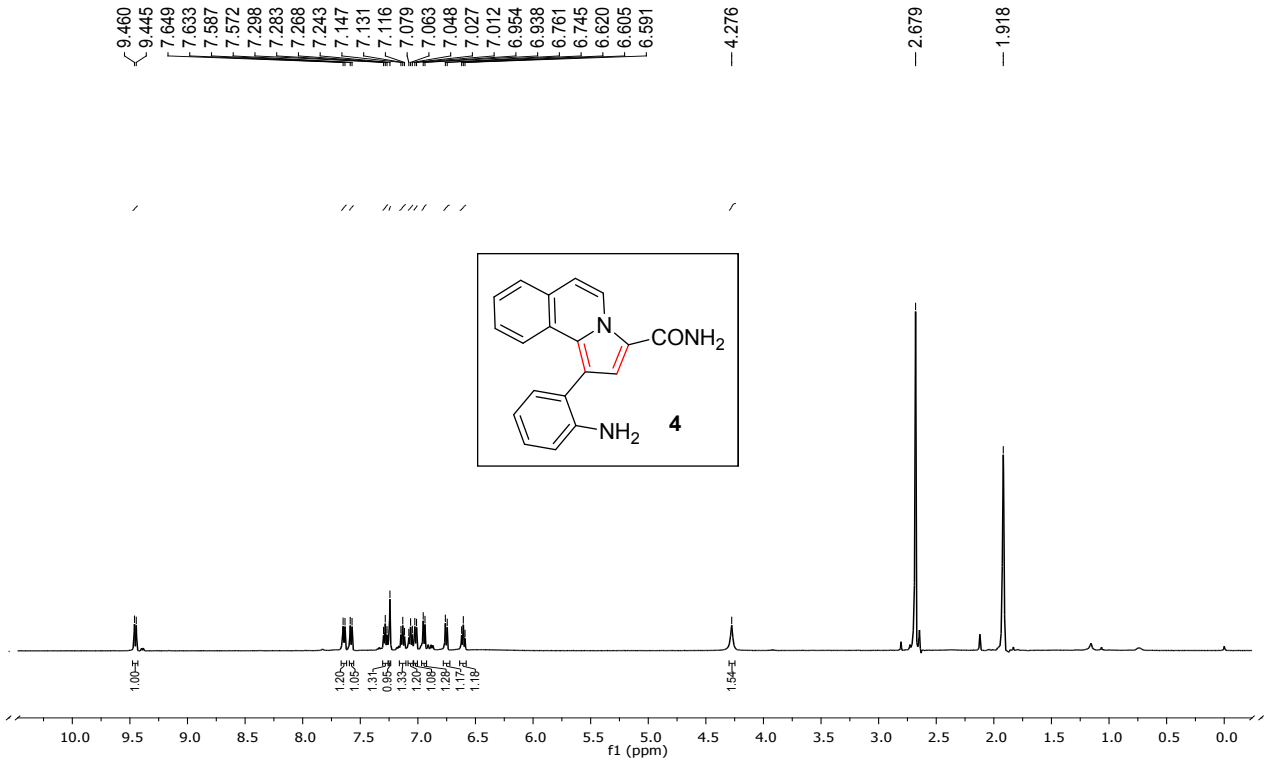
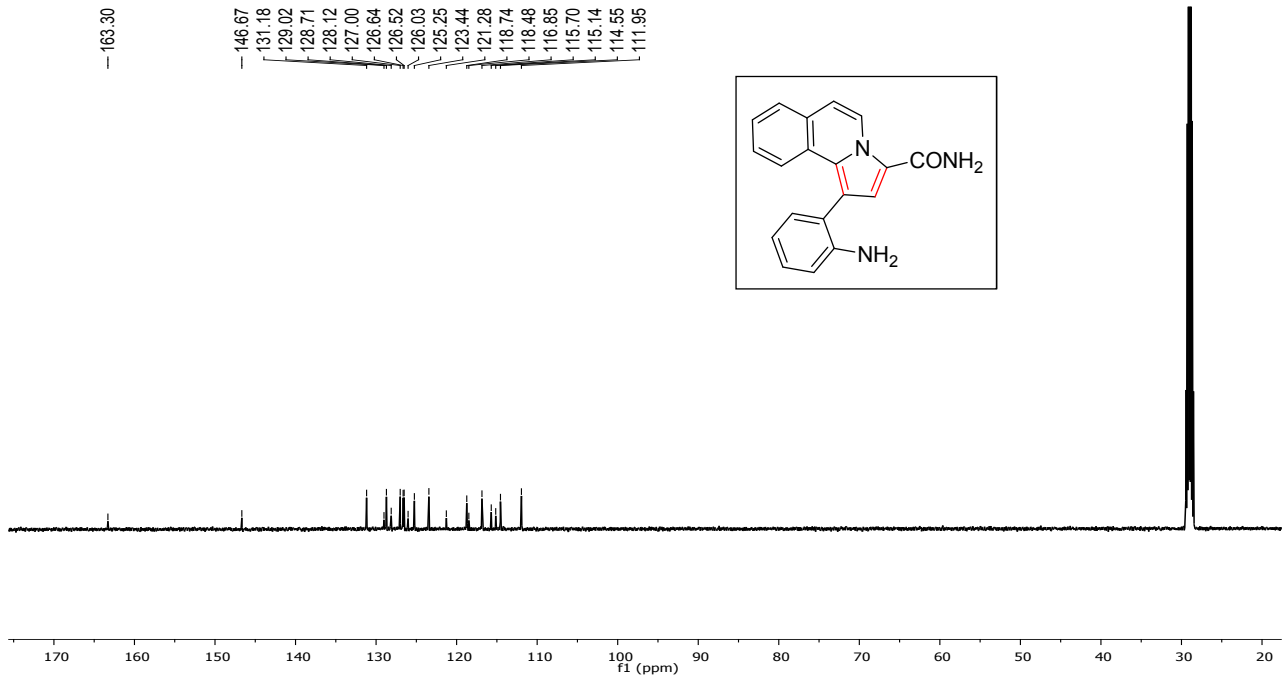


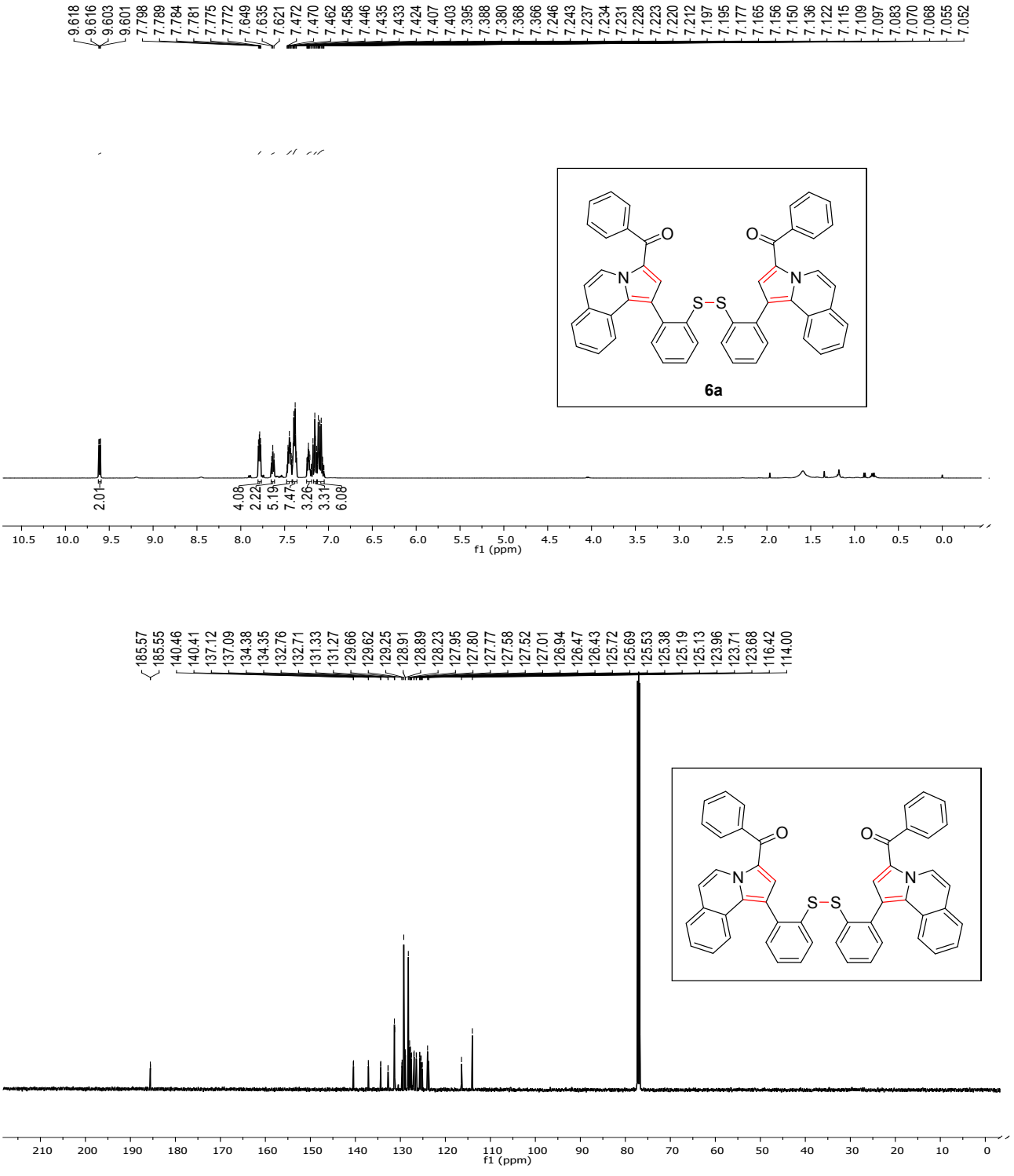


^{1}H NMR (500 MHz, $(CD_3)_2CO$) &^{13}C{^{1}H} (125 MHz, $(CD_3)_2CO$) Spectra of **4**

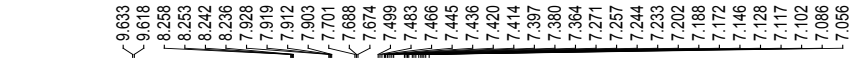


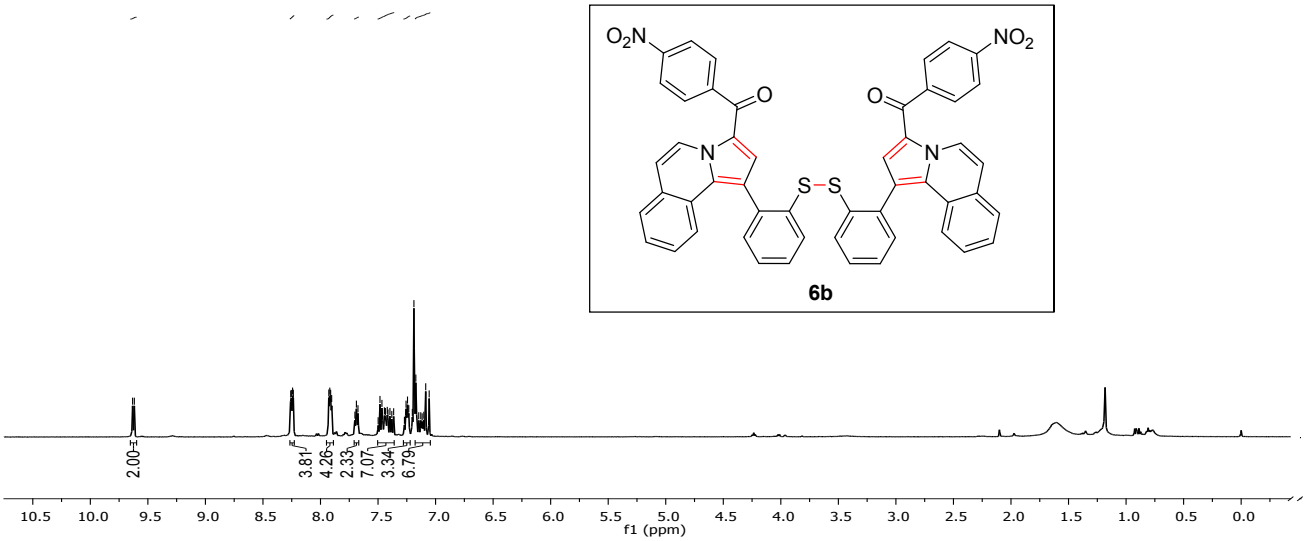


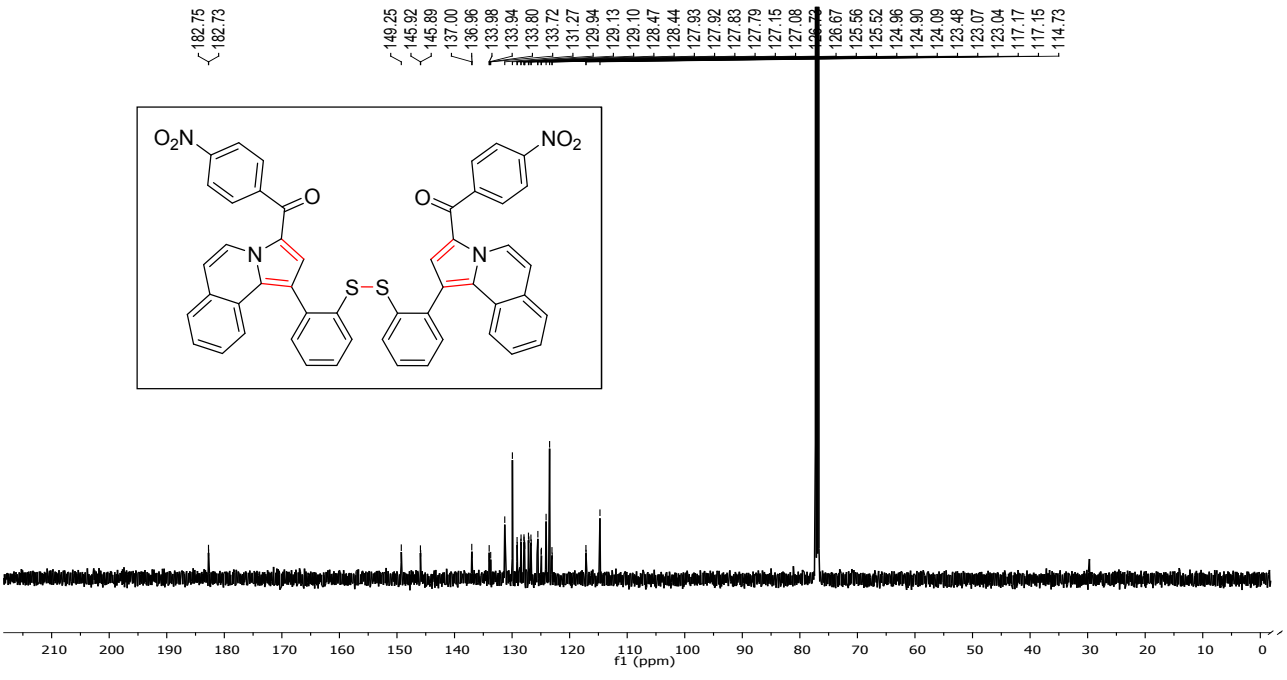
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **6a**



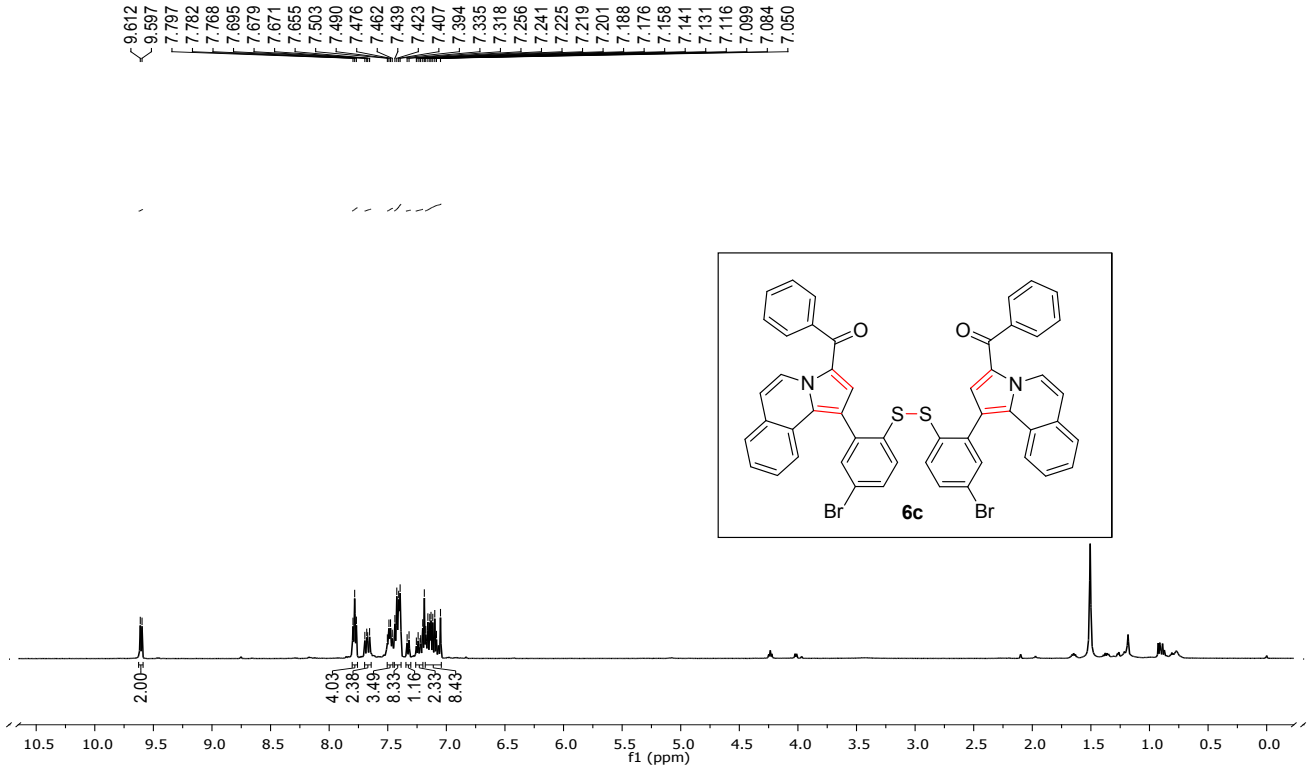
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C (125 MHz, $CDCl_3$) Spectra of **6b**

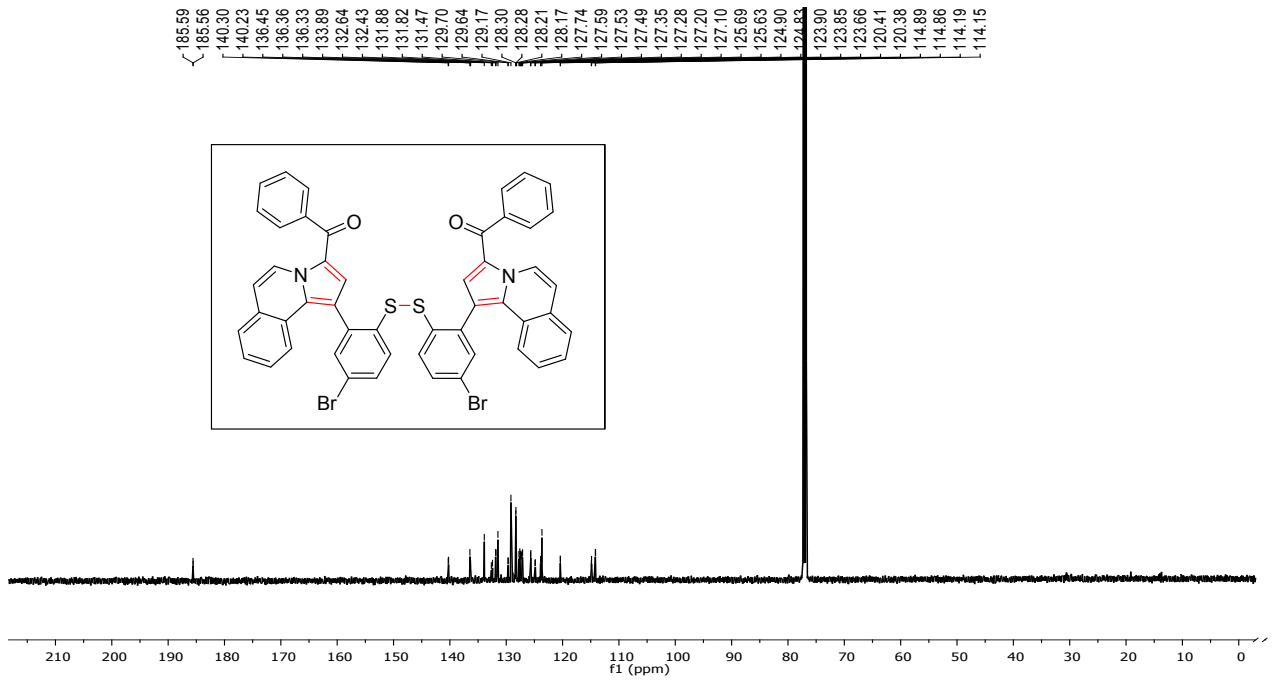




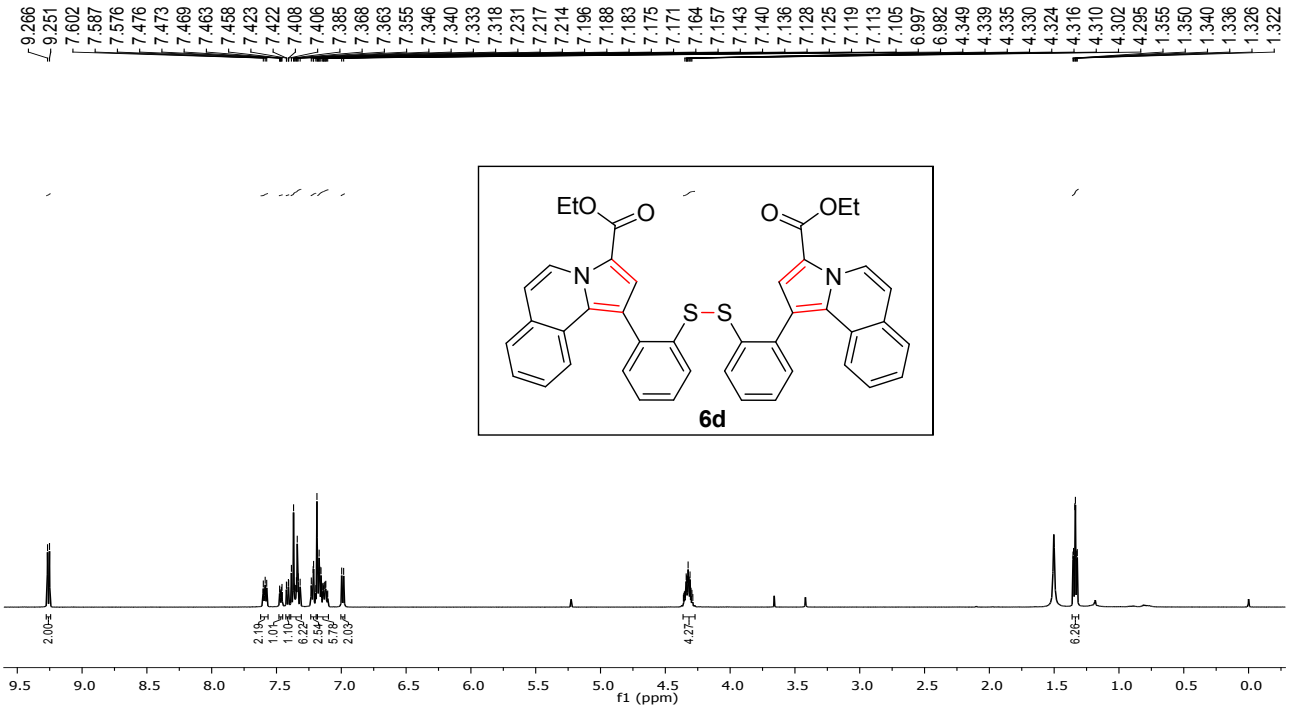


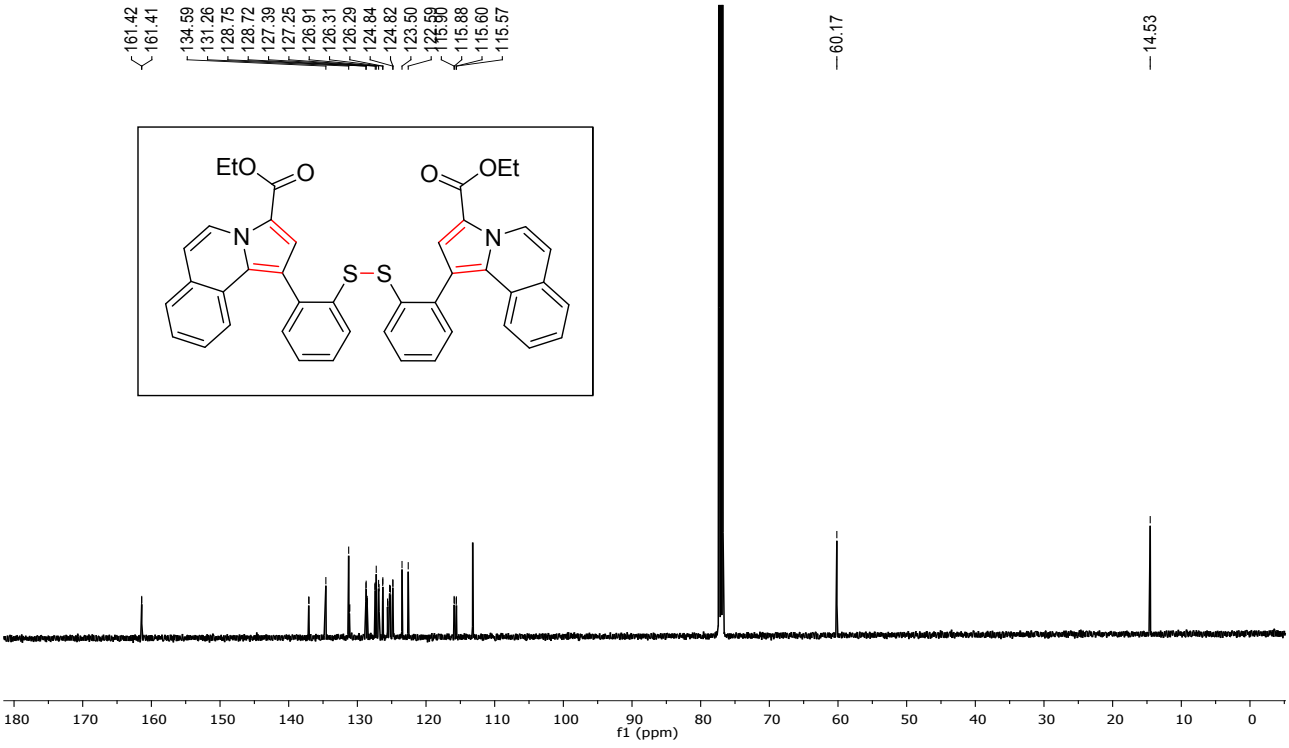
^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **6c**



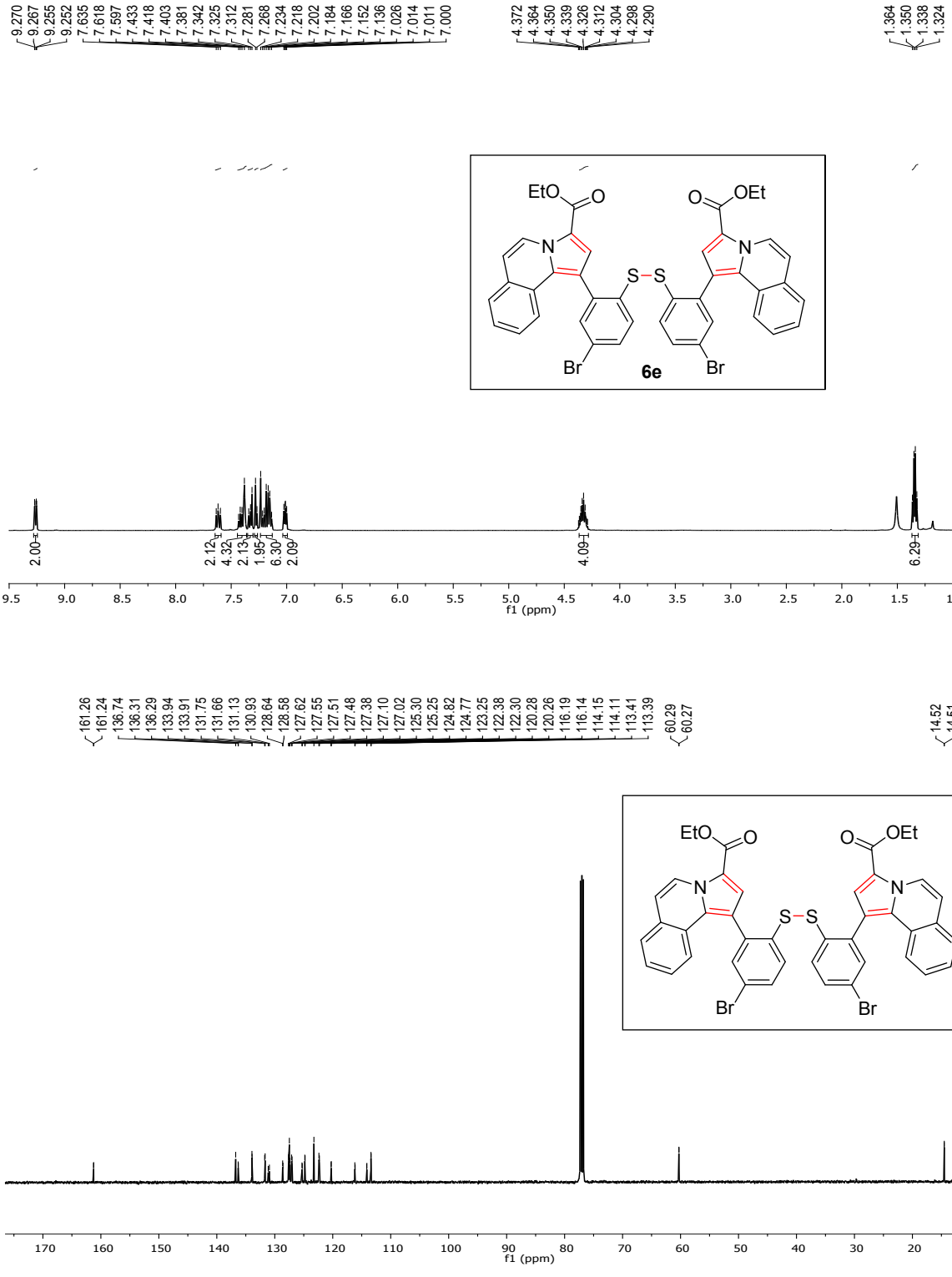


^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$)Spectra of **6d**





^{1}H NMR (500 MHz, $CDCl_3$) &^{13}C{^{1}H} (125 MHz, $CDCl_3$) Spectra of **6e**



4. Single crystal X-ray of 3a and 6a

Single crystal X-ray of 3a (CCDC: 2042168, 30% ellipsoid contour probability level)

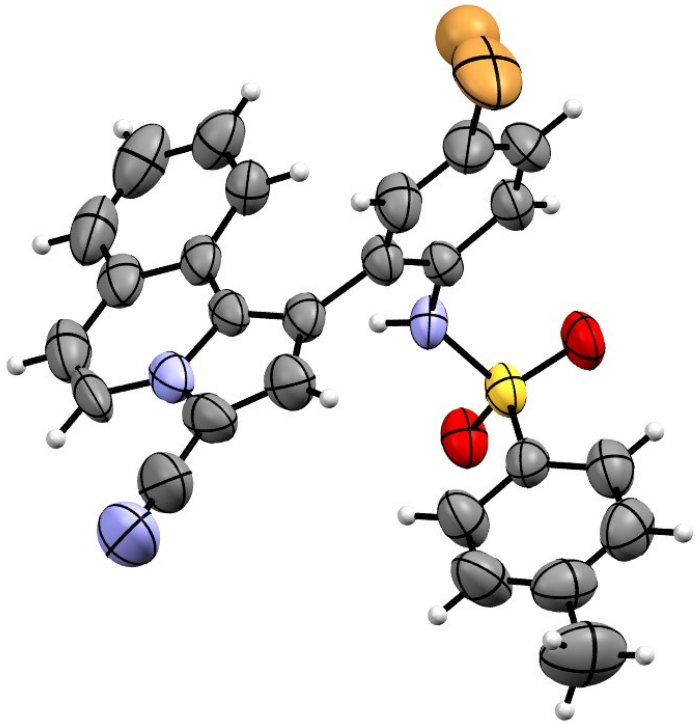


Table 1 Crystal data and structure refinement for DATAM.

Identification code	DATAM
Empirical formula	$C_{26}H_{18}BrN_3O_2S$
Formula weight	516.40
Temperature/K	298
Crystal system	triclinic
Space group	P-1
a/Å	10.479(6)
b/Å	11.171(5)
c/Å	12.250(6)
α/°	64.87(5)
β/°	73.59(6)
γ/°	66.24(5)
Volume/Å^3	1177.5(12)
Z	2

ρ_{calc}g/cm^3	1.456
μ/mm^{-1}	1.863
F(000)	524.0
Crystal size/mm^3	0.22 × 0.2 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.032 to 51
Index ranges	-12 ≤ h ≤ 11, -13 ≤ k ≤ 7, -14 ≤ l ≤ 14
Reflections collected	9288
Independent reflections	4280 [R_{int} = 0.0495, R_{sigma} = 0.0897]
Data/restraints/parameters	4280/0/304
Goodness-of-fit on F^2	1.070
Final R indexes [I>=2σ (I)]	R_1 = 0.0729, wR_2 = 0.1374
Final R indexes [all data]	R_1 = 0.1614, wR_2 = 0.1722
Largest diff. peak/hole / e Å^{-3}	0.38/-0.40

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

Atom	*x*	*y*	*z*	U(eq)
S23	4149.5(15)	3823.3(13)	4378.7(11)	58.0(4)
O24	3512(4)	2838(3)	4516(3)	72.4(11)
O25	5015(4)	3500(3)	5262(3)	66.3(10)
N1	3108(5)	9508(4)	3506(5)	66.6(12)
N15	5168(7)	11193(6)	1015(6)	129(2)
N22	2883(4)	5301(4)	4413(3)	53.0(11)
C2	2238(5)	8668(4)	3947(5)	54.9(13)
C3	1529(6)	8443(5)	5169(5)	56.5(14)
C4	1840(6)	8951(5)	5909(5)	68.1(15)
C5	2801(7)	9741(6)	5390(7)	83.4(19)
C6	3375(6)	10019(5)	4250(7)	77.2(18)
C7	513(6)	7772(5)	5649(5)	63.2(15)
C8	-130(6)	7574(5)	6818(5)	78.2(18)
C9	200(9)	8024(7)	7574(6)	98(2)
C10	1168(8)	8710(7)	7109(7)	92(2)
C11	3643(6)	9636(6)	2301(6)	77.8(17)
C12	3161(6)	8885(5)	1985(5)	72.9(17)
C13	2299(6)	8269(5)	2976(5)	56.7(14)
C14	4495(8)	10483(7)	1597(7)	104(2)

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

Atom	*x*	*y*	*z*	U(eq)
C16	1510(6)	7419(5)	2971(4)	54.9(13)
C17	462(6)	8063(6)	2233(5)	73.1(16)
C18	-326(6)	7340(7)	2208(6)	82.6(18)
C19	-78(6)	5949(6)	2922(5)	73.6(16)
C20	975(6)	5283(5)	3645(4)	60.9(14)
C21	1808(5)	5990(5)	3656(4)	48.2(12)
C26	5139(6)	4202(5)	2933(4)	57.4(14)
C27	5862(6)	5138(6)	2564(5)	77.6(18)
C28	6691(7)	5384(7)	1456(6)	90(2)
C29	6833(7)	4710(8)	695(5)	86.6(19)
C30	6107(7)	3790(7)	1064(5)	85.6(19)
C31	5265(6)	3530(5)	2167(5)	73.2(17)
C32	7794(8)	4975(8)	-516(5)	135(3)
Br1	-1703(2)	8309.4(11)	1108(3)	130.0(10)
Br1A	-2194(8)	8205(8)	1873(11)	104(3)

Table 3 Anisotropic Displacement Parameters (Å^2×10^3) for DATAM. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
S23	70.4(11)	42.0(7)	67.4(8)	-17.0(7)	-18.7(7)	-20.2(7)
O24	86(3)	46(2)	96(2)	-22.2(19)	-18(2)	-31(2)
O25	84(3)	52(2)	67(2)	-15.4(18)	-35.8(19)	-16(2)
N1	61(3)	42(3)	98(3)	-22(3)	-23(3)	-13(2)
N15	121(6)	107(5)	169(6)	-58(4)	26(5)	-69(4)
N22	69(3)	40(2)	57(2)	-22(2)	-18(2)	-13(2)
C2	50(4)	33(3)	82(4)	-17(3)	-20(3)	-11(3)
C3	58(4)	37(3)	75(4)	-22(3)	-22(3)	-5(3)
C4	66(4)	48(3)	92(4)	-28(3)	-32(3)	-1(3)
C5	93(6)	66(4)	111(5)	-41(4)	-48(4)	-12(4)
C6	71(5)	52(3)	133(5)	-35(4)	-40(4)	-24(3)
C7	76(4)	56(3)	65(3)	-29(3)	-6(3)	-22(3)
C8	89(5)	57(3)	76(4)	-25(3)	-2(4)	-16(3)
C9	123(7)	70(4)	78(4)	-31(4)	-25(4)	2(4)
C10	108(6)	72(4)	102(5)	-53(4)	-40(4)	4(4)
C11	64(5)	55(4)	109(5)	-16(4)	-10(4)	-29(3)
C12	79(5)	56(3)	79(4)	-16(3)	-8(3)	-29(3)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for DATAM. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C13	58(4)	41(3)	71(3)	-21(3)	-18(3)	-9(3)
C14	97(6)	74(4)	144(6)	-43(5)	5(5)	-41(5)
C16	62(4)	44(3)	64(3)	-19(3)	-14(3)	-19(3)
C17	84(5)	54(3)	88(4)	-26(3)	-32(3)	-13(3)
C18	63(5)	79(4)	121(5)	-53(4)	-39(4)	-1(4)
C19	63(5)	79(4)	99(4)	-42(4)	-19(3)	-27(4)
C20	69(4)	58(3)	66(3)	-25(3)	-8(3)	-29(3)
C21	52(4)	51(3)	49(3)	-21(3)	-9(2)	-20(3)
C26	58(4)	58(3)	66(3)	-31(3)	-13(3)	-15(3)
C27	92(5)	93(4)	72(4)	-35(3)	-5(3)	-52(4)
C28	89(5)	120(5)	82(4)	-38(4)	6(4)	-64(5)
C29	70(5)	117(6)	70(4)	-39(4)	-8(3)	-22(4)
C30	94(6)	99(5)	76(4)	-47(4)	-15(4)	-24(4)
C31	86(5)	67(4)	81(4)	-29(3)	-24(4)	-26(3)
C32	112(7)	197(8)	85(5)	-53(5)	12(4)	-51(6)
Br1	119.2(15)	113.9(8)	174(2)	-40.1(8)	-97.4(15)	-14.3(7)

Table 4 Bond Lengths for DATAM.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S23	O24	1.435(3)	C11	C12	1.357(7)
S23	O25	1.443(3)	C11	C14	1.410(9)
S23	N22	1.658(4)	C12	C13	1.391(7)
S23	C26	1.752(5)	C13	C16	1.492(6)
N1	C2	1.408(6)	C16	C17	1.383(7)
N1	C6	1.396(6)	C16	C21	1.399(6)
N1	C11	1.390(7)	C17	C18	1.382(7)
N15	C14	1.149(7)	C18	C19	1.377(8)
N22	C21	1.417(6)	C18	Br1	1.916(6)
C2	C3	1.434(6)	C18	Br1A	1.877(10)
C2	C13	1.415(6)	C19	C20	1.374(7)
C3	C4	1.416(7)	C20	C21	1.399(6)
C3	C7	1.398(7)	C26	C27	1.384(7)
C4	C5	1.441(8)	C26	C31	1.382(6)
C4	C10	1.400(8)	C27	C28	1.372(7)
C5	C6	1.311(7)	C28	C29	1.374(8)
C7	C8	1.363(6)	C29	C30	1.371(8)
C8	C9	1.395(8)	C29	C32	1.526(8)

Table 4 Bond Lengths for DATAM.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C9	C10	1.368(9)	C30	C31	1.374(7)

Table 5 Bond Angles for DATAM.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O24	S23	O25	119.7(2)	C2	C13	C16	126.7(5)
O24	S23	N22	108.5(2)	C12	C13	C2	108.0(5)
O24	S23	C26	108.2(2)	C12	C13	C16	125.2(5)
O25	S23	N22	104.5(2)	N15	C14	C11	178.7(9)
O25	S23	C26	108.3(2)	C17	C16	C13	118.6(5)
N22	S23	C26	106.9(2)	C17	C16	C21	118.6(5)
C6	N1	C2	121.8(5)	C21	C16	C13	122.8(5)
C11	N1	C2	108.5(4)	C18	C17	C16	121.3(5)
C11	N1	C6	129.6(5)	C17	C18	Br1	118.0(5)
C21	N22	S23	122.5(3)	C17	C18	Br1A	122.8(5)
N1	C2	C3	117.8(5)	C19	C18	C17	120.3(6)
N1	C2	C13	105.9(5)	C19	C18	Br1	121.7(5)
C13	C2	C3	136.3(5)	C19	C18	Br1A	111.0(6)
C4	C3	C2	118.9(5)	C20	C19	C18	119.3(5)
C7	C3	C2	122.6(5)	C19	C20	C21	121.1(5)
C7	C3	C4	118.5(5)	C16	C21	N22	119.8(4)
C3	C4	C5	118.9(5)	C20	C21	N22	120.8(4)
C10	C4	C3	119.0(6)	C20	C21	C16	119.3(5)
C10	C4	C5	122.1(6)	C27	C26	S23	120.0(4)
C6	C5	C4	121.8(5)	C31	C26	S23	121.0(4)
C5	C6	N1	120.5(5)	C31	C26	C27	118.9(5)
C8	C7	C3	120.6(5)	C28	C27	C26	120.1(5)
C7	C8	C9	121.6(6)	C27	C28	C29	121.3(6)
C10	C9	C8	118.5(6)	C28	C29	C32	120.2(7)
C9	C10	C4	121.7(6)	C30	C29	C28	118.2(6)
N1	C11	C14	121.4(6)	C30	C29	C32	121.6(6)
C12	C11	N1	108.6(5)	C29	C30	C31	121.6(5)
C12	C11	C14	129.9(7)	C30	C31	C26	119.9(5)
C11	C12	C13	109.0(5)				

Table 6 Torsion Angles for DATAM.

A	B	C	D	Angle/°	A	B	C	D	Angle/°

Table 6 Torsion Angles for DATAM.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S23	N22	C21	C16	-129.7(4)	C7	C3	C4	C10	2.9(7)
S23	N22	C21	C20	54.6(6)	C7	C8	C9	C10	1.7(9)
S23	C26	C27	C28	176.8(5)	C8	C9	C10	C4	-0.9(10)
S23	C26	C31	C30	-176.6(5)	C10	C4	C5	C6	-176.7(6)
O24	S23	N22	C21	-52.2(4)	C11	N1	C2	C3	-177.7(4)
O24	S23	C26	C27	179.7(5)	C11	N1	C2	C13	1.5(6)
O24	S23	C26	C31	-3.3(5)	C11	N1	C6	C5	-177.4(6)
O25	S23	N22	C21	179.1(3)	C11	C12	C13	C2	0.5(6)
O25	S23	C26	C27	-49.1(5)	C11	C12	C13	C16	176.7(5)
O25	S23	C26	C31	127.8(4)	C12	C13	C16	C17	-64.2(7)
N1	C2	C3	C4	-6.1(7)	C12	C13	C16	C21	114.1(6)
N1	C2	C3	C7	172.1(5)	C13	C2	C3	C4	175.1(5)
N1	C2	C13	C12	-1.2(6)	C13	C2	C3	C7	-6.7(9)
N1	C2	C13	C16	-177.4(5)	C13	C16	C17	C18	-178.6(5)
N1	C11	C12	C13	0.4(7)	C13	C16	C21	N22	1.3(7)
N22	S23	C26	C27	63.0(5)	C13	C16	C21	C20	177.0(4)
N22	S23	C26	C31	-120.0(4)	C14	C11	C12	C13	-177.1(7)
C2	N1	C6	C5	-0.8(8)	C16	C17	C18	C19	-0.2(9)
C2	N1	C11	C12	-1.2(6)	C16	C17	C18	Br1	-177.7(4)
C2	N1	C11	C14	176.6(6)	C16	C17	C18	Br1A	150.3(6)
C2	C3	C4	C5	3.2(7)	C17	C16	C21	N22	179.5(4)
C2	C3	C4	C10	-178.9(5)	C17	C16	C21	C20	-4.7(7)
C2	C3	C7	C8	179.7(5)	C17	C18	C19	C20	-1.0(9)
C2	C13	C16	C17	111.3(6)	C18	C19	C20	C21	-0.8(8)
C2	C13	C16	C21	-70.4(7)	C19	C20	C21	N22	179.4(4)
C3	C2	C13	C12	177.7(5)	C19	C20	C21	C16	3.7(7)
C3	C2	C13	C16	1.5(9)	C21	C16	C17	C18	3.1(8)
C3	C4	C5	C6	1.2(9)	C26	S23	N22	C21	64.4(4)
C3	C4	C10	C9	-1.4(9)	C26	C27	C28	C29	-0.4(10)
C3	C7	C8	C9	-0.2(8)	C27	C26	C31	C30	0.5(8)
C4	C3	C7	C8	-2.1(8)	C27	C28	C29	C30	0.8(10)
C4	C5	C6	N1	-2.4(9)	C27	C28	C29	C32	-178.3(6)
C5	C4	C10	C9	176.5(6)	C28	C29	C30	C31	-0.5(10)
C6	N1	C2	C3	5.1(7)	C29	C30	C31	C26	-0.1(10)
C6	N1	C2	C13	-175.8(4)	C31	C26	C27	C28	-0.2(9)
C6	N1	C11	C12	175.8(5)	C32	C29	C30	C31	178.5(6)
C6	N1	C11	C14	-6.4(9)	Br1	C18	C19	C20	176.4(4)
C7	C3	C4	C5	-175.1(5)	Br1A	C18	C19	C20	-154.6(6)

Table 7 Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for DATAM.

Atom	*x*	*y*	*z*	U(eq)
H22	2879.15	5662.71	4910.04	64
H5	3020.86	10061.74	5878.42	100
H6	3963.74	10561.8	3933.25	93
H7	273.97	7458.84	5166.81	76
H8	-805.18	7128.62	7117.85	94
H9	-228.27	7860.3	8376.23	117
H10	1385.58	9025.19	7602.61	110
H12	3371.67	8795.68	1226.95	87
H17	285.03	9001.29	1743.62	88
H19	-617.65	5465.04	2914.26	88
H20	1137.13	4346.95	4135.55	73
H27	5785.1	5601.13	3068.45	93
H28	7167.08	6020.22	1216.01	108
H30	6185.61	3331.81	555.15	103
H31	4781.28	2902.48	2397.55	88
H32A	7872.84	4335.23	-882.09	203
H32B	8709.42	4838.22	-379.99	203
H32C	7406.02	5917.34	-1049.33	203

Table 8 Atomic Occupancy for DATAM.

Atom	*Occupancy*	Atom	*Occupancy*	Atom	*Occupancy*
Br1	0.865(6)	Br1A	0.135(6)		

Experimental

Single crystals of $C_{26}H_{18}BrN_3O_2S$ **[DATAM]** were **[]**. A suitable crystal was selected and **[]** on a **Rigaku Saturn 724+ HG** diffractometer. The crystal was kept at 298 K during data collection. Using Olex2 [1], the structure was solved with the olex2.solve [2] structure solution program using Charge Flipping and refined with the SHELXL [3] refinement package using Least Squares minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. &Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. (2015). Acta Cryst. A71, 59-75.
3. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of [DATAM]

Crystal Data for $C_{26}H_{18}BrN_3O_2S$ (M =516.40 g/mol): triclinic, space group P-1 (no. 2), a = 10.479(6) Å, b = 11.171(5) Å, c = 12.250(6) Å, α = 64.87(5)°, β = 73.59(6)°, γ = 66.24(5)°, V = 1177.5(12) Å^3, Z = 2, T = 298 K, μ(MoKα) = 1.863 mm^{-1}, *Dcalc* = 1.456 g/cm^3, 9288 reflections measured (6.032° ≤ 2Θ ≤ 51°), 4280 unique (R_{int} = 0.0495, R_{sigma} = 0.0897) which were used in all calculations. The final R_1 was 0.0729 (I > 2σ(I)) and wR_2 was 0.1722 (all data).

Single crystal X-ray of 6a (CCDC: 2042169, 20% ellipsoid contour probability levels)

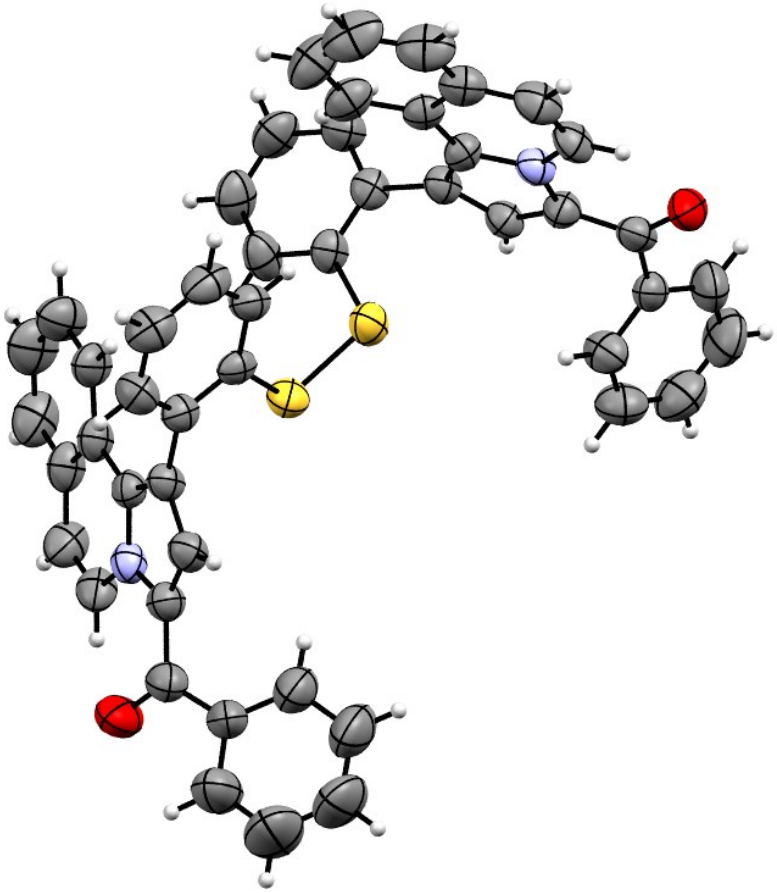


Table 1 Crystal data and structure refinement for sab.

Identification code	sab
Empirical formula	$C_{50}H_{32}N_2O_2S_2$
Formula weight	756.89
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.230(9)
b/Å	14.373(8)
c/Å	18.320(11)
α/°	90
β/°	106.462(15)
γ/°	90
Volume/Å^3	3846(4)
Z	4

ρ_{calc}g/cm^3	1.307
μ/mm^{-1}	0.183
F(000)	1576.0
Crystal size/mm^3	0.182 × 0.085 × 0.045
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.636 to 50
Index ranges	$-18 \le h \le 18$, $-17 \le k \le 17$, $-21 \le l \le 21$
Reflections collected	45854
Independent reflections	4764 [R_{int} = 0.2127, R_{sigma} = 0.1817]
Data/restraints/parameters	4764/0/505
Goodness-of-fit on F^2	0.987
Final R indexes [I>=2σ (I)]	R_1 = 0.0669, wR_2 = 0.1278
Final R indexes [all data]	R_1 = 0.2278, wR_2 = 0.1889
Largest diff. peak/hole / e Å^{-3}	0.26/-0.27

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

Atom	*x*	*y*	*z*	U(eq)
C1	5188(4)	5768(3)	2194(3)	52.8(14)
C2	5600(4)	5710(4)	1610(3)	69.8(17)
C3	5339(5)	5028(5)	1065(3)	78.7(19)
C4	4658(5)	4412(4)	1088(3)	77.9(19)
C5	4244(4)	4477(4)	1679(3)	65.2(16)
C6	4515(4)	5157(4)	2234(3)	51.2(14)
C7	4056(4)	5239(3)	2850(3)	48.6(14)
C8	4195(4)	4724(3)	3520(3)	49.1(14)
C9	4789(4)	3959(3)	3848(3)	50.1(14)
C10	5425(4)	3578(4)	3508(3)	70.7(17)
C11	5993(4)	2856(4)	3859(4)	90(2)
C12	5934(5)	2506(4)	4547(4)	95(2)
C13	5321(5)	2865(4)	4888(4)	86(2)
C14	4743(4)	3595(4)	4559(3)	61.8(16)
C15	4143(4)	4021(4)	4930(3)	69.0(17)
C16	3614(4)	4749(4)	4627(3)	60.9(16)
C17	3170(4)	5860(3)	3538(3)	53.0(14)
C18	2515(4)	6413(4)	3788(3)	56.6(15)
C19	2224(4)	7307(4)	3375(3)	55.2(15)

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

Atom	*x*	*y*	*z*	U(eq)
C20	1323(5)	7555(5)	3165(4)	89(2)
C21	1025(5)	8371(6)	2785(4)	106(2)
C22	1640(6)	8952(5)	2623(4)	96(2)
C23	2549(6)	8739(4)	2833(4)	84(2)
C24	2851(4)	7915(4)	3211(3)	69.5(17)
C25	3427(4)	5929(3)	2878(3)	53.4(14)
C26	7548(4)	6477(3)	3334(3)	47.2(14)
C27	7415(4)	5632(3)	3659(3)	57.3(15)
C28	8166(5)	5101(4)	4032(3)	74.2(19)
C29	9041(5)	5413(4)	4090(3)	76.6(19)
C30	9173(4)	6244(4)	3761(3)	64.5(16)
C31	8428(4)	6788(3)	3380(3)	50.4(14)
C32	8568(3)	7690(3)	3023(3)	51.1(14)
C33	8799(3)	8539(4)	3400(3)	57.7(15)
C34	8857(4)	9215(4)	2888(3)	58.2(15)
C35	9195(4)	10179(4)	3006(4)	67.4(17)
C36	9035(4)	10719(4)	3637(4)	68.4(17)
C37	8309(5)	10563(4)	3928(4)	92(2)
C38	8147(6)	11153(5)	4485(5)	119(3)
C39	8718(7)	11902(6)	4739(5)	130(3)
C40	9419(7)	12083(6)	4446(5)	142(3)
C41	9581(5)	11489(5)	3894(4)	106(2)
C42	8637(4)	9180(4)	1477(4)	64.6(17)
C43	8408(4)	8668(4)	854(4)	75.5(19)
C44	8169(4)	7703(4)	872(3)	63.2(16)
C45	7897(4)	7173(5)	198(3)	83(2)
C46	7715(5)	6252(5)	231(4)	93(2)
C47	7788(4)	5821(4)	930(4)	86(2)
C48	8052(4)	6333(4)	1595(3)	69.2(17)
C49	8233(3)	7280(4)	1574(3)	55.8(15)
C50	8481(3)	7843(3)	2255(3)	50.8(14)
N1	3642(3)	5101(3)	3926(2)	51.4(11)
N2	8670(3)	8781(3)	2180(3)	54.6(12)
O1	2182(3)	6176(2)	4300(2)	78.3(13)
O2	9576(3)	10531(3)	2570(3)	98.1(15)
S1	5479.9(10)	6626.6(10)	2929.8(8)	64.5(5)
S2	6647.1(10)	7226.4(9)	2831.6(8)	63.0(5)

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

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	61(4)	66(4)	32(4)	2(3)	14(3)	4(3)
C2	66(4)	100(5)	48(4)	-8(4)	24(4)	-12(4)
C3	83(5)	109(5)	50(4)	-12(4)	28(4)	2(4)
C4	93(6)	81(4)	57(5)	-20(3)	17(4)	2(4)
C5	73(5)	65(4)	56(4)	0(3)	16(4)	-7(3)
C6	62(4)	58(3)	33(4)	10(3)	13(3)	6(3)
C7	58(4)	54(3)	35(4)	3(3)	16(3)	-4(3)
C8	54(4)	51(3)	41(4)	-1(3)	12(3)	1(3)
C9	55(4)	48(3)	42(4)	-4(3)	6(3)	-4(3)
C10	85(5)	66(4)	56(4)	-7(3)	10(4)	6(4)
C11	106(6)	87(5)	68(5)	1(4)	9(4)	38(4)
C12	108(7)	79(5)	76(6)	14(4)	-9(5)	25(4)
C13	98(6)	75(5)	70(5)	25(4)	-2(4)	6(4)
C14	70(5)	61(4)	48(4)	3(3)	6(4)	-7(3)
C15	84(5)	74(4)	48(4)	17(3)	18(4)	-10(4)
C16	70(4)	70(4)	50(4)	11(3)	28(3)	-10(3)
C17	61(4)	48(3)	54(4)	6(3)	22(3)	3(3)
C18	65(4)	54(4)	53(4)	-5(3)	21(3)	-16(3)
C19	64(4)	56(4)	52(4)	-5(3)	27(3)	-2(3)
C20	65(5)	94(5)	121(6)	5(4)	46(5)	10(4)
C21	79(6)	104(6)	138(7)	13(5)	37(5)	38(5)
C22	113(7)	77(5)	96(6)	7(4)	26(6)	25(5)
C23	99(6)	63(5)	88(6)	12(4)	25(5)	-4(4)
C24	61(4)	66(4)	78(5)	13(3)	13(4)	3(4)
C25	57(4)	55(3)	50(4)	7(3)	19(3)	-4(3)
C26	72(4)	41(3)	31(3)	-4(2)	18(3)	-3(3)
C27	79(5)	50(3)	49(4)	-2(3)	27(3)	-7(3)
C28	120(6)	53(4)	56(4)	9(3)	35(4)	7(4)
C29	99(6)	70(4)	55(4)	8(3)	13(4)	10(4)
C30	63(4)	69(4)	59(4)	5(3)	14(3)	-5(3)
C31	68(4)	50(3)	37(4)	2(3)	20(3)	-1(3)
C32	63(4)	54(3)	39(4)	-1(3)	20(3)	-8(3)
C33	62(4)	62(4)	50(4)	0(3)	17(3)	-6(3)
C34	68(4)	56(4)	55(4)	-2(3)	26(3)	-5(3)
C35	70(5)	57(4)	80(5)	6(4)	29(4)	0(3)
C36	70(5)	55(4)	87(5)	-10(3)	34(4)	-7(3)
C37	113(6)	72(4)	106(6)	-7(4)	57(5)	5(4)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for sab. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C38	159(8)	91(5)	135(8)	-16(5)	89(6)	12(6)
C39	174(10)	104(7)	131(8)	-52(6)	76(7)	-14(6)
C40	166(10)	127(7)	147(9)	-68(6)	66(7)	-40(7)
C41	120(7)	94(5)	116(7)	-29(5)	56(5)	-34(5)
C42	78(5)	58(4)	65(5)	24(4)	32(4)	17(3)
C43	110(6)	66(4)	60(5)	13(4)	39(4)	10(4)
C44	68(4)	84(4)	41(4)	2(4)	19(3)	11(3)
C45	108(6)	96(5)	48(5)	15(4)	28(4)	21(5)
C46	123(6)	116(6)	44(5)	-14(4)	29(4)	-4(5)
C47	118(6)	83(4)	63(5)	-16(4)	35(4)	-22(4)
C48	95(5)	71(4)	53(4)	-11(3)	41(4)	-8(3)
C49	62(4)	68(4)	42(4)	1(3)	21(3)	5(3)
C50	56(4)	50(3)	52(4)	2(3)	24(3)	3(3)
N1	64(3)	53(3)	40(3)	5(2)	20(3)	-8(2)
N2	58(3)	58(3)	52(3)	8(3)	24(3)	5(2)
O1	105(4)	64(2)	88(3)	2(2)	64(3)	-5(2)
O2	135(4)	72(3)	113(4)	-4(3)	77(3)	-25(3)
S1	71.0(11)	72.8(10)	55.7(11)	-9.2(8)	27.7(8)	-6.5(8)
S2	68.9(11)	55.9(9)	67.2(11)	7.3(8)	24.3(9)	-0.8(8)

Table 4 Bond Lengths for sab.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.388(7)	C26	C31	1.392(6)
C1	C6	1.367(6)	C26	S2	1.781(5)
C1	S1	1.789(5)	C27	C28	1.384(7)
C2	C3	1.374(7)	C28	C29	1.381(8)
C3	C4	1.373(7)	C29	C30	1.378(7)
C4	C5	1.401(7)	C30	C31	1.391(6)
C5	C6	1.385(7)	C31	C32	1.495(6)
C6	C7	1.491(6)	C32	C33	1.397(6)
C7	C8	1.397(6)	C32	C50	1.391(6)
C7	C25	1.391(6)	C33	C34	1.371(6)
C8	C9	1.443(6)	C34	C35	1.472(7)
C8	N1	1.381(6)	C34	N2	1.395(6)
C9	C10	1.401(7)	C35	C36	1.469(7)
C9	C14	1.424(7)	C35	O2	1.221(6)
C10	C11	1.387(7)	C36	C37	1.376(7)

Table 4 Bond Lengths for sab.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C11	C12	1.384(8)	C36	C41	1.384(7)
C12	C13	1.364(8)	C37	C38	1.401(8)
C13	C14	1.393(7)	C38	C39	1.379(9)
C14	C15	1.423(7)	C39	C40	1.350(9)
C15	C16	1.340(6)	C40	C41	1.398(9)
C16	N1	1.393(6)	C42	C43	1.319(7)
C17	C18	1.449(7)	C42	N2	1.397(6)
C17	C25	1.375(6)	C43	C44	1.436(7)
C17	N1	1.387(6)	C44	C45	1.409(7)
C18	C19	1.493(7)	C44	C49	1.401(7)
C18	O1	1.235(6)	C45	C46	1.357(7)
C19	C20	1.364(7)	C46	C47	1.397(7)
C19	C24	1.388(7)	C47	C48	1.383(7)
C20	C21	1.374(8)	C48	C49	1.391(6)
C21	C22	1.350(8)	C49	C50	1.446(7)
C22	C23	1.362(8)	C50	N2	1.393(6)
C23	C24	1.383(7)	S1	S2	2.029(2)
C26	C27	1.393(6)			

Table 5 Bond Angles for sab.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	S1	123.5(5)	C29	C28	C27	120.2(6)
C6	C1	C2	120.8(5)	C30	C29	C28	120.4(6)
C6	C1	S1	115.7(4)	C29	C30	C31	120.4(6)
C3	C2	C1	120.0(6)	C26	C31	C32	120.3(5)
C4	C3	C2	120.3(6)	C30	C31	C26	119.0(5)
C3	C4	C5	119.2(6)	C30	C31	C32	120.6(5)
C6	C5	C4	120.6(5)	C33	C32	C31	126.0(5)
C1	C6	C5	119.0(5)	C50	C32	C31	126.5(5)
C1	C6	C7	120.6(5)	C50	C32	C33	107.5(4)
C5	C6	C7	120.4(5)	C34	C33	C32	109.6(5)
C8	C7	C6	129.6(5)	C33	C34	C35	130.9(6)
C25	C7	C6	124.0(5)	C33	C34	N2	106.5(5)
C25	C7	C8	106.3(5)	N2	C34	C35	121.9(5)
C7	C8	C9	133.6(5)	C36	C35	C34	118.9(5)
N1	C8	C7	107.6(5)	O2	C35	C34	120.3(6)
N1	C8	C9	118.8(5)	O2	C35	C36	120.7(5)
C10	C9	C8	123.0(5)	C37	C36	C35	123.3(6)

Table 5 Bond Angles for sab.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C10	C9	C14	118.9(5)	C37	C36	C41	118.0(6)
C14	C9	C8	118.2(5)	C41	C36	C35	118.2(6)
C11	C10	C9	120.3(6)	C36	C37	C38	120.7(7)
C12	C11	C10	120.1(6)	C39	C38	C37	119.5(7)
C13	C12	C11	120.6(7)	C40	C39	C38	120.7(8)
C12	C13	C14	121.1(7)	C39	C40	C41	119.5(8)
C13	C14	C9	118.9(6)	C36	C41	C40	121.4(7)
C13	C14	C15	122.0(6)	C43	C42	N2	119.9(5)
C15	C14	C9	119.0(5)	C42	C43	C44	121.8(6)
C16	C15	C14	122.0(6)	C45	C44	C43	121.1(6)
C15	C16	N1	119.5(5)	C49	C44	C43	119.1(6)
C25	C17	C18	129.1(5)	C49	C44	C45	119.8(6)
C25	C17	N1	105.8(5)	C46	C45	C44	120.0(6)
N1	C17	C18	125.0(5)	C45	C46	C47	120.6(6)
C17	C18	C19	116.4(5)	C48	C47	C46	119.9(6)
O1	C18	C17	123.8(5)	C47	C48	C49	120.4(6)
O1	C18	C19	119.8(5)	C44	C49	C50	118.9(5)
C20	C19	C18	119.9(6)	C48	C49	C44	119.1(5)
C20	C19	C24	118.3(5)	C48	C49	C50	121.9(5)
C24	C19	C18	121.9(5)	C32	C50	C49	135.3(5)
C19	C20	C21	121.8(6)	C32	C50	N2	106.9(5)
C22	C21	C20	119.3(7)	N2	C50	C49	117.8(5)
C21	C22	C23	120.8(7)	C8	N1	C16	122.5(5)
C22	C23	C24	120.1(6)	C8	N1	C17	109.8(4)
C23	C24	C19	119.7(6)	C17	N1	C16	127.7(5)
C17	C25	C7	110.5(5)	C34	N2	C42	128.2(5)
C27	C26	S2	124.3(5)	C50	N2	C34	109.5(4)
C31	C26	C27	120.5(5)	C50	N2	C42	122.3(5)
C31	C26	S2	115.2(4)	C1	S1	S2	105.3(2)
C28	C27	C26	119.5(6)	C26	S2	S1	105.3(2)

Table 6 Hydrogen Bonds for sab.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C2	H2	S2	0.93	2.71	3.206(6)	114.6
C2	H2	S2	0.93	2.71	3.206(6)	114.6
C15	H15	S1[1]	0.93	3.01	3.911(6)	163.4
C15	H15	S1[1]	0.93	3.01	3.911(6)	163.4
C16	H16	O1	0.93	2.35	2.929(7)	120.5

Table 6 Hydrogen Bonds for sab.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
C16	H16	O1	0.93	2.35	2.929(7)	120.5
C27	H27	S1	0.93	2.71	3.207(6)	114.6
C27	H27	S1	0.93	2.71	3.207(6)	114.6
C42	H42	O1[2]	0.93	2.60	3.287(6)	131.4
C42	H42	O1[2]	0.93	2.60	3.287(6)	131.4
C42	H42	O2	0.93	2.32	2.864(8)	117.1
C42	H42	O2	0.93	2.32	2.864(8)	117.1

[1]1-X,1-Y,1-Z; [2]1-X,1/2+Y,1/2-Z

Table 7 Torsion Angles for sab.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	1.1(9)	C30	C31	C32	C33	-80.6(7)
C1	C6	C7	C8	-101.7(7)	C30	C31	C32	C50	100.3(6)
C1	C6	C7	C25	73.2(7)	C31	C26	C27	C28	0.3(7)
C2	C1	C6	C5	-0.4(8)	C31	C26	S2	S1	-176.3(3)
C2	C1	C6	C7	-178.3(5)	C31	C32	C33	C34	-179.2(5)
C2	C1	S1	S2	-11.7(5)	C31	C32	C50	C49	1.6(10)
C2	C3	C4	C5	-1.0(9)	C31	C32	C50	N2	179.9(5)
C3	C4	C5	C6	0.2(9)	C32	C33	C34	C35	-170.6(5)
C4	C5	C6	C1	0.5(8)	C32	C33	C34	N2	-0.8(6)
C4	C5	C6	C7	178.5(5)	C32	C50	N2	C34	-1.1(6)
C5	C6	C7	C8	80.4(7)	C32	C50	N2	C42	-179.3(4)
C5	C6	C7	C25	-104.7(6)	C33	C32	C50	C49	-177.7(5)
C6	C1	C2	C3	-0.4(9)	C33	C32	C50	N2	0.6(6)
C6	C1	S1	S2	168.6(4)	C33	C34	C35	C36	-35.7(9)
C6	C7	C8	C9	-0.8(10)	C33	C34	C35	O2	146.6(6)
C6	C7	C8	N1	176.5(5)	C33	C34	N2	C42	179.2(5)
C6	C7	C25	C17	-176.0(5)	C33	C34	N2	C50	1.2(6)
C7	C8	C9	C10	2.1(9)	C34	C35	C36	C37	-27.5(9)
C7	C8	C9	C14	-179.7(5)	C34	C35	C36	C41	160.0(6)
C7	C8	N1	C16	-180.0(4)	C35	C34	N2	C42	-9.8(8)
C7	C8	N1	C17	-1.5(6)	C35	C34	N2	C50	172.2(5)
C8	C7	C25	C17	-0.1(6)	C35	C36	C37	C38	-174.4(6)
C8	C9	C10	C11	178.4(5)	C35	C36	C41	C40	174.4(7)
C8	C9	C14	C13	-179.1(5)	C36	C37	C38	C39	0.6(11)
C8	C9	C14	C15	-2.4(7)	C37	C36	C41	C40	1.5(11)
C9	C8	N1	C16	-2.2(7)	C37	C38	C39	C40	1.2(14)

Table 7 Torsion Angles for sab.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C9	C8	N1	C17	176.3(4)	C38	C39	C40	C41	-1.6(15)
C9	C10	C11	C12	0.2(9)	C39	C40	C41	C36	0.2(14)
C9	C14	C15	C16	0.6(8)	C41	C36	C37	C38	-1.9(10)
C10	C9	C14	C13	-0.9(8)	C42	C43	C44	C45	177.9(6)
C10	C9	C14	C15	175.8(5)	C42	C43	C44	C49	-3.9(9)
C10	C11	C12	C13	-0.2(10)	C43	C42	N2	C34	-177.0(5)
C11	C12	C13	C14	-0.4(11)	C43	C42	N2	C50	0.9(8)
C12	C13	C14	C9	0.9(9)	C43	C44	C45	C46	176.9(6)
C12	C13	C14	C15	-175.6(6)	C43	C44	C49	C48	-176.3(5)
C13	C14	C15	C16	177.2(5)	C43	C44	C49	C50	3.9(8)
C14	C9	C10	C11	0.3(8)	C44	C45	C46	C47	0.4(10)
C14	C15	C16	N1	0.5(8)	C44	C49	C50	C32	176.4(6)
C15	C16	N1	C8	0.3(7)	C44	C49	C50	N2	-1.8(7)
C15	C16	N1	C17	-177.9(5)	C45	C44	C49	C48	1.9(8)
C17	C18	C19	C20	136.3(6)	C45	C44	C49	C50	-177.8(5)
C17	C18	C19	C24	-45.3(7)	C45	C46	C47	C48	-0.3(10)
C18	C17	C25	C7	-178.0(5)	C46	C47	C48	C49	1.0(9)
C18	C17	N1	C8	178.7(5)	C47	C48	C49	C44	-1.8(8)
C18	C17	N1	C16	-2.9(8)	C47	C48	C49	C50	177.9(5)
C18	C19	C20	C21	179.9(6)	C48	C49	C50	C32	-3.4(10)
C18	C19	C24	C23	-179.4(5)	C48	C49	C50	N2	178.5(5)
C19	C20	C21	C22	-0.9(11)	C49	C44	C45	C46	-1.2(9)
C20	C19	C24	C23	-1.0(8)	C49	C50	N2	C34	177.5(4)
C20	C21	C22	C23	-0.2(11)	C49	C50	N2	C42	-0.7(7)
C21	C22	C23	C24	0.7(11)	C50	C32	C33	C34	0.1(6)
C22	C23	C24	C19	-0.1(9)	N1	C8	C9	C10	-174.9(5)
C24	C19	C20	C21	1.5(9)	N1	C8	C9	C14	3.2(7)
C25	C7	C8	C9	-176.4(5)	N1	C17	C18	C19	168.1(5)
C25	C7	C8	N1	0.9(6)	N1	C17	C18	O1	-13.4(9)
C25	C17	C18	C19	-15.2(8)	N1	C17	C25	C7	-0.8(6)
C25	C17	C18	O1	163.3(6)	N2	C34	C35	C36	155.8(5)
C25	C17	N1	C8	1.4(5)	N2	C34	C35	O2	-22.0(9)
C25	C17	N1	C16	179.8(5)	N2	C42	C43	C44	1.4(9)
C26	C27	C28	C29	0.8(8)	O1	C18	C19	C20	-42.2(8)
C26	C31	C32	C33	99.6(6)	O1	C18	C19	C24	136.2(6)
C26	C31	C32	C50	-79.5(7)	O2	C35	C36	C37	150.2(7)
C27	C26	C31	C30	-0.5(7)	O2	C35	C36	C41	-22.3(9)
C27	C26	C31	C32	179.3(4)	S1	C1	C2	C3	179.9(4)
C27	C26	S2	S1	4.4(4)	S1	C1	C6	C5	179.3(4)
C27	C28	C29	C30	-1.5(9)	S1	C1	C6	C7	1.4(7)

Table 7 Torsion Angles for sab.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C28	C29	C30	C31	1.3(8)	S2	C26	C27	C28	179.5(4)
C29	C30	C31	C26	-0.2(8)	S2	C26	C31	C30	-179.9(4)
C29	C30	C31	C32	180.0(5)	S2	C26	C31	C32	-0.1(6)

Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for sab.

Atom	*x*	*y*	*z*	U(eq)
H2	6054.37	6132.24	1587.29	84
H3	5623.75	4984.25	679.98	94
H4	4473.95	3955.9	715.76	93
H5	3784.18	4061.01	1698.58	78
H10	5465.23	3809.98	3044.9	85
H11	6414.76	2607.77	3632.12	108
H12	6316.08	2020.68	4779.02	114
H13	5288.34	2617.56	5349.24	103
H15	4116.33	3787.76	5396.45	83
H16	3231.73	5017.99	4883.98	73
H20	897.95	7160.77	3282.36	107
H21	405.53	8522.31	2641.02	127
H22	1441.8	9504.29	2363.76	115
H23	2966.89	9148.16	2722.92	101
H24	3471.07	7768.36	3353.92	83
H25	3208.94	6374.82	2502.13	64
H27	6826.29	5425.47	3624.64	69
H28	8081.77	4532.59	4244.68	89
H29	9543.19	5060.43	4351.79	92
H30	9764.63	6442.92	3794.14	77
H33	8899.23	8630.78	3919.93	69
H37	7921.37	10060.95	3753.46	110
H38	7658.15	11039.3	4683.16	142
H39	8617.7	12287.47	5115.22	156
H40	9792.5	12597.99	4610.83	171
H41	10066.68	11614.53	3694.29	127
H42	8775.2	9806.92	1448.04	77
H43	8400.88	8938.32	391.73	91
H45	7842.45	7454.73	-269.92	99
H46	7540.03	5905.2	-215.03	112
H47	7659.67	5190.38	946.65	103

Table 8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for sab.

Atom	*x*	*y*	*z*	U(eq)
H48	8109.37	6042.67	2059.75	83

Experimental

Single crystals of $C_{50}H_{32}N_2O_2S_2$ **[sab]** were **[]**. A suitable crystal was selected and **[]** on a diffractometer. The crystal was kept at 296.15 K during data collection. Using Olex2 [1], the structure was solved with the olex2.solve [2] structure solution program using Charge Flipping and refined with the olex2.refine [3] refinement package using Gauss-Newton minimisation.

1. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. &Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
2. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. (2015). Acta Cryst. A71, 59-75.
3. Bourhis, L.J., Dolomanov, O.V., Gildea, R.J., Howard, J.A.K., Puschmann, H. (2015). Acta Cryst. A71, 59-75.

Crystal structure determination of [sab]

Crystal Data for $C_{50}H_{32}N_2O_2S_2$ (M =756.89 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 15.230(9) Å, b = 14.373(8) Å, c = 18.320(11) Å, β = 106.462(15)°, V = 3846(4) Å^3, Z = 4, T = 296.15 K, μ(MoKα) = 0.183 mm^{-1}, *Dcalc* = 1.307 g/cm^3, 45854 reflections measured (4.636° ≤ 2Θ ≤ 50°), 4764 unique (R_{int} = 0.2127, R_{sigma} = 0.1817) which were used in all calculations. The final R_1 was 0.0669 (I > 2σ(I)) and wR_2 was 0.1889 (all data).