

Supplementary Material

Design, Synthesis, Molecular docking and Anti-proliferative activity of novel phenothiazine containing imidazo[1,2-a]pyridine derivatives against MARK4 Protein

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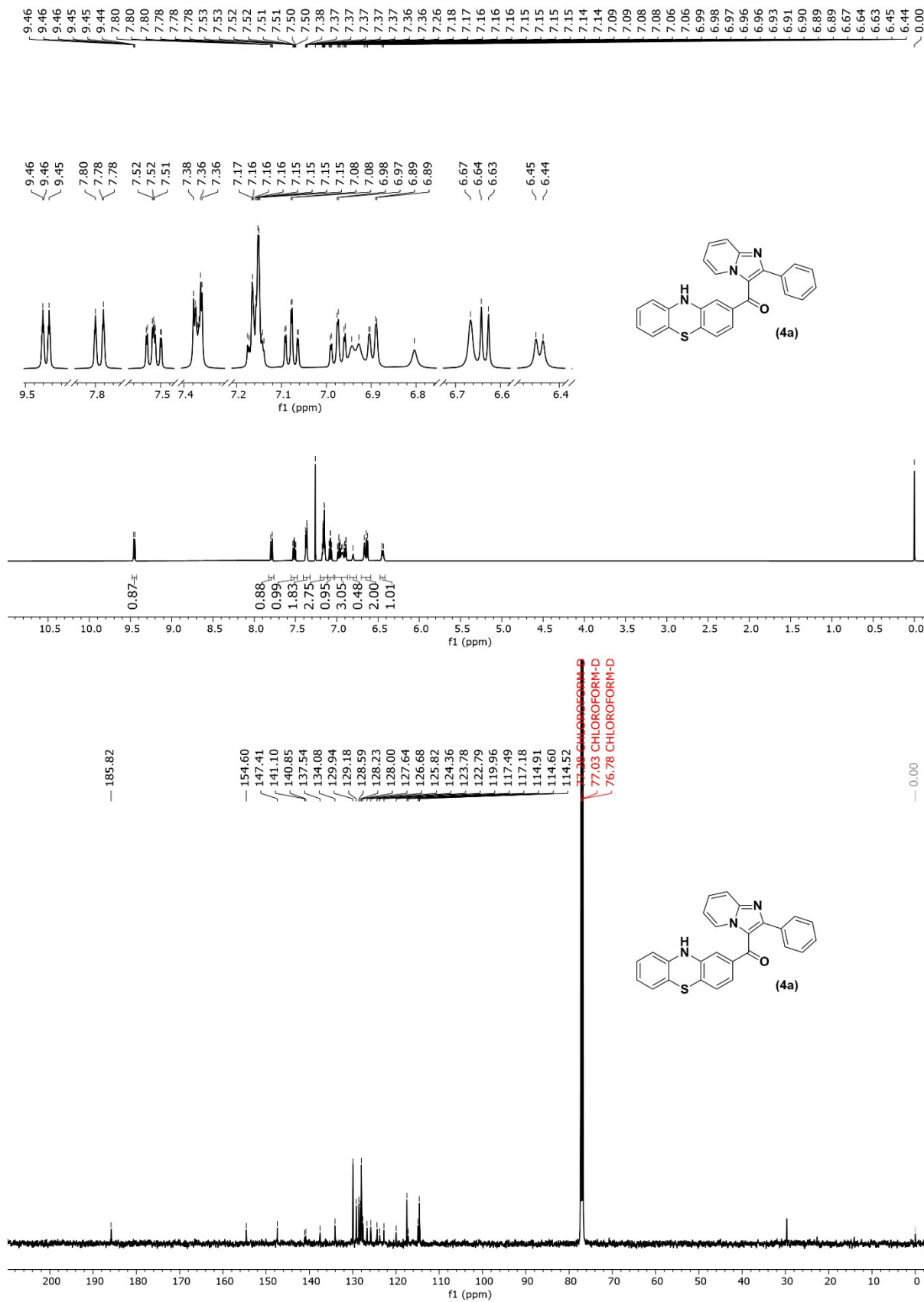
*Corresponding authors: e-mail: naseem.ahmed@cy.iitr.ac.in

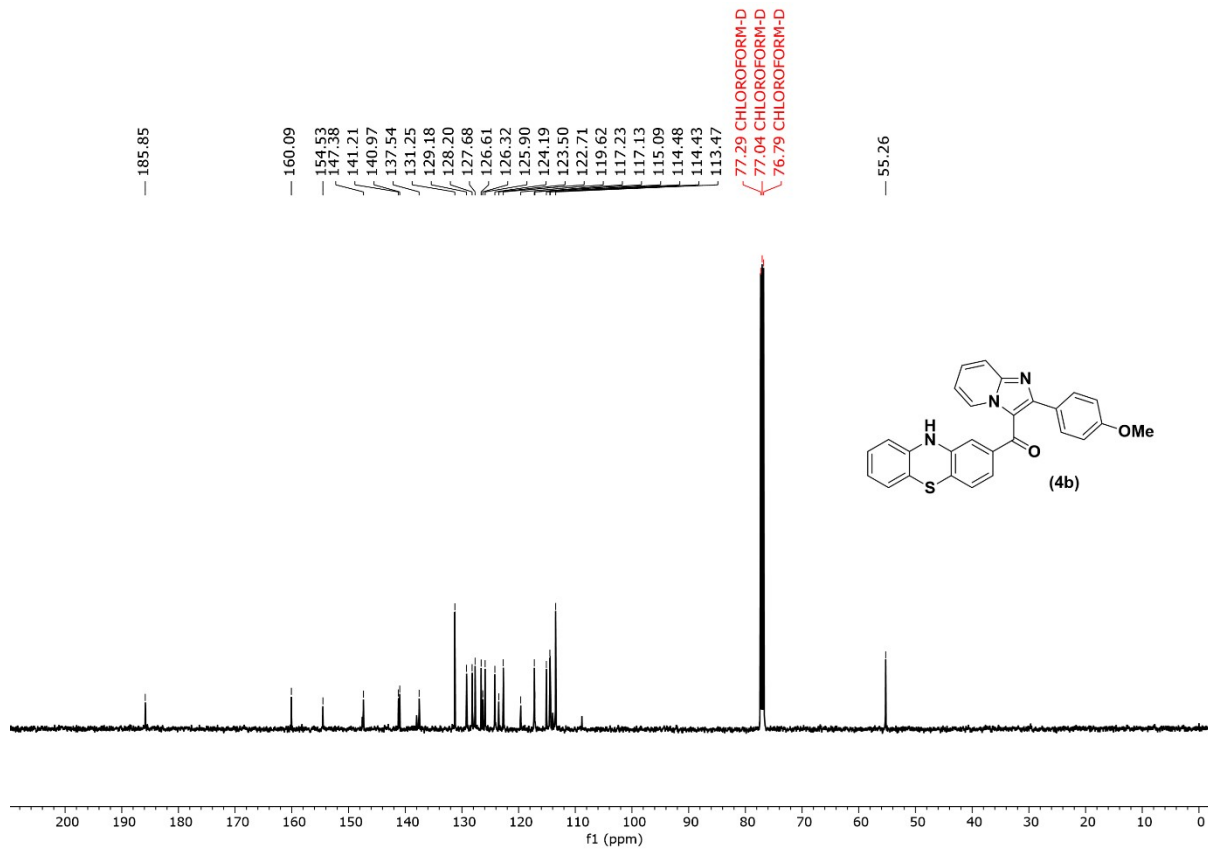
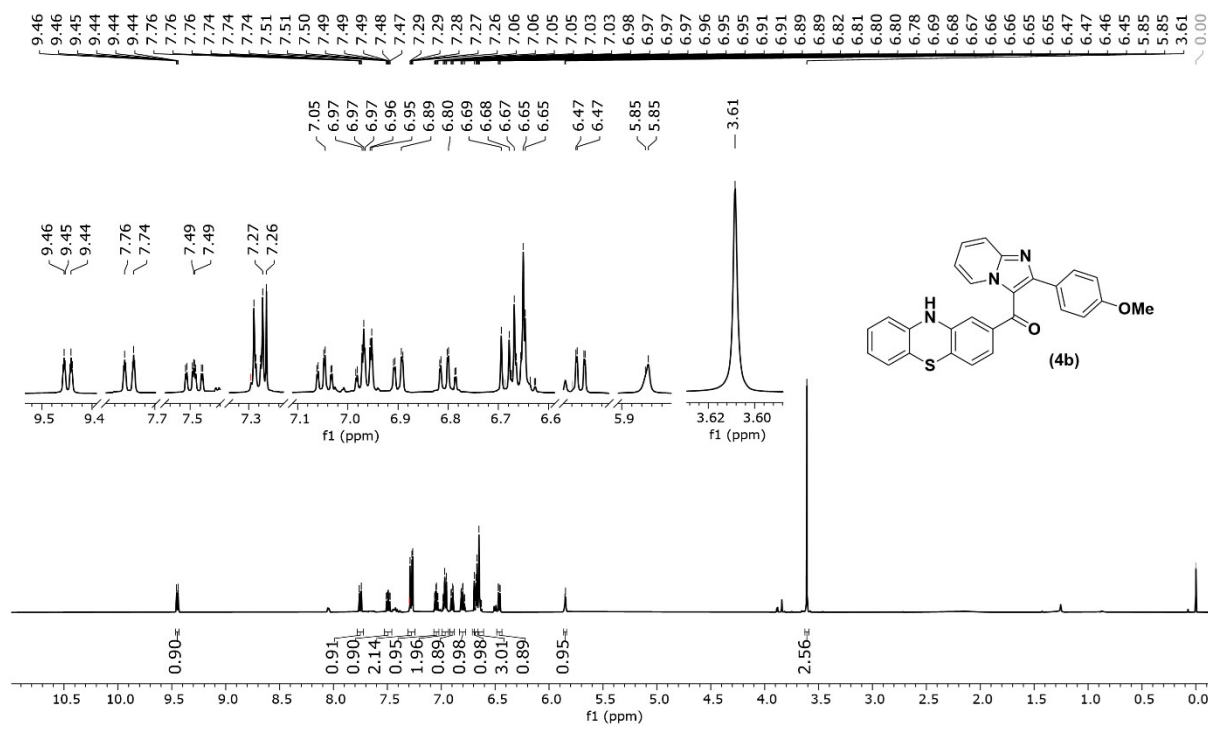
§*Sharing First Co-author:* Authors equally contributed to this work

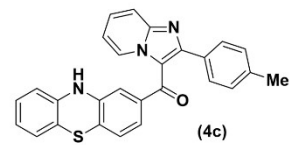
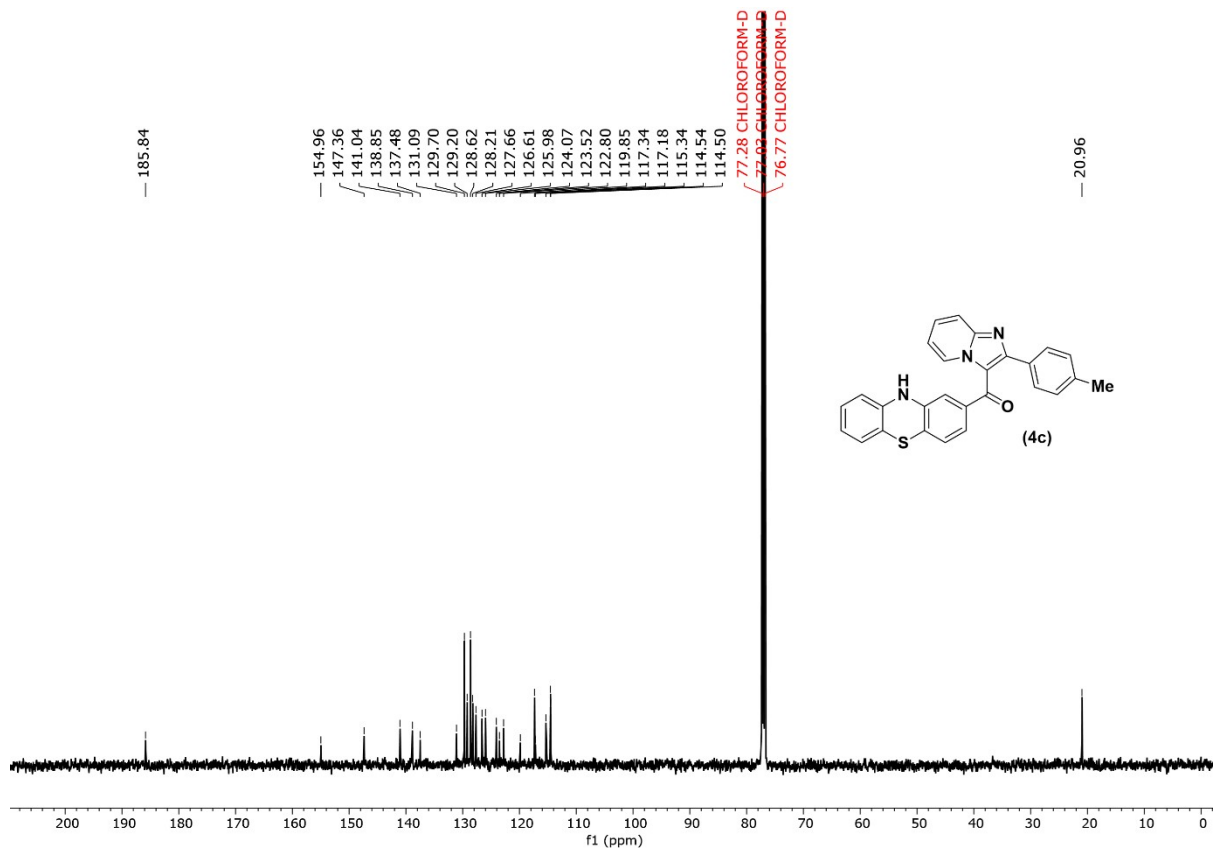
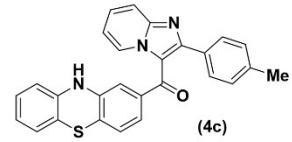
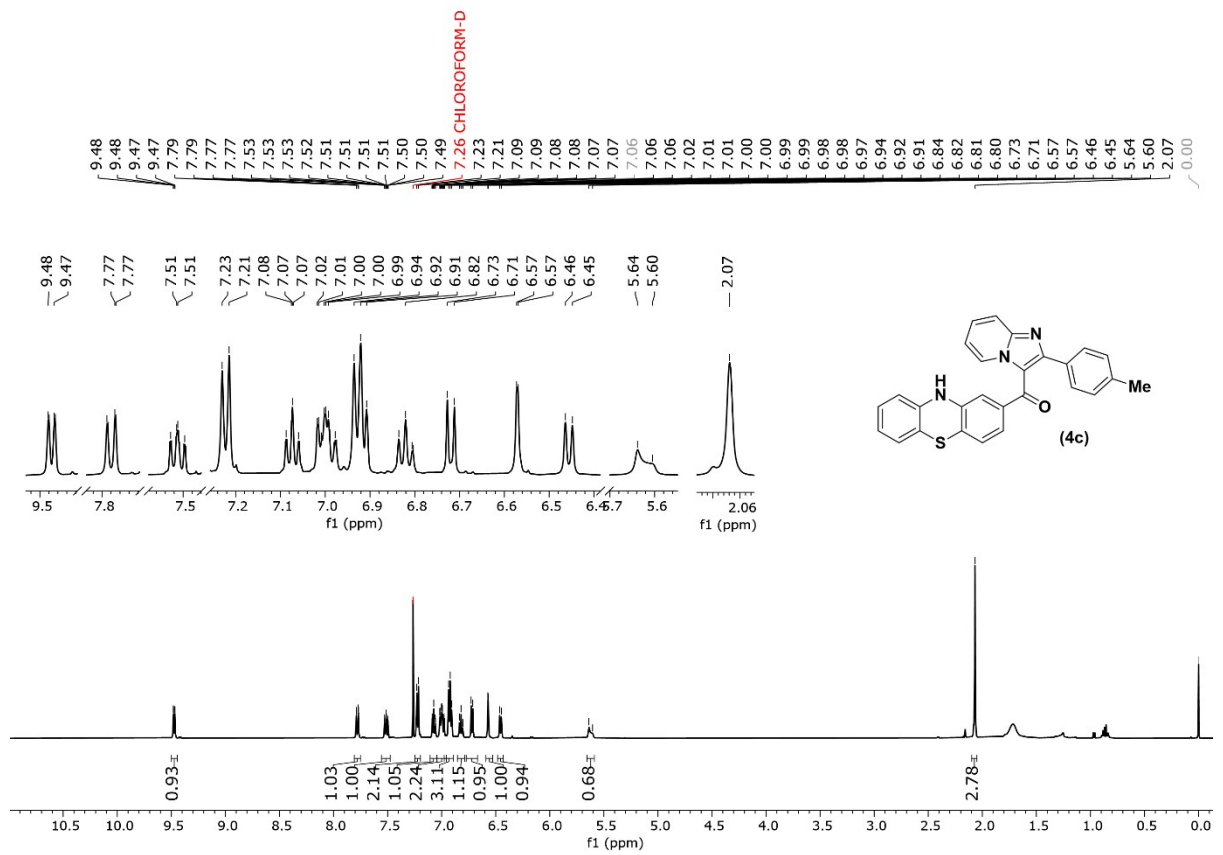
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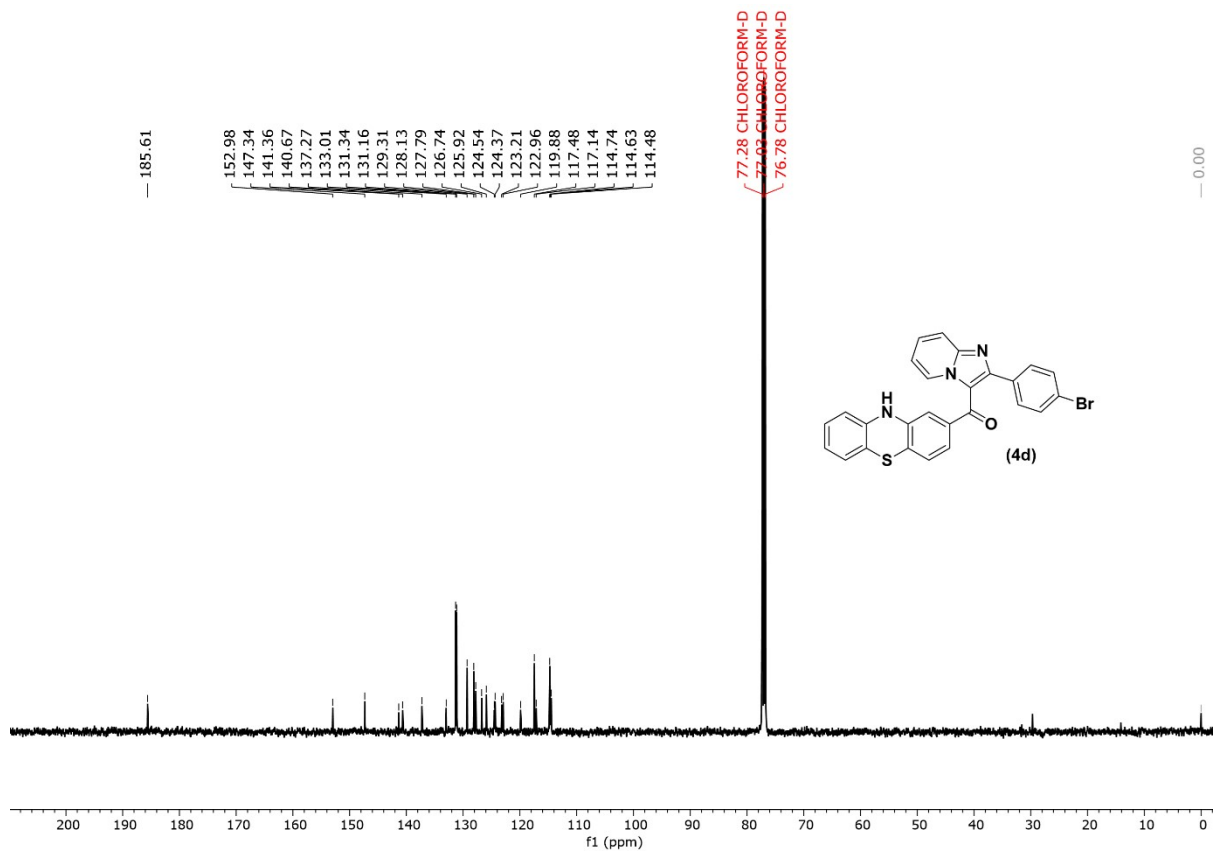
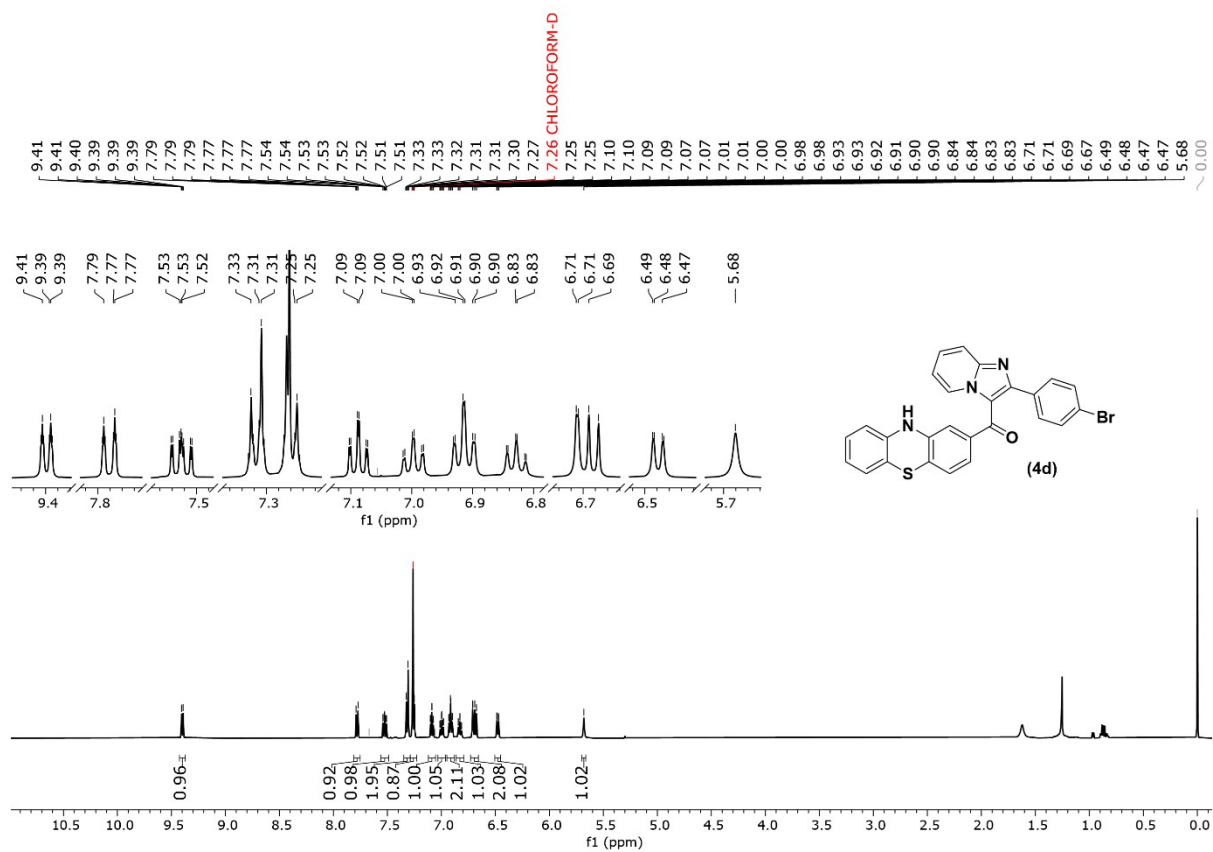
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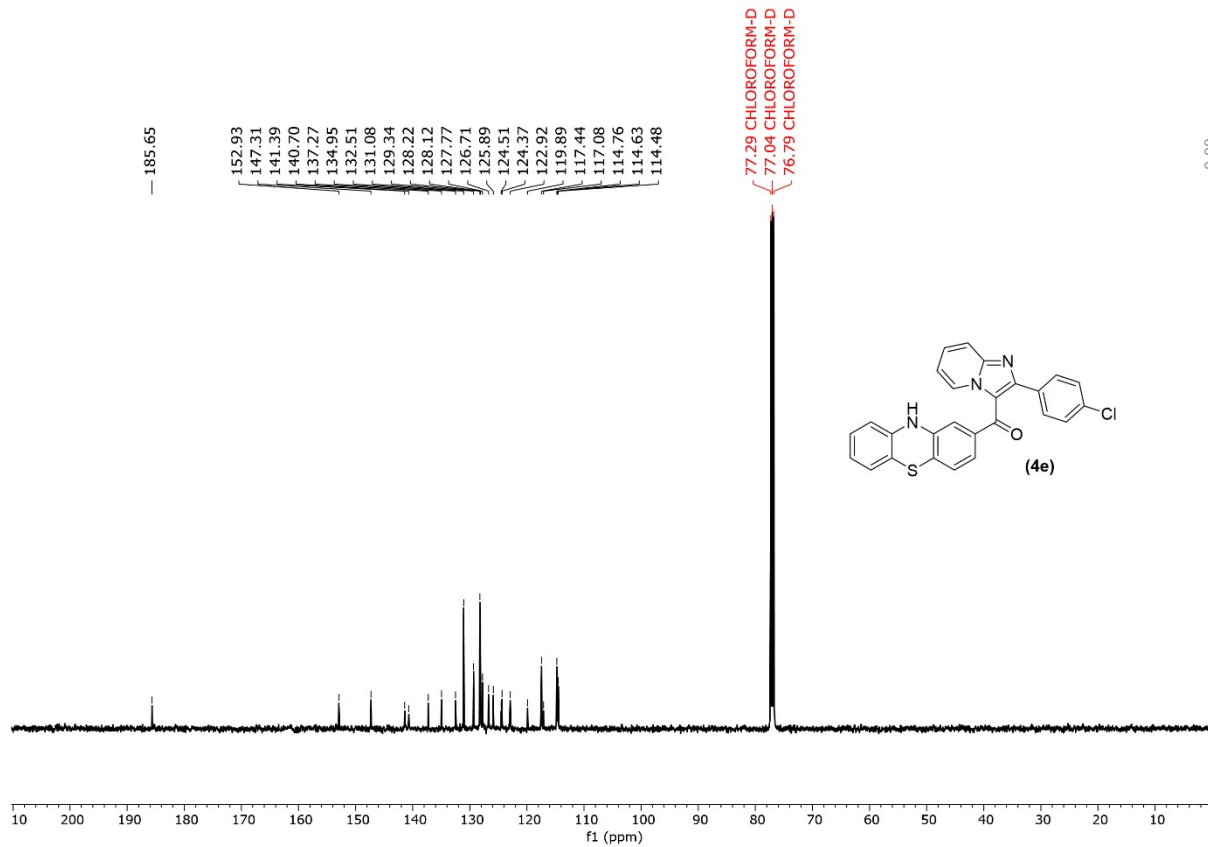
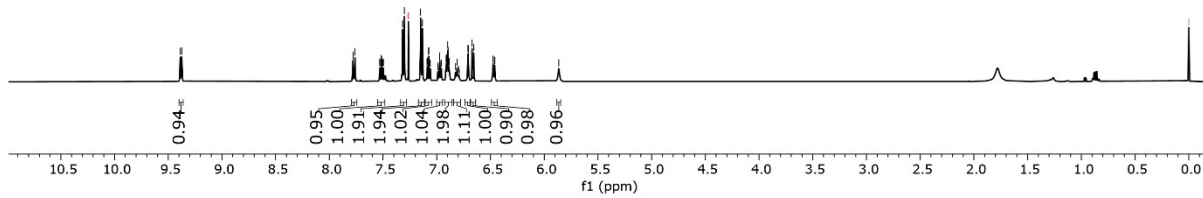
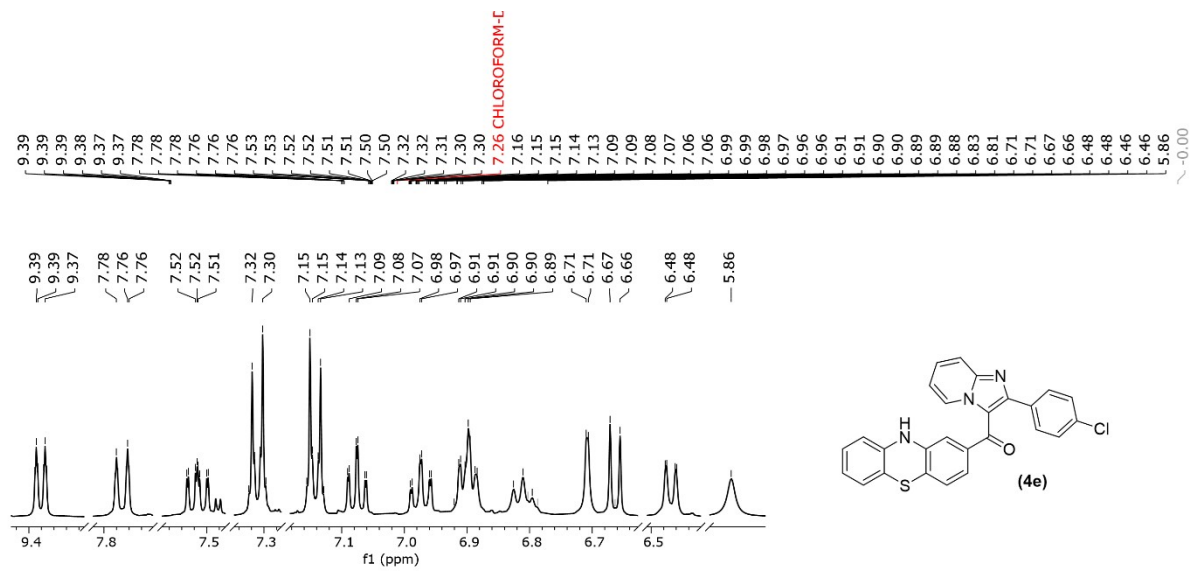
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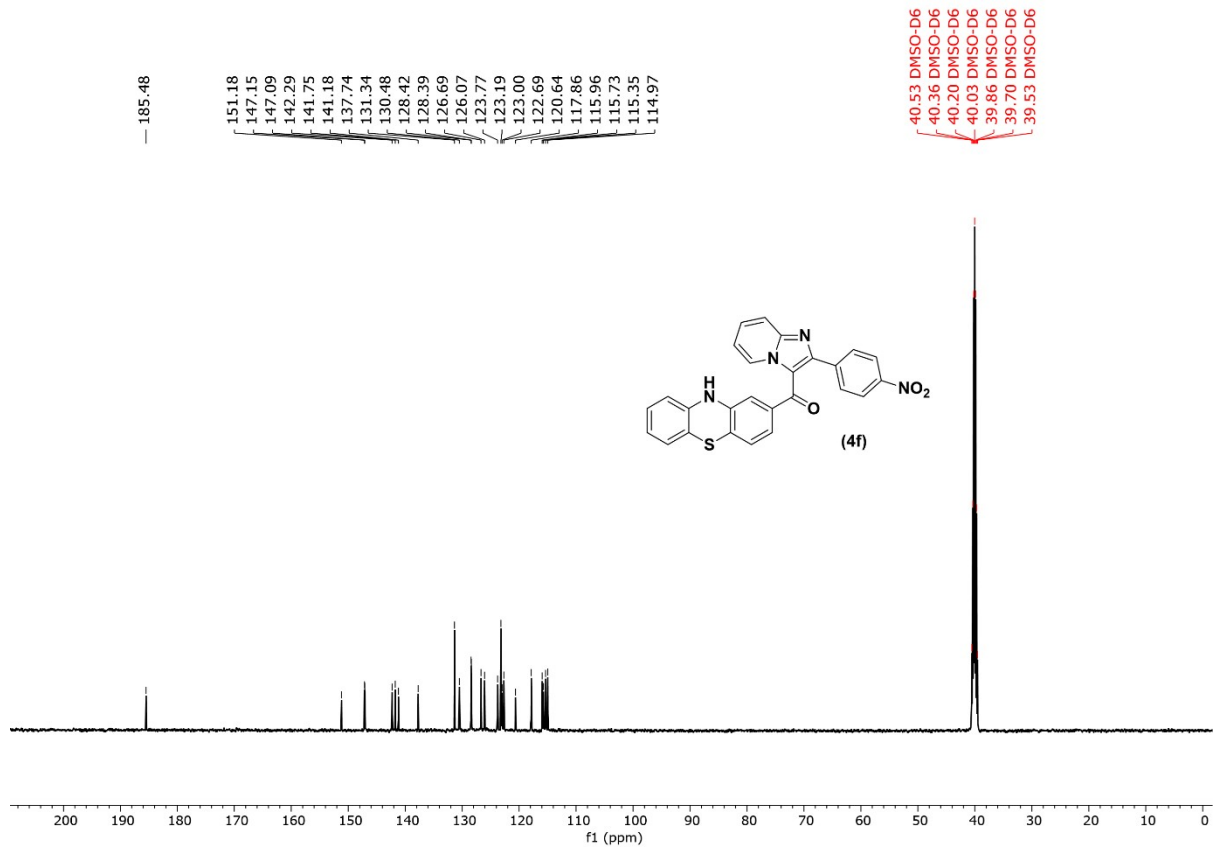
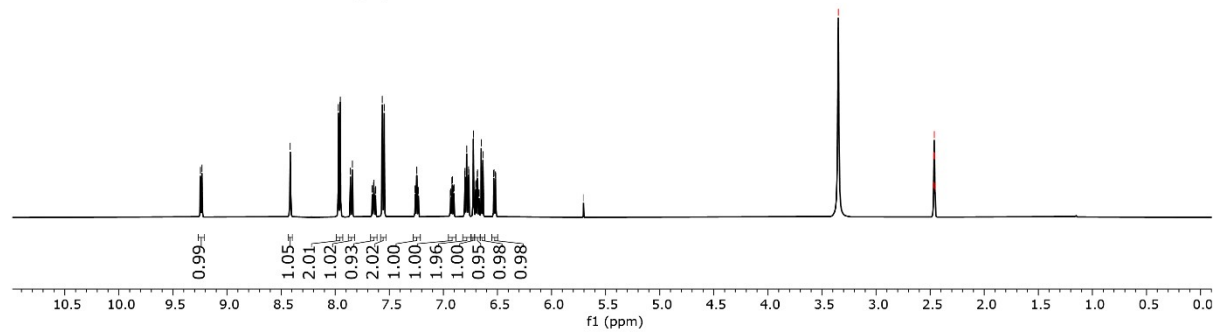
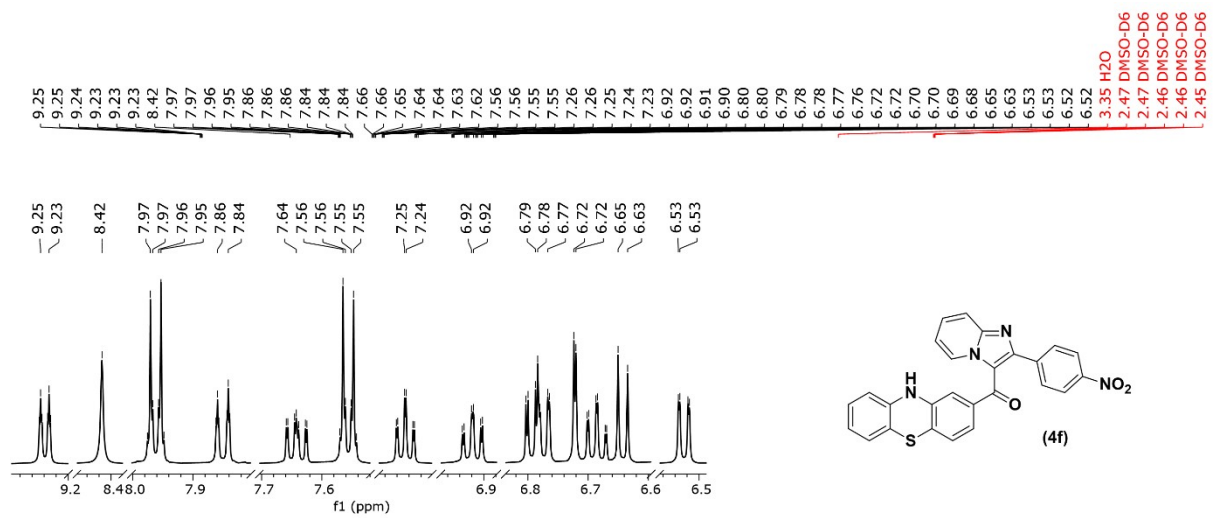


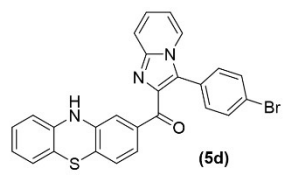
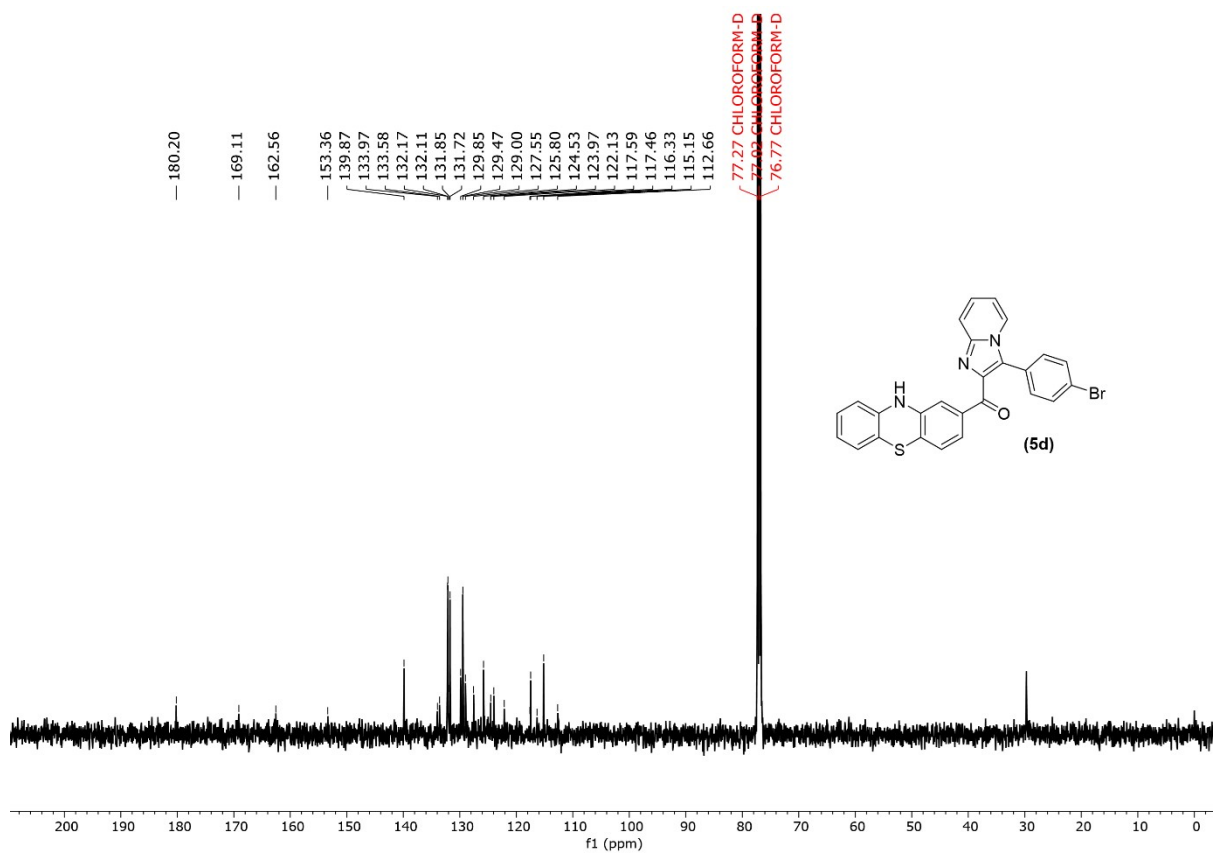
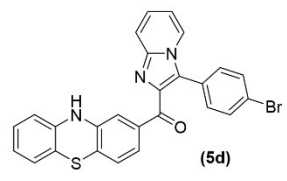
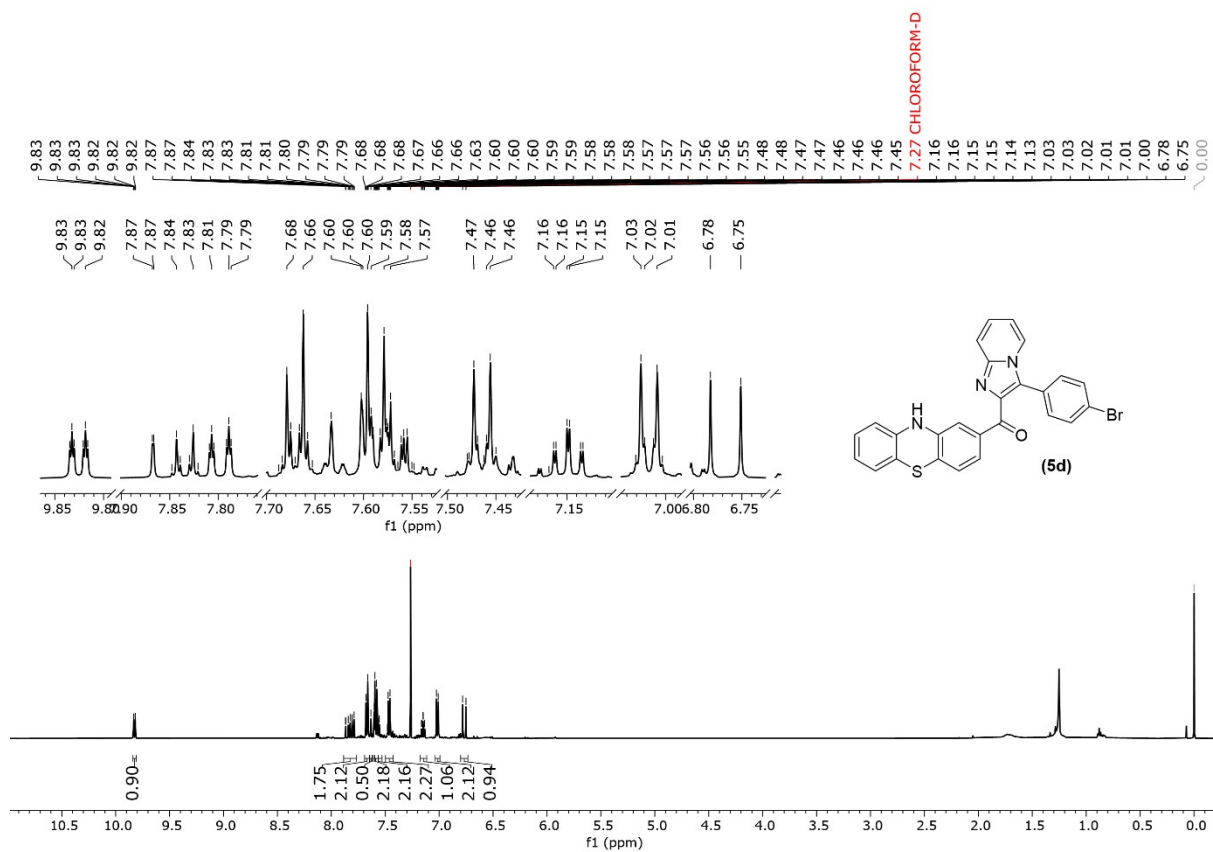


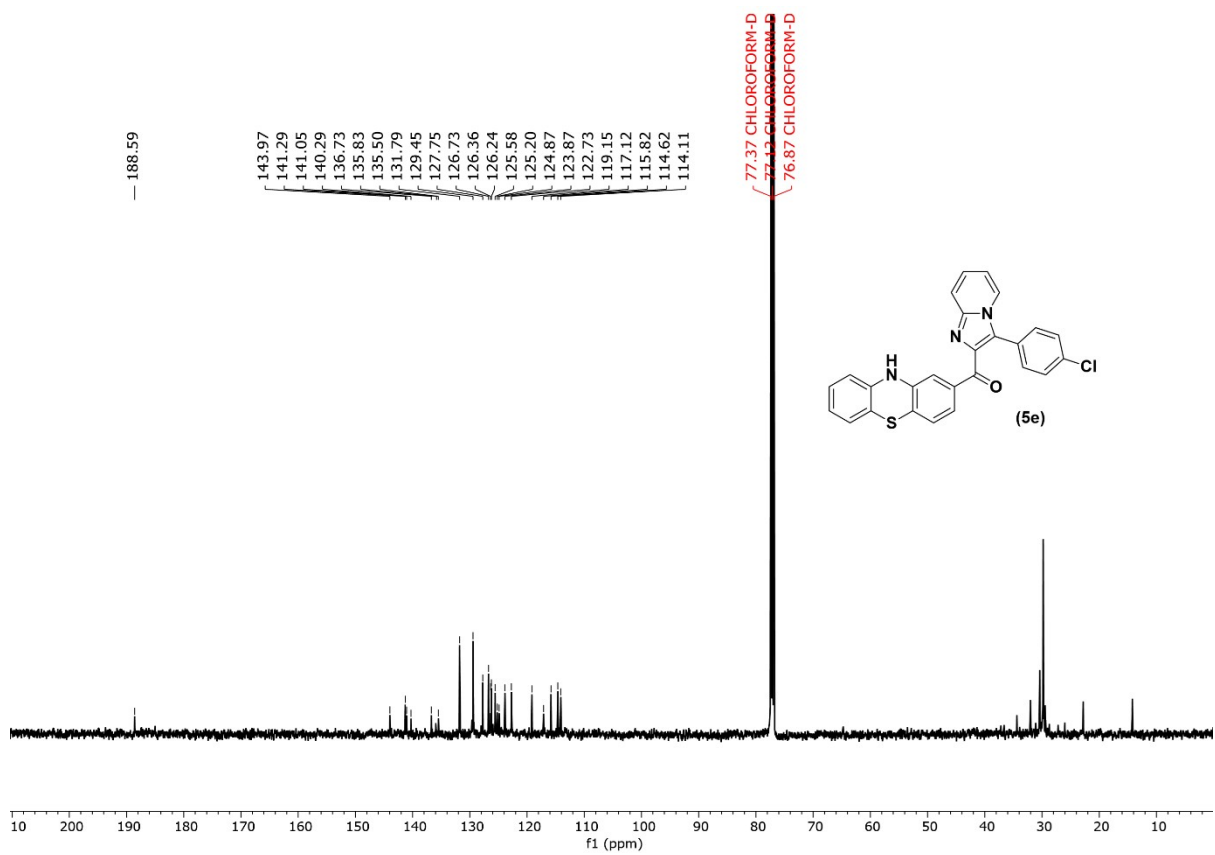
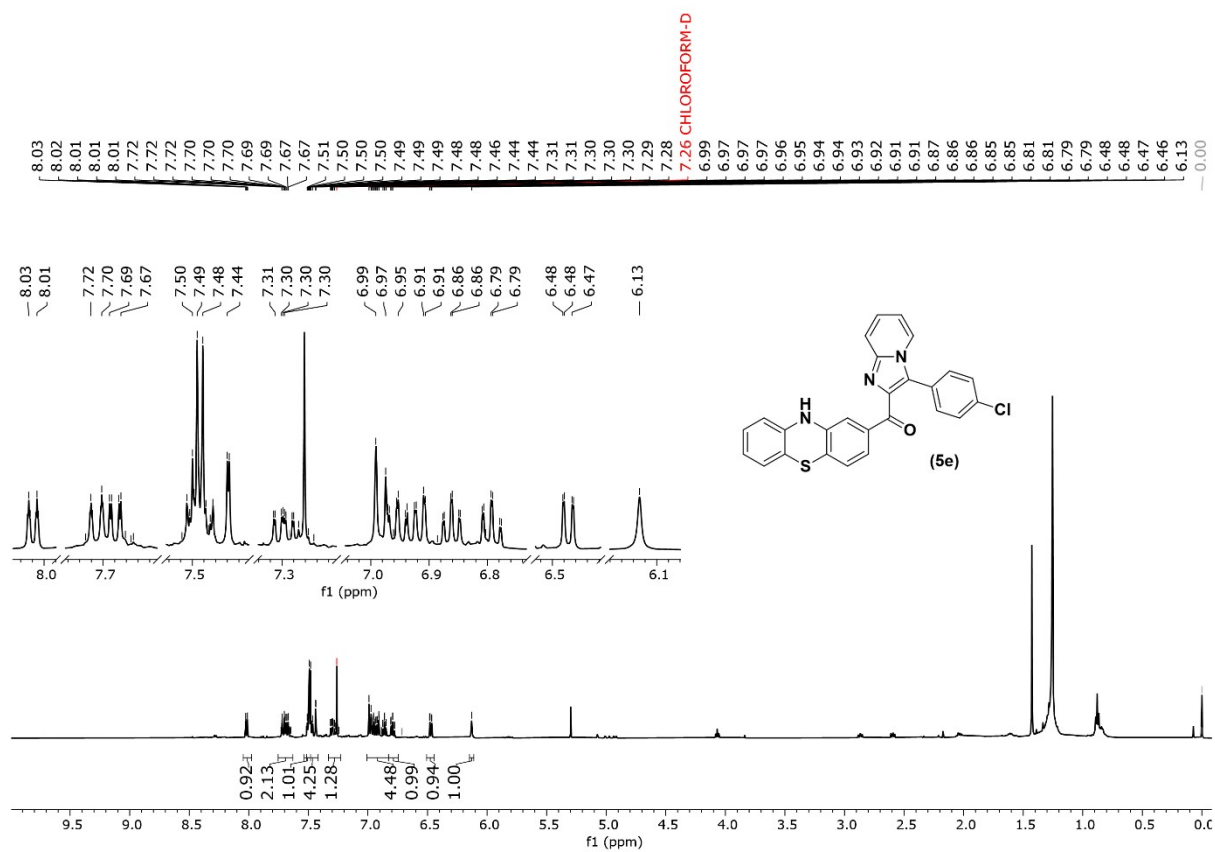


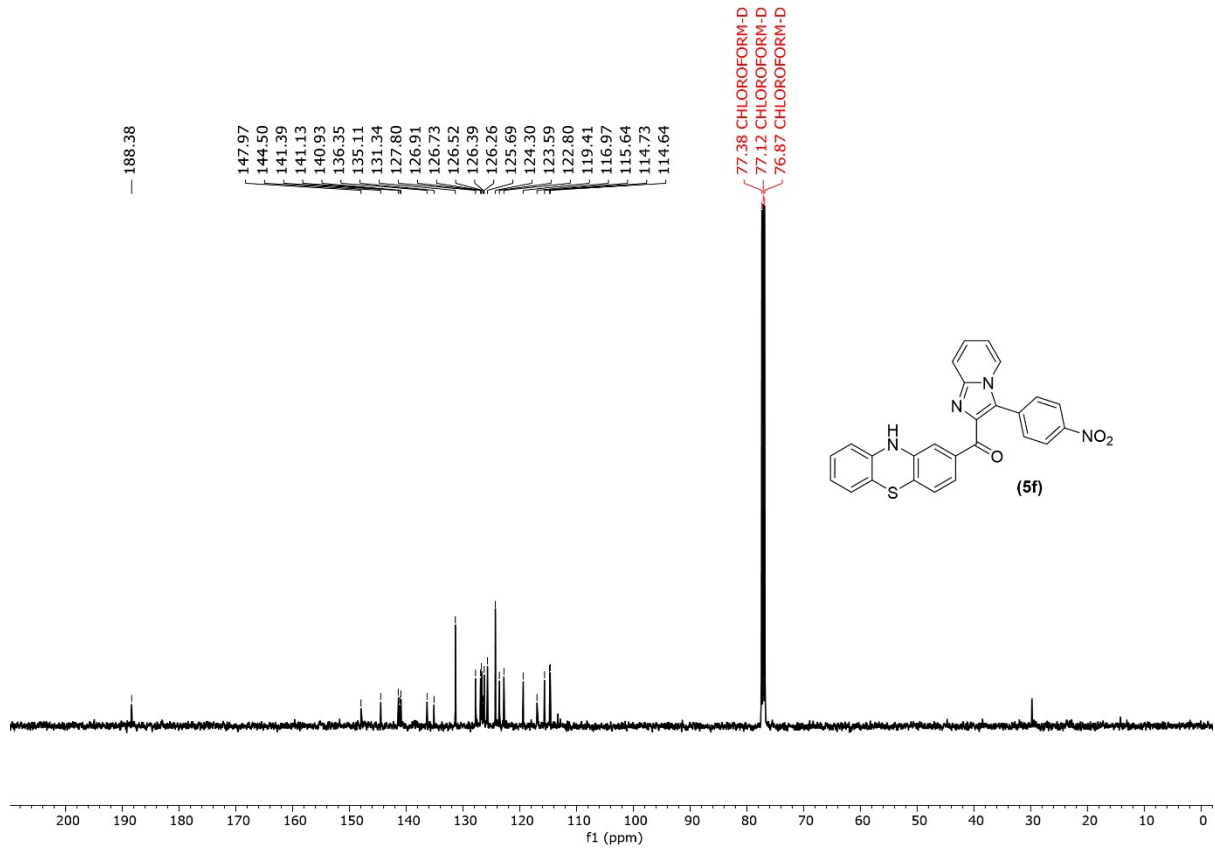
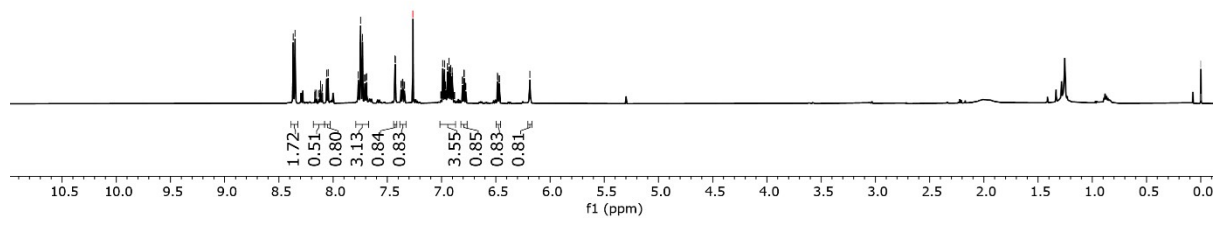
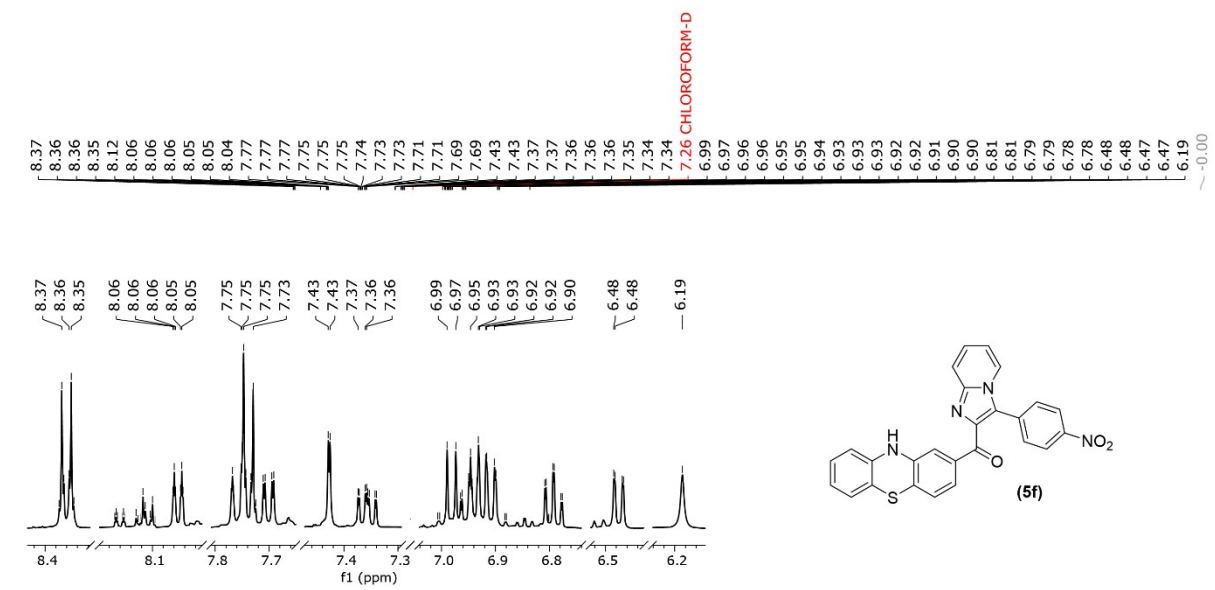


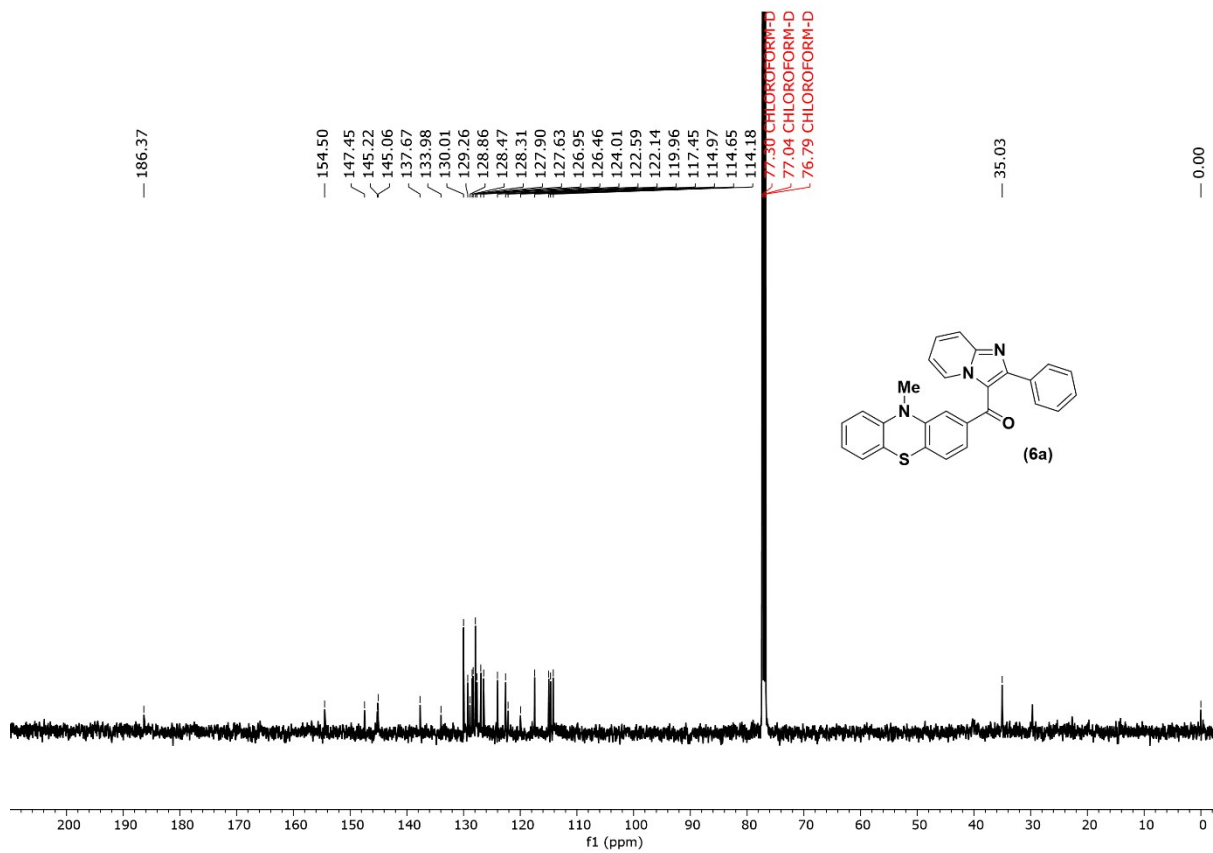
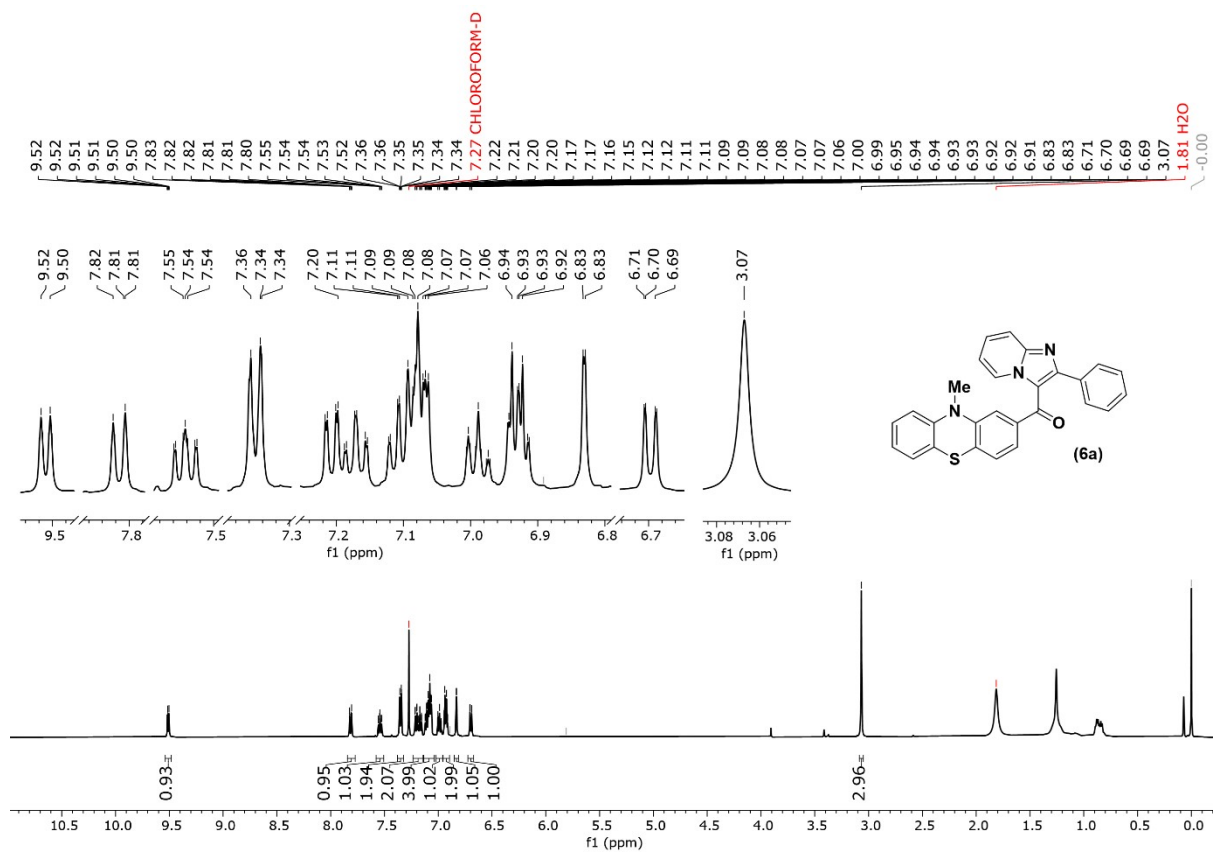


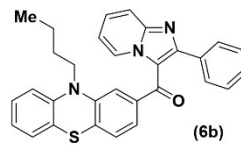
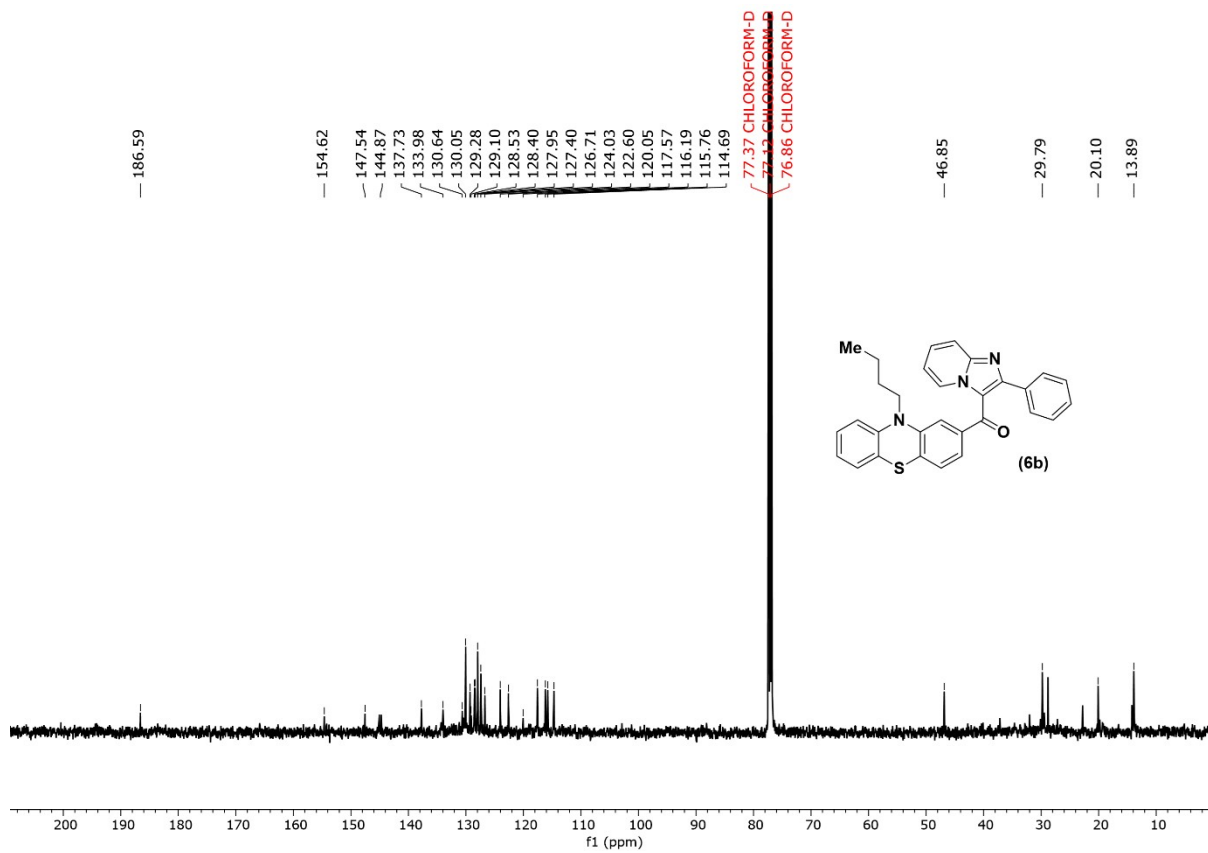
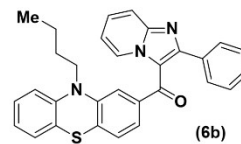
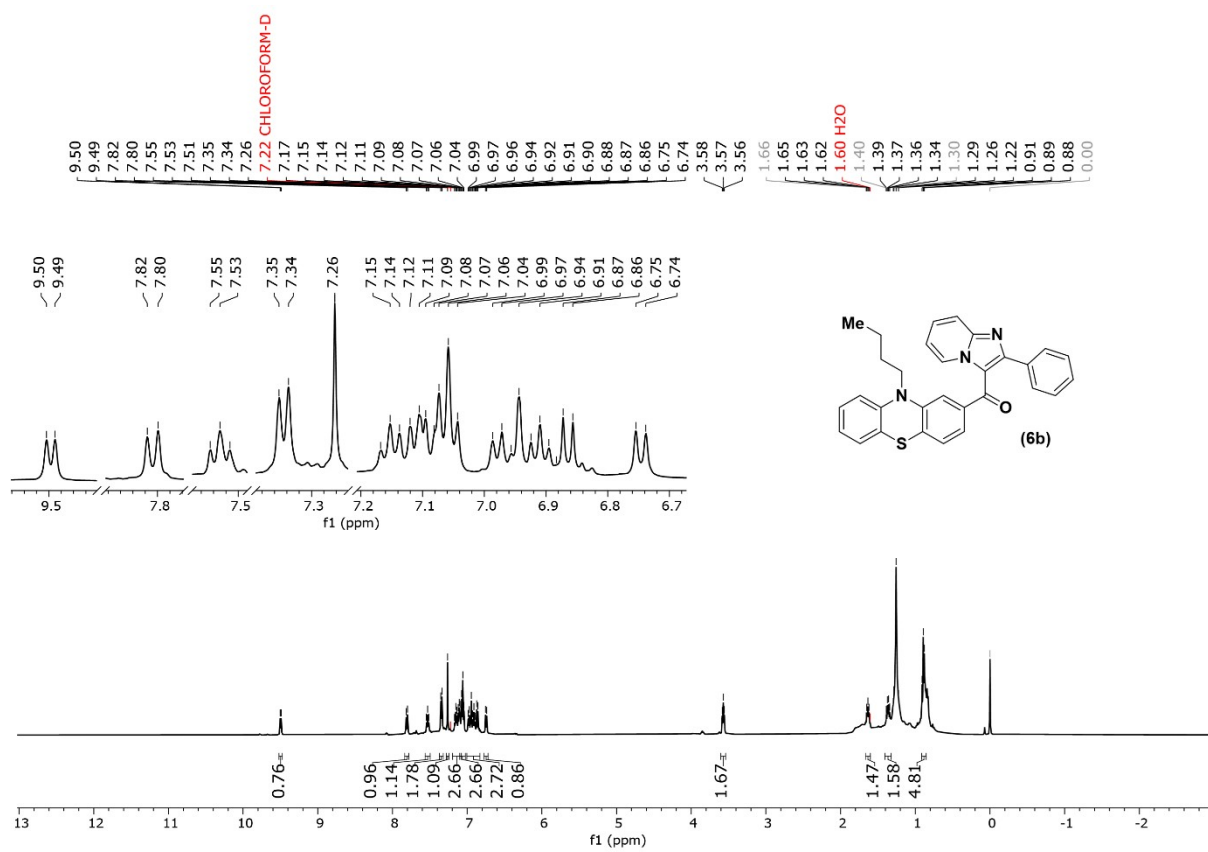


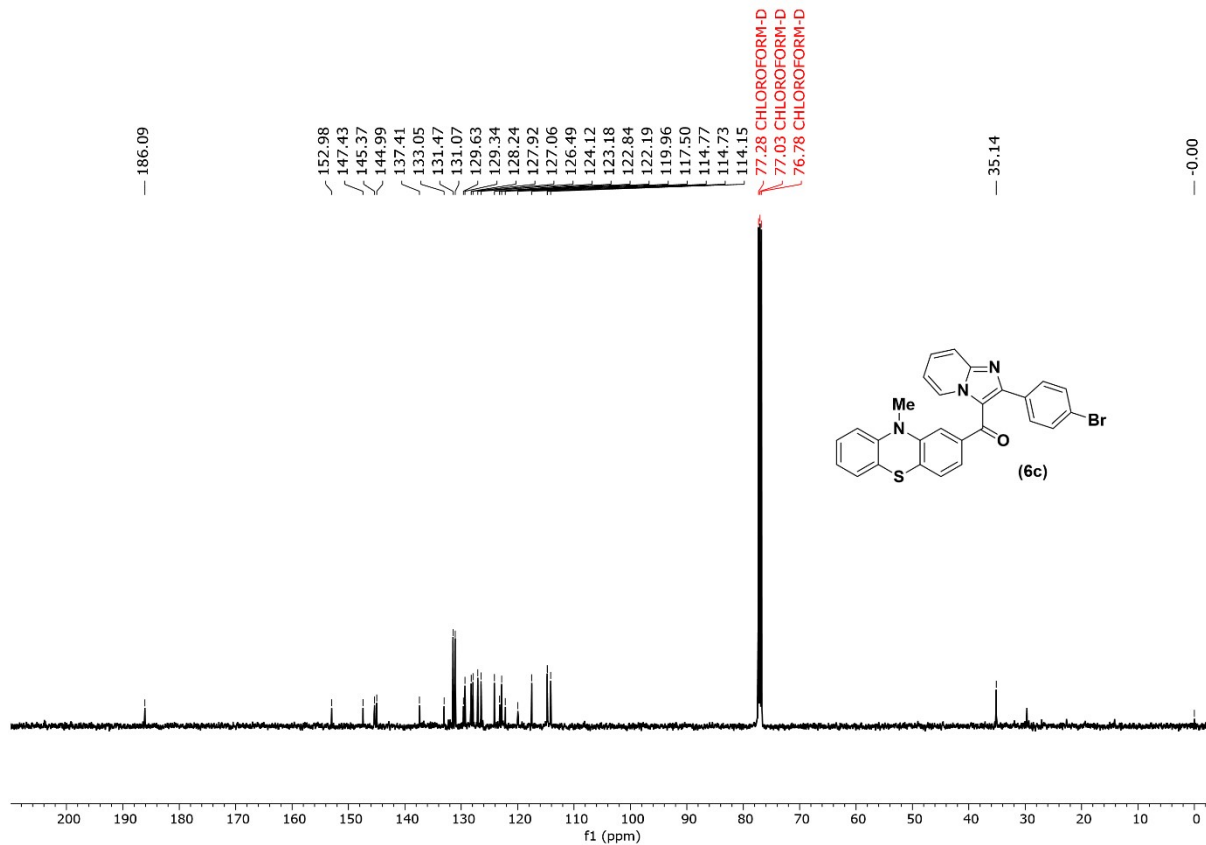
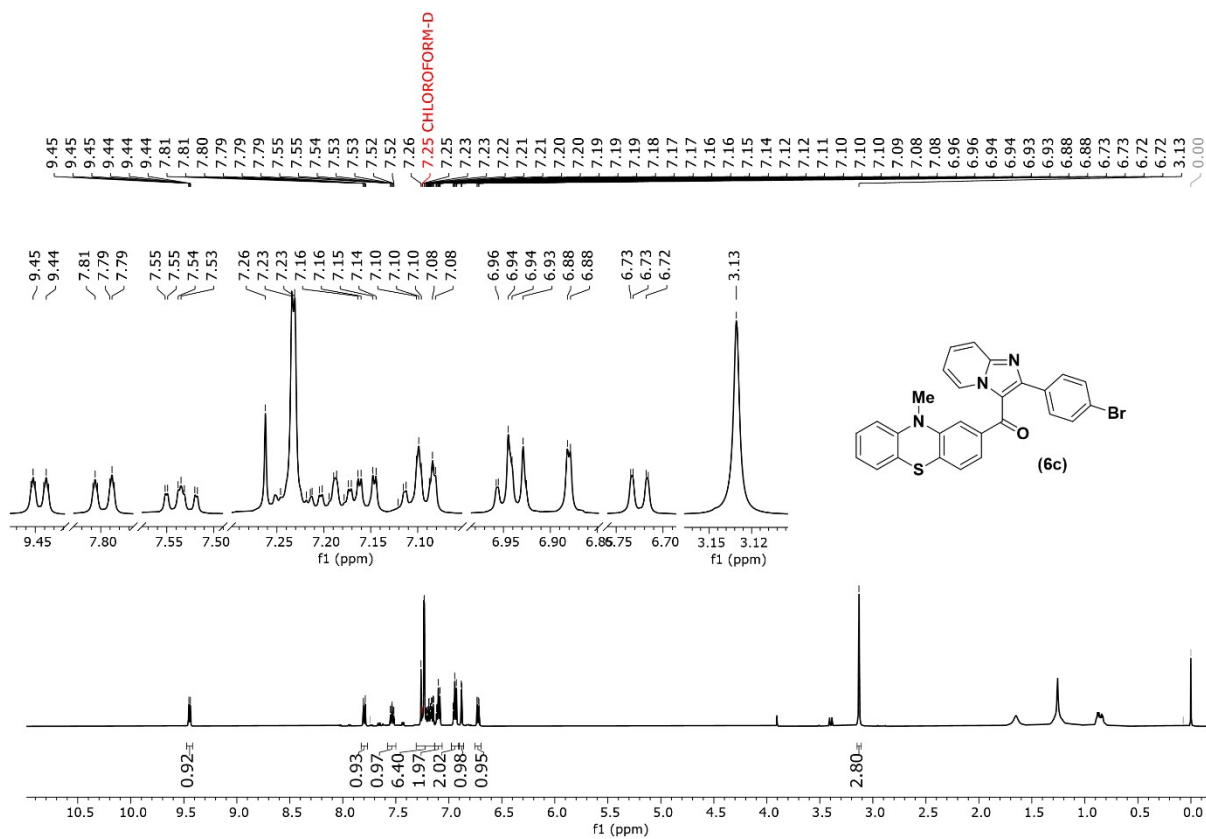


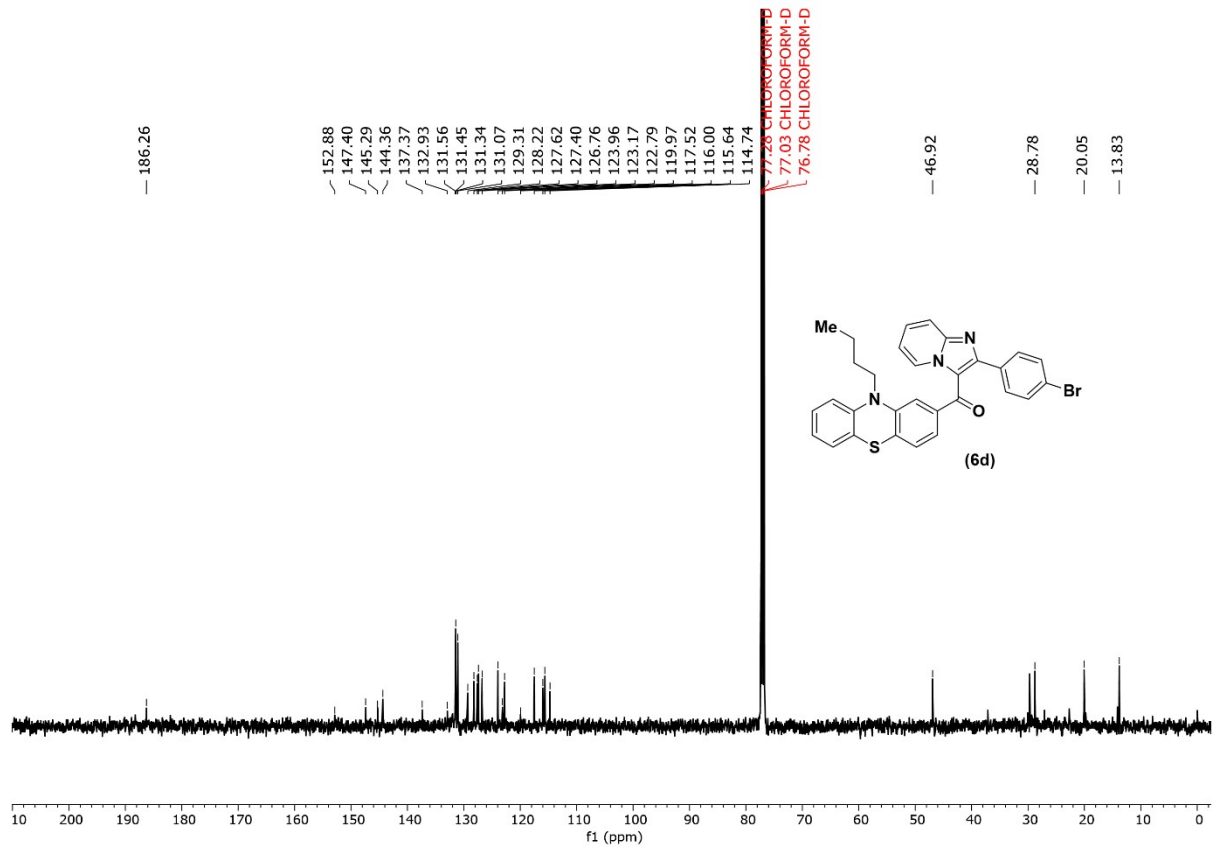
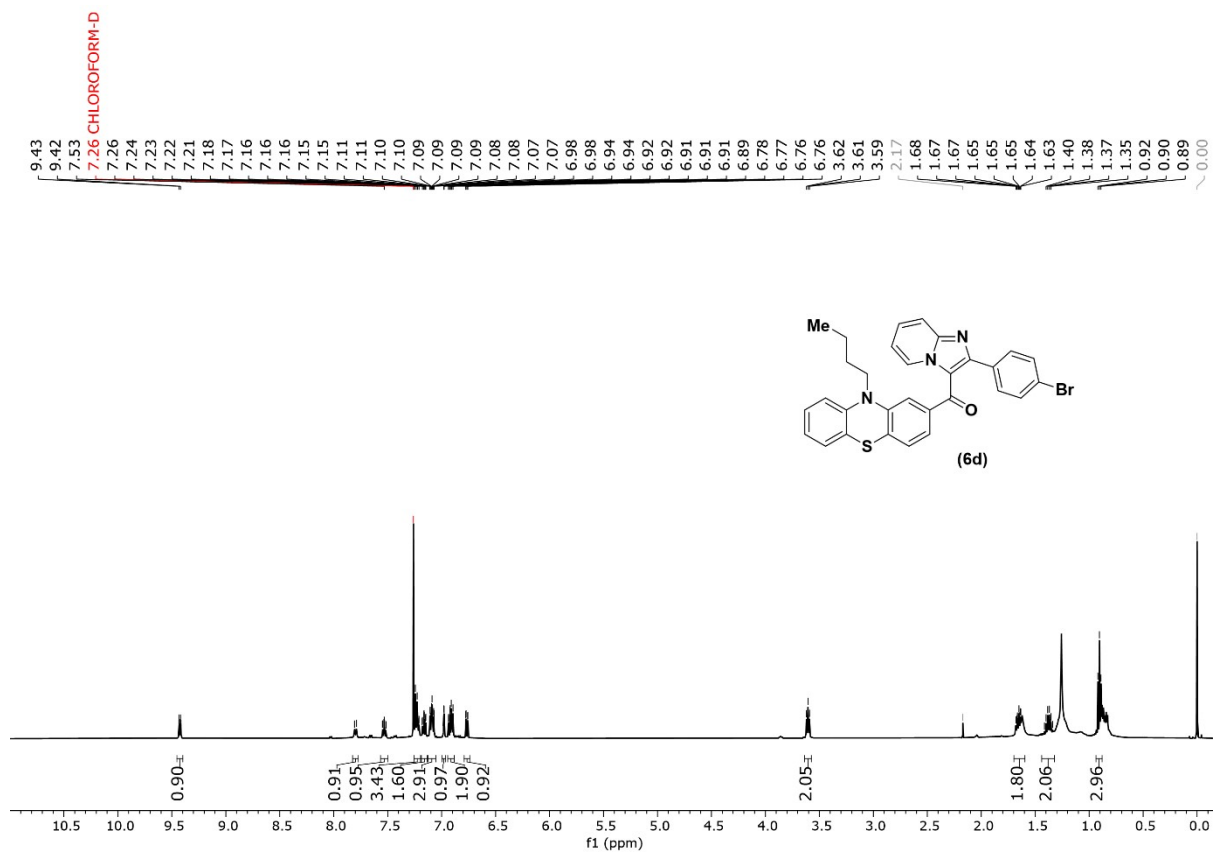


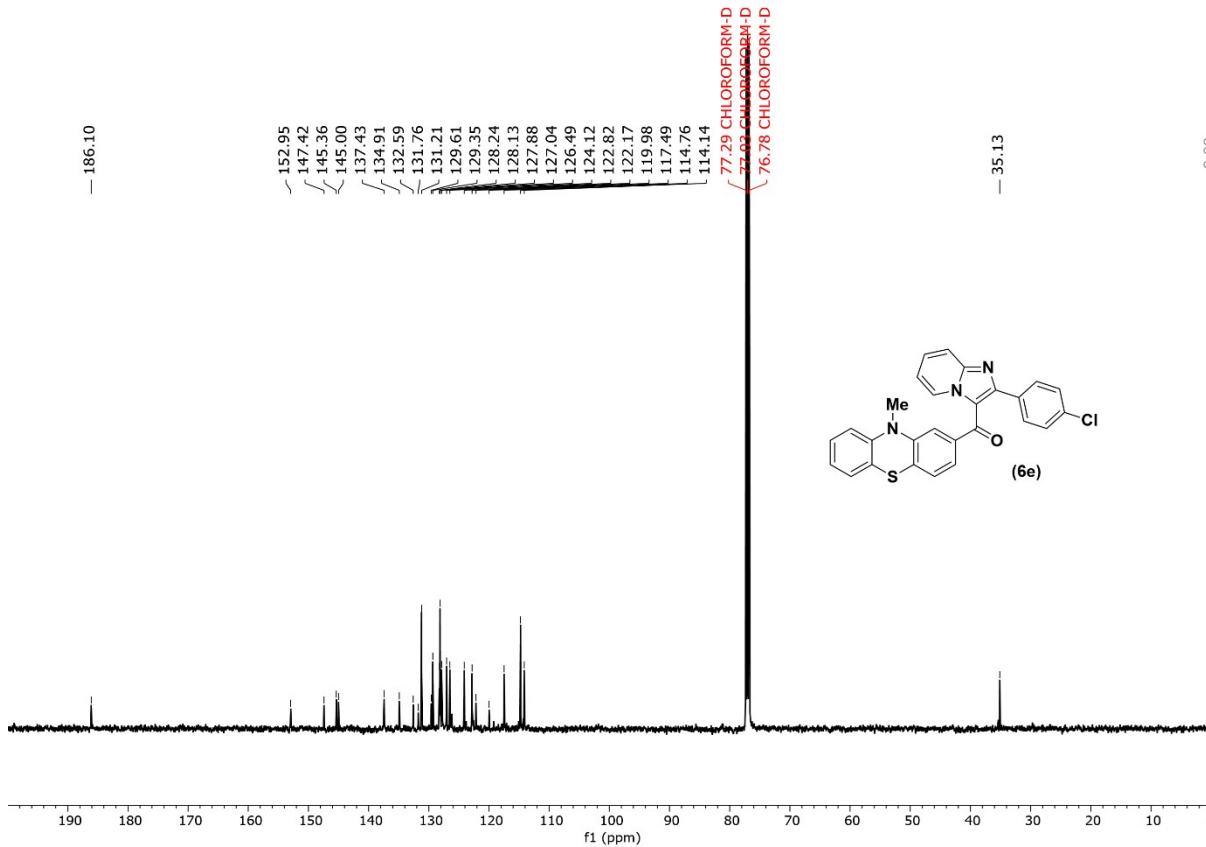
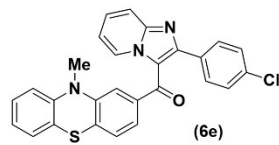
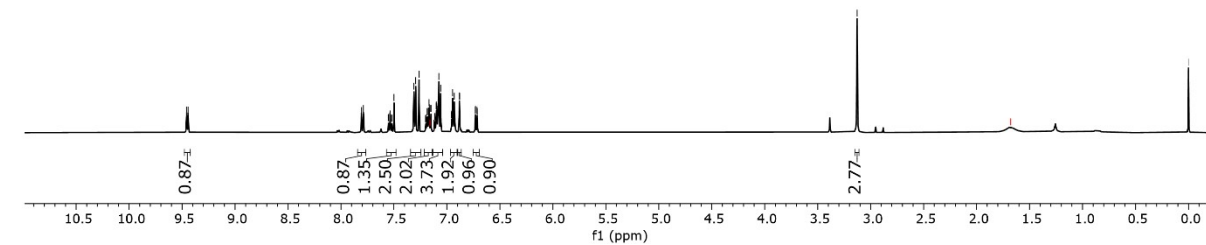
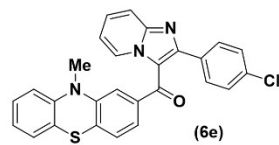
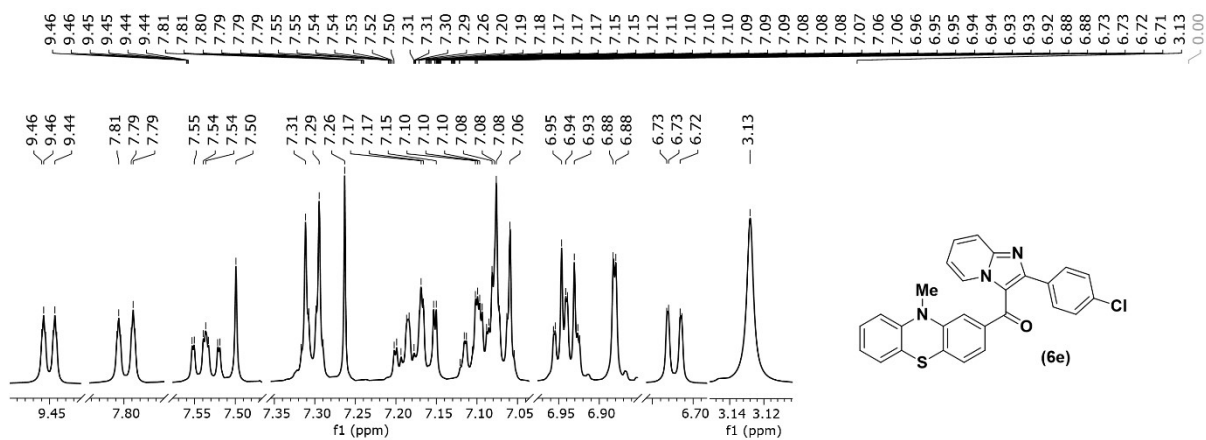


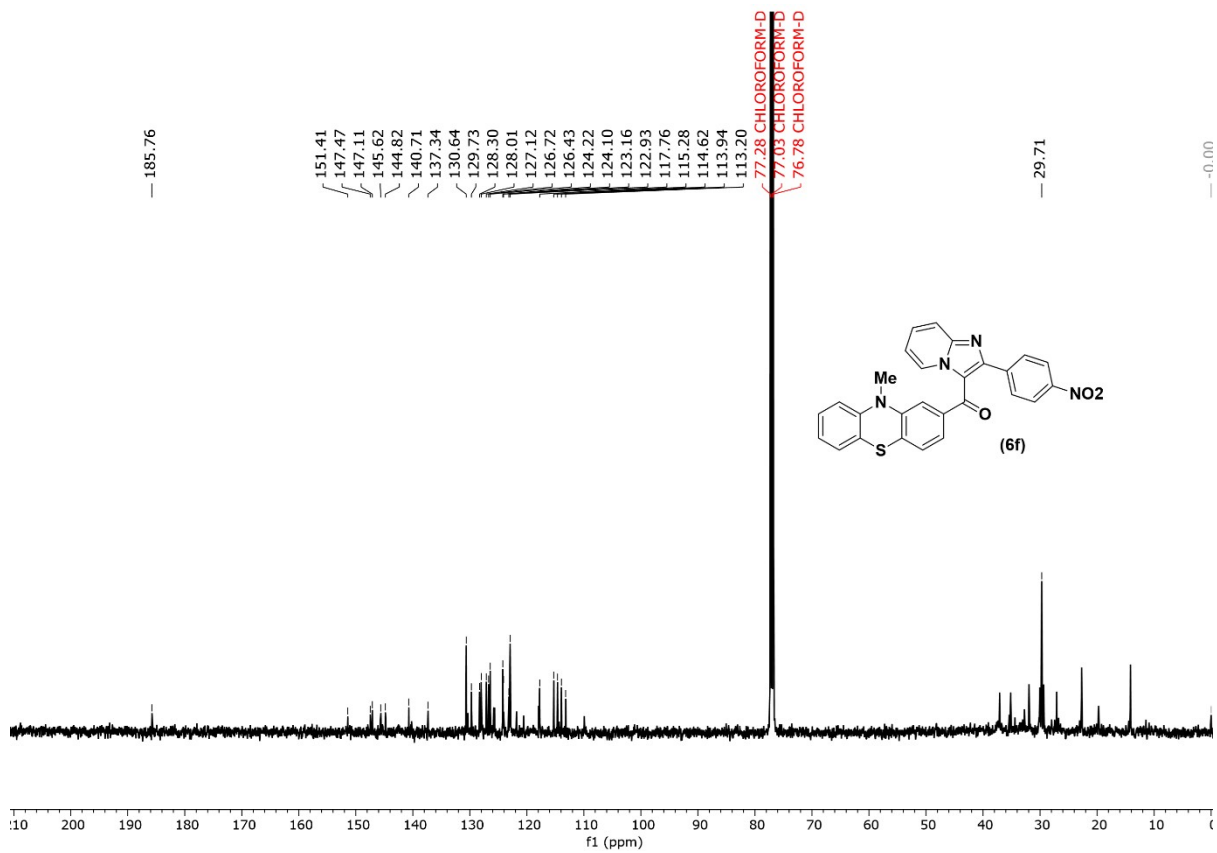
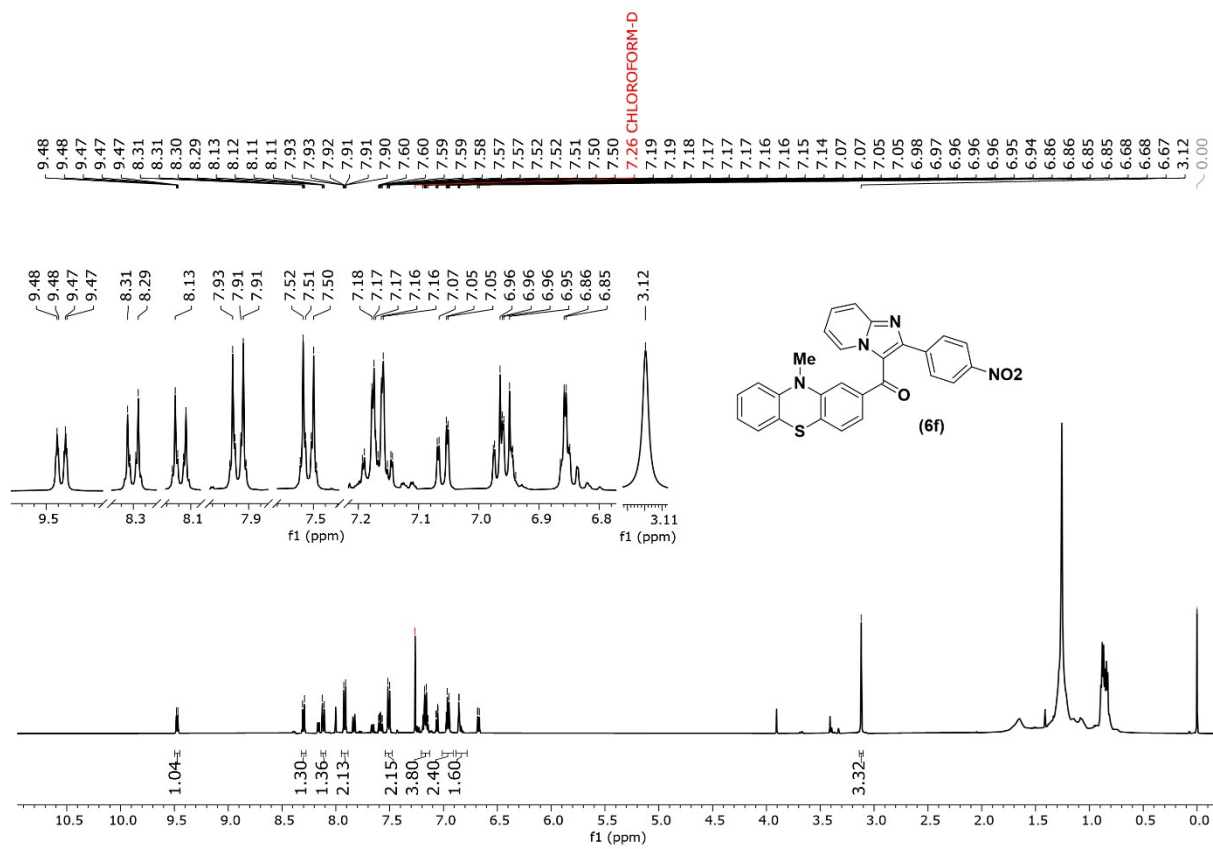


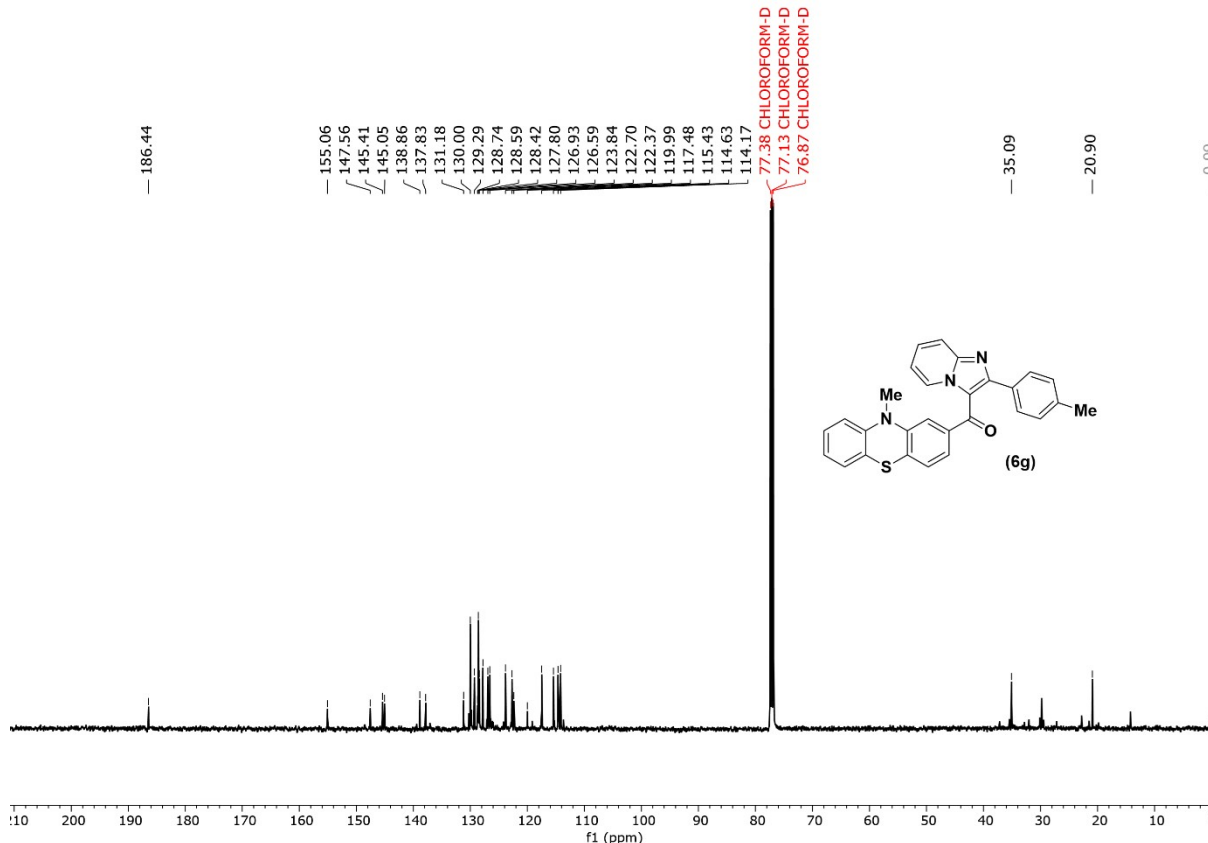
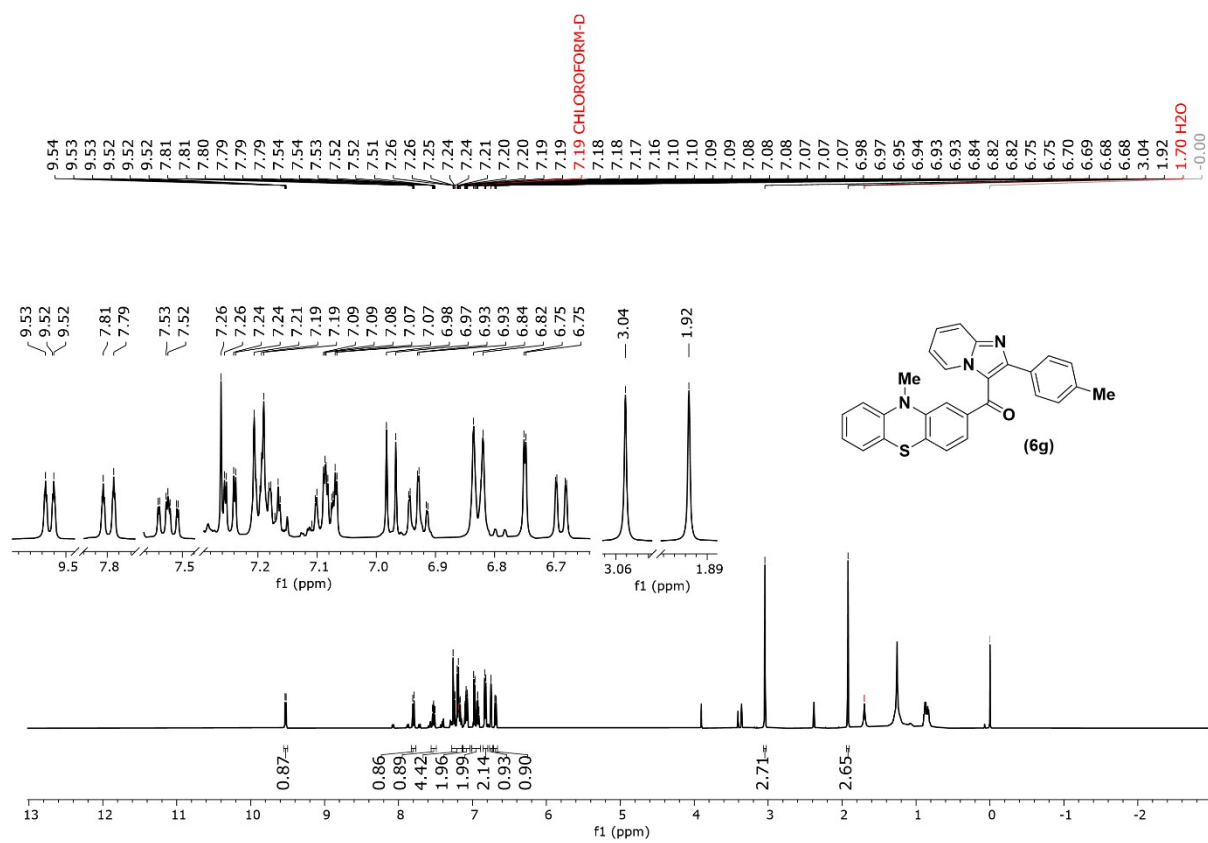


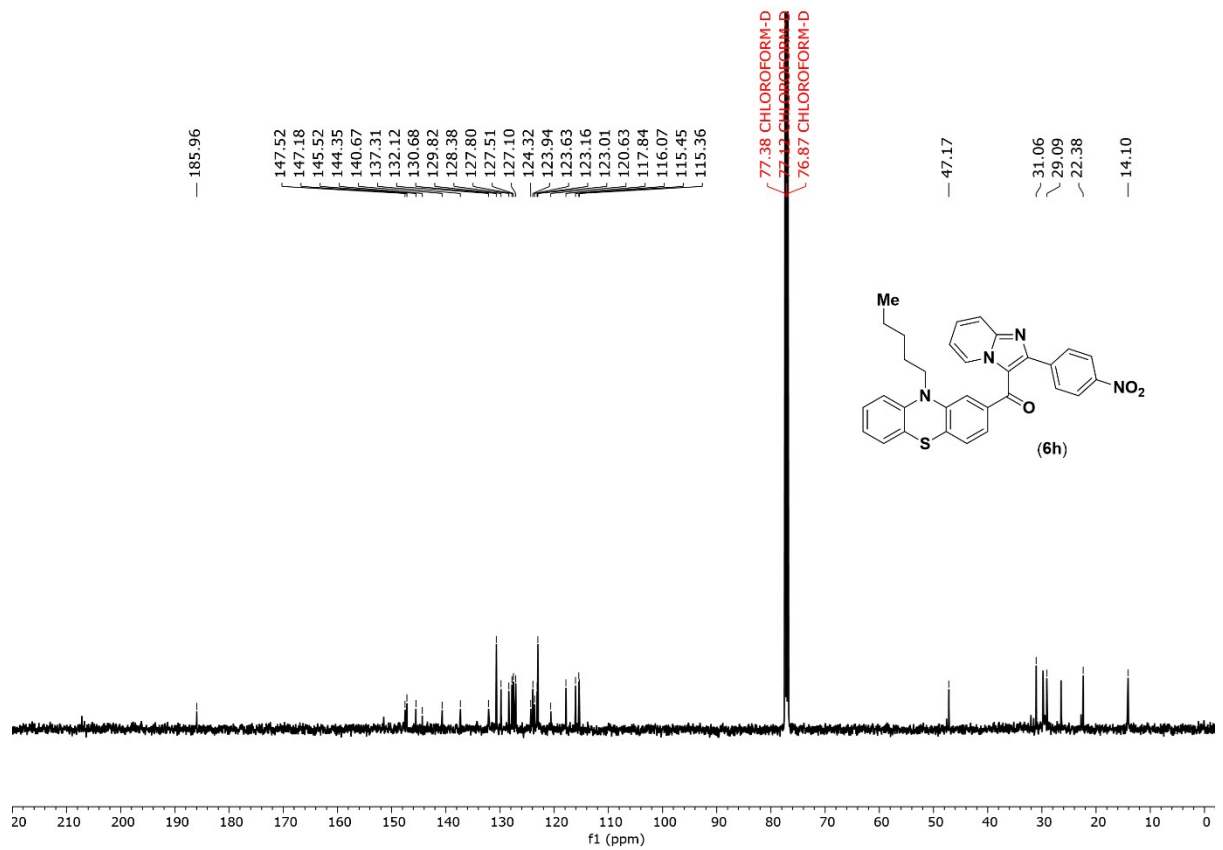
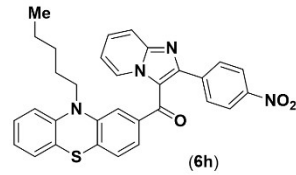
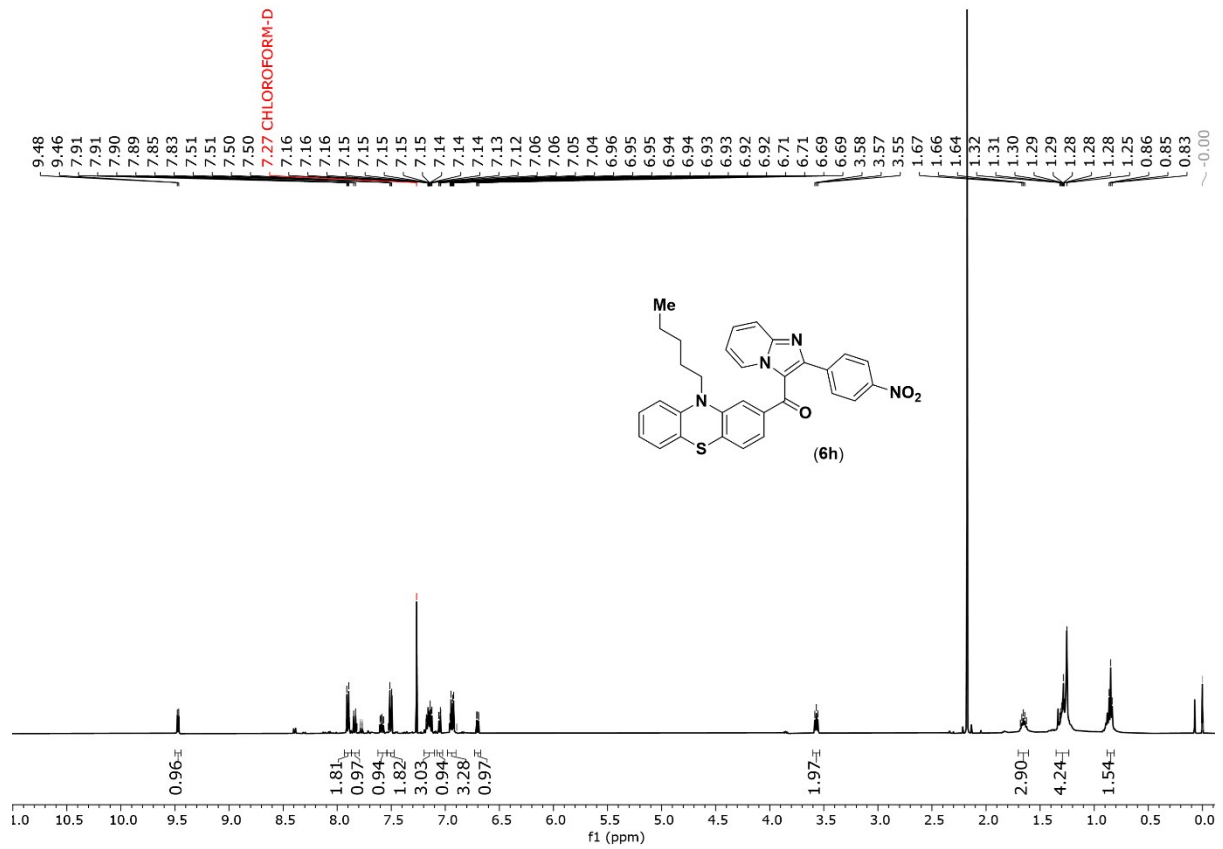


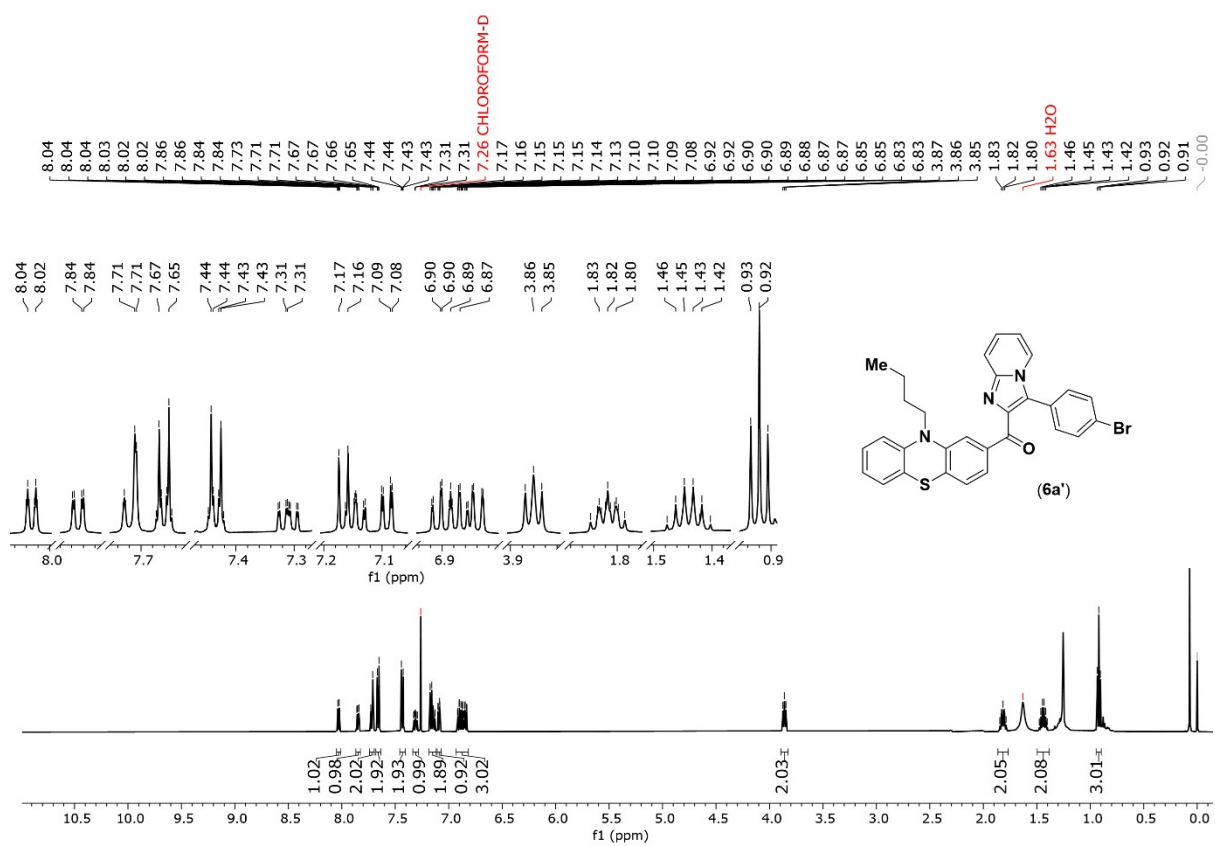


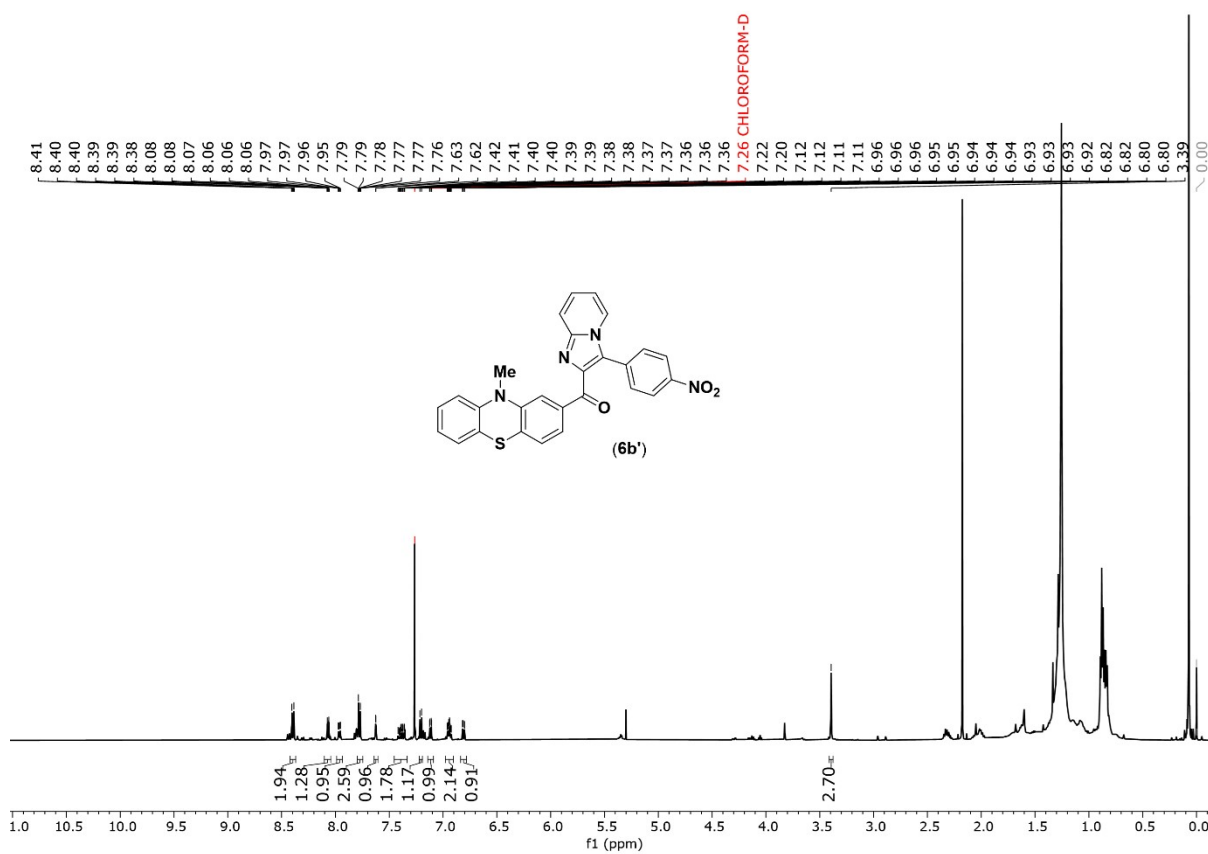
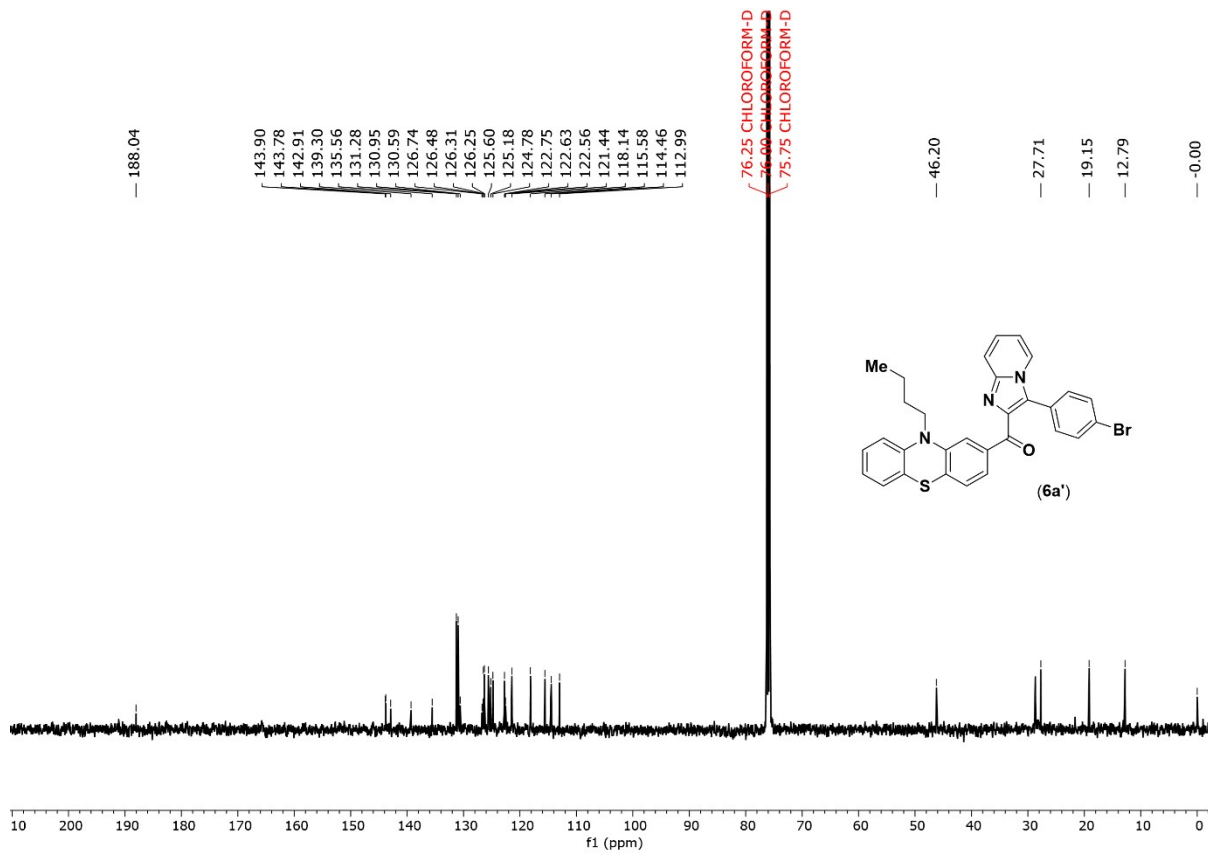


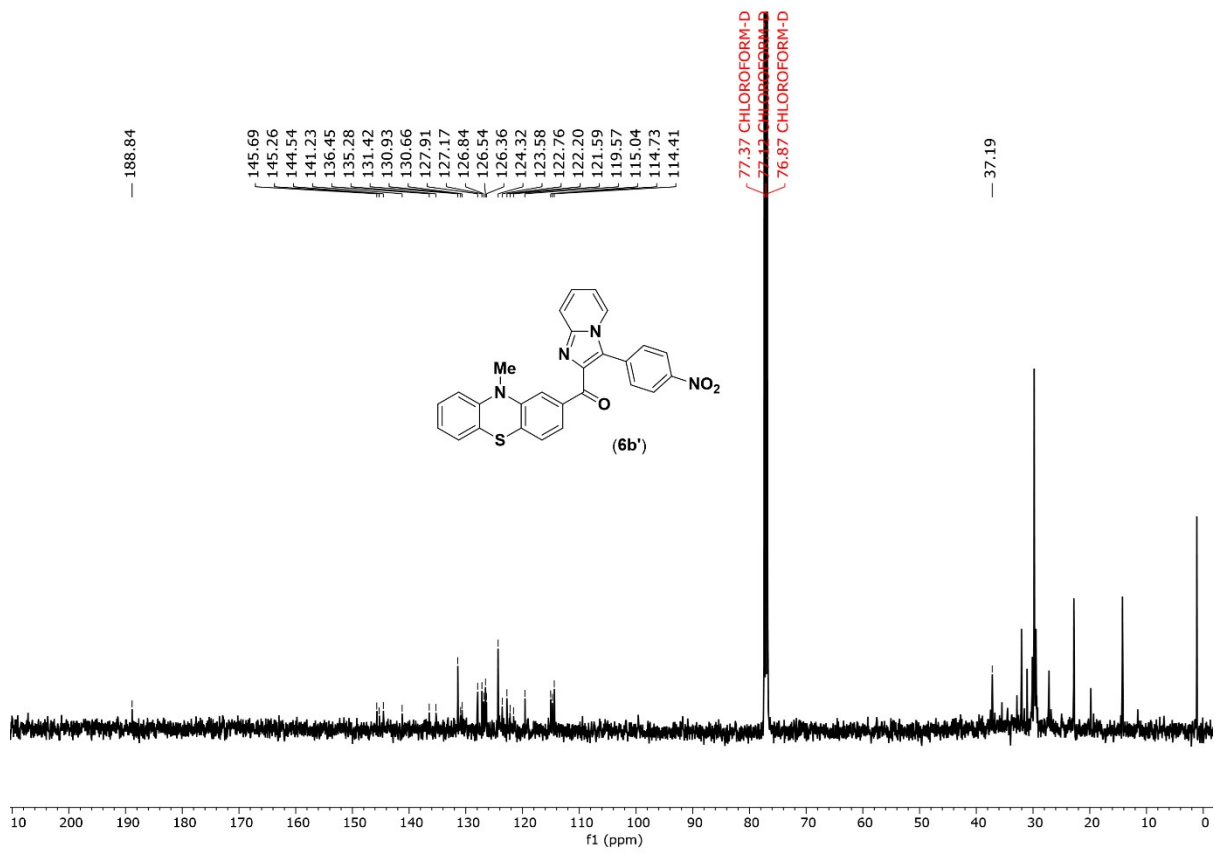


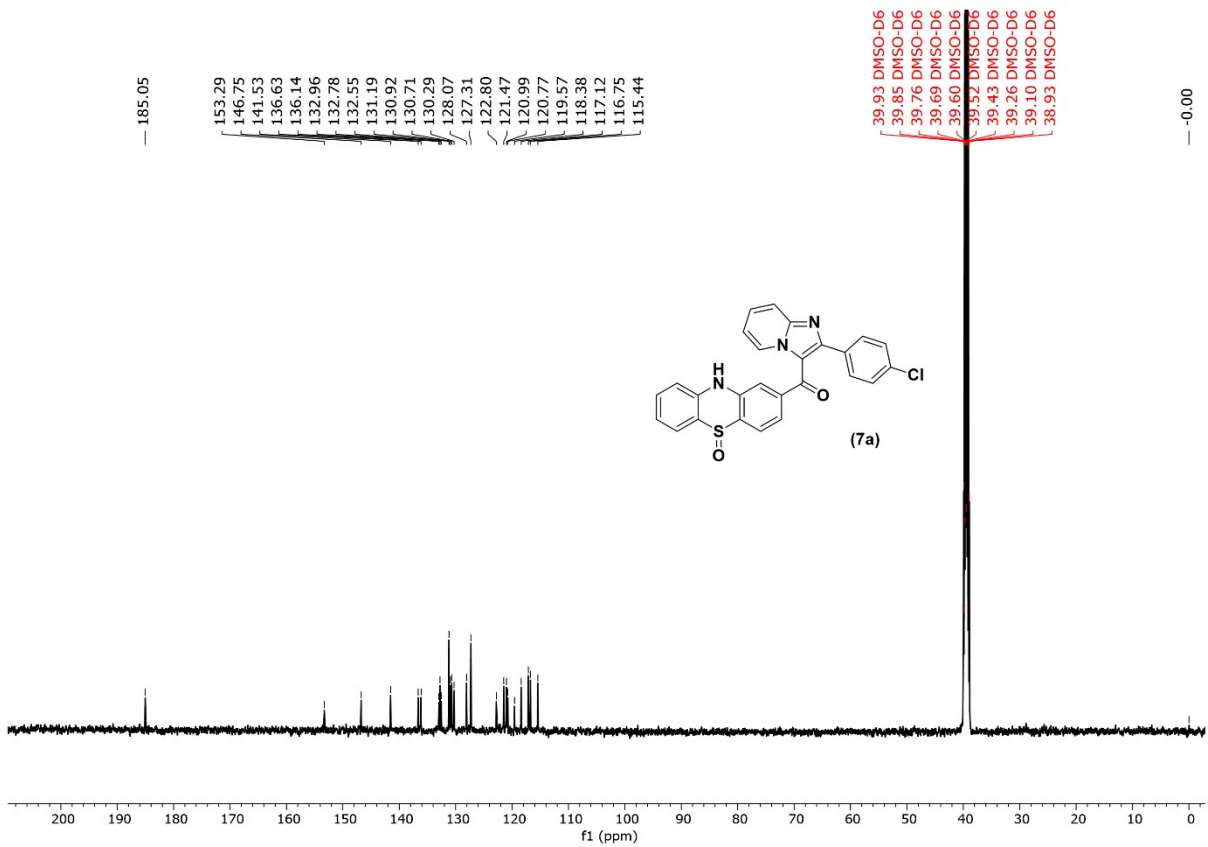
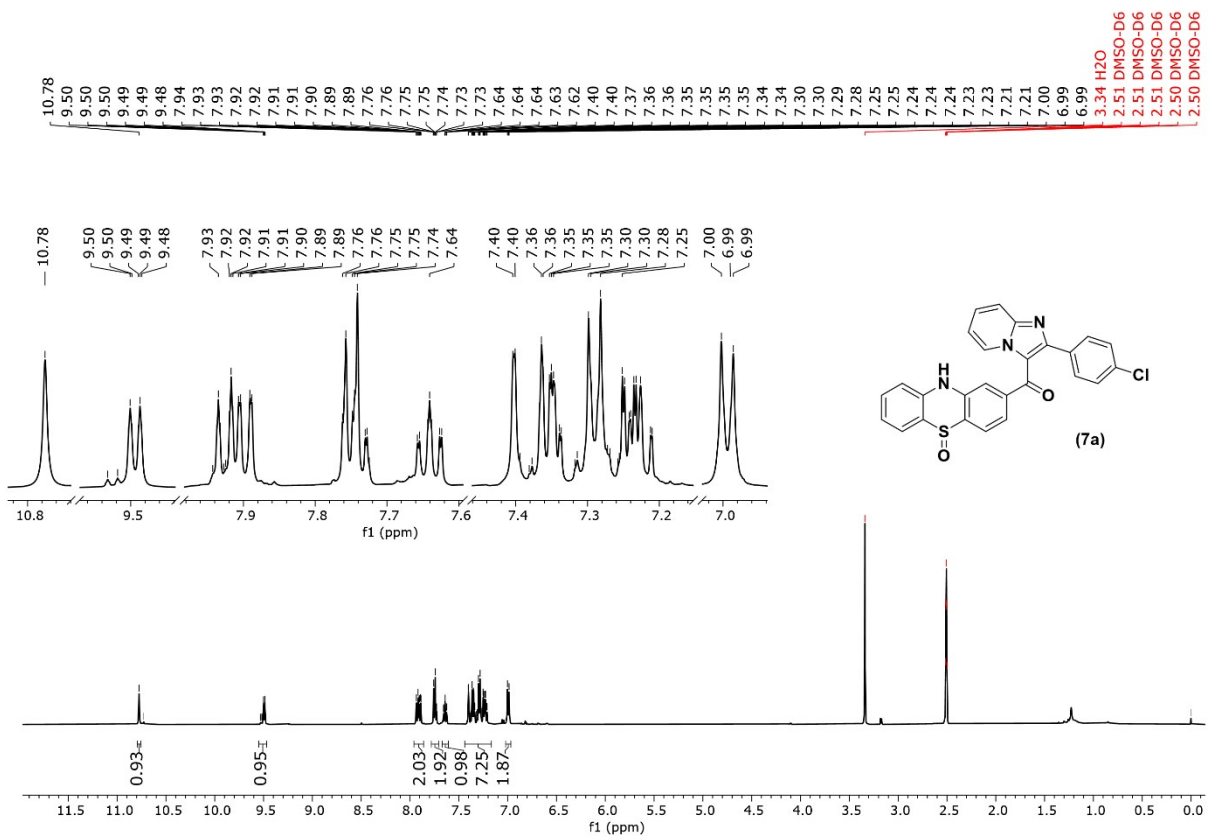


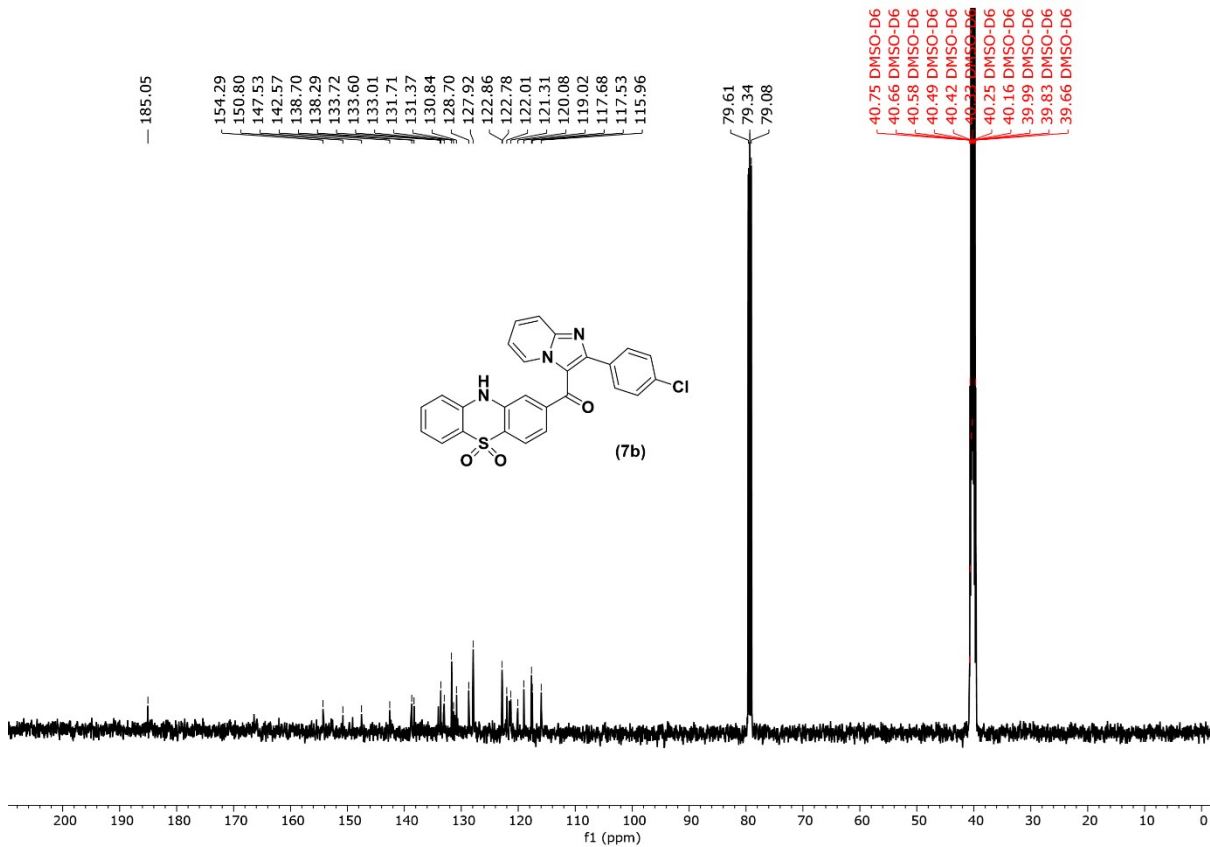
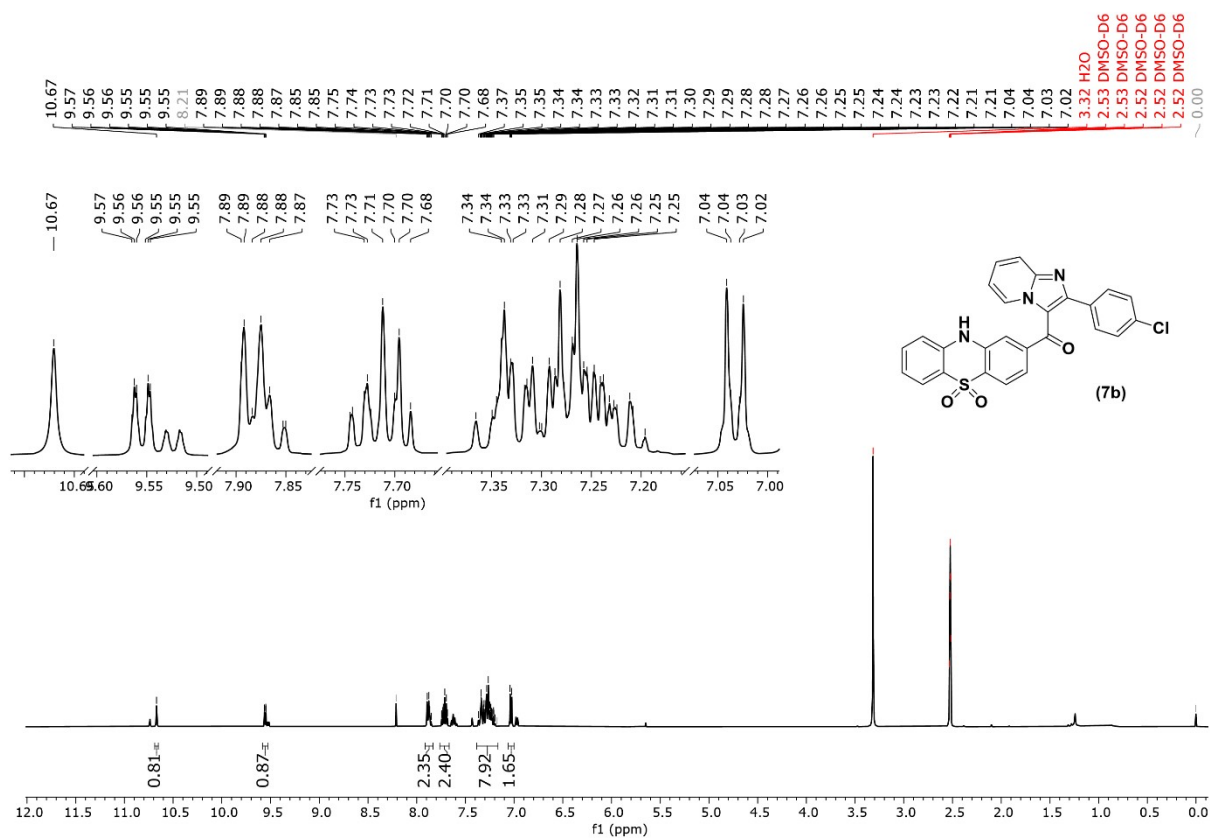


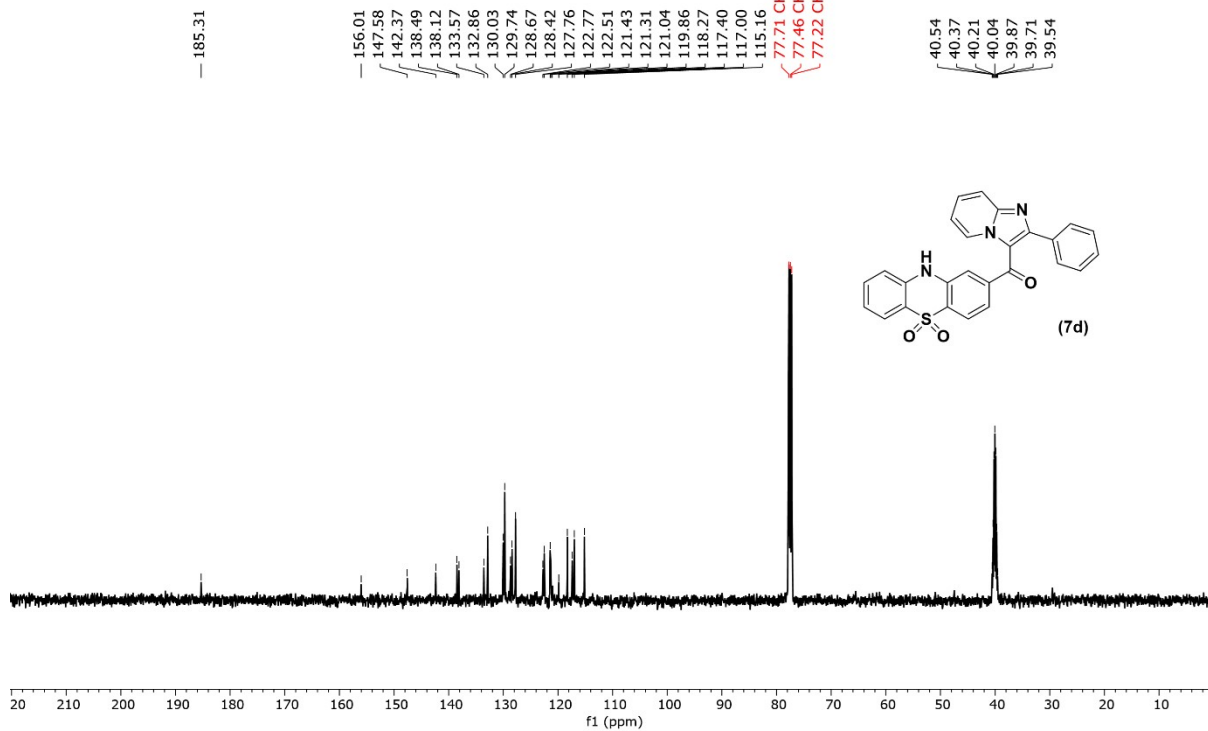
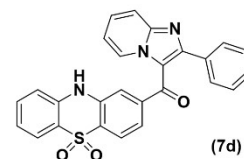
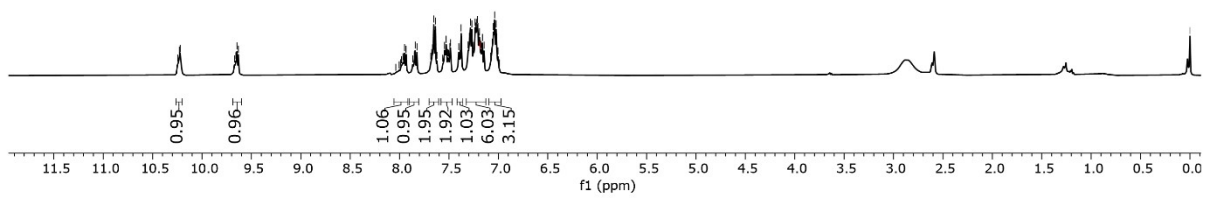
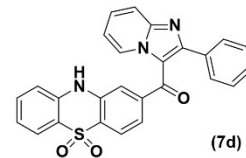
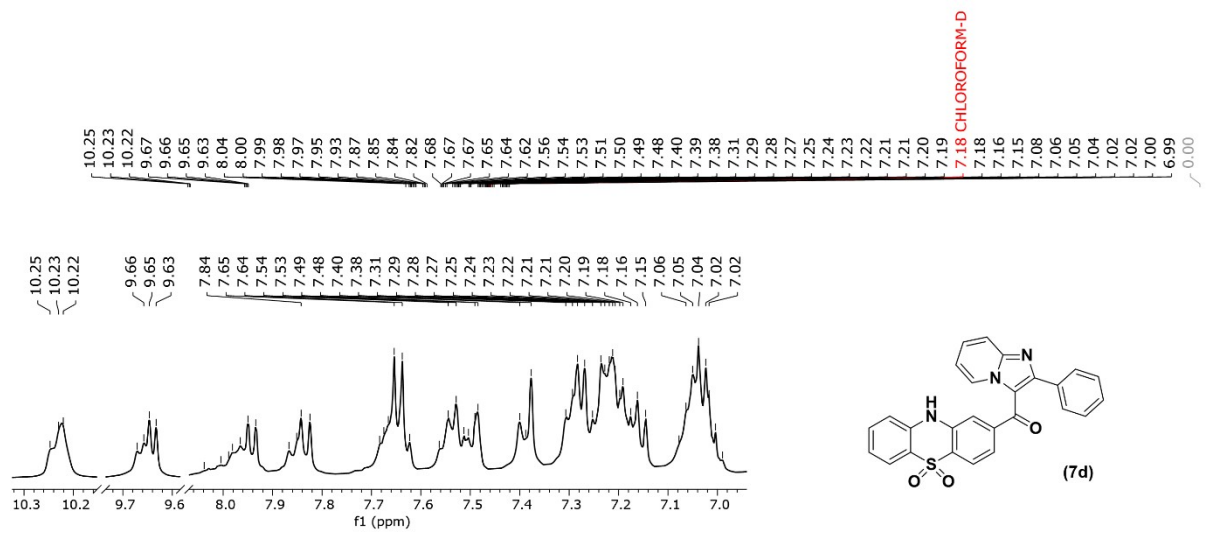


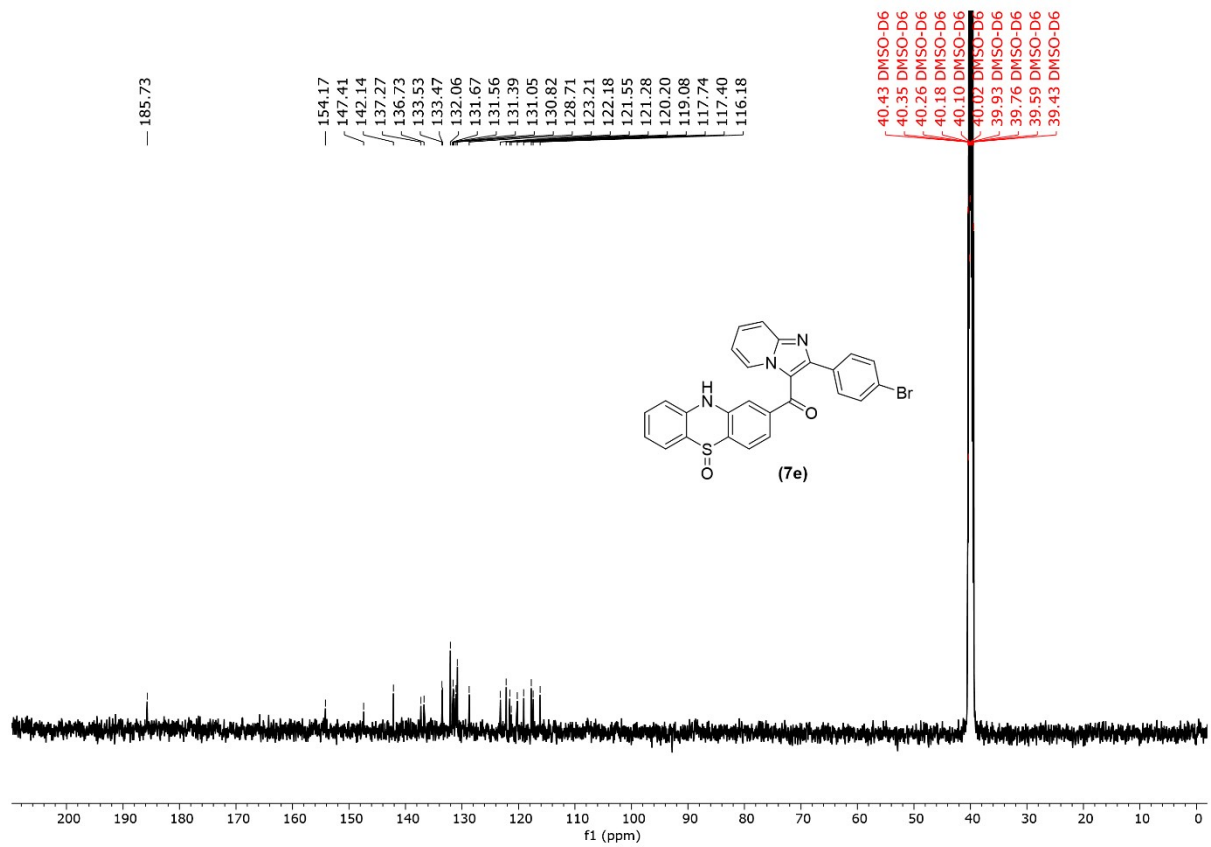
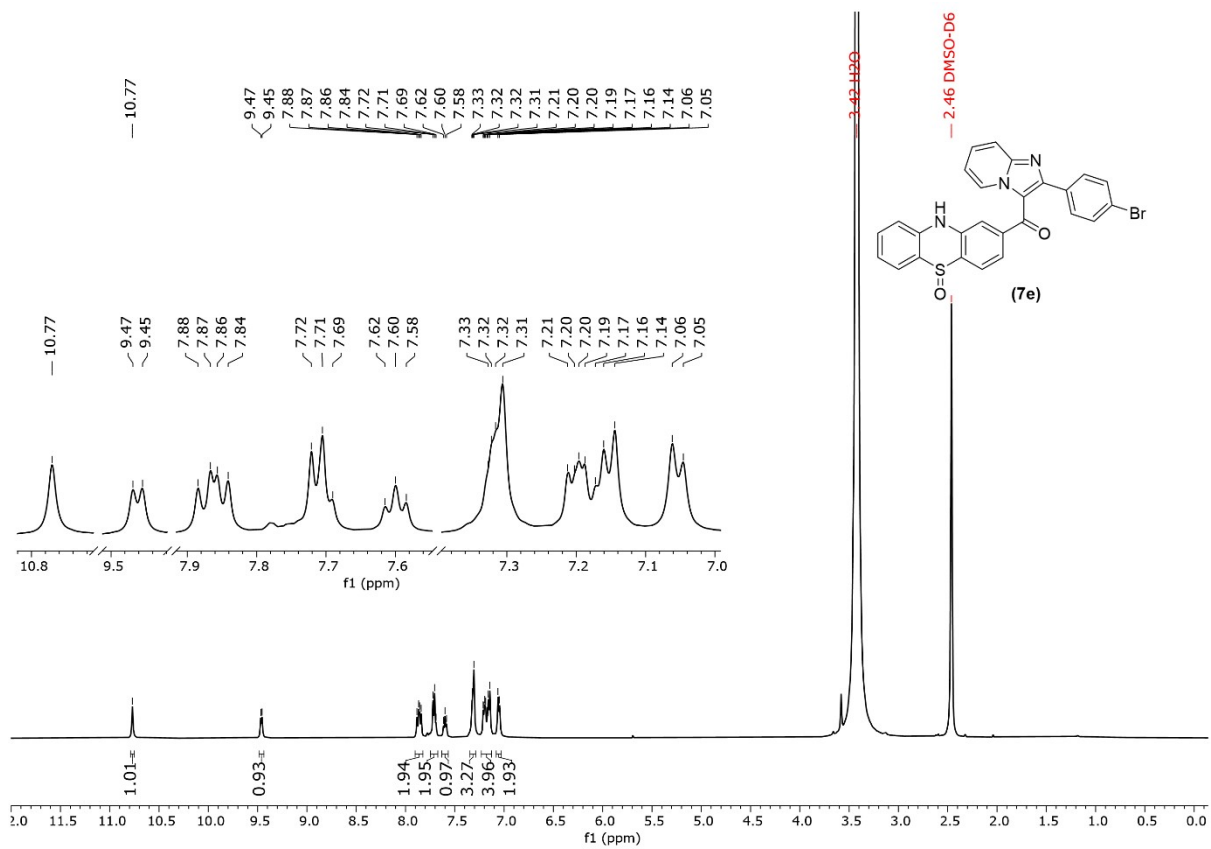


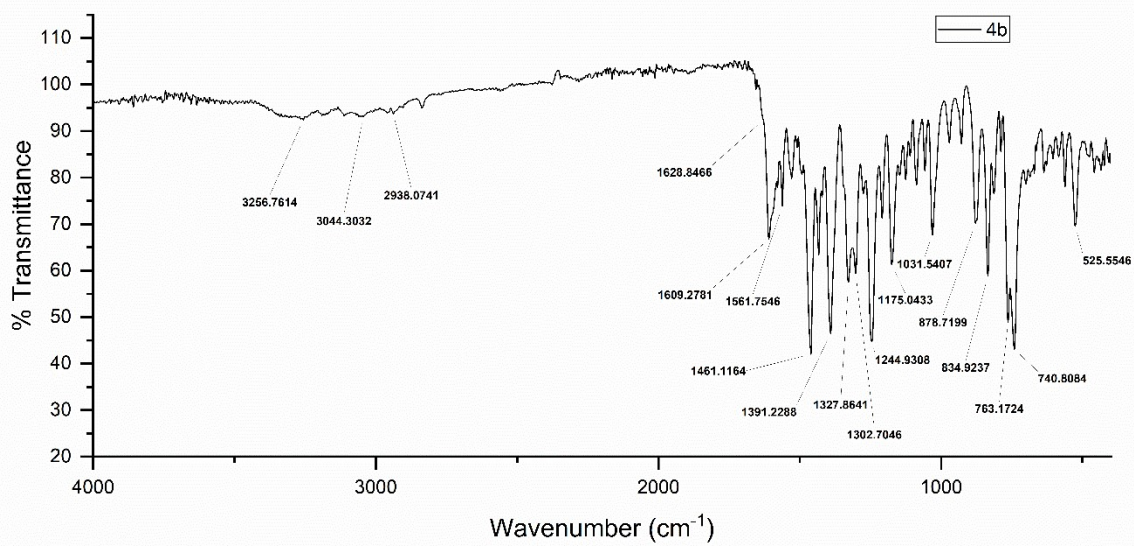
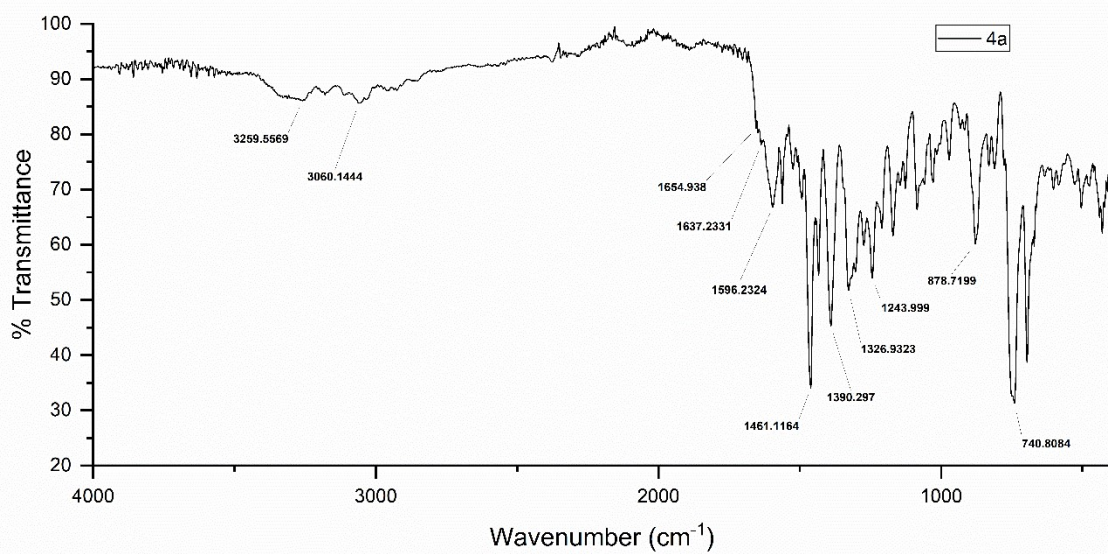


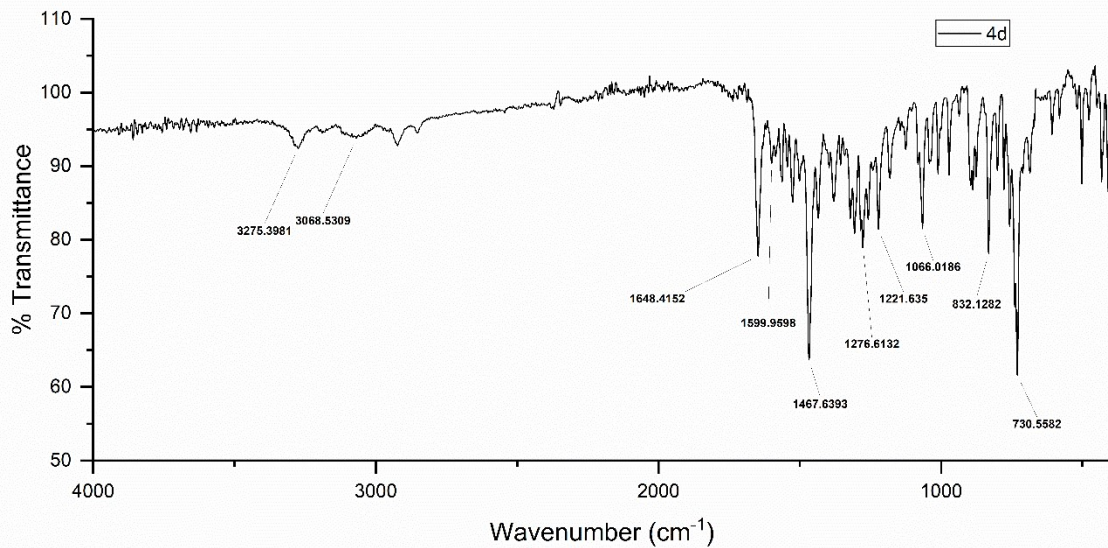
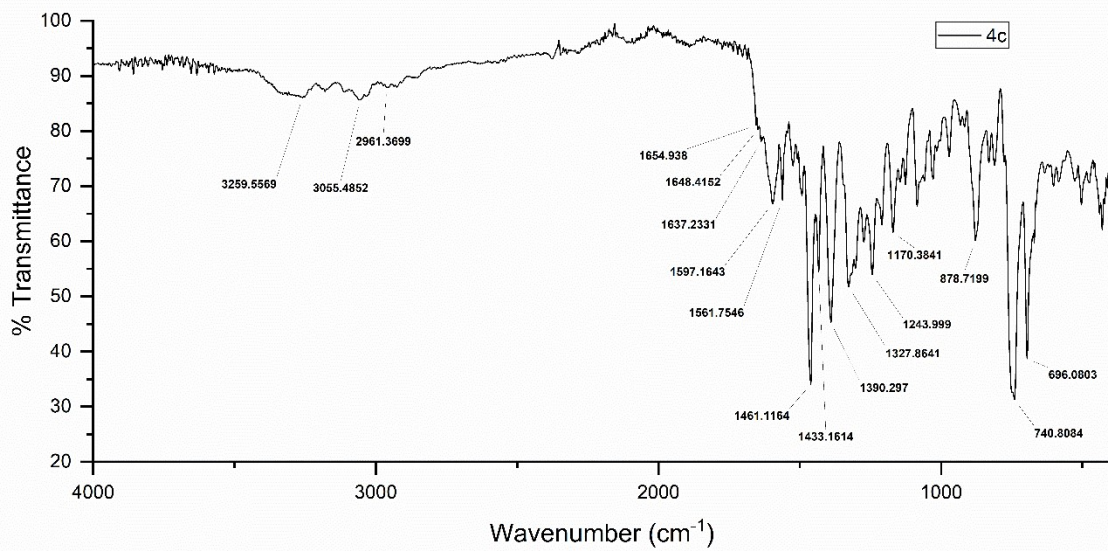


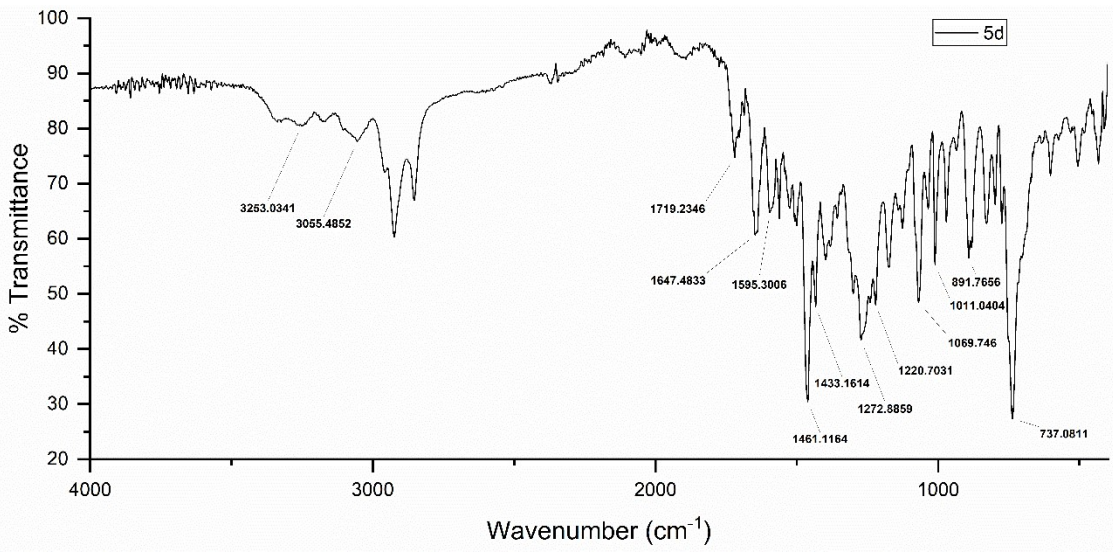
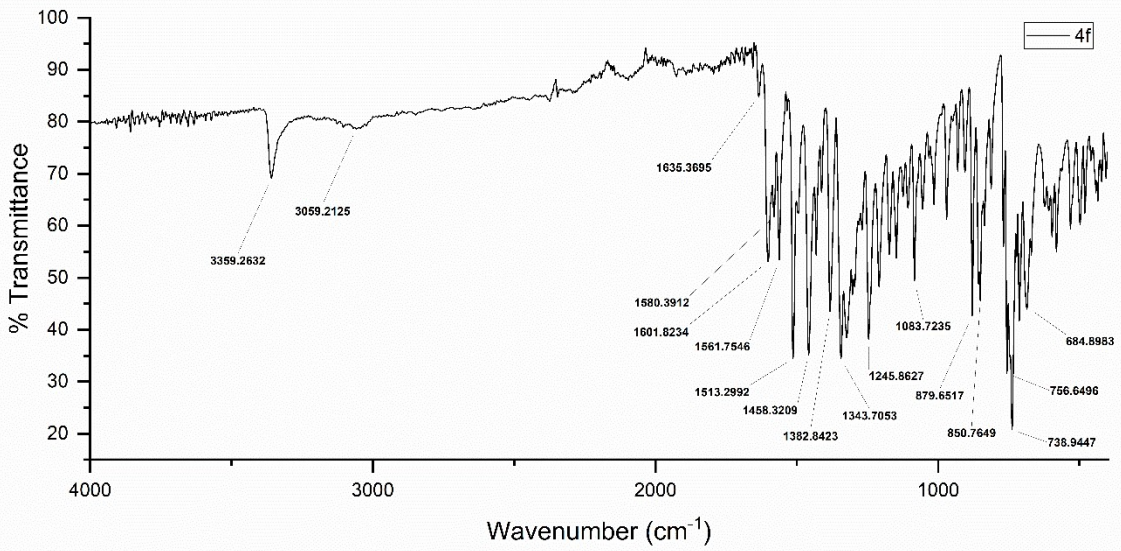
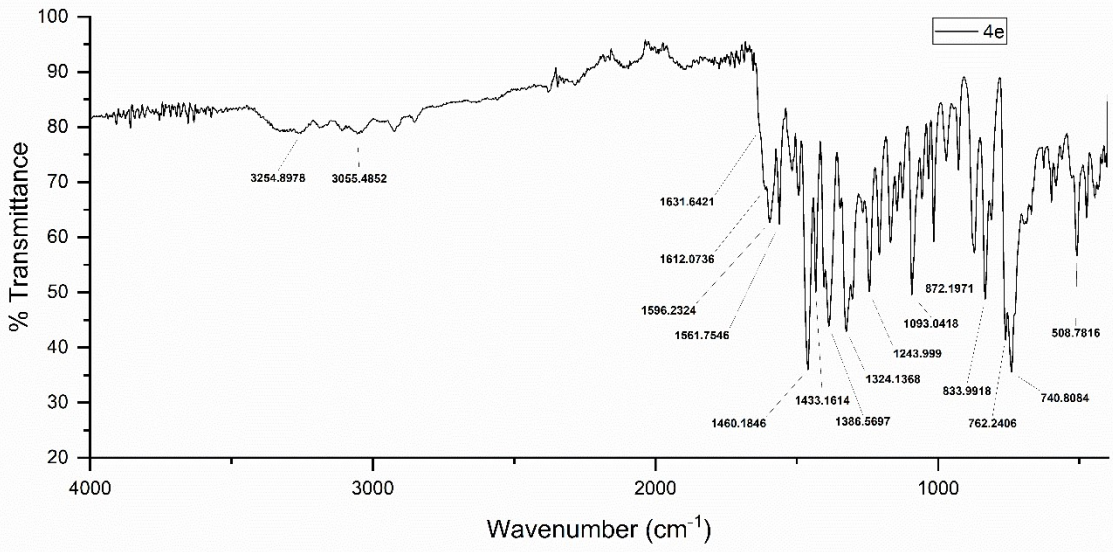


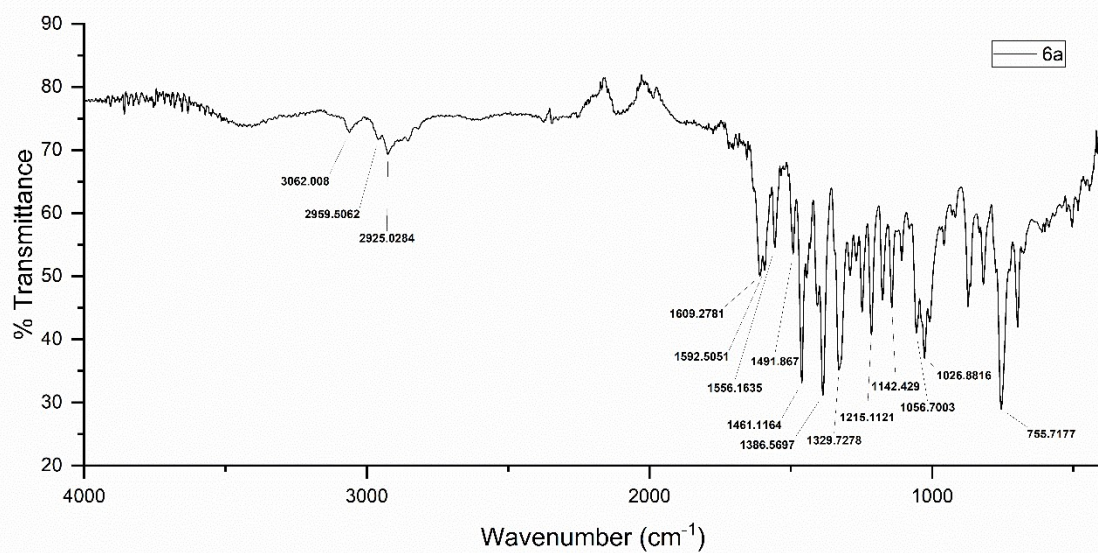
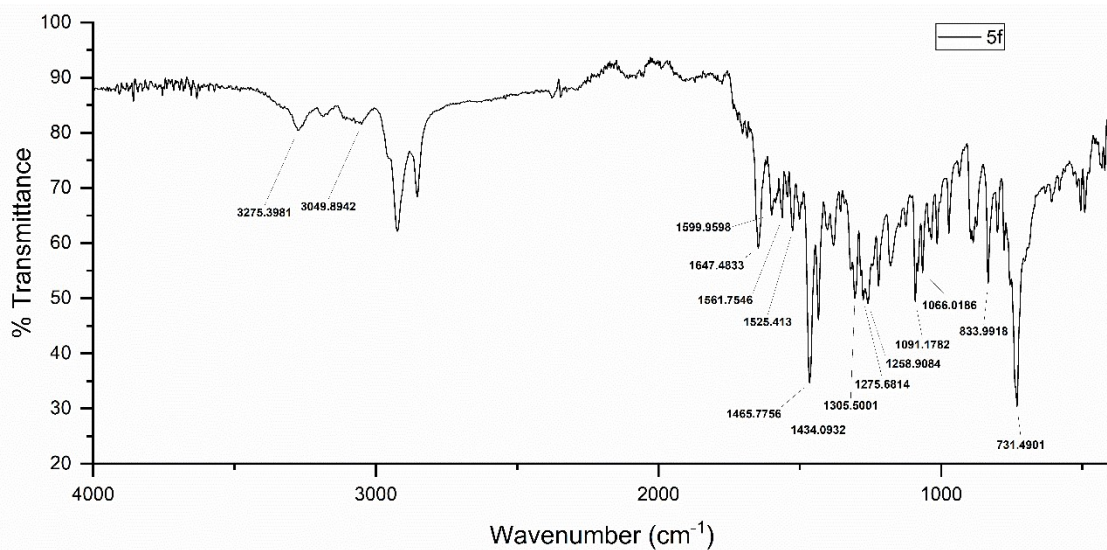


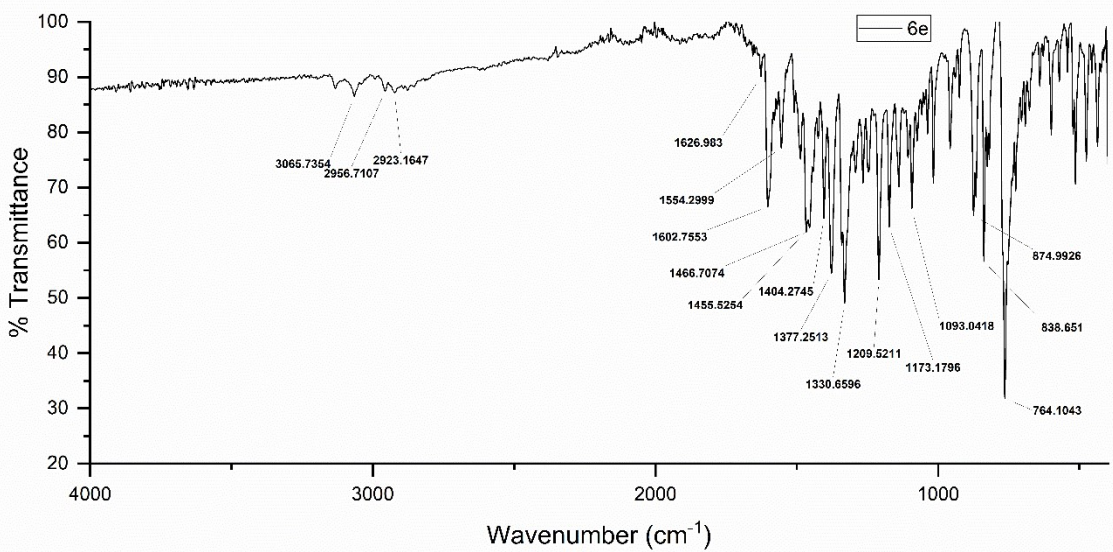
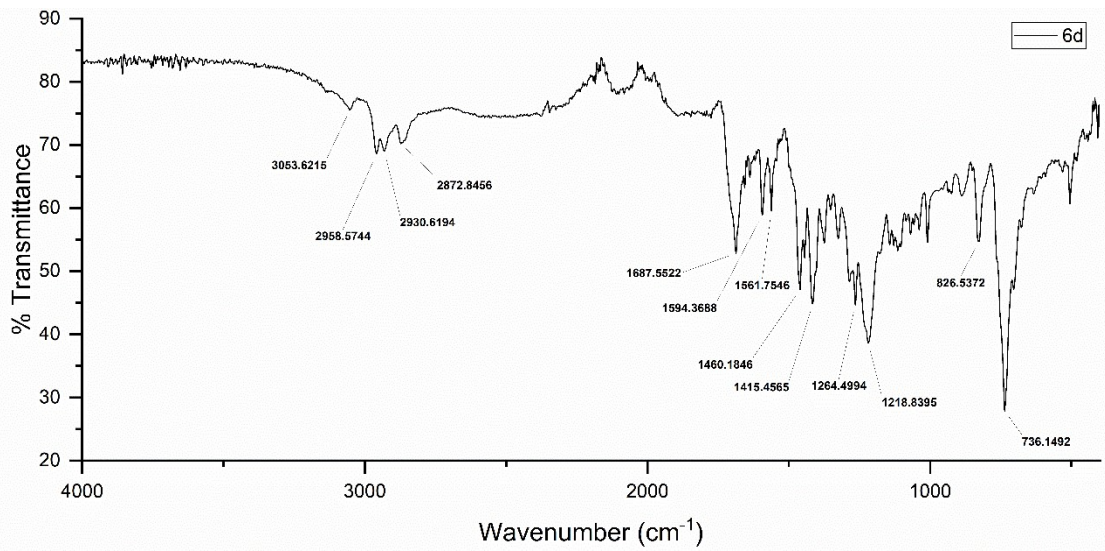
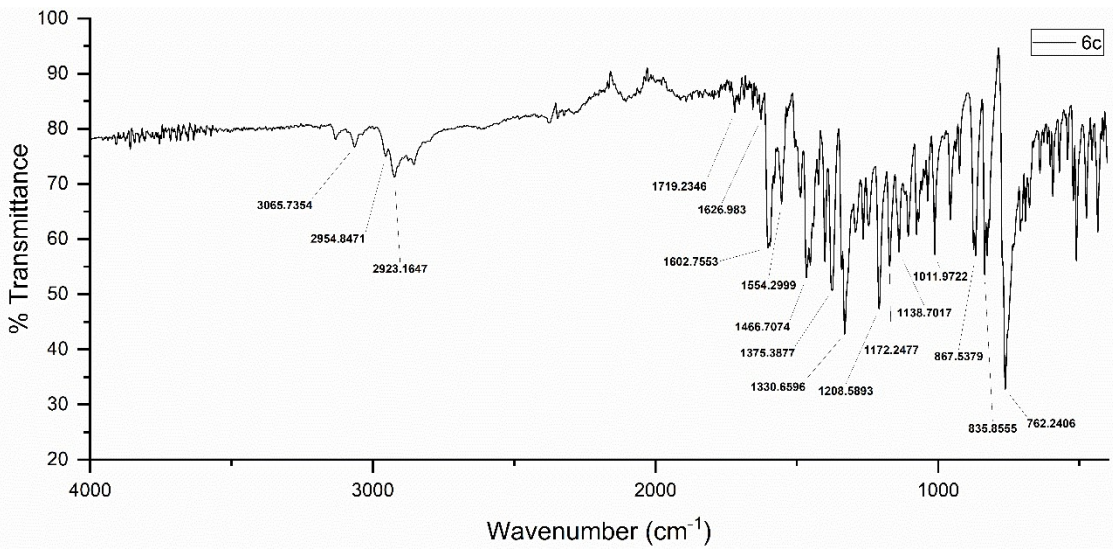


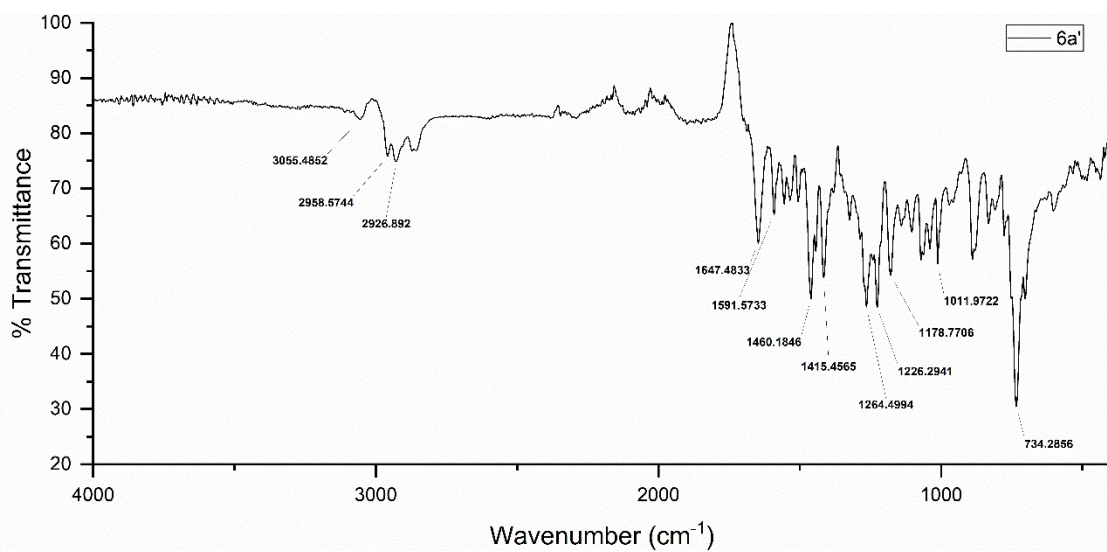
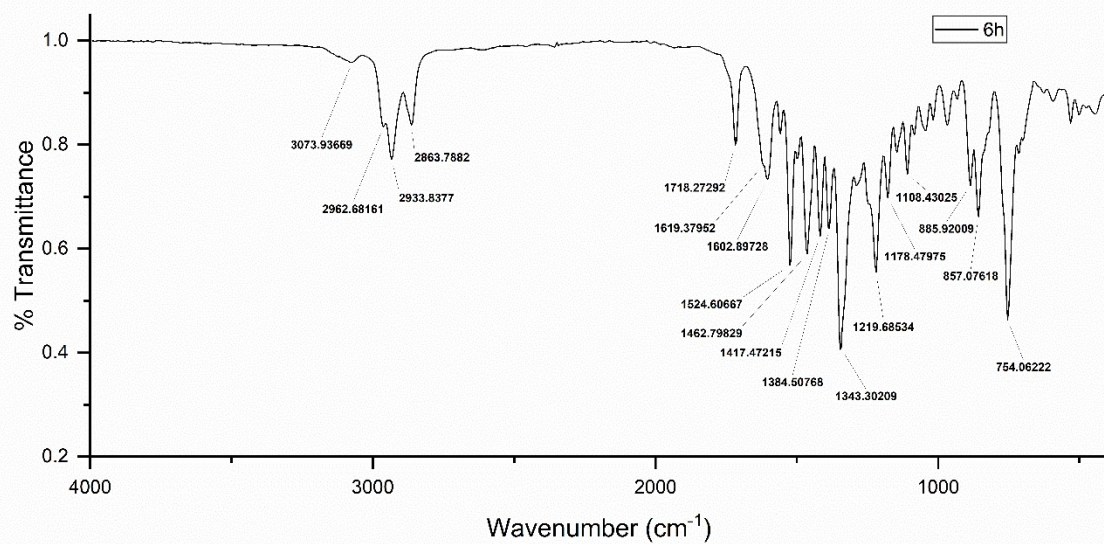
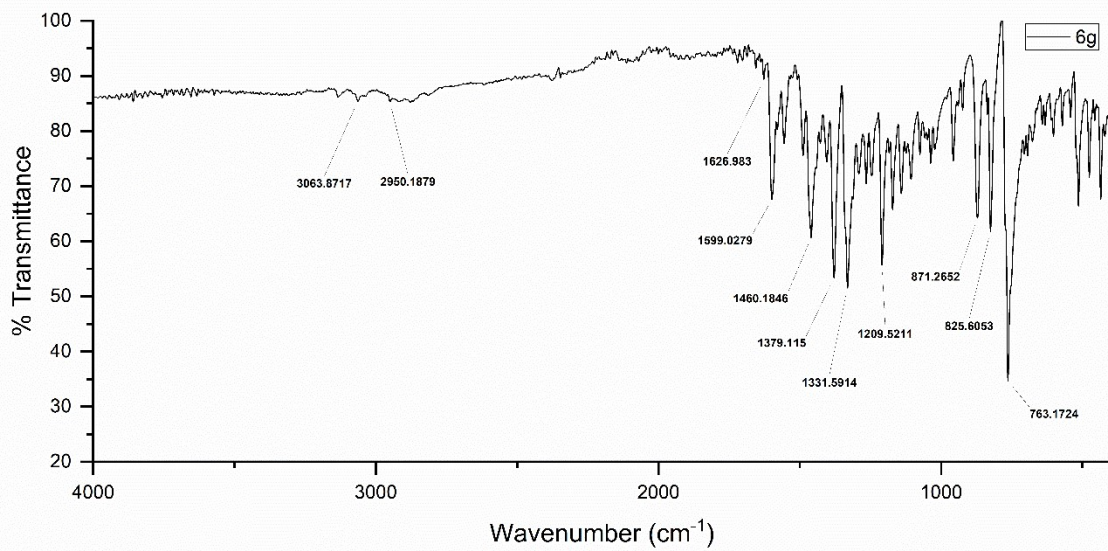


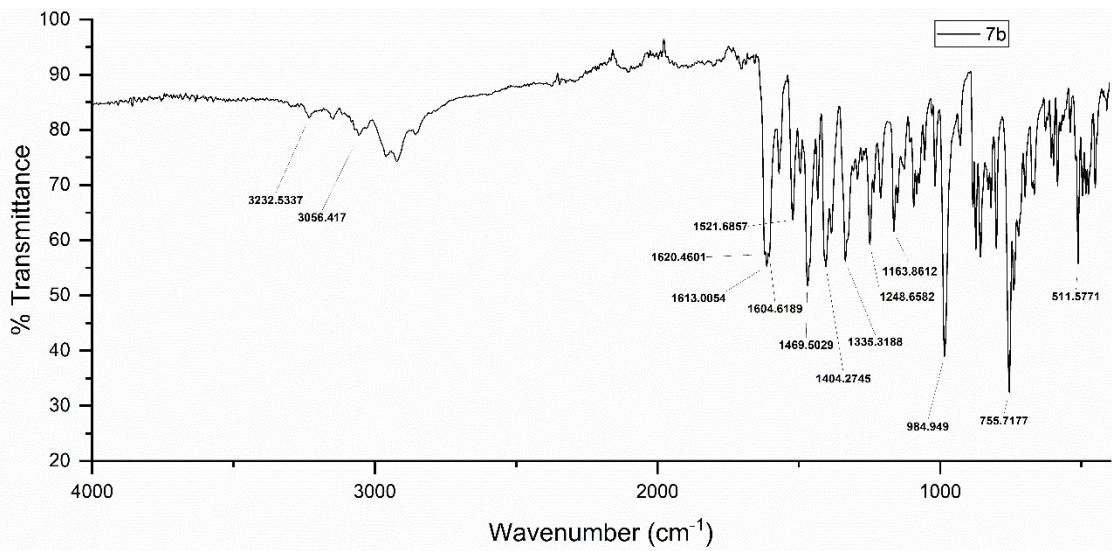
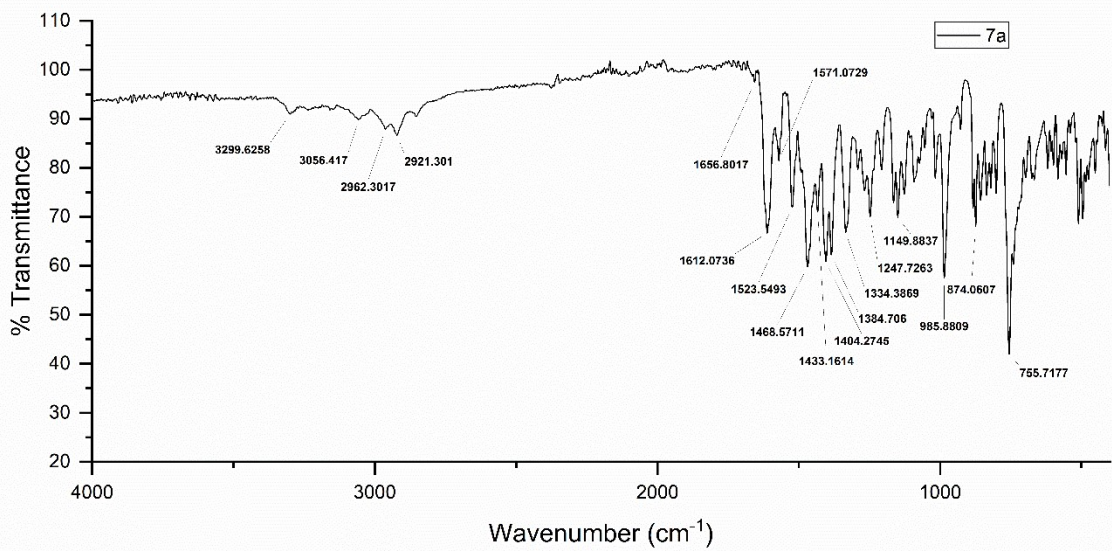
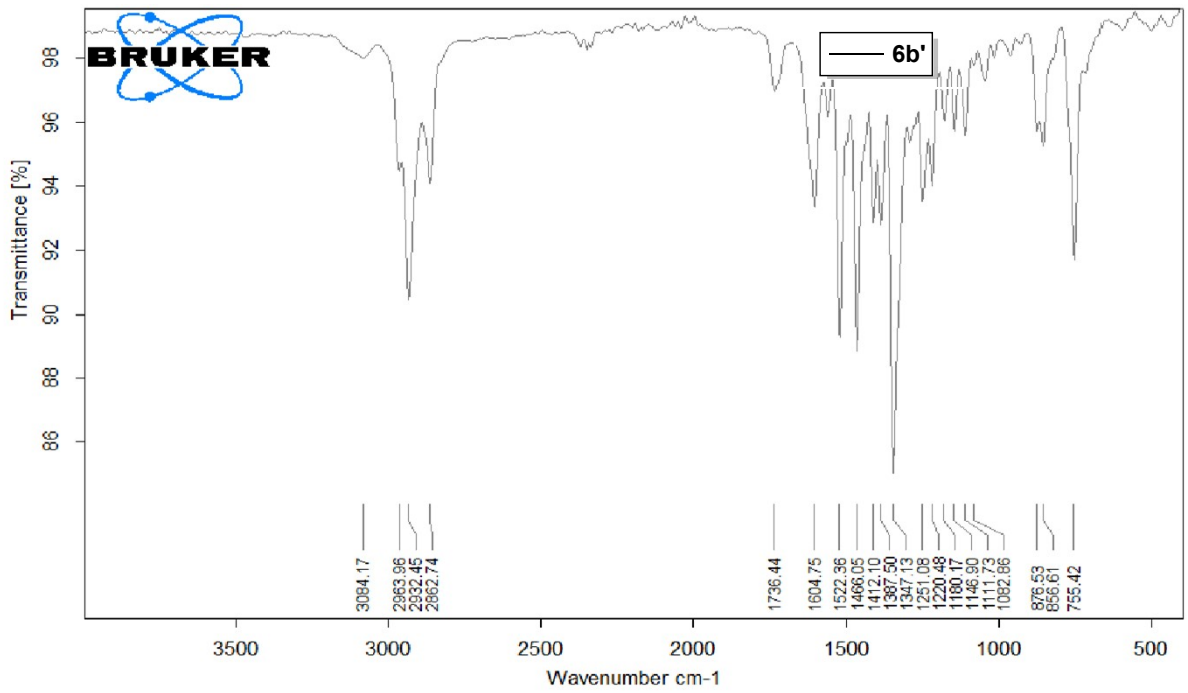


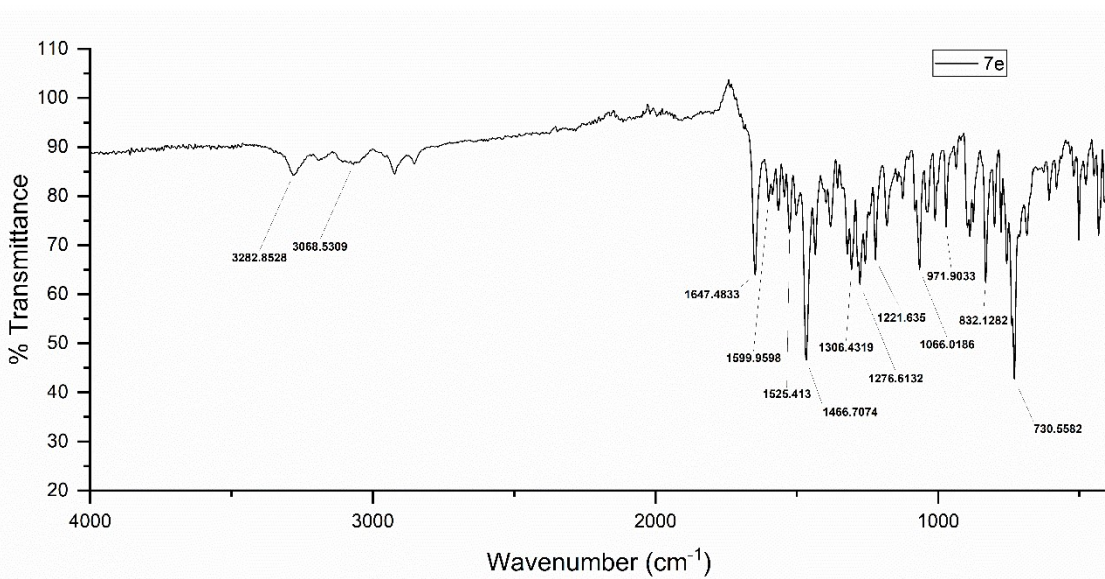
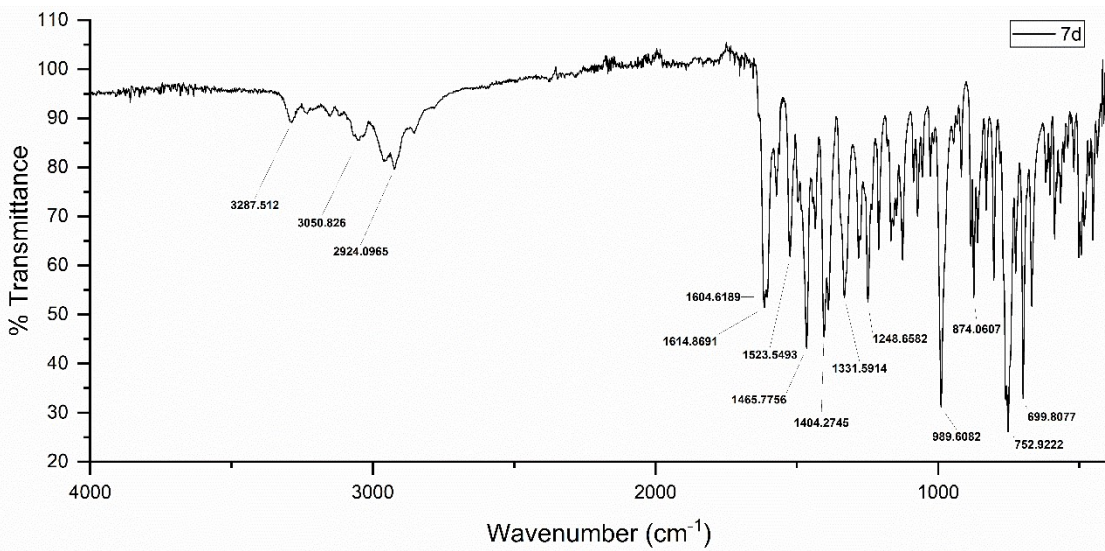
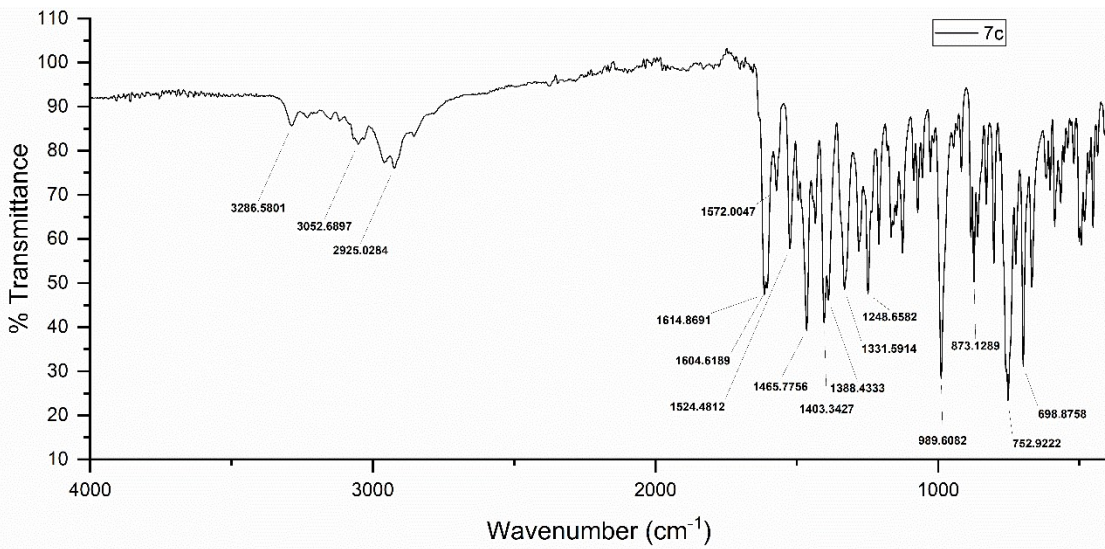












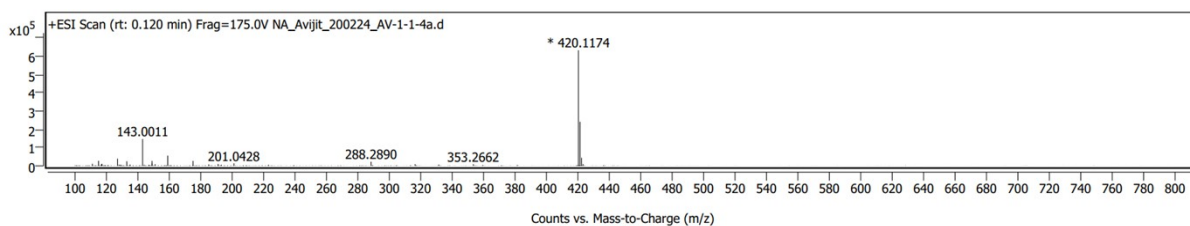


Figure S1: HRMS-ESI spectra of **4a**

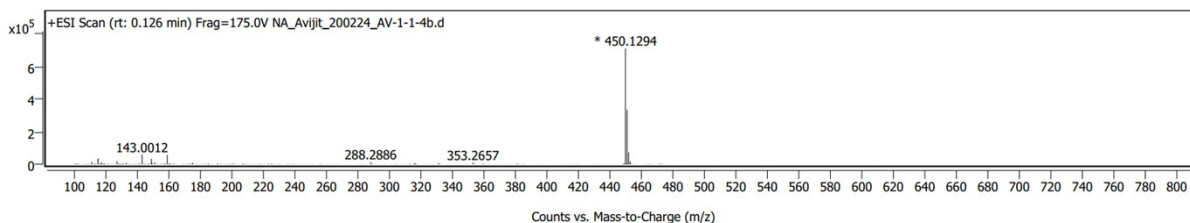


Figure S2: HRMS-ESI spectra of **4b**

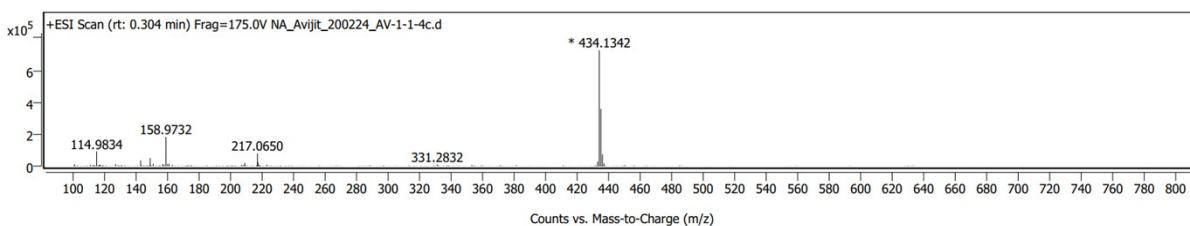


Figure S3: HRMS-ESI spectra of **4c**

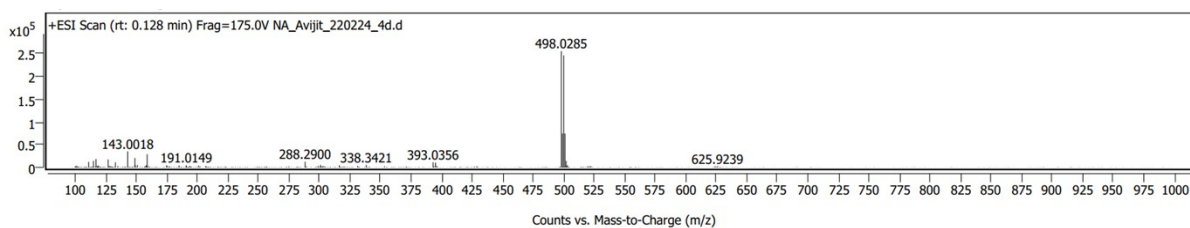


Figure S4: HRMS-ESI spectra of **4d**

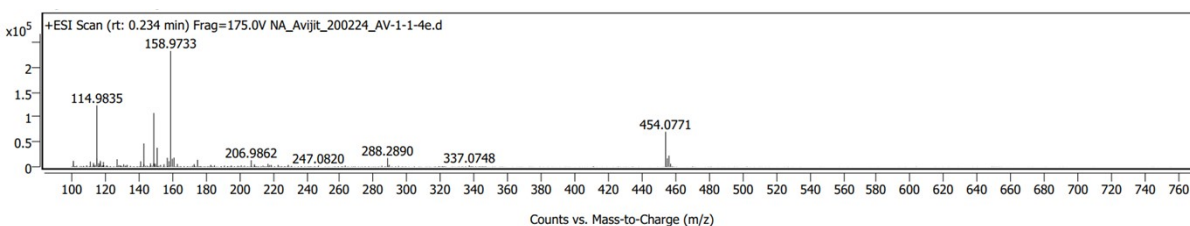


Figure S5: HRMS-ESI spectra of **4e**

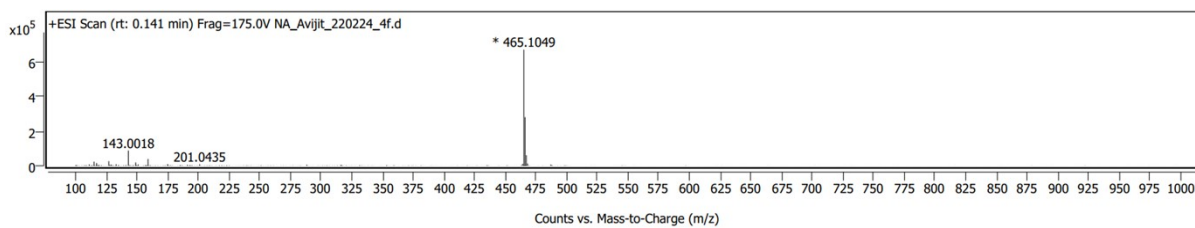


Figure S6: HRMS-ESI spectra of **4f**

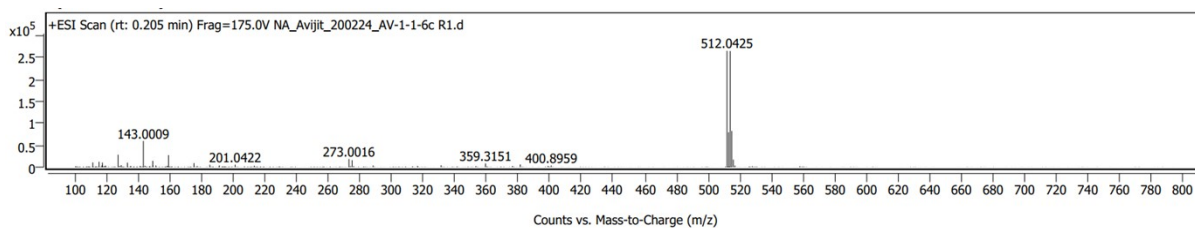


Figure S7: HRMS-ESI spectra of **6c**

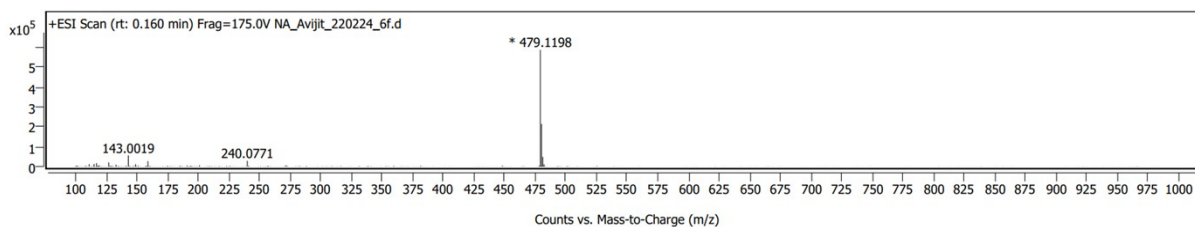


Figure S8: HRMS-ESI spectra of **6f**

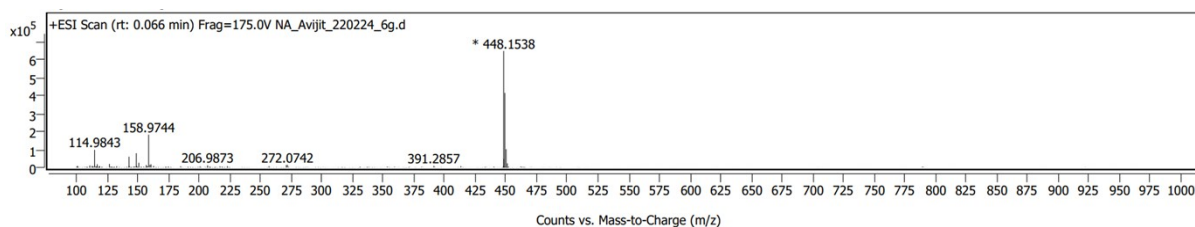


Figure S9: HRMS-ESI spectra of **6g**

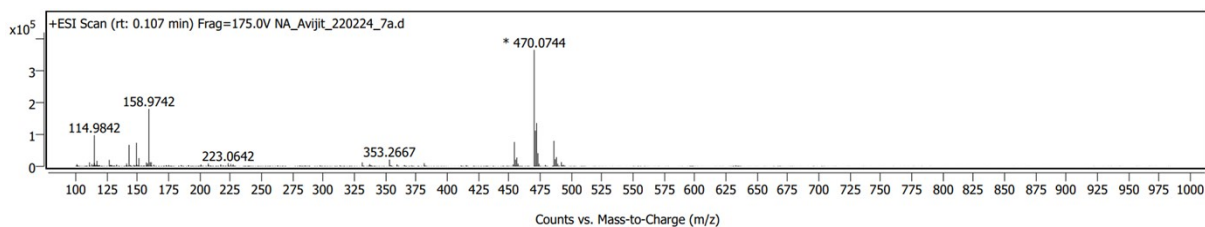


Figure S10: HRMS-ESI spectra of **7a**

Table S1: MTT assay against MDA-MB-231 and A549

	MDA-MB-231		A549	
	6h	6a	6h	6a
IC50 μM	24.72	38.9	42.96	58.57

Table S2: Determination of MitoSOX in MDA-MB-231 and A549

MitoSOX	Control	3 h	6 h
MDA-MB-231	14.991	26.688	39.007
A549	17.422	25.057	34.617

Table S3: TMRM imaging of MDA-MB-231 and A549

TMRM	Control	3 h	6 h
MDA-MB-231	49.023	33.118	33.768
A549	43.34	21.782	22.341

SINGLE CRYSTAL-XRD DATA OF MOLECULE 4a

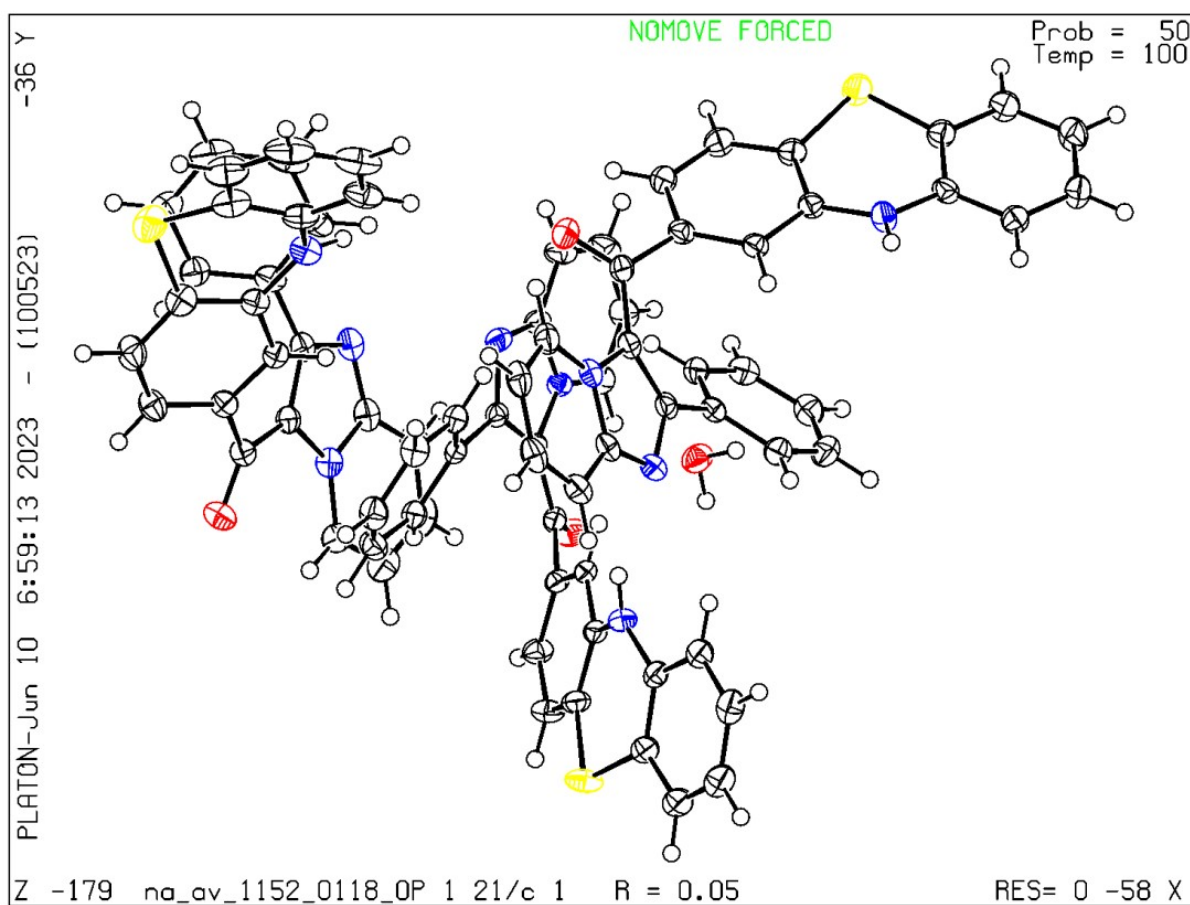


Figure 2: Ortep diagram of compound 4a (CCDC 2289193).

Table S4: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for NA_AV_1152_0118_0ma. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
S001	5684.0 (5)	4588.7 (2)	1680.4 (4)	34.12 (14)
S002	3683.1 (5)	1508.4 (2)	6920.9 (4)	36.74 (15)
S003	10755.4 (6)	4518.3 (2)	8883.6 (4)	40.85 (16)
O006	8267.2 (13)	2910.5 (5)	2813.3 (9)	28.4 (3)
O007	11520.2 (13)	4318.3 (5)	4779.4 (9)	30.3 (3)
O008	5794.9 (13)	3332.1 (5)	7305.9 (10)	31.0 (3)
N00A	8145.1 (13)	2696.7 (5)	4497.0 (10)	19.5 (3)
N00B	8114.4 (14)	3105.0 (5)	5599.3 (10)	22.1 (4)
N00C	5007.3 (14)	4175.7 (5)	3280.8 (11)	23.4 (4)
N00D	4819.5 (14)	3910.0 (5)	6203.8 (11)	23.3 (4)
N00E	11076.9 (14)	3478.9 (5)	4428.7 (11)	24.1 (4)
N00F	4383.0 (15)	3821.3 (5)	4851.2 (11)	23.9 (4)
N00G	11160.1 (15)	2971.3 (5)	5348.6 (12)	27.5 (4)
N00H	2324.6 (15)	2215.0 (5)	6148.2 (12)	27.3 (4)
N00I	9235.4 (15)	3978.0 (6)	7869.1 (11)	28.2 (4)
C00J	8054.3 (16)	3091.1 (6)	4193.2 (12)	19.3 (4)
C00K	8149.2 (16)	2720.7 (6)	5350.4 (12)	21.5 (4)
C00L	7950.2 (16)	3161.8 (6)	3301.6 (12)	20.7 (4)
C00M	7412.6 (17)	3534.8 (6)	2968.5 (12)	21.2 (4)
C00N	5920.6 (17)	4017.7 (6)	2923.2 (12)	20.8 (4)
C00O	6481.7 (16)	3695.6 (6)	3302.9 (12)	19.7 (4)
C00P	8028.5 (16)	3776.3 (6)	4978.3 (12)	19.9 (4)
C00Q	4579.8 (16)	3089.9 (6)	4691.6 (12)	21.2 (4)
C00R	8585.1 (17)	4028.0 (6)	4454.3 (13)	23.1 (4)
C00S	4192.8 (18)	4400.3 (6)	2855.5 (13)	23.3 (4)
C00T	1894.5 (18)	1831.4 (6)	6012.7 (13)	24.0 (4)
C00U	8054.4 (16)	3333.3 (6)	4898.9 (12)	19.1 (4)
C00V	10991.1 (17)	4243.6 (6)	6165.3 (13)	23.2 (4)
C00W	4610.1 (16)	3457.5 (6)	5203.7 (13)	22.0 (4)
C00X	7473.3 (17)	3949.3 (6)	5624.7 (13)	23.4 (4)
C00Y	3797.7 (17)	2688.6 (6)	6351.9 (12)	21.7 (4)
C00Z	11250.3 (17)	4091.1 (6)	5333.7 (13)	23.4 (4)
C010	11207.1 (17)	3654.3 (6)	5212.8 (13)	22.3 (4)
C011	4503.2 (17)	4093.0 (6)	5463.4 (13)	24.1 (4)
C012	11270.5 (17)	3326.5 (6)	5758.8 (13)	23.2 (4)
C013	5215.9 (17)	3213.3 (7)	6701.0 (13)	23.4 (4)
C014	6316.4 (19)	4173.0 (6)	2189.3 (12)	25.5 (4)
C015	10157.8 (17)	4070.6 (6)	6600.6 (12)	21.9 (4)
C016	8159.4 (17)	2331.3 (6)	4095.0 (13)	24.5 (4)
C017	3414.4 (17)	2297.7 (6)	6392.3 (13)	23.2 (4)

C018	4858.4 (17)	2788.8 (6)	6652.6 (12)	22.8 (4)
C019	11030.8 (17)	3069.2 (6)	4543.5 (14)	26.6 (5)
C01A	8134.1 (18)	2364.4 (7)	5820.1 (14)	28.5 (5)
C01B	5357.9 (17)	2785.8 (6)	4814.5 (13)	24.2 (4)
C01C	4873.4 (17)	3495.9 (6)	6049.7 (13)	22.6 (4)
C01D	4381.6 (19)	4593.7 (6)	2106.8 (13)	25.9 (5)
C01E	8758.4 (19)	4153.2 (7)	8541.7 (13)	29.4 (5)
C01F	11472.9 (18)	3332.0 (6)	6663.9 (13)	25.7 (4)
C01G	10027.2 (18)	4170.1 (6)	7424.7 (13)	24.1 (4)
C01H	5273.8 (19)	2431.1 (7)	4367.3 (13)	28.3 (5)
C01I	7245 (2)	4011.8 (7)	1857.6 (13)	29.7 (5)
C01J	8585.8 (19)	4441.6 (7)	4570.7 (14)	29.2 (5)
C01K	7473.1 (18)	4363.5 (7)	5735.7 (14)	28.6 (5)
C01L	3171.2 (18)	4445.5 (6)	3194.8 (14)	26.5 (5)
C01M	4137.8 (18)	1998.8 (6)	6712.6 (14)	26.8 (5)
C01N	882.5 (18)	1784.4 (7)	5581.8 (13)	26.8 (5)
C01O	2431.2 (18)	1486.4 (7)	6320.7 (14)	27.5 (5)
C01P	5211.9 (19)	2095.1 (7)	6955.8 (14)	30.3 (5)
C01Q	8104.5 (19)	2005.6 (7)	5419.5 (15)	31.8 (5)
C01R	10978.4 (18)	3648.2 (7)	3650.4 (13)	28.5 (5)
C01S	3737.7 (18)	3037.9 (7)	4081.6 (13)	26.4 (5)
C01T	11638.1 (19)	4549.3 (7)	6526.8 (14)	29.9 (5)
C01U	4961.7 (19)	4126.7 (7)	6927.5 (14)	29.1 (5)
C01V	8029.4 (19)	4611.3 (7)	5212.4 (15)	30.8 (5)
C01W	12339.0 (18)	3551.0 (7)	7027.6 (14)	28.8 (5)
C01X	4354.6 (18)	4513.2 (7)	5437.9 (14)	28.5 (5)
C01Y	7799.0 (18)	3694.8 (7)	2243.6 (13)	26.6 (5)
C01Z	5571.1 (18)	2488.9 (7)	6952.7 (13)	26.8 (5)
C020	8132.1 (19)	1990.0 (7)	4548.5 (15)	29.8 (5)
C021	2366 (2)	4687.1 (7)	2806.7 (15)	32.6 (5)
C022	412 (2)	1407.5 (7)	5478.4 (15)	32.3 (5)
C023	3554 (2)	4824.9 (6)	1711.0 (15)	31.3 (5)
C024	1949 (2)	1110.9 (7)	6217.6 (15)	32.7 (5)
C025	3656.9 (19)	2679.6 (7)	3633.7 (14)	30.6 (5)
C026	4506.4 (19)	4727.2 (7)	6155.3 (15)	31.4 (5)
C027	10811.3 (19)	3403.0 (8)	2986.9 (15)	34.6 (5)
C028	2555 (2)	4875.5 (7)	2066.0 (15)	35.0 (6)
C029	932 (2)	1069.6 (7)	5800.8 (15)	34.8 (5)
C02A	4414.9 (19)	2375.4 (7)	3786.7 (14)	30.5 (5)
C02B	10759 (2)	3129.6 (7)	7165.5 (15)	32.4 (5)
C02C	4801 (2)	4530.4 (7)	6905.0 (15)	33.6 (5)
C02D	10741.7 (19)	4455.2 (7)	7798.7 (14)	30.0 (5)
C02E	11507 (2)	4651.6 (7)	7346.0 (15)	34.2 (5)
C02F	7686 (2)	4062.7 (8)	8719.4 (15)	35.8 (6)
C02G	9359 (2)	4423.6 (7)	9049.0 (14)	34.6 (5)
C02H	10880 (2)	2816.1 (7)	3853.5 (16)	34.6 (5)
C02I	10770 (2)	2981.3 (8)	3084.6 (16)	38.8 (6)
C02J	12491 (2)	3569.6 (8)	7884.7 (15)	38.3 (6)

C02K	10898 (2)	3160.8 (8)	8012.4 (16)	40.2 (6)
C02L	7210 (2)	4239.8 (9)	9389.9 (17)	44.7 (7)
C02M	8860 (2)	4609.2 (8)	9706.1 (15)	42.7 (6)
C02N	7793 (3)	4516.4 (9)	9871.5 (16)	46.5 (7)
C02O	11764 (2)	3378.0 (9)	8376.2 (16)	42.9 (6)
O1	8093.6 (13)	1761.0 (5)	2344.1 (9)	31.7 (4)

Table S5: Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for NA_AV_1152_0118_0ma. The Anisotropic displacement factor exponent takes the form: - $2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U₁₁	U₂₂	U₃₃	U₂₃	U₁₃	U₁₂
S001	44.3 (4)	28.2 (3)	30.2 (3)	13.1 (2)	5.5 (2)	7.6 (3)
S002	38.8 (3)	20.8 (3)	48.7 (4)	7.8 (2)	-15.6 (3)	0.0 (2)
S003	43.5 (4)	50.6 (4)	28.6 (3)	-13.4 (3)	2.9 (3)	-1.0 (3)
O006	36.7 (9)	27.4 (8)	21.1 (7)	-3.3 (6)	1.0 (6)	4.5 (7)
O007	37.7 (9)	24.0 (8)	30.1 (8)	2.1 (6)	9.0 (7)	-1.2 (7)
O008	28.3 (8)	33.1 (9)	31.0 (8)	-0.3 (7)	-4.8 (6)	-2.9 (7)
N00A	19.3 (8)	18.2 (8)	20.8 (8)	1.4 (6)	0.8 (6)	2.2 (7)
N00B	21.6 (9)	24.3 (9)	20.1 (8)	2.6 (7)	-0.7 (7)	2.8 (7)
N00C	26.0 (9)	23.1 (9)	20.8 (8)	3.7 (7)	-0.3 (7)	3.0 (7)
N00D	21.5 (9)	21.4 (9)	27.0 (9)	-1.0 (7)	3.2 (7)	-5.0 (7)
N00E	22.8 (9)	22.9 (9)	26.8 (9)	-4.4 (7)	3.0 (7)	2.5 (7)
N00F	24.9 (9)	20.0 (9)	27.0 (9)	2.4 (7)	4.0 (7)	-1.5 (7)
N00G	22.1 (9)	21.7 (9)	38.7 (10)	-2.4 (8)	2.0 (8)	1.7 (7)
N00H	20.5 (9)	17.7 (9)	43.4 (11)	3.8 (8)	-2.9 (8)	2.0 (7)
N00I	29.3 (10)	26.6 (10)	29.2 (10)	-0.3 (7)	6.5 (8)	3.9 (8)
C00J	19.1 (10)	17.1 (9)	21.4 (9)	1.3 (7)	-0.5 (7)	1.6 (8)
C00K	19.3 (10)	24.4 (11)	21.0 (10)	2.6 (8)	1.7 (8)	3.3 (8)
C00L	19.5 (10)	22.0 (10)	20.4 (9)	-1.4 (8)	-0.7 (7)	-1.5 (8)
C00M	24.1 (10)	22.1 (10)	17.0 (9)	0.6 (7)	-2.7 (7)	-1.2 (8)
C00N	25.1 (10)	18.6 (10)	18.4 (9)	0.7 (7)	-2.4 (8)	-3.2 (8)
C00O	21.3 (10)	20.7 (10)	16.7 (9)	1.0 (7)	-2.2 (7)	-3.2 (8)
C00P	18.6 (10)	19.5 (10)	21.0 (9)	-1.2 (7)	-4.2 (7)	-0.1 (8)
C00Q	19.5 (10)	21.3 (10)	23.3 (10)	1.7 (8)	4.9 (8)	-1.8 (8)
C00R	20.4 (10)	24.3 (11)	24.6 (10)	-1.9 (8)	0.9 (8)	0.3 (8)
C00S	27.3 (11)	15.5 (10)	26.2 (10)	-1.3 (8)	-7.0 (8)	0.4 (8)
C00T	25.3 (11)	19.0 (10)	28.0 (11)	3.7 (8)	2.3 (8)	-0.3 (8)
C00U	15.4 (9)	21.9 (10)	19.9 (9)	0.2 (7)	0.4 (7)	0.8 (8)
C00V	25.4 (11)	18.1 (10)	25.9 (10)	-0.6 (8)	1.3 (8)	2.6 (8)
C00W	15.8 (9)	23.2 (10)	27.1 (10)	1.7 (8)	2.7 (8)	-3.1 (8)
C00X	20.4 (10)	24.9 (11)	24.9 (10)	-1.9 (8)	0.1 (8)	0.4 (8)
C00Y	18.8 (10)	22.1 (10)	24.3 (10)	4.3 (8)	2.2 (8)	2.3 (8)
C00Z	21.7 (10)	20.7 (10)	27.8 (11)	0.4 (8)	1.9 (8)	1.1 (8)
C010	20.0 (10)	22.7 (10)	24.4 (10)	-1.7 (8)	2.1 (8)	-0.2 (8)
C011	19.8 (10)	21.8 (11)	31.2 (11)	1.6 (8)	5.8 (8)	-4.0 (8)
C012	17.8 (10)	20.2 (10)	31.7 (11)	-0.9 (8)	2.7 (8)	2.1 (8)

C013	16.9 (10)	28.2 (11)	25.2 (10)	1.2 (8)	2.2 (8)	-1.5 (8)
C014	32.0 (12)	23.6 (11)	20.3 (10)	4.8 (8)	-2.4 (8)	0.5 (9)
C015	21.7 (10)	18.7 (10)	24.9 (10)	-1.3 (8)	-1.4 (8)	3.2 (8)
C016	24.3 (11)	21.4 (10)	27.4 (11)	-1.5 (8)	-0.8 (8)	2.7 (8)
C017	21.1 (10)	21.1 (10)	27.4 (10)	3.8 (8)	0.4 (8)	1.6 (8)
C018	21.4 (10)	24.9 (11)	22.5 (10)	3.0 (8)	4.5 (8)	0.0 (8)
C019	20.5 (10)	22.7 (11)	36.7 (12)	-4.9 (9)	3.5 (9)	1.6 (8)
C01A	26.9 (11)	31.3 (12)	27.6 (11)	9.6 (9)	3.8 (9)	6.9 (9)
C01B	19.8 (10)	26.5 (11)	26.3 (10)	2.5 (8)	0.6 (8)	-1.0 (8)
C01C	19.4 (10)	20.5 (10)	27.8 (10)	0.7 (8)	2.0 (8)	-3.4 (8)
C01D	35.0 (12)	15.6 (10)	26.6 (11)	-0.6 (8)	-4.6 (9)	0.6 (9)
C01E	34.7 (13)	27.6 (12)	26.4 (11)	6.3 (9)	6.8 (9)	13.4 (10)
C01F	23.9 (11)	22.1 (11)	31.6 (11)	5.7 (8)	5.3 (9)	8.6 (9)
C01G	23.6 (10)	22.3 (10)	26.4 (10)	1.5 (8)	2.6 (8)	4.7 (8)
C01H	27.1 (12)	28.0 (12)	30.2 (11)	3.0 (9)	6.1 (9)	4.3 (9)
C01I	38.1 (13)	31.2 (12)	20.2 (10)	6.4 (8)	5.0 (9)	0.7 (10)
C01J	29.5 (12)	24.1 (11)	33.9 (12)	2.5 (9)	2.3 (9)	-3.3 (9)
C01K	26.4 (11)	26.6 (12)	32.7 (12)	-7.3 (9)	1.8 (9)	3.3 (9)
C01L	30.5 (12)	17.8 (10)	30.8 (11)	-1.5 (8)	-3.3 (9)	0.7 (9)
C01M	27.7 (11)	21.1 (11)	31.1 (11)	3.4 (8)	-2.9 (9)	2.9 (9)
C01N	23.6 (11)	26.3 (11)	30.2 (11)	1.9 (9)	-0.1 (9)	1.7 (9)
C01O	28.5 (12)	22.5 (11)	31.0 (11)	1.3 (9)	-3.6 (9)	2.0 (9)
C01P	25.0 (11)	27.8 (12)	37.3 (12)	5.7 (9)	-4.6 (9)	6.1 (9)
C01Q	30.8 (12)	23.5 (12)	41.5 (13)	10.4 (9)	4.4 (10)	6.1 (9)
C01R	24.5 (11)	34.3 (12)	26.9 (11)	-0.2 (9)	3.7 (9)	4.5 (9)
C01S	23.9 (11)	27.0 (11)	28.3 (11)	1.4 (8)	1.6 (8)	2.4 (9)
C01T	31.4 (12)	24.6 (11)	34.1 (12)	-3.7 (9)	5.8 (9)	-3.6 (9)
C01U	28.3 (12)	29.1 (12)	29.9 (11)	-4.0 (9)	2.3 (9)	-7.8 (9)
C01V	31.3 (12)	20.3 (11)	40.3 (13)	-4.9 (9)	-1.5 (10)	1.5 (9)
C01W	22.2 (11)	33.8 (12)	30.4 (11)	1.1 (9)	3.0 (9)	5.3 (9)
C01X	26.5 (11)	23.4 (11)	35.9 (12)	2.8 (9)	5.3 (9)	-2.1 (9)
C01Y	27.4 (11)	31.9 (12)	20.8 (10)	2.1 (8)	3.5 (8)	3.5 (9)
C01Z	20.0 (10)	30.1 (12)	30.0 (11)	3.6 (9)	-0.7 (8)	0.6 (9)
C020	28.7 (12)	20.3 (11)	40.1 (13)	1.0 (9)	-0.3 (10)	3.3 (9)
C021	29.9 (12)	22.5 (11)	44.5 (14)	-4.8 (10)	-6.8 (10)	3.2 (9)
C022	28.4 (12)	29.7 (12)	38.1 (13)	-4.3 (10)	-5.1 (10)	-3.0 (9)
C023	43.1 (14)	15.6 (10)	34.0 (12)	1.6 (8)	-8.7 (10)	0.7 (9)
C024	37.4 (13)	19.3 (11)	40.6 (13)	2.8 (9)	-6.3 (10)	1.8 (9)
C025	29.2 (12)	35.9 (13)	26.4 (11)	-3.7 (9)	-1.5 (9)	-0.5 (10)
C026	28.1 (12)	21.0 (11)	45.6 (14)	-4.3 (9)	6.6 (10)	-4.3 (9)
C027	28.9 (12)	45.8 (15)	29.2 (12)	-6.0 (10)	3.3 (9)	4.3 (11)
C028	41.1 (14)	19.6 (11)	42.6 (14)	-0.1 (9)	-	4.7 (10)
					13.3 (11)	
C029	39.6 (14)	20.2 (11)	43.8 (14)	-3.6 (10)	-4.0 (11)	-3.4 (10)
C02A	35.1 (13)	27.2 (12)	29.6 (11)	-6.1 (9)	6.1 (9)	-3.5 (10)
C02B	30.9 (12)	21.9 (11)	45.1 (14)	9.0 (10)	7.3 (10)	4.8 (9)
C02C	31.6 (13)	28.9 (12)	40.4 (13)	-9.8 (10)	3.3 (10)	-9.7 (10)
C02D	32.6 (12)	30.4 (12)	27.4 (11)	-7.5 (9)	4.0 (9)	3.5 (10)

C02E	39.1 (14)	27.1 (12)	36.6 (13)	-9.4 (10)	2.7 (10)	-6.8 (10)
C02F	35.9 (13)	33.8 (13)	38.5 (13)	14.1 (10)	11.1 (10)	13.3 (11)
C02G	43.0 (14)	34.7 (13)	26.5 (11)	2.1 (9)	5.4 (10)	13.1 (11)
C02H	29.7 (12)	28.8 (12)	45.2 (14)	- 10.9 (10)	2.6 (10)	0.8 (10)
C02I	31.6 (13)	43.3 (15)	41.3 (14)	- 18.7 (11)	0.9 (10)	1.3 (11)
C02J	33.3 (13)	49.1 (16)	32.0 (13)	-1.2 (11)	-3.5 (10)	7.8 (11)
C02K	43.1 (15)	35.8 (14)	43.3 (14)	20.3 (11)	15.8 (12)	13.5 (12)
C02L	48.5 (16)	46.0 (16)	41.7 (14)	20.0 (12)	21.7 (12)	22.0 (13)
C02M	59.1 (18)	41.4 (15)	28.3 (12)	-0.7 (10)	9.8 (11)	15.1 (13)
C02N	59.0 (18)	49.5 (17)	33.1 (13)	14.4 (12)	21.1 (13)	29.2 (14)
C02O	49.9 (16)	52.8 (17)	26.5 (12)	10.1 (11)	5.7 (11)	17.4 (13)
O1	27.2 (8)	44.1 (10)	23.7 (8)	0.7 (7)	1.2 (6)	1.7 (7)

Table S6: Bond Lengths for NA_AV_1152_0118_0ma.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S001	C014	1.765 (2)	C00Y	C017	1.383 (3)
S001	C01D	1.765 (2)	C00Y	C018	1.397 (3)
S002	C01M	1.760 (2)	C00Z	C010	1.465 (3)
S002	C01O	1.766 (2)	C010	C012	1.403 (3)
S003	C02D	1.769 (2)	C011	C01X	1.409 (3)
S003	C02G	1.765 (3)	C012	C01F	1.473 (3)
O006	C00L	1.227 (2)	C013	C018	1.477 (3)
O007	C00Z	1.231 (2)	C013	C01C	1.456 (3)
O008	C013	1.241 (2)	C014	C01I	1.386 (3)
N00A	C00J	1.402 (2)	C015	C01G	1.392 (3)
N00A	C00K	1.384 (2)	C016	C020	1.353 (3)
N00A	C016	1.378 (3)	C017	C01M	1.409 (3)
N00B	C00K	1.340 (3)	C018	C01Z	1.392 (3)
N00B	C00U	1.363 (2)	C019	C02H	1.403 (3)
N00C	C00N	1.385 (3)	C01A	C01Q	1.357 (3)
N00C	C00S	1.394 (3)	C01B	C01H	1.384 (3)
N00D	C011	1.381 (3)	C01D	C023	1.396 (3)
N00D	C01C	1.401 (3)	C01E	C02F	1.387 (3)
N00D	C01U	1.378 (3)	C01E	C02G	1.398 (4)
N00E	C010	1.398 (3)	C01F	C01W	1.388 (3)
N00E	C019	1.376 (3)	C01F	C02B	1.395 (3)
N00E	C01R	1.379 (3)	C01G	C02D	1.402 (3)
N00F	C00W	1.359 (3)	C01H	C02A	1.382 (3)
N00F	C011	1.343 (3)	C01I	C01Y	1.383 (3)
N00G	C012	1.358 (3)	C01J	C01V	1.390 (3)
N00G	C019	1.345 (3)	C01K	C01V	1.385 (3)
N00H	C00T	1.391 (3)	C01L	C021	1.392 (3)
N00H	C017	1.393 (3)	C01M	C01P	1.384 (3)
N00I	C01E	1.390 (3)	C01N	C022	1.384 (3)
N00I	C01G	1.390 (3)	C01O	C024	1.386 (3)

C00J	C00L	1.462 (3)		C01P	C01Z	1.380 (3)
C00J	C00U	1.398 (3)		C01Q	C020	1.414 (3)
C00K	C01A	1.408 (3)		C01R	C027	1.355 (3)
C00L	C00M	1.490 (3)		C01S	C025	1.395 (3)
C00M	C00O	1.390 (3)		C01T	C02E	1.387 (3)
C00M	C01Y	1.394 (3)		C01U	C02C	1.356 (3)
C00N	C00O	1.395 (3)		C01W	C02J	1.392 (3)
C00N	C014	1.405 (3)		C01X	C026	1.366 (3)
C00P	C00R	1.393 (3)		C021	C028	1.384 (4)
C00P	C00U	1.478 (3)		C022	C029	1.379 (3)
C00P	C00X	1.400 (3)		C023	C028	1.384 (4)
C00Q	C00W	1.476 (3)		C024	C029	1.386 (3)
C00Q	C01B	1.393 (3)		C025	C02A	1.383 (3)
C00Q	C01S	1.397 (3)		C026	C02C	1.408 (3)
C00R	C01J	1.387 (3)		C027	C02I	1.412 (4)
C00S	C01D	1.402 (3)		C02B	C02K	1.377 (4)
C00S	C01L	1.396 (3)		C02D	C02E	1.381 (3)
C00T	C01N	1.393 (3)		C02F	C02L	1.389 (4)
C00T	C01O	1.399 (3)		C02G	C02M	1.397 (3)
C00V	C00Z	1.488 (3)		C02H	C02I	1.361 (4)
C00V	C015	1.392 (3)		C02J	C02O	1.378 (4)
C00V	C01T	1.396 (3)		C02K	C02O	1.384 (4)
C00W	C01C	1.396 (3)		C02L	C02N	1.378 (4)
C00X	C01K	1.388 (3)		C02M	C02N	1.377 (4)

Table S7: Bond Angles for NA_AV_1152_0118_0ma.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C014	S001	C01D	101.79 (10)	N00H	C017	C01M	122.28 (19)
C01M	S002	C01O	101.80 (10)	C00Y	C017	N00H	119.42 (18)
C02G	S003	C02D	99.88 (11)	C00Y	C017	C01M	118.25 (19)
C00K	N00A	C00J	107.00 (16)	C00Y	C018	C013	120.72 (18)
C016	N00A	C00J	131.35 (17)	C01Z	C018	C00Y	120.0 (2)
C016	N00A	C00K	121.53 (17)	C01Z	C018	C013	119.22 (19)
C00K	N00B	C00U	106.34 (17)	N00E	C019	C02H	119.4 (2)
C00N	N00C	C00S	124.29 (17)	N00G	C019	N00E	111.53 (18)
C011	N00D	C01C	106.95 (17)	N00G	C019	C02H	129.1 (2)
C01U	N00D	C011	121.65 (19)	C01Q	C01A	C00K	118.8 (2)
C01U	N00D	C01C	131.27 (19)	C01H	C01B	C00Q	120.8 (2)
C019	N00E	C010	107.06 (18)	N00D	C01C	C013	121.26 (18)
C019	N00E	C01R	121.66 (19)	C00W	C01C	N00D	104.71 (17)
C01R	N00E	C010	131.27 (19)	C00W	C01C	C013	133.91 (19)
C011	N00F	C00W	106.05 (17)	C00S	C01D	S001	121.79 (16)
C019	N00G	C012	105.51 (18)	C023	C01D	S001	117.94 (17)
C00T	N00H	C017	124.83 (18)	C023	C01D	C00S	120.1 (2)
C01E	N00I	C01G	123.0 (2)	N00I	C01E	C02G	120.1 (2)
N00A	C00J	C00L	119.86 (17)	C02F	C01E	N00I	120.7 (2)

C00U	C00J	N00A	104.78 (16)	C02F	C01E	C02G	119.2 (2)
C00U	C00J	C00L	135.33 (18)	C01W	C01F	C012	120.8 (2)
N00A	C00K	C01A	119.43 (19)	C01W	C01F	C02B	119.3 (2)
N00B	C00K	N00A	110.90 (17)	C02B	C01F	C012	119.8 (2)
N00B	C00K	C01A	129.59 (19)	N00I	C01G	C015	120.4 (2)
O006	C00L	C00J	120.90 (18)	N00I	C01G	C02D	121.28 (19)
O006	C00L	C00M	118.74 (18)	C015	C01G	C02D	118.3 (2)
C00J	C00L	C00M	120.31 (17)	C02A	C01H	C01B	120.1 (2)
C00O	C00M	C00L	122.10 (18)	C01Y	C01I	C014	120.6 (2)
C00O	C00M	C01Y	120.07 (19)	C00R	C01J	C01V	120.4 (2)
C01Y	C00M	C00L	117.43 (19)	C01V	C01K	C00X	120.5 (2)
N00C	C00N	C00O	119.51 (18)	C021	C01L	C00S	120.5 (2)
N00C	C00N	C014	122.30 (18)	C017	C01M	S002	121.75 (17)
C00O	C00N	C014	118.18 (19)	C01P	C01M	S002	117.54 (16)
C00M	C00O	C00N	120.96 (18)	C01P	C01M	C017	120.4 (2)
C00R	C00P	C00U	122.11 (18)	C022	C01N	C00T	120.8 (2)
C00R	C00P	C00X	118.64 (19)	C00T	C01O	S002	122.42 (17)
C00X	C00P	C00U	119.18 (18)	C024	C01O	S002	116.87 (17)
C01B	C00Q	C00W	121.60 (18)	C024	C01O	C00T	120.5 (2)
C01B	C00Q	C01S	118.71 (19)	C01Z	C01P	C01M	120.9 (2)
C01S	C00Q	C00W	119.67 (19)	C01A	C01Q	C020	120.5 (2)
C01J	C00R	C00P	120.6 (2)	C027	C01R	N00E	118.8 (2)
N00C	C00S	C01D	121.8 (2)	C025	C01S	C00Q	120.1 (2)
N00C	C00S	C01L	119.34 (19)	C02E	C01T	C00V	119.2 (2)
C01L	C00S	C01D	118.83 (19)	C02C	C01U	N00D	118.9 (2)
N00H	C00T	C01N	119.87 (19)	C01K	C01V	C01J	119.4 (2)
N00H	C00T	C01O	121.99 (19)	C01F	C01W	C02J	120.3 (2)
C01N	C00T	C01O	118.1 (2)	C026	C01X	C011	118.7 (2)
N00B	C00U	C00J	110.93 (18)	C01I	C01Y	C00M	119.5 (2)
N00B	C00U	C00P	118.84 (17)	C01P	C01Z	C018	119.2 (2)
C00J	C00U	C00P	130.21 (18)	C016	C020	C01Q	120.9 (2)
C015	C00V	C00Z	120.91 (18)	C028	C021	C01L	120.4 (2)
C015	C00V	C01T	119.99 (19)	C029	C022	C01N	120.8 (2)
C01T	C00V	C00Z	119.00 (19)	C028	C023	C01D	120.4 (2)
N00F	C00W	C00Q	120.14 (18)	C01O	C024	C029	120.7 (2)
N00F	C00W	C01C	111.21 (18)	C02A	C025	C01S	120.2 (2)
C01C	C00W	C00Q	128.64 (19)	C01X	C026	C02C	120.5 (2)
C01K	C00X	C00P	120.5 (2)	C01R	C027	C02I	120.9 (2)
C017	C00Y	C018	121.05 (19)	C021	C028	C023	119.8 (2)
O007	C00Z	C00V	121.92 (19)	C022	C029	C024	119.0 (2)
O007	C00Z	C010	121.28 (19)	C01H	C02A	C025	119.9 (2)
C010	C00Z	C00V	116.76 (18)	C02K	C02B	C01F	119.8 (2)
N00E	C010	C00Z	122.40 (18)	C01U	C02C	C026	120.8 (2)
N00E	C010	C012	104.37 (18)	C01G	C02D	S003	118.80 (18)
C012	C010	C00Z	133.23 (19)	C02E	C02D	S003	120.03 (18)
N00D	C011	C01X	119.4 (2)	C02E	C02D	C01G	120.8 (2)
N00F	C011	N00D	111.05 (18)	C02D	C02E	C01T	120.5 (2)
N00F	C011	C01X	129.5 (2)	C01E	C02F	C02L	120.5 (3)

N00G	C012	C010	111.49 (19)	C01E	C02G	S003	120.30 (18)
N00G	C012	C01F	120.30 (19)	C02M	C02G	S003	120.0 (2)
C010	C012	C01F	128.17 (19)	C02M	C02G	C01E	119.7 (3)
O008	C013	C018	119.96 (19)	C02I	C02H	C019	119.3 (2)
O008	C013	C01C	119.69 (19)	C02H	C02I	C027	120.0 (2)
C01C	C013	C018	120.34 (18)	C02O	C02J	C01W	120.0 (2)
C00N	C014	S001	121.44 (17)	C02B	C02K	C02O	120.9 (2)
C01I	C014	S001	117.83 (16)	C02N	C02L	C02F	120.1 (3)
C01I	C014	C00N	120.69 (19)	C02N	C02M	C02G	120.3 (3)
C00V	C015	C01G	120.76 (19)	C02M	C02N	C02L	120.2 (2)
C020	C016	N00A	118.8 (2)	C02J	C02O	C02K	119.6 (2)

Table S8: Torsion Angles for NA_AV_1152_0118_0ma.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S001	C014	C01I	C01Y	177.78 (18)	C00Z	C010	C012	C01F	-4.0 (4)
S001	C01D	C023	C028	172.91 (17)	C010	N00E	C019	N00G	-2.1 (2)
S002	C01M	C01P	C01Z	168.17 (18)	C010	N00E	C019	C02H	178.8 (2)
S002	C01O	C024	C029	175.9 (2)	C010	N00E	C01R	C027	-177.2 (2)
S003	C02D	C02E	C01T	168.07 (19)	C010	C012	C01F	C01W	-49.2 (3)
S003	C02G	C02M	C02N	175.72 (19)	C010	C012	C01F	C02B	128.0 (2)
O006	C00L	C00M	C00O	137.7 (2)	C011	N00D	C01C	C00W	1.6 (2)
O006	C00L	C00M	C01Y	-35.1 (3)	C011	N00D	C01C	C013	178.25 (18)
O007	C00Z	C010	N00E	-23.3 (3)	C011	N00D	C01U	C02C	-1.0 (3)
O007	C00Z	C010	C012	156.8 (2)	C011	N00F	C00W	C00Q	-178.53 (18)
O008	C013	C018	C00Y	140.2 (2)	C011	N00F	C00W	C01C	0.3 (2)
O008	C013	C018	C01Z	-36.3 (3)	C011	C01X	C026	C02C	-0.3 (3)
O008	C013	C01C	N00D	-23.7 (3)	C012	N00G	C019	N00E	1.1 (2)
O008	C013	C01C	C00W	151.8 (2)	C012	N00G	C019	C02H	-179.8 (2)
N00A	C00J	C00L	O006	-22.5 (3)	C012	C01F	C01W	C02J	176.9 (2)

N00A	C00J	C00L	C00M	154.99(18)	C012	C01F	C02B	C02K	-174.9(2)
N00A	C00J	C00U	N00B	-1.4(2)	C013	C018	C01Z	C01P	175.9(2)
N00A	C00J	C00U	C00P	176.93(19)	C014	S001	C01D	C00S	19.9(2)
N00A	C00K	C01A	C01Q	-0.7(3)	C014	S001	C01D	C023	-165.25(17)
N00A	C016	C020	C01Q	-0.9(3)	C014	C00N	C00O	C00M	0.5(3)
N00B	C00K	C01A	C01Q	175.7(2)	C014	C01I	C01Y	C00M	0.5(3)
N00C	C00N	C00O	C00M	-178.81(18)	C015	C00V	C00Z	O007	143.1(2)
N00C	C00N	C014	S001	1.1(3)	C015	C00V	C00Z	C010	-39.0(3)
N00C	C00N	C014	C01I	178.8(2)	C015	C00V	C01T	C02E	5.9(3)
N00C	C00S	C01D	S001	-3.5(3)	C015	C01G	C02D	S003	-168.65(16)
N00C	C00S	C01D	C023	-178.25(19)	C015	C01G	C02D	C02E	4.2(3)
N00C	C00S	C01L	C021	176.29(19)	C016	N00A	C00J	C00L	0.1(3)
N00D	C011	C01X	C026	-1.4(3)	C016	N00A	C00J	C00U	178.2(2)
N00D	C01U	C02C	C026	-0.7(3)	C016	N00A	C00K	N00B	-178.96(18)
N00E	C010	C012	N00G	-1.5(2)	C016	N00A	C00K	C01A	-1.9(3)
N00E	C010	C012	C01F	176.1(2)	C017	N00H	C00T	C01N	-164.3(2)
N00E	C019	C02H	C02I	-0.7(3)	C017	N00H	C00T	C01O	17.9(3)
N00E	C01R	C027	C02I	-1.8(3)	C017	C00Y	C018	C013	-172.52(19)
N00F	C00W	C01C	N00D	-1.2(2)	C017	C00Y	C018	C01Z	4.0(3)
N00F	C00W	C01C	C013	-177.2(2)	C017	C01M	C01P	C01Z	5.2(4)
N00F	C011	C01X	C026	178.7(2)	C018	C00Y	C017	N00H	174.83(19)
N00G	C012	C01F	C01W	128.2(2)	C018	C00Y	C017	C01M	-2.7(3)
N00	C012	C01F	C02B	-54.6(3)	C018	C013	C01	N00D	155.06(1)

G							C		9)	
N00G	C019	C02H	C02I	-179.7 (2)		C018	C013	C01C	C00W	-29.5 (3)
N00H	C00T	C01N	C022	-176.5 (2)		C019	N00E	C010	C00Z	-177.85 (19)
N00H	C00T	C01O	S002	1.1 (3)		C019	N00E	C010	C012	2.1 (2)
N00H	C00T	C01O	C024	176.1 (2)		C019	N00E	C01R	C027	1.3 (3)
N00H	C017	C01M	S002	-6.2 (3)		C019	N00G	C012	C010	0.2 (2)
N00H	C017	C01M	C01P	-179.3 (2)		C019	N00G	C012	C01F	-177.58 (19)
N00I	C01E	C02F	C02L	-179.7 (2)		C019	C02H	C02I	C027	0.2 (4)
N00I	C01E	C02G	S003	-4.4 (3)		C01A	C01Q	C020	C016	-1.7 (4)
N00I	C01E	C02G	C02M	177.7 (2)		C01B	C00Q	C00W	N00F	140.0 (2)
N00I	C01G	C02D	S003	8.8 (3)		C01B	C00Q	C00W	C01C	-38.6 (3)
N00I	C01G	C02D	C02E	-178.4 (2)		C01B	C00Q	C01S	C025	2.9 (3)
C00J	N00A	C00K	N00B	-2.6 (2)		C01B	C01H	C02A	C025	2.0 (3)
C00J	N00A	C00K	C01A	174.36 (18)		C01C	N00D	C011	N00F	-1.6 (2)
C00J	N00A	C016	C020	-172.6 (2)		C01C	N00D	C011	C01X	178.44 (19)
C00J	C00L	C00M	C00O	-39.8 (3)		C01C	N00D	C01U	C02C	-176.4 (2)
C00J	C00L	C00M	C01Y	147.4 (2)		C01C	C013	C018	C00Y	-38.5 (3)
C00K	N00A	C00J	C00L	-175.68 (18)		C01C	C013	C018	C01Z	145.0 (2)
C00K	N00A	C00J	C00U	2.4 (2)		C01D	S001	C014	C00N	-18.7 (2)
C00K	N00A	C016	C020	2.7 (3)		C01D	S001	C014	C01I	163.50 (18)
C00K	N00B	C00U	C00J	-0.2 (2)		C01D	C00S	C01L	C021	-1.7 (3)
C00K	N00B	C00U	C00P	-178.72 (17)		C01D	C023	C028	C021	-1.7 (3)
C00K	C01A	C01Q	C020	2.5 (3)		C01E	N00I	C01G	C015	-153.8 (2)
C00L	C00J	C00	N00B	176.2 (2)		C01E	N00I	C01	C02D	28.8 (3)

		U					G			
C00L	C00J	C00U	C00P	-5.5 (4)		C01E	C02F	C02L	C02N	1.8 (4)
C00L	C00M	C00O	C00N	-172.60 (18)		C01E	C02G	C02M	C02N	2.2 (4)
C00L	C00M	C01Y	C01I	172.4 (2)		C01F	C01W	C02J	C02O	-1.6 (4)
C00N	N00C	C00S	C01D	-20.6 (3)		C01F	C02B	C02K	C02O	-2.6 (4)
C00N	N00C	C00S	C01L	161.50 (19)		C01G	N00I	C01E	C02F	148.9 (2)
C00N	C014	C01I	C01Y	0.0 (3)		C01G	N00I	C01E	C02G	-31.1 (3)
C00O	C00M	C01Y	C01I	-0.5 (3)		C01G	C02D	C02E	C01T	-4.7 (4)
C00O	C00N	C014	S001	-178.24 (15)		C01L	C00S	C01D	S001	174.42 (16)
C00O	C00N	C014	C01I	-0.5 (3)		C01L	C00S	C01D	C023	-0.3 (3)
C00P	C00R	C01J	C01V	-0.1 (3)		C01L	C021	C028	C023	-0.3 (3)
C00P	C00X	C01K	C01V	-0.5 (3)		C01M	S002	C01O	C00T	-16.8 (2)
C00Q	C00W	C01C	N00D	177.45 (19)		C01M	S002	C01O	C024	168.09 (19)
C00Q	C00W	C01C	C013	1.5 (4)		C01M	C01P	C01Z	C018	-3.9 (3)
C00Q	C01B	C01H	C02A	0.4 (3)		C01N	C00T	C01O	S002	-176.74 (17)
C00Q	C01S	C025	C02A	-0.5 (3)		C01N	C00T	C01O	C024	-1.8 (3)
C00R	C00P	C00U	N00B	141.19 (19)		C01N	C022	C029	C024	-1.3 (4)
C00R	C00P	C00U	C00J	-37.0 (3)		C01O	S002	C01M	C017	19.1 (2)
C00R	C00P	C00X	C01K	0.4 (3)		C01O	S002	C01M	C01P	-167.56 (19)
C00R	C01J	C01V	C01K	0.0 (3)		C01O	C00T	C01N	C022	1.4 (3)
C00S	N00C	C00N	C00O	-158.76 (19)		C01O	C024	C029	C022	0.9 (4)
C00S	N00C	C00N	C014	21.9 (3)		C01R	N00E	C010	C00Z	0.8 (3)
C00S	C01D	C023	C028	2.0 (3)		C01R	N00E	C010	C012	-179.3 (2)
C00S	C01L	C021	C028	2.0 (3)		C01R	N00E	C019	N00G	179.15 (1)

						R	E		9)	
C00T	N00 H	C017	C00Y	167.4 (2)		C01 R	N00 E	C019	C02H	0.0 (3)
C00T	N00 H	C017	C01 M	-15.2 (3)		C01 R	C027	C02I	C02H	1.1 (4)
C00T	C01 N	C022	C029	0.1 (4)		C01S	C00 Q	C00 W	N00F	-41.7 (3)
C00T	C01 O	C024	C029	0.7 (4)		C01S	C00 Q	C00 W	C01C	139.7 (2)
C00 U	N00 B	C00 K	N00 A	1.8 (2)		C01S	C00 Q	C01 B	C01H	-2.8 (3)
C00 U	N00 B	C00 K	C01A	- 174.9 (2)		C01S	C025	C02 A	C01H	-1.9 (3)
C00 U	C00J	C00 L	O006	160.2 (2)		C01T	C00 V	C00Z	O007	-40.5 (3)
C00 U	C00J	C00 L	C00 M	-22.3 (3)		C01T	C00 V	C00Z	C010	137.4 (2)
C00 U	C00P	C00 R	C01J	- 176.94 (1 9)		C01T	C00 V	C015	C01G	-6.4 (3)
C00 U	C00P	C00 X	C01K	177.32 (1 9)		C01 U	N00 D	C011	N00F	- 177.98 (1 8)
C00 V	C00Z	C010	N00E	158.79 (1 9)		C01 U	N00 D	C011	C01X	2.1 (3)
C00 V	C00Z	C010	C012	-21.1 (3)		C01 U	N00 D	C01 C	C00 W	177.6 (2)
C00 V	C015	C01 G	N00I	- 176.11 (1 9)		C01 U	N00 D	C01 C	C013	-5.9 (3)
C00 V	C015	C01 G	C02D	1.3 (3)		C01 W	C01F	C02 B	C02K	2.3 (3)
C00 V	C01T	C02 E	C02D	-0.4 (4)		C01 W	C02J	C02 O	C02K	1.3 (4)
C00 W	N00F	C011	N00 D	0.8 (2)		C01 X	C026	C02 C	C01U	1.3 (4)
C00 W	N00F	C011	C01X	- 179.2 (2)		C01 Y	C00 M	C00 O	C00N	0.0 (3)
C00 W	C00 Q	C01 B	C01H	175.52 (1 9)		C02 B	C01F	C01 W	C02J	-0.2 (3)
C00 W	C00 Q	C01S	C025	- 175.5 (2)		C02 B	C02 K	C02 O	C02J	0.7 (4)
C00 X	C00P	C00 R	C01J	-0.1 (3)		C02 D	S003	C02 G	C01E	31.7 (2)
C00 X	C00P	C00 U	N00B	-35.6 (3)		C02 D	S003	C02 G	C02 M	- 150.4 (2)
C00 X	C00P	C00 U	C00J	146.2 (2)		C02F	C01E	C02 G	S003	175.54 (1 7)
C00 X	C01 K	C01 V	C01J	0.3 (3)		C02F	C01E	C02 G	C02 M	-2.3 (3)

C00 Y	C017	C01 M	S002	171.25 (1 7)		C02F	C02L	C02 N	C02 M	-2.0 (4)
C00 Y	C017	C01 M	C01P	-1.9 (3)		C02 G	S003	C02 D	C01G	-33.6 (2)
C00 Y	C018	C01 Z	C01P	-0.6 (3)		C02 G	S003	C02 D	C02E	153.5 (2)
C00Z	C00 V	C015	C01G	169.98 (1 9)		C02 G	C01E	C02F	C02L	0.4 (3)
C00Z	C00 V	C01 T	C02E	- 170.5 (2)		C02 G	C02 M	C02 N	C02L	0.0 (4)
C00Z	C010	C012	N00 G	178.4 (2)						

Table S9: Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for NA_AV_1152_0118_0ma.

Atom	x	y	z	U(eq)
H00C	4936.71	4131.44	3811.08	28
H00H	1874.94	2420.58	6074.37	33
H00I	9026.6	3734.23	7717.72	34
H00O	6223.76	3584.55	3797.11	24
H00R	8967.49	3915.37	4013.43	28
H00X	7093.78	3782.01	5990	28
H00Y	3332.29	2892.25	6115.92	26
H015	9672.4	3882.35	6332.43	26
H016	8187.98	2319.44	3510.42	29
H01A	8144.48	2375.02	6406.7	34
H01B	5953.55	2822.3	5210.13	29
H01H	5807.91	2225.56	4459.9	34
H01I	7502.41	4120.06	1360.72	36
H01J	8968.97	4609.97	4209.54	35
H01K	7088.67	4477.76	6173.75	34
H01L	3024.62	4310.47	3694.14	32
H01N	510.89	2013.83	5356.17	32
H01P	5708.48	1887.26	7127.17	36
H01Q	8064.98	1763.02	5726.81	38
H01R	11026.88	3931.37	3580.84	34
H01S	3218.82	3246.94	3971.54	32
H01T	12161.99	4685.81	6215.36	36
H01U	5168.45	3995.44	7433.32	35
H01V	8030.88	4894.56	5291.02	37
H01W	12830.6	3688.89	6690.29	35
H01X	4152.8	4645.17	4931.95	34
H01Y	8438.45	3586.94	2016.27	32
H01Z	6295.88	2554.59	7152.8	32
H020	8131.4	1736.34	4277.95	36
H021	1681.68	4722.76	3051.86	39

H022	-278.44	1381.33	5181.74	39
H023	3677.54	4948.18	1194.92	38
H024	2319.01	879.43	6434.93	39
H025	3079.42	2644.41	3222.43	37
H026	4412.4	5010.92	6148.38	38
H027	10720.8	3516.37	2449	42
H028	2002.21	5039.13	1801.87	42
H029	598.88	812.19	5738.12	42
H02A	4345.18	2128.5	3492.94	37
H02B	10179.19	2970.7	6923.53	39
H02C	4888.87	4682.41	7400.99	40
H02E	11947.74	4858.26	7597.69	41
H02F	7272.92	3878	8379.82	43
H02H	10854.29	2532.46	3922.27	41
H02I	10665.59	2812.64	2613.2	47
H02J	13095.22	3714.35	8131.14	46
H02K	10392.16	3031.52	8351.73	48
H02L	6482.03	4170.19	9516.63	54
H02M	9258	4800.04	10040.17	51
H02N	7457.05	4643.54	10318.94	56
H02O	11856.37	3394.95	8961.45	52
H1A	7397.22	1736.17	2424.58	47
H1B	8124.67	1779.83	1809.9	47

Table S10: Solvent masks information for NA_AV_1152_0118_0ma.

Number	X	Y	Z	Volume	Electron count	Content
1	0.035	-0.053	0.273	38.2	0.0	?
2	-0.035	0.053	0.727	38.2	0.0	?
3	-0.035	0.447	0.227	38.2	0.0	?
4	0.035	0.553	0.773	38.2	0.0	?
5	0.500	0.000	0.500	266.6	91.5	?
6	0.500	0.500	1.000	266.6	91.5	?

Experimental

A suitable Single crystal of $C_{26}H_{17}N_3OS$ [**4a**] crystal was selected on a Bruker APEX-IV CCD diffractometer. The crystal was kept at 100.00 K during data collection. Using Olex2 [1], the structure was solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using LS minimization.

References

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2. Sheldrick, G. M. (2015). *Acta Cryst.* A71, 3–8
3. Sheldrick, G. M. (2008). *Acta Cryst.* A64, 112–122.