

Electronic Supplementary Information

Discovery of 2,3-dihydro-1*H*-pyrrolo[3,4-*b*]quinolin-1-one derivatives as possible anti-leishmanial agents

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Table S1. *In vitro* cytotoxicity of compounds **5a-p**, **6a-i**, **7a-c**, and **8a-b**^[a]

Code	% Inhibition on host J774 macrophage cell line				
	6.25 μ M	12.5 μ M	25 μ M	50 μ M	100 μ M
5a	14.43 \pm 0.39	15.62 \pm 1.26	14.17 \pm 5.26	55.74 \pm 3.97	69.88 \pm 6.11
5b	6.77 \pm 0.28	11.45 \pm 9.19	24.17 \pm 1.87	34.33 \pm 2.35	59.28 \pm 4.95
5c	15.64 \pm 4.18	17.81 \pm 3.21	22.34 \pm 2.4	59.97 \pm 2.29	68.21 \pm 5.54
5d	14.53 \pm 2.63	19.96 \pm 3.45	23.11 \pm 4.19	58.07 \pm 4.98	81.47 \pm 6.24
5e	4.72 \pm 3.01	22.57 \pm 4.41	13.46 \pm 1.29	67.62 \pm 5.30	87.14 \pm 5.42
5f	3.54 \pm 2.47	19.21 \pm 0.94	26.46 \pm 1.46	47.55 \pm 2.39	50.56 \pm 6.17
5g	8.72 \pm 5.65	13.47 \pm 1.55	24.93 \pm 2.95	28.51 \pm 2.64	56.37 \pm 4.82
5h	12.31 \pm 1.64	16.77 \pm 1.22	21.25 \pm 1.69	41.27 \pm 3.36	73.48 \pm 2.87
5i	6.37 \pm 1.08	19.25 \pm 1.04	48.45 \pm 3.34	59.13 \pm 1.57	62.35 \pm 3.57
5j	13.25 \pm 1.01	18.49 \pm 0.91	25.33 \pm 1.80	36.24 \pm 4.02	59.61 \pm 2.32
5k	9.63 \pm 1.01	15.62 \pm 0.97	23.95 \pm 1.46	38.48 \pm 3.44	51.64 \pm 4.72
5l	11.16 \pm 0.71	12.43 \pm 2.28	26.67 \pm 2.43	46.97 \pm 1.81	68.15 \pm 2.91
5m	8.45 \pm 0.86	11.09 \pm 0.82	27.65 \pm 3.91	23.36 \pm 1.52	41.55 \pm 2.93
5n	9.16 \pm 0.79	13.59 \pm 1.06	25.61 \pm 2.23	46.18 \pm 1.01	63.97 \pm 4.97
5o	12.05 \pm 1.62	22.18 \pm 2.64	24.16 \pm 2.51	67.92 \pm 1.79	73.45 \pm 2.12
5p	9.04 \pm 4.76	16.71 \pm 3.30	20.33 \pm 1.13	51.46 \pm 4.76	77.32 \pm 6.16
6a	9.26 \pm 5.47	17.65 \pm 4.45	22.37 \pm 1.89	42.19 \pm 3.76	61.52 \pm 4.40
6b	12.34 \pm 2.77	15.86 \pm 3.45	20.47 \pm 2.13	63.89 \pm 5.36	90.52 \pm 7.60
6c	10.53 \pm 2.41	14.37 \pm 5.67	25.76 \pm 2.36	27.54 \pm 3.16	63.39 \pm 5.70
6d	5.65 \pm 2.28	16.34 \pm 6.21	26.65 \pm 3.44	45.83 \pm 5.62	65.32 \pm 5.62
6e	15.46 \pm 2.23	19.08 \pm 8.19	23.61 \pm 1.12	43.26 \pm 3.45	71.58 \pm 6.65
6f	7.88 \pm 6.71	5.32 \pm 7.33	26.09 \pm 0.95	58.29 \pm 5.46	67.43 \pm 5.32
6g	11.82 \pm 4.53	19.07 \pm 6.65	24.88 \pm 2.33	36.44 \pm 2.93	59.81 \pm 4.46
6h	9.74 \pm 5.16	12.37 \pm 5.28	24.31 \pm 3.67	53.15 \pm 5.16	68.34 \pm 7.12
6i	8.79 \pm 4.33	12.45 \pm 8.17	23.31 \pm 1.89	34.55 \pm 2.88	48.61 \pm 3.35
7a	12.34 \pm 2.95	19.76 \pm 4.51	21.33 \pm 4.15	62.57 \pm 3.21	74.05 \pm 7.61

7b	17.65±6.71	22.15±3.32	26.42±2.31	44.52±4.61	58.16±5.94
7c	19.16±8.89	13.28±5.61	21.17±0.95	49.11±5.61	62.37±4.55
8a	14.53±5.54	19.22±6.65	23.74±3.14	37.31±3.45	54.47±6.81
8b	15.14±6.14	13.69±5.13	18.05±2.11	43.28±5.16	59.83±6.32
Miltefosine	5.66±3.6	11.09±4.3	17.19±6.4	24.22±8.3	62.11 ±4.35

^[a]Percentages of inhibition are expressed as mean ± standard deviation for each compound of three individual experiments performed in duplicates.

Table S2. *In vitro* anti-promastigote and anti-amastigote activities of compounds **5a-p**, **6a-i**, **7a-c**, and **8a-b**^[a]

Code	Anti-promastigote activity			Anti-amastigote activity		
	6.25 µM	12.5 µM	25 µM	6.25 µM	12.5 µM	25 µM
5a	63.3±5.4	65.9±5.1	70.2±6.1	51.2±3.1	62.5±6.7	68.5±7.8
5b	12.0±2.3	22.8±3.2	40.7±5.4	47.4±4.3	58.3±7.2	68.2±4.5
5c	43.3±5.2	54.3±4.8	63.8±4.5	52.9±6.6	66.3±6.7	74.9±8.5
5d	46.2±4.6	53.4±7.9	70.1±3.9	55.6±2.5	49.7±5.5	64.8±5.7
5e	29.7±1.1	55.1±8.1	61.9±2.7	29.7±3.1	55.1±4.4	61.9±6.0
5f	36.6±3.5	41.3±6.7	69.2±1.5	29.4±7.6	59.6±6.1	69.6±7.2
5g	25.6±4.4	36.8±4.4	45.9±3.3	26.8±8.8	37.8±4.4	46.72±3.5
5h	47.1±3.6	55.3±5.6	67.2±4.5	41.6±2.4	55.3±6.2	45.5±0.9
5i	53.3±6.7	58.3±6.1	64.1±7.3	53.3±6.2	58.3±6.3	74.1±1.1
5j	52.1±4.1	64.8±3.3	68.3±4.4	64.8±4.8	68.3±6.5	72.7±6.8
5k	55.6±1.0	66.2±7.7	71.7±8.2	76.1±8.8	78.7±7.2	75.7±7.2
5l	49.8±0.7	56.4±8.2	69.4±5.4	47.6±5.3	62.8±5.4	66.6±5.4
5m	69.8±0.4	76.9±4.6	85.4±7.7	57.8±6.6	65.3±7.3	85.6±9.3
5n	65.1±0.8	73.5±3.3	78.6±3.1	27.4±2.9	64.3±5.6	75.9±6.4
5o	53.5±1.6	51.9±6.4	60.9±5.4	41.7±3.7	52.9±4.5	56.0±5.2
5p	58.9±0.8	61.0±2.2	70.0±6.6	58.9±1.6	62.1±7.1	75.8±8.4
6a	27.9±0.5	33.3±4.9	40.7±3.4	29.2±3.1	34.4±3.1	60.0±6.6
6b	21.3±0.8	32.7±5.7	47.4±4.6	16.6±0.5	25.2±1.0	41.1±9.7

6c	11.2±1.4	12.4±7.7	39.8±6.1	12.6±1.4	14.3±1.5	42.9±4.6
6d	10.0±1.3	23.7±8.3	43.4±3.2	11.4±2.3	27.2±3.2	46.9±4.2
6e	8.2±2.2	24.4±3.3	41.2±1.0	9.7±8.2	25.6±2.3	42.1±3.9
6f	29.8±0.7	41.4±1.2	50.2±1.2	21.0±9.0	42.9±5.5	53.9±6.2
6g	27.6±1.5	32.9±2.3	40.6±2.	28.2±2.3	34.0±4.7	31.7±2.7
6h	25.2±1.0	36.2±4.6	45.9±0.9	16.5±7.1	35.3±3.4	47.0±4.4
6i	46.0±3.4	46.7±5.0	52.0±5.5	21.7±6.5	31.5±2.8	47.5±5.4
7a	29.7±3.9	55.1±4.5	61.9±6.2	63.3±3.2	76.0±7.1	75.0±7.6
7b	55.4±4.6	76.1±7.1	79.6±8.1	45.4±2.9	54.1±5.0	72.2±6.8
7c	42.9±3.8	46.9±3.9	76.5±3.6	37.8±4.1	53.2±7.7	46.3±5.1
8a	52.0±7.0	62.8±5.6	72.7±6.9	42.2±5.6	54.8±4.9	71.3±6.9
8b	63.4±7.5	73.8±7.1	77.2±4.2	32.1±4.1	47.6±3.2	69.4±8.2
Miltefosine	49.56± 4.61	85.01±1.61	91.95± 3.52	49.3± 12 .04	76.49± 10.1	93.11± 1.81

^[a]Percentages of inhibition are expressed as mean ± standard deviation for each compound of three individual experiments performed in duplicates.

Table S3. Docking scores and binding interaction with LdTOP1.

Code	LdTOP1	Hydrogen Bond Interactions	Arene-arene / Arene-H Interactions	Secondary Residues
5m	-8.4789	Lys352	Tgp11	Asn178, Ala177, Met254, Tyr252, Thr246, Pro257, Lys250, His453, Arg314, Thr217, Asp353, DT10, DG12, DA113, Ile220, Asn221
5n	-8.5766	Asn221	Tgp11, DT10	Lys352, His453, Arg314, Thr217, Asp353, Ile355, DG12, DC112, Asn178, Ala177, DA113, Tyr222, Ile220
7a	-8.3910	Asn221	DT10, Tgp11	Asn178, DC112, Pro257, Ala177, DA113, Tyr252, Lys251, DT9, Lys352, Arg314, His453, Thr217, Tyr222, Ile220
8a	-9.4846	Asn178	Tgp11, DC112	Ala177, Tyr252, DT9, Pro257, DT10, Ile220, Asn221, DA113, Lys200, Glu182, Met254, Lys251
Camptothecin	-7.7961	Lys352, Asp353, Arg314	Tgp11	Thr217, Ile220, His453, Asn221, Tyr222, DT10, DC112, DG12, DA113, Asn178

➤ **¹H, ¹³C, and ¹⁹F NMR Spectra:**

Figure S1: ¹H NMR of compound 5a

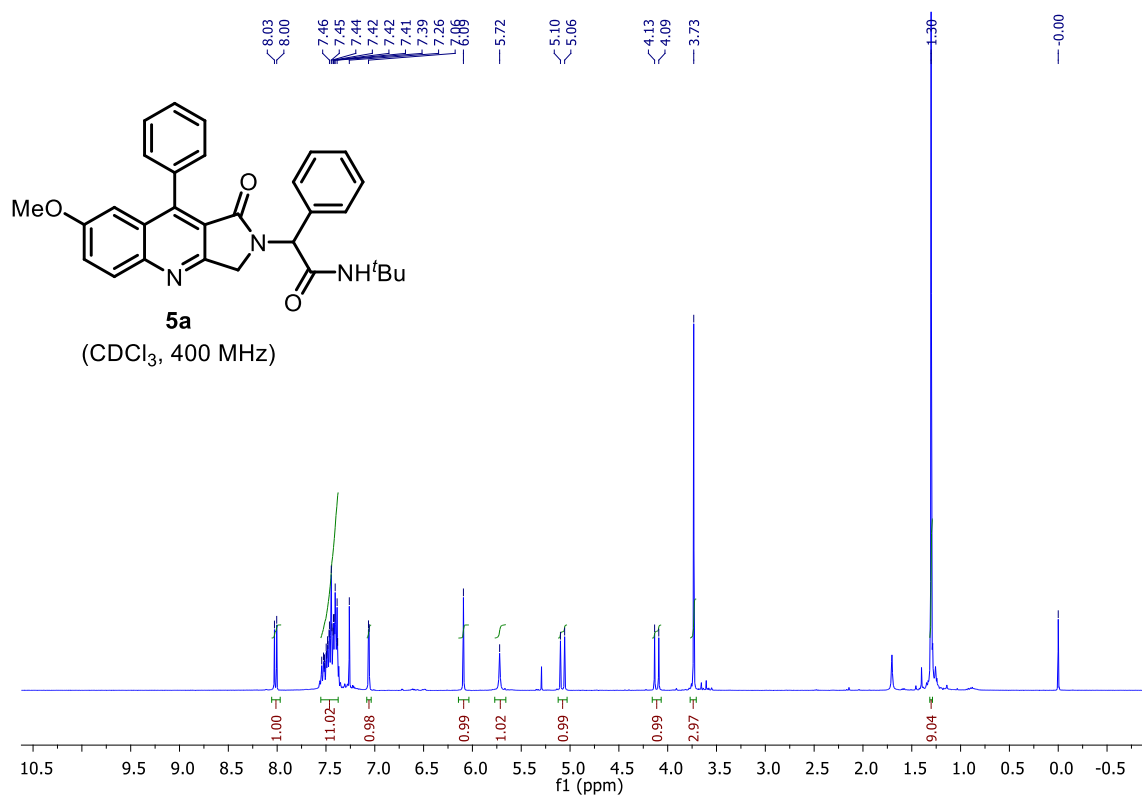


Figure S2: ¹³C NMR of compound 5a

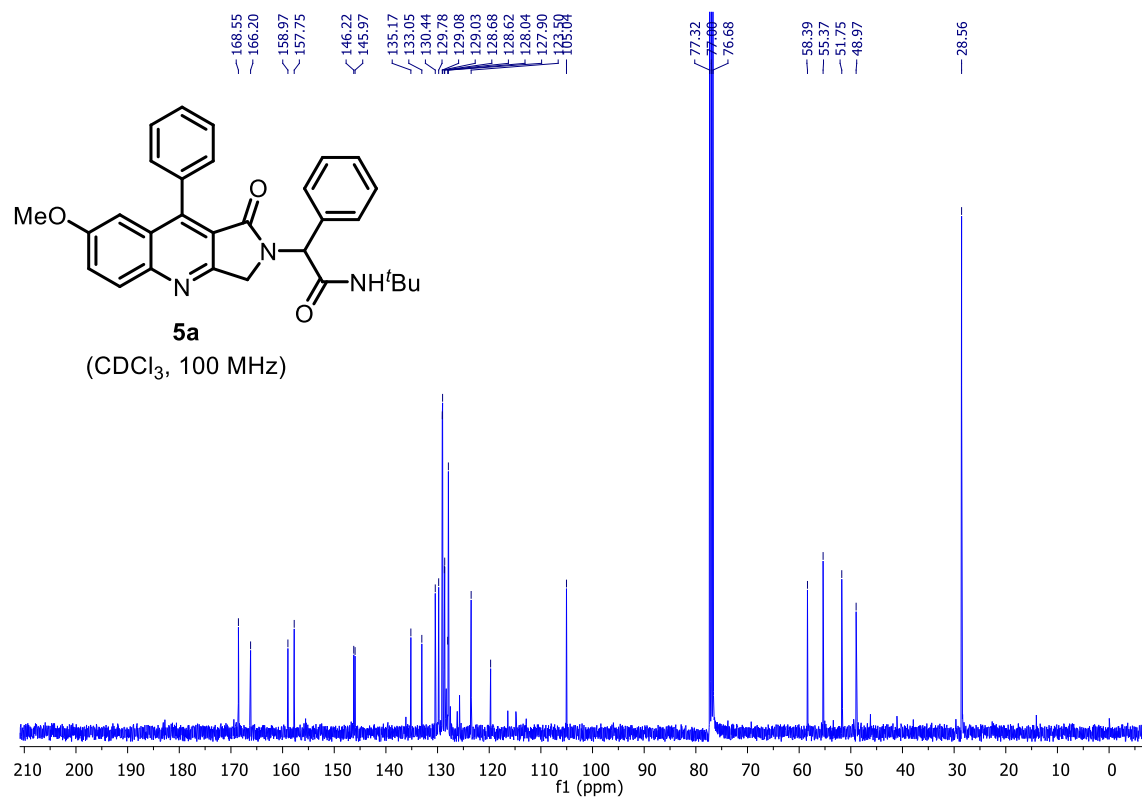


Figure S3: ^1H NMR of compound **5e**

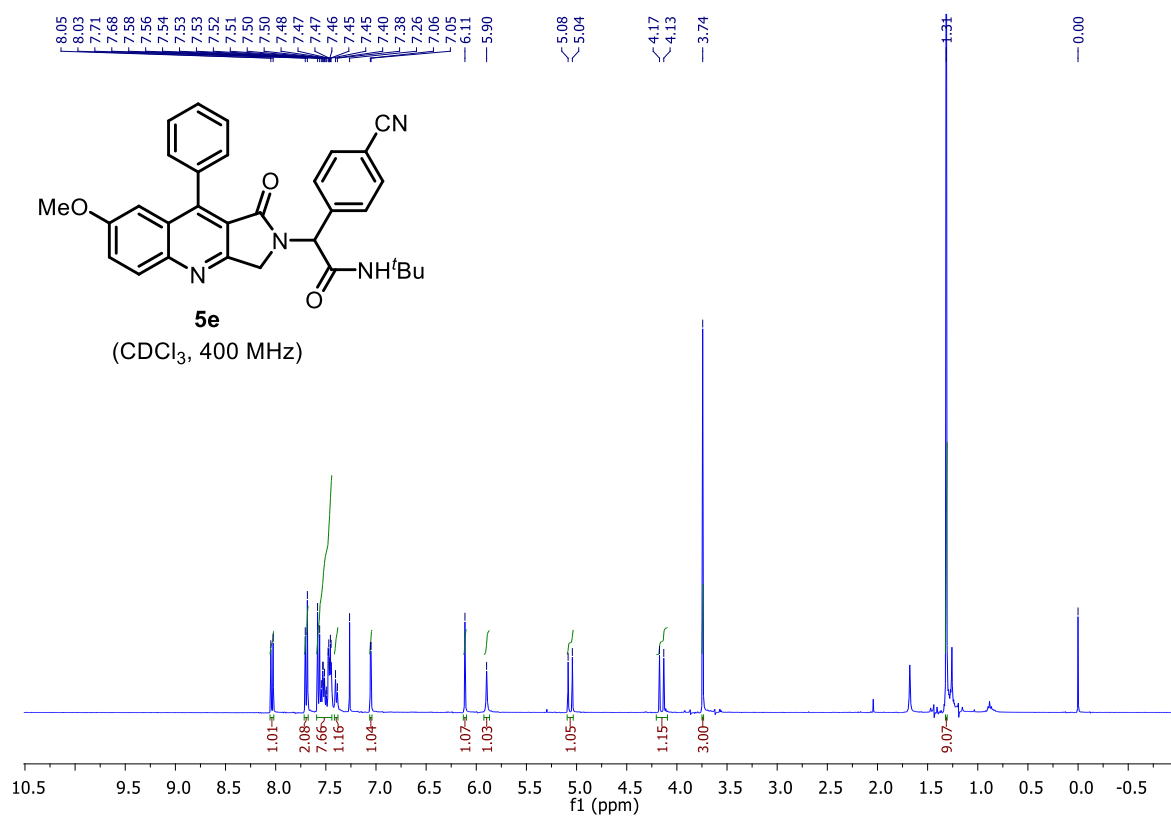


Figure S4: ^{13}C NMR of compound **5e**

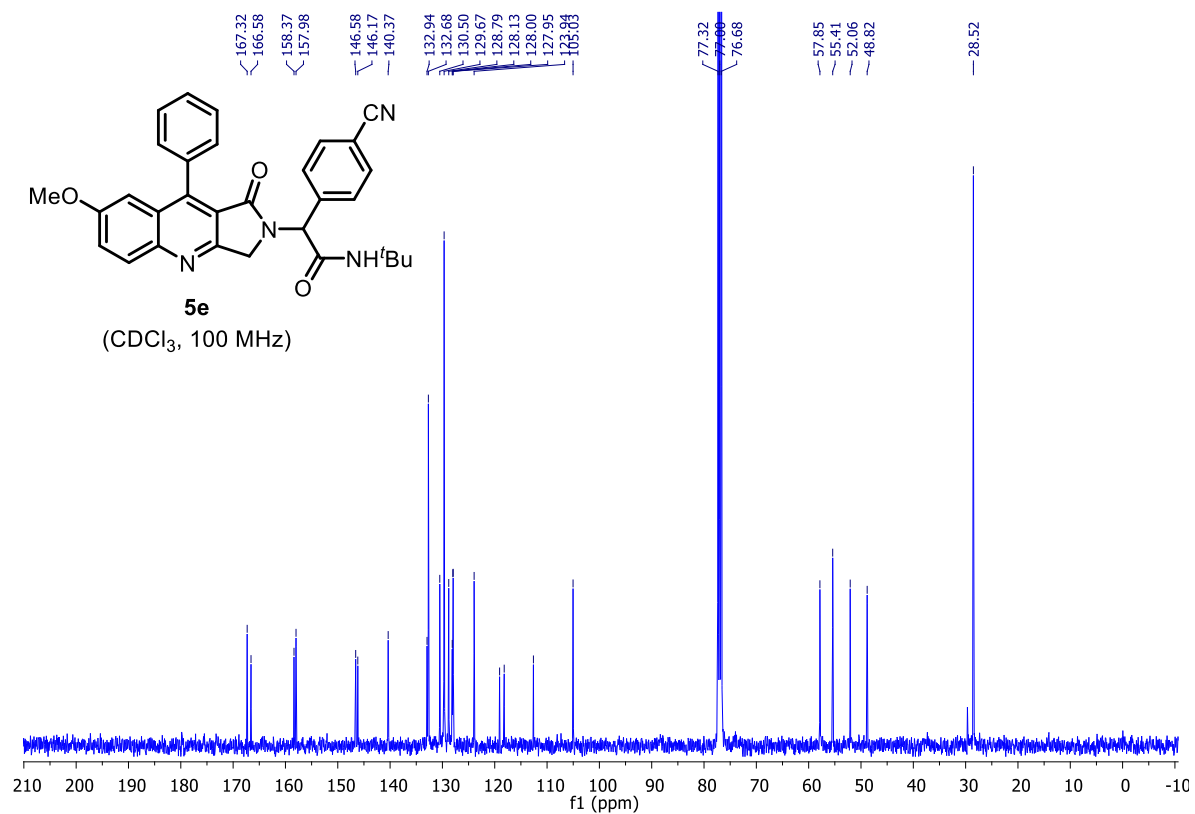


Figure S5: ^1H NMR of compound **5i**

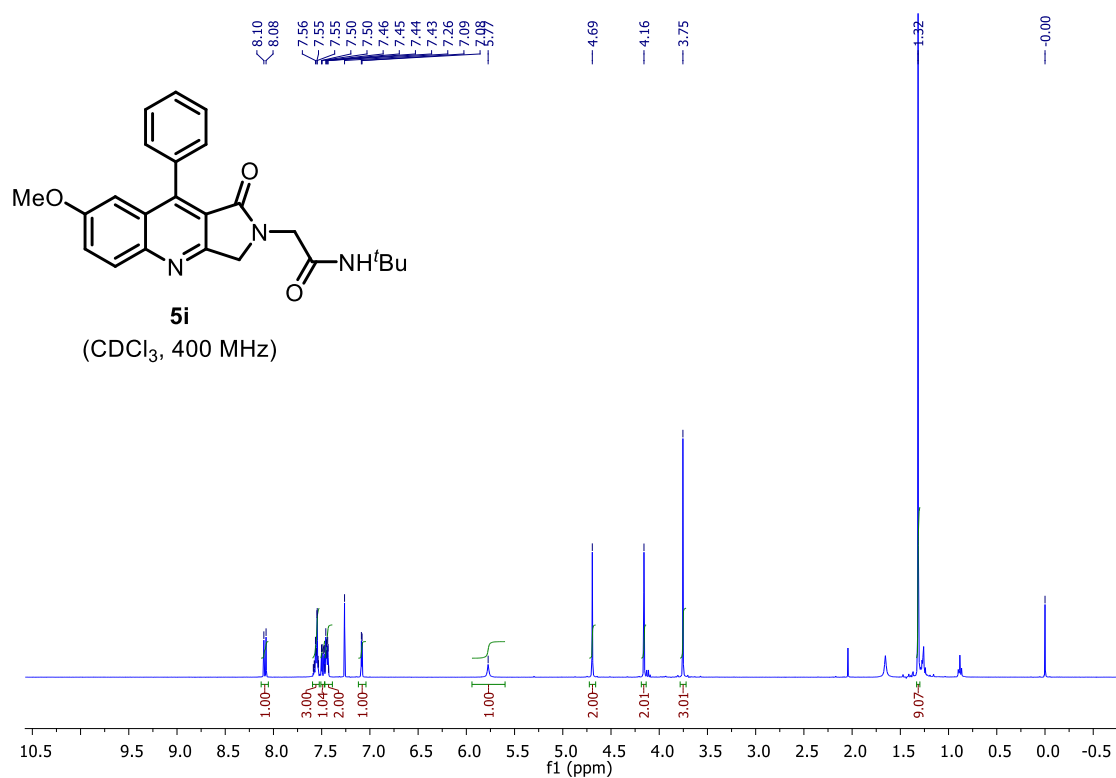


Figure S6: ^{13}C NMR of compound **5i**

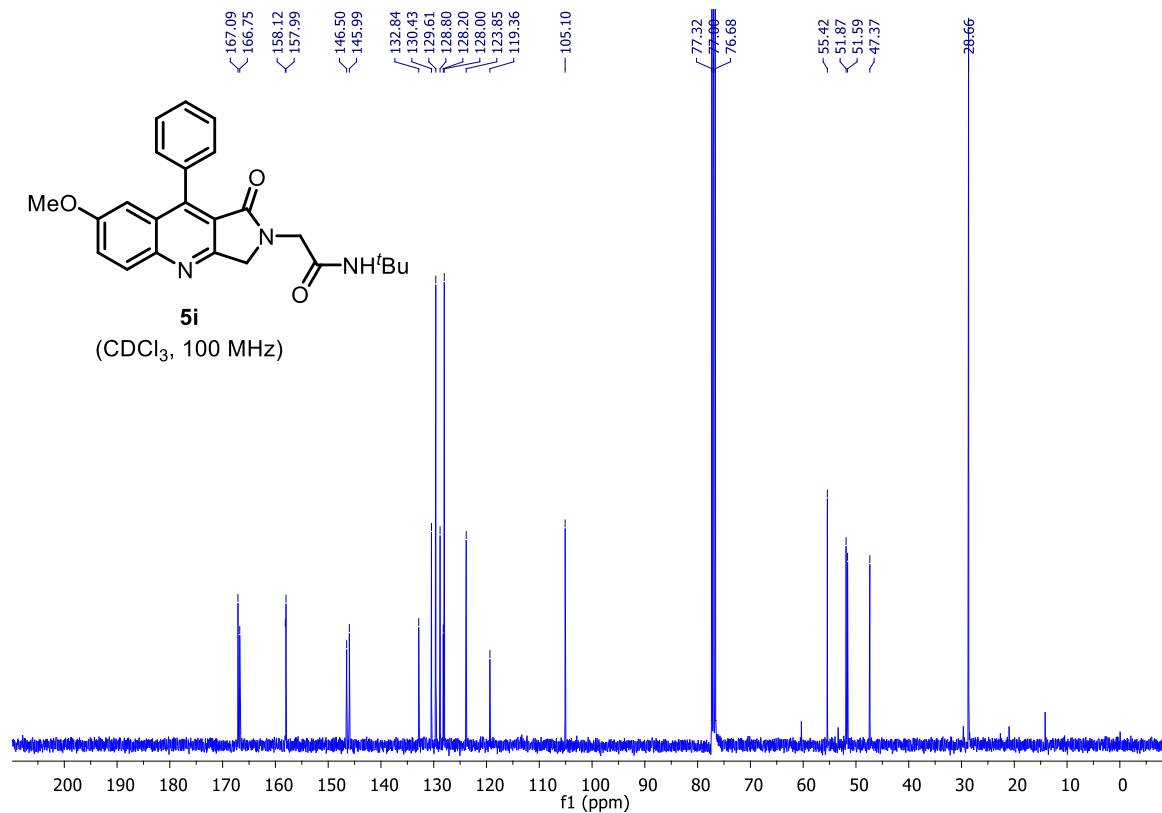


Figure S7: ^1H NMR of compound **5m**

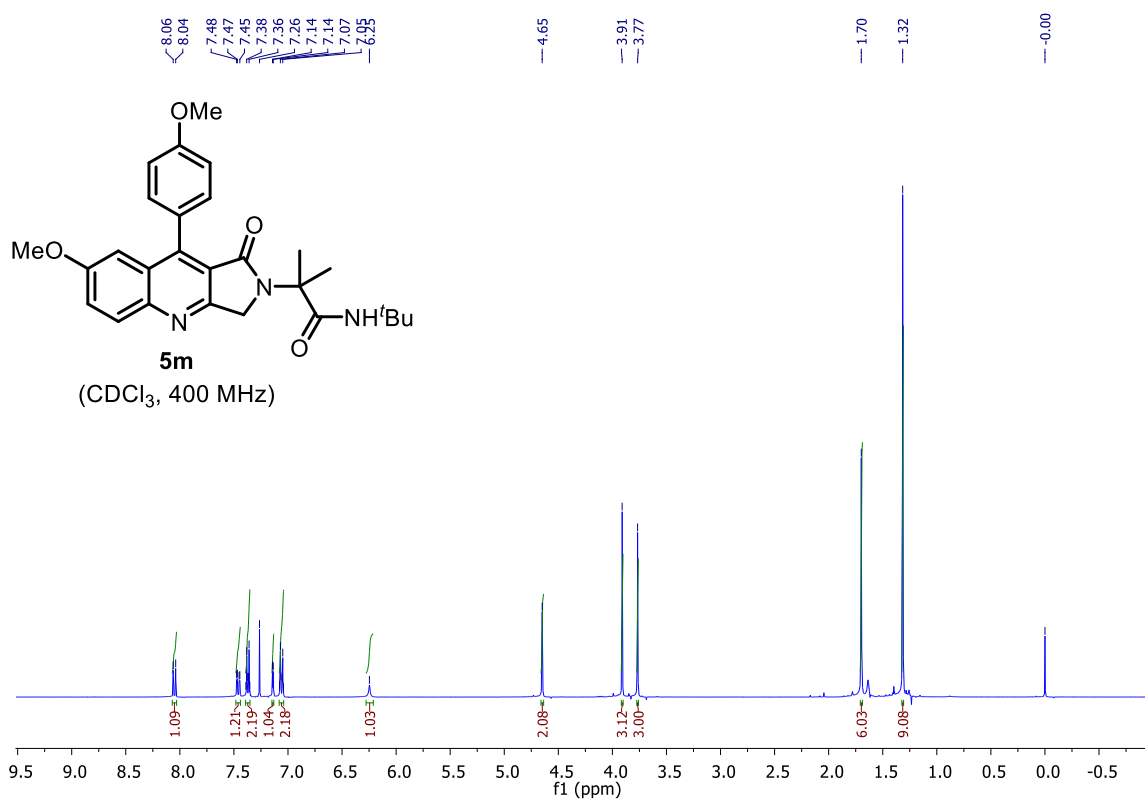


Figure S8: ^{13}C NMR of compound **5m**

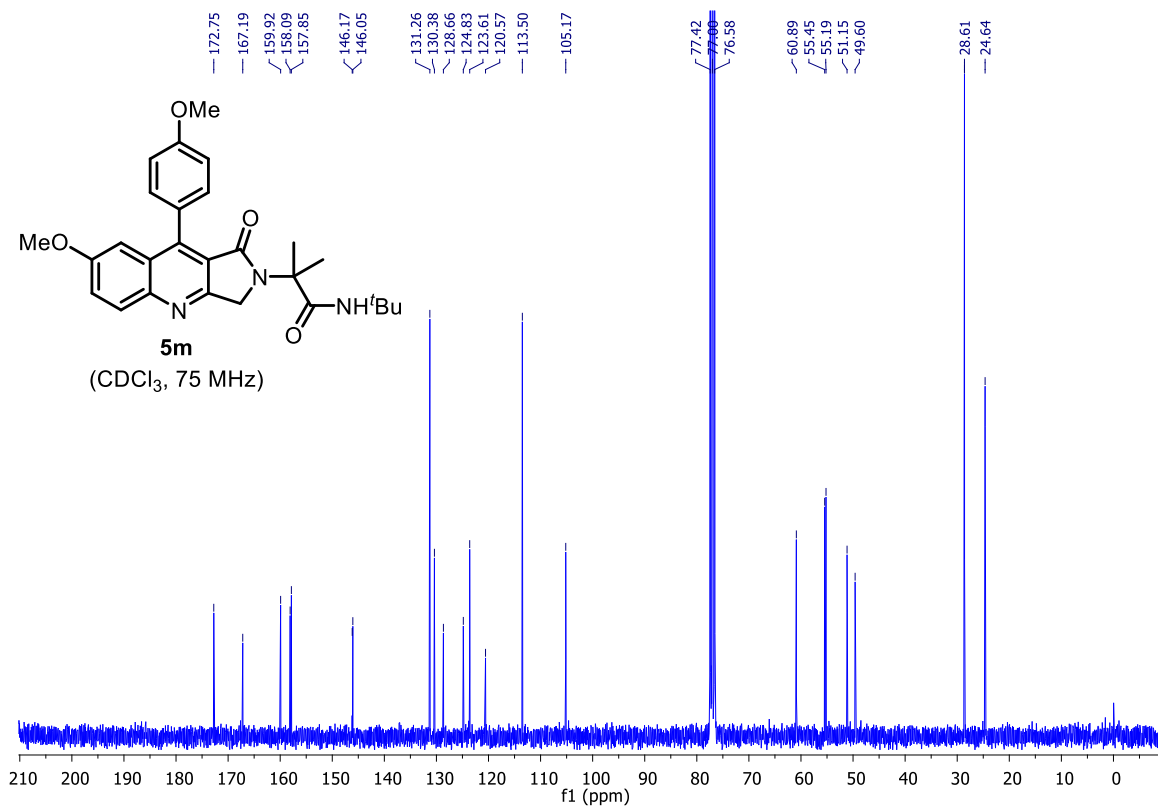


Figure S9: ^1H NMR of compound **5n**

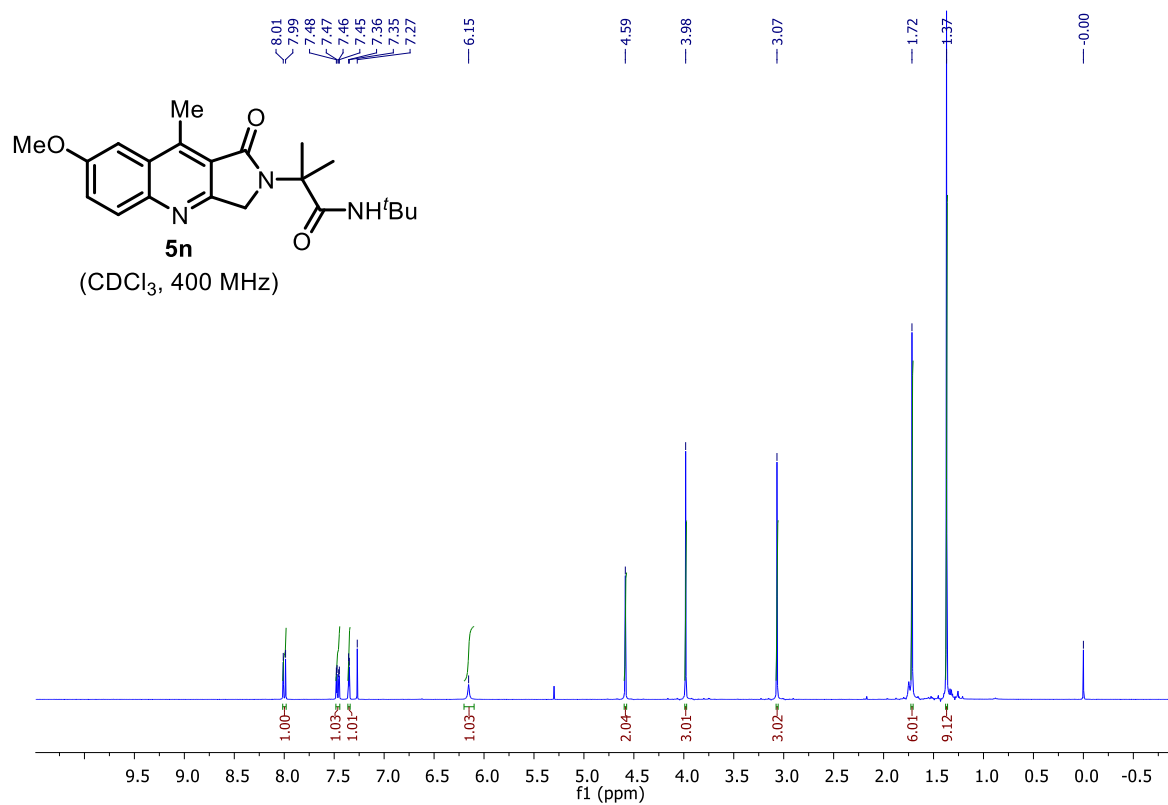


Figure S10: ^{13}C NMR of compound **5n**

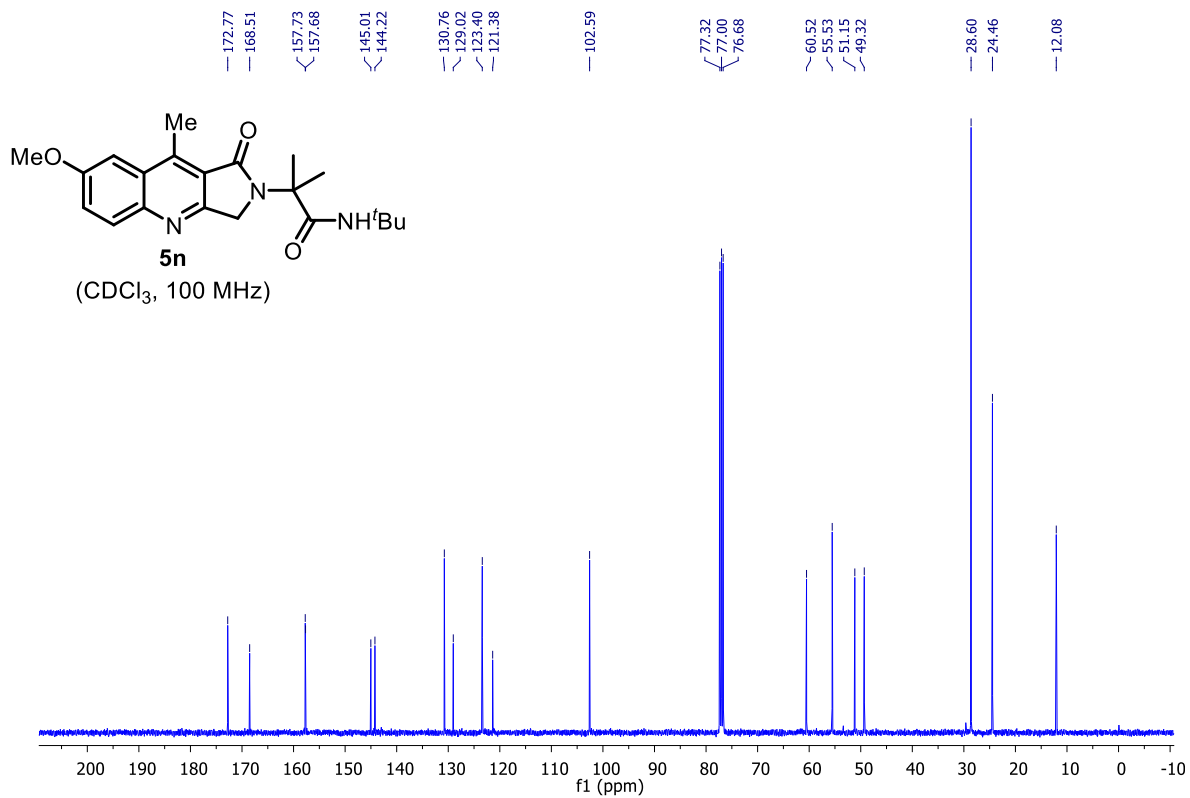


Figure S11: ^1H NMR of compound **5o**

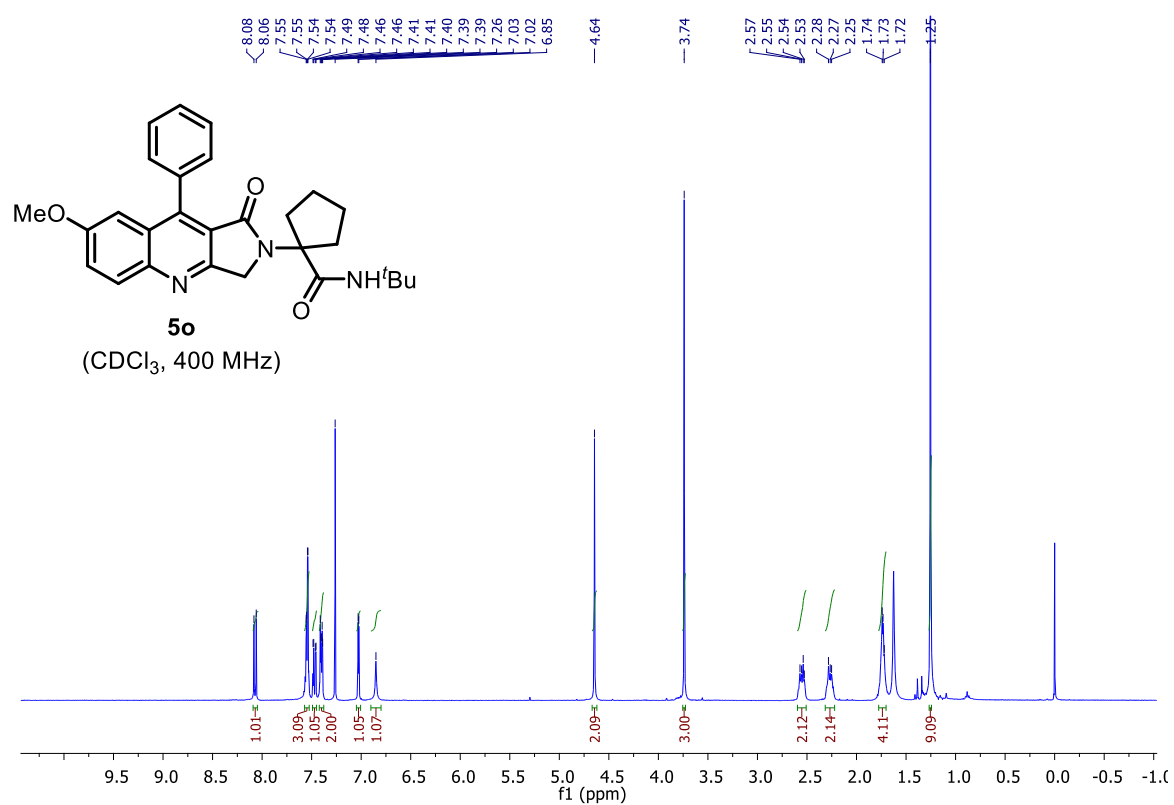


Figure S12: ^{13}C NMR of compound **5o**

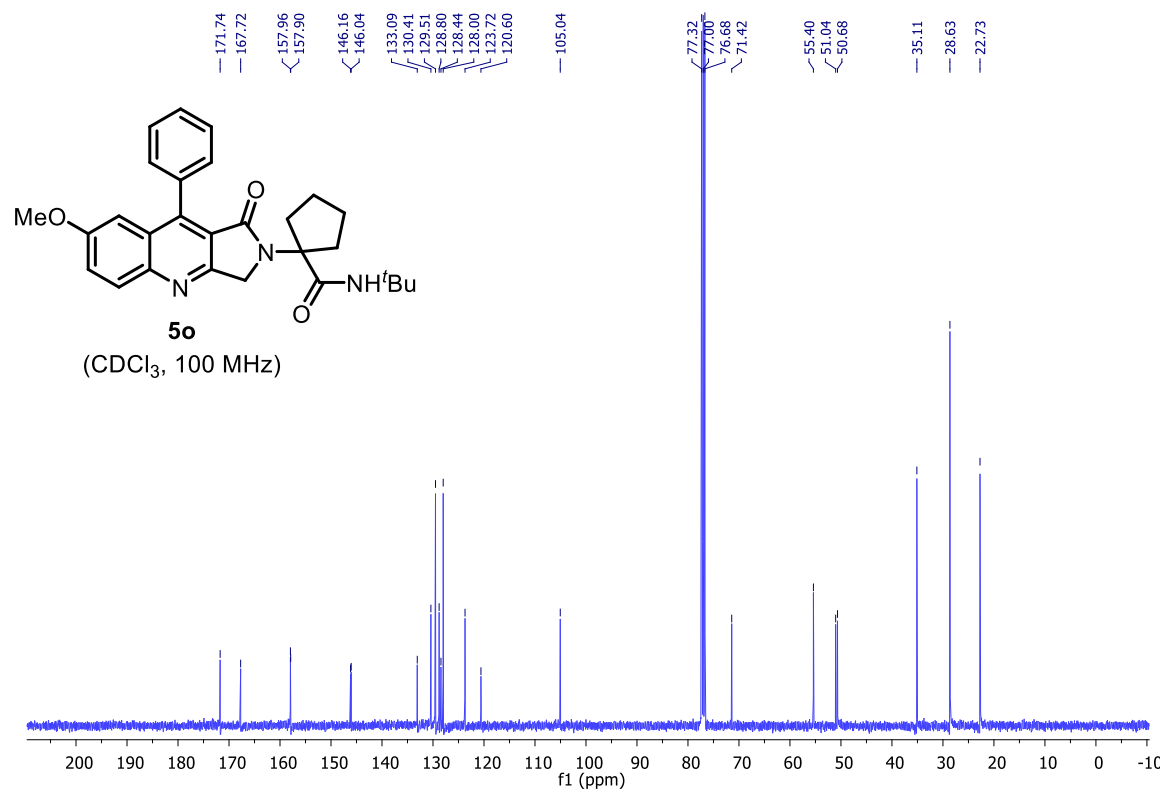


Figure S13: ^1H NMR of compound **5p**

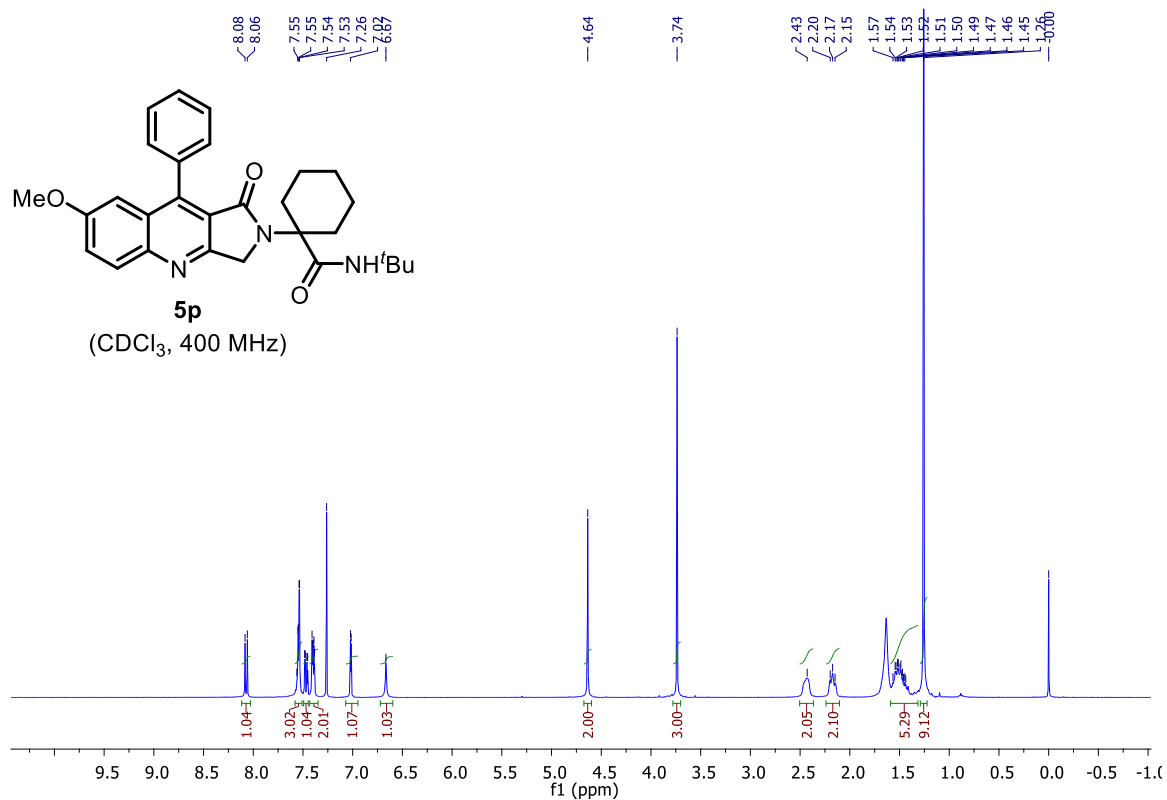


Figure S14: ^{13}C NMR of compound **5p**

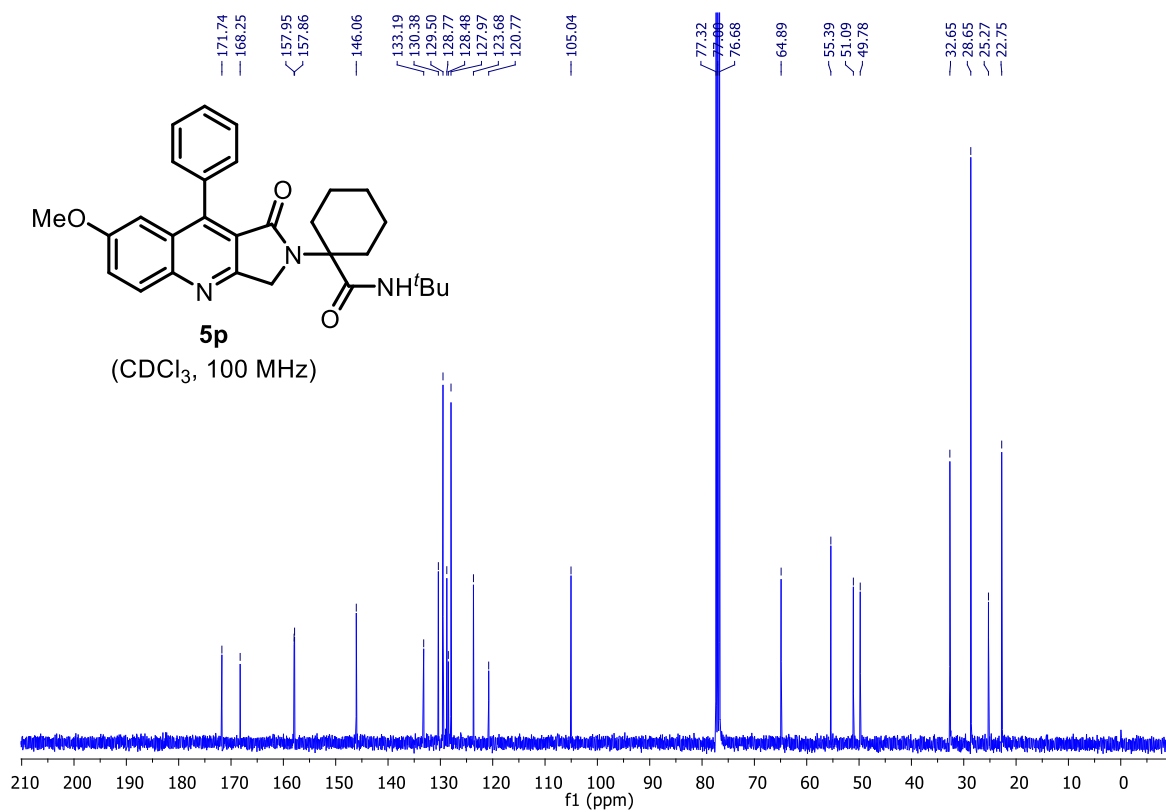


Figure S15: ^1H NMR of compound **5q**

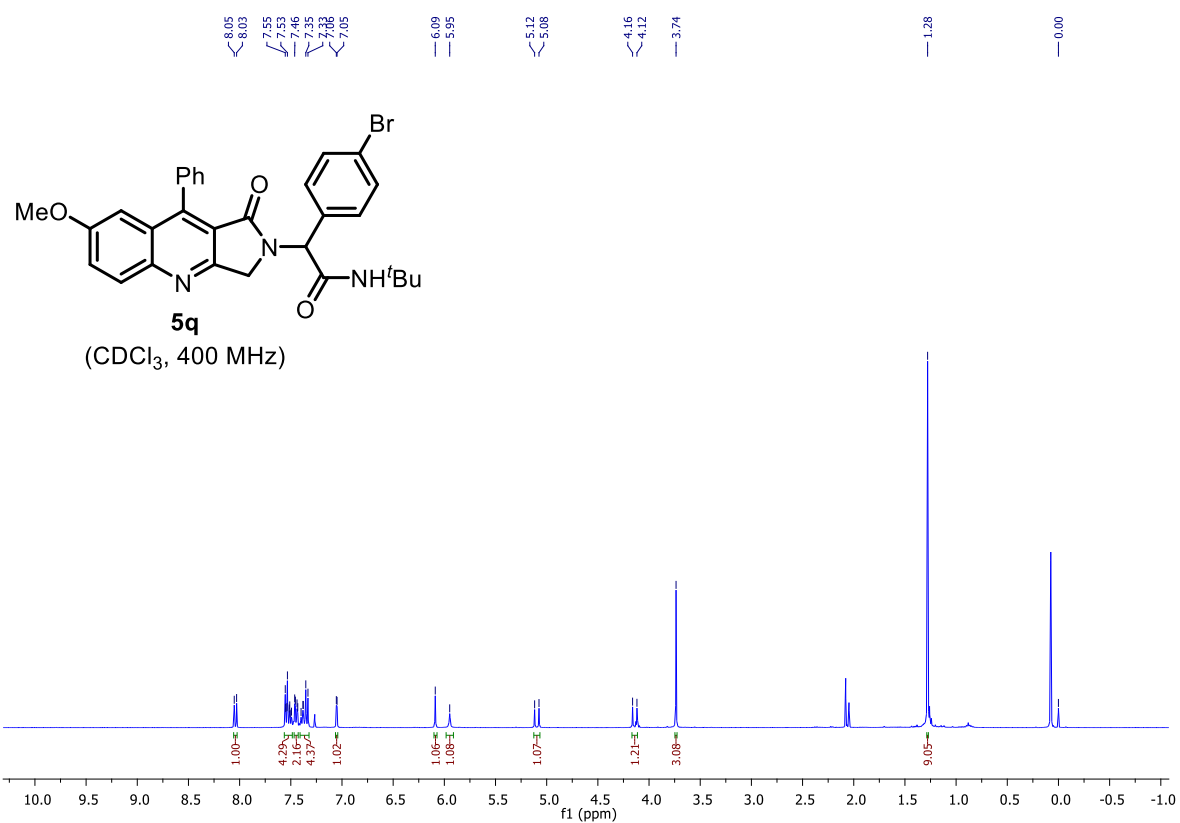


Figure S16: ^{13}C NMR of compound **5q**

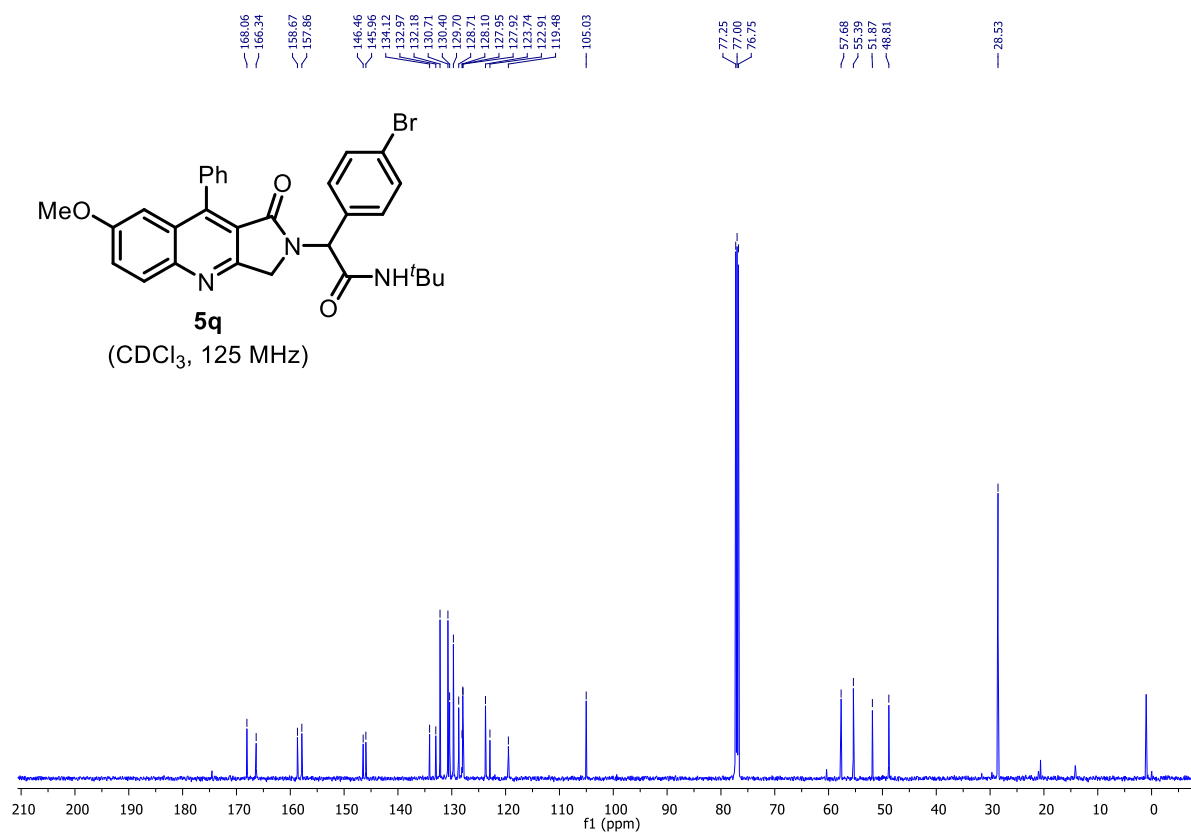


Figure S17: ^1H NMR of compound **5r**

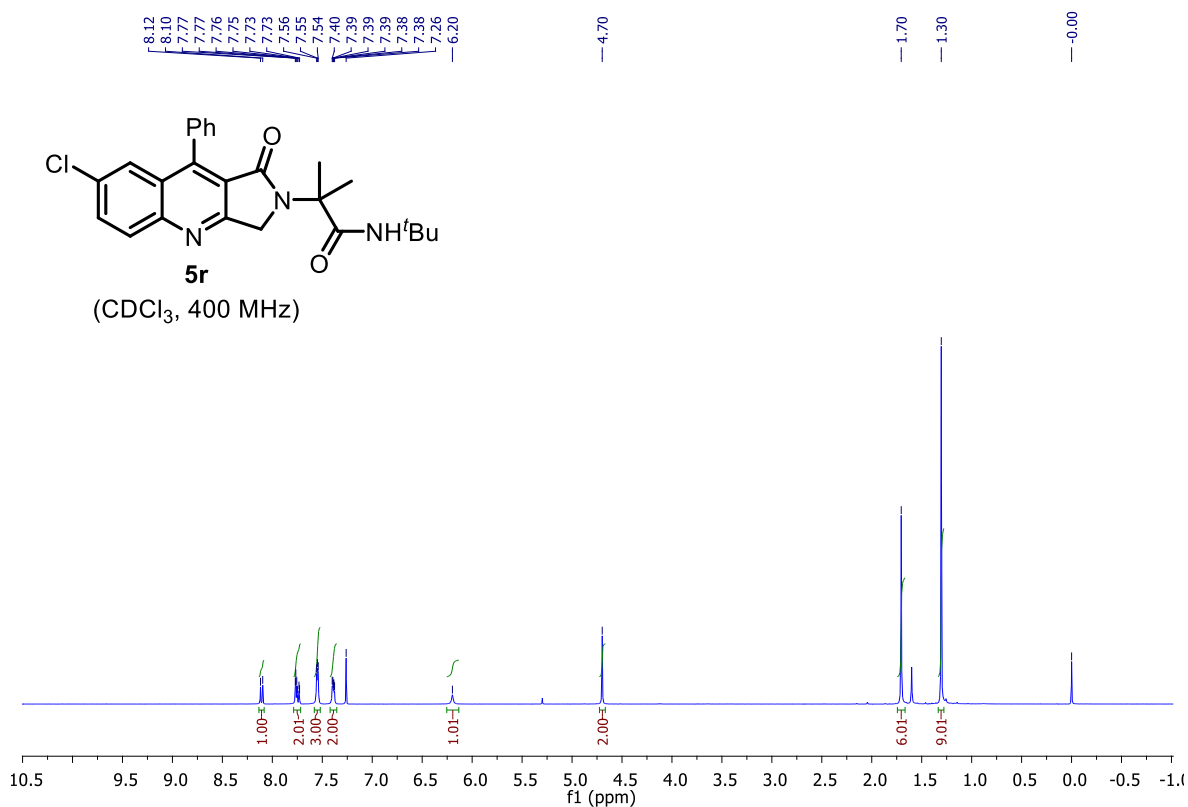


Figure S18: ^{13}C NMR of compound **5r**

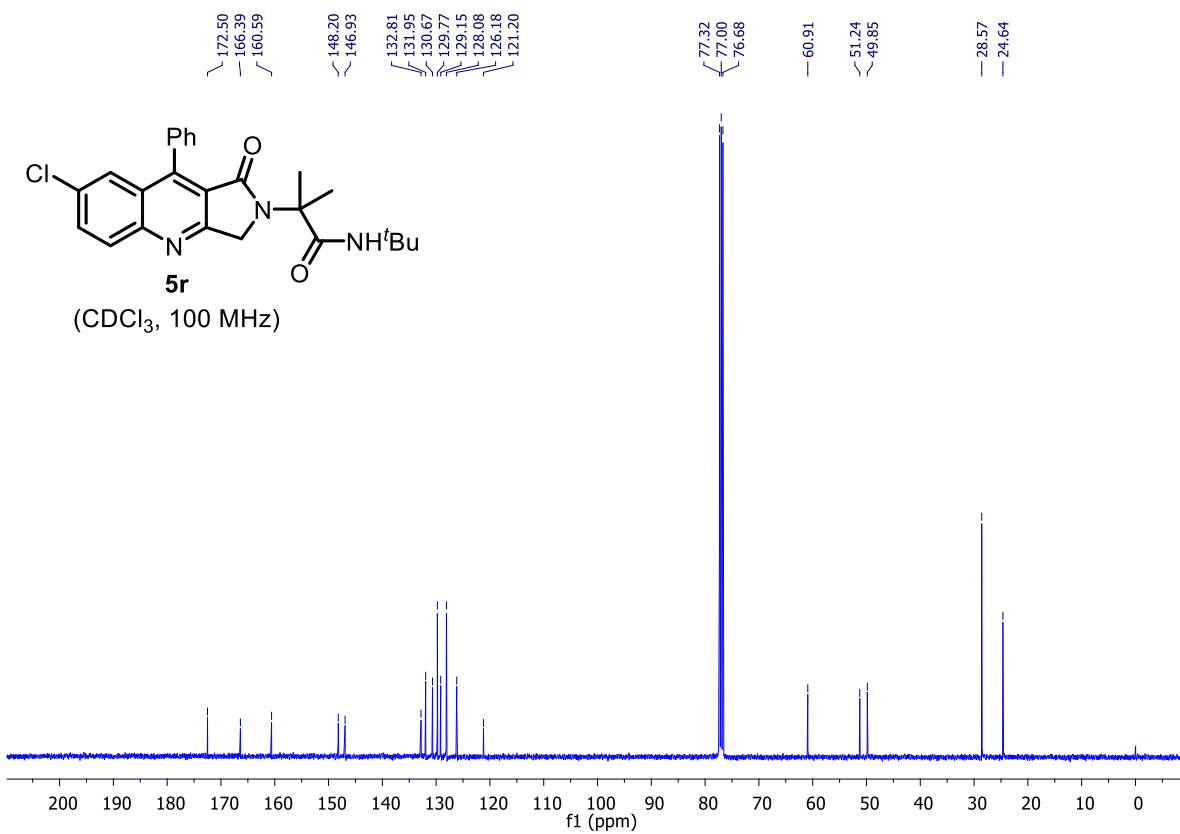


Figure S19: ^1H NMR of compound **6a**

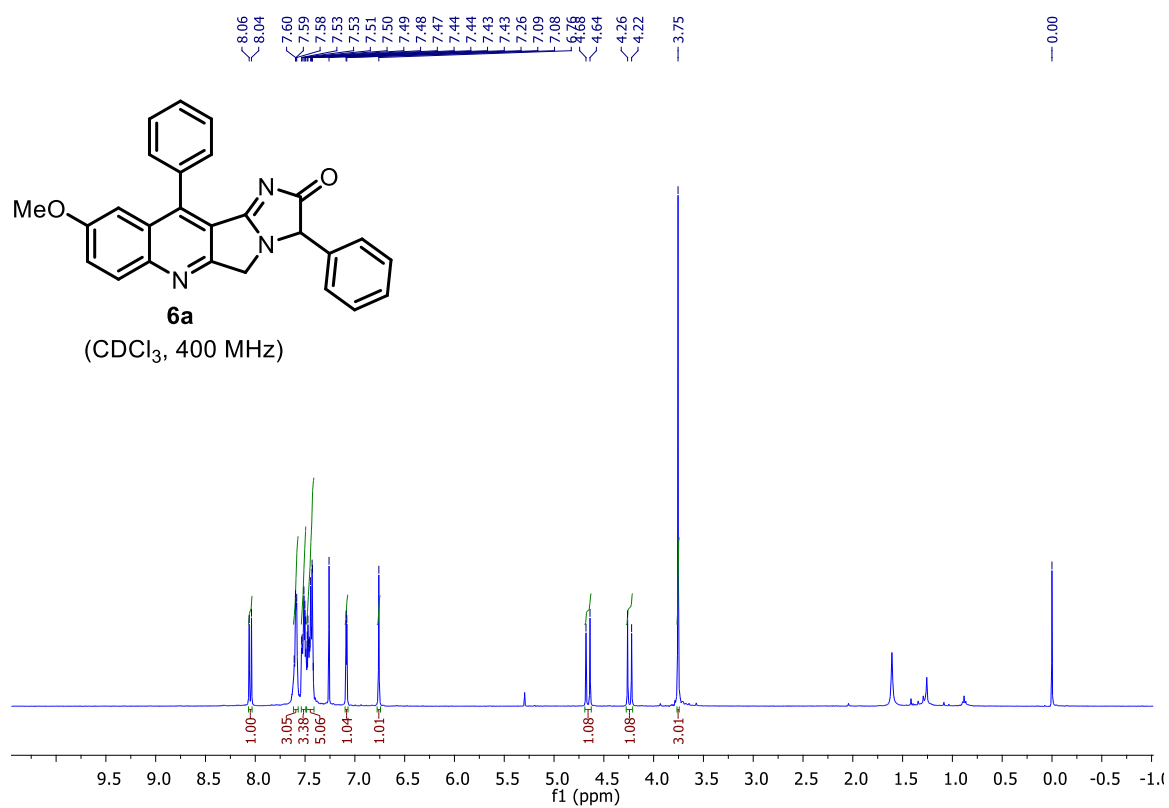


Figure S20: ^{13}C NMR of compound **6a**

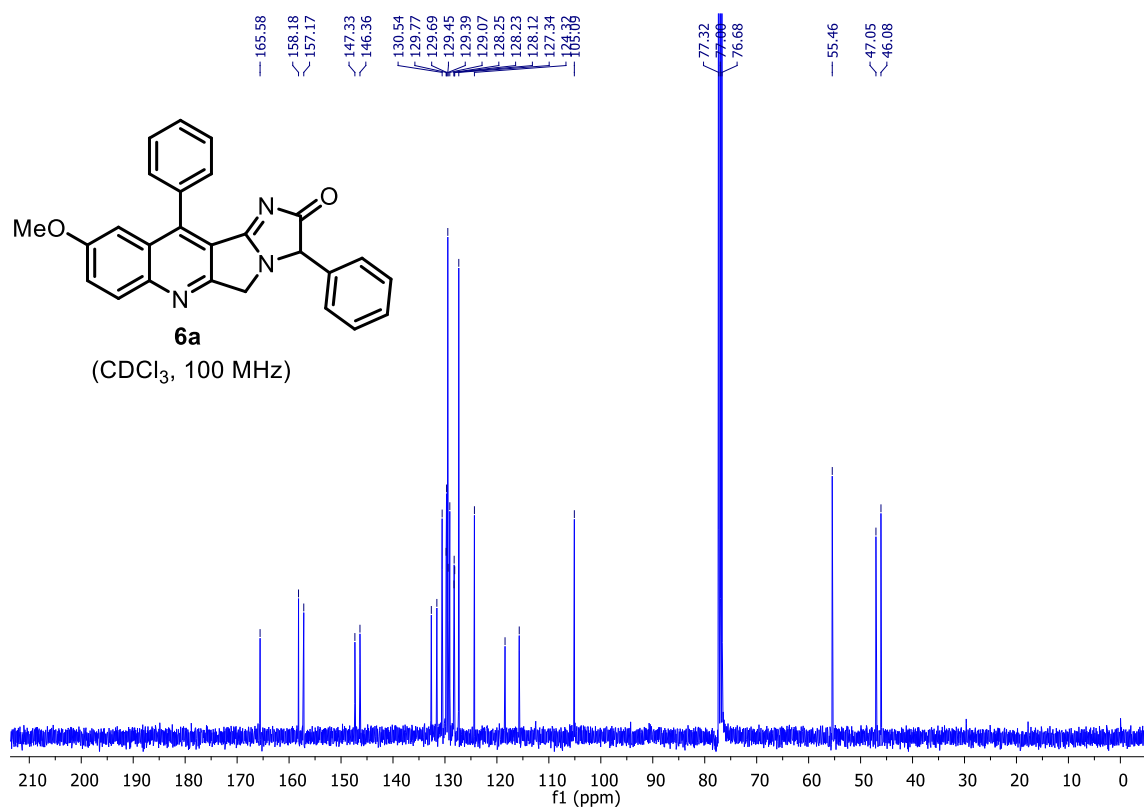


Figure S21: ^1H NMR of compound **6b**

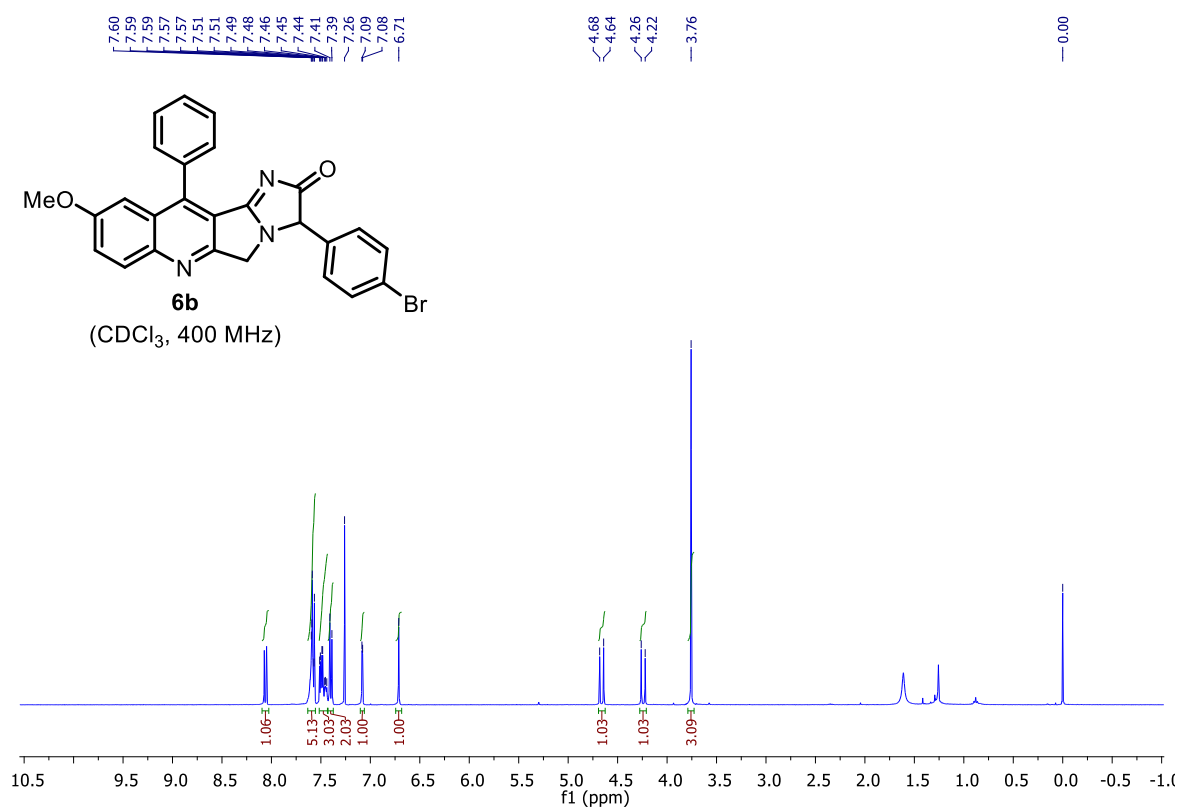


Figure S22: ^{13}C NMR of compound **6b**

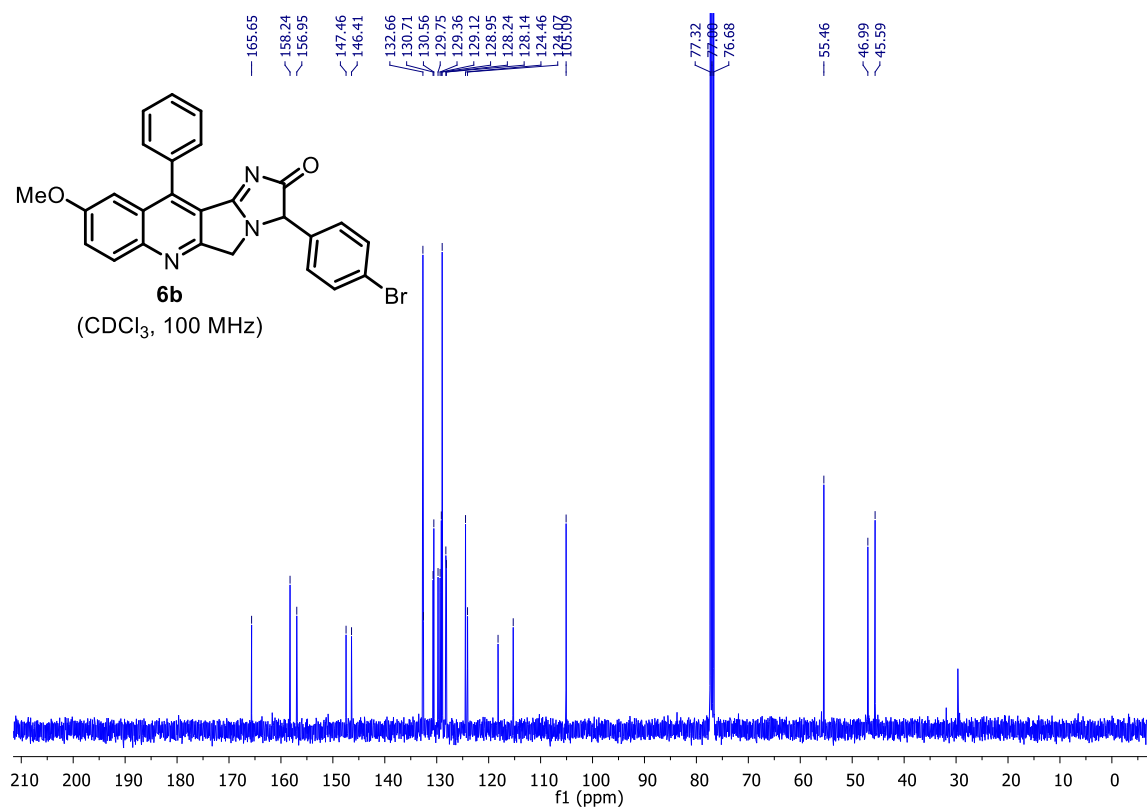


Figure S23: ^1H NMR of compound **6c**

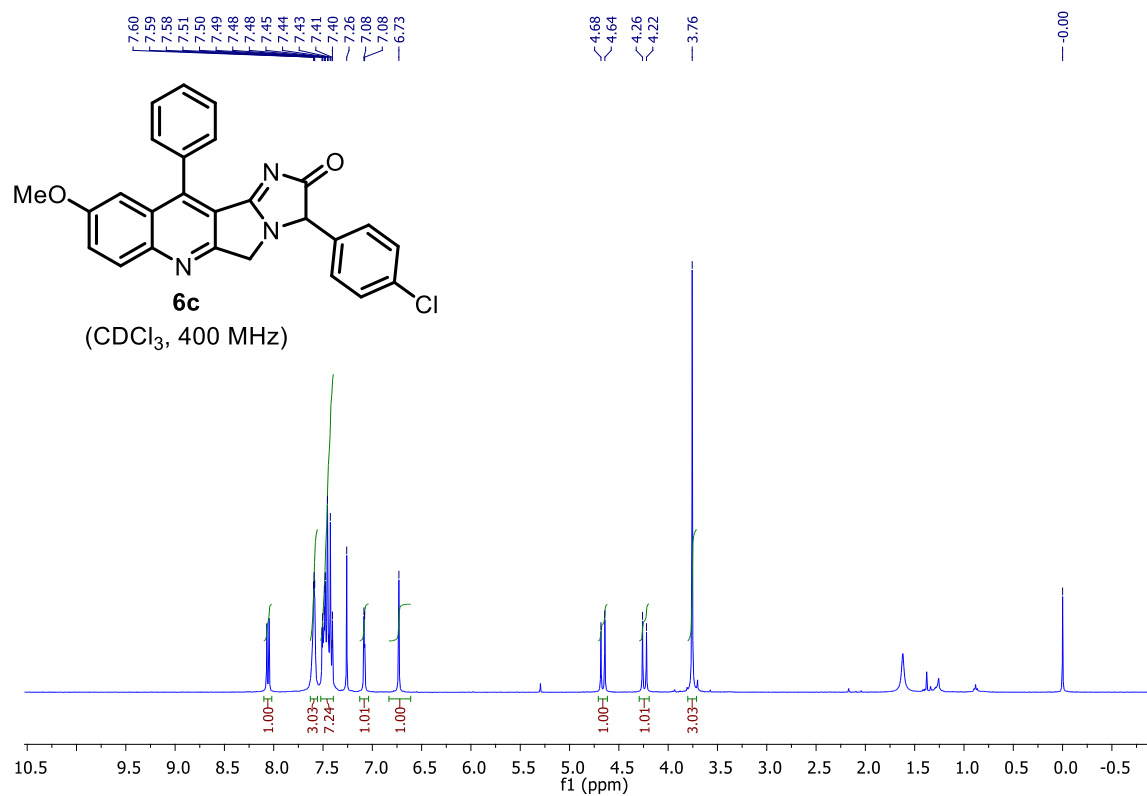


Figure S24: ^{13}C NMR of compound **6c**

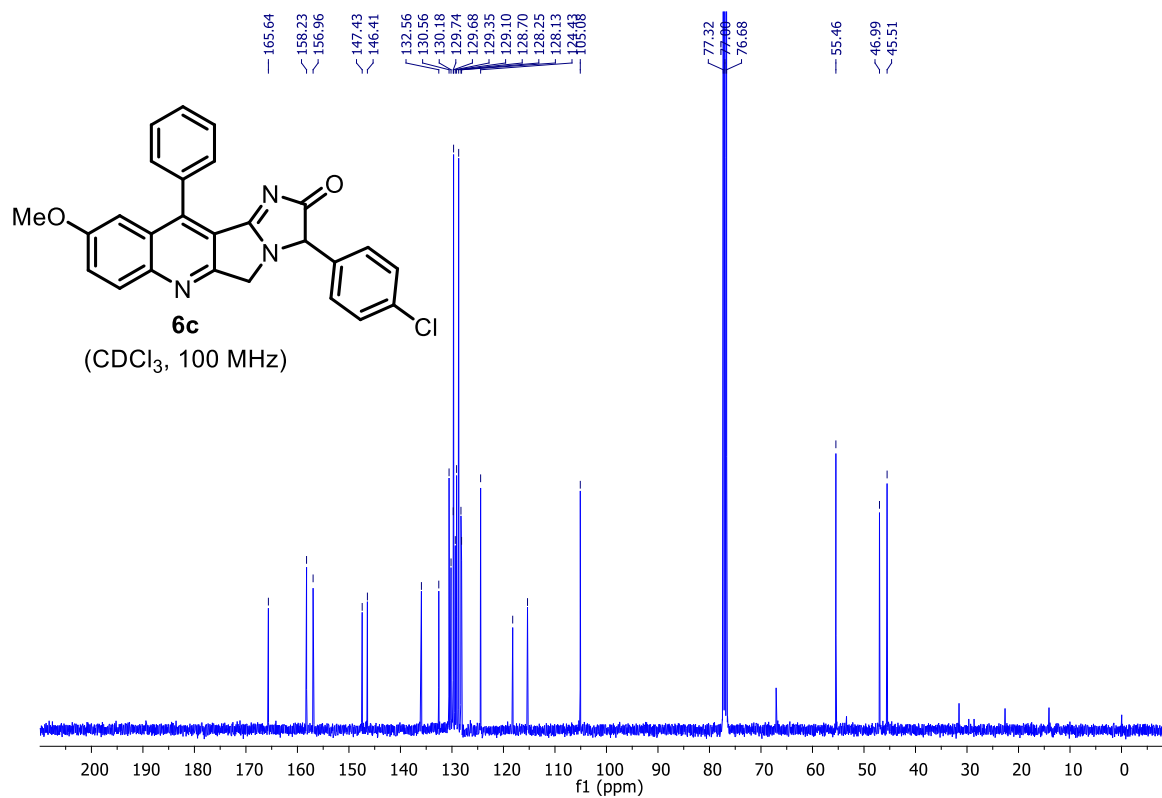


Figure S25: ^1H NMR of compound **6d**

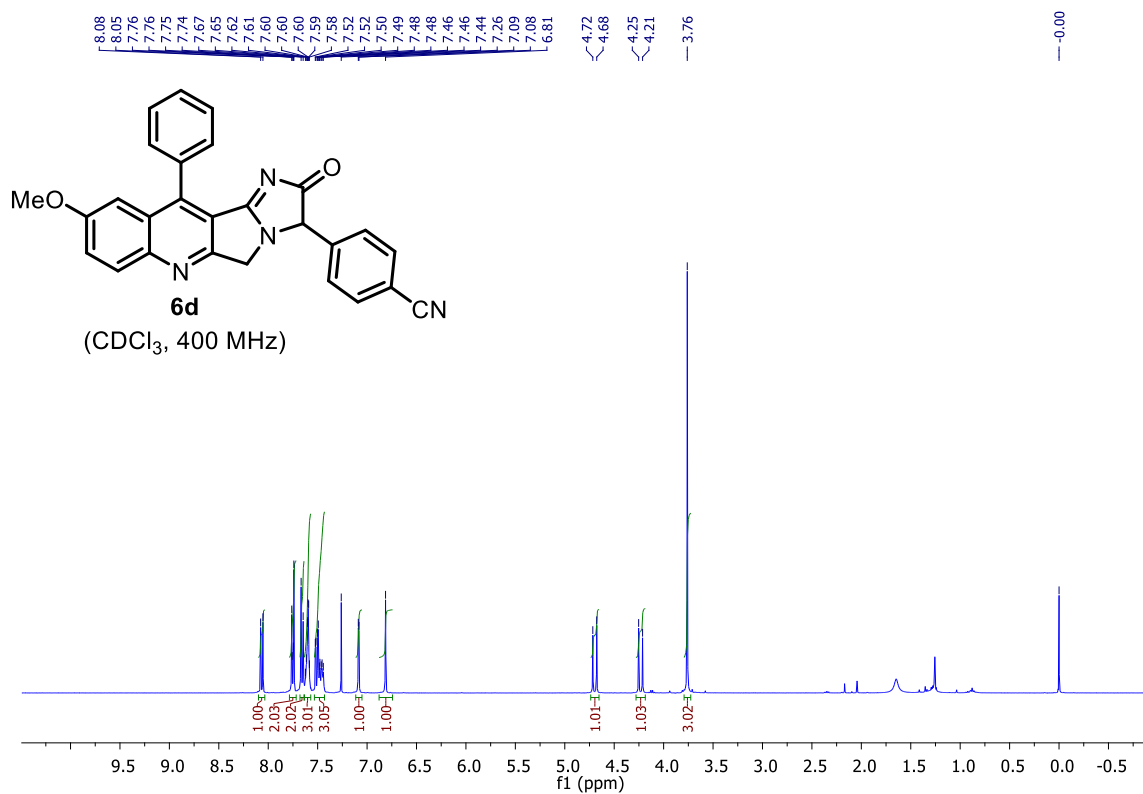


Figure S26: ^{13}C NMR of compound **6d**

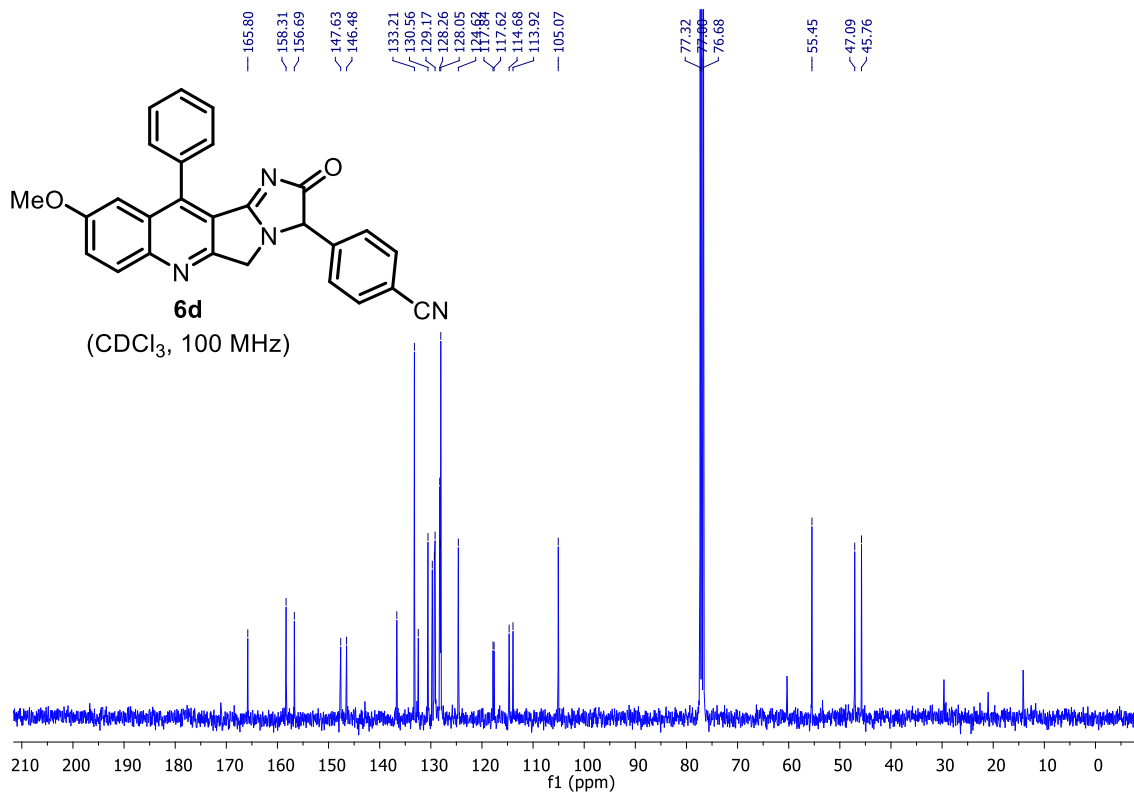


Figure S27: ^1H NMR of compound **6e**

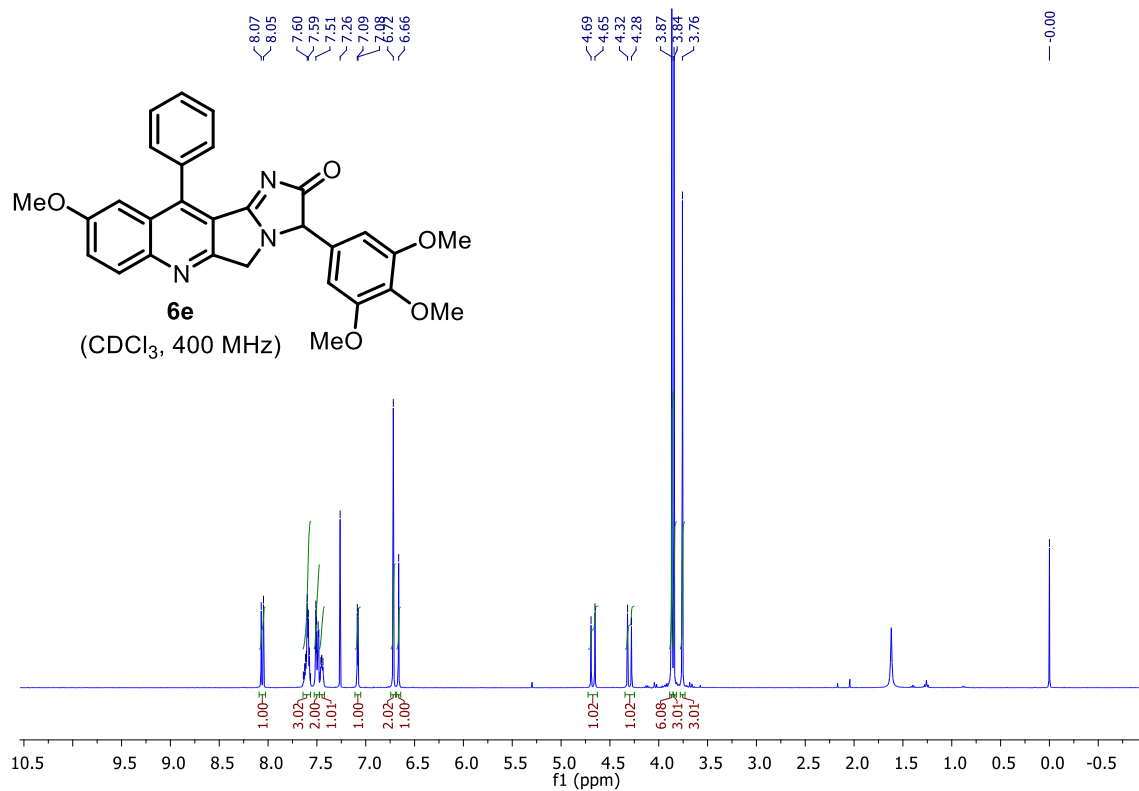


Figure S28: ^{13}C NMR of compound **6e**

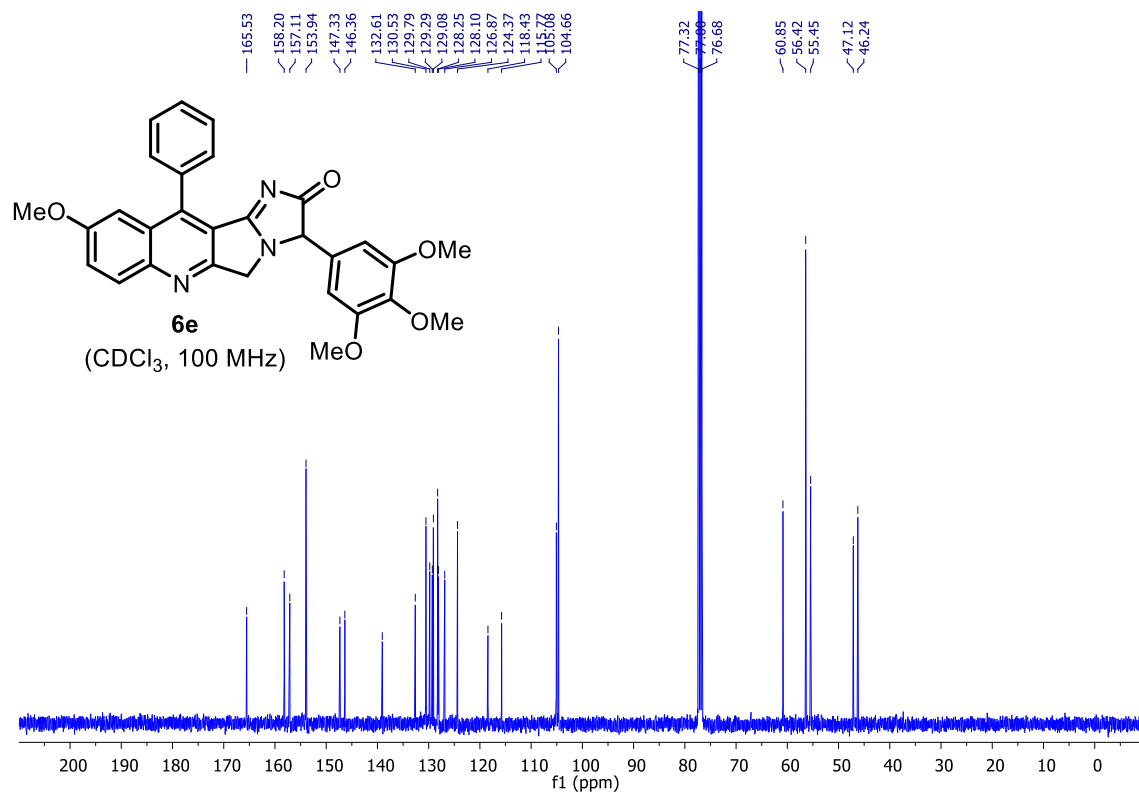


Figure S29: ^1H NMR of compound **6f**

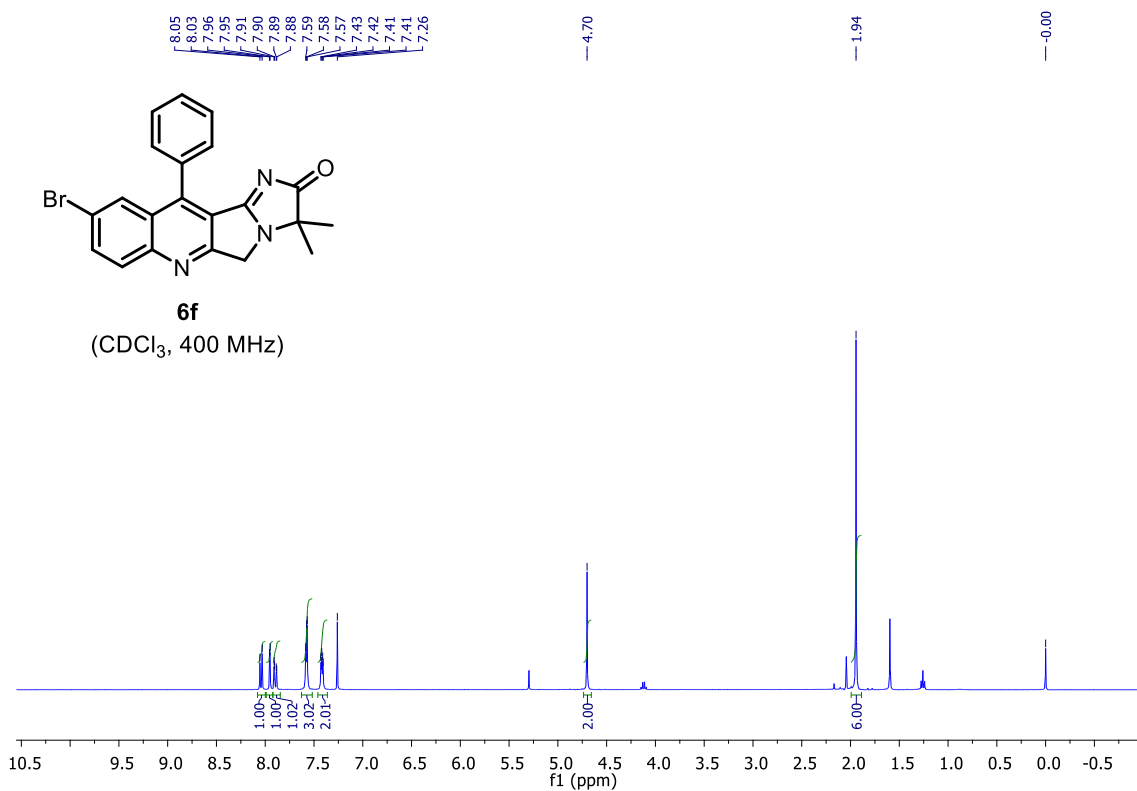


Figure S30: ^{13}C NMR of compound **6f**

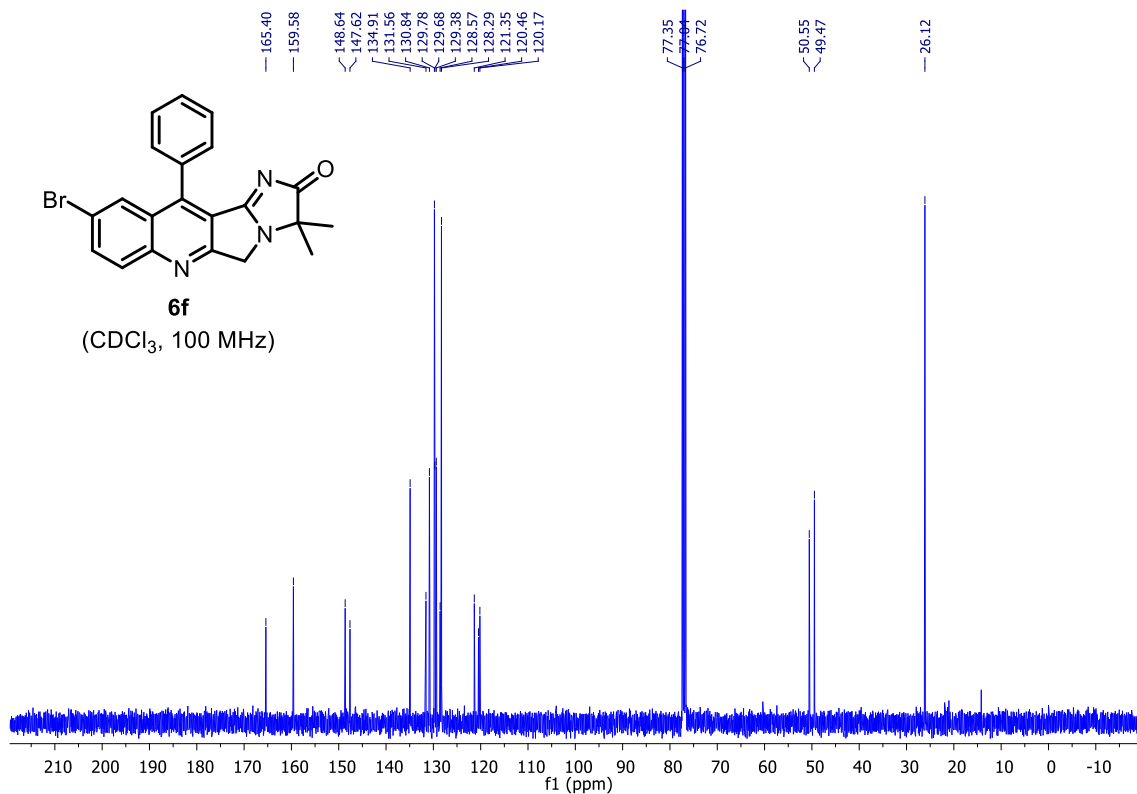


Figure S31: ^1H NMR of compound **6g**

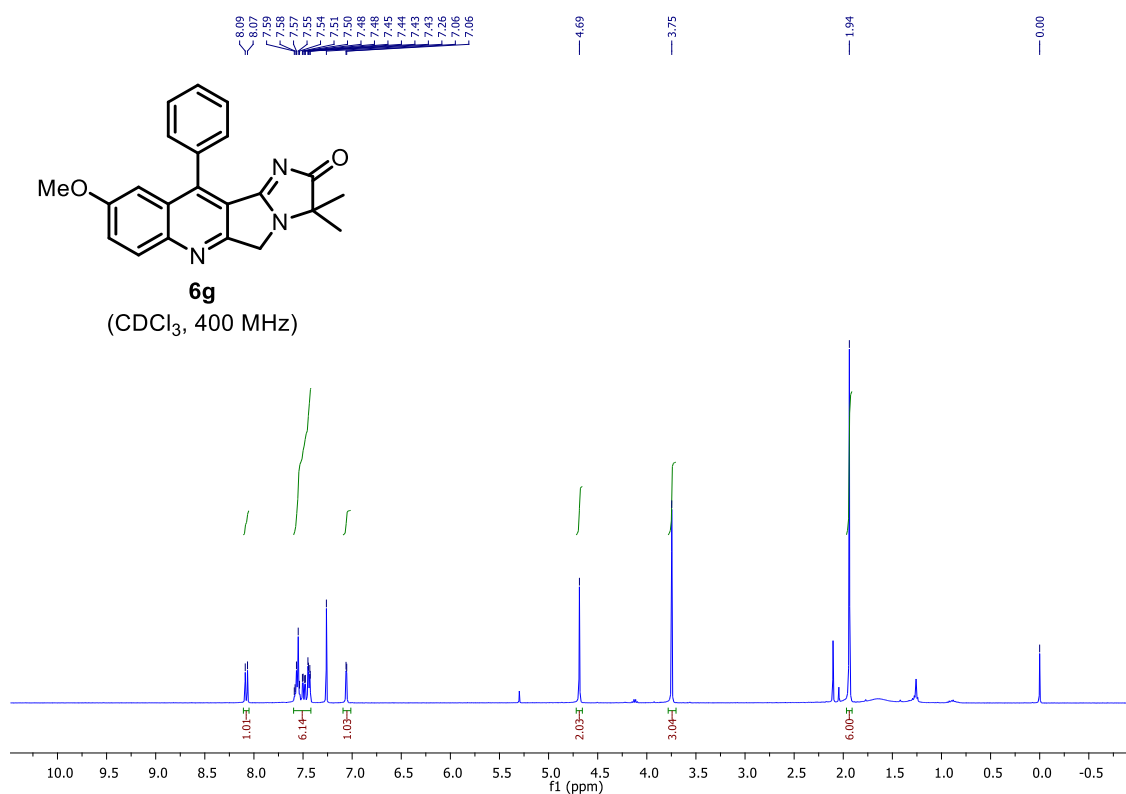


Figure S32: ^{13}C NMR of compound **6g**

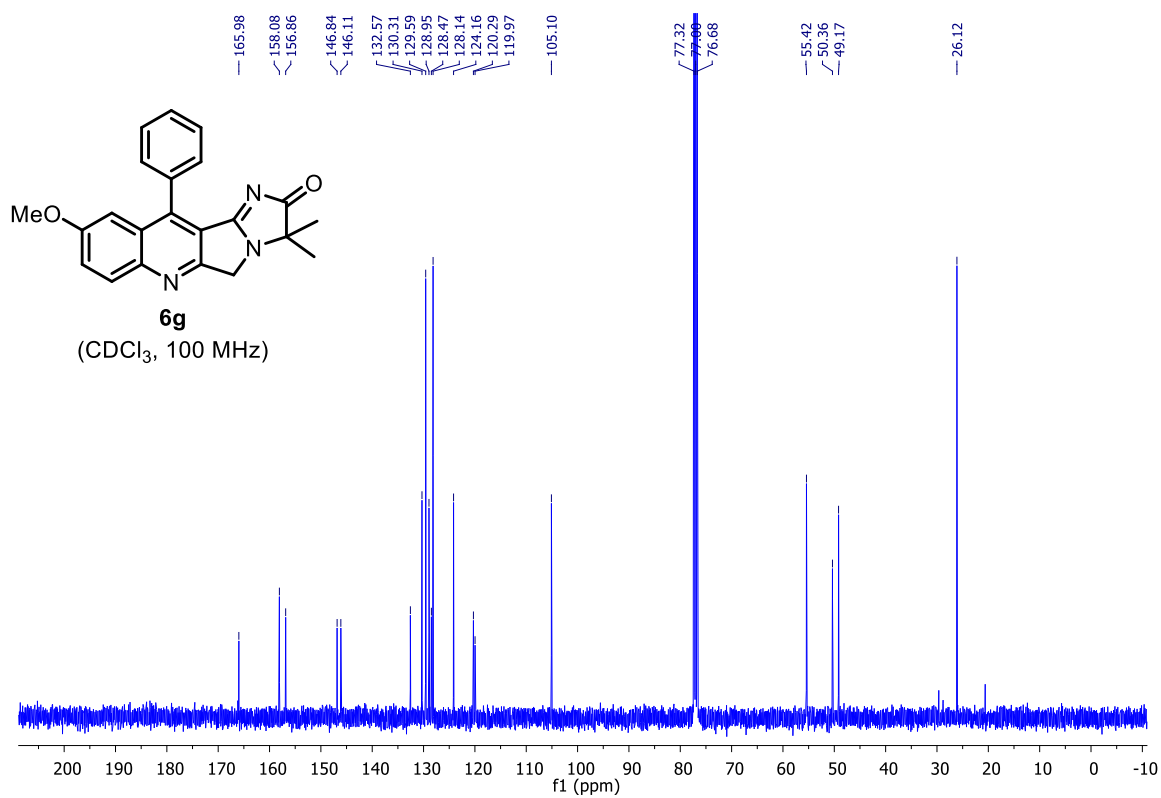


Figure S33: ^1H NMR of compound **6h**

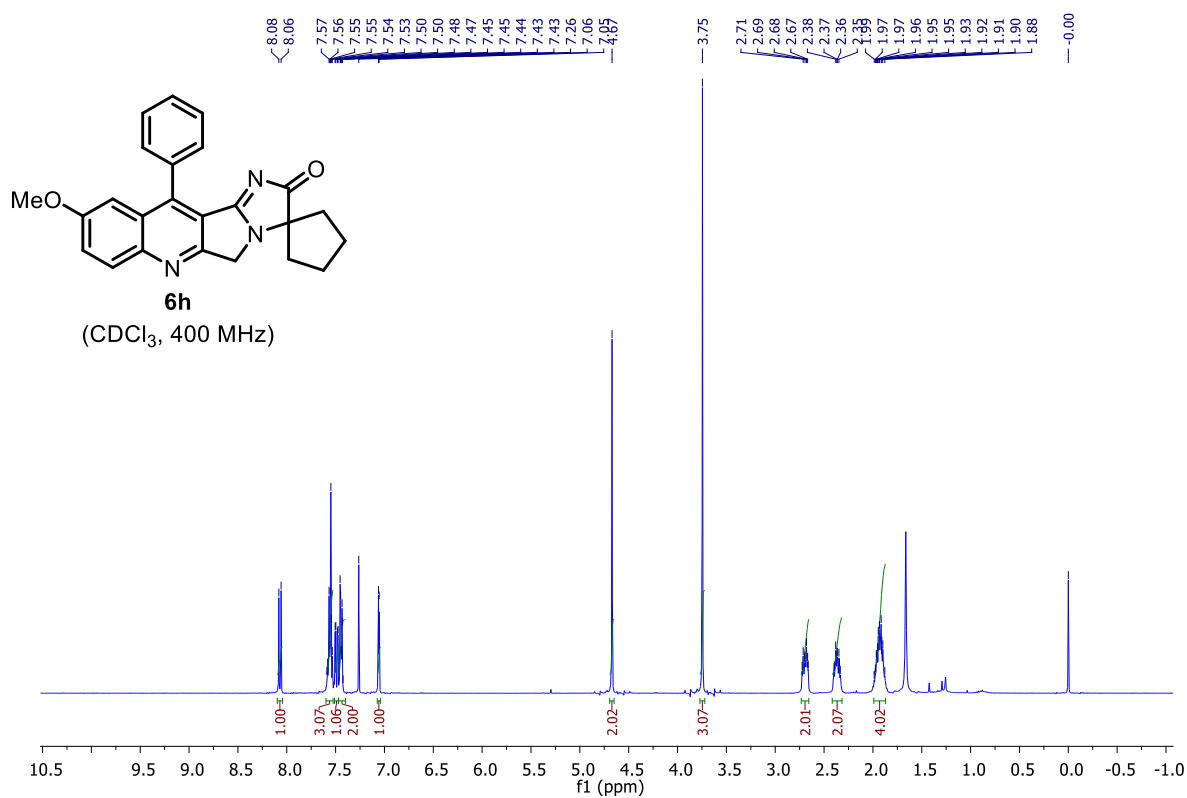


Figure S34: ^{13}C NMR of compound **6h**

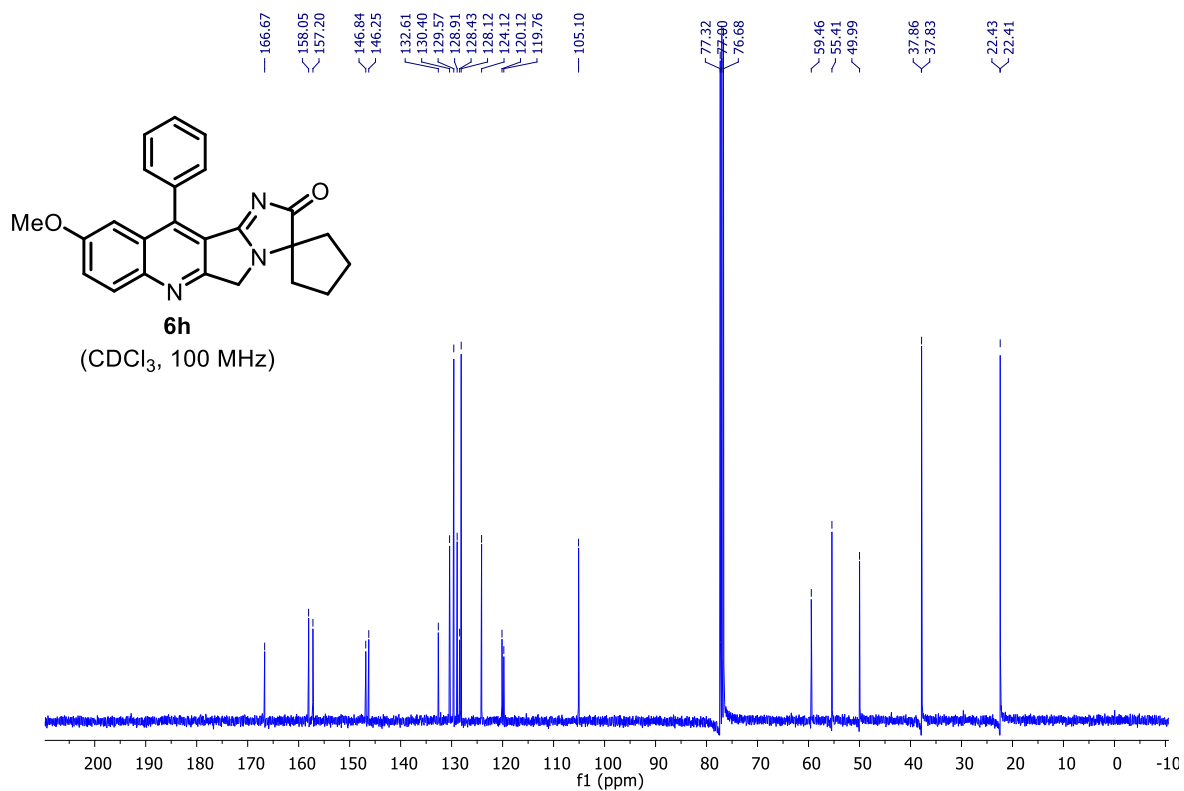


Figure S35: ^1H NMR of compound **6i**

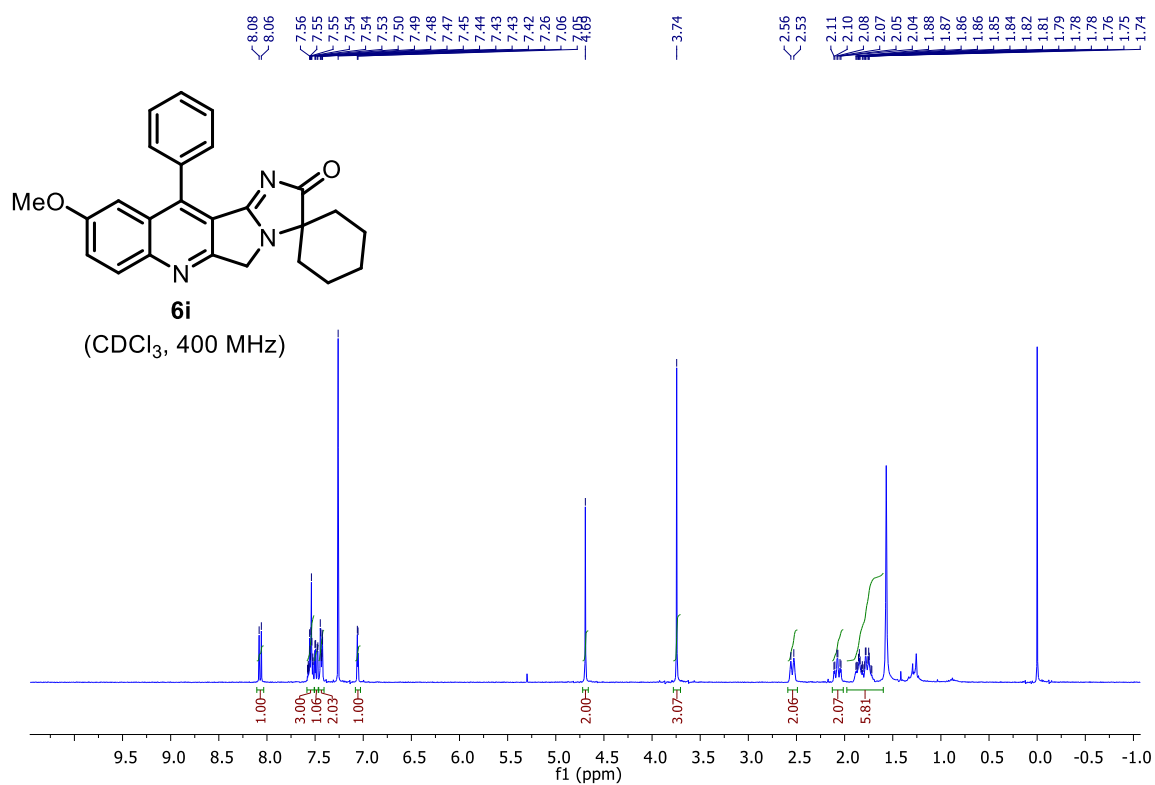


Figure S36: ^{13}C NMR of compound **6i**

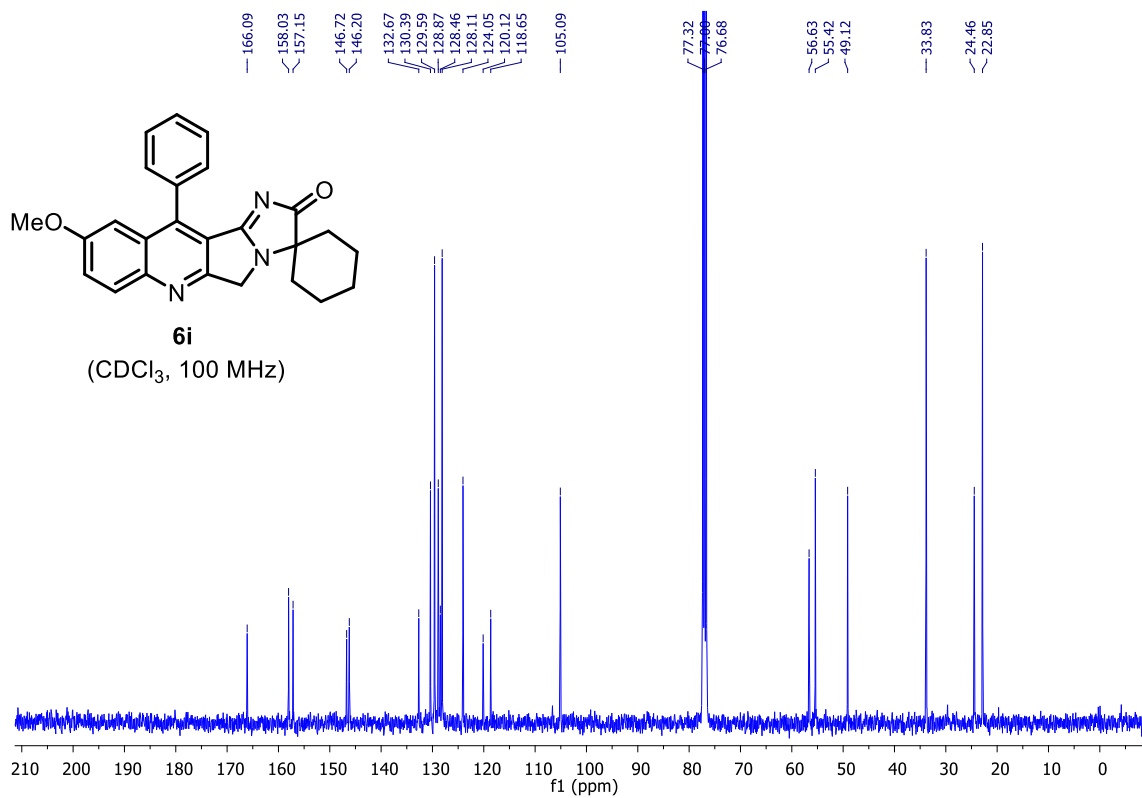


Figure S37: ¹H NMR of compound 7a

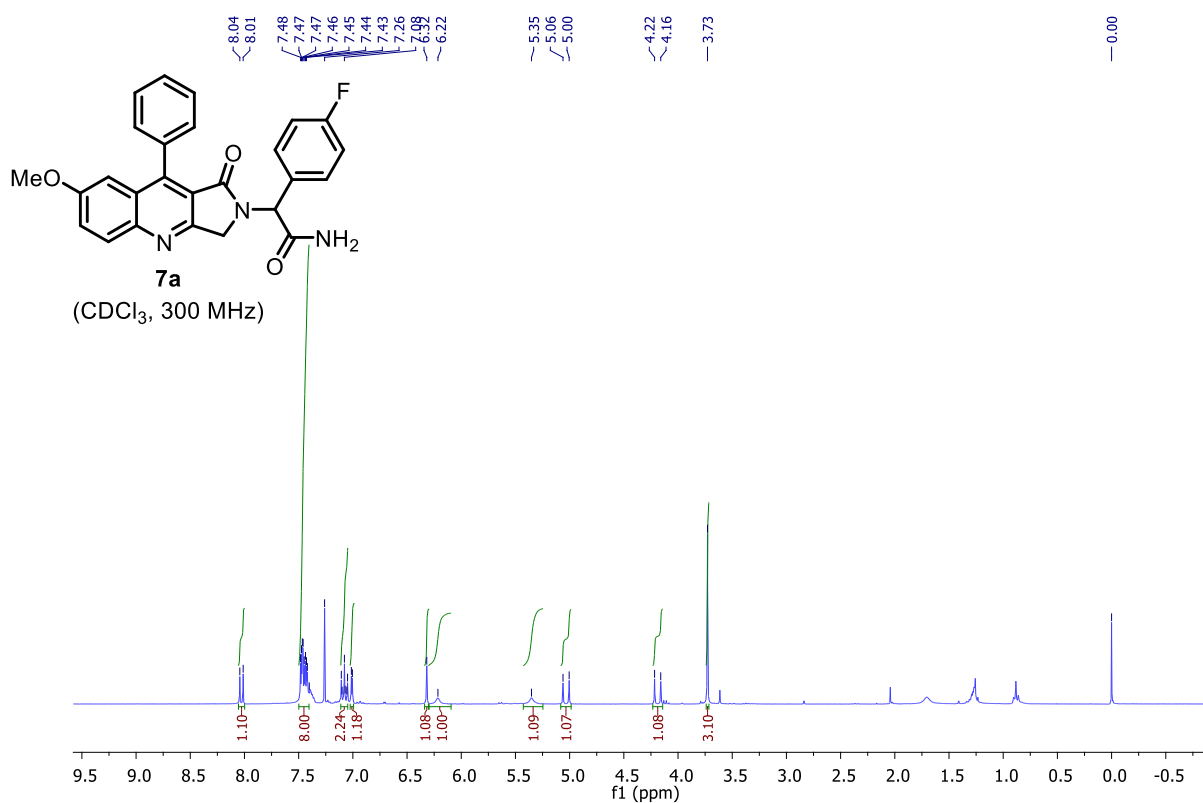


Figure S38: ¹³C NMR of compound 7a

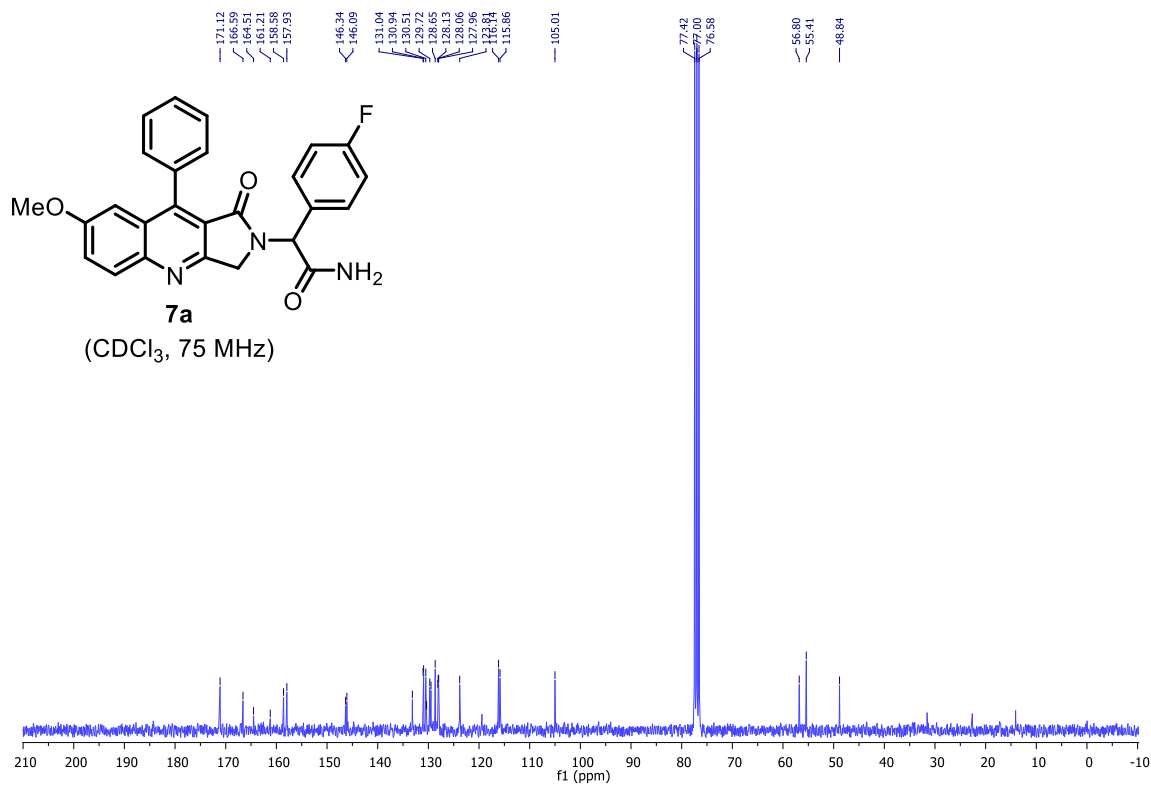


Figure S39: ^{19}F NMR of compound **7a**

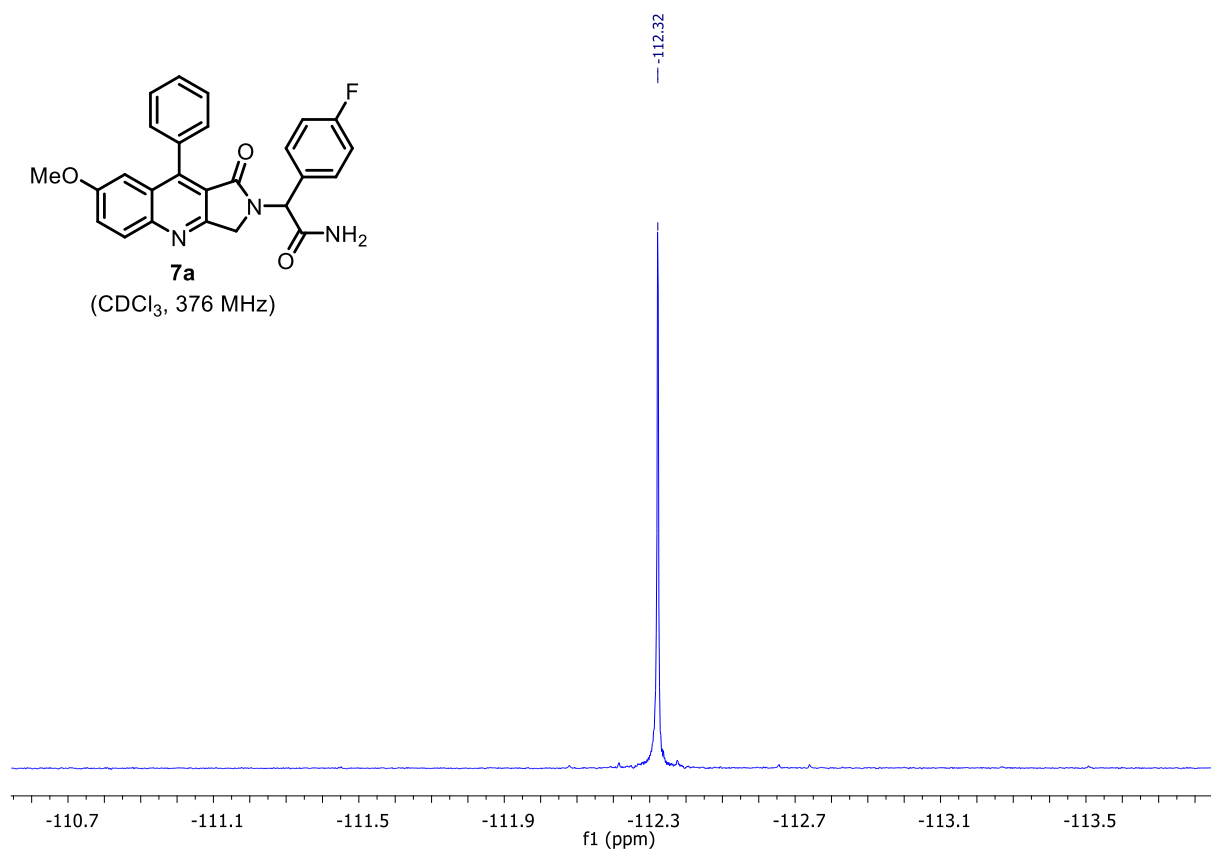


Figure S40: ^1H NMR of compound **7b**

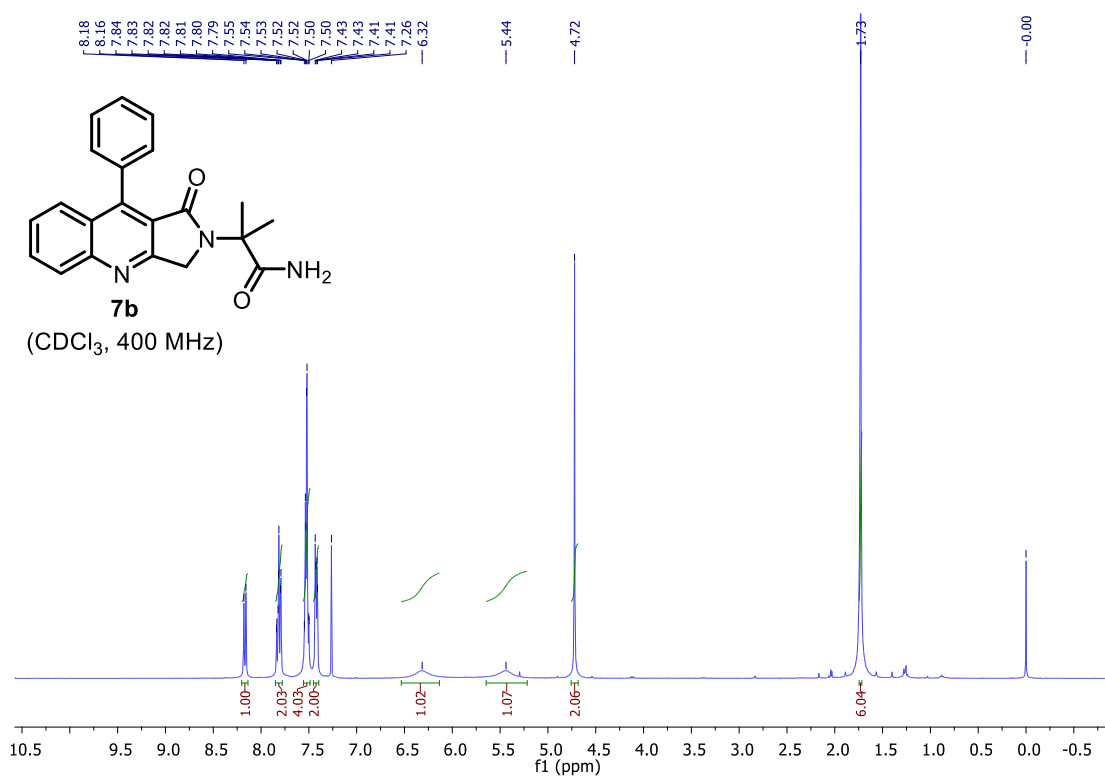


Figure S41: ^{13}C NMR of compound **7b**

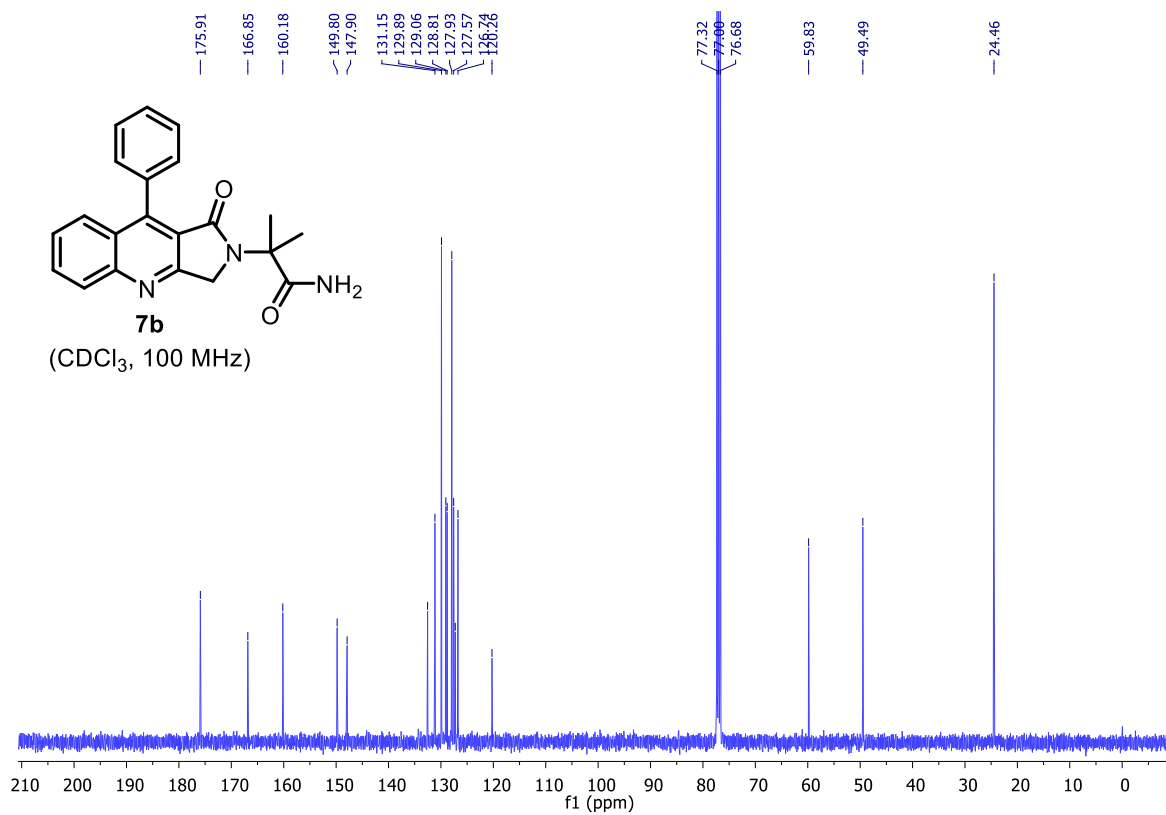


Figure S42: ^1H NMR of compound **7c**

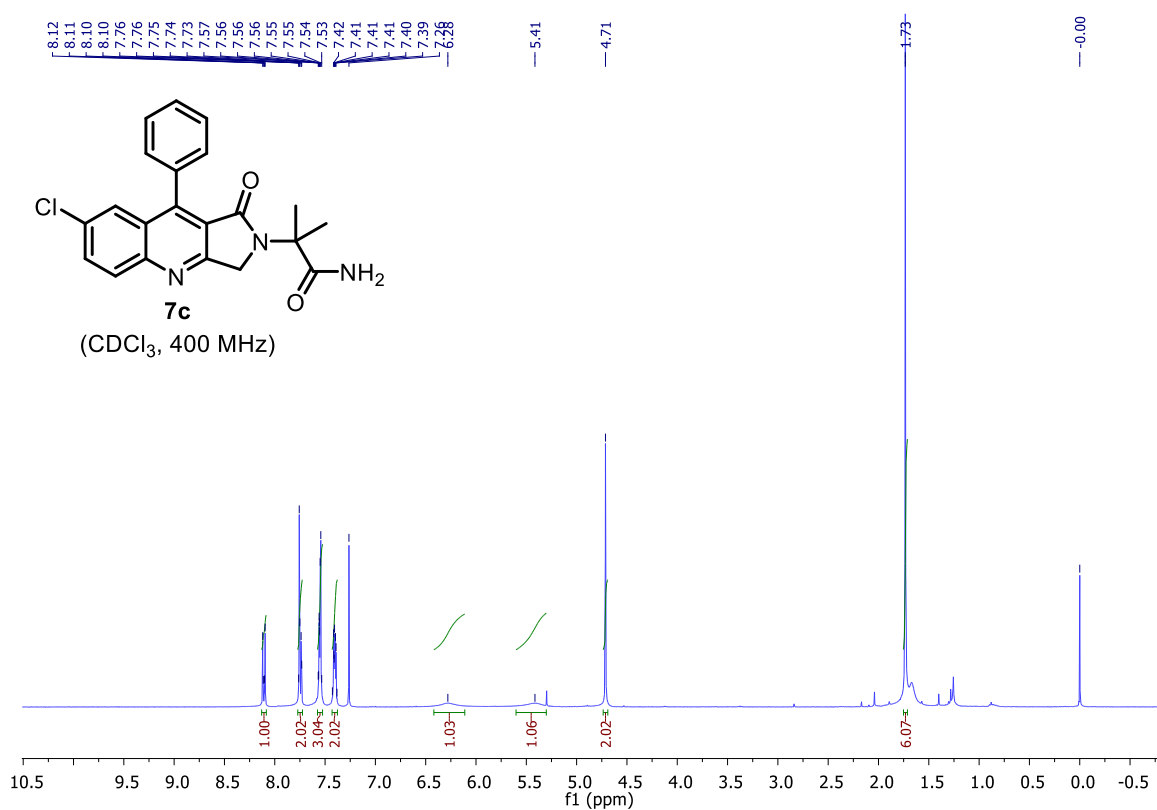


Figure S43: ^{13}C NMR of compound **7c**

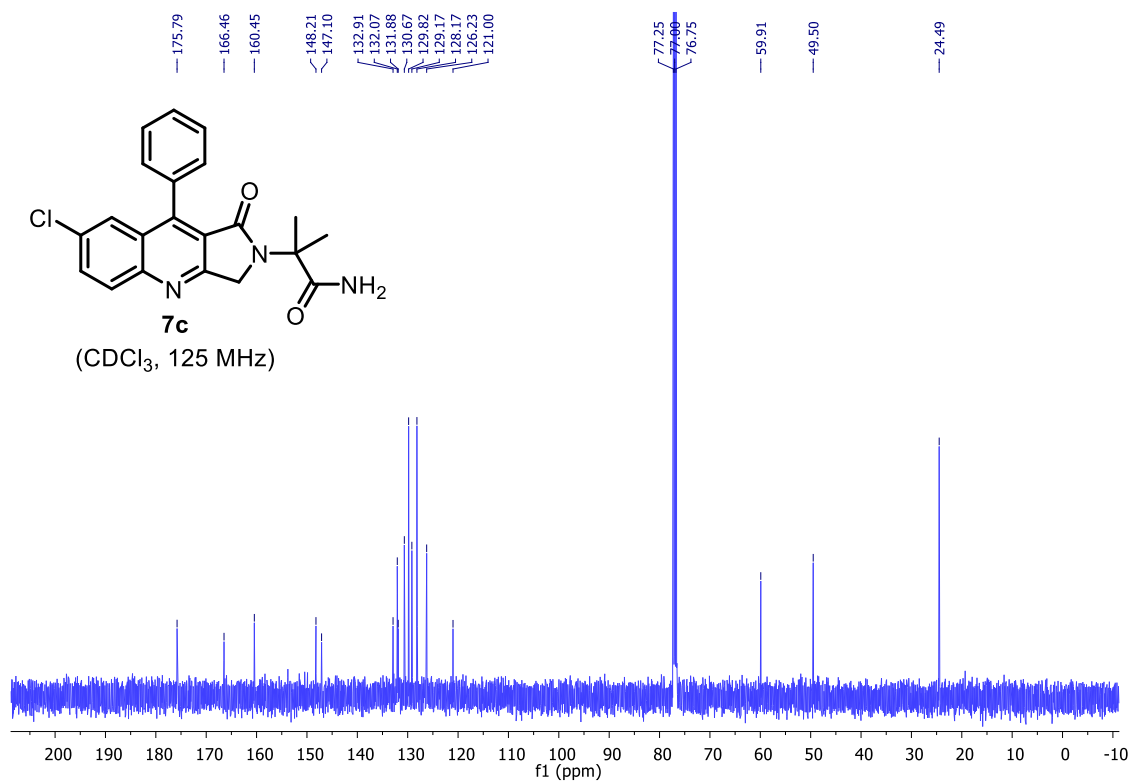


Figure S44: ^1H NMR of compound **8a**

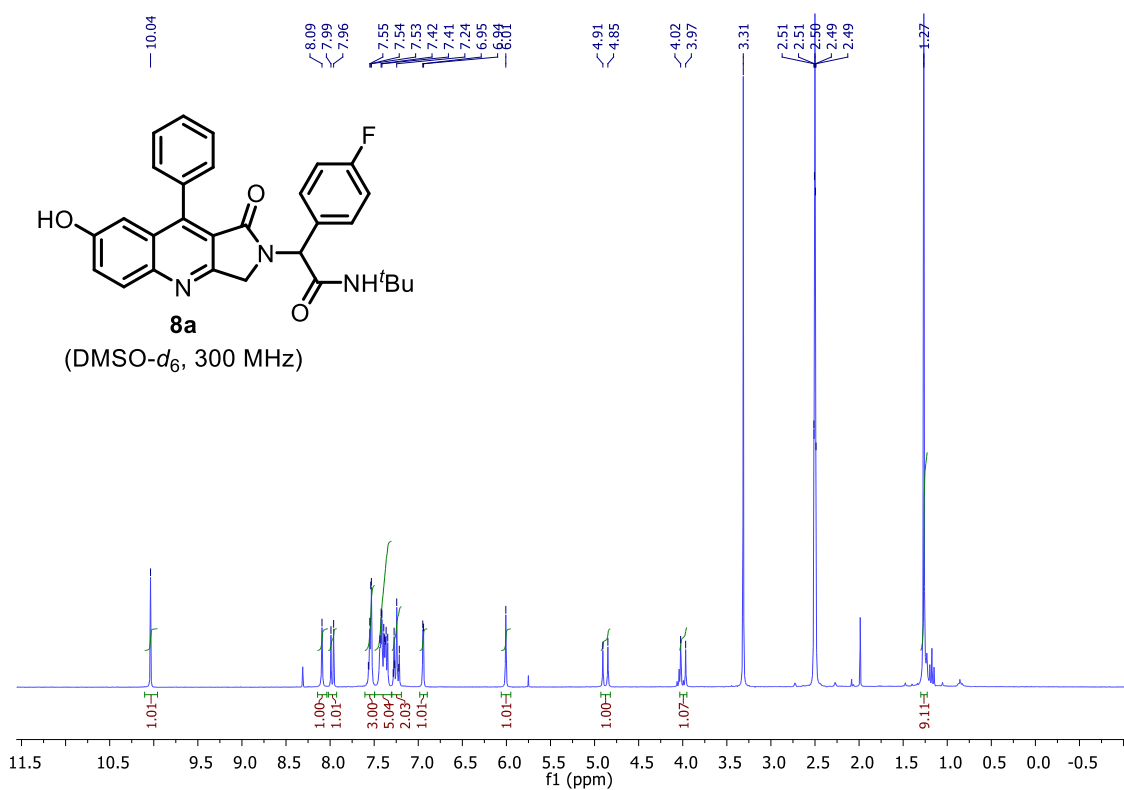


Figure S45: ^{13}C NMR of compound **8a**

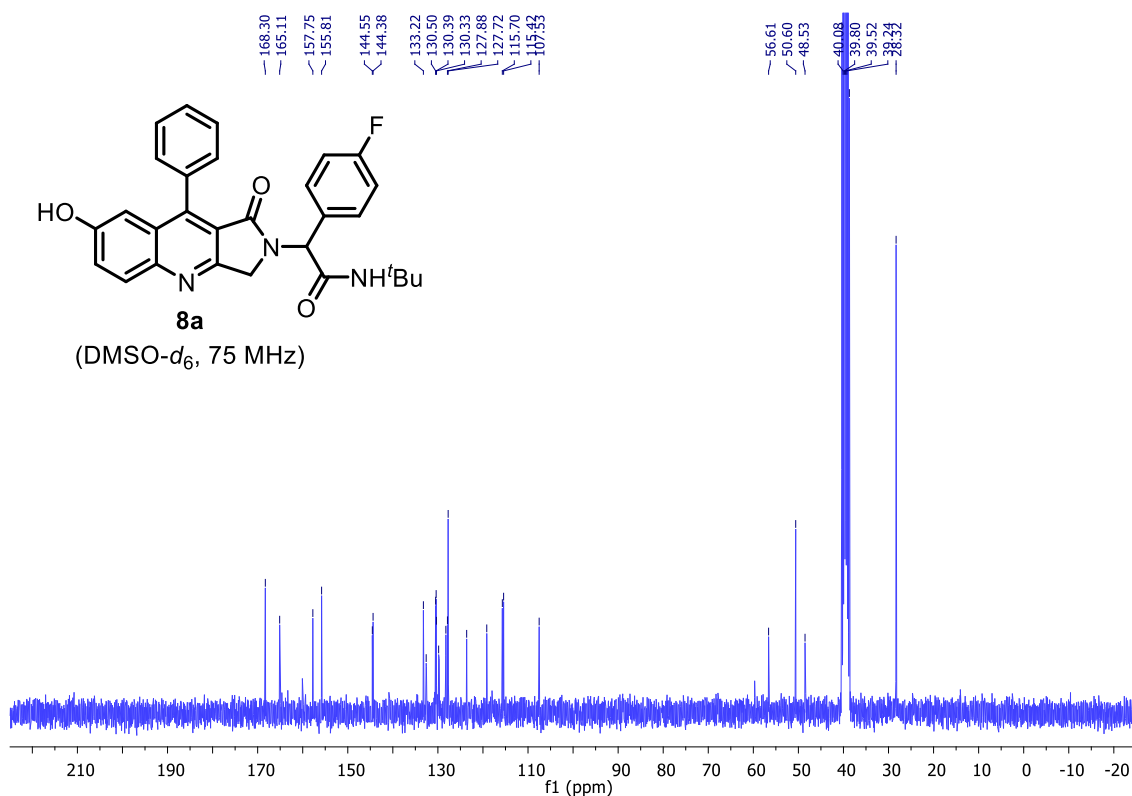


Figure S46: ^{19}F NMR of compound **8a**

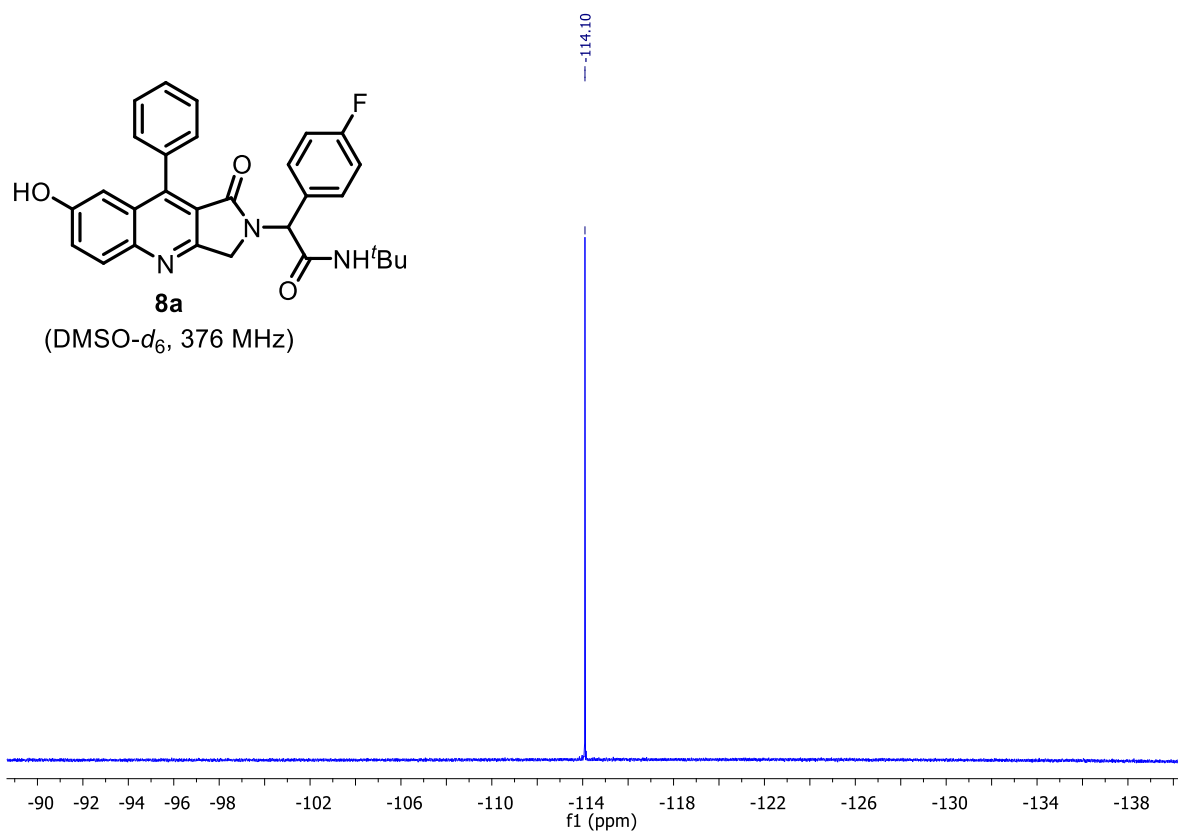


Figure S47: ^1H NMR of compound **8b**

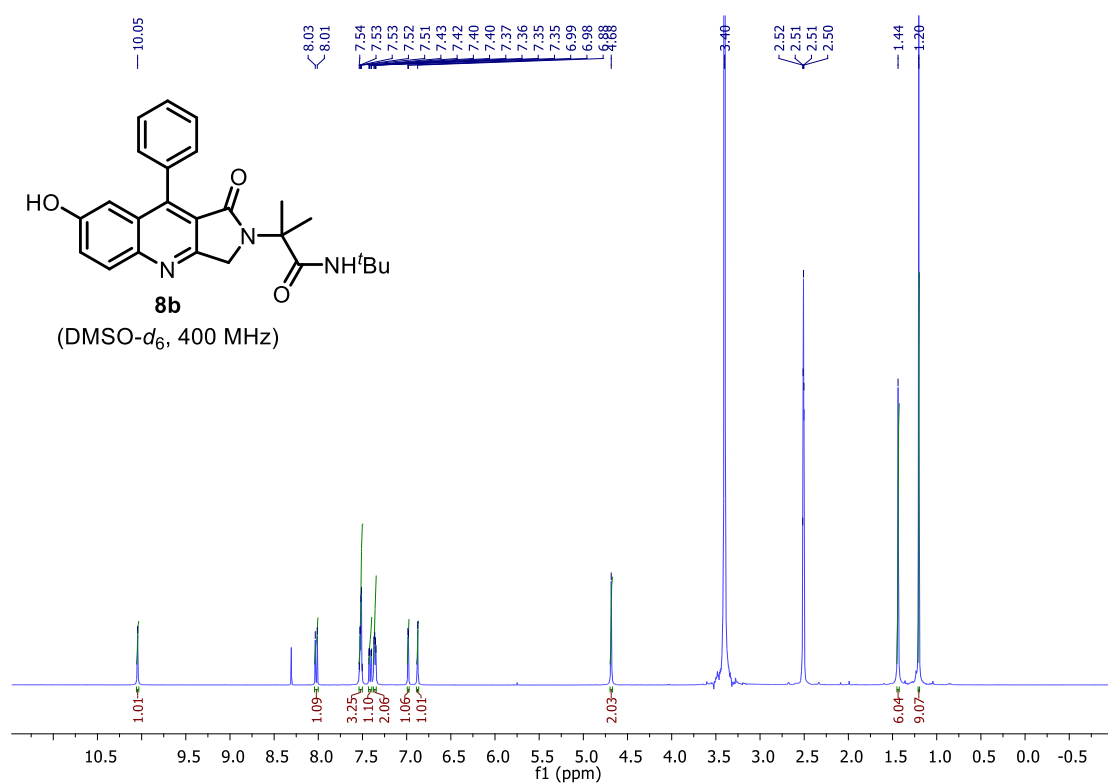
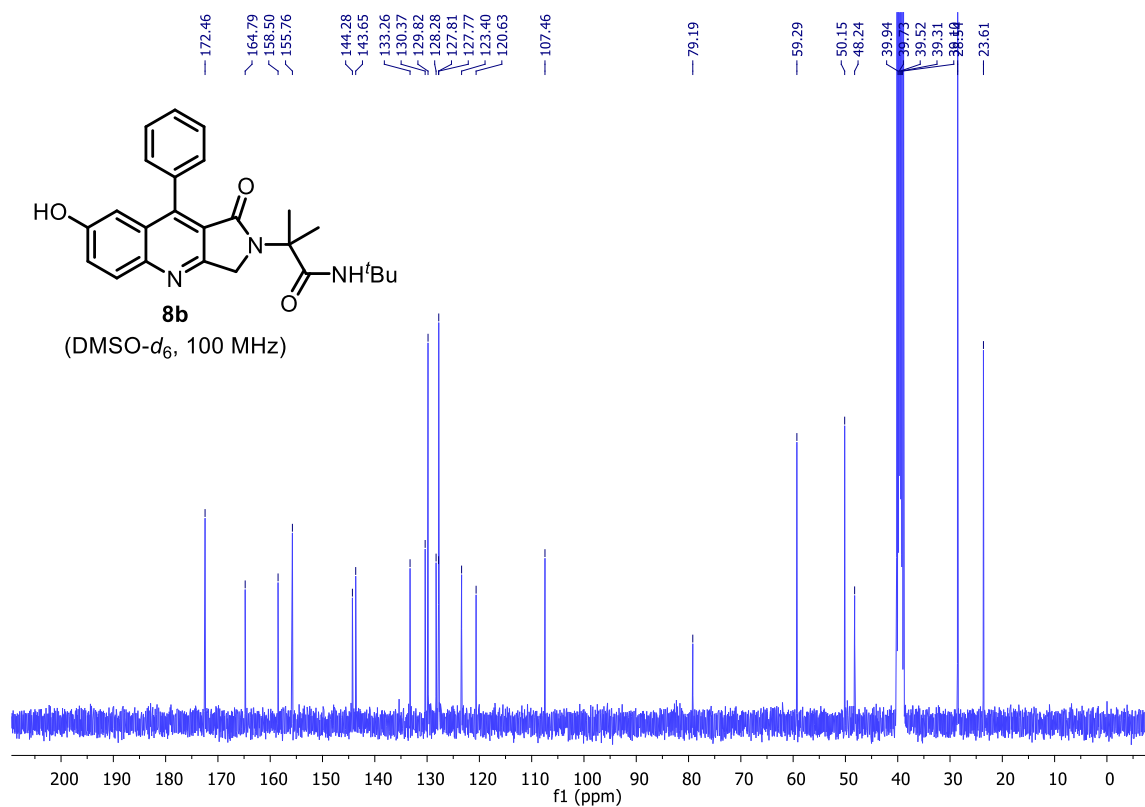


Figure S48: ^{13}C NMR of compound **8b**



➤ **HRMS Spectra:**

Figure S49: HRMS Spectrum of compound 5a

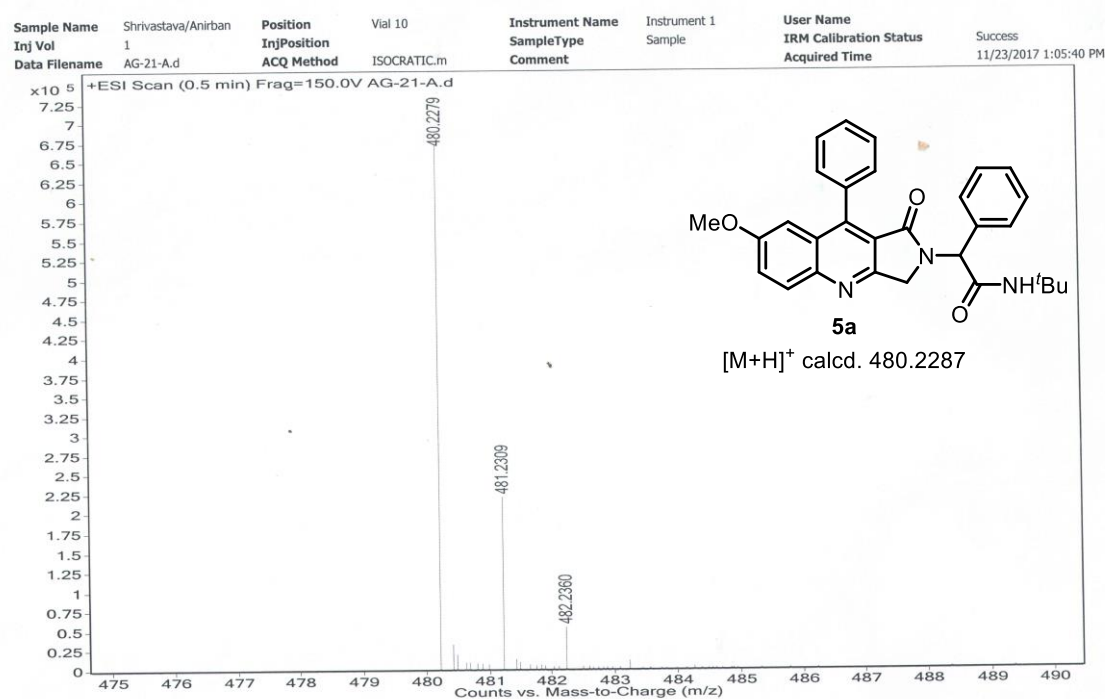


Figure S50: HRMS Spectrum of compound 5e

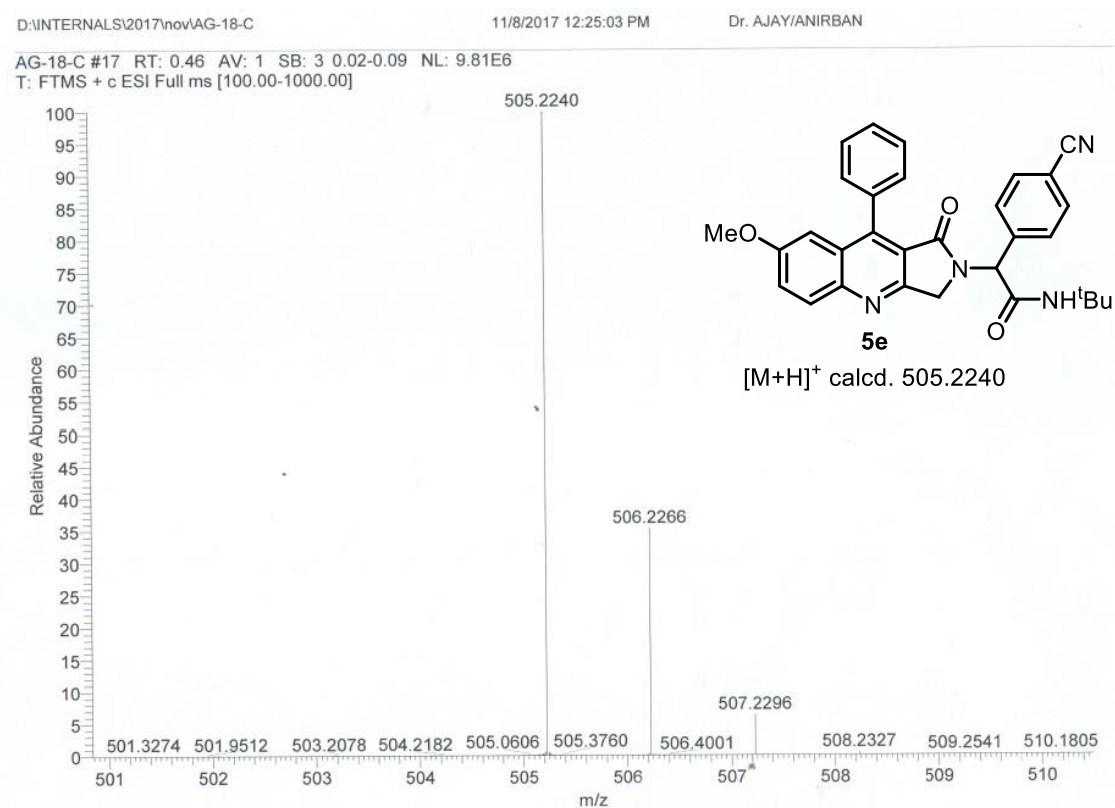


Figure S51: HRMS Spectrum of compound 5i

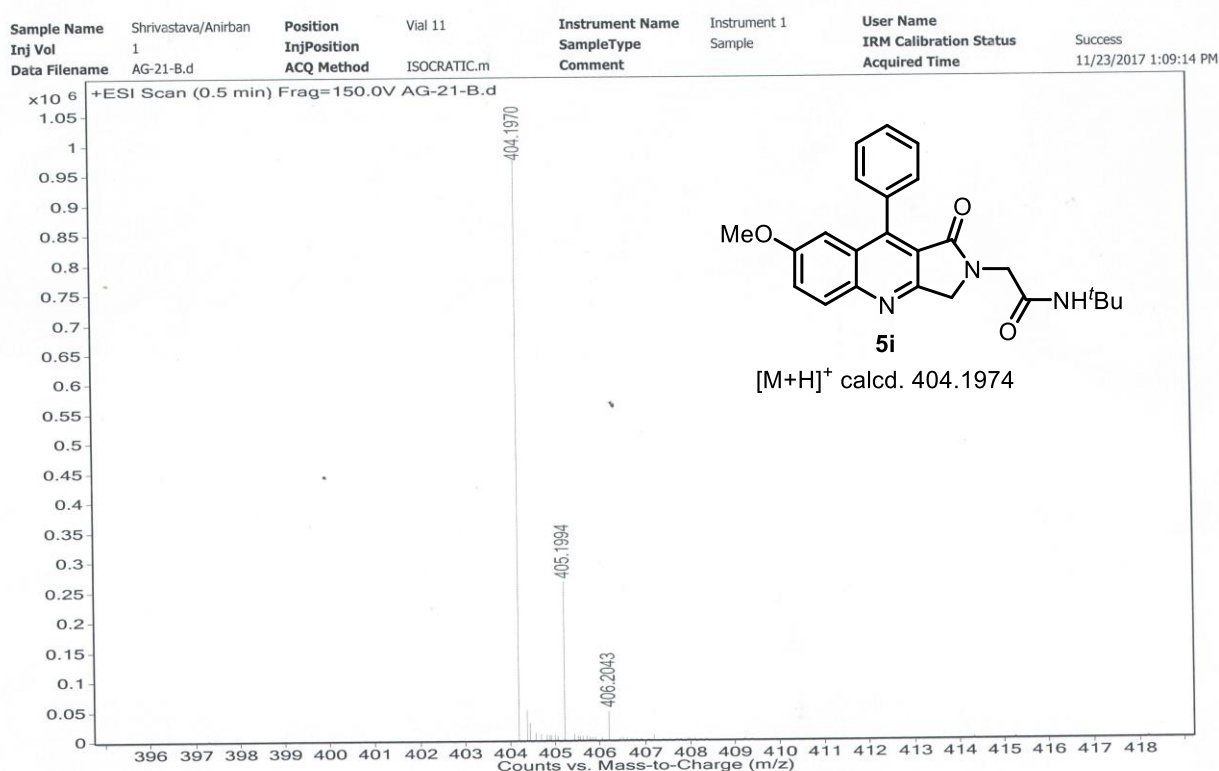


Figure S52: HRMS Spectrum of compound 5m

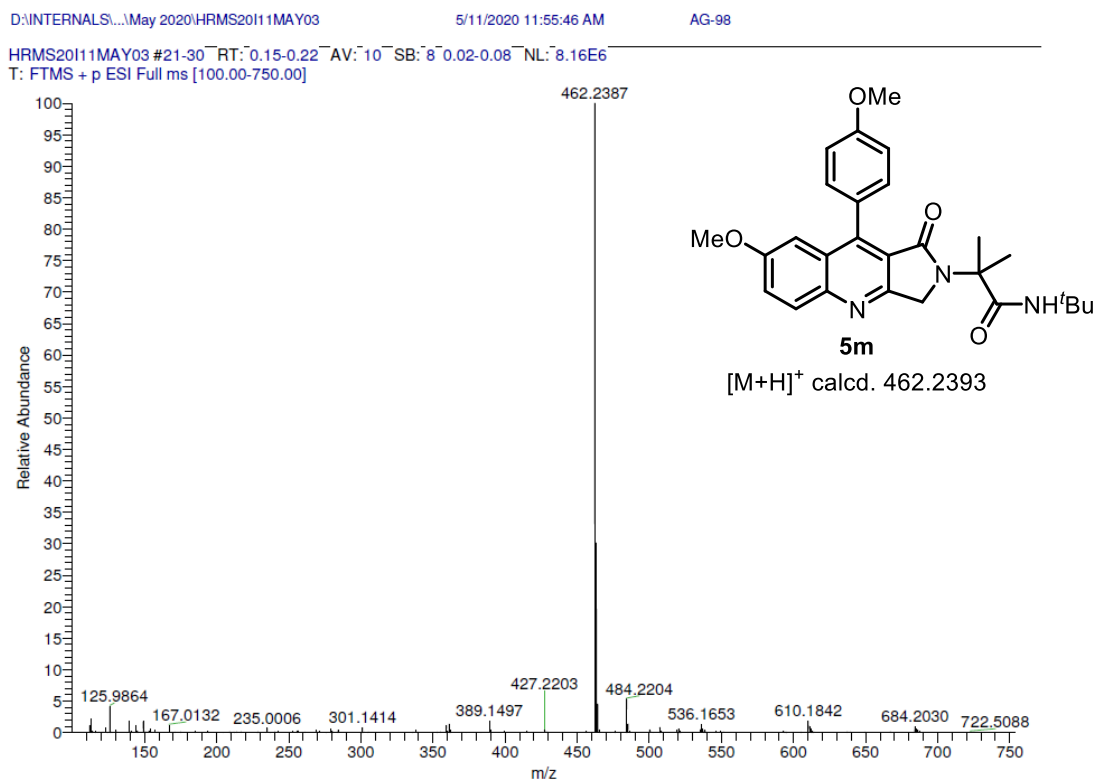


Figure S53: HRMS Spectrum of compound 5n

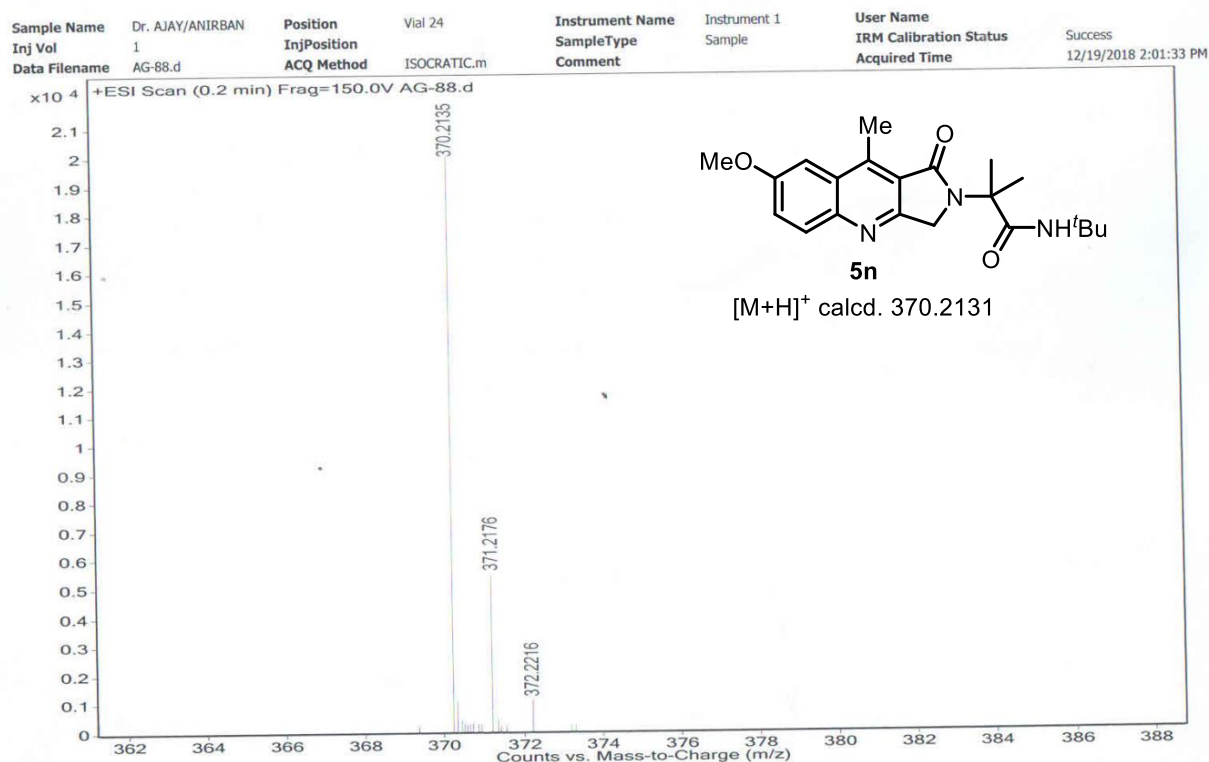


Figure S54: HRMS Spectrum of compound 5o

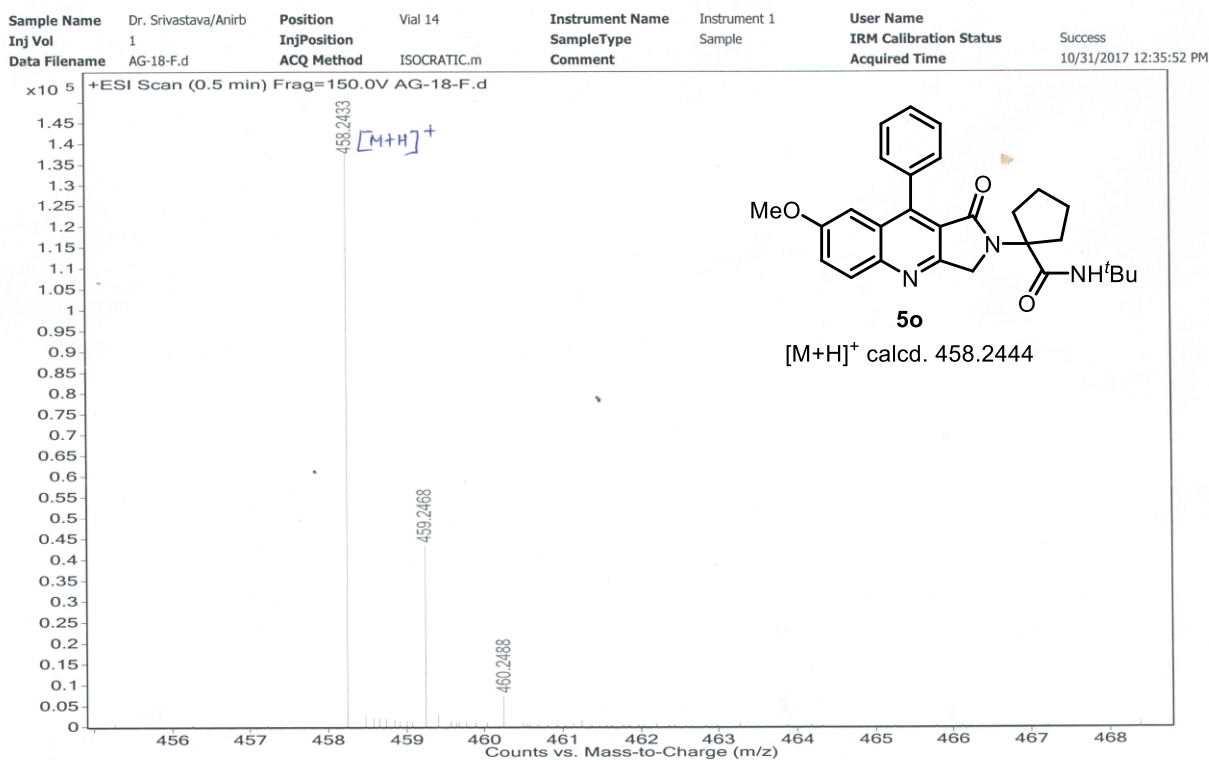


Figure S55: HRMS Spectrum of compound 5p

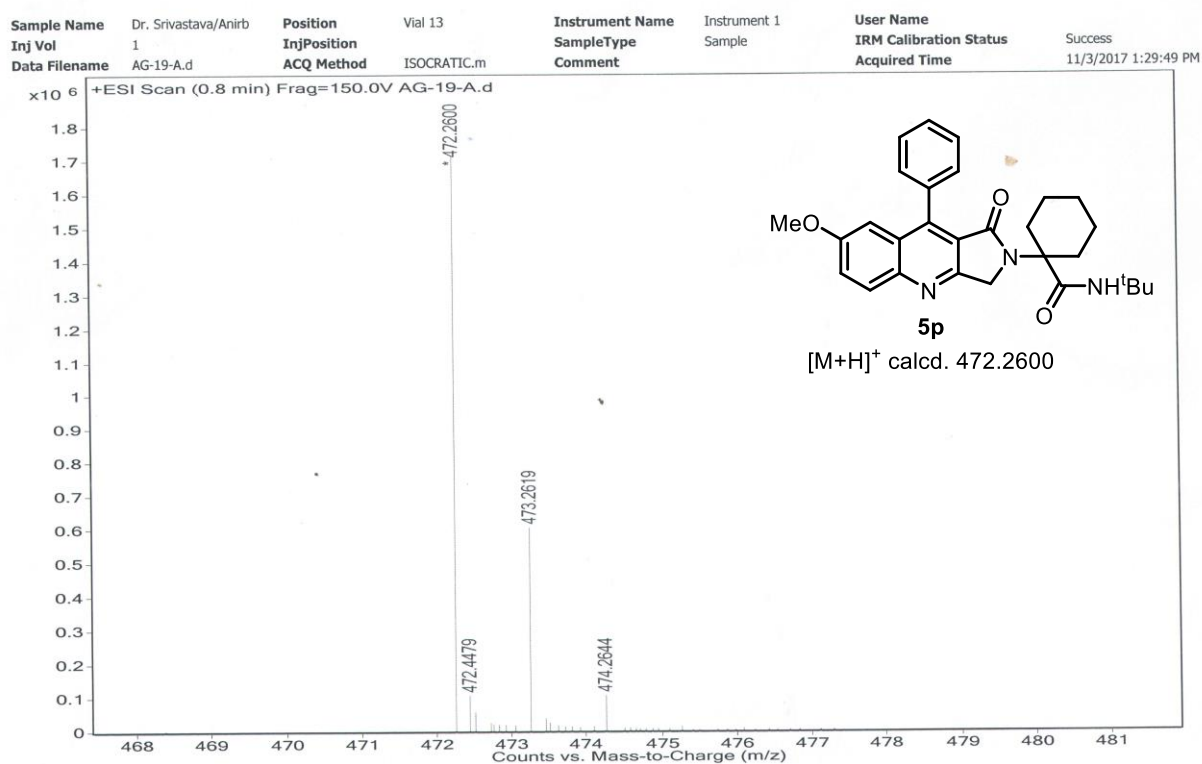


Figure S56: HRMS Spectrum of compound 5q

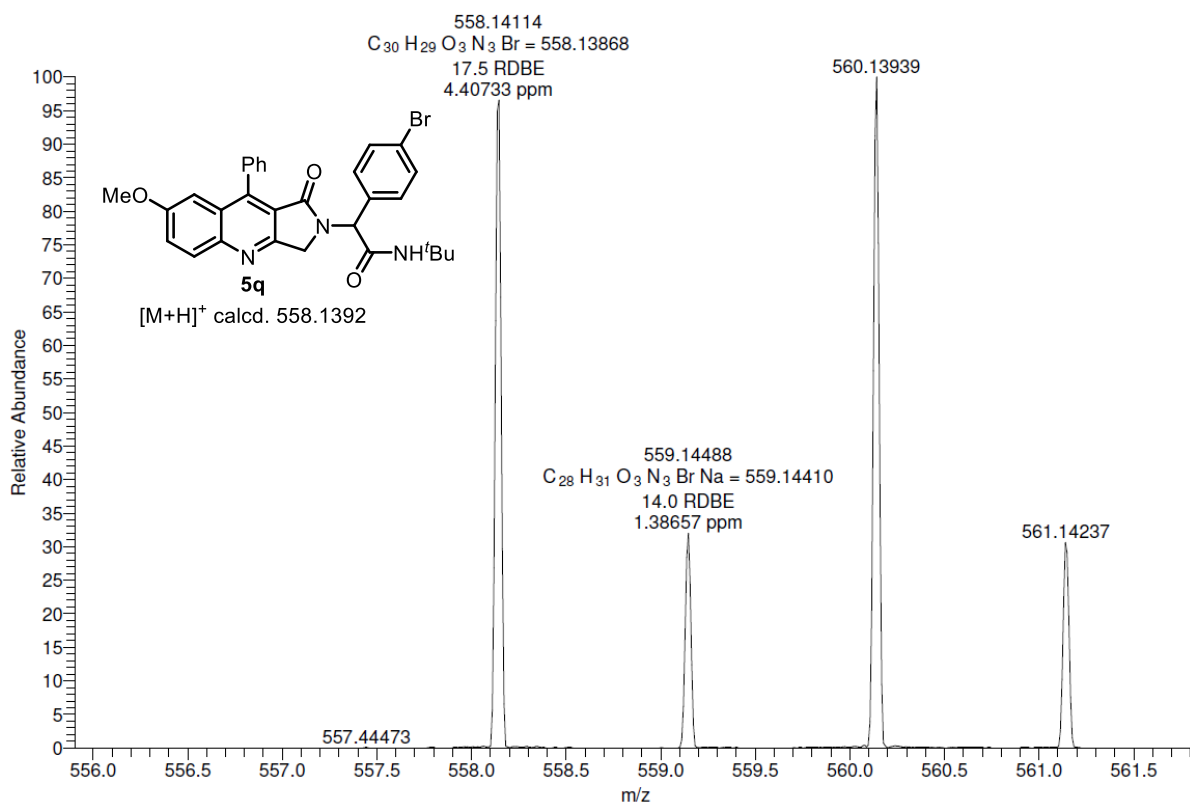


Figure S57: HRMS Spectrum of compound 6a

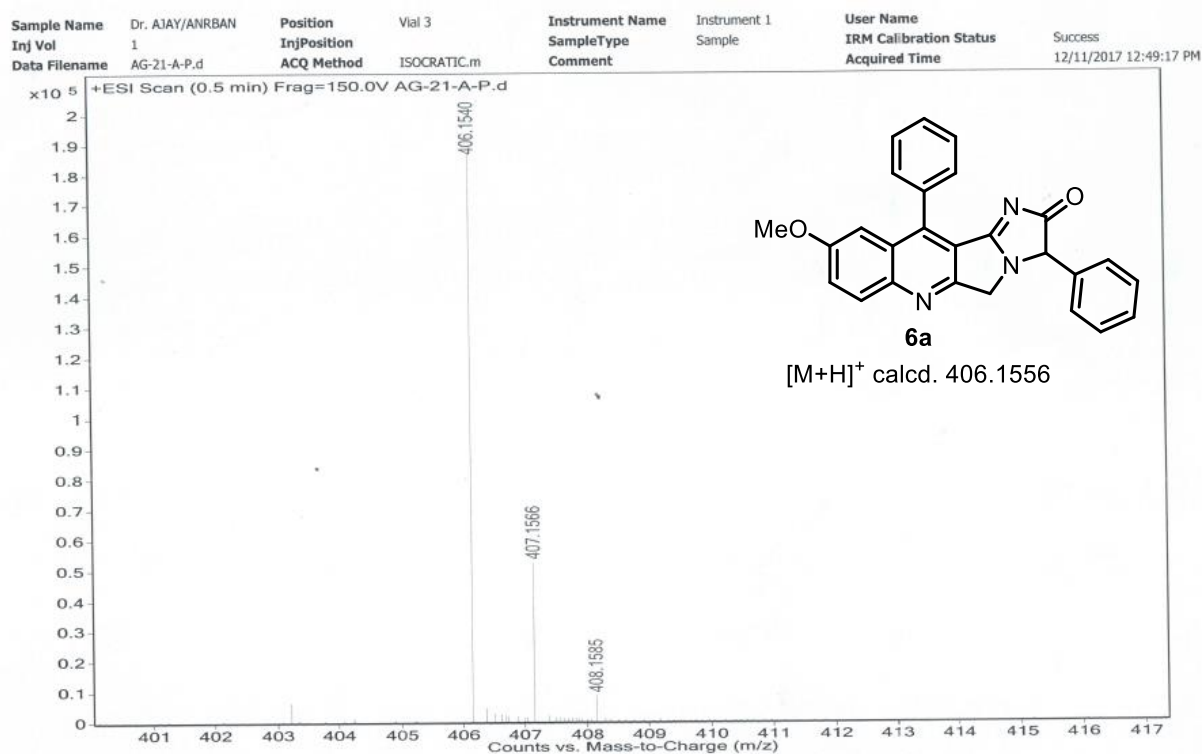


Figure S58: HRMS Spectrum of compound 6b

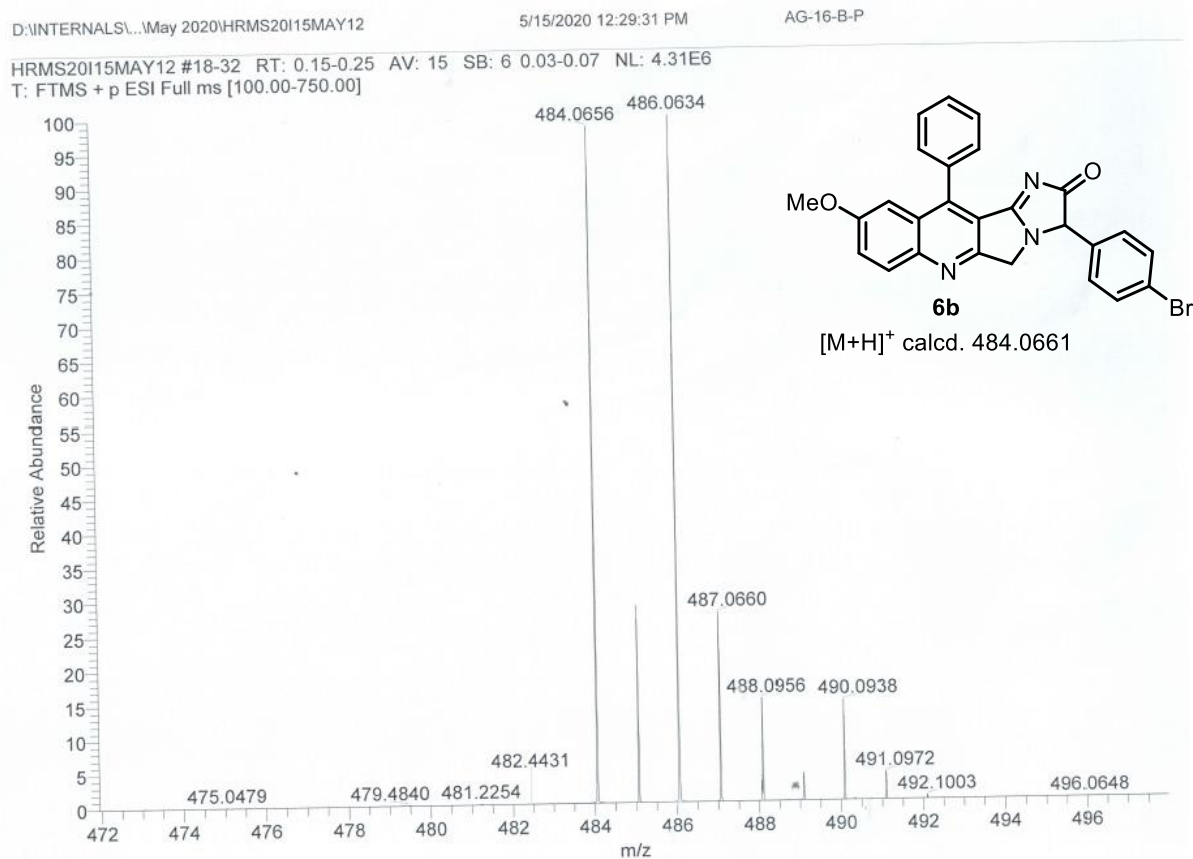


Figure S59: HRMS Spectrum of compound 6c

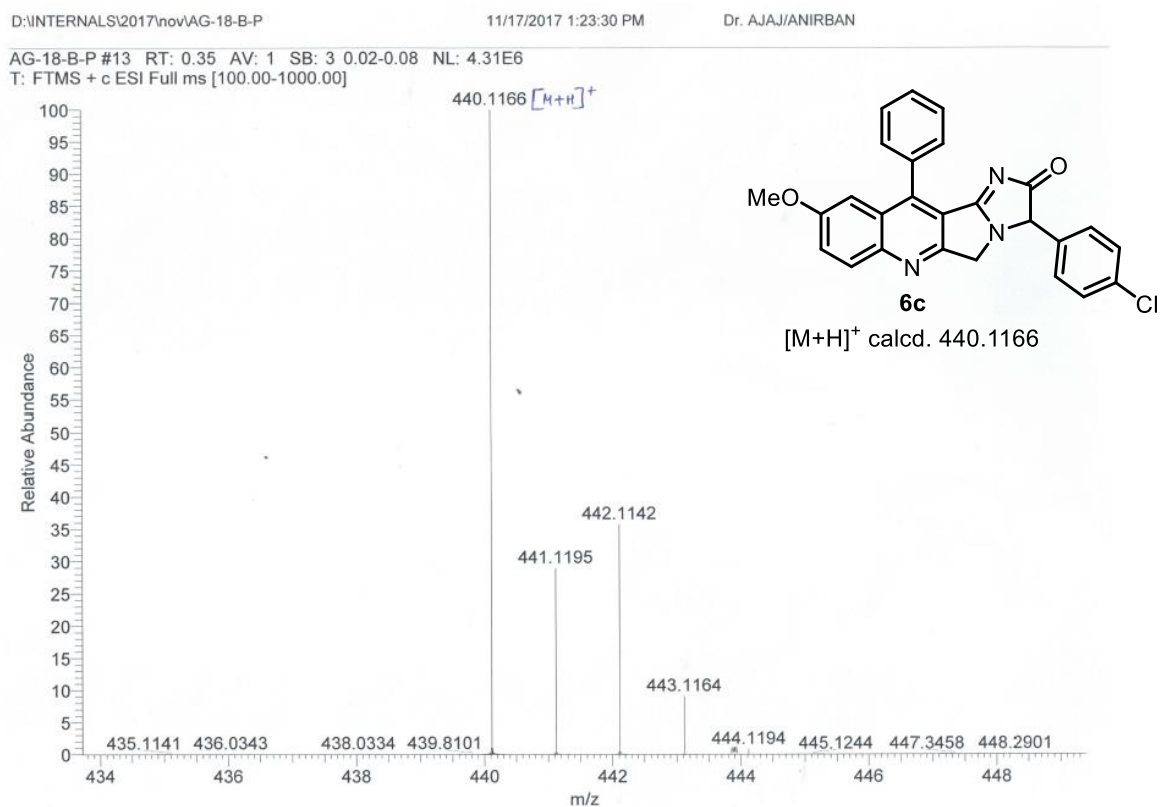


Figure S60: HRMS Spectrum of compound 6d

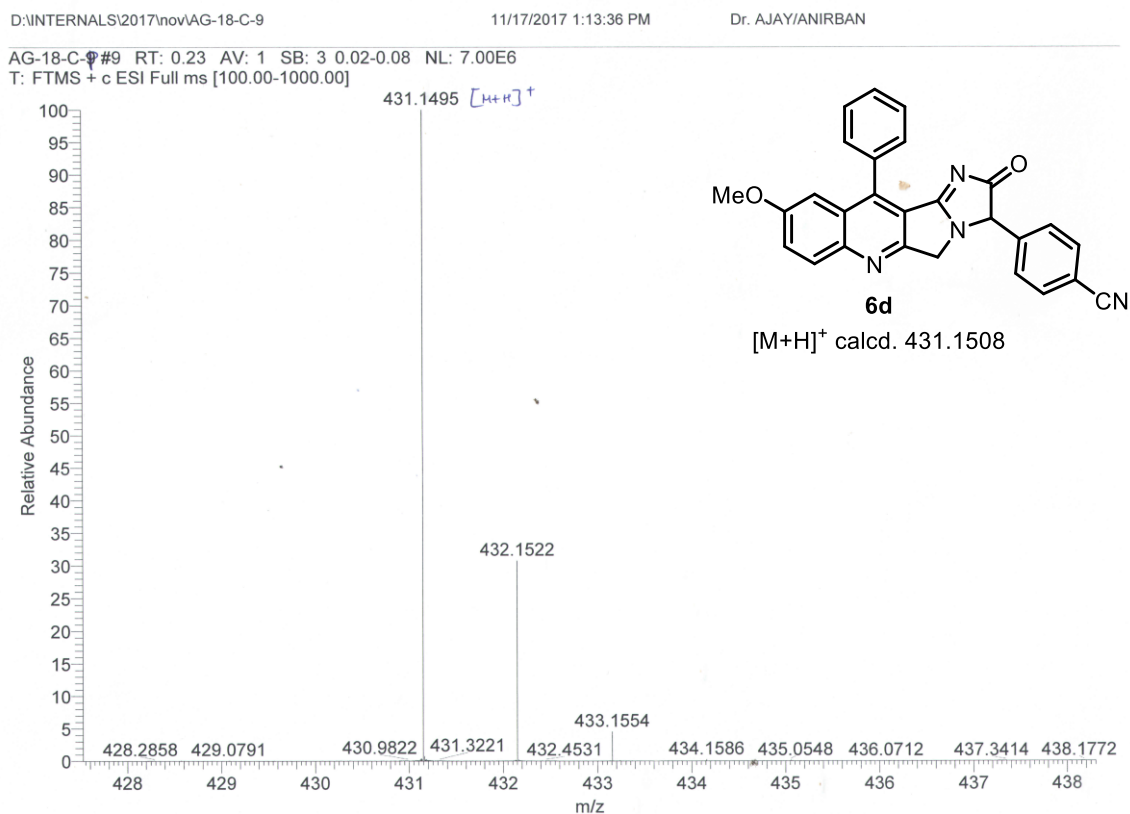


Figure S61: HRMS Spectrum of compound 6e

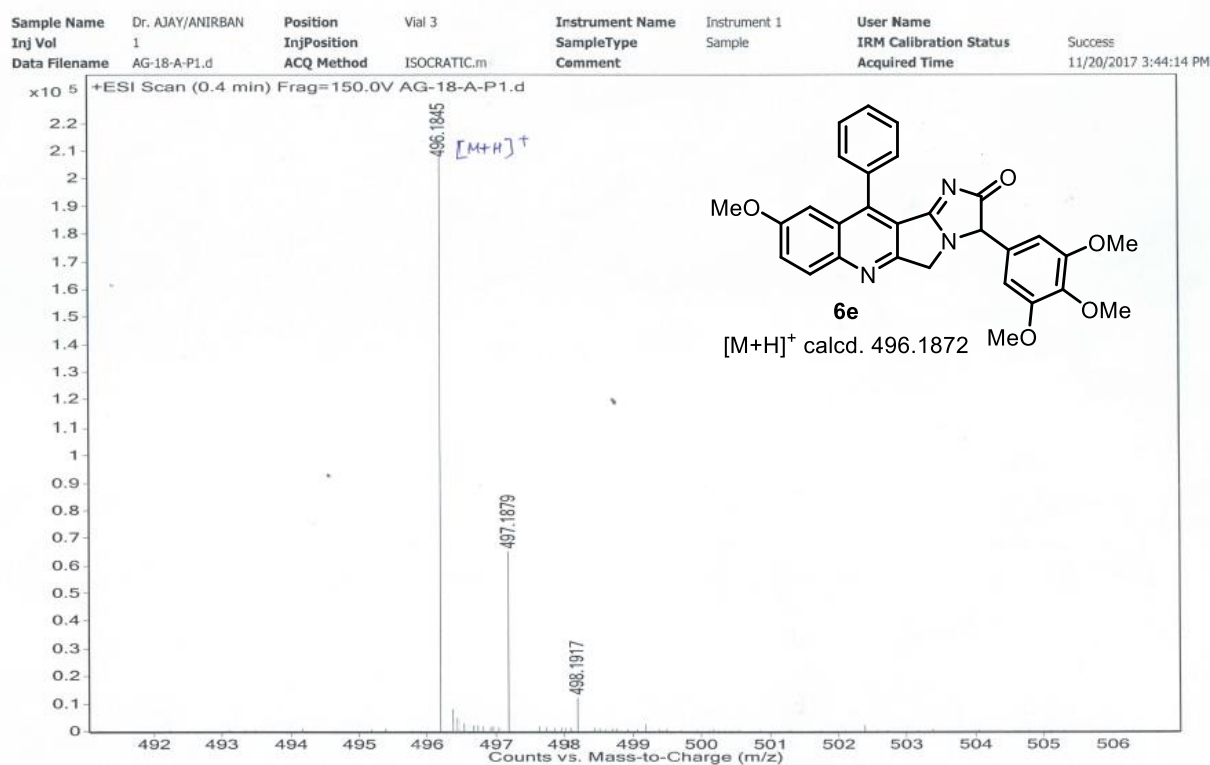


Figure S62: HRMS Spectrum of compound 6f

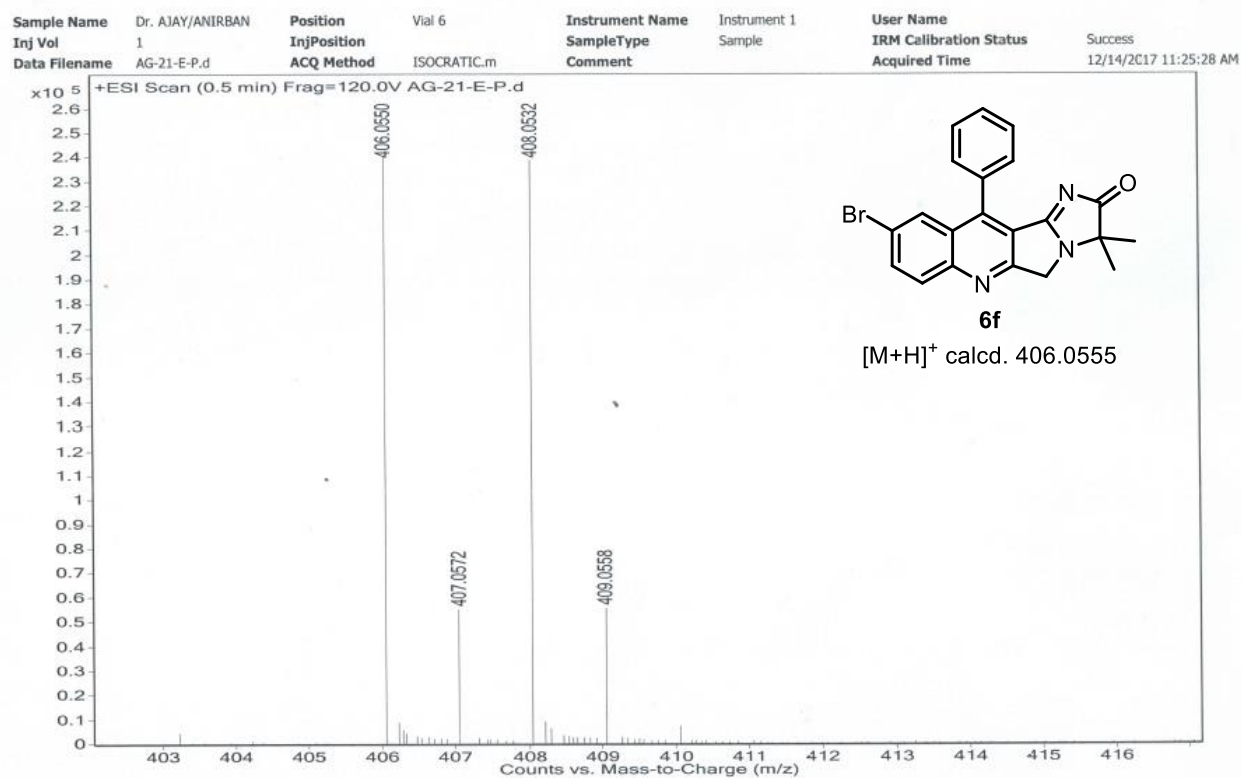


Figure S63: HRMS Spectrum of compound 6g

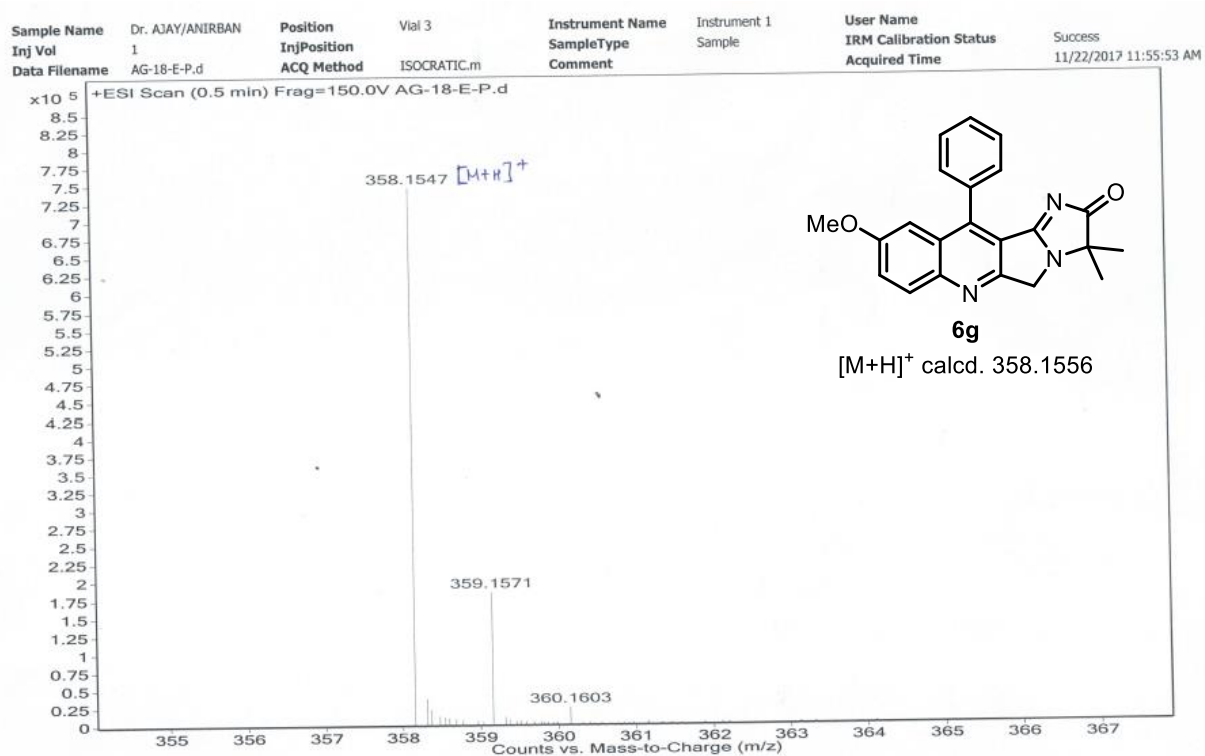


Figure S64: HRMS Spectrum of compound 6h

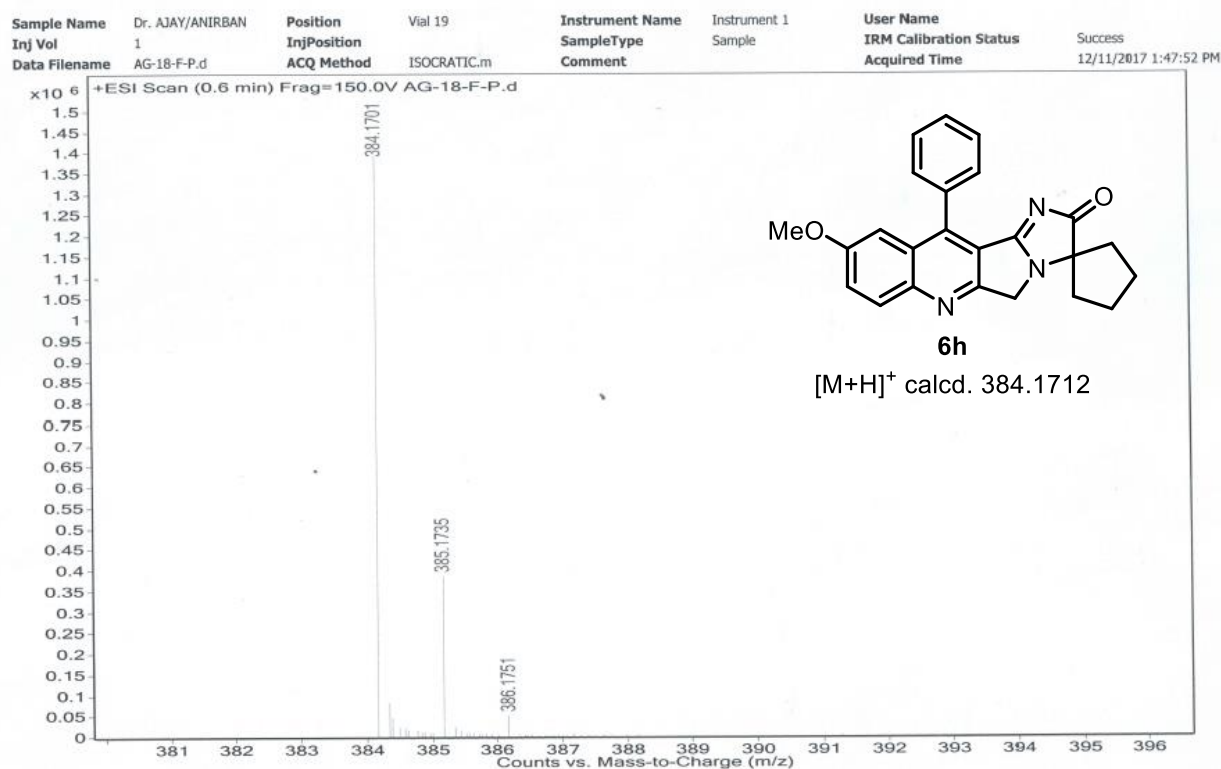


Figure S65: HRMS Spectrum of compound 6i

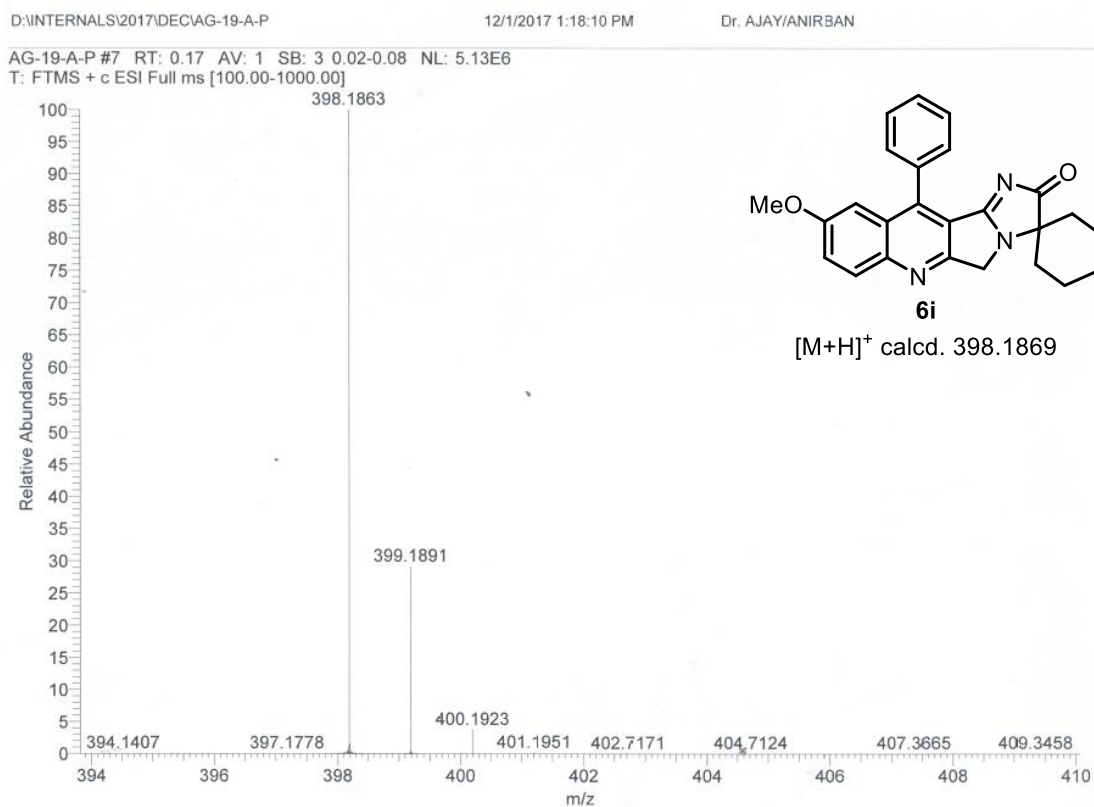


Figure S66: HRMS Spectrum of compound 7a

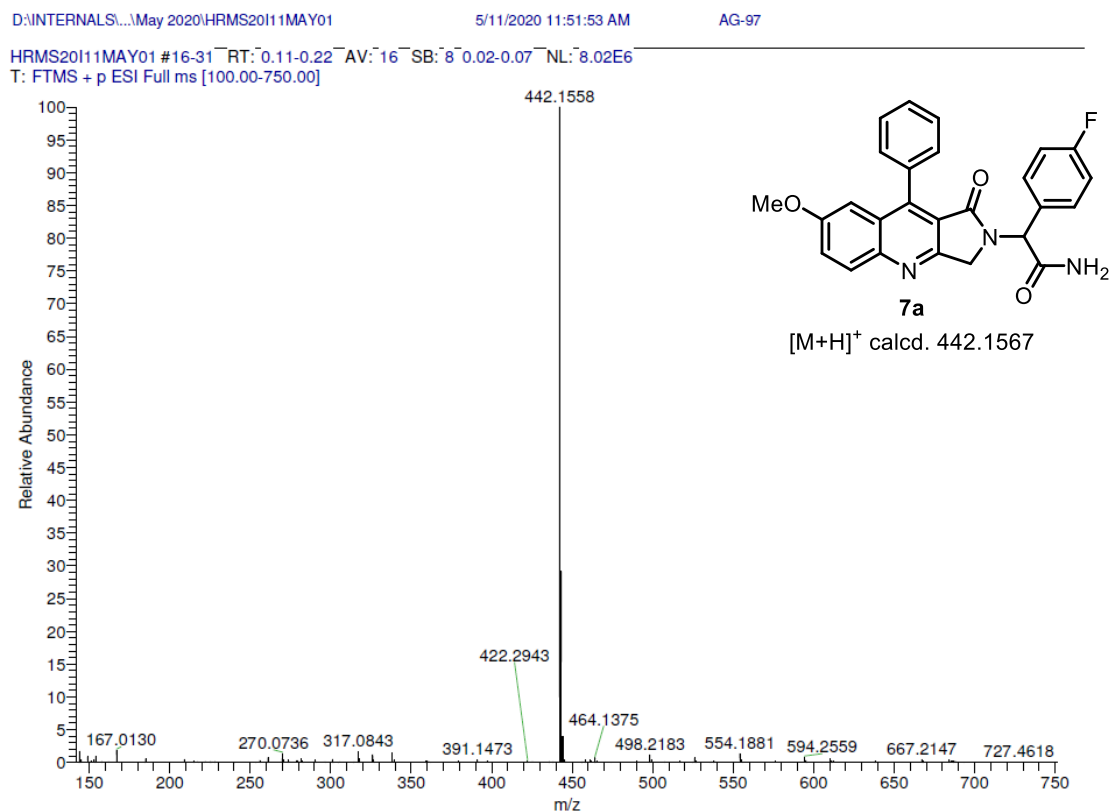


Figure S67: HRMS Spectrum of compound 7b

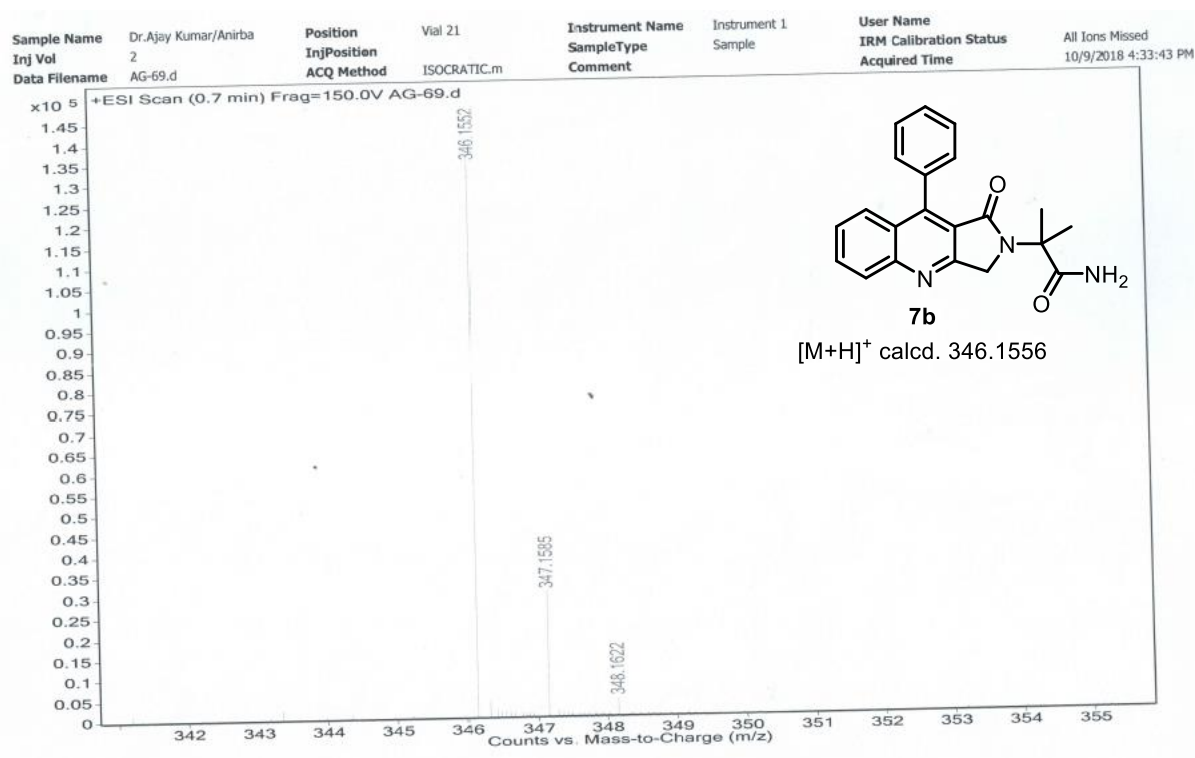


Figure S68: HRMS Spectrum of compound 7c

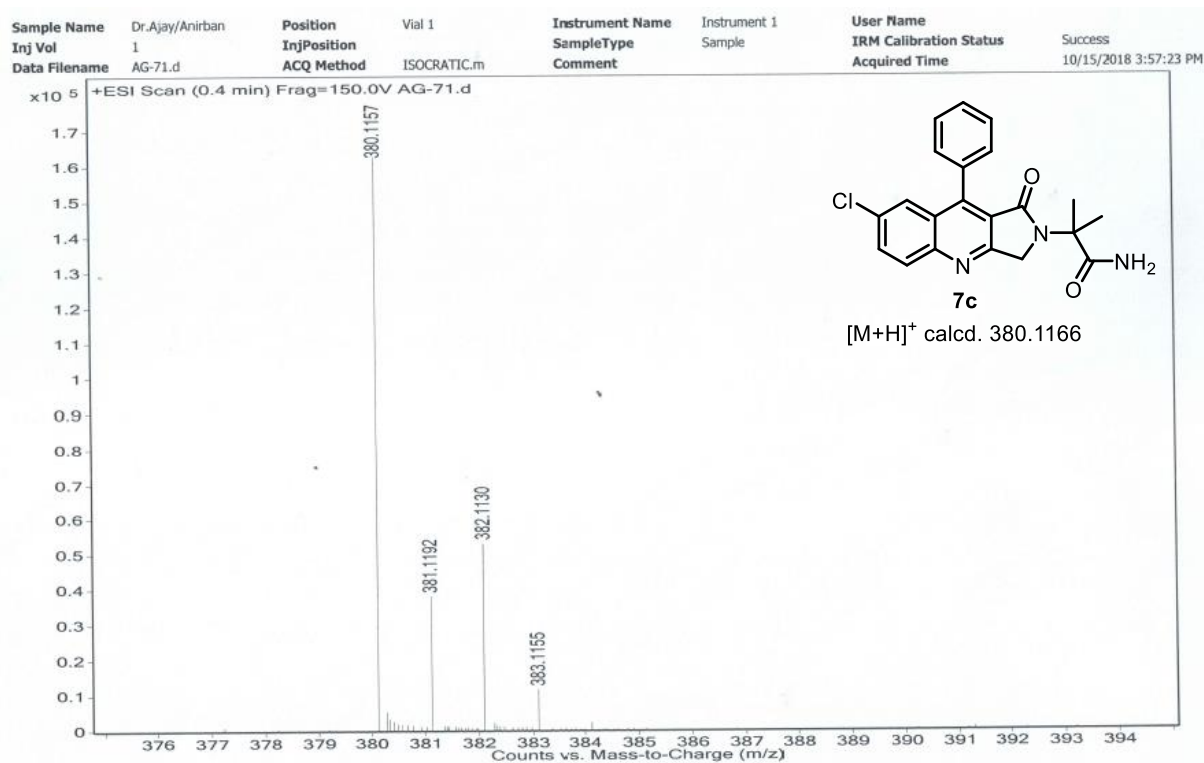


Figure S69: HRMS Spectrum of compound **8a**

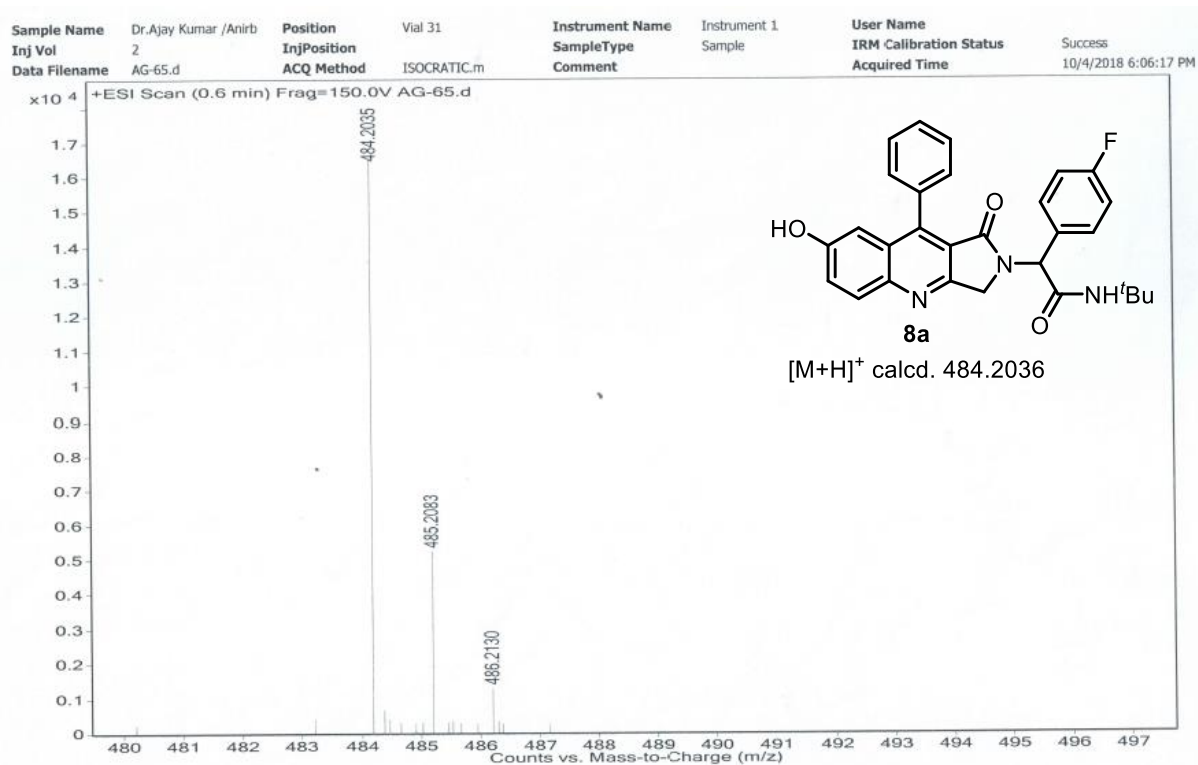
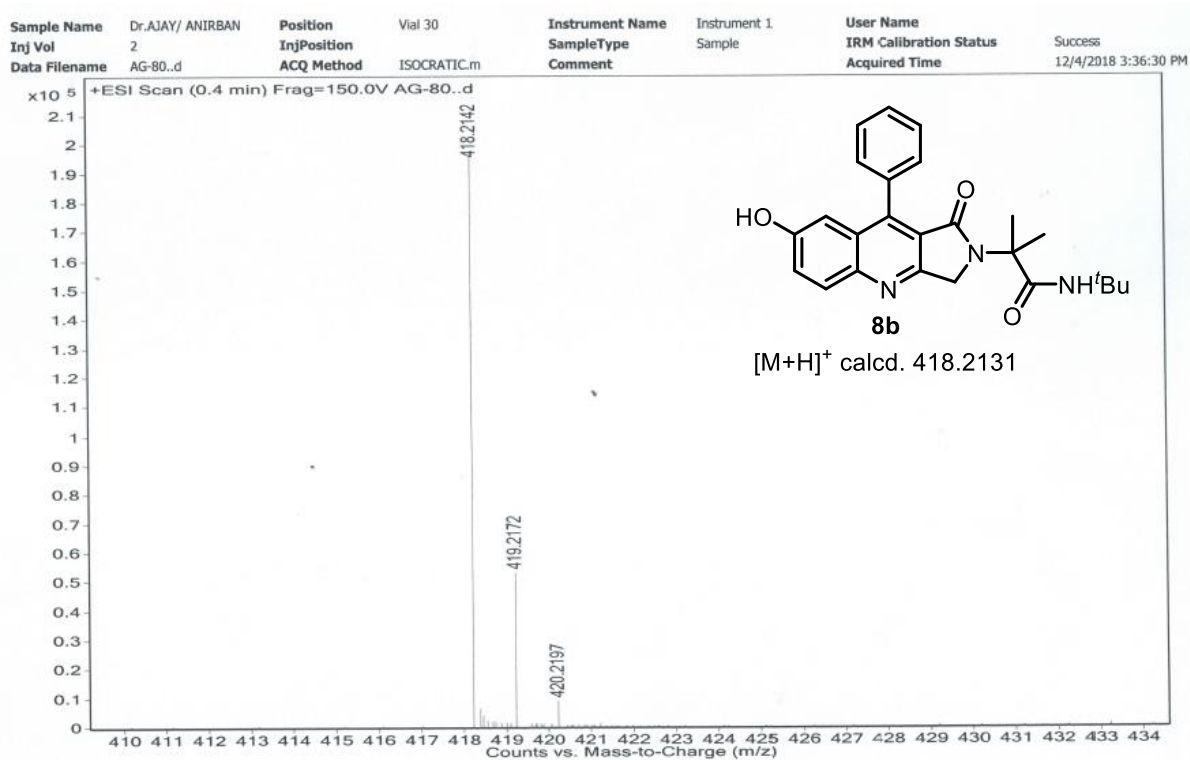


Figure S70: HRMS Spectrum of compound **8b**



➤ **HPLC Chromatograms:**

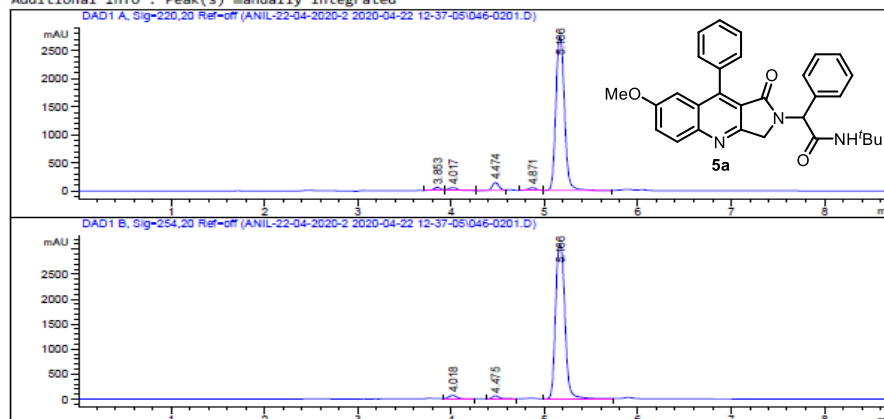
Figure S71. HPLC of compound **5a**

Data File C:\CHEM32\1\DATA\ANIL-22-04-2020-2 2020-04-22 12-37-05\046-0201.D
 Sample Name: S-017-0970

```

=====
Acq. Operator   : CBRS-REPOSITORY           Seq. Line :    2
Acq. Instrument : Instrument 1              Location  : Vial 46
Injection Date  : 4/22/2020 12:51:04 PM    Inj       :    1
                                           Inj Volume: 5.000 µl
Acq. Method    : C:\CHEM32\1\DATA\ANIL-22-04-2020-2 2020-04-22 12-37-05\ACN-WATER-90-10.M
Last changed   : 4/20/2020 3:41:17 PM by CBRS-REPOSITORY
Analysis Method: C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 4/20/2020 3:41:17 PM by CBRS-REPOSITORY
Method Info    : OSDD
  
```

Additional Info : Peak(s) manually integrated



Area Percent Report

```

=====
Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=220,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.853	BV	0.0790	305.30634	58.34921	1.5944
2	4.017	VB	0.1004	344.22580	52.54739	1.7977
3	4.474	BV	0.0803	725.13135	140.39035	3.7869
4	4.871	VB	0.0909	289.94571	49.09618	1.5142
5	5.166	BV	0.1000	1.74836e4	2755.58032	91.3067

Instrument 1 4/22/2020 1:01:54 PM CBRS-REPOSITORY

Page 1 of 2

Data File C:\CHEM32\1\DATA\ANIL-22-04-2020-2 2020-04-22 12-37-05\046-0201.D
 Sample Name: S-017-0970

Totals : 1.91482e4 3055.96345

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.018	BB	0.0951	400.85669	67.67677	1.8098
2	4.475	VV	0.0870	349.72238	60.88288	1.5789
3	5.166	BV	0.1105	2.13987e4	3100.92920	96.6113

Totals : 2.21493e4 3229.48886

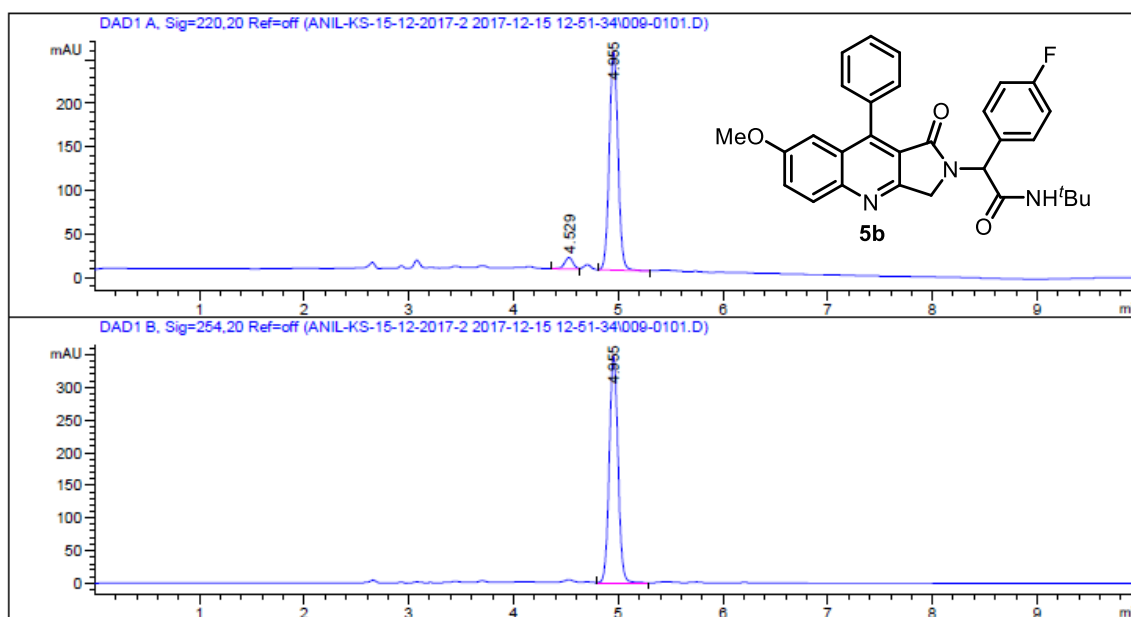
Figure S72. HPLC of compound 5b

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\009-0101.D

Sample Name: AG-16-A

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 9
Injection Date  : 12/15/2017 12:53:24 PM       Inj       :    1
                                                    Inj Volume: 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.529	BV	0.0877	74.75621	13.28310	4.9067
2	4.955	BV	0.0894	1448.79443	250.87790	95.0933

Totals : 1523.55064 264.16099

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.955	BB	0.0893	1999.90173	346.87448	100.0000

Totals : 1999.90173 346.87448

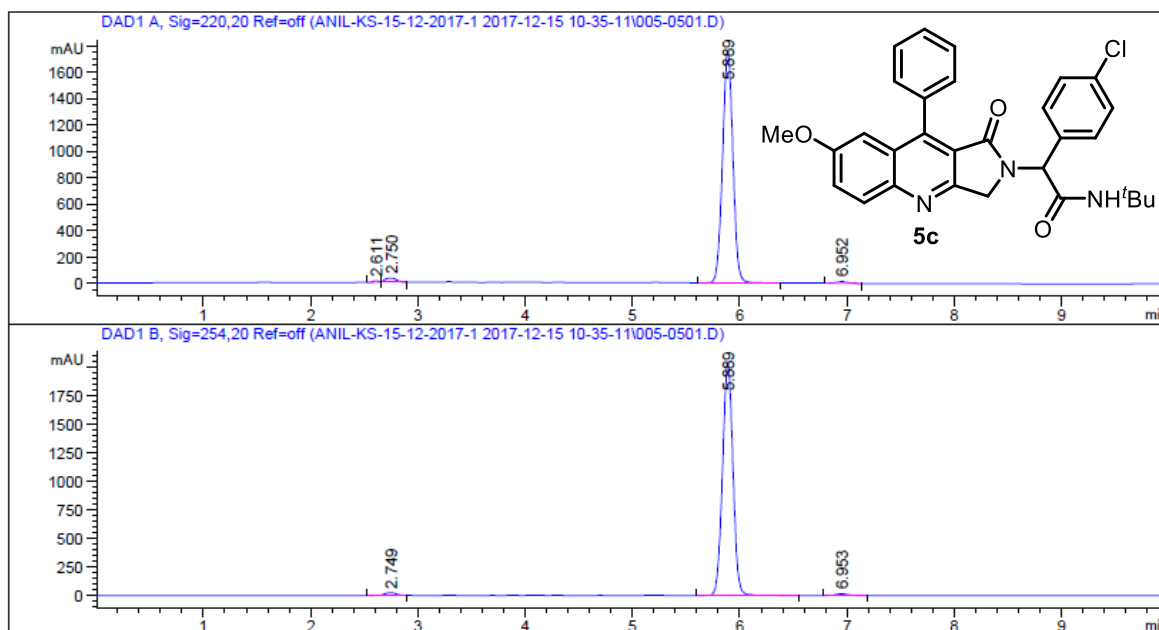
Figure S73. HPLC of compound 5c

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\005-0501.D

Sample Name: AG-18-B

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    5
Acq. Instrument : Instrument 1                   Location  : Vial 5
Injection Date  : 12/15/2017 11:24:59 AM       Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method: C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
    
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.611	VV	0.0536	42.89240	12.63753	0.3528
2	2.750	VB	0.1211	238.73804	31.98623	1.9639
3	5.889	BV	0.1044	1.17859e4	1753.70935	96.9545
4	6.952	BB	0.1168	88.57812	11.90393	0.7287

Totals : 1.21561e4 1810.23704

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.749	VV	0.1286	180.87119	22.78513	1.2834
2	5.889	BB	0.1049	1.37997e4	2041.10522	97.9162
3	6.953	BB	0.1180	112.80927	14.95814	0.8004

Totals : 1.40934e4 2078.84849

Figure S74. HPLC of compound 5d

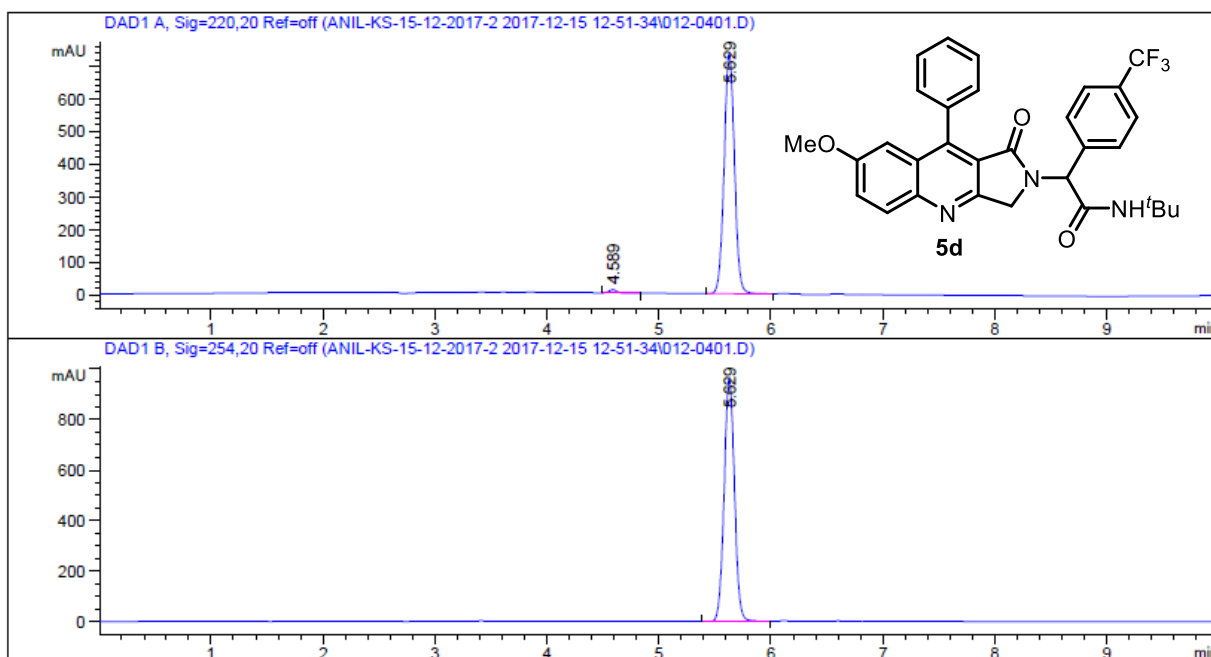
Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\012-0401.D

Sample Name: AG-16-D

```

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Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    4
Acq. Instrument : Instrument 1                   Location  : Vial 12
Injection Date  : 12/15/2017 1:29:21 PM        Inj       :    1
                                                    Inj Volume: 3.000 µl

Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
    
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.589	VB	0.0735	49.19337	10.34305	1.0353
2	5.629	VV	0.1007	4702.18848	733.96106	98.9647

Totals : 4751.38185 744.30411

Signal 2: DAD1 B, Sig=254,20 Ref=off

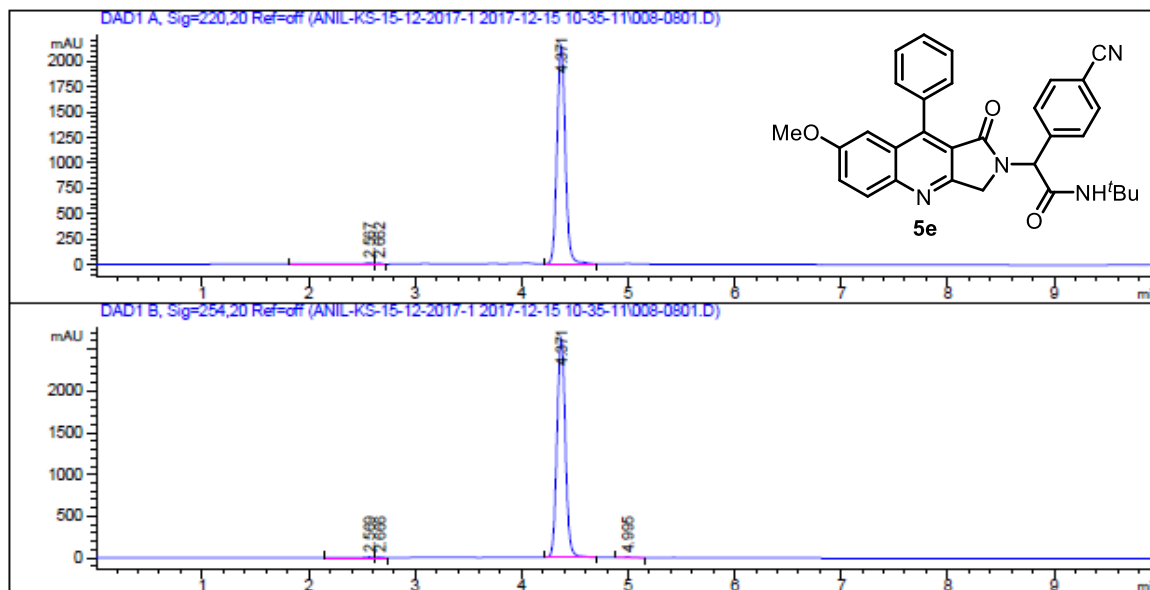
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.629	BV	0.1007	6156.72510	961.58978	100.0000

Totals : 6156.72510 961.58978

Figure S75. HPLC of compound 5e

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\008-0801.D
 Sample Name: AG-18-C

```
=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    8
Acq. Instrument : Instrument 1                  Location  : Vial 8
Injection Date  : 12/15/2017 12:00:57 PM      Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
=====
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.567	VV	0.1949	224.47668	14.63903	1.9014
2	2.662	VB	0.0554	37.57271	10.58339	0.3183
3	4.371	BV	0.0851	1.15436e4	2134.05884	97.7803
Totals :				1.18056e4	2159.28126	

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.569	BV	0.0643	29.10434	6.74852	0.2012
2	2.666	VB	0.0546	22.12838	6.36094	0.1530
3	4.371	BV	0.0861	1.43707e4	2617.52319	99.3653
4	4.995	BB	0.0915	40.56085	7.01396	0.2805
Totals :				1.44625e4	2637.64661	

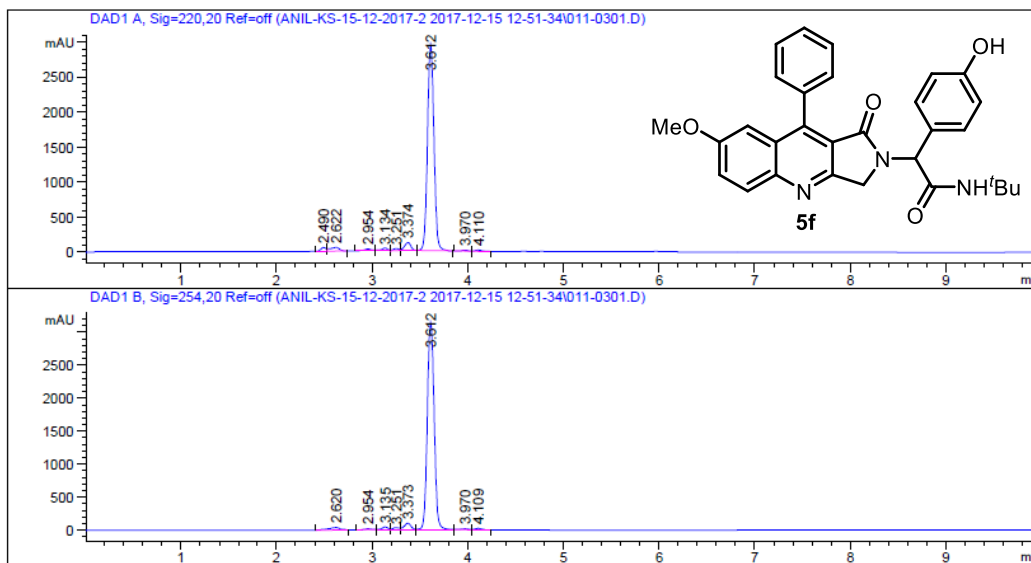
Figure S76. HPLC of compound 5f

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\011-0301.D
 Sample Name: AG-16-C

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.          Seq. Line :    3
Acq. Instrument : Instrument 1                 Location  : Vial 11
Injection Date  : 12/15/2017 1:17:24 PM      Inj       :    1
                                           Inj Volume: 3.000 µl

Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.490	BV	0.0601	221.87688	56.20625	1.4357
2	2.622	VB	0.0964	368.11603	54.76589	2.3820
3	2.954	BV	0.0744	138.84819	26.80680	0.8985
4	3.134	VV	0.0745	183.18430	36.55915	1.1853
5	3.251	VV	0.0622	119.30866	28.90448	0.7720
6	3.374	VB	0.0723	535.85718	115.05862	3.4674
7	3.612	BB	0.0726	1.37379e4	2935.39307	88.8951
8	3.970	BV	0.0812	64.03028	11.82412	0.4143
9	4.110	VB	0.0788	84.93763	16.85517	0.5496

Totals : 1.54540e4 3282.37354

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.620	BV	0.1155	321.04678	38.40248	1.9249
2	2.954	BV	0.0682	74.12491	15.96286	0.4444
3	3.135	VV	0.0654	171.70801	40.57630	1.0295
4	3.251	VV	0.0610	119.41612	29.66819	0.7160
5	3.373	VB	0.0735	446.52136	93.80724	2.6772
6	3.612	BB	0.0793	1.53550e4	3129.08081	92.0628
7	3.970	BV	0.0788	75.03034	14.38816	0.4499
8	4.109	VB	0.0780	115.98534	23.31987	0.6954

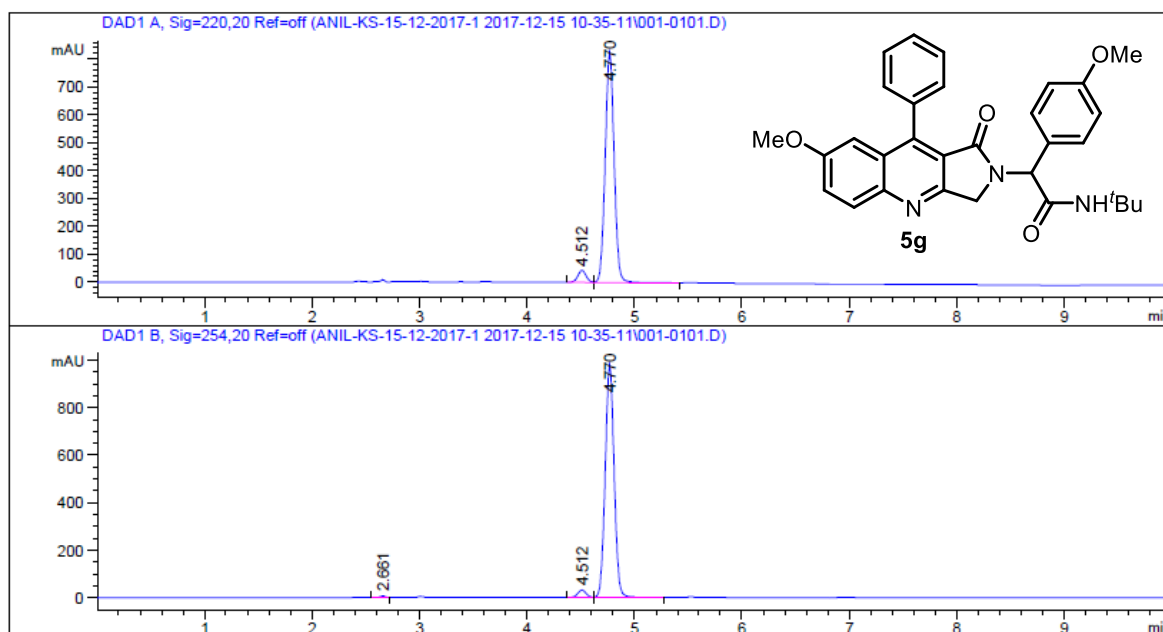
Totals : 1.66788e4 3385.20592

Figure S77. HPLC of compound 5g

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\001-0101.D
 Sample Name: AG-136

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 1
Injection Date  : 12/15/2017 10:36:55 AM       Inj       :    1
                                                    Inj Volume: 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
  
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.512	VV	0.0822	230.72125	43.26201	4.6156
2	4.770	VB	0.0894	4768.02051	825.53345	95.3844

Totals : 4998.74176 868.79546

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.661	VV	0.0509	21.22003	6.71313	0.3626
2	4.512	VV	0.0823	168.00214	31.45425	2.8707
3	4.770	VB	0.0894	5663.09131	980.83392	96.7667

Totals : 5852.31347 1019.00130

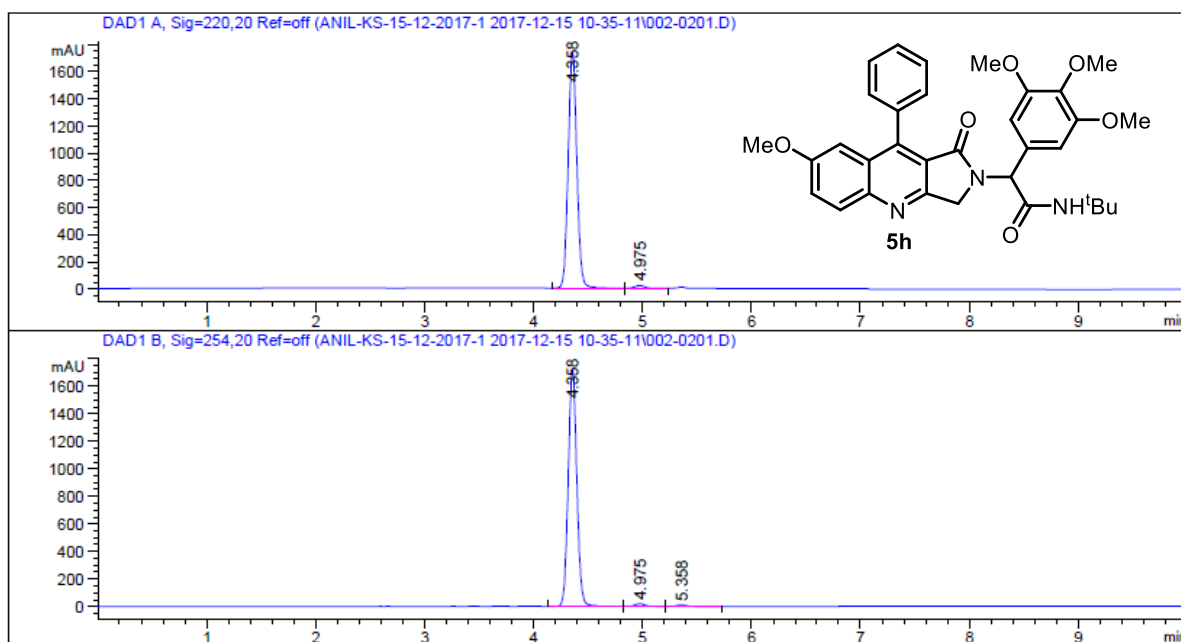
Figure S78. HPLC of compound 5h

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\002-0201.D

Sample Name: AG-18-A

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    2
Acq. Instrument : Instrument 1                  Location  : Vial 2
Injection Date  : 12/15/2017 10:48:53 AM      Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
    
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.358	BV	0.0863	9576.26074	1736.92810	98.6785
2	4.975	VV	0.1007	128.24675	19.50057	1.3215

Totals : 9704.50749 1756.42867

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.358	BV	0.0838	9417.81641	1723.43262	98.0696
2	4.975	VV	0.0966	120.32935	19.32729	1.2530
3	5.358	VB	0.0936	65.05067	10.90698	0.6774

Totals : 9603.19642 1753.66689

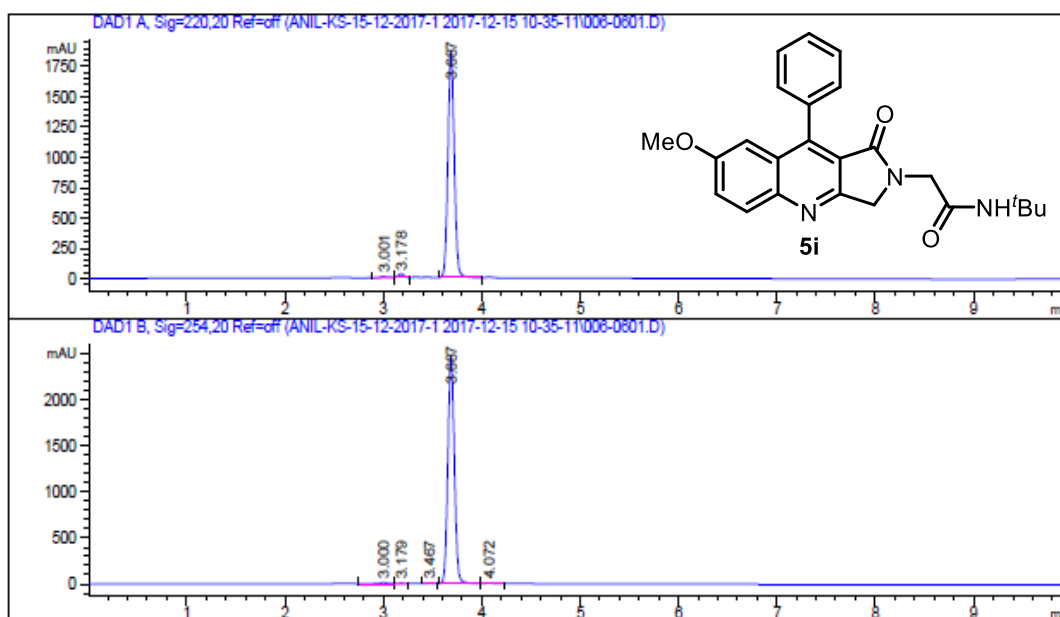
Figure S79. HPLC of compound 5i

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\006-0601.D
 Sample Name: AG-21-B

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    6
Acq. Instrument : Instrument 1                   Location  : Vial 6
Injection Date  : 12/15/2017 11:36:57 AM       Inj       :    1
                                                    Inj Volume: 3.000 µl

Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method: C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.001	VV	0.0783	61.49919	11.15435	0.7148
2	3.178	VB	0.0641	125.84449	30.50060	1.4628
3	3.687	BV	0.0685	8415.78418	1870.13306	97.8224

Totals : 8603.12786 1911.78800

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.000	BV	0.0695	65.43272	14.26784	0.5651
2	3.179	VV	0.0723	26.98400	5.59539	0.2330
3	3.467	VB	0.0688	23.95547	5.29011	0.2069
4	3.687	BV	0.0737	1.14160e4	2479.01758	98.5917
5	4.072	VB	0.0838	46.69102	8.54166	0.4032

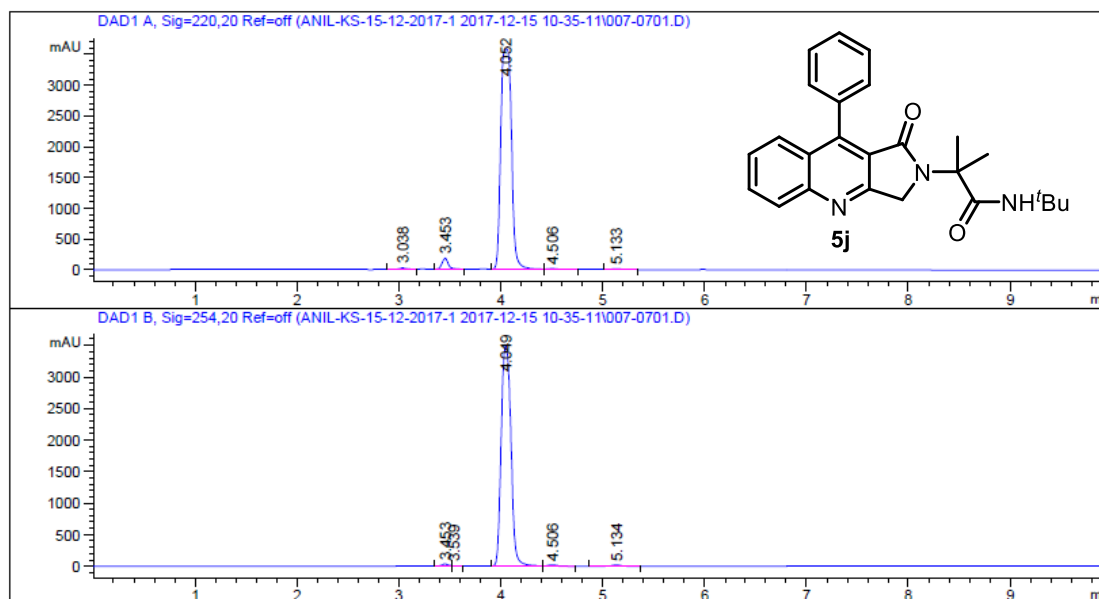
Totals : 1.15791e4 2512.71257

Figure S80. HPLC of compound 5j

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\007-0701.D
 Sample Name: AG-21-D

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    7
Acq. Instrument : Instrument 1                   Location  : Vial 7
Injection Date  : 12/15/2017 11:48:57 AM       Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.038	VV	0.0996	159.76851	23.40314	0.5866
2	3.453	VV	0.0692	812.05127	178.08176	2.9817
3	4.052	BV	0.1172	2.60986e4	3574.22852	95.8305
4	4.506	VB	0.0916	83.07650	13.92503	0.3050
5	5.133	VB	0.0903	80.64246	13.76763	0.2961

Totals : 2.72341e4 3803.40607

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.453	BV	0.0658	135.58652	31.73555	0.5782
2	3.539	VB	0.0483	19.77046	6.36127	0.0843
3	4.049	BV	0.1089	2.30717e4	3501.33618	98.3828
4	4.506	VB	0.0897	115.86201	19.96015	0.4941
5	5.134	BB	0.0916	108.02787	18.10634	0.4607

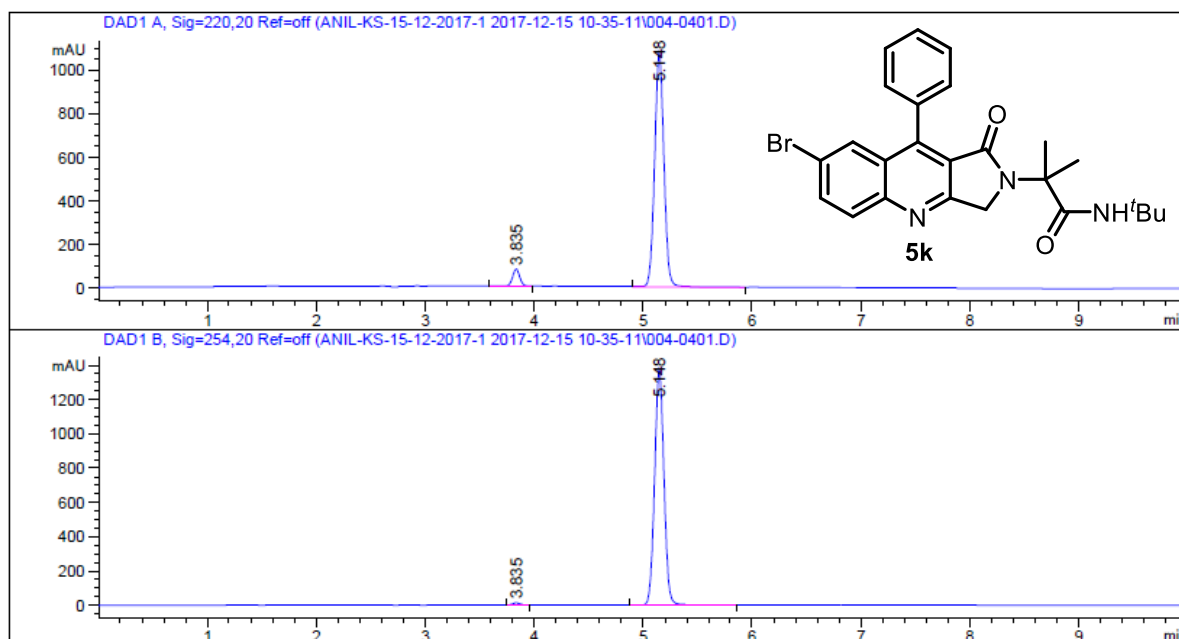
Totals : 2.34510e4 3577.49950

Figure S81. HPLC of compound 5k

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\004-0401.D
 Sample Name: AG-21-E

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    4
Acq. Instrument : Instrument 1                   Location  : Vial 4
Injection Date  : 12/15/2017 11:12:59 AM       Inj       :    1
                                                    Inj Volume: 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-1 2017-12-15 10-35-11\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.835	VV	0.0767	397.71454	78.99175	5.8764
2	5.148	VV	0.0911	6370.28857	1075.61047	94.1236

Totals : 6768.00311 1154.60223

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.835	VV	0.0721	62.74902	13.53850	0.7582
2	5.148	BB	0.0915	8212.81348	1377.84229	99.2418

Totals : 8275.56250 1391.38078

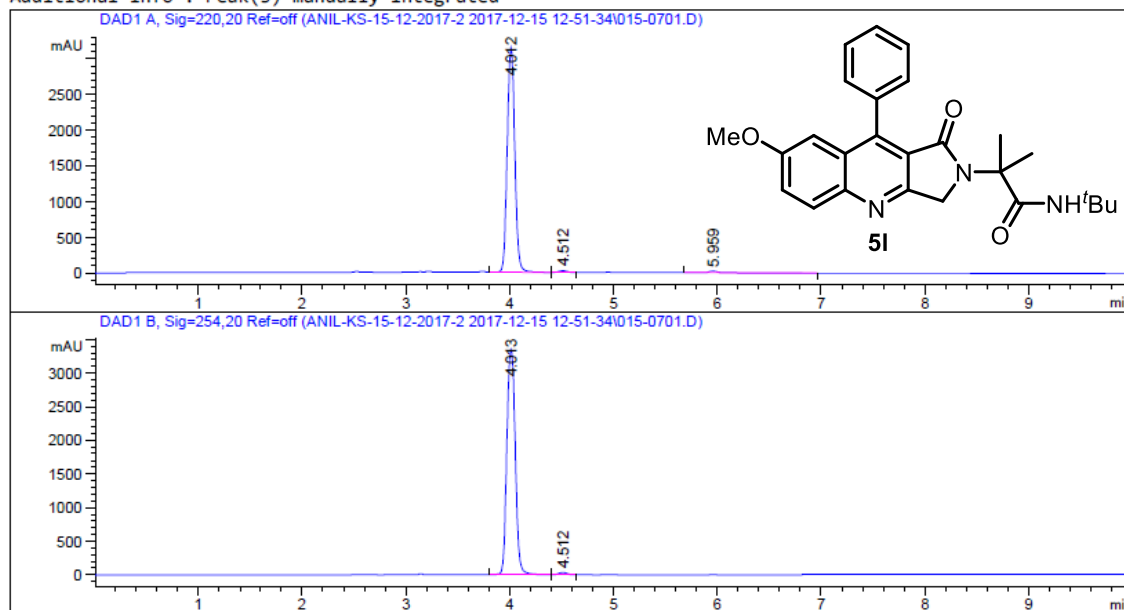
Figure S82. HPLC of compound 5I

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\015-0701.D
 Sample Name: AG-18-E

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    7
Acq. Instrument : Instrument 1                  Location  : Vial 15
Injection Date  : 12/15/2017 2:05:15 PM        Inj       :    1
                                           Inj Volume: 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
  
```

Additional Info : Peak(s) manually integrated



Signal 1: DAD1 A, Sig=220,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.012	VV	0.0814	1.59636e4	3137.04468	98.1641
2	4.512	VB	0.0835	135.55725	25.69749	0.8336
3	5.959	BB	0.1036	162.99409	23.30471	1.0023

Totals : 1.62622e4 3186.04688

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.013	VV	0.0917	1.88305e4	3343.33594	99.0521
2	4.512	VB	0.0840	180.20427	33.89356	0.9479

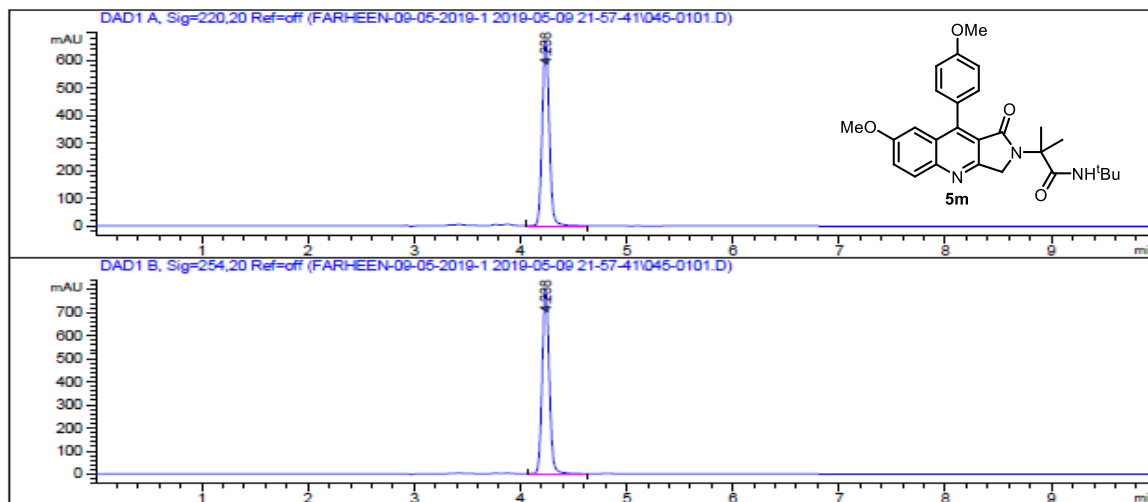
Totals : 1.90107e4 3377.22950

Figure S83. HPLC of compound 5m

Data File C:\CHEM32\1\DATA\FARHEEN-09-05-2019-1 2019-05-09 21-57-41\045-0101.D
 Sample Name: S-019-0009

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 45
Injection Date  : 5/9/2019 9:59:24 PM          Inj       :    1
                                                    Inj Volume: 4.000 µl
Acq. Method    : C:\CHEM32\1\DATA\FARHEEN-09-05-2019-1 2019-05-09 21-57-41\ACN-WATER-90-10.M
Last changed   : 5/3/2019 10:08:39 AM by Dr. Anil Kumar K.S.
Analysis Method: C:\CHEM32\1\DATA\FARHEEN-09-05-2019-2 2019-05-09 23-31-20\METH-WATER-90-10-NEW.M
Last changed   : 4/29/2019 11:34:05 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
  
```



=====
 Area Percent Report
 =====

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=220,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.238	BB	0.0720	3103.95850	670.56421	100.0000

Totals : 3103.95850 670.56421

Instrument 1 5/10/2019 3:05:47 AM Dr. Anil Kumar K.S.

Page 1 of 2

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.238	W	0.0720	3719.73022	802.90283	100.0000

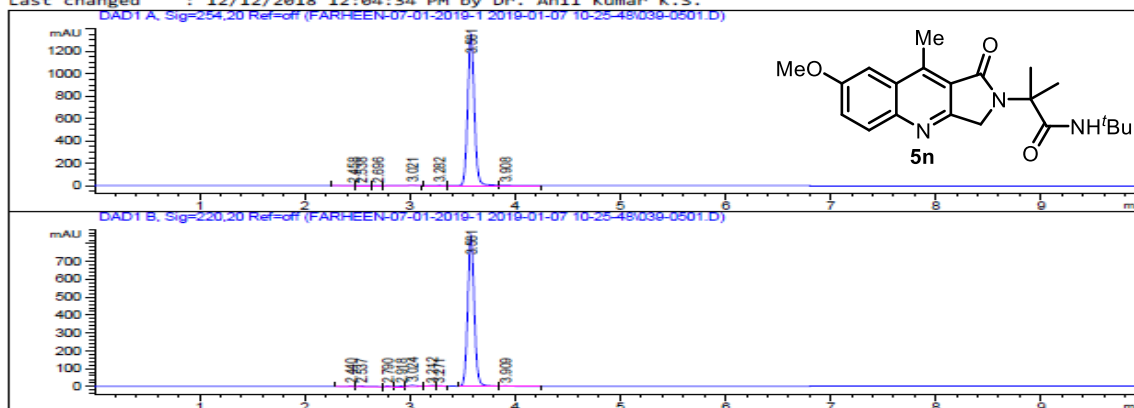
Totals : 3719.73022 802.90283

Figure S84. HPLC of compound 5n

Data File C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\039-0501.D
 Sample Name: S-019-0006

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    5
Acq. Instrument : Instrument 1                  Location  : Vial 39
Injection Date  : 1/7/2019 11:13:01 AM         Inj       :    1
                                                    Inj Volume: 5.000 µl
Method         : C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\ACN-WATER-90-10.M
                (Sequence Method)
Last changed   : 12/12/2018 12:04:34 PM by Dr. Anil Kumar K.S.
=====
  
```



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.458	BV	0.0836	7.30253	1.33934	0.1213
2	2.538	VV	0.0748	14.82715	2.84650	0.2464
3	2.696	VB	0.0722	6.17382	1.32817	0.1026
4	3.021	BB	0.0932	24.08361	3.54556	0.4002
5	3.282	BV	0.0725	9.51162	1.96451	0.1581
6	3.581	VV	0.0697	5925.78467	1338.45410	98.4701
7	3.908	VB	0.0911	30.17077	4.68942	0.5014
Totals :				6017.85417	1354.16760	

Instrument 1 1/7/2019 12:21:48 PM Dr. Anil Kumar K.S.

Page 1 of 2

Signal 2: DAD1 B, Sig=220,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.440	BV	0.0974	14.80971	2.29225	0.3856
2	2.537	VB	0.1279	34.53092	3.53680	0.8991
3	2.790	BV	0.0656	17.40842	4.09395	0.4533
4	2.918	W	0.0774	15.77617	2.81533	0.4108
5	3.024	W	0.0830	44.95138	7.60114	1.1705
6	3.212	W	0.0736	26.98288	5.27958	0.7026
7	3.271	VB	0.0509	12.80687	3.83900	0.3335
8	3.581	BV	0.0689	3655.98633	837.20837	95.1975
9	3.909	VB	0.0964	17.17186	2.49043	0.4471
Totals :				3840.42453	869.15685	

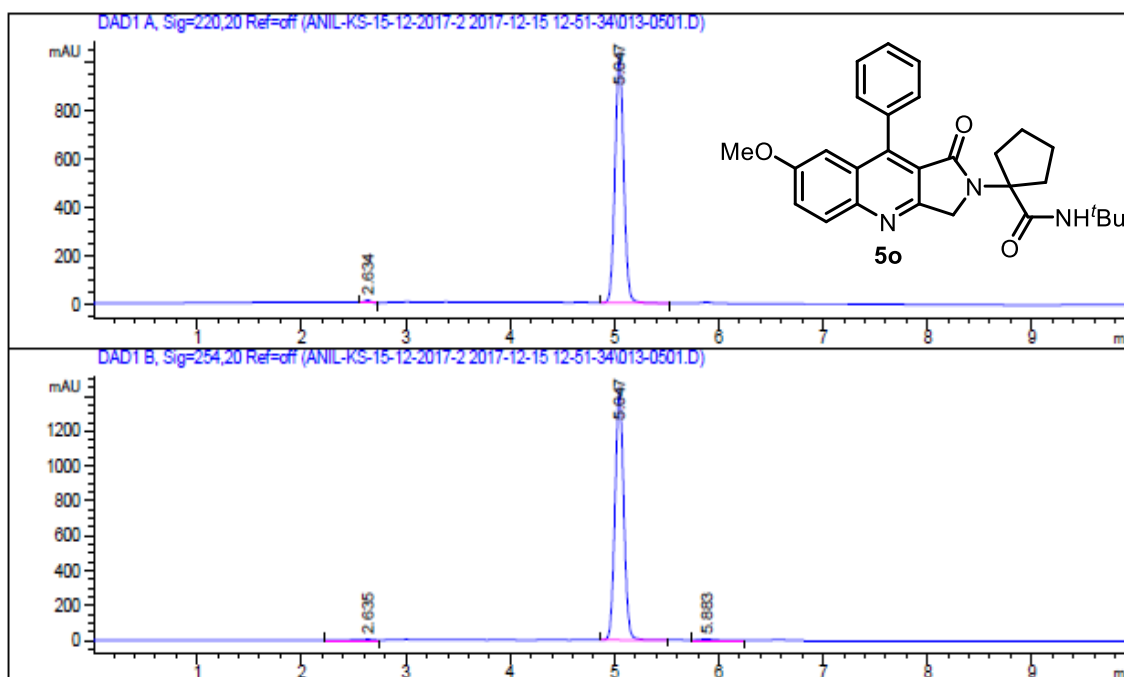
Figure S85. HPLC of compound 5o

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\013-0501.D

Sample Name: AG-18-F

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    5
Acq. Instrument : Instrument 1                   Location  : Vial 13
Injection Date  : 12/15/2017 1:41:18 PM        Inj       :    1
                                                    Inj Volume: 3.000 µl
Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method: C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
    
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.634	VB	0.0706	60.06581	12.38757	0.9960
2	5.047	BV	0.0899	5970.51514	1026.19019	99.0040

Totals : 6030.58094 1038.57775

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.635	BB	0.0751	27.41661	5.23576	0.3252
2	5.047	BV	0.0901	8365.23145	1434.04065	99.2327
3	5.883	BB	0.1008	37.26209	5.66331	0.4420

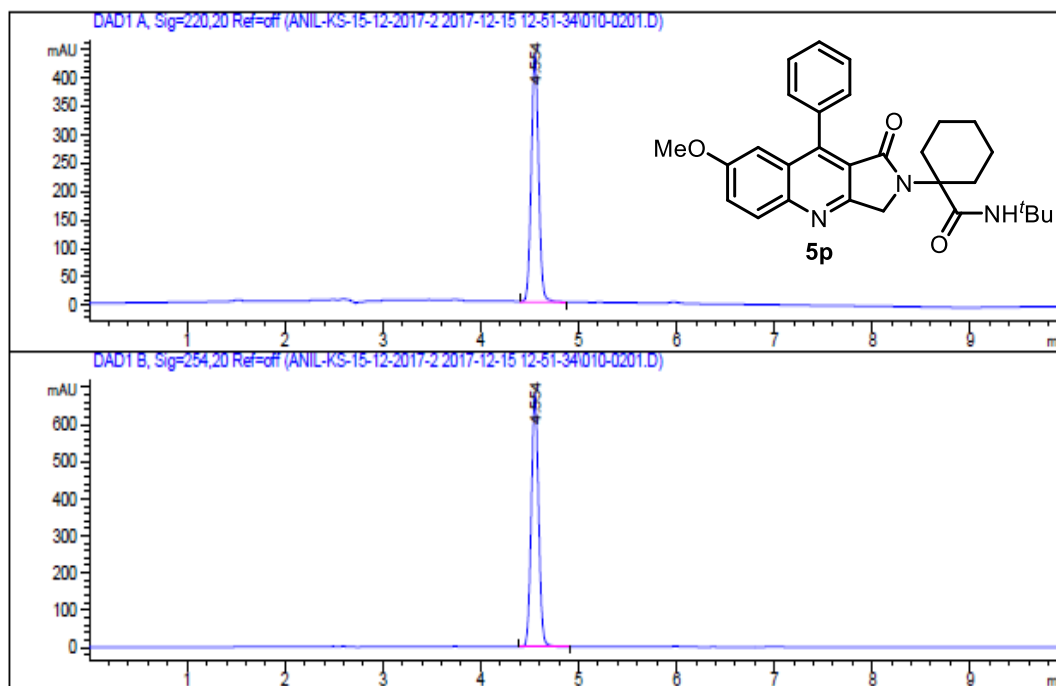
Totals : 8429.91014 1444.93972

Figure S86. HPLC of compound 5p

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\010-0201.D

Sample Name: A9-19-A

```
=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    2
Acq. Instrument : Instrument 1                  Location  : Vial 10
Injection Date  : 12/15/2017 1:05:27 PM       Inj       :    1
                                                    Inj Volume: 3.000 µl
Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.554	WV	0.0810	2280.25098	435.94400	100.0000

Totals : 2280.25098 435.94400

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.554	BB	0.0805	3534.63086	681.92010	100.0000

Totals : 3534.63086 681.92010

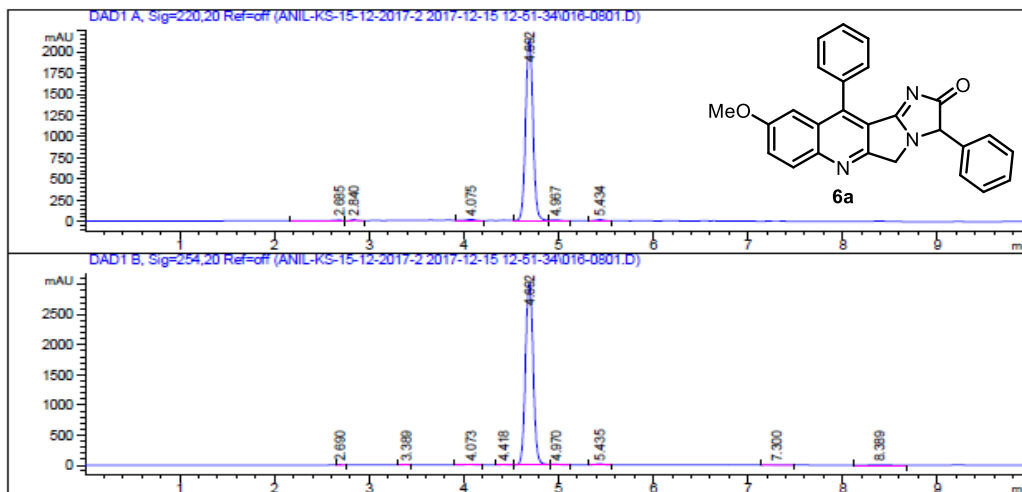
Figure S87. HPLC of compound 6a

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\016-0801.D
 Sample Name: AG-21-A-P

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    8
Acq. Instrument : Instrument 1                   Location  : Vial 16
Injection Date  : 12/15/2017 2:17:15 PM        Inj       :    1
                                           Inj Volume: 3.000 µl

Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSOD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.685	VB	0.1152	103.02876	11.87425	0.8617
2	2.840	BV	0.0778	72.20421	14.08029	0.6039
3	4.075	VB	0.0975	96.57744	14.52980	0.8078
4	4.692	VV	0.0829	1.15376e4	2138.82104	96.4997
5	4.967	VB	0.0989	66.05271	10.01547	0.5525
6	5.434	BV	0.0908	80.64073	13.67817	0.6745

Totals : 1.19561e4 2202.99903

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.690	VB	0.0519	27.11286	7.93599	0.1541
2	3.389	BV	0.0654	24.60736	5.81327	0.1399
3	4.073	BB	0.0933	59.43724	9.45979	0.3378
4	4.418	VV	0.0830	38.43474	7.11383	0.2185
5	4.692	VV	0.0901	1.71339e4	3022.39673	97.3911
6	4.970	VB	0.0948	83.26785	12.98086	0.4733
7	5.435	BV	0.0912	132.75661	22.39119	0.7546
8	7.300	BV	0.1195	41.14302	5.36498	0.2339
9	8.389	BV	0.1298	52.21698	6.23127	0.2968

Totals : 1.75929e4 3099.68791

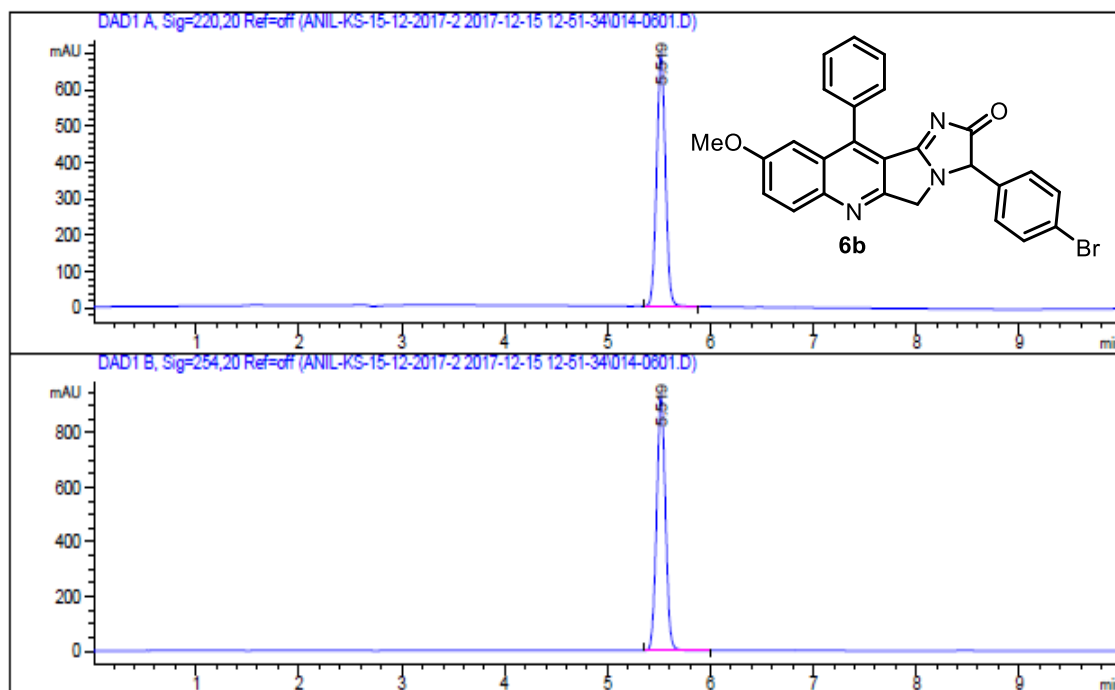
Figure S88. HPLC of compound 6b

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\014-0601.D

Sample Name: AG-16-B-P

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.          Seq. Line :    6
Acq. Instrument : Instrument 1                 Location  : Vial 14
Injection Date  : 12/15/2017 1:53:16 PM      Inj       :    1
                                                Inj Volume: 3.000 µl
Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method: C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
    
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.519	W	0.0919	4149.05469	692.43347	100.0000

Totals : 4149.05469 692.43347

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.519	W	0.0920	5610.87549	935.17145	100.0000

Totals : 5610.87549 935.17145

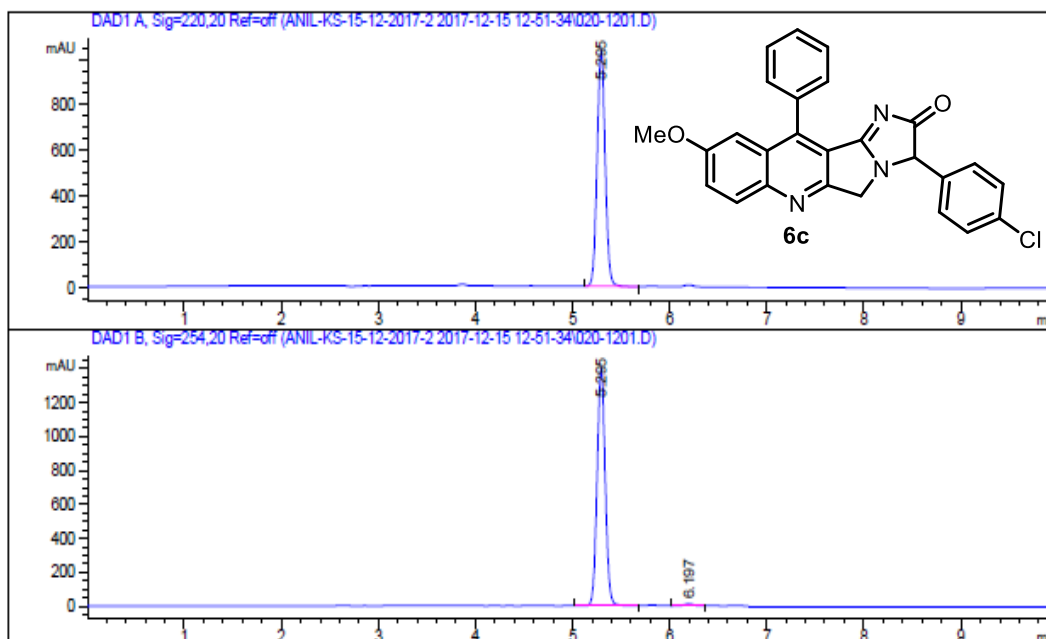
Figure S89. HPLC of compound 6c

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\020-1201.D
 Sample Name: AG-18-B-P

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :   12
Acq. Instrument : Instrument 1                  Location  : Vial 20
Injection Date  : 12/15/2017 3:05:20 PM        Inj       :    1
                                                    Inj Volume: 3.000 µl

Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.295	VB	0.0898	5982.72314	1029.17029	100.0000

Totals : 5982.72314 1029.17029

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.295	BV	0.0900	8163.41992	1400.07507	99.0790
2	6.197	BB	0.1009	75.88558	11.81718	0.9210

Totals : 8239.30550 1411.89225

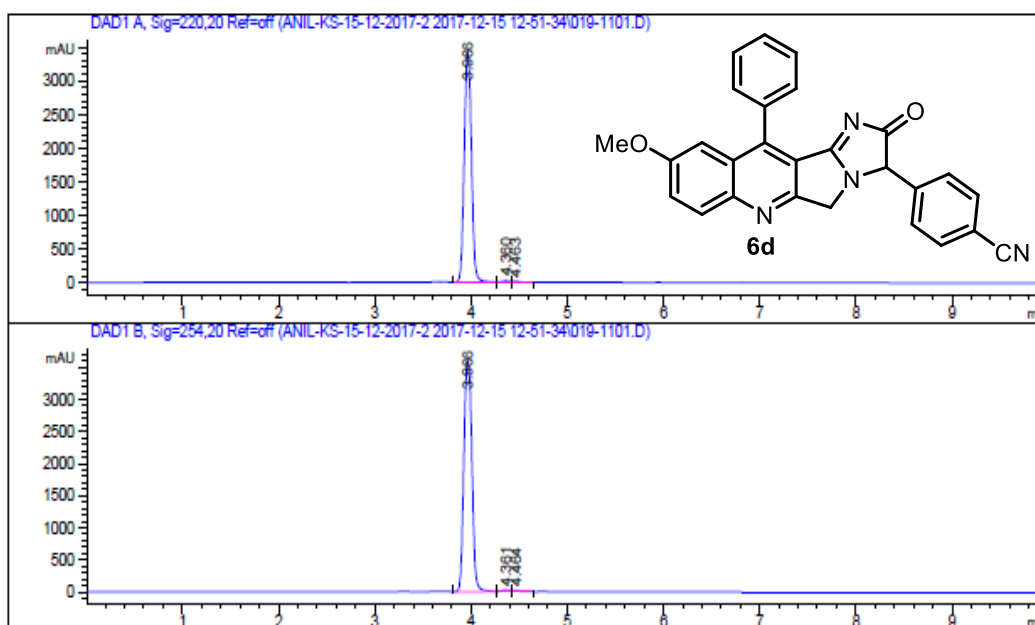
Figure S90. HPLC of compound 6d

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\019-1101.D
 Sample Name: AG-18-C-P

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :   11
Acq. Instrument : Instrument 1                  Location  : Vial 19
Injection Date  : 12/15/2017 2:53:18 PM        Inj       :    1
                                           Inj Volume: 3.000 µl

Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method: C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.966	BB	0.0849	1.78302e4	3417.97974	99.1765
2	4.360	BV	0.0777	89.34116	17.44733	0.4969
3	4.463	VB	0.0752	58.70437	11.97353	0.3265

Totals : 1.79783e4 3447.40060

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.966	BB	0.0958	2.08845e4	3593.79395	99.0360
2	4.361	BV	0.0770	113.42193	22.41887	0.5379
3	4.464	VB	0.0769	89.86758	17.79210	0.4262

Totals : 2.10878e4 3634.00492

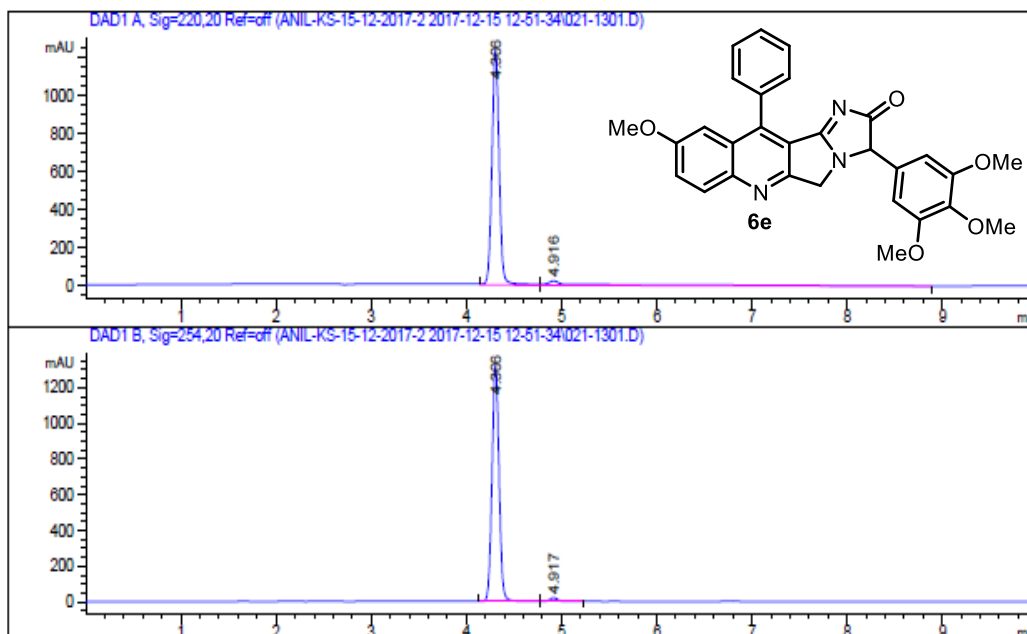
Figure S91. HPLC of compound 6e

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\021-1301.D
 Sample Name: AG-18-A-P

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :   13
Acq. Instrument : Instrument 1                  Location  : Vial 21
Injection Date  : 12/15/2017 3:17:17 PM       Inj       :    1
                                                    Inj Volume: 3.000 µl

Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.306	WV	0.0817	6547.84961	1237.75269	90.0686
2	4.916	VB	0.3824	721.99658	23.37426	9.9314

Totals : 7269.84619 1261.12694

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.306	BV	0.0801	6823.17090	1324.72534	98.2684
2	4.917	WV	0.0901	120.22906	20.59347	1.7316

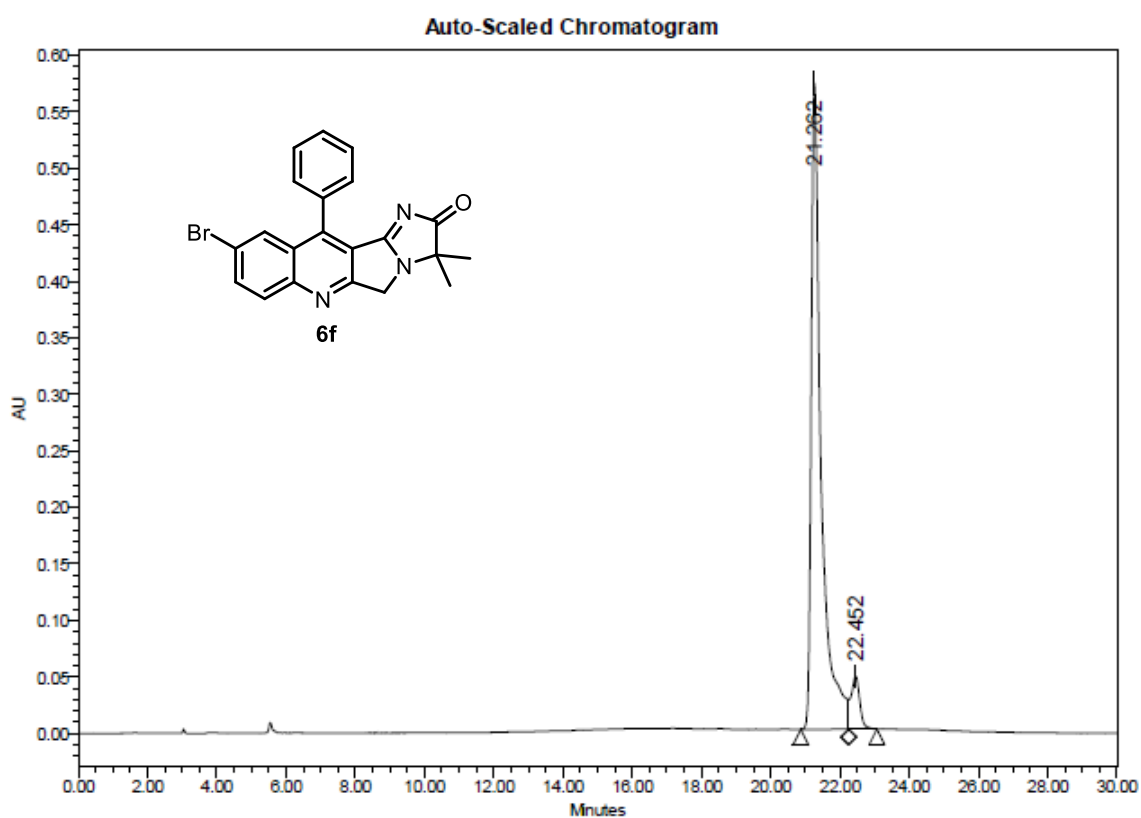
Totals : 6943.39996 1345.31881

Figure S92. HPLC of compound **6f**



SAF_CDRI_GSC and HPLC LAB, LUCKNOW

SAMPLE INFORMATION			
Sample Name:	AG-21-E-P	Acquired By:	System
Sample Type:	Unknown	Acq. Method Set:	NEW GENERAL HPLC
Vial:	1	Processing Method:	AG_21_E_P
Injection #:	12	Channel Name:	254.0nm
Injection Volume:	10.00 ul	Proc. Chnl. Descr.:	PDA 254.0 nm
Run Time:	30.0 Minutes		
Date Acquired:	7/1/2020 4:00:45 PM IST		
Date Processed:	7/3/2020 2:35:18 PM IST		



Peak Results

Name	RT	Area	Height	% Area
1	21.262	11357125	572057	93.24
2	22.452	823921	46776	6.76

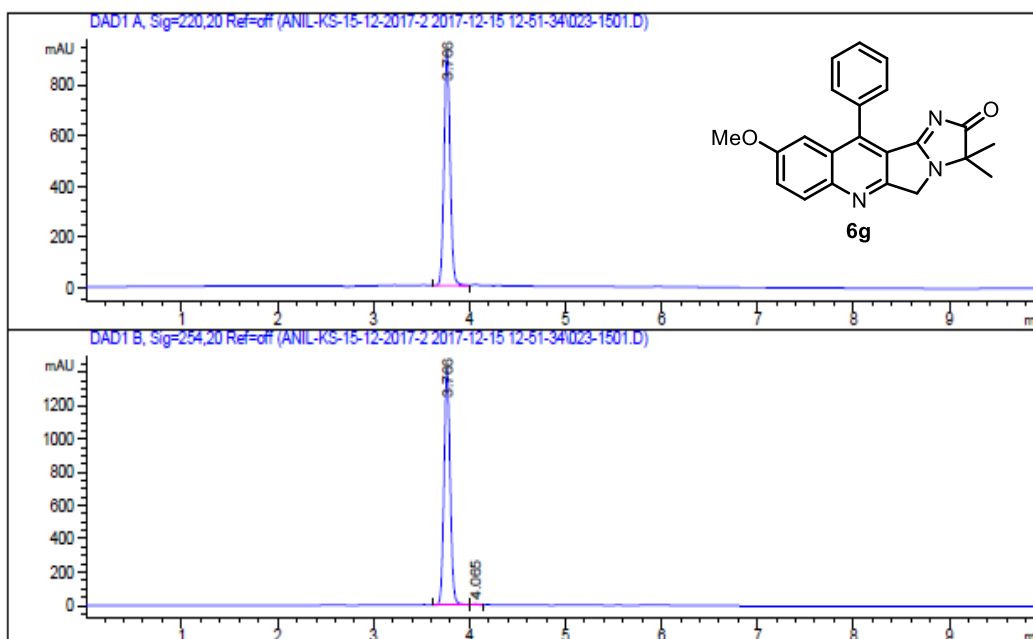
Figure S93. HPLC of compound 6g

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\023-1501.D
 Sample Name: AG-18-E-P

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :   15
Acq. Instrument : Instrument 1                  Location  : Vial 23
Injection Date  : 12/15/2017 3:41:13 PM        Inj       :    1
                                                    Inj Volume: 3.000 µl

Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.766	BV	0.0679	4122.53613	927.59344	100.0000

Totals : 4122.53613 927.59344

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.766	BV	0.0680	6352.28467	1425.41724	99.4520
2	4.065	WV	0.0760	35.00503	6.80146	0.5480

Totals : 6387.28970 1432.21870

Figure S94. HPLC of compound 6h

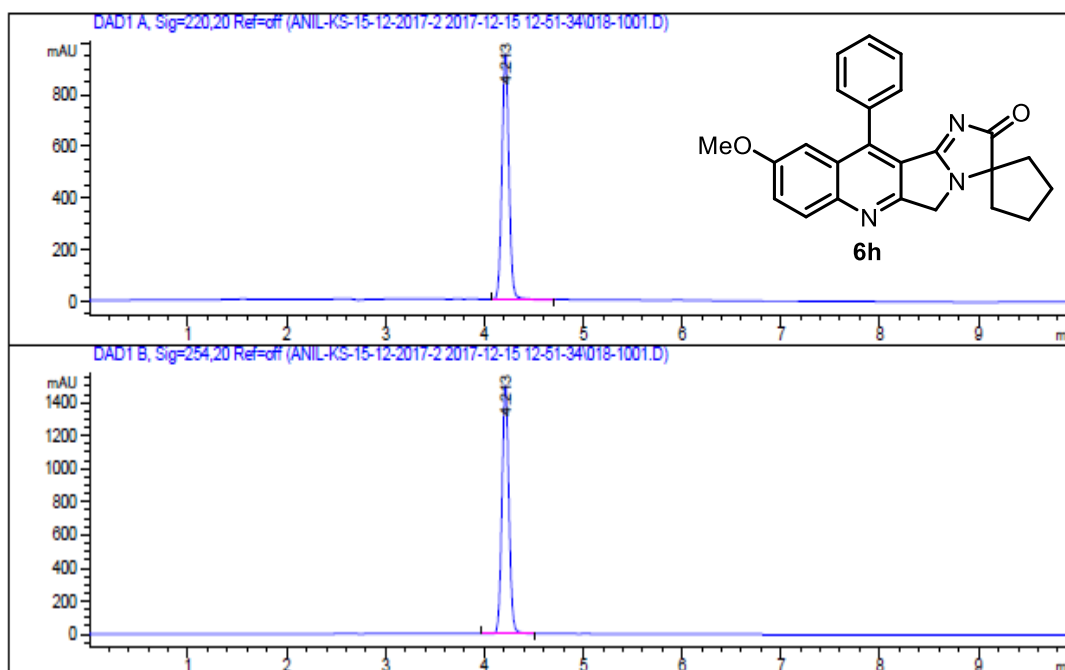
Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\018-1001.D

Sample Name: AG-18-F-P

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line : 10
Acq. Instrument : Instrument 1                  Location  : Vial 18
Injection Date  : 12/15/2017 2:41:15 PM        Inj       : 1
                                           Inj Volume: 3.000 µl

Acq. Method     : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method : C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed    : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info     : OSDD
    
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.213	WV	0.0774	4691.17920	954.21094	100.0000

Totals : 4691.17920 954.21094

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.213	BV	0.0771	7372.19385	1505.42444	100.0000

Totals : 7372.19385 1505.42444

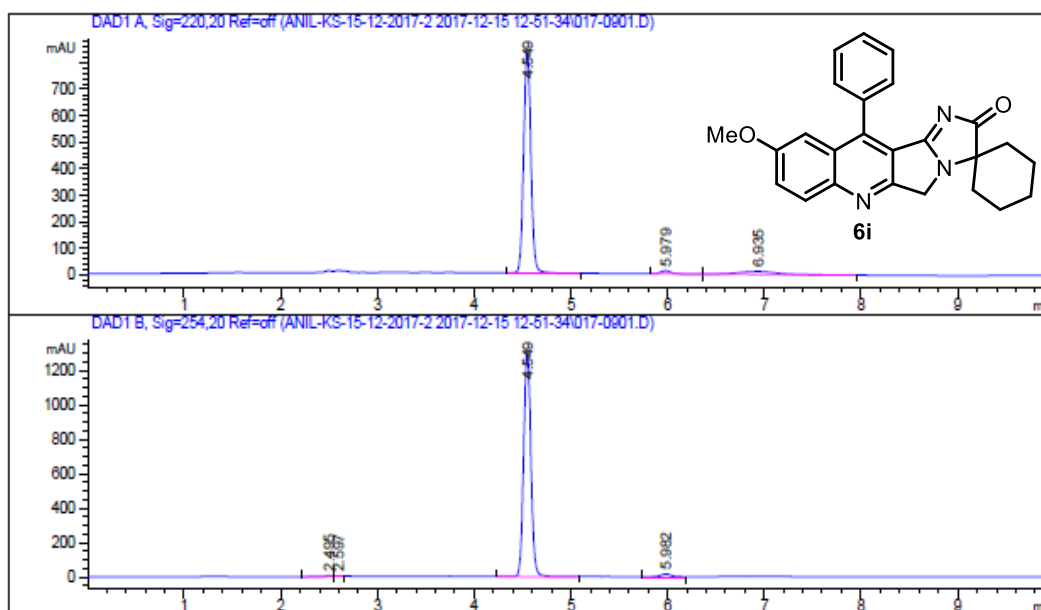
Figure S95. HPLC of compound **6i**

Data File C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\017-0901.D
 Sample Name: AG-19-A-P

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.          Seq. Line :    9
Acq. Instrument : Instrument 1                 Location  : Vial 17
Injection Date  : 12/15/2017 2:29:15 PM       Inj       :    1
                                           Inj Volume: 3.000 µl

Acq. Method    : C:\CHEM32\1\DATA\ANIL-KS-15-12-2017-2 2017-12-15 12-51-34\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Analysis Method: C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/15/2017 10:35:01 AM by Dr. Anil Kumar K.S.
Method Info    : OSDD
  
```



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.549	W	0.0830	4384.64551	837.99878	91.5577
2	5.979	BV	0.1083	86.36610	12.55259	1.8034
3	6.935	VB	0.4269	317.92987	11.48540	6.6388
Totals :				4788.94147	862.03677	

Signal 2: DAD1 B, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.495	BV	0.0704	28.29429	5.85662	0.4061
2	2.597	W	0.0758	28.55070	5.38616	0.4098
3	4.549	BV	0.0828	6801.49365	1304.23962	97.6230
4	5.982	BB	0.1041	108.76447	16.24367	1.5611
Totals :				6967.10310	1331.72608	

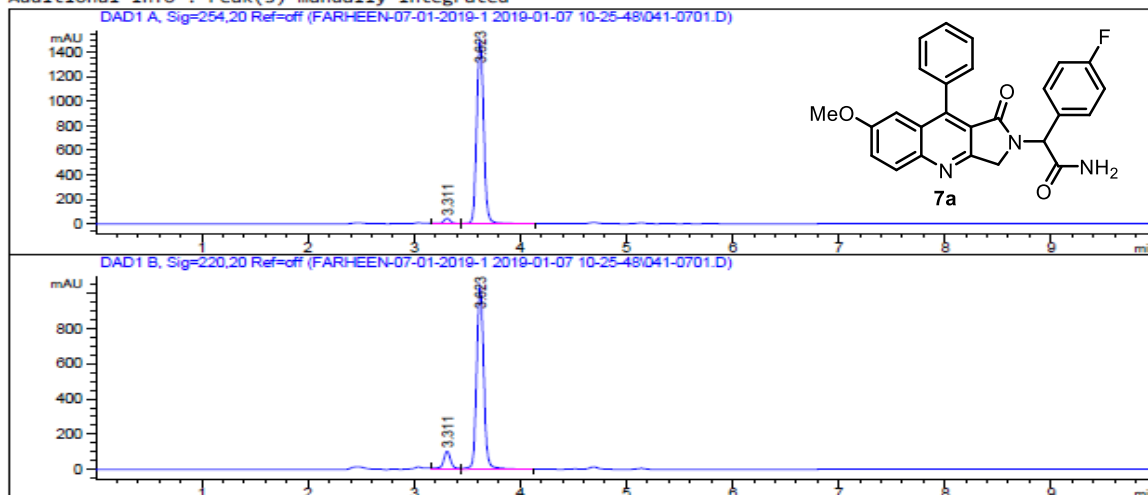
Figure S96. HPLC of compound 7a

Data File C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\041-0701.D
 Sample Name: S-019-0008

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    7
Acq. Instrument : Instrument 1                  Location  : Vial 41
Injection Date  : 1/7/2019 11:36:01 AM         Inj       :    1
                                           Inj Volume: 5.000 µl

Method         : C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\ACN-WATER-90-10.M
                (Sequence Method)
Last changed   : 12/12/2018 12:04:34 PM by Dr. Anil Kumar K.S.
Additional Info: Peak(s) manually integrated
  
```



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution      : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.311	W	0.0736	228.13037	46.23408	3.2276
2	3.623	VB	0.0714	6840.02051	1495.67200	96.7724

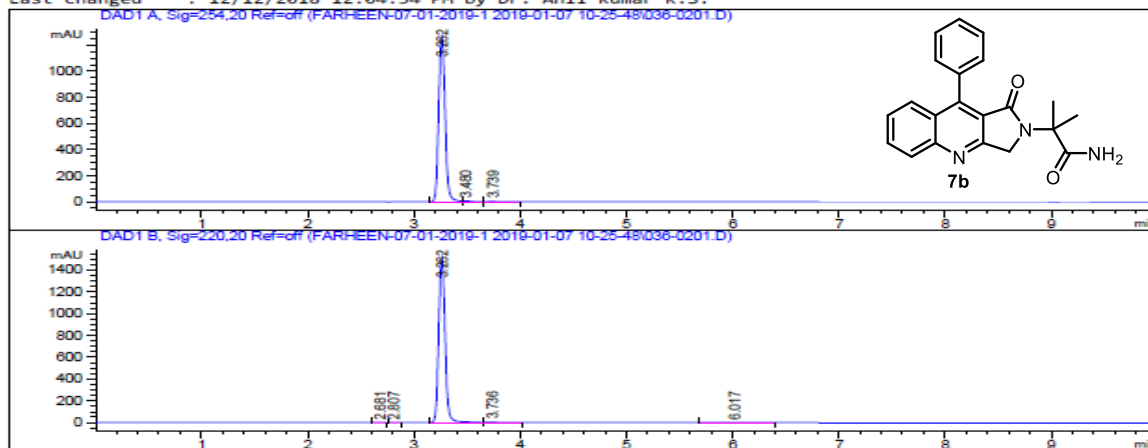
Totals : 7068.15088 1541.90608

Figure S97. HPLC of compound 7b

Data File C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\036-0201.D
 Sample Name: S-019-0003

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    2
Acq. Instrument : Instrument 1                 Location  : Vial 36
Injection Date  : 1/7/2019 10:38:31 AM        Inj       :    1
                                                Inj Volume: 5.000 µl
Method         : C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\ACN-WATER-90-10.M
                (Sequence Method)
Last changed   : 12/12/2018 12:04:34 PM by Dr. Anil Kumar K.S.
  
```



Area Percent Report

```

=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution      :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.262	VV	0.0646	5270.99756	1264.93420	98.8703
2	3.480	VV	0.0831	38.41008	6.67493	0.7205
3	3.739	VB	0.0783	21.81442	4.08745	0.4092

Totals : 5331.22206 1275.69659

Instrument 1 1/7/2019 12:15:50 PM Dr. Anil Kumar K.S.

Page 1 of 2

Signal 2: DAD1 B, Sig=220,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.681	BB	0.0759	7.09305	1.42895	0.1128
2	2.807	BB	0.0614	9.14099	2.34993	0.1453
3	3.262	VV	0.0641	6240.91650	1513.67029	99.2294
4	3.736	VB	0.0877	22.84978	3.82422	0.3633
5	6.017	BB	0.1322	9.38072	1.03008	0.1492

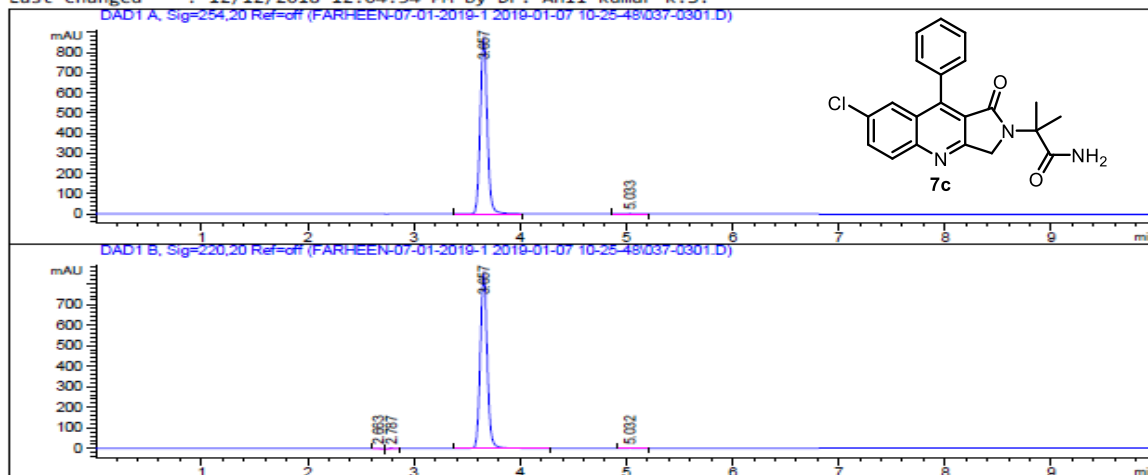
Totals : 6289.38104 1522.30347

Figure S98. HPLC of compound 7c

Data File C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\037-0301.D
 Sample Name: S-019-0004

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    3
Acq. Instrument : Instrument 1                 Location  : Vial 37
Injection Date  : 1/7/2019 10:50:01 AM        Inj       :    1
                                                Inj Volume: 5.000 µl
Method         : C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\ACN-WATER-90-10.M
                (Sequence Method)
Last changed   : 12/12/2018 12:04:34 PM by Dr. Anil Kumar K.S.
  
```



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.657	BB	0.0713	3970.32495	868.97247	99.8229
2	5.033	BB	0.0909	7.04517	1.19238	0.1771

Totals : 3977.37012 870.16485

Instrument 1 1/7/2019 12:20:43 PM Dr. Anil Kumar K.S.

Page 1 of 2

Signal 2: DAD1 B, Sig=220,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.663	BB	0.0725	6.88353	1.47320	0.1762
2	2.787	BB	0.0591	11.17208	3.02201	0.2860
3	3.657	BB	0.0714	3881.49805	848.52203	99.3683
4	5.032	BB	0.0893	6.61964	1.14768	0.1695

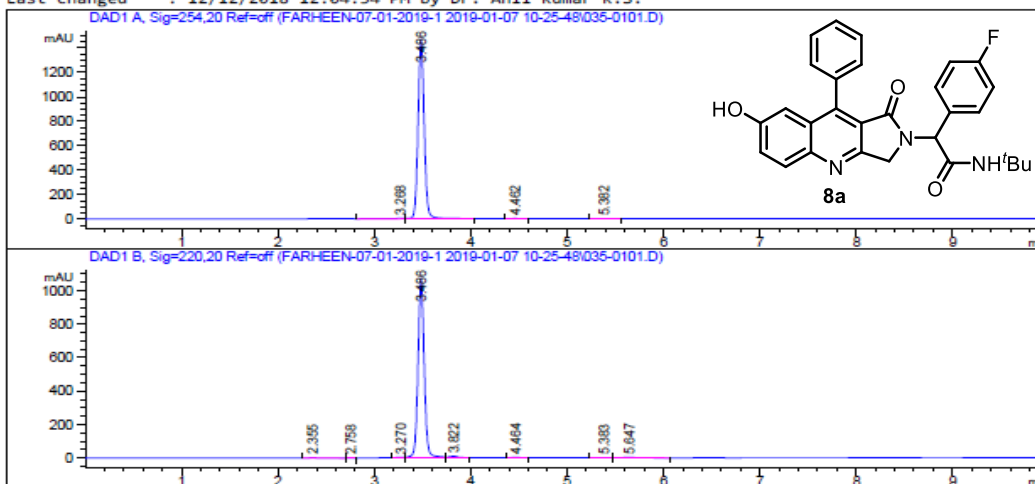
Totals : 3906.17330 854.16492

Figure S99. HPLC of compound 8a

Data File C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\035-0101.D
 Sample Name: S-019-0002

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    1
Acq. Instrument : Instrument 1                   Location  : Vial 35
Injection Date  : 1/7/2019 10:26:59 AM          Inj       :    1
                                                    Inj Volume: 5.000 µl
Acq. Method    : C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\ACN-WATER-90-10.M
Last changed   : 12/12/2018 12:04:34 PM by Dr. Anil Kumar K.S.
Analysis Method: C:\CHEM32\1\METHODS\ACN-WATER-90-10.M
Last changed   : 12/12/2018 12:04:34 PM by Dr. Anil Kumar K.S.
  
```



Area Percent Report

```

Sorted By      : Signal
Multiplier     : 1.0000
Dilution       : 1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.268	BV	0.1134	32.70513	3.91652	0.4948
2	3.486	VB	0.0683	6547.66309	1461.54419	99.0623
3	4.462	BB	0.1008	10.74677	1.67659	0.1626
4	5.382	BV	0.1333	18.52433	2.17581	0.2803

Totals : 6609.63932 1469.31312

Signal 2: DAD1 B, Sig=220,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.355	BV	0.2264	33.66593	1.86660	0.6821
2	2.758	VB	0.0712	11.41082	2.40979	0.2312
3	3.270	BV	0.0695	11.36731	2.48075	0.2303
4	3.486	WV	0.0683	4774.40039	1065.34521	96.7399
5	3.822	VB	0.0875	41.48795	6.96486	0.8406
6	4.464	BB	0.1034	9.85346	1.52455	0.1997
7	5.383	BV	0.1298	16.62584	1.98339	0.3369
8	5.647	VB	0.1320	36.48479	3.86806	0.7393

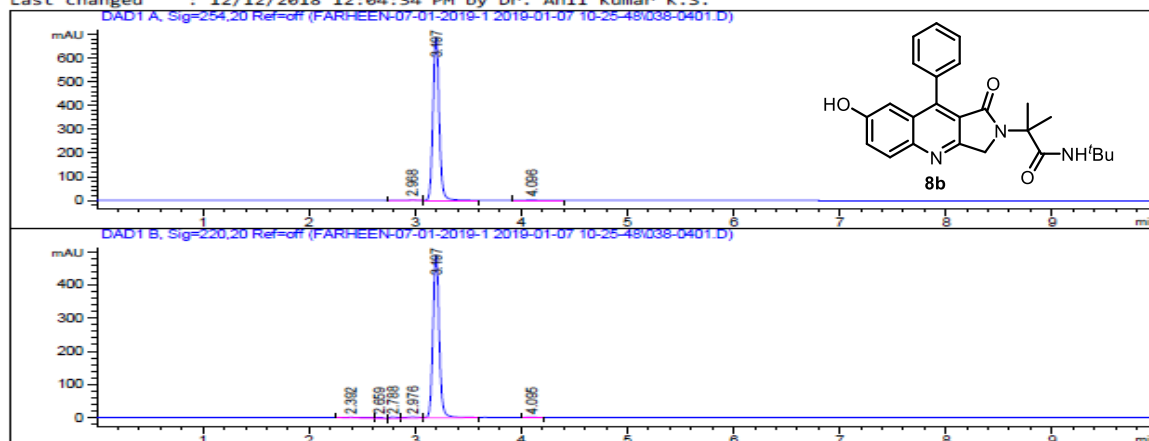
Totals : 4935.29649 1086.44322

Figure S100. HPLC of compound 8b

Data File C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\038-0401.D
 Sample Name: S-019-0005

```

=====
Acq. Operator   : Dr. Anil Kumar K.S.           Seq. Line :    4
Acq. Instrument : Instrument 1                  Location  : Vial 38
Injection Date  : 1/7/2019 11:01:30 AM         Inj       :    1
                                                Inj Volume: 5.000 µl
Method         : C:\CHEM32\1\DATA\FARHEEN-07-01-2019-1 2019-01-07 10-25-48\ACN-WATER-90-10.M
                (Sequence Method)
Last changed   : 12/12/2018 12:04:34 PM by Dr. Anil Kumar K.S.
  
```



Area Percent Report

```

=====
Sorted By      :      Signal
Multiplier     :      1.0000
Dilution       :      1.0000
Use Multiplier & Dilution Factor with ISTDs
  
```

Signal 1: DAD1 A, Sig=254,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.968	BV	0.1678	22.11630	1.69949	0.7762
2	3.197	VV	0.0636	2818.83057	691.14648	98.9256
3	4.096	BB	0.0796	8.49724	1.66354	0.2982

Totals : 2849.44410 694.50952

Instrument 1 1/7/2019 12:21:16 PM Dr. Anil Kumar K.S.

Page 1 of 2

Signal 2: DAD1 B, Sig=220,20 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.392	BV	0.2123	25.19151	1.48190	1.1881
2	2.659	VB	0.0825	13.54921	2.53064	0.6390
3	2.788	BV	0.0791	23.62584	4.36741	1.1142
4	2.976	W	0.1197	34.83565	3.92096	1.6429
5	3.197	VB	0.0638	2017.82727	492.11786	95.1629
6	4.095	BB	0.0741	5.36289	1.15544	0.2529

Totals : 2120.39238 505.57421