Supporting Information

Novel Approach Toward Synthesis of Skeletally Diverse Benzimidazole-pyrrolo[1,2-a]quinoxalines by S_NAr / Pictet-Spengler Reaction Under Focused Microwave Irradiation

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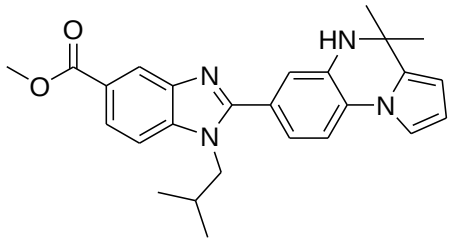
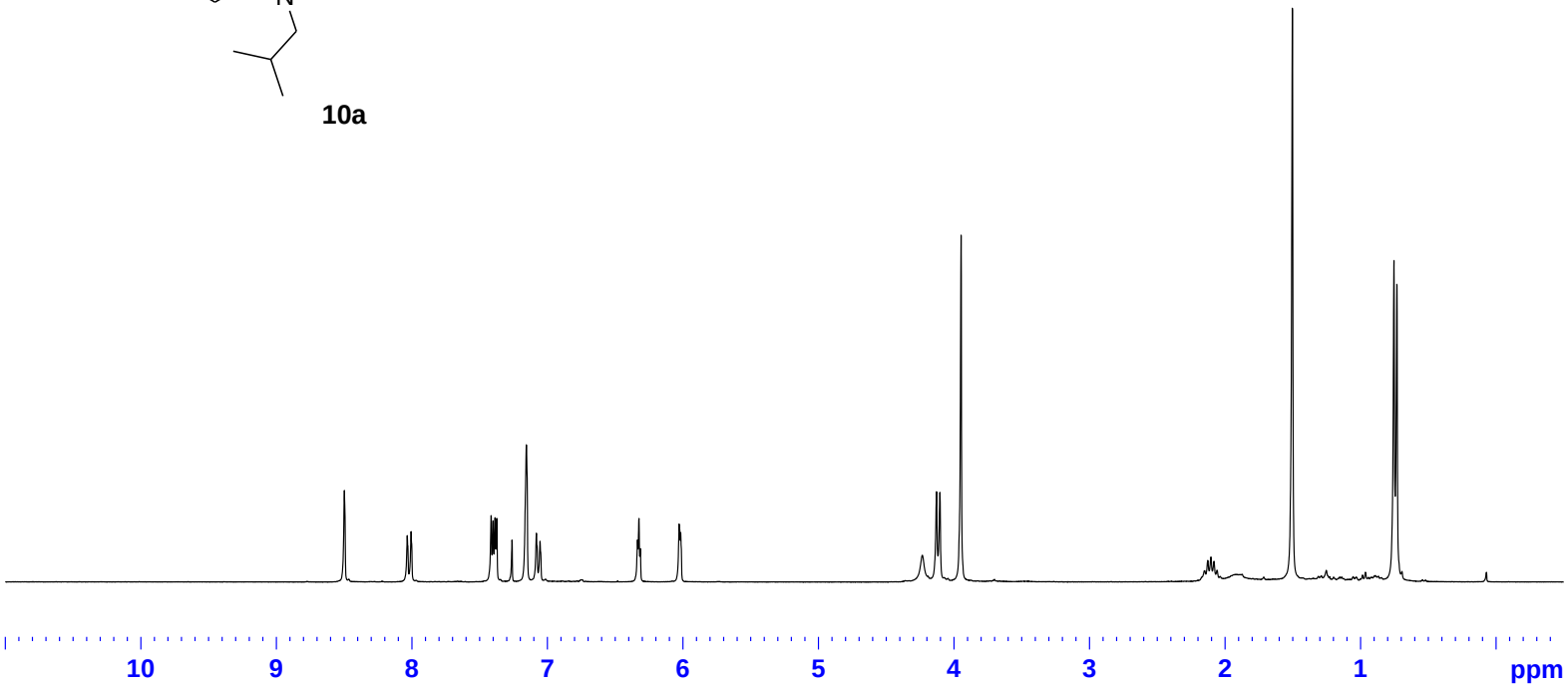
General Methods

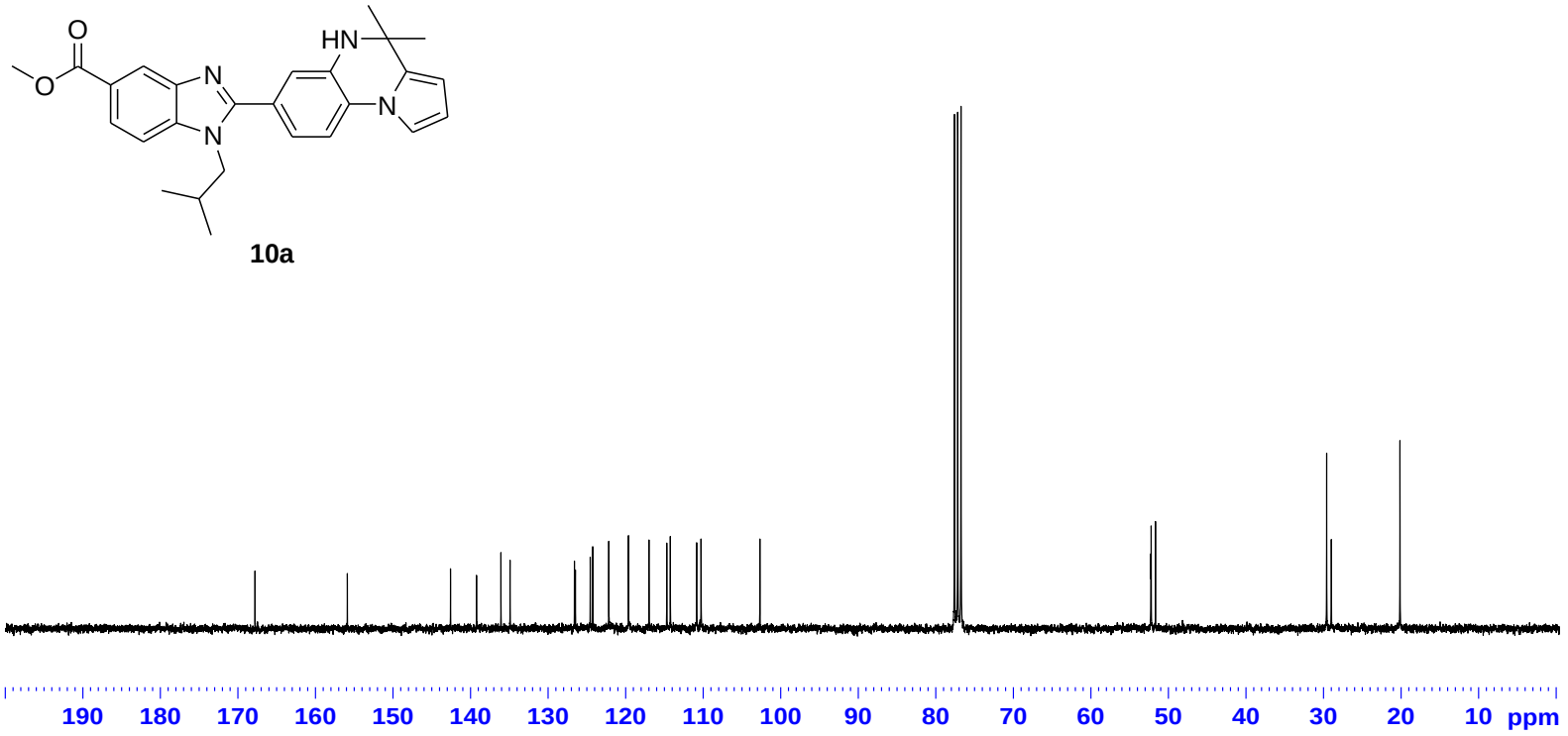
Dichloromethane and chloroform was distilled from calcium hydride before use. All reactions were performed under an inert atmosphere with unpurified reagents and dry solvents. Analytical thin-layer chromatography (TLC) was performed using 0.25 mm silica gel-coated Kieselgel 60 F254 plates. Flash chromatography was performed using the indicated solvent and silica gel 60 (Merck, 230-400 mesh). All the microwave experiments were conducted in a Biotage initiator sealed vessel under optimized reaction conditions of power and pressure. ^{1}H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded on a Bruker DRX-300 spectrometer. Chemical shifts are reported in parts per million (ppm) on the δ scale from an internal standard. High-resolution mass spectra (HRMS) were recorded on a JEOL TMS-HX 110 mass spectrometer. Analytical HPLC analyses were recorded with UV detection at λ=254nm (column: Sphereclone 5μ Si (250 x 4.6 mm).



10a

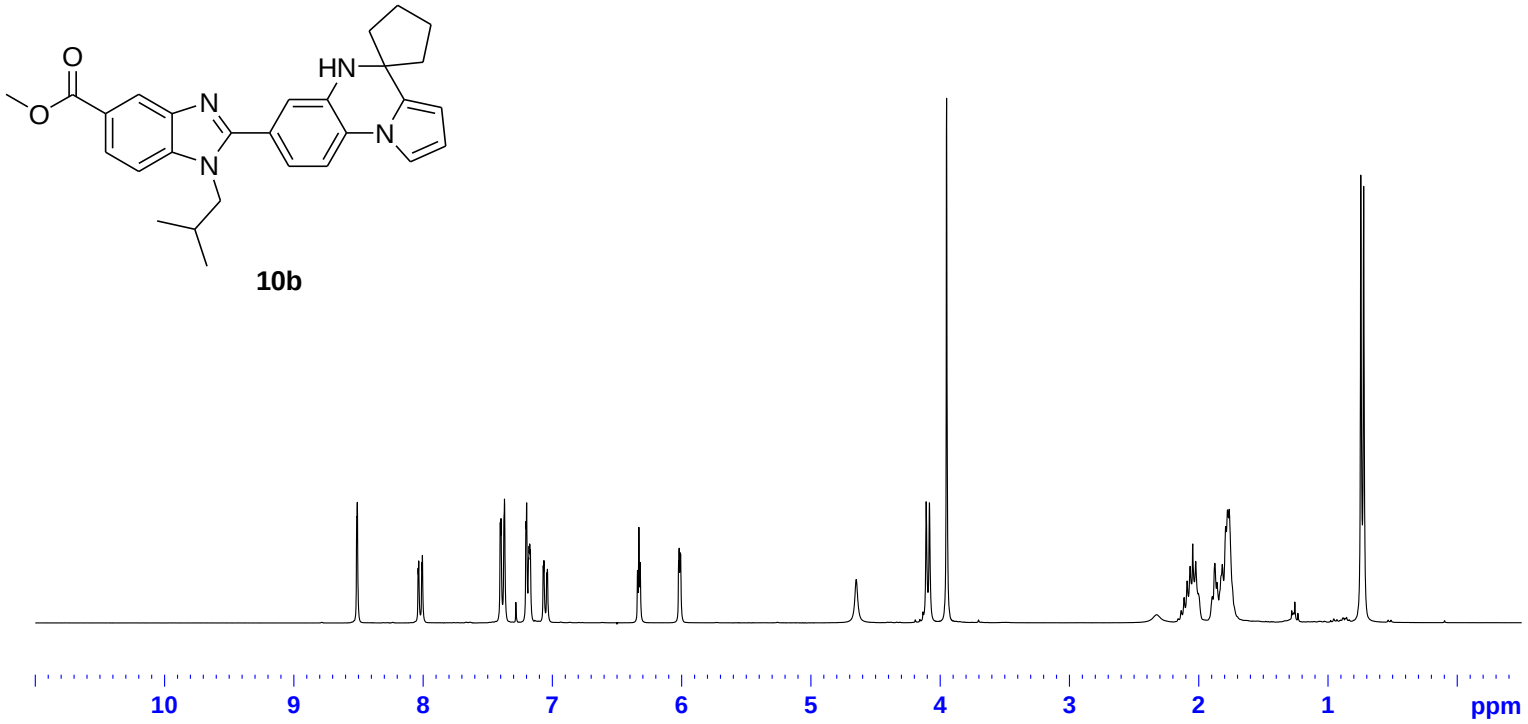


^{1}HNMR spectrum (300 MHz) of compound 10a in $CDCl_3$



10a

^{13}C NMR spectrum (75 MHz) of compound 10a in $CDCl_3$



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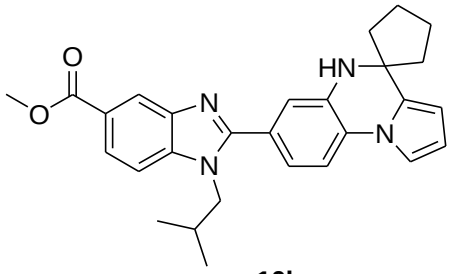
^{1}HNMR spectrum (300 MHz) of compound 10b in $CDCl_3$



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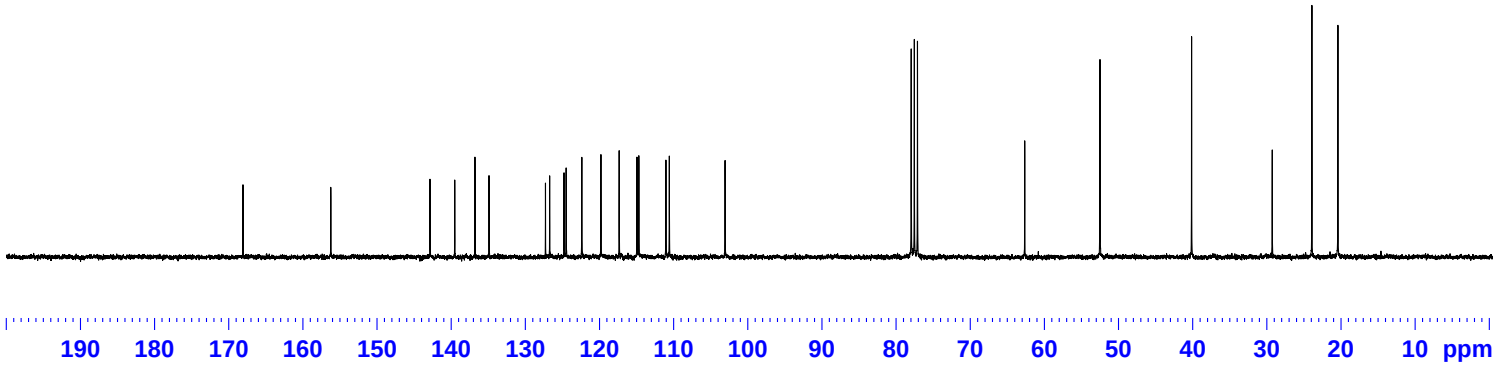

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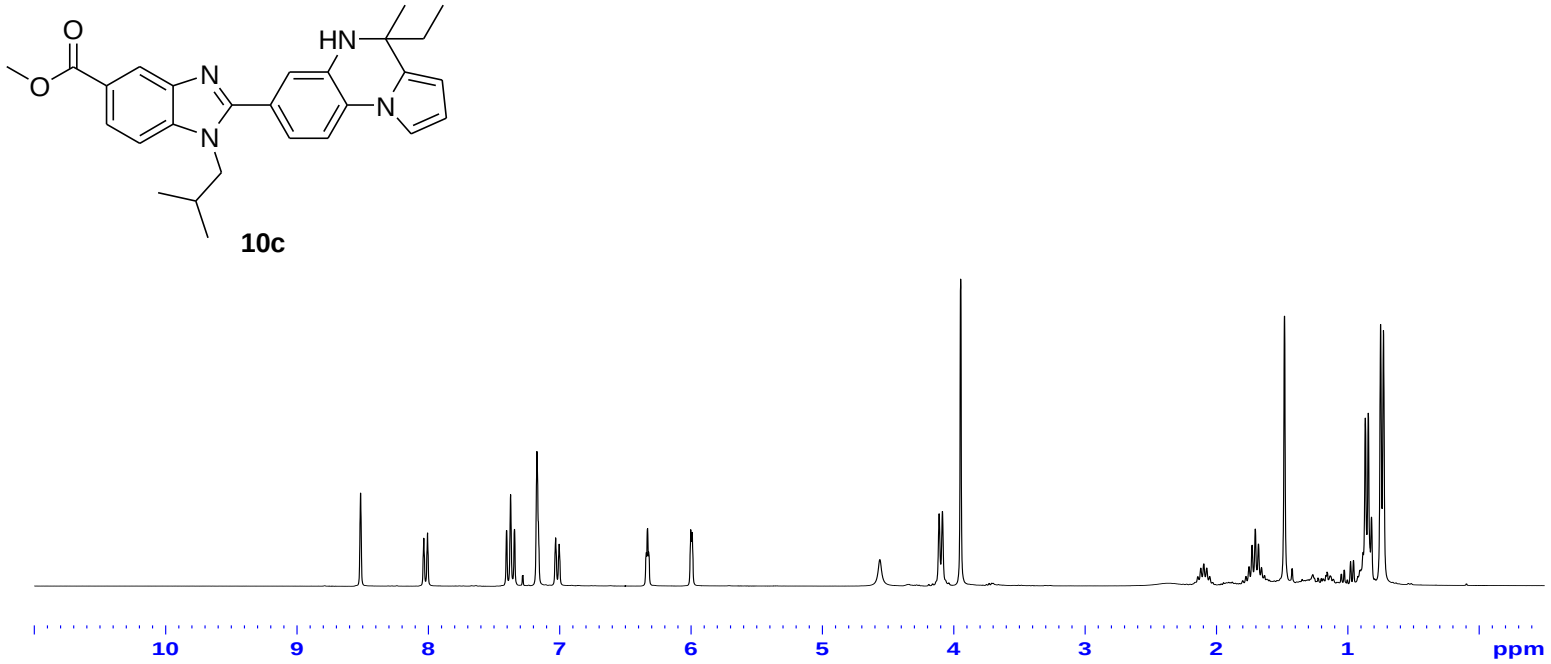

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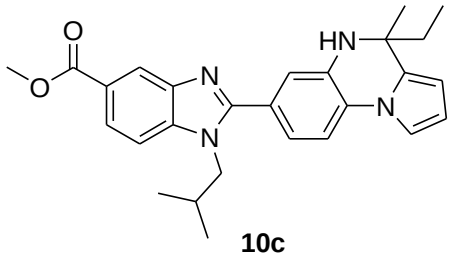
^{1}HNMR spectrum (300 MHz) of compound 10c in $CDCl_3$



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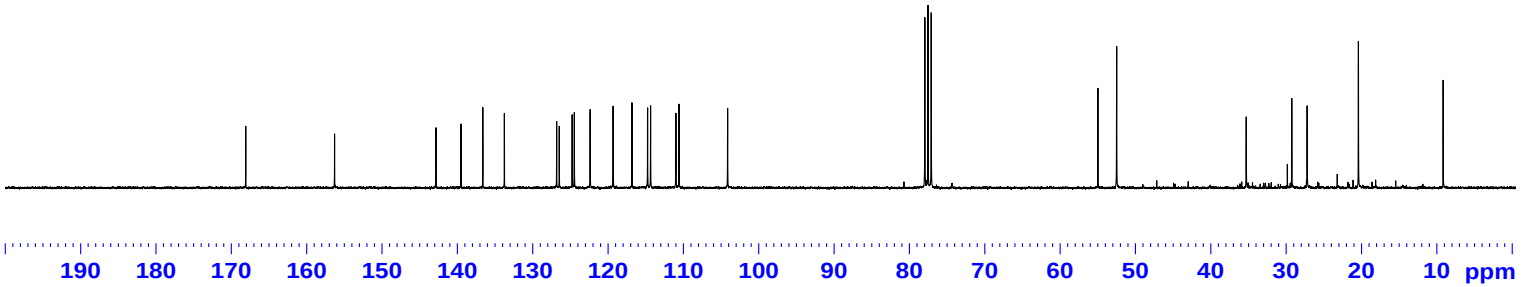
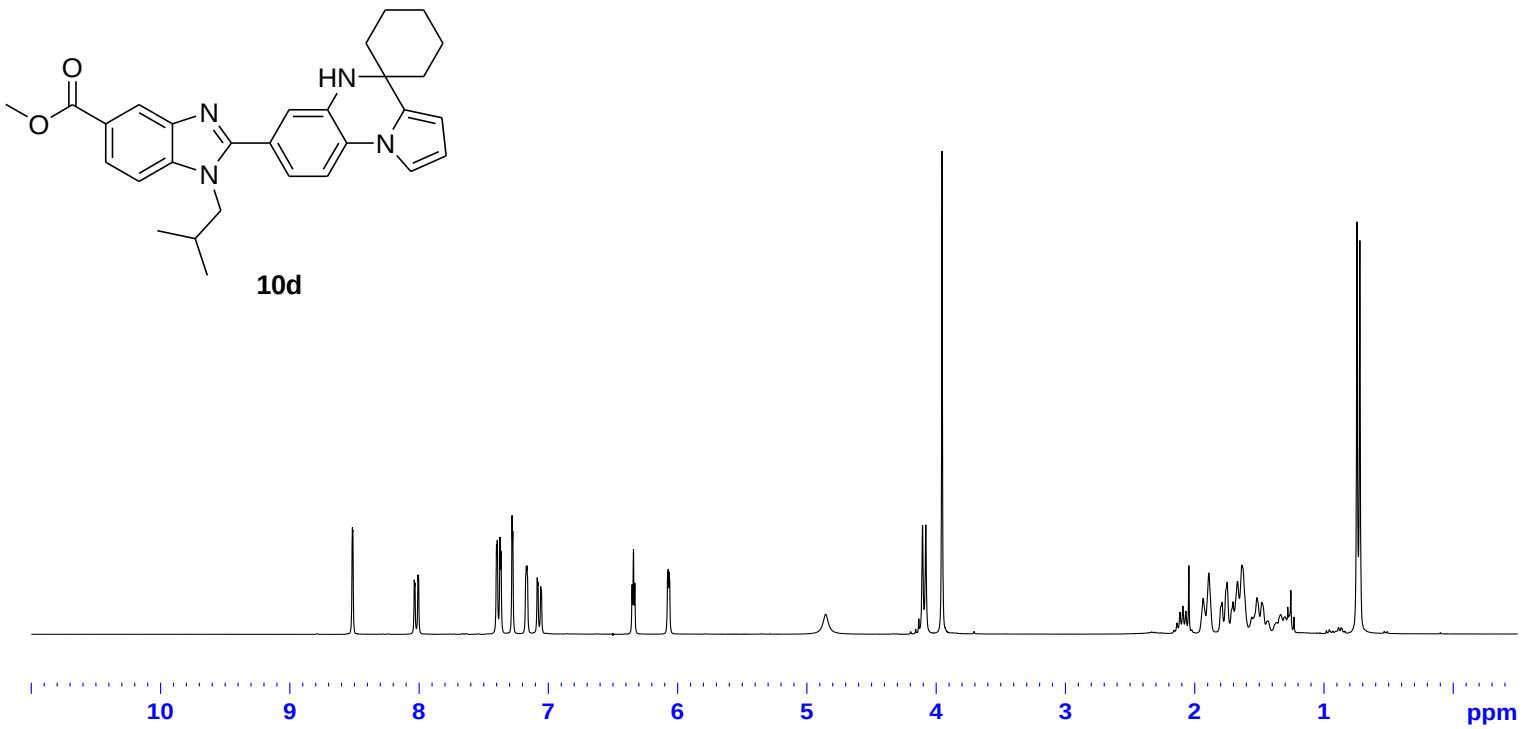


^{13}C NMR spectrum (75 MHz) of compound 10c in $CDCl_3$



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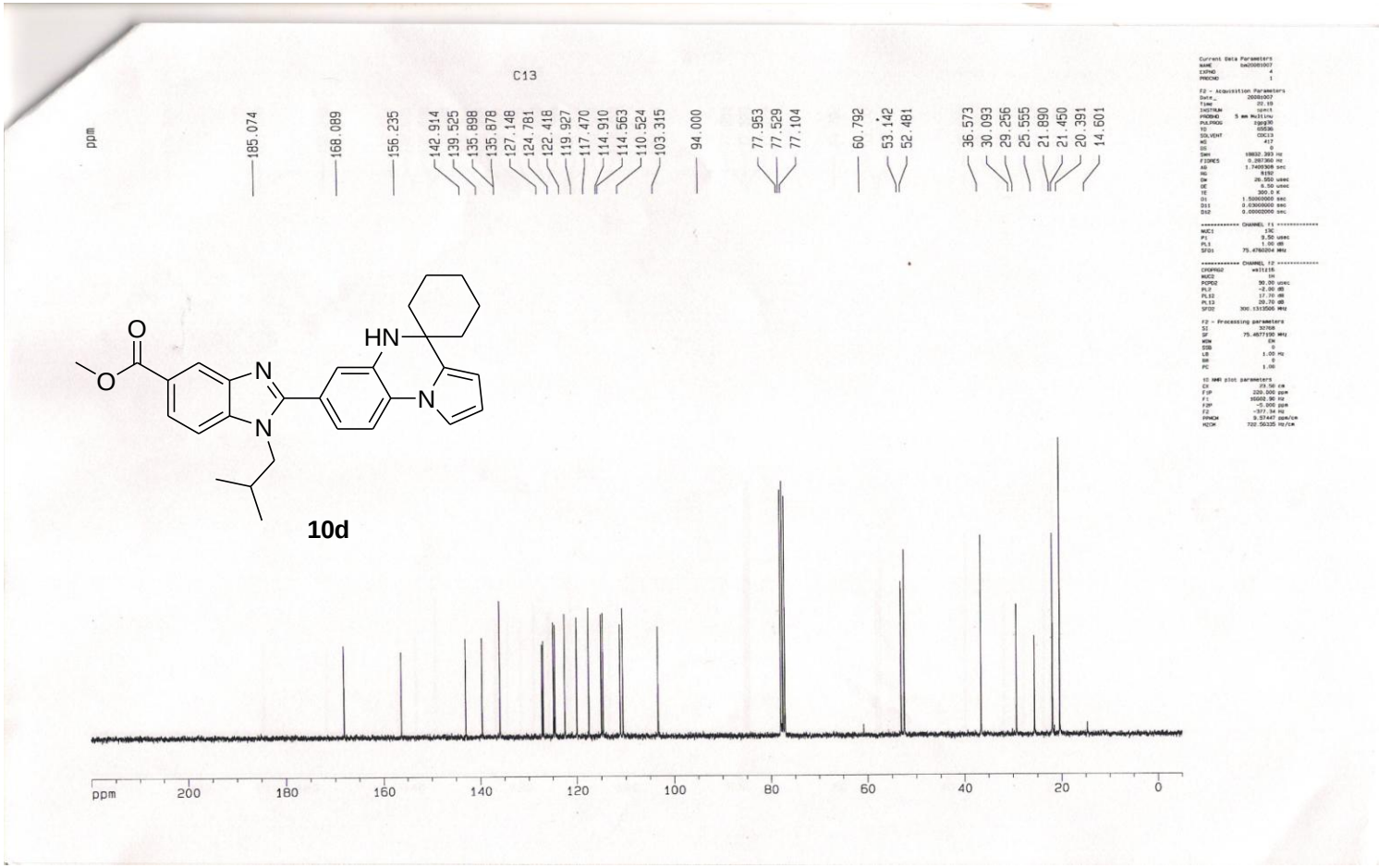
^{1}HNMR spectrum (300 MHz) of compound 10d in $CDCl_3$



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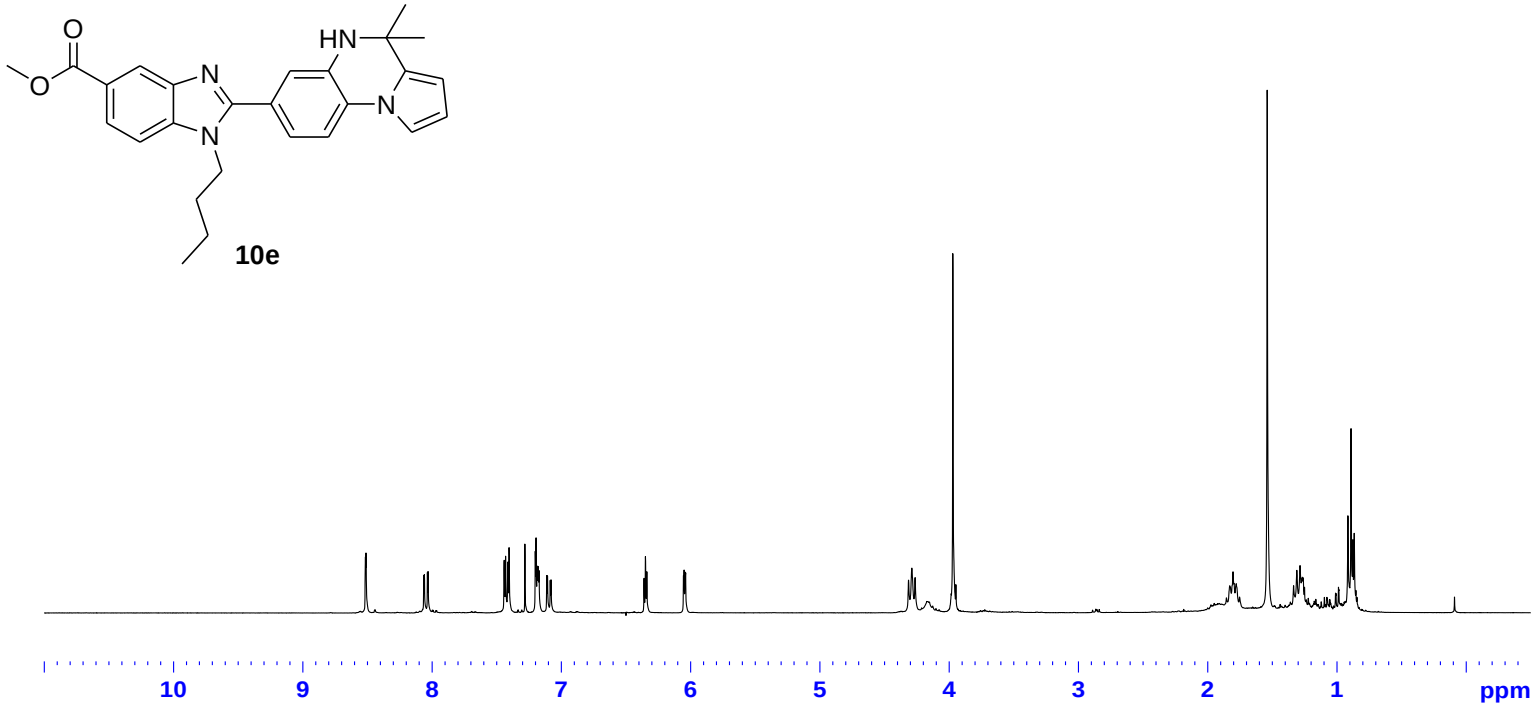

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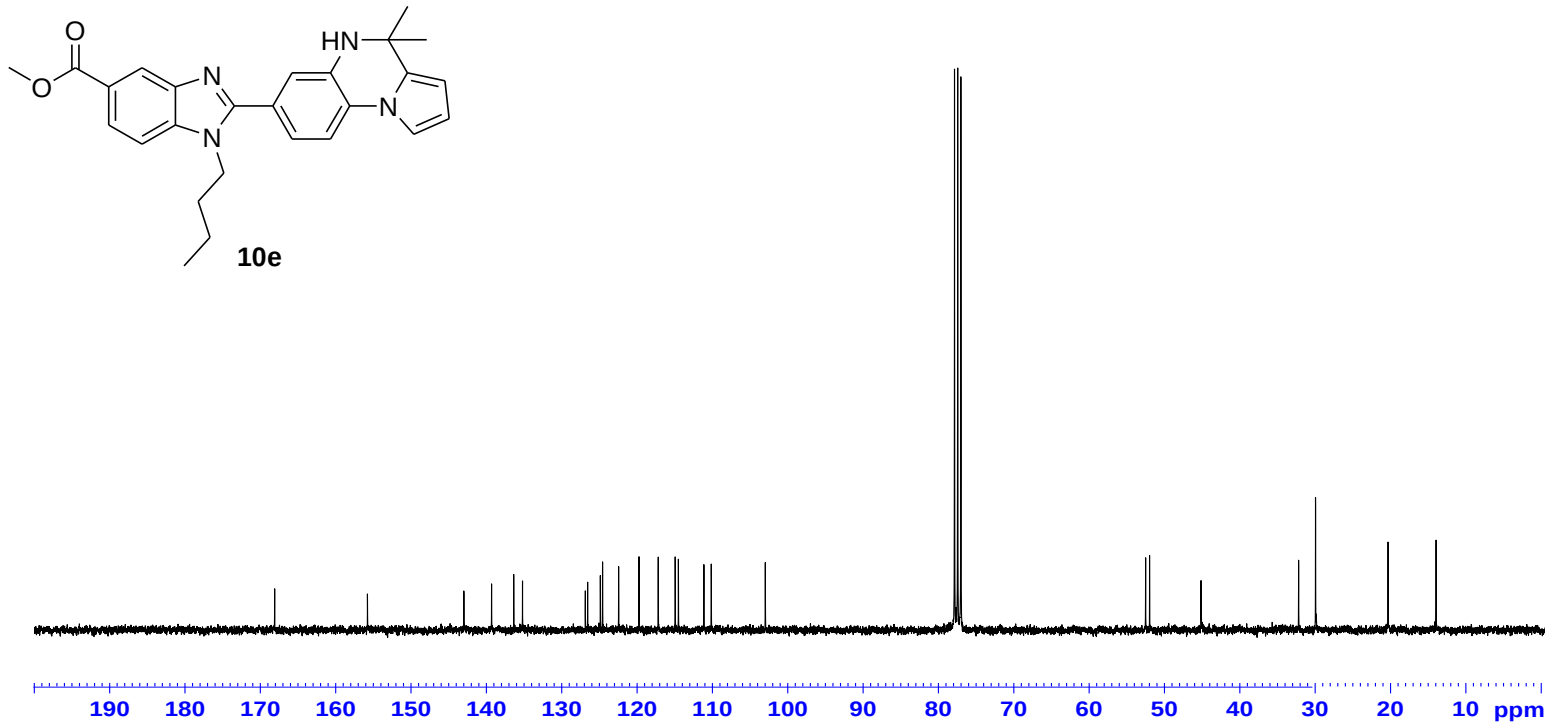

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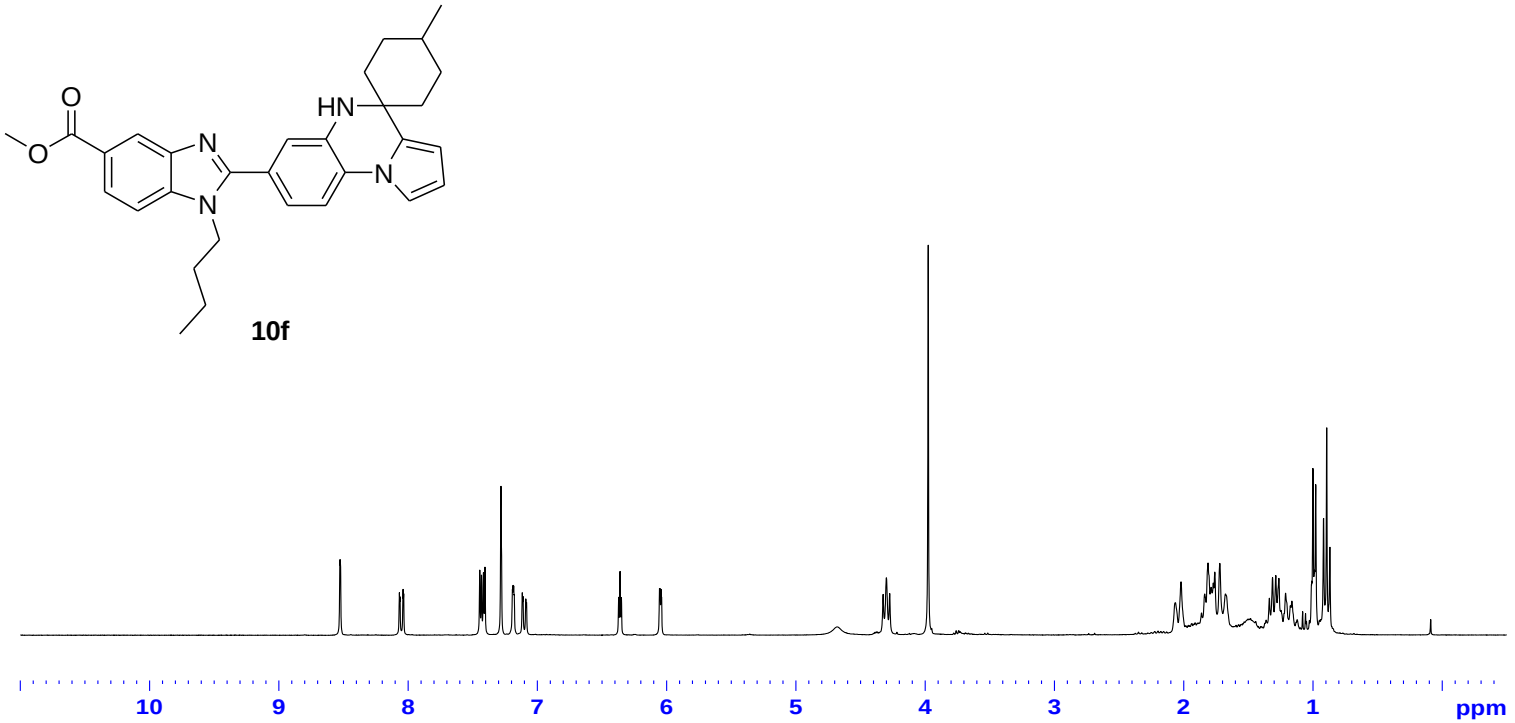

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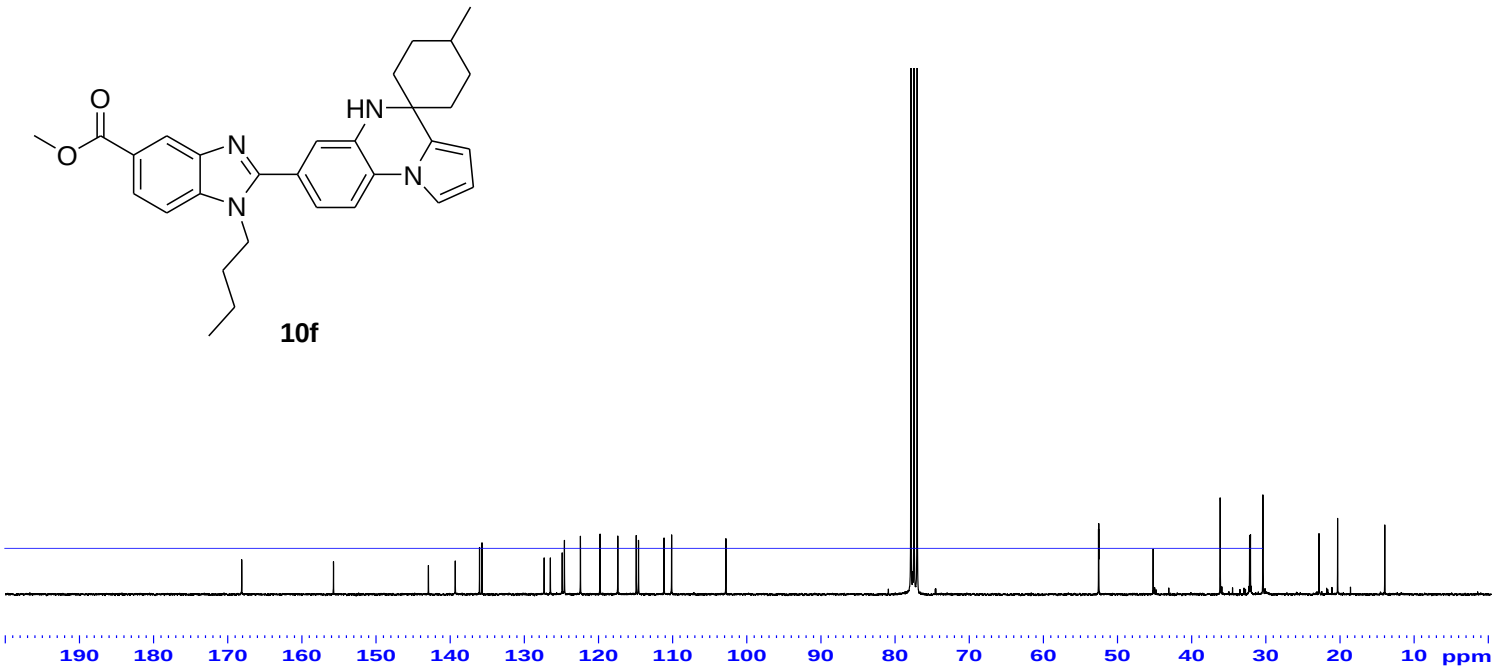

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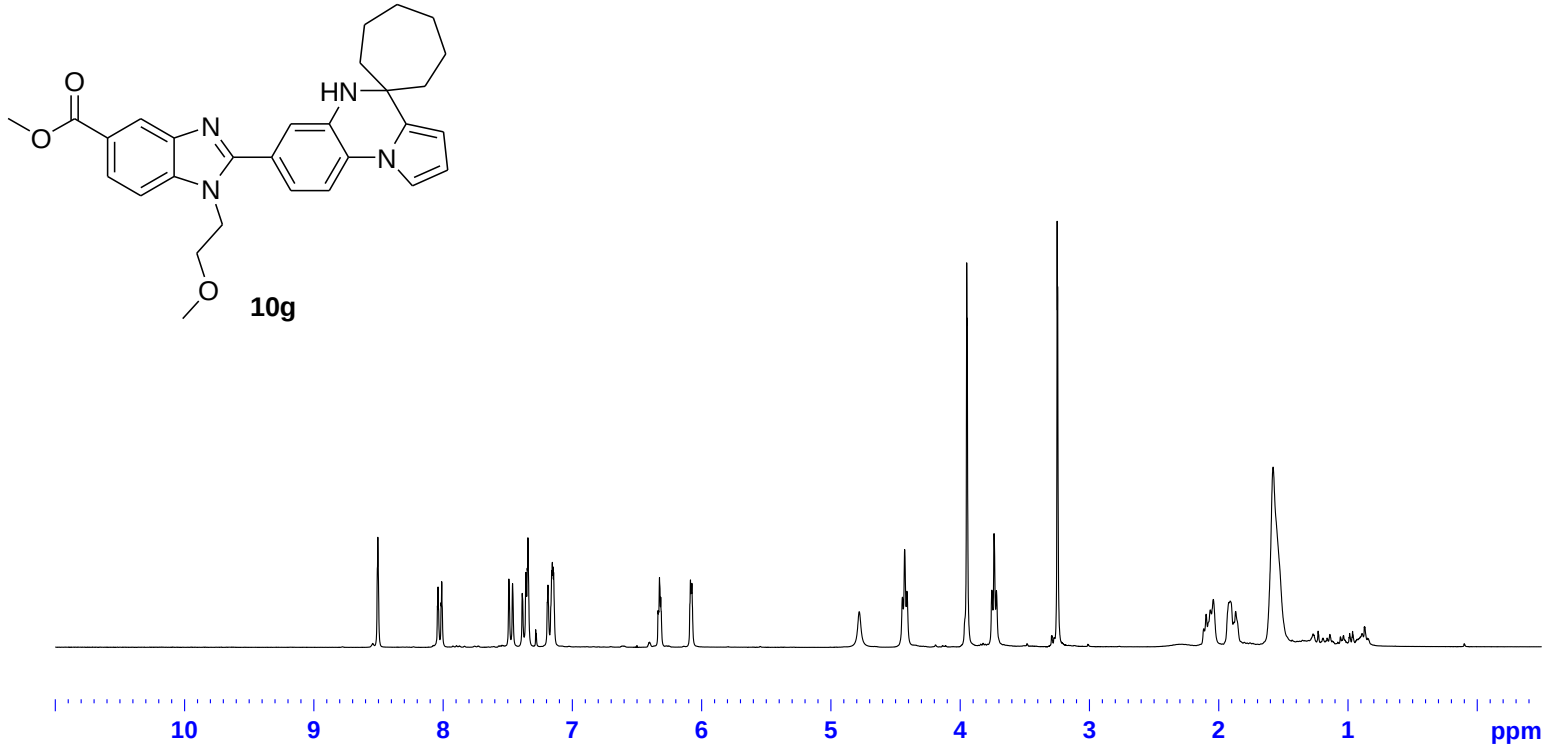
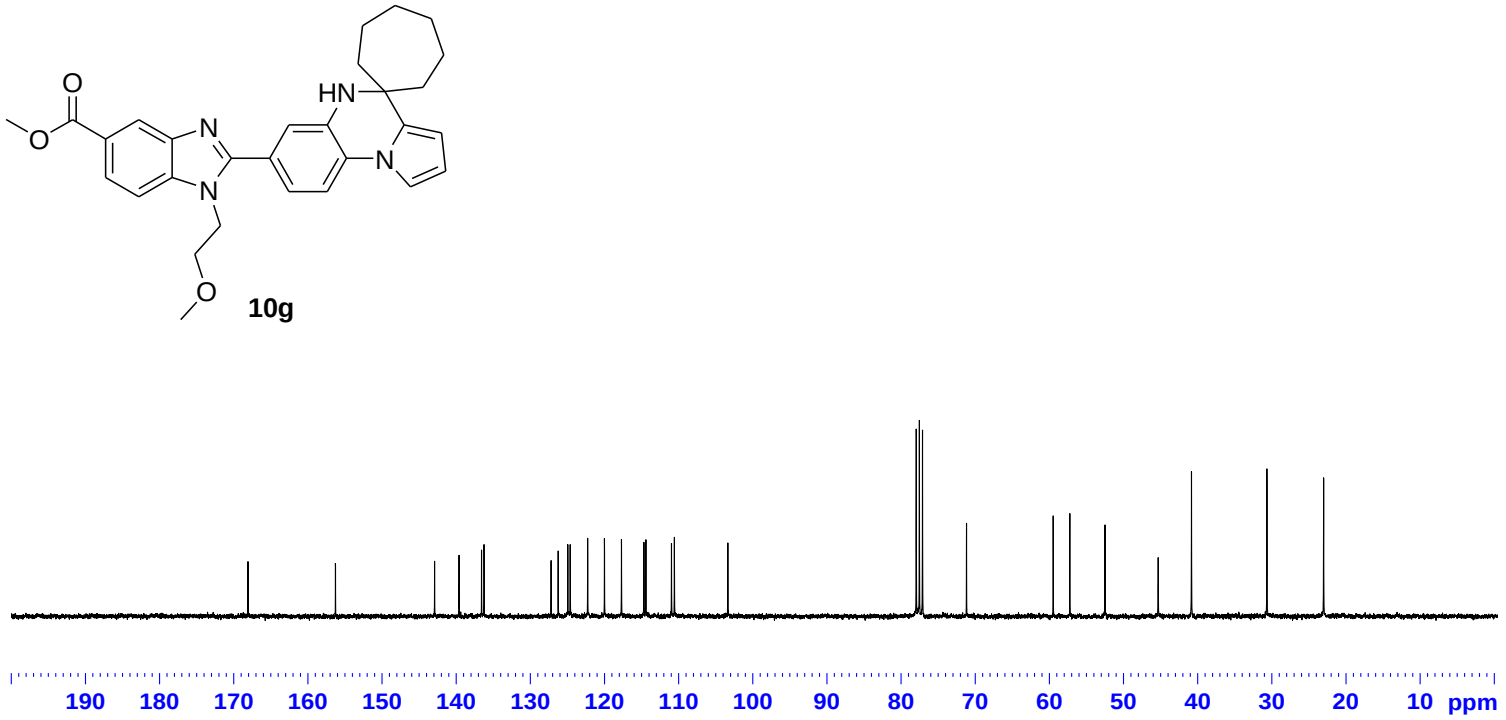
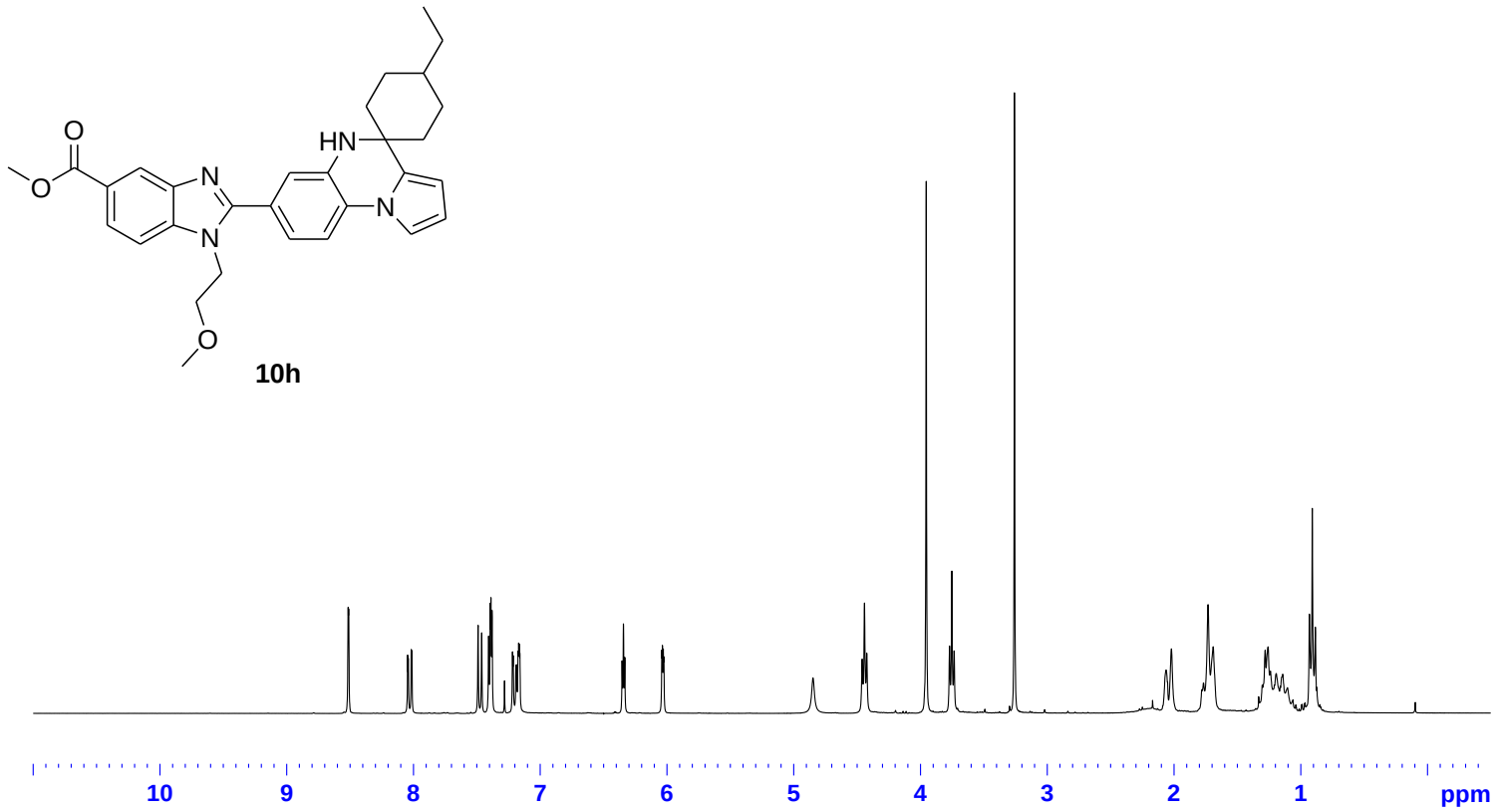


^{1}HNMR spectrum (300 MHz) of compound 10g in $CDCl_3$



^{13}C NMR spectrum (75 MHz) of compound 10g in $CDCl_3$



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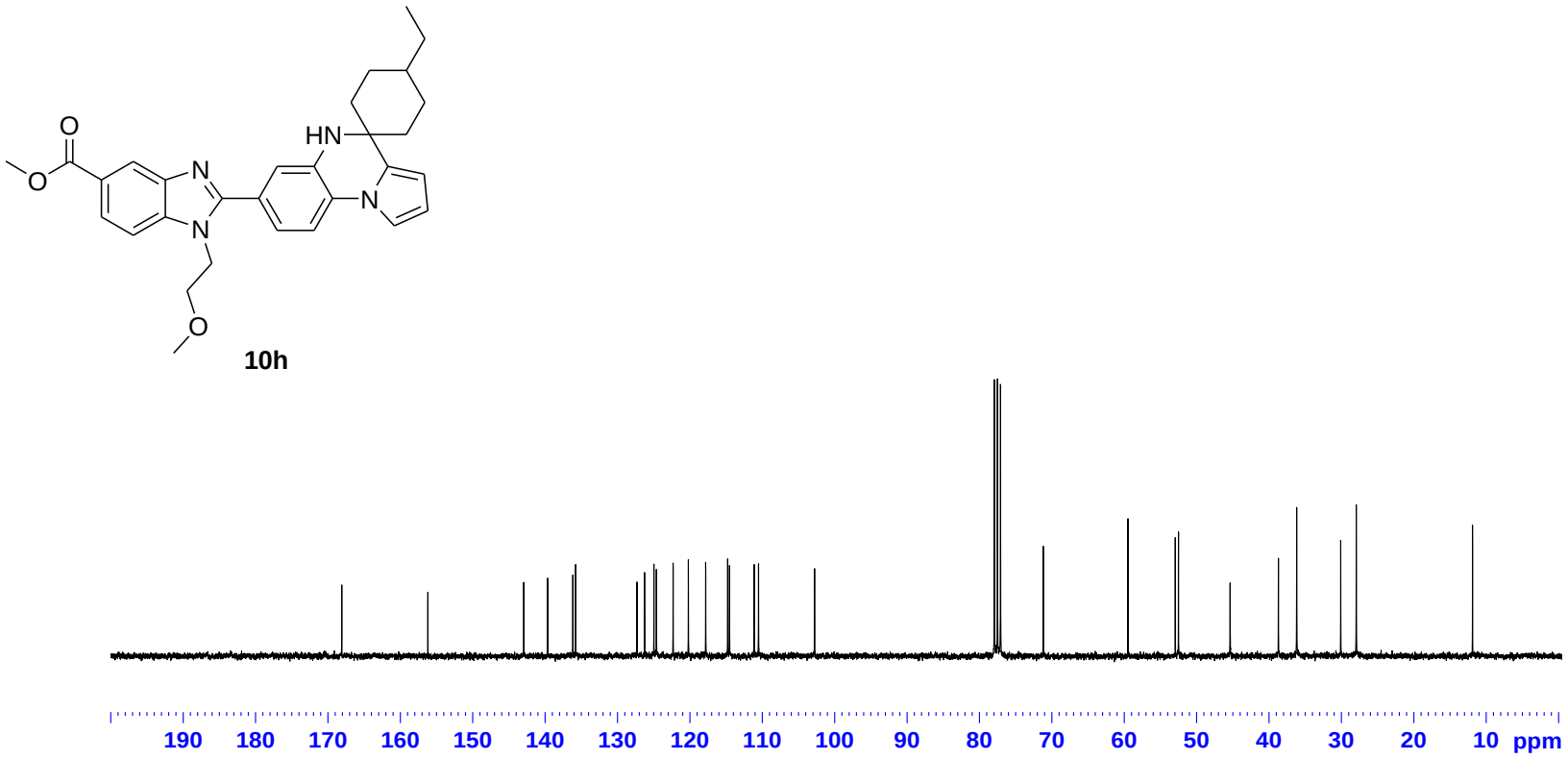

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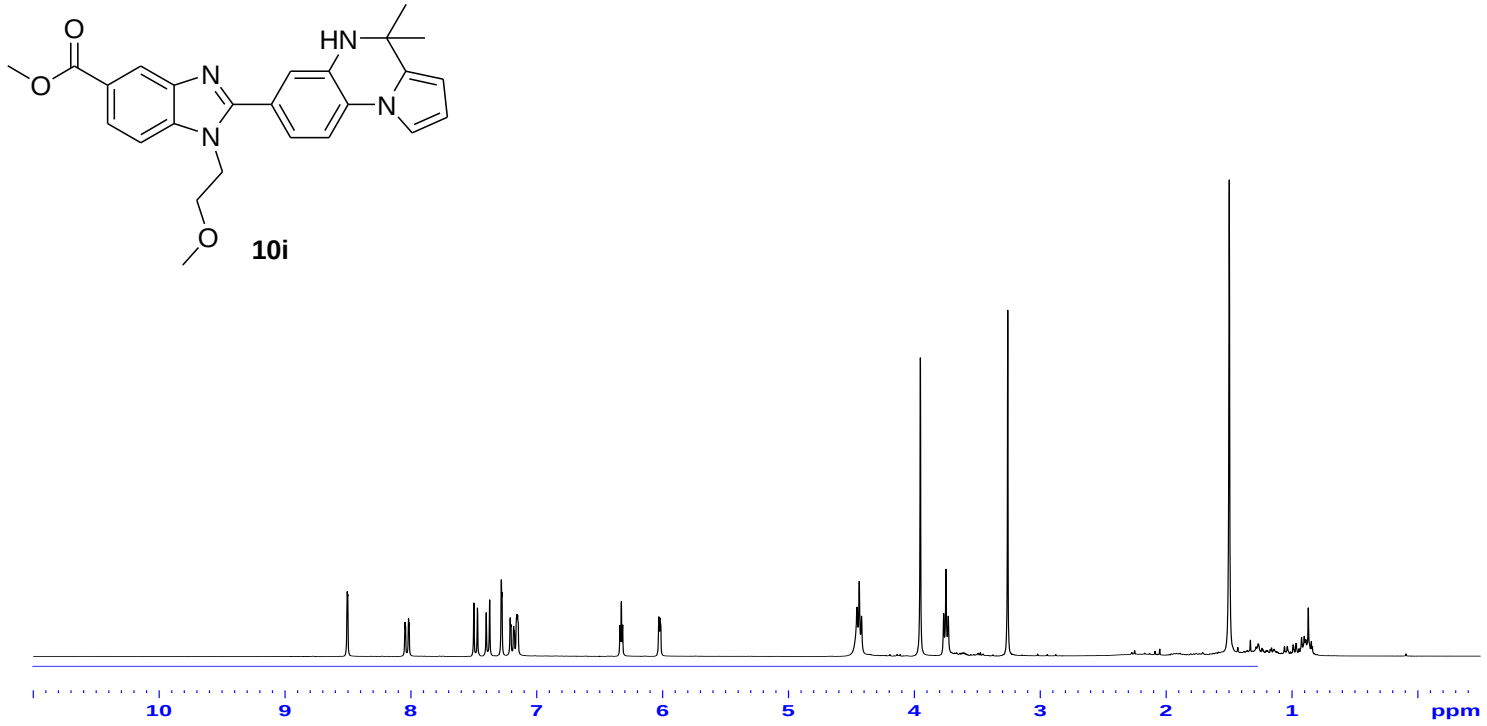

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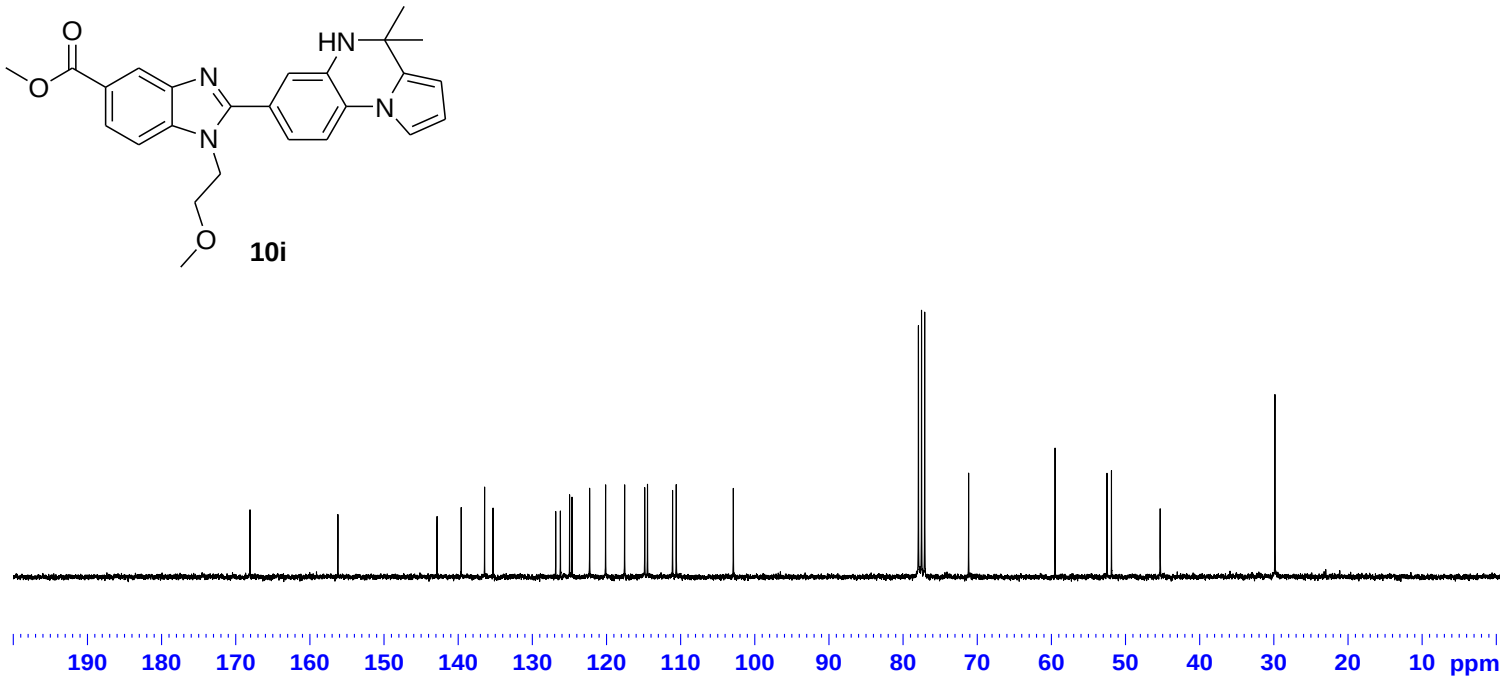

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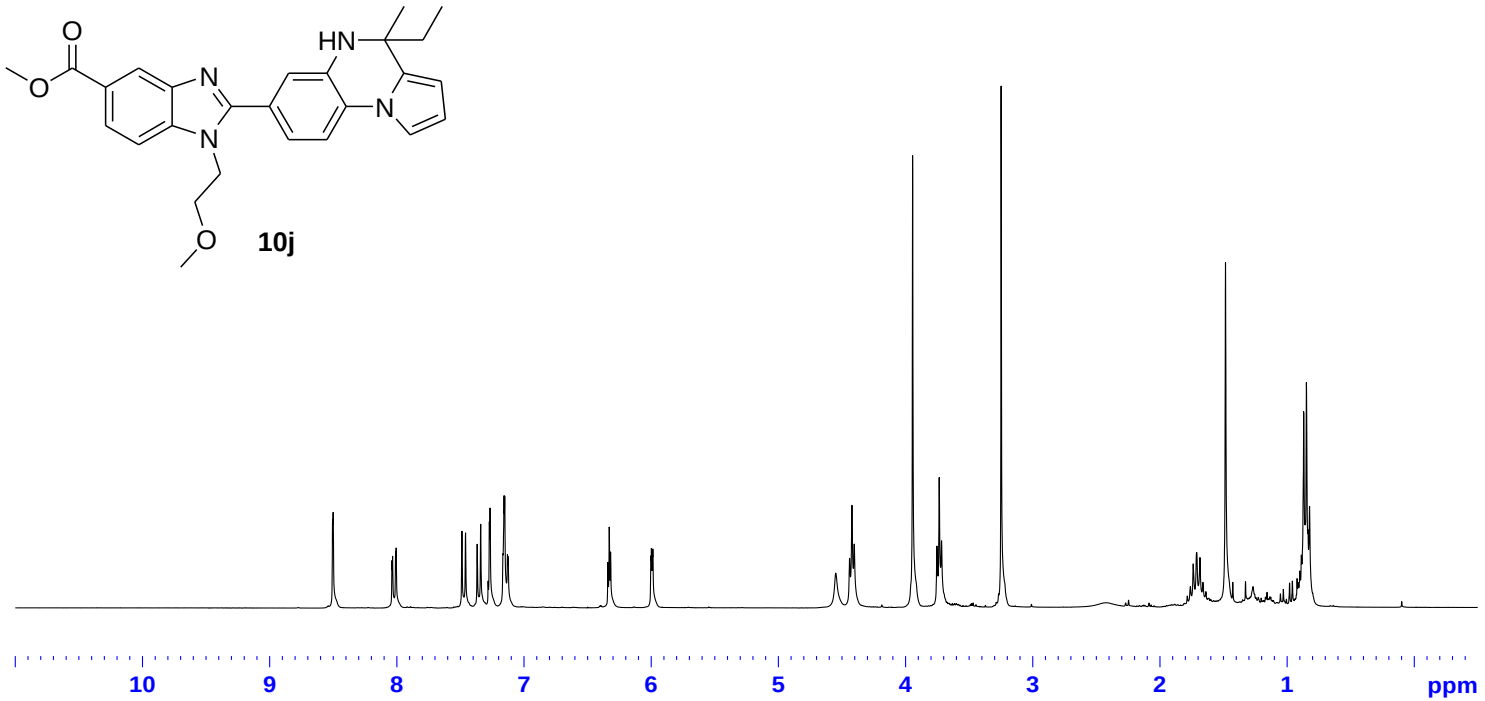

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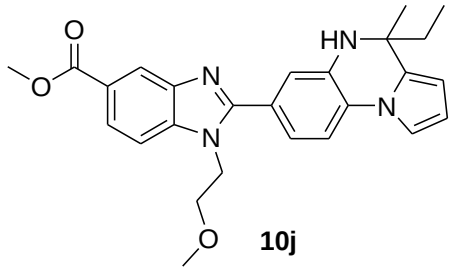
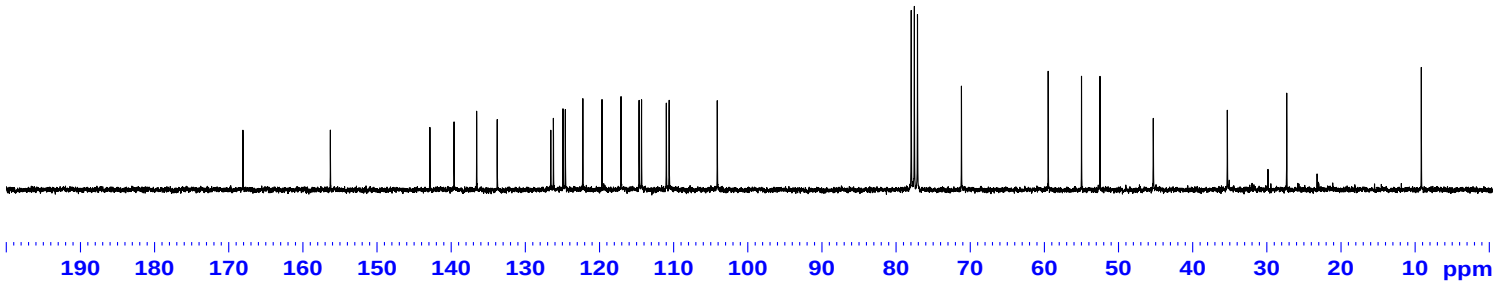


10j



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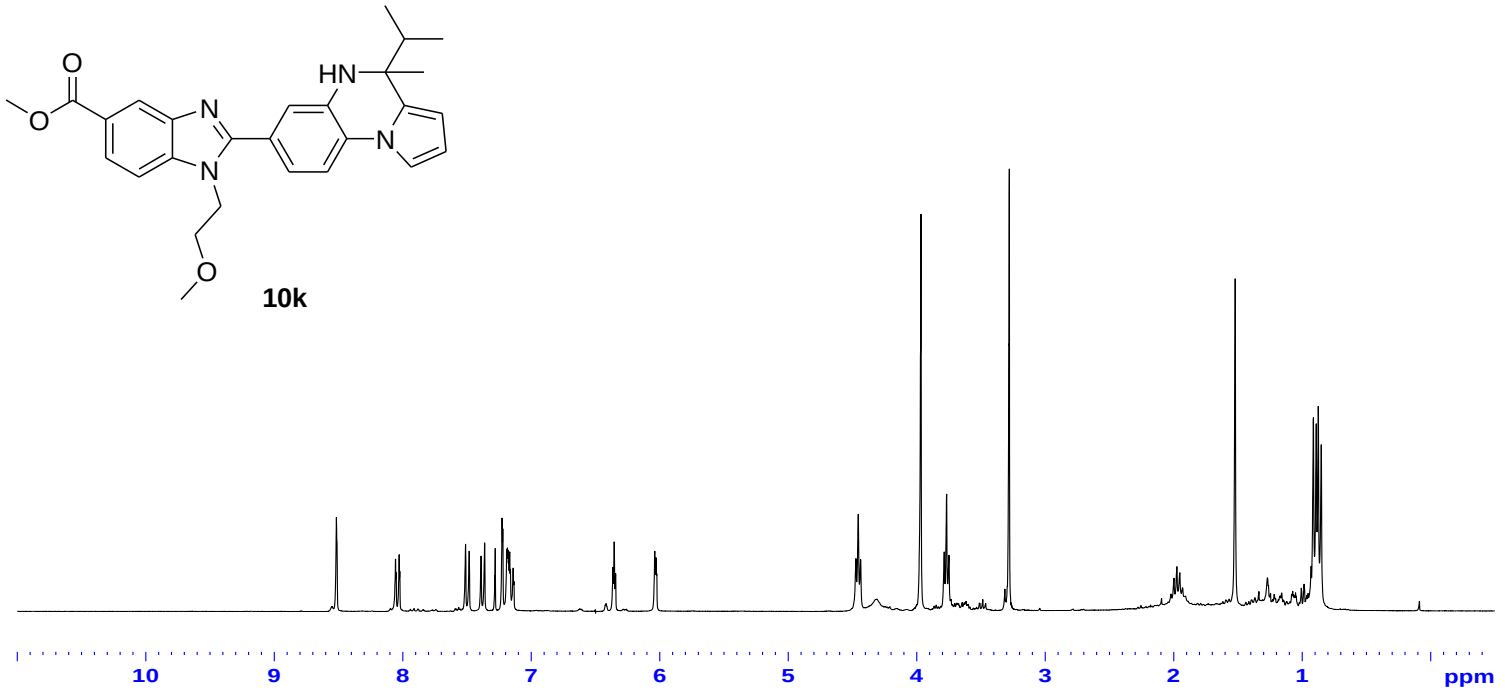

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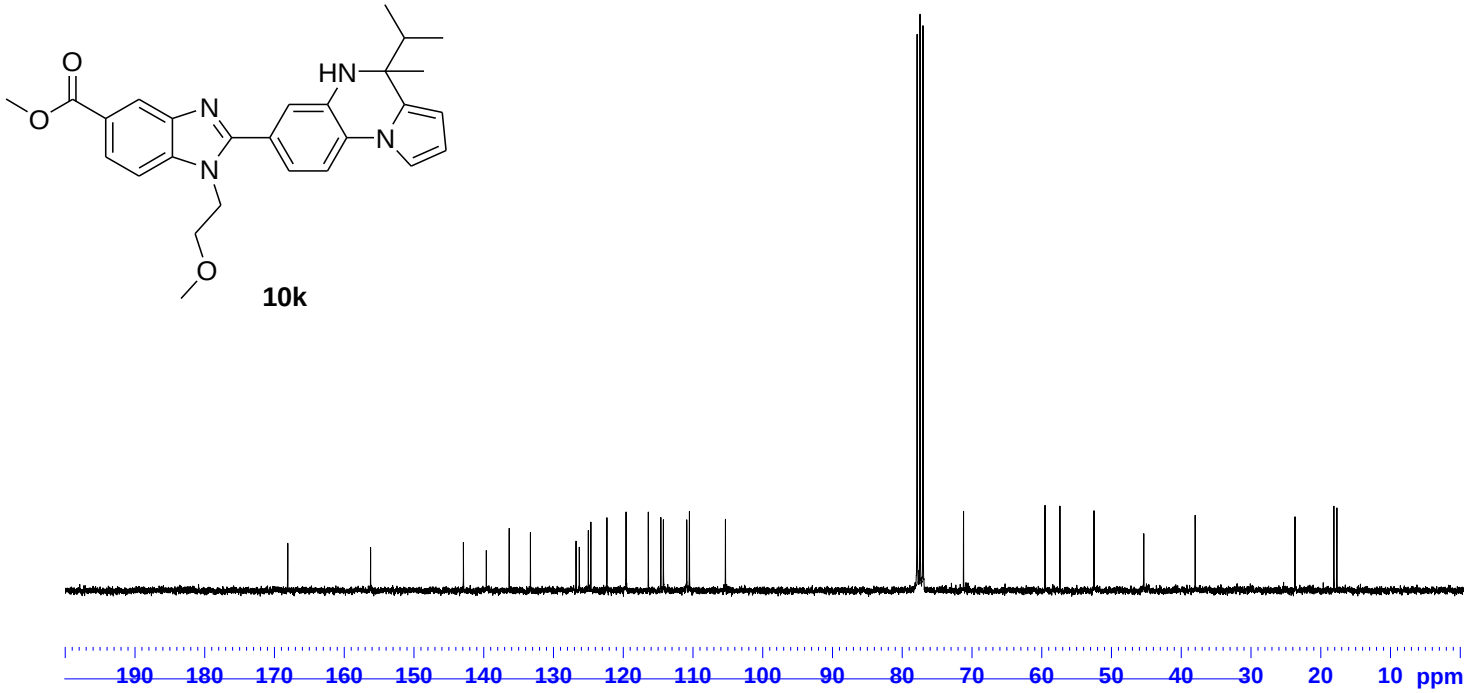

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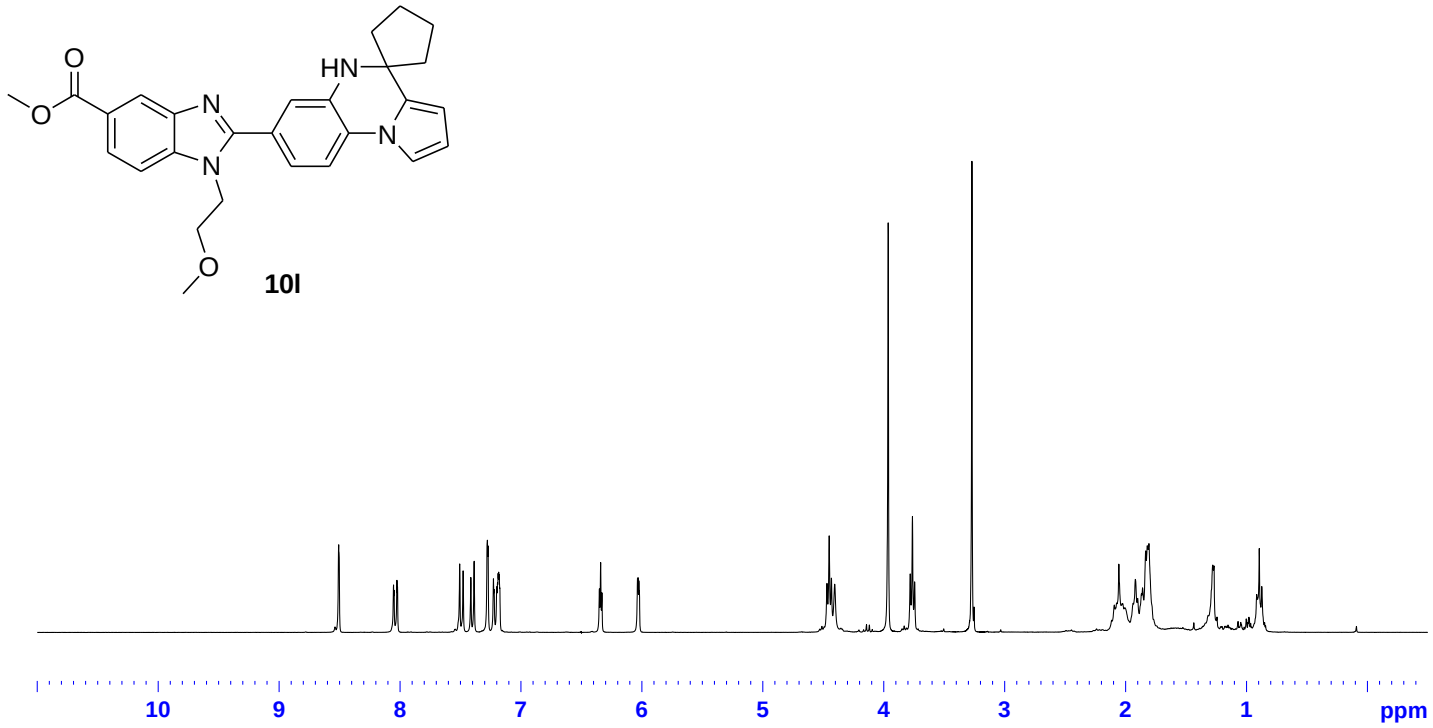

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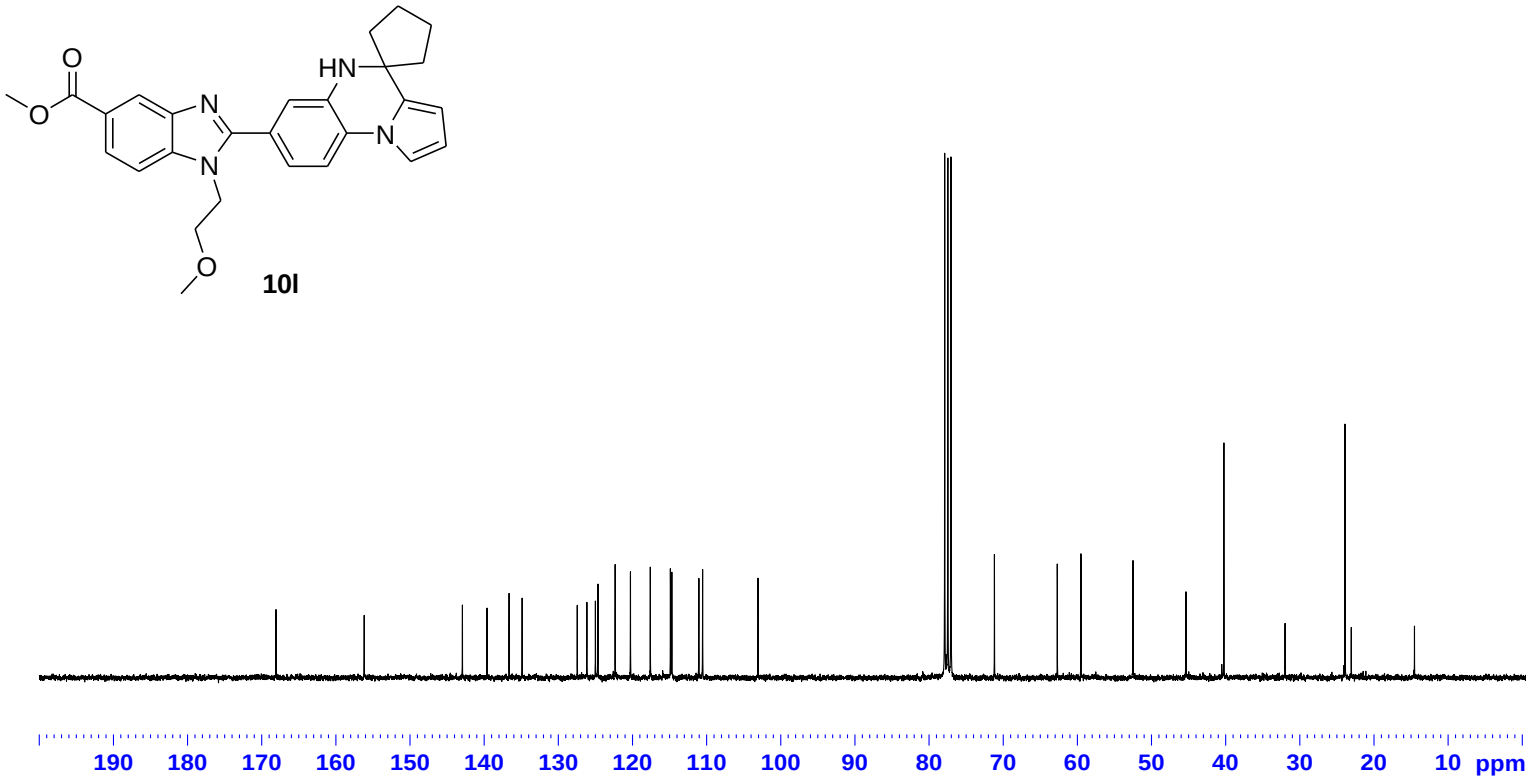

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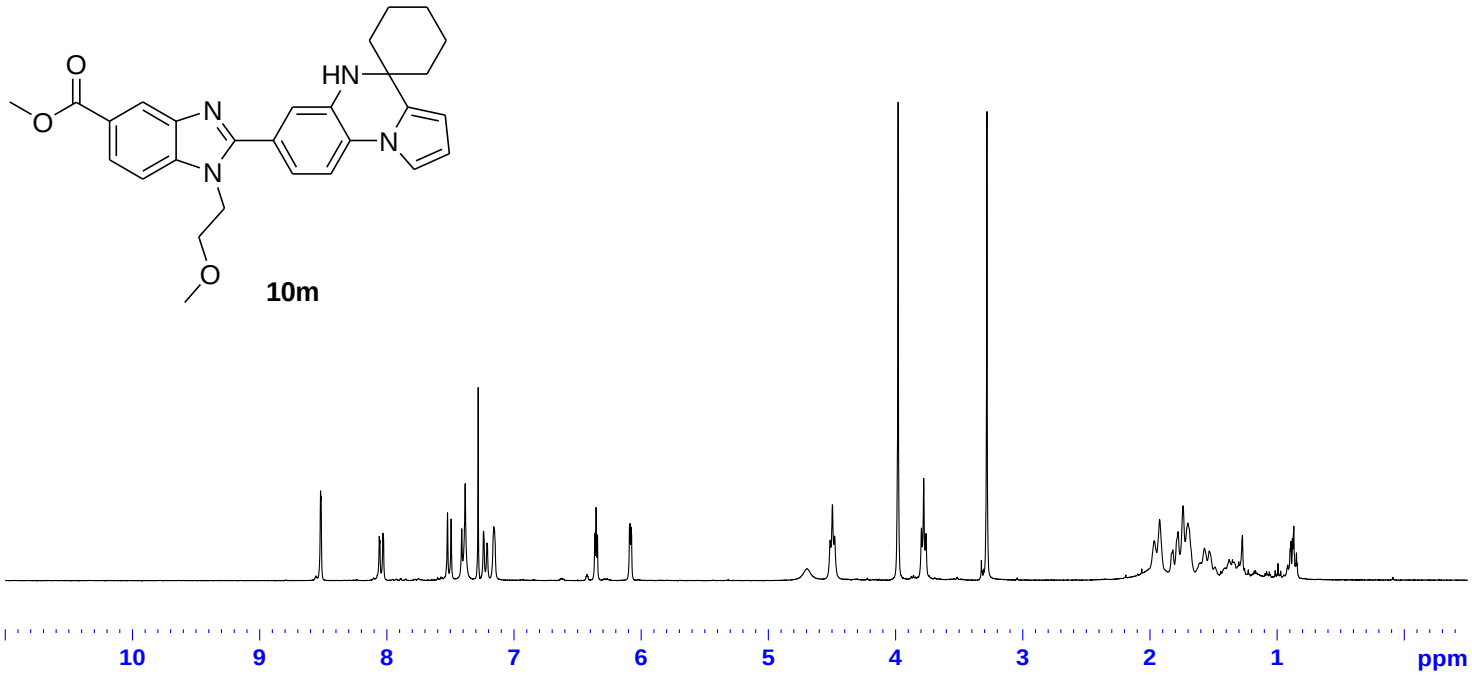

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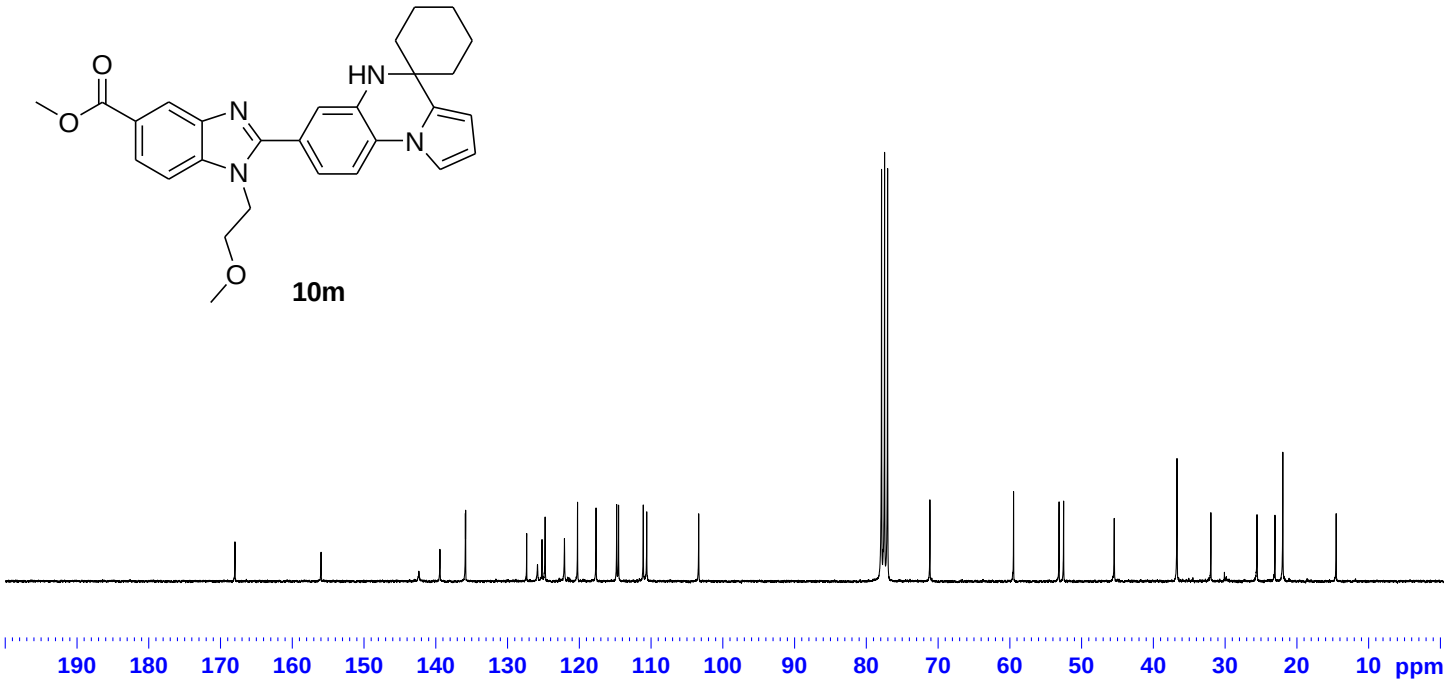

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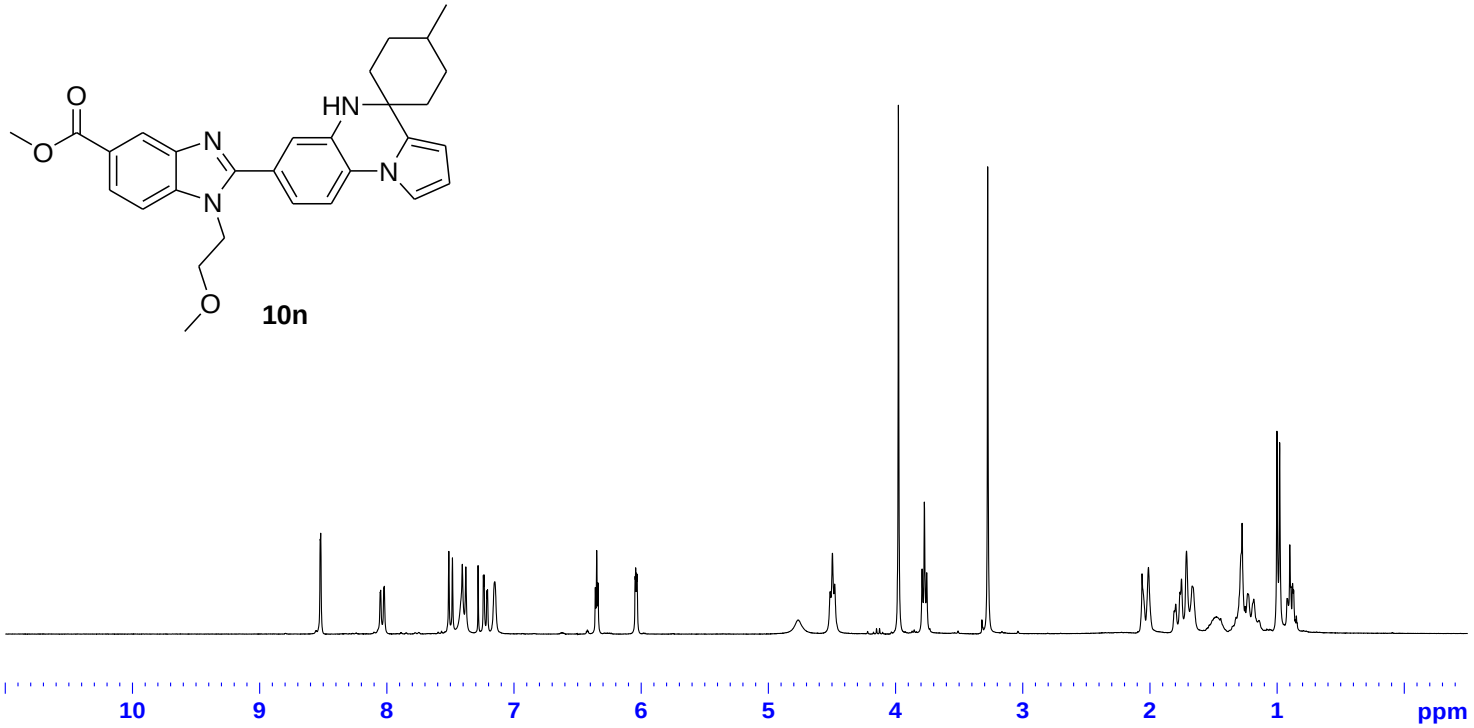

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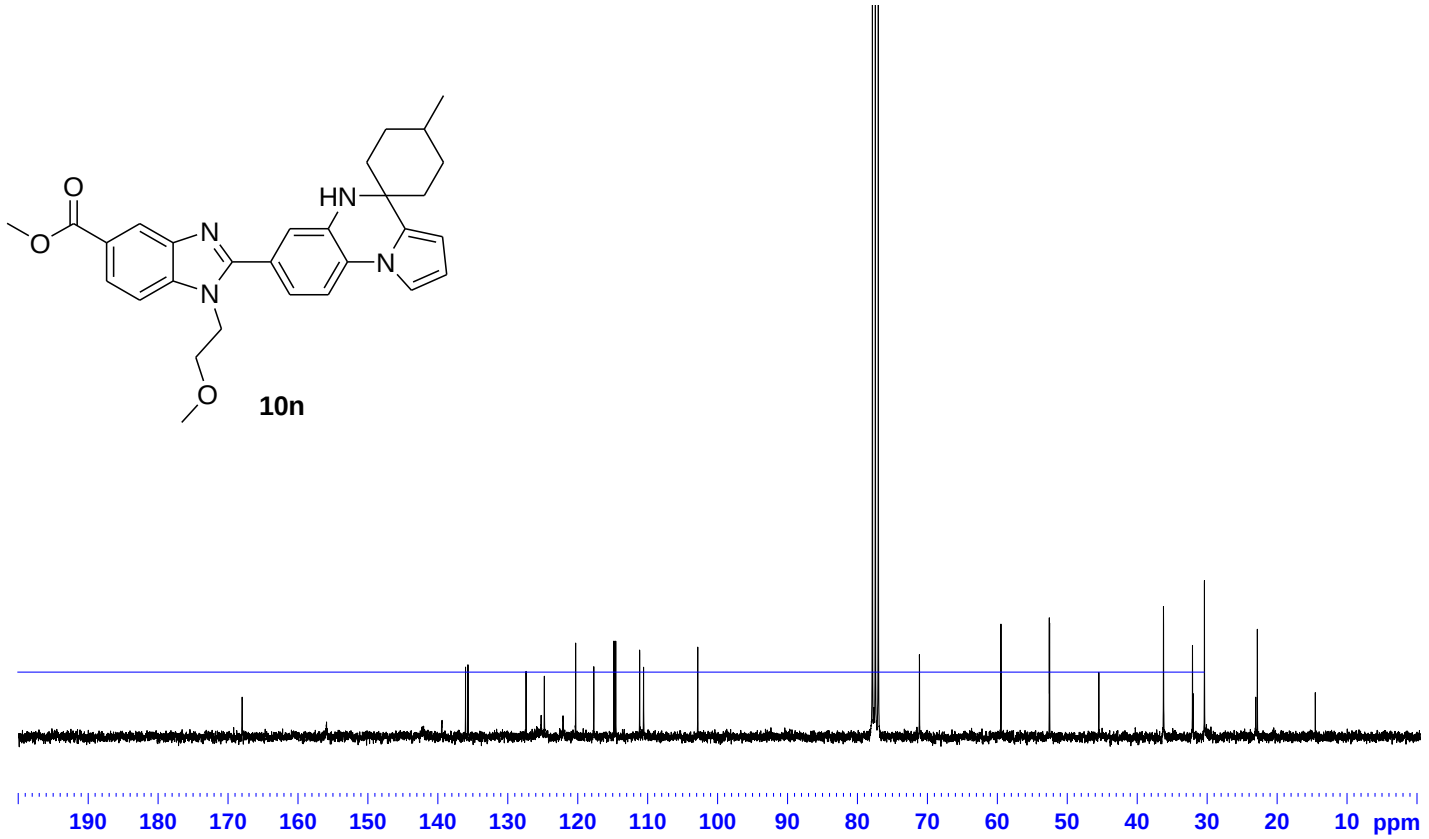

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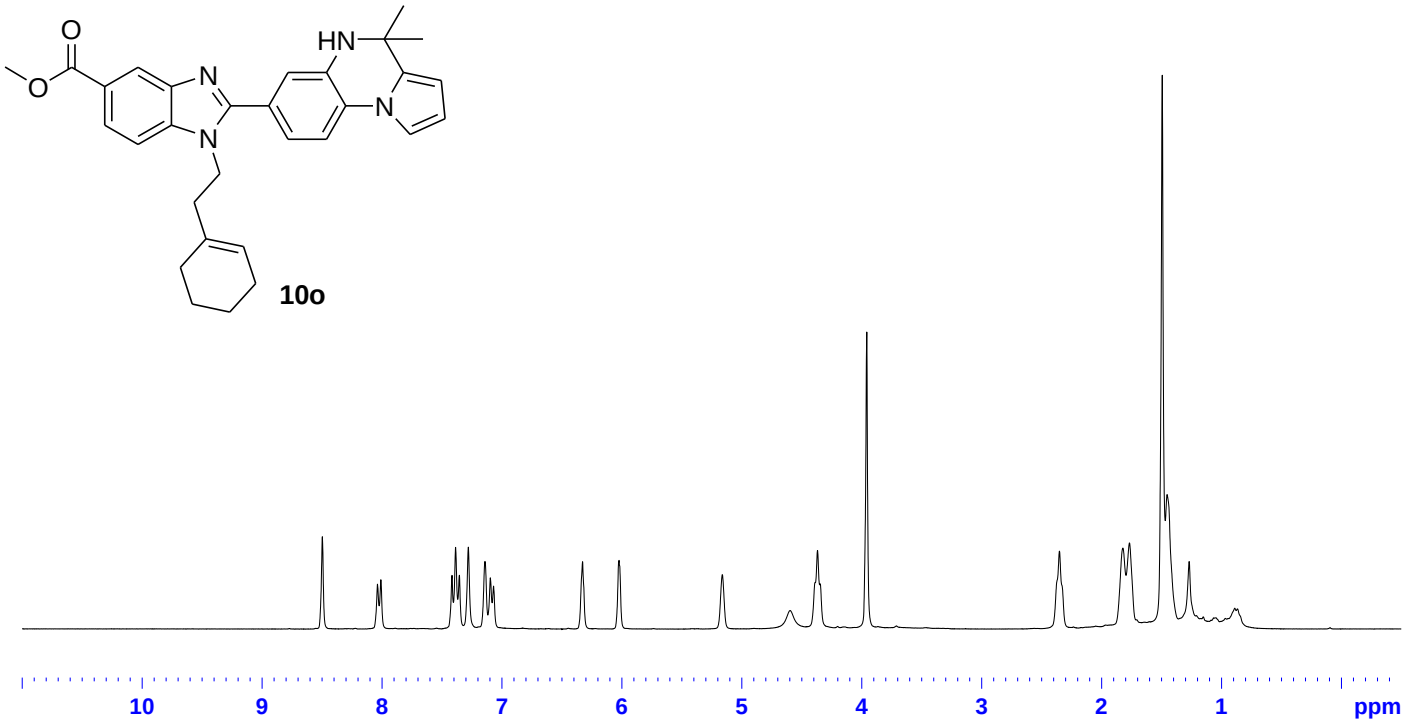

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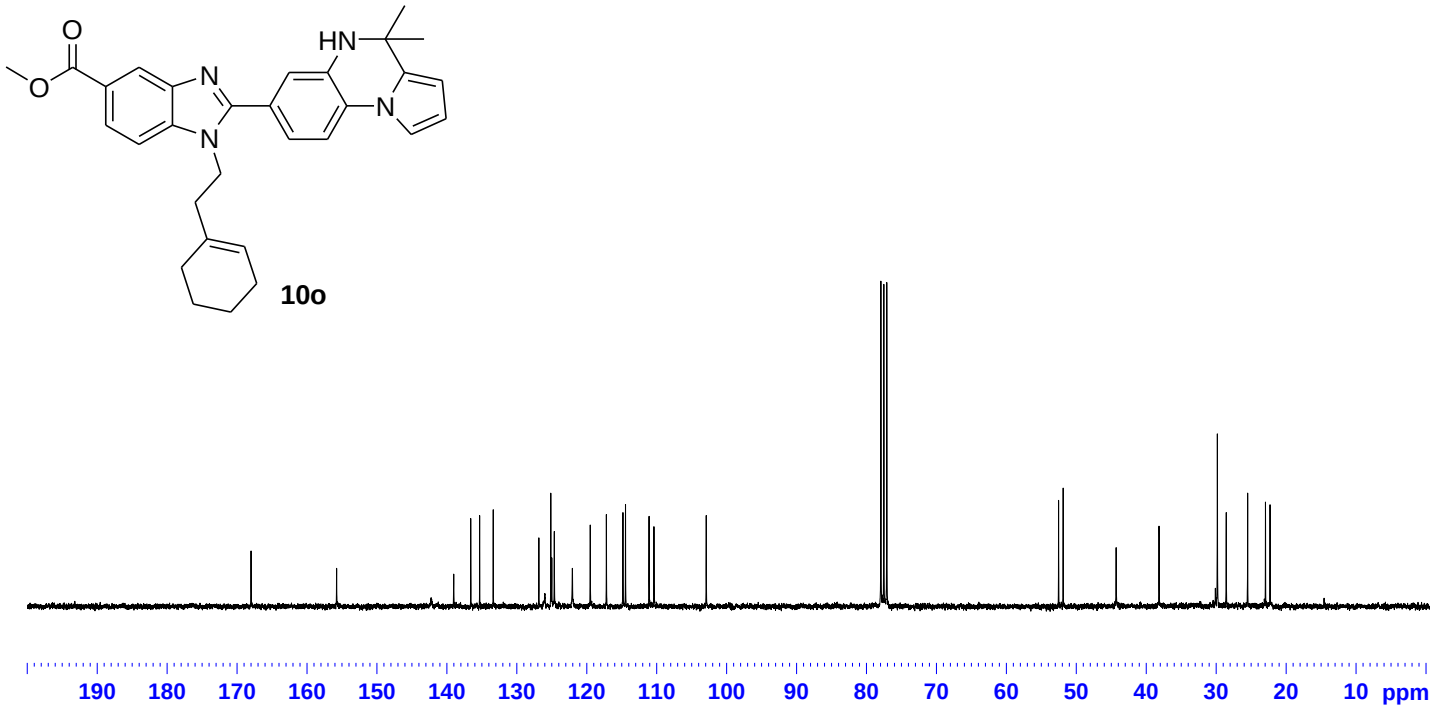

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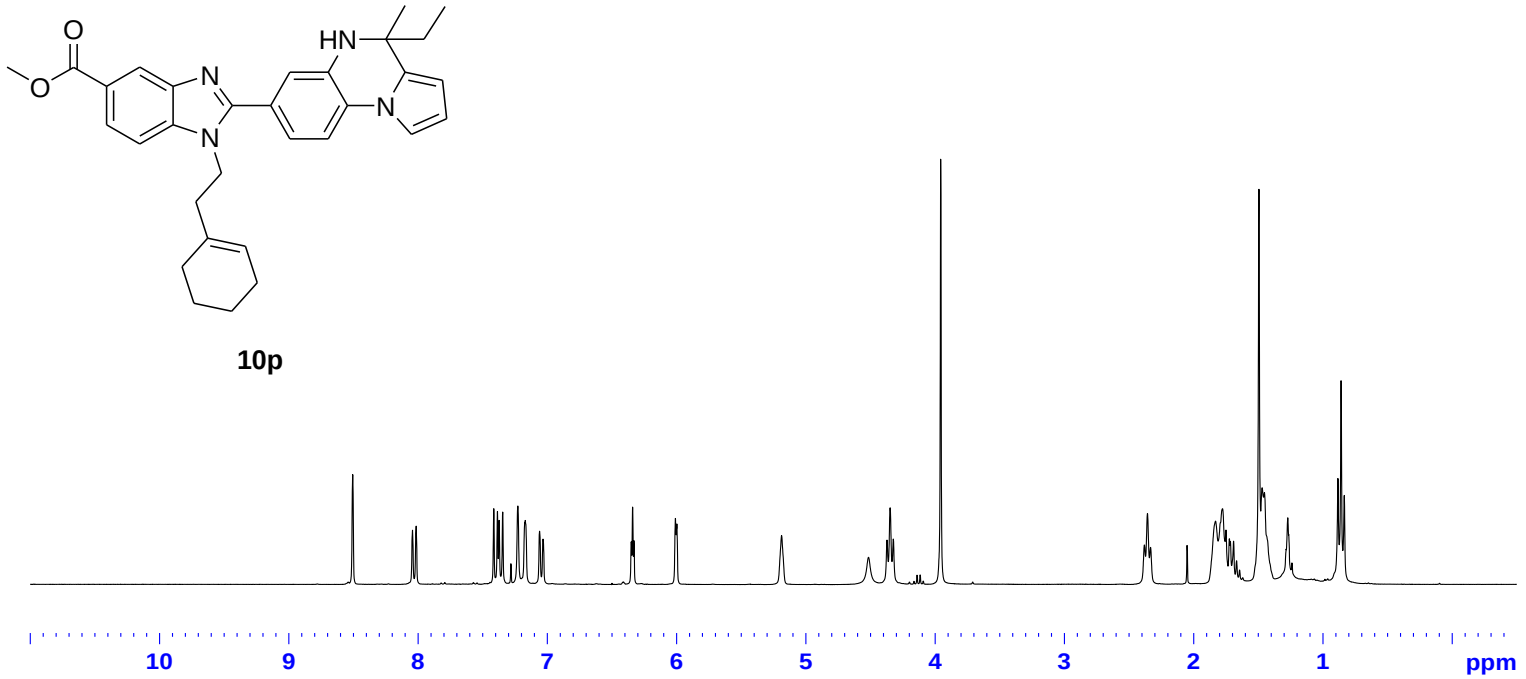

10p

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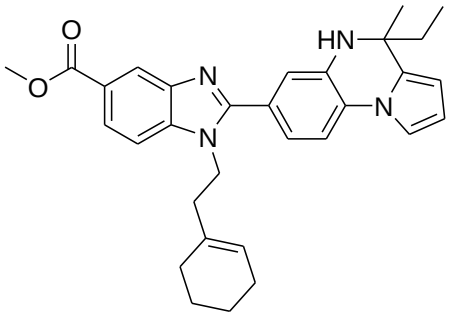
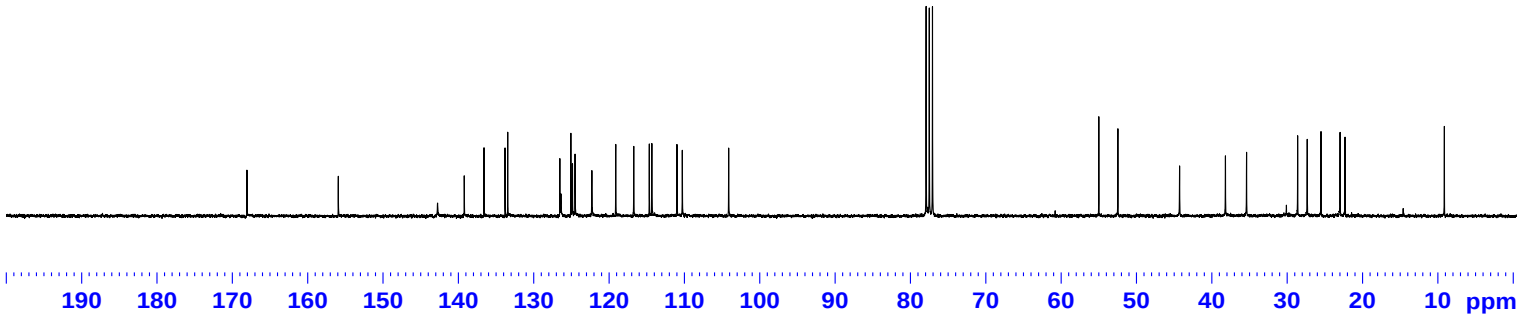
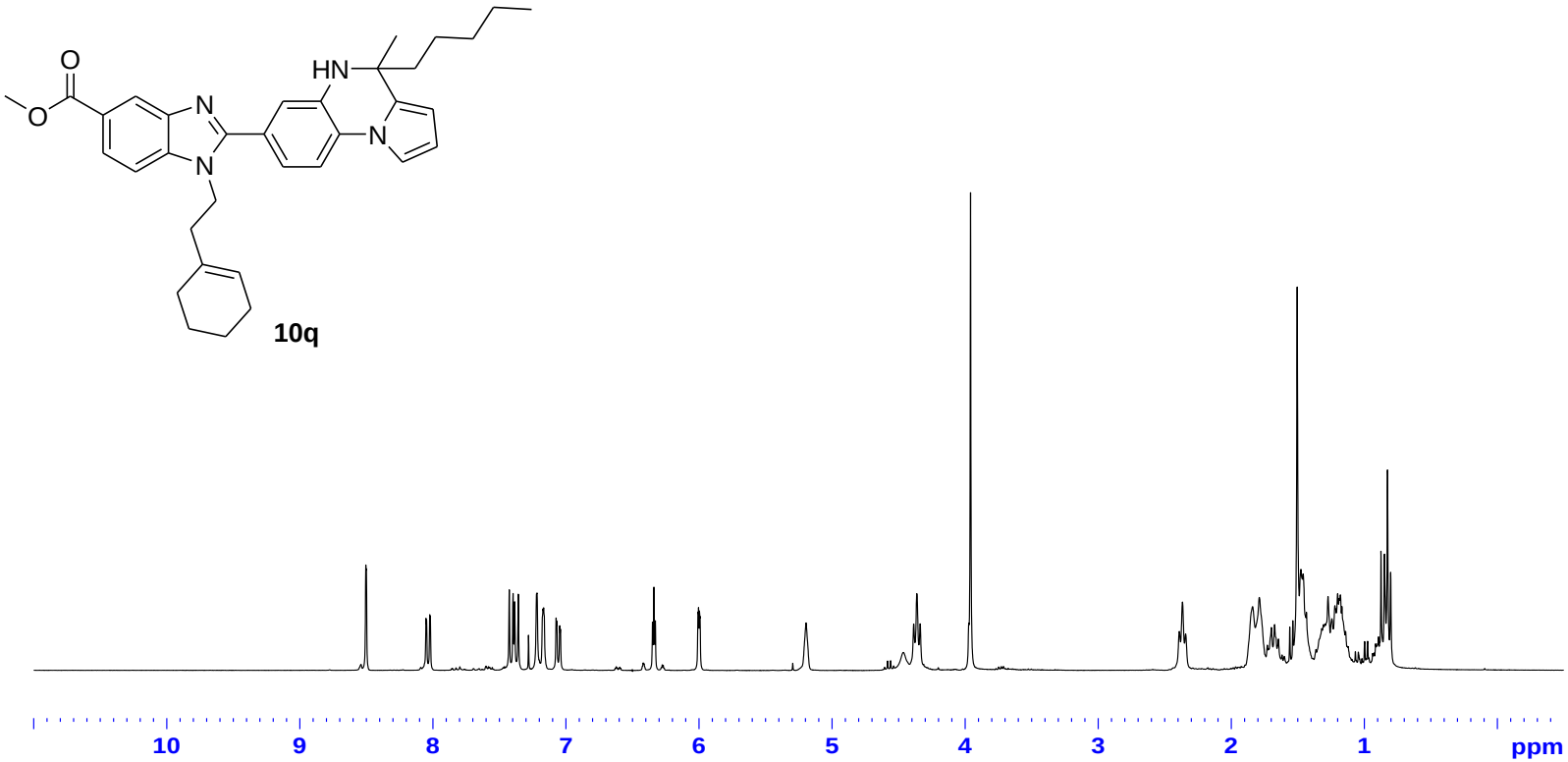


10p



^{13}C NMR spectrum (75 MHz) of compound 10p in $CDCl_3$



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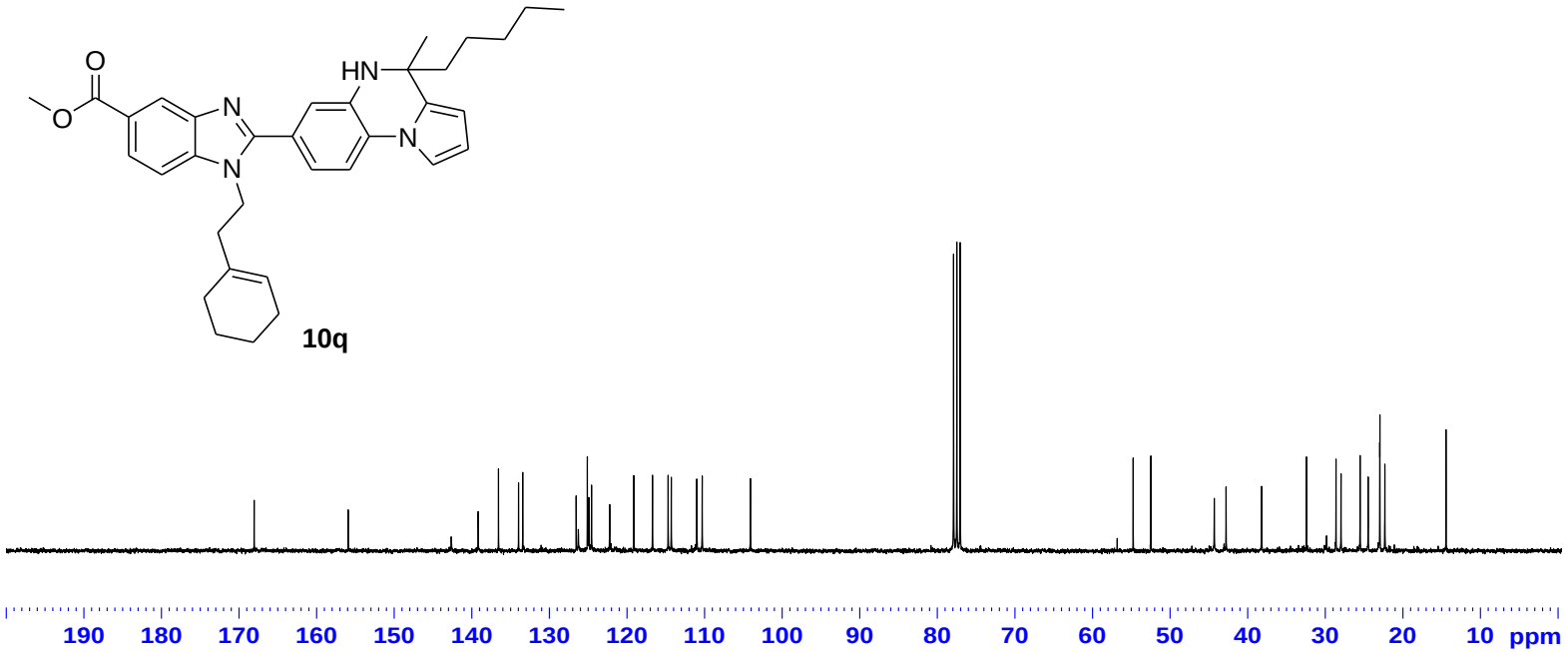
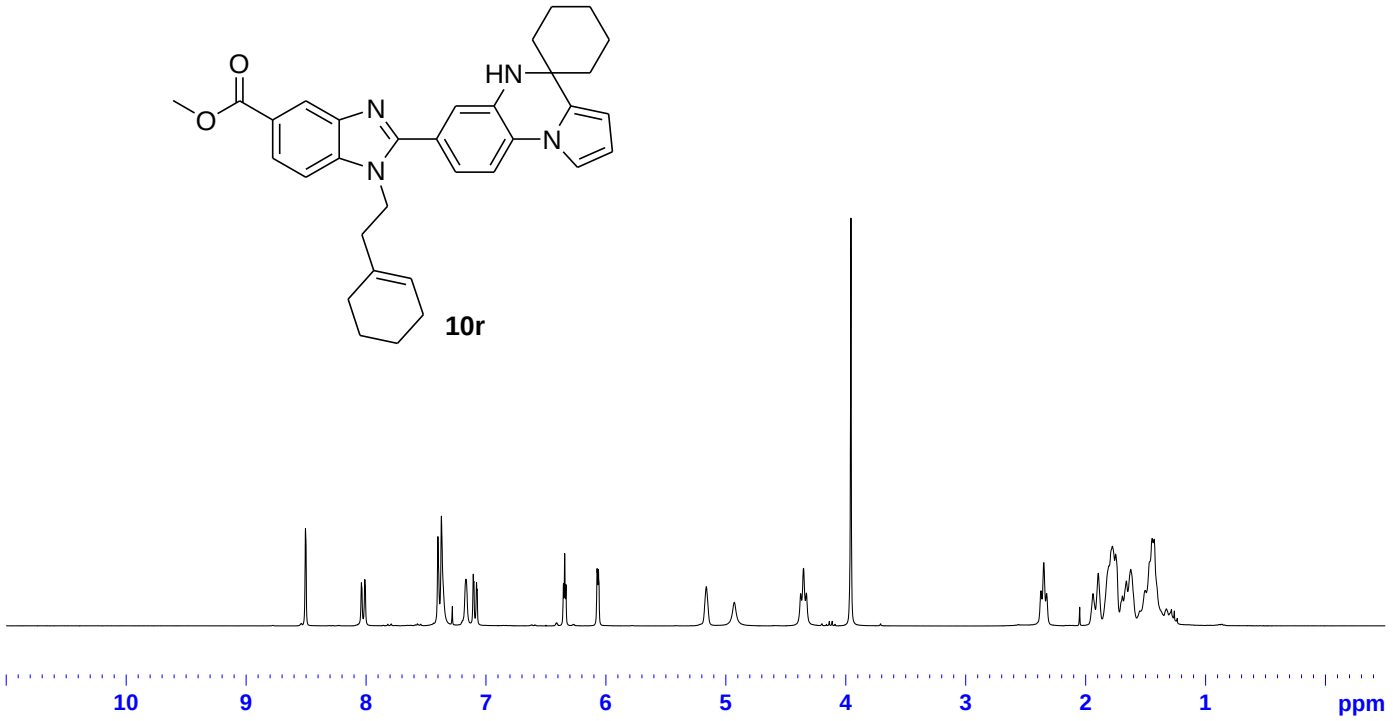


^{13}C NMR spectrum (75 MHz) of compound 10q in $CDCl_3$



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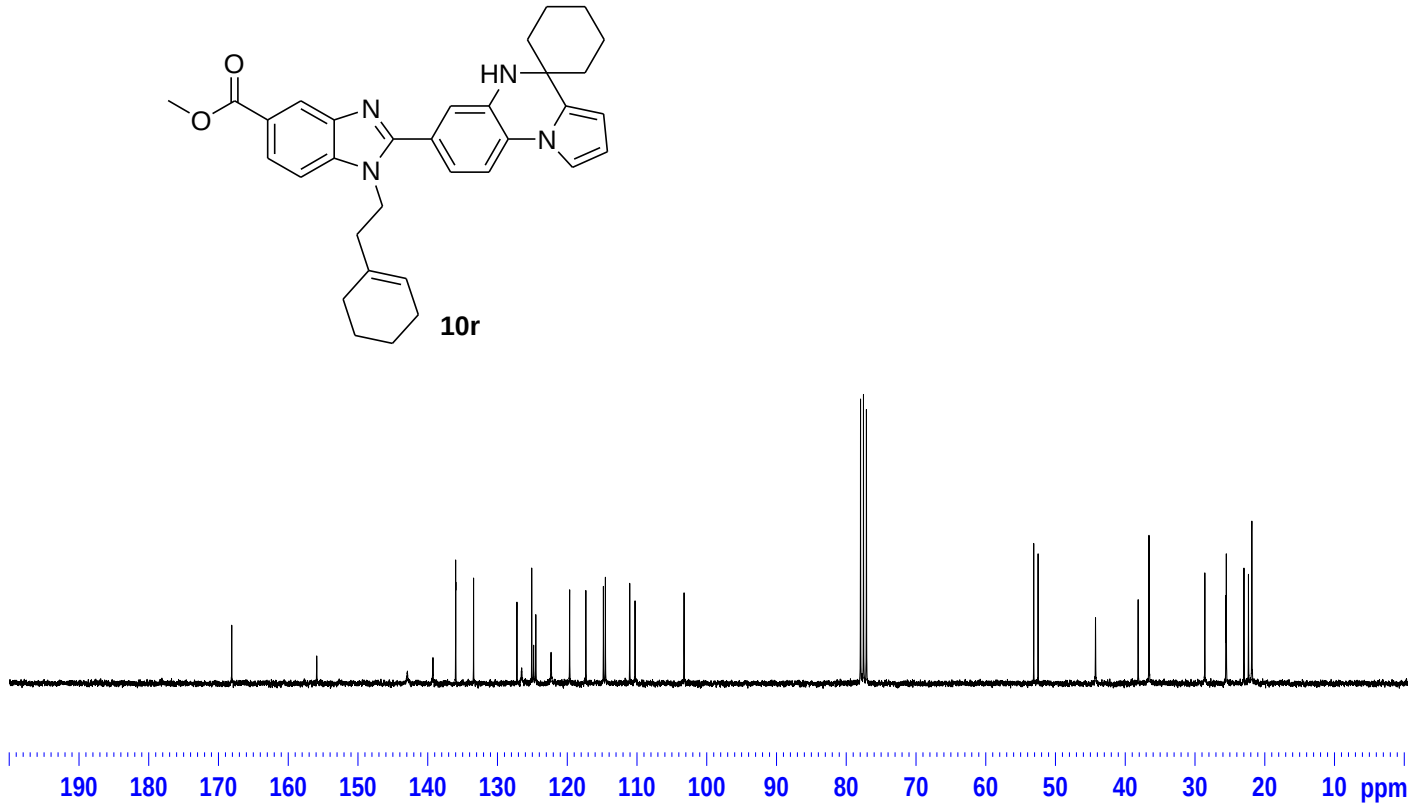

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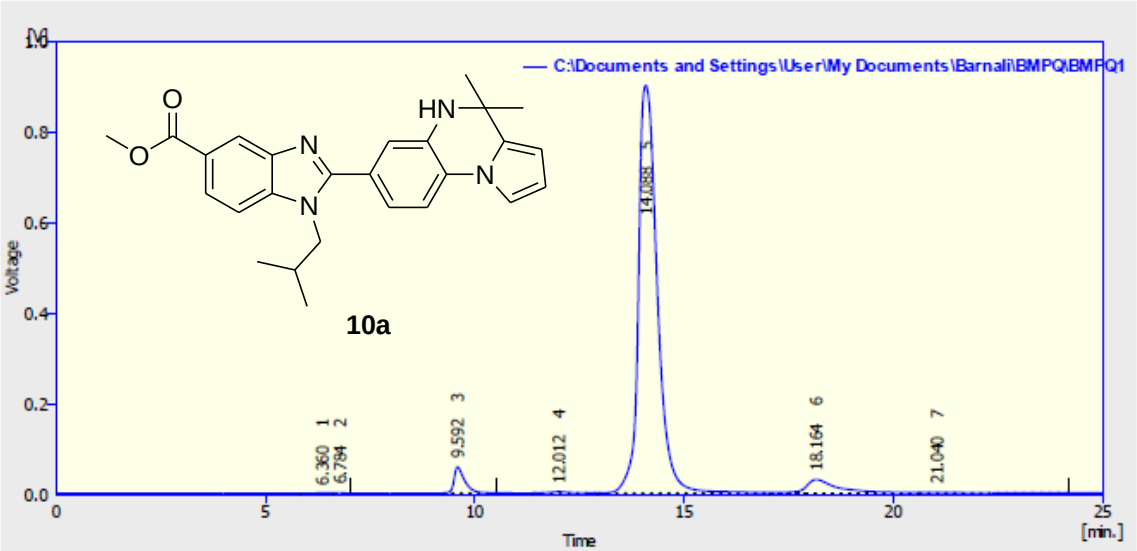

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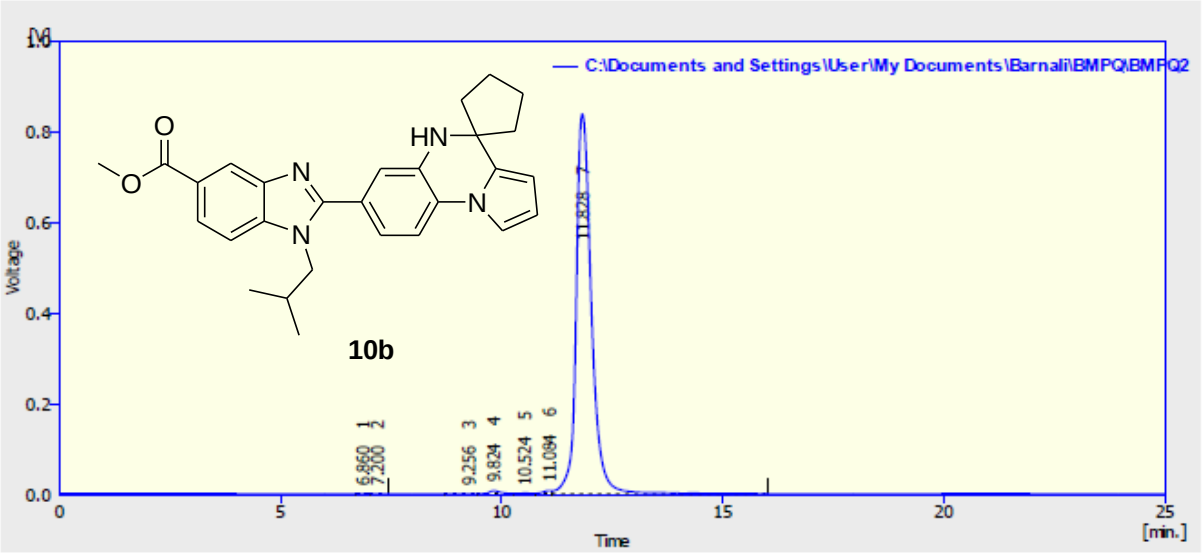
2	6.784	12.286	1.172	0.0	0.1	0.16
3	9.592	1012.364	57.906	3.3	5.0	0.26
4	12.012	108.684	3.228	0.3	0.3	0.42
5	14.088	28214.612	901.293	90.7	90.5	0.46
6	18.164	1620.693	29.851	5.2	3.0	0.66
7	21.040	108.541	1.504	0.3	0.2	1.06
	Total	31091.219	995.669	100.0	100.0	

Crude HPLC Spectra of Compounds 10a



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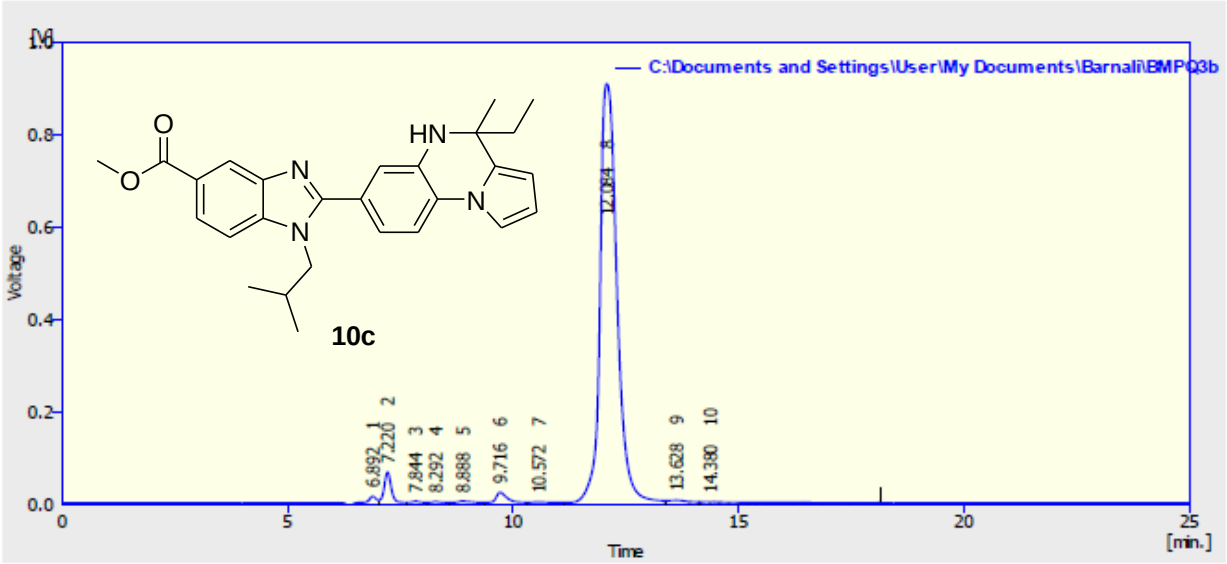
1	6.860	2.202	0.232	0.0	0.0	0.15
2	7.200	2.942	0.270	0.0	0.0	0.16
3	9.256	4.230	0.222	0.0	0.0	0.20
4	9.824	118.044	6.802	0.6	0.8	0.26
5	10.524	27.639	1.323	0.1	0.2	0.39
6	11.084	101.455	7.106	0.5	0.8	0.23
7	11.828	20176.711	838.575	98.7	98.1	0.34
	Total	20433.223	854.529	100.0	100.0	

Crude HPLC Spectra of Compounds 10b



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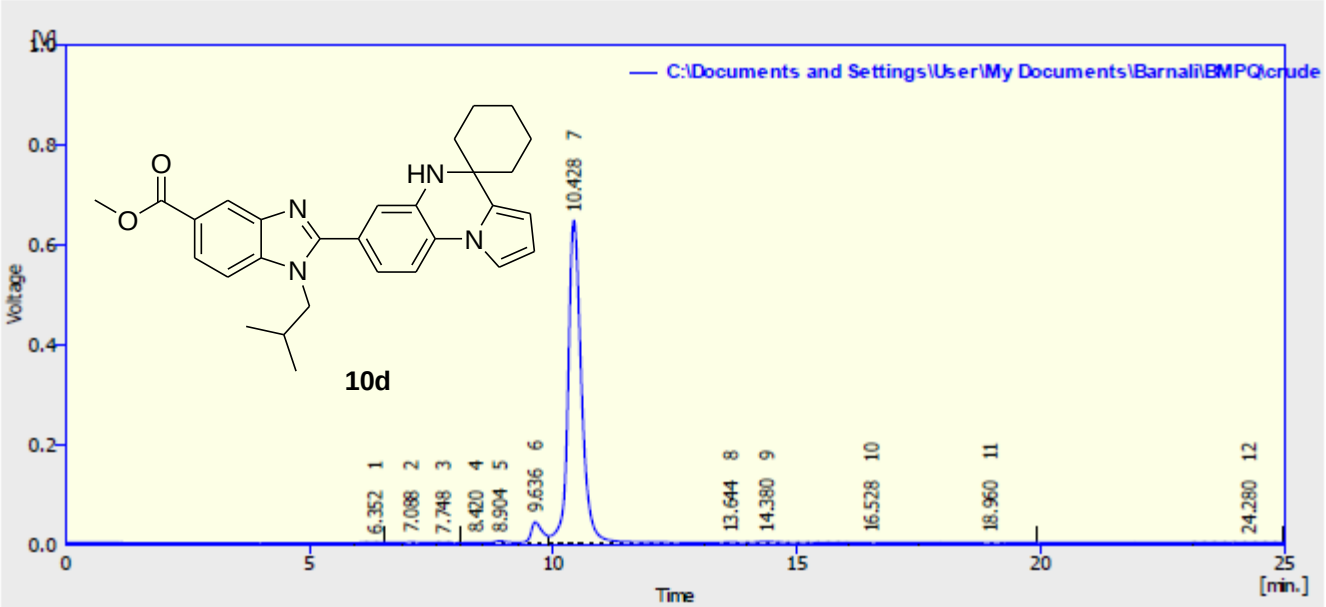
1	6.892	337.924	19.551	1.2	1.8	0.24
2	7.220	915.612	71.819	3.3	6.7	0.17
3	7.844	174.690	8.327	0.6	0.8	0.44
4	8.292	169.756	7.077	0.6	0.7	0.49
5	8.888	280.636	8.162	1.0	0.8	0.79
6	9.716	604.420	26.551	2.2	2.5	0.28
7	10.572	209.948	5.300	0.8	0.5	0.60
8	12.084	24144.714	911.319	87.9	85.2	0.38

Crude HPLC Spectra of Compounds 10c



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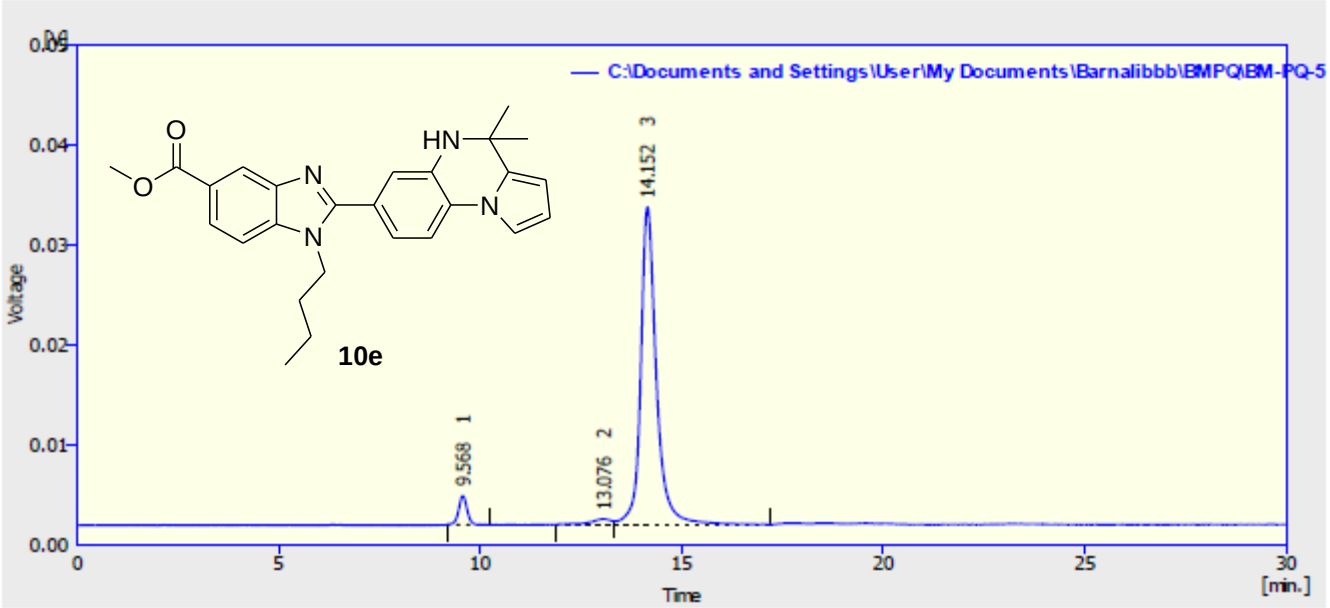
1	6.352	9.195	0.426	0.1	0.1	0.36
2	7.088	23.992	1.476	0.2	0.2	0.22
3	7.748	4.677	0.430	0.0	0.1	0.17
4	8.420	10.067	0.714	0.1	0.1	0.24
5	8.904	70.781	3.705	0.5	0.5	0.28
6	9.636	681.882	41.721	5.1	6.0	0.26
7	10.428	12429.524	646.151	92.1	92.2	0.28
8	13.644	44.309	1.506	0.3	0.2	0.47

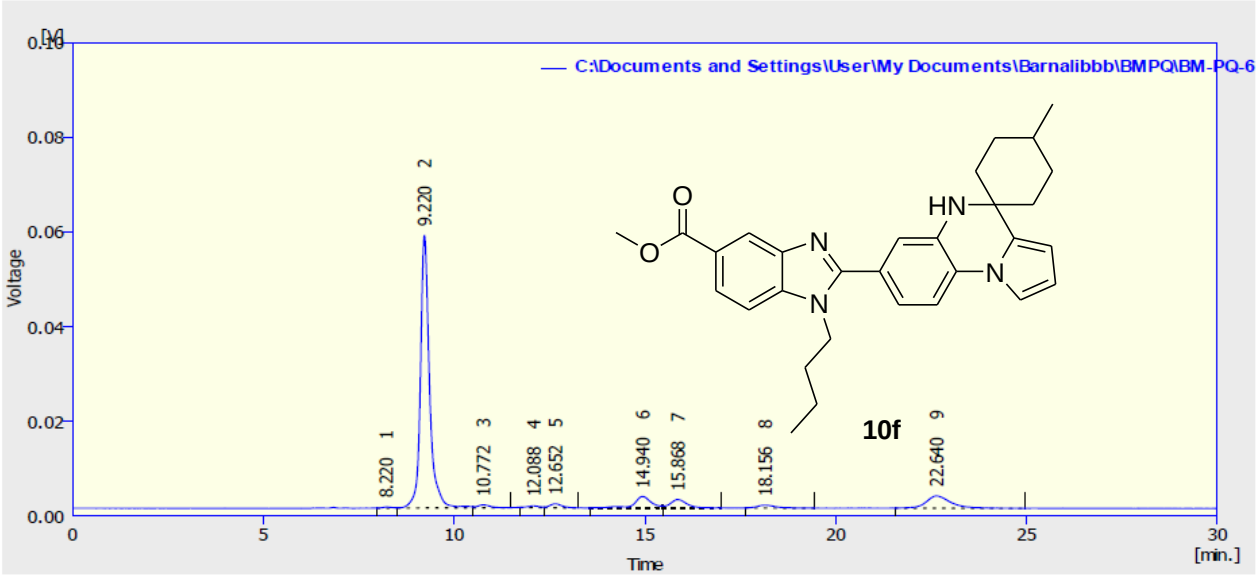
Crude HPLC Spectra of Compounds 10d



Result Table (Uncal - C:\Documents and Settings\User\My Documents\Barnalibbb\BMPQ\BM-PQ-5)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.568	42.762	2.906	4.6	8.2	0.22
2	13.076	21.693	0.582	2.3	1.6	0.57
3	14.152	863.858	31.818	93.1	90.1	0.38
	Total	928.312	35.306	100.0	100.0	

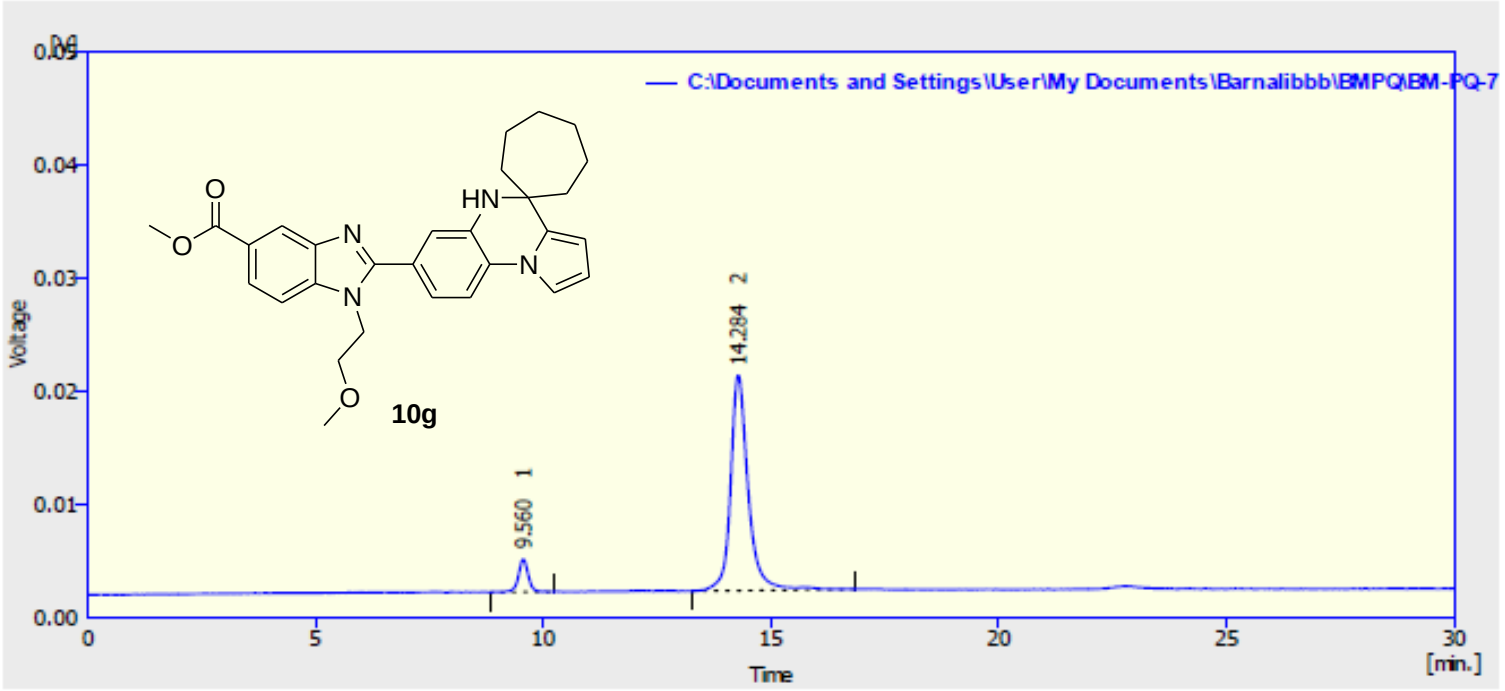
Crude HPLC Spectra of Compounds 10e



Result Table (Uncal - C:|Documents and Settings|User|My Documents|Barnalibbb|BMPQ|BM-PQ-6)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	8.220	3.924	0.225	0.3	0.3	0.29
2	9.220	955.024	57.614	74.9	85.8	0.23
3	10.772	14.575	0.640	1.1	1.0	0.33
4	12.088	7.819	0.375	0.6	0.6	0.33
5	12.652	18.904	0.846	1.5	1.3	0.34
6	14.940	78.358	2.454	6.1	3.7	0.41
7	15.868	54.661	1.802	4.3	2.7	0.44
8	18.156	21.663	0.620	1.7	0.9	0.50

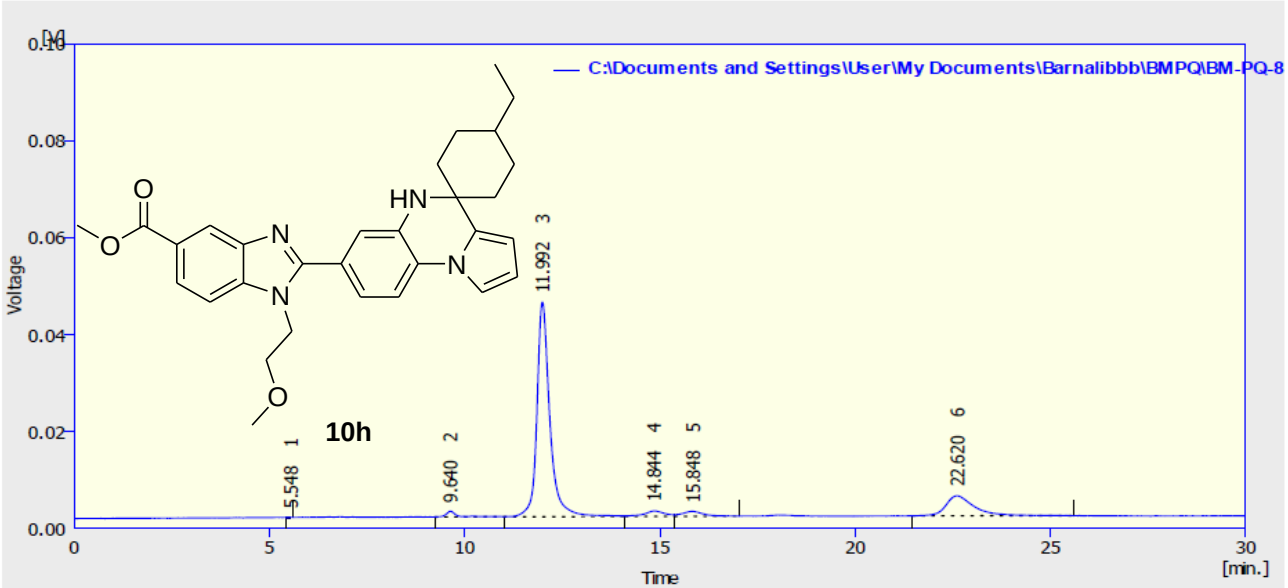
Crude HPLC Spectra of Compounds 10f



Result Table (Uncal - C:\Documents and Settings\User\My Documents\Barnalibbb\BMPQ\BM-PQ-7)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.560	44.229	2.898	7.9	13.2	0.22
2	14.284	517.539	19.052	92.1	86.8	0.38
	Total	561.768	21.950	100.0	100.0	

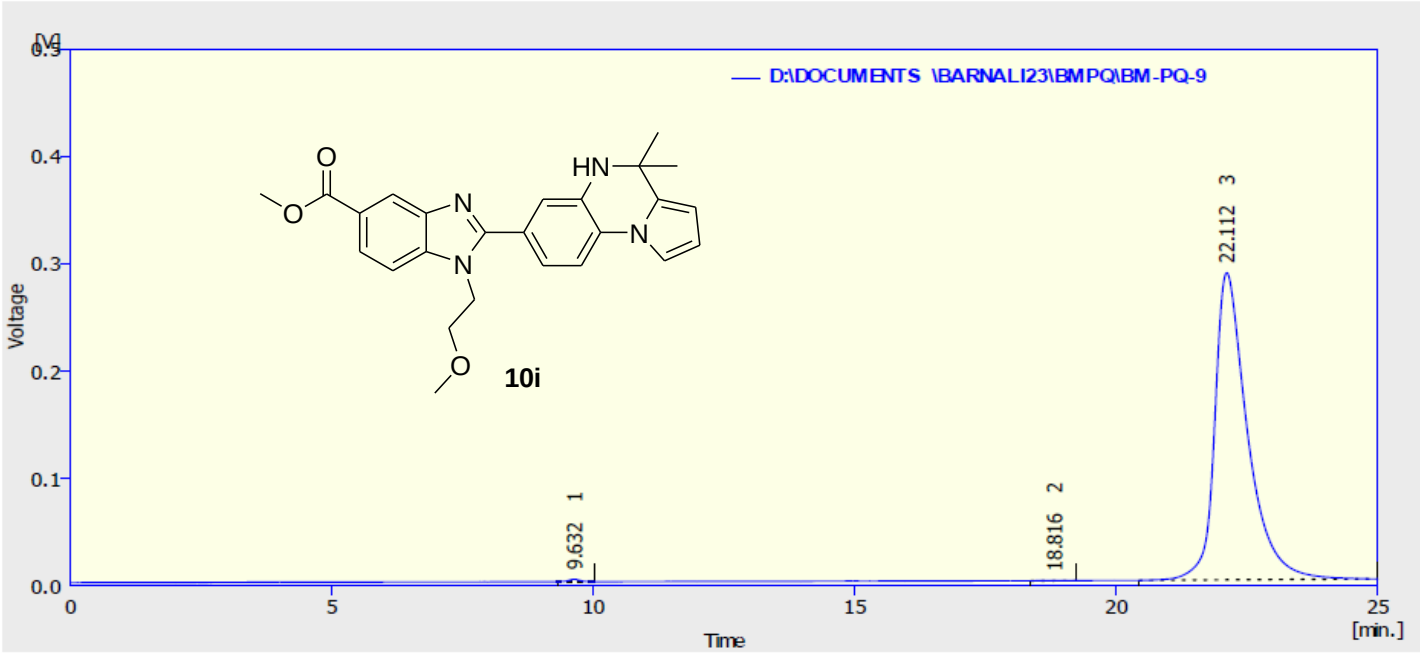
Crude HPLC Spectra of Compounds 10g



Result Table (Uncal - C:|Documents and Settings|User|My Documents|Barnalibbb|BMPQ|BM-PQ-8)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	5.548	0.282	0.048	0.0	0.1	0.05
2	9.640	22.762	1.182	1.7	2.3	0.22
3	11.992	1021.803	44.328	76.3	85.5	0.32
4	14.844	41.233	1.126	3.1	2.2	0.52
5	15.848	38.360	1.012	2.9	2.0	0.57
6	22.620	214.426	4.128	16.0	8.0	0.72
	Total	1338.866	51.824	100.0	100.0	

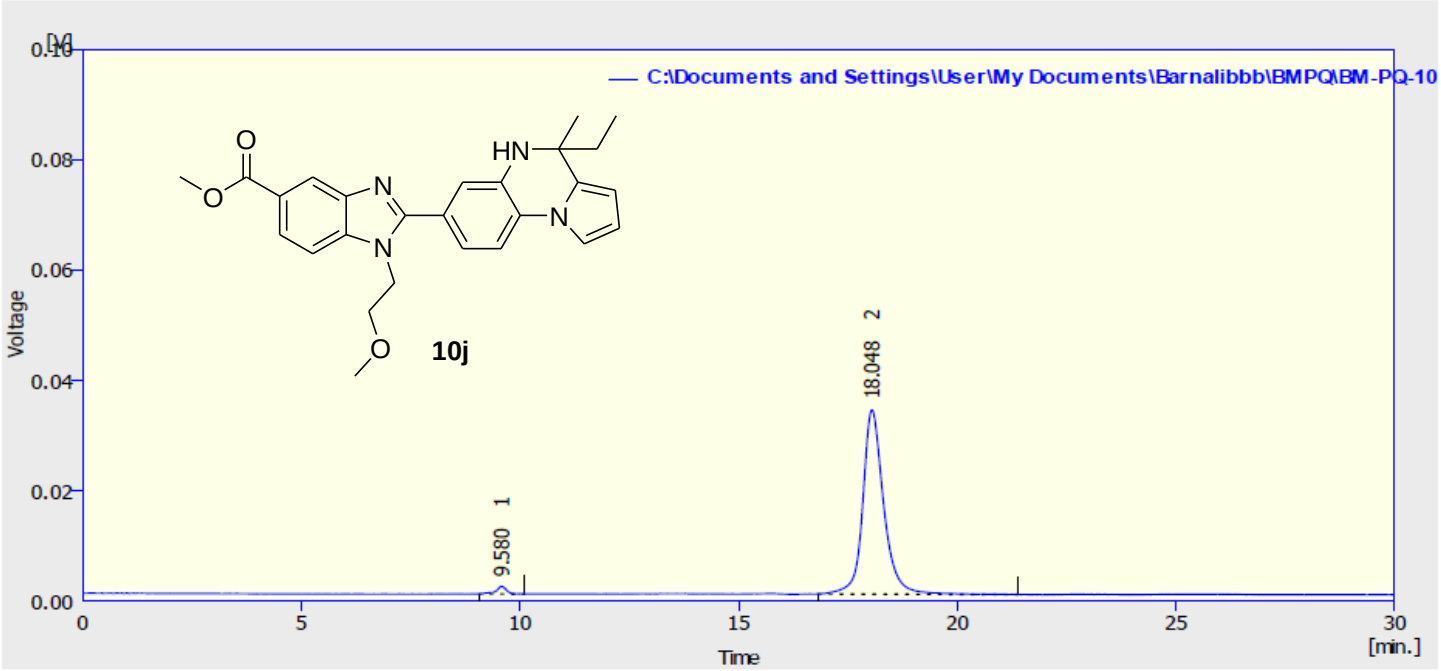
Crude HPLC Spectra of Compounds 10h



Result Table (Uncal - D:|DOCUMENTS |BARNALI23|BMPQ|BM-PQ-9)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.632	32.720	2.288	0.3	0.8	0.22
2	18.816	3.115	0.108	0.0	0.0	0.53
3	22.112	12521.821	286.273	99.7	99.2	0.62
	Total	12557.656	288.669	100.0	100.0	

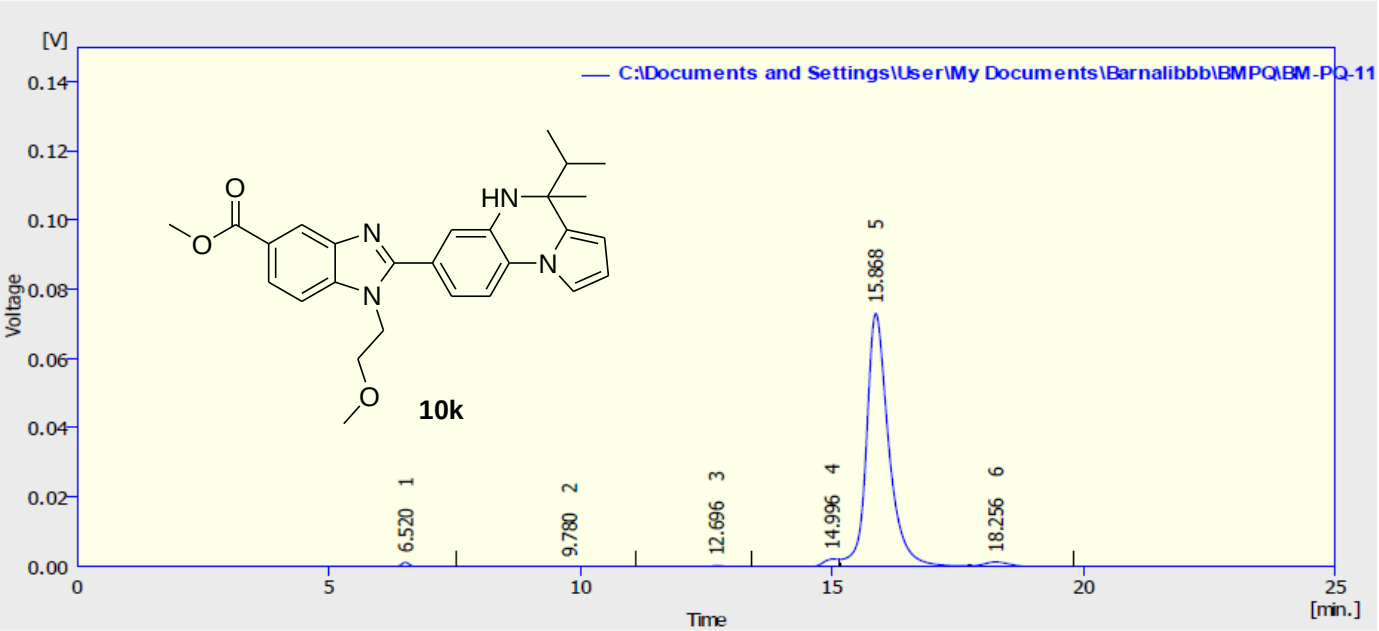
Crude HPLC Spectra of Compounds 10i



Result Table (Uncal - C:|Documents and Settings|User|My Documents|Barnalibbb|BMPQ|BM-PQ-10)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.580	23.152	1.362	2.0	3.9	0.22
2	18.048	1118.414	33.413	98.0	96.1	0.47
	Total	1141.567	34.775	100.0	100.0	

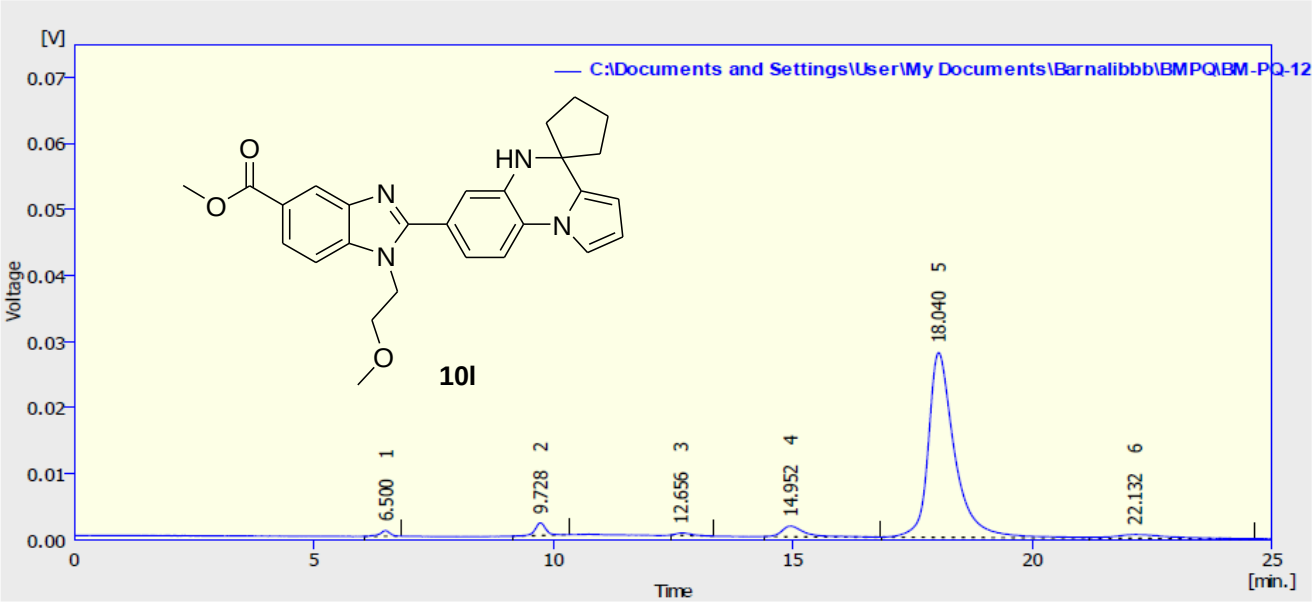
Crude HPLC Spectra of Compounds 10j



Result Table (Uncal - C:|Documents and Settings|User|My Documents|Barnalibbb|BMPQ|BM-PQ-11)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.520	29.174	1.594	1.2	2.0	0.21
2	9.780	8.158	0.278	0.3	0.3	0.23
3	12.696	15.695	0.661	0.6	0.8	0.36
4	14.996	55.430	2.527	2.2	3.2	0.35
5	15.868	2305.682	73.488	92.7	91.6	0.44
6	18.256	74.332	1.644	3.0	2.1	0.66
	Total	2488.472	80.193	100.0	100.0	

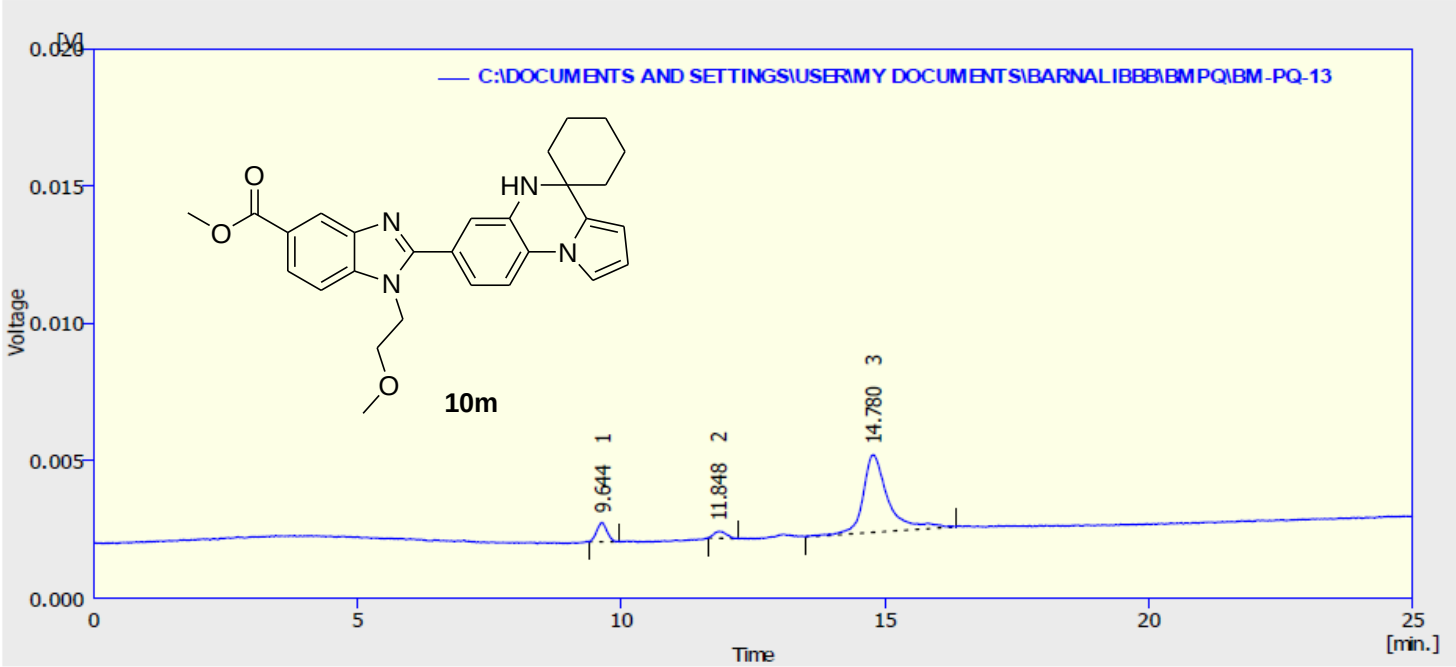
Crude HPLC Spectra of Compounds 10k



Result Table (Uncal - C:|Documents and Settings|User|My Documents|Barnalibbb|BMPQ|BM-PQ-12)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.500	12.799	0.838	1.0	2.5	0.21
2	9.728	30.263	1.906	2.5	5.7	0.23
3	12.656	8.256	0.360	0.7	1.1	0.31
4	14.952	54.471	1.602	4.4	4.8	0.46
5	18.040	1076.216	27.969	87.7	84.1	0.53
6	22.132	45.651	0.570	3.7	1.7	1.04
	Total	1227.655	33.244	100.0	100.0	

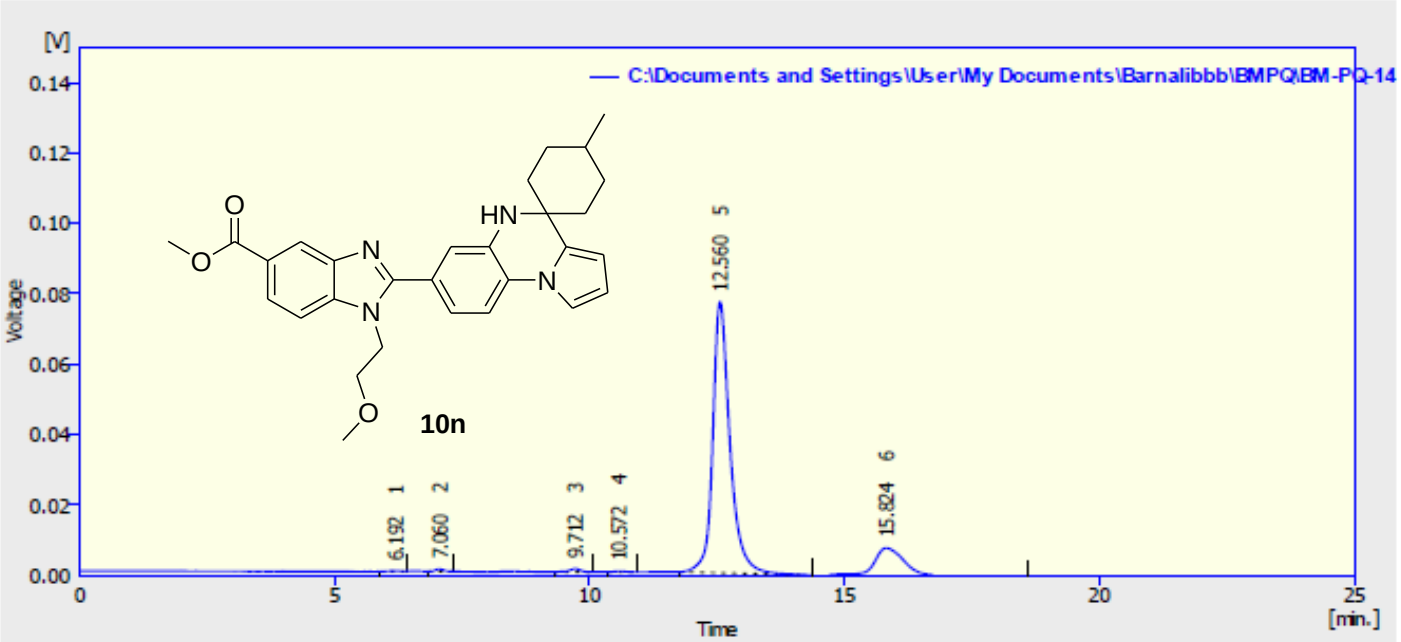
Crude HPLC Spectra of Compounds 10l



Result Table (Uncal - C:|DOCUMENTS AND SETTINGS|USER|MY DOCUMENTS|BARNALIBBB|BMPQ|BM-PQ-13)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.644	9.624	0.706	9.0	18.7	0.22
2	11.848	4.163	0.240	3.9	6.4	0.26
3	14.780	93.377	2.826	87.1	74.9	0.43
	Total	107.163	3.772	100.0	100.0	

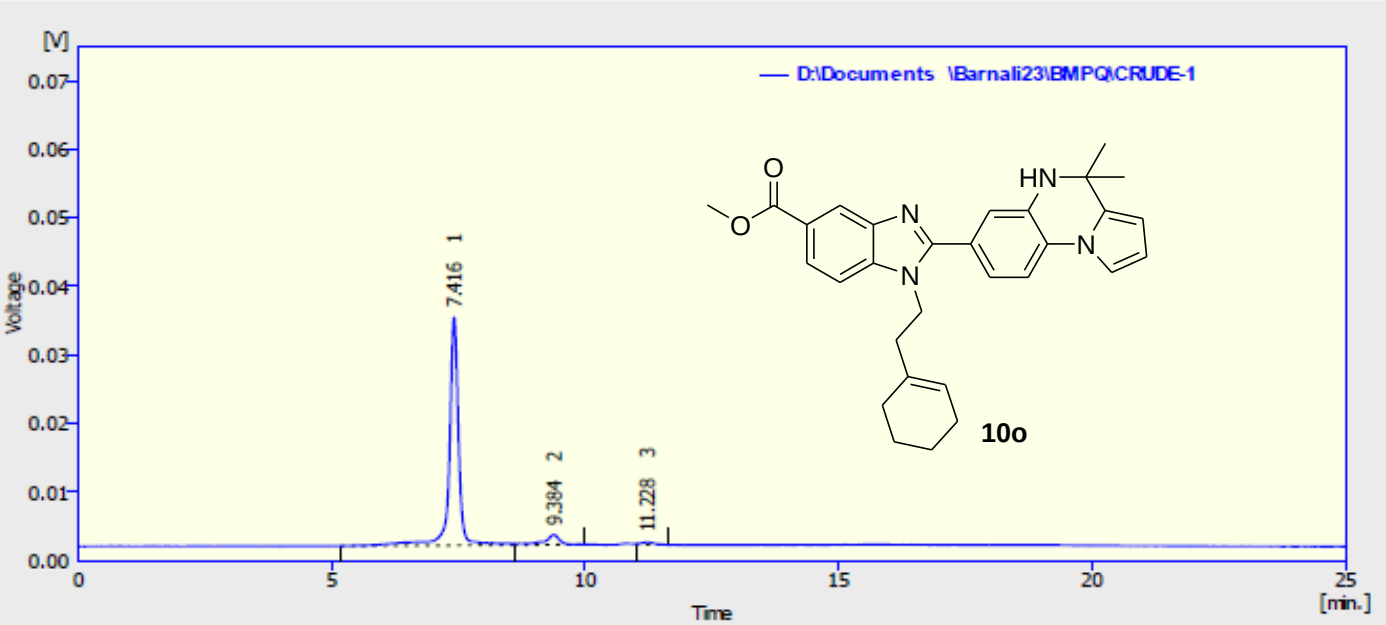
Crude HPLC Spectra of Compounds 10m



Result Table (Uncal - C:\Documents and Settings\User\My Documents\Barnalibbb\BMPQ\BM-PQ-14)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.192	2.875	0.182	0.1	0.2	0.24
2	7.060	8.003	0.687	0.4	0.8	0.18
3	9.712	14.533	0.926	0.7	1.1	0.23
4	10.572	4.449	0.301	0.2	0.3	0.24
5	12.560	1810.996	77.123	83.2	88.5	0.33
6	15.824	335.780	7.914	15.4	9.1	0.60
	Total	2176.636	87.133	100.0	100.0	

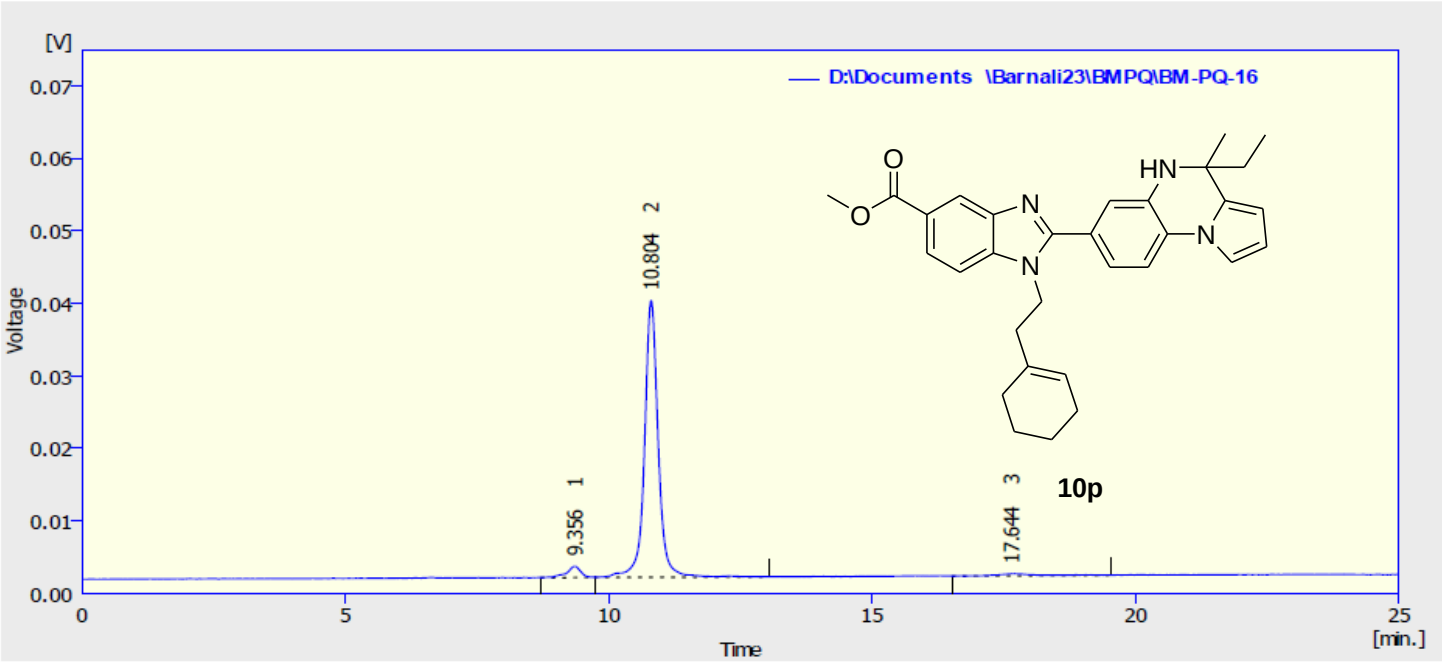
Crude HPLC Spectra of Compounds 10n



Result Table (Uncal - D:\Documents \Barnali23\BMPQ\CRUDE-1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	7.416	433.877	33.306	92.1	94.9	0.16
2	9.384	31.917	1.468	6.8	4.2	0.24
3	11.228	5.079	0.328	1.1	0.9	0.25
	Total	470.873	35.102	100.0	100.0	

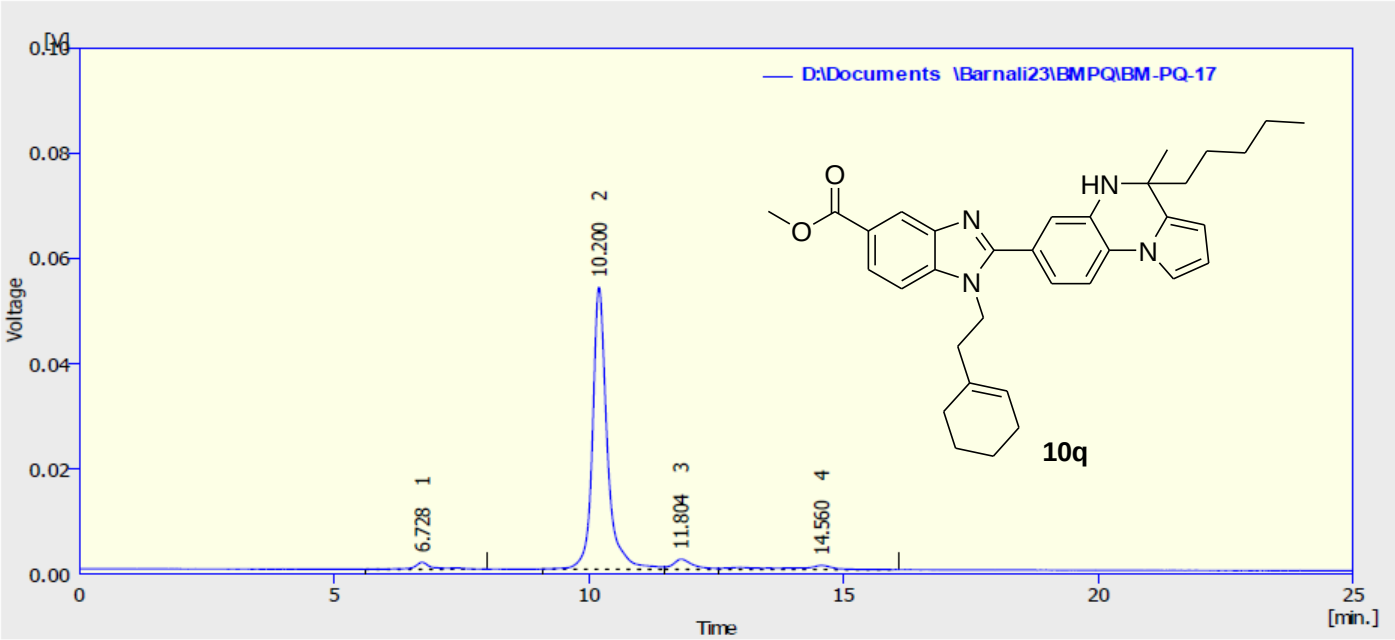
Crude HPLC Spectra of Compounds 10o



Result Table (Uncal - D:|Documents |Barnali23|BMPQ|BM-PQ-16)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.356	29.230	1.554	3.9	3.9	0.26
2	10.804	696.300	38.174	94.0	95.4	0.26
3	17.644	15.163	0.286	2.0	0.7	0.54
	Total	740.693	40.013	100.0	100.0	

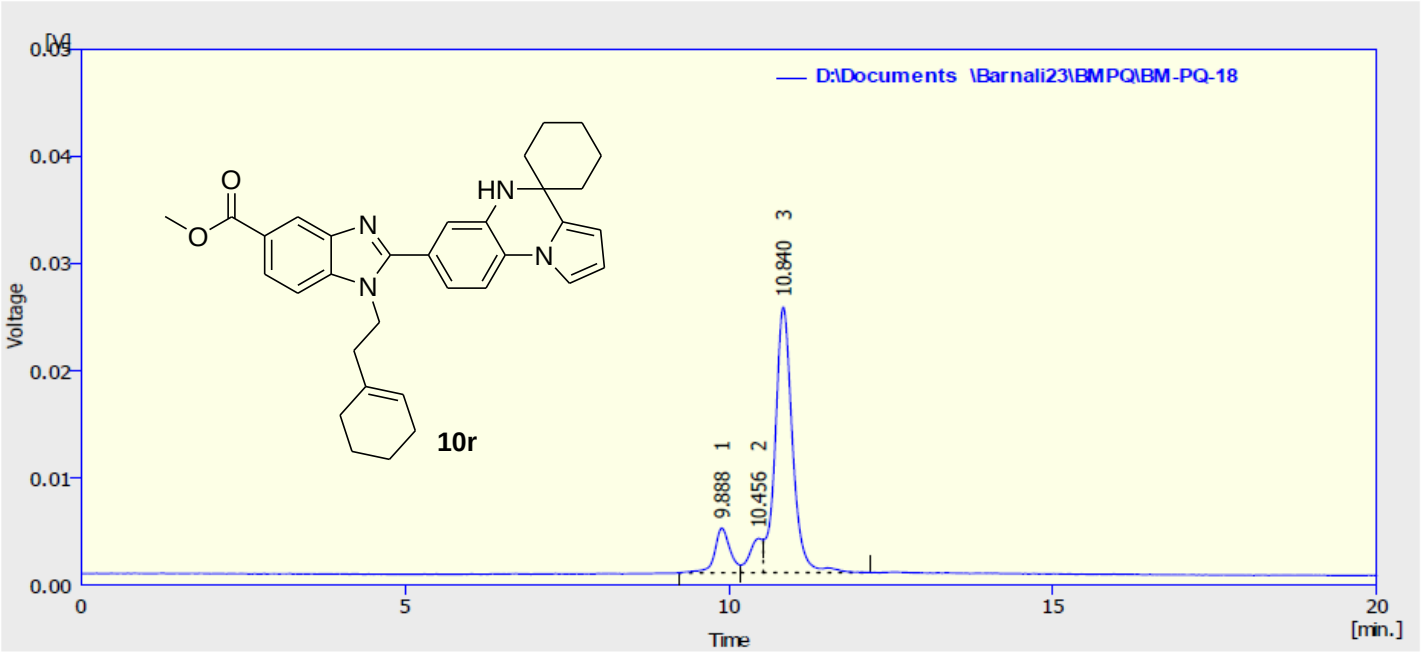
Crude HPLC Spectra of Compounds 10p



Result Table (Uncal - D:\Documents \Barnali23\BMPQ\BM-PQ-17)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.728	34.020	1.323	2.8	2.3	0.25
2	10.200	1076.661	53.601	88.4	92.9	0.28
3	11.804	52.935	1.940	4.3	3.4	0.38
4	14.560	54.854	0.805	4.5	1.4	0.43
	Total	1218.470	57.669	100.0	100.0	

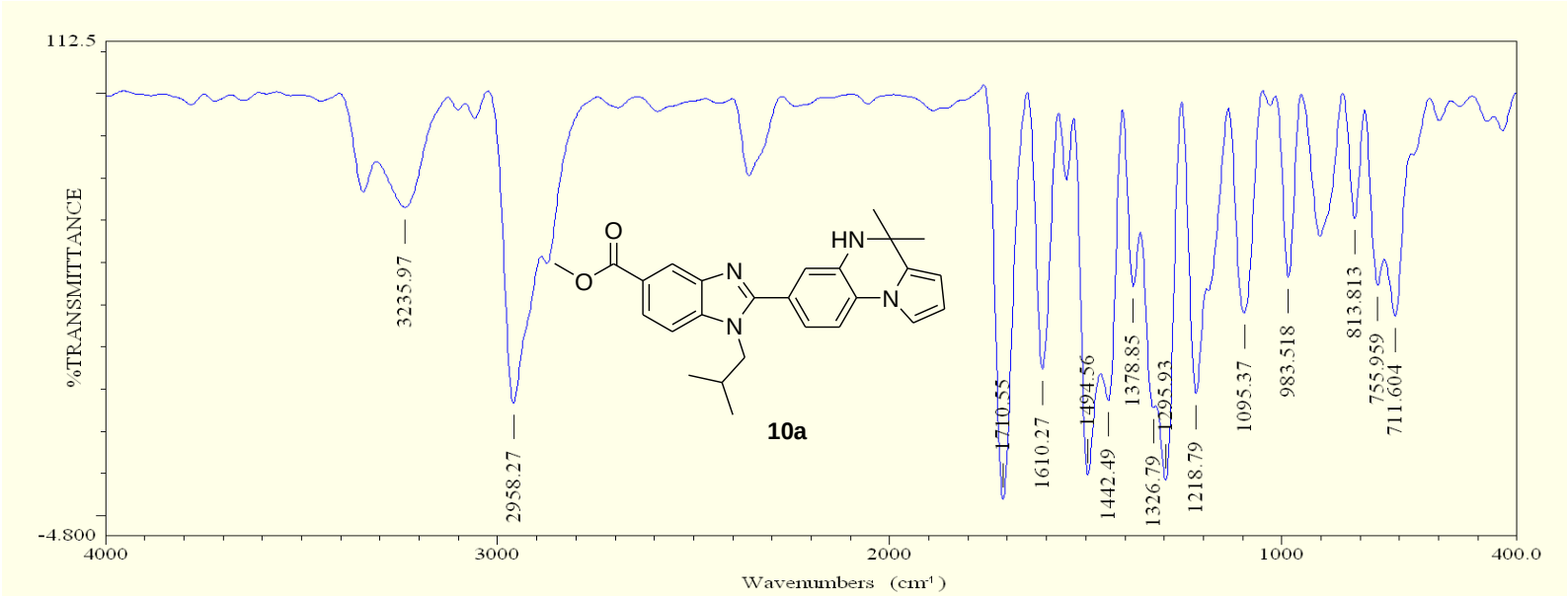
Crude HPLC Spectra of Compounds 10q



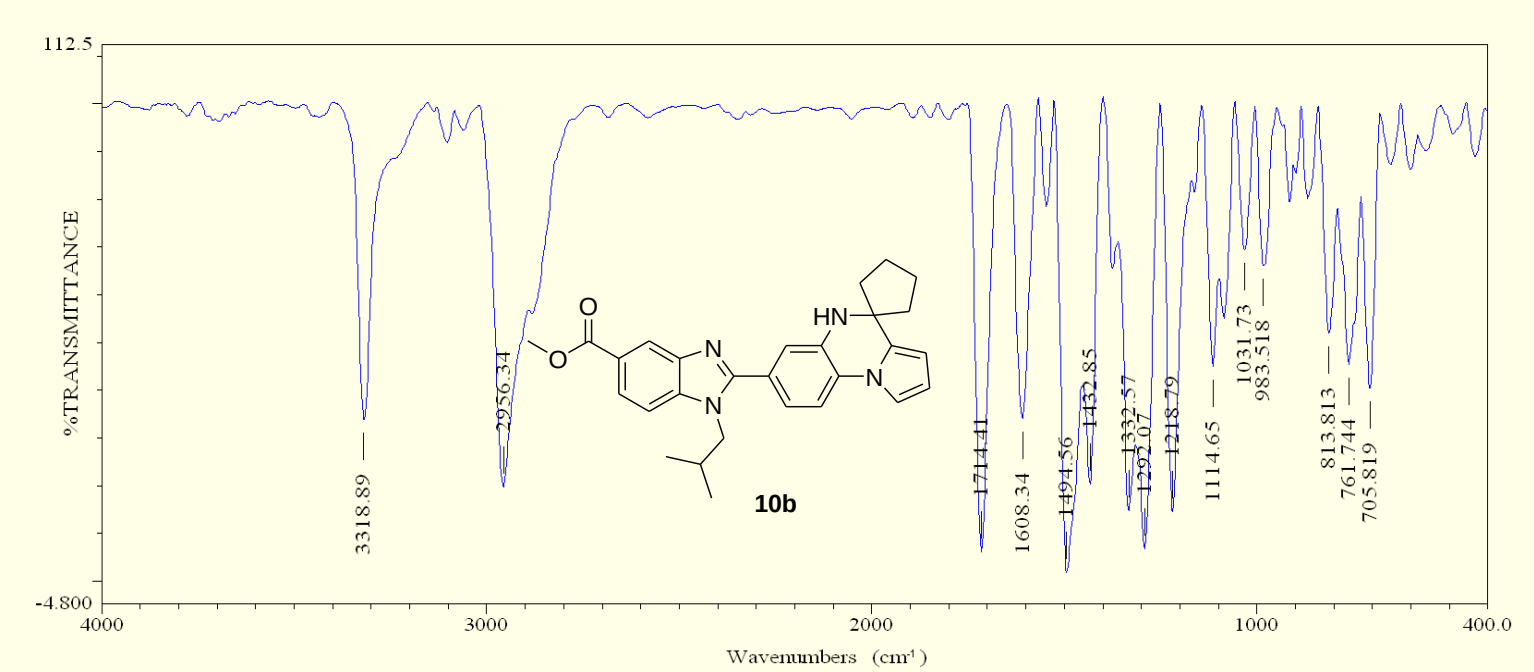
Result Table (Uncal - D:|Documents |Barnali23|BMPQ|BM-PQ-18)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	9.888	70.440	4.181	12.2	13.0	0.24
2	10.456	43.981	3.207	7.6	10.0	0.22
3	10.840	463.854	24.786	80.2	77.0	0.27
	Total	578.274	32.174	100.0	100.0	

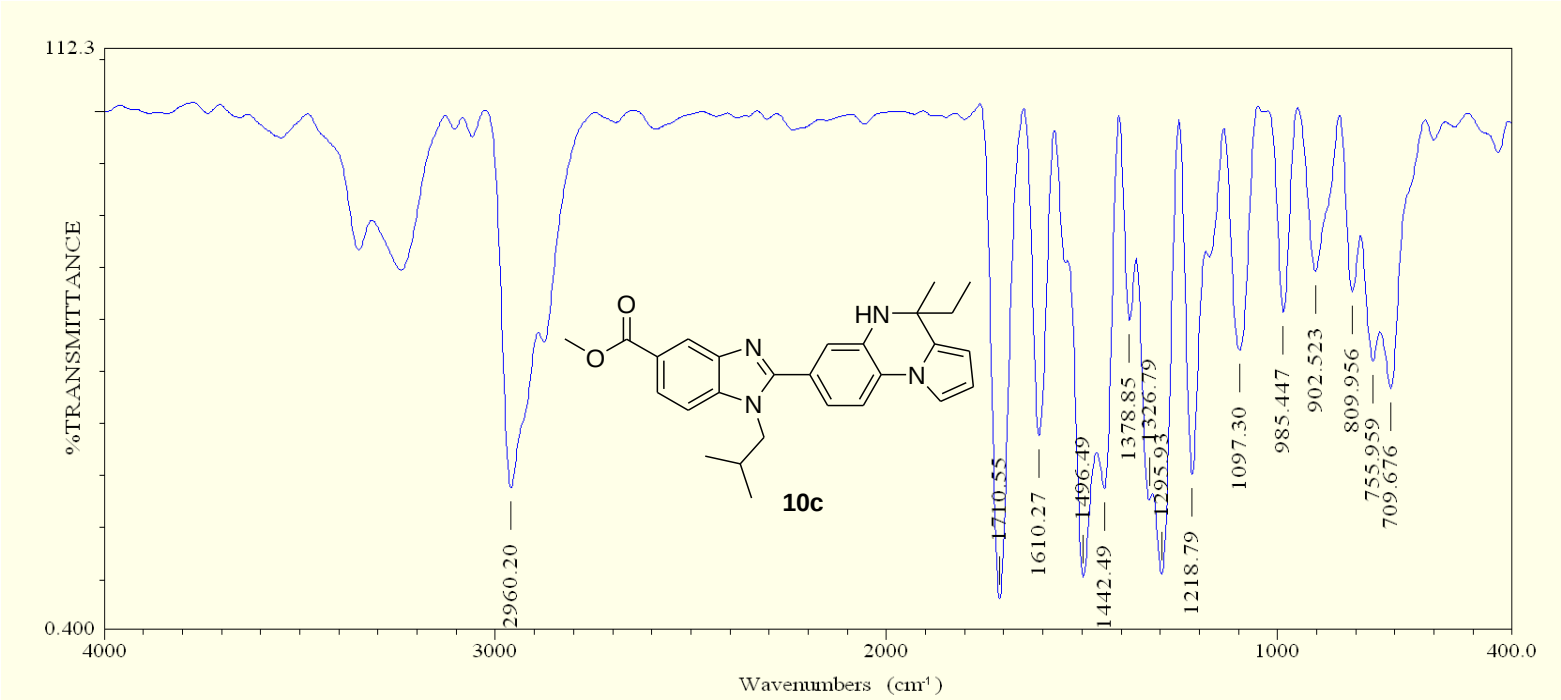
Crude HPLC Spectra of Compounds 10r



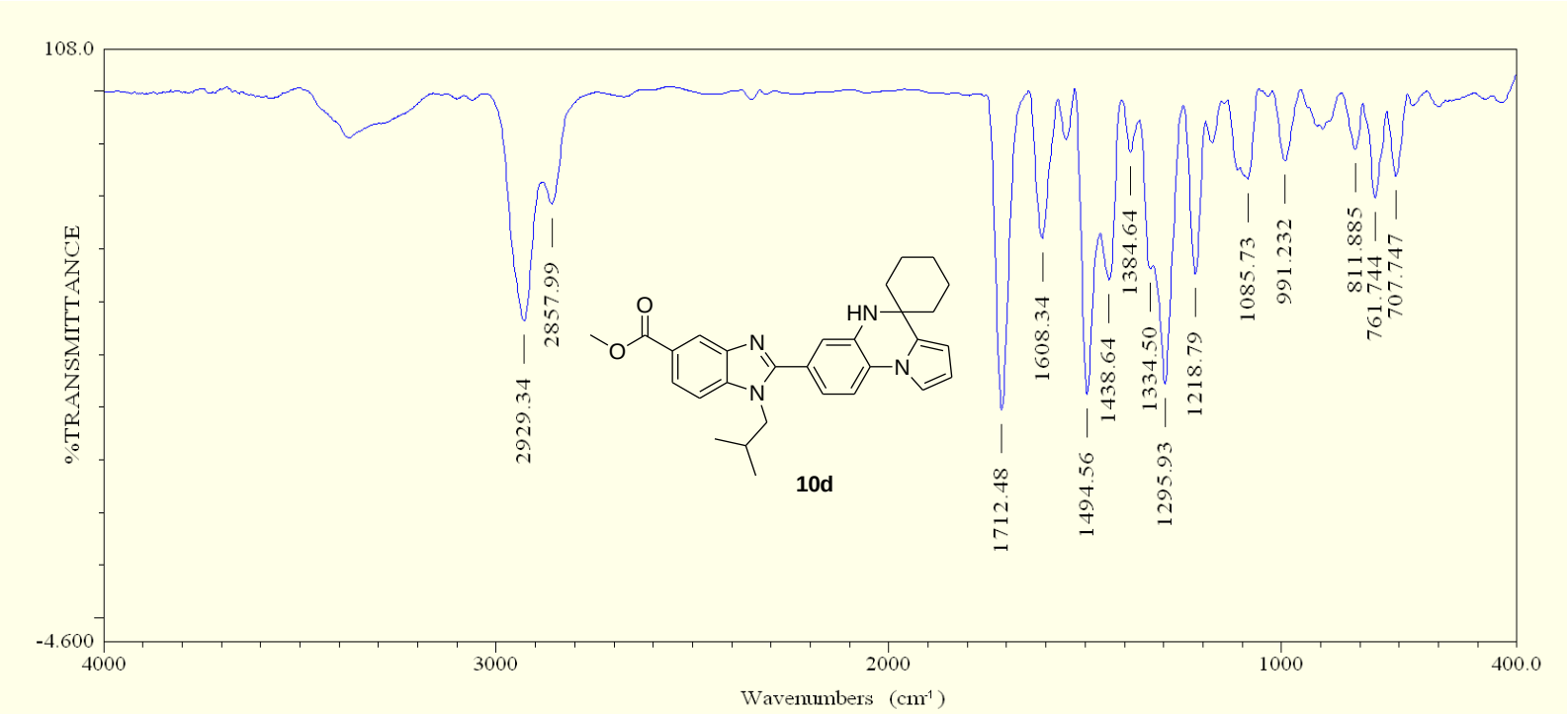
IR spectra of Compounds 10a



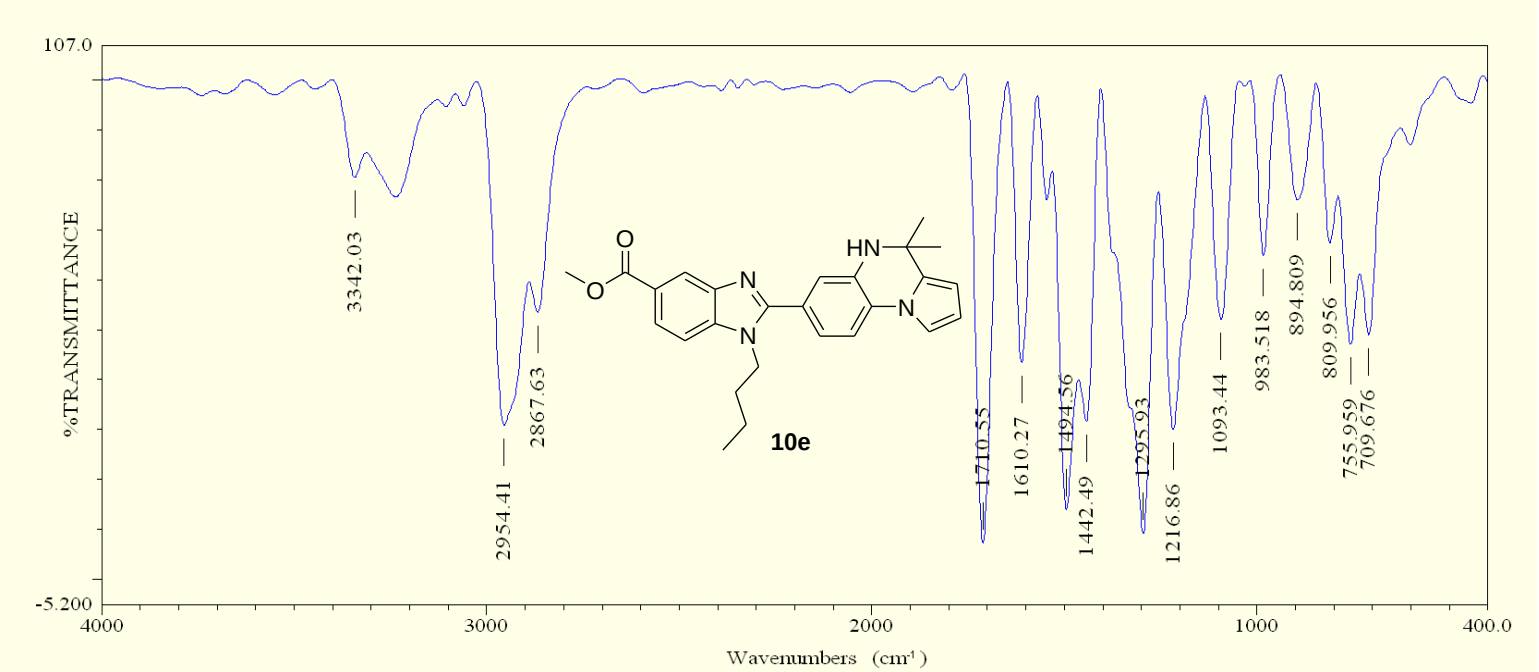
IR spectra of Compounds 10b



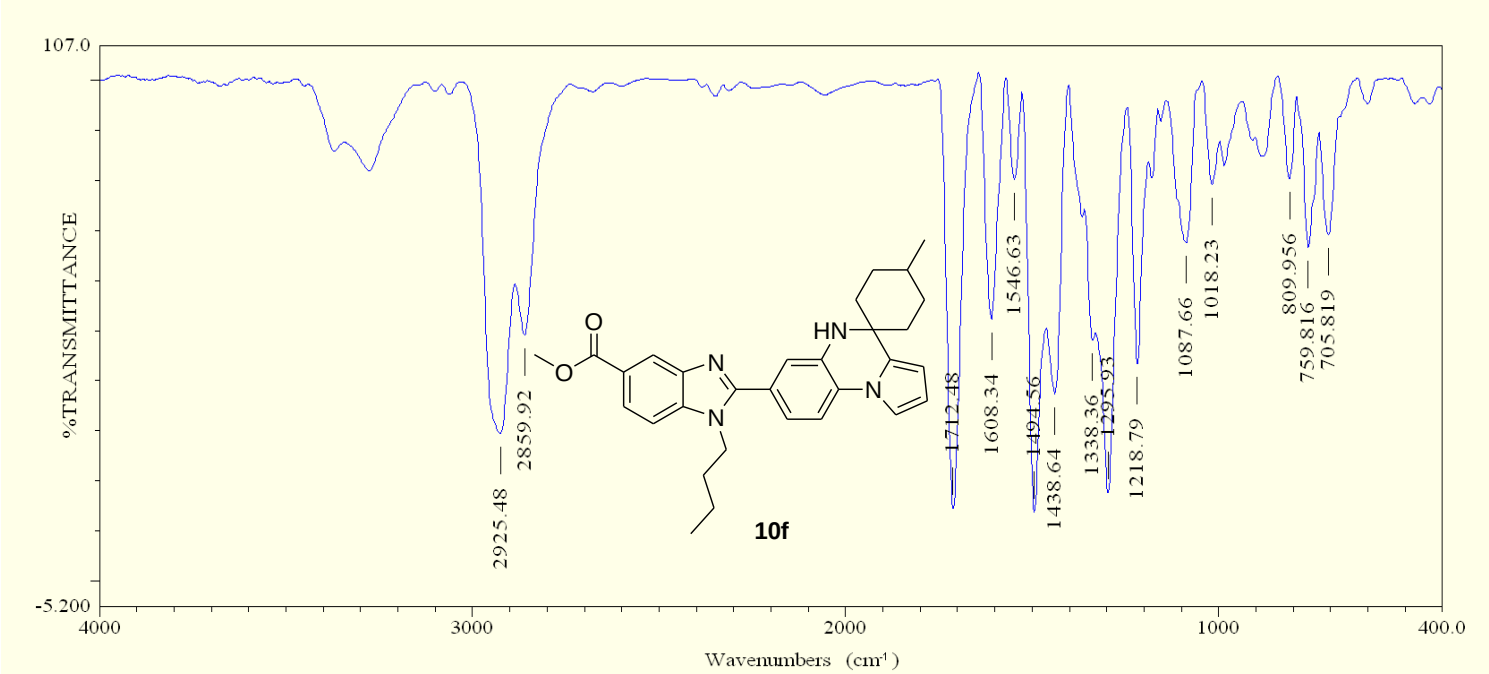
IR spectra of Compounds 10c



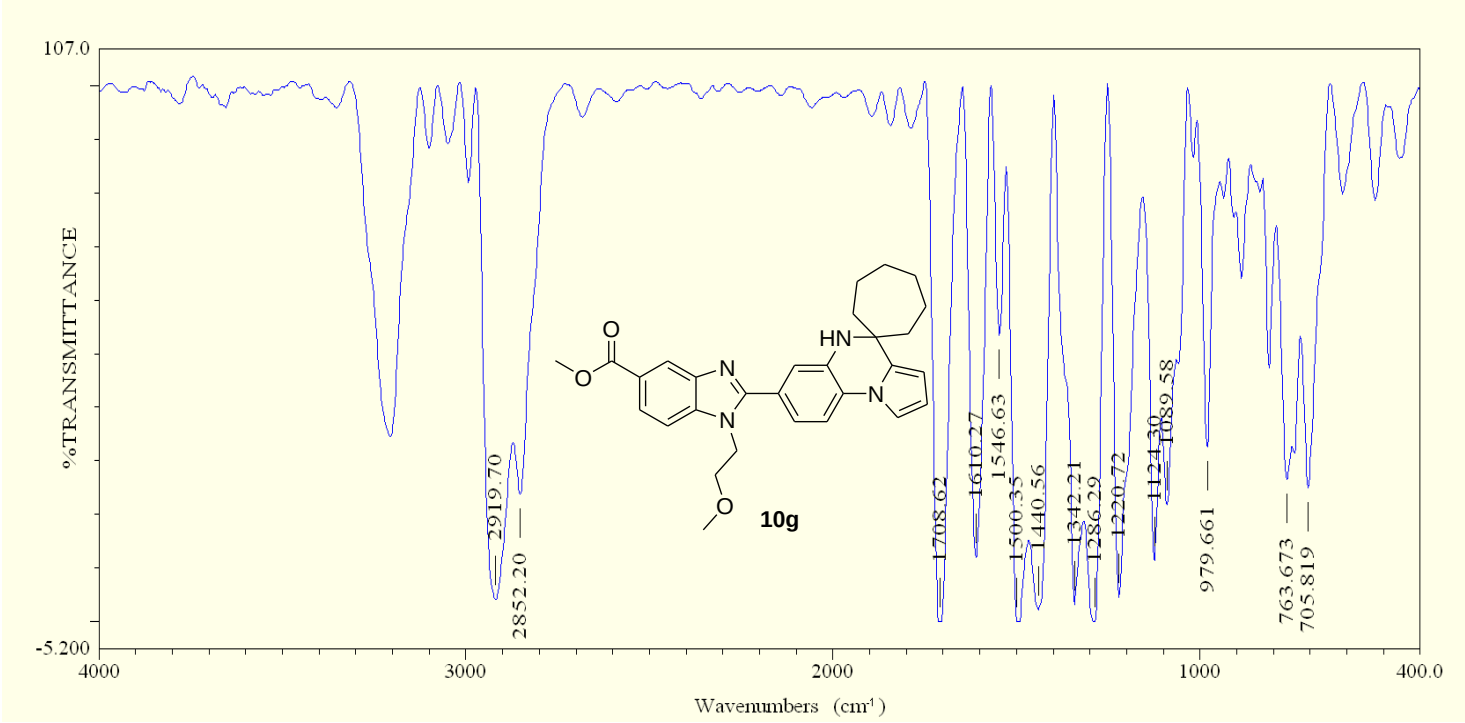
IR spectra of Compounds 10d



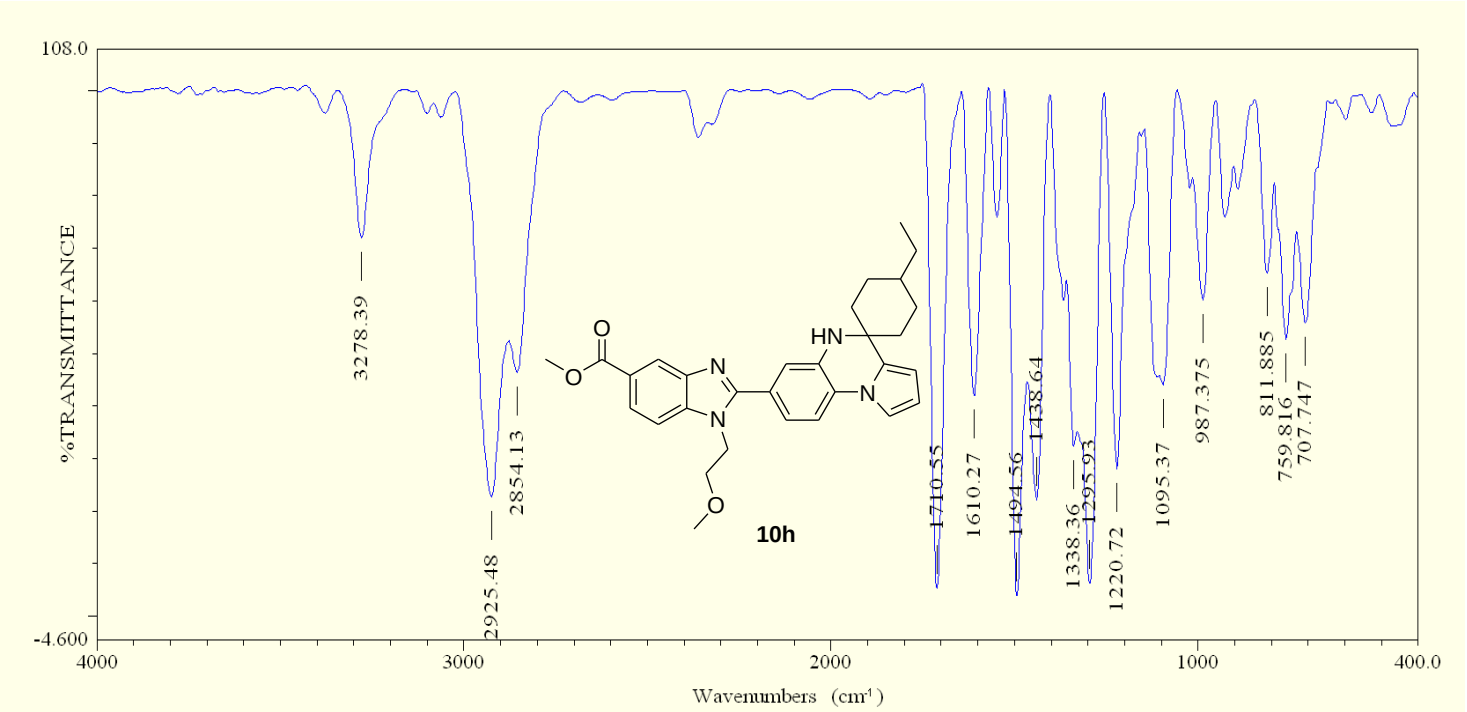
IR spectra of Compounds 10e



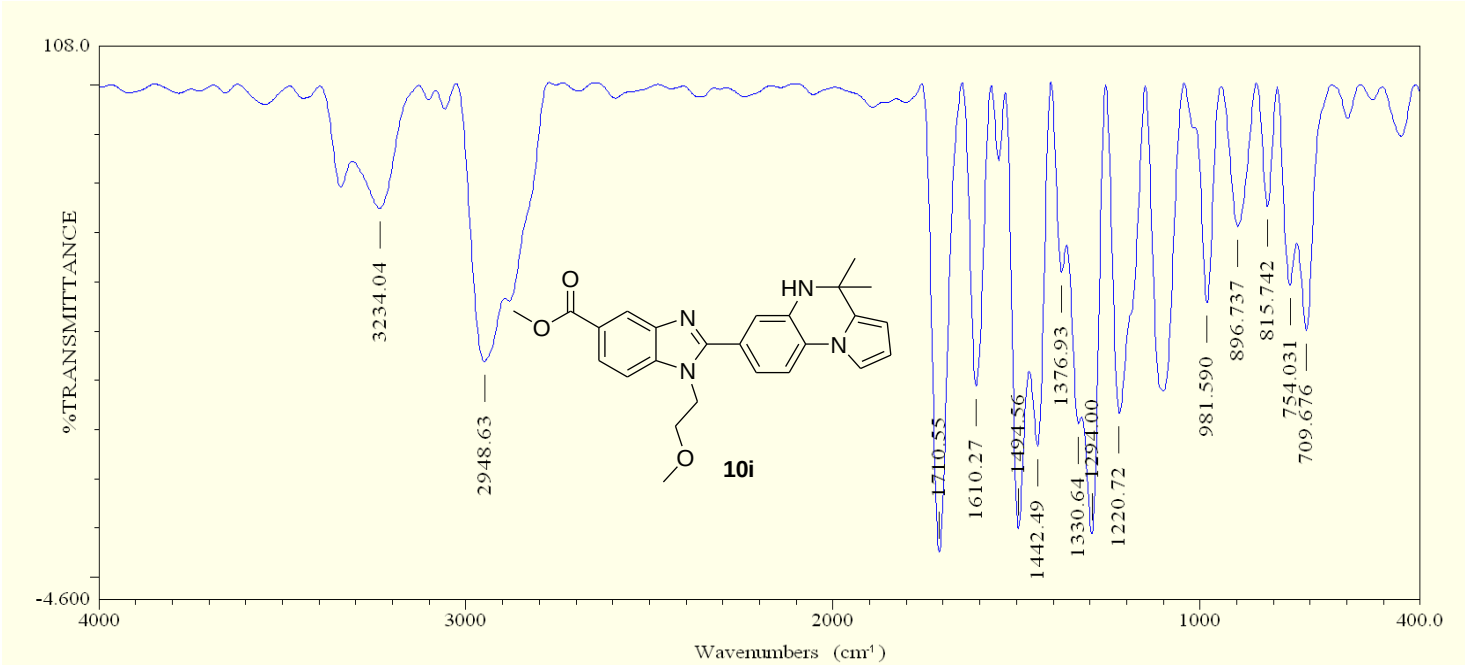
IR spectra of Compounds 10f



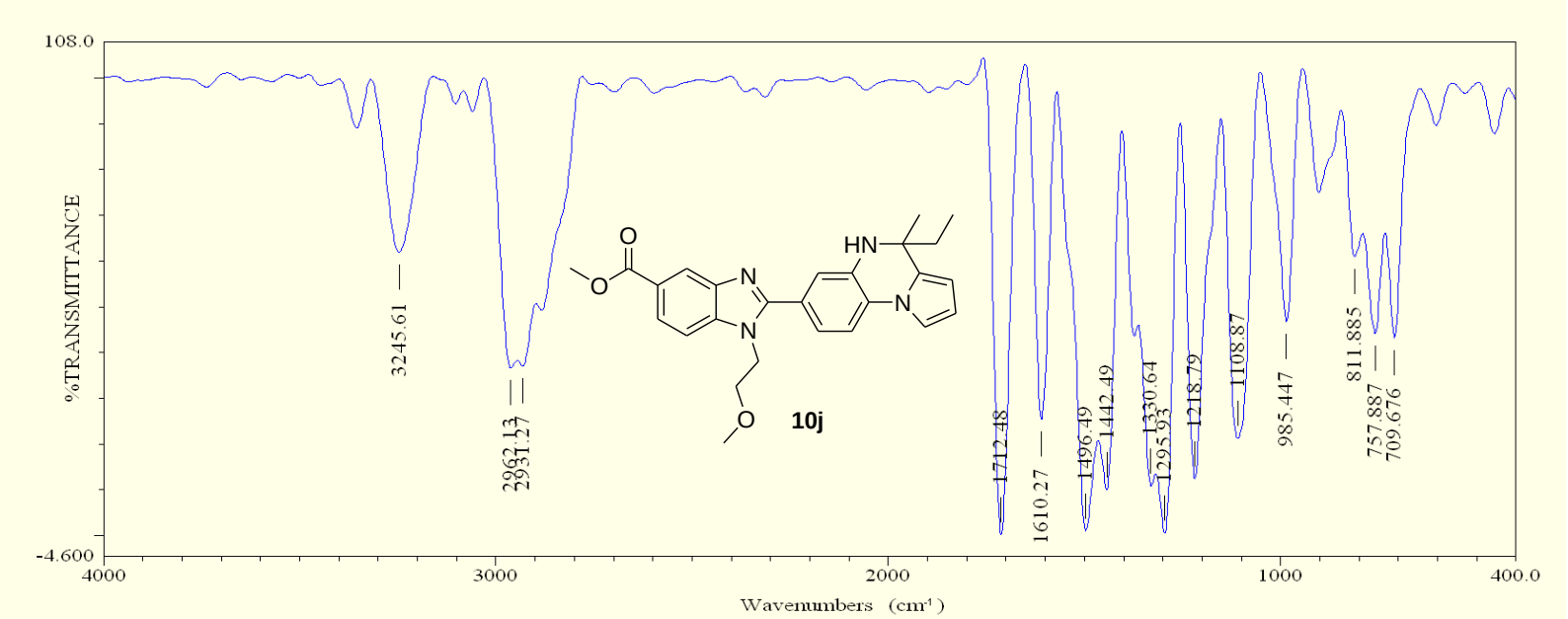
IR spectra of Compounds 10g



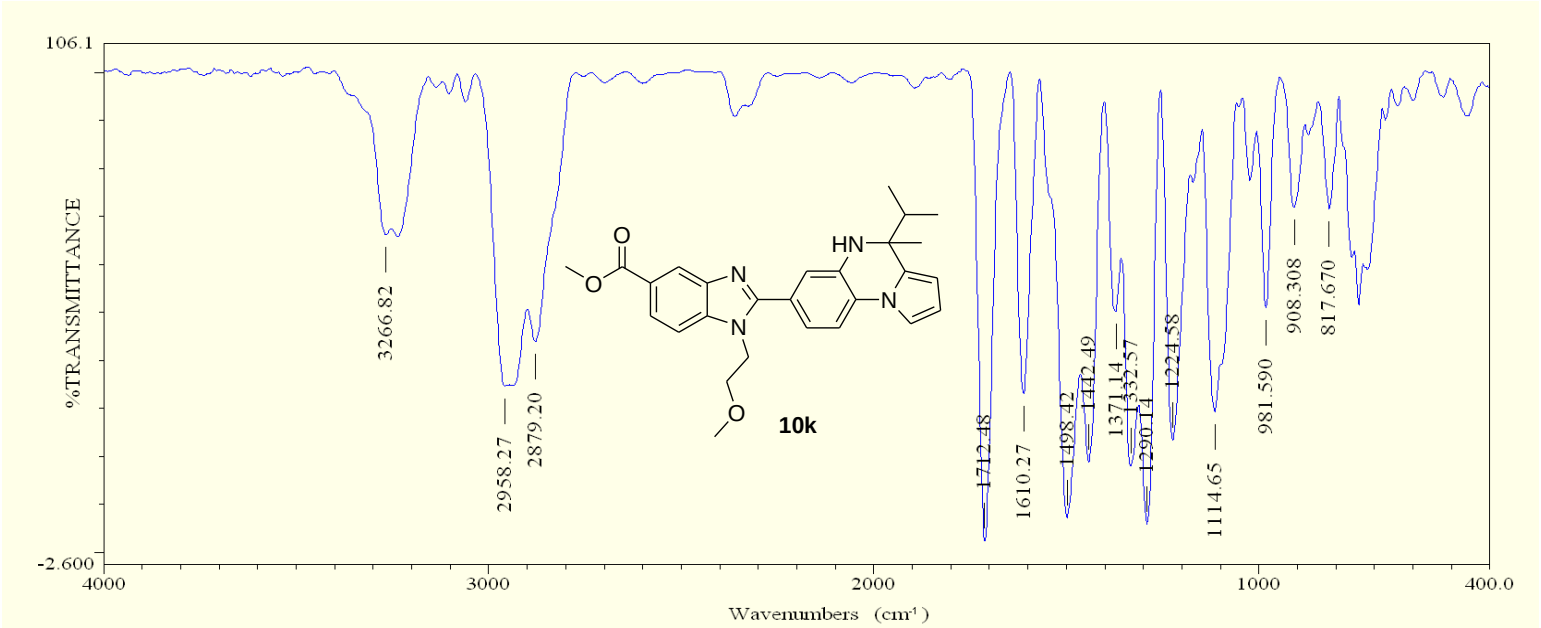
IR spectra of Compounds 10h



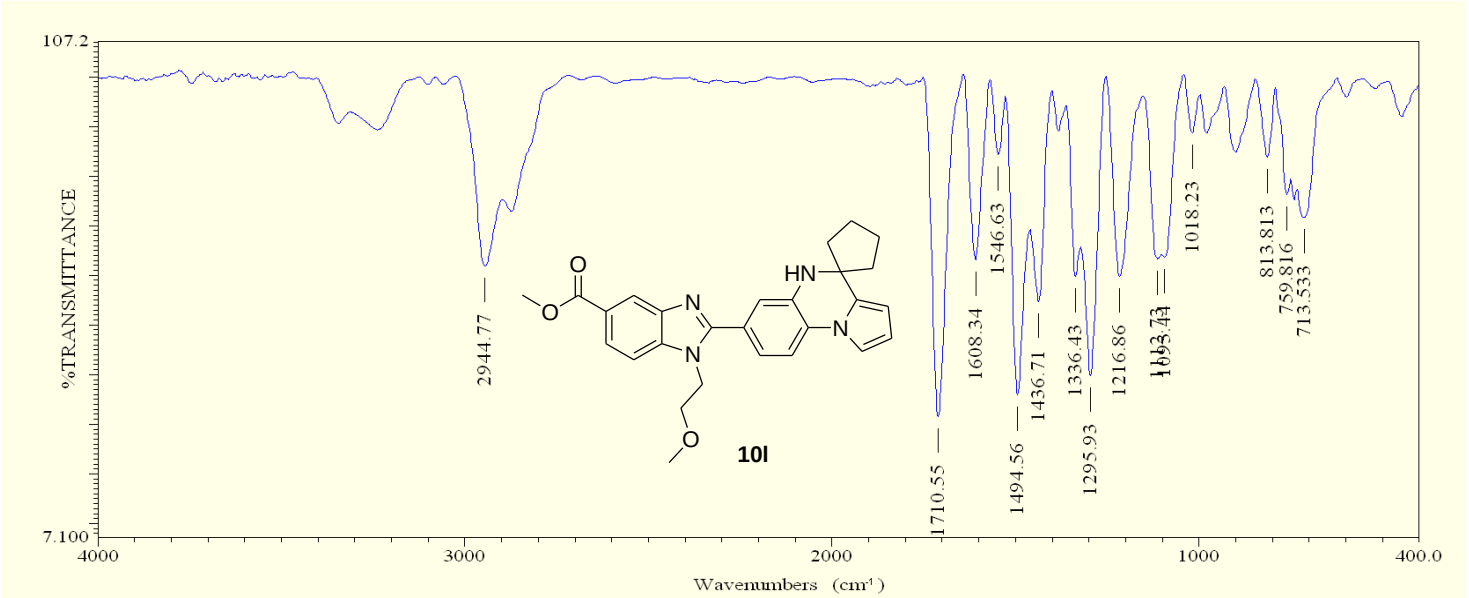
IR spectra of Compounds 10i



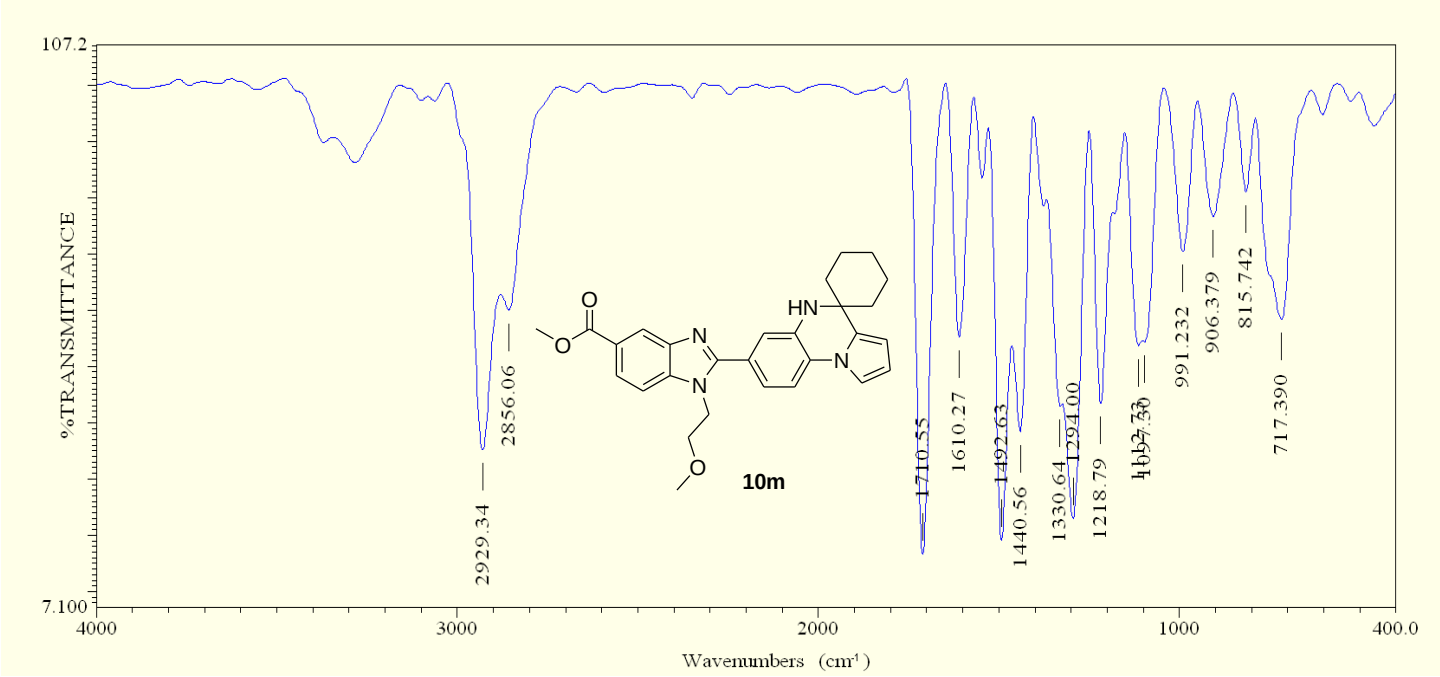
IR spectra of Compounds 10j



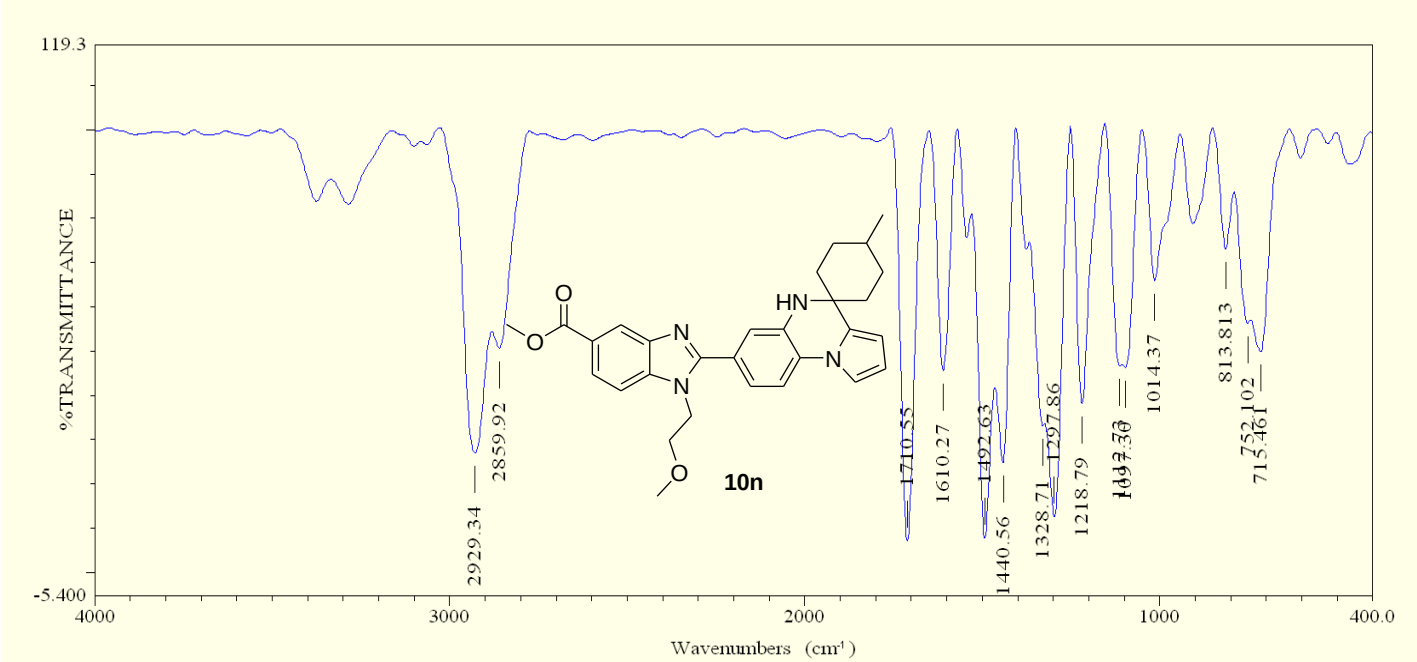
IR spectra of Compounds 10k



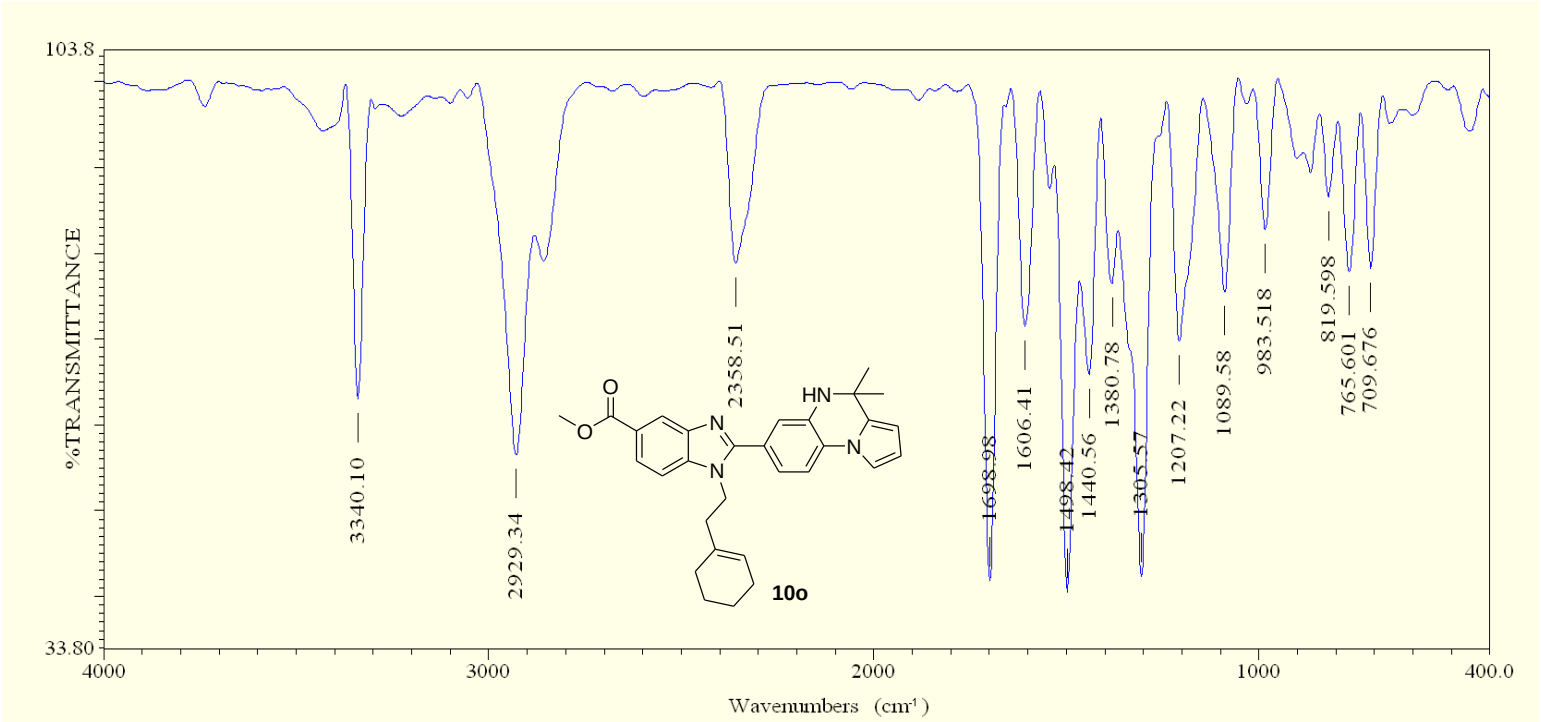
IR spectra of Compounds 10l



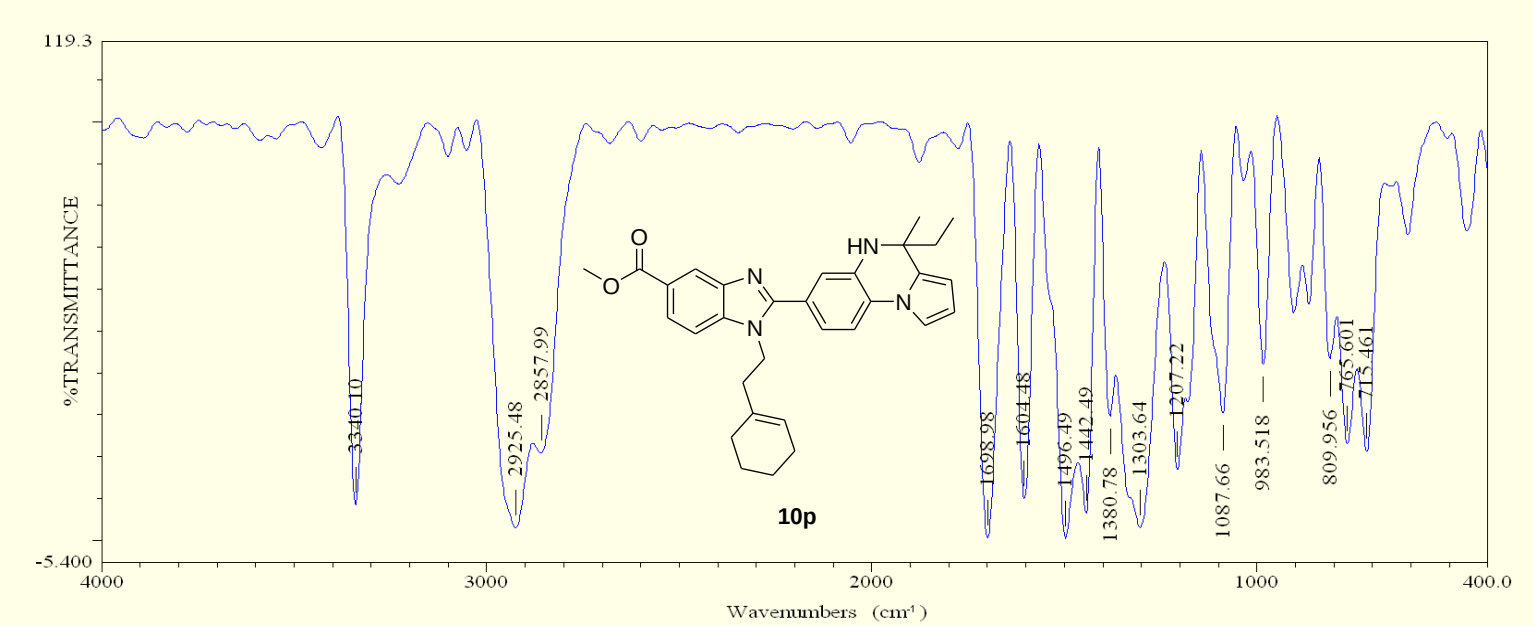
IR spectra of Compounds 10m



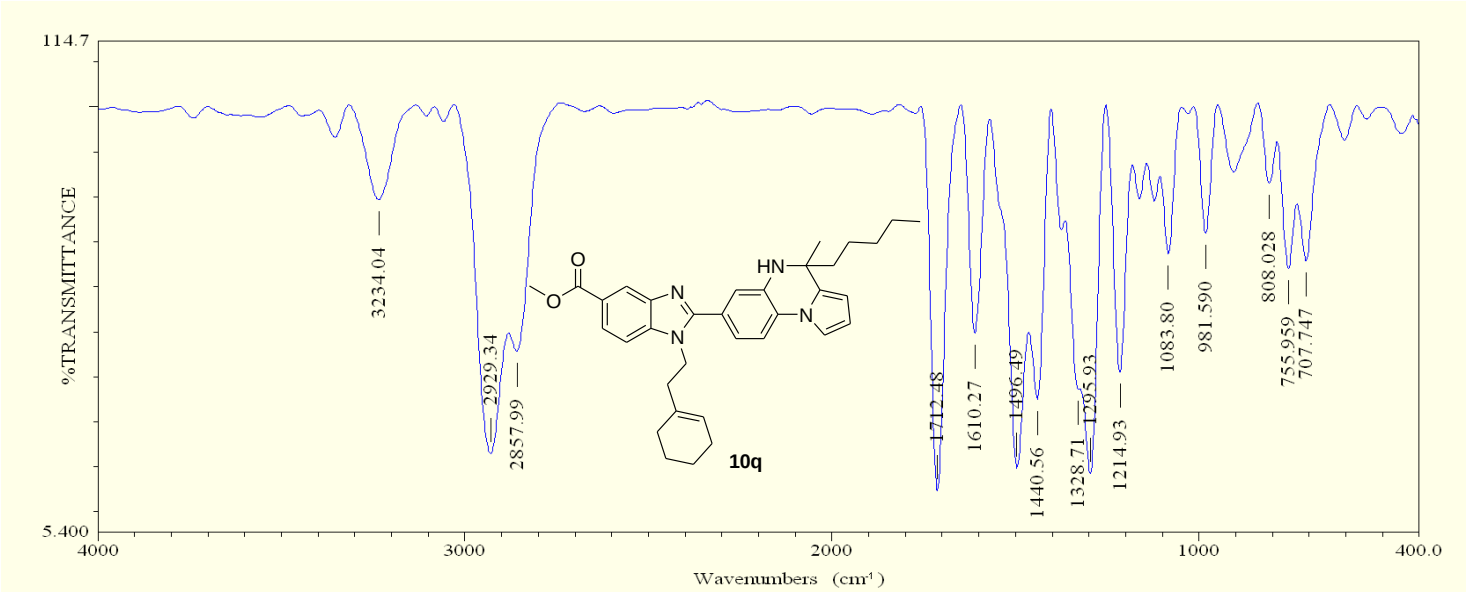
IR spectra of Compounds 10n



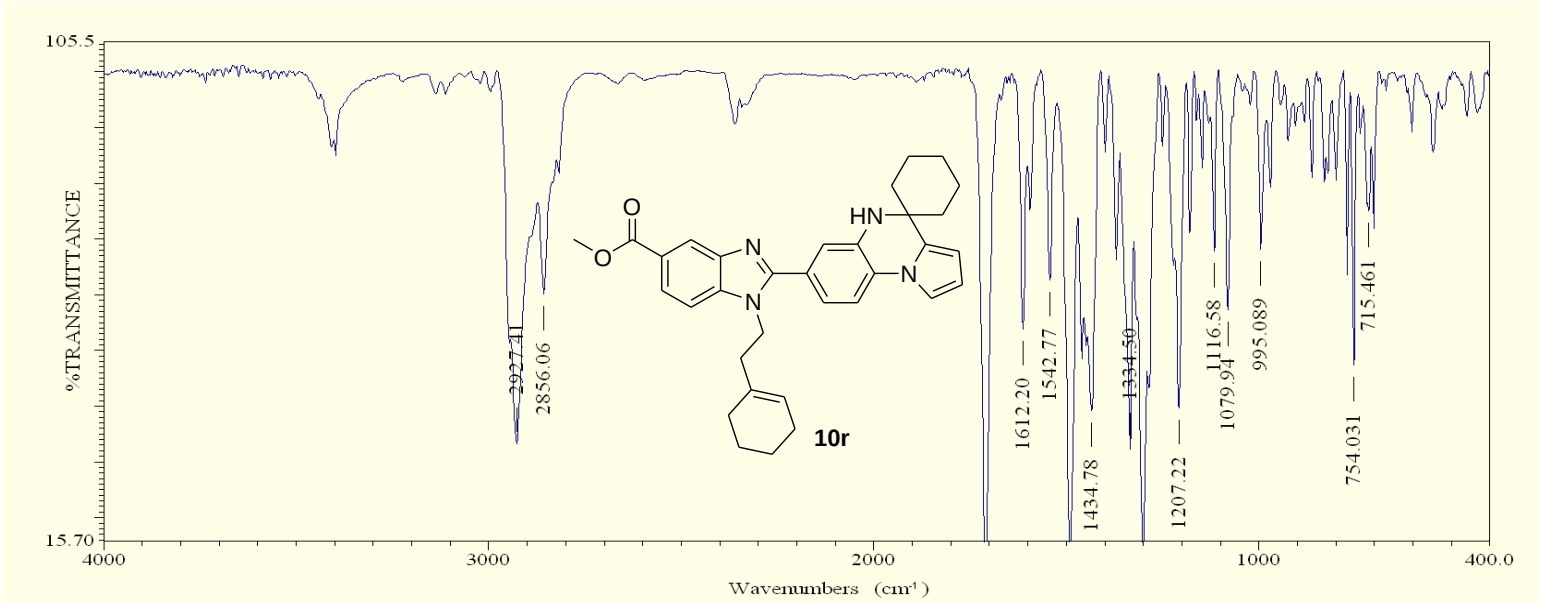
IR spectra of Compounds 10o



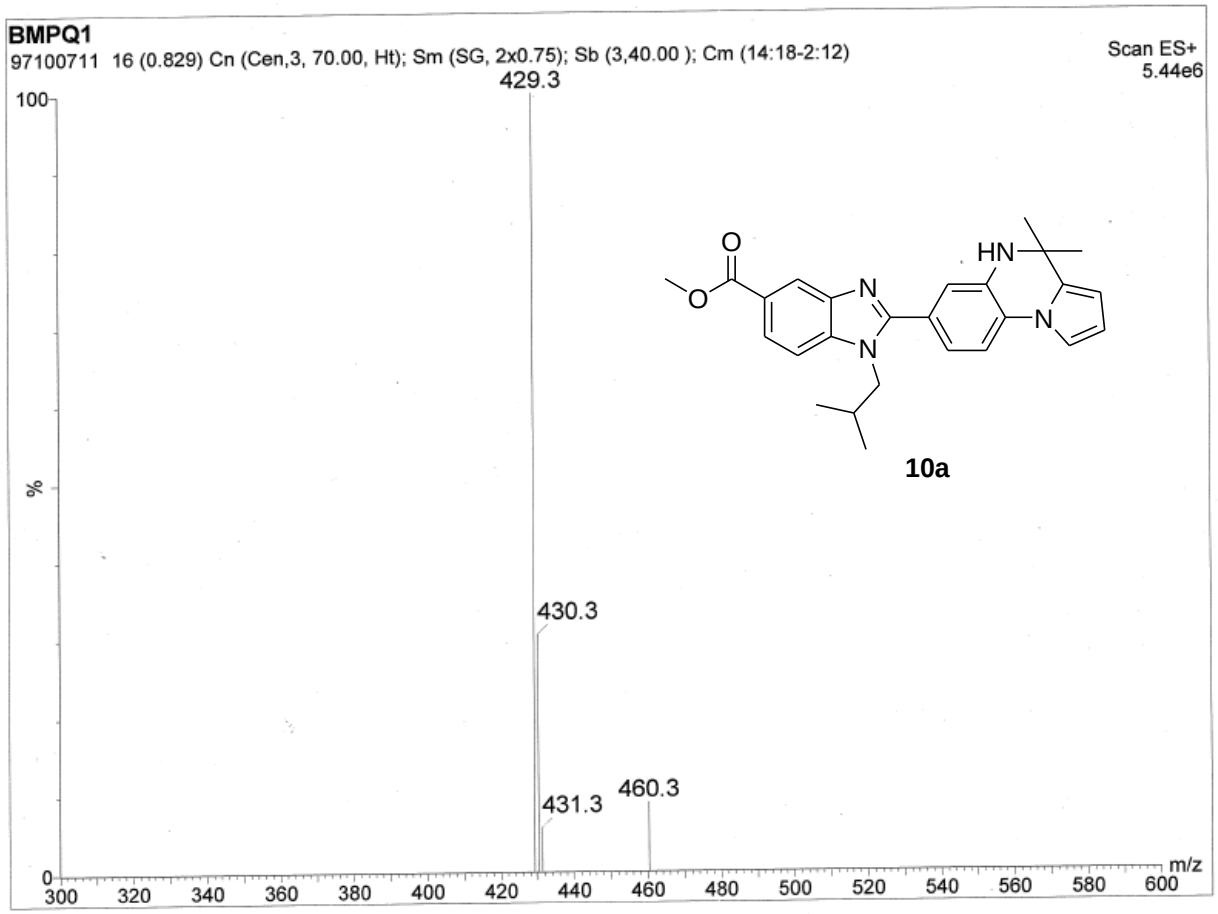
IR spectra of Compounds 10p



IR spectra of Compounds 10q

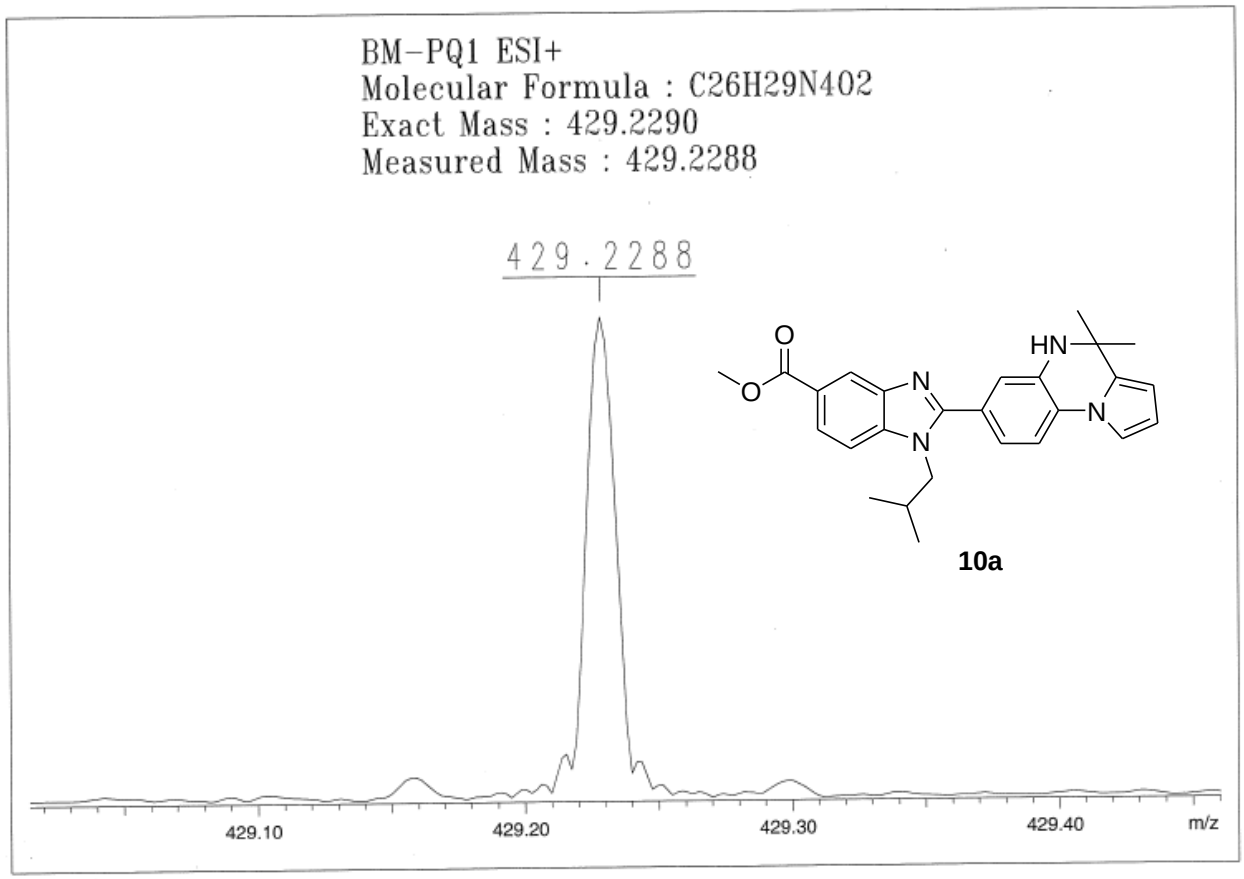


IR spectra of Compounds 10r

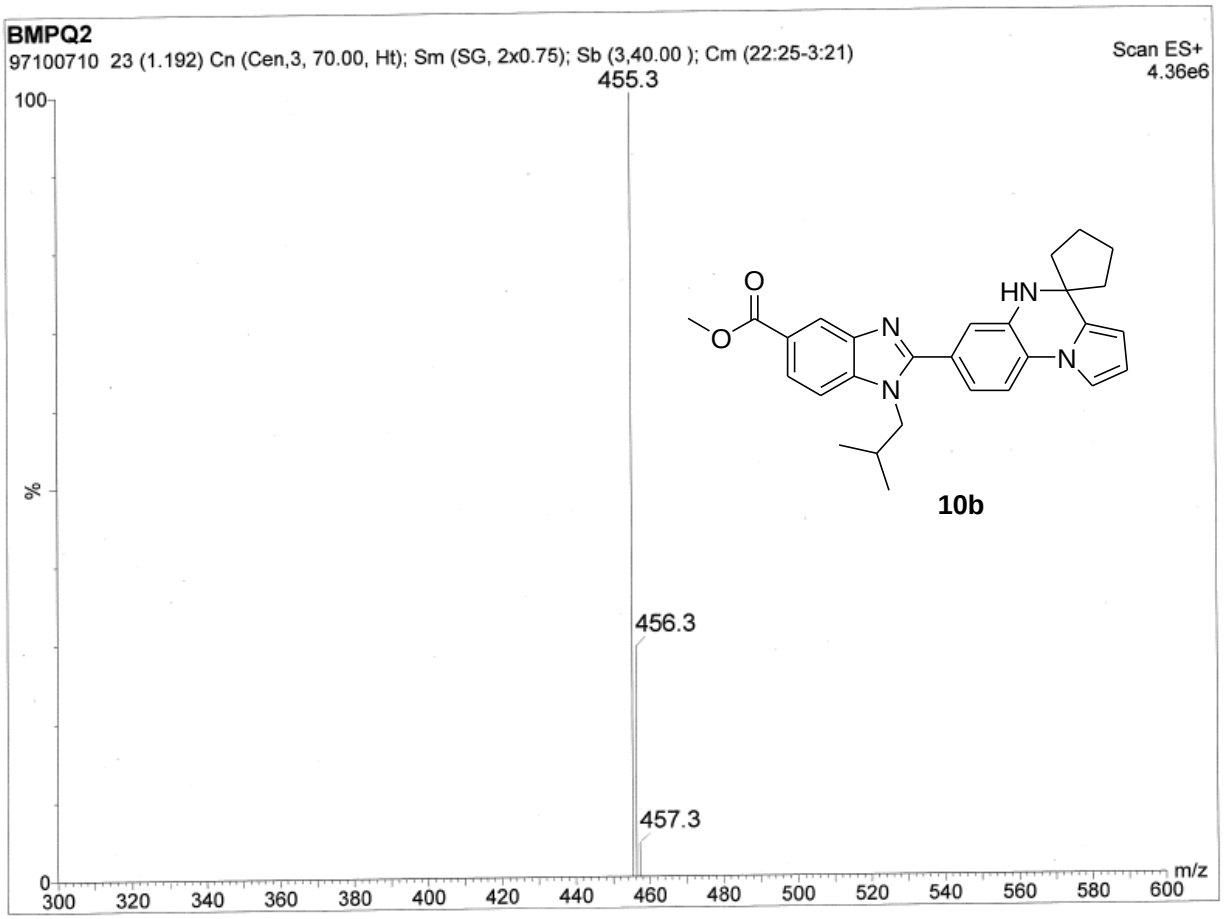


10a

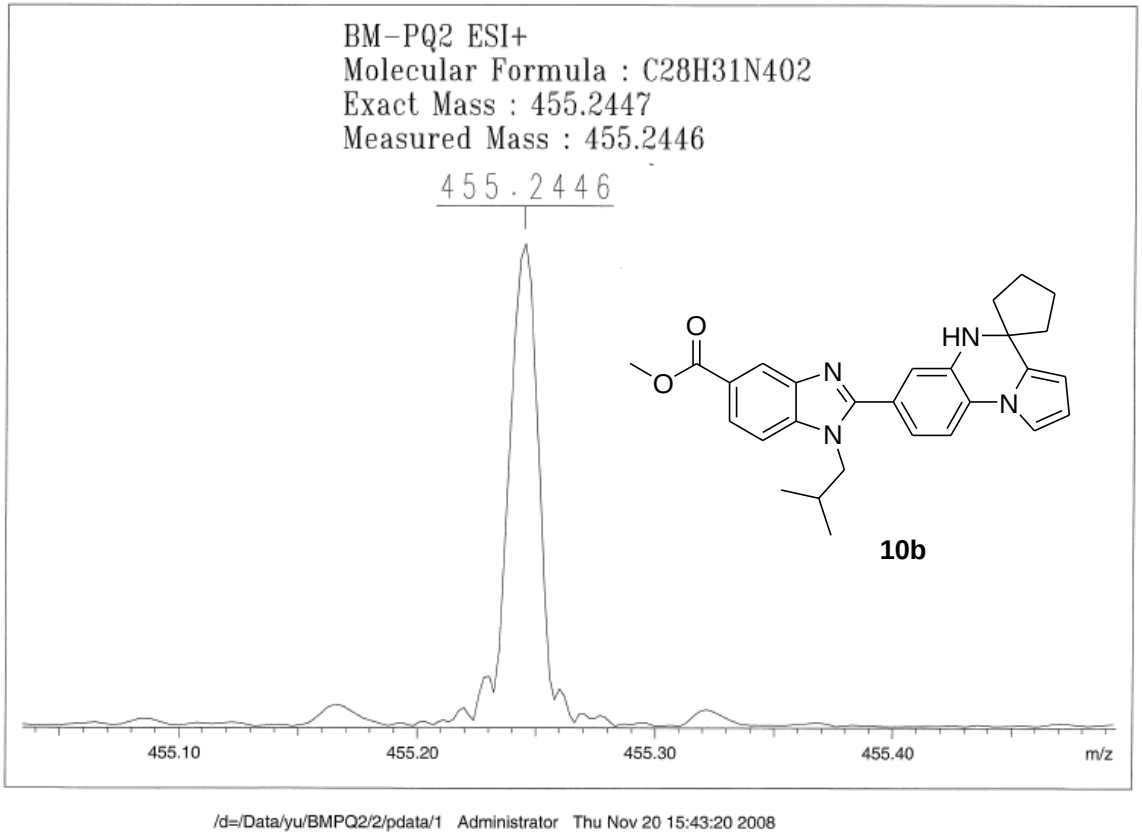
LR Mass spectra of Compounds 10a



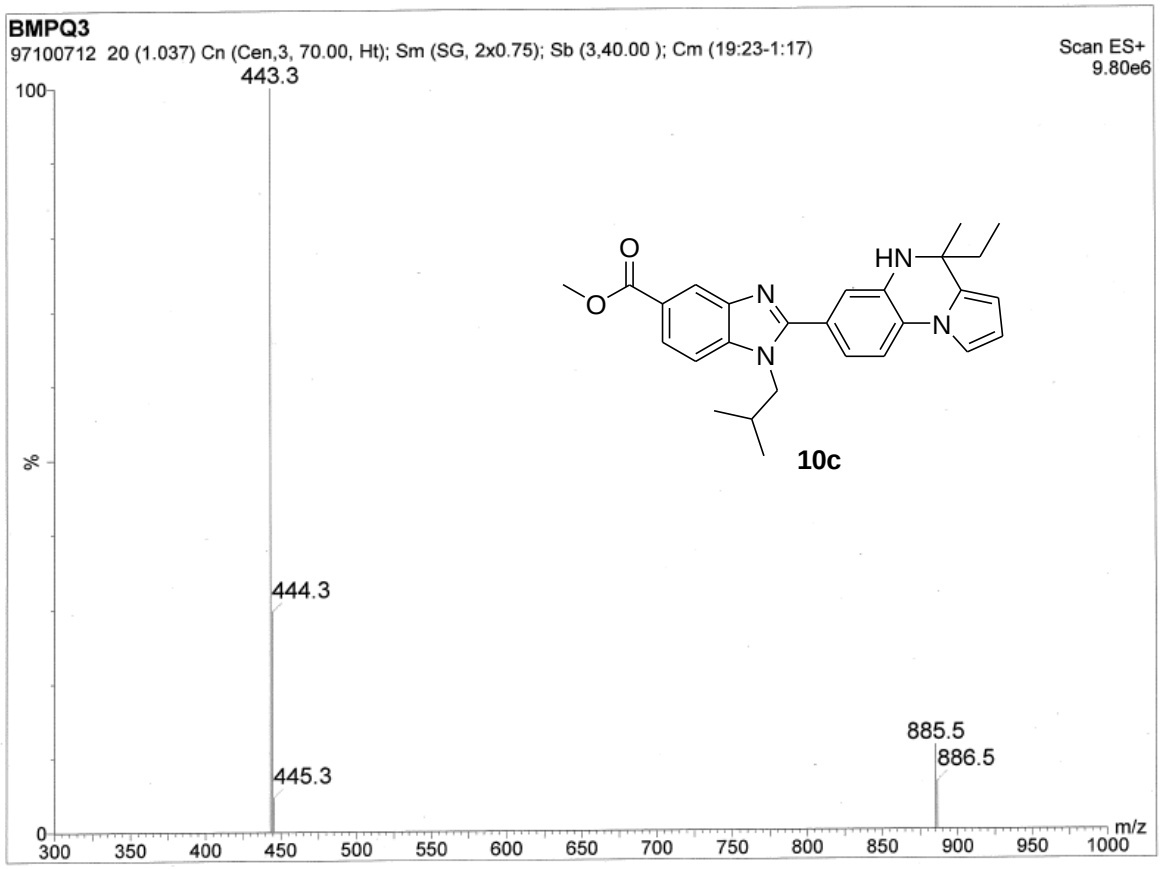
HR Mass spectra of Compounds 10a



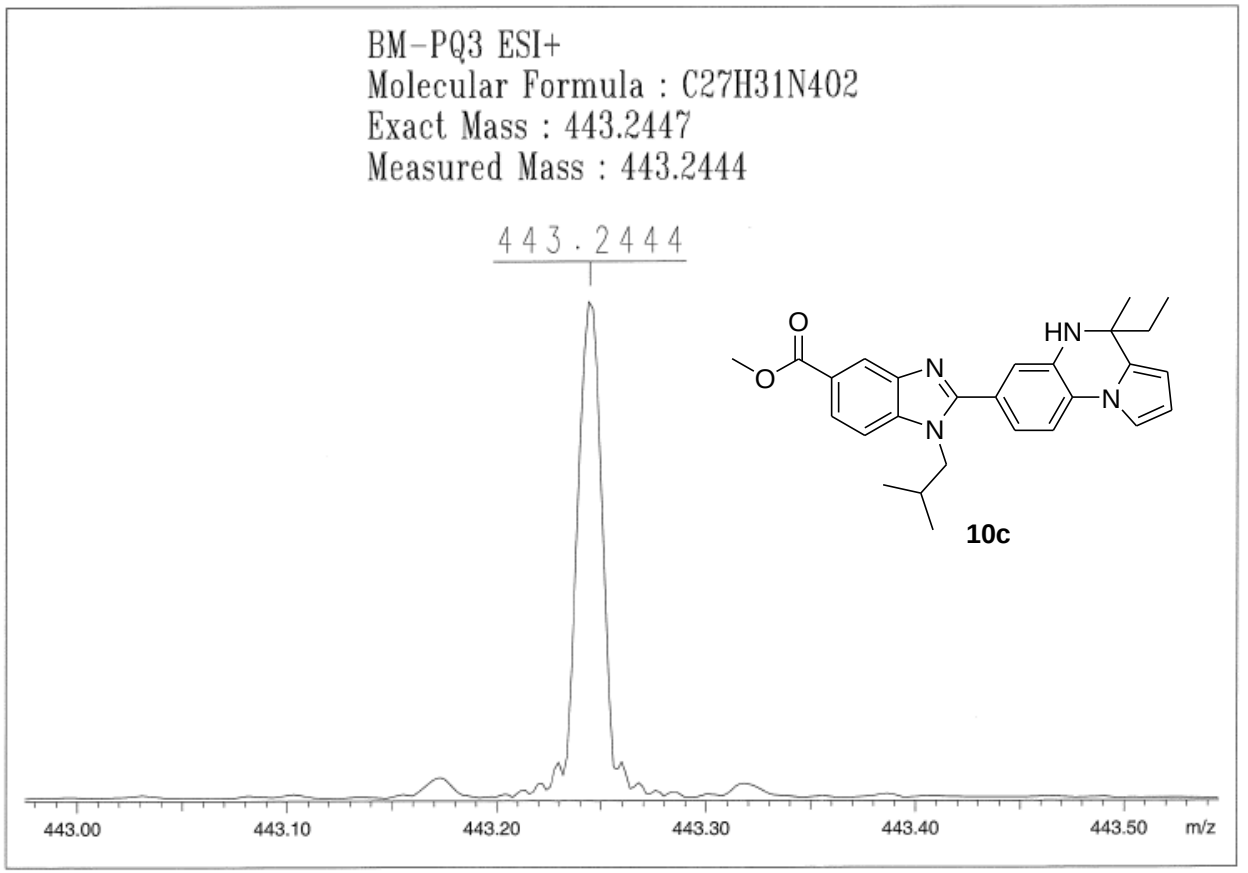
LR Mass spectra of Compounds 10b



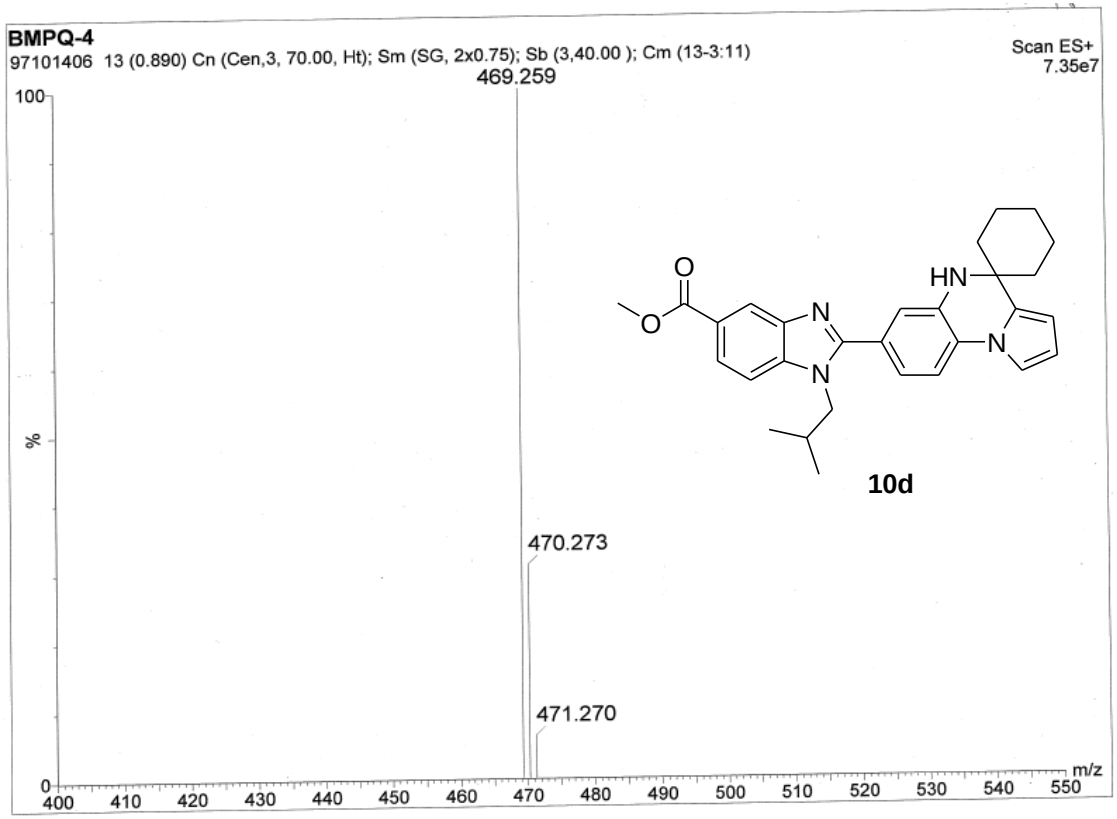
HR Mass spectra of Compounds 10b



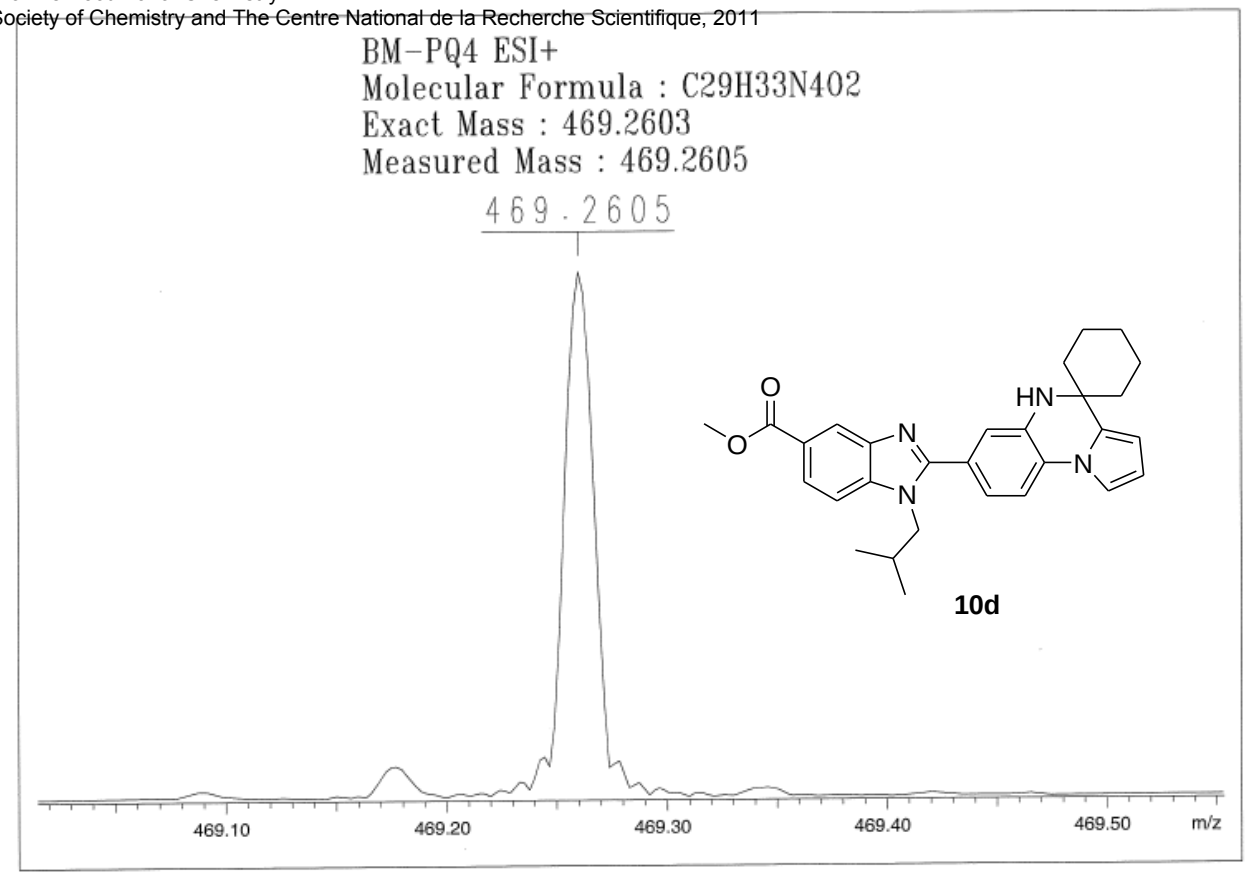
LR Mass spectra of Compounds 10c



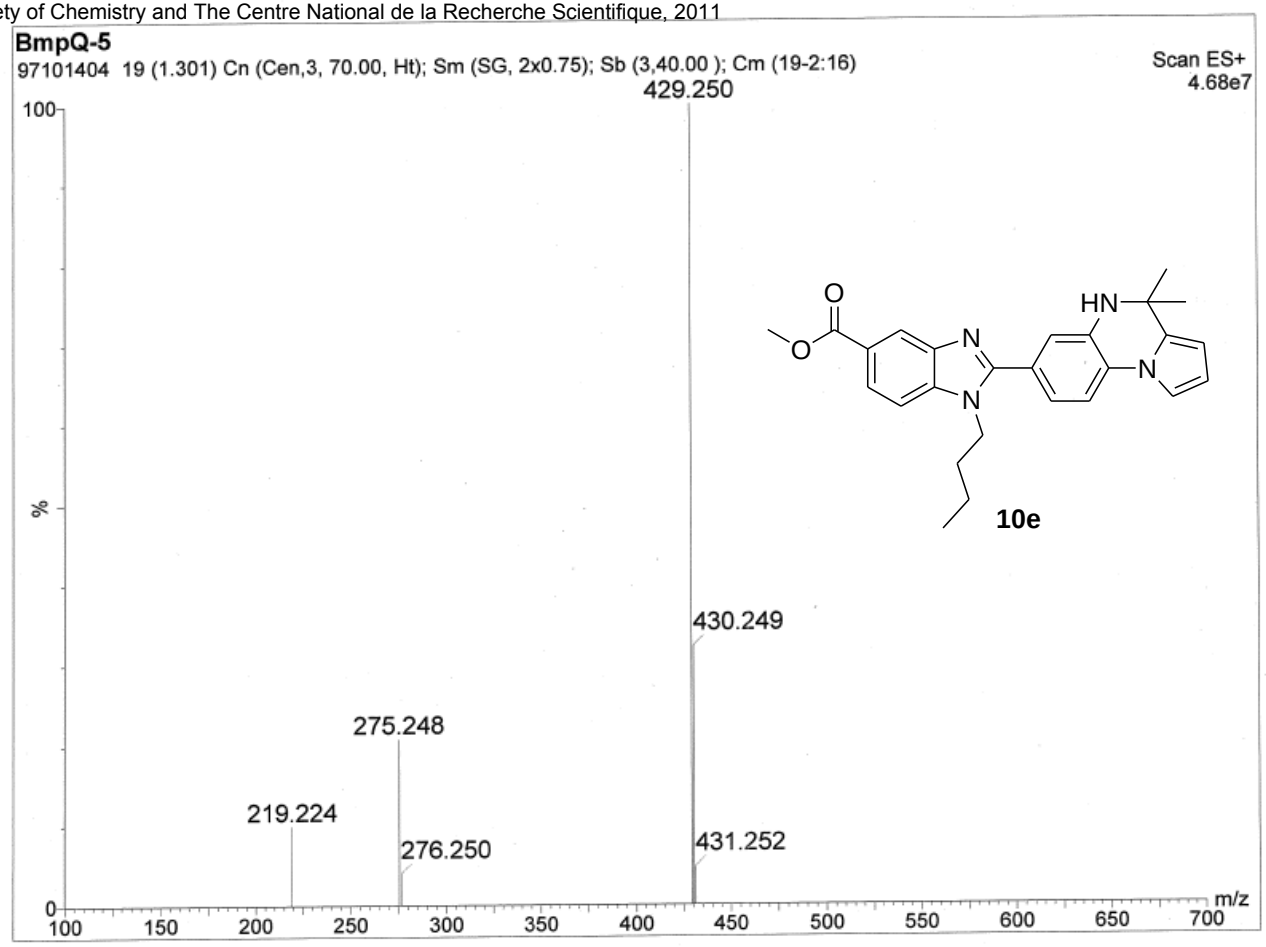
HR Mass spectra of Compounds 10c



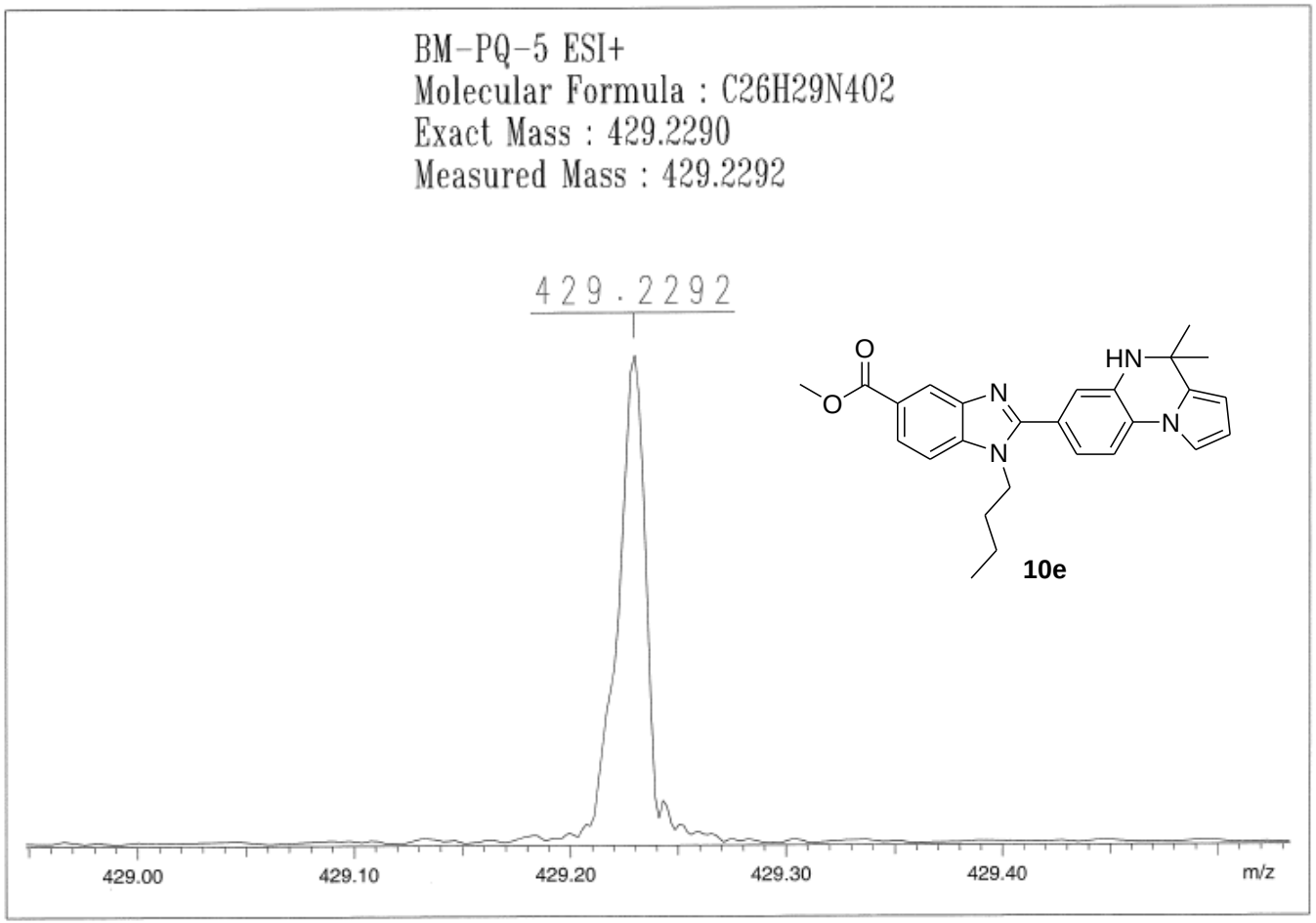
LR Mass spectra of Compounds 10d



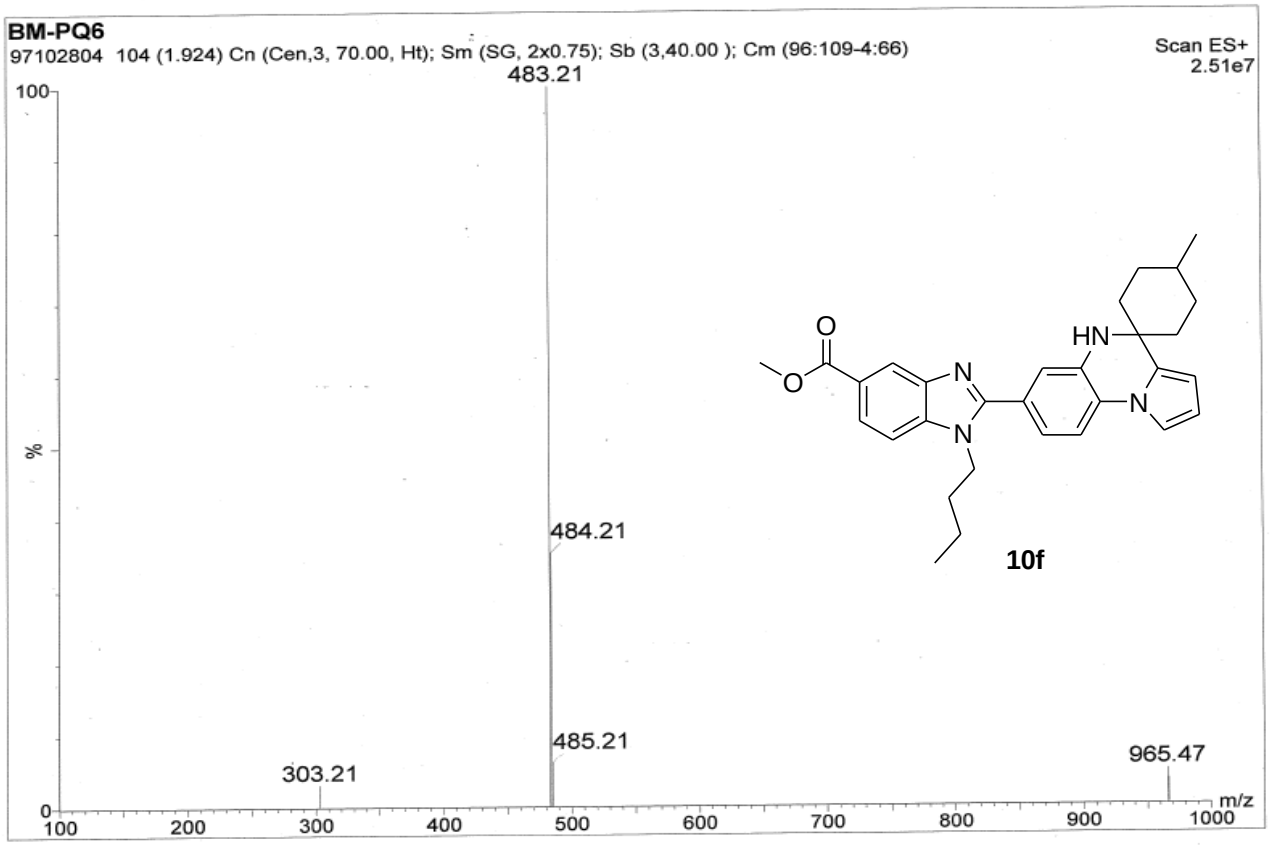
HR Mass spectra of Compounds 10d



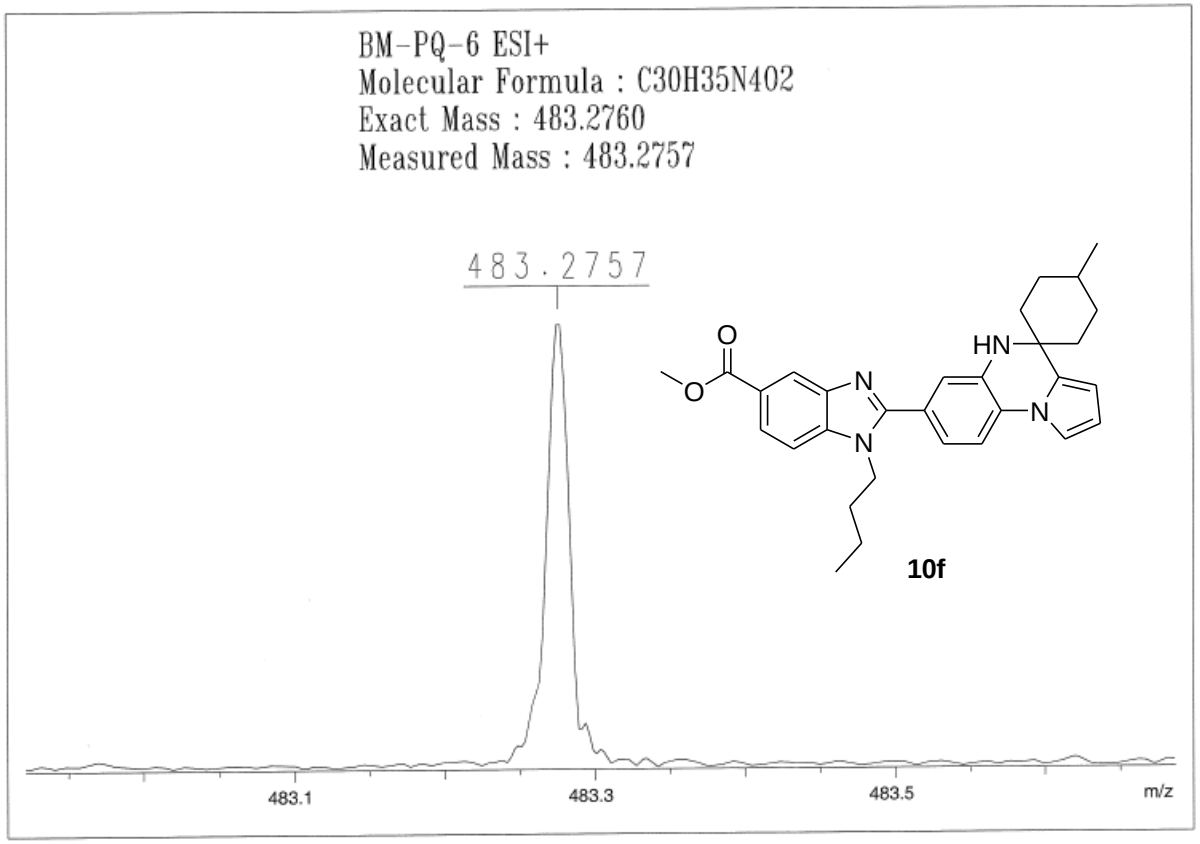
LR Mass spectra of Compounds 10e



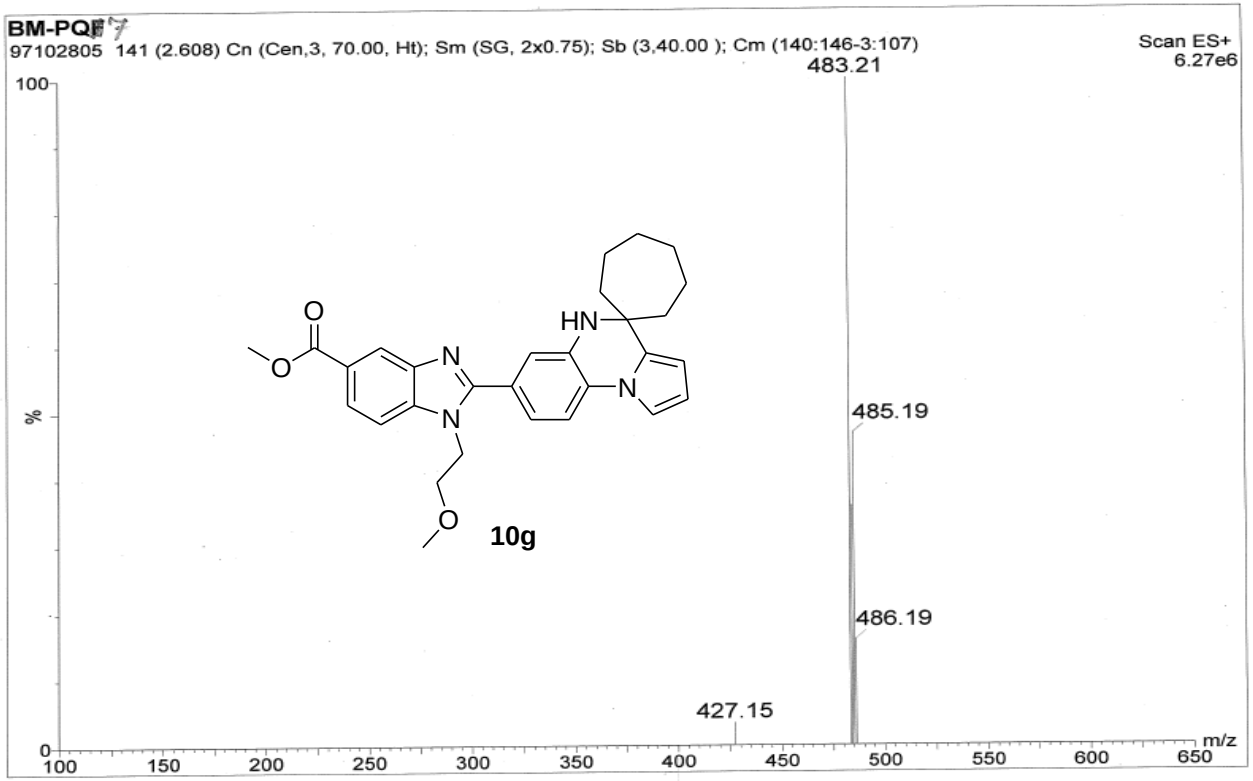
HR Mass spectra of Compounds 10e



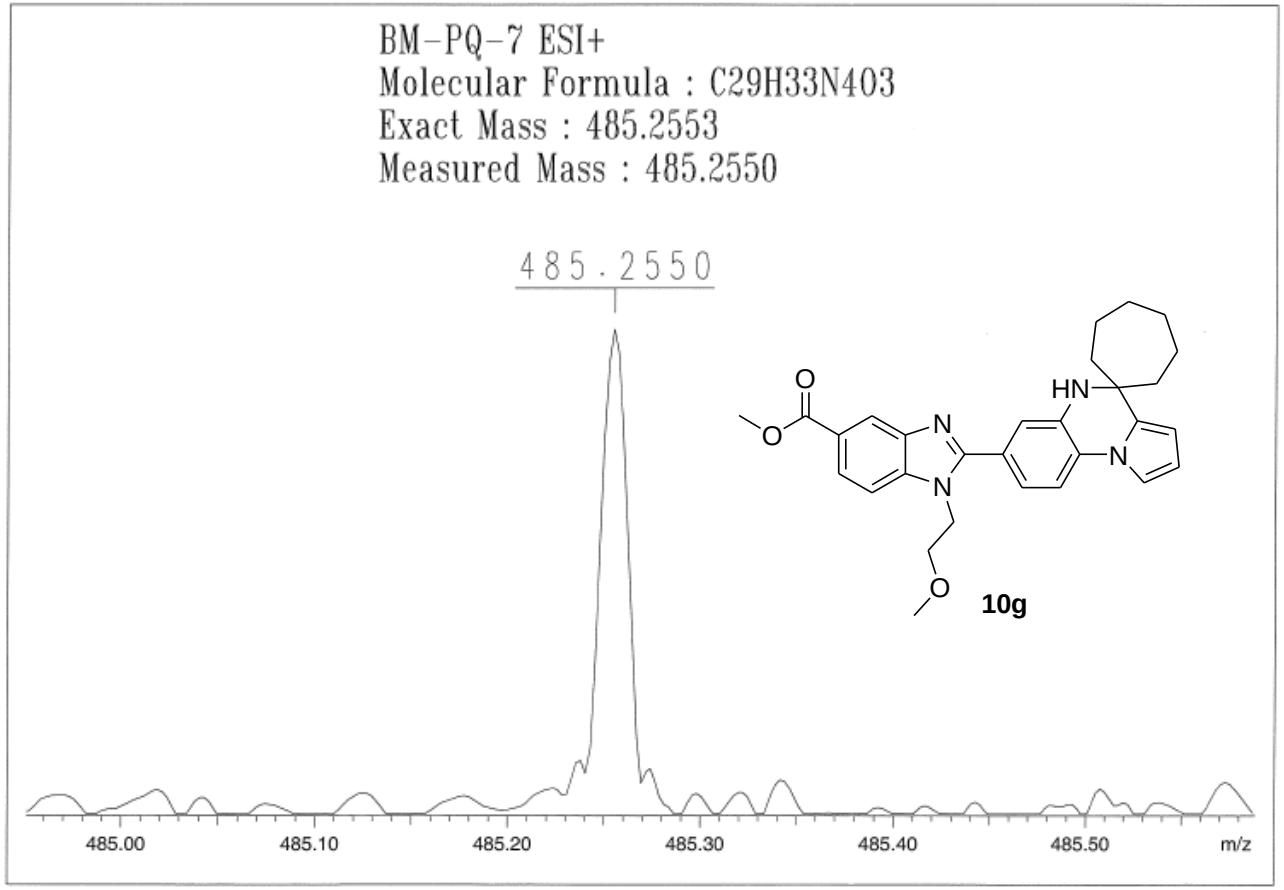
LR Mass spectra of Compounds 10f



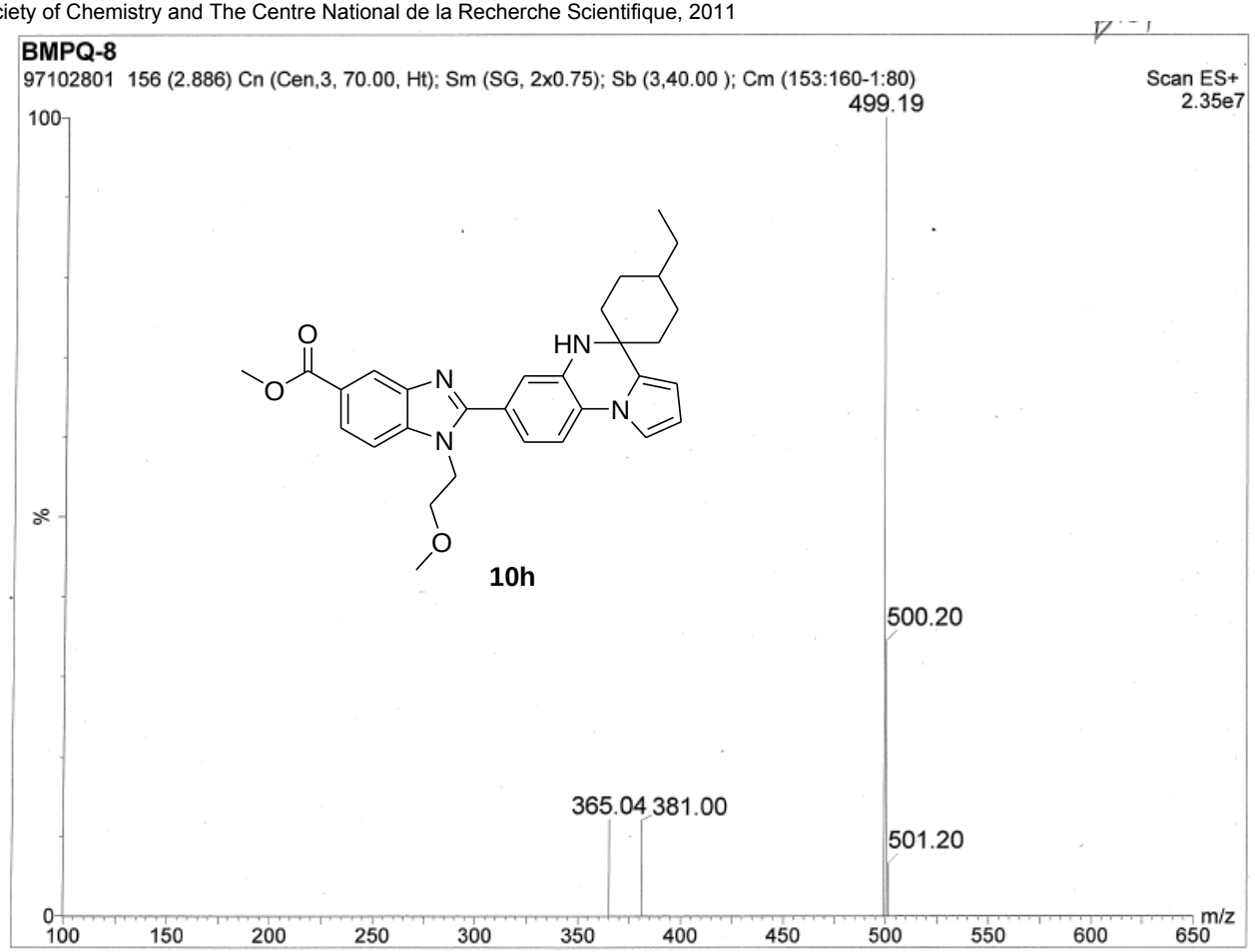
HR Mass spectra of Compounds 10f



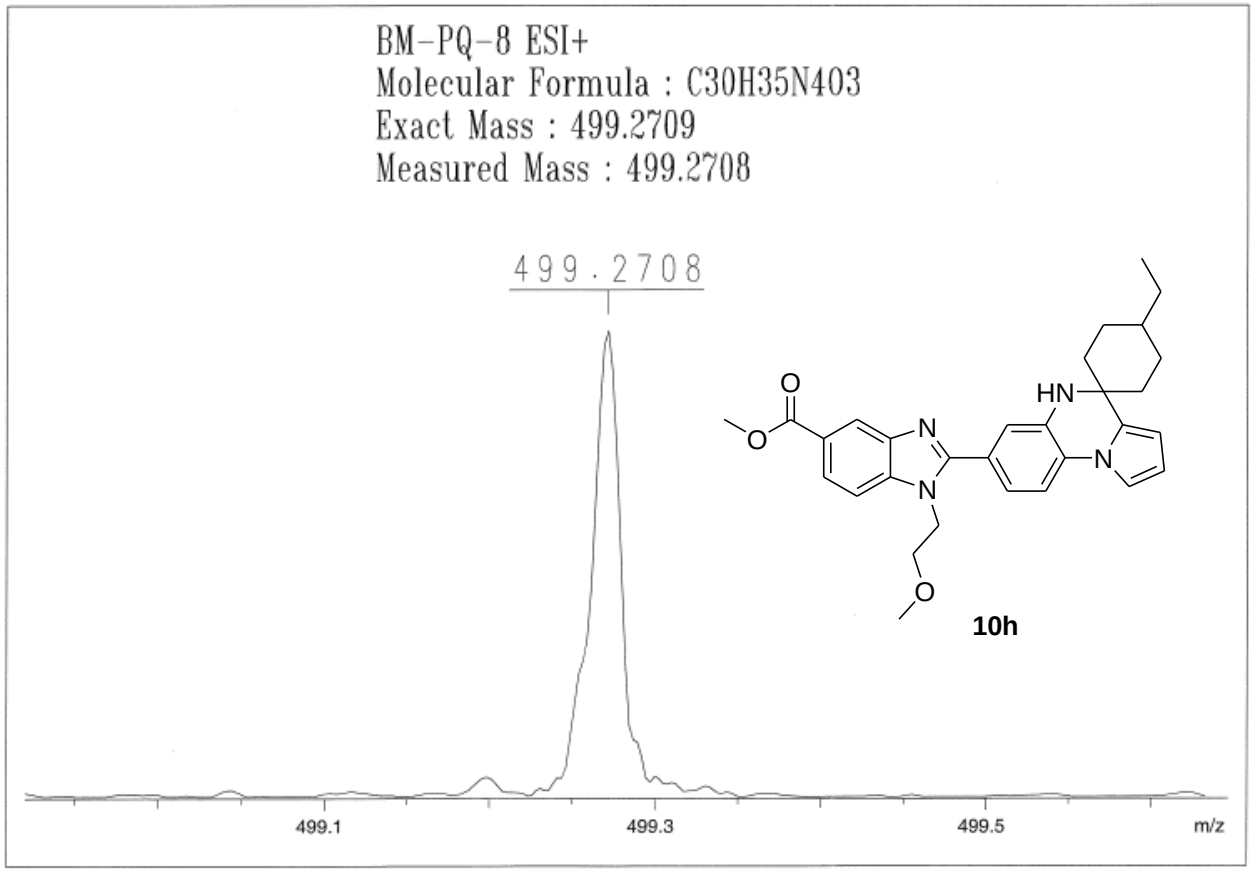
LR Mass spectra of Compounds 10g



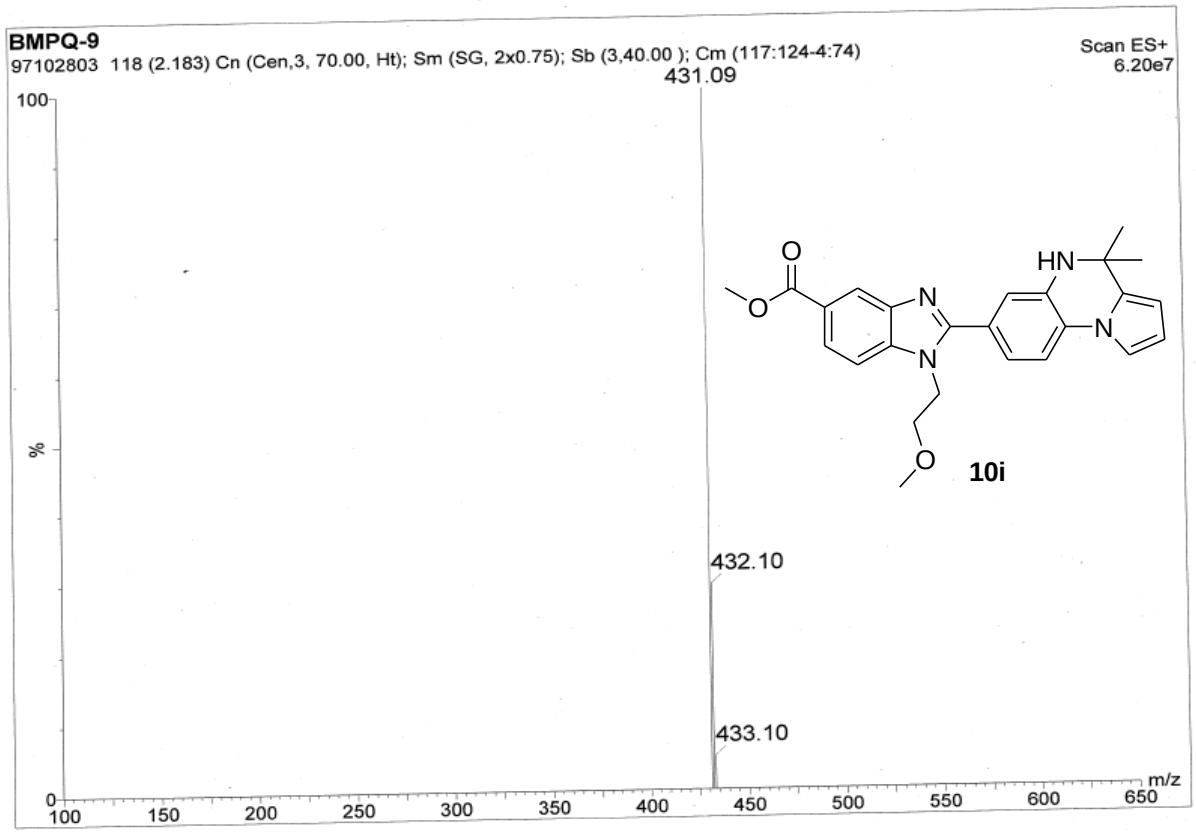
HR Mass spectra of Compounds 10g



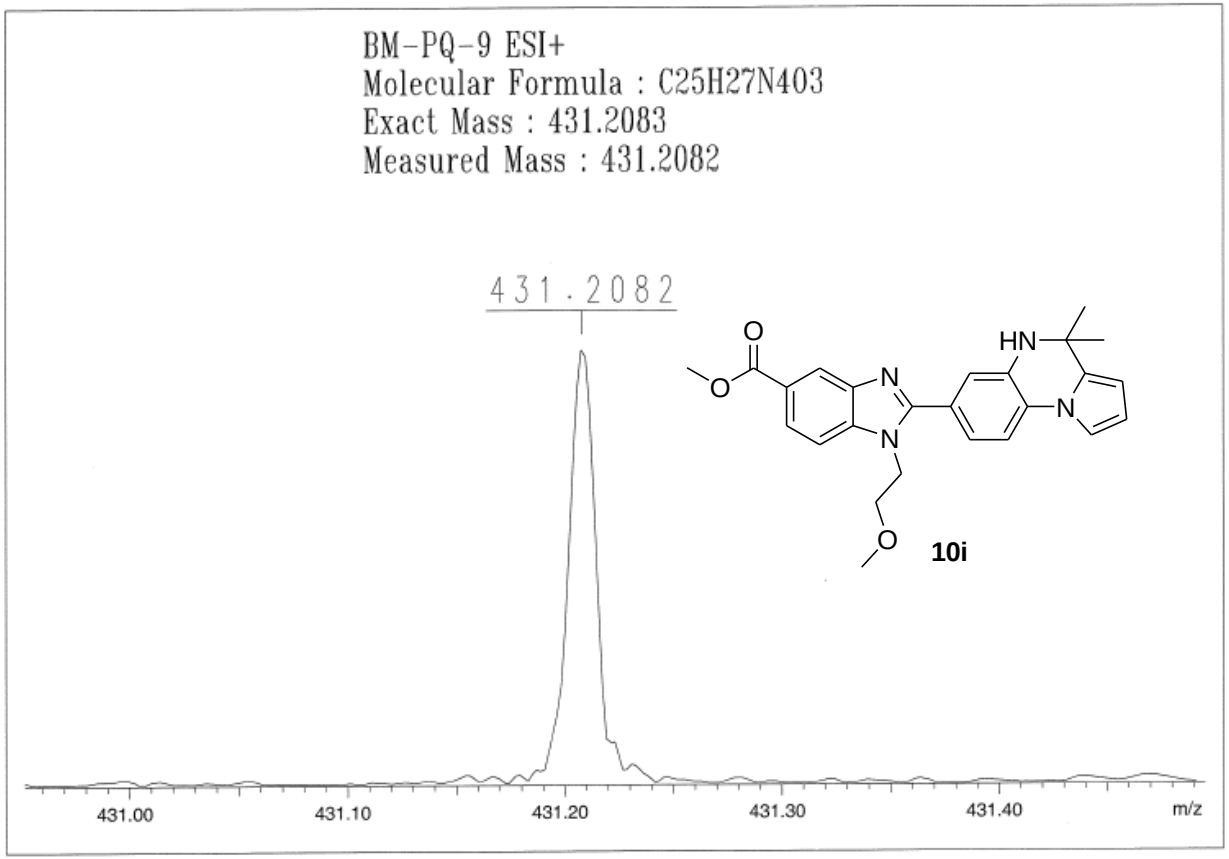
LR Mass spectra of Compounds 10h



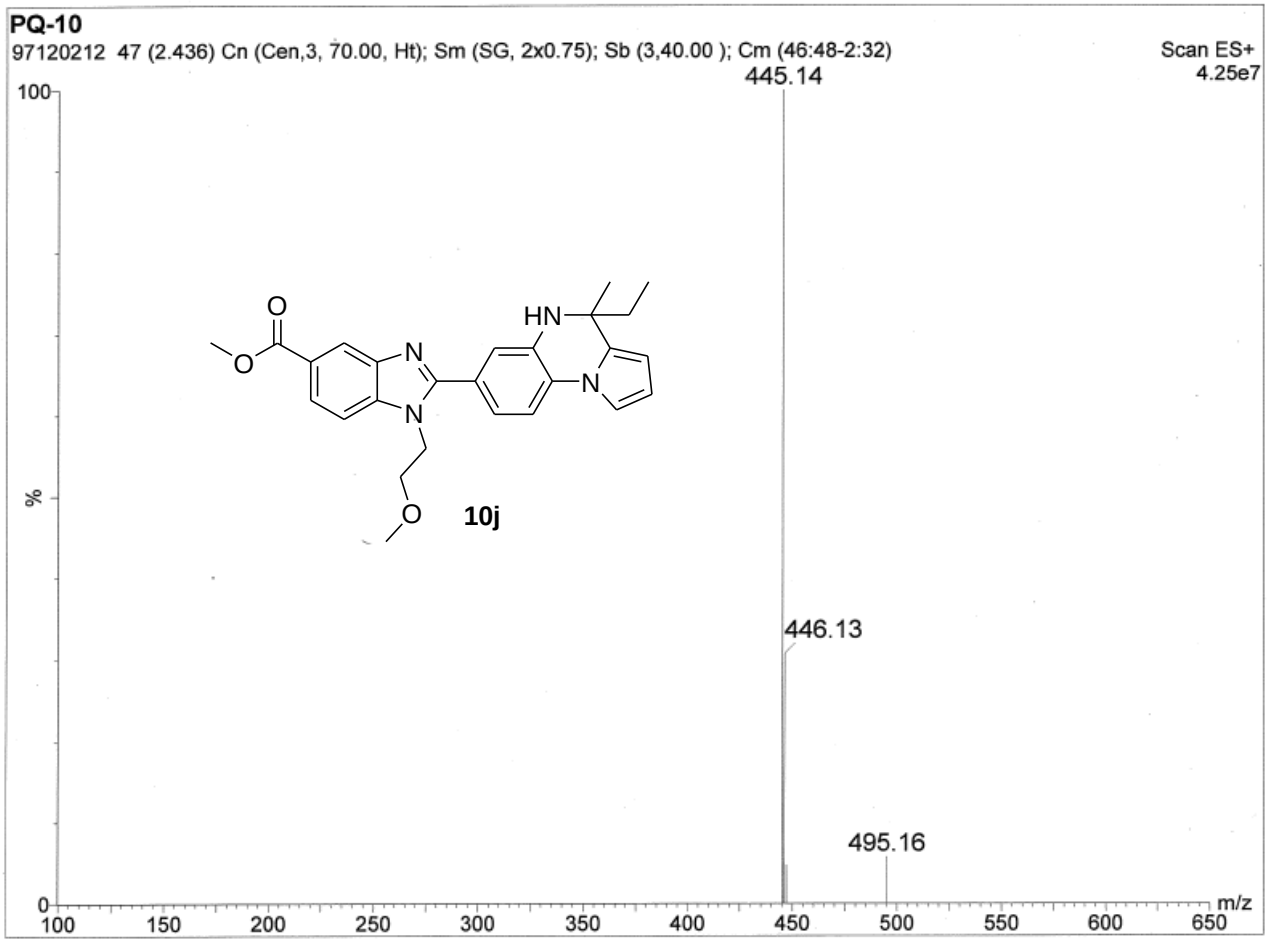
HR Mass spectra of Compounds 10h



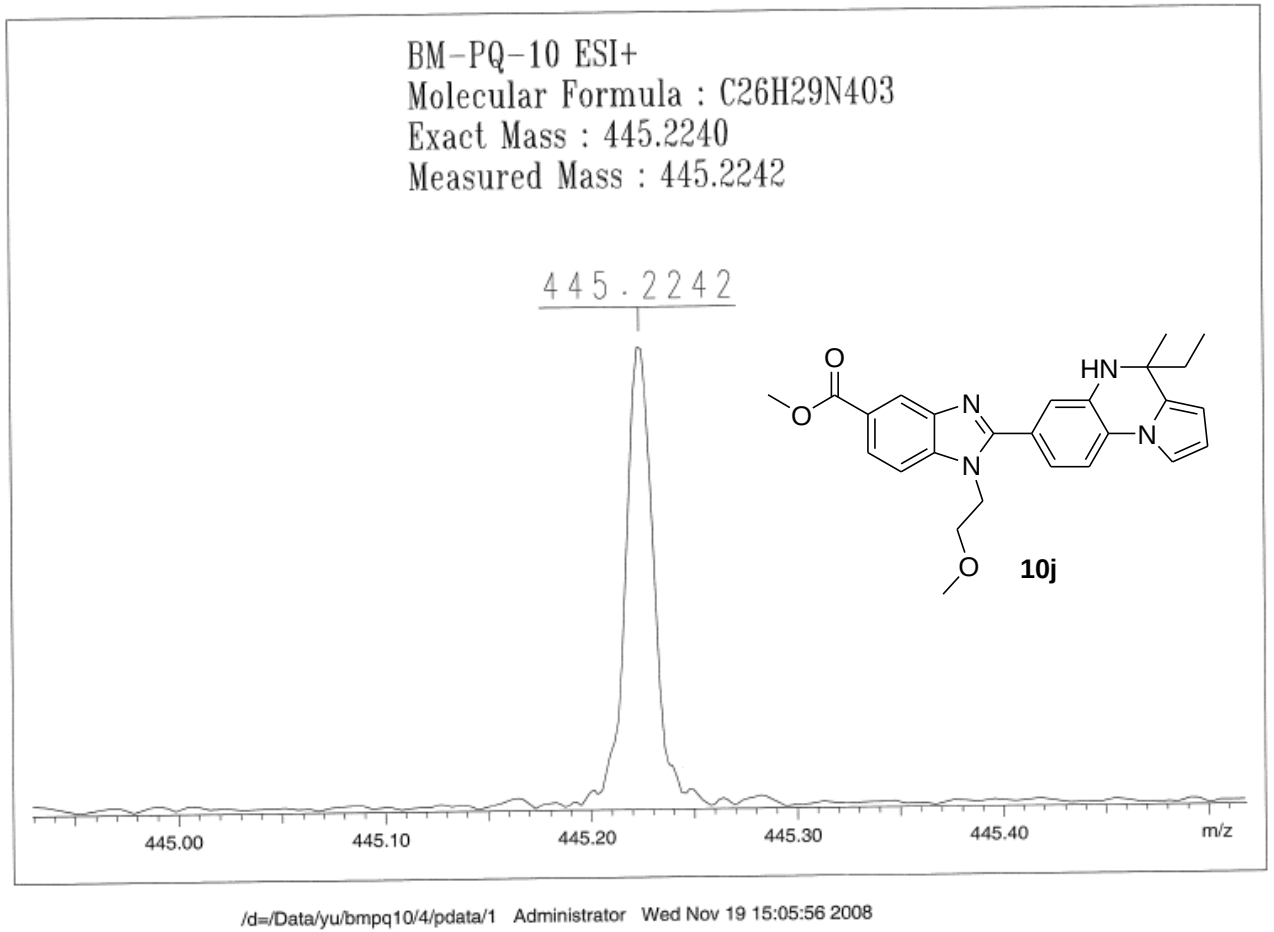
LR Mass spectra of Compounds 10i



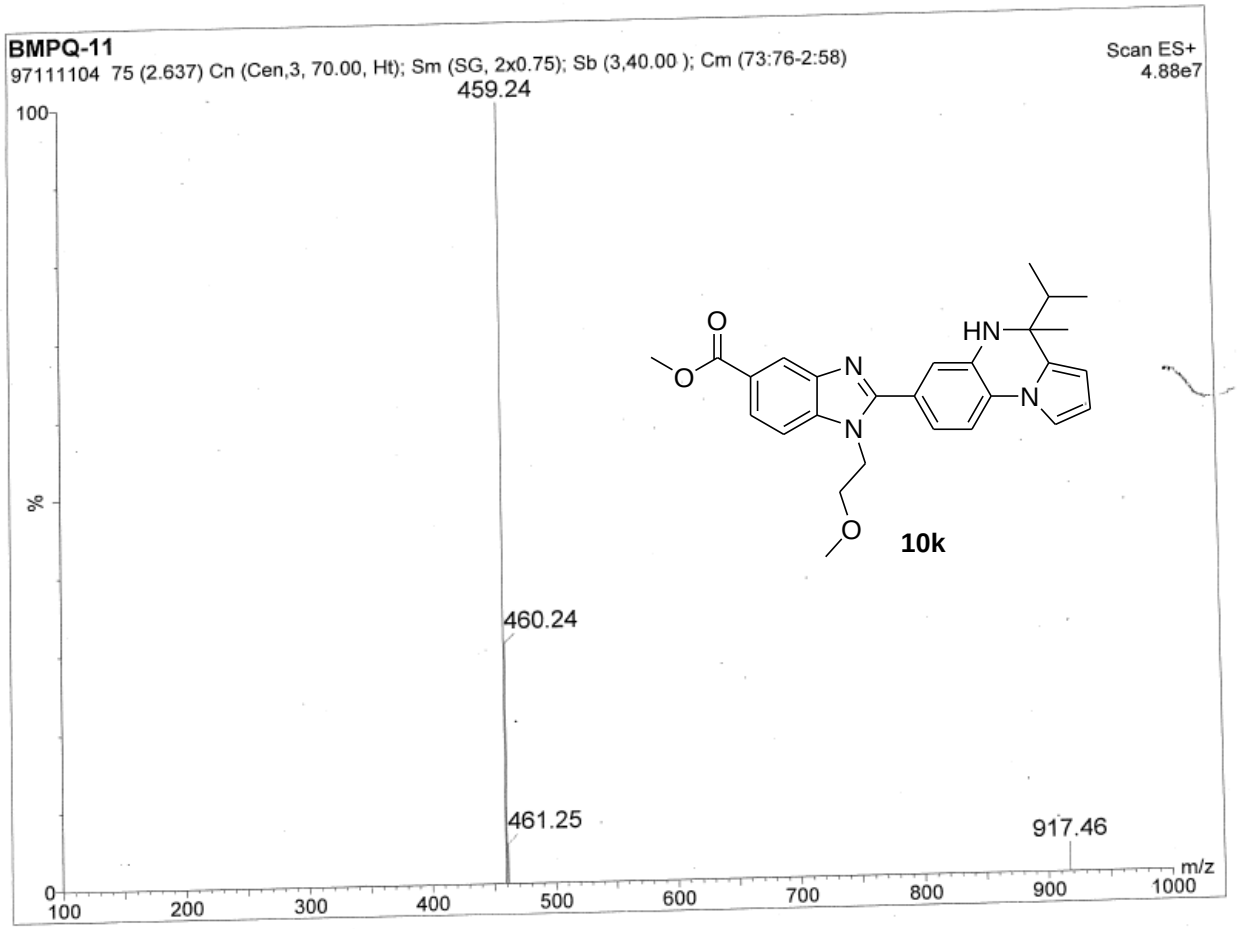
HR Mass spectra of Compounds 10i



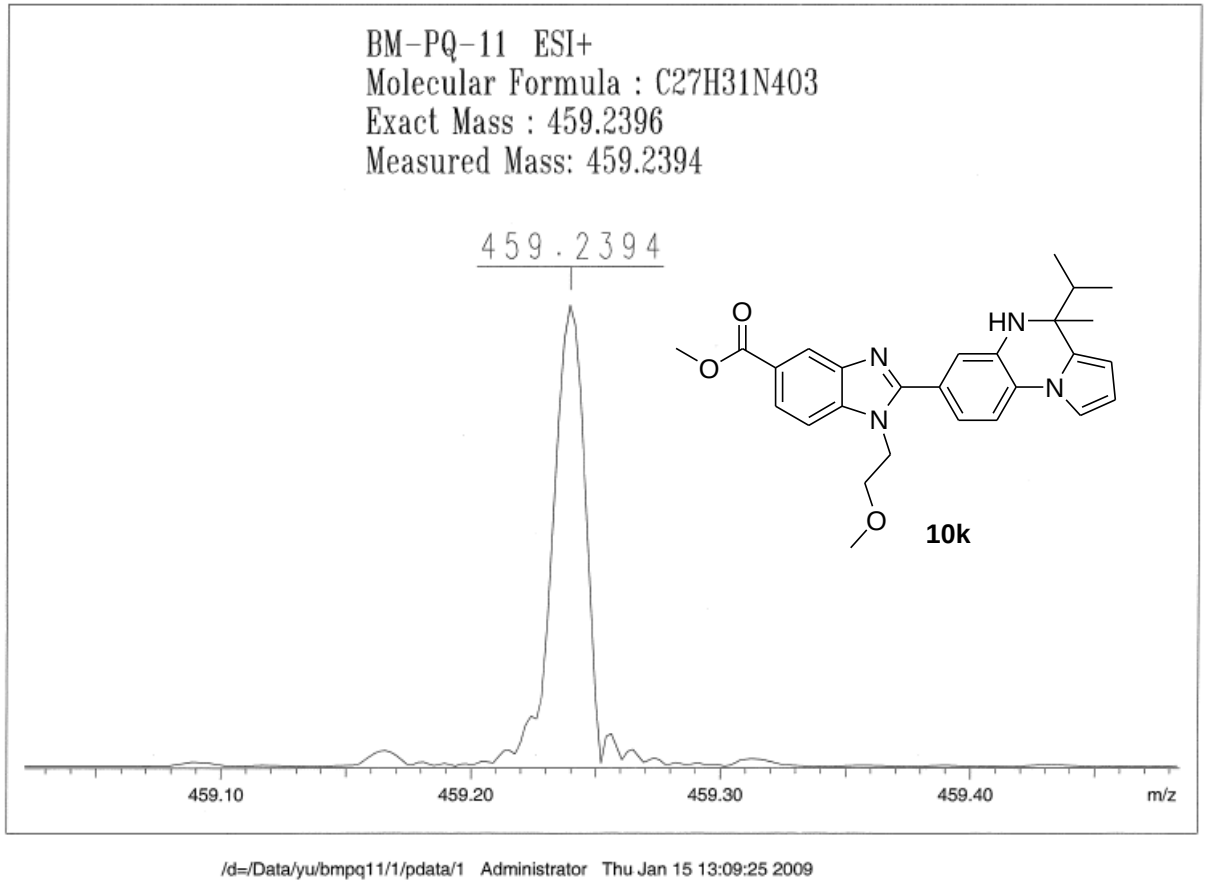
LR Mass spectra of Compounds 10j



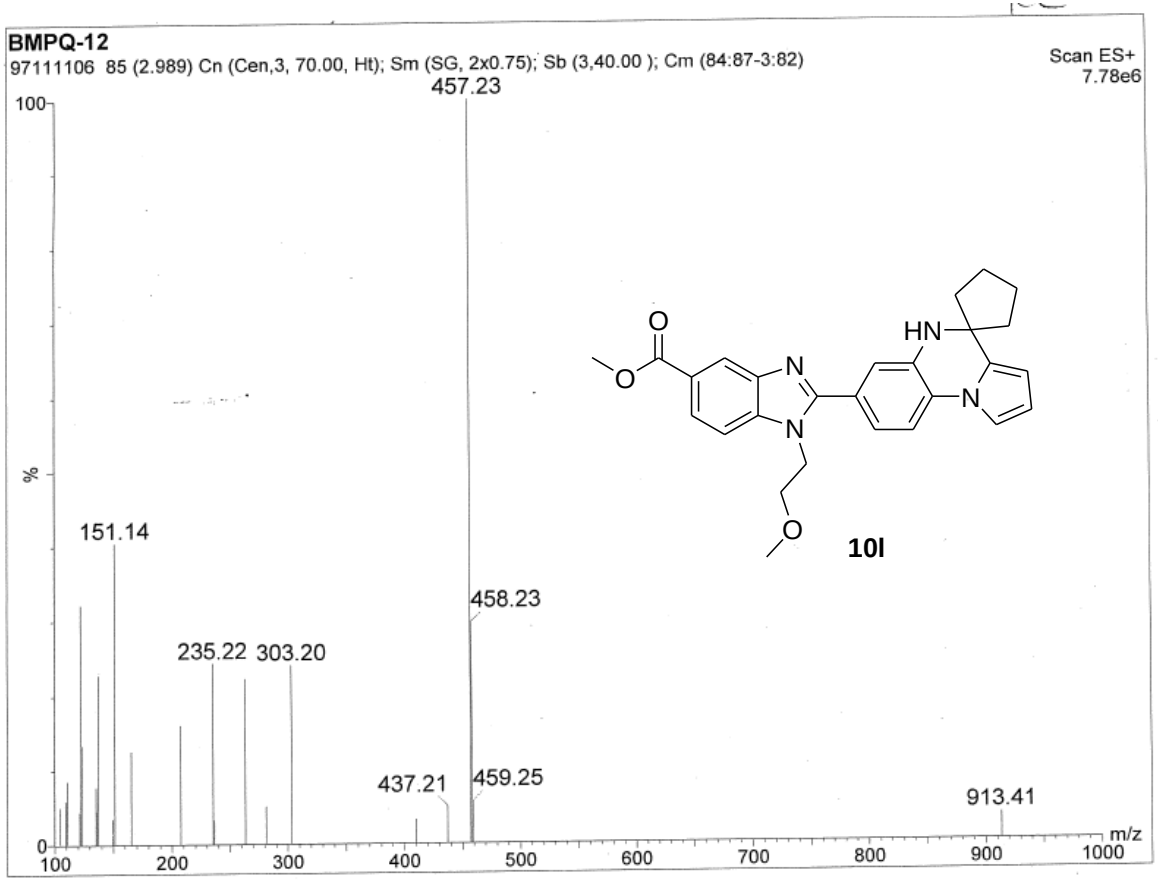
HR Mass spectra of Compounds 10j



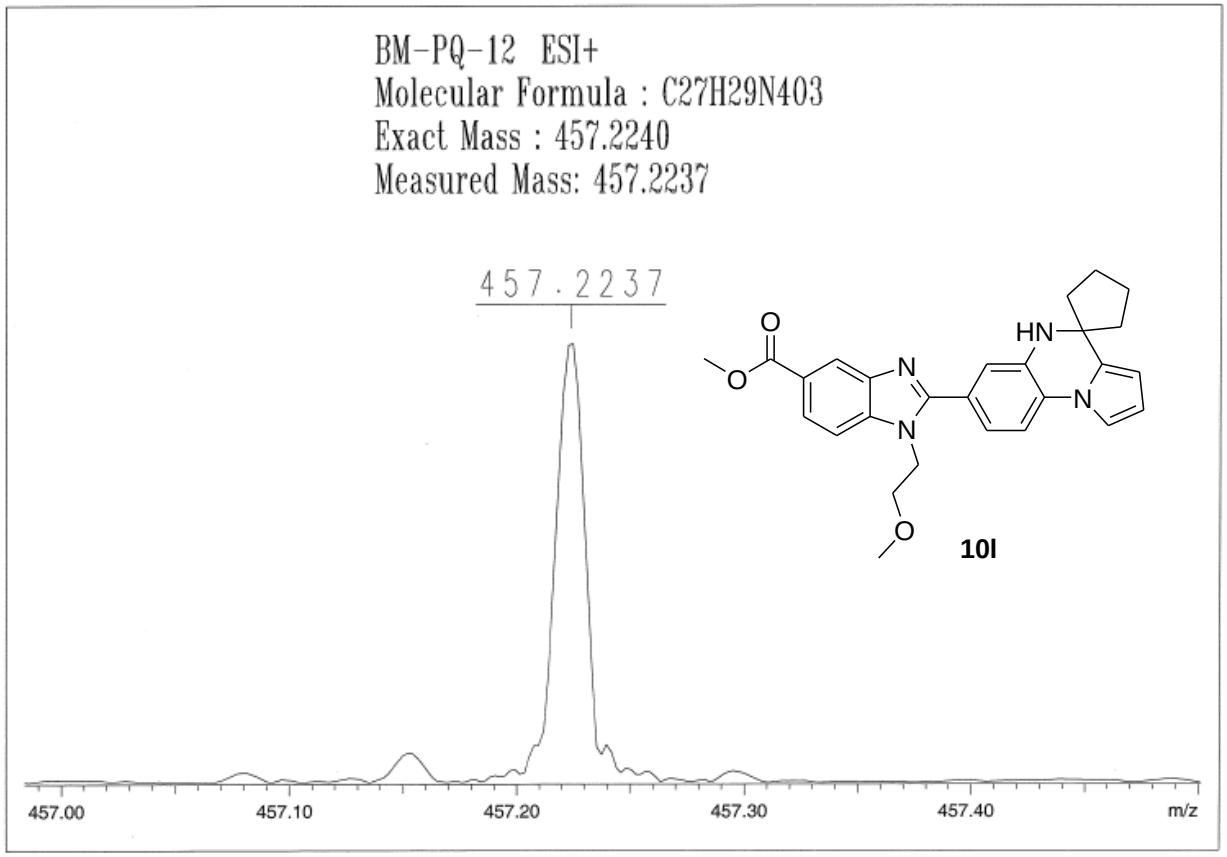
LR Mass spectra of Compounds 10k



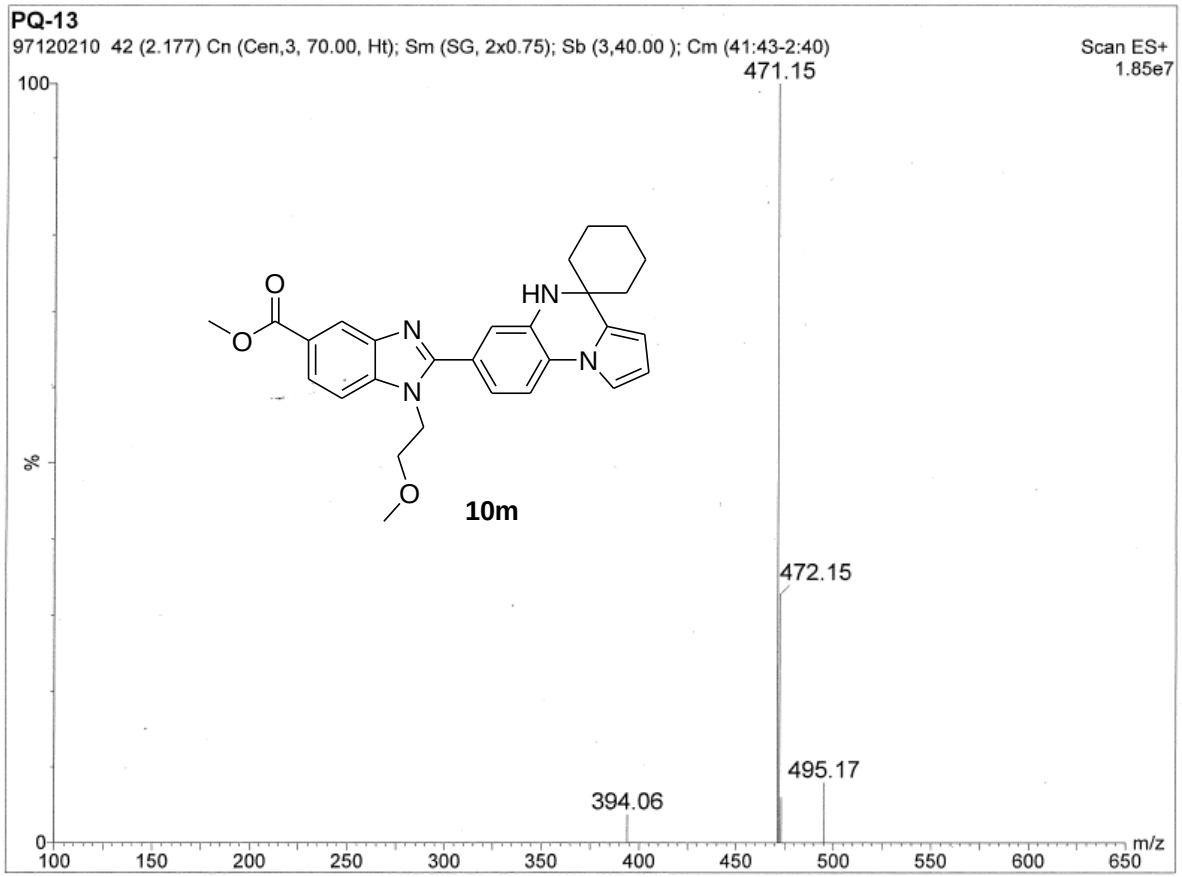
HR Mass spectra of Compounds 10k



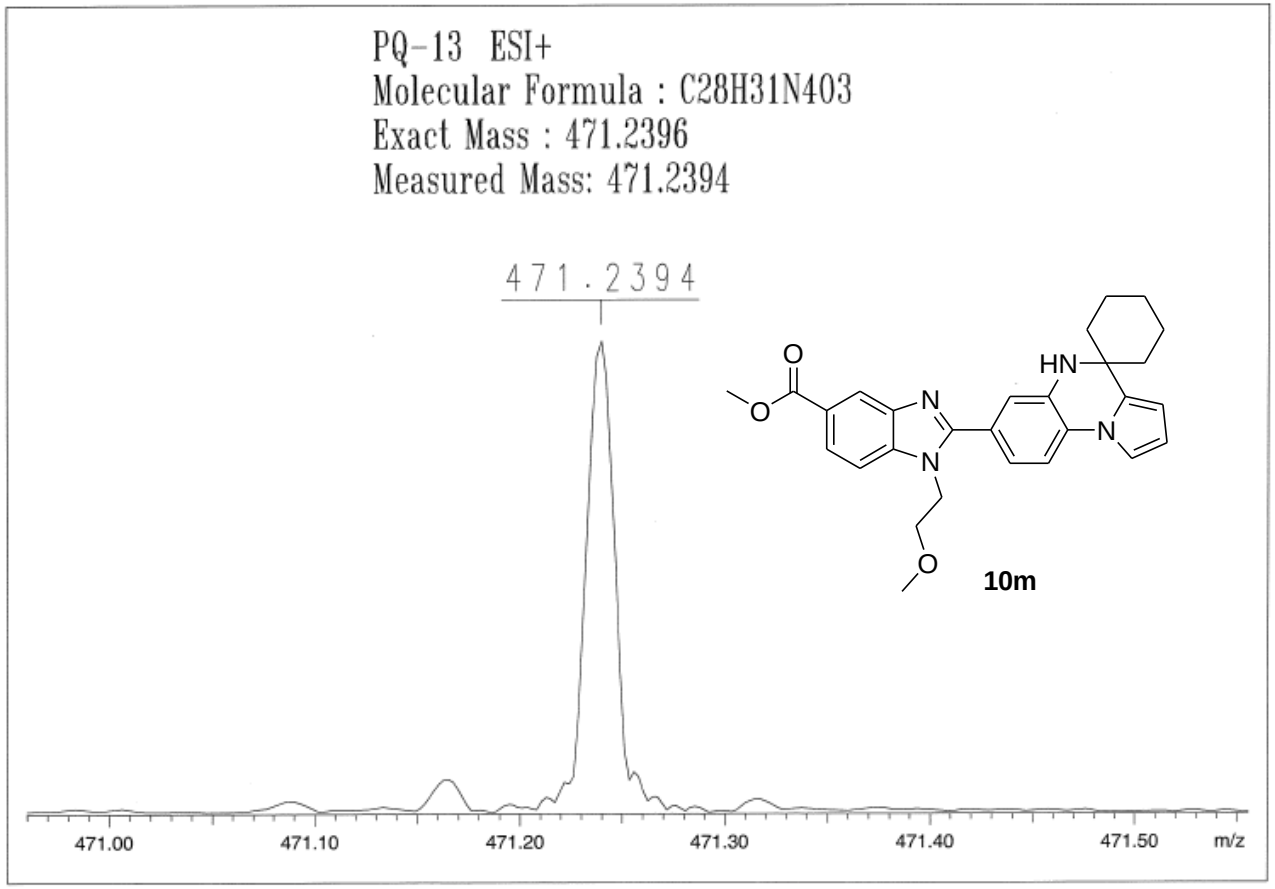
LR Mass spectra of Compounds 10l



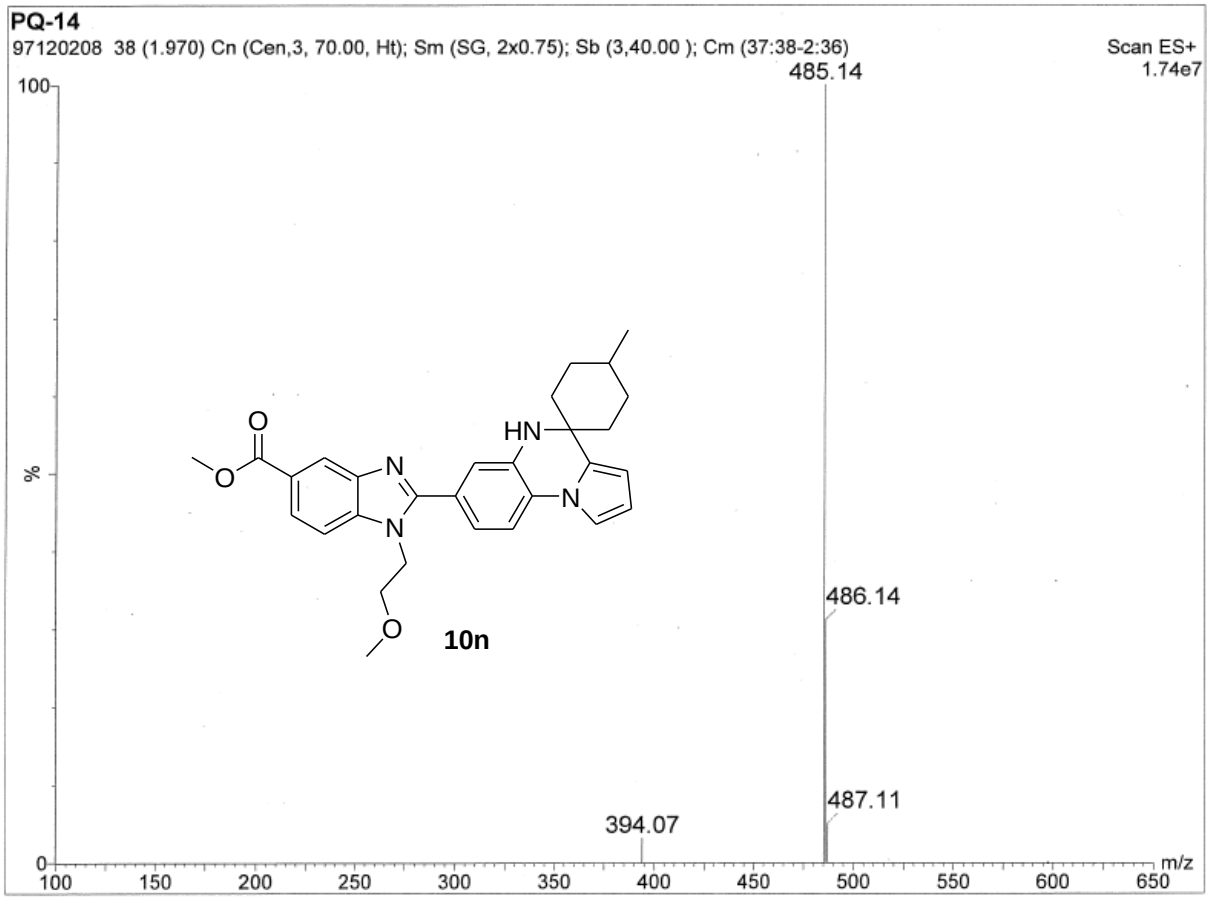
HR Mass spectra of Compounds 10l



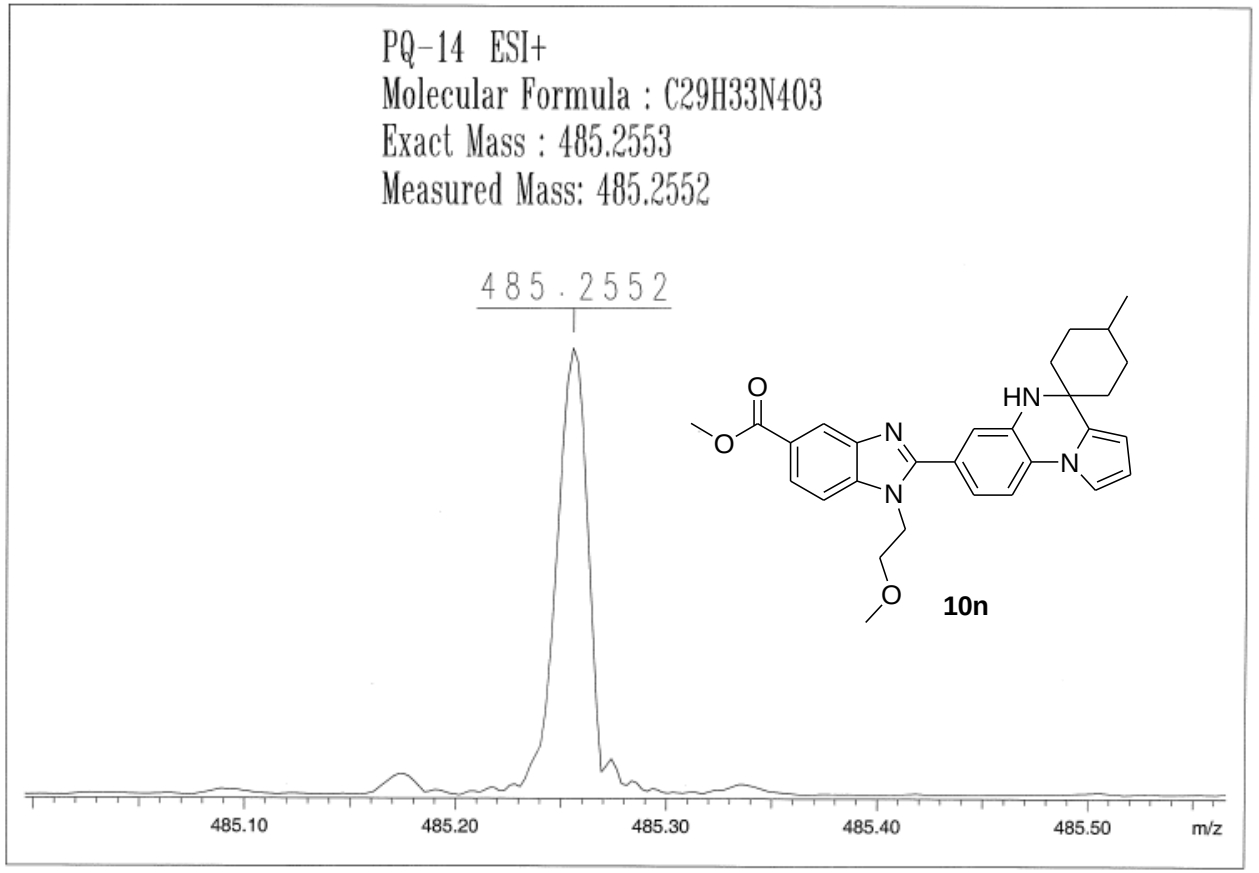
LR Mass spectra of Compounds 10m



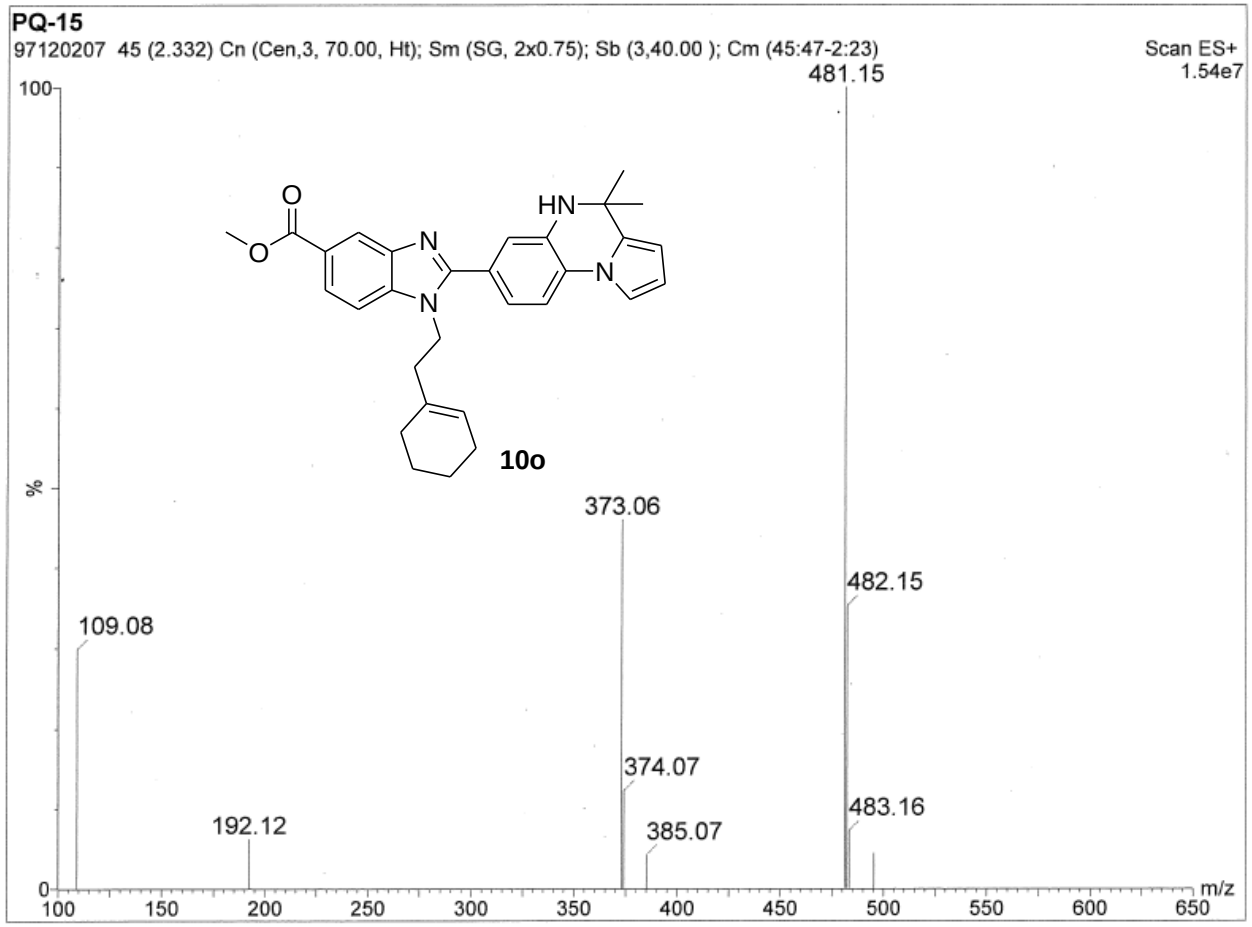
HR Mass spectra of Compounds 10m



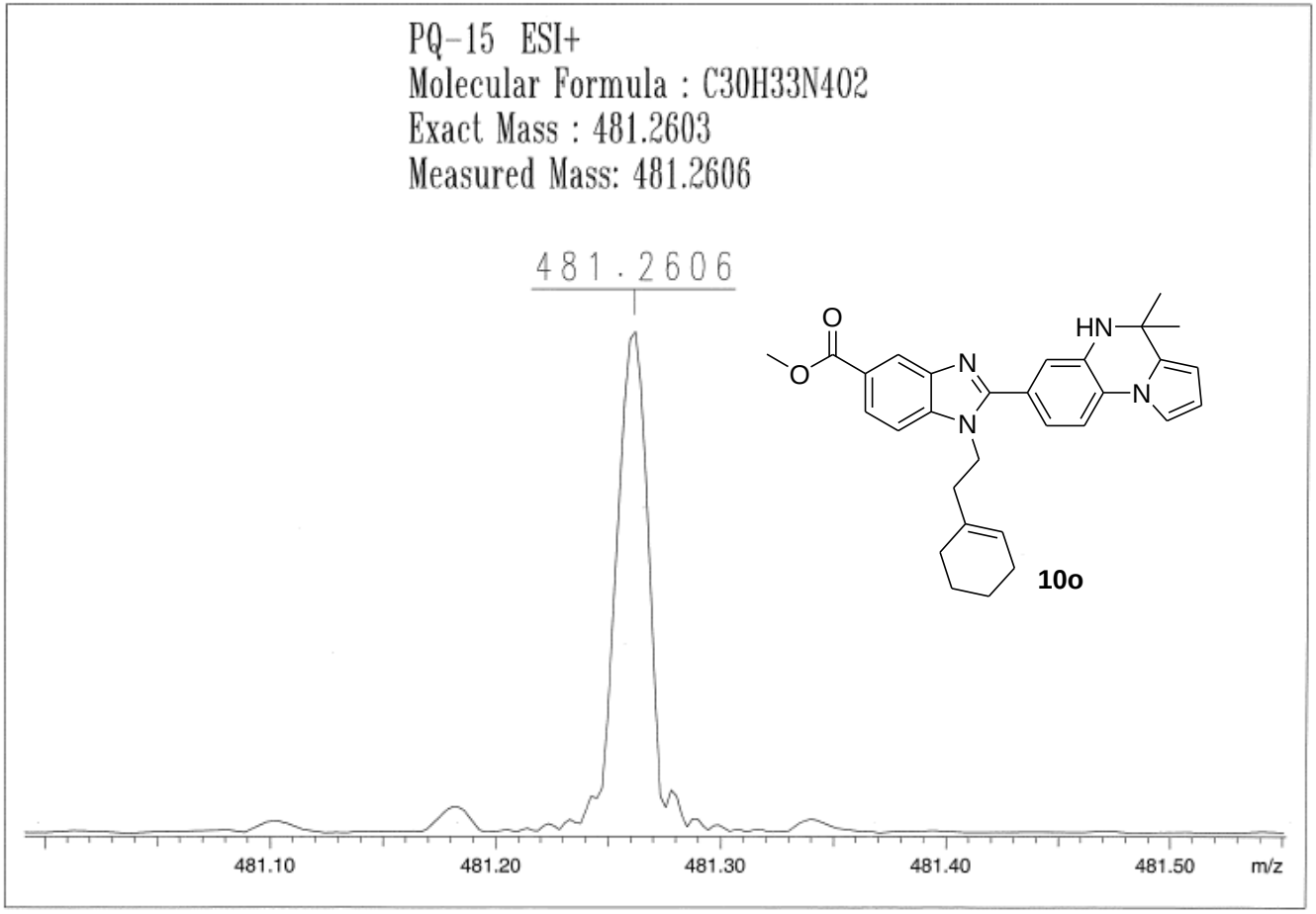
LR Mass spectra of Compounds 10n



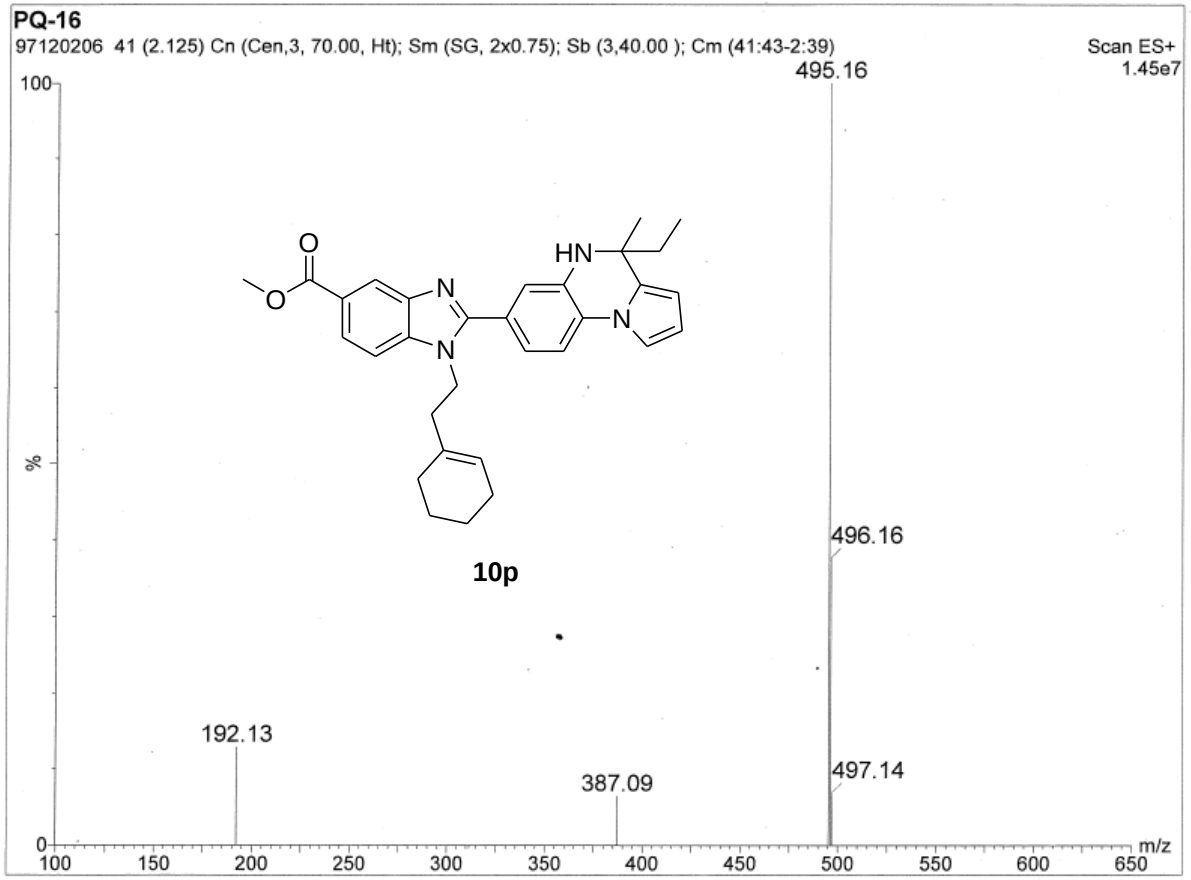
HR Mass spectra of Compounds 10n



LR Mass spectra of Compounds 10o

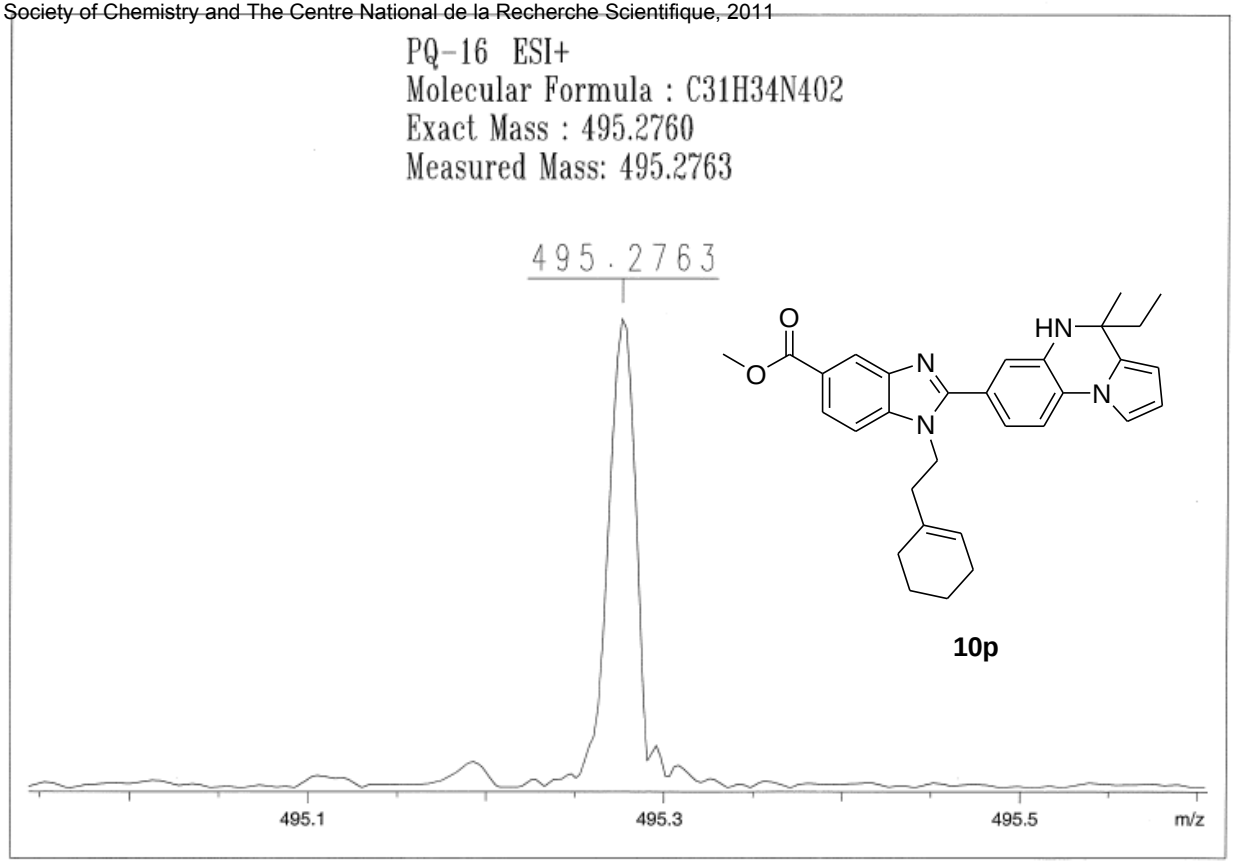


HR Mass spectra of Compounds 10o

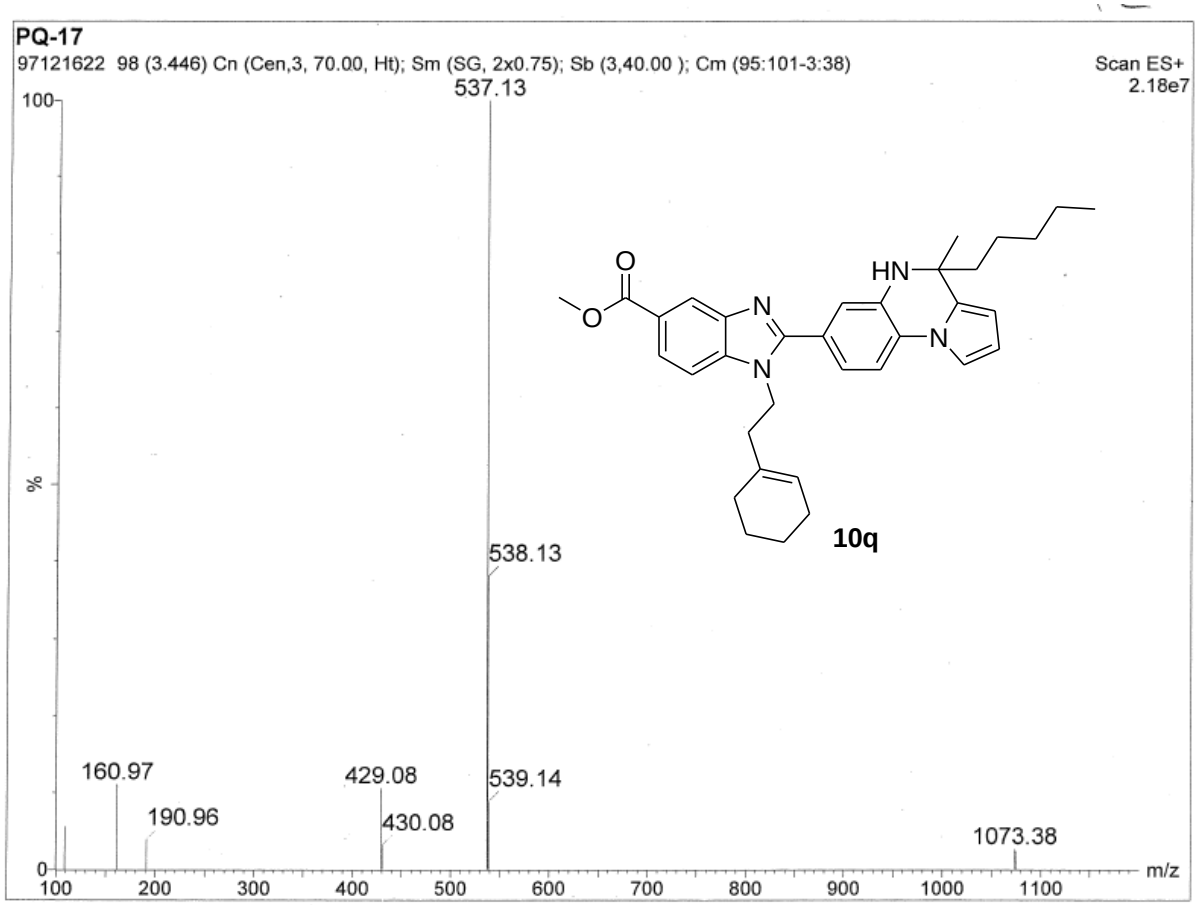


10p

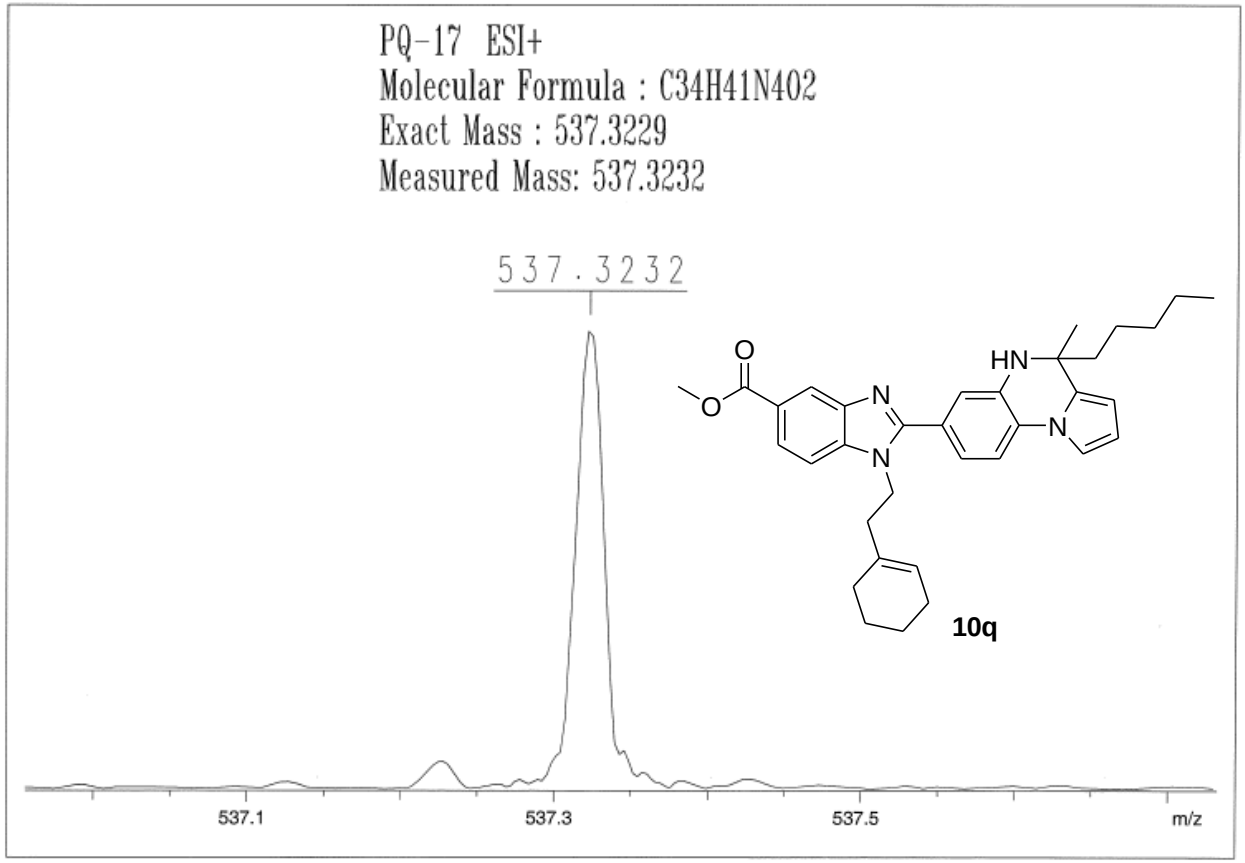
LR Mass spectra of Compounds 10p



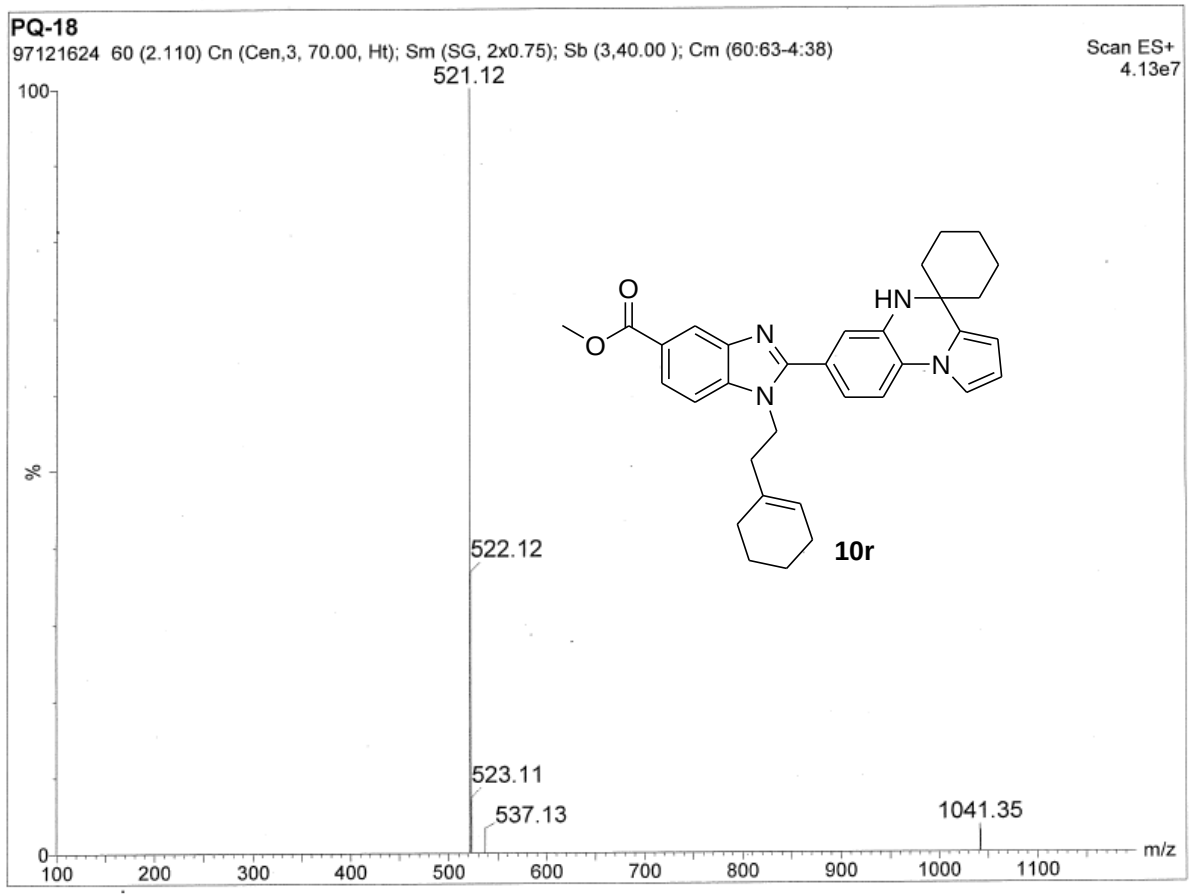
HR Mass spectra of Compounds 10p



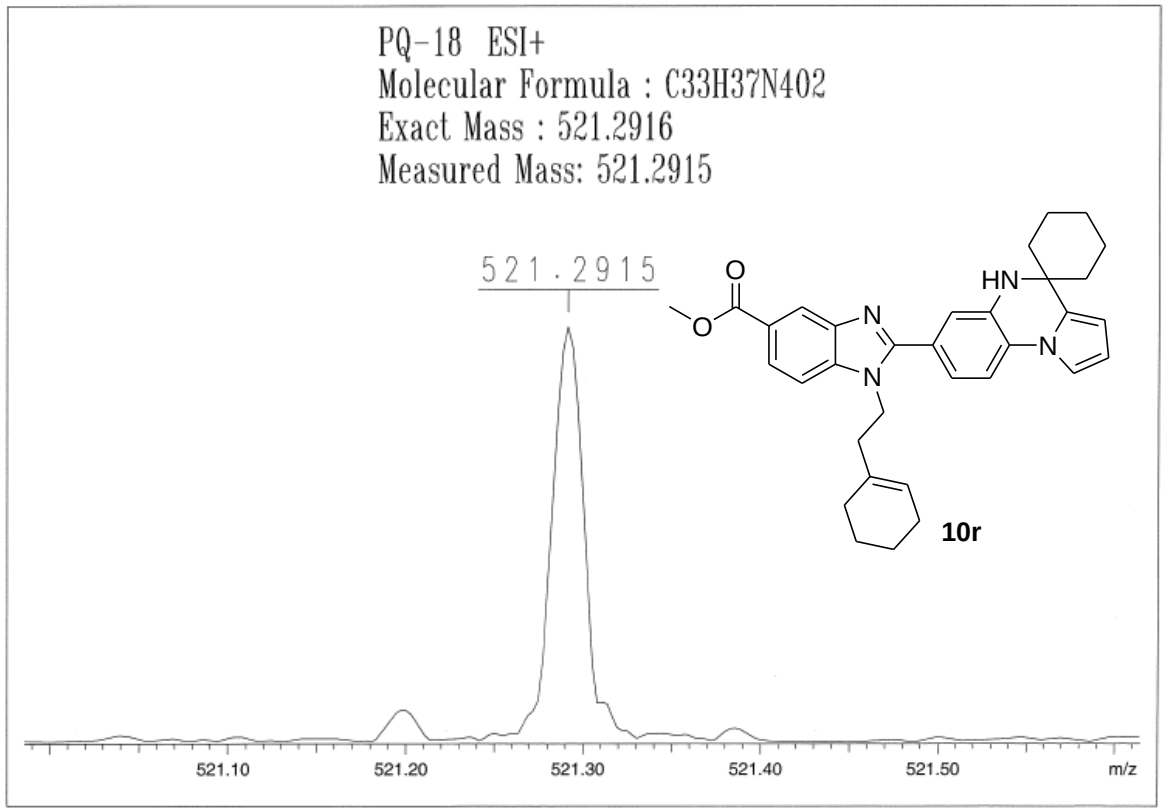
LR Mass spectra of Compounds 10q



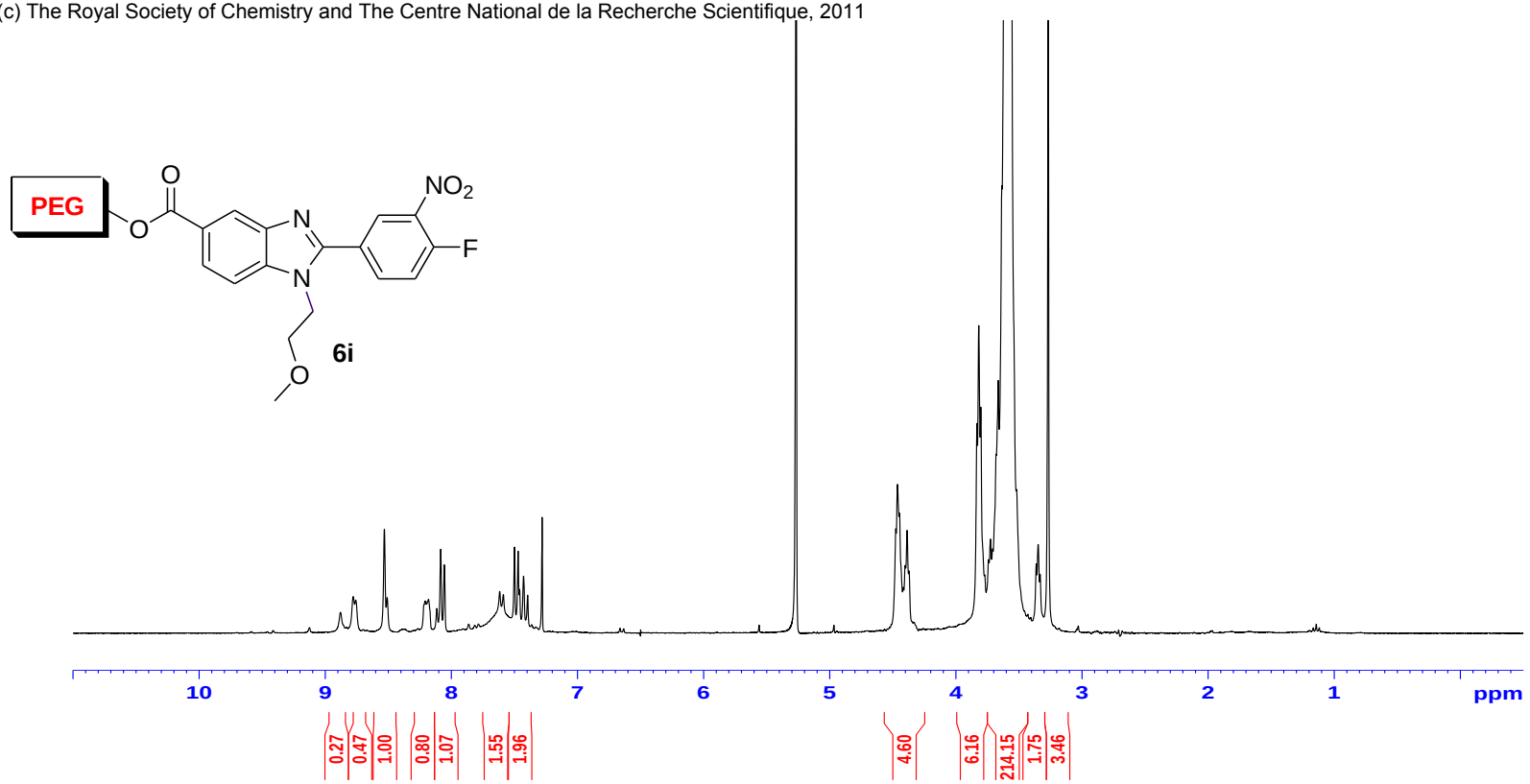
HR Mass spectra of Compounds 10q



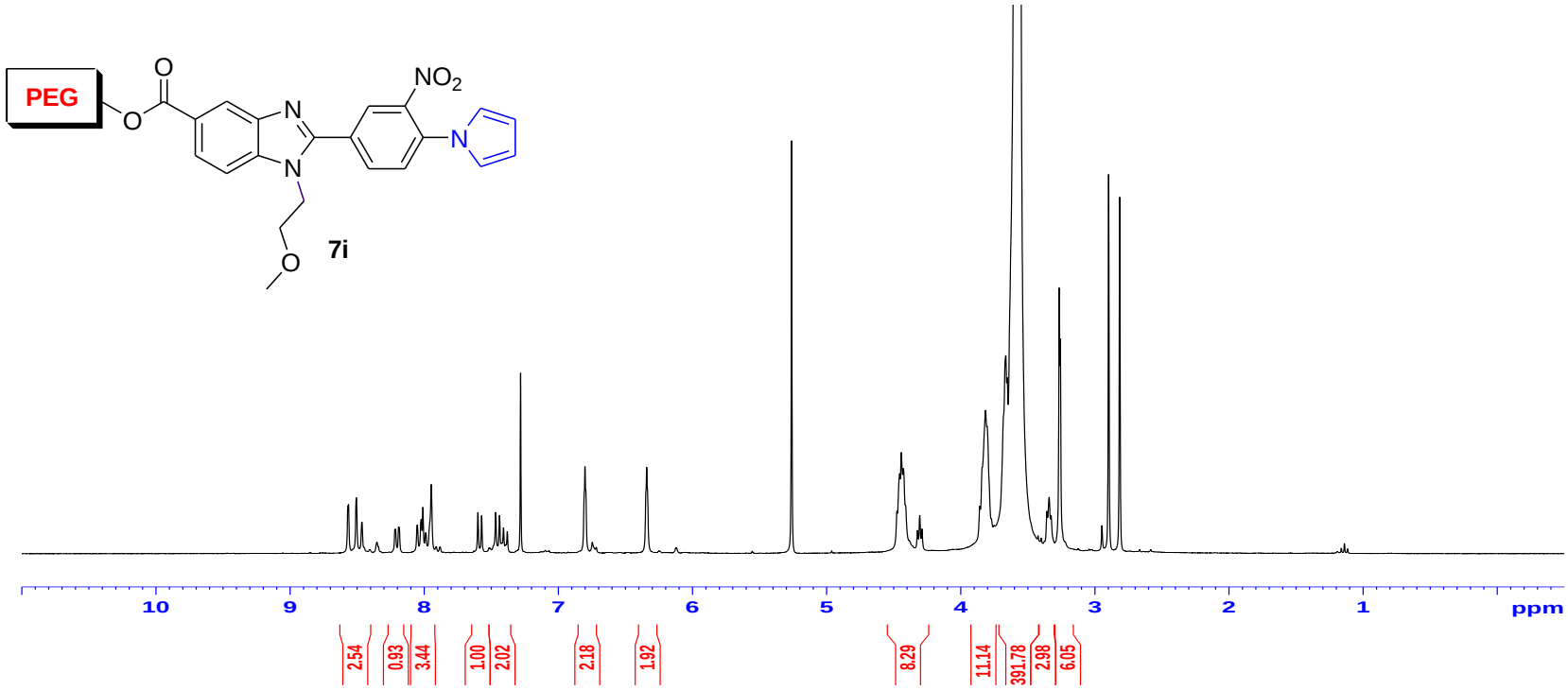
LR Mass spectra of Compounds 10r



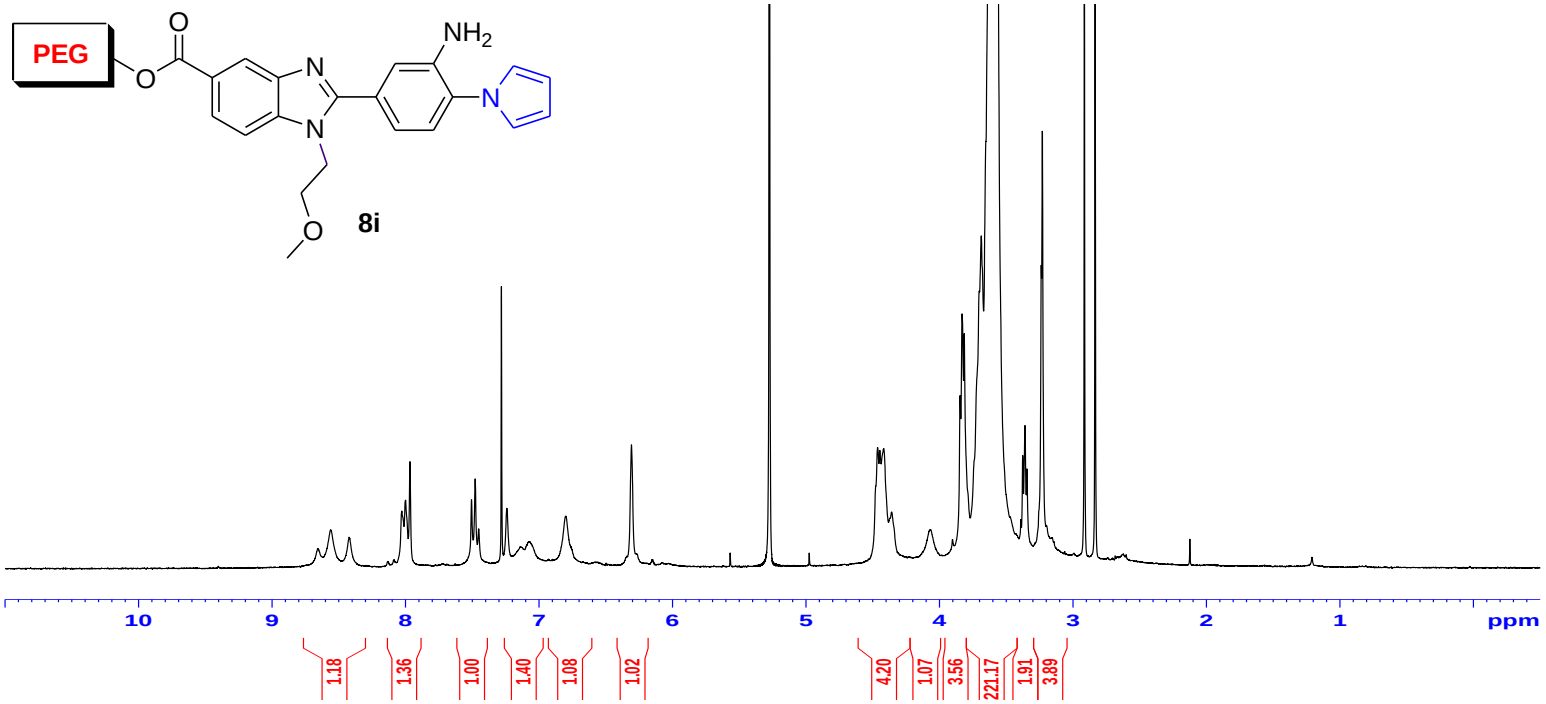
HR Mass spectra of Compounds 10r



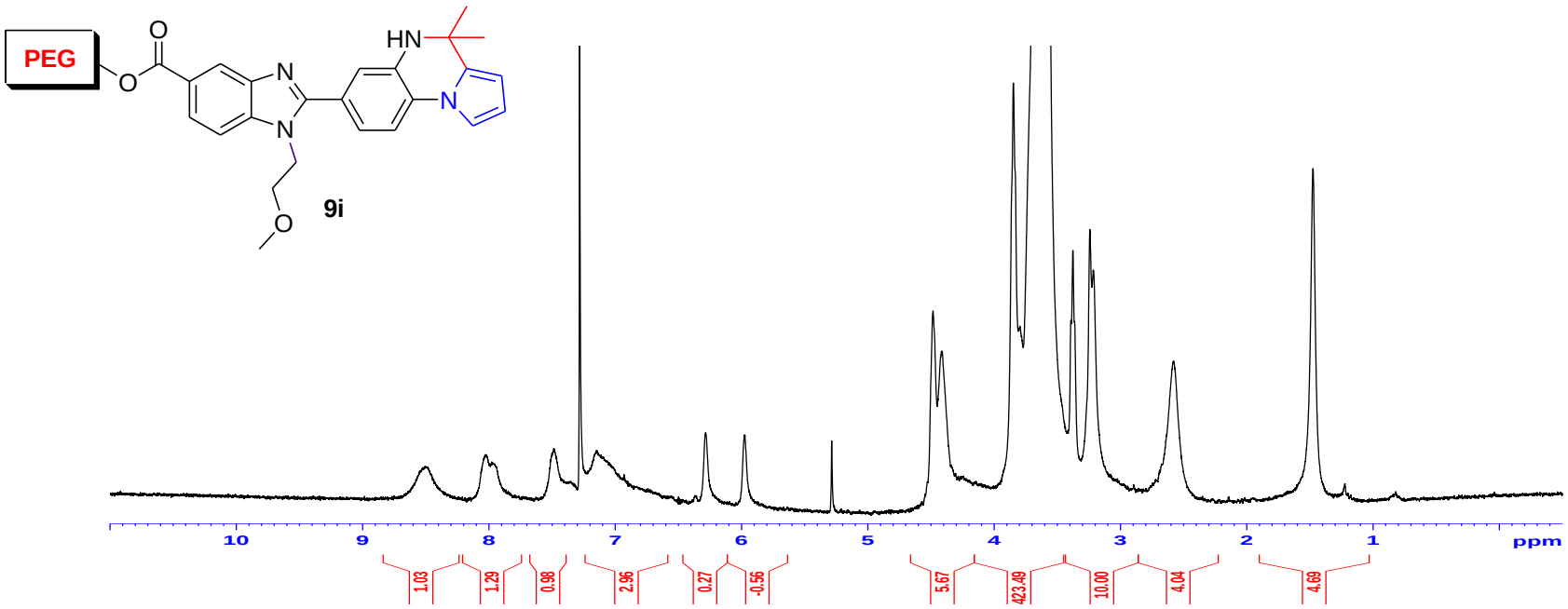
^{1}HNMR spectrum (300 MHz) of intermediate compound 6i in $CDCl_3$



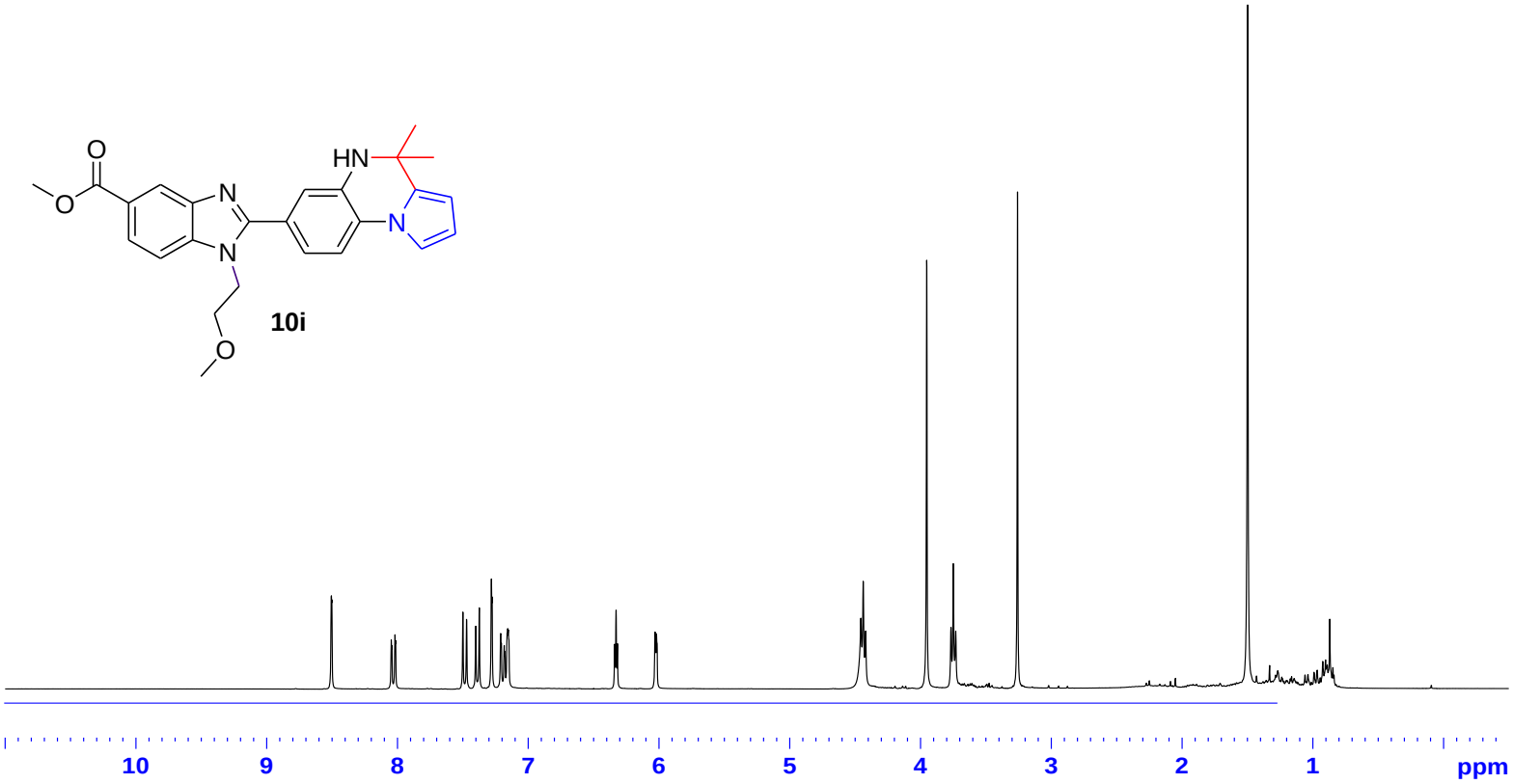
^{1}HNMR spectrum (300 MHz) of intermediate compound 7i in $CDCl_3$



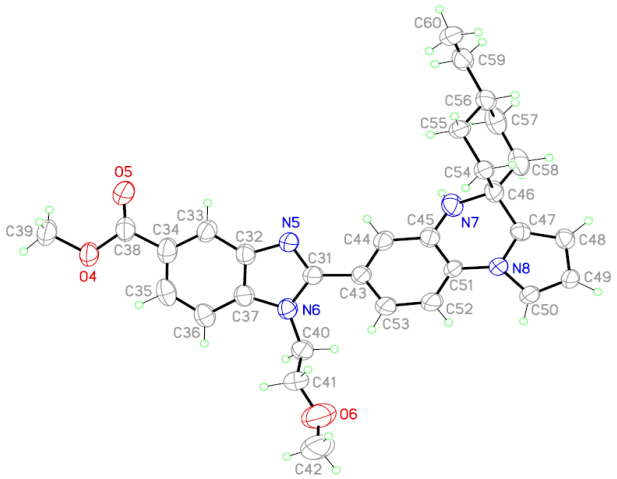
^{1}HNMR spectrum (300 MHz) of intermediate compound 8i in $CDCl_3$

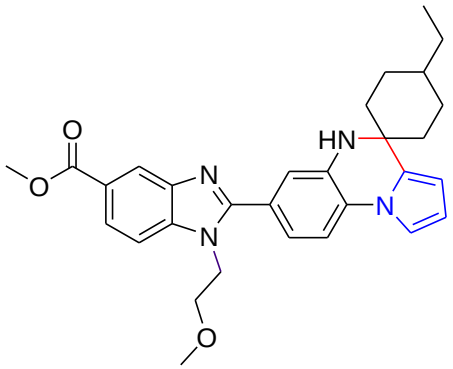


^{1}HNMR spectrum (300 MHz) of intermediate compound 9i in $CDCl_3$



^{1}HNMR spectrum (300 MHz) of final compound 10i in $CDCl_3$





10h

ORTEP diagram of Methyl

2-(4-ethyl-5'*H*-spiro[cyclohexane-1,4'-pyrrolo[1,2-*a*]quinoxalin]-7'-yl)

-1-(2-methoxyethyl)-1*H*-benzimidazole-5-carboxylate (10h)

Table 1. Crystal data and structure refinement for **10h**

Identification code	101119lts	
Empirical formula	C30 H34 N4 O3	
Formula weight	498.61	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.3481(6) Å	α= 105.903(2)°.
	b = 15.7551(8) Å	β= 108.938(2)°.
	c = 16.7496(9) Å	γ = 93.046(2)°.
Volume	2927.8(3) Å^3	
Z	4	
Density (calculated)	1.131 Mg/m^3	
Absorption coefficient	0.074 mm^{-1}	
F(000)	1064	
Crystal size	0.15 x 0.15 x 0.05 mm^3	
Theta range for data collection	1.77 to 26.42°.	
Index ranges	-15<=h<=15, -19<=k<=17, -20<=l<=18	
Reflections collected	43472	
Independent reflections	11900 [R(int) = 0.0937]	
Completeness to theta = 26.42°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9486 and 0.6811	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11900 / 20 / 717	
Goodness-of-fit on F^2	0.956	
Final R indices [I>2sigma(I)]	R1 = 0.0861, wR2 = 0.2406	
R indices (all data)	R1 = 0.1378, wR2 = 0.2707	
Largest diff. peak and hole	0.823 and -0.380 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for 101119LTs. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	806(3)	3630(2)	1630(2)	54(1)
C(2)	1736(3)	4440(2)	1144(2)	57(1)
C(3)	2503(4)	4795(2)	825(2)	73(1)
C(4)	2306(5)	5590(3)	638(3)	79(1)
C(5)	1365(5)	6018(3)	752(3)	96(2)
C(6)	602(4)	5658(3)	1063(3)	87(2)
C(7)	791(4)	4862(2)	1244(2)	68(1)
C(10)	-701(3)	4603(3)	1901(3)	79(1)
C(11)	-202(4)	5285(3)	2818(3)	87(2)
C(12)	52(4)	4418(3)	3800(3)	92(2)
C(13)	492(3)	2923(2)	1979(2)	53(1)
C(14)	-623(3)	2436(3)	1642(2)	59(1)
C(15)	-851(3)	1775(2)	1990(2)	57(1)
C(16)	5(3)	1598(2)	2665(2)	53(1)
C(17)	-1241(3)	532(3)	3010(3)	70(1)
C(18)	-1020(3)	-12(3)	3519(3)	75(1)
C(19)	211(3)	80(3)	3930(3)	67(1)
C(20)	692(3)	687(2)	3639(2)	54(1)
C(21)	1925(3)	1011(2)	3781(2)	48(1)
C(22)	1137(3)	2085(2)	3006(2)	49(1)
C(23)	1361(3)	2736(2)	2646(2)	47(1)
C(24)	2719(3)	1033(2)	4704(2)	52(1)
C(25)	3997(3)	1273(2)	4848(2)	48(1)
C(26)	4364(3)	665(2)	4135(2)	46(1)
C(27)	3573(3)	639(2)	3215(2)	47(1)
C(28)	2299(3)	382(2)	3069(2)	49(1)
C(29)	5639(3)	953(2)	4314(2)	52(1)
C(30)	6133(3)	358(3)	3692(3)	66(1)
C(31)	4777(3)	6894(2)	6276(2)	42(1)
C(32)	5351(3)	6314(2)	5201(2)	44(1)
C(33)	6002(3)	6022(2)	4663(2)	51(1)
C(34)	5418(3)	5473(2)	3807(2)	57(1)

C(35)	4213(3)	5209(2)	3486(2)	58(1)
C(36)	3563(3)	5488(2)	4012(2)	53(1)
C(37)	4157(3)	6046(2)	4872(2)	44(1)
C(40)	2598(3)	6279(2)	5548(2)	55(1)
C(41)	1829(3)	6853(3)	5106(3)	68(1)
C(42)	4(4)	7333(4)	4919(4)	127(2)
C(43)	4796(2)	7357(2)	7166(2)	44(1)
C(44)	5732(3)	7292(2)	7891(2)	45(1)
C(45)	5833(3)	7734(2)	8757(2)	51(1)
C(46)	7149(3)	8379(2)	10305(2)	51(1)
C(51)	5005(3)	8266(3)	8898(2)	72(1)
C(52)	4106(3)	8345(3)	8201(3)	81(1)
C(53)	3977(3)	7894(2)	7332(2)	60(1)
C(54)	7877(2)	9123(2)	10192(2)	45(1)
C(55)	8994(2)	8855(2)	10071(2)	46(1)
C(56)	9736(3)	8583(2)	10852(2)	50(1)
C(57)	9047(3)	7829(2)	10973(2)	63(1)
C(58)	7896(3)	8062(2)	11057(2)	63(1)
C(59)	10875(3)	8315(3)	10761(2)	66(1)
C(60)	11644(3)	9011(3)	10644(3)	80(1)
N(1)	1722(3)	3661(2)	1377(2)	56(1)
N(2)	207(3)	4332(2)	1557(2)	64(1)
N(3)	1975(2)	1927(2)	3713(2)	49(1)
N(4)	-197(2)	960(2)	3068(2)	54(1)
N(5)	5720(2)	6842(2)	6074(2)	43(1)
N(6)	3791(2)	6428(2)	5568(2)	45(1)
N(7)	6702(2)	7613(2)	9478(2)	54(1)
O(3)	593(2)	4954(2)	3438(2)	76(1)
O(6)	810(3)	6777(2)	5280(3)	106(1)
C(8)	2901(15)	5999(11)	334(12)	64(3)
C(9)	3645(8)	7225(6)	24(6)	74(2)
O(1)	2800(5)	6803(3)	317(4)	58(1)
O(2)	3529(6)	5546(5)	-34(5)	83(1)
C(8')	3339(12)	6008(11)	293(11)	64(3)
C(9')	5257(7)	6218(6)	307(6)	74(2)
O(1')	4347(5)	5783(3)	509(3)	58(1)
O(2')	3102(6)	6593(5)	-103(5)	83(1)

C(38)	6004(9)	5085(7)	3212(7)	50(2)
C(39)	5891(8)	4333(7)	1735(5)	72(2)
O(4)	5289(6)	4698(5)	2348(4)	59(2)
O(5)	7037(6)	5167(5)	3450(5)	63(2)
C(38')	6321(12)	5318(12)	3307(11)	50(2)
C(39')	6525(11)	4285(10)	2043(8)	72(2)
O(4')	5793(8)	4622(8)	2556(7)	59(2)
O(5')	7346(9)	5554(6)	3561(8)	63(2)
N(8)	5105(5)	8873(4)	9724(4)	36(1)
C(47)	6060(8)	8858(5)	10435(6)	36(2)
C(48)	5883(7)	9297(5)	11198(6)	44(2)
C(49)	4791(5)	9622(5)	10936(4)	44(1)
C(50)	4338(5)	9349(4)	10046(4)	44(1)
N(8')	5161(5)	8500(4)	9863(4)	36(1)
C(47')	6186(9)	8570(6)	10548(6)	36(2)
C(48')	6017(8)	8958(5)	11329(6)	44(2)
C(49')	4842(5)	9124(5)	11100(4)	44(1)
C(50')	4337(5)	8826(5)	10216(4)	44(1)

Table 3. Bond lengths [Å] and angles [°] for 101119LTs.

C(1)-N(1)	1.333(5)
C(1)-N(2)	1.375(4)
C(1)-C(13)	1.480(5)
C(2)-N(1)	1.388(5)
C(2)-C(3)	1.389(6)
C(2)-C(7)	1.407(5)
C(3)-C(4)	1.387(5)
C(3)-H(3)	0.9500
C(4)-C(8)	1.259(14)
C(4)-C(5)	1.414(7)
C(4)-C(8')	1.730(12)
C(5)-C(6)	1.380(7)
C(5)-H(5)	0.9500
C(6)-C(7)	1.383(6)
C(6)-H(6)	0.9500
C(7)-N(2)	1.383(6)
C(10)-N(2)	1.452(5)
C(10)-C(11)	1.518(5)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-O(3)	1.416(5)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-O(3)	1.418(5)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(23)	1.387(4)
C(13)-C(14)	1.395(5)
C(14)-C(15)	1.382(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.379(5)
C(15)-H(15)	0.9500
C(16)-N(4)	1.408(5)
C(16)-C(22)	1.413(4)

C(17)-C(18)	1.346(6)
C(17)-N(4)	1.384(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.431(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.374(5)
C(19)-H(19)	0.9500
C(20)-N(4)	1.377(4)
C(20)-C(21)	1.501(4)
C(21)-N(3)	1.478(4)
C(21)-C(24)	1.529(4)
C(21)-C(28)	1.541(4)
C(22)-C(23)	1.382(5)
C(22)-N(3)	1.389(4)
C(23)-H(23)	0.9500
C(24)-C(25)	1.526(4)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.524(4)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.521(4)
C(26)-C(29)	1.523(4)
C(26)-H(26)	1.0000
C(27)-C(28)	1.525(4)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.508(5)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-N(5)	1.313(4)
C(31)-N(6)	1.385(4)

C(31)-C(43)	1.461(4)
C(32)-N(5)	1.377(4)
C(32)-C(37)	1.391(4)
C(32)-C(33)	1.397(4)
C(33)-C(34)	1.382(5)
C(33)-H(33)	0.9500
C(34)-C(35)	1.403(5)
C(34)-C(38)	1.439(11)
C(34)-C(38')	1.589(16)
C(35)-C(36)	1.377(5)
C(35)-H(35)	0.9500
C(36)-C(37)	1.391(4)
C(36)-H(36)	0.9500
C(37)-N(6)	1.383(4)
C(40)-N(6)	1.467(4)
C(40)-C(41)	1.506(5)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-O(6)	1.387(4)
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(42)-O(6)	1.454(6)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-C(53)	1.400(4)
C(43)-C(44)	1.411(4)
C(44)-C(45)	1.387(4)
C(44)-H(44)	0.9500
C(45)-C(51)	1.395(5)
C(45)-N(7)	1.397(4)
C(46)-C(47')	1.398(11)
C(46)-N(7)	1.482(4)
C(46)-C(58)	1.526(5)
C(46)-C(54)	1.530(5)
C(46)-C(47)	1.622(9)
C(51)-C(52)	1.366(6)

C(51)-N(8)	1.413(7)
C(51)-N(8')	1.499(7)
C(52)-C(53)	1.386(5)
C(52)-H(52)	0.9500
C(53)-H(53)	0.9500
C(54)-C(55)	1.522(4)
C(54)-H(54A)	0.9900
C(54)-H(54B)	0.9900
C(55)-C(56)	1.517(4)
C(55)-H(55A)	0.9900
C(55)-H(55B)	0.9900
C(56)-C(57)	1.522(5)
C(56)-C(59)	1.531(5)
C(56)-H(56)	1.0000
C(57)-C(58)	1.527(5)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-C(60)	1.506(6)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800
N(3)-H(3A)	0.8800
N(7)-H(7)	0.8800
C(8)-O(2)	1.272(12)
C(8)-O(1)	1.287(16)
C(9)-O(1)	1.487(9)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(8')-O(2')	1.271(17)
C(8')-O(1')	1.276(15)
C(9')-O(1')	1.462(8)
C(9')-H(9'1)	0.9800

C(9')-H(9'2)	0.9800
C(9')-H(9'3)	0.9800
C(38)-O(5)	1.194(10)
C(38)-O(4)	1.370(10)
C(39)-O(4)	1.468(8)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(38')-O(5')	1.198(12)
C(38')-O(4')	1.358(12)
C(39')-O(4')	1.464(11)
C(39')-H(39D)	0.9800
C(39')-H(39E)	0.9800
C(39')-H(39F)	0.9800
N(8)-C(47)	1.385(9)
N(8)-C(50)	1.392(8)
C(47)-C(48)	1.369(10)
C(48)-C(49)	1.444(9)
C(48)-H(48)	0.9500
C(49)-C(50)	1.342(8)
C(49)-H(49)	0.9500
C(50)-H(50)	0.9500
N(8')-C(47')	1.381(10)
N(8')-C(50')	1.389(8)
C(47')-C(48')	1.371(10)
C(48')-C(49')	1.434(10)
C(48')-H(48')	0.9500
C(49')-C(50')	1.338(8)
C(49')-H(49')	0.9500
C(50')-H(50')	0.9500
N(1)-C(1)-N(2)	113.2(4)
N(1)-C(1)-C(13)	123.1(3)
N(2)-C(1)-C(13)	123.7(3)
N(1)-C(2)-C(3)	128.9(3)
N(1)-C(2)-C(7)	110.1(4)
C(3)-C(2)-C(7)	120.9(4)
C(4)-C(3)-C(2)	116.7(4)

C(4)-C(3)-H(3)	121.6
C(2)-C(3)-H(3)	121.6
C(8)-C(4)-C(3)	125.4(8)
C(8)-C(4)-C(5)	112.5(8)
C(3)-C(4)-C(5)	122.1(5)
C(8)-C(4)-C(8')	12.3(12)
C(3)-C(4)-C(8')	113.5(7)
C(5)-C(4)-C(8')	124.3(6)
C(6)-C(5)-C(4)	120.8(4)
C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
C(5)-C(6)-C(7)	117.2(5)
C(5)-C(6)-H(6)	121.4
C(7)-C(6)-H(6)	121.4
C(6)-C(7)-N(2)	132.0(4)
C(6)-C(7)-C(2)	122.2(5)
N(2)-C(7)-C(2)	105.8(3)
N(2)-C(10)-C(11)	111.2(3)
N(2)-C(10)-H(10A)	109.4
C(11)-C(10)-H(10A)	109.4
N(2)-C(10)-H(10B)	109.4
C(11)-C(10)-H(10B)	109.4
H(10A)-C(10)-H(10B)	108.0
O(3)-C(11)-C(10)	112.4(3)
O(3)-C(11)-H(11A)	109.1
C(10)-C(11)-H(11A)	109.1
O(3)-C(11)-H(11B)	109.1
C(10)-C(11)-H(11B)	109.1
H(11A)-C(11)-H(11B)	107.9
O(3)-C(12)-H(12A)	109.5
O(3)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
O(3)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(23)-C(13)-C(14)	120.2(4)
C(23)-C(13)-C(1)	117.5(3)

C(14)-C(13)-C(1)	122.2(3)
C(15)-C(14)-C(13)	119.2(3)
C(15)-C(14)-H(14)	120.4
C(13)-C(14)-H(14)	120.4
C(16)-C(15)-C(14)	120.9(3)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(15)-C(16)-N(4)	123.0(3)
C(15)-C(16)-C(22)	120.3(4)
N(4)-C(16)-C(22)	116.7(3)
C(18)-C(17)-N(4)	108.6(3)
C(18)-C(17)-H(17)	125.7
N(4)-C(17)-H(17)	125.7
C(17)-C(18)-C(19)	107.9(4)
C(17)-C(18)-H(18)	126.1
C(19)-C(18)-H(18)	126.1
C(20)-C(19)-C(18)	106.9(4)
C(20)-C(19)-H(19)	126.6
C(18)-C(19)-H(19)	126.6
C(19)-C(20)-N(4)	108.1(3)
C(19)-C(20)-C(21)	132.2(3)
N(4)-C(20)-C(21)	119.6(3)
N(3)-C(21)-C(20)	107.3(3)
N(3)-C(21)-C(24)	109.3(3)
C(20)-C(21)-C(24)	110.2(3)
N(3)-C(21)-C(28)	111.0(3)
C(20)-C(21)-C(28)	109.4(3)
C(24)-C(21)-C(28)	109.7(3)
C(23)-C(22)-N(3)	121.8(3)
C(23)-C(22)-C(16)	118.5(3)
N(3)-C(22)-C(16)	119.6(3)
C(22)-C(23)-C(13)	120.9(3)
C(22)-C(23)-H(23)	119.5
C(13)-C(23)-H(23)	119.5
C(25)-C(24)-C(21)	112.2(3)
C(25)-C(24)-H(24A)	109.2
C(21)-C(24)-H(24A)	109.2

C(25)-C(24)-H(24B)	109.2
C(21)-C(24)-H(24B)	109.2
H(24A)-C(24)-H(24B)	107.9
C(26)-C(25)-C(24)	112.8(3)
C(26)-C(25)-H(25A)	109.0
C(24)-C(25)-H(25A)	109.0
C(26)-C(25)-H(25B)	109.0
C(24)-C(25)-H(25B)	109.0
H(25A)-C(25)-H(25B)	107.8
C(27)-C(26)-C(29)	113.2(3)
C(27)-C(26)-C(25)	110.7(3)
C(29)-C(26)-C(25)	109.8(3)
C(27)-C(26)-H(26)	107.7
C(29)-C(26)-H(26)	107.7
C(25)-C(26)-H(26)	107.7
C(26)-C(27)-C(28)	112.0(3)
C(26)-C(27)-H(27A)	109.2
C(28)-C(27)-H(27A)	109.2
C(26)-C(27)-H(27B)	109.2
C(28)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(27)-C(28)-C(21)	112.0(2)
C(27)-C(28)-H(28A)	109.2
C(21)-C(28)-H(28A)	109.2
C(27)-C(28)-H(28B)	109.2
C(21)-C(28)-H(28B)	109.2
H(28A)-C(28)-H(28B)	107.9
C(30)-C(29)-C(26)	114.8(3)
C(30)-C(29)-H(29A)	108.6
C(26)-C(29)-H(29A)	108.6
C(30)-C(29)-H(29B)	108.6
C(26)-C(29)-H(29B)	108.6
H(29A)-C(29)-H(29B)	107.5
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5

H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
N(5)-C(31)-N(6)	112.5(3)
N(5)-C(31)-C(43)	122.9(3)
N(6)-C(31)-C(43)	124.6(3)
N(5)-C(32)-C(37)	110.7(3)
N(5)-C(32)-C(33)	129.2(3)
C(37)-C(32)-C(33)	120.0(3)
C(34)-C(33)-C(32)	117.8(3)
C(34)-C(33)-H(33)	121.1
C(32)-C(33)-H(33)	121.1
C(33)-C(34)-C(35)	121.4(3)
C(33)-C(34)-C(38)	122.7(5)
C(35)-C(34)-C(38)	115.8(4)
C(33)-C(34)-C(38')	108.0(5)
C(35)-C(34)-C(38')	130.4(6)
C(38)-C(34)-C(38')	17.1(6)
C(36)-C(35)-C(34)	121.4(3)
C(36)-C(35)-H(35)	119.3
C(34)-C(35)-H(35)	119.3
C(35)-C(36)-C(37)	116.9(3)
C(35)-C(36)-H(36)	121.6
C(37)-C(36)-H(36)	121.6
N(6)-C(37)-C(32)	105.3(3)
N(6)-C(37)-C(36)	132.1(3)
C(32)-C(37)-C(36)	122.6(3)
N(6)-C(40)-C(41)	113.0(3)
N(6)-C(40)-H(40A)	109.0
C(41)-C(40)-H(40A)	109.0
N(6)-C(40)-H(40B)	109.0
C(41)-C(40)-H(40B)	109.0
H(40A)-C(40)-H(40B)	107.8
O(6)-C(41)-C(40)	107.2(3)
O(6)-C(41)-H(41A)	110.3
C(40)-C(41)-H(41A)	110.3
O(6)-C(41)-H(41B)	110.3
C(40)-C(41)-H(41B)	110.3

H(41A)-C(41)-H(41B)	108.5
O(6)-C(42)-H(42A)	109.5
O(6)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
O(6)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(53)-C(43)-C(44)	118.9(3)
C(53)-C(43)-C(31)	123.6(3)
C(44)-C(43)-C(31)	117.4(3)
C(45)-C(44)-C(43)	121.0(3)
C(45)-C(44)-H(44)	119.5
C(43)-C(44)-H(44)	119.5
C(44)-C(45)-C(51)	118.6(3)
C(44)-C(45)-N(7)	121.3(3)
C(51)-C(45)-N(7)	120.0(3)
C(47')-C(46)-N(7)	105.5(4)
C(47')-C(46)-C(58)	102.5(4)
N(7)-C(46)-C(58)	109.1(3)
C(47')-C(46)-C(54)	119.1(4)
N(7)-C(46)-C(54)	110.8(3)
C(58)-C(46)-C(54)	109.3(3)
C(47')-C(46)-C(47)	19.2(5)
N(7)-C(46)-C(47)	108.0(4)
C(58)-C(46)-C(47)	118.0(4)
C(54)-C(46)-C(47)	101.5(4)
C(52)-C(51)-C(45)	120.9(3)
C(52)-C(51)-N(8)	113.7(4)
C(45)-C(51)-N(8)	124.6(4)
C(52)-C(51)-N(8')	130.0(4)
C(45)-C(51)-N(8')	107.6(4)
N(8)-C(51)-N(8')	27.1(2)
C(51)-C(52)-C(53)	121.4(3)
C(51)-C(52)-H(52)	119.3
C(53)-C(52)-H(52)	119.3
C(52)-C(53)-C(43)	119.2(3)
C(52)-C(53)-H(53)	120.4

C(43)-C(53)-H(53)	120.4
C(55)-C(54)-C(46)	112.8(3)
C(55)-C(54)-H(54A)	109.0
C(46)-C(54)-H(54A)	109.0
C(55)-C(54)-H(54B)	109.0
C(46)-C(54)-H(54B)	109.0
H(54A)-C(54)-H(54B)	107.8
C(56)-C(55)-C(54)	111.2(3)
C(56)-C(55)-H(55A)	109.4
C(54)-C(55)-H(55A)	109.4
C(56)-C(55)-H(55B)	109.4
C(54)-C(55)-H(55B)	109.4
H(55A)-C(55)-H(55B)	108.0
C(55)-C(56)-C(57)	109.8(3)
C(55)-C(56)-C(59)	112.9(3)
C(57)-C(56)-C(59)	110.5(3)
C(55)-C(56)-H(56)	107.8
C(57)-C(56)-H(56)	107.8
C(59)-C(56)-H(56)	107.8
C(56)-C(57)-C(58)	112.5(3)
C(56)-C(57)-H(57A)	109.1
C(58)-C(57)-H(57A)	109.1
C(56)-C(57)-H(57B)	109.1
C(58)-C(57)-H(57B)	109.1
H(57A)-C(57)-H(57B)	107.8
C(46)-C(58)-C(57)	113.8(3)
C(46)-C(58)-H(58A)	108.8
C(57)-C(58)-H(58A)	108.8
C(46)-C(58)-H(58B)	108.8
C(57)-C(58)-H(58B)	108.8
H(58A)-C(58)-H(58B)	107.7
C(60)-C(59)-C(56)	115.7(3)
C(60)-C(59)-H(59A)	108.3
C(56)-C(59)-H(59A)	108.3
C(60)-C(59)-H(59B)	108.3
C(56)-C(59)-H(59B)	108.3
H(59A)-C(59)-H(59B)	107.4

C(59)-C(60)-H(60A)	109.5
C(59)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(59)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(1)-N(1)-C(2)	104.6(3)
C(1)-N(2)-C(7)	106.3(3)
C(1)-N(2)-C(10)	128.6(4)
C(7)-N(2)-C(10)	123.9(3)
C(22)-N(3)-C(21)	118.2(2)
C(22)-N(3)-H(3A)	120.9
C(21)-N(3)-H(3A)	120.9
C(20)-N(4)-C(17)	108.6(3)
C(20)-N(4)-C(16)	122.3(3)
C(17)-N(4)-C(16)	129.0(3)
C(31)-N(5)-C(32)	105.2(2)
C(37)-N(6)-C(31)	106.3(2)
C(37)-N(6)-C(40)	124.9(2)
C(31)-N(6)-C(40)	128.6(3)
C(45)-N(7)-C(46)	117.2(3)
C(45)-N(7)-H(7)	121.4
C(46)-N(7)-H(7)	121.4
C(11)-O(3)-C(12)	113.4(3)
C(41)-O(6)-C(42)	112.8(4)
C(4)-C(8)-O(2)	116.3(13)
C(4)-C(8)-O(1)	122.1(9)
O(2)-C(8)-O(1)	121.2(11)
C(8)-O(1)-C(9)	115.6(7)
O(2')-C(8')-O(1')	121.7(10)
O(2')-C(8')-C(4)	118.5(9)
O(1')-C(8')-C(4)	119.5(12)
O(1')-C(9')-H(9'1)	109.5
O(1')-C(9')-H(9'2)	109.5
H(9'1)-C(9')-H(9'2)	109.5
O(1')-C(9')-H(9'3)	109.5
H(9'1)-C(9')-H(9'3)	109.5

H(9'2)-C(9')-H(9'3)	109.5
C(8')-O(1')-C(9')	119.2(9)
O(5)-C(38)-O(4)	123.5(9)
O(5)-C(38)-C(34)	121.7(8)
O(4)-C(38)-C(34)	114.5(8)
C(38)-O(4)-C(39)	114.5(6)
O(5')-C(38')-O(4')	120.2(13)
O(5')-C(38')-C(34)	131.6(12)
O(4')-C(38')-C(34)	105.9(8)
O(4')-C(39')-H(39D)	109.5
O(4')-C(39')-H(39E)	109.5
H(39D)-C(39')-H(39E)	109.5
O(4')-C(39')-H(39F)	109.5
H(39D)-C(39')-H(39F)	109.5
H(39E)-C(39')-H(39F)	109.5
C(38')-O(4')-C(39')	115.5(10)
C(47)-N(8)-C(50)	108.9(6)
C(47)-N(8)-C(51)	115.1(5)
C(50)-N(8)-C(51)	134.1(5)
C(48)-C(47)-N(8)	107.9(7)
C(48)-C(47)-C(46)	129.8(7)
N(8)-C(47)-C(46)	122.3(7)
C(47)-C(48)-C(49)	106.9(7)
C(47)-C(48)-H(48)	126.6
C(49)-C(48)-H(48)	126.6
C(50)-C(49)-C(48)	108.1(6)
C(50)-C(49)-H(49)	126.0
C(48)-C(49)-H(49)	126.0
C(49)-C(50)-N(8)	108.2(6)
C(49)-C(50)-H(50)	125.9
N(8)-C(50)-H(50)	125.9
C(47')-N(8')-C(50')	109.0(6)
C(47')-N(8')-C(51)	125.9(6)
C(50')-N(8')-C(51)	124.3(5)
C(48')-C(47')-N(8')	107.6(8)
C(48')-C(47')-C(46)	135.4(8)
N(8')-C(47')-C(46)	116.1(7)

C(47')-C(48')-C(49')	107.0(7)
C(47')-C(48')-H(48')	126.5
C(49')-C(48')-H(48')	126.5
C(50')-C(49')-C(48')	108.3(6)
C(50')-C(49')-H(49')	125.8
C(48')-C(49')-H(49')	125.8
C(49')-C(50')-N(8')	108.1(6)
C(49')-C(50')-H(50')	126.0
N(8')-C(50')-H(50')	126.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å ^{2}x 10^3) for 101119LTs. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	51(2)	53(2)	38(2)	-3(2)	0(2)	20(2)
C(2)	77(2)	44(2)	34(2)	0(1)	6(2)	20(2)
C(3)	122(4)	50(2)	43(2)	10(2)	24(2)	30(2)
C(4)	117(4)	45(2)	46(2)	8(2)	-2(2)	7(2)
C(5)	124(4)	38(2)	72(3)	6(2)	-26(3)	13(3)
C(6)	91(3)	42(2)	76(3)	-6(2)	-20(3)	18(2)
C(7)	76(3)	44(2)	45(2)	-9(2)	-12(2)	21(2)
C(10)	49(2)	60(2)	90(3)	-13(2)	2(2)	23(2)
C(11)	55(2)	71(3)	101(3)	-25(2)	28(2)	6(2)
C(12)	73(3)	96(3)	88(3)	-23(3)	50(3)	-14(2)
C(13)	48(2)	52(2)	42(2)	-6(2)	10(2)	14(2)
C(14)	45(2)	69(2)	42(2)	-5(2)	4(2)	22(2)
C(15)	40(2)	64(2)	50(2)	0(2)	8(2)	8(2)
C(16)	35(2)	65(2)	46(2)	-1(2)	12(2)	8(2)
C(17)	39(2)	87(3)	66(3)	3(2)	17(2)	1(2)
C(18)	53(2)	91(3)	83(3)	23(3)	33(2)	0(2)
C(19)	53(2)	83(3)	64(2)	16(2)	25(2)	2(2)
C(20)	38(2)	69(2)	49(2)	6(2)	18(2)	4(2)
C(21)	42(2)	55(2)	41(2)	6(1)	15(1)	3(1)
C(22)	39(2)	56(2)	39(2)	-5(2)	14(1)	7(1)
C(23)	39(2)	52(2)	37(2)	-4(1)	11(1)	9(1)
C(24)	46(2)	64(2)	41(2)	8(2)	16(2)	6(2)
C(25)	41(2)	56(2)	38(2)	6(1)	10(1)	4(1)
C(26)	44(2)	45(2)	45(2)	9(1)	16(1)	6(1)
C(27)	44(2)	47(2)	47(2)	7(1)	19(2)	8(1)
C(28)	43(2)	58(2)	39(2)	8(1)	14(1)	5(2)
C(29)	43(2)	55(2)	57(2)	17(2)	14(2)	9(2)
C(30)	52(2)	77(3)	81(3)	27(2)	33(2)	22(2)
C(31)	39(2)	42(2)	42(2)	6(1)	15(1)	7(1)
C(32)	52(2)	43(2)	38(2)	11(1)	18(1)	15(1)
C(33)	56(2)	58(2)	44(2)	15(2)	24(2)	23(2)
C(34)	78(3)	51(2)	47(2)	12(2)	28(2)	25(2)

C(35)	84(3)	42(2)	38(2)	2(1)	18(2)	6(2)
C(36)	60(2)	44(2)	45(2)	4(1)	13(2)	4(2)
C(37)	50(2)	37(2)	42(2)	9(1)	15(1)	4(1)
C(40)	43(2)	57(2)	51(2)	-1(2)	16(2)	-6(2)
C(41)	38(2)	94(3)	63(2)	11(2)	19(2)	8(2)
C(42)	80(3)	144(5)	123(5)	-9(4)	29(3)	54(3)
C(43)	36(2)	45(2)	44(2)	-1(1)	16(1)	-2(1)
C(44)	41(2)	41(2)	49(2)	-1(1)	23(2)	-3(1)
C(45)	40(2)	56(2)	44(2)	-4(2)	18(2)	-15(2)
C(46)	48(2)	56(2)	37(2)	-4(1)	16(2)	-8(2)
C(51)	29(2)	110(3)	48(2)	-24(2)	17(2)	-6(2)
C(52)	34(2)	107(3)	59(2)	-32(2)	11(2)	7(2)
C(53)	36(2)	71(2)	50(2)	-10(2)	12(2)	4(2)
C(54)	37(2)	45(2)	44(2)	0(1)	13(1)	3(1)
C(55)	36(2)	46(2)	50(2)	4(1)	16(1)	4(1)
C(56)	48(2)	47(2)	41(2)	0(1)	10(2)	11(1)
C(57)	86(3)	46(2)	43(2)	3(2)	15(2)	5(2)
C(58)	78(3)	57(2)	42(2)	2(2)	20(2)	-12(2)
C(59)	66(2)	76(2)	43(2)	2(2)	10(2)	40(2)
C(60)	40(2)	110(3)	65(3)	-13(2)	19(2)	10(2)
N(1)	75(2)	47(2)	39(2)	6(1)	16(1)	22(1)
N(2)	66(2)	44(2)	50(2)	-10(1)	0(2)	19(1)
N(3)	35(1)	59(2)	35(1)	-2(1)	4(1)	6(1)
N(4)	36(2)	68(2)	49(2)	3(1)	17(1)	0(1)
N(5)	41(1)	45(1)	40(1)	5(1)	15(1)	9(1)
N(6)	45(2)	41(1)	42(1)	-1(1)	17(1)	0(1)
N(7)	55(2)	49(2)	44(2)	0(1)	17(1)	-12(1)
O(3)	52(2)	85(2)	64(2)	-21(1)	23(1)	-8(1)
O(6)	70(2)	101(2)	134(3)	7(2)	44(2)	5(2)
C(8)	106(11)	55(3)	51(3)	10(2)	52(6)	43(6)
C(9)	78(4)	70(4)	82(4)	27(3)	37(3)	-2(3)
O(1)	68(2)	50(2)	59(2)	13(2)	30(2)	-2(2)
O(2)	89(3)	81(3)	88(4)	33(3)	39(3)	6(3)
C(8')	106(11)	55(3)	51(3)	10(2)	52(6)	43(6)
C(9')	78(4)	70(4)	82(4)	27(3)	37(3)	-2(3)
O(1')	68(2)	50(2)	59(2)	13(2)	30(2)	-2(2)
O(2')	89(3)	81(3)	88(4)	33(3)	39(3)	6(3)

C(38)	62(6)	40(6)	47(3)	5(4)	29(4)	-2(4)
C(39)	82(6)	81(4)	53(5)	1(4)	41(5)	8(6)
O(4)	63(5)	64(2)	44(3)	-3(2)	26(3)	2(4)
O(5)	65(4)	69(5)	55(3)	4(4)	33(3)	13(3)
C(38')	62(6)	40(6)	47(3)	5(4)	29(4)	-2(4)
C(39')	82(6)	81(4)	53(5)	1(4)	41(5)	8(6)
O(4')	63(5)	64(2)	44(3)	-3(2)	26(3)	2(4)
O(5')	65(4)	69(5)	55(3)	4(4)	33(3)	13(3)
N(8)	34(2)	39(3)	35(2)	10(2)	14(2)	9(2)
C(47)	37(3)	30(5)	38(3)	5(3)	13(2)	-4(3)
C(48)	41(3)	46(5)	38(3)	5(3)	13(2)	-1(3)
C(49)	41(2)	48(3)	39(3)	2(2)	20(2)	3(3)
C(50)	35(2)	48(3)	43(3)	3(2)	16(2)	5(3)
N(8')	34(2)	39(3)	35(2)	10(2)	14(2)	9(2)
C(47')	37(3)	30(5)	38(3)	5(3)	13(2)	-4(3)
C(48')	41(3)	46(5)	38(3)	5(3)	13(2)	-1(3)
C(49')	41(2)	48(3)	39(3)	2(2)	20(2)	3(3)
C(50')	35(2)	48(3)	43(3)	3(2)	16(2)	5(3)

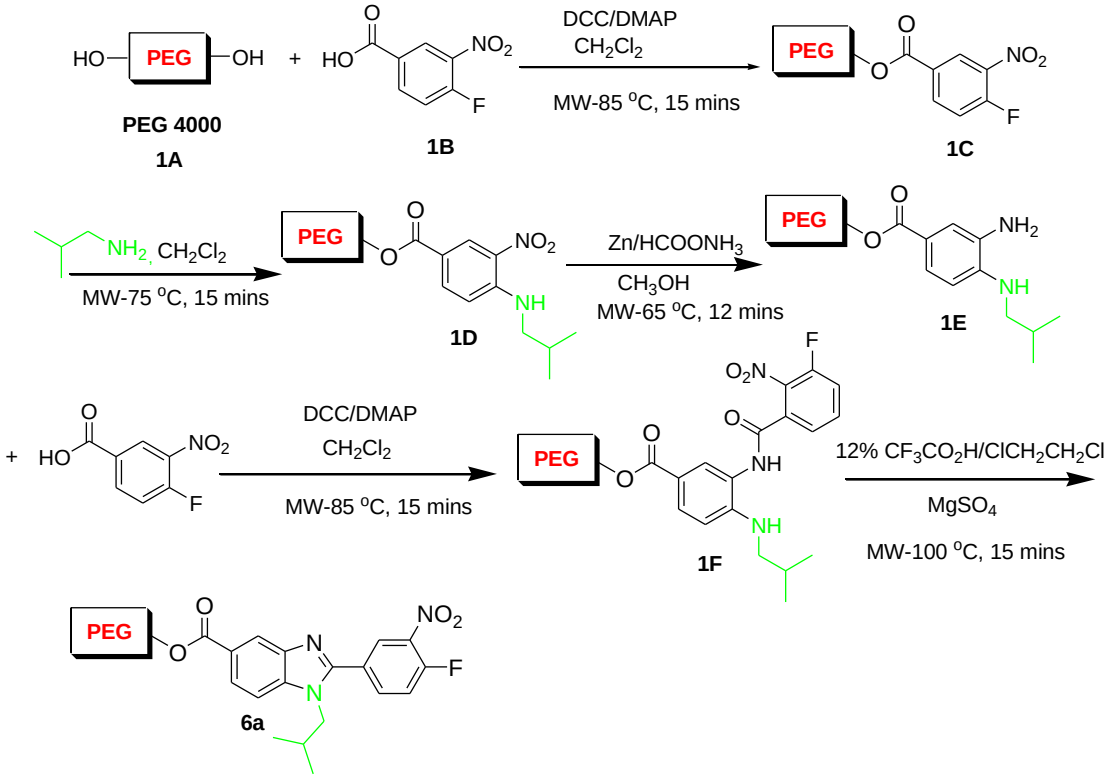
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10 ^{3}) for 101119LTs.

	x	y	z	U(eq)
H(3)	3131	4507	739	88
H(5)	1257	6560	614	115
H(6)	-27	5945	1150	105
H(10A)	-1132	4072	1932	95
H(10B)	-1253	4863	1493	95
H(11A)	196	5827	2779	104
H(11B)	-842	5459	3031	104
H(12A)	-465	4753	4057	139
H(12B)	645	4258	4264	139
H(12C)	-399	3874	3331	139
H(14)	-1218	2558	1180	71
H(15)	-1607	1439	1761	69
H(17)	-1989	610	2669	84
H(18)	-1581	-390	3593	90
H(19)	618	-221	4327	81
H(23)	2122	3061	2859	57
H(24A)	2516	1477	5157	62
H(24B)	2591	440	4783	62
H(25A)	4146	1899	4854	58
H(25B)	4475	1233	5435	58
H(26)	4278	46	4179	55
H(27A)	3785	201	2763	56
H(27B)	3689	1233	3137	56
H(28A)	2167	-238	3082	58
H(28B)	1815	403	2476	58
H(29A)	5739	1566	4274	63
H(29B)	6094	976	4928	63
H(30A)	6008	-258	3704	100
H(30B)	6966	564	3881	100
H(30C)	5745	379	3088	100
H(33)	6818	6196	4879	61

H(35)	3837	4831	2894	69
H(36)	2748	5308	3798	64
H(40A)	2612	6406	6164	66
H(40B)	2265	5643	5229	66
H(41A)	2214	7483	5345	81
H(41B)	1664	6646	4458	81
H(42A)	364	7962	5185	190
H(42B)	-702	7249	5054	190
H(42C)	-193	7162	4274	190
H(44)	6302	6941	7784	54
H(52)	3557	8717	8314	97
H(53)	3341	7949	6854	72
H(54A)	7411	9289	9669	54
H(54B)	8071	9656	10720	54
H(55A)	8804	8349	9519	56
H(55B)	9435	9363	10012	56
H(56)	9933	9109	11397	60
H(57A)	9516	7692	11513	75
H(57B)	8894	7287	10460	75
H(58A)	7453	7528	11073	76
H(58B)	8055	8536	11627	76
H(59A)	11317	8160	11297	80
H(59B)	10689	7770	10246	80
H(60A)	11257	9117	10077	120
H(60B)	12378	8799	10649	120
H(60C)	11798	9568	11130	120
H(3A)	2520	2361	4110	58
H(7)	6973	7104	9442	64
H(9A)	4420	7097	308	111
H(9B)	3653	7872	192	111
H(9C)	3419	6983	-622	111
H(9'1)	5215	5899	-296	111
H(9'2)	6016	6208	732	111
H(9'3)	5147	6838	349	111
H(39A)	6247	4821	1600	108
H(39B)	5334	3918	1185	108
H(39C)	6494	4015	2010	108

H(39D)	6711	4733	1781	108
H(39E)	6110	3732	1569	108
H(39F)	7243	4165	2434	108
H(48)	6383	9374	11788	53
H(49)	4453	9968	11325	53
H(50)	3617	9463	9696	53
H(48')	6572	9091	11910	53
H(49')	4483	9399	11507	53
H(50')	3552	8835	9888	53

Scheme 5. Synthetic scheme for the polymer Polymer Bound Benzimidazole Derivatives 6.



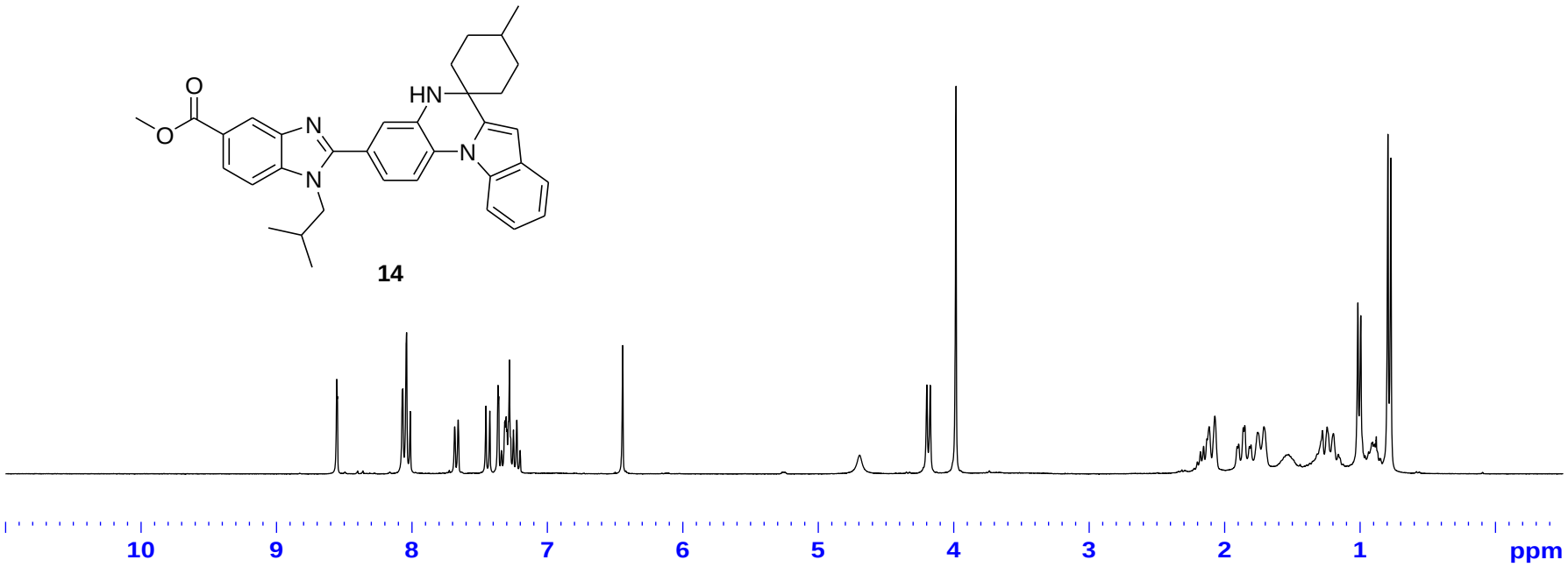
General Procedure for the Preparation of Polymer Bound Benzimidazole Derivatives 6.

Polyethylene glycol **1A** (PEG 4000) (1.0 g, 0.25 mmol, 1.0 equiv) dissolved in (5 mL) of dichloromethane was added to a solution of 4-fluoro-3-nitrobenzoic acid **1B** (0.11 g, 0.60 mmol, 2.4 equiv) in dichloromethane (5 mL) in the presence of *N*,*N*′-dicyclohexylcarbodiimide (DCC) (0.144 g, 0.70 mmol, 2.4 equiv) and *N*,*N*′-dimethylamino pyridine (DMAP) (3 mg). The reaction mixture was stirred at room temperature for 10 mins and subsequently irradiated in sealed microwave biotage vial (10 ml) at 85 ^{o}C for 15 mins. After completion of the reaction, the insoluble

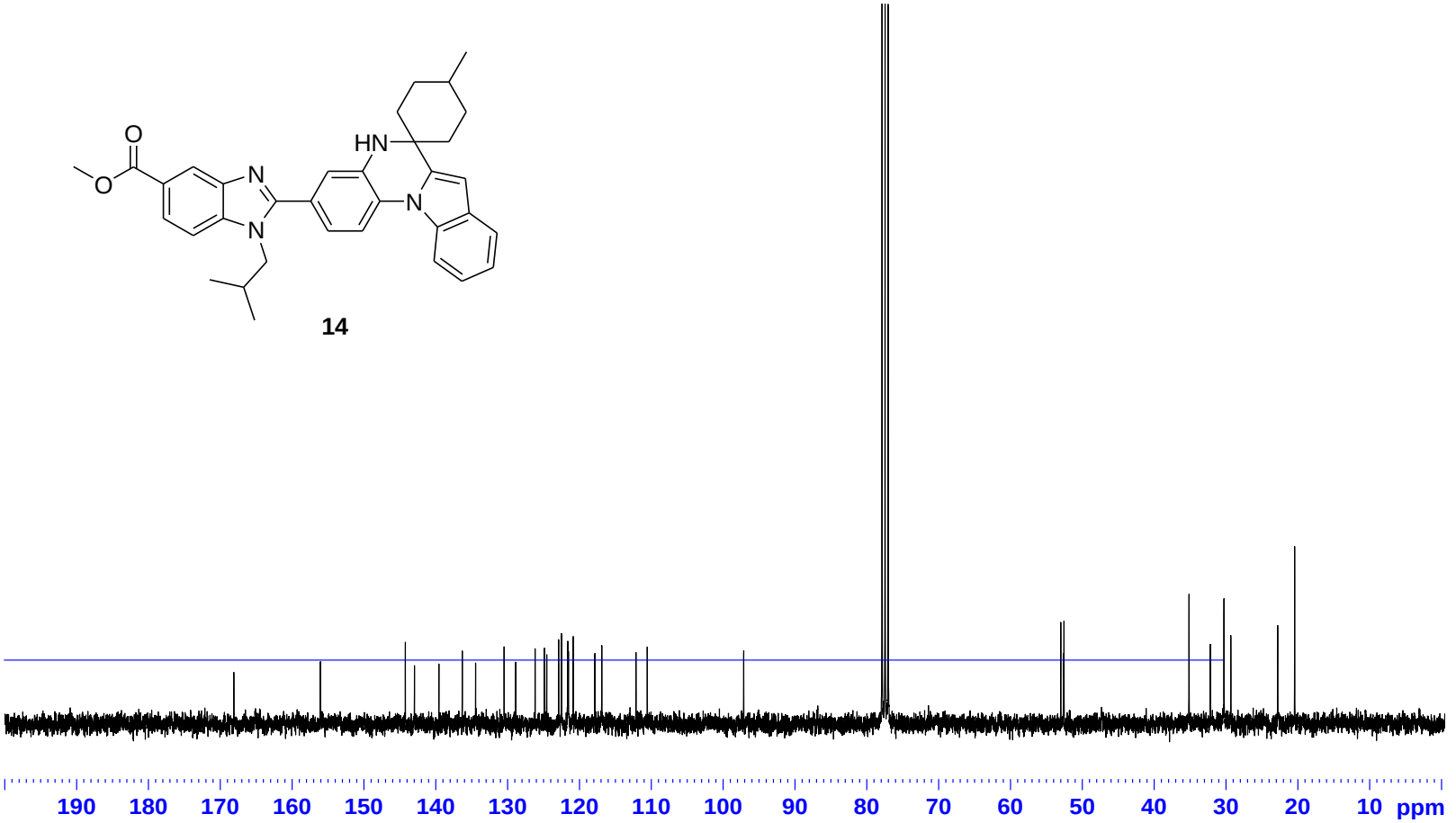
dicyclohexyl urea (DCU) was filtered through filter paper. The reaction mixtures were precipitated by slow addition of cold ether and precipitated polymer conjugate **1C** was filtered through fritted funnel. The crude product was washed successively with cold ether (50 mL × 3) to remove the undesired impurity and dried for further steps. To the polymer conjugate **1C** (1.1 gm, 0.25 mmol, 1.0 equiv) dissolved in (6 mL) of dichloromethane was added isobutyl amine (0.07 gm, 1.01 mmol, 4.0 equiv). The reaction mixture was stirred at room temperature and subsequently irradiated under sealed microwave vial (10 ml) at 75 ^{o}C for 15 mins to obtain the polymer bound conjugates **1D**. After completion of the reaction, the reaction mixtures were precipitated by slow addition of cold ether and precipitated polymer conjugate **1D** was filtered through fritted funnel. The crude product was washed successively with ether (50 mL × 3) to remove the undesired impurity and dried for further steps. Subsequently to the polymer conjugate **1D** (1.2 gm, 0.27 mmol, 1.0 equiv) dissolved in (6 mL) of methanol was added Zn (0.26 gm, 4.05 mmol, 15.0 equiv) and ammonium formate (0.17 gm, 2.70 mmol, 10.0 equiv). The reaction mixture was stirred at room temperature and subsequently irradiated in sealed microwave vial (10 ml) at 65 ^{o}C for 12 mins to obtain the polymer bound conjugates **1E**. After completion, the mixtures were filtered with Celite

to remove zinc and the filtrate was collected and concentrated under reduced pressure. Then dichloromethane (25 mL) was added to precipitate ammonium formate, and the mixture was again passed through a thin layer of Celite to remove ammonium formate and dried. Polymer bound *o*-phenylene diamine **1E** (1.0 g, 0.23 mmol, 1.0 equiv) dissolved in (5 mL) of dichloromethane was added to a solution of 4-fluoro-3-nitrobenzoic acid (0.11 g, 0.60 mmol, 2.6 equiv) in dichloromethane (5 mL) in the presence of *N*,*N*′-dicyclohexylcarbodiimide (DCC) (0.12 g, 0.60 mmol, 2.6 equiv) and *N*,*N*′- dimethylamino pyridine (DMAP) (2 mg). The reaction mixture was stirred at room temperature and subsequently irradiated in sealed microwave vial (10 ml) for 85 ^{o}C 15 mins to obtain the polymer bound amide conjugates **3**. After completion of the reaction, the suspensible dicyclohexyl urea (DCU) was filtered through filter paper. The reaction mixtures were precipitated by slow addition of cold ether and precipitated amide conjugate **1F** was filtered through fritted funnel. The crude product was washed successively with ether (50 mL × 3) to remove the undesired impurity and dried for further steps. To a solution of **1F** in 1, 2-dichloroethane, trifluoroacetic acid (0.5 mL) and MgSO4 (0.5 g) were added and irradiated under sealed microwave vial (10 ml) 100 ^{o}C for 15 mins. After completion of the reaction, MgSO4 was removed through celite. The reaction mixtures were

precipitated by slow addition of excess of cold ether (100 mL) and filtered through a fritted funnel to obtain the compound **6a** in high purity in quantitative yields

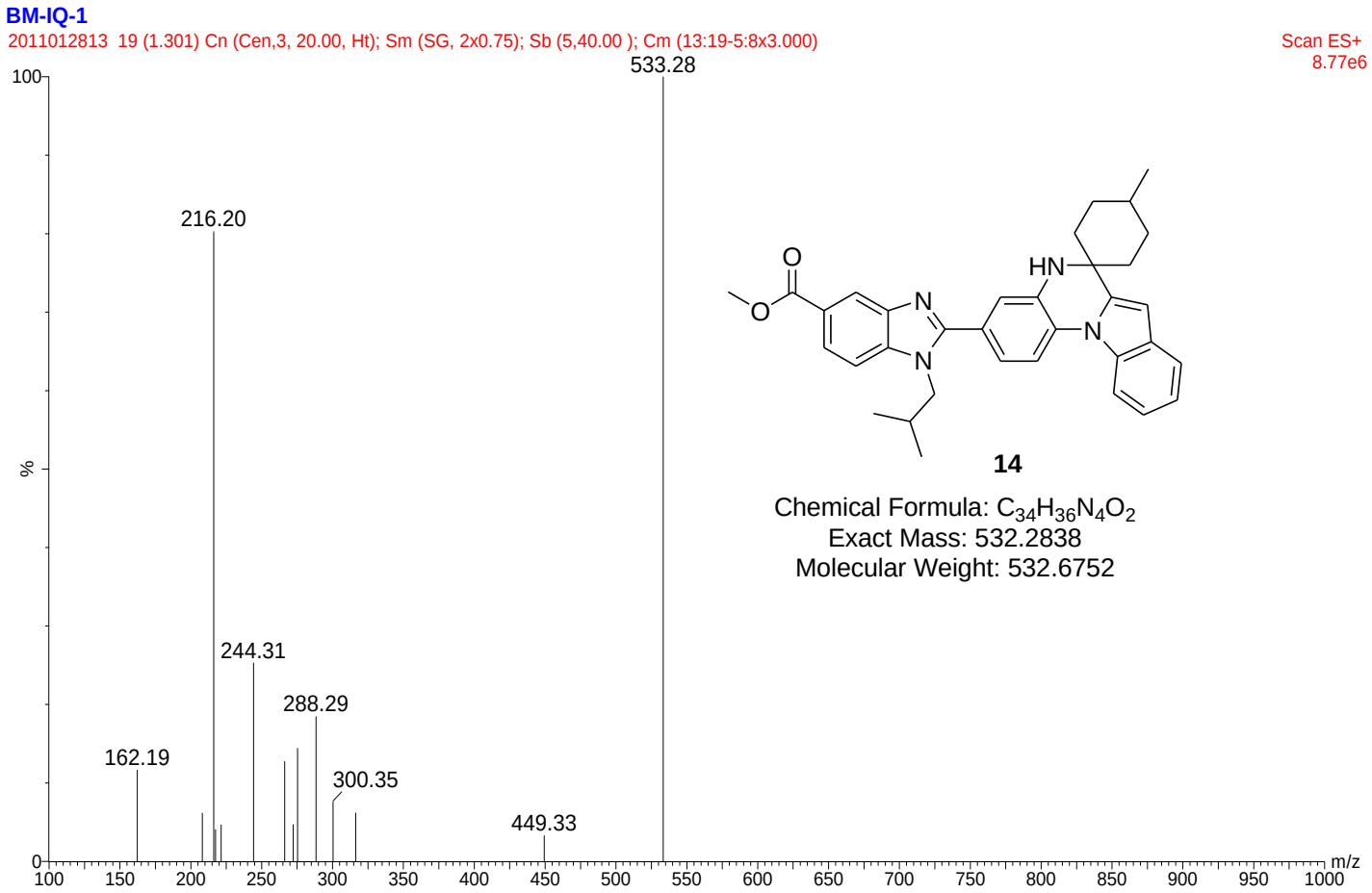


^{1}H NMR Spectrum of Compound 14 in $CDCl_3$

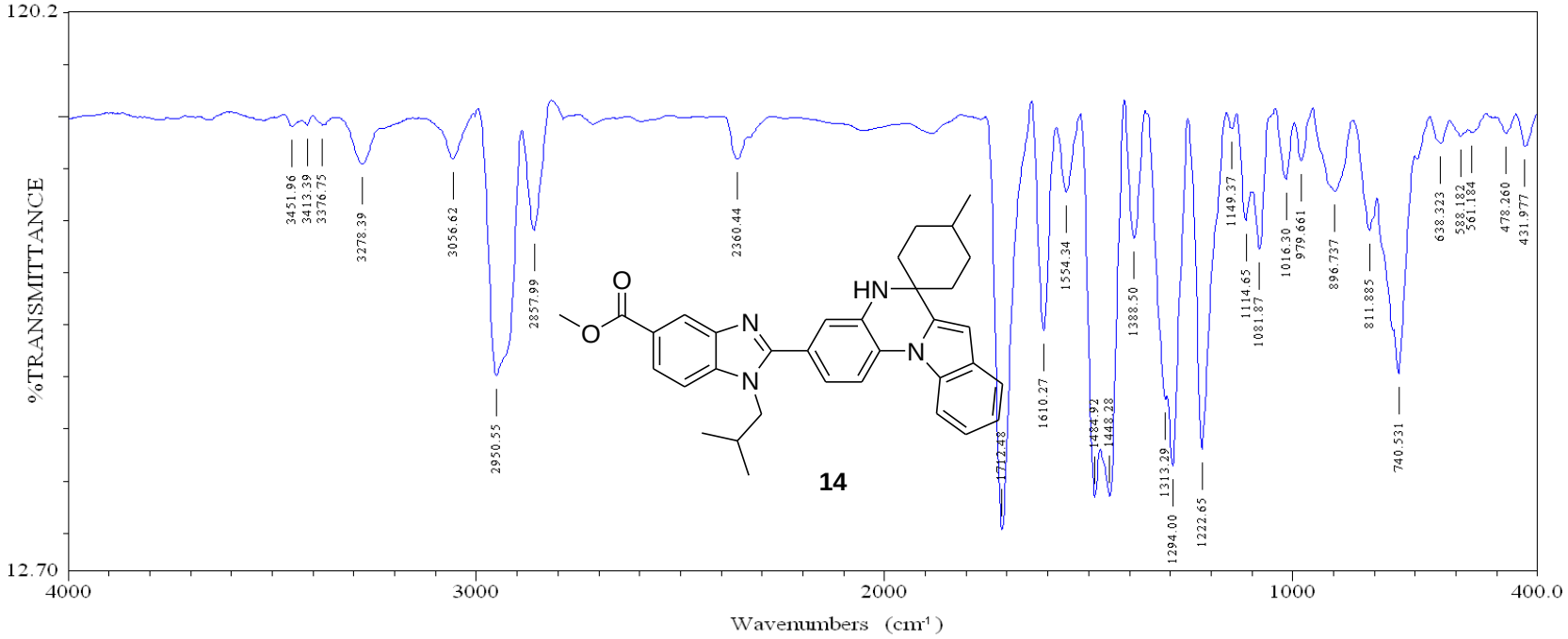


14

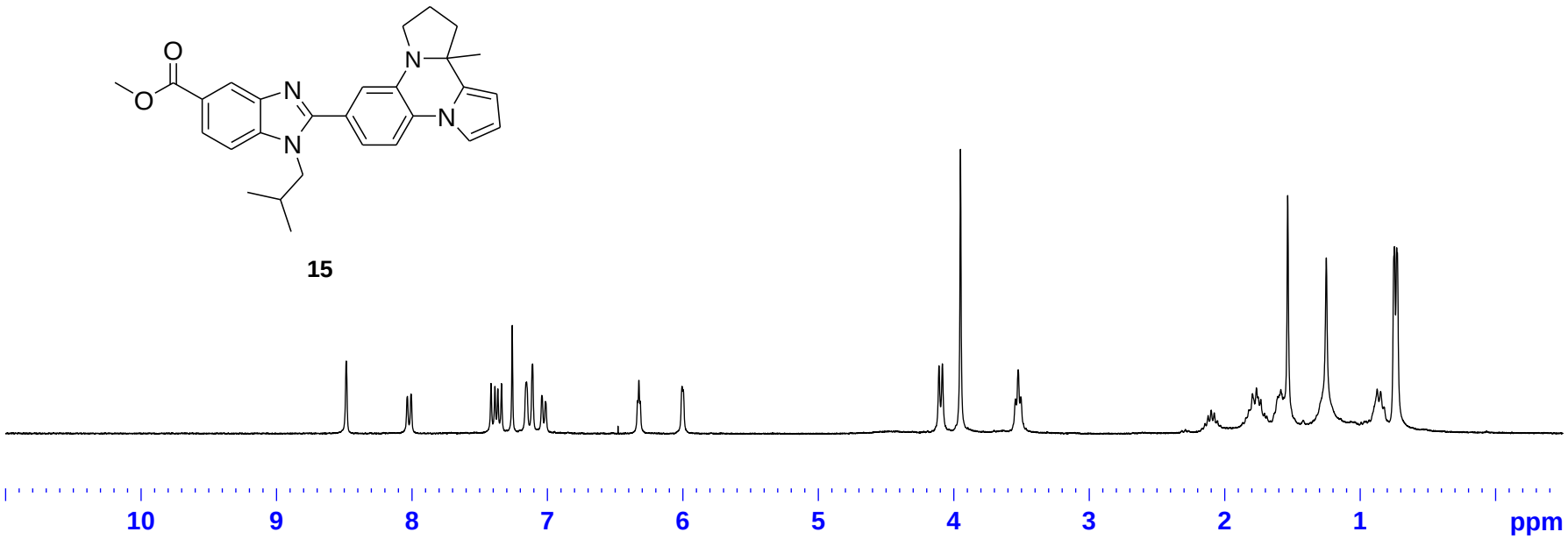
^{13}C NMR Spectrum of Compound 14 in $CDCl_3$



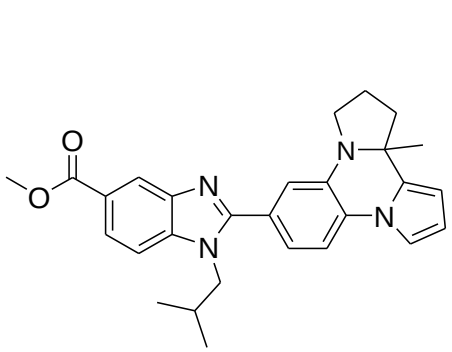
LR Mass Spectrum of Compound 14



IR Spectrum of Compound 14

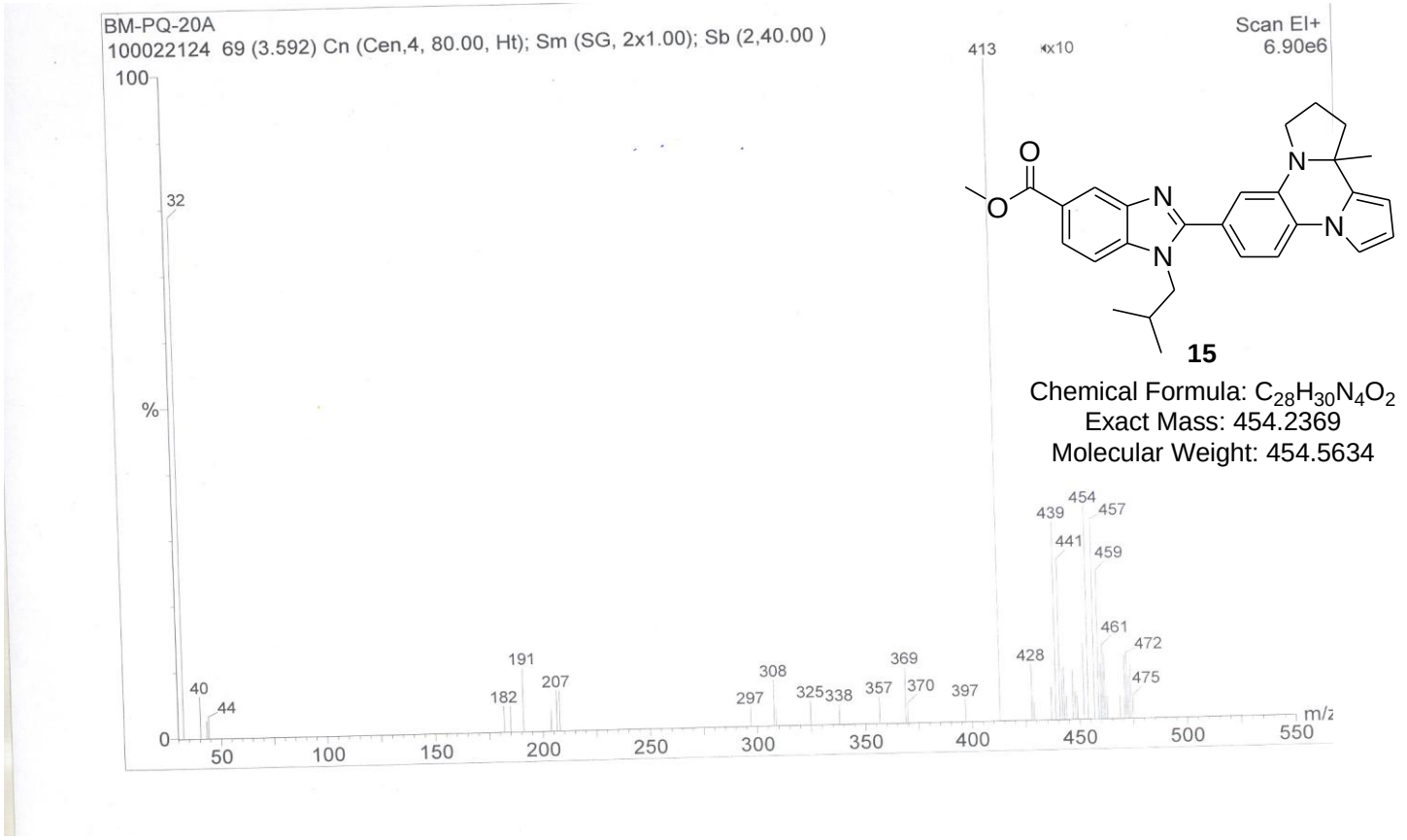


^{1}H NMR Spectrum of Compound 15 in $CDCl_3$



15

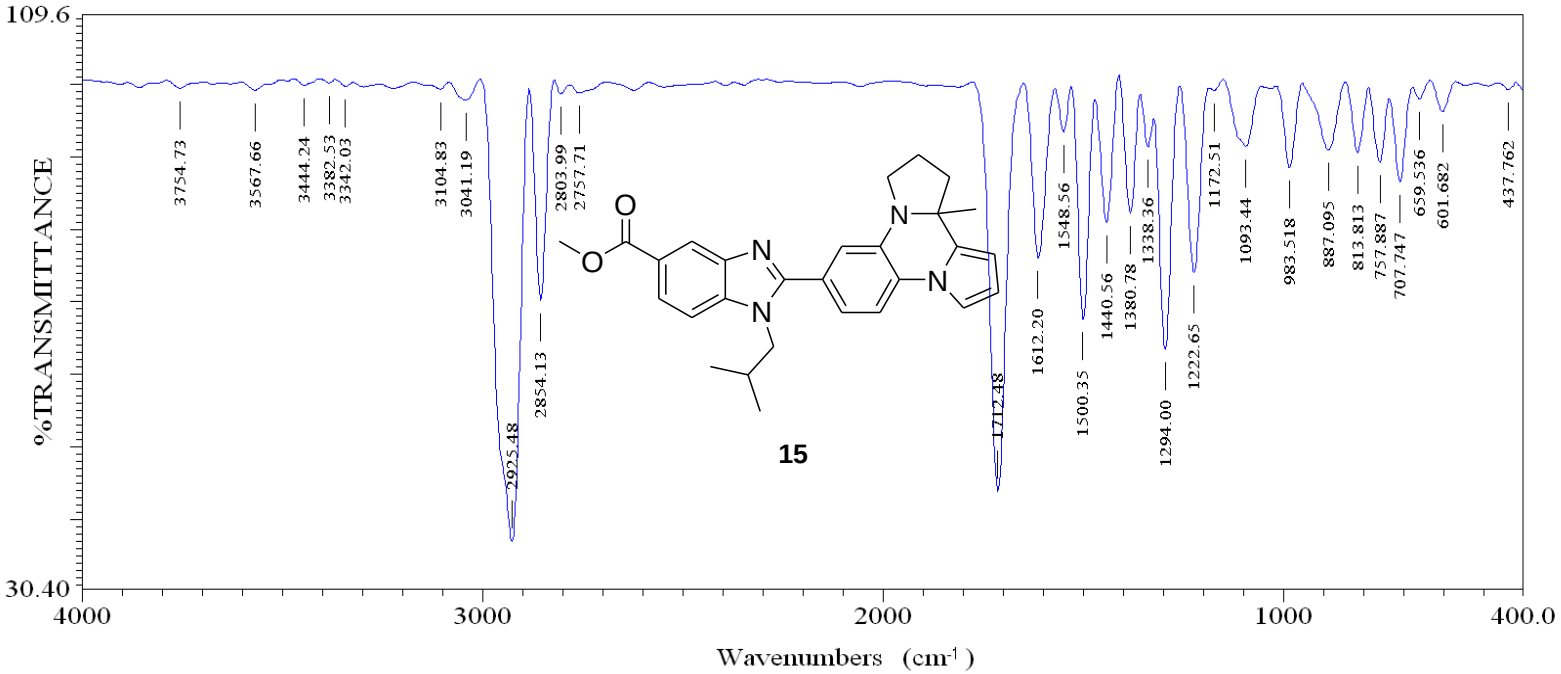
^{13}C NMR Spectrum of Compound 14 in $CDCl_3$



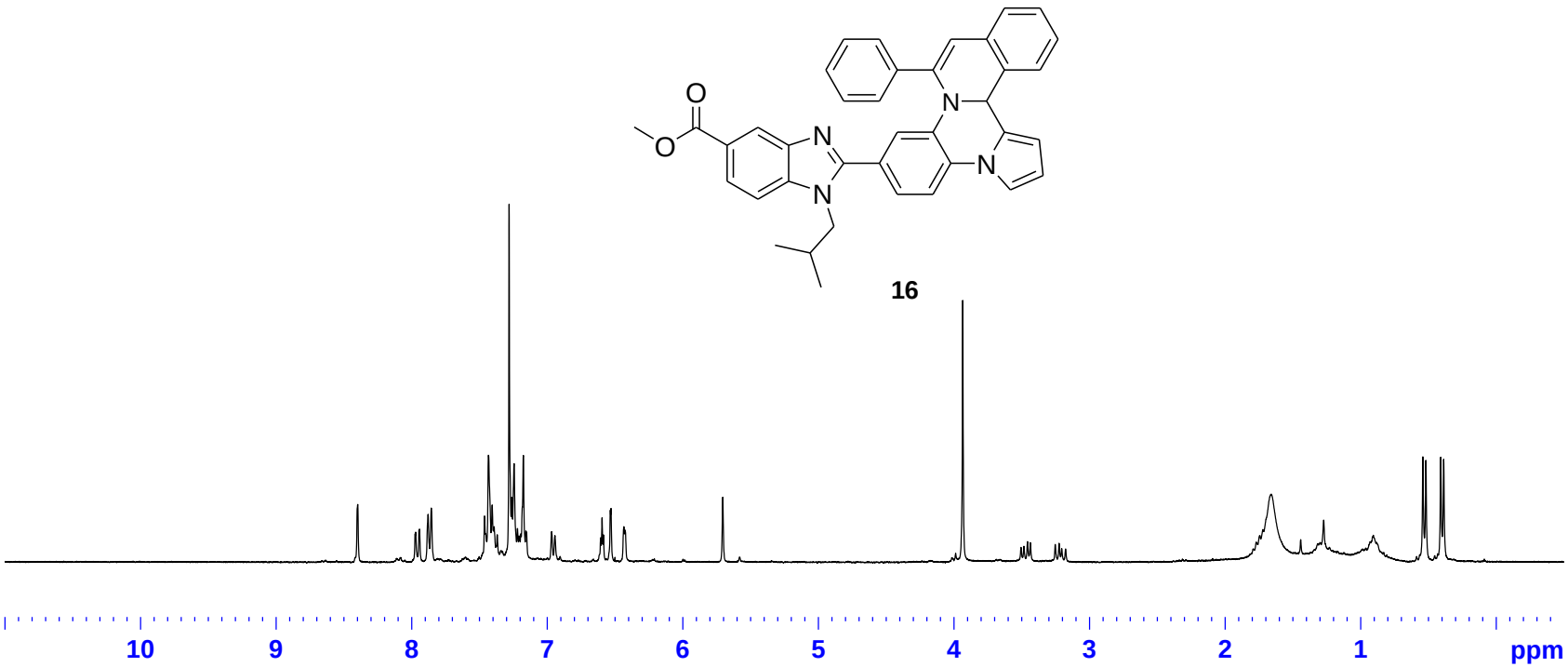
15

Chemical Formula: $C_{28}H_{30}N_4O_2$
Exact Mass: 454.2369
Molecular Weight: 454.5634

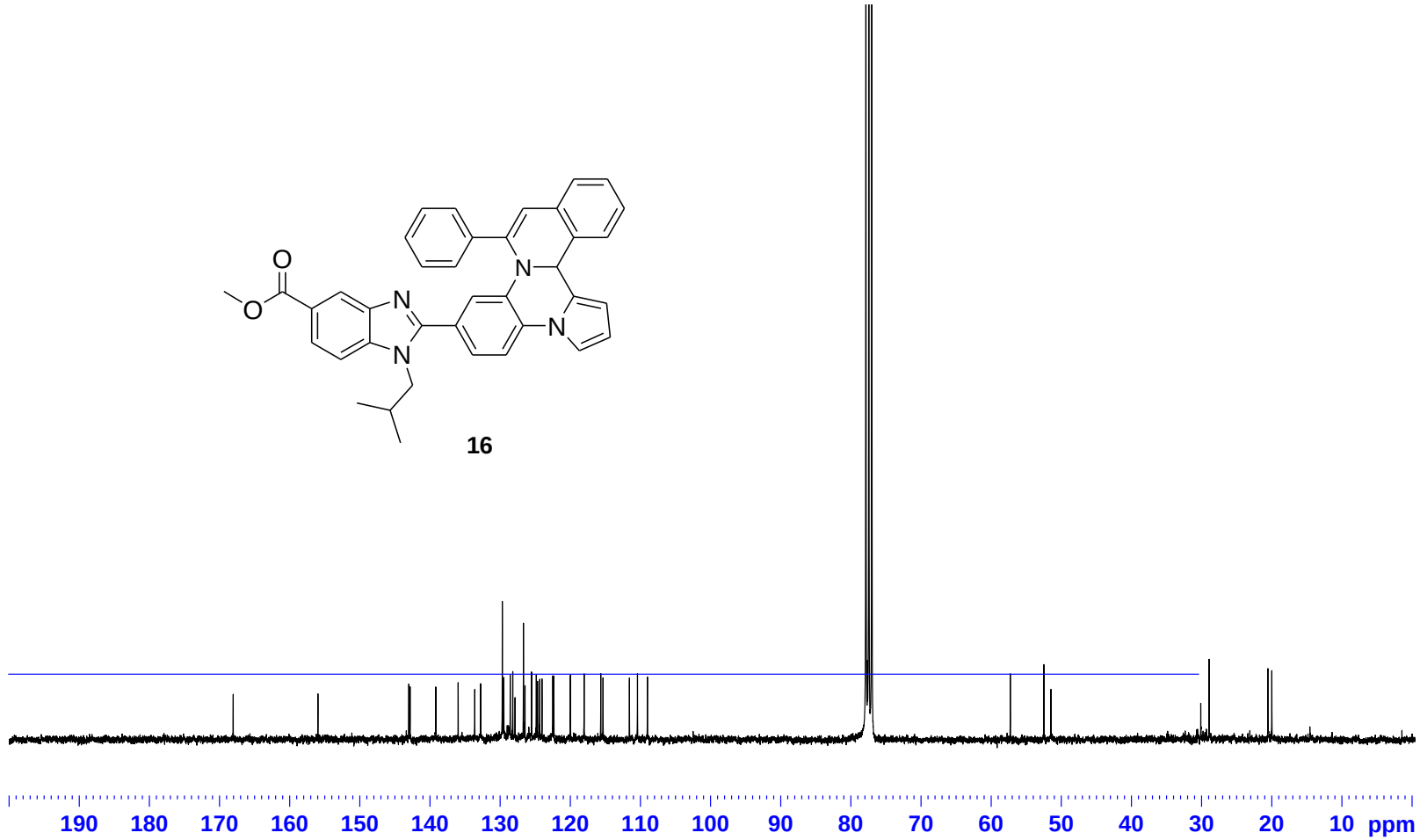
LR Mass Spectrum of Compound 15 in $CDCl_3$



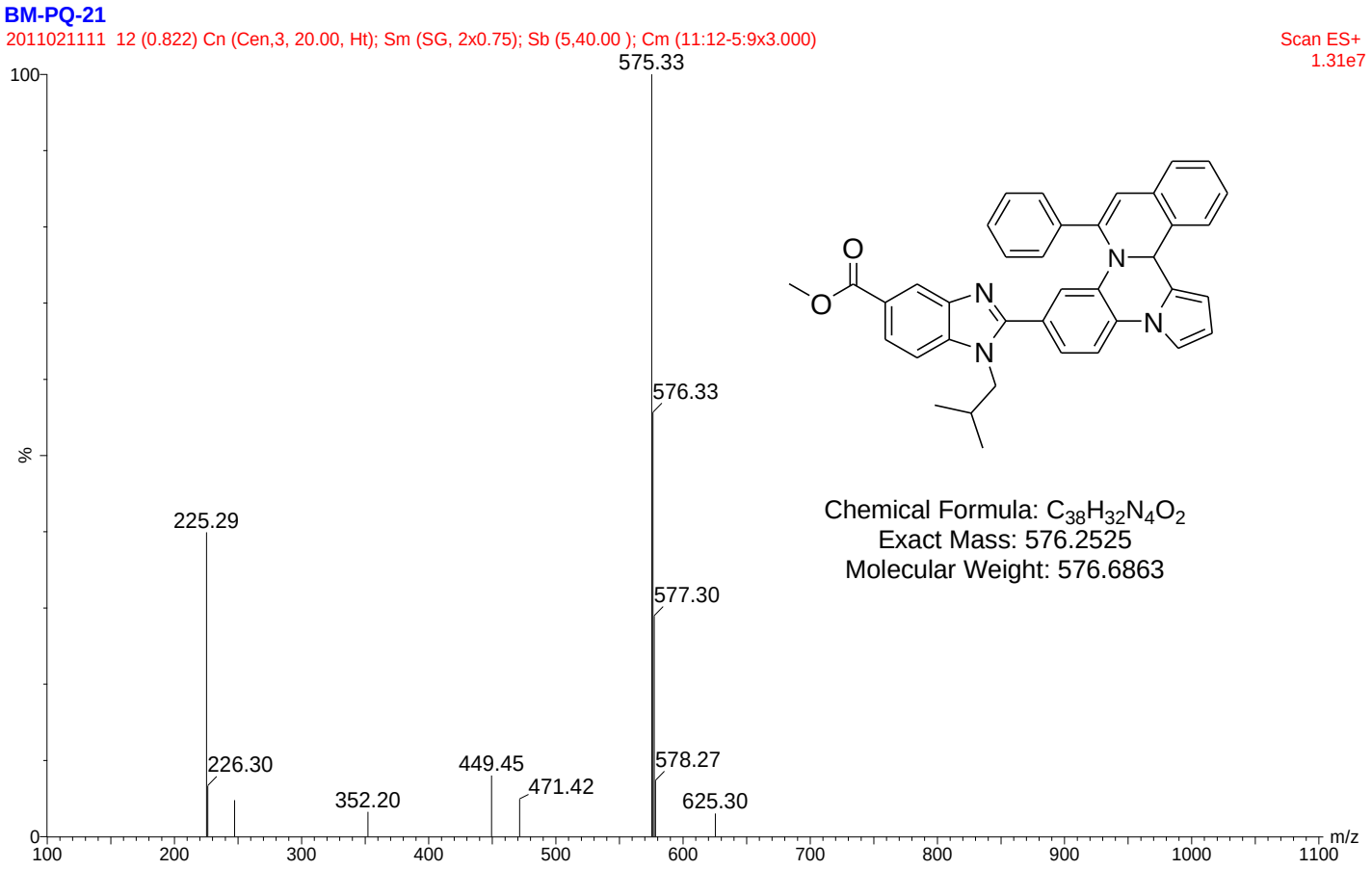
IR Spectrum of Compound 15



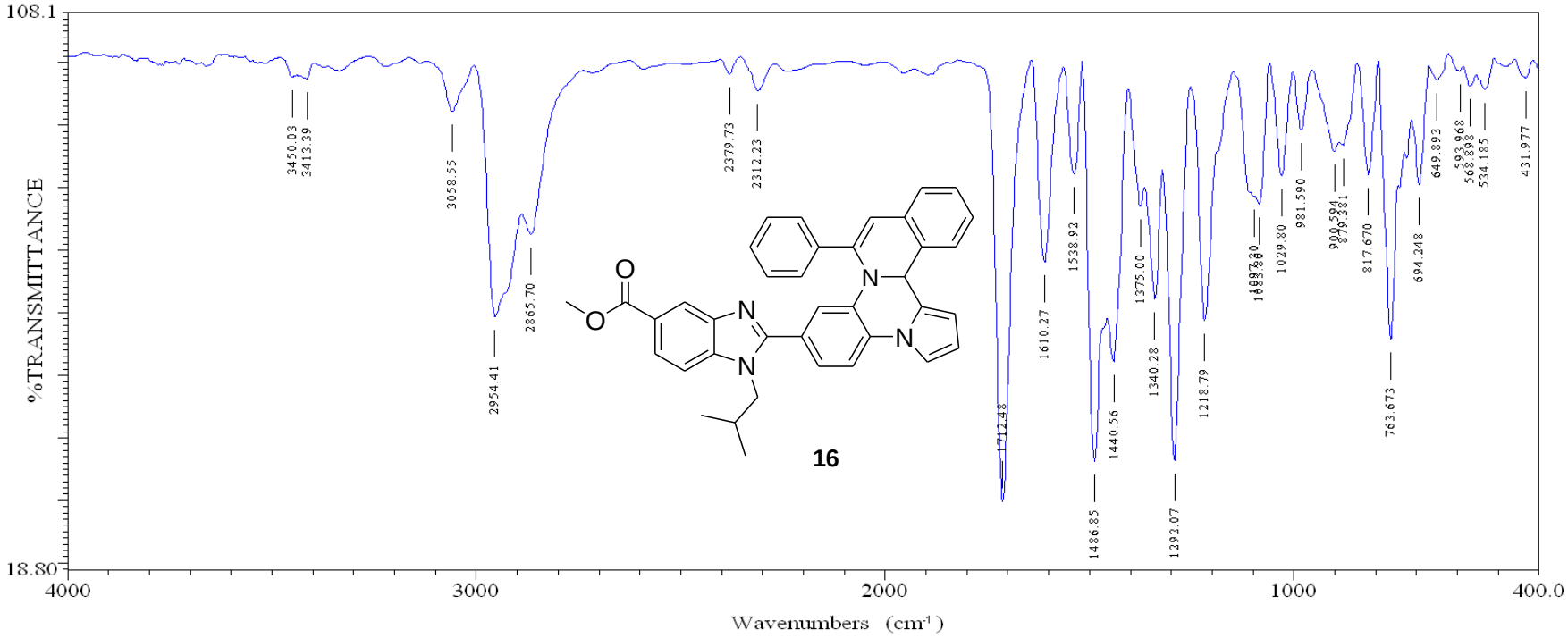
^{1}H NMR Spectrum of Compound 16 in $CDCl_3$



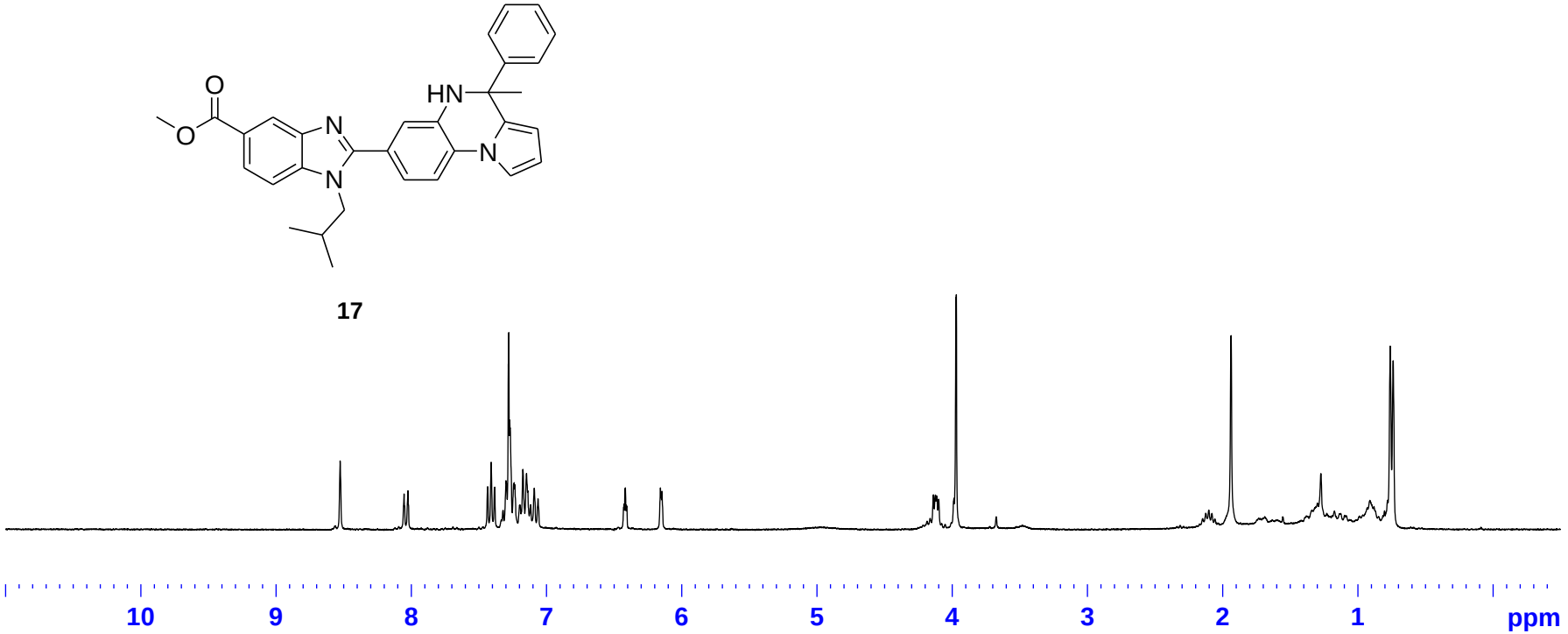
^{13}C NMR Spectrum of Compound 16 in $CDCl_3$



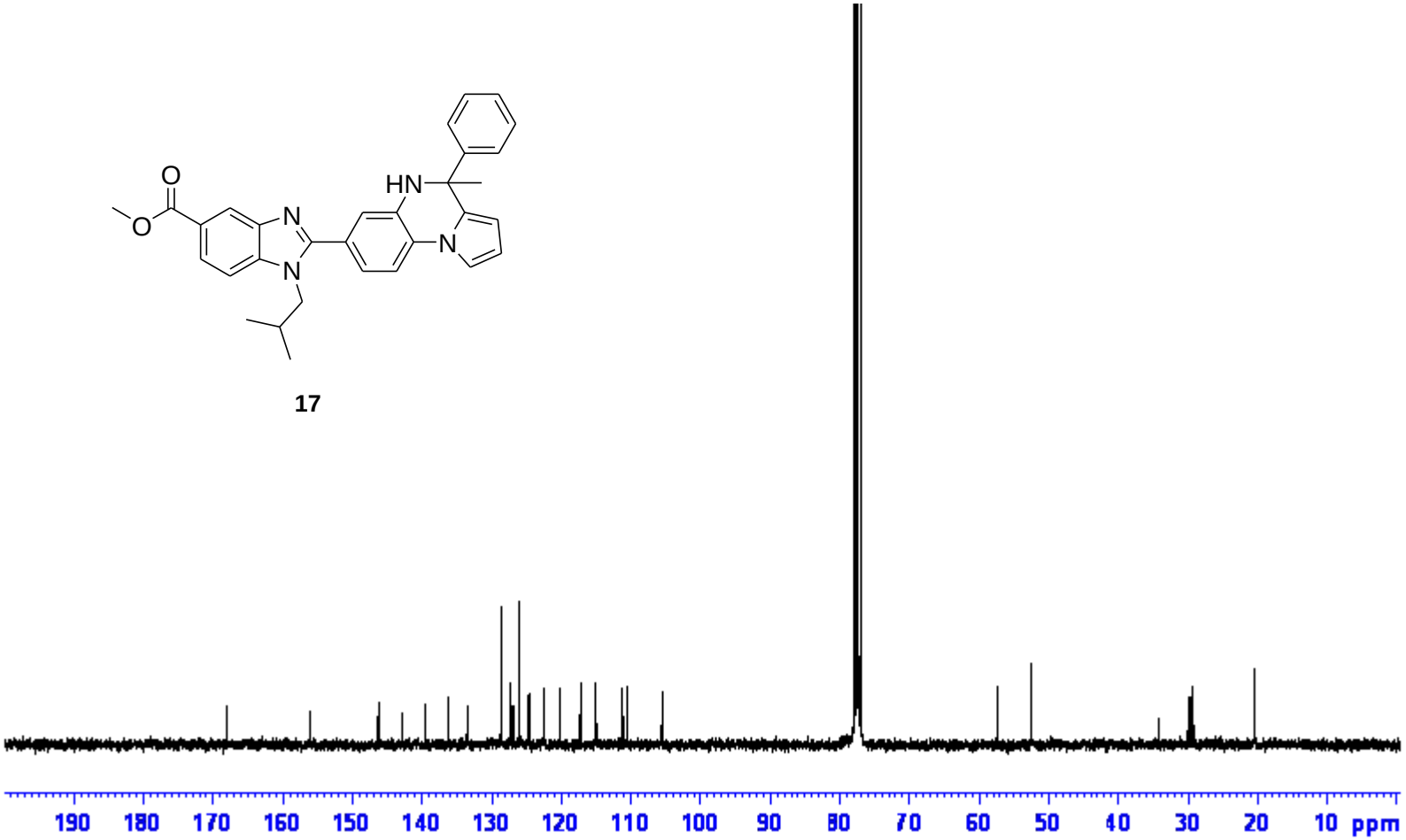
LR Mass Spectrum of Compound 16 in $CDCl_3$



IR Spectrum of Compound 16 in $CDCl_3$

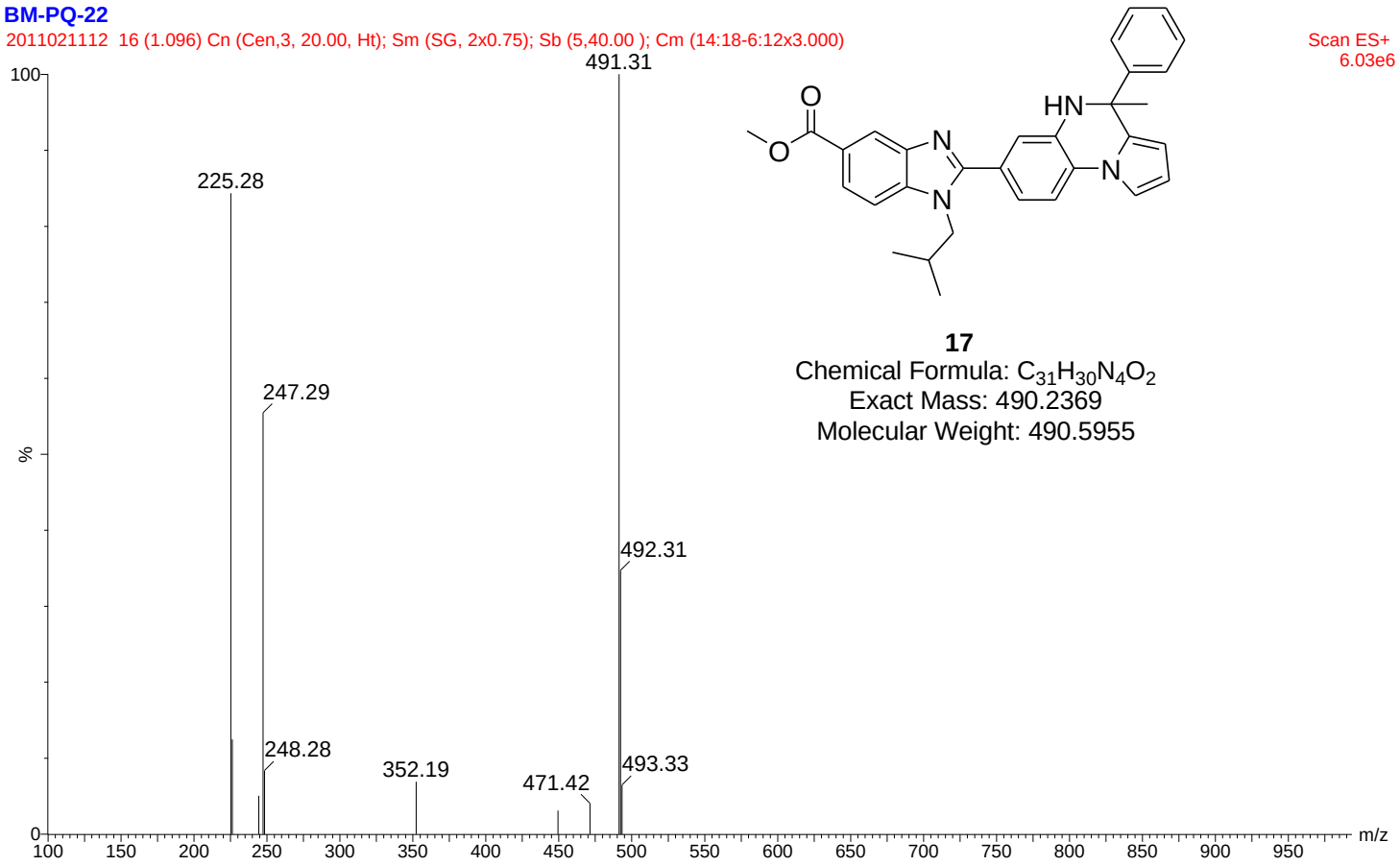


^{1}H NMR Spectrum of Compound 17 in $CDCl_3$

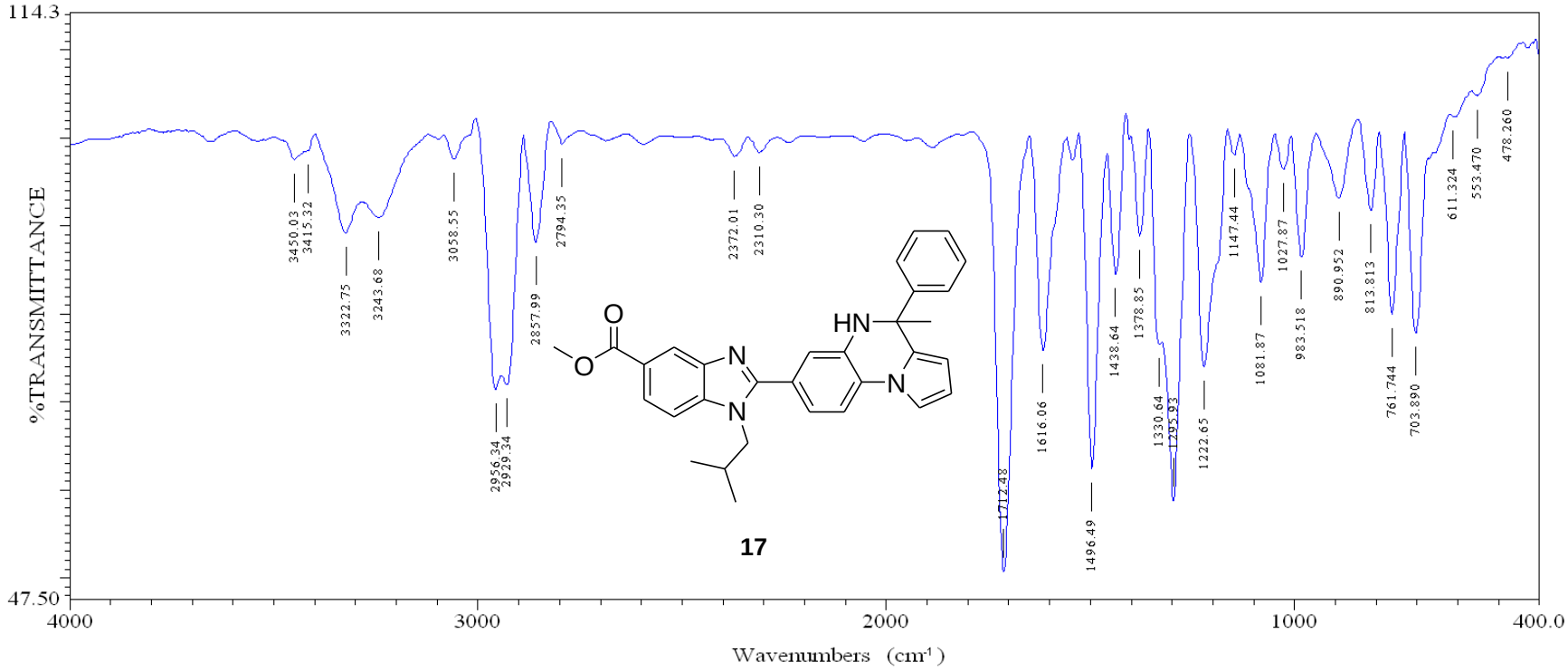


17

^{13}C NMR Spectrum of Compound 17 in $CDCl_3$



LR Mass Spectrum of Compound 17 in $CDCl_3$



IR Spectrum of Compound 17 in $CDCl_3$

General Procedure for the Preparation of Polymer Bound 1-isobutyl-2-(3-nitro-4-(1H-indole-1-yl)phenyl)-1H-benzo[d]imidazole-5-carboxyl ate 11. Indole (0.24 g, 2.14 mmol, 5 equiv) and Cs_2CO_3 (0.69 g, 2.14 mmol, 5 equiv) was added to the solution of **6a** (2.0 g, 0.43 mmol, 1 equiv) in dimethyl formamide (10 mL) in a 20 mL microwave vial. The vial was sealed and the reaction mixtures were irradiated in a microwave reactor at 135 ℃ for 10 minutes to obtain the polymer conjugate **11.** After being cooled to room temperature, the reaction mixtures were precipitated by slow addition of cold ether and precipitated pyrrole bound polymer conjugates **11** were filtered through fritted funnel. The crude product was washed in succession with ether (100 mL×3) to remove the undesired impurity and dried for next steps.

General Procedure for the Preparation of Polymer Bound 2-(3-amino-4-(1H-indole-1-yl)phenyl)-1-isobutyl -1H-benzo[d]imidazole-5-carboxylate 12. To a solution of **11** (2.00 g, 0.41 mmol) in methanol (10 ml), zinc dust (0.53 g, 8.20 mmol, 20.0 equiv) and ammonium formate (0.27 g, 4.10 mmol, and 10.0 equiv) were added in a 20 mL microwave vial. The vial was sealed and the reaction mixtures were irradiated in a microwave reactor at 60 ℃ for 10 minutes. After being cooled to ambient temperature, the reaction

mixtures were then subjected to centrifugation for removal of Zn and filtered through fritted funnel and the supernatant liquid was concentrated by rotary evaporation. Dichloromethane (10 mL) was then added to salt out ammonium formate. The reaction mixtures were filtered through fritted funnel again to remove ammonium formate to obtain the polymer bound 2-(3-amino-4-(1H-indole-1-yl)phenyl)-1-isobutyl-1H-benzo[d]imidazole-5-carboxylate **12.**

General Procedure for the Preparation of Polymer Bound 2-(4,4-dialkyl-4,5-dihydropyrrolo[1,2-a]quinoxalin-7-yl)-1-methyl-1H-benzo[d]imidazole-5-carboxylate 13. To a stirred solution of polymer bound 2-(3-amino-4-(1H-indole-1-yl)phenyl)-1-isobutyl-1H-benzo[d]imidazole-5-carboxylate conjugates **12** in $CHCl_3$ (10 mL), 4-methylcyclohexanone (1.05 mmol, 5.0 equiv), trifluoro acetic acid (TFA) 0.05 ml and $MgSO_4$ (20 mg) were added in 20 mL microwave vial. The vial was sealed and the reaction mixtures were irradiated in a microwave reactor at 85 ℃ for 12 minutes. After cooling to room tempaeratue, the crude product mixtures were purified by precipitation with cold ether (100 mL×3) and dried to obtain the conjugate **13** in high purity.

General Procedure for the Cleavage of Polymer Bound Substituted alkyl 2-(4,4-alkyl-4,5-dihydropyrrolo[1,2-a]quinoxalin-7-yl)-1-methyl-1H-benzo[d]imidazole-5-carboxylate 14. To a solution of conjugates **13** in methanol (20 mL), KCN (100 mg) was added and stirred for 24 hours at room temperature. After completion of the reaction, excess of cold ether (100 mL) was added, the polymer was filtered off and filtrate was subjected to evaporation. The residue was dried under vacuum, and and was purified by silica gel column and eluted with a mixture of ethyl acetate and hexane (1:4) to get the title compounds **14** as a pale yellow solid in 94 % yield.

General Procedure for the synthesis of methyl 2-(12b-methyl-1,2,3,12b-tetrahydrodipyrrolo[1,2-*a*:2,1-*c*]quinoxalin-6-yl)-1-isobutyl-1*H*-benzo[*d*]imidazole-5-carboxylate 15.

To a stirred solution of polymer bound 2-(3-amino-4-(1H-pyrrol-1-yl)phenyl)-1-isobutyl-1H-benzo[d]imidazole-5-carboxylate conjugates 8a (1.5 gm, 0.32 mm, 1.0 equiv) in MeOH (10 mL), pent-4-yn-1-ol (0.08 gm, 0.95 mmol, 3.0 equiv), $PtCl_4$ (5.3 mg, 5 mol-%) were added in 50 mL flask under argon atmosphere. The mixture was stirred at at 100 ^oC for 24 h. After completion of the reaction time, reaction mixture was filtered through celite pad. The crude product mixtures were purified by precipitation with cold ether (100 mL×3) and dried to obtain the polymer bound conjugate **15** in high purity. To a solution of

conjugates **15** in methanol (20 mL), KCN (100 mg) was added and stirred for 24 hours at room temperature. After completion of the reaction, excess of cold ether (100 mL) was added, the polymer was filtered off and filtrate was subjected to evaporation. The residue was dried under vacuum. The residue was purified by flash silica gel column chromatography as a white solid in 81 % yield.

General Procedure for the synthesis of methyl 1-isobutyl-2-(10-phenyl-15b*H*-isoquino[2,1-*a*]pyrrolo[2,1-*c*]quinoxalin-7-yl)-1*H*-benzimidazole-5-carboxylate 16.

To a stirred solution of polymer bound 2-(3-amino-4-(1H-pyrrol-1-yl)phenyl)-1-isobutyl-1H-benzo[d]imidazole-5-carboxylate conjugates 8a (1.5 gm, 0.32 mm, 1.0 equiv) in DCE (10 mL), 2-(phenylethynyl)benzaldehyde (0.19 gm, 0.95 mmol, 3.0 equiv), AuCl (3.6 mg, 5 mol-%) were added in 50 mL flask under nitrogen atmosphere. The mixture was stirred at room temperaturefor 12 h. After completion of the reaction time, reaction mixture was filtered through celite pad. The crude product mixtures were purified by precipitation with cold ether (100 mL×3) and dried to obtain the polymer bound conjugate **16** in high purity. To a solution of conjugates **15** in methanol (20 mL), KCN (100 mg) was added and stirred for 24 hours at room temperature. After completion of the reaction, excess of cold ether (100 mL) was added, the polymer was filtered off and filtrate was subjected to evaporation. The residue was dried under vacuum. The

residue was purified by flash silica gel column chromatography as a pale yellow solid in 79 % yield.

General Procedure for the synthesis of methyl 1-isobutyl-2-(4-methyl-4-phenyl-4,5-dihydropyrrolo[1,2-*a*]quinoxalin-7-yl)-1*H*-benzimidazole-5-carboxylate 17. To a stirred solution of polymer bound 2-(3-amino-4-(1H-pyrrol-1-yl)phenyl)-1-isobutyl-1H-benzo[d]imidazole-5-carboxylate conjugates 8a (1.5 gm, 0.32 mm, 1.0 equiv) in toluene (10 mL), phenyl acetylene (0.10 gm, 0.95 mmol, 3.0 equiv), AgOTf (8.1 mg, 10 mol-%) were added in 50 mL flask under nitrogen atmosphere. The mixture was heated with stirring for 24 h. After completion of the reaction time, reaction mixture was filtered through celite pad. The crude product mixtures were purified by precipitation with cold ether (100 mL×3) and dried to obtain the polymer bound conjugate **17** in high purity. To a solution of conjugates **15** in methanol (20 mL), KCN (100 mg) was added and stirred for 24 hours at room temperature. After completion of the reaction, excess of cold ether (100 mL) was added, the polymer was filtered off and filtrate was subjected to evaporation. The residue was dried under vacuum. The residue was purified by flash silica gel column chromatography as a white solid in 65 % yield.