

Supporting Information

Polymer supported synthesis of novel benzoxazole linked benzimidazoles under microwave conditions: *In vitro* evaluation of VEGFR-3 kinase inhibition activity

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Contents

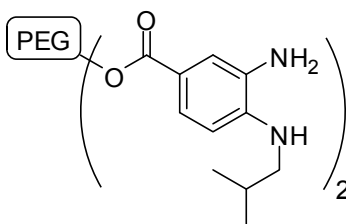
General Methods	S3
Spectral Data for polymer supported intermediates 9a-14a	S4-S6
Copies of ^1H NMR and ^{13}C NMR of Compounds 15a- 15p	S7-S38
Copies of HPLC Spectra of Compounds 15a- 15p	S39-S54
Copies of LR and HR Mass Spectra of Compound.15a- 15p	S55-S86
Copies of IR Spectra of Compounds 15a- 15p	S87-S102
^1H , ^{13}C and Mass Data of Intermediate 'a'	S103
Copies of ^1H NMR and ^{13}C NMR of Intermediate 'a'	S104-105
Elemental Analysis of Compound 15n	S106-S107
X-Ray Crystallographic data of Compound 15n	S108-S119
^{19}F NMR Spectra of Compound 15d and 15e	S120-S121
Copies of ^1H NMR spectrum of Intermediates 9a-14a	S122-S126
Copies of ^1H NMR spectrum of Intermediates 9f-14f	S127-S131
Copies of ^1H NMR spectrum of Intermediates 9n-14n	S132-S136
Microwave data (Time vs. pressure, temperature, power graphs) for synthesis of compound 11a-14a	S137-S140

General Methods

Dichloromethane 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. All the microwave experiments were conducted in Biotage initiator under optimized reaction condition of power and pressure. Flash chromatography was performed using the indicated solvent and silica gel 60 (Merck, 230-400 mesh). ^1H NMR (300 MHz) and ^{13}C NMR (75 MHz) spectra were recorded on a Bruker DX-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. PEG was purchased from SHOWA.

Spectral data of polymer supported intermediates:

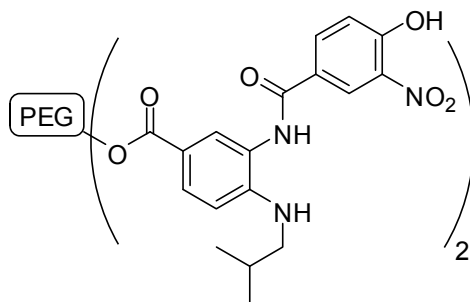
Polymer bound 3-amino-(4-isobutylamino) benzene carboxylates 9a.



^1H NMR (300 MHz, CDCl_3) δ 7.58 (d, $J = 8.5$ Hz, 1H), 7.42 (s, 1H), 6.55 (d, $J = 8.5$ Hz, 1H), 4.40 (t, $J = 6.5$ Hz, 2H), 3.89-3.40 (m, PEG), 2.98 (d, $J = 6.2$ Hz, 2H), 1.94 (sext, $J = 6.2$ Hz, 1H), 1.01 (d, $J = 6.2$ Hz, 6H).

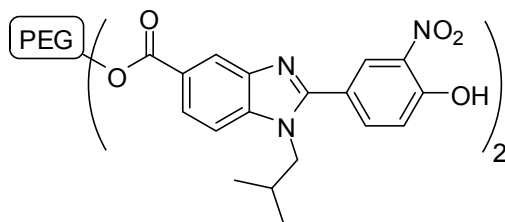
Polymer bound 3-(4-Hydroxy-3-nitrobenzamido)-4-(isobutylamino) carboxylates

11a.



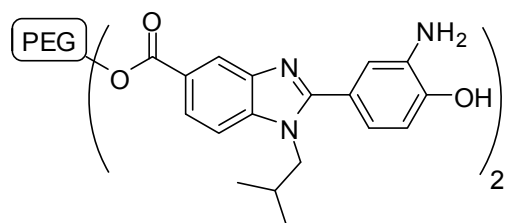
^1H NMR (300 MHz, CDCl_3) δ 9.18 (s, NH), 8.79 (s, 1H), 8.22 (d, $J = 8.4$ Hz, 1H), 7.79-7.70 (m, 2H), 7.10 (d, $J = 8.4$ Hz, 1H), 6.56 (d, $J = 8.7$ Hz, 1H), 5.11 (s, NH), 4.26 (t, $J = 6.9$ Hz, 2H), 3.87-3.20 (m, PEG), 1.81 (sext, $J = 6.5$ Hz, 1H), 1.01 (d, $J = 6.5$ Hz, 6H).

2-(4-Hydroxy-3-nitrophenyl)-1-isobutyl-1H-benzo[d]imidazole carboxylates 12a.



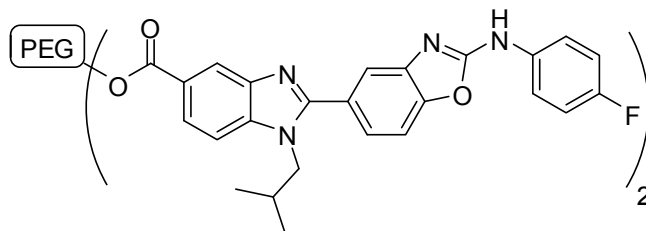
^1H NMR (300 MHz, CDCl_3) δ 8.38 (s, 1H), 8.35 (m, 1H), 7.94 (d, $J = 8.7$ Hz, 1H), 7.86 (d, $J = 8.6$ Hz, 1H), 7.37 (d, $J = 8.7$ Hz, 1H), 7.23 (d, $J = 8.6$ Hz, 1H), 4.36 (d, $J = 6.2$ Hz, 2H), 4.01 (d, $J = 6.6$ Hz, 2H), 3.74-3.25 (m, PEG), 1.99 (m, 1H), 0.69 (d, $J = 6.6$ Hz, 6H).

Polymer bound 2-(3-Amino-4-hydroxyphenyl)-1-isobutyl-1H-benzo[d]imidazole carboxylates 13a.

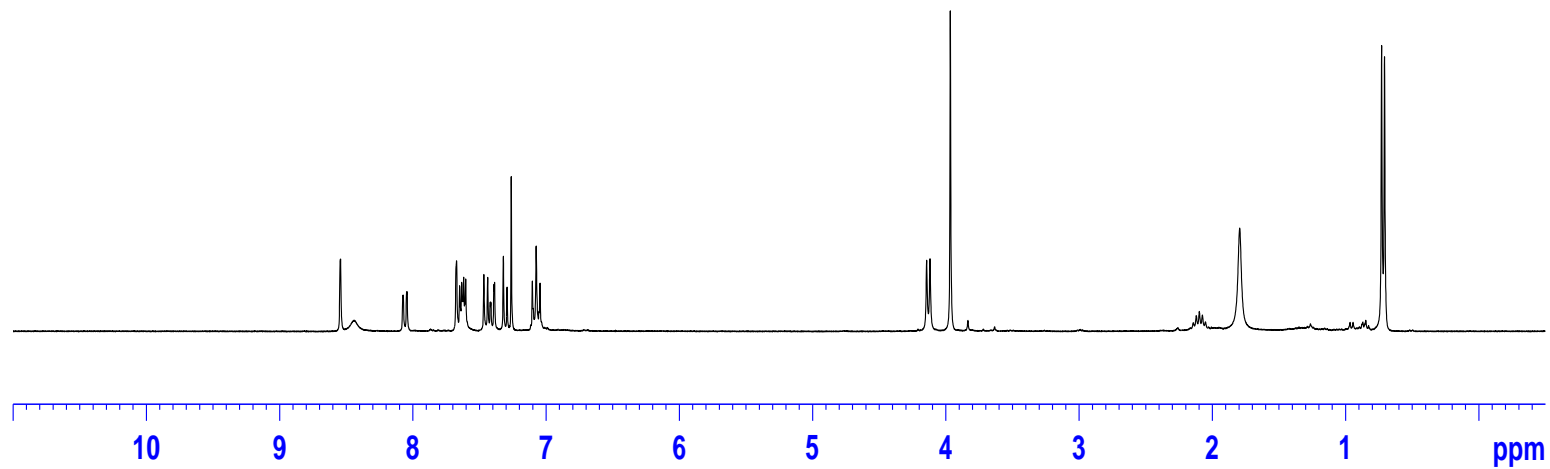
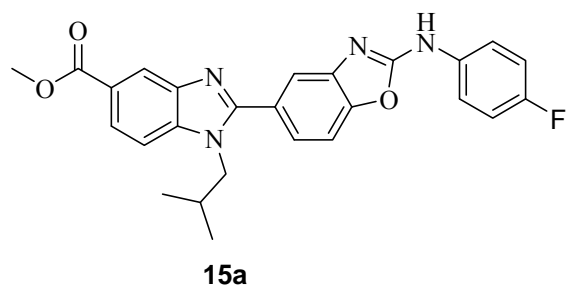


^1H NMR (300 MHz, CDCl_3) δ 8.40 (s, 1H), 7.96 (d, $J = 8.5$ Hz, 1H), 7.39 (d, $J = 8.4$ Hz, 1H), 6.97 (s, 1H), 6.92 (d, $J = 8.5$ Hz, 1H), 6.80 (m, 1H), 4.47-4.37 (m, 2H), 4.08 (d, $J = 6.2$ Hz, 2H), 3.99-3.39 (m, PEG), 2.01 (m, 1H), 0.70 (d, $J = 6.5$ Hz, 6H).

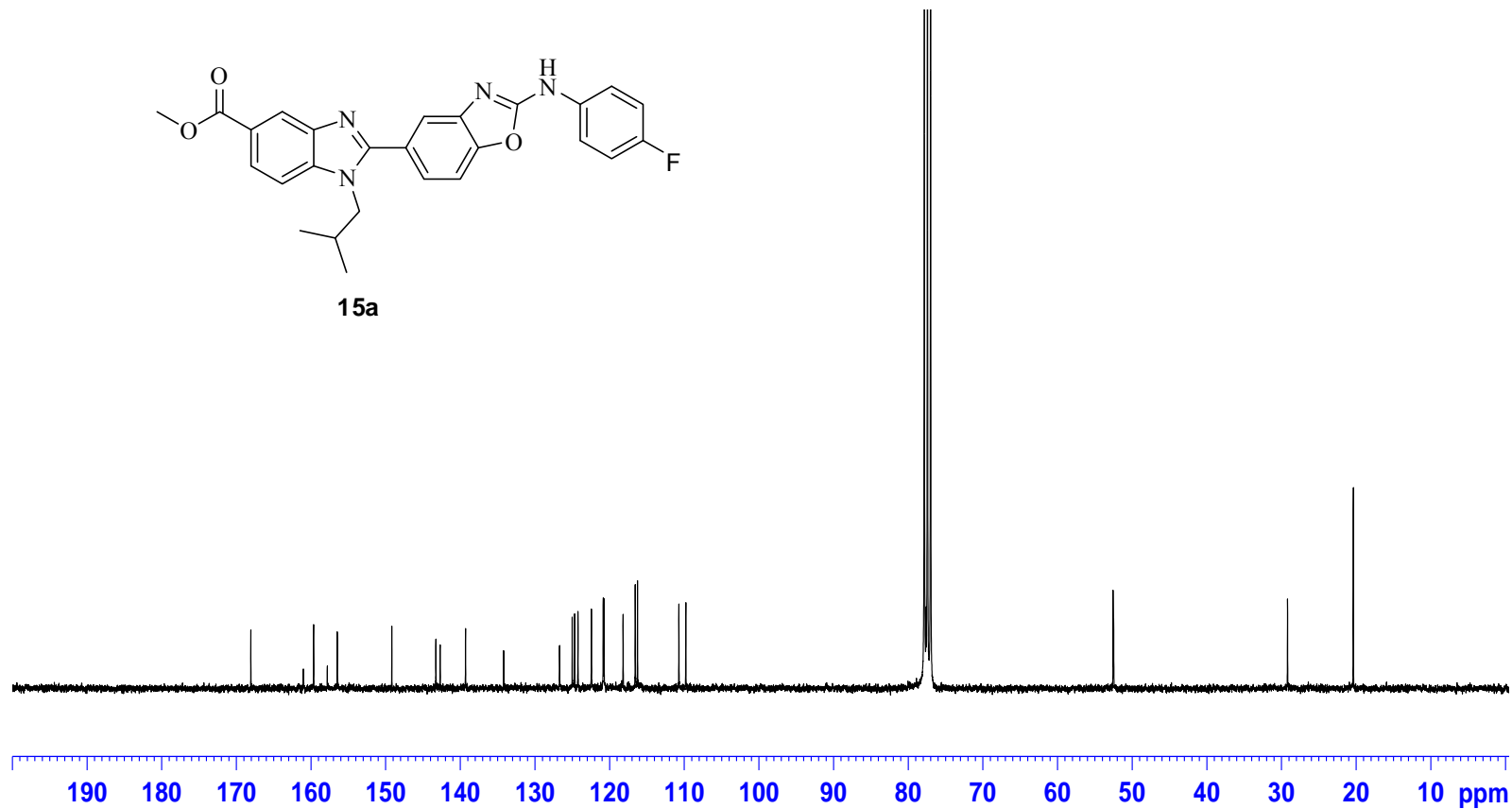
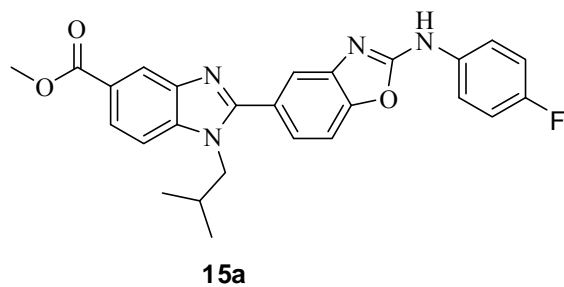
Polymer bound 1-Isobutyl-2-(2-(phenylamino)benzo[d]oxazol-5-yl)-1H-benzo[d]imidazole-carboxylate 14a.



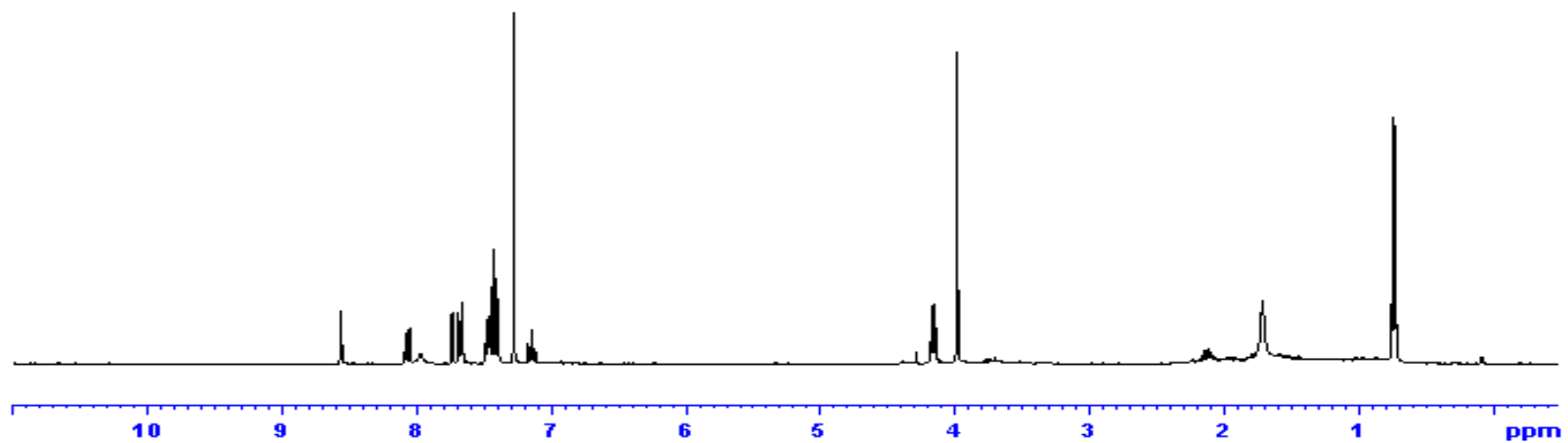
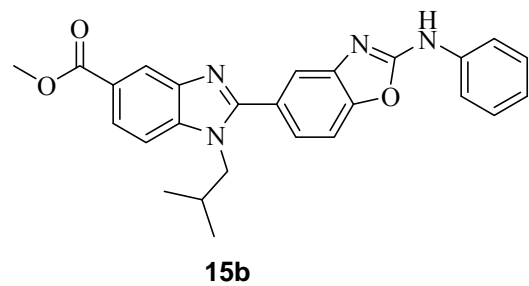
^1H NMR (300 MHz, CDCl_3) δ 8.75 (s, NH), 8.50 (d, $J = 1.5$ Hz, 1H), 8.08-7.99 (m, 2H), 7.72-7.60 (m, 2H), 7.55 (d, $J = 8.3$ Hz, 1H), 7.43-7.42 (m, 4H), 7.05 (t, $J = 7.4$ Hz, 1H), 4.54-4.50 (m, 2H), 4.12 (d, $J = 6.2$ Hz, 2H), 3.91-3.36 (m, PEG), 2.19 (m, 1H), 0.77 (d, $J = 6.5$ Hz, 6H).



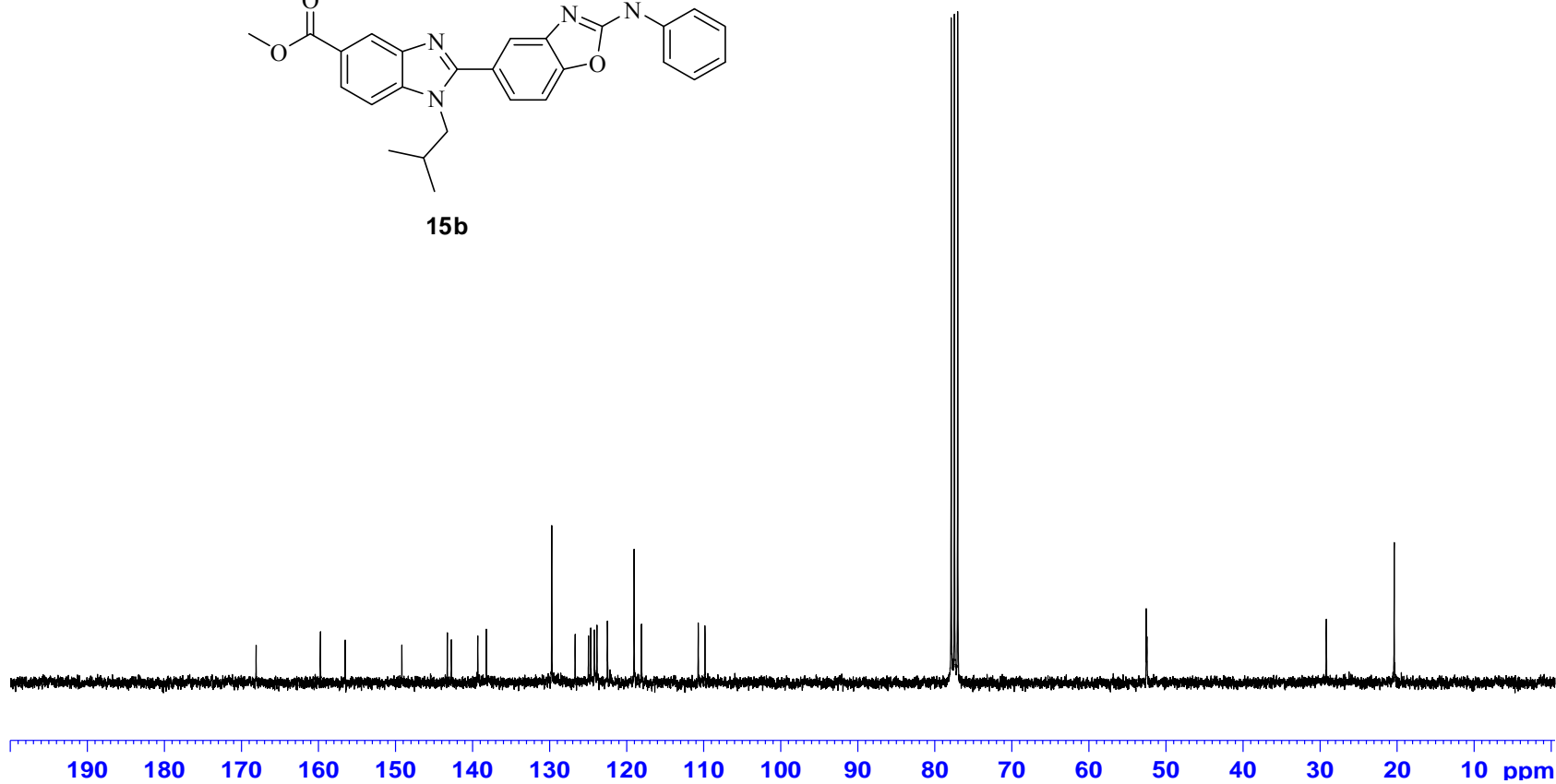
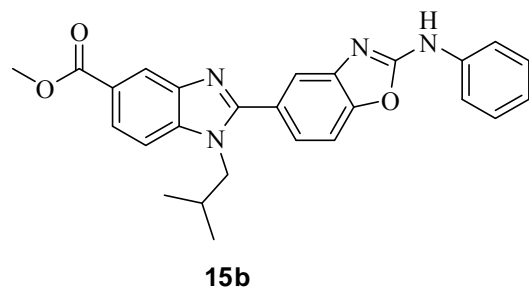
^1H NMR spectrum (300 MHz) of compound 15a in CDCl_3



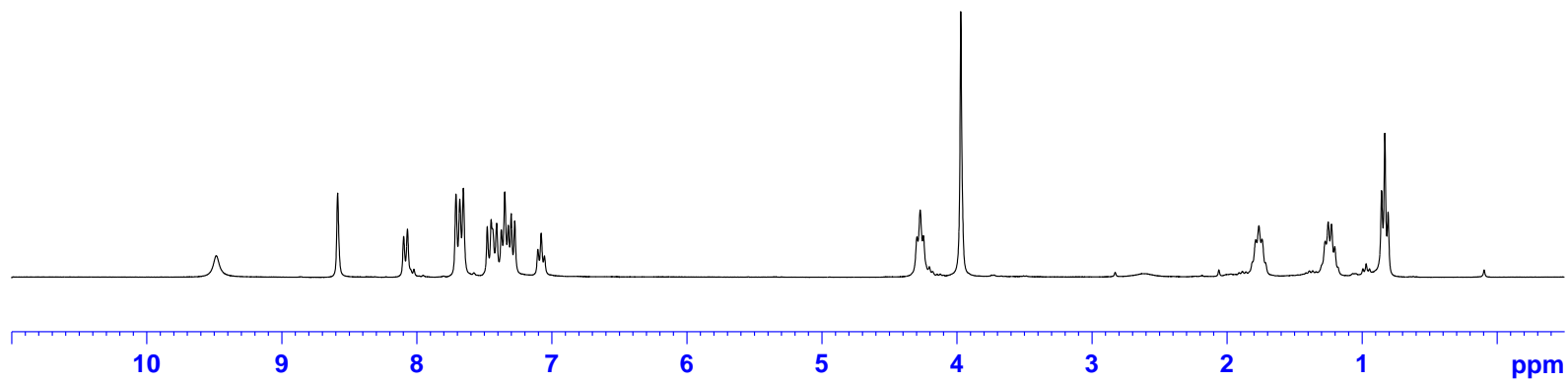
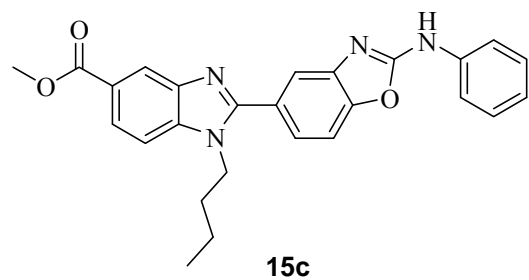
^{13}C NMR spectrum (75 MHz) of compound 15a in CDCl_3



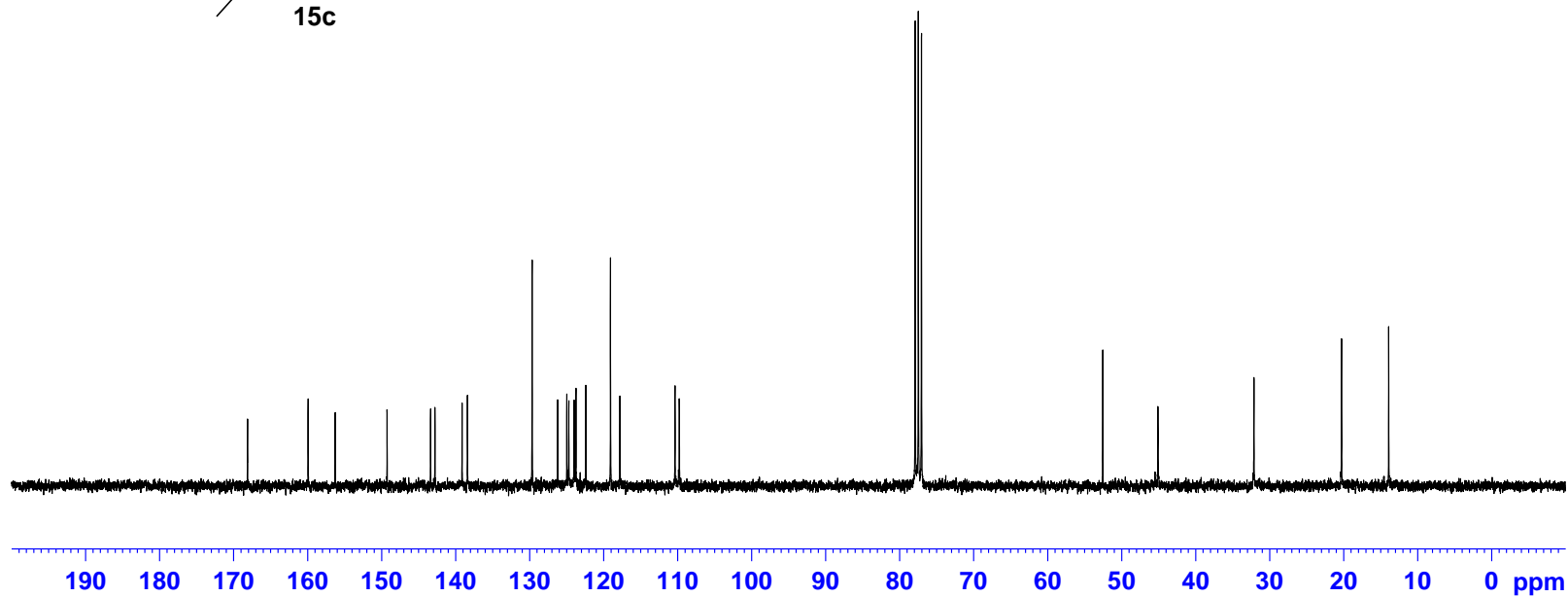
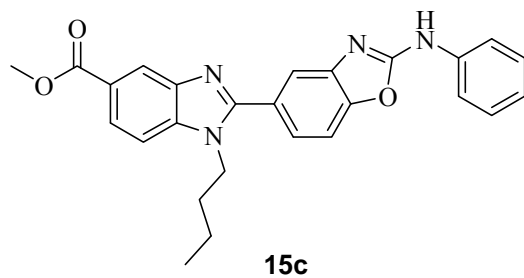
¹H NMR spectrum (300 MHz) of compound 15b in CDCl₃



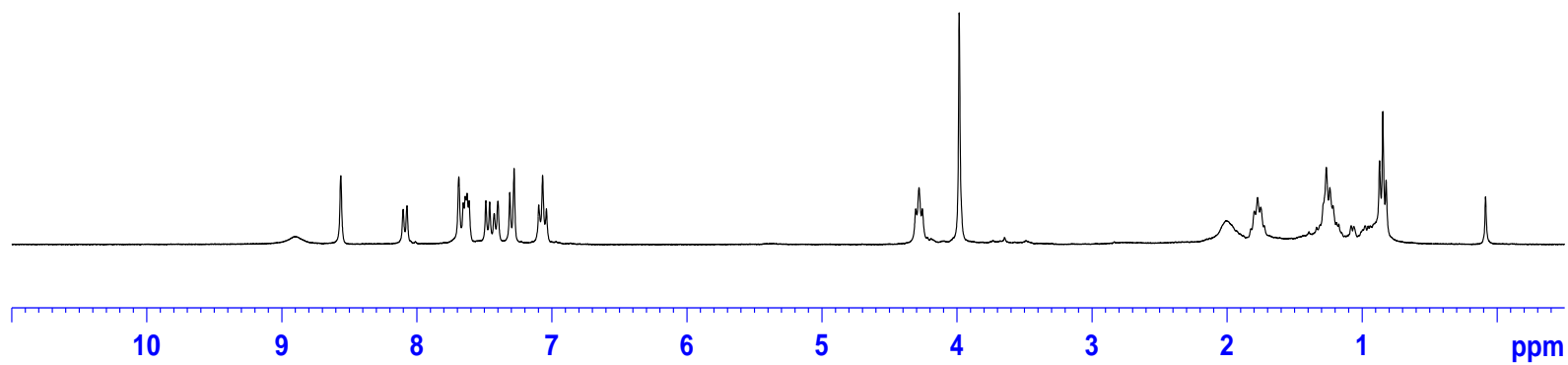
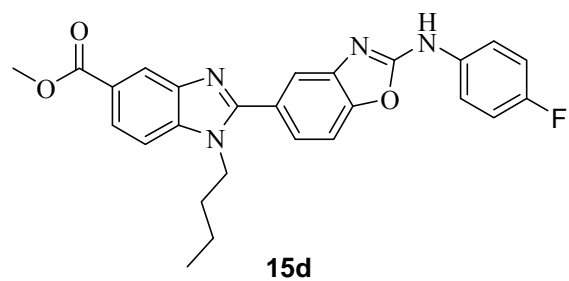
¹³C NMR spectrum (75 MHz) of compound 15b in CDCl₃



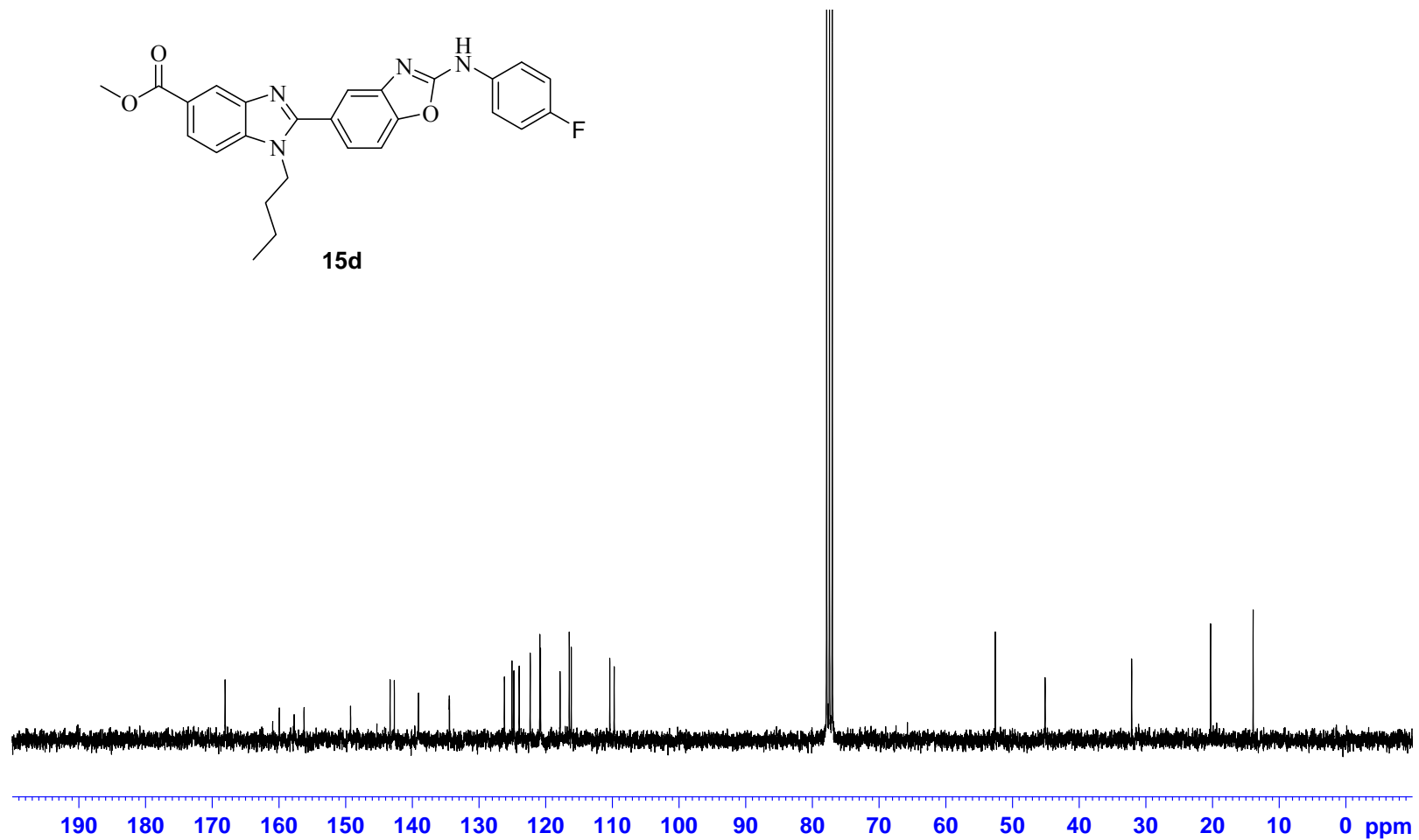
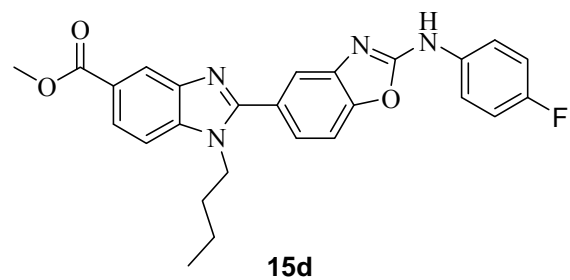
¹H NMR spectrum (300 MHz) of compound 15c in CDCl₃



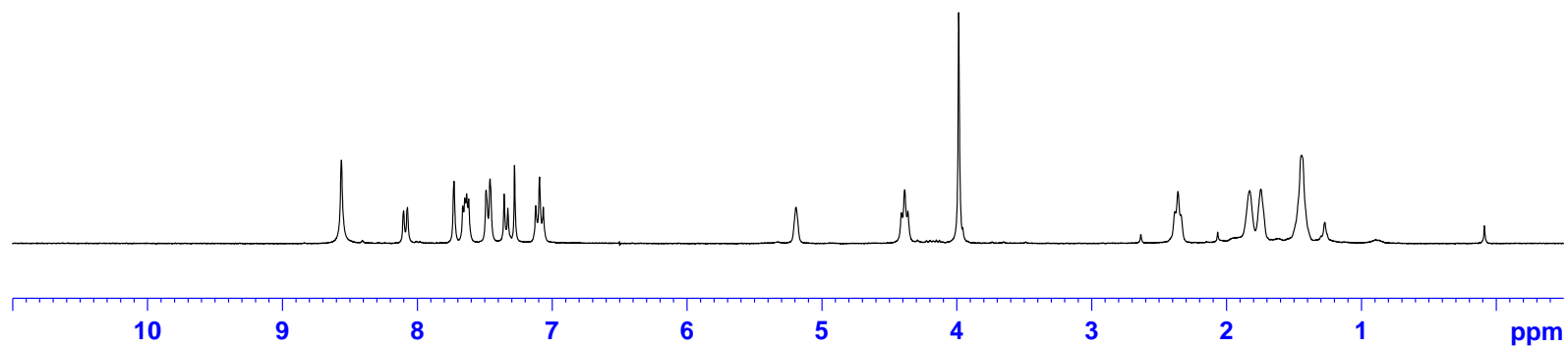
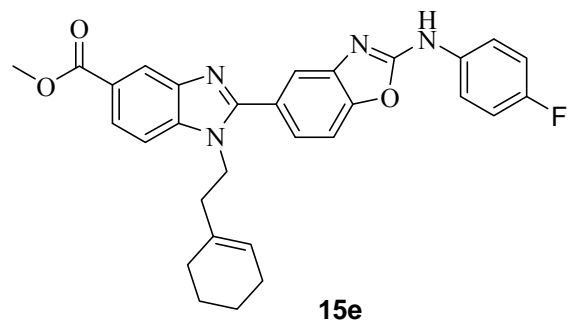
¹³C NMR spectrum (75 MHz) of compound 15c in CDCl₃



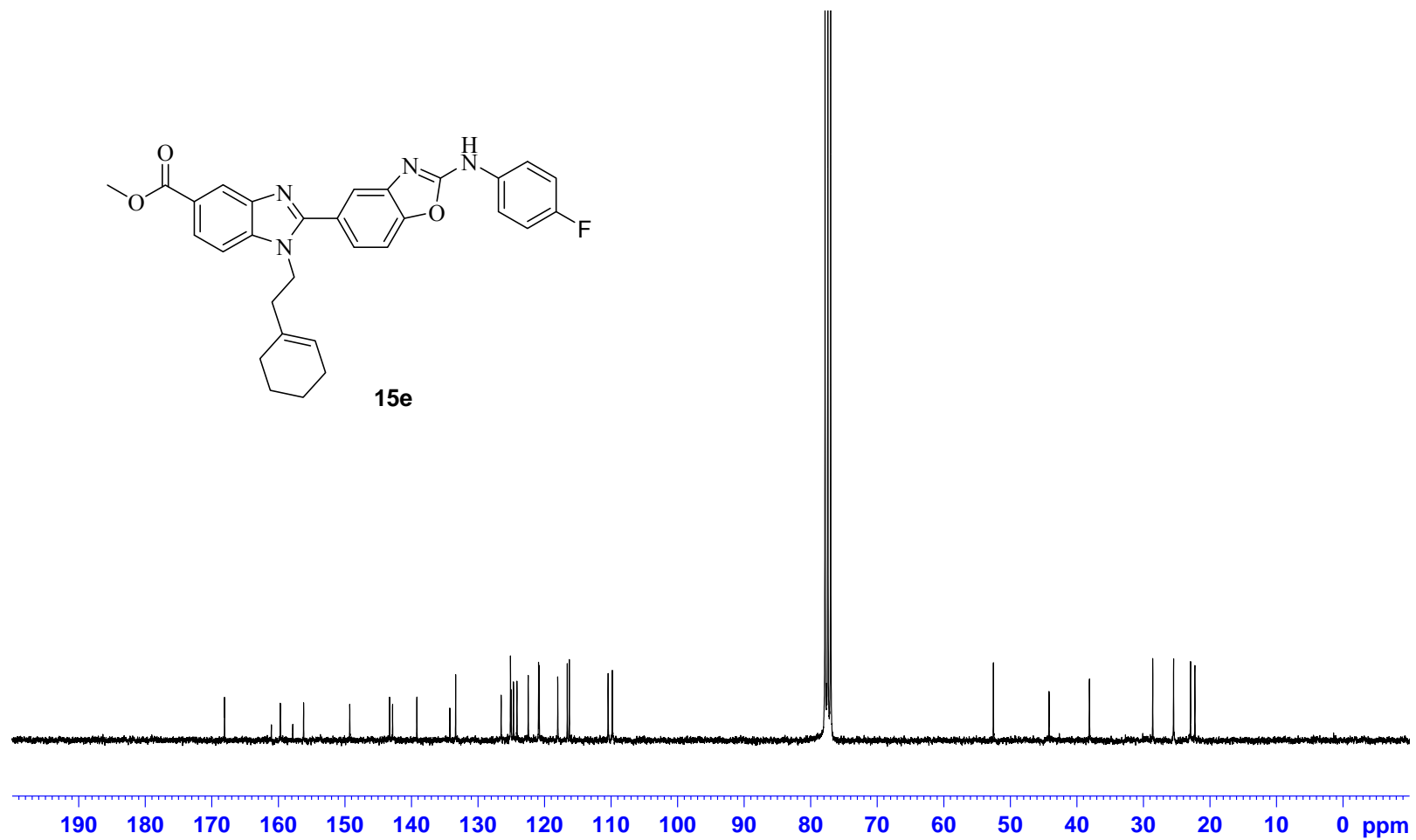
^1H NMR spectrum (300 MHz) of compound 15d in CDCl_3



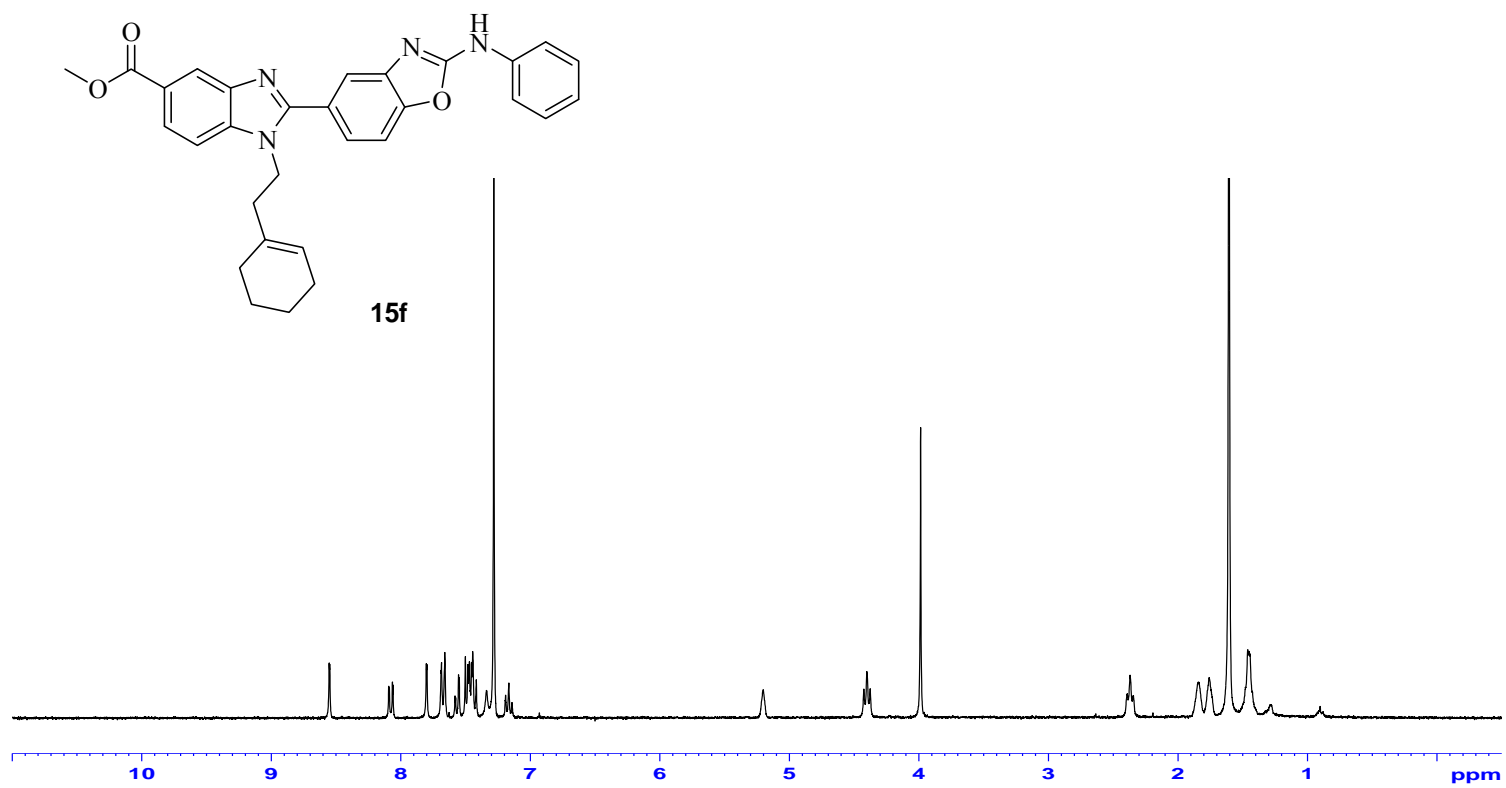
¹³C NMR spectrum (75 MHz) of compound 15d in CDCl₃



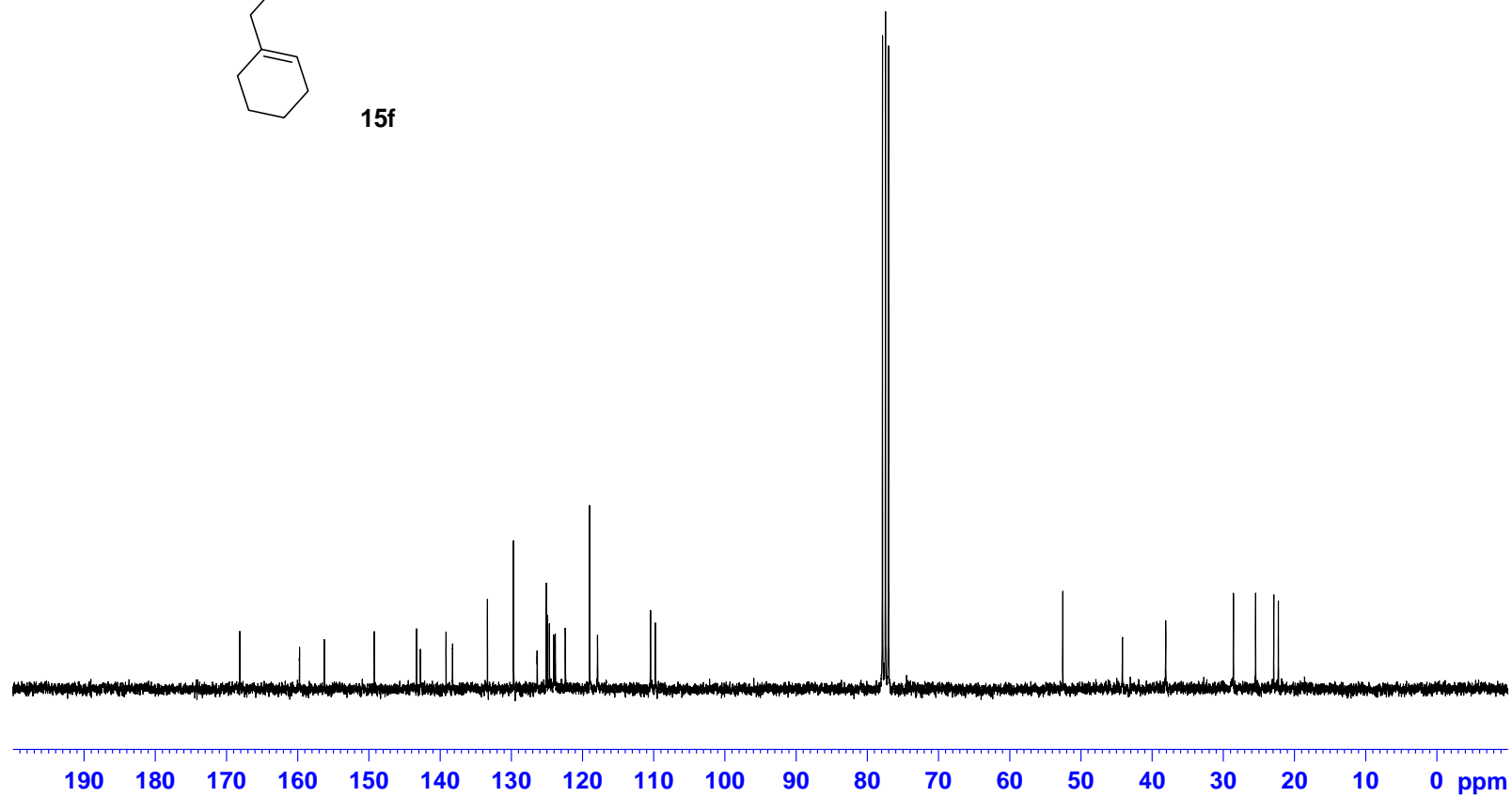
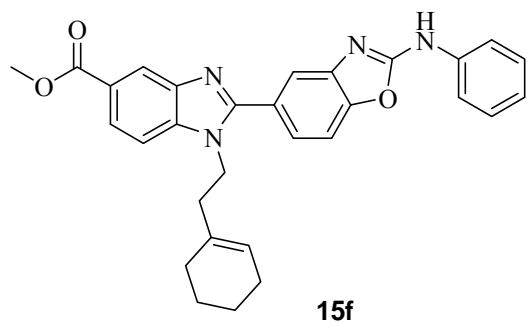
¹H NMR spectrum (300 MHz) of compound 15e in CDCl₃



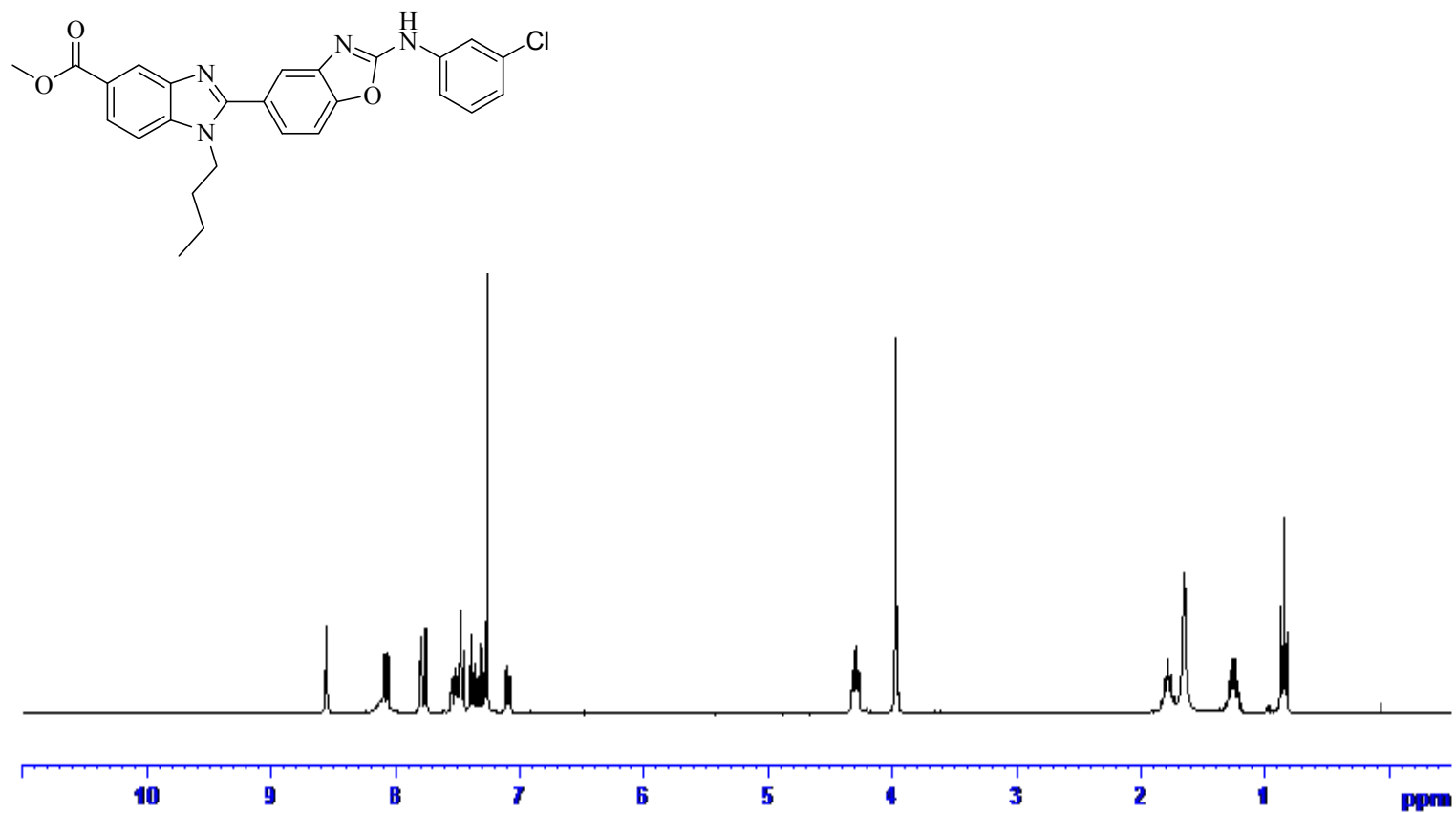
¹³C NMR spectrum (75 MHz) of compound 15e in CDCl₃



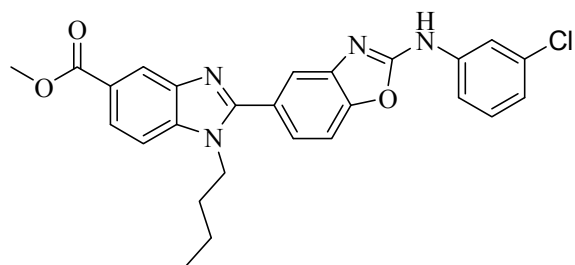
¹H NMR spectrum (300 MHz) of compound 15f in CDCl₃



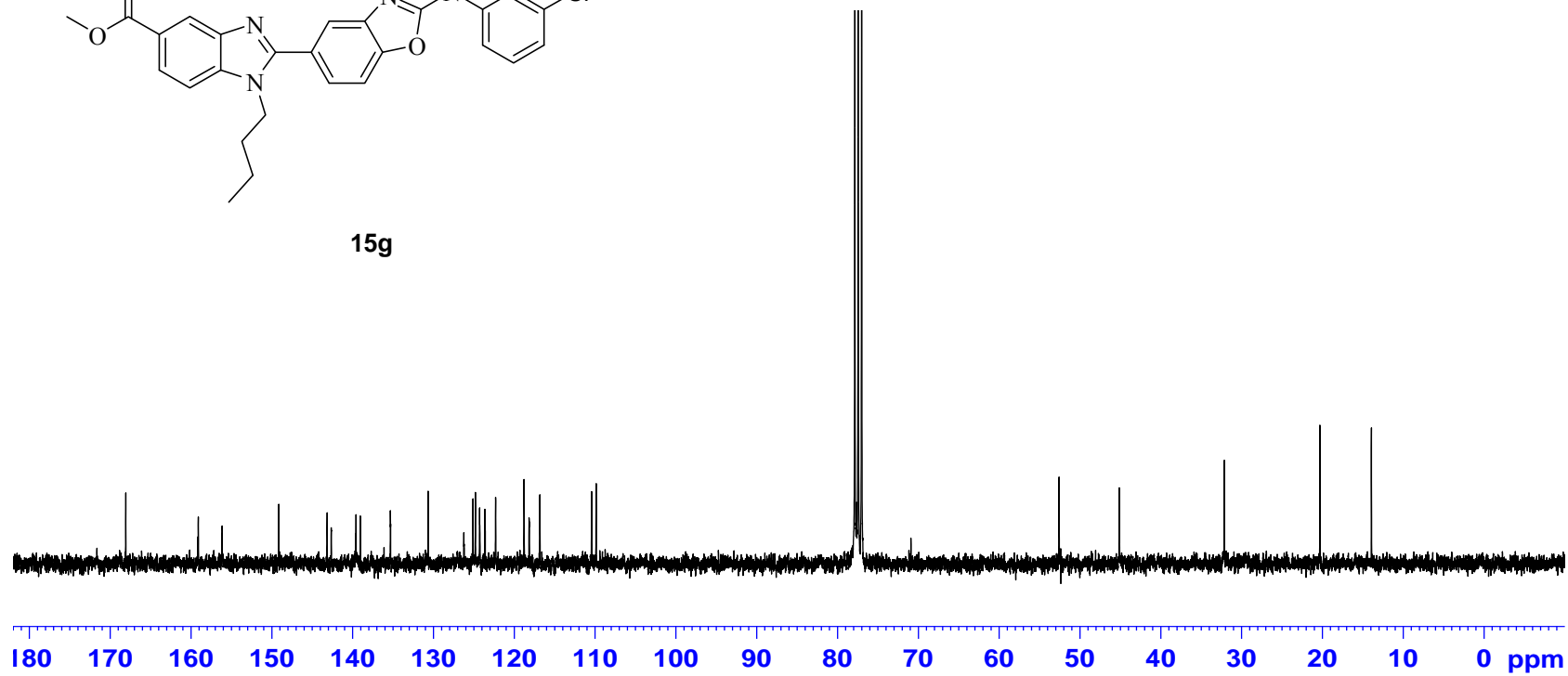
^{13}C NMR spectrum (75 MHz) of compound 15f in CDCl_3



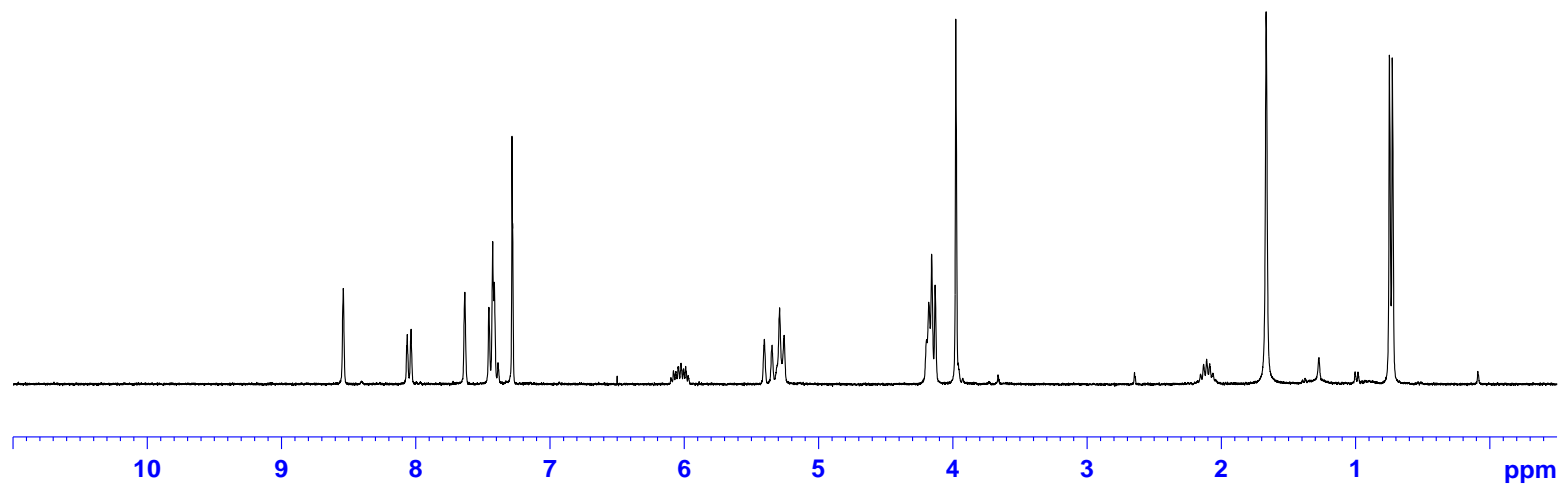
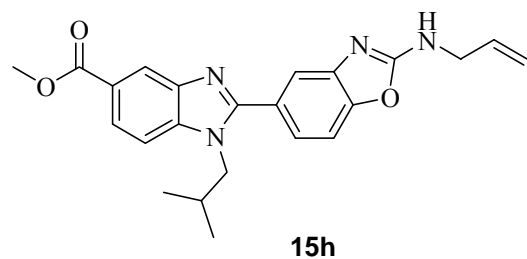
¹H NMR spectrum (300 MHz) of compound 15g in CDCl₃



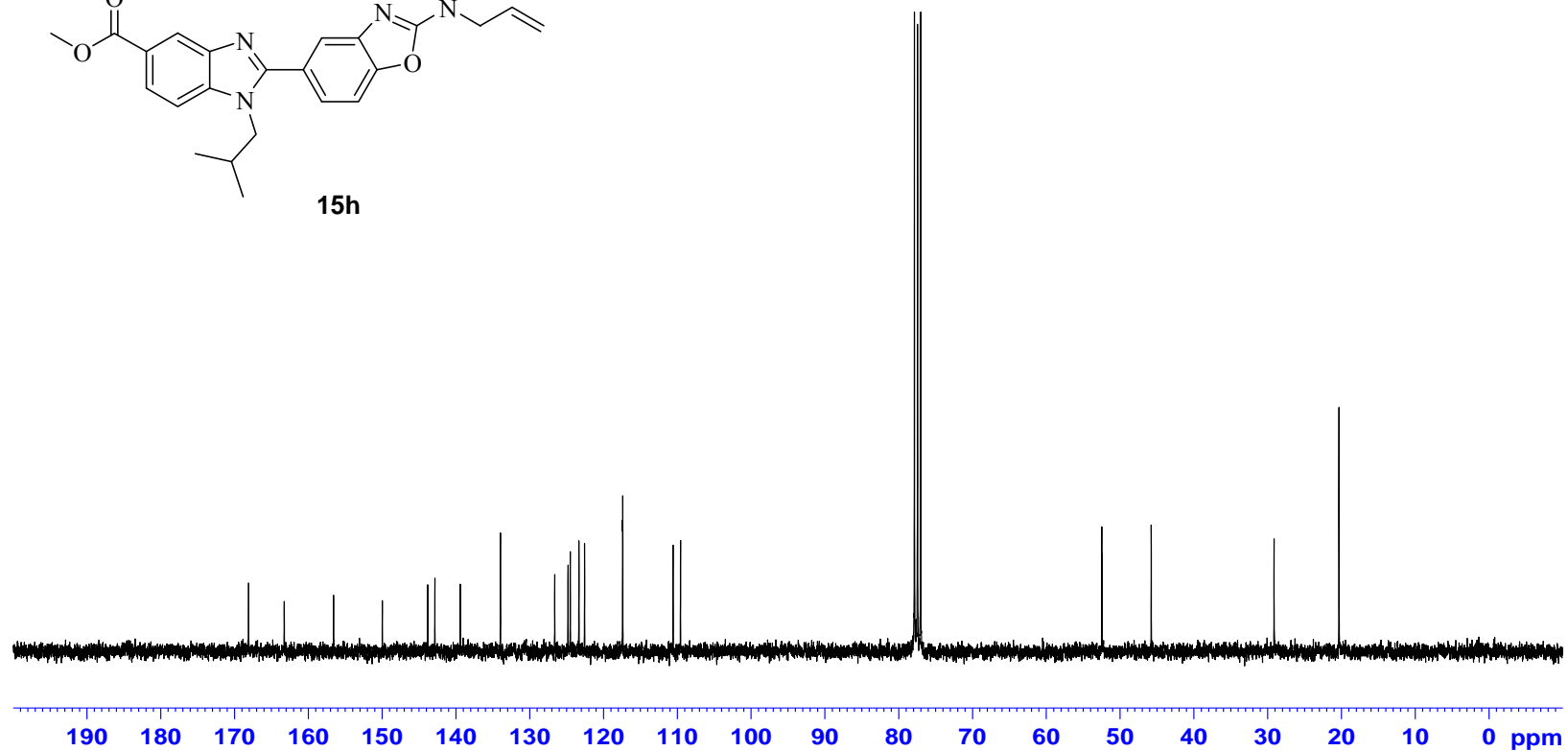
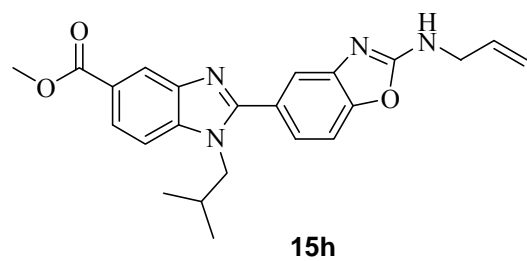
15g



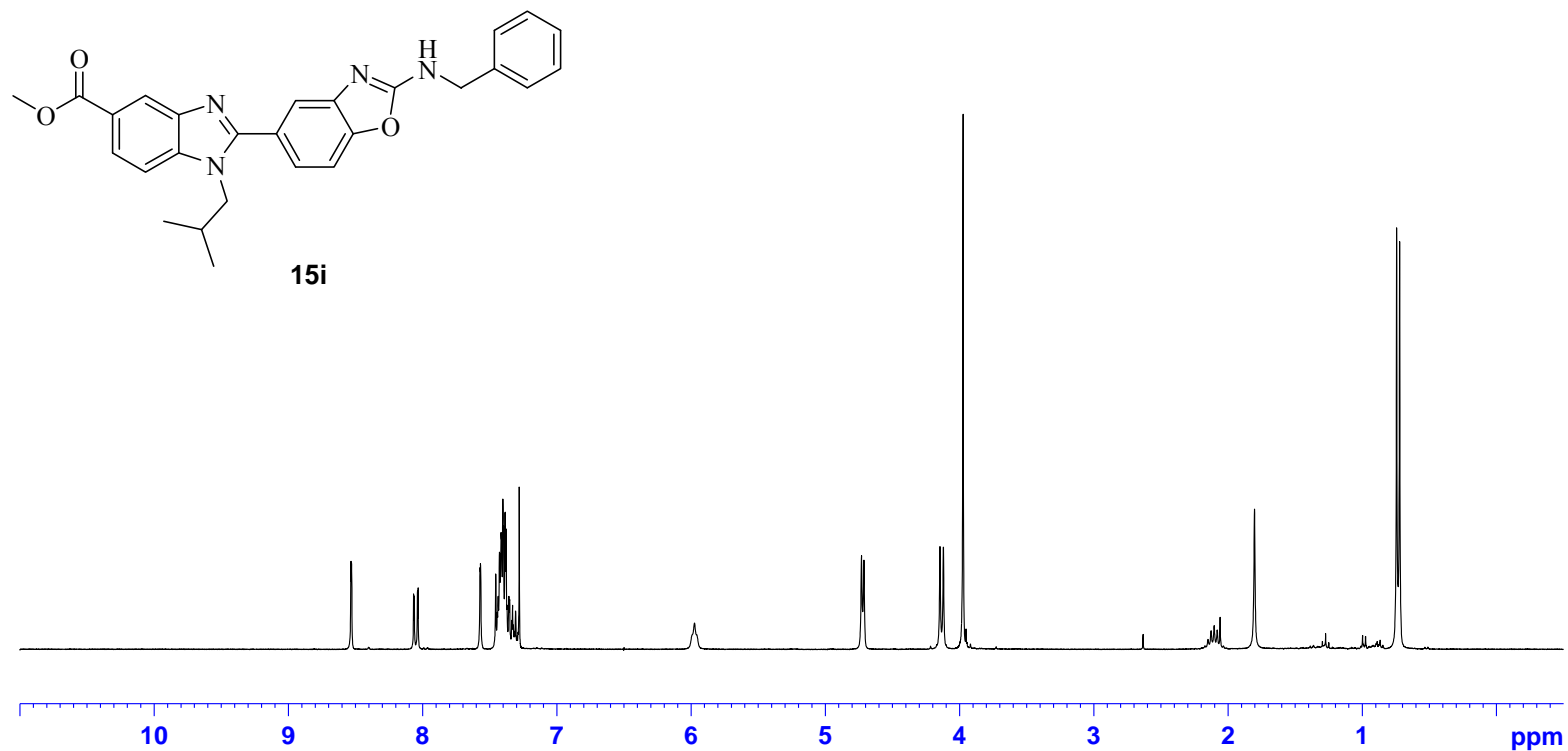
¹³C NMR spectrum (75 MHz) of compound 15g in CDCl₃



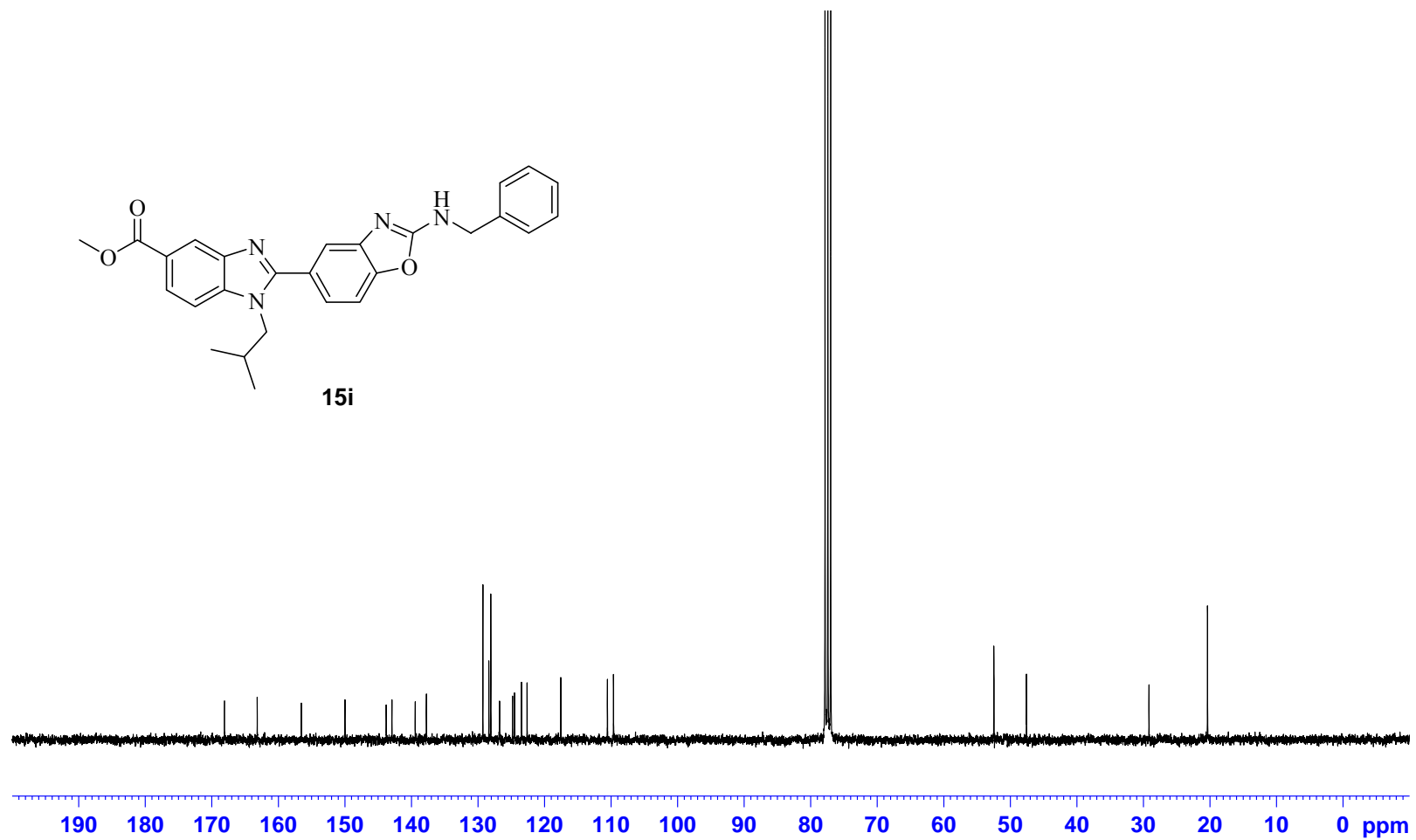
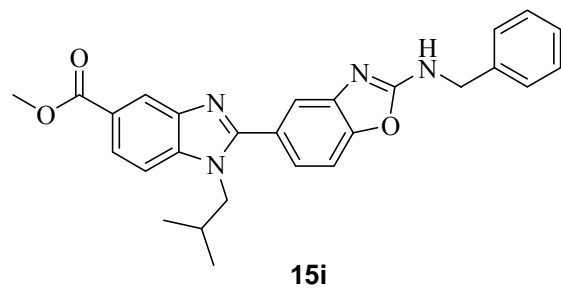
¹H NMR spectrum (300 MHz) of compound 15h in CDCl₃



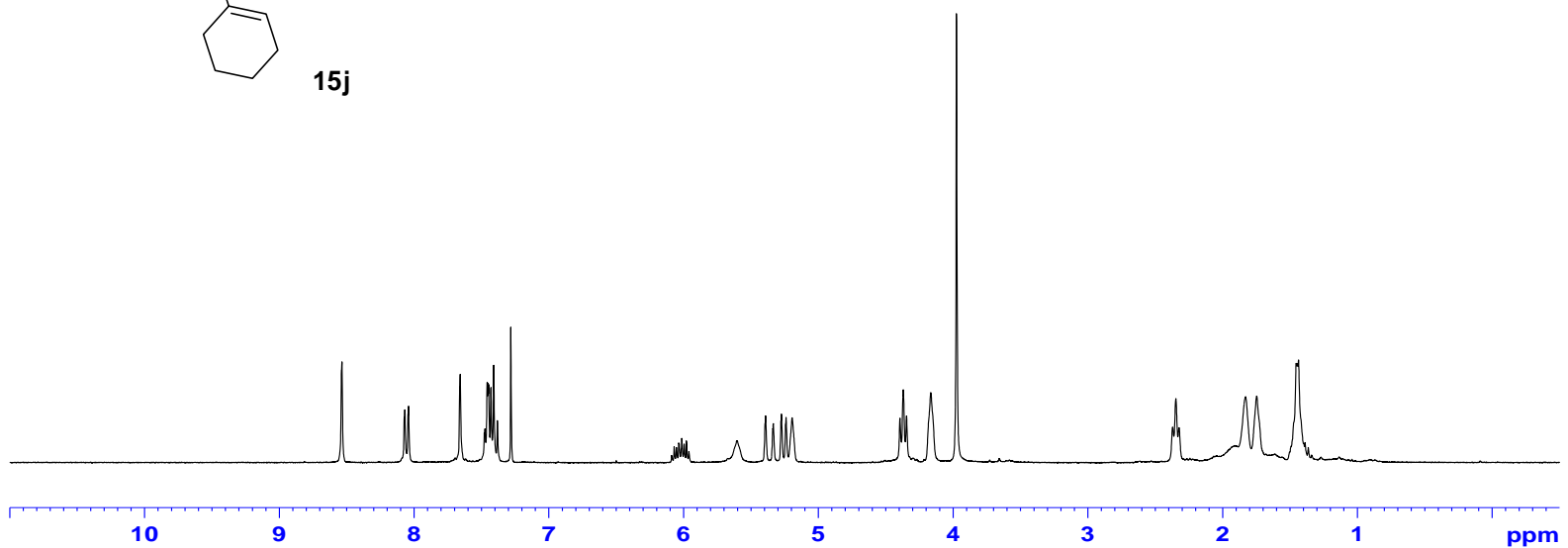
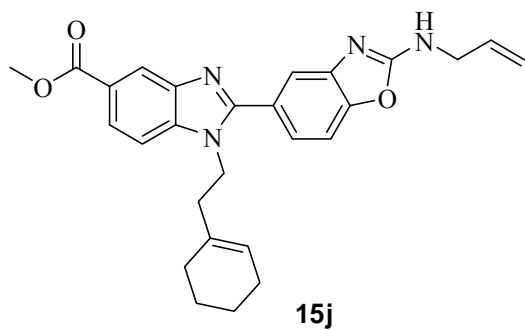
¹³C NMR spectrum (75 MHz) of compound 15h in CDCl₃



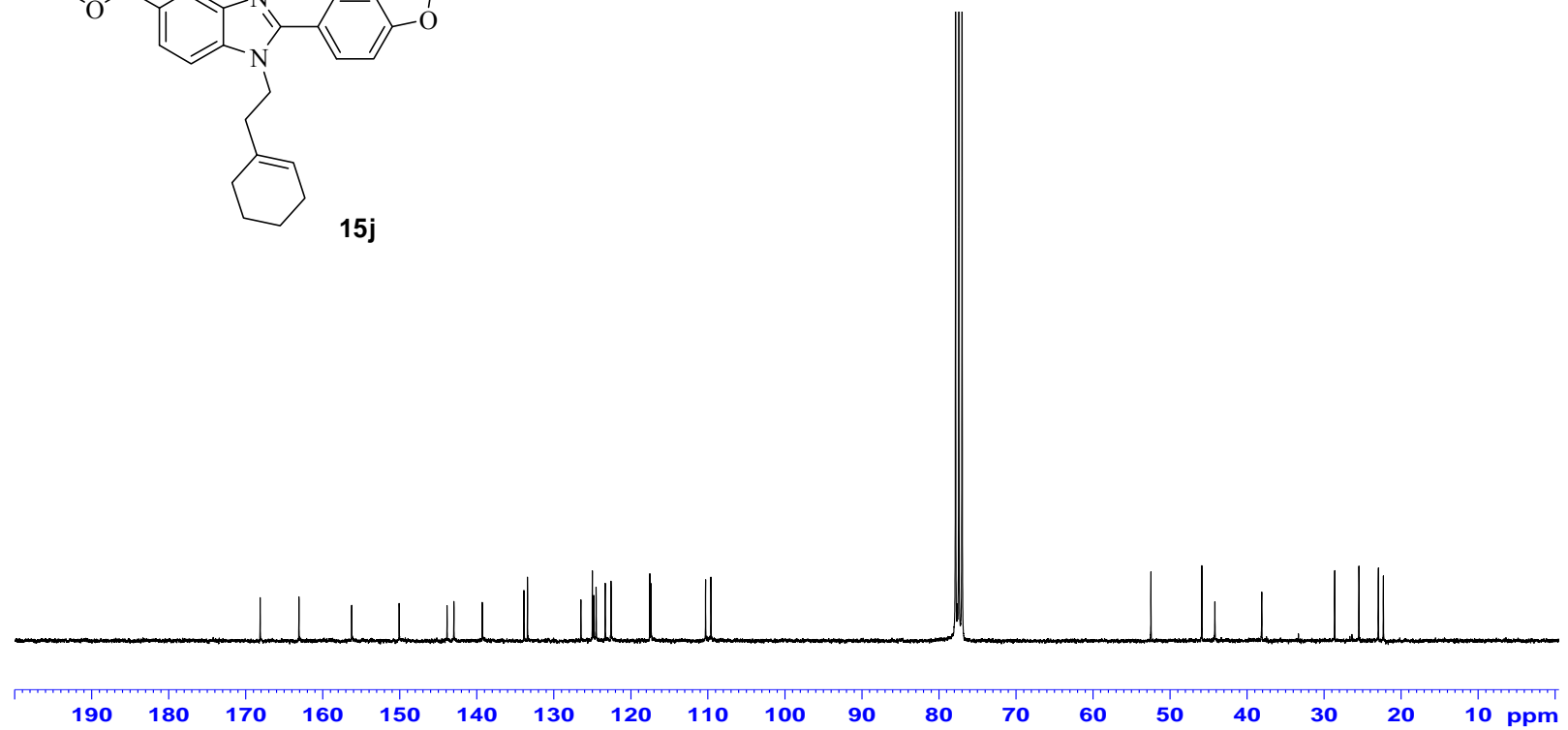
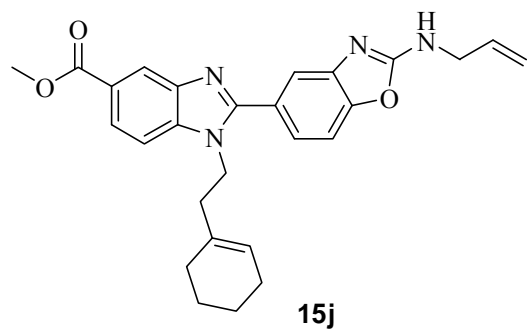
¹H NMR spectrum (300 MHz) of compound 15i in CDCl₃



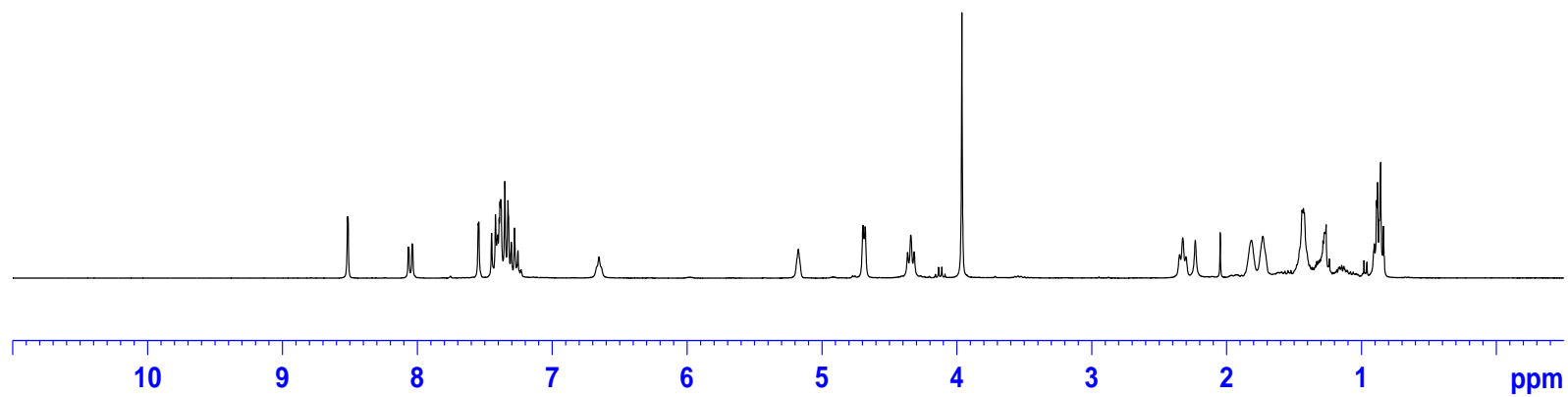
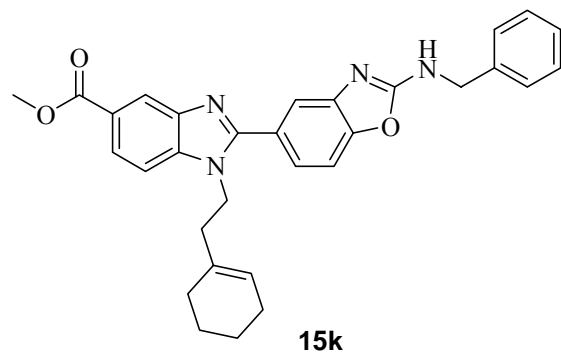
^{13}C NMR spectrum (75 MHz) of compound 15i in CDCl_3



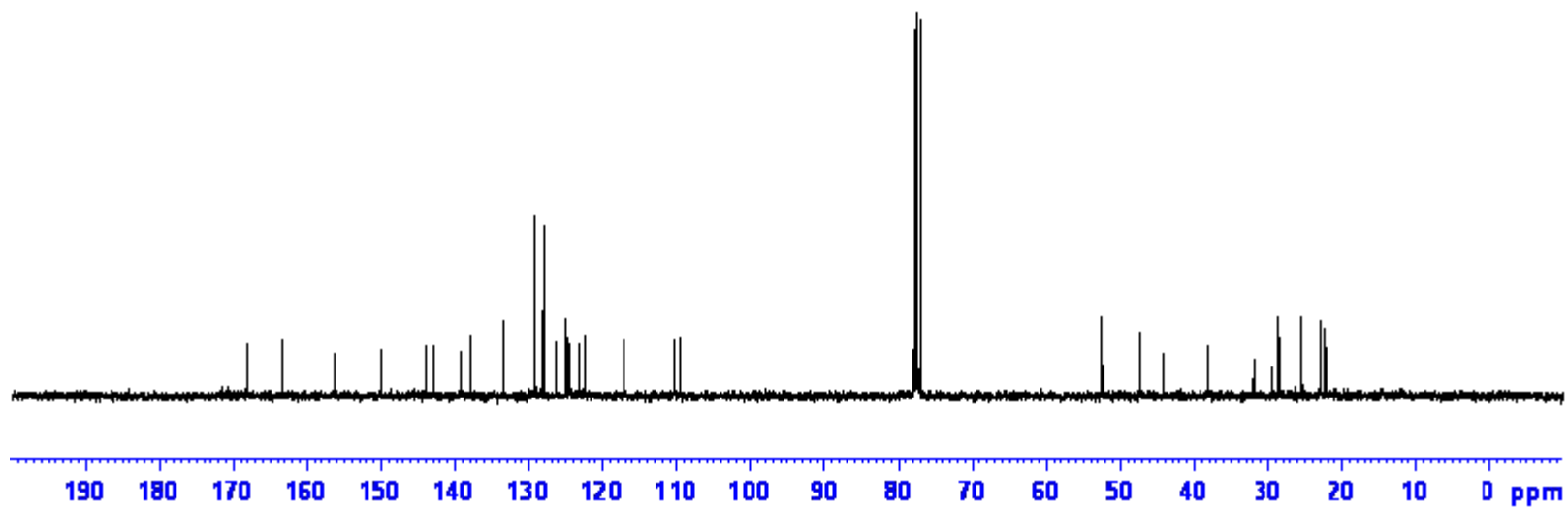
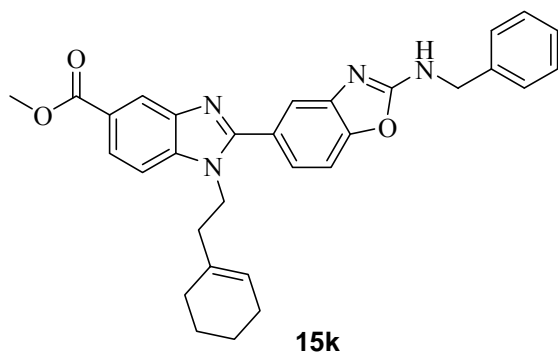
¹H NMR spectrum (300 MHz) of compound 15j in CDCl₃



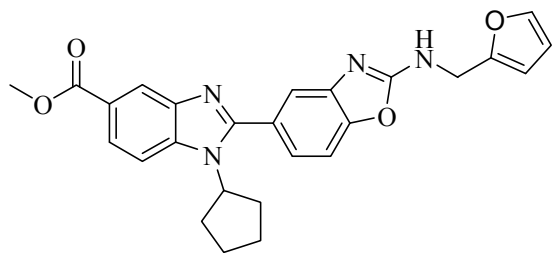
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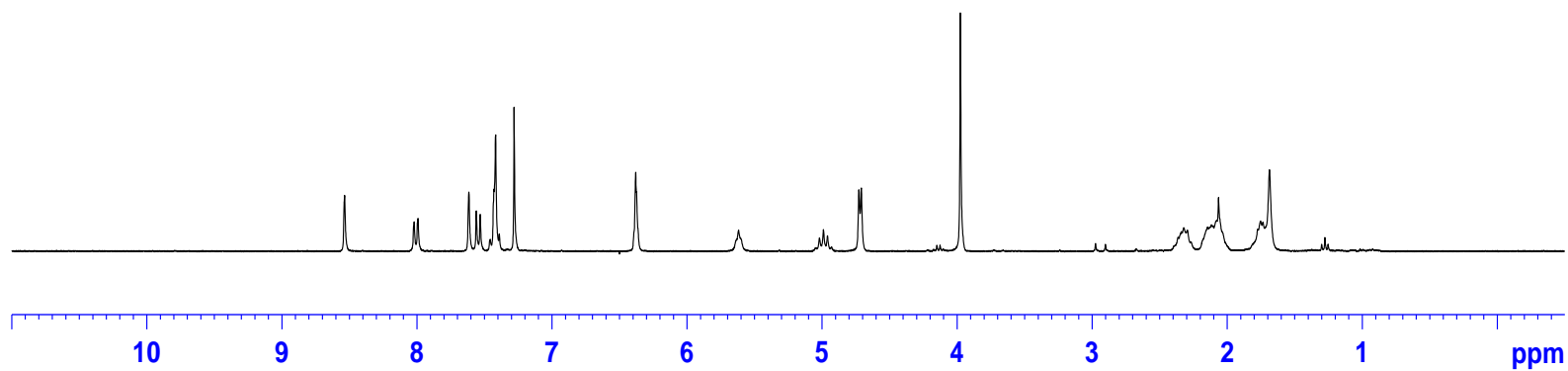
^1H NMR spectrum (300 MHz) of compound 15k in CDCl_3



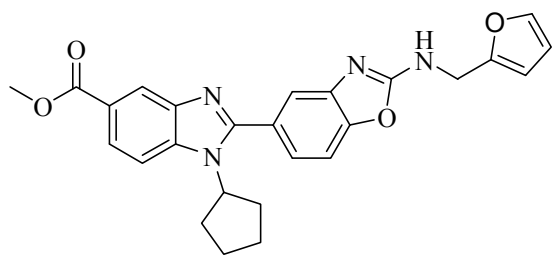
^{13}C NMR spectrum (75 MHz) of compound 15k in CDCl_3



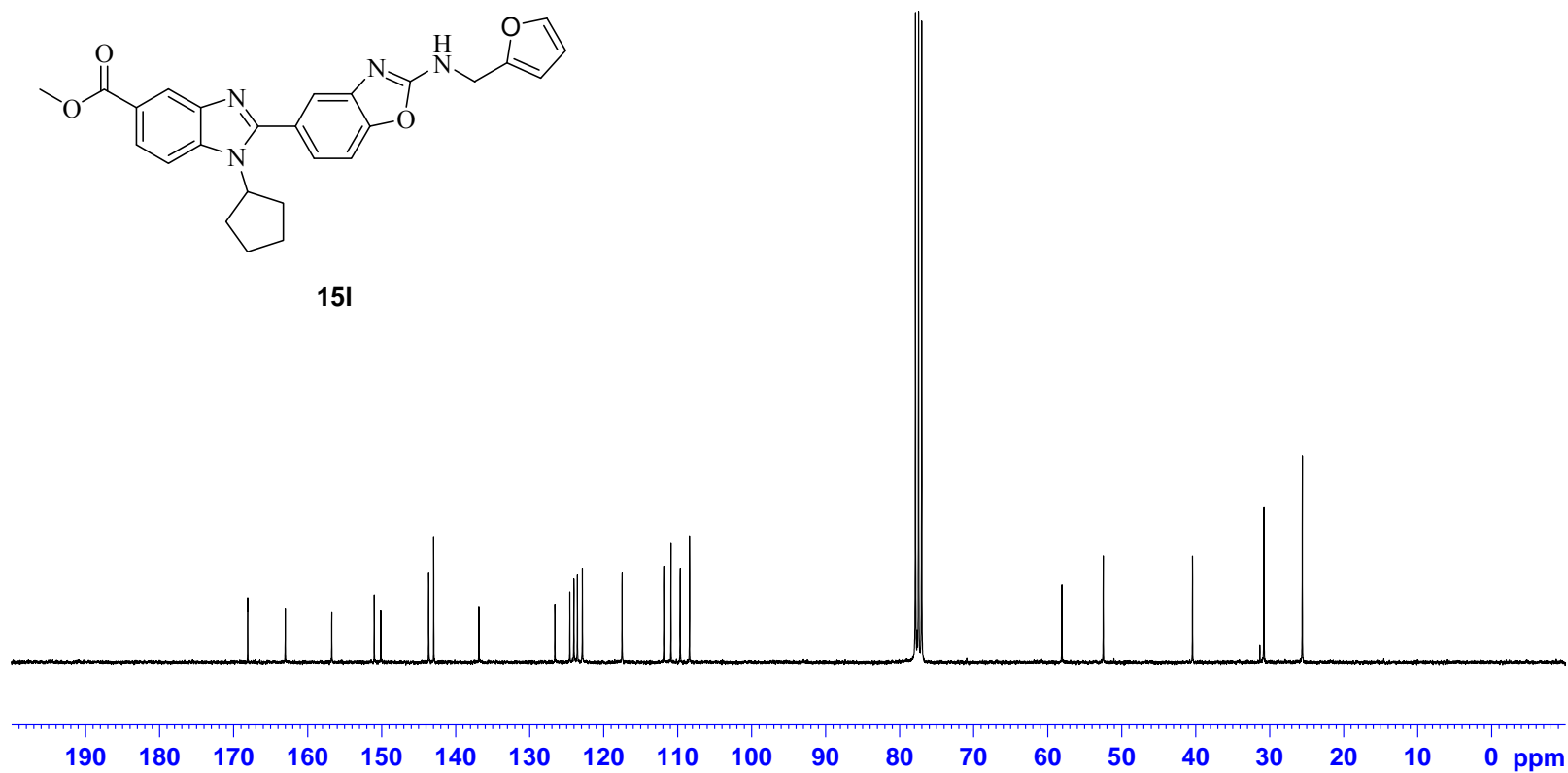
15l



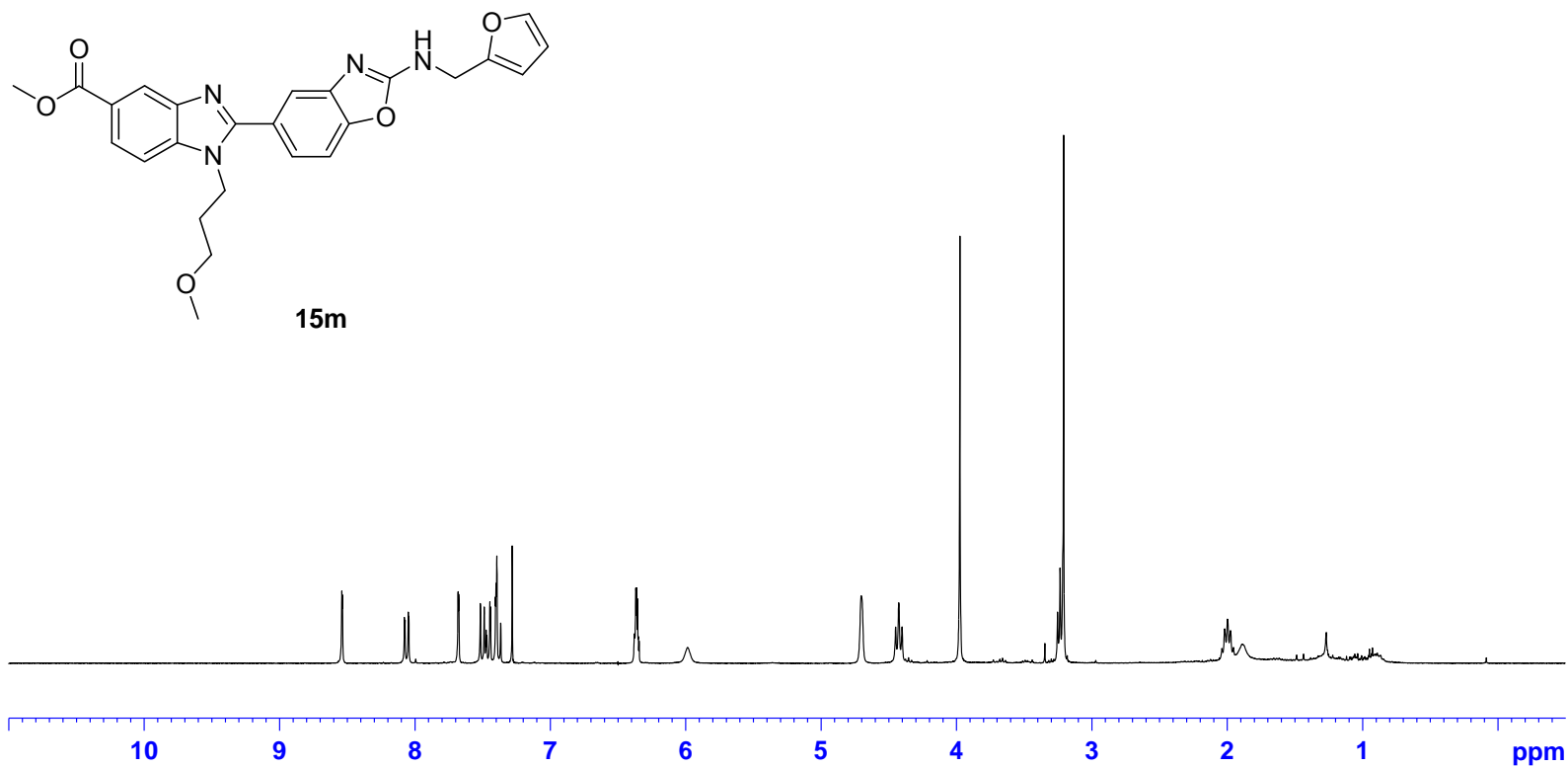
¹H NMR spectrum (300 MHz) of compound 15l in CDCl₃



15l

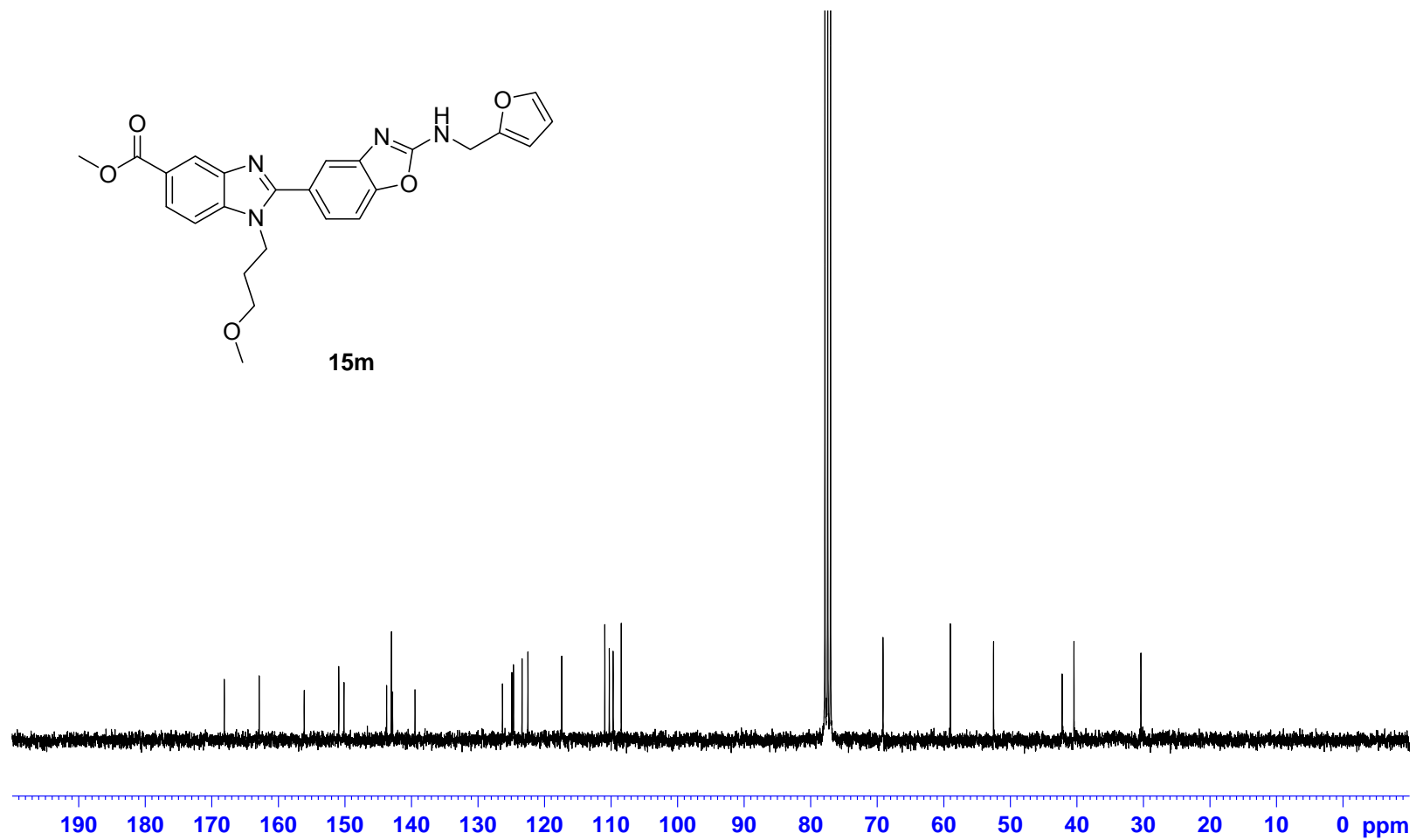
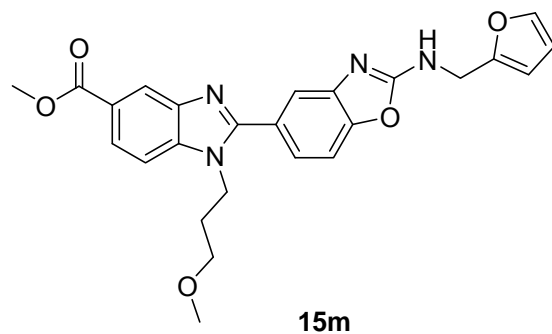


^{13}C NMR spectrum (75 MHz) of compound 15l in CDCl_3

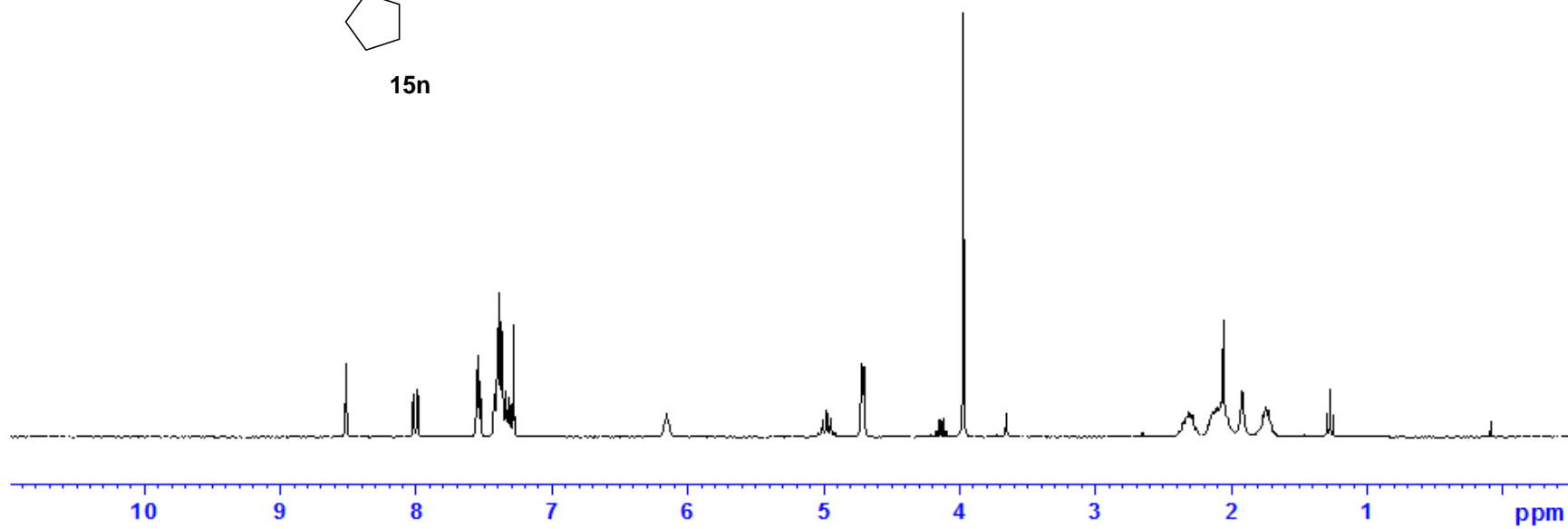
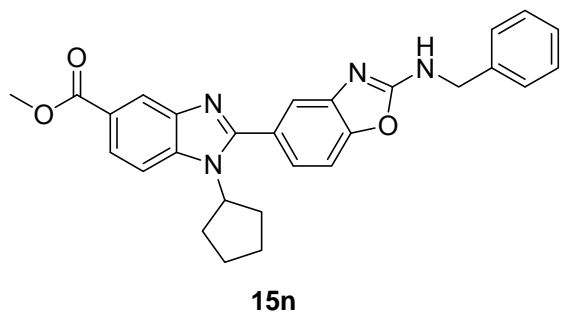


15m

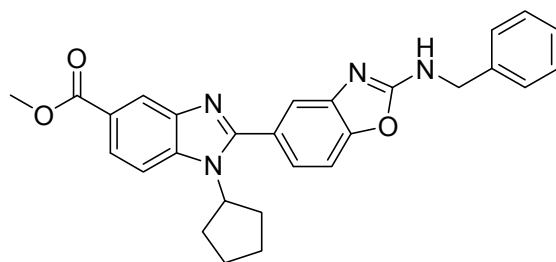
¹H NMR spectrum (300 MHz) of compound 15m in CDCl₃



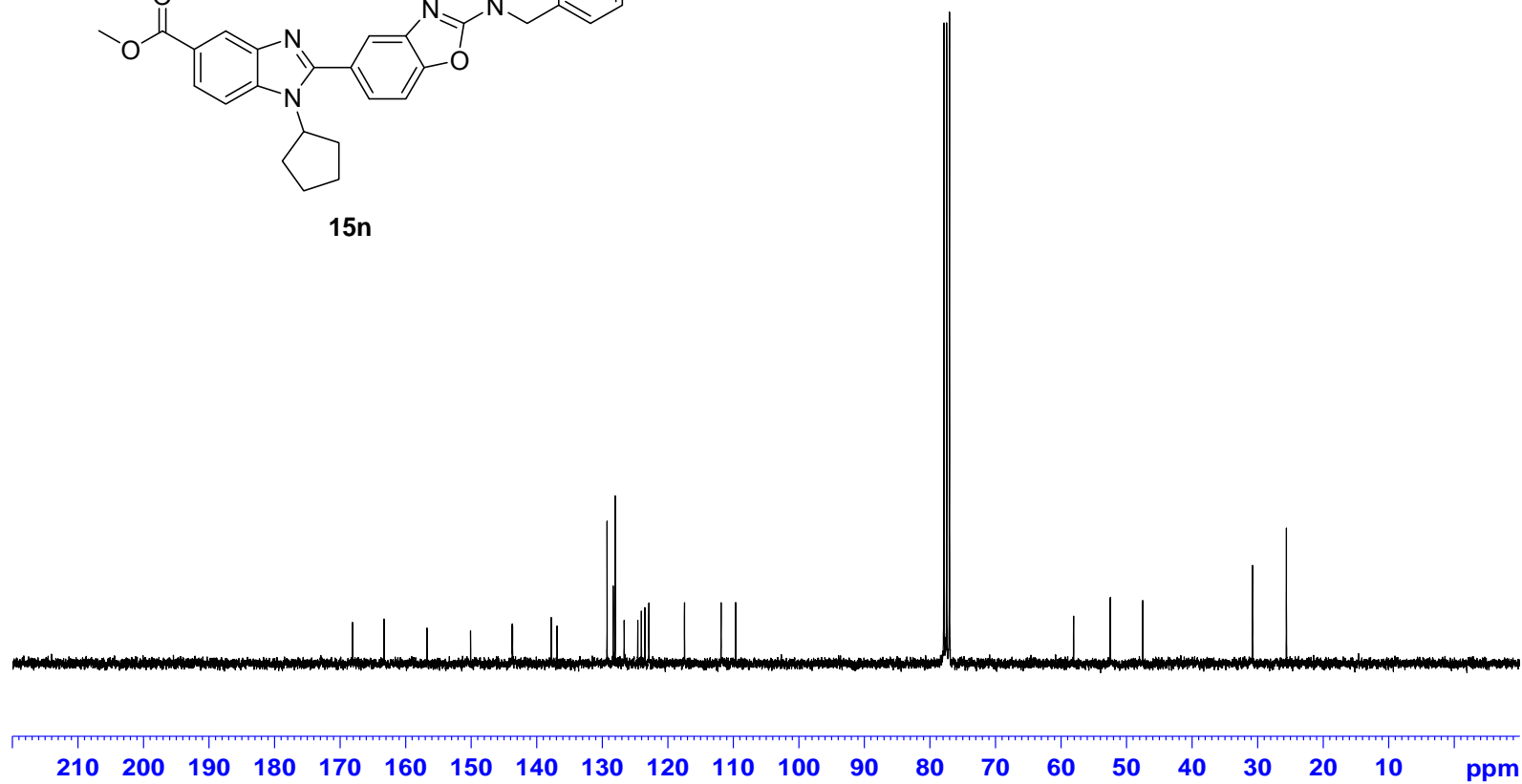
^{13}C NMR spectrum (75 MHz) of compound 15m in CDCl_3



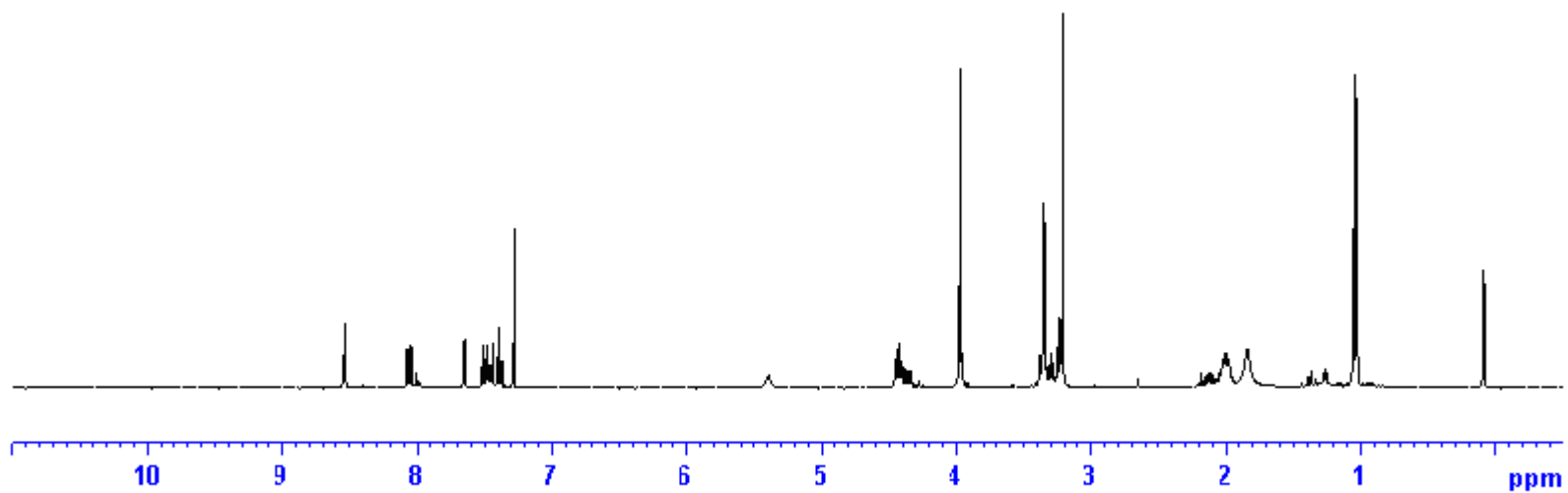
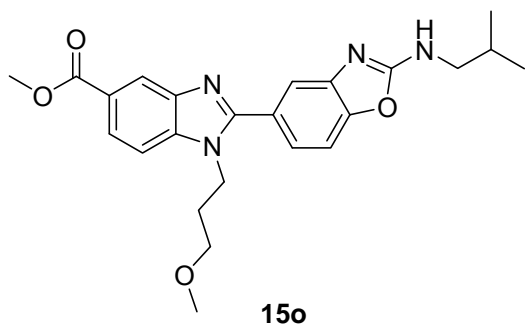
¹H NMR spectrum (300 MHz) of compound 15n in CDCl₃



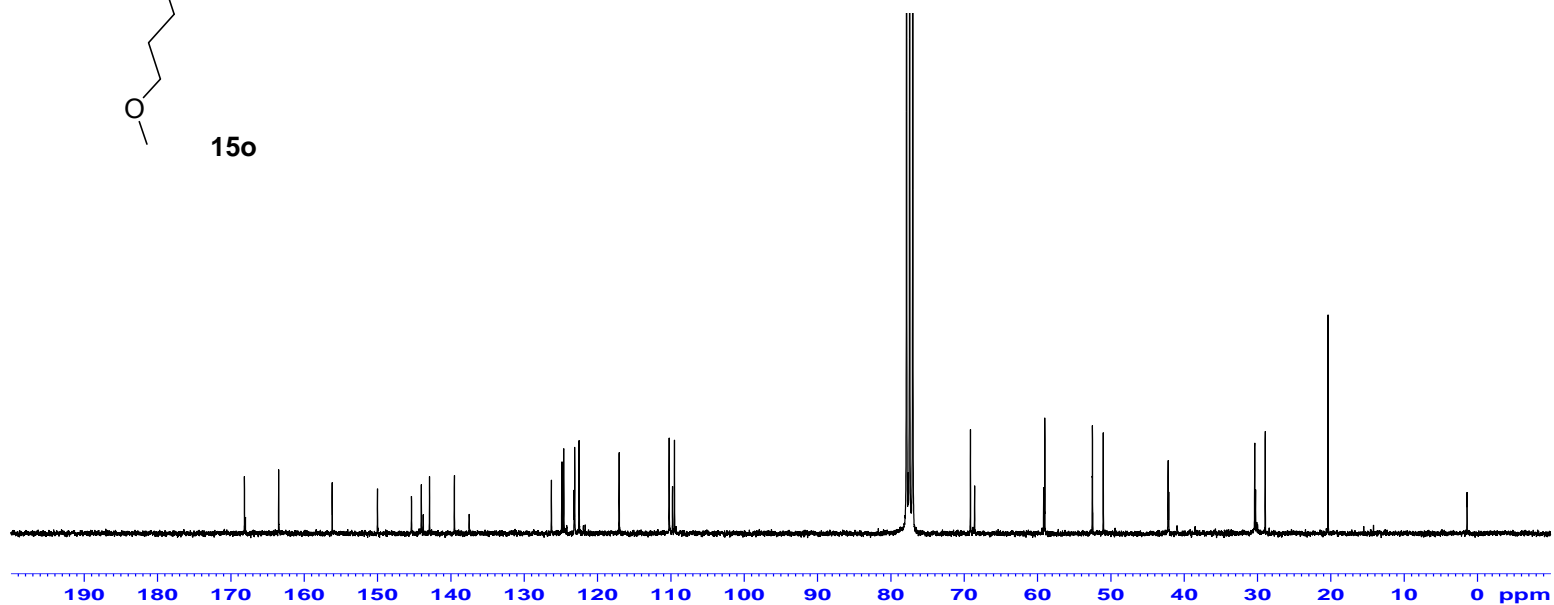
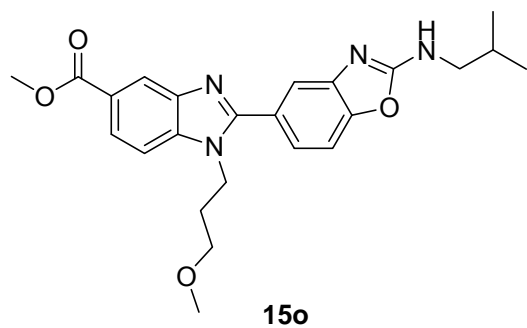
15n



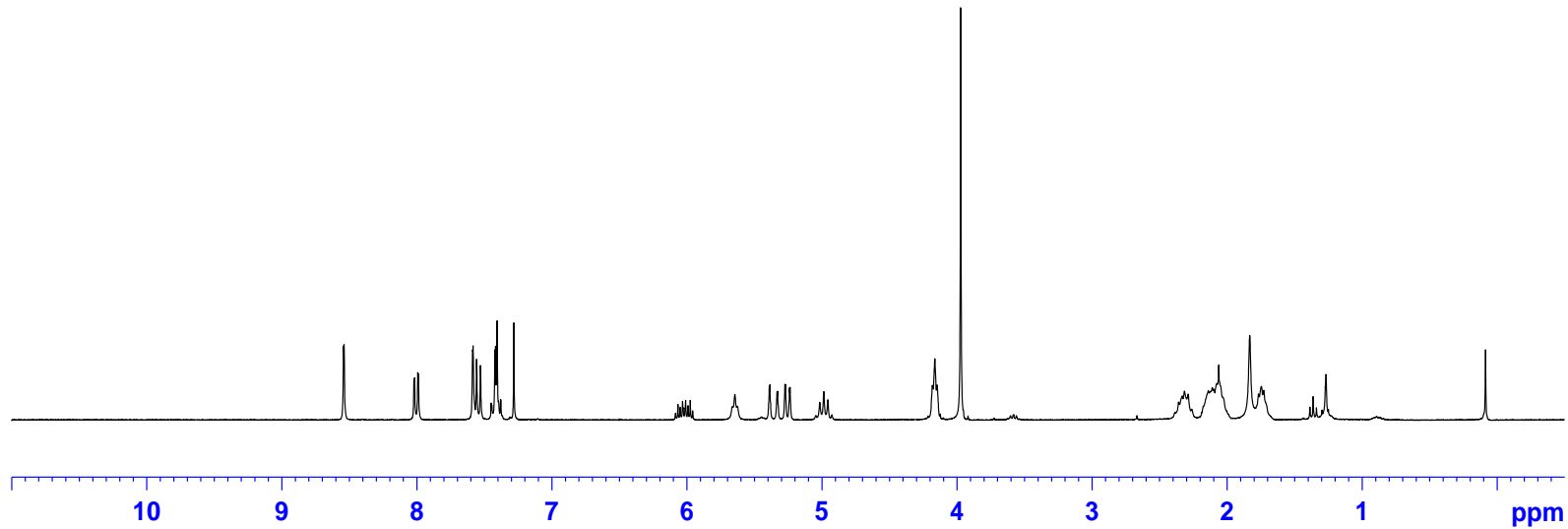
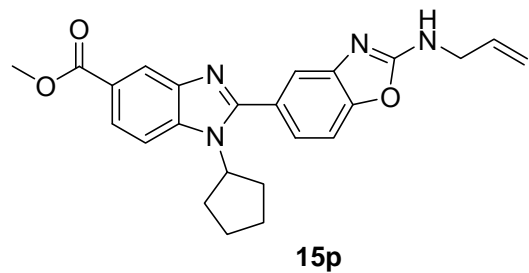
¹³C NMR spectrum (75 MHz) of compound 15n in CDCl₃



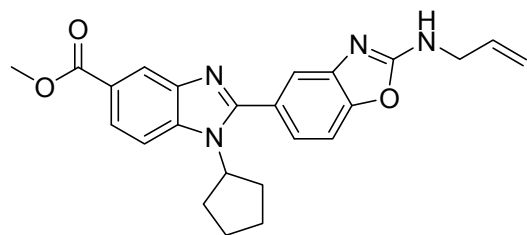
¹H NMR spectrum (300 MHz) of compound 15o in CDCl₃



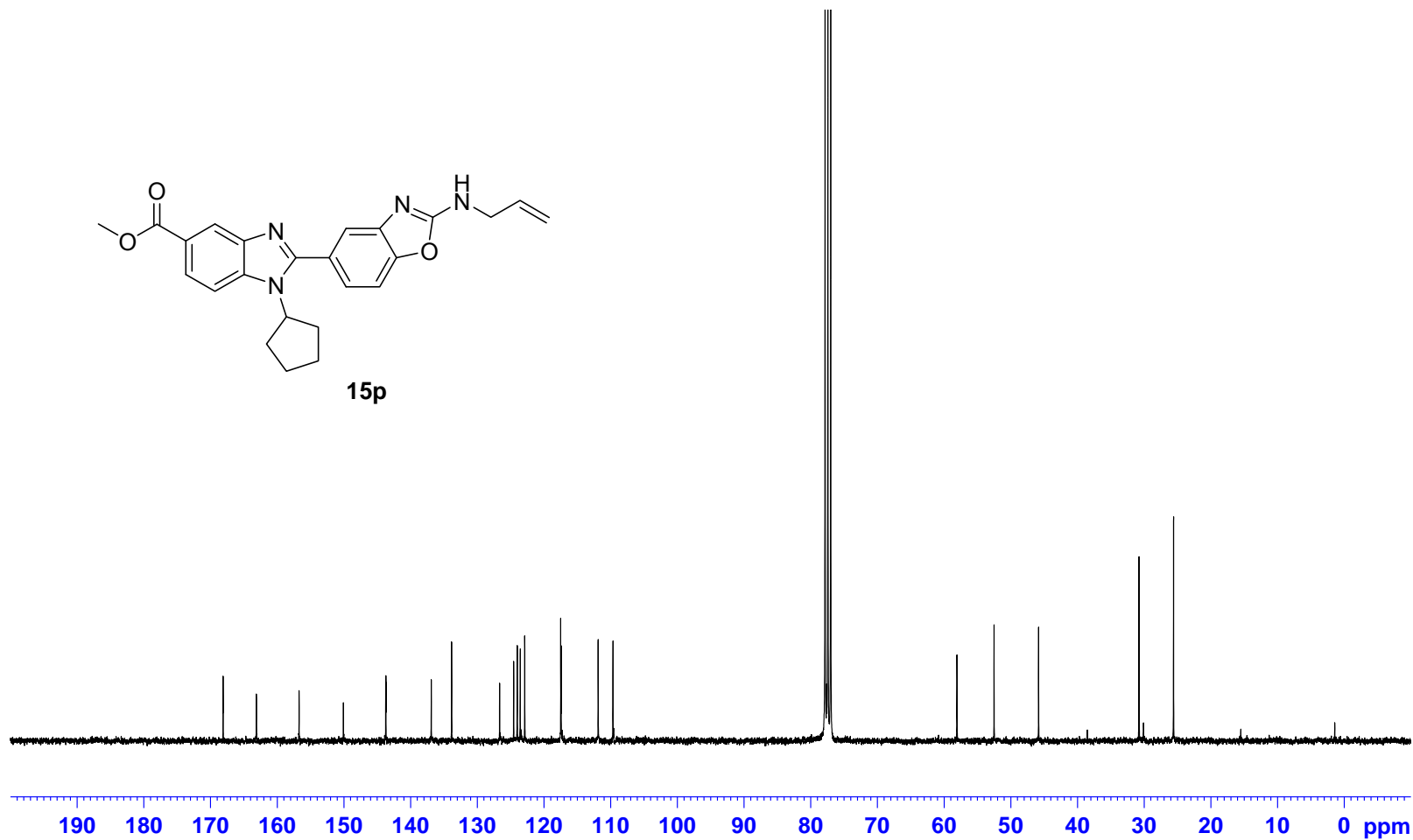
^{13}C NMR spectrum (75 MHz) of compound 15o in CDCl_3



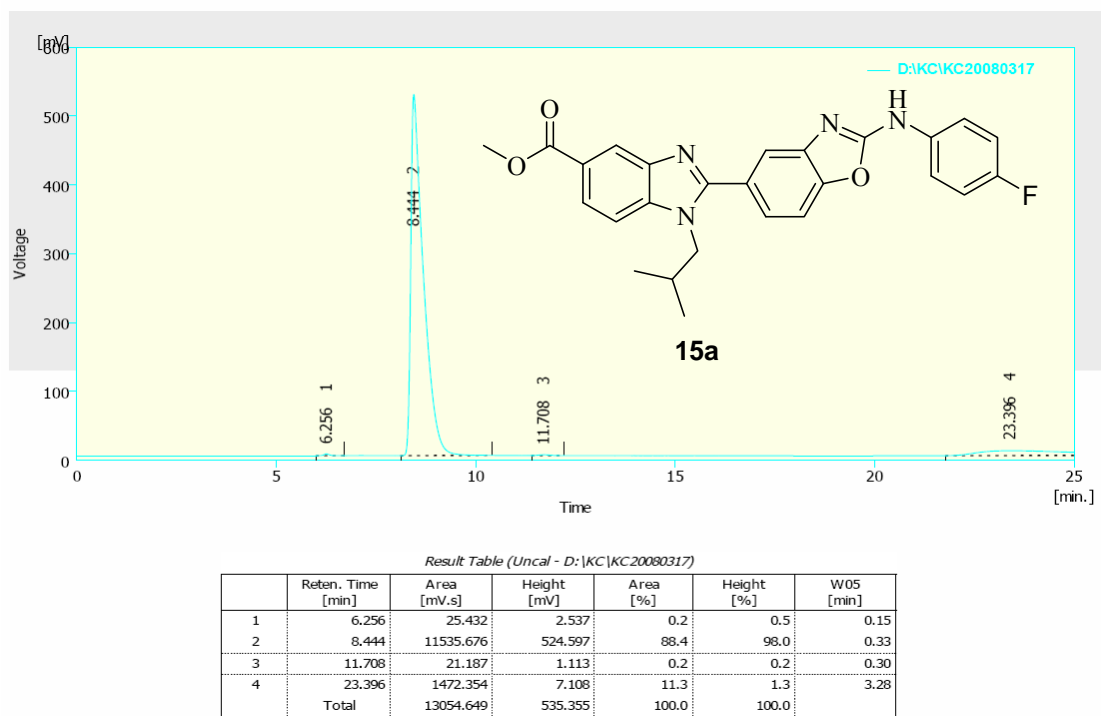
¹H NMR spectrum (300 MHz) of compound 15p in CDCl₃



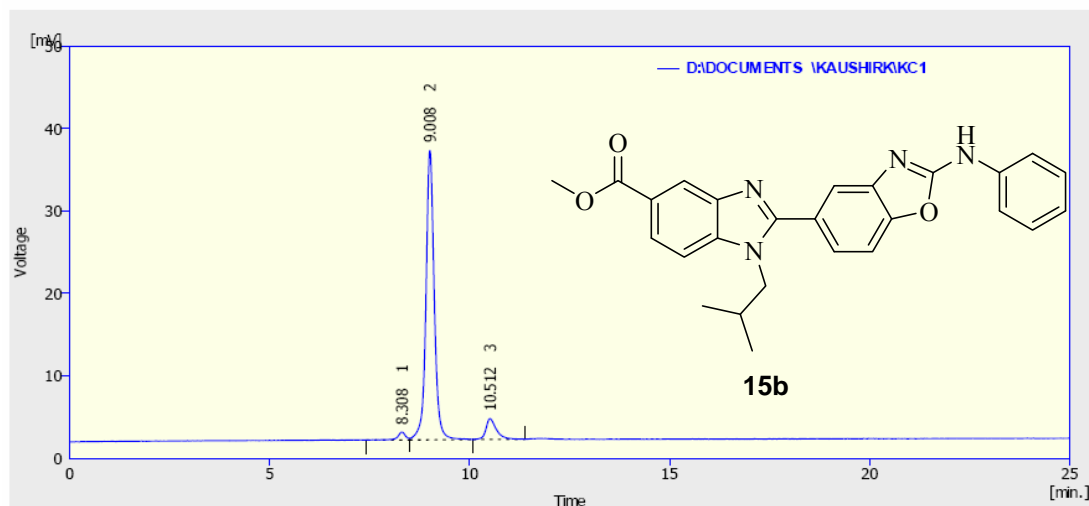
15p



¹³C NMR spectrum (75 MHz) of compound 15p in CDCl₃



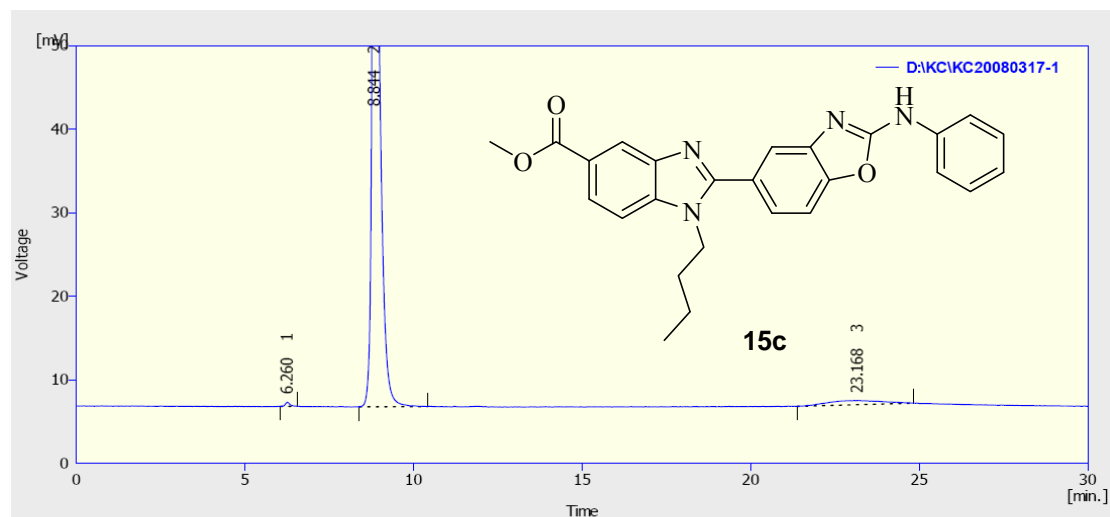
Crude HPLC Spectra of Compound 15a



Result Table (Uncal - D:\DOCUMENTS \KAUSHIRK\KC1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	8.308	13.685	0.945	2.4	2.4	0.19
2	9.008	506.734	35.125	89.4	91.0	0.21
3	10.512	46.271	2.515	8.2	6.5	0.26
	Total	566.690	38.585	100.0	100.0	

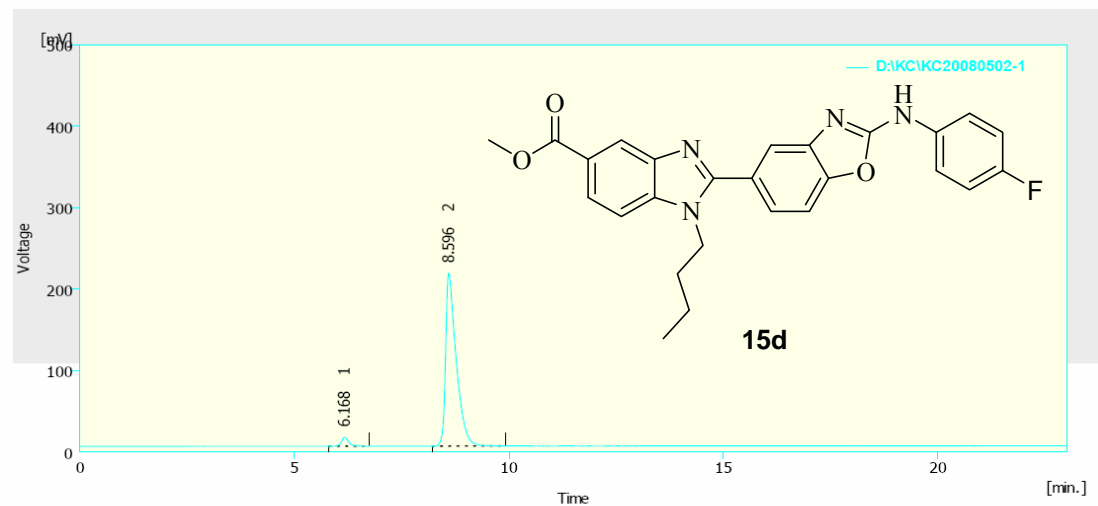
Crude HPLC Spectra of Compound 15b



Result Table (Uncal - D:\KC\KC20080317-1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.260	4.605	0.488	0.3	0.6	0.14
2	8.844	1355.025	87.533	95.5	98.9	0.22
3	23.168	58.555	0.519	4.1	0.6	2.12
	Total	1418.185	88.539	100.0	100.0	

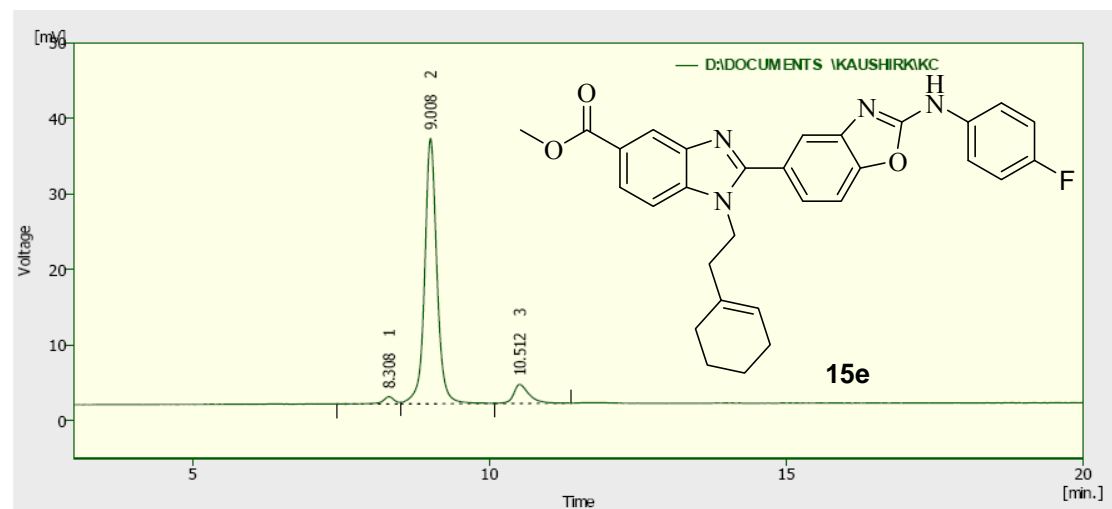
Crude HPLC Spectra of Compound 15c



Result Table (Uncal - D:\KC\KC20080502-1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.168	130.059	10.941	3.4	4.9	0.18
2	8.596	3660.406	212.303	96.6	95.1	0.26
	Total	3790.465	223.244	100.0	100.0	

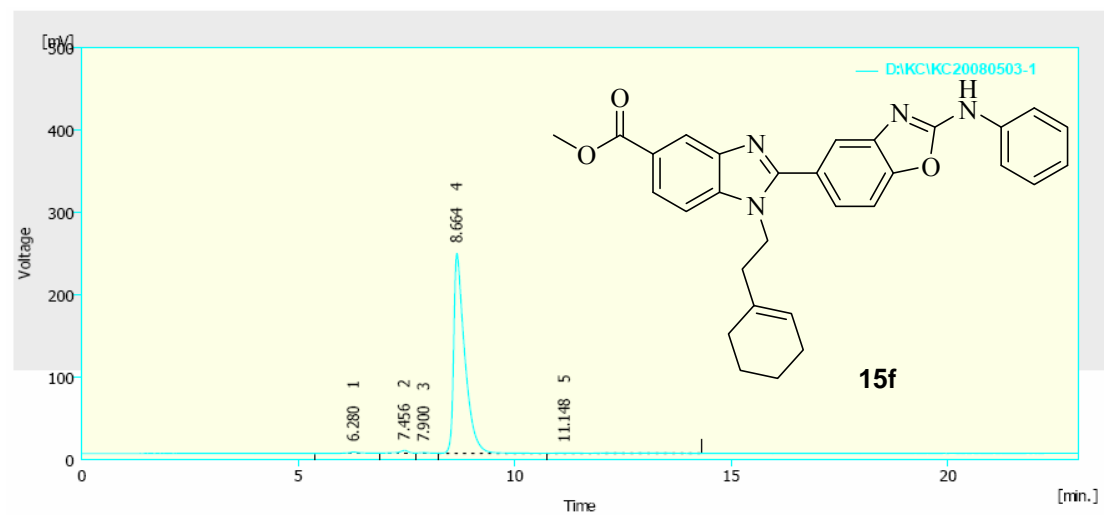
Crude HPLC Spectra of Compound 15d



Result Table (Uncal - D:\DOCUMENTS [KAUSHIRK]KC)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	8.308	13.685	0.945	2.4	2.4	0.19
2	9.008	506.734	35.125	89.4	91.0	0.21
3	10.512	46.271	2.515	8.2	6.5	0.26
Total		566.690	38.585	100.0	100.0	

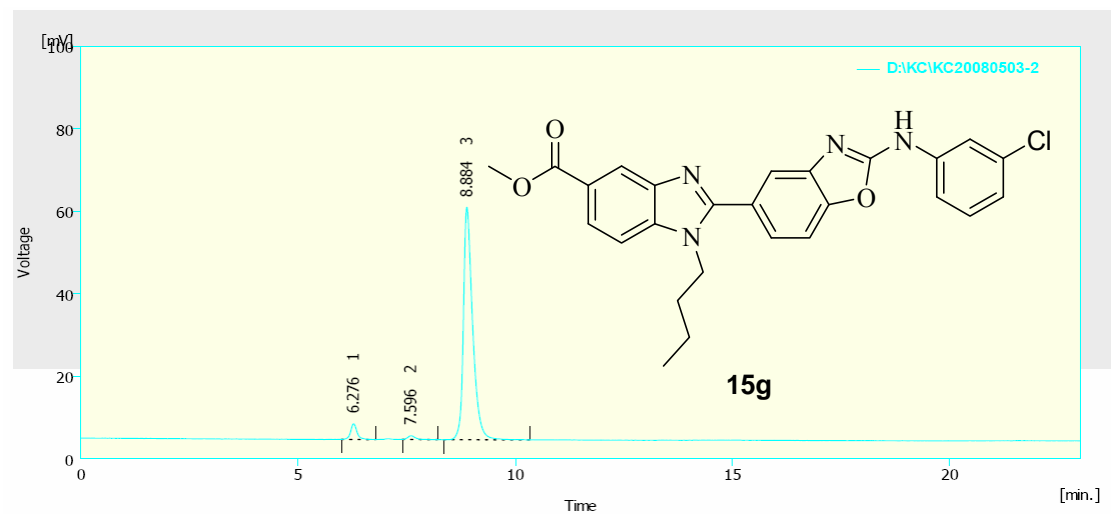
Crude HPLC Spectra of Compound 15e



Result Table (Uncal - D:\KC\KC20080503-1)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.280	41.406	1.800	0.9	0.7	0.26
2	7.456	67.098	3.705	1.5	1.5	0.21
3	7.900	19.332	1.072	0.4	0.4	0.28
4	8.664	4337.877	242.558	96.2	97.2	0.26
5	11.148	42.654	0.423	0.9	0.2	0.56
	Total	4508.367	249.558	100.0	100.0	

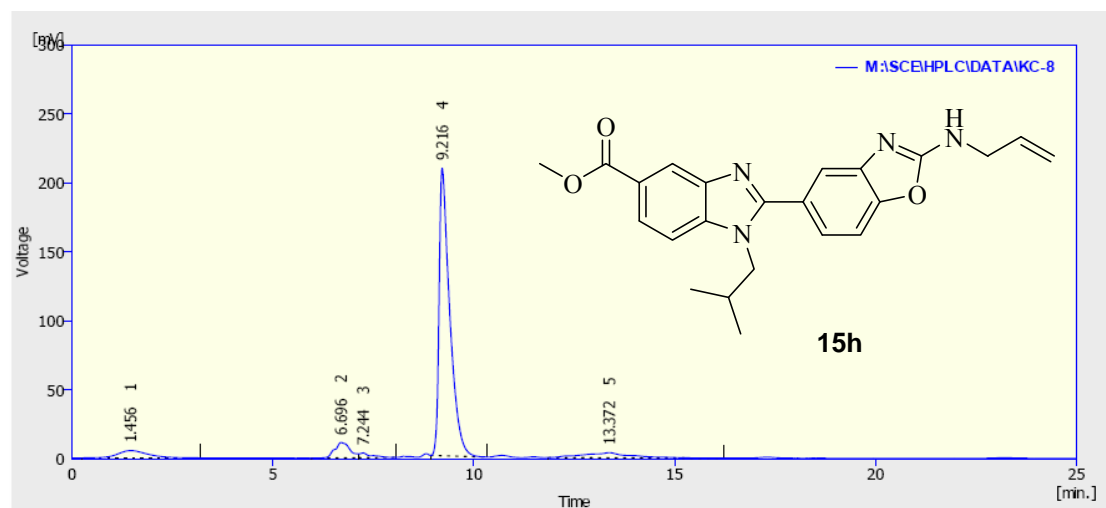
Crude HPLC Spectra of Compound 15f



Result Table (Uncal - D:\KC\KC20080503-2)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.276	39.677	3.821	4.5	6.3	0.15
2	7.596	11.512	0.909	1.3	1.5	0.18
3	8.884	836.037	56.372	94.2	92.3	0.22
Total		887.226	61.102	100.0	100.0	

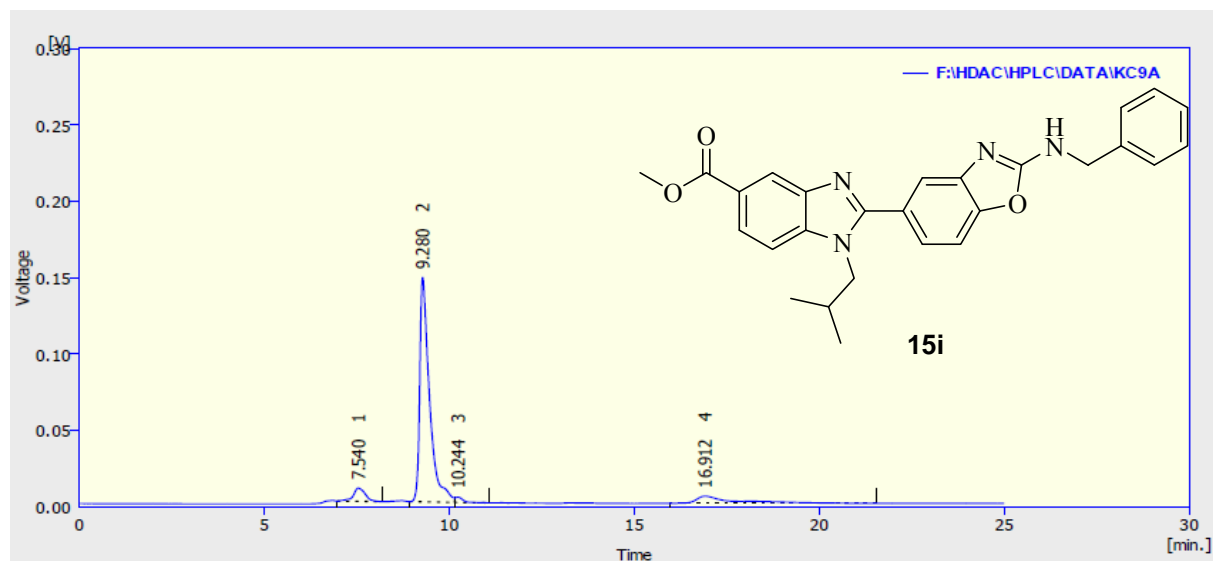
Crude HPLC Spectra of Compound 15g



Result Table (Uncal - M: [SCE]HPLC [DATA] [KC-8])

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	1.456	282.773	5.362	5.9	2.3	0.78
2	6.696	297.736	11.159	6.2	4.8	0.44
3	7.244	69.912	3.476	1.5	1.5	0.23
4	9.216	3845.604	208.590	80.0	89.8	0.27
5	13.372	309.267	3.727	6.4	1.6	1.09
	Total	4805.292	232.315	100.0	100.0	

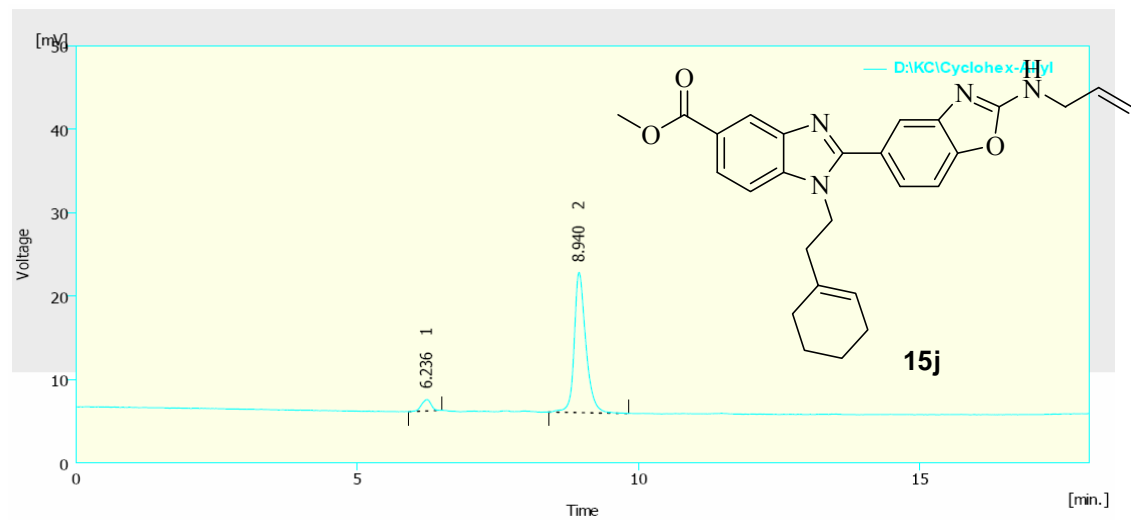
Crude HPLC Spectra of Compound 15h



Result Table (Uncal - F:\HPLC\HPLC\DATA\KC9A)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	7.540	195.148	8.655	5.9	5.3	0.33
2	9.280	2702.245	146.947	82.0	89.7	0.26
3	10.244	51.085	3.437	1.6	2.1	0.23
4	16.912	347.151	4.744	10.5	2.9	0.67
	Total	3295.629	163.783	100.0	100.0	

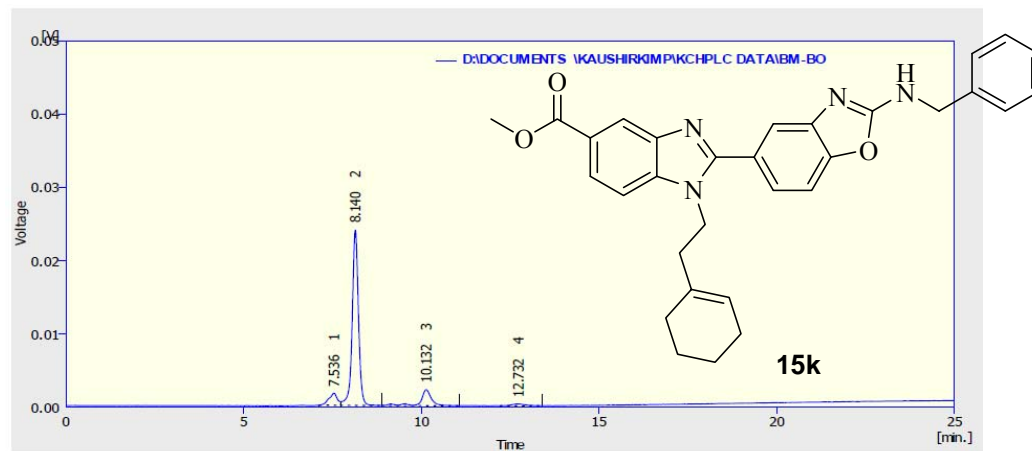
Crude HPLC Spectra of Compound 15i



Result Table (Uncal - D:\KC\Cyclohex-Allyl)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.236	16.068	1.367	6.2	7.5	0.19
2	8.940	242.098	16.808	93.8	92.5	0.21
	Total	258.166	18.175	100.0	100.0	

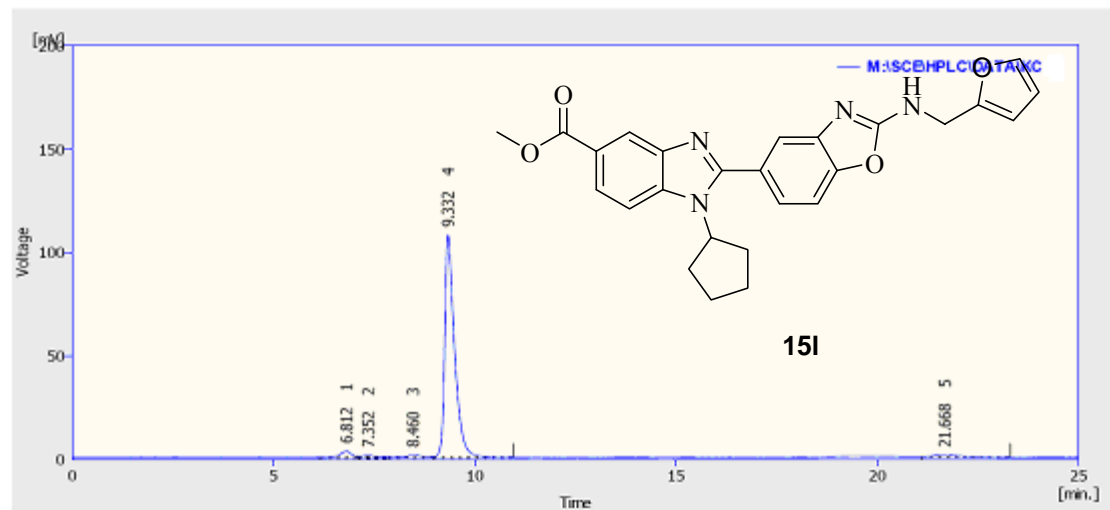
Crude HPLC Spectra of Compound 15j



Result Table (Uncal - D:\DOCUMENTS\KAUSHIRKIMP\KCHPLC DATA\BM-BO)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	7.536	27.189	1.636	7.3	5.8	0.27
2	8.140	294.262	23.943	79.0	85.4	0.18
3	10.132	44.222	2.185	11.9	7.8	0.25
4	12.732	6.847	0.256	1.8	0.9	0.37
	Total	372.519	28.020	100.0	100.0	

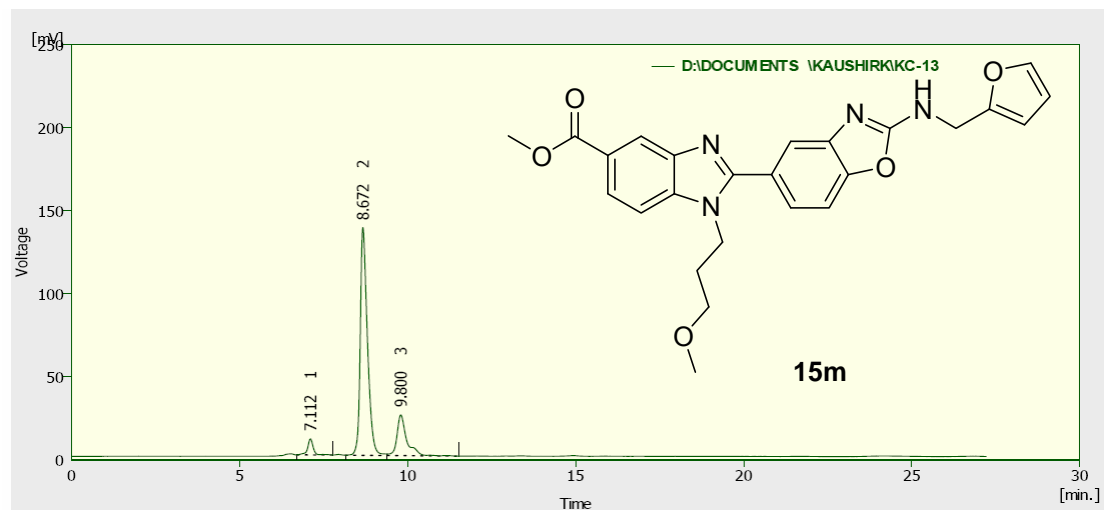
Crude HPLC Spectra of Compound 15k



Result Table (Uncaf - M: [SCE]HPLC [DATA] KC

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.812	60.139	3.020	3.0	2.7	0.29
2	7.352	25.410	1.006	1.3	0.9	0.42
3	8.460	34.916	1.222	1.8	1.1	0.30
4	9.332	1819.470	107.475	92.0	94.7	0.25
5	21.668	38.463	0.727	1.9	0.6	0.76
	Total	1978.399	113.450	100.0	100.0	

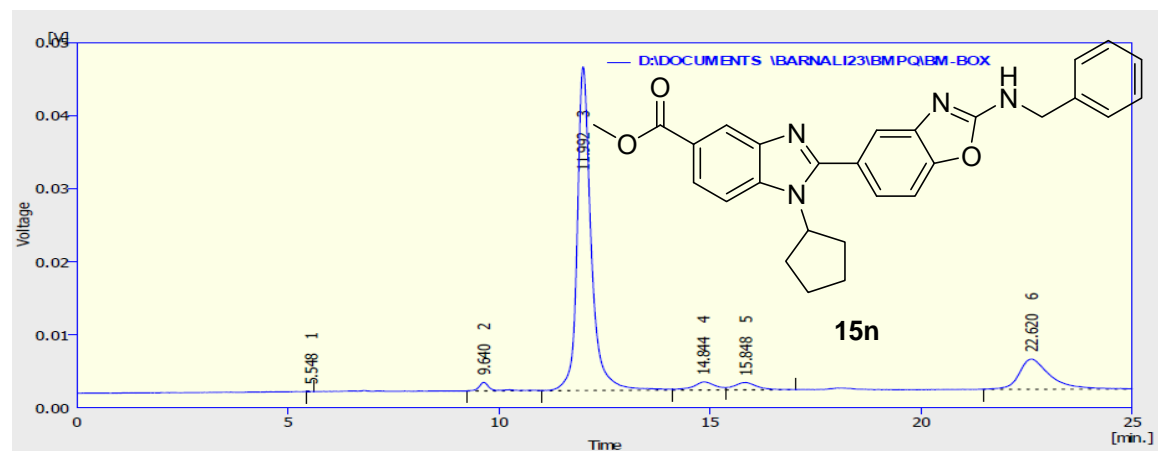
Crude HPLC Spectra of Compound 151



Result Table (Uncal - D:\DOCUMENTS \KAUSHIRK\KC-13)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	7.112	114.549	9.701	4.3	5.7	0.16
2	8.672	2037.194	137.056	76.7	80.0	0.22
3	9.800	503.670	24.499	19.0	14.3	0.26
	Total	2655.413	171.256	100.0	100.0	

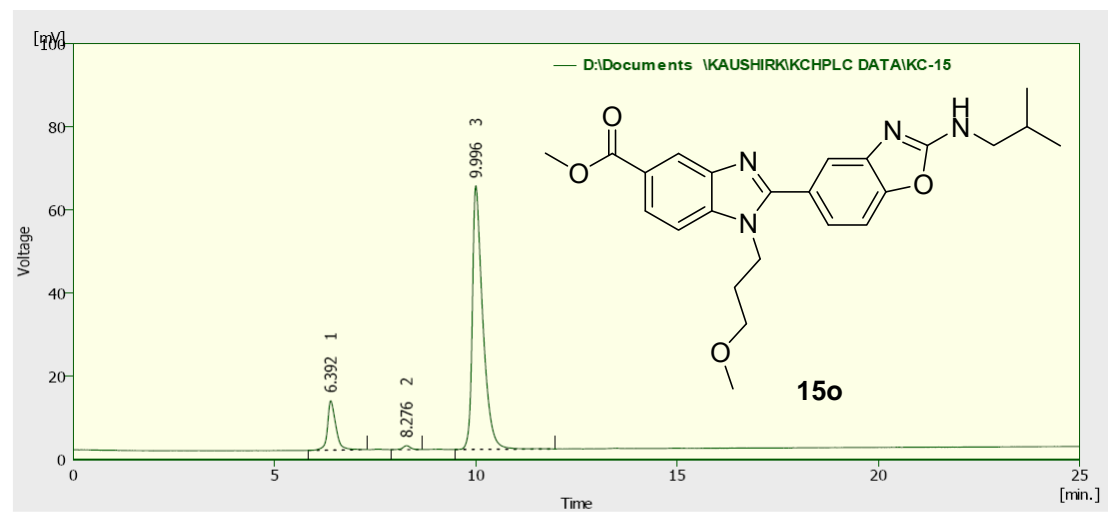
Crude HPLC Spectra of Compound 15m



Result Table (Uncal - D: [DOCUMENTS] [BARNALI23] [BMPQ] [BM-BOX])

	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	

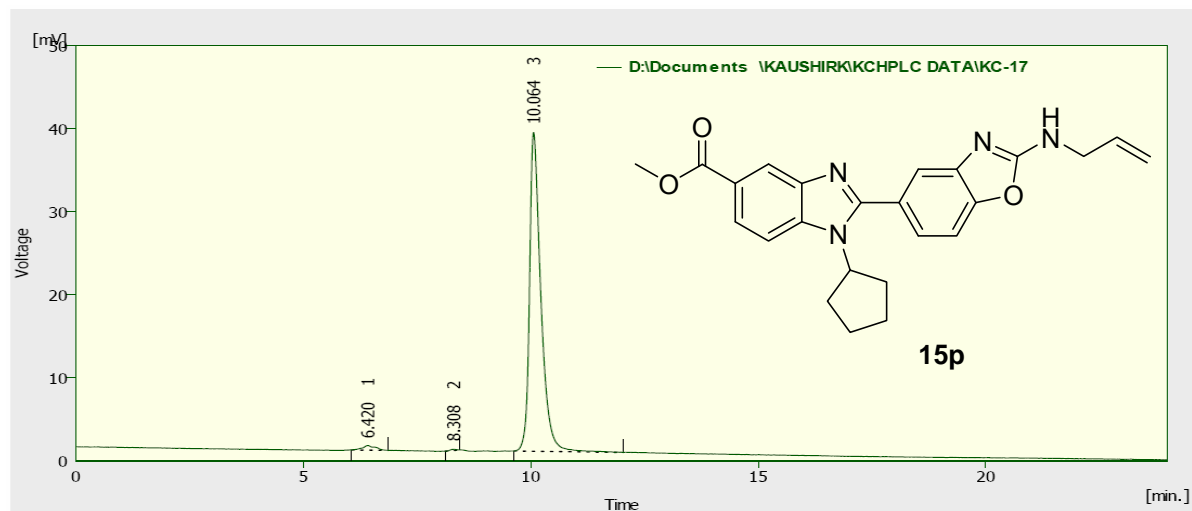
Crude HPLC Spectra of Compound 15n



Result Table (Uncal - D:\Documents\KAUSHIRK\KCHPLC DATA\KC-15)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.392	170.136	11.846	12.8	15.6	0.21
2	8.276	12.574	0.952	0.9	1.3	0.19
3	9.996	1150.216	63.316	86.3	83.2	0.27
	Total	1332.926	76.114	100.0	100.0	

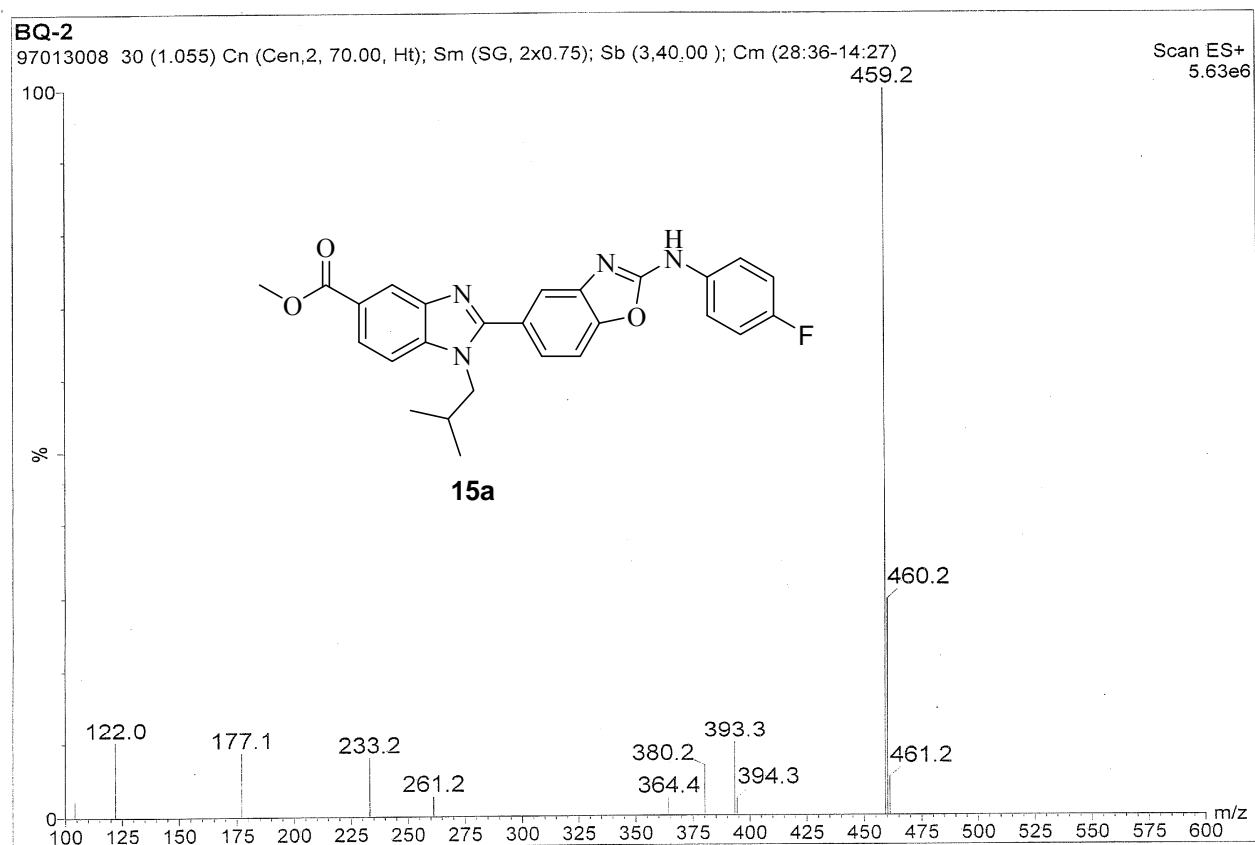
Crude HPLC Spectra of Compound 15o



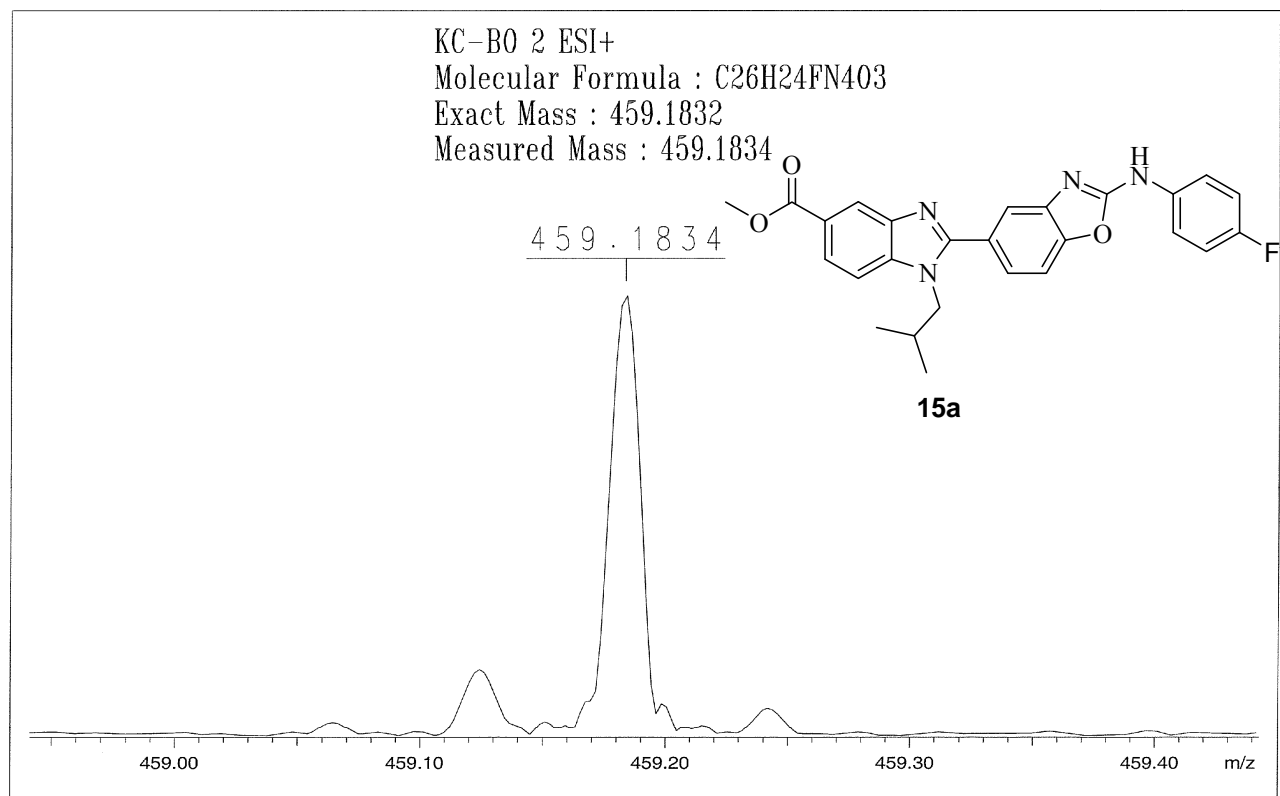
Result Table (Uncal - D:\Documents\KAUSHIRK\KCHPLC DATA\KC-17)

	Reten. Time [min]	Area [mV.s]	Height [mV]	Area [%]	Height [%]	W05 [min]
1	6.420	10.996	0.547	1.6	1.4	0.33
2	8.308	1.326	0.159	0.2	0.4	0.16
3	10.064	666.548	38.359	98.2	98.2	0.25
	Total	678.870	39.066	100.0	100.0	

Crude HPLC Spectra of Compound 15p

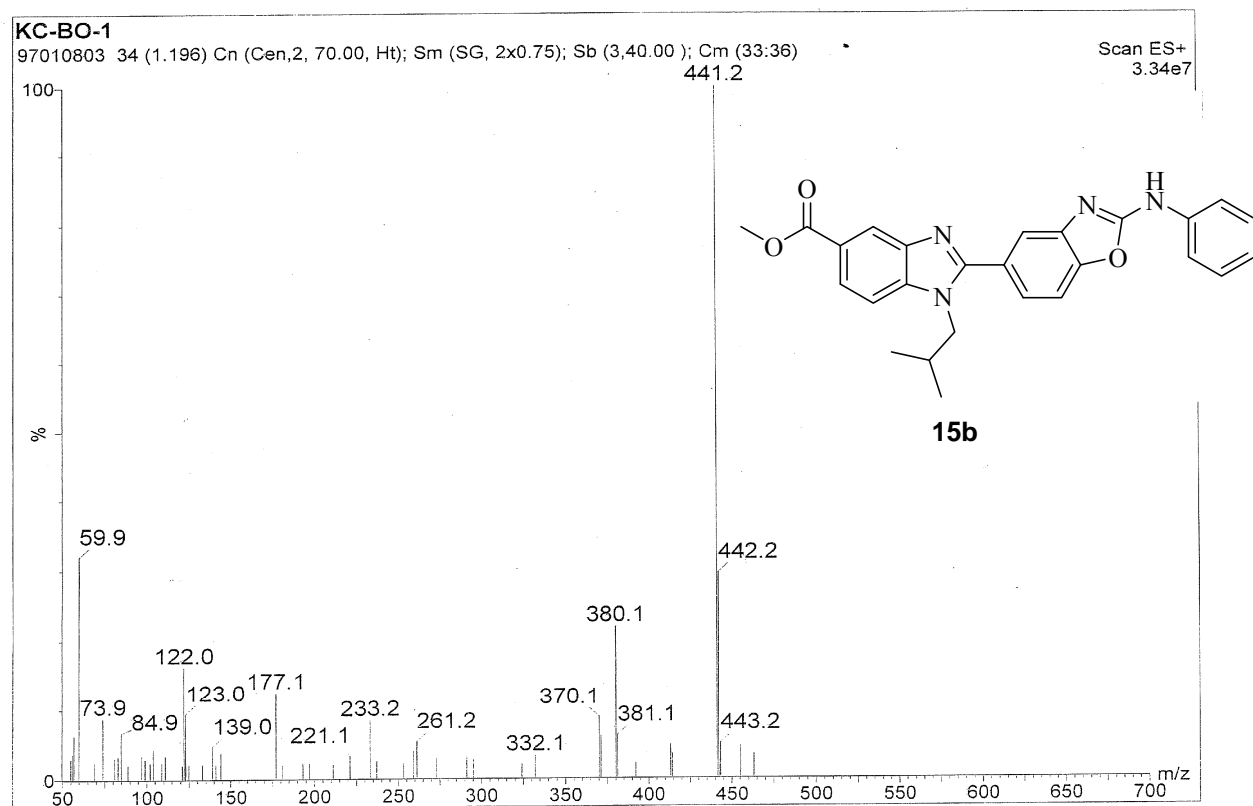


LR Mass Spectra of Compound 15a

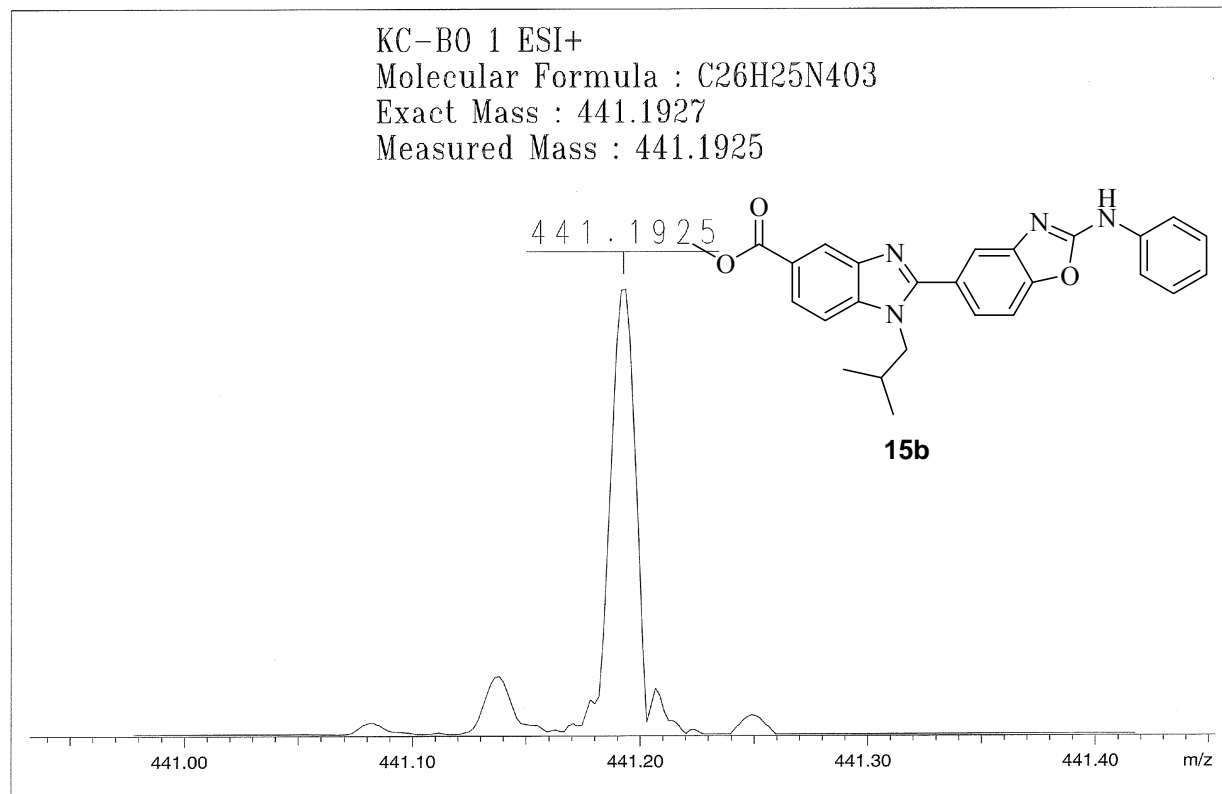


/d=/Data/yl/KCBO2/1/pdata/1 Administrator Thu Aug 7 15:22:16 2008

HR Mass Spectra of Compound 15a

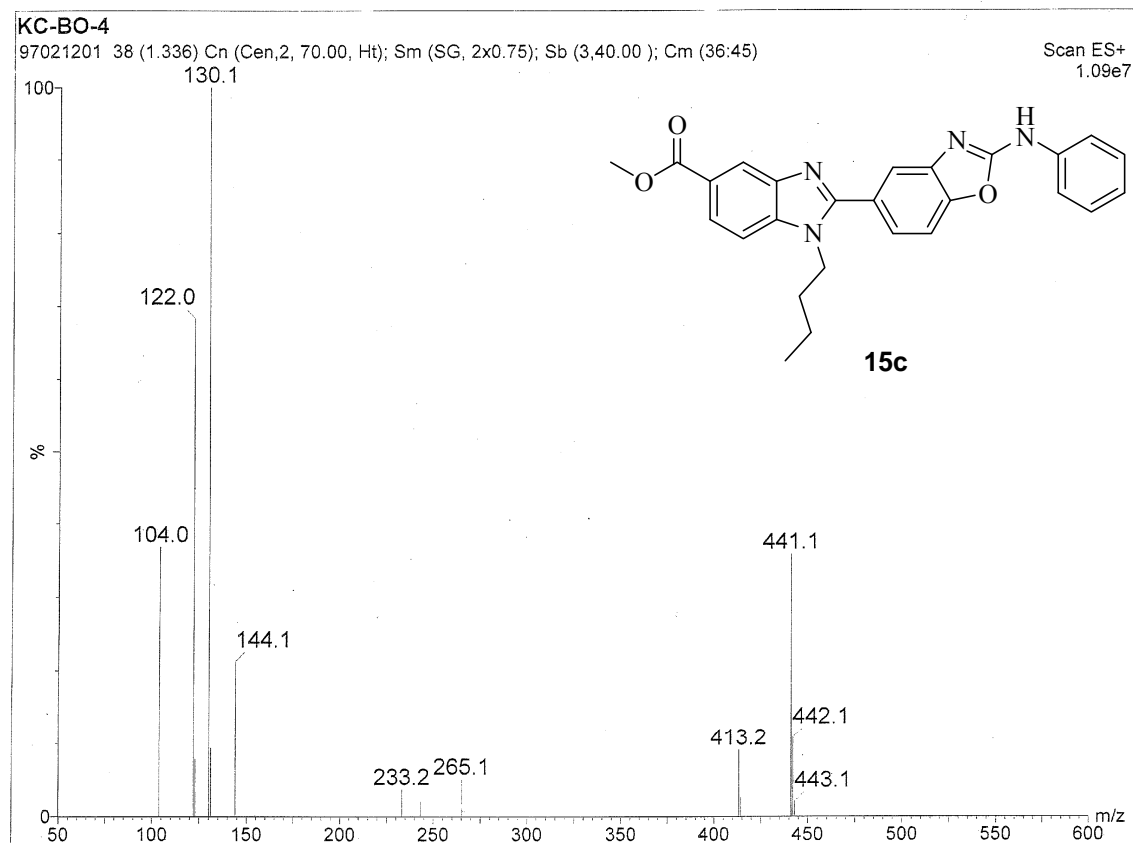


LR Mass Spectra of Compound 15b

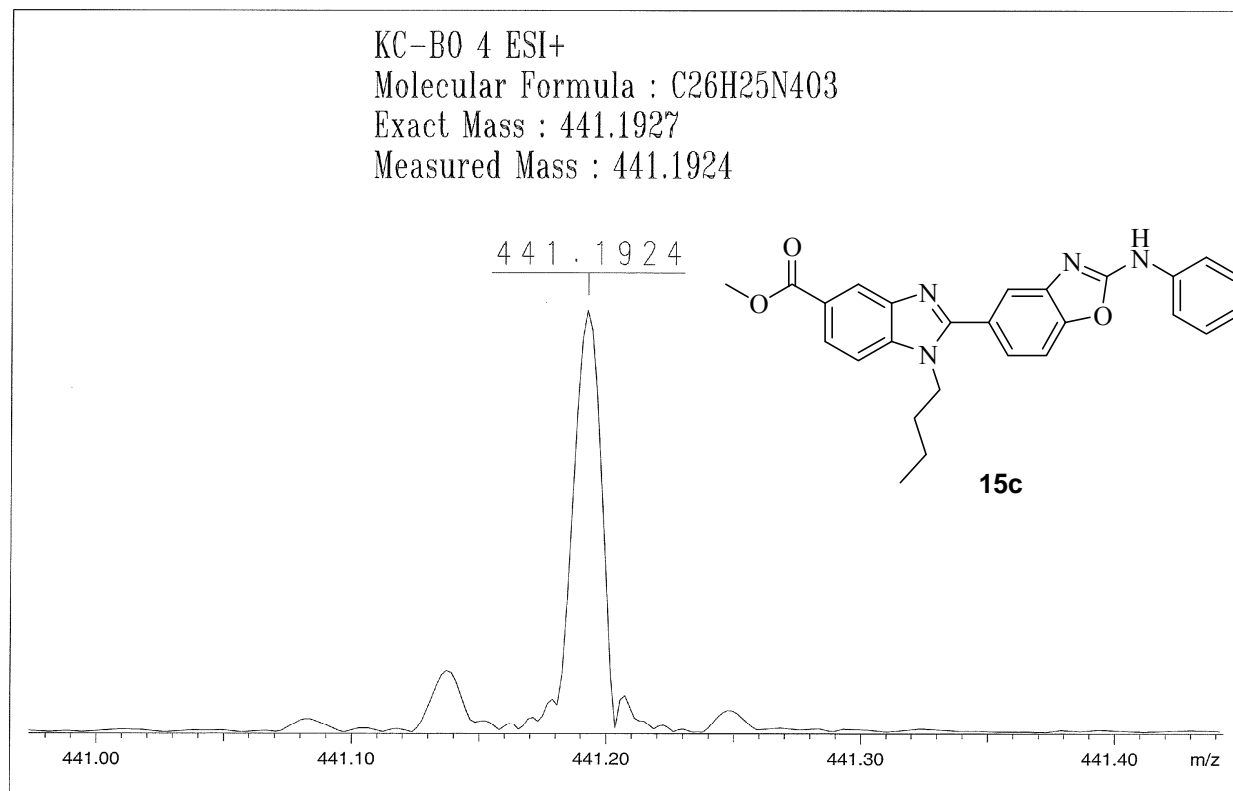


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HR Mass Spectra of Compound 15b

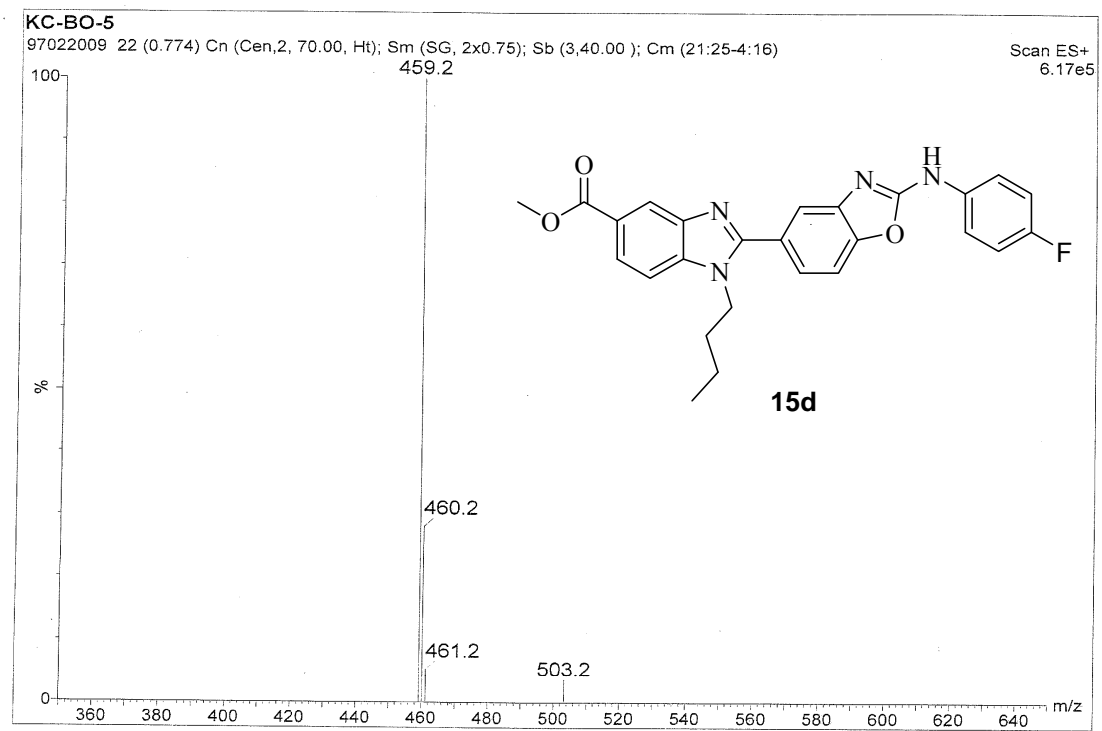


LR Mass Spectra of Compound 15c

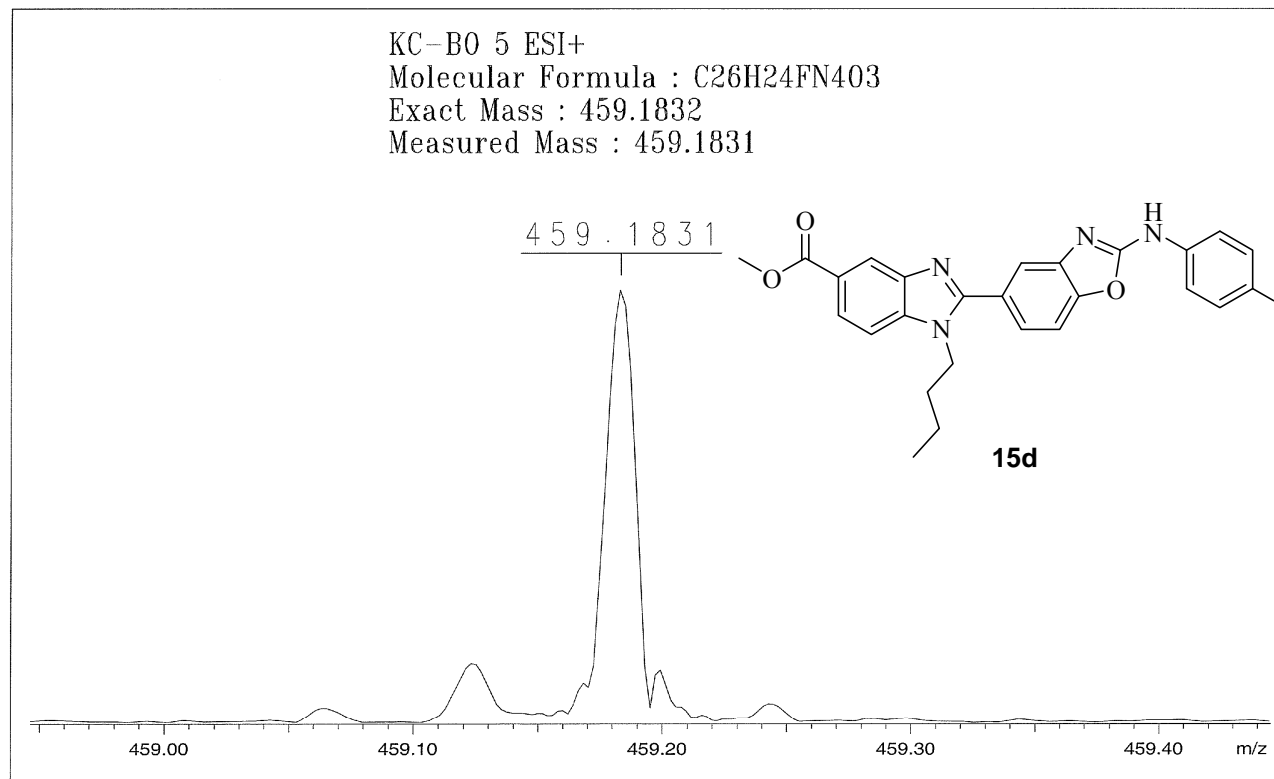


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HR Mass Spectra of Compound 15c

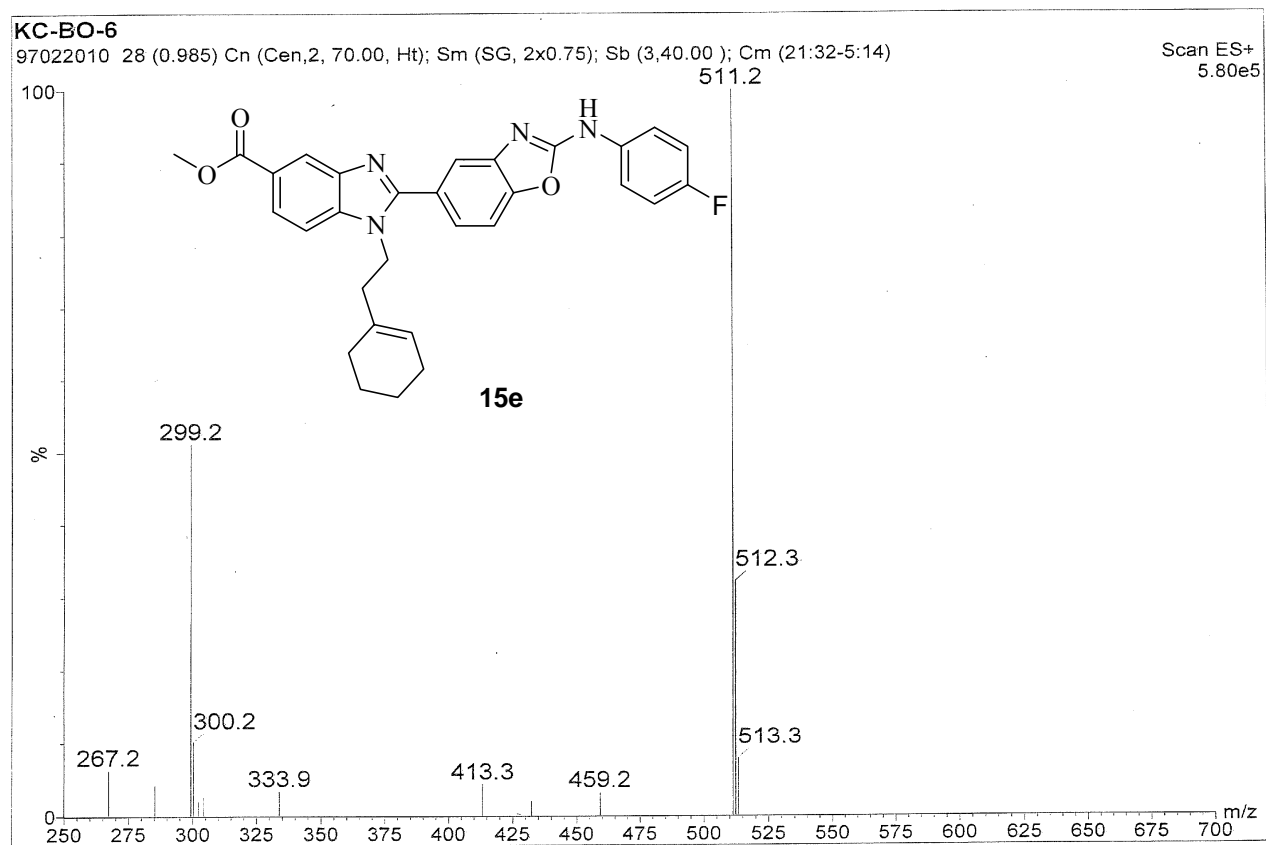


LR Mass Spectra of Compound 15d

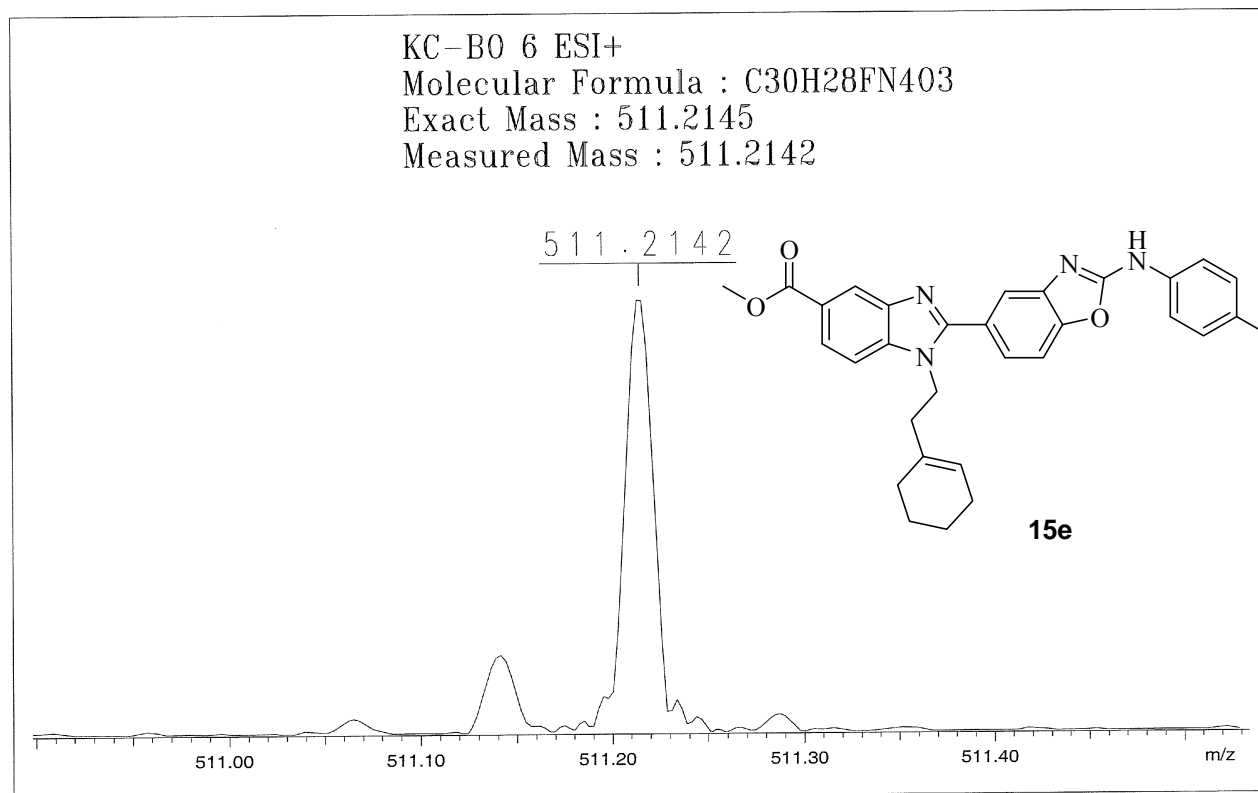


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HR Mass Spectra of Compound 15d

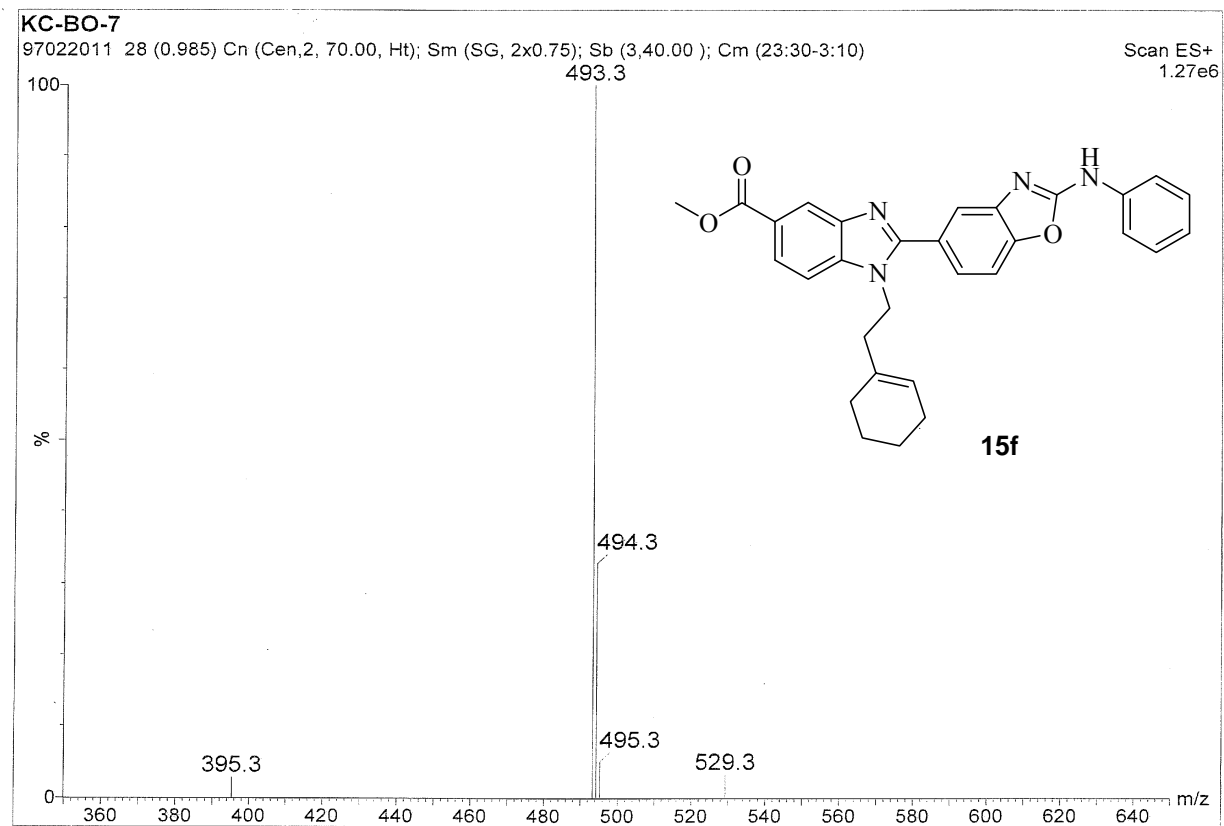


LR Mass Spectra of Compound 15e

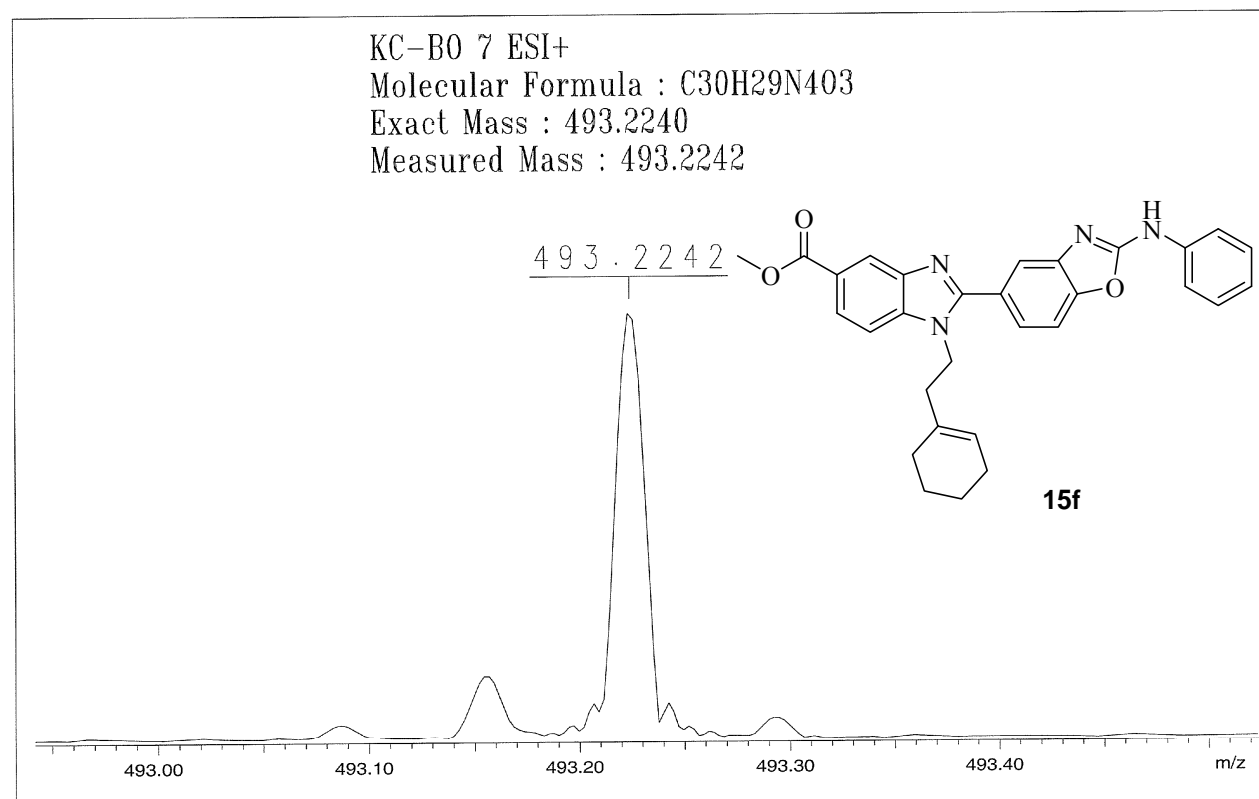


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HR Mass Spectra of Compound 15e

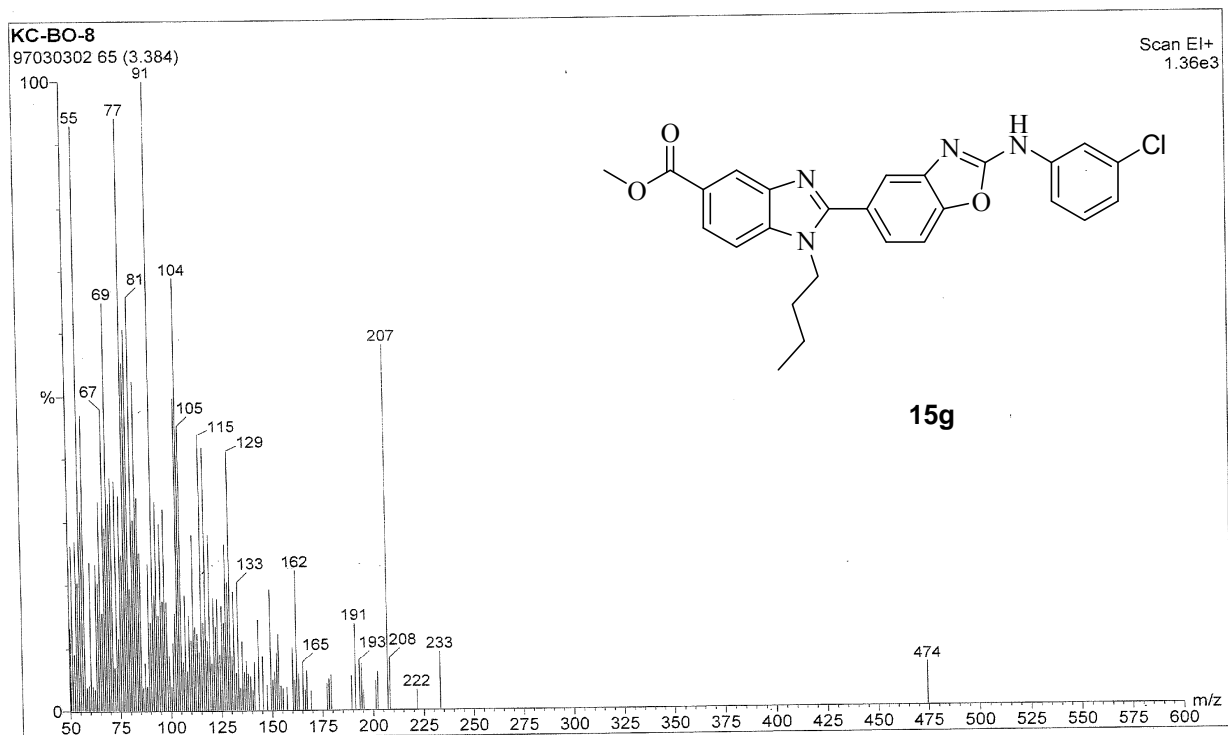


LR Mass Spectra of Compound 15f

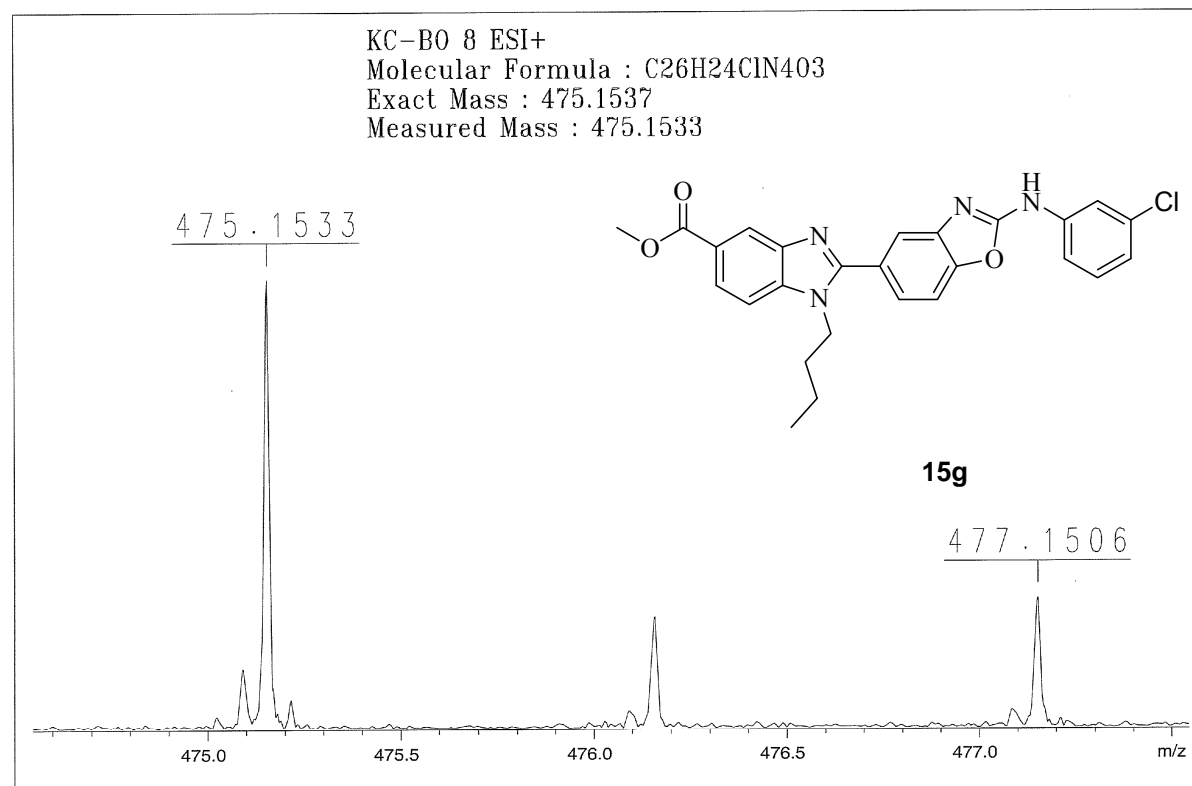


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HR Mass Spectra of Compound 15f

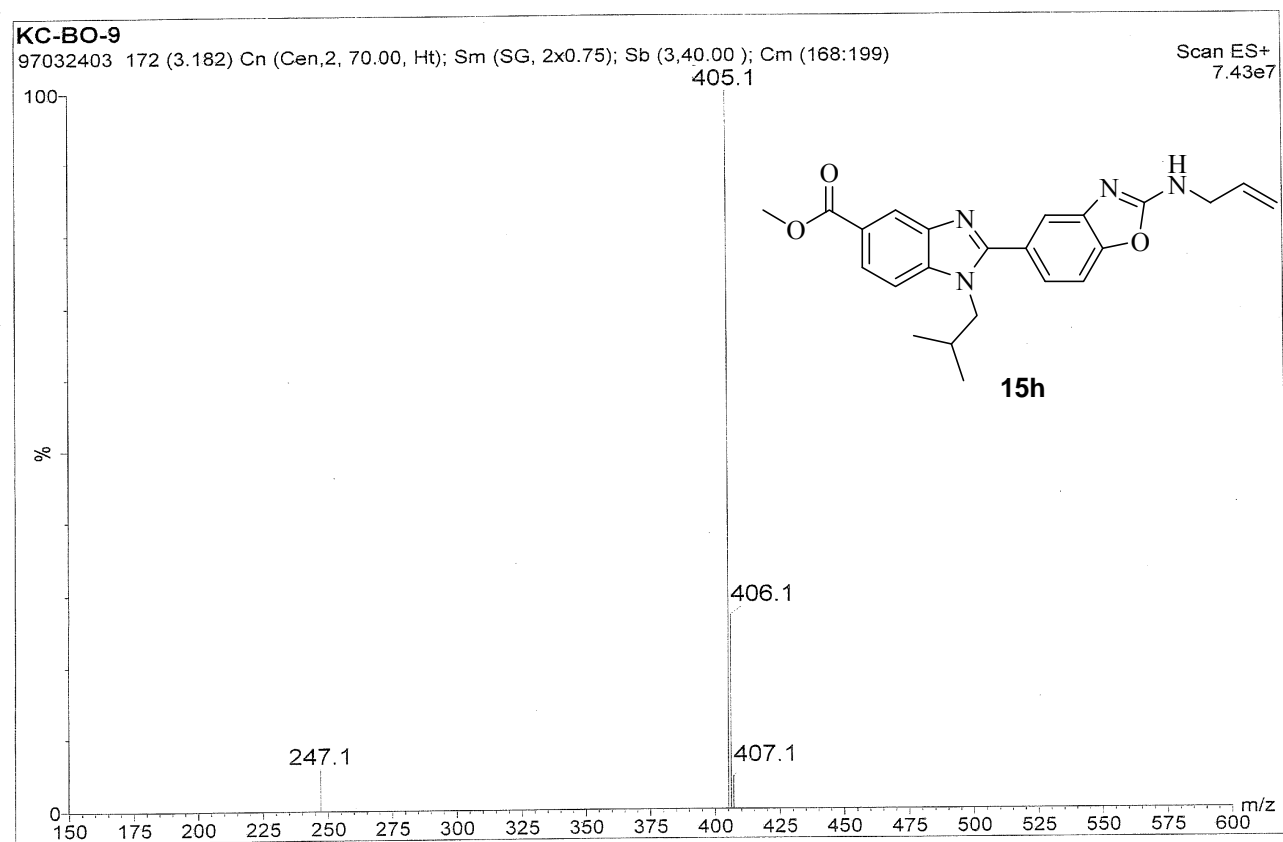


LR Mass Spectra of Compound 15g

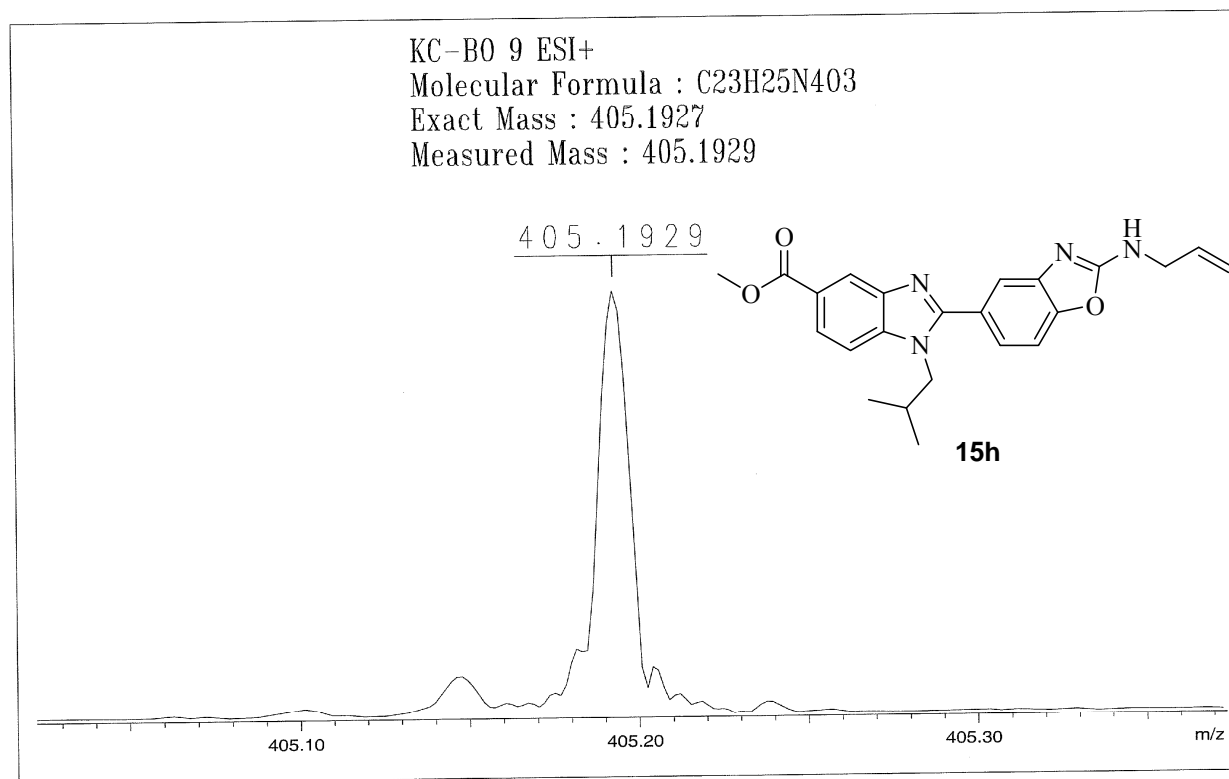


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HR Mass Spectra of Compound 15g

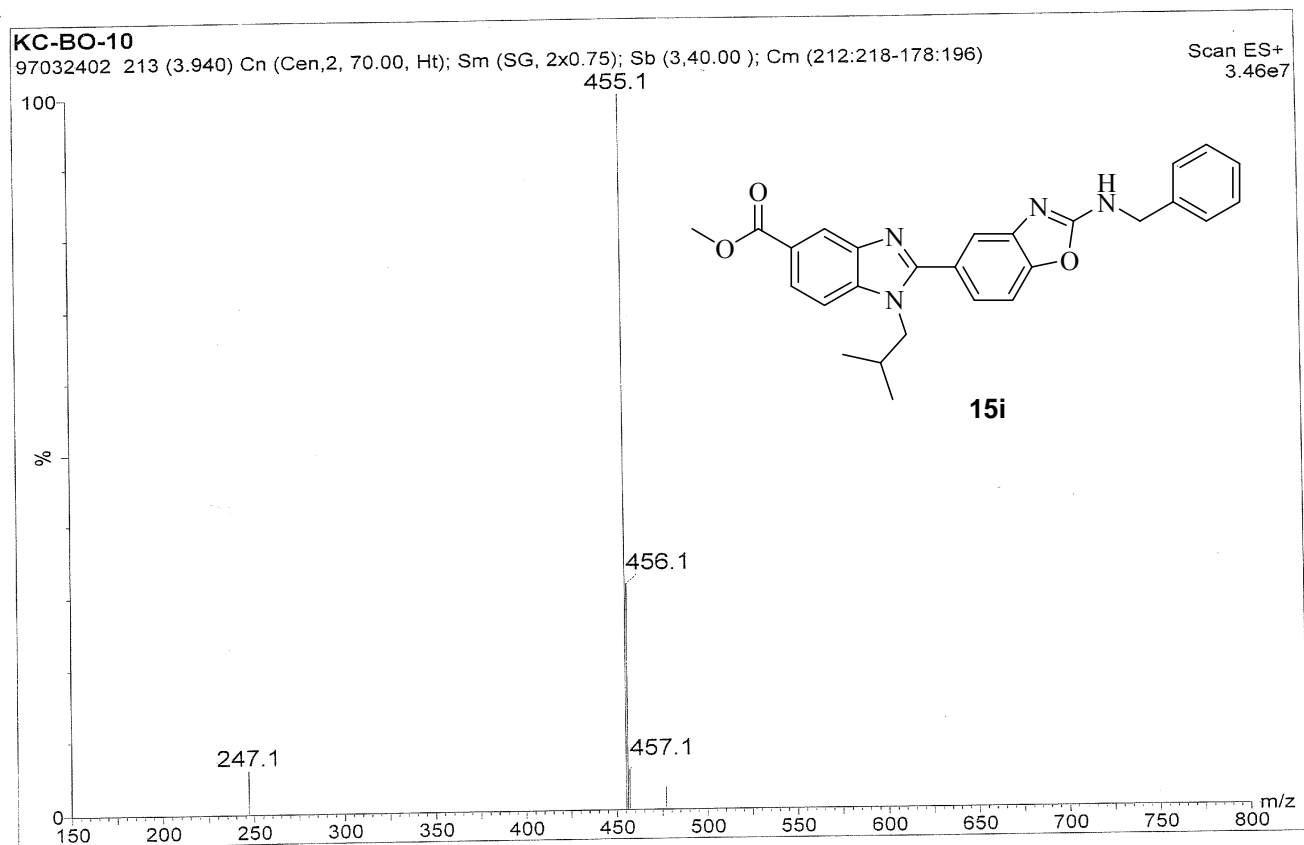


LR Mass Spectra of Compound 15h

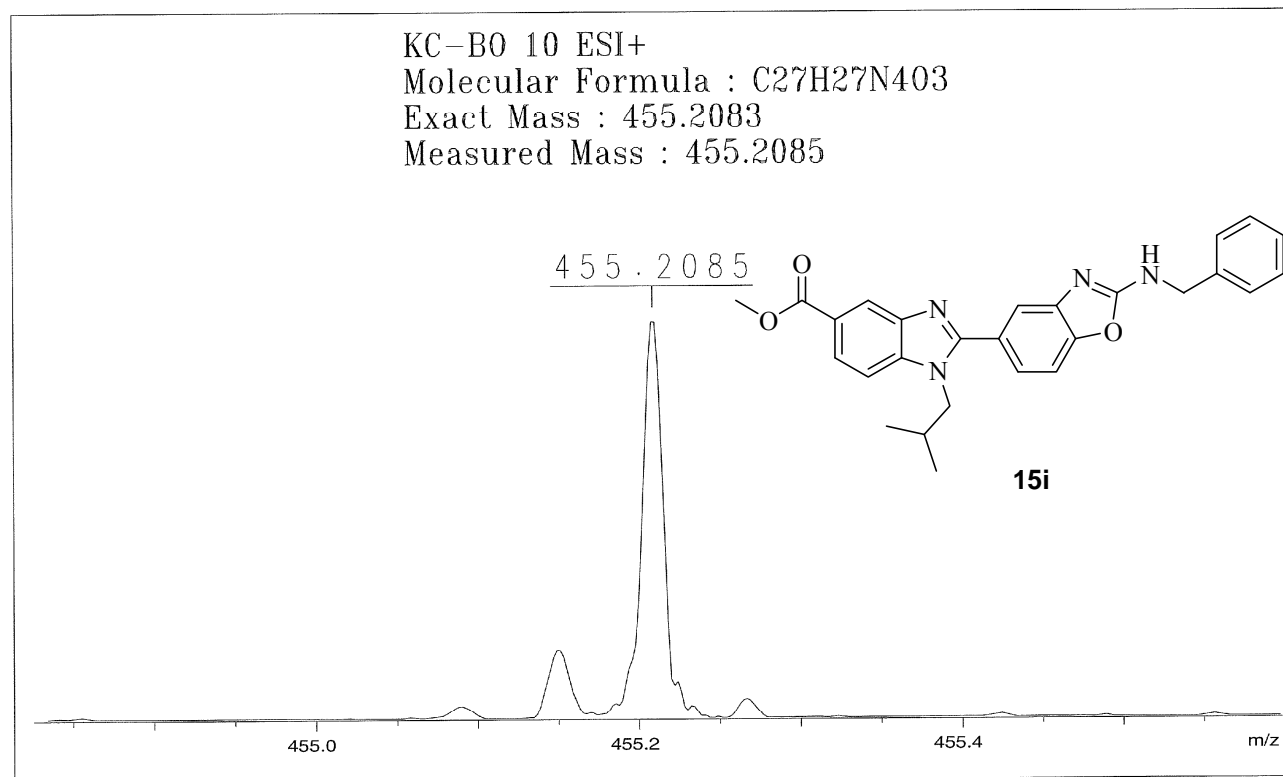


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HR Mass Spectra of Compound 15h

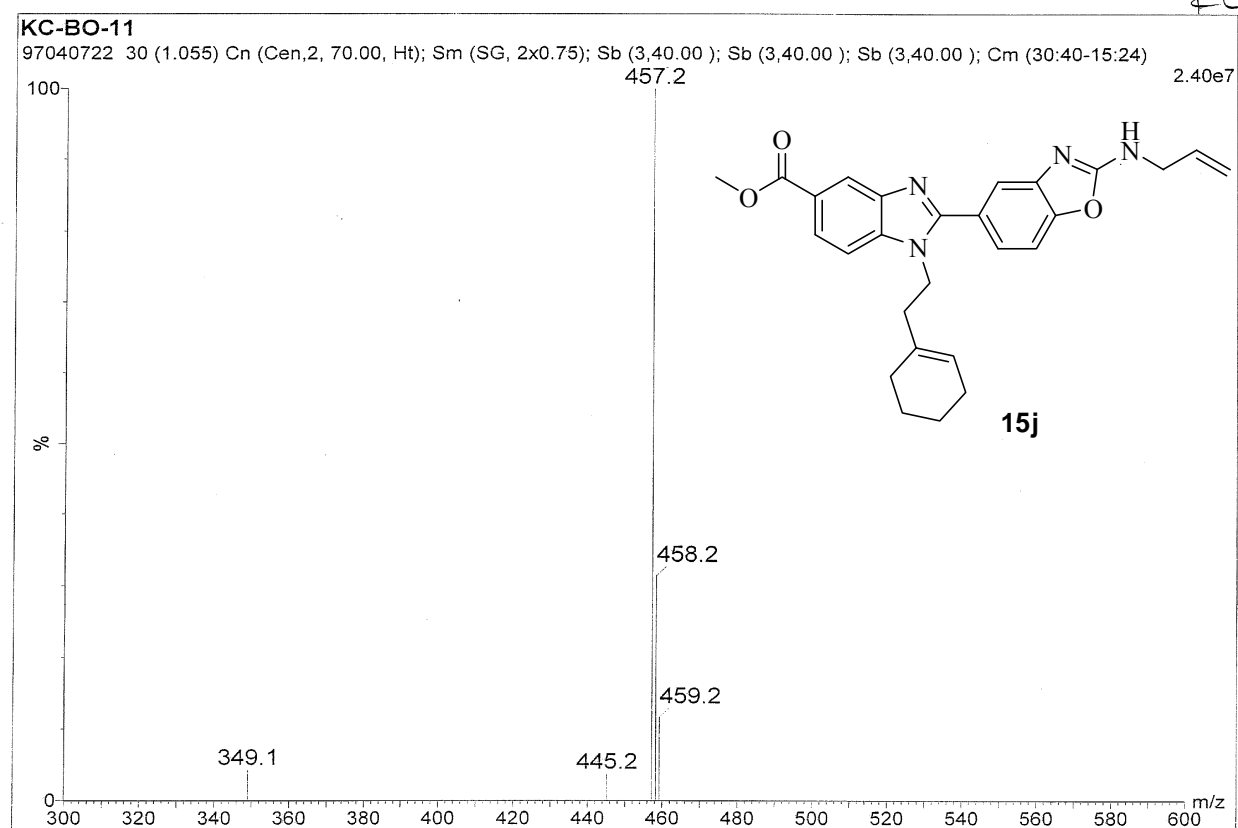


LR Mass Spectra of Compound 15i

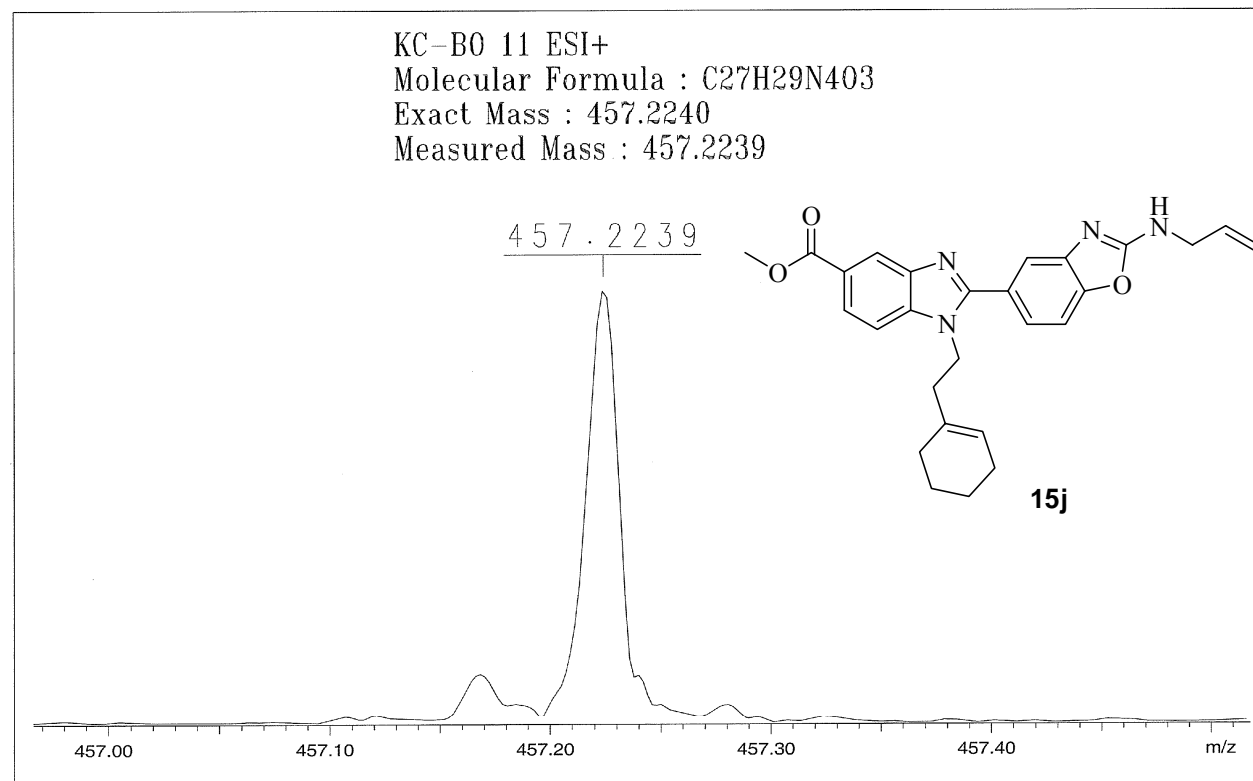


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HR Mass Spectra of Compound 15i

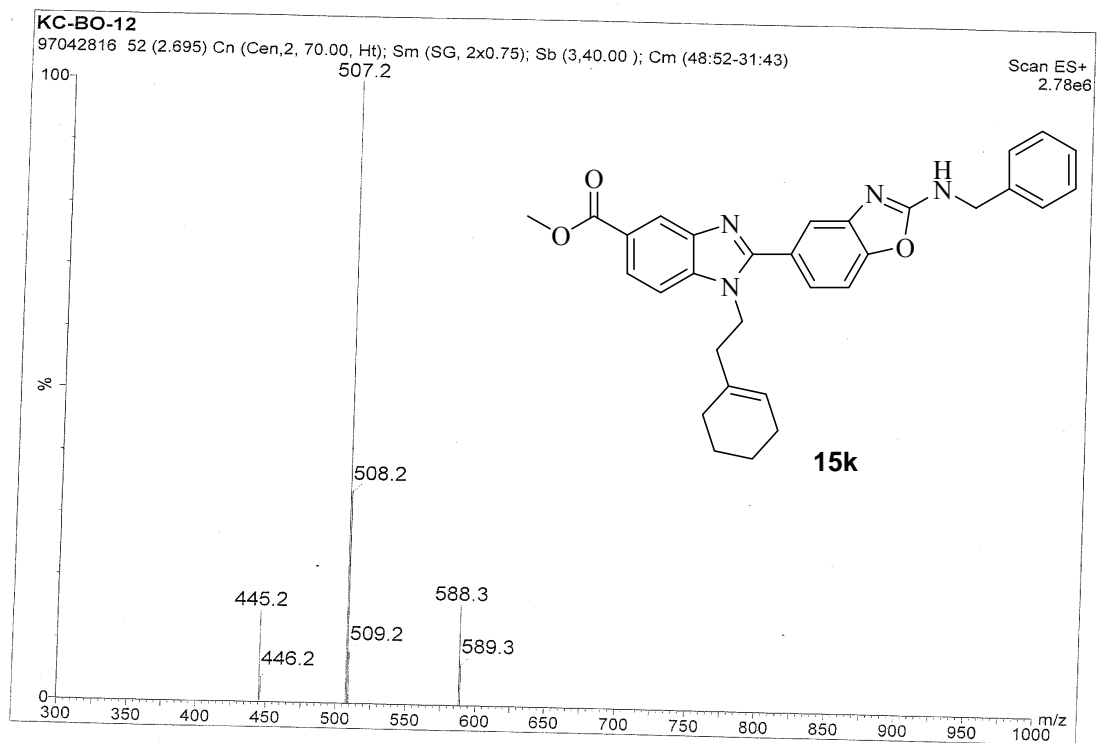


LR Mass Spectra of Compound 15j

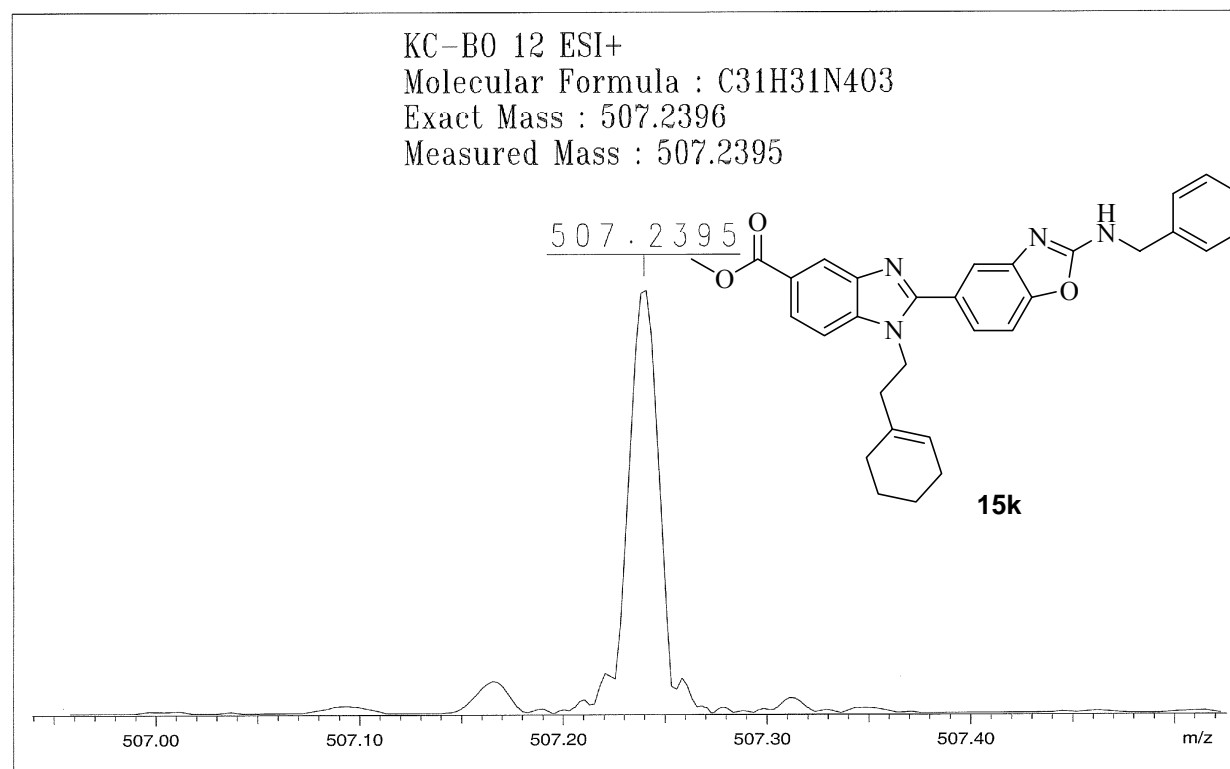


/d=/Data/yl/KCBO11/1/pdata/1 Administrator Thu Aug 7 17:23:48 2008

HR Mass Spectra of Compound 15j

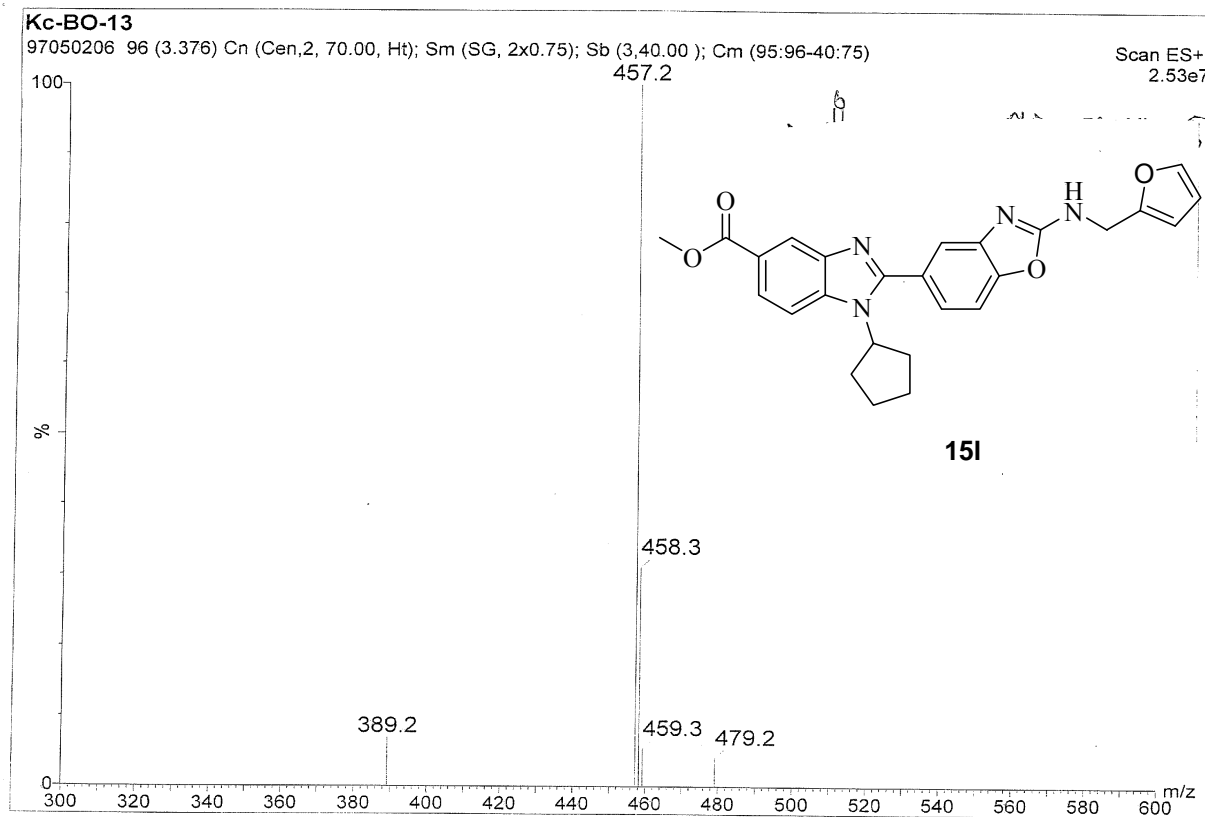


LR Mass Spectra of Compound 15k

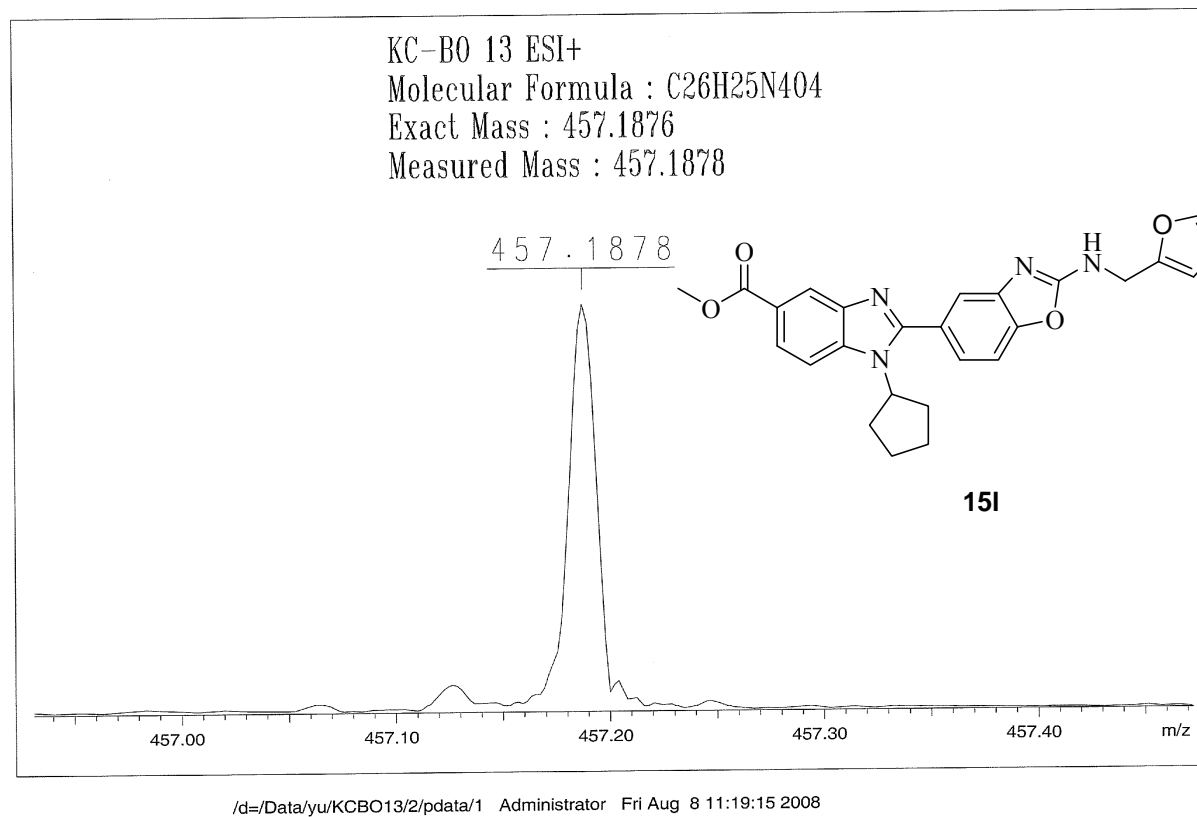


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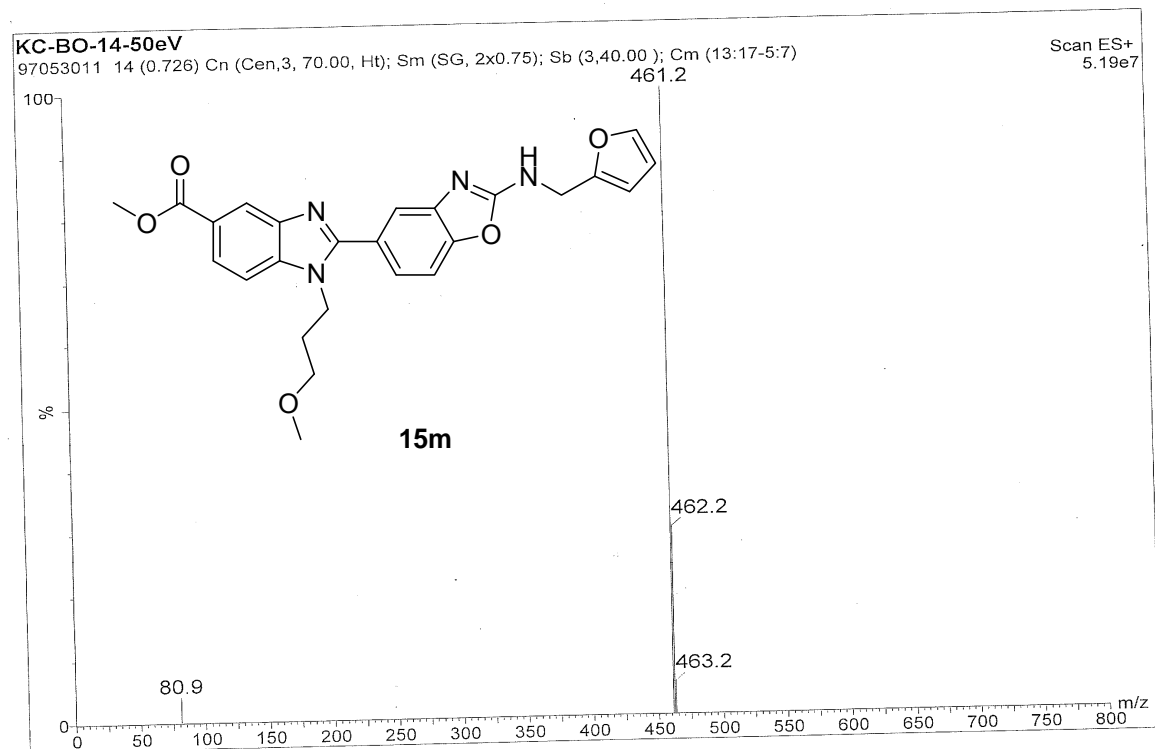
HR Mass Spectra of Compound 15k



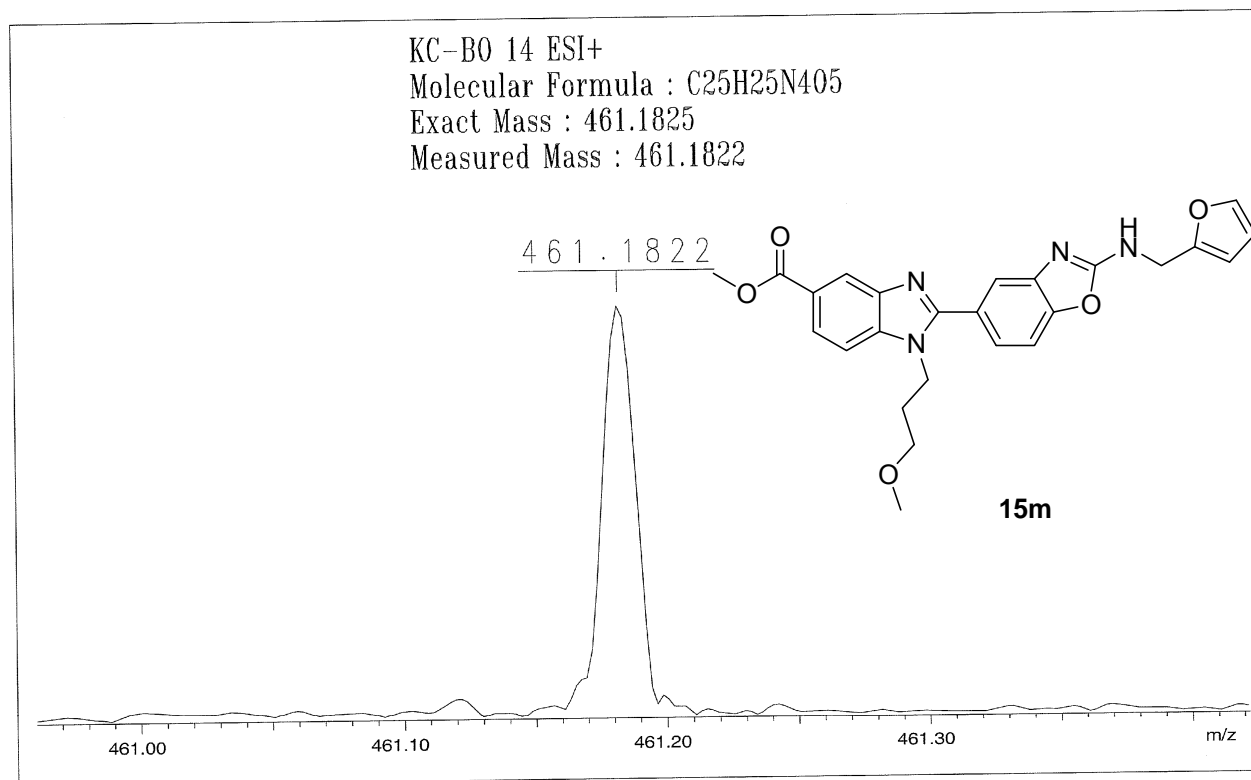
LR Mass Spectra of Compound 15l



HR Mass Spectra of Compound 15I

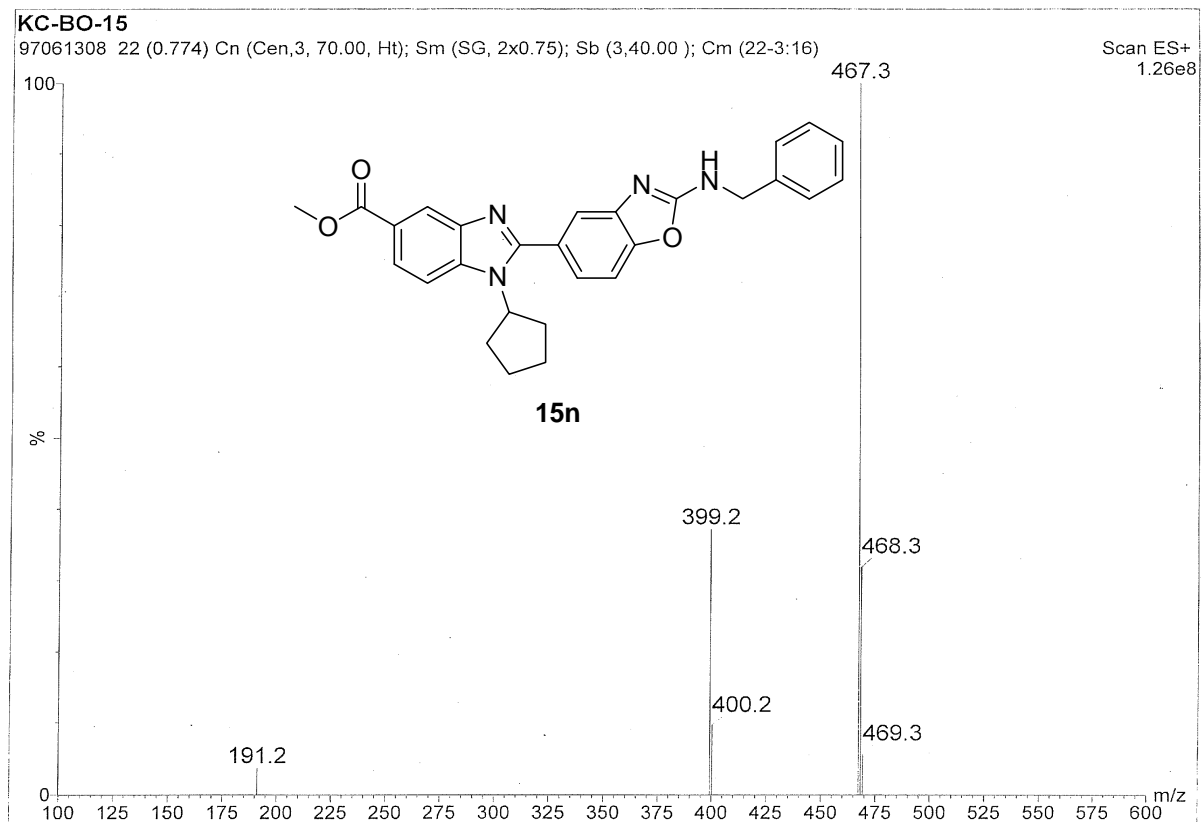


LR Mass Spectra of Compound 15m

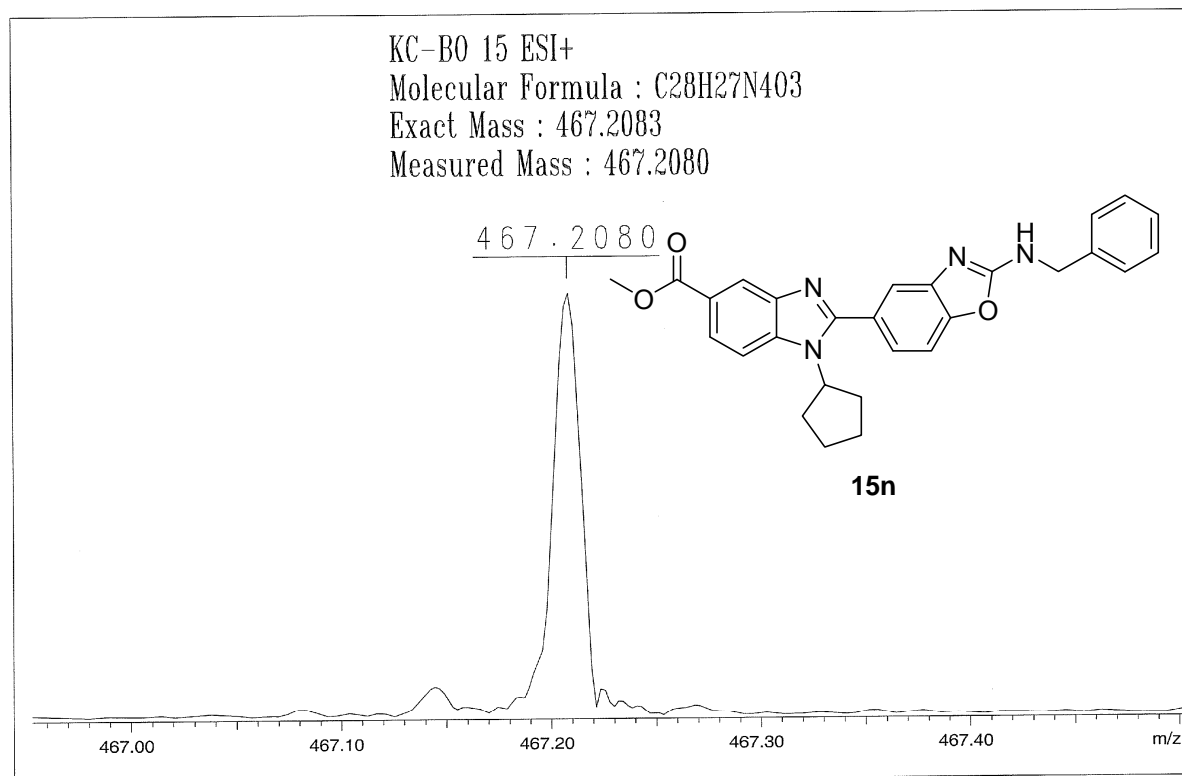


/d=/Data/you/KCBO14/2/pdata/1 Administrator Fri Aug 8 11:28:30 2008

HR Mass Spectra of Compound 15m

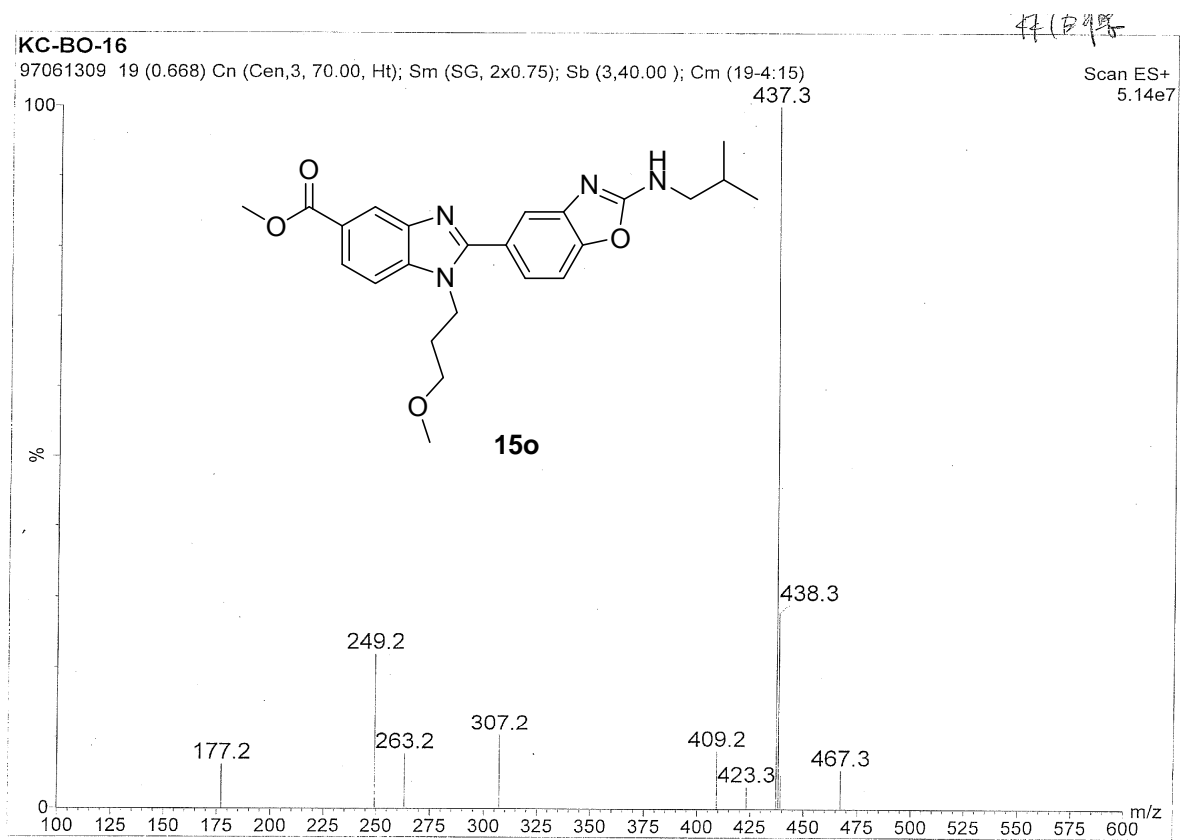


LR Mass Spectra of Compound 15n

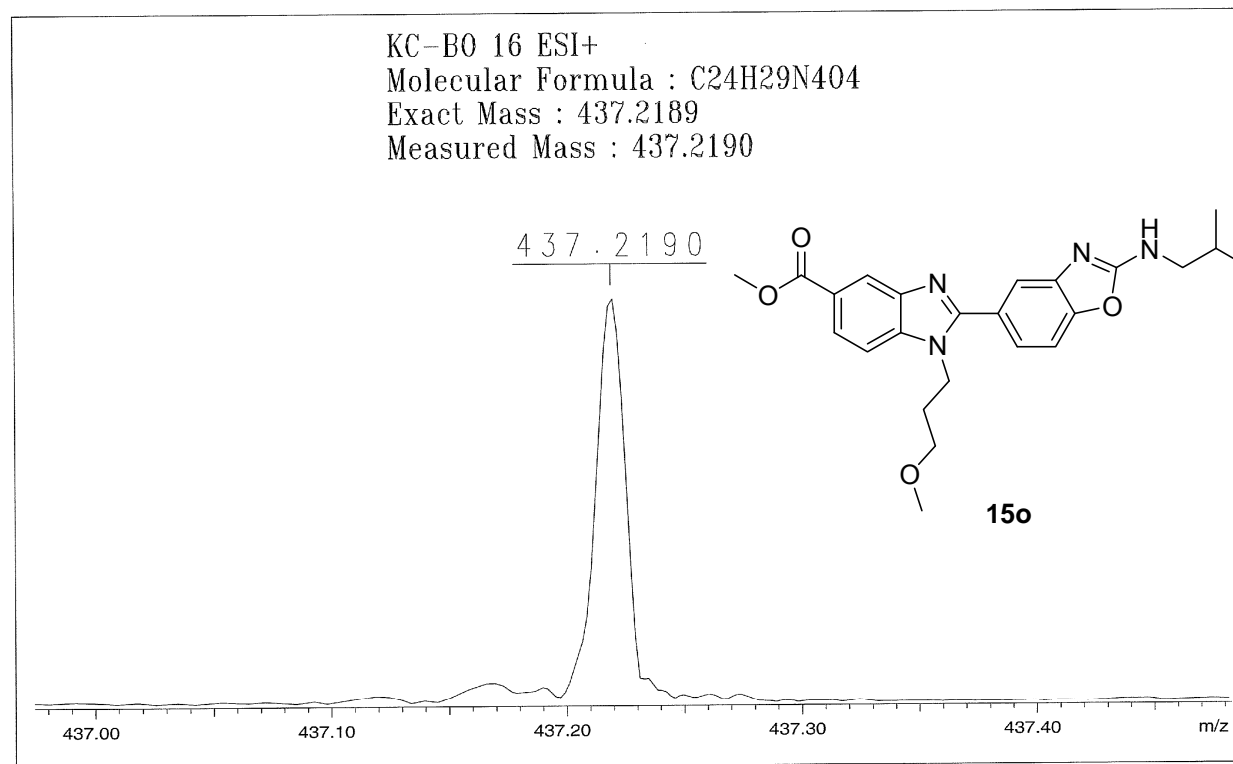


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HR Mass Spectra of Compound 15n

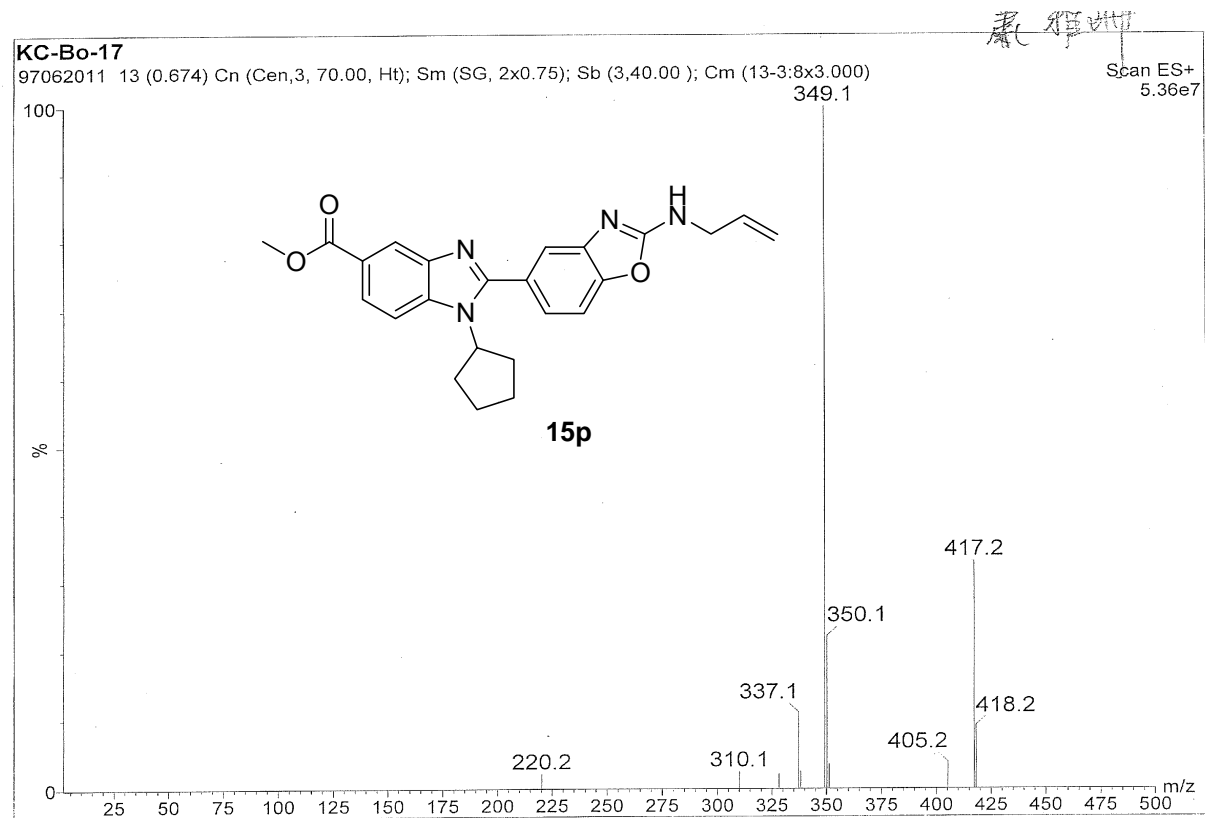


LR Mass Spectra of Compound 15o

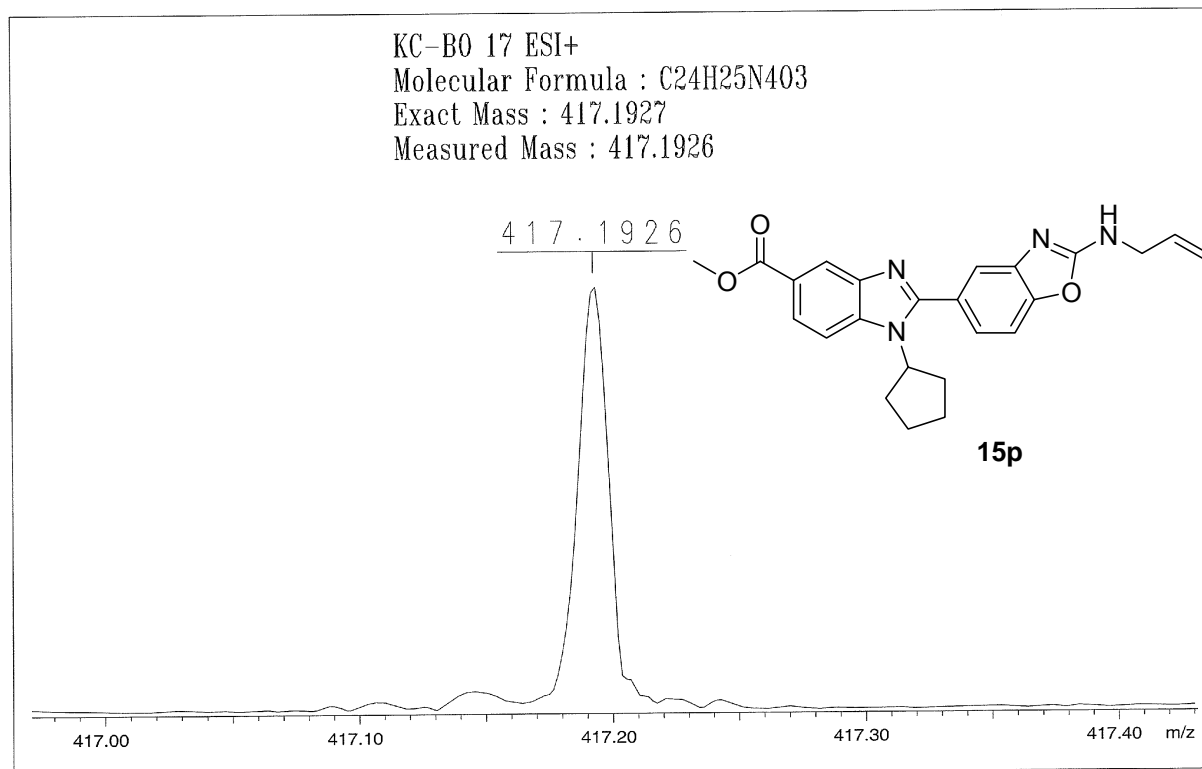


/d=/Data/yy/KCBO16/1/pdata/1 Administrator Fri Aug 8 11:59:16 2008

HR Mass Spectra of Compound 15o

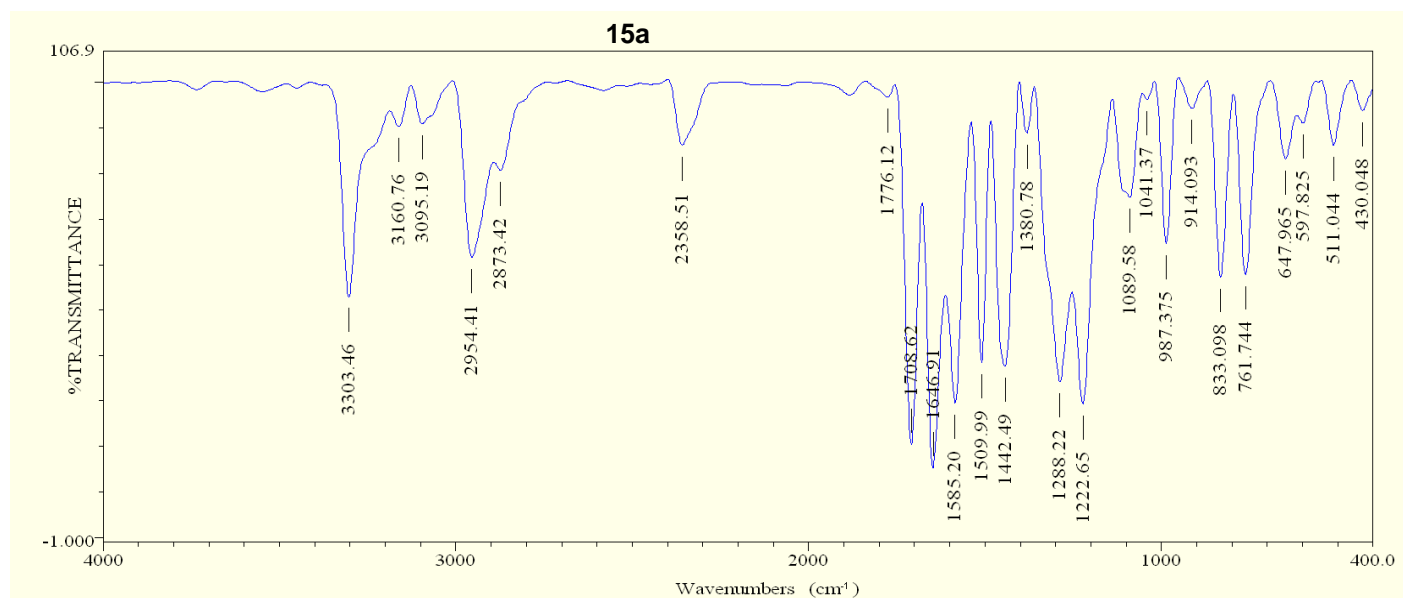
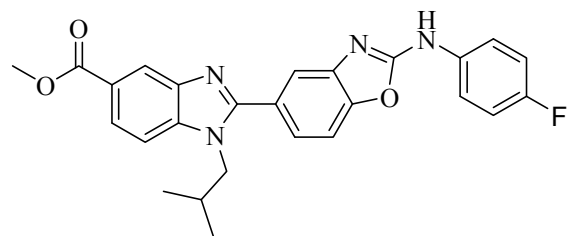


LR Mass Spectra of Compound 15p

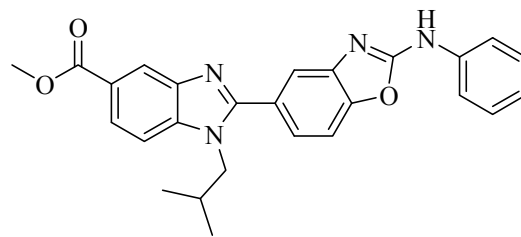


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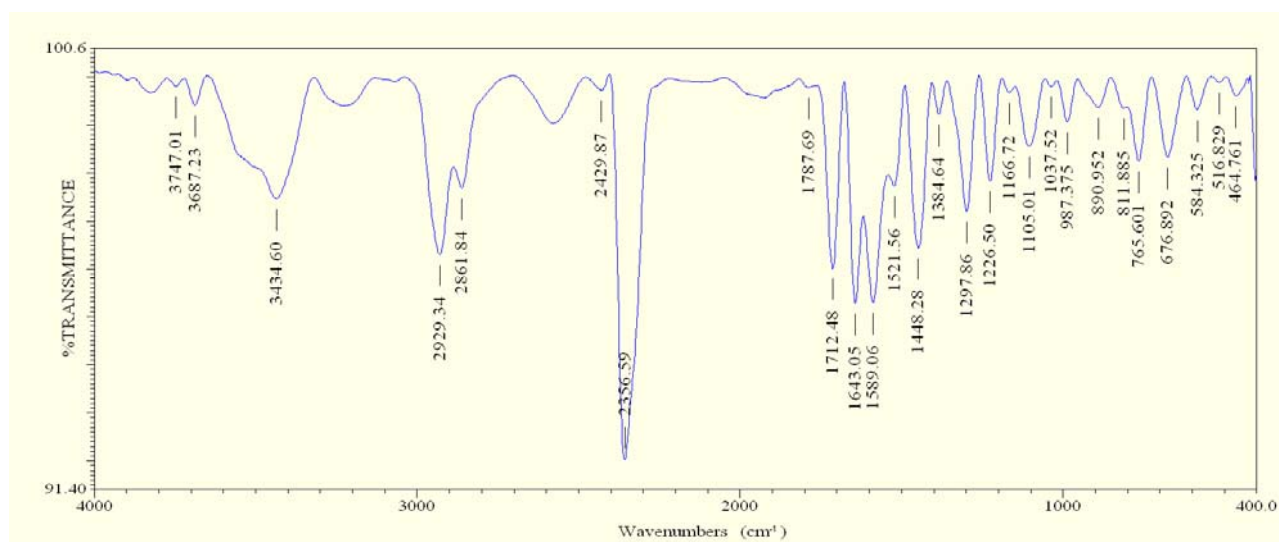
HR Mass Spectra of Compound 15p



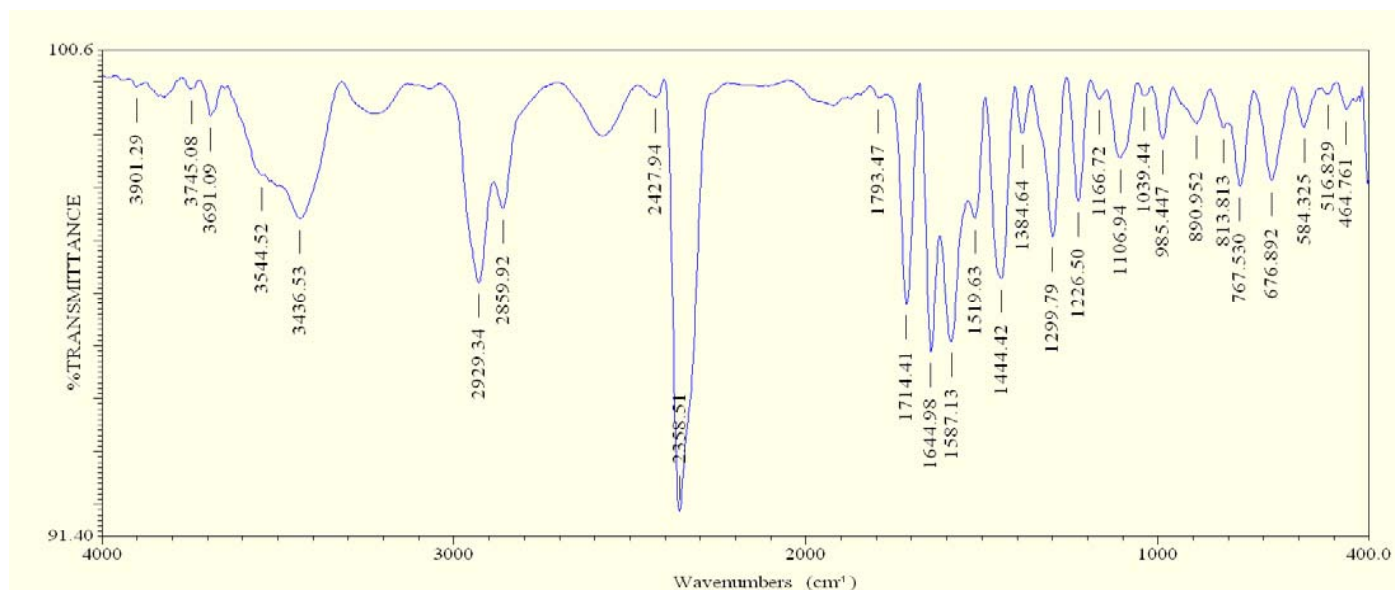
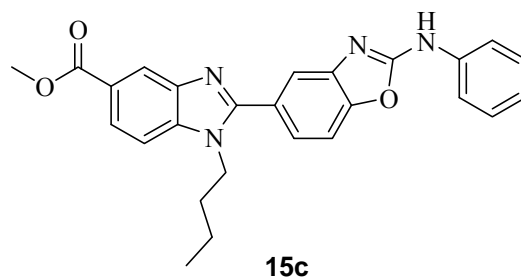
IR Spectra of Compound 15a



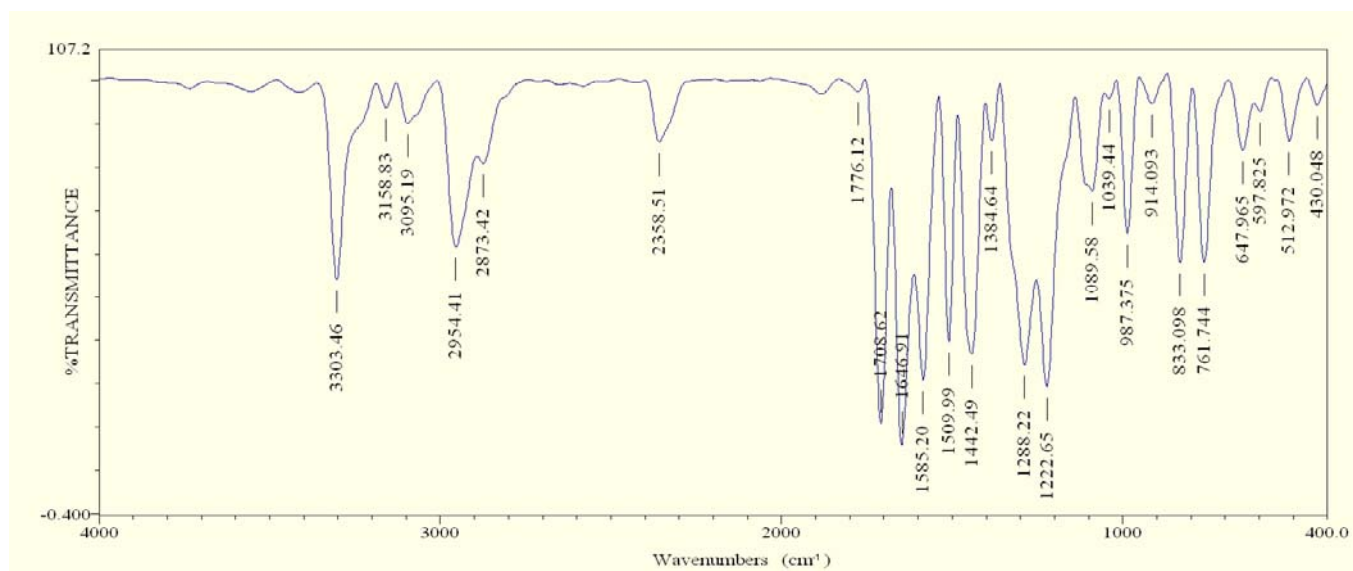
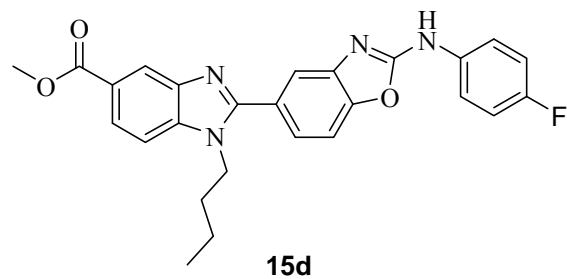
15b



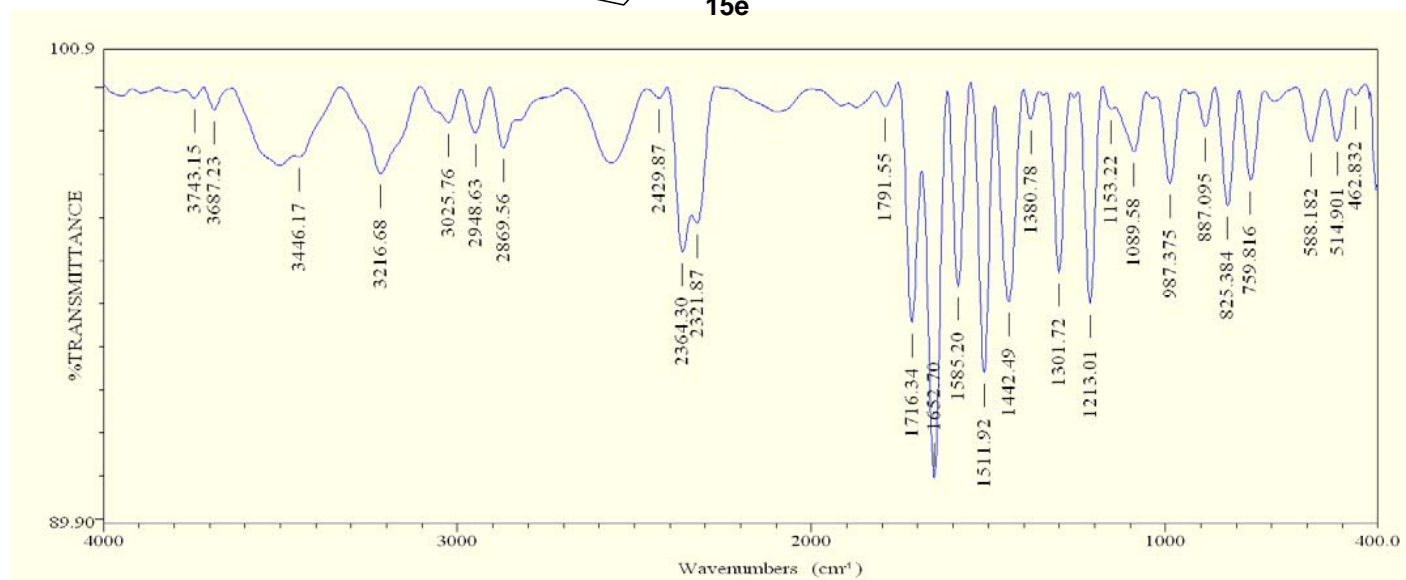
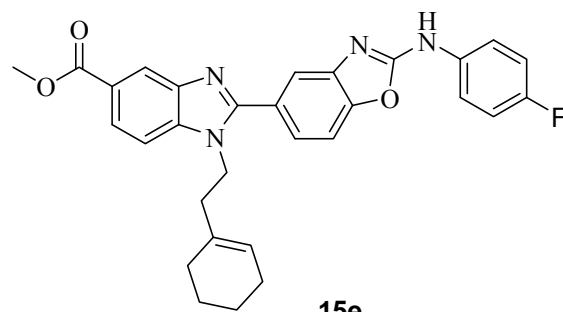
IR Spectra of Compound 15b



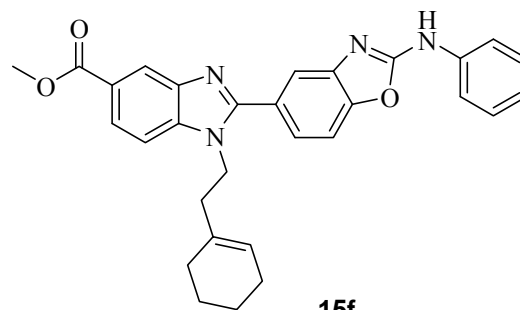
IR Spectra of Compound 15c



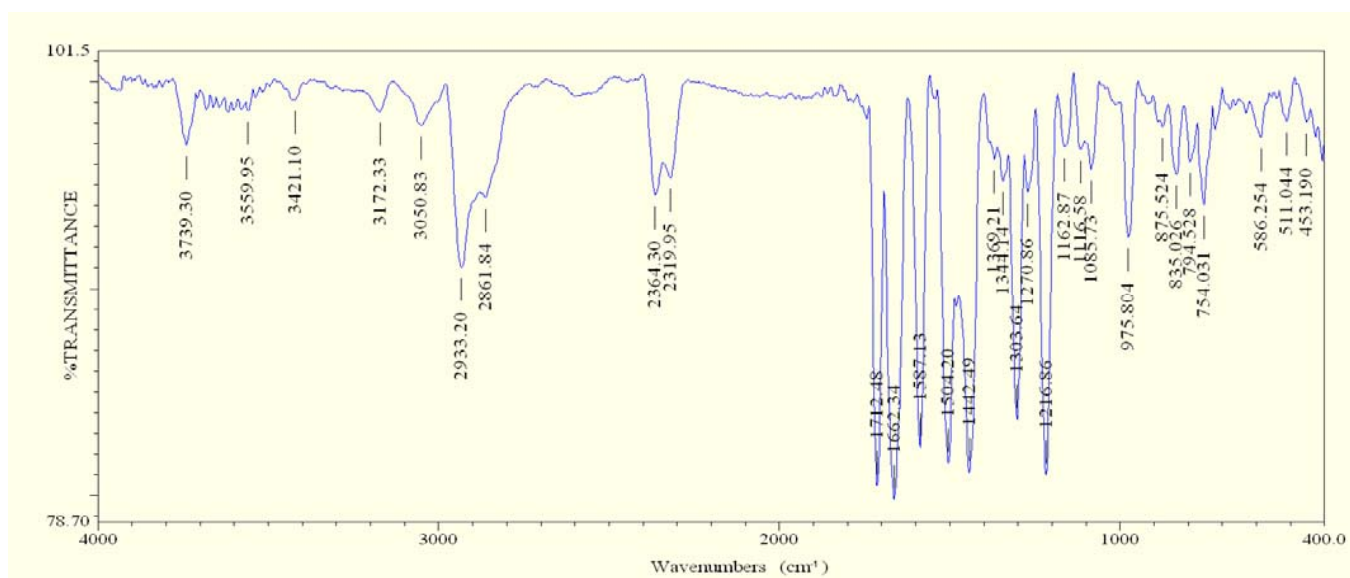
IR Spectra of Compound 15d



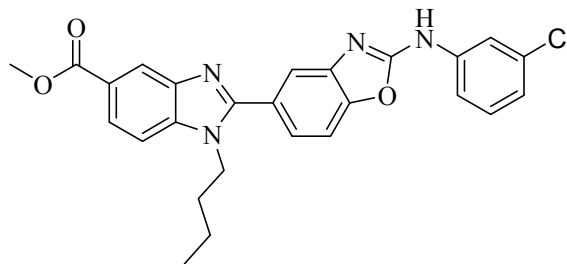
IR Spectra of Compound 15e



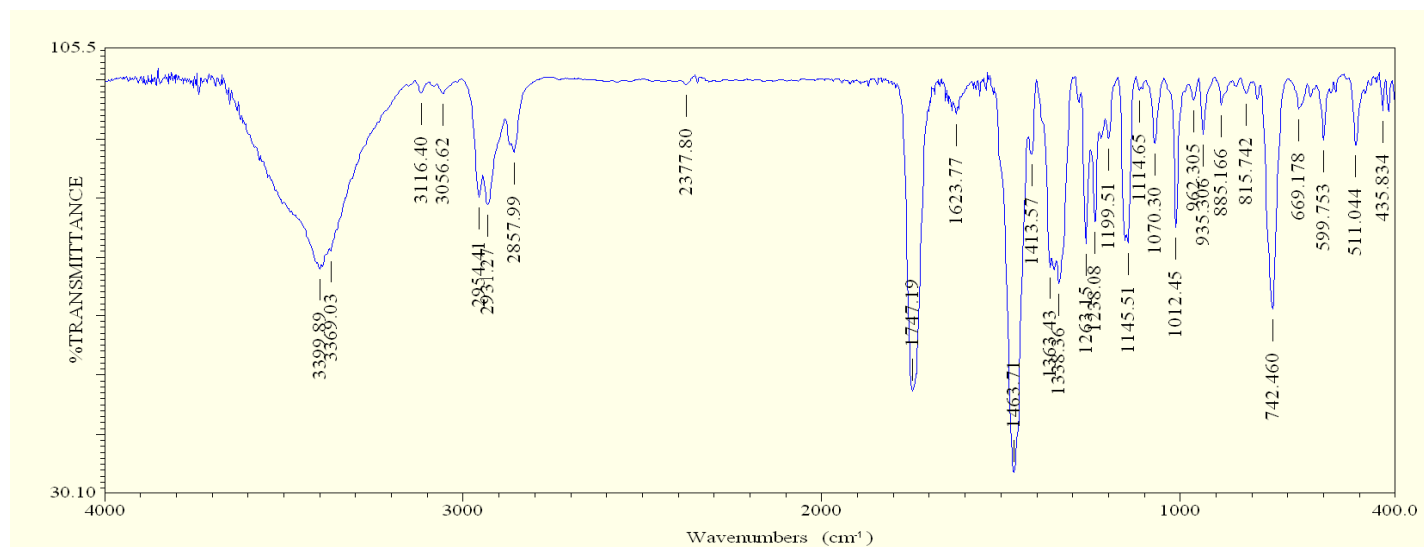
15f



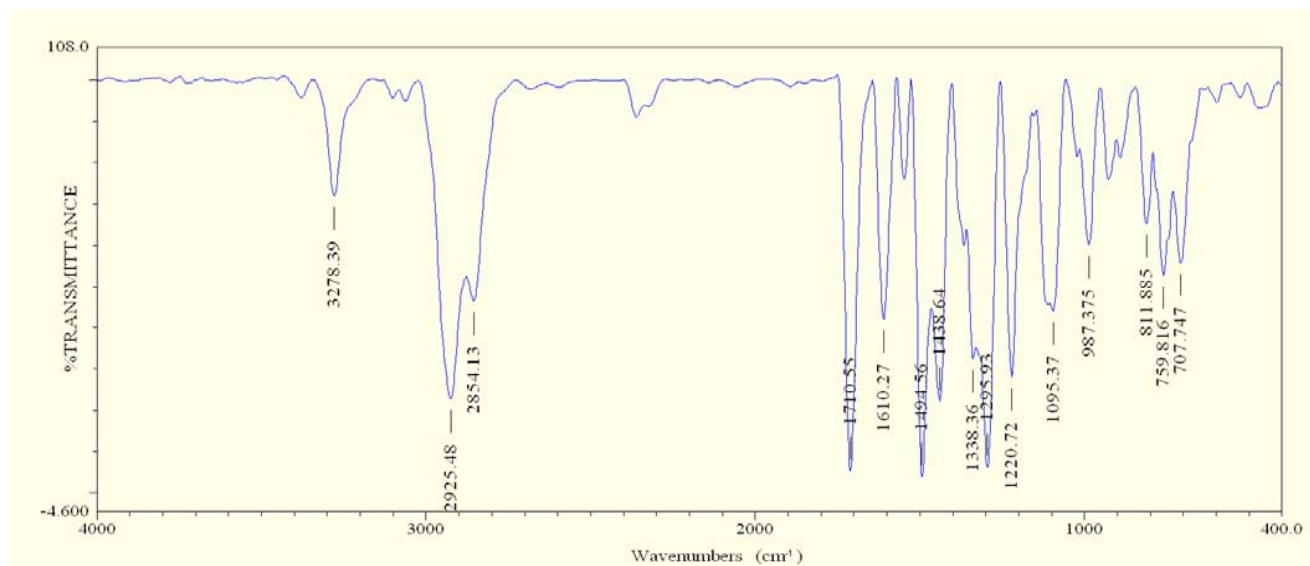
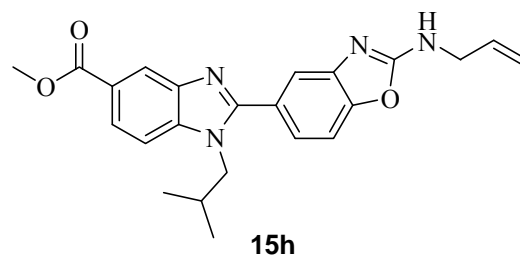
IR Spectra of Compound 15f



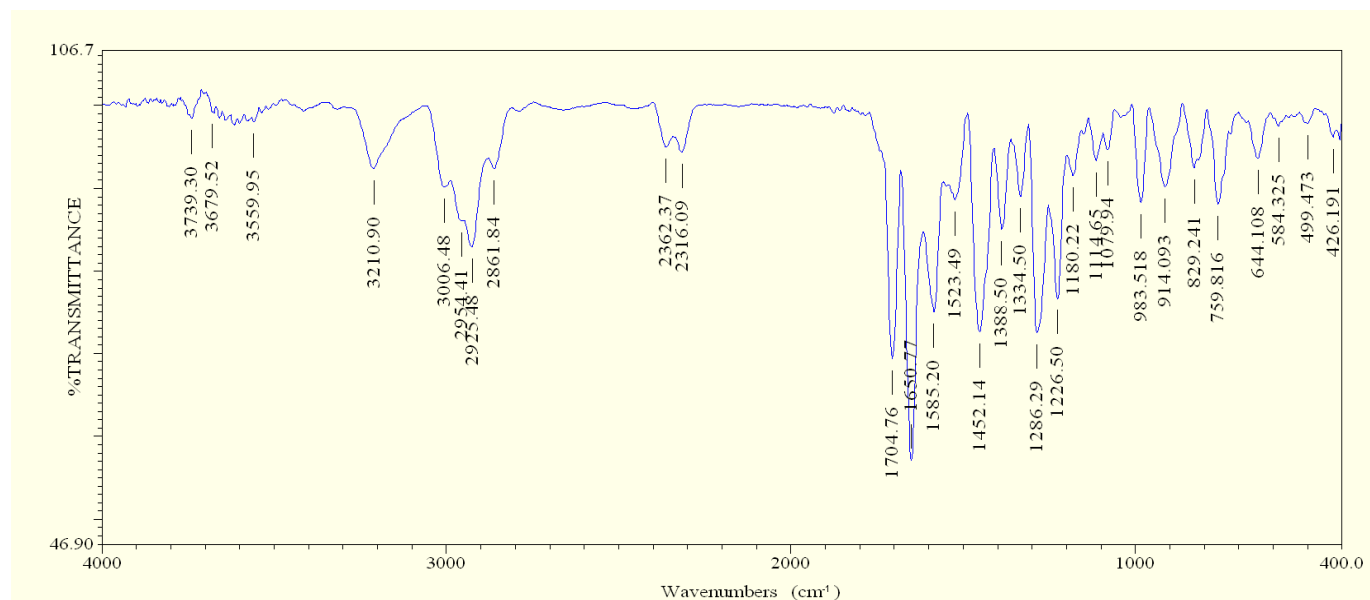
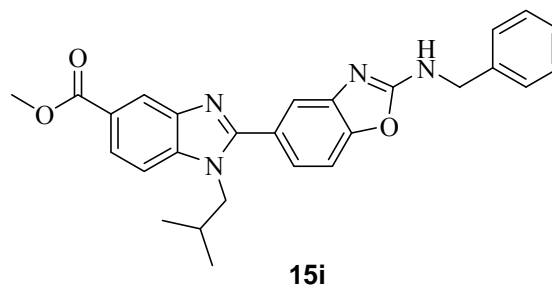
15g



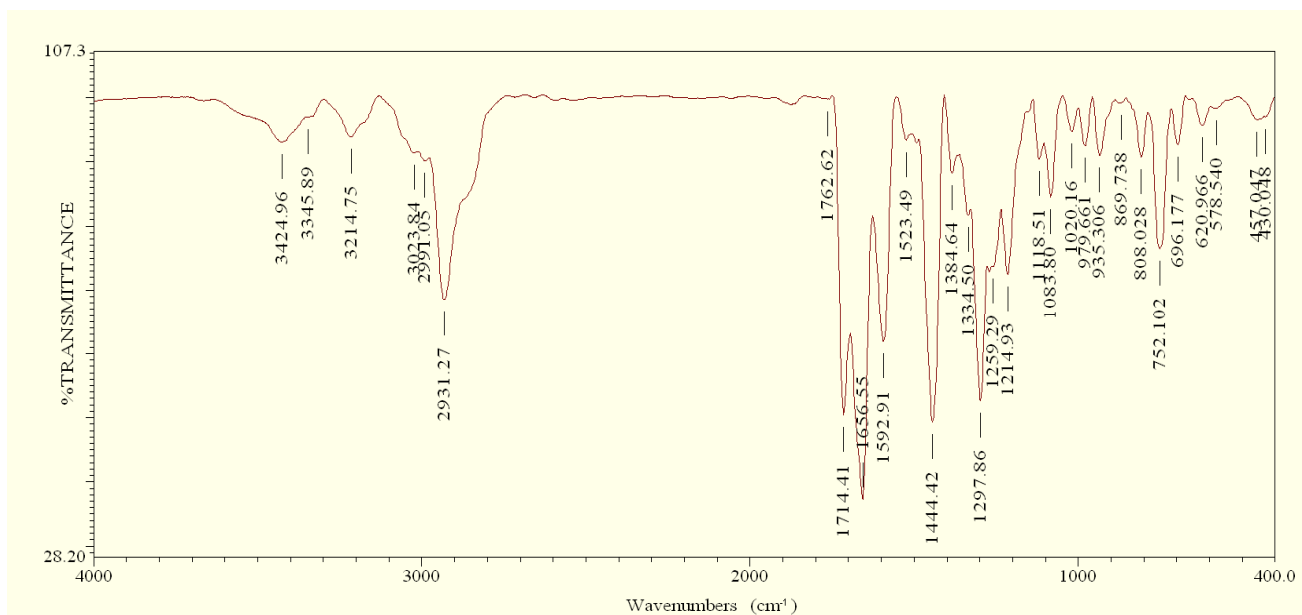
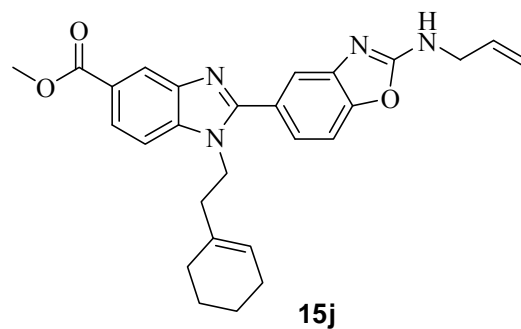
IR Spectra of Compound 15g



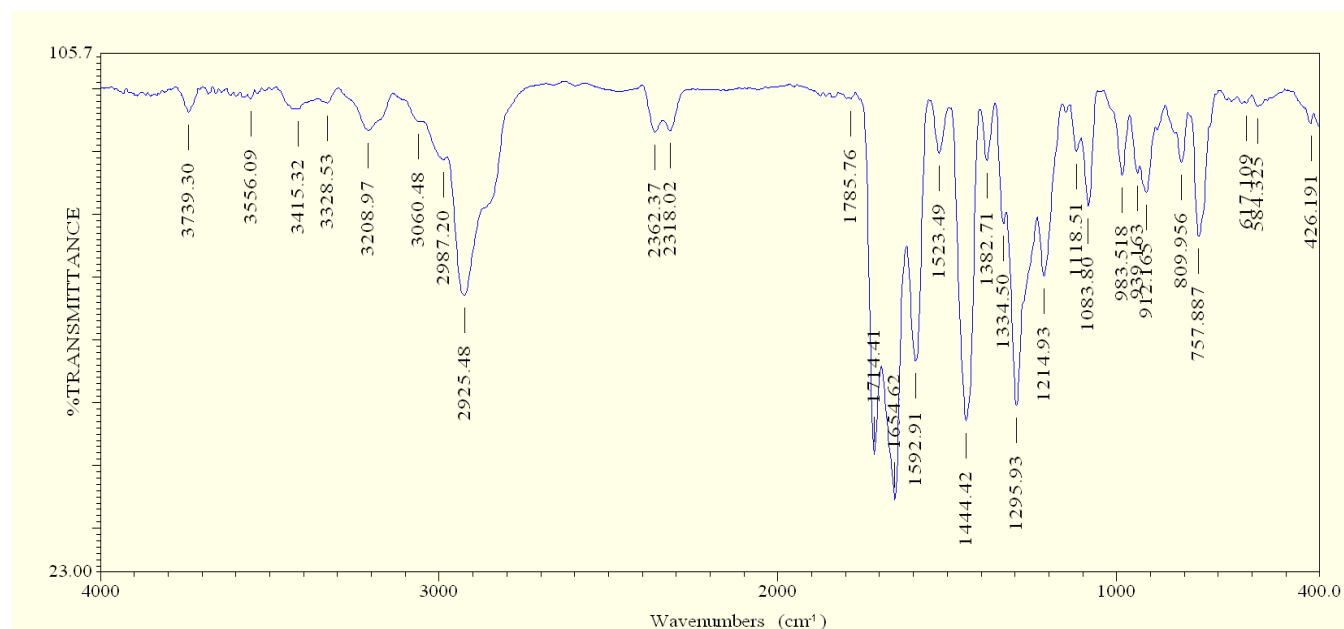
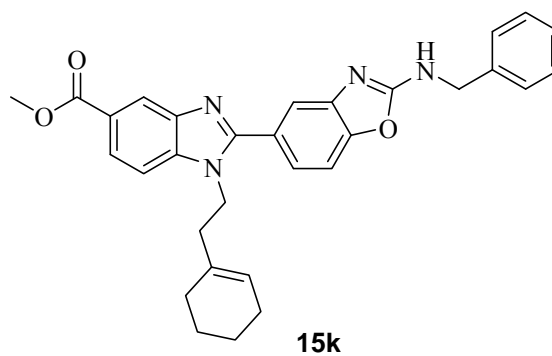
IR Spectra of Compound 15h



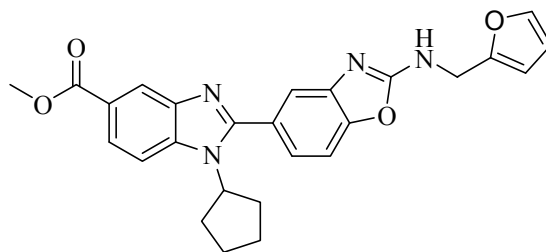
IR Spectra of Compound 15i



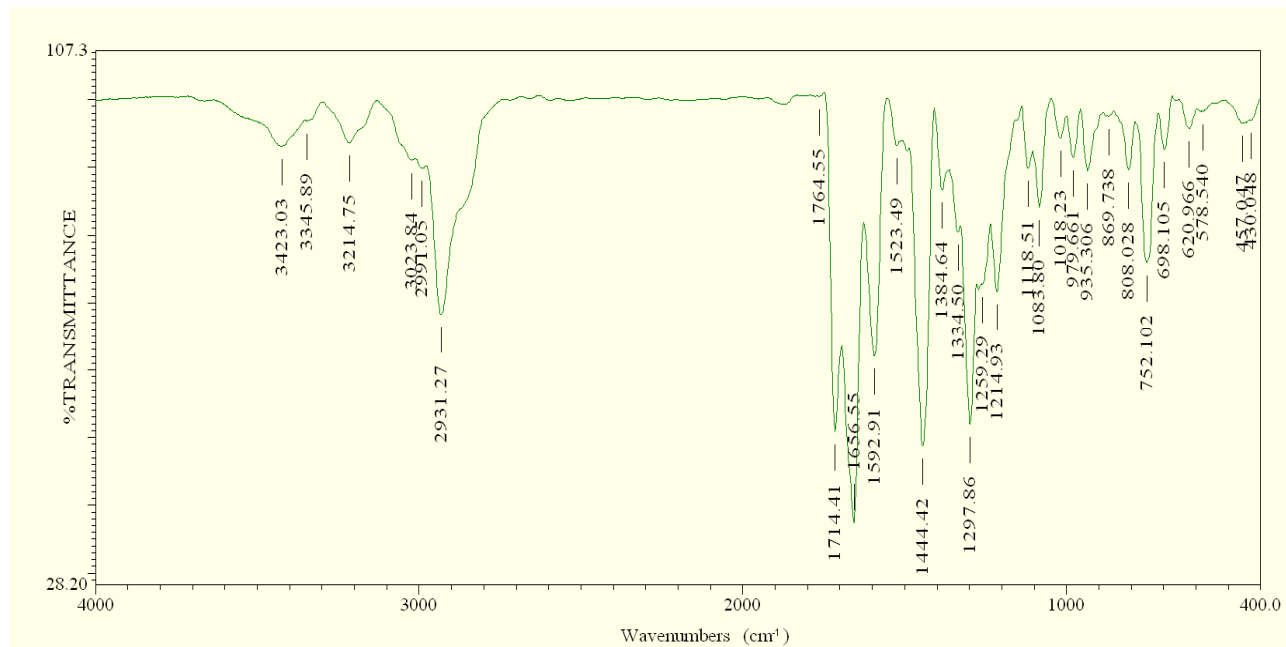
IR Spectra of Compound 15j



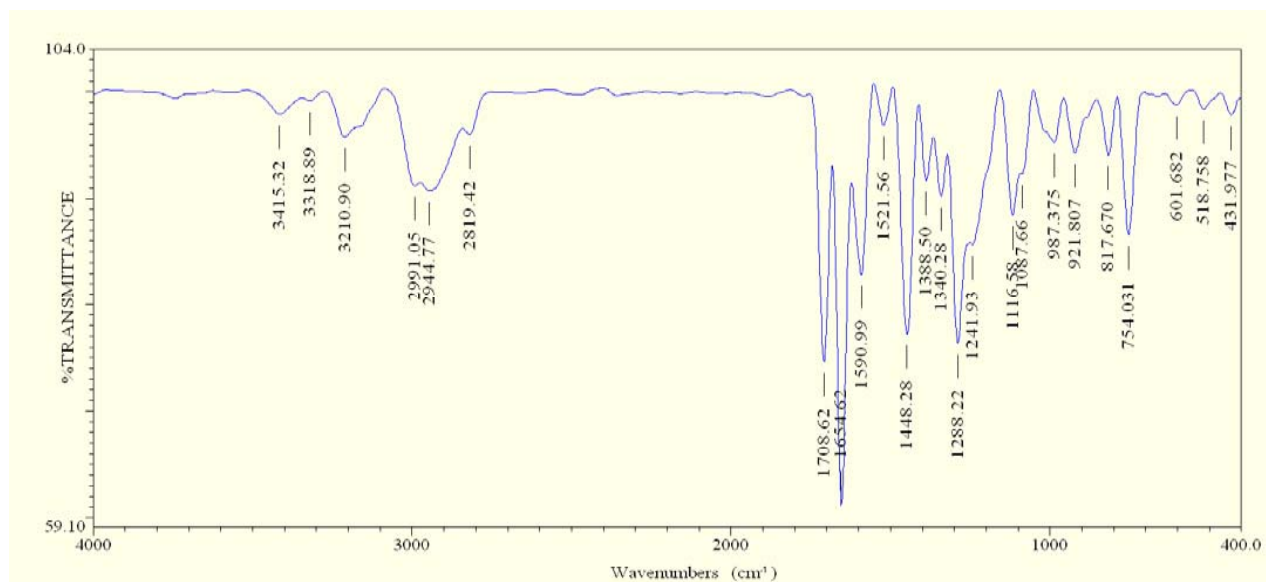
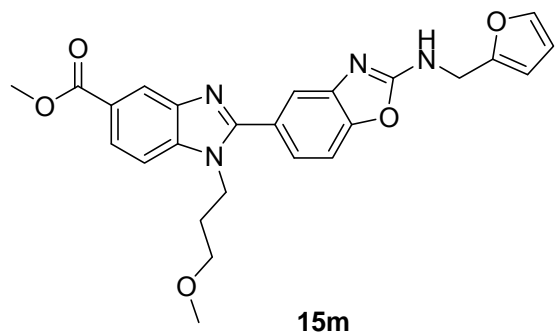
IR Spectra of Compound 15k



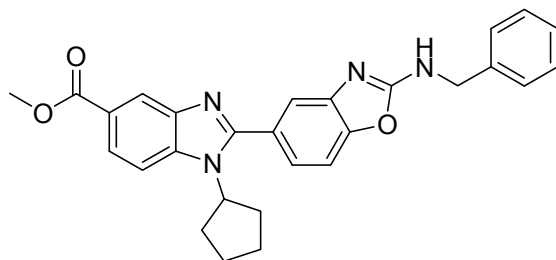
15l



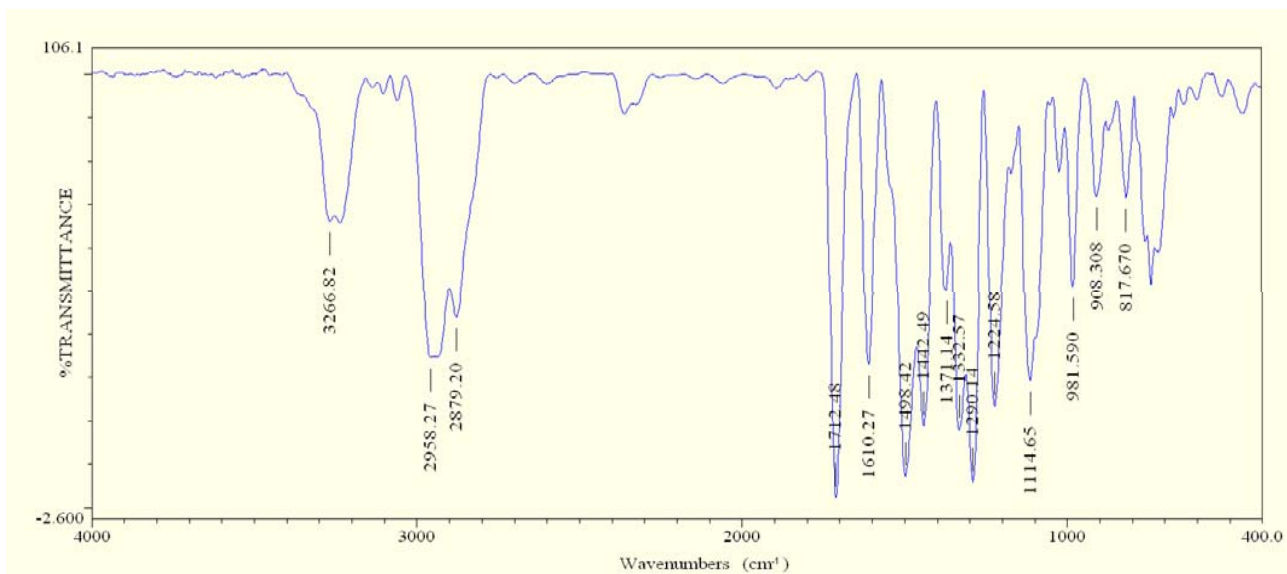
IR Spectra of Compound 15l



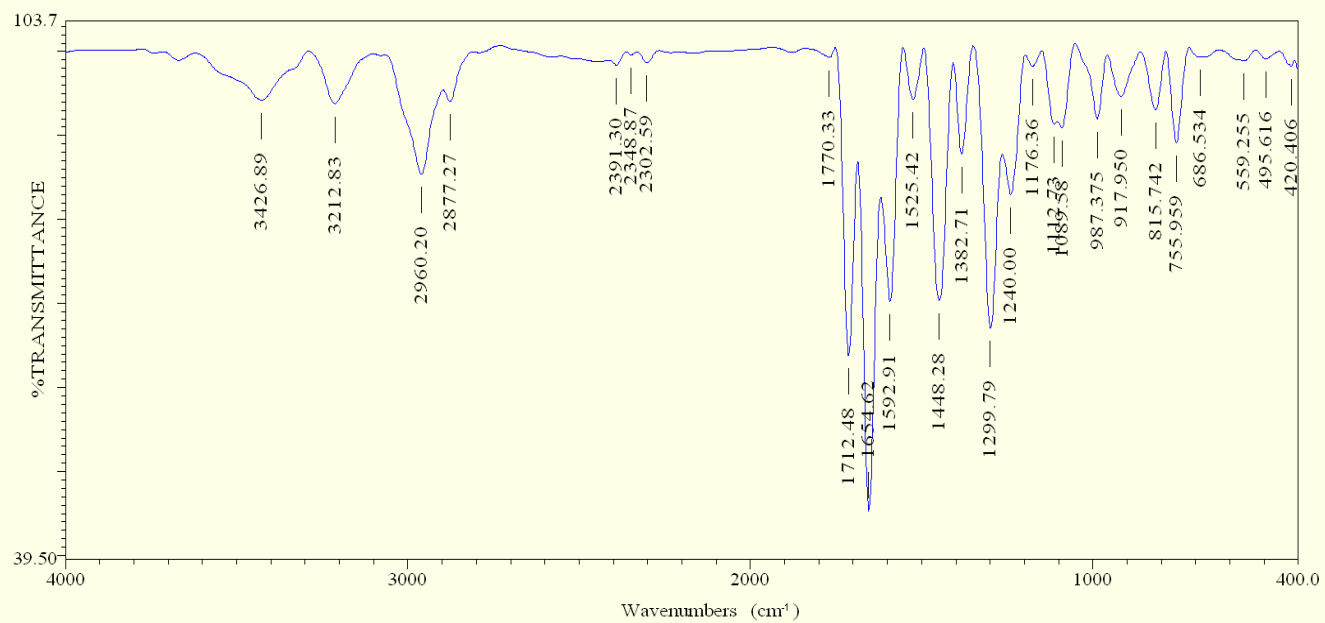
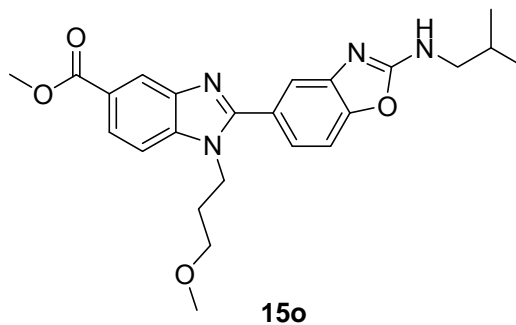
IR Spectra of Compound 15m



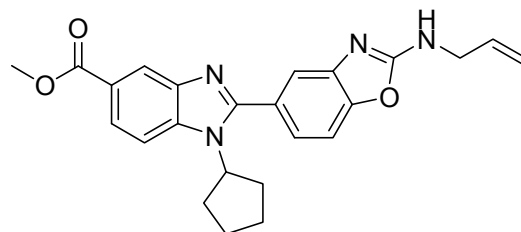
15n



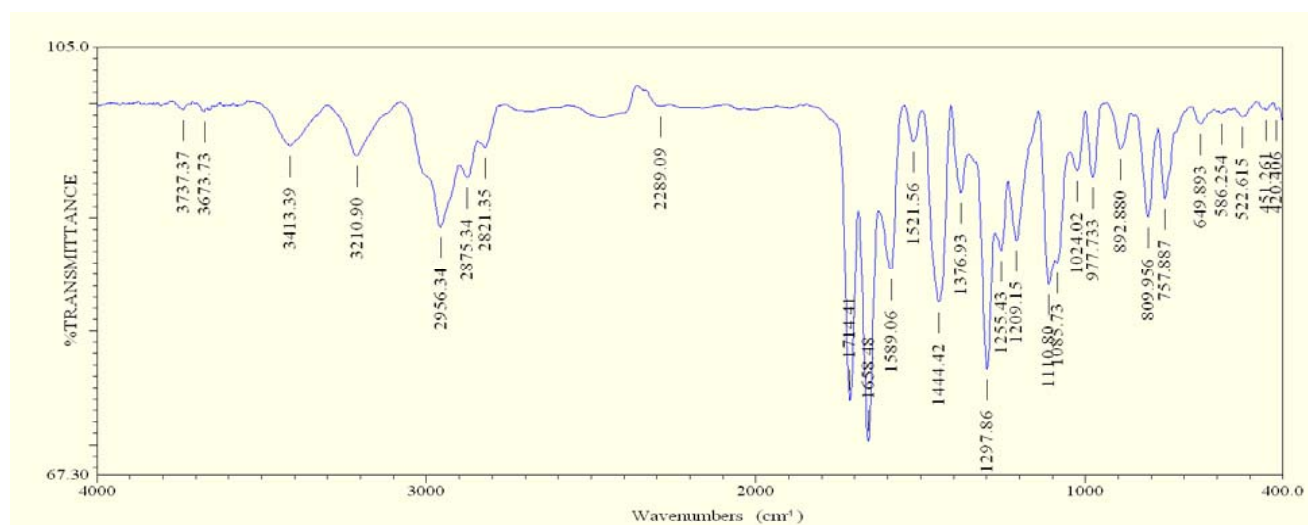
IR Spectra of Compound 15n



IR Spectra of Compound 15o

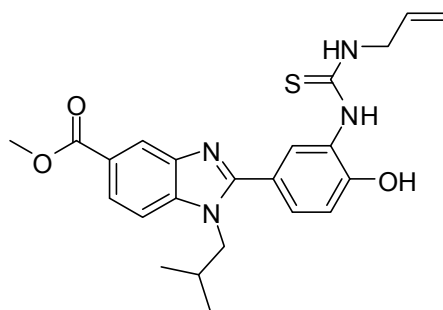


15p



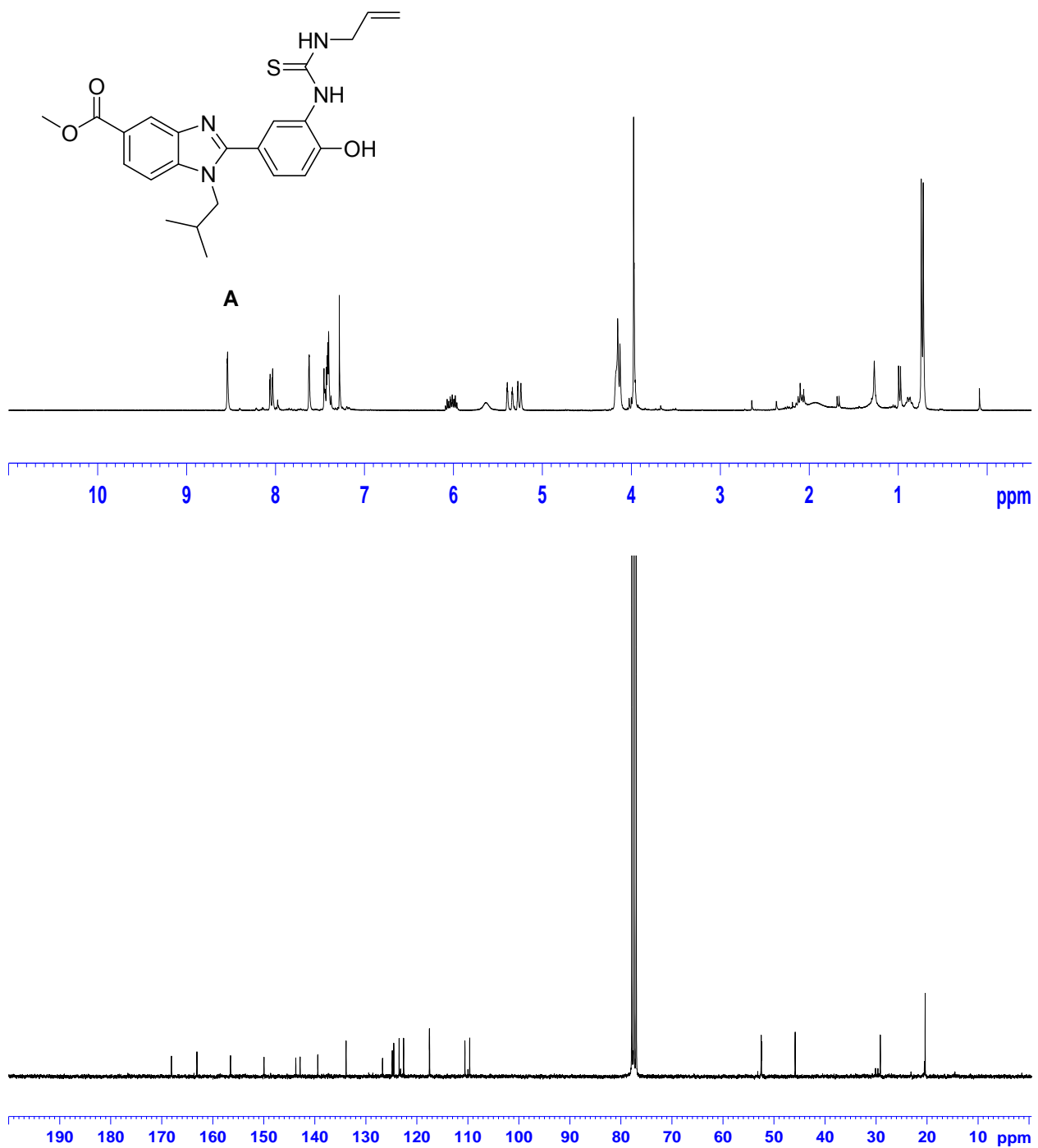
IR Spectra of Compound 15p

Methyl 2-(3-(3-allylthioureido)-4-hydroxyphenyl)-1-isobutyl-1H-benzo[d]imidazole-5-carboxylate (**a**):

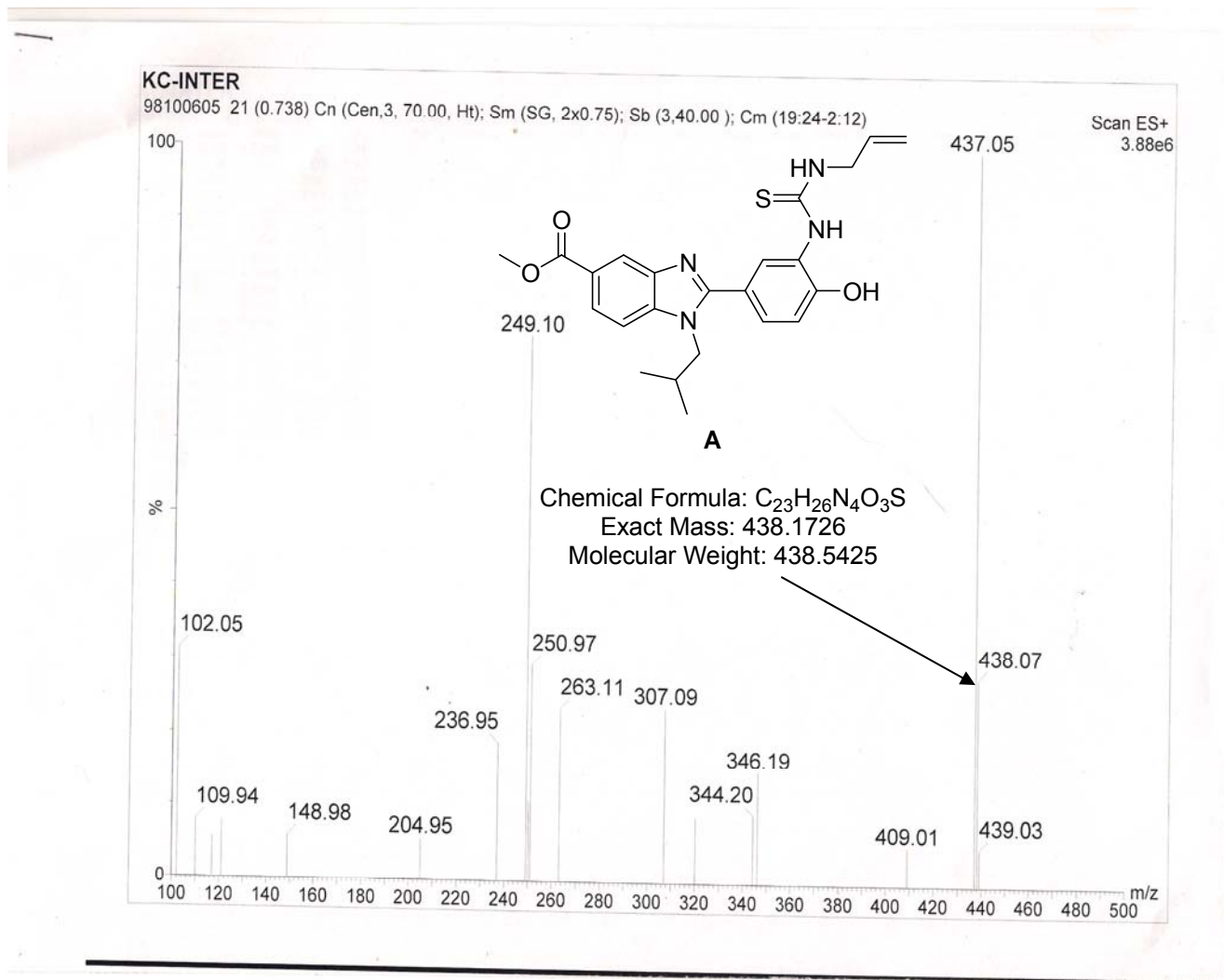


a

^1H NMR (300 MHz, CDCl_3) δ 8.53 (d, $J = 1.3$ Hz, 1H), 8.04 (dd, $J = 8.5, 1.3$ Hz, 1H), 7.68 (s, 1H), 7.46-7.40 (m, 3H), 6.03 (m, 1H), 5.59 (brs, OH), 5.36 (dd, $J = 17.2, 1.2$ Hz, 1H), 5.26 (dd, $J = 10.3, 1.2$ Hz, 1H), 4.29-4.04 (m, 4H), 3.93 (s, 3H), 2.10(sept, $J = 6.6$ Hz, 1H), 0.72 (d, $J = 6.6$ Hz, 6H); ^{13}C NMR (75 MHz, CDCl_3): δ 168.1, 163.1, 156.5, 149.9, 143.7, 142.9, 139.4, 133.8, 126.7, 124.6, 124.5, 123.4, 123.2, 122.6, 117.8, 110.5, 109.6, 52.5, 52.4, 45.0, 29.1, 20.5; MS (ESI) m/z : 438 (M^+), 439 ($\text{M}+\text{H}$);





^1H and ^{13}C Spectra of Intermediate 'a'



LR Mass Spectral Data of Intermediate 'a'

Elemental Analysis of Compound 15n

中興大學研發處貴重儀器使用中心					
元素分析儀 Elementar vario EL III CHN-OS Rapid 服務報告書 NO. 1					
NAME: <u>Barnab</u>					
使用者姓名:	<u>馬娜莉</u>	中心編號:	_____		
服務單位:	<u>交大應化所</u>	名稱或代號:	<u>Kr-B0-15 [15n]</u>		
主管姓名:	<u>孫仲銘</u>				
收件日期:	<u>99年11月4日</u>	完成日期:	<u>99年11月4日</u>		
分析結果:					
樣品重量:	1) <u>3.566 mg</u>	2) <u>3.516 mg</u>	3) _____	mg	
<i>Weight</i>	N %	C %	H %	S %	O %
實驗值:	1) <u>11.81</u>	<u>72.05</u>	<u>5.68</u>	_____	_____
<i>experimental value</i>	2) <u>11.81</u>	<u>72.00</u>	<u>5.77</u>	_____	_____
	3) _____	_____	_____	_____	_____
推測值:	<u>12.01</u>	<u>72.09</u>	<u>5.62</u>	_____	_____
<i>Calculated Value</i>					
本日所用之 Standard:					
★ <input type="checkbox"/> Acetanilid <input type="checkbox"/> 4-Nitroaniline <input type="checkbox"/> Benzoic acid					
<input type="checkbox"/> Sulfanilic acid <input type="checkbox"/> 1-Chloro-2,4-dinitrobenzene					
	N %	C %	H %	S %	O %
理論值:	<u>10.36</u>	<u>71.09</u>	<u>6.71</u>	_____	_____
測出值:	<u>10.29</u>	<u>71.07</u>	<u>6.63</u>	_____	_____
建議:					
費用核算: C H N: <u>1000</u>					
O: _____					
S: _____ 合計台幣: <u>1000</u>					
儀器負責人簽章: 鄭政峯  技術員簽章: 陳宜絹 					
報告日期: 99年11月5日					

中興大學研發處貴重儀器使用中心

元素分析儀 Elementar vario EL III CHN-OS Rapid 服務報告書 NO. 1

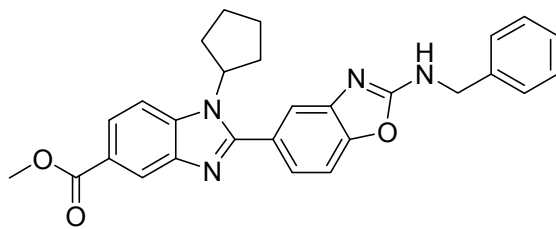
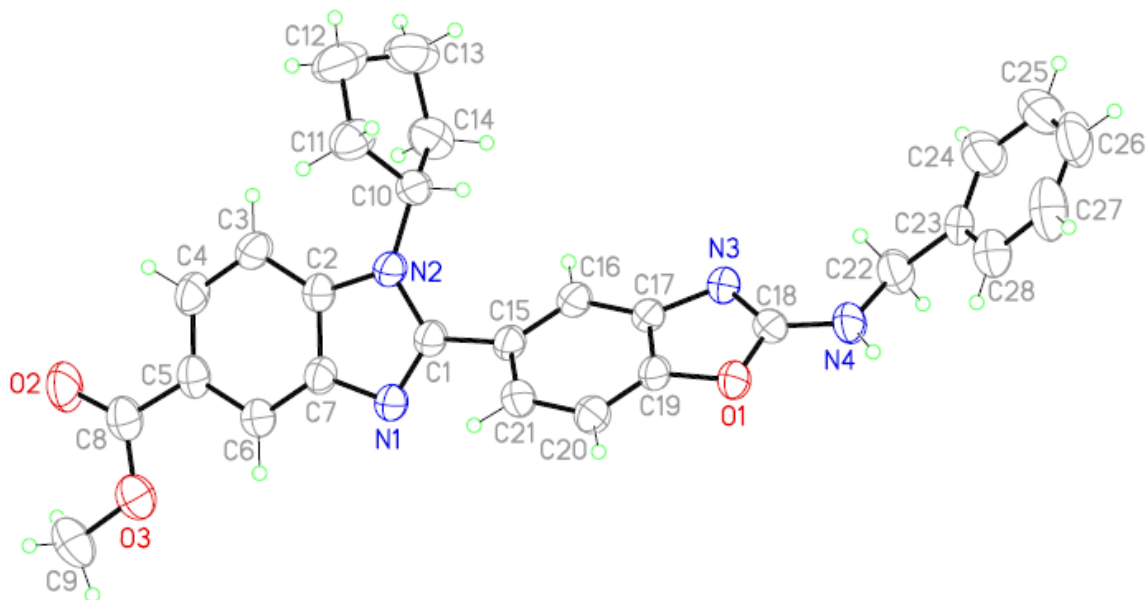
Name: <i>Bornali</i>					
使用者姓名:	<u>馬娜莉</u>	中心編號:	_____		
服務單位:	<u>交大應化所</u>	名稱或代號:	<u>Kr-B0-15 [15H]</u>		
主管姓名:	<u>孫仲銘</u>				
收件日期:	<u>99年11月4日</u>	完成日期:	<u>99年</u>	<u>11月</u>	<u>5日</u>
分析結果:					
樣品重量:	1) <u>2.115 mg</u>	2) <u>2.105 mg</u>	3) _____	mg	
<i>Weight</i>	N %	C %	H %	S %	O %
實驗值:	1) _____	_____	_____	_____	<u>10.45</u>
<i>experimental value</i>	2) _____	_____	_____	_____	<u>10.41</u>
	3) _____	_____	_____	_____	_____
推測值:	_____	_____	_____	_____	<u>10.29</u>
<i>Calculated value</i>					
本日所用之 Standard:					
<input type="checkbox"/>	Acetanilid	<input type="checkbox"/>	4-Nitroaniline	<input checked="" type="checkbox"/>	Benzoic acid
<input type="checkbox"/>	Sulfanilic acid	<input type="checkbox"/>	1-Chloro-2,4-dinitrobenzene		
	N %	C %	H %	S %	O %
理論值:	_____	_____	_____	_____	<u>26.20</u>
測出值:	_____	_____	_____	_____	<u>26.14</u>
建議:					
費用核算: C H N: _____					
	O:	<u>1000</u>	_____		
	S:	_____	合計台幣:	<u>1000</u>	_____

儀器負責人簽章: 鄭政峯  技術員簽章: 陳宜絹

 技術員
陳宜絹

報告日期: 99年11月6日

X ray crystallographic data of compound 15n



15n

ORTEP diagram of Compound 15n

Table 1. Crystal data and structure refinement for 100220_0m.

Identification code	100220_0m
Empirical formula	C ₂₈ H ₂₆ N ₄ O ₃
Formula weight	466.53
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 11.2213(3) Å, $\alpha = 90^\circ$. b = 11.0837(2) Å, $\beta = 100.1810(10)^\circ$. c = 18.7917(5) Å, $\gamma = 90^\circ$.
Volume	2300.39(10) Å ³
Z	4
Density (calculated)	1.347 Mg/m ³
Absorption coefficient	0.089 mm ⁻¹
F(000)	984
Crystal size	0.30 x 0.10 x 0.10 mm ³
Theta range for data collection	2.14 to 26.38°.
Index ranges	-11 ≤ h ≤ 14, -13 ≤ k ≤ 13, - 23 ≤ l ≤ 22
Reflections collected	17349
Independent reflections	4699 [R(int) = 0.0355]
Completeness to theta = 26.38°	99.8 %
Absorption correction	Empirical
Max. and min. transmission	0.7454 and 0.6978
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4699 / 12 / 336
Goodness-of-fit on F ²	1.032
Final R indices [I > 2σ(I)]	R1 = 0.0473, wR2 = 0.1126
R indices (all data)	R1 = 0.0844, wR2 = 0.1300
Largest diff. peak and hole	0.268 and -0.299 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 100220_0m. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3423(2)	3441(2)	479(1)	37(1)
C(2)	2816(2)	5347(2)	440(1)	38(1)
C(3)	2606(2)	6576(2)	522(1)	47(1)
C(4)	1644(2)	7076(2)	67(1)	49(1)
C(5)	895(2)	6397(2)	-460(1)	43(1)
C(6)	1107(2)	5175(2)	-532(1)	44(1)
C(7)	2070(2)	4654(2)	-75(1)	38(1)
C(8)	-123(2)	7014(2)	-929(1)	47(1)
C(9)	-1688(2)	6808(2)	-1939(1)	64(1)
C(10)	4641(2)	4848(2)	1417(1)	42(1)
C(11)	4190(2)	5479(2)	2048(1)	57(1)
C(12)	4965(3)	6613(2)	2214(2)	79(1)
C(13)	6076(3)	6382(2)	1901(2)	75(1)
C(14)	5614(2)	5679(2)	1216(1)	59(1)
C(15)	4107(2)	2317(2)	684(1)	37(1)
C(16)	5363(2)	2254(2)	739(1)	39(1)
C(17)	5905(2)	1123(2)	846(1)	37(1)
C(18)	7063(2)	-399(2)	926(1)	42(1)
C(19)	5187(2)	113(2)	882(1)	38(1)
C(20)	3961(2)	145(2)	848(1)	44(1)
C(21)	3426(2)	1277(2)	748(1)	41(1)
C(22)	9181(2)	-827(2)	916(1)	52(1)
C(23)	10128(16)	-1440(5)	1491(10)	44(1)
C(24)	11199(4)	-864(4)	1724(3)	78(2)
C(25)	12073(5)	-1408(4)	2235(3)	104(2)
C(26)	11885(5)	-2508(5)	2512(3)	79(2)
C(27)	10809(5)	-3080(5)	2303(3)	74(2)
C(28)	9937(4)	-2562(4)	1776(3)	54(1)
C(23')	10070(50)	-1262(17)	1510(30)	44(1)
C(24')	10817(12)	-596(12)	2003(8)	78(2)

C(25')	11603(13)	-1115(12)	2565(9)	104(2)
C(26')	11595(16)	-2297(14)	2671(9)	79(2)
C(27')	11028(18)	-3033(17)	2112(9)	74(2)
C(28')	10222(13)	-2501(14)	1550(7)	54(1)
N(1)	2469(1)	3463(1)	-42(1)	41(1)
N(2)	3686(1)	4556(1)	799(1)	38(1)
O(1)	5933(1)	-886(1)	941(1)	44(1)
N(4)	7952(1)	-1210(1)	963(1)	49(1)
N(3)	7112(1)	770(1)	884(1)	42(1)
O(2)	-405(1)	8053(1)	-869(1)	63(1)
O(3)	-716(1)	6278(1)	-1437(1)	59(1)

Table 3. Bond lengths [Å] and angles [°] for 100220_0m.

C(1)-N(1)	1.317(2)
C(1)-N(2)	1.383(2)
C(1)-C(15)	1.479(2)
C(2)-N(2)	1.394(2)
C(2)-C(7)	1.395(3)
C(2)-C(3)	1.396(3)
C(3)-C(4)	1.370(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.399(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.386(2)
C(5)-C(8)	1.482(3)
C(6)-C(7)	1.382(2)
C(6)-H(6)	0.9300
C(7)-N(1)	1.392(2)
C(8)-O(2)	1.204(2)
C(8)-O(3)	1.340(2)
C(9)-O(3)	1.435(2)
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600

C(9)-H(9C)	0.9600
C(10)-N(2)	1.469(2)
C(10)-C(14)	1.525(3)
C(10)-C(11)	1.538(3)
C(10)-H(10)	0.9800
C(11)-C(12)	1.529(3)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(12)-C(13)	1.491(4)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.516(3)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.397(3)
C(15)-C(21)	1.400(3)
C(16)-C(17)	1.393(2)
C(16)-H(16)	0.9300
C(17)-C(19)	1.387(3)
C(17)-N(3)	1.400(2)
C(18)-N(3)	1.300(2)
C(18)-N(4)	1.336(2)
C(18)-O(1)	1.383(2)
C(19)-C(20)	1.366(3)
C(19)-O(1)	1.381(2)
C(20)-C(21)	1.390(2)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-C(23')	1.44(2)
C(22)-N(4)	1.460(3)
C(22)-C(23)	1.534(7)
C(22)-H(22A)	0.9699
C(22)-H(22B)	0.9697

C(23)-C(24)	1.363(12)
C(23)-C(28)	1.385(12)
C(24)-C(25)	1.383(5)
C(24)-H(24)	0.9300
C(25)-C(26)	1.357(6)
C(25)-H(25)	0.9300
C(26)-C(27)	1.359(6)
C(26)-H(26)	0.9300
C(27)-C(28)	1.387(5)
C(27)-H(27)	0.9300
C(28)-H(28)	0.9300
C(23')-C(24')	1.357(17)
C(23')-C(28')	1.384(17)
C(24')-C(25')	1.376(13)
C(24')-H(24')	0.9300
C(25')-C(26')	1.326(14)
C(25')-H(25')	0.9300
C(26')-C(27')	1.392(15)
C(26')-H(26')	0.9300
C(27')-C(28')	1.395(14)
C(27')-H(27')	0.9300
C(28')-H(28')	0.9300
N(4)-H(4A)	0.8600
N(1)-C(1)-N(2)	112.98(14)
N(1)-C(1)-C(15)	121.68(15)
N(2)-C(1)-C(15)	125.33(15)
N(2)-C(2)-C(7)	105.81(15)
N(2)-C(2)-C(3)	132.71(17)
C(7)-C(2)-C(3)	121.48(16)
C(4)-C(3)-C(2)	117.09(18)
C(4)-C(3)-H(3)	121.5
C(2)-C(3)-H(3)	121.5
C(3)-C(4)-C(5)	122.19(17)
C(3)-C(4)-H(4)	118.9
C(5)-C(4)-H(4)	118.9

C(6)-C(5)-C(4)	120.24(17)
C(6)-C(5)-C(8)	121.35(18)
C(4)-C(5)-C(8)	118.41(17)
C(7)-C(6)-C(5)	118.39(18)
C(7)-C(6)-H(6)	120.8
C(5)-C(6)-H(6)	120.8
C(6)-C(7)-N(1)	129.33(17)
C(6)-C(7)-C(2)	120.61(16)
N(1)-C(7)-C(2)	110.05(15)
O(2)-C(8)-O(3)	122.90(18)
O(2)-C(8)-C(5)	125.0(2)
O(3)-C(8)-C(5)	112.09(17)
O(3)-C(9)-H(9A)	109.5
O(3)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
O(3)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(2)-C(10)-C(14)	113.10(17)
N(2)-C(10)-C(11)	114.57(17)
C(14)-C(10)-C(11)	105.25(16)
N(2)-C(10)-H(10)	107.9
C(14)-C(10)-H(10)	107.9
C(11)-C(10)-H(10)	107.9
C(12)-C(11)-C(10)	106.2(2)
C(12)-C(11)-H(11A)	110.5
C(10)-C(11)-H(11A)	110.5
C(12)-C(11)-H(11B)	110.5
C(10)-C(11)-H(11B)	110.5
H(11A)-C(11)-H(11B)	108.7
C(13)-C(12)-C(11)	105.3(2)
C(13)-C(12)-H(12A)	110.7
C(11)-C(12)-H(12A)	110.7
C(13)-C(12)-H(12B)	110.7
C(11)-C(12)-H(12B)	110.7

H(12A)-C(12)-H(12B)	108.8
C(12)-C(13)-C(14)	103.8(2)
C(12)-C(13)-H(13A)	111.0
C(14)-C(13)-H(13A)	111.0
C(12)-C(13)-H(13B)	111.0
C(14)-C(13)-H(13B)	111.0
H(13A)-C(13)-H(13B)	109.0
C(13)-C(14)-C(10)	104.7(2)
C(13)-C(14)-H(14A)	110.8
C(10)-C(14)-H(14A)	110.8
C(13)-C(14)-H(14B)	110.8
C(10)-C(14)-H(14B)	110.8
H(14A)-C(14)-H(14B)	108.9
C(16)-C(15)-C(21)	120.83(16)
C(16)-C(15)-C(1)	122.14(16)
C(21)-C(15)-C(1)	116.69(17)
C(17)-C(16)-C(15)	117.65(17)
C(17)-C(16)-H(16)	121.2
C(15)-C(16)-H(16)	121.2
C(19)-C(17)-C(16)	119.43(17)
C(19)-C(17)-N(3)	109.71(15)
C(16)-C(17)-N(3)	130.74(17)
N(3)-C(18)-N(4)	129.38(19)
N(3)-C(18)-O(1)	116.08(16)
N(4)-C(18)-O(1)	114.54(16)
C(20)-C(19)-O(1)	127.96(16)
C(20)-C(19)-C(17)	124.42(16)
O(1)-C(19)-C(17)	107.60(16)
C(19)-C(20)-C(21)	115.94(17)
C(19)-C(20)-H(20)	122.0
C(21)-C(20)-H(20)	122.0
C(20)-C(21)-C(15)	121.67(18)
C(20)-C(21)-H(21)	119.2
C(15)-C(21)-H(21)	119.2
C(23')-C(22)-N(4)	113(3)

C(23')-C(22)-C(23)	7(2)
N(4)-C(22)-C(23)	111.9(8)
C(23')-C(22)-H(22A)	104.0
N(4)-C(22)-H(22A)	109.2
C(23)-C(22)-H(22A)	110.8
C(23')-C(22)-H(22B)	113.3
N(4)-C(22)-H(22B)	109.2
C(23)-C(22)-H(22B)	107.9
H(22A)-C(22)-H(22B)	107.9
C(24)-C(23)-C(28)	118.9(5)
C(24)-C(23)-C(22)	118.7(8)
C(28)-C(23)-C(22)	122.3(8)
C(23)-C(24)-C(25)	119.7(5)
C(23)-C(24)-H(24)	120.1
C(25)-C(24)-H(24)	120.1
C(26)-C(25)-C(24)	121.3(4)
C(26)-C(25)-H(25)	119.4
C(24)-C(25)-H(25)	119.4
C(25)-C(26)-C(27)	119.9(4)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.1
C(26)-C(27)-C(28)	119.4(5)
C(26)-C(27)-H(27)	120.3
C(28)-C(27)-H(27)	120.3
C(23)-C(28)-C(27)	120.7(5)
C(23)-C(28)-H(28)	119.7
C(27)-C(28)-H(28)	119.7
C(24')-C(23')-C(28')	116.3(15)
C(24')-C(23')-C(22)	127.5(15)
C(28')-C(23')-C(22)	116.1(15)
C(23')-C(24')-C(25')	122.3(13)
C(23')-C(24')-H(24')	118.8
C(25')-C(24')-H(24')	118.8
C(26')-C(25')-C(24')	120.5(12)
C(26')-C(25')-H(25')	119.7

C(24')-C(25')-H(25')	119.7
C(25')-C(26')-C(27')	118.7(14)
C(25')-C(26')-H(26')	120.7
C(27')-C(26')-H(26')	120.7
C(26')-C(27')-C(28')	118.2(14)
C(26')-C(27')-H(27')	120.9
C(28')-C(27')-H(27')	120.9
C(23')-C(28')-C(27')	121.4(15)
C(23')-C(28')-H(28')	119.3
C(27')-C(28')-H(28')	119.3
C(1)-N(1)-C(7)	105.25(14)
C(1)-N(2)-C(2)	105.91(14)
C(1)-N(2)-C(10)	127.60(14)
C(2)-N(2)-C(10)	126.41(14)
C(19)-O(1)-C(18)	103.26(13)
C(18)-N(4)-C(22)	120.43(16)
C(18)-N(4)-H(4A)	119.8
C(22)-N(4)-H(4A)	119.8
C(18)-N(3)-C(17)	103.31(16)
C(8)-O(3)-C(9)	116.28(17)

Symmetry transformations used to generate equivalent atoms:

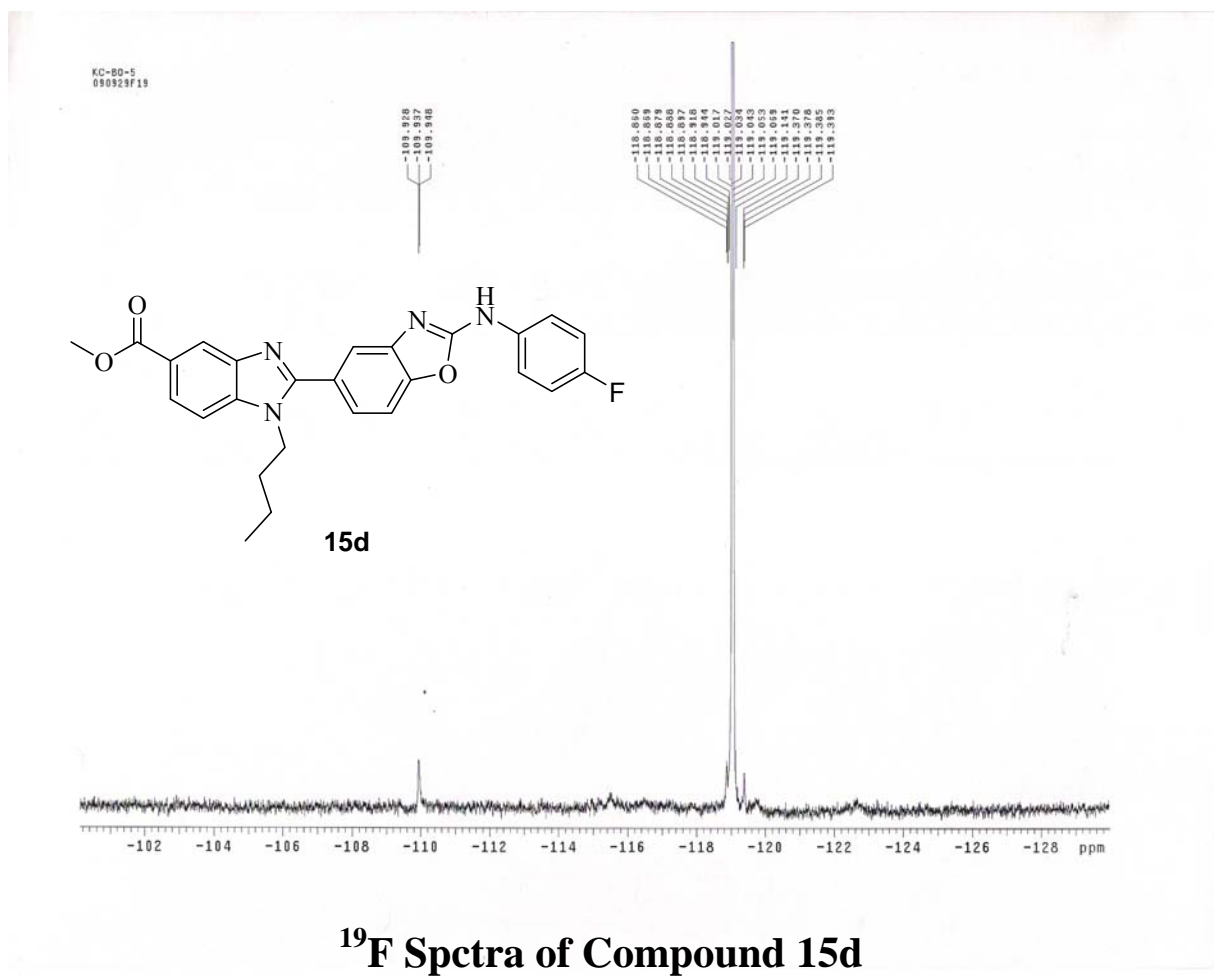
Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 100220_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

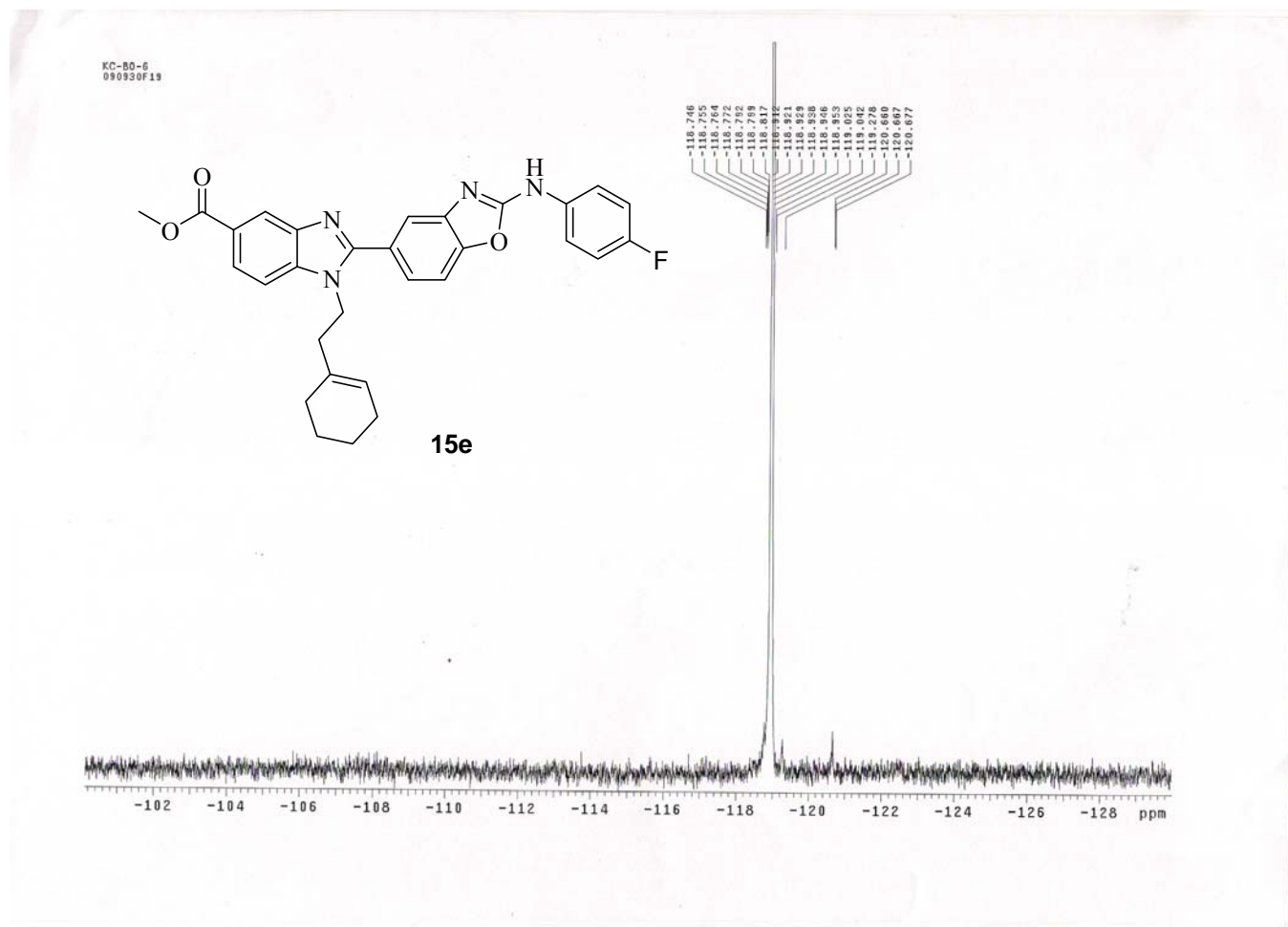
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(1)	31(1)	40(1)	0(1)	6(1)	4(1)
C(2)	39(1)	33(1)	42(1)	3(1)	8(1)	6(1)
C(3)	54(1)	30(1)	53(1)	-4(1)	1(1)	4(1)
C(4)	52(1)	31(1)	62(1)	3(1)	9(1)	9(1)
C(5)	40(1)	38(1)	52(1)	8(1)	11(1)	8(1)
C(6)	42(1)	40(1)	48(1)	-1(1)	1(1)	6(1)
C(7)	40(1)	31(1)	43(1)	0(1)	7(1)	5(1)

C(8)	42(1)	44(1)	56(1)	10(1)	11(1)	5(1)
C(9)	49(1)	80(2)	60(2)	16(1)	-1(1)	13(1)
C(10)	44(1)	37(1)	41(1)	-1(1)	-1(1)	4(1)
C(11)	71(2)	56(1)	42(1)	-6(1)	7(1)	0(1)
C(12)	104(2)	61(2)	64(2)	-19(1)	-5(2)	-5(2)
C(13)	76(2)	56(1)	83(2)	-1(1)	-15(2)	-15(1)
C(14)	50(1)	62(1)	62(2)	0(1)	4(1)	-5(1)
C(15)	41(1)	32(1)	36(1)	-2(1)	3(1)	7(1)
C(16)	43(1)	31(1)	42(1)	-2(1)	4(1)	2(1)
C(17)	39(1)	34(1)	37(1)	-4(1)	1(1)	4(1)
C(18)	39(1)	39(1)	42(1)	-4(1)	-5(1)	5(1)
C(19)	42(1)	30(1)	38(1)	0(1)	-1(1)	8(1)
C(20)	43(1)	32(1)	53(1)	2(1)	4(1)	0(1)
C(21)	38(1)	38(1)	46(1)	1(1)	2(1)	4(1)
C(22)	43(1)	52(1)	60(1)	6(1)	4(1)	9(1)
C(23)	38(2)	38(2)	53(2)	-6(3)	6(2)	13(3)
C(24)	58(3)	53(2)	112(4)	-1(2)	-16(3)	3(2)
C(25)	69(3)	75(3)	145(5)	-18(3)	-44(3)	15(2)
C(26)	68(3)	94(3)	68(3)	-1(2)	-5(2)	44(2)
C(27)	72(3)	77(2)	77(4)	28(2)	27(2)	33(2)
C(28)	52(3)	55(2)	57(3)	8(2)	13(2)	12(2)
C(23')	38(2)	38(2)	53(2)	-6(3)	6(2)	13(3)
C(24')	58(3)	53(2)	112(4)	-1(2)	-16(3)	3(2)
C(25')	69(3)	75(3)	145(5)	-18(3)	-44(3)	15(2)
C(26')	68(3)	94(3)	68(3)	-1(2)	-5(2)	44(2)
C(27')	72(3)	77(2)	77(4)	28(2)	27(2)	33(2)
C(28')	52(3)	55(2)	57(3)	8(2)	13(2)	12(2)
N(1)	43(1)	33(1)	46(1)	-2(1)	0(1)	7(1)
N(2)	42(1)	30(1)	40(1)	-1(1)	2(1)	4(1)
O(1)	43(1)	30(1)	56(1)	1(1)	0(1)	7(1)
N(4)	42(1)	37(1)	65(1)	1(1)	-1(1)	10(1)
N(3)	39(1)	34(1)	50(1)	-4(1)	1(1)	7(1)
O(2)	54(1)	42(1)	90(1)	10(1)	3(1)	15(1)
O(3)	58(1)	57(1)	57(1)	6(1)	-6(1)	15(1)

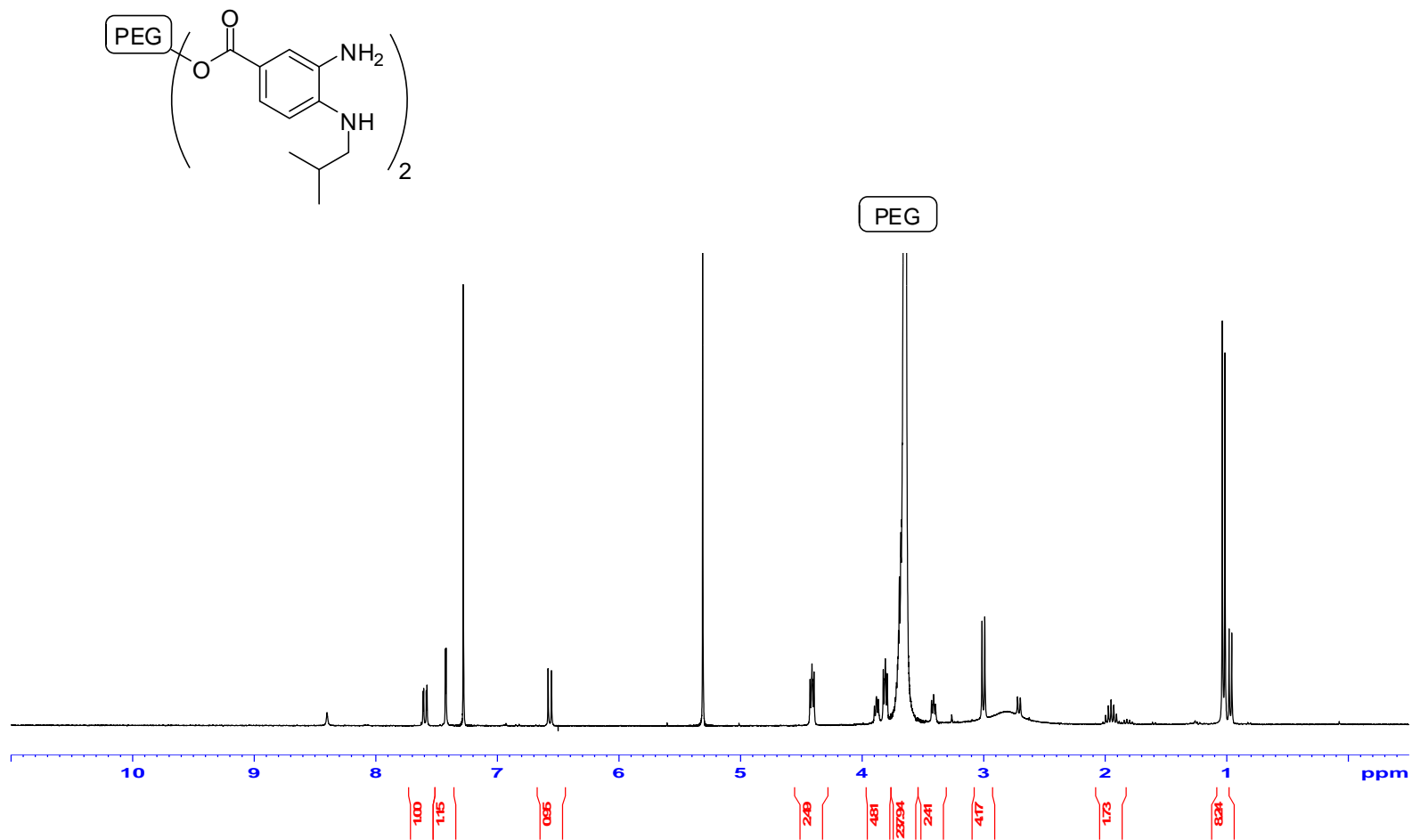
Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for 100220_0m.

	x	y	z	U(eq)
H(3)	3098	7036	871	56
H(4)	1483	7893	110	58
H(6)	613	4716	-880	53
H(9A)	-2371	6935	-1704	97
H(9B)	-1914	6277	-2344	97
H(9C)	-1429	7567	-2104	97
H(10)	5033	4091	1599	50
H(11A)	3342	5691	1913	68
H(11B)	4285	4954	2467	68
H(12A)	4538	7317	1993	95
H(12B)	5171	6743	2732	95
H(13A)	6661	5913	2231	91
H(13B)	6450	7133	1793	91
H(14A)	6261	5215	1068	70
H(14B)	5274	6218	826	70
H(16)	5822	2944	705	47
H(20)	3512	-549	889	52
H(21)	2593	1346	722	50
H(22A)	9235	44	961	63
H(22B)	9356	-1045	445	63
H(24)	11342	-109	1540	94
H(25)	12802	-1011	2392	124
H(26)	12492	-2869	2845	95
H(27)	10659	-3813	2511	88
H(28)	9217	-2971	1614	65
H(24')	10797	240	1963	94
H(25')	12144	-632	2872	124
H(26')	11961	-2628	3110	95
H(27')	11182	-3858	2114	88
H(28')	9777	-2988	1197	65
H(4A)	7800	-1962	1014	59

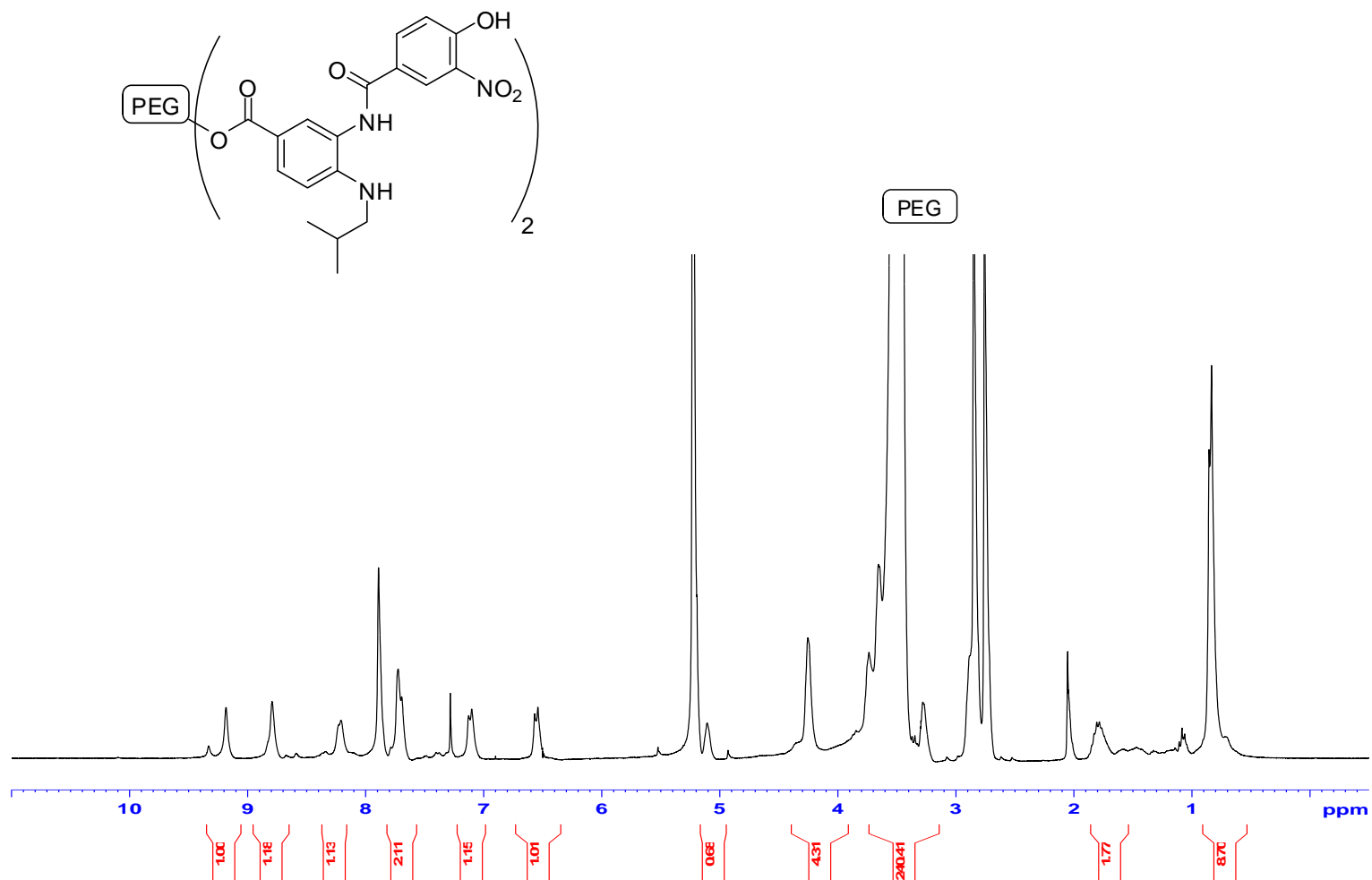




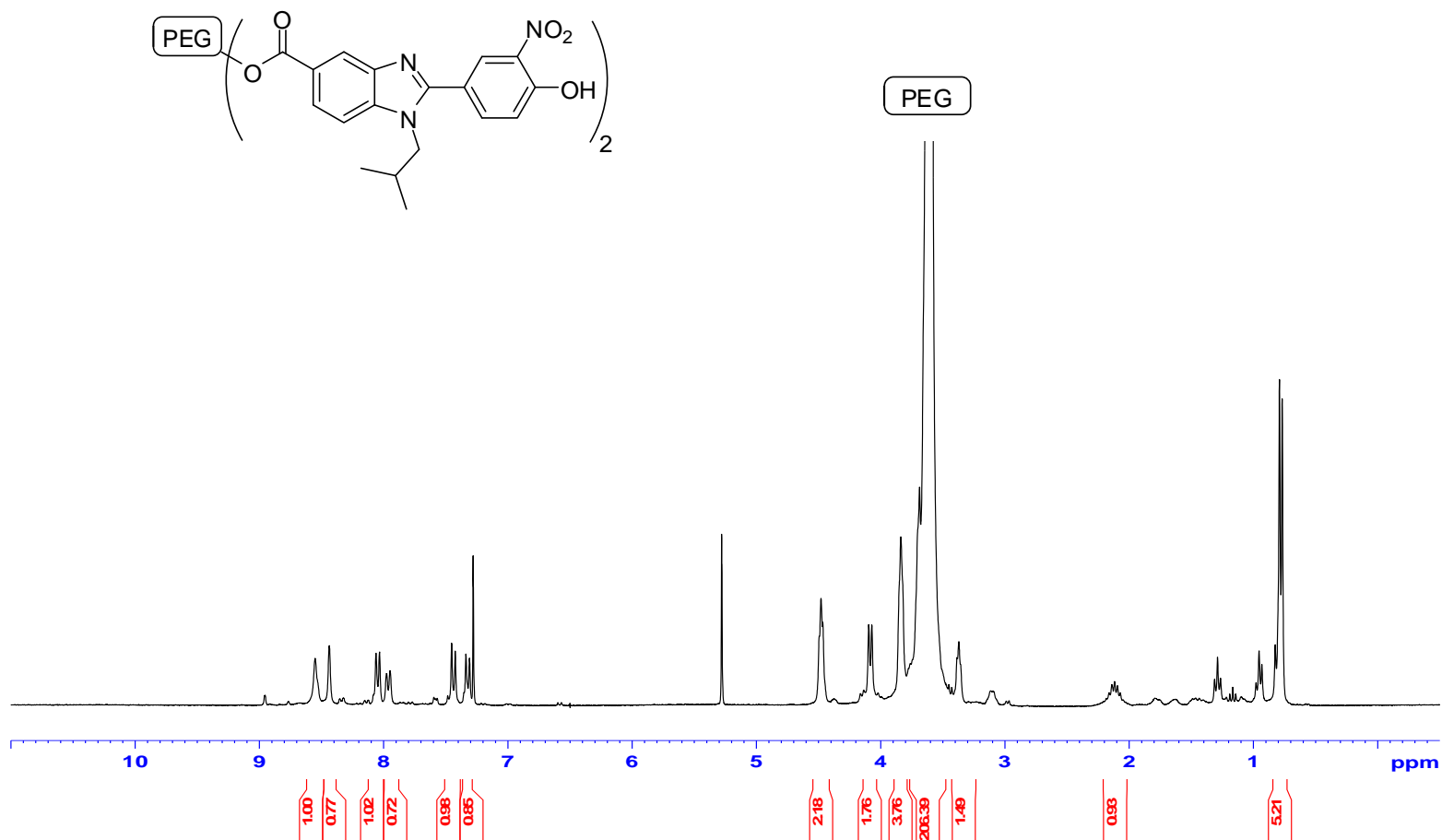
^{19}F Spectra of Compound 15e



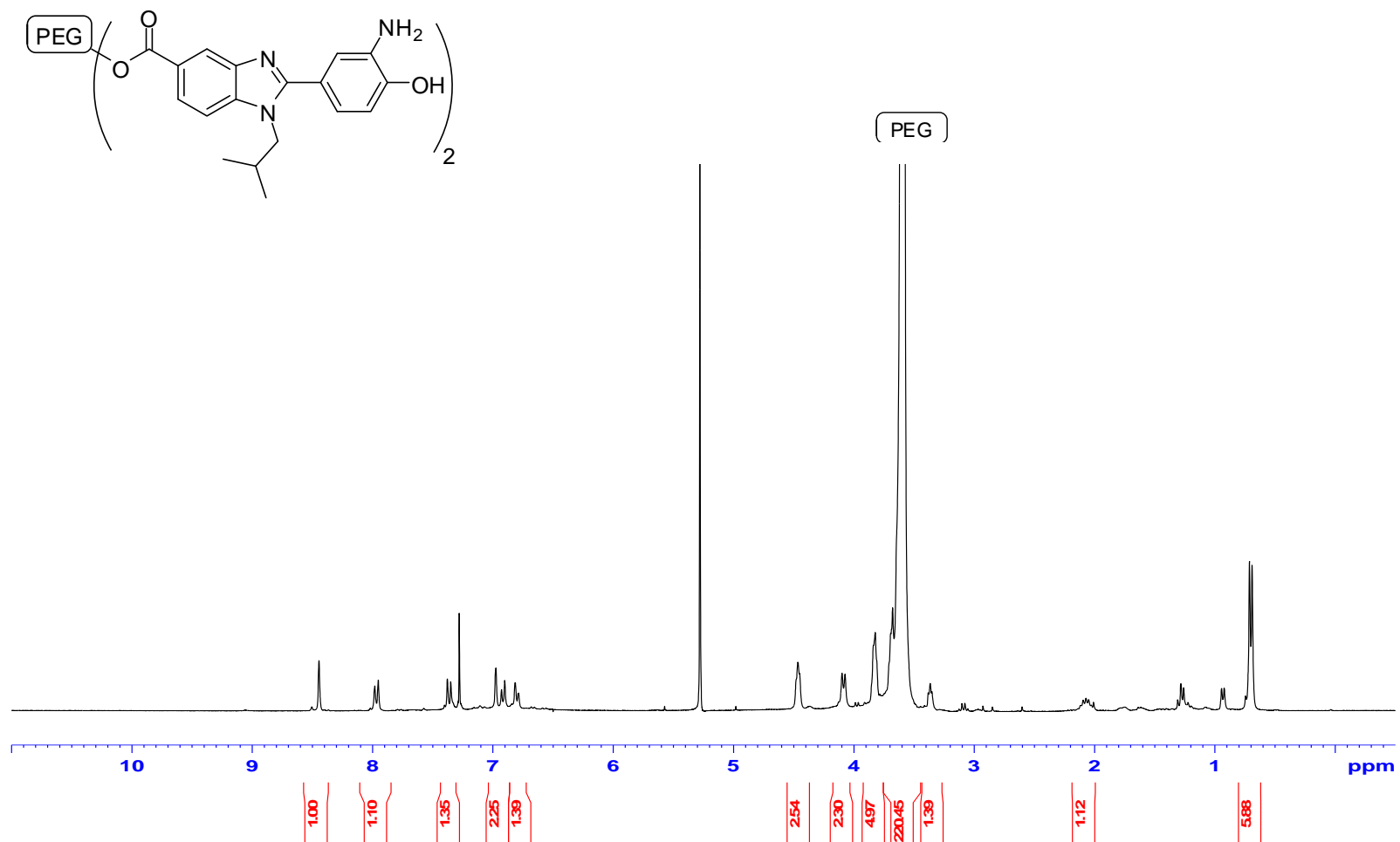
¹H NMR Spectrum (300 MHz) of compound 9a in CDCl₃



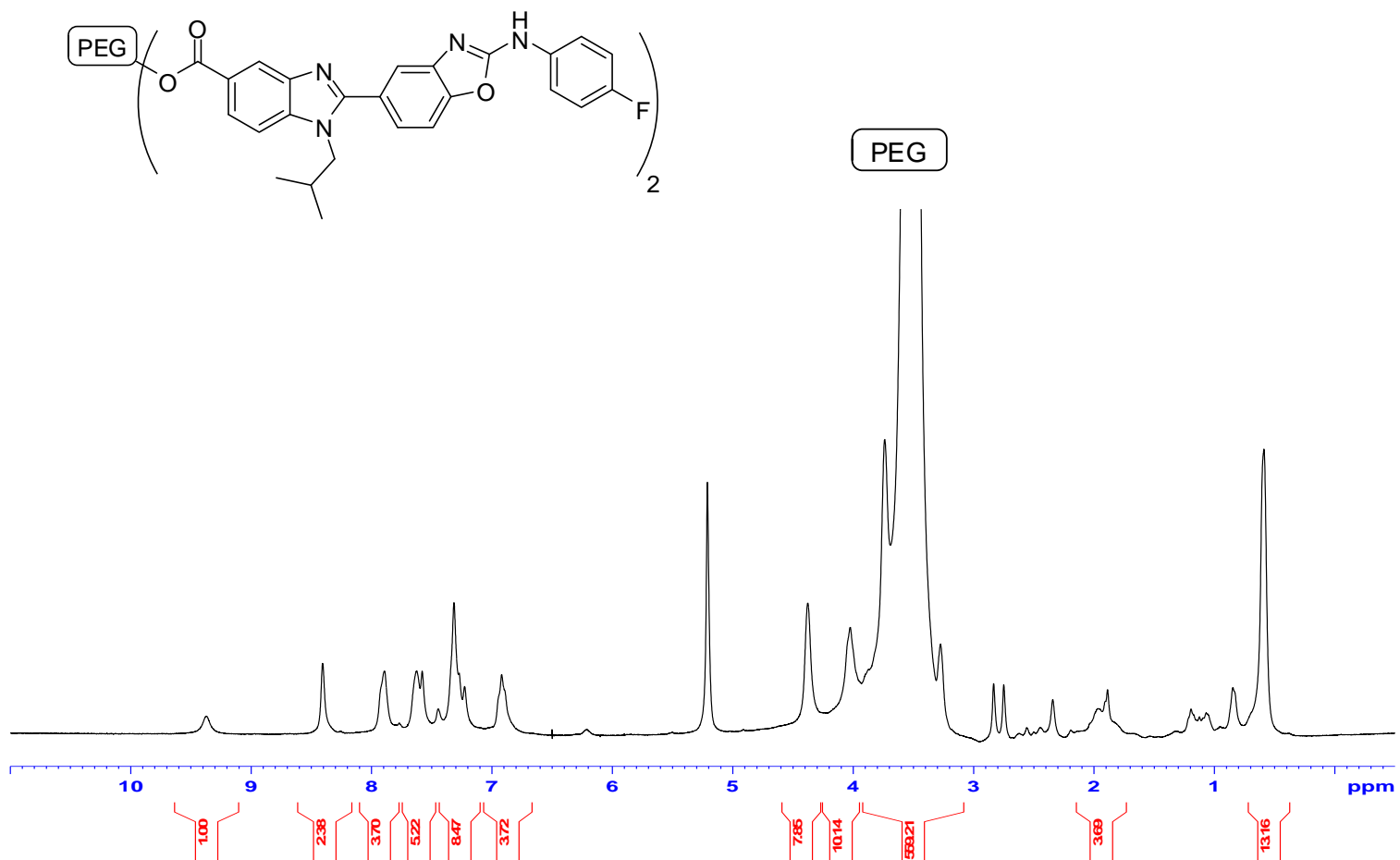
¹H NMR Spectrum (300 MHz) of compound 11a in CDCl₃



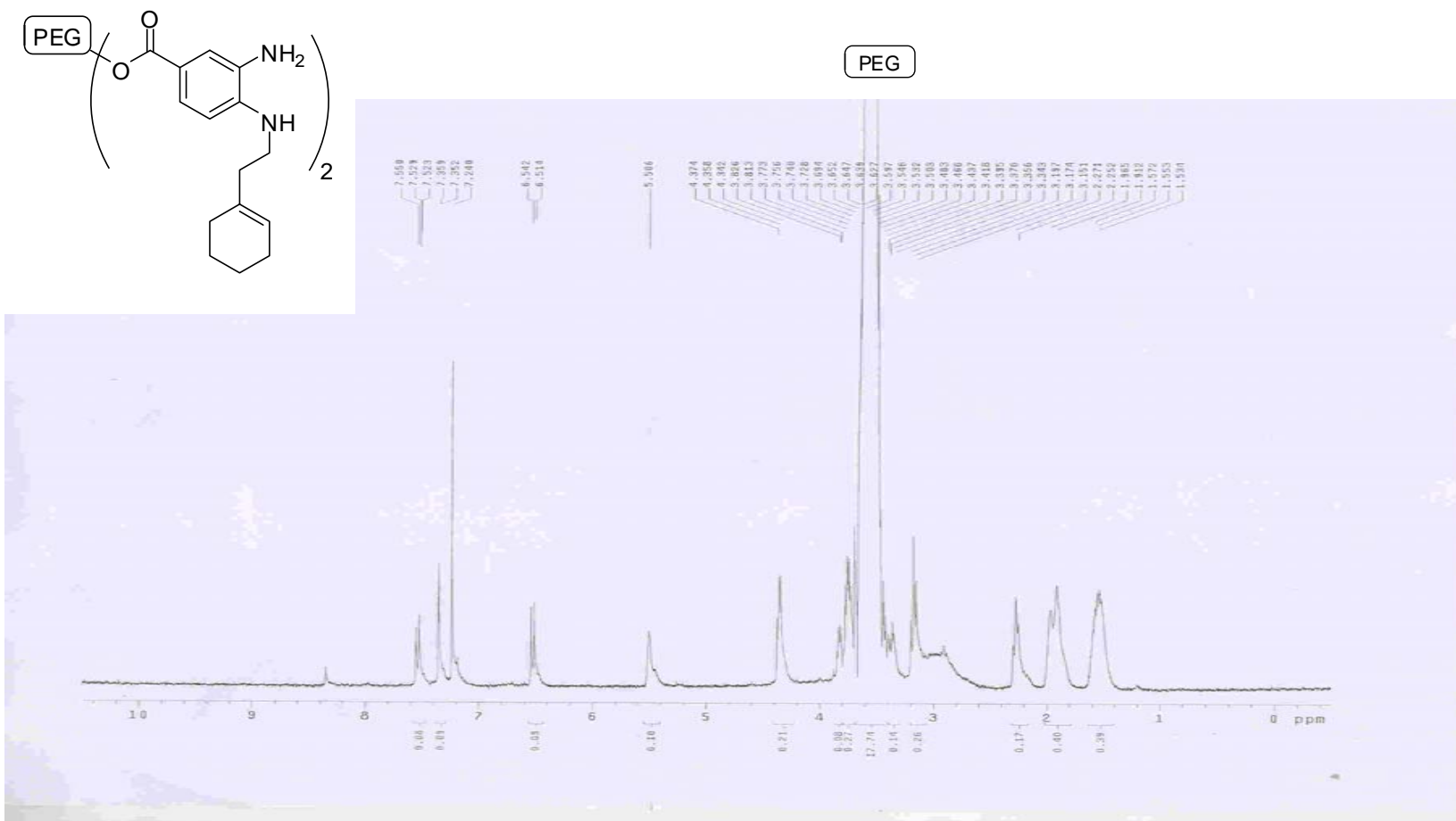
¹H NMR Spectrum (300 MHz) of compound 12a in CDCl₃



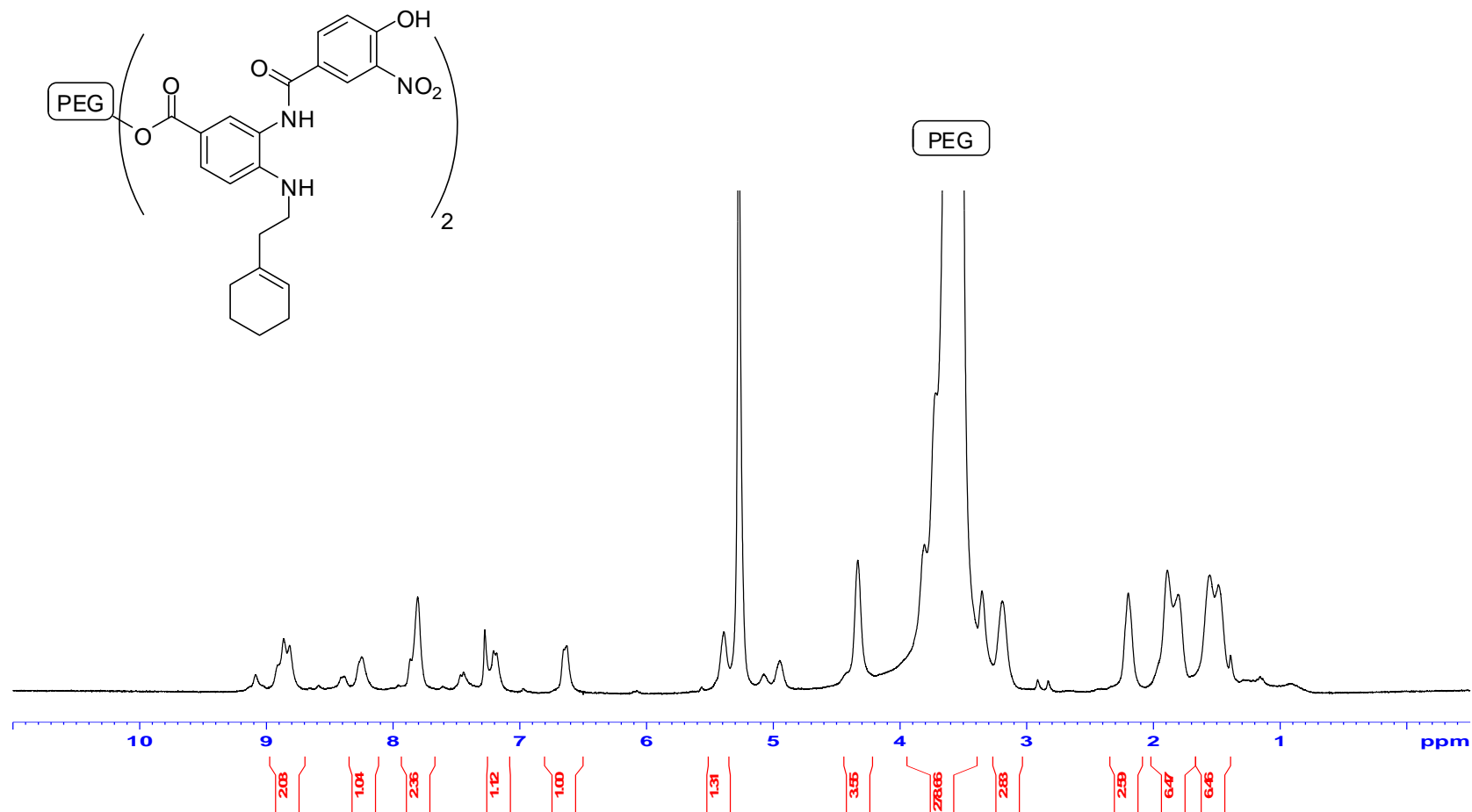
¹H NMR Spectrum (300 MHz) of compound 13a in CDCl₃



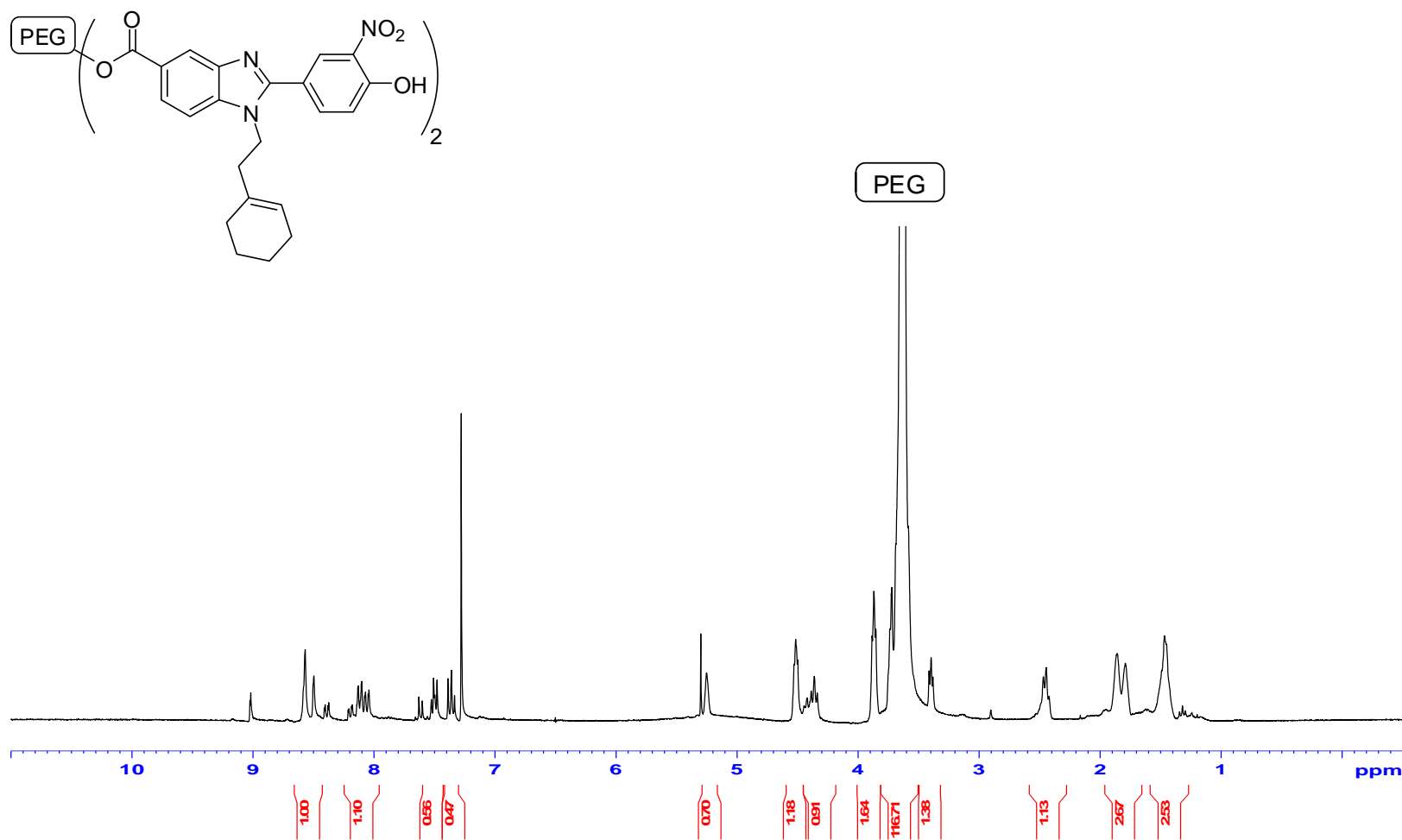
¹H NMR Spectrum (300 MHz) of compound 14a in CDCl₃



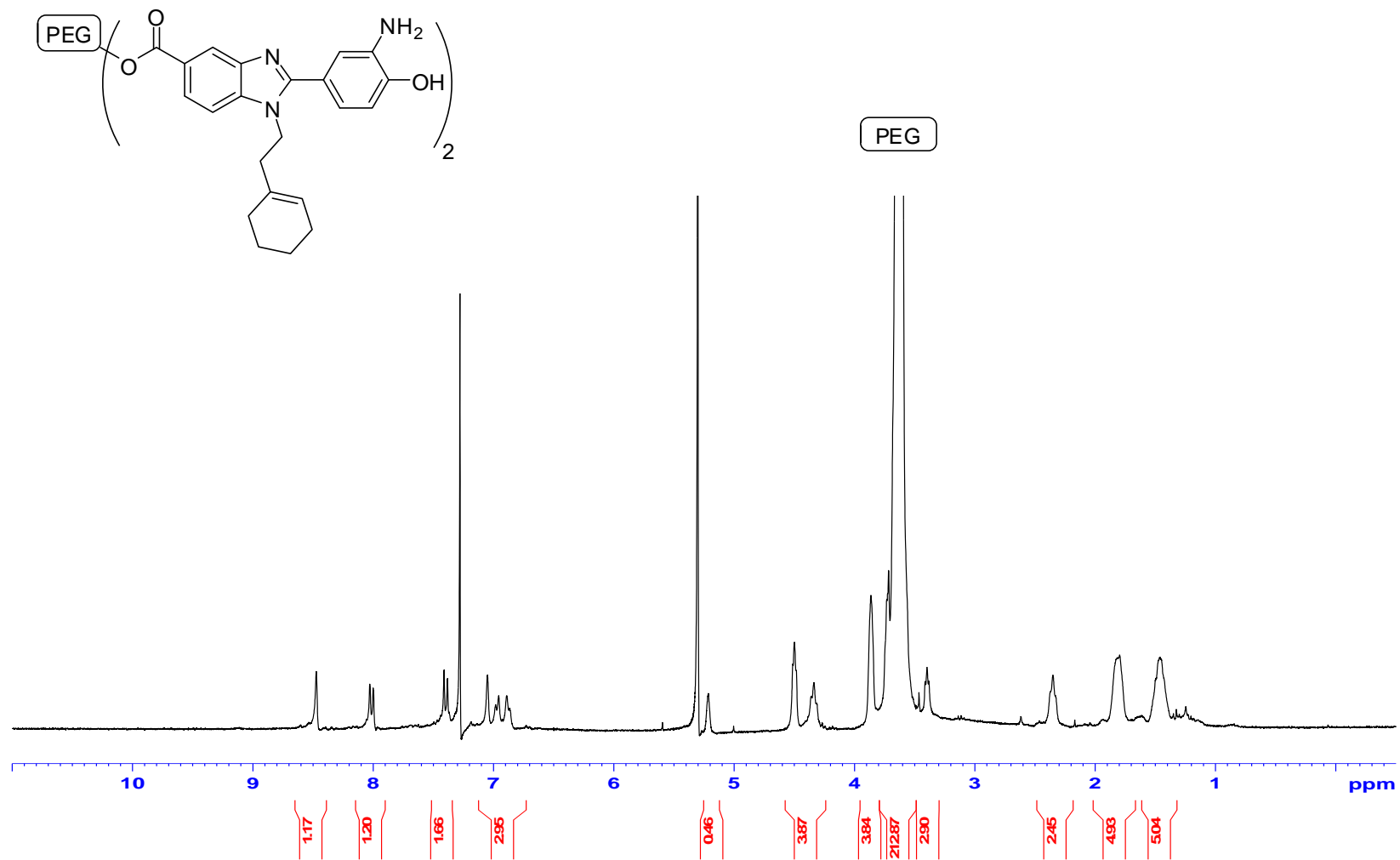
¹H NMR Spectrum (300 MHz) of compound 9f in CDCl₃



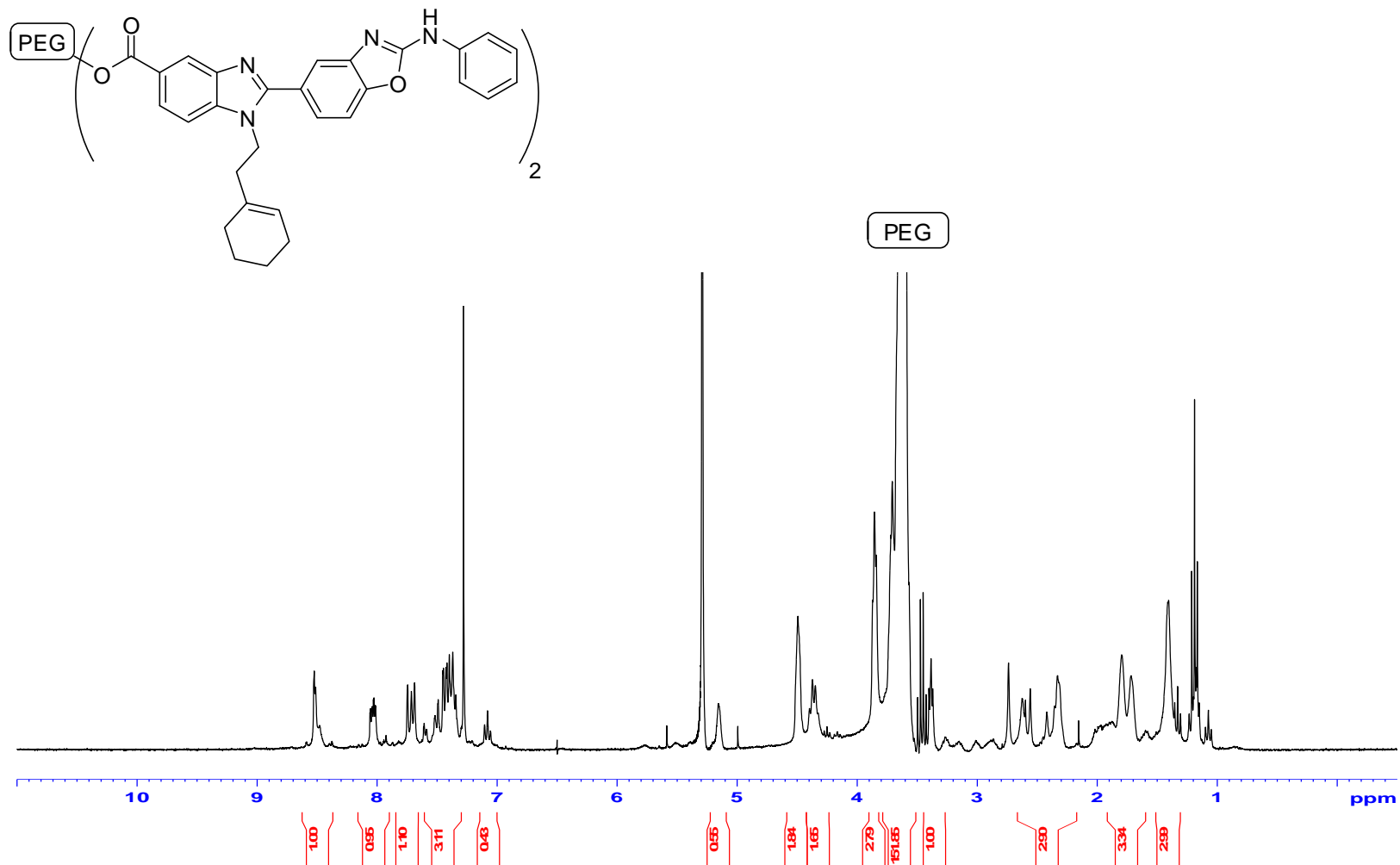
¹H NMR Spectrum (300 MHz) of compound 11f in CDCl₃



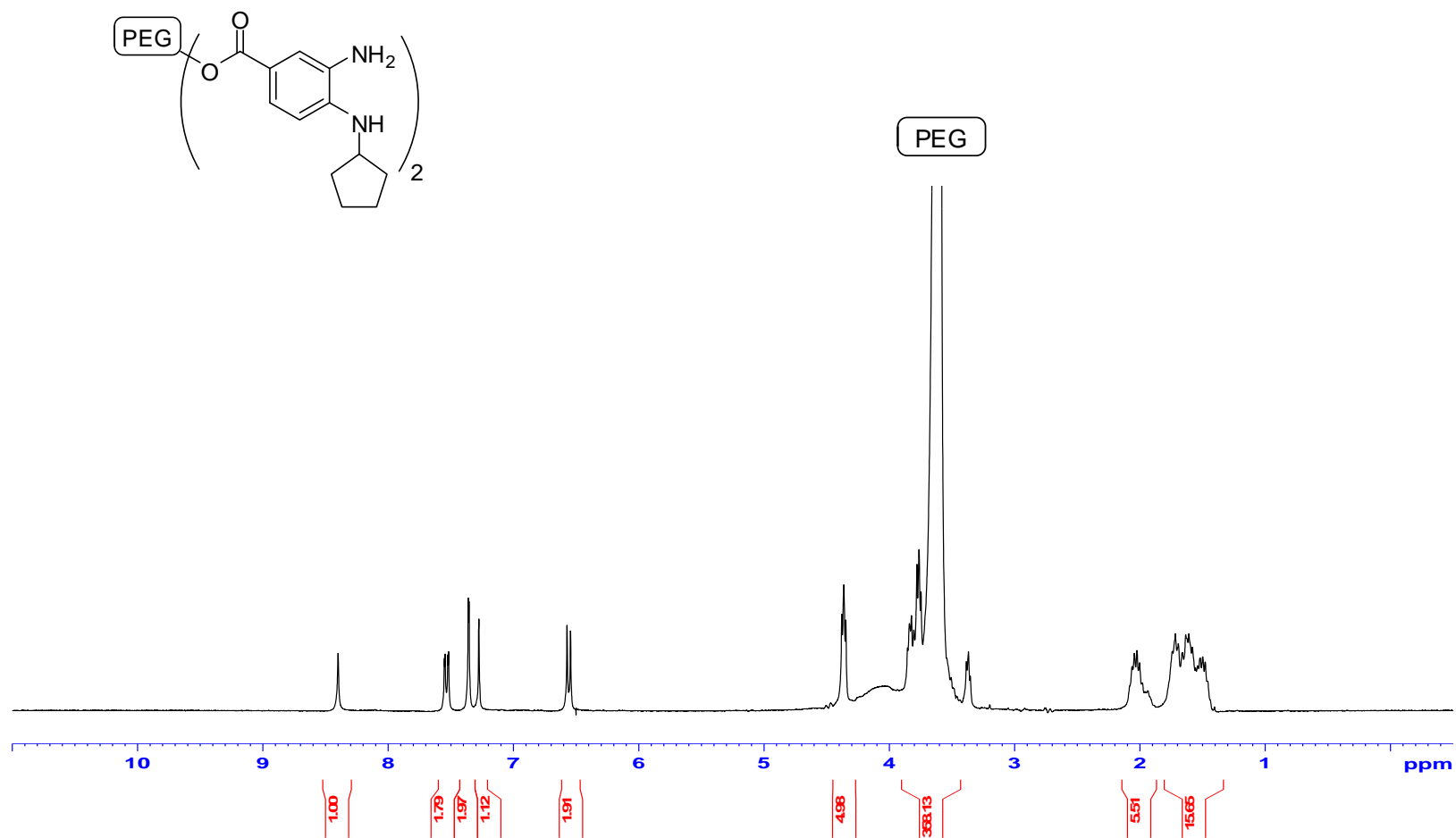
¹H NMR Spectrum (300 MHz) of compound 12f in CDCl₃



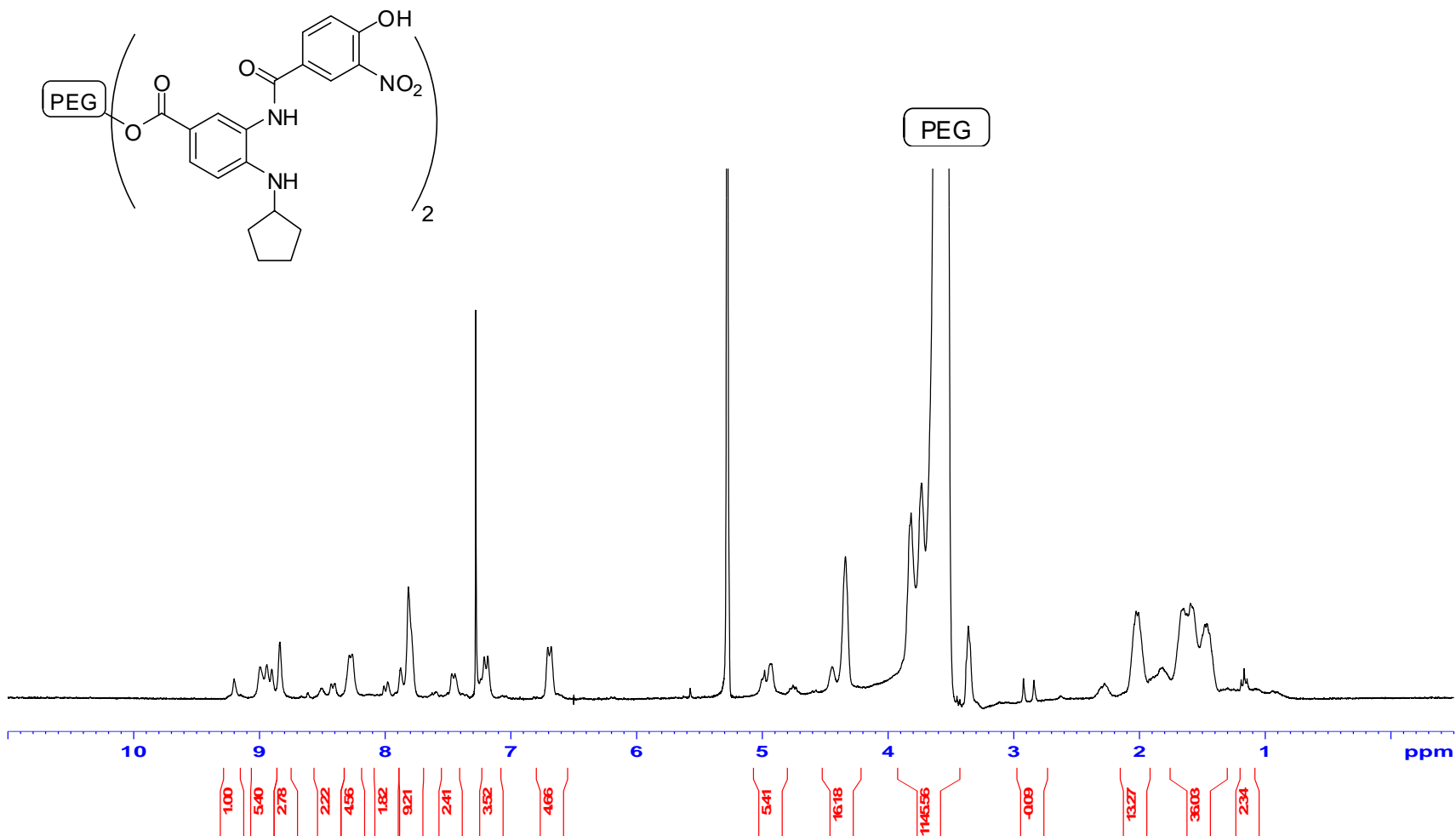
¹H NMR Spectrum (300 MHz) of compound 13f in CDCl₃



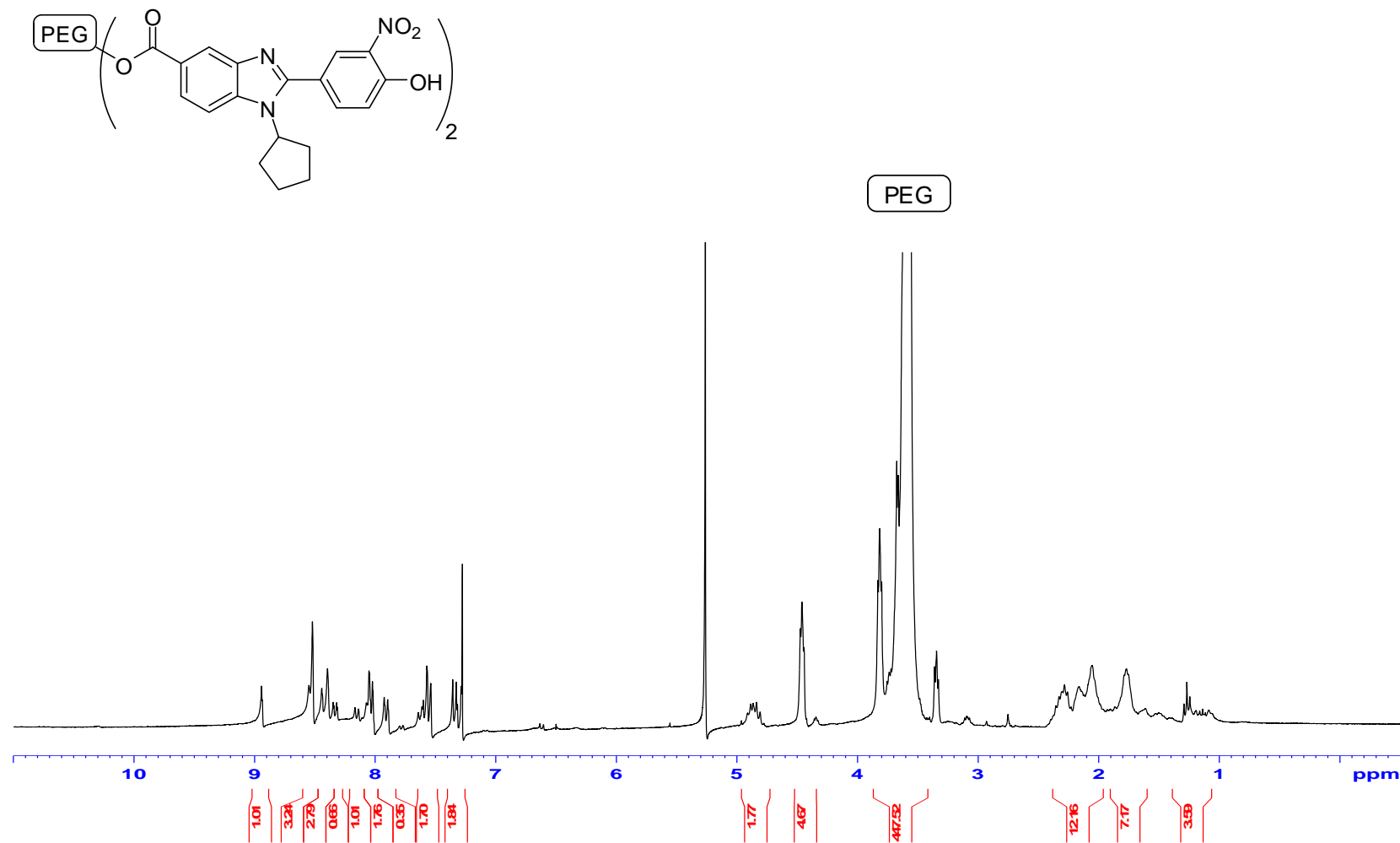
¹H NMR Spectrum (300 MHz) of compound 14f in CDCl₃



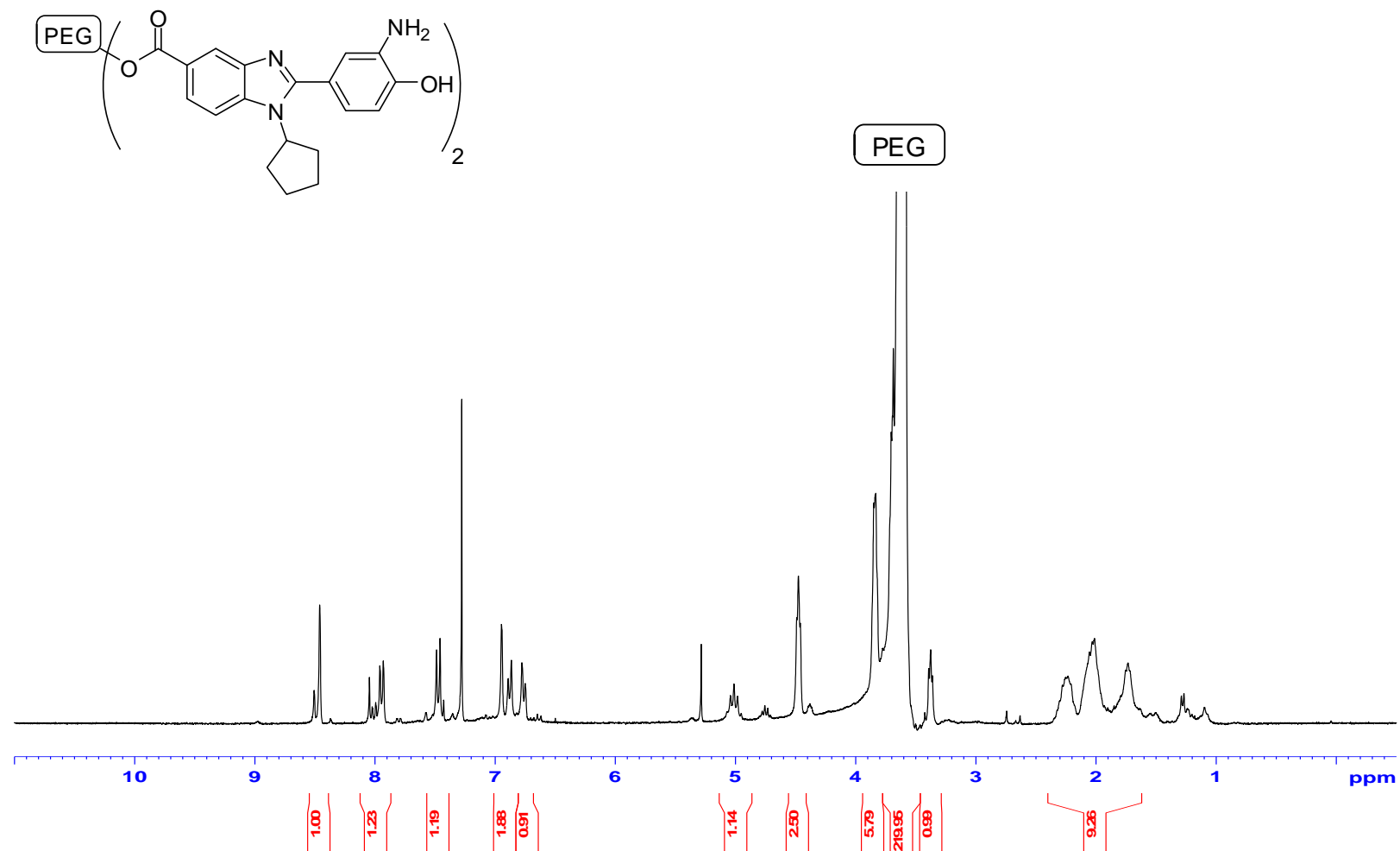
¹H NMR Spectrum (300 MHz) of compound 9n in CDCl₃



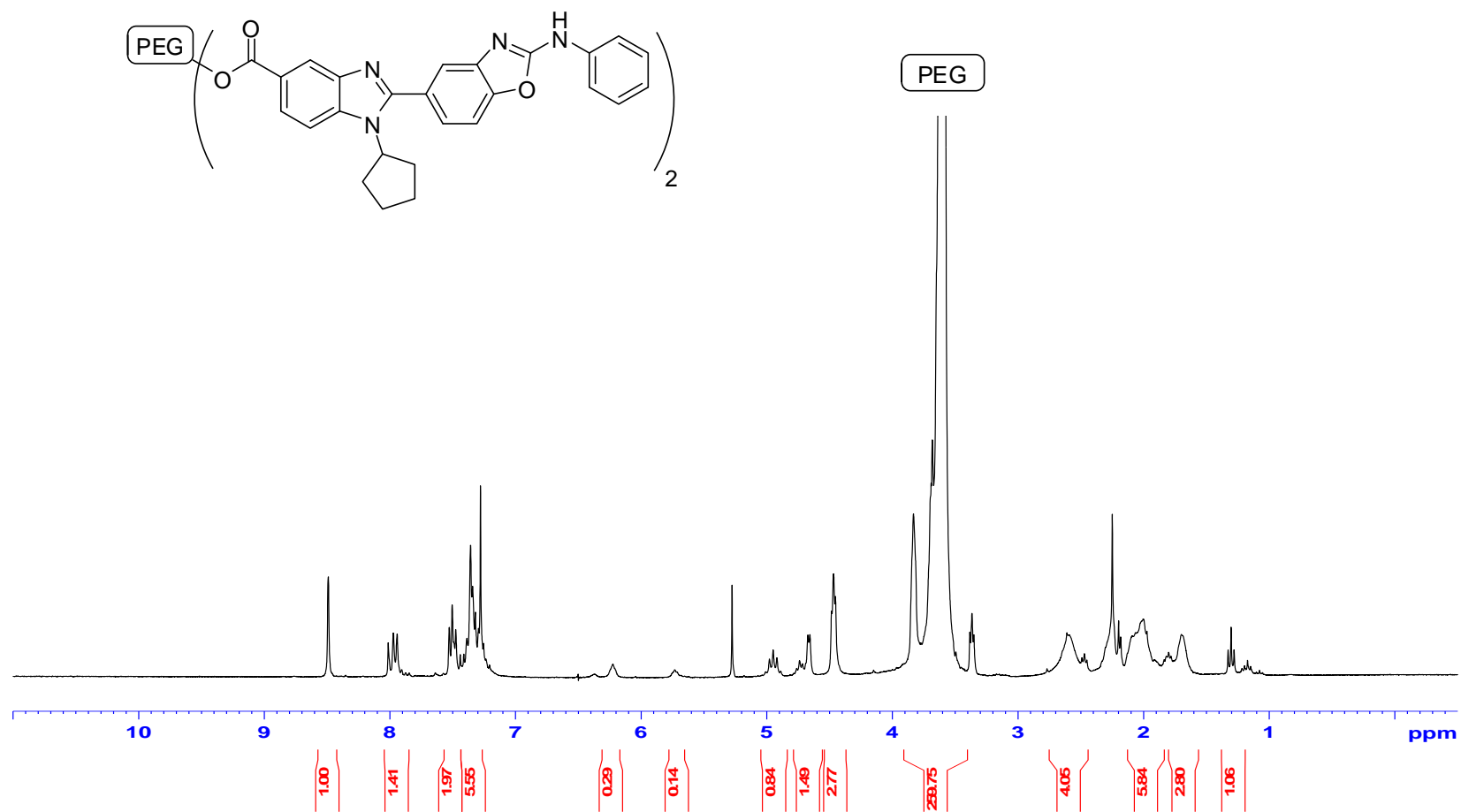
¹H NMR Spectrum (300 MHz) of compound 11n in CDCl₃



¹H NMR Spectrum (300 MHz) of compound 12n in CDCl₃



¹H NMR Spectrum (300 MHz) of compound 13n in CDCl₃



¹H NMR Spectrum (300 MHz) of compound 14n in CDCl₃

Synthesis of Polymer bound 3-(4-Hydroxy-3- nitrobenzamido)-4-(isobutylamino) carboxylates 11a.

Status: OK

Absorption level: Normal

Vial type: 10-20 ml

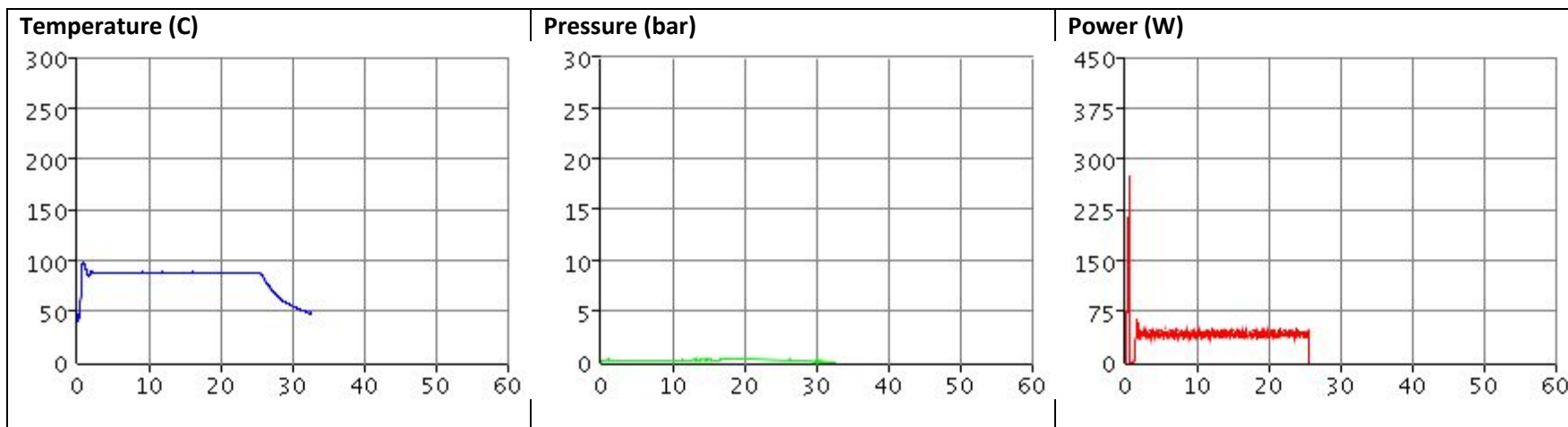
Pre-stirring: 0

Initial power: 0

Dynamic deflector optimization: Off

Step Time ?C bar W FHT Cooling Stir Rate

1	00:25:00	90	Off	Off	On	On	600
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Synthesis of 2-(4-Hydroxy-3-nitrophenyl)-1-isobutyl-1H-benzo[d]imidazole carboxylates 12a.

Status: OK

Absorption level: Normal

Vial type: 10-20 ml

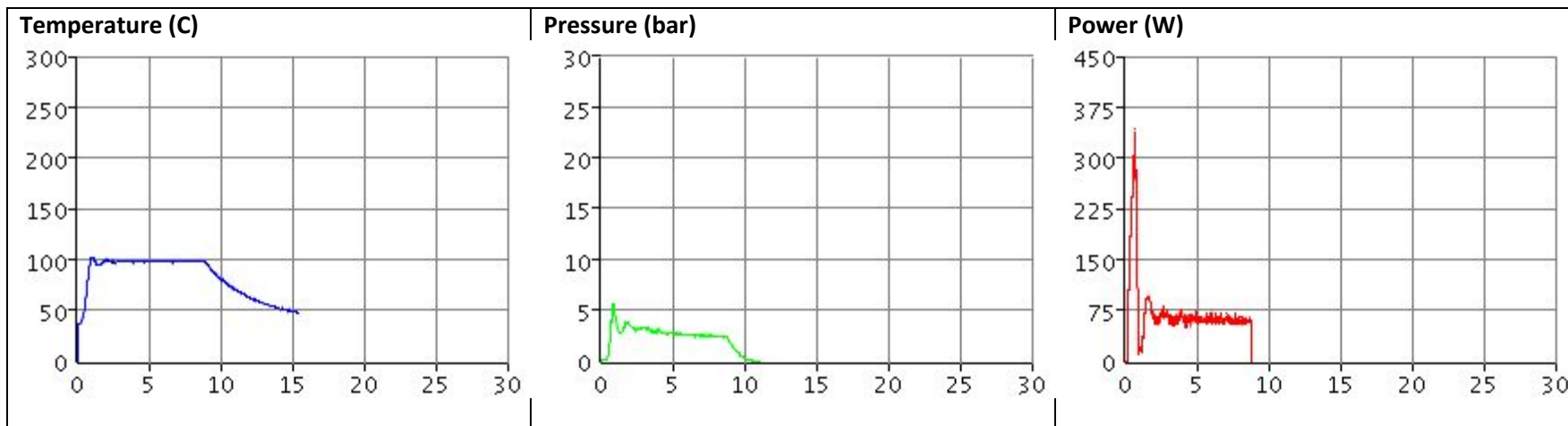
Pre-stirring: 0

Initial power: 0

Dynamic deflector optimization: Off

Step Time ?C bar W FHT Cooling Stir Rate

1	00:08:00	100	8	Off	On	On	600
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Synthesis of Polymer bound 2-(3-Amino-4-hydroxyphenyl)-1-isobutyl-1H-benzo[d]imidazole carboxylates 13a.

Status: OK

Absorption level: Normal

Vial type: 10-20 ml

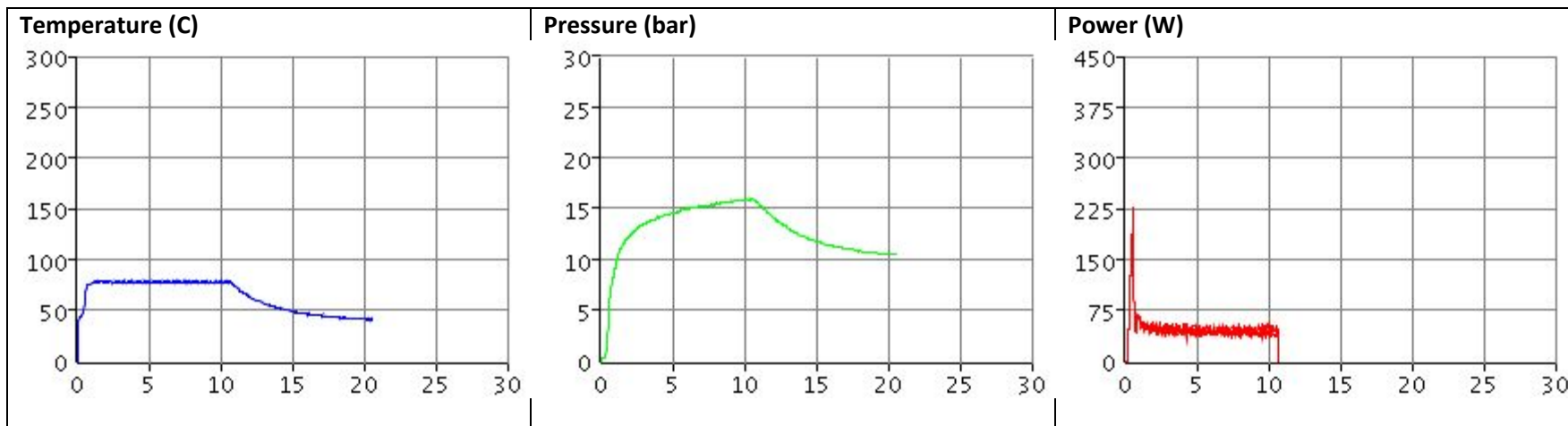
Pre-stirring: 10

Initial power: 0

Dynamic deflector optimization: Off

Step Time ?C bar W FHT Cooling Stir Rate

1	00:10:00	80	Off	Off	On	On	600
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Synthesis of Polymer bound 1-Isobutyl-2-(2-(phenylamino) benzo[d]oxazol-5-yl)-1H-benzo[d]imidazole-carboxylate 14a.

Status: OK

Absorption level: Normal

Vial type: 10-20 ml

Pre-stirring: 0

Initial power: 0

Dynamic deflector optimization: Off

Step Time ?C bar W FHT Cooling Stir Rate

1	00:10:00	100	5	Off	On	On	600
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