Supporting Information

Design and Synthesis of Benzimidazole-Chalcone Derivatives as Potential Anticancer Agents

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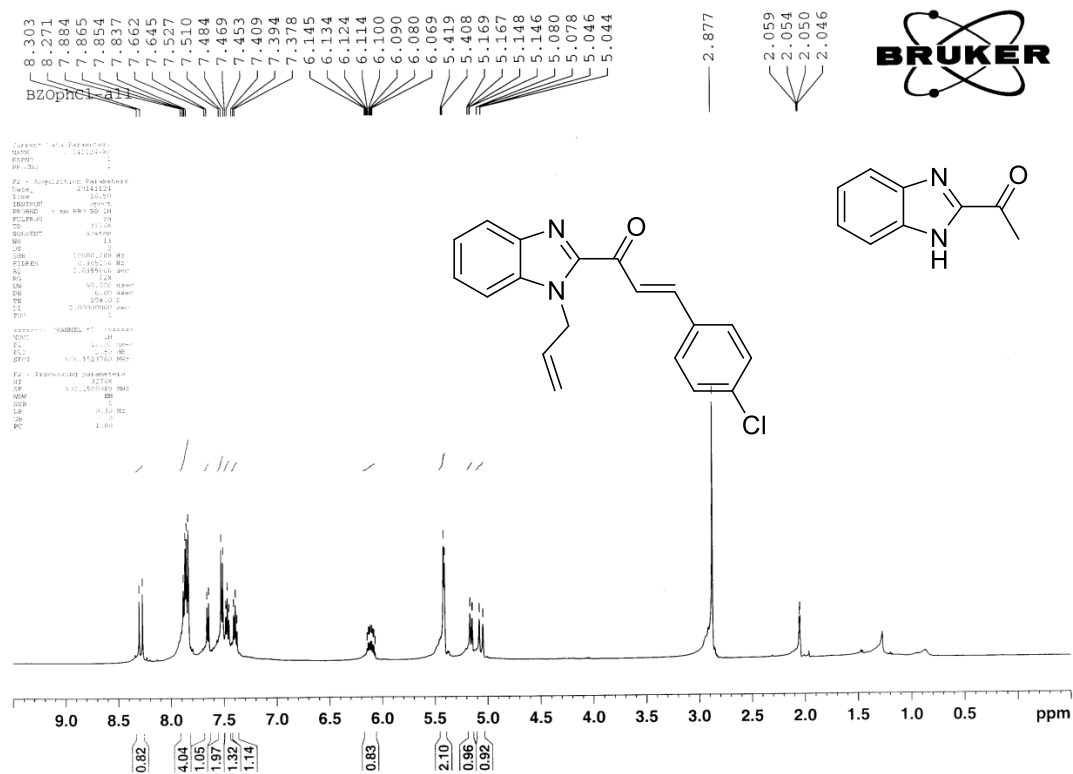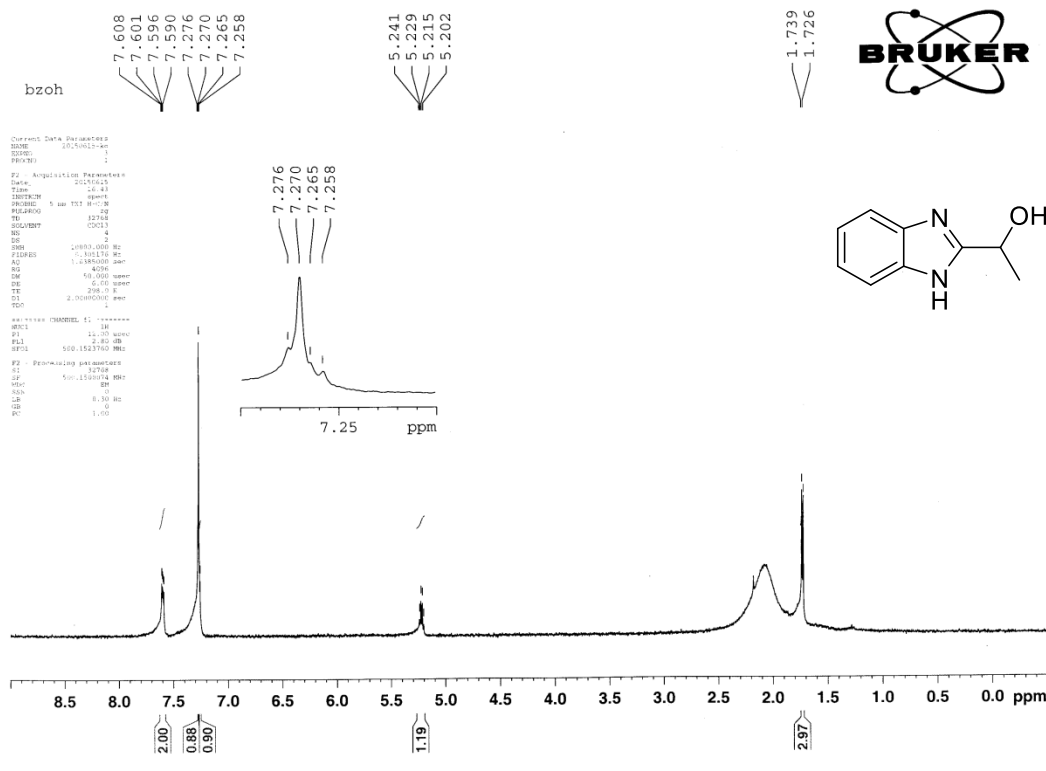These authors contributed equally to this work.

Contents

(1) Characterization Data:

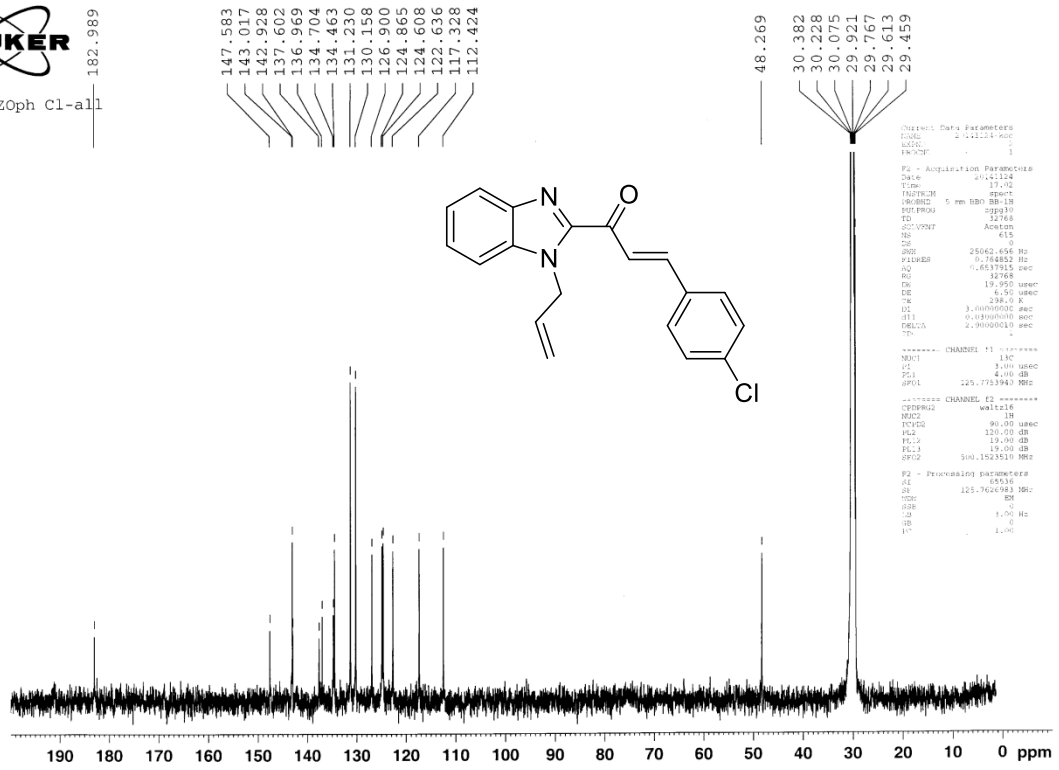 ^{1}H-NMR, ^{13}C-NMR, IR, HPLC

(2) Flow Cytometry Data

(1) Characterization Data

bzoh

7.608
7.601
7.596
7.590
7.276
7.270
7.265
7.258

5.241
5.229
5.215
5.202

1.739
1.726

BRUKER

7.276
7.270
7.265
7.258

7.25 ppm

8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm

2.00 0.88 0.90 1.19 2.97

8.303
8.271
7.884
7.865
7.854
7.837
7.662
7.645
7.527
7.510
7.484
7.469
7.453
7.409
7.394
7.378
6.145
6.134
6.124
6.114
6.100
6.090
6.080
6.069
5.419
5.408
5.167
5.148
5.146
5.080
5.078
5.046
5.044

2.877

2.059
2.054
2.050
2.046

BRUKER

BZOphCl-all

9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

0.82 4.04 1.05 1.97 1.32 1.14 0.83 2.10 0.96 0.92

¹H-NMR spectrum of compound **19d**

^{13}C-NMR spectrum of compound **19d**
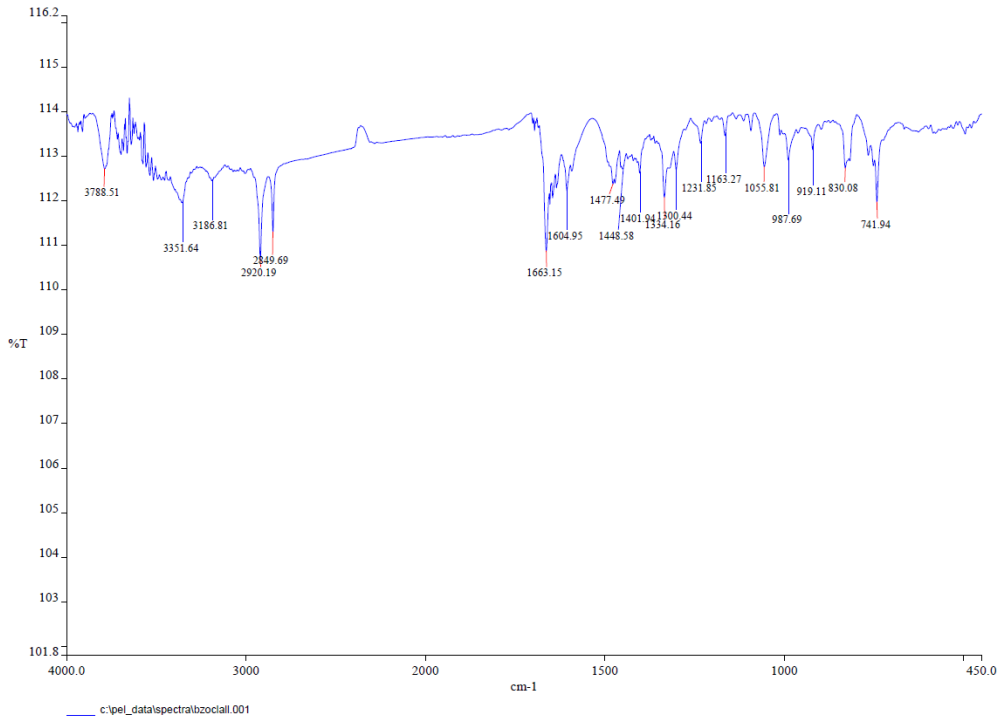
IR spectrum of compound **19d**
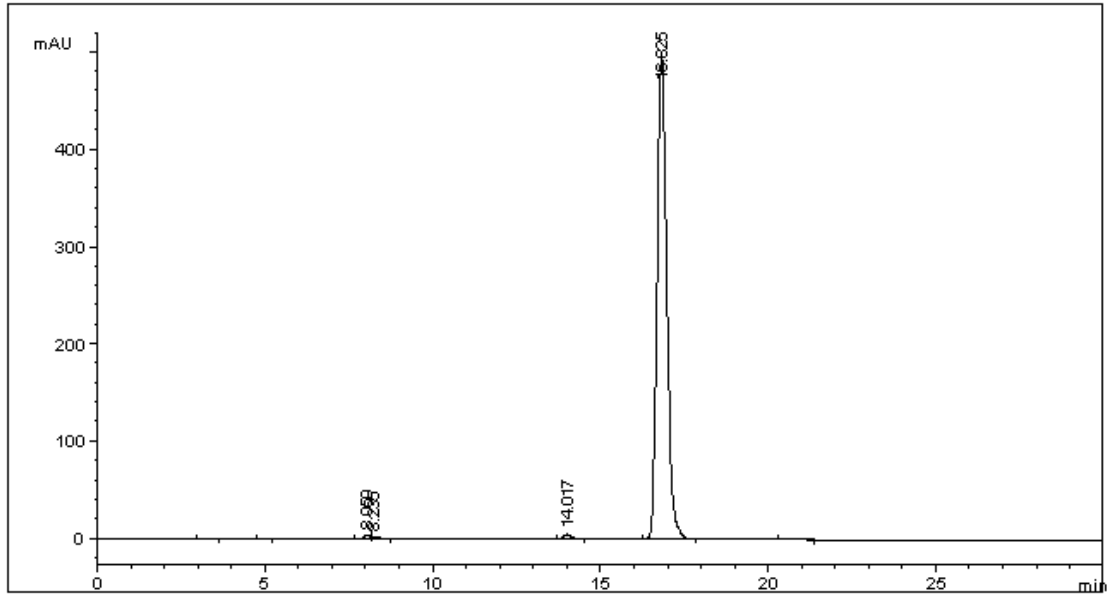
HPLC spectrum of compound **19d**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	8.05	0.2178	56.94883	0.5562
2	8.235	0.2043	36.42011	0.3557
3	14.017	0.2913	94.06382	0.9187
4	16.825	0.3131	10051.4	98.169
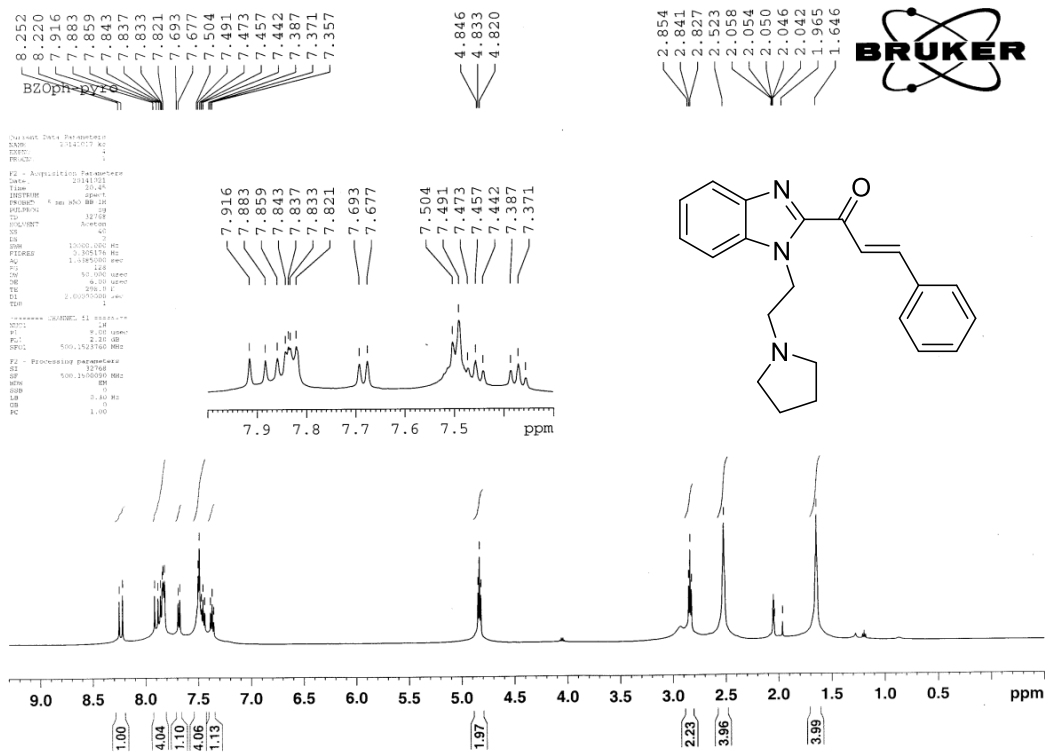
^{1}H-NMR spectrum of compound **20a**
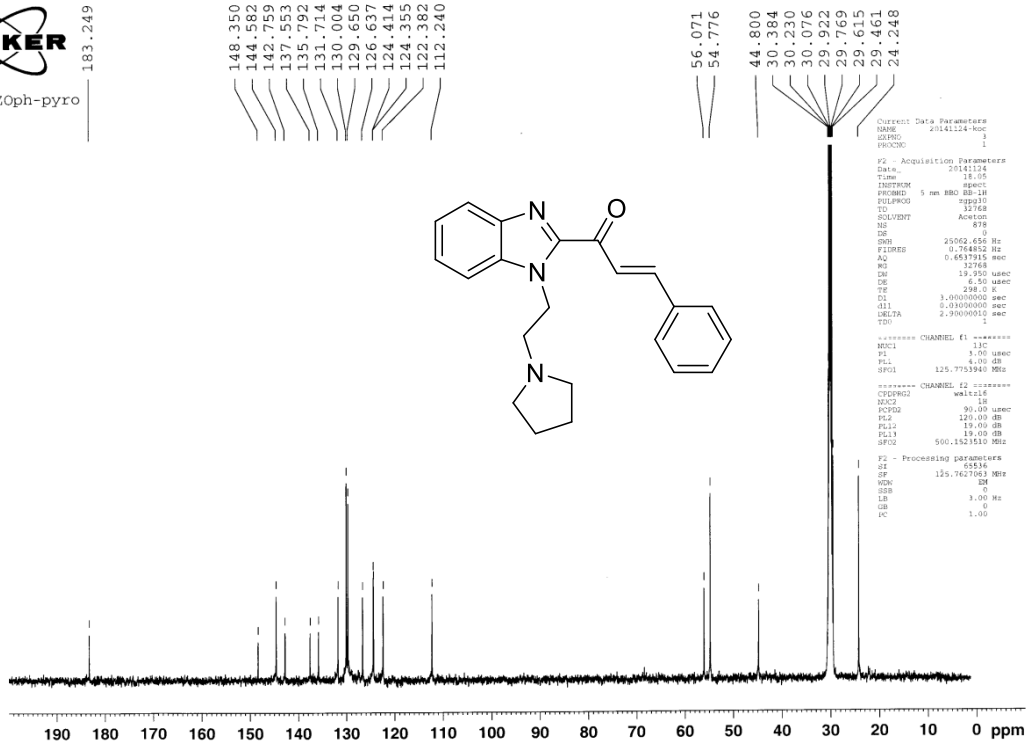
13C-NMR spectrum of compound **20a**
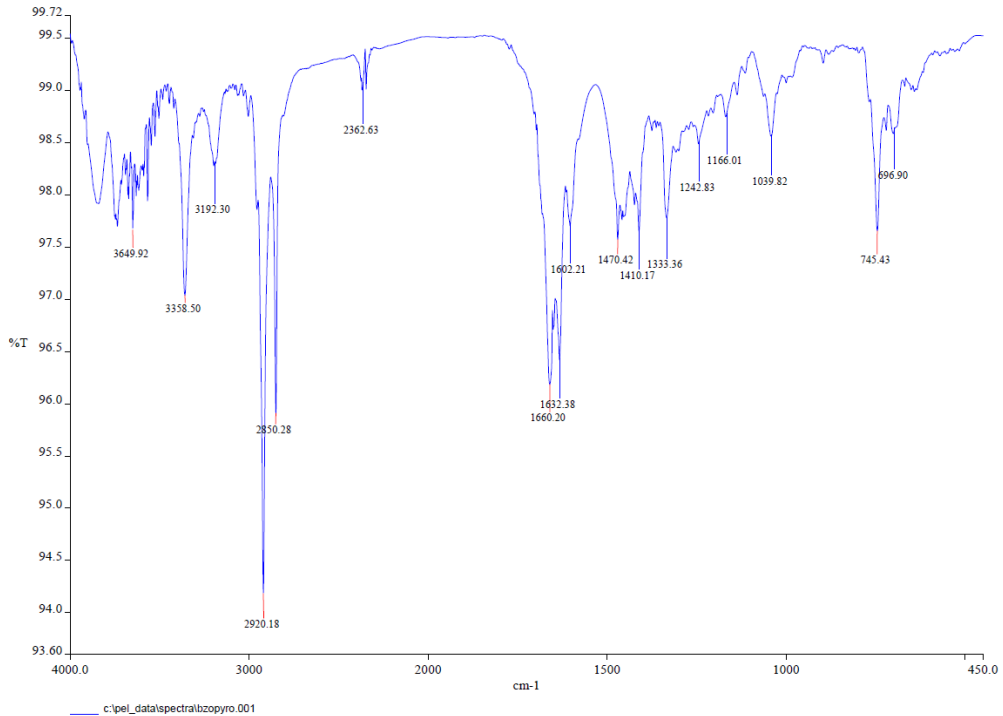
IR spectrum of compound **20a**
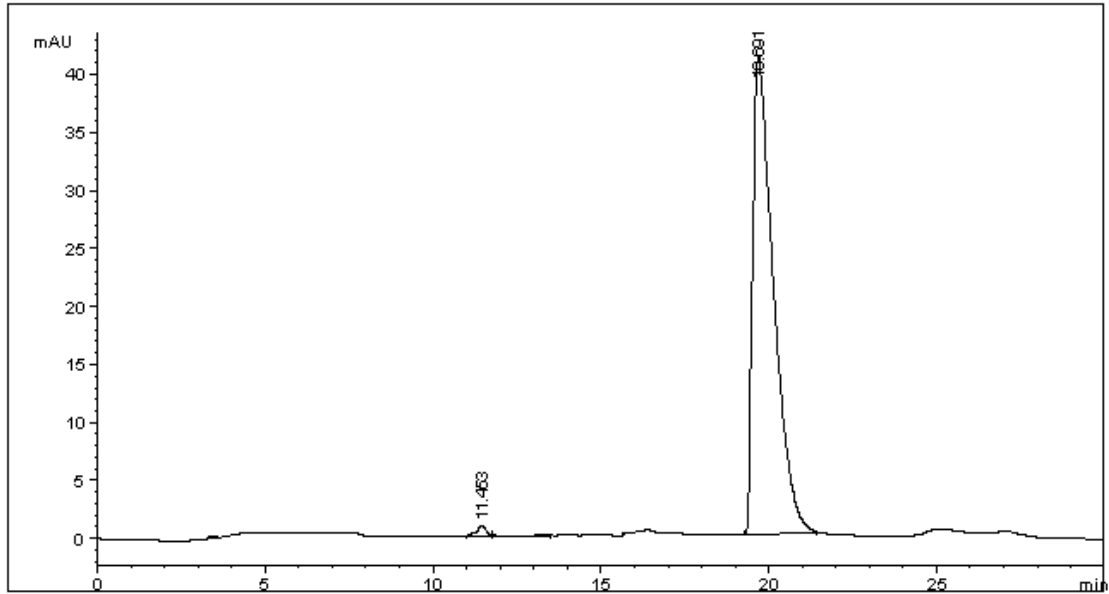
HPLC spectrum of compound **20a**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	11.453	0.3000	71.80160	3.8726
2	19.691	0.6477	1782.26953	96.1274
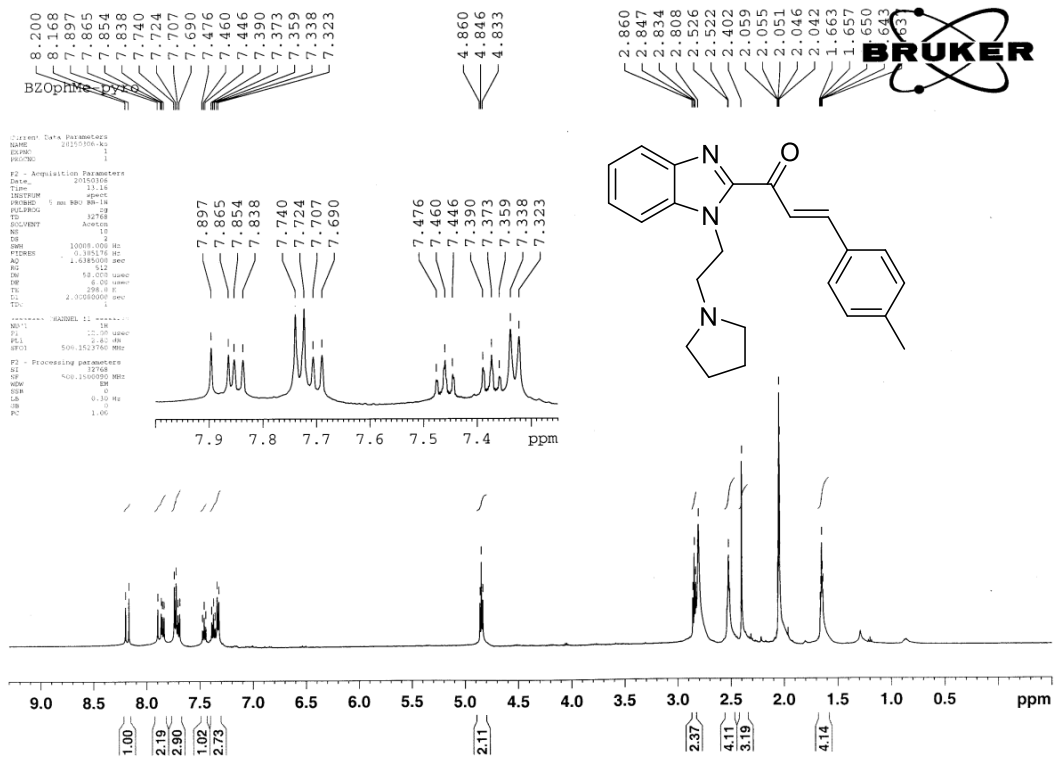
^{1}H-NMR spectrum of compound **20b**
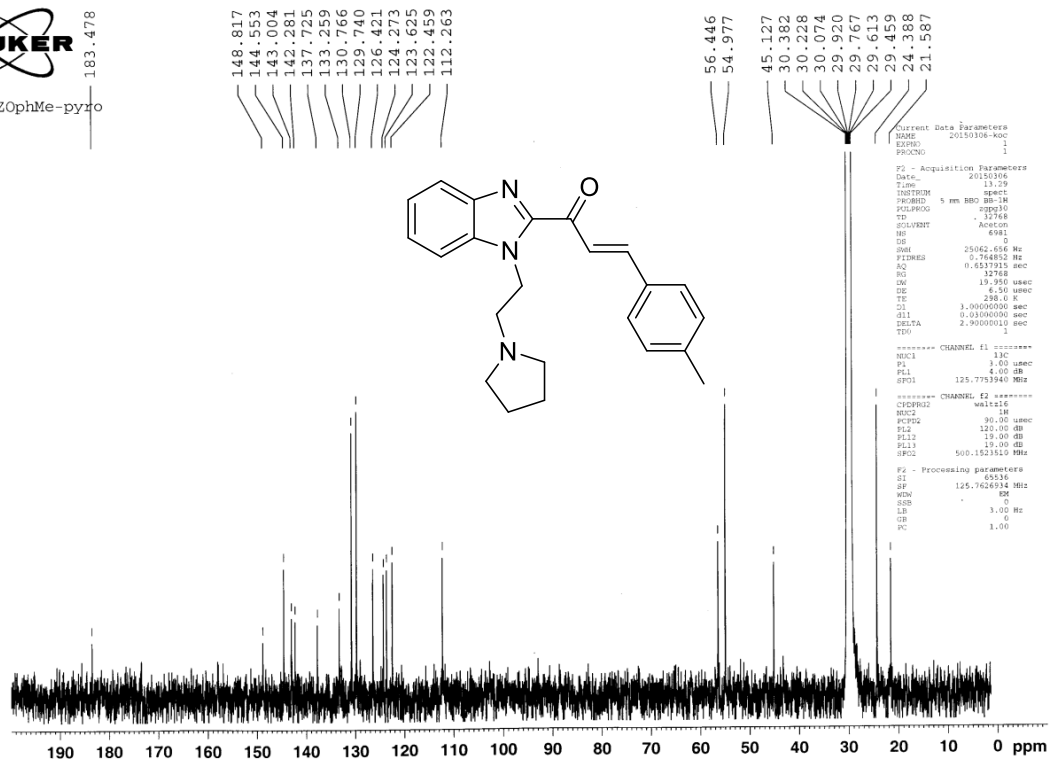
^{13}C-NMR spectrum of compound **20b**
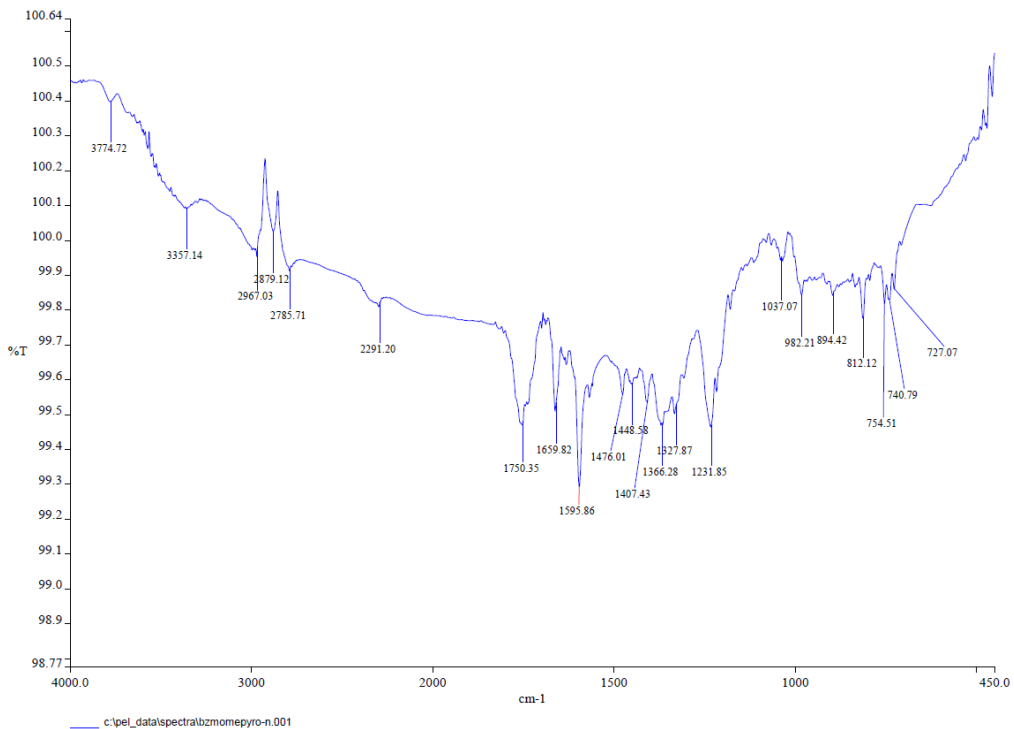
IR spectrum of compound **20b**
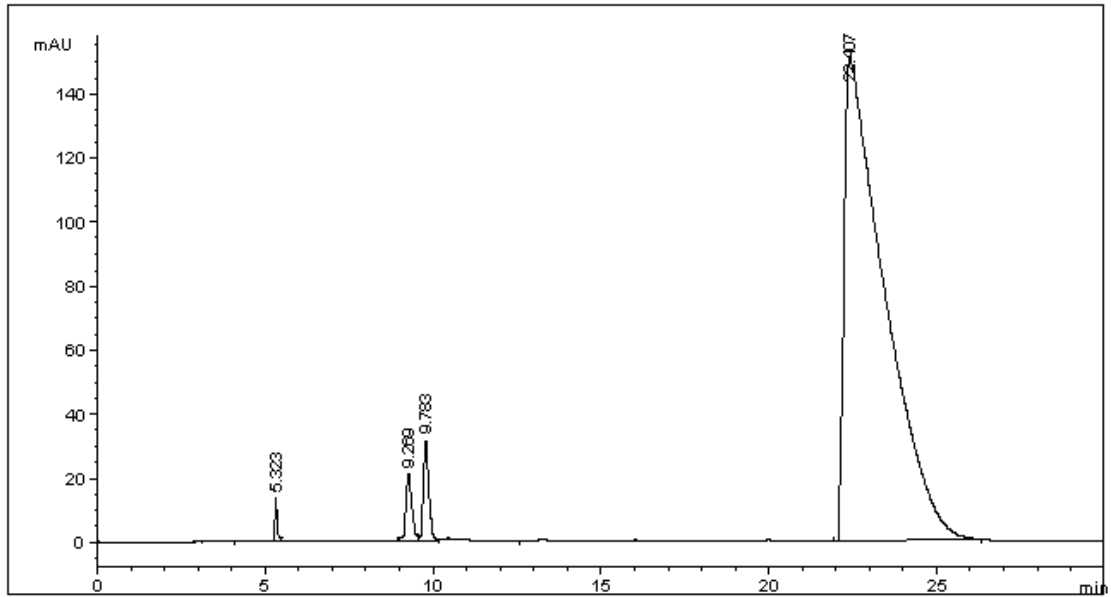
HPLC spectrum of compound **20b**

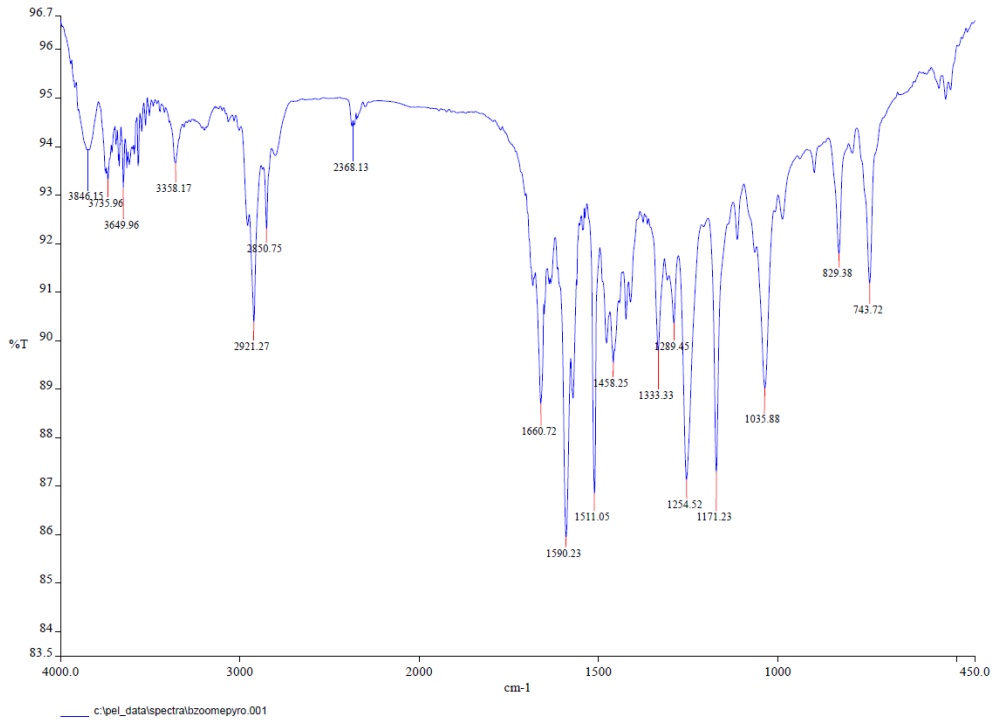| Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	5.323	0.0522	36.09950	0.2756
2	9.270	0.1684	180.59157	1.3785
3	9.783	0.1675	287.45895	2.1943
4	22.407	1.3899	12596.0	96.1516
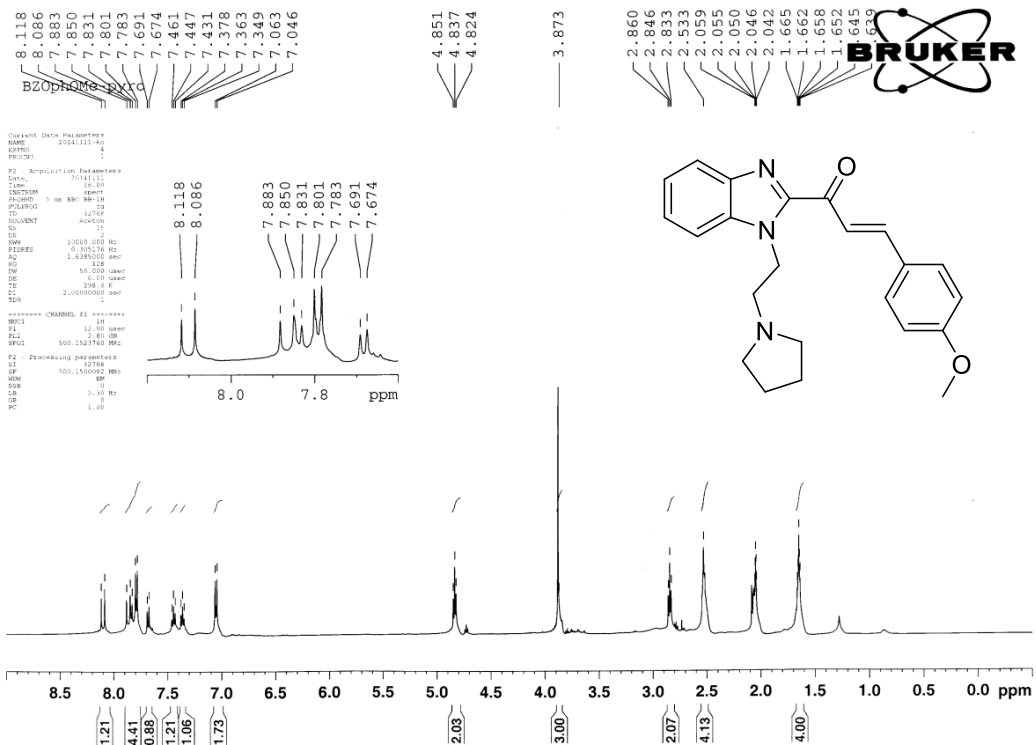
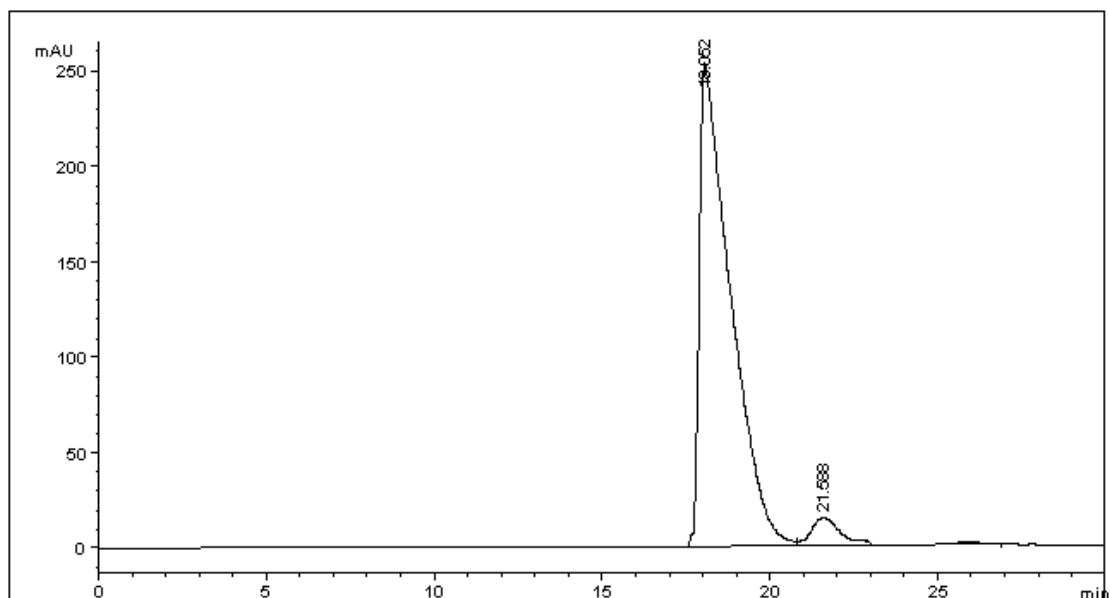¹H-NMR spectrum of compound **20c**
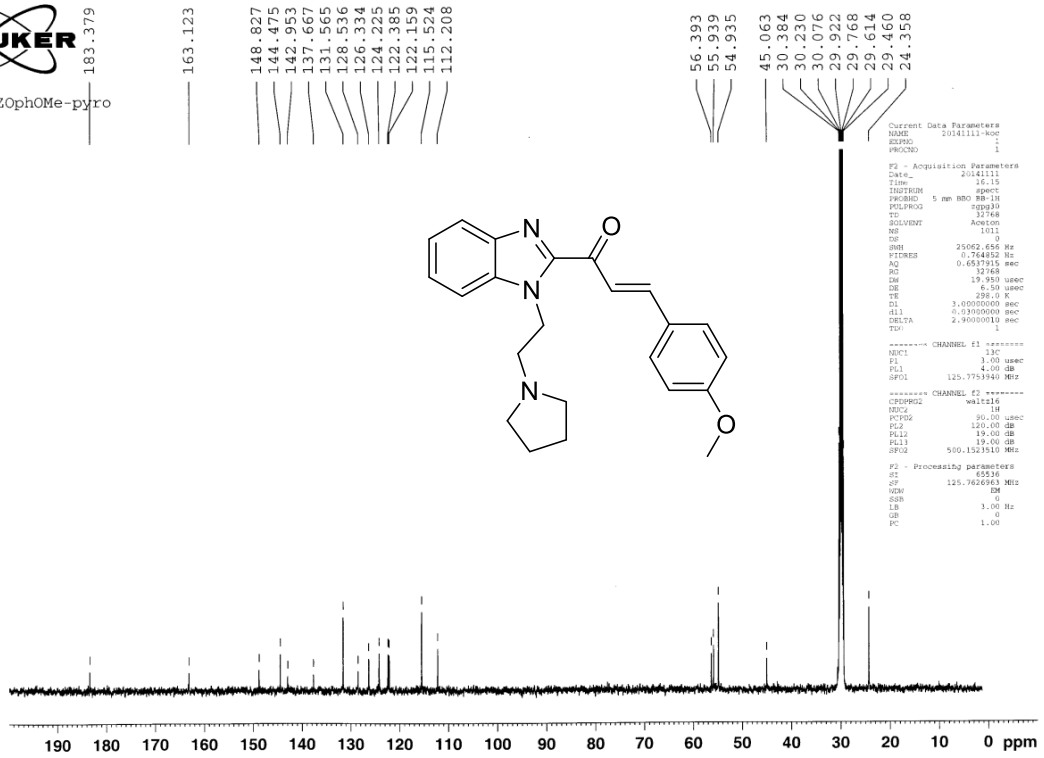
¹³C-NMR spectrum of compound **20c**

IR spectrum of compound **20c**

HPLC spectrum of compound **20c**
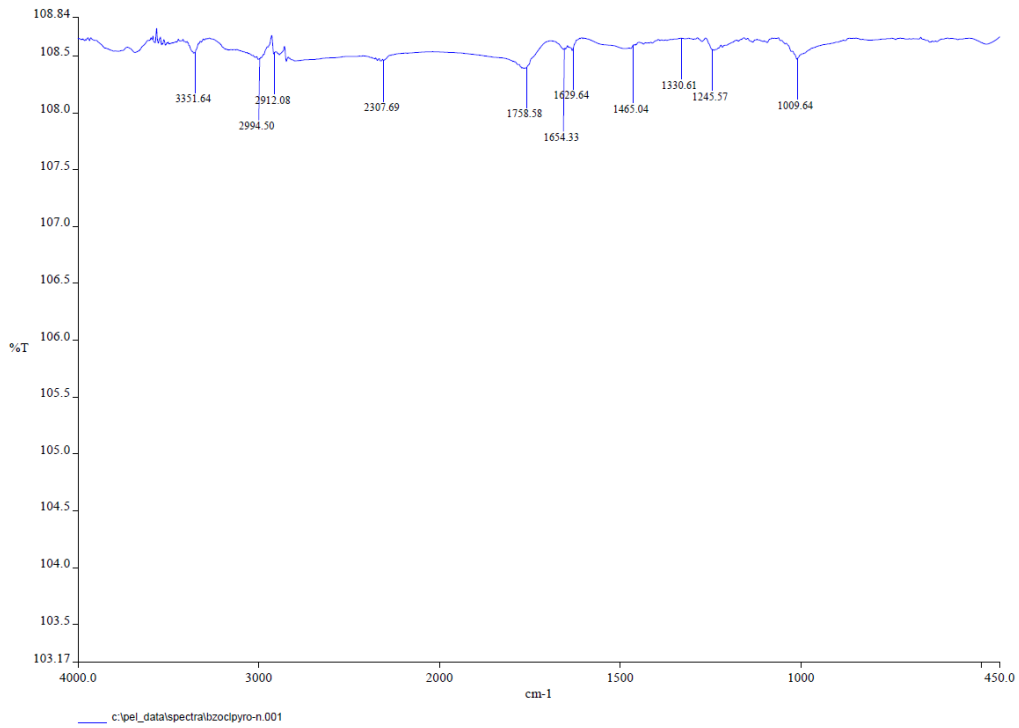
Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	18.052	0.8788	16437.4	95.0057
2	21.588	0.9133	864.08667	4.9943

¹H-NMR spectrum of compound **20d**

BZpy

183.230

142.917
140.460
136.946
134.806
131.237
130.208
126.609
125.274
124.397
122.486
112.325

77.318

56.387
54.955

45.087
30.383
30.229
30.075
29.921
29.767
29.613
29.459
24.364

Current Data Parameters
NAME   CARBON_01.fid
EXPNO   1
PROCNO   1

F2 - Processing parameters
SI   131072
SF   125.6965872 MHz
WDW   EM
SSB   0
LB   0.30 Hz
GB   0
PC   1.00

BRUKER

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
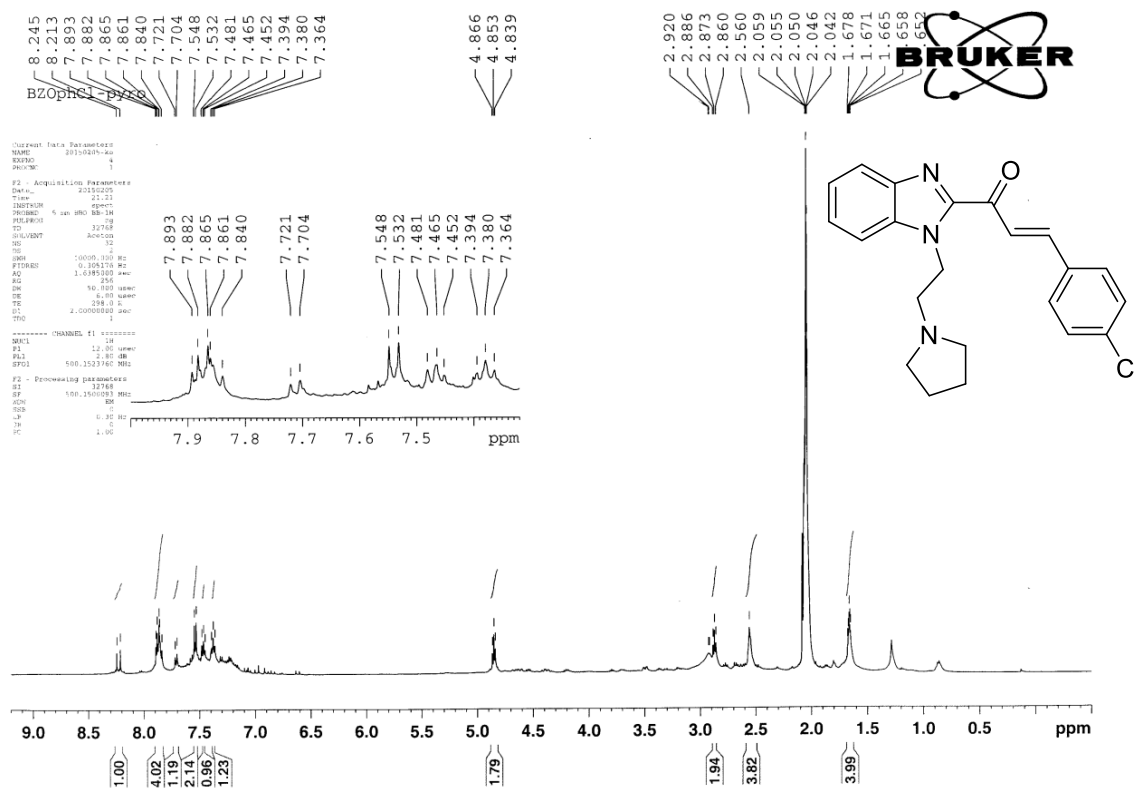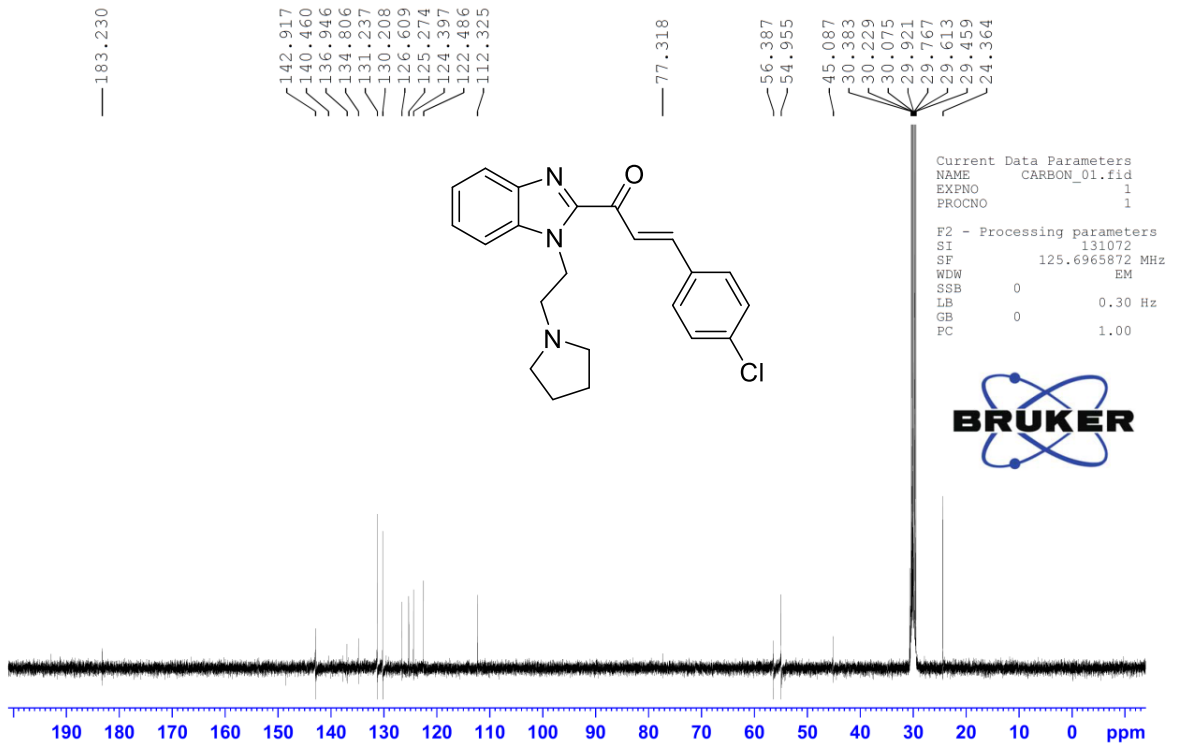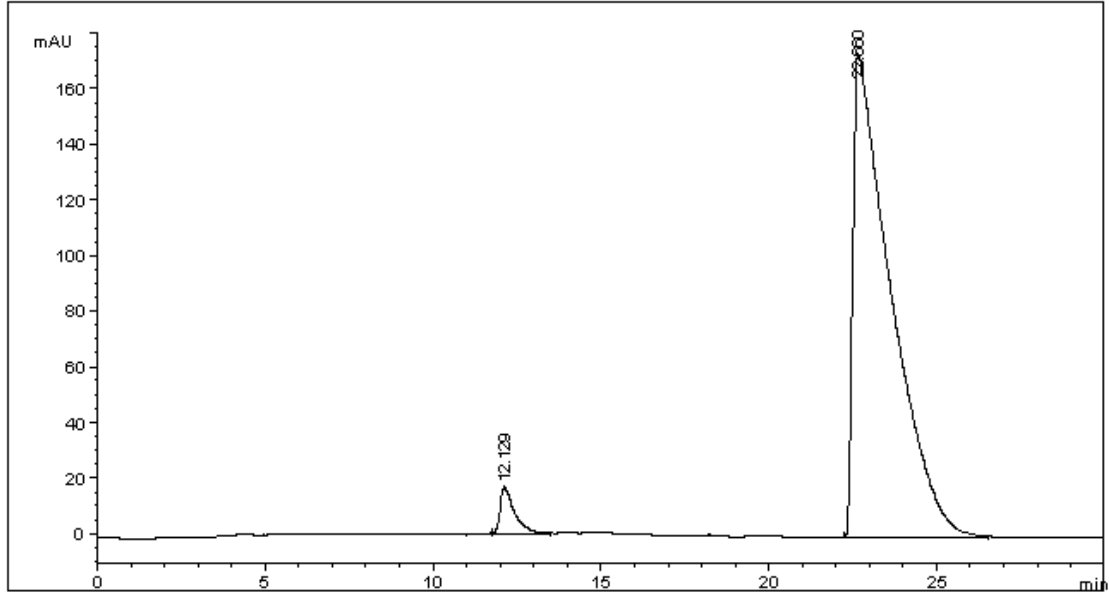
¹³C-NMR spectrum of compound **20d**

IR spectrum of compound **20d**

HPLC spectrum of compound **20d**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	12.129	0.4295	491.38254	3.5048
2	22.660	1.0394	13528.9	96.4953

¹H-NMR spectrum of compound **21a**

183.324

148.508
144.411
142.876
137.760
135.892
131.647
130.006
129.619
126.422
124.552
124.265
122.438
112.362

59.388
55.665

43.840
30.384
30.230
30.076
29.922
29.768
29.614
29.461
26.827
25.032

Current Data Parameters
NAME   20141011-ku
EXPNO   5
PROCNO   1

F2 - Acquisition Parameters
Date_   20141012
Time   22.33
INSTRUM   spect
PROBHD   5 mm BBO BB-1H
PULPROG   zgpg30
TD   32768
SOLVENT   Aceton
NS   267
DS   0
SWH   25062.656 Hz
FIDRES   0.764852 Hz
AQ   0.6537915 sec
RG   32768
DW   19.950 usec
DE   6.50 usec
TE   298.0 K
D1   3.00000000 sec
d11   0.03000000 sec
DELTA   2.90000010 sec
TD0   1

======== CHANNEL f1 ========
NUC1   13C
P1   3.00 usec
PL1   4.00 dB
SFO1   125.7753940 MHz

======== CHANNEL f2 ========
CPDPRG2   waltz16
NUC2   1H
PCPD2   90.00 usec
PL2   120.00 dB
PL12   19.00 dB
PL13   19.00 dB
SFO2   500.1523510 MHz

F2 - Processing parameters
SI   65536
SF   125.7627037 MHz
WDW   EM
SSB   0
LB   3.00 Hz
GB   0
PC   1.00

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

^{13}C-NMR spectrum of compound **21a**

IR spectrum of compound **21a**
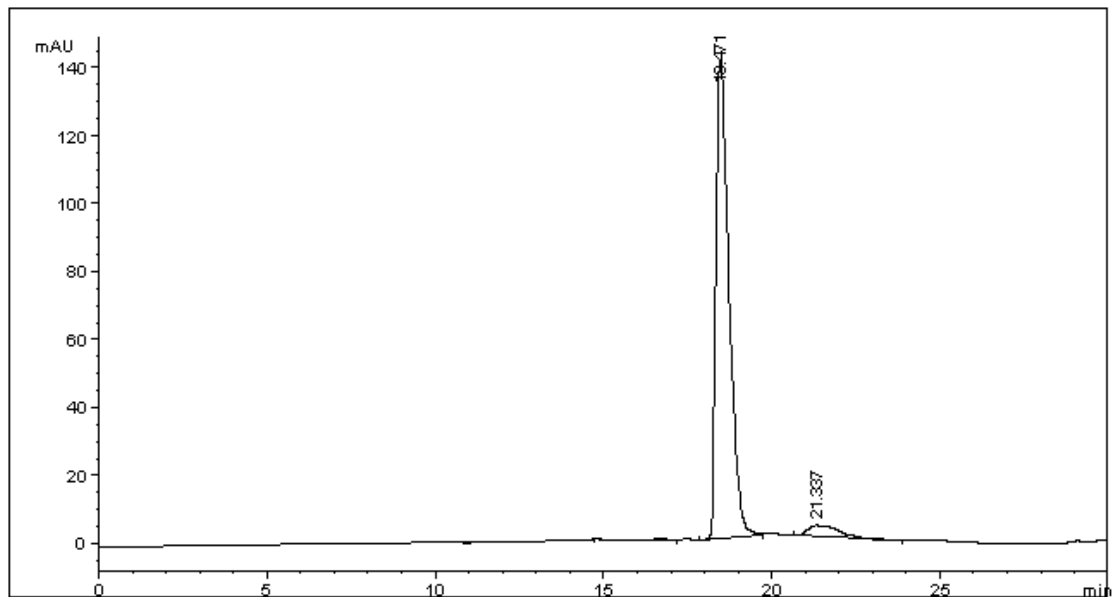
HPLC spectrum of compound **21a**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	18.471	0.4193	3837.38745	95.0169
2	21.337	0.9008	201.24811	4.9831
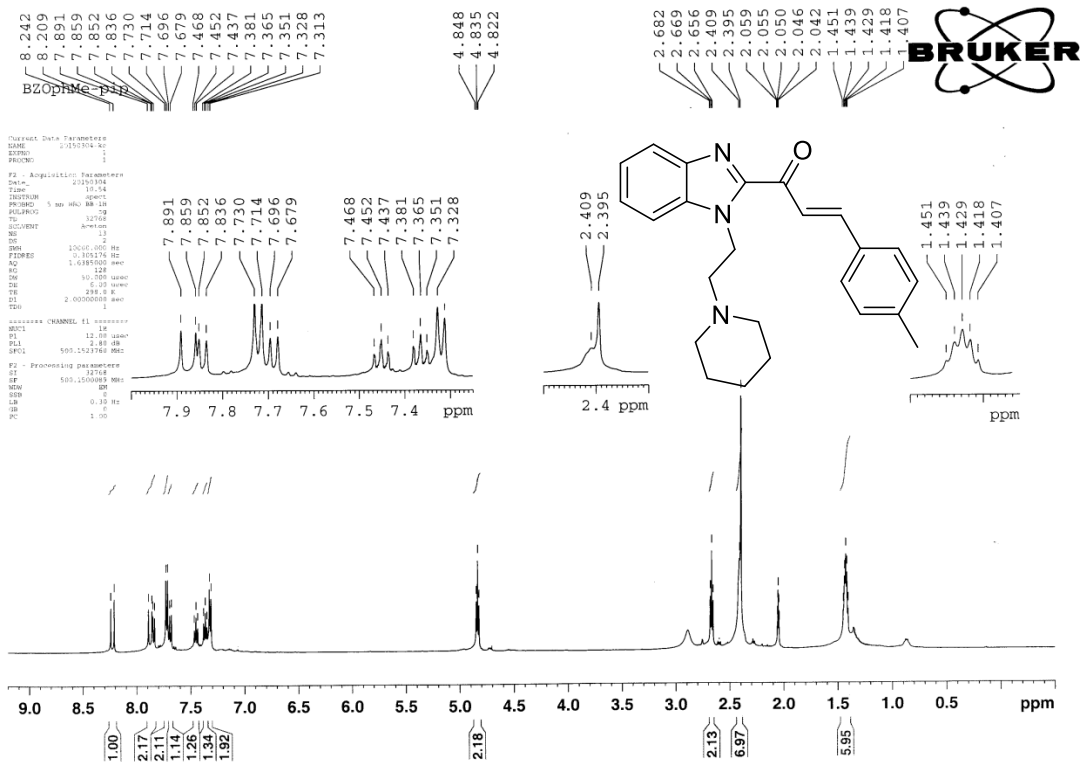
¹H-NMR spectrum of compound **21b**
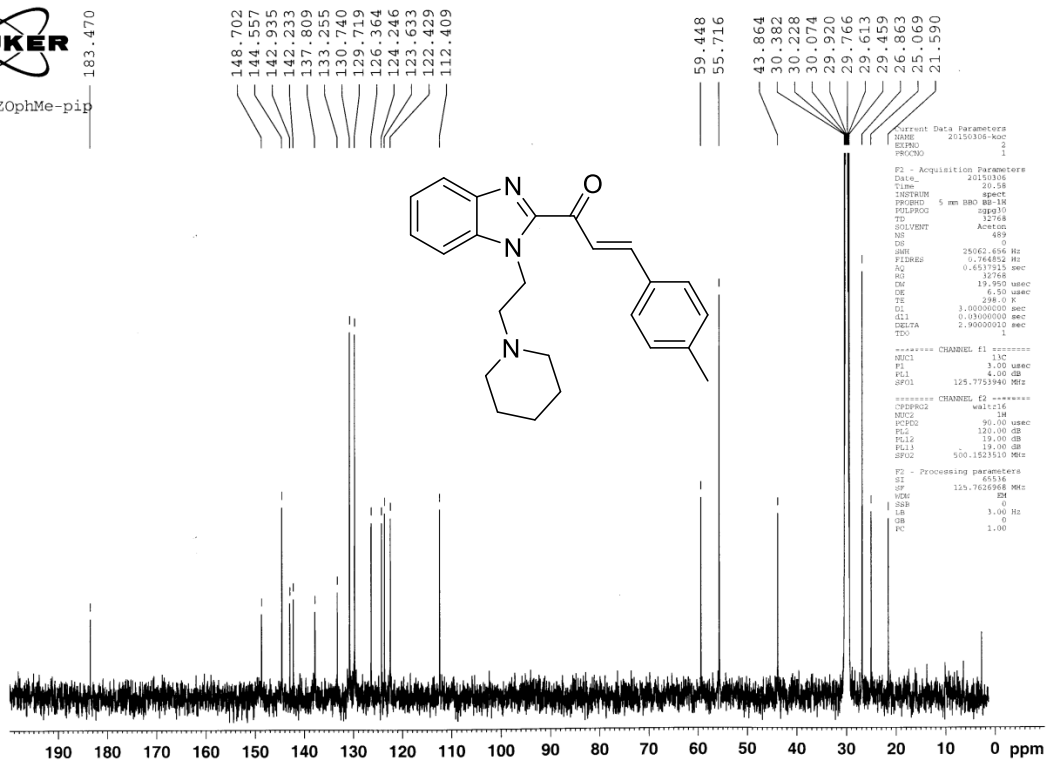
^{13}C-NMR spectrum of compound **21b**
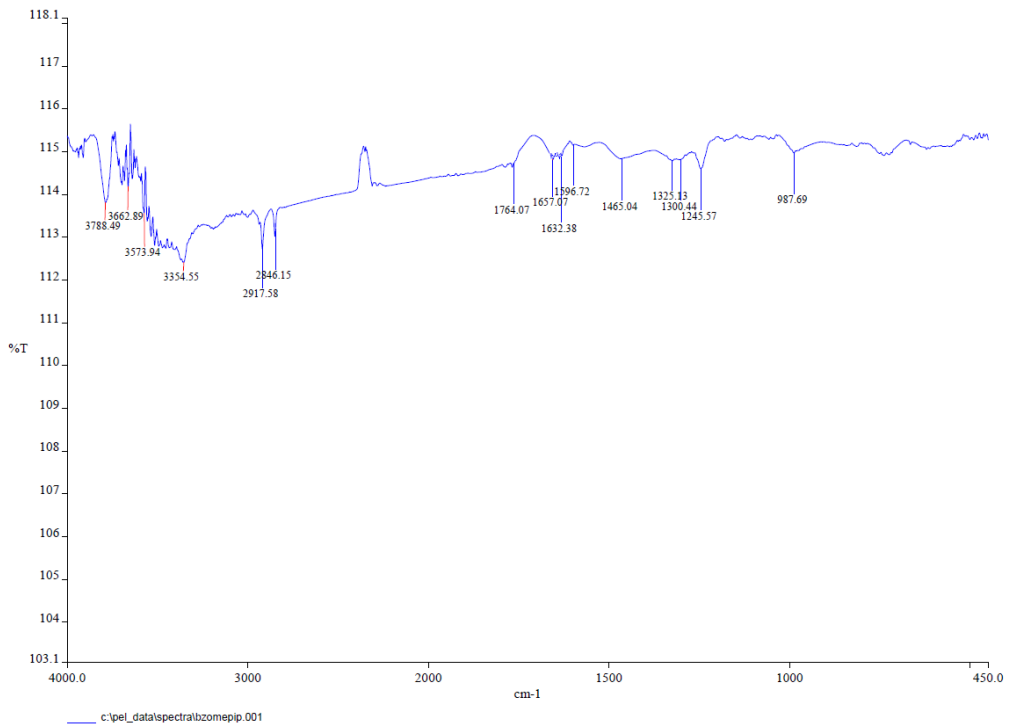
IR spectrum of compound **21b**

HPLC spectrum of compound **21b**
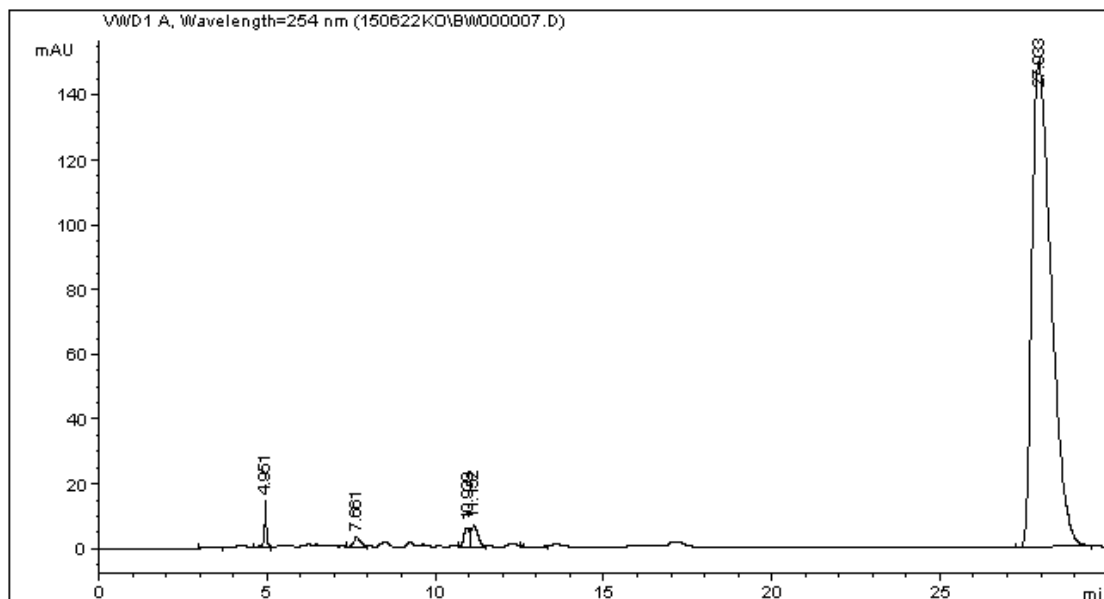
Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	4.951	0.0699	68.29758	1.0947
2	7.661	0.1966	38.23409	0.6129
3	10.939	0.1666	64.38687	1.0320
4	11.152	0.2067	91.49991	1.4666
5	27.933	0.6205	5976.29102	95.7937
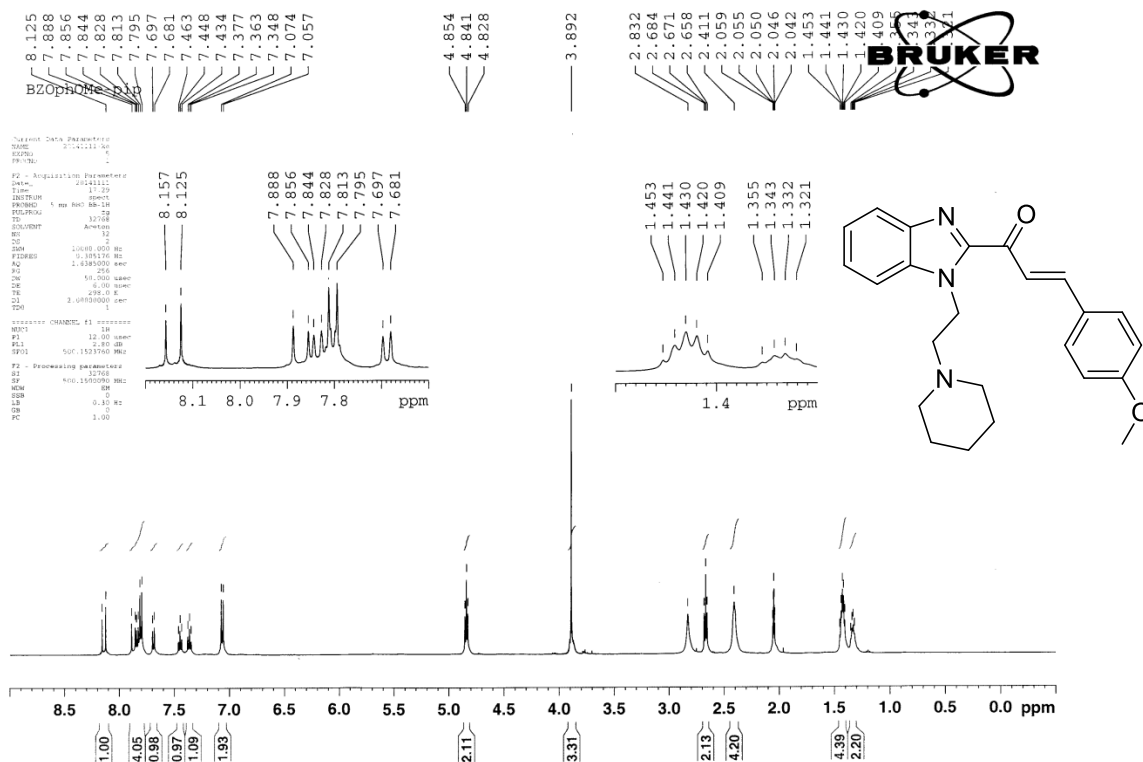
^{1}H-NMR spectrum of compound **21c**
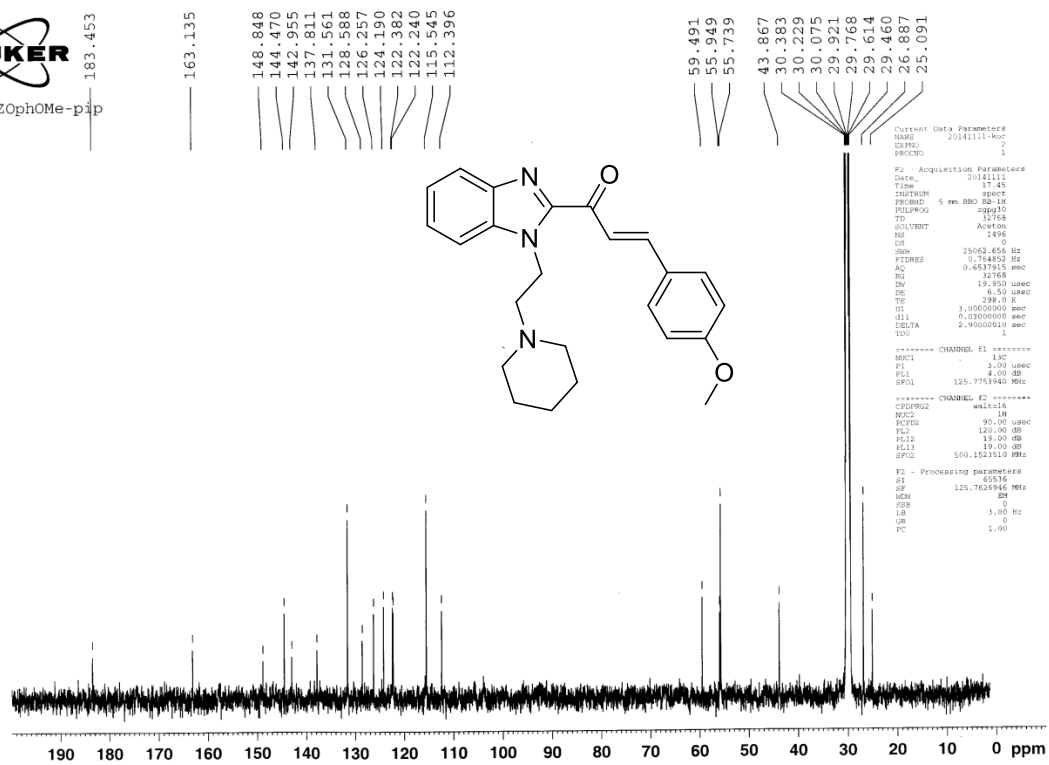
^{13}C-NMR spectrum of compound **21c**
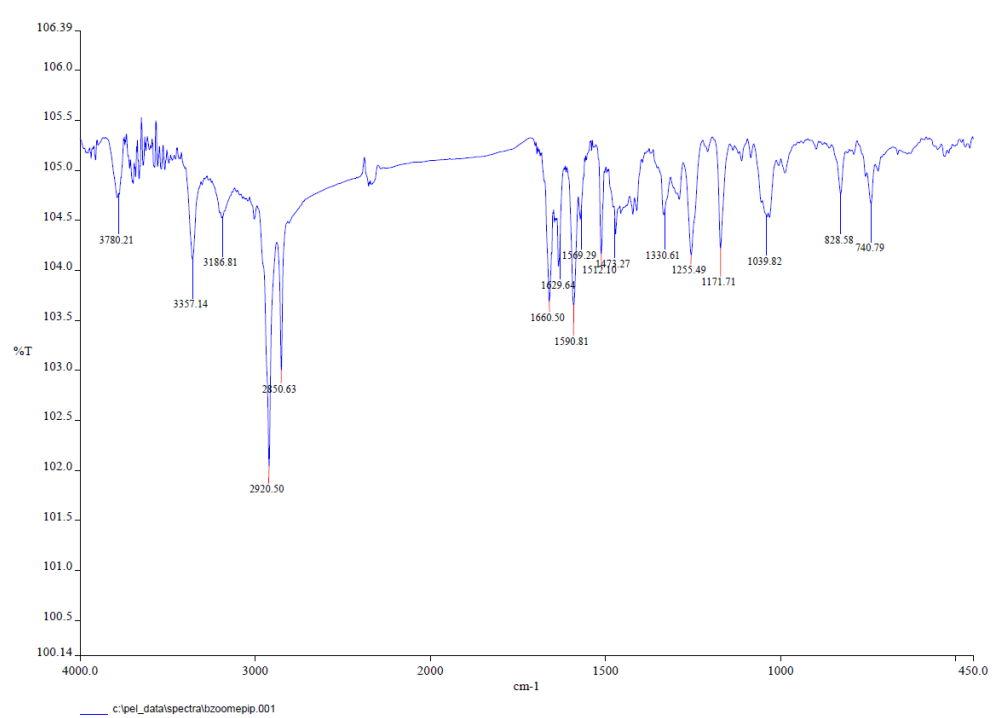
IR spectrum of compound **21c**
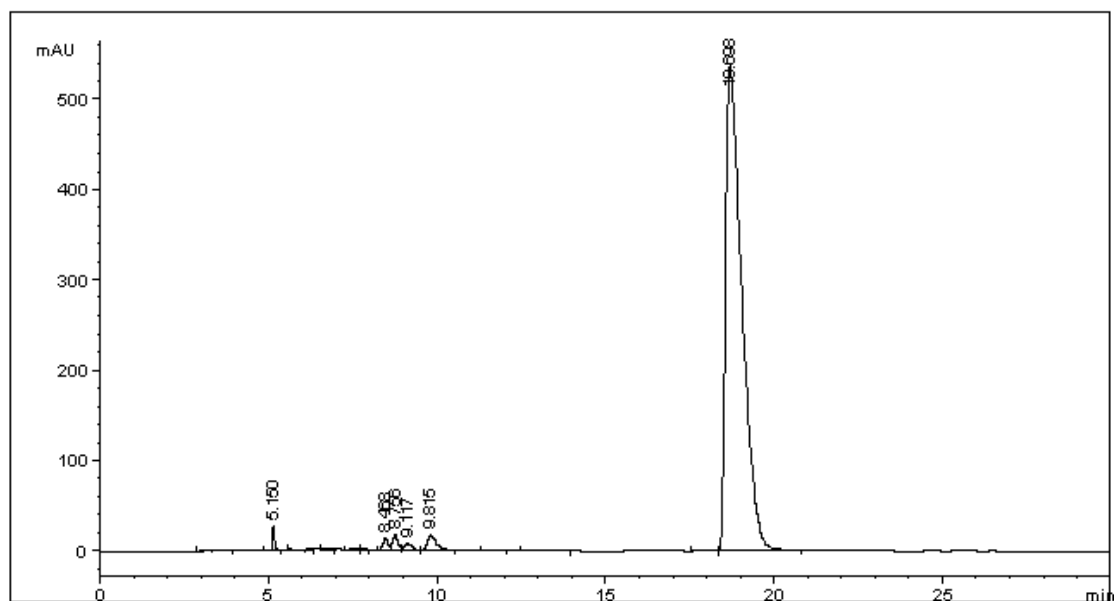
HPLC spectrum of compound **21c**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	5.150	0.0654	120.31086	0.6396
2	8.468	0.1586	143.72900	0.7641
3	8.756	0.1657	182.23738	0.9688
4	9.117	0.2214	113.33360	0.6025
5	9.815	0.2669	299.16333	1.5904
6	18.698	0.4951	17951.6	95.4346
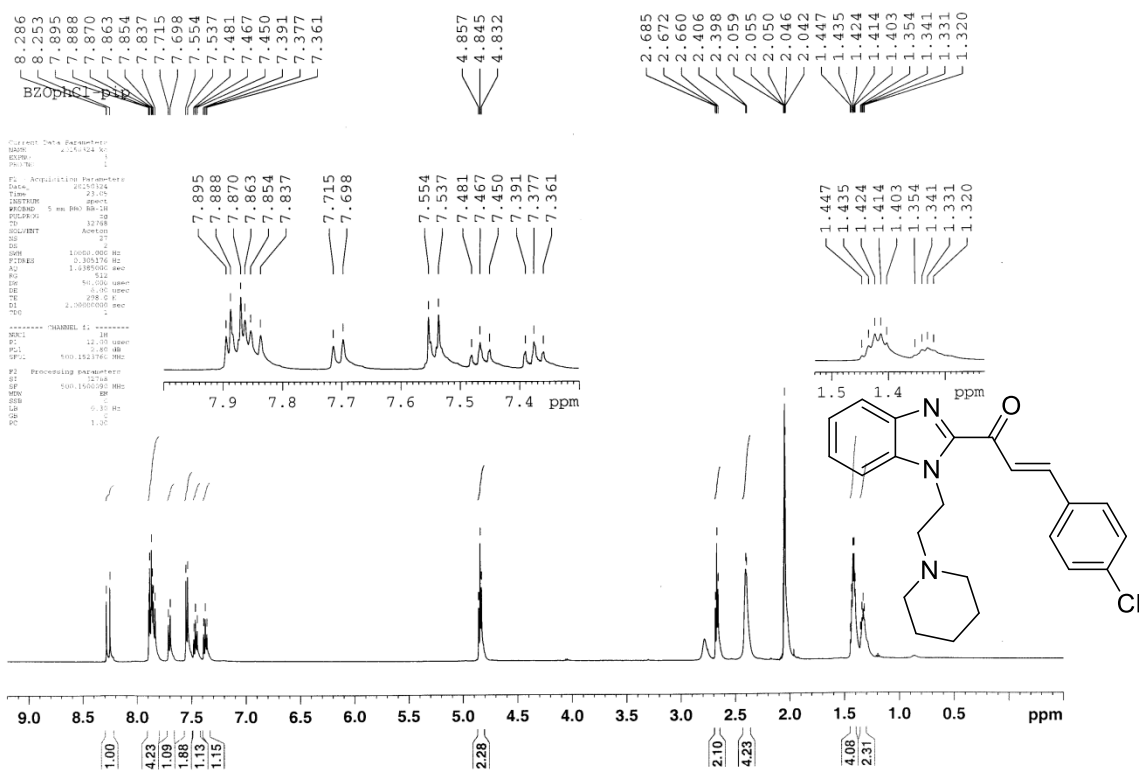
^{1}H-NMR spectrum of compound **21d**
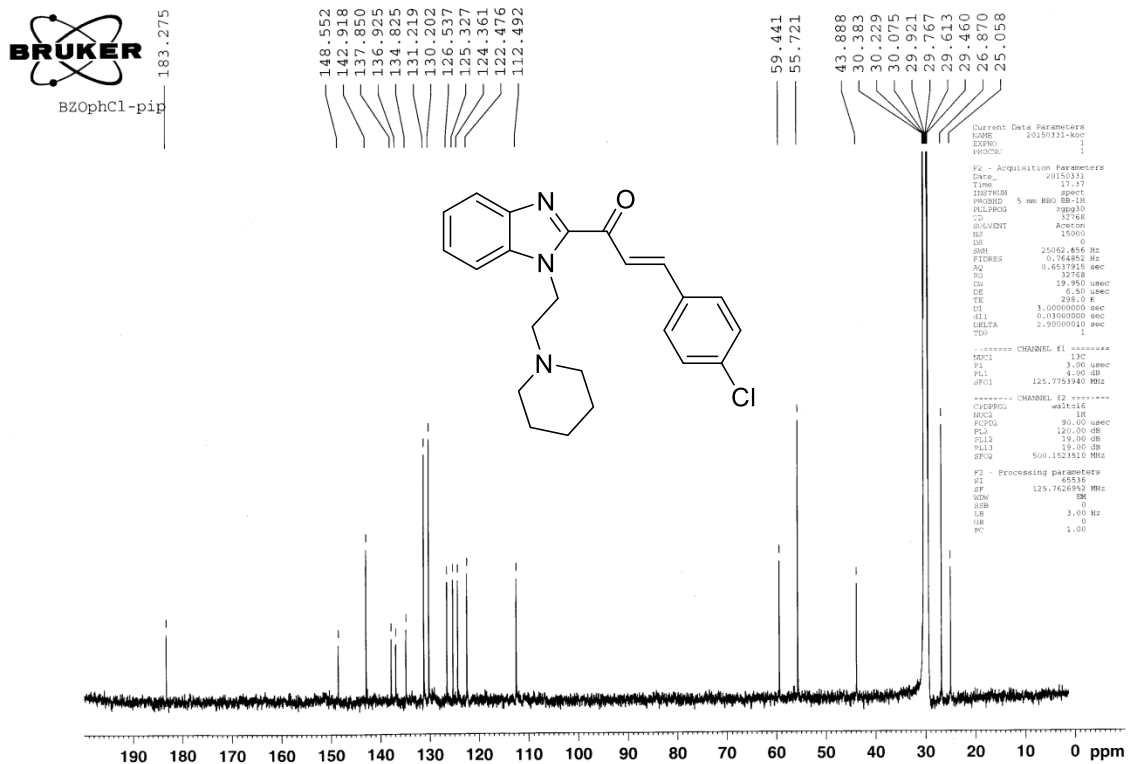
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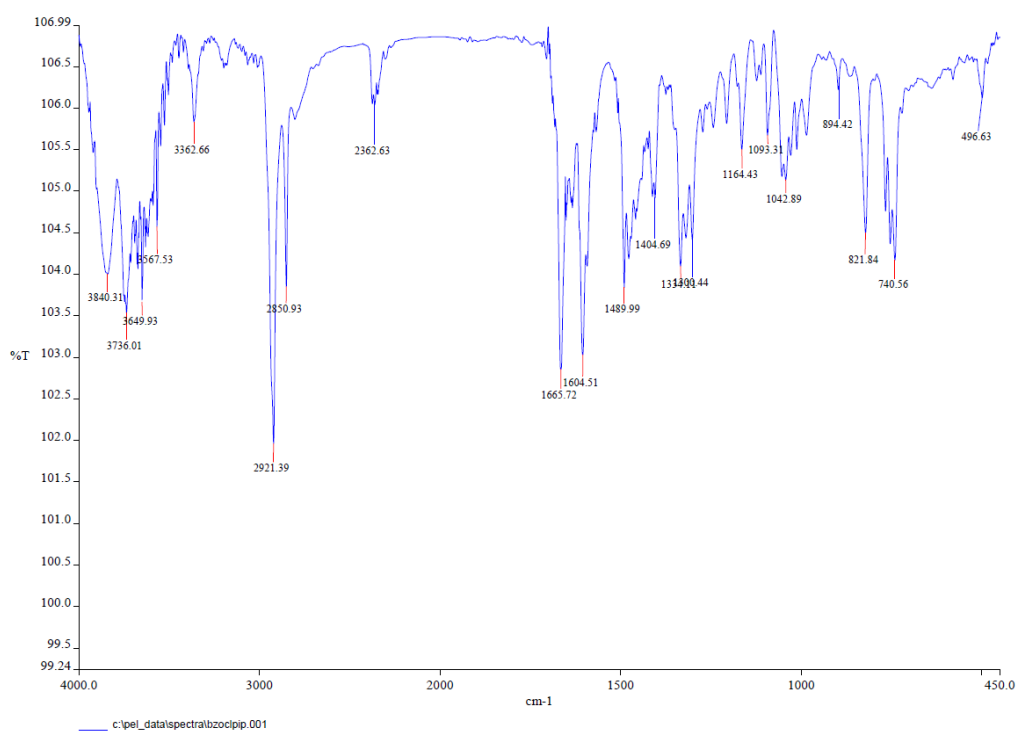
IR spectrum of compound **21d**
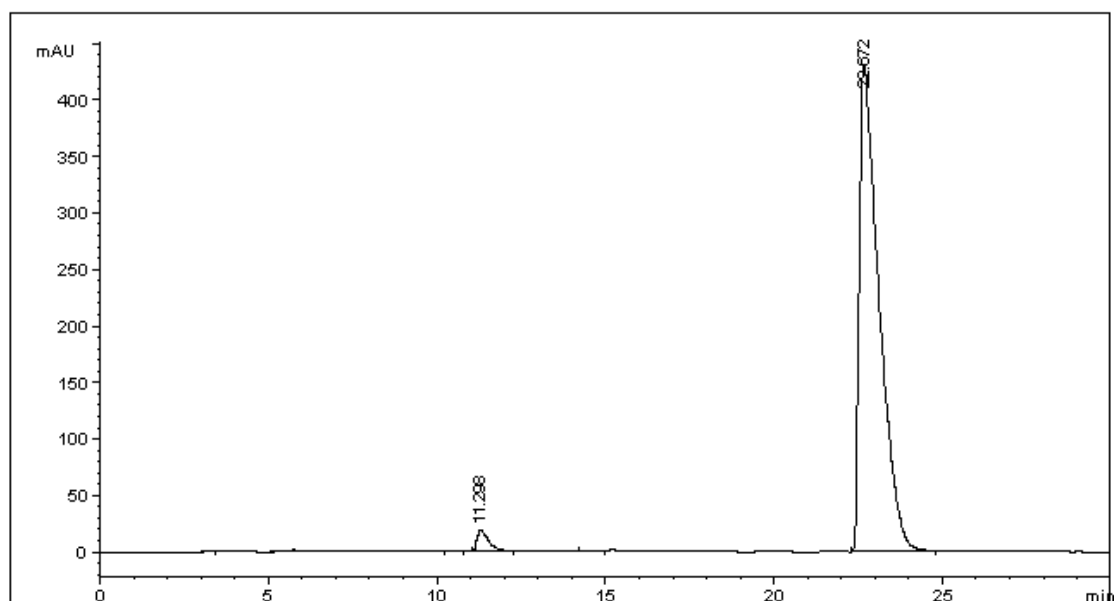
HPLC spectrum of compound **21d**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	11.298	0.3362	439.36765	2.4527
2	22.672	0.5824	17474.1	97.5473
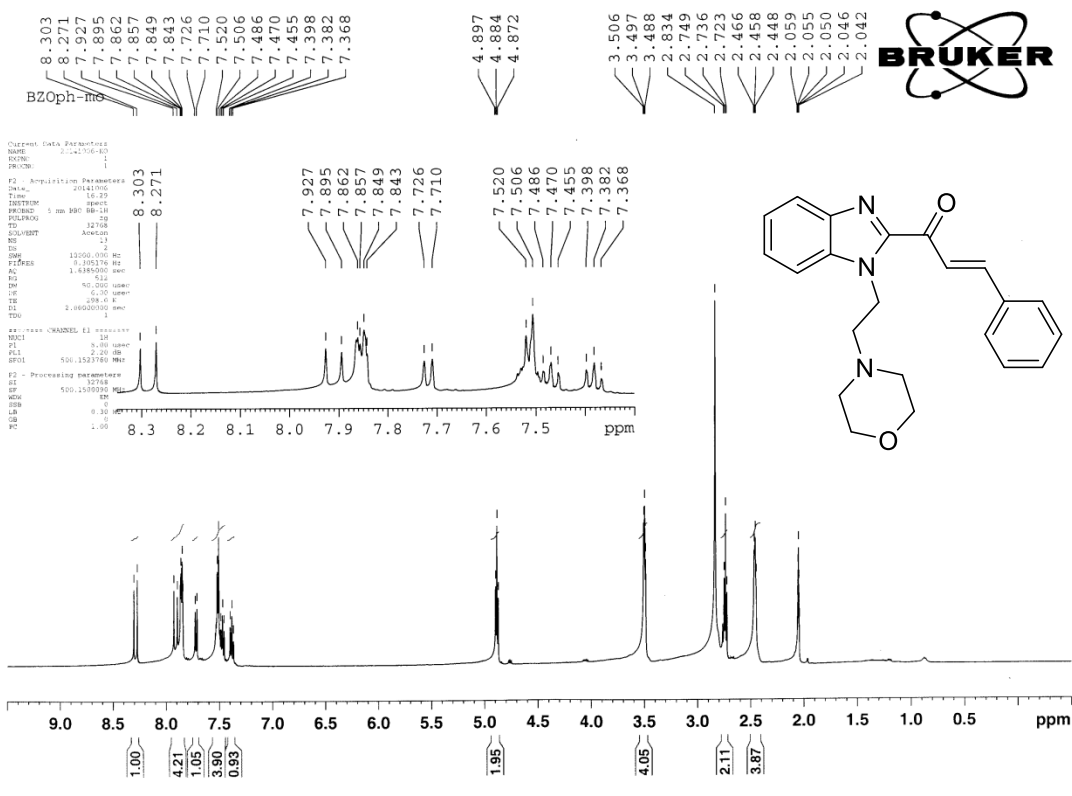
^{1}H-NMR spectrum of compound **22a**
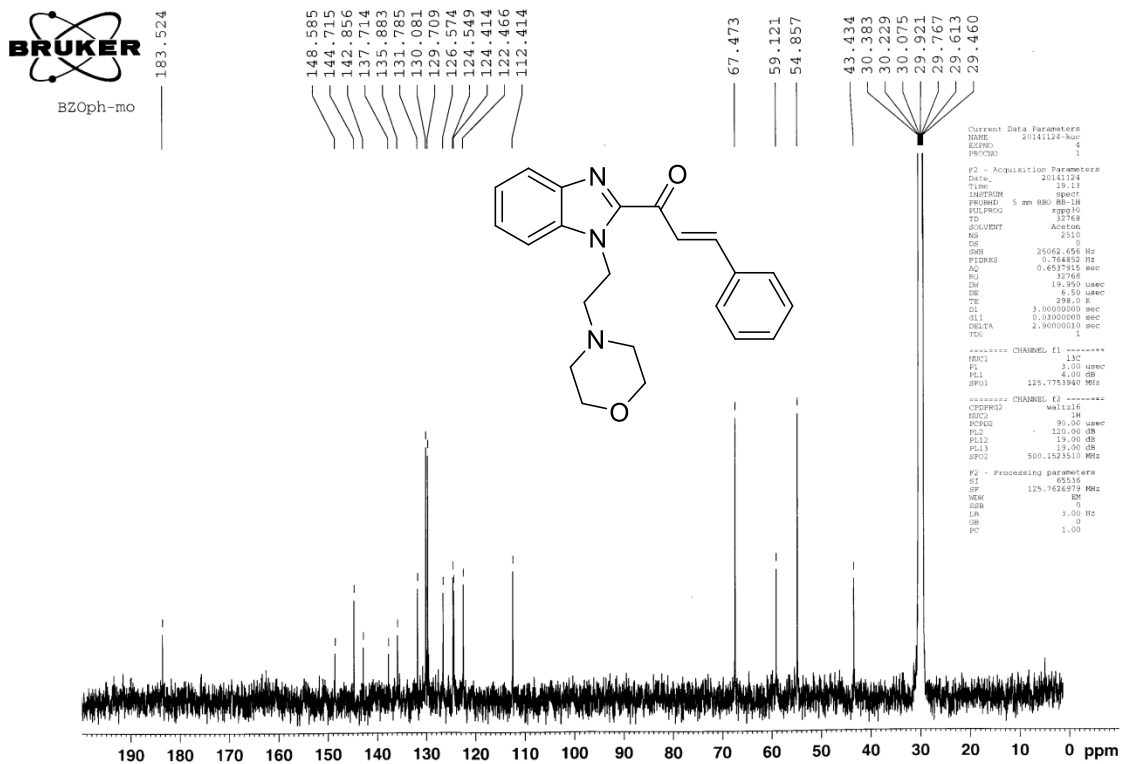
^{13}C-NMR spectrum of compound **22a**
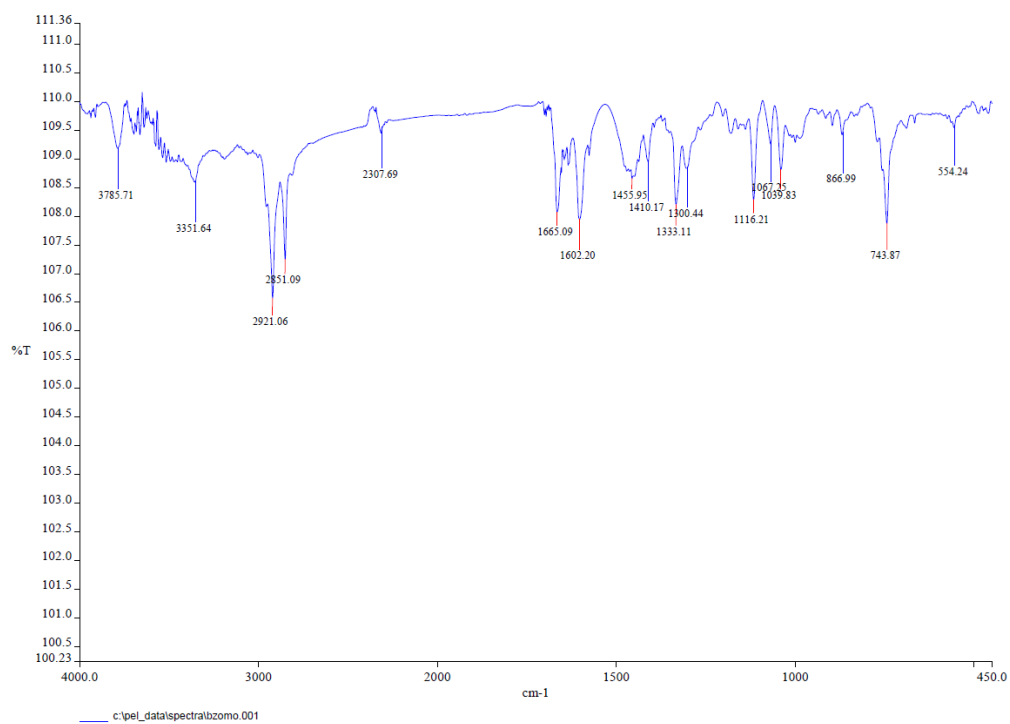
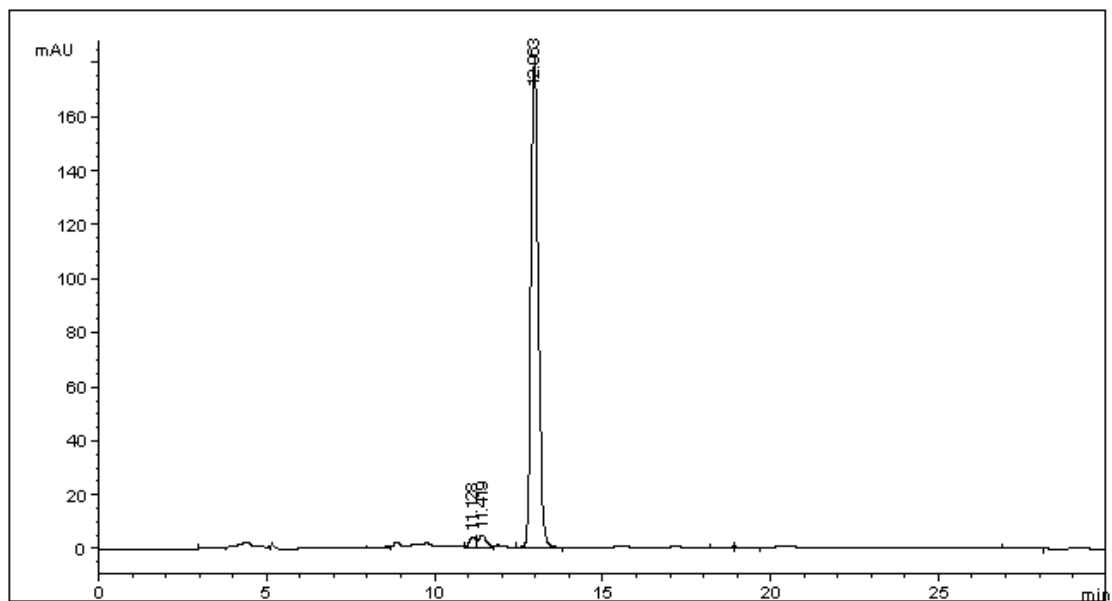IR spectrum of compound **22a**
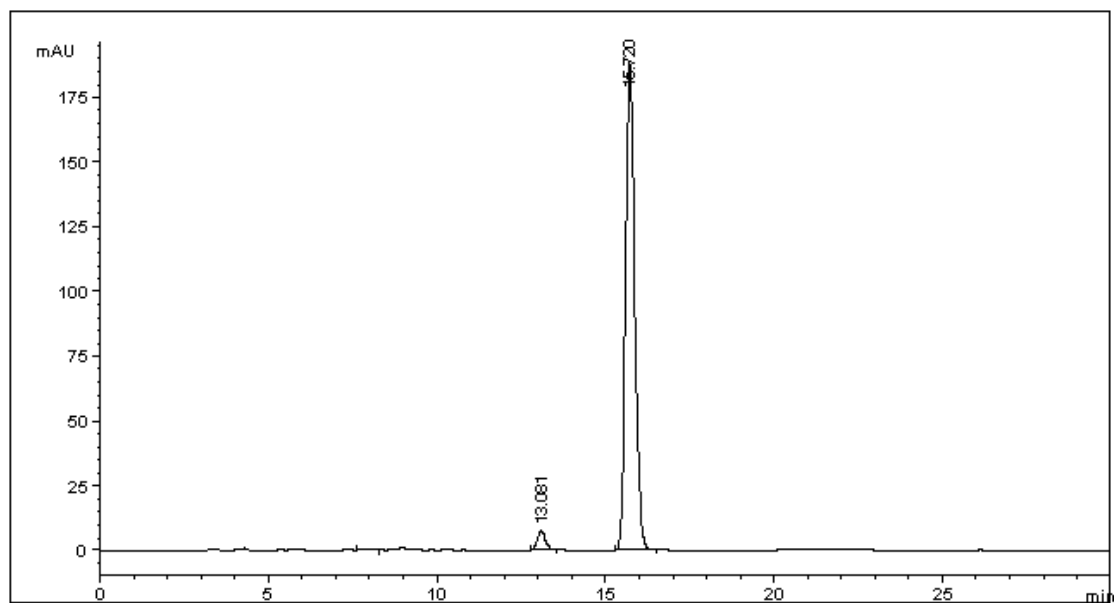
HPLC spectrum of compound **22a**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	13.081	0.263	131.5152	3.5487
2	15.72	0.2962	3574.548	96.4513
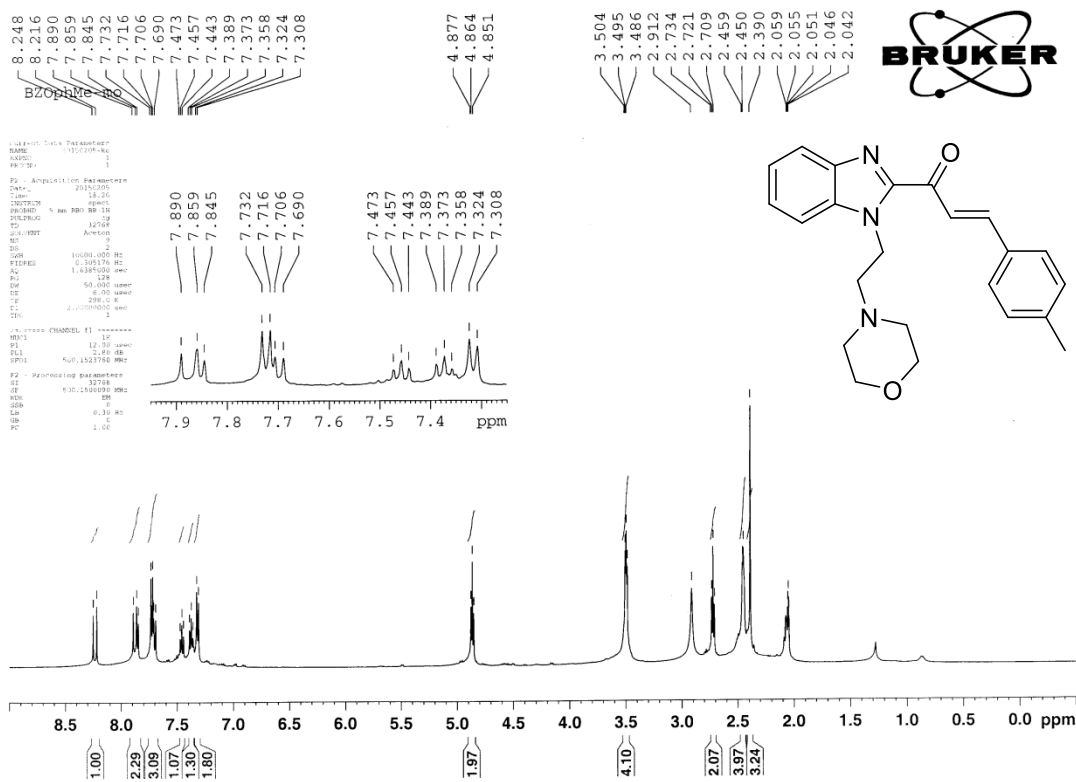
^{1}H-NMR spectrum of compound **22b**
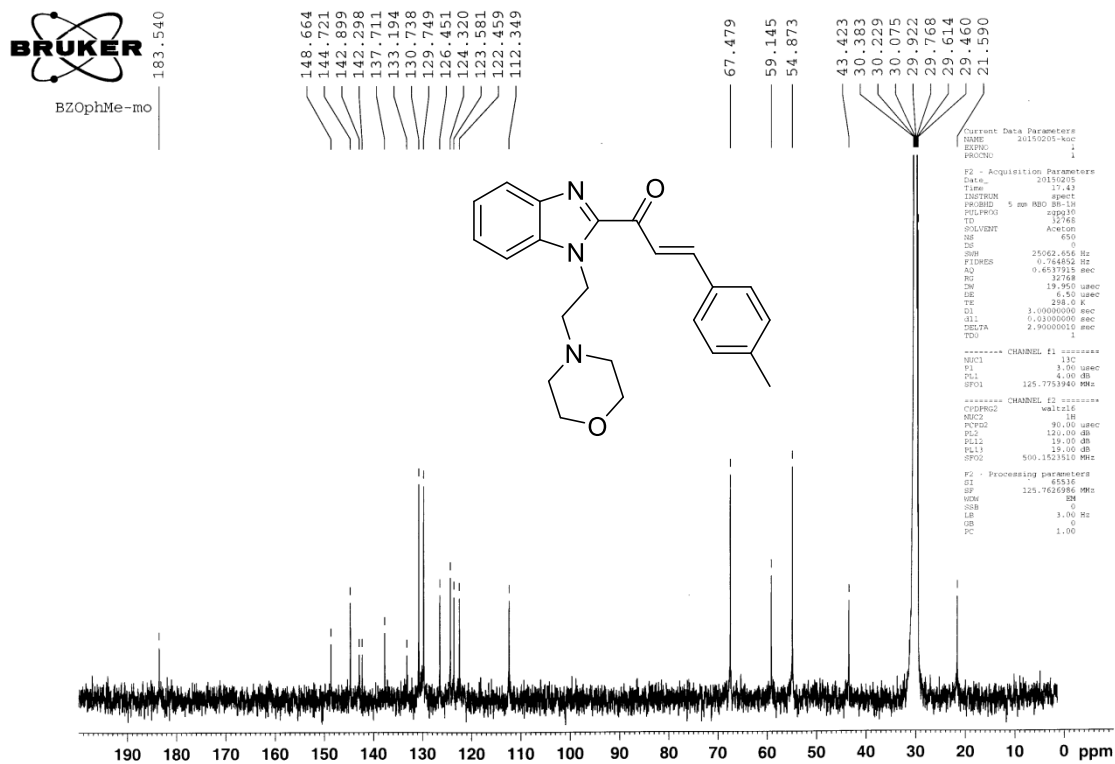
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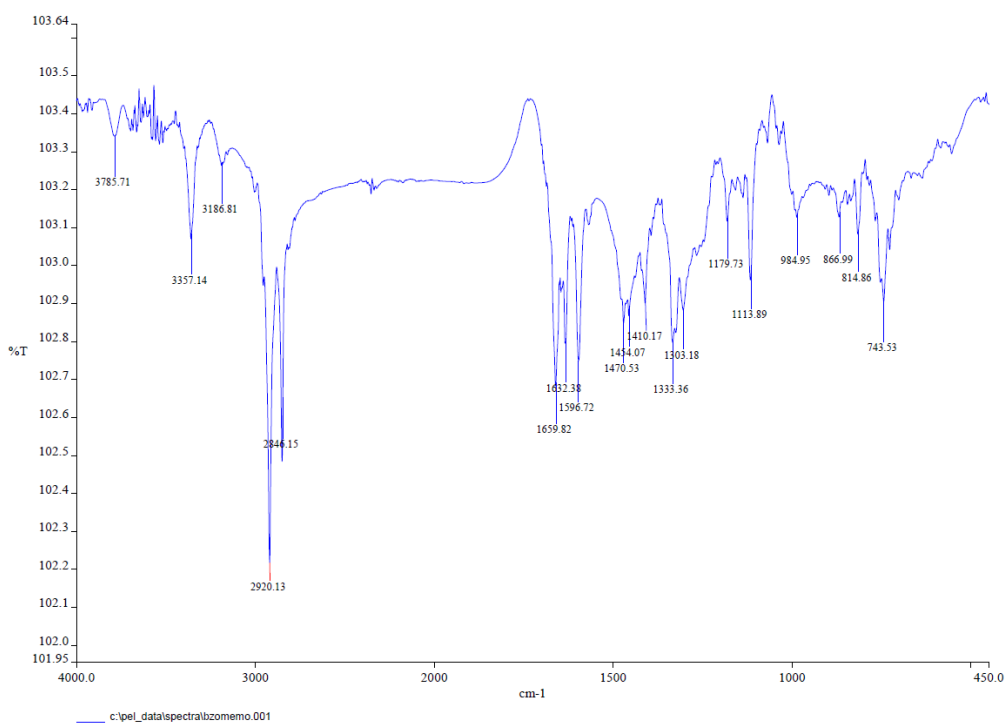
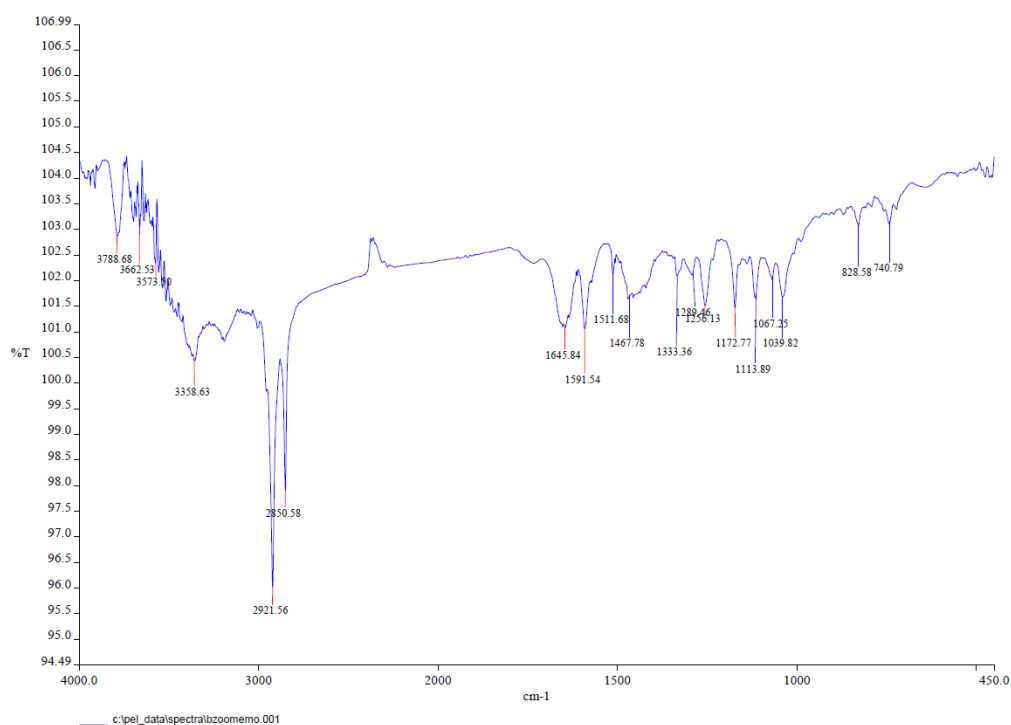IR spectrum of compound **22b**

HPLC spectrum of compound **22b**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	11.128	0.2204	51.86035	1.8558
2	11.419	0.2363	68.21777	2.4412
3	12.963	0.2307	2674.29761	95.7029
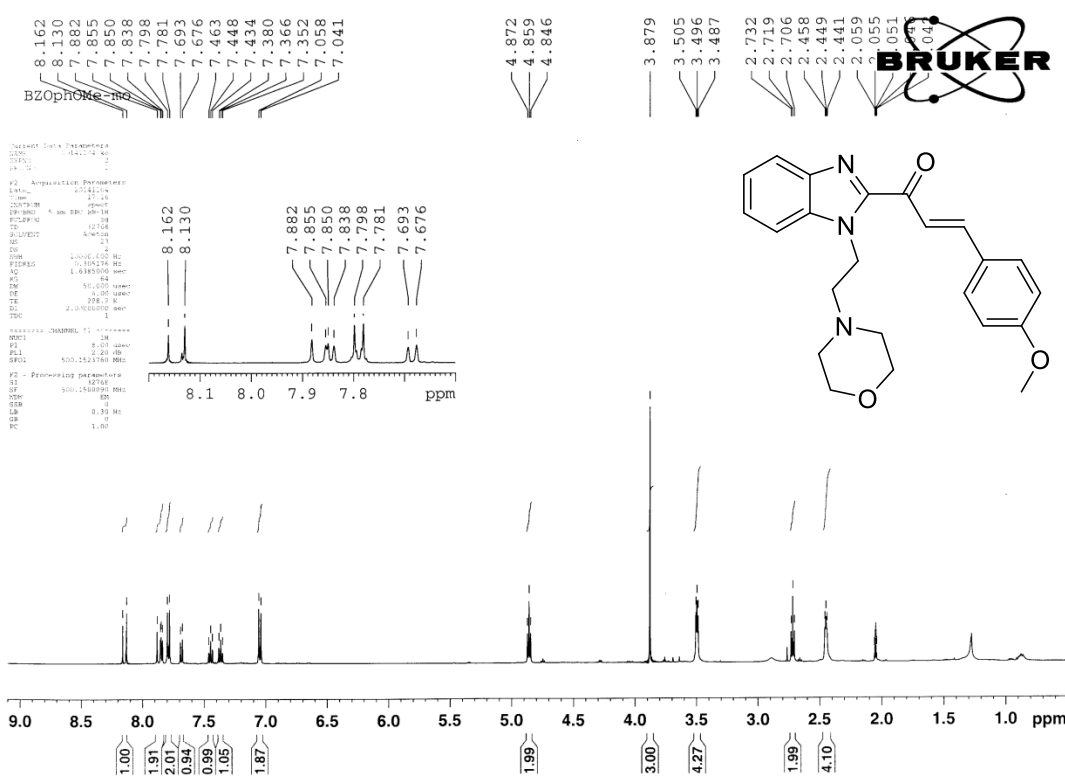
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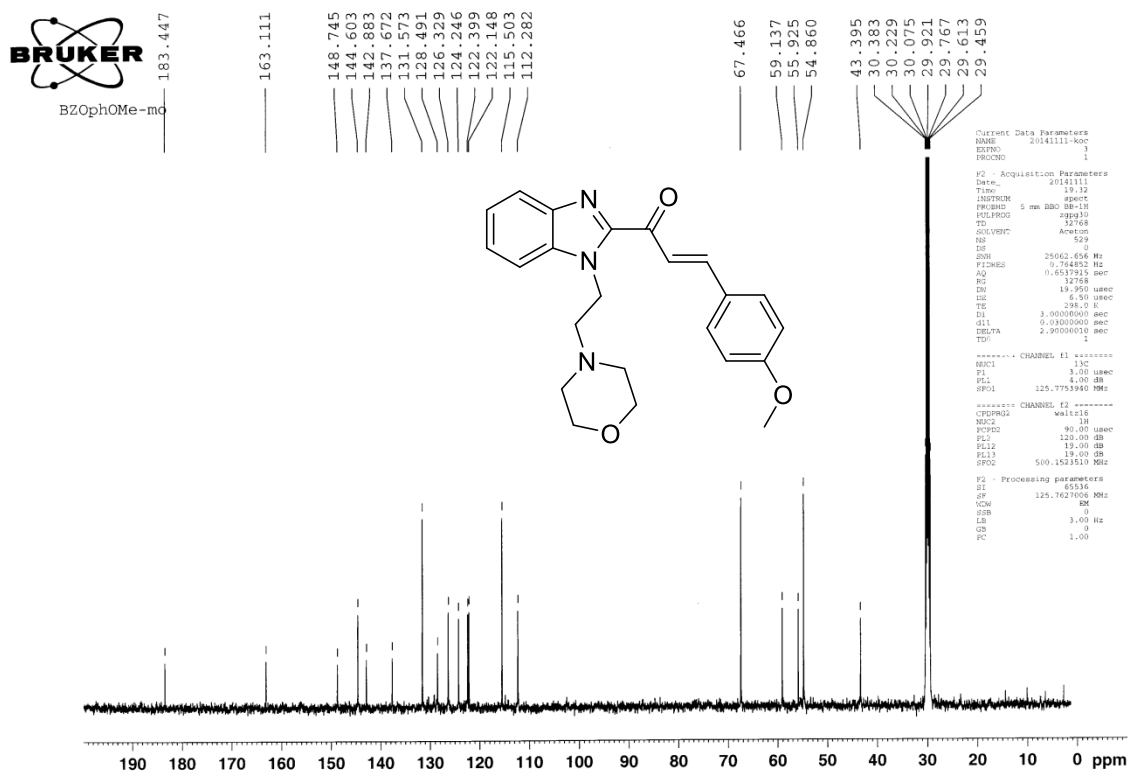
^{13}C-NMR spectrum of compound **22c**

IR spectrum of compound **22c**
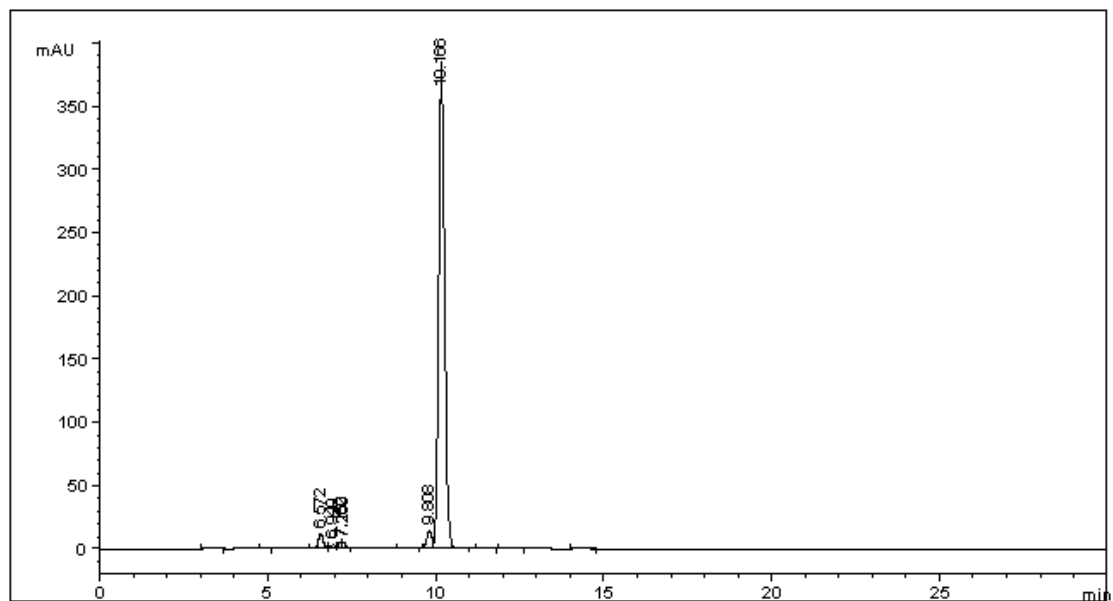
HPLC spectrum of compound **22c**

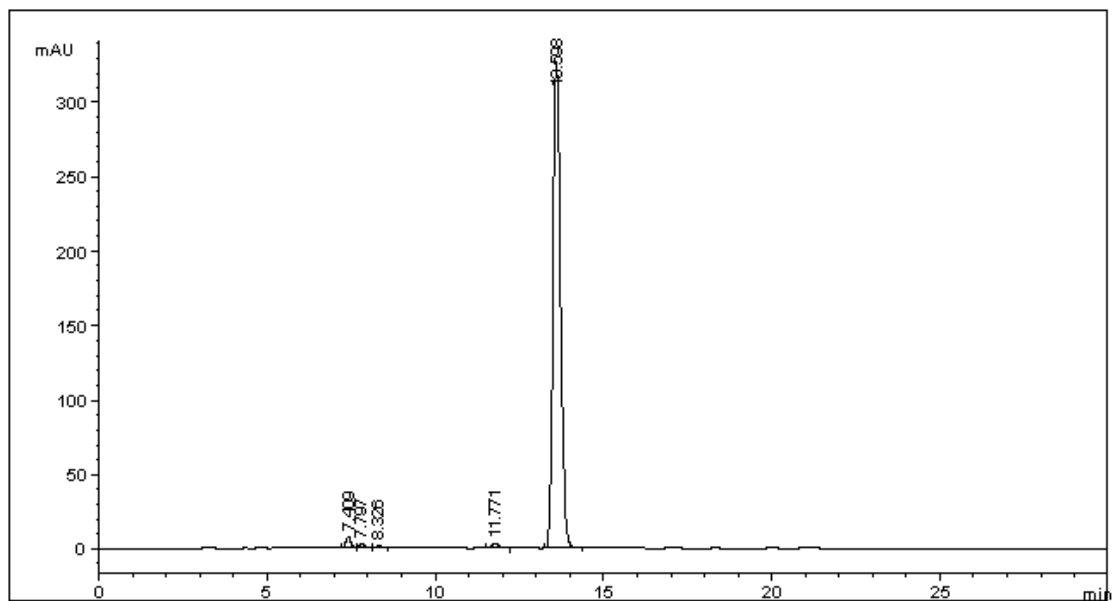| Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	6.949	0.1349	25.79159	0.5232
2	7.162	0.1196	32.28178	0.6549
3	7.25	0.1134	27.91112	0.5662
4	9.808	0.1719	153.38657	3.1118
5	10.166	0.1891	4689.81201	95.1438
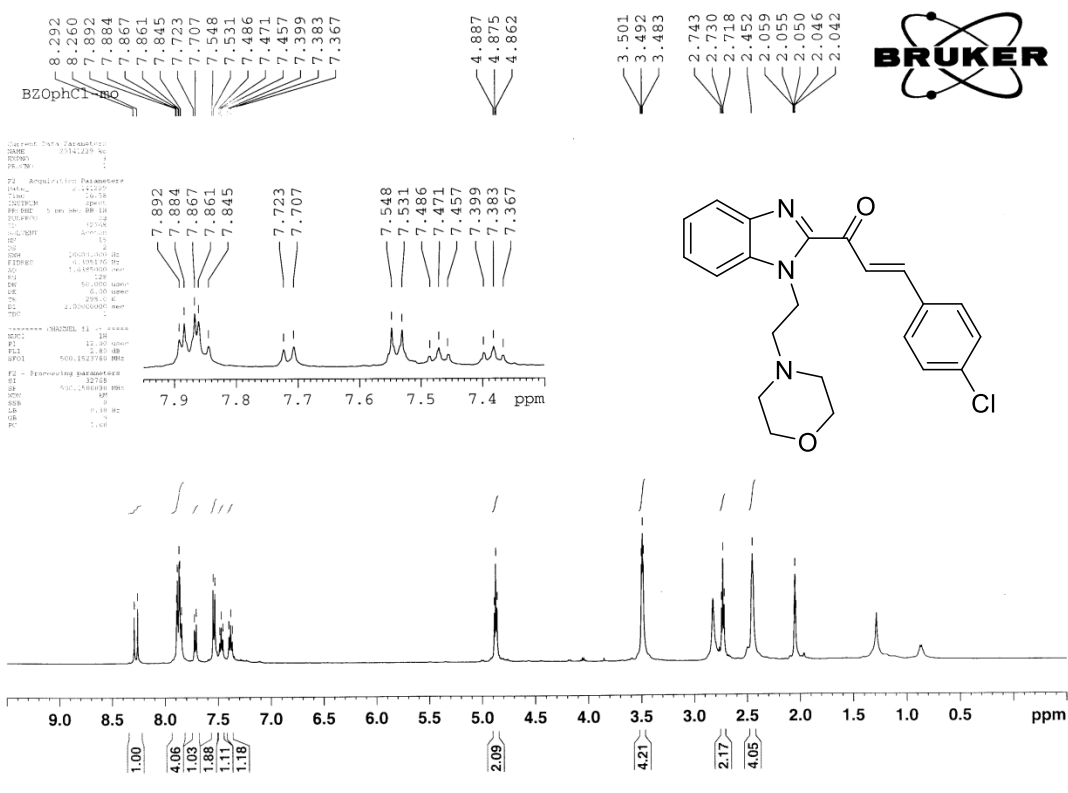
¹H-NMR spectrum of compound **22d**
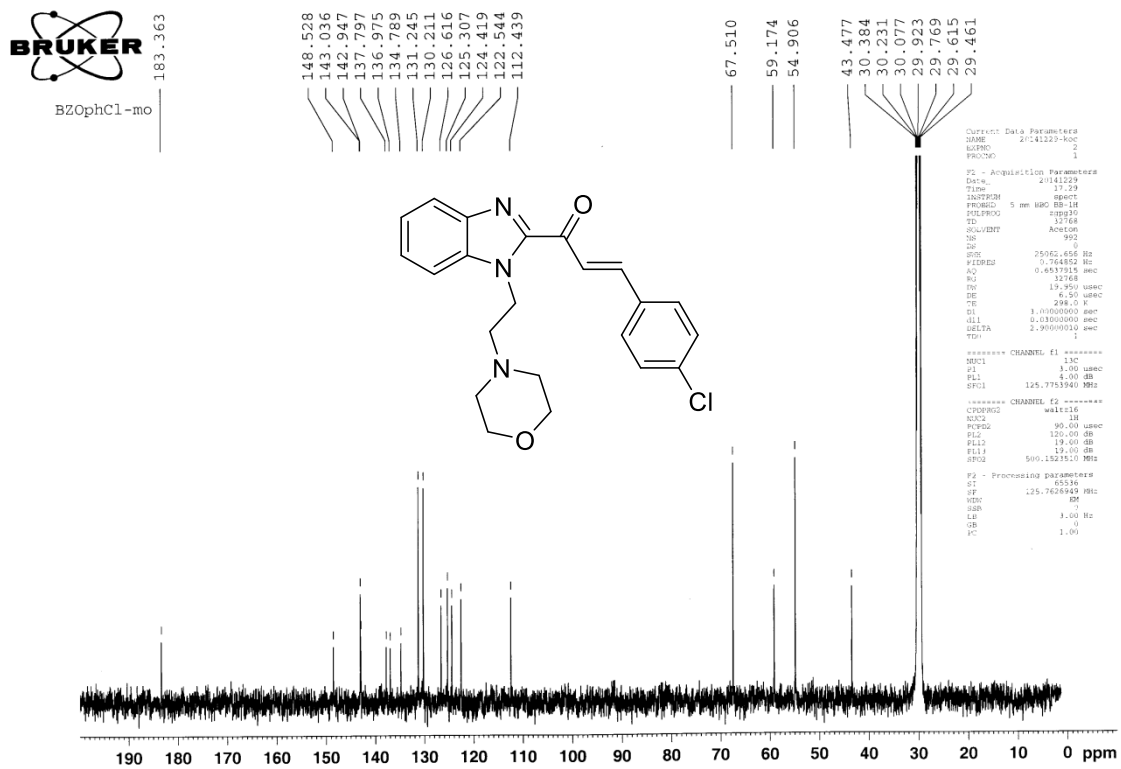
¹³C-NMR spectrum of compound **22d**
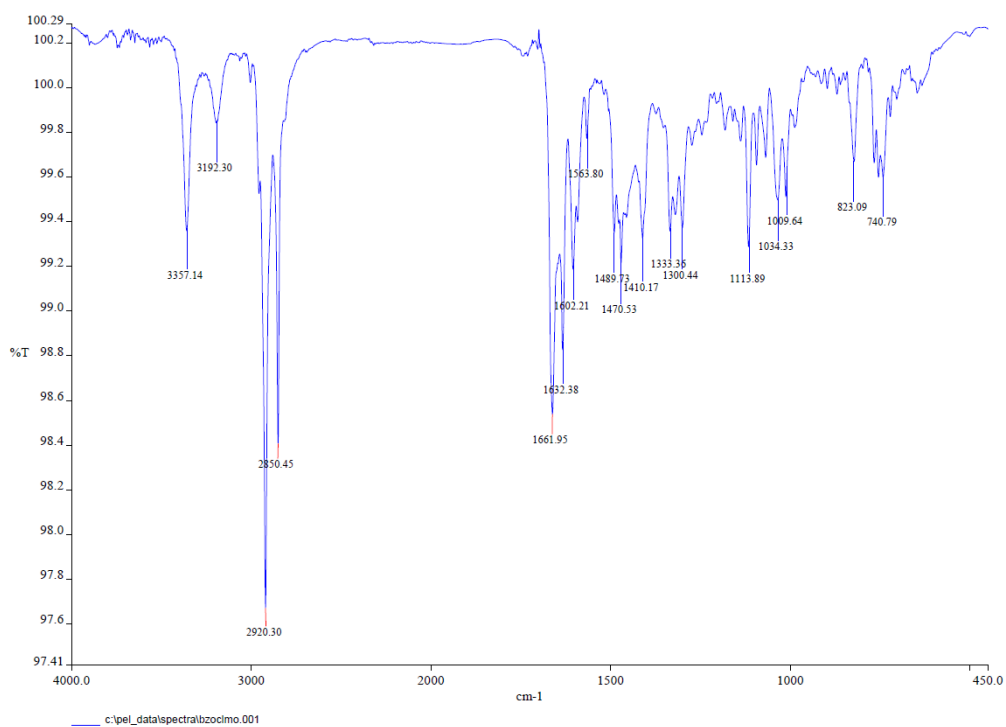
IR spectrum of compound **22d**

HPLC spectrum of compound **22d**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	7.409	0.1596	80.65369	1.5400
2	7.797	0.1728	40.02195	0.7642
3	8.326	0.1800	26.33945	0.5029
4	11.771	0.2311	50.84013	0.9708
5	13.598	0.2397	5039.33447	96.2221
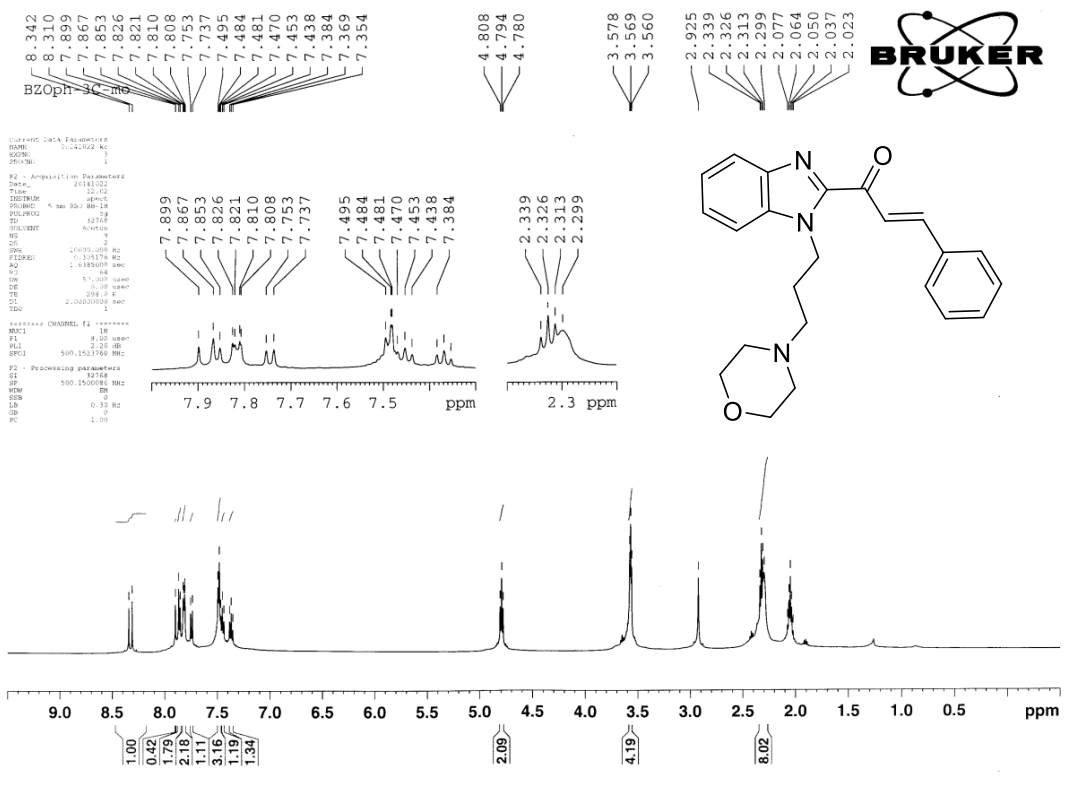
^{1}H-NMR spectrum of compound **23a**
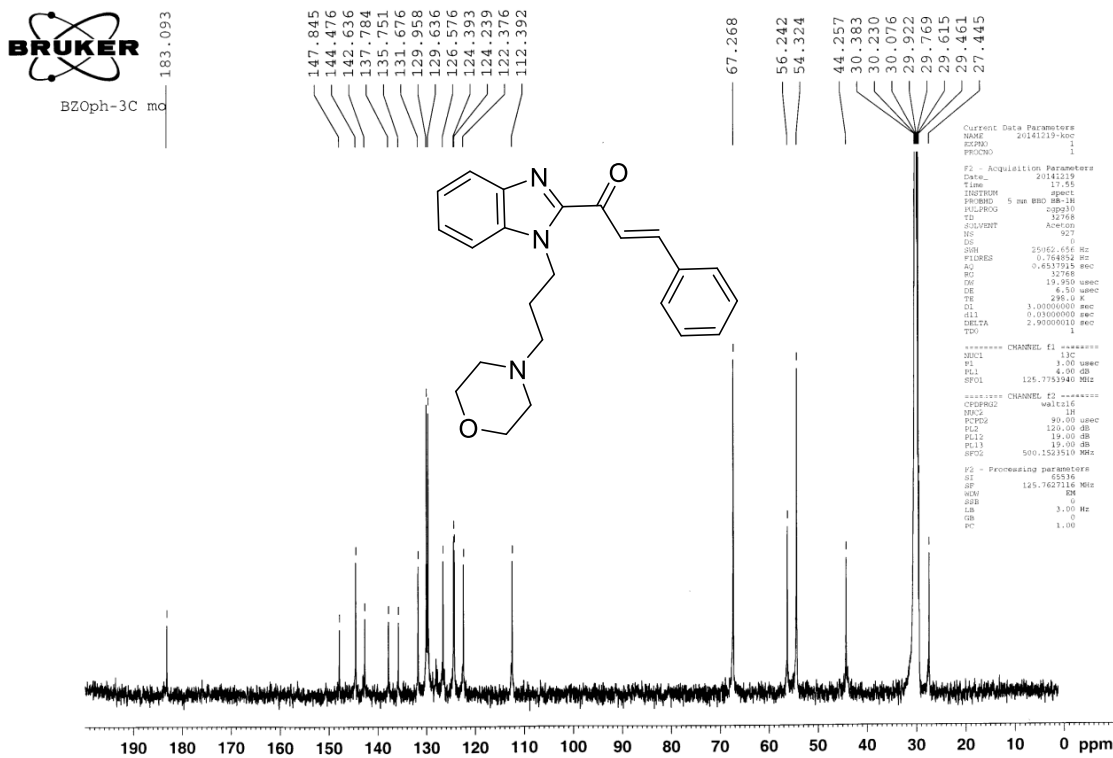
^{13}C-NMR spectrum of compound **23a**
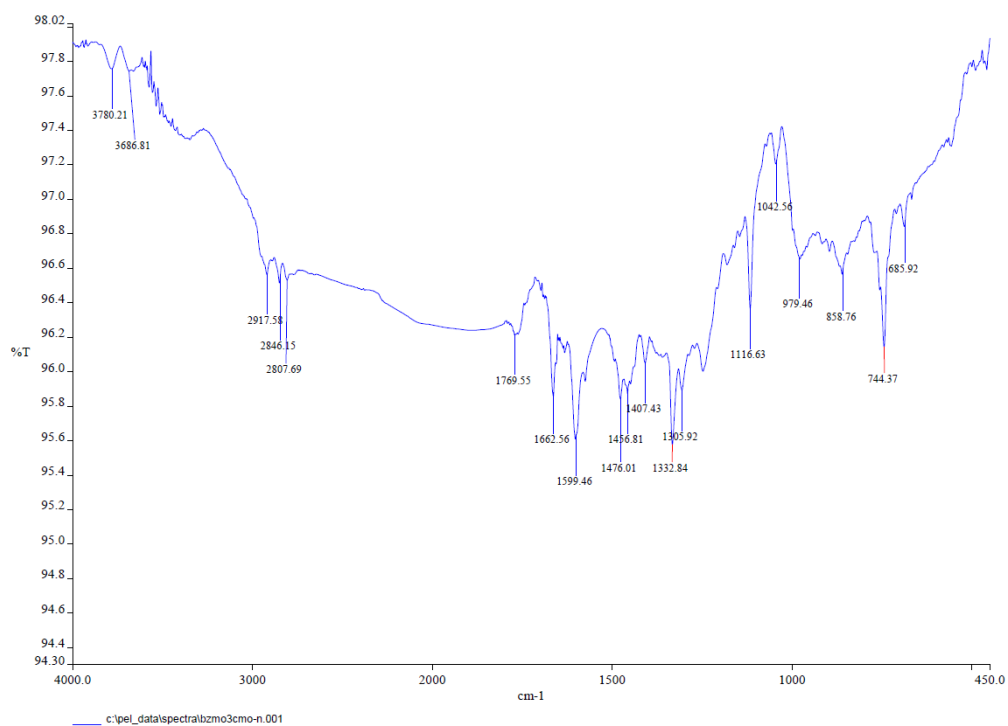
IR spectrum of compound **23a**
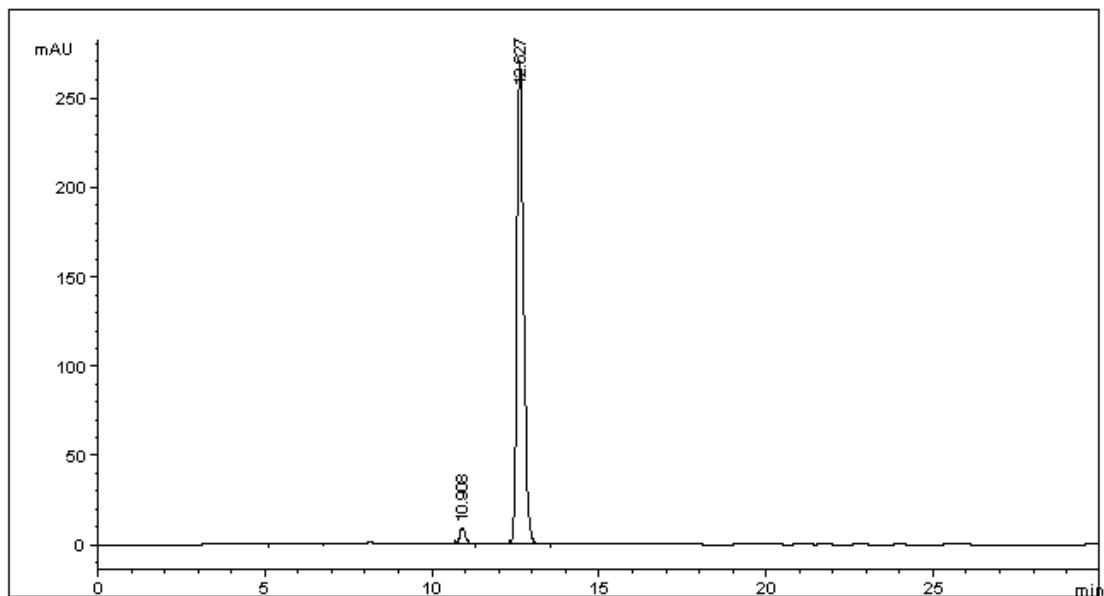
HPLC spectrum of compound **23a**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	10.908	0.1868	105.05498	2.6781
2	12.627	0.2189	3817.72192	97.3219
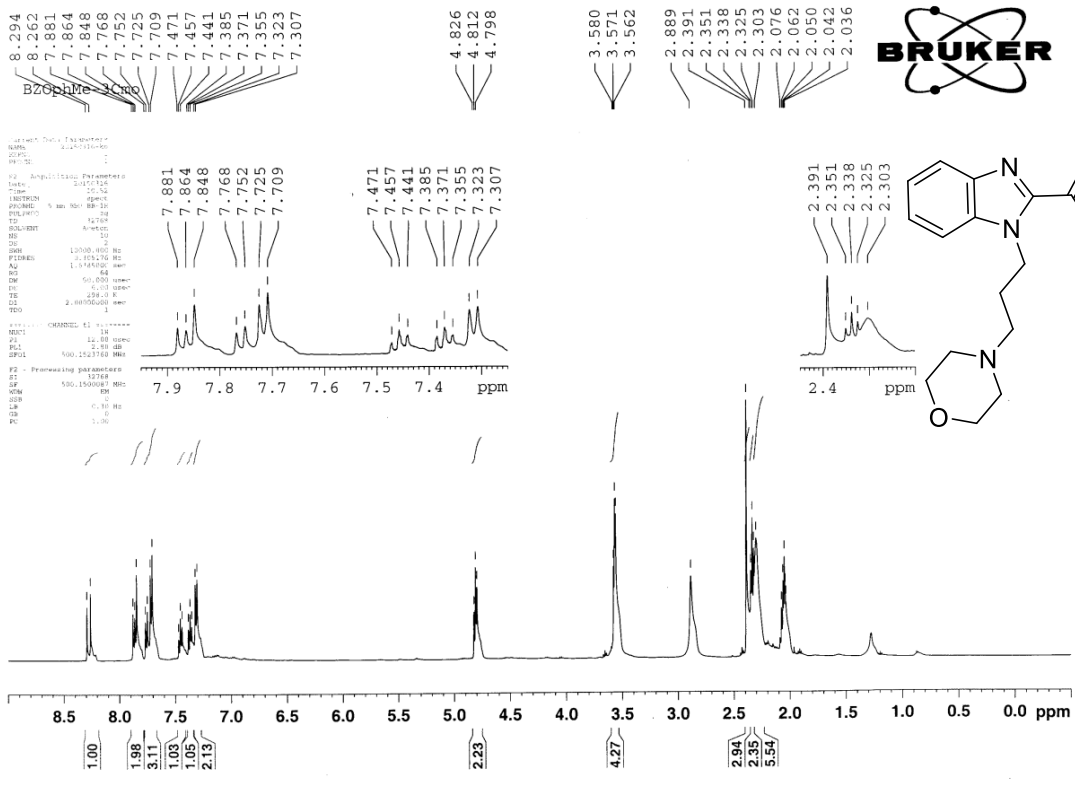
¹H-NMR spectrum of compound **23b**
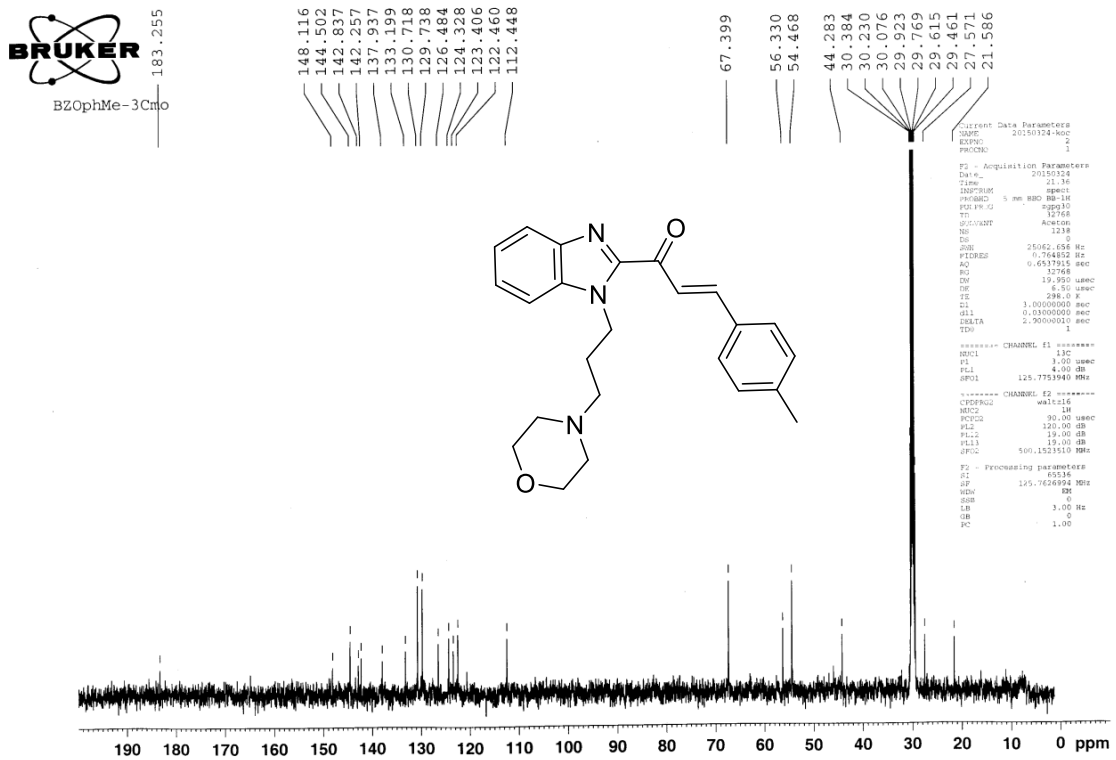
¹³C-NMR spectrum of compound **23b**
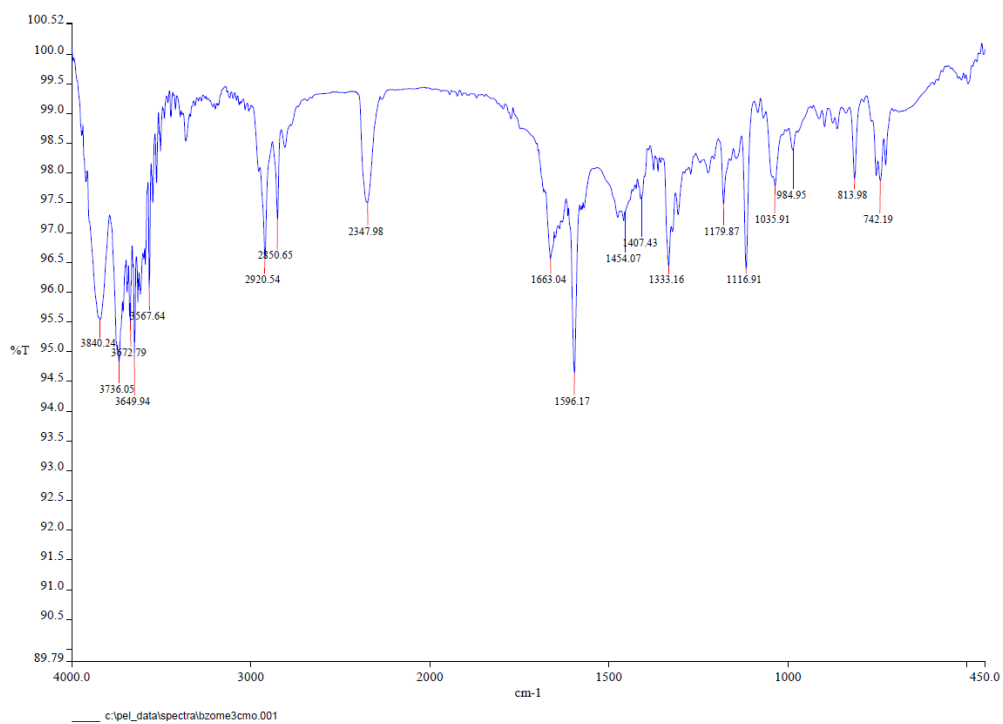
IR spectrum of compound **23b**

HPLC spectrum of compound **23b**
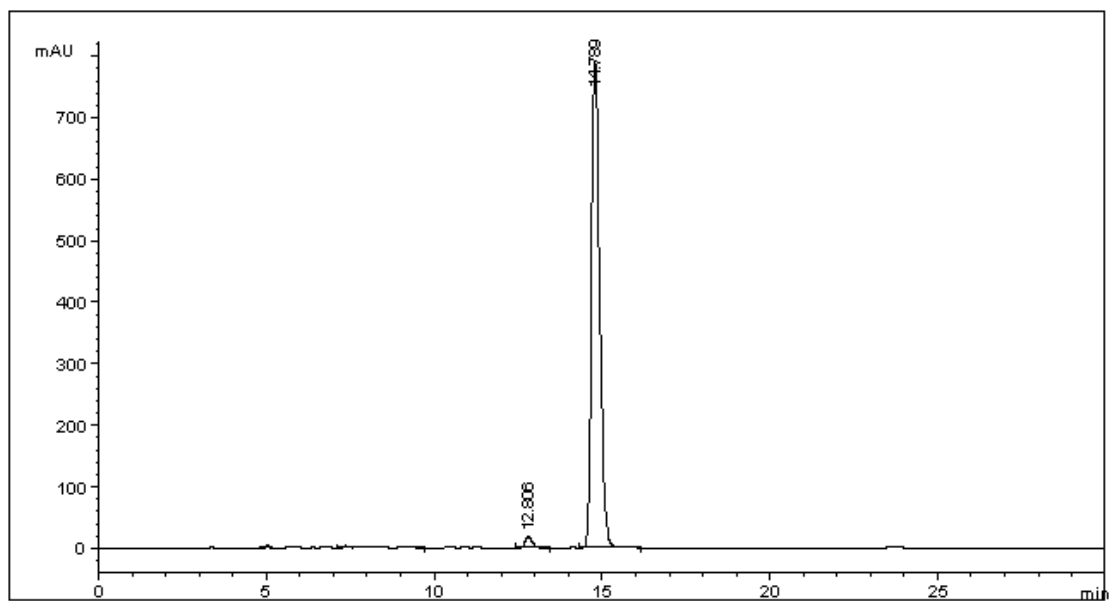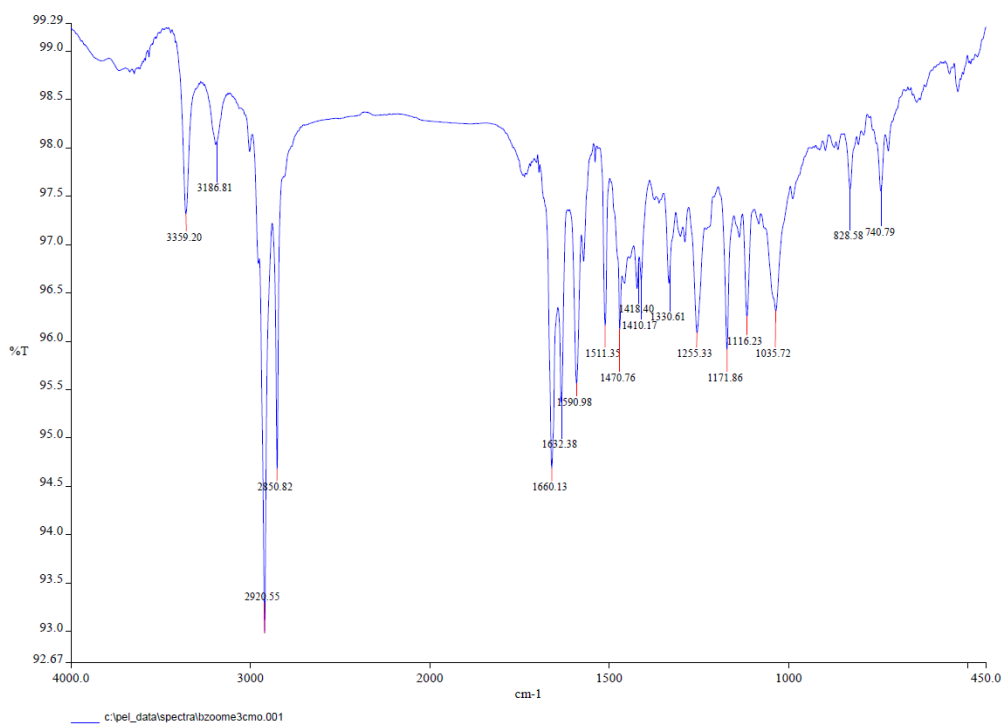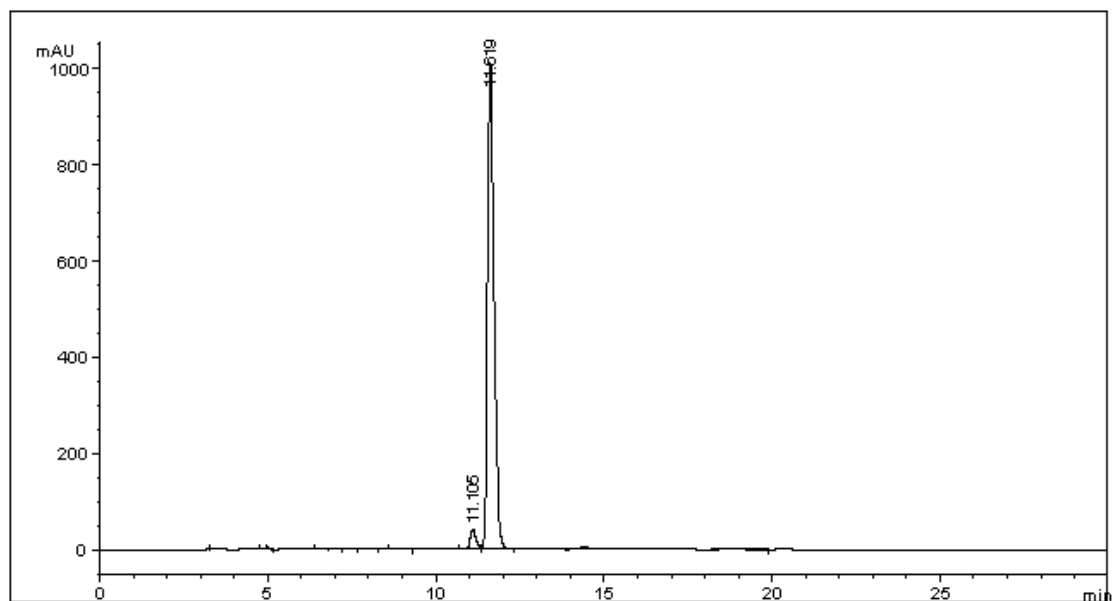
Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	12.806	0.2203	278.77322	2.0574
2	14.789	0.2576	13271.3	97.9426

¹H-NMR chemical shifts (ppm):
8.200, 8.168, 7.866, 7.834, 7.850, 7.789, 7.771, 7.752, 7.736, 7.457, 7.442, 7.427, 7.373, 7.357, 7.342, 7.053, 7.036

4.814, 4.800, 4.786

3.874, 3.574, 3.565, 3.556

2.339, 2.327, 2.313, 2.077, 2.064, 2.051, 2.044, 2.039

BZOphOMe-3Cmo

Integrations: 0.84, 2.34, 2.88, 2.33, 1.99, 2.02, 3.12, 4.29, 8.32
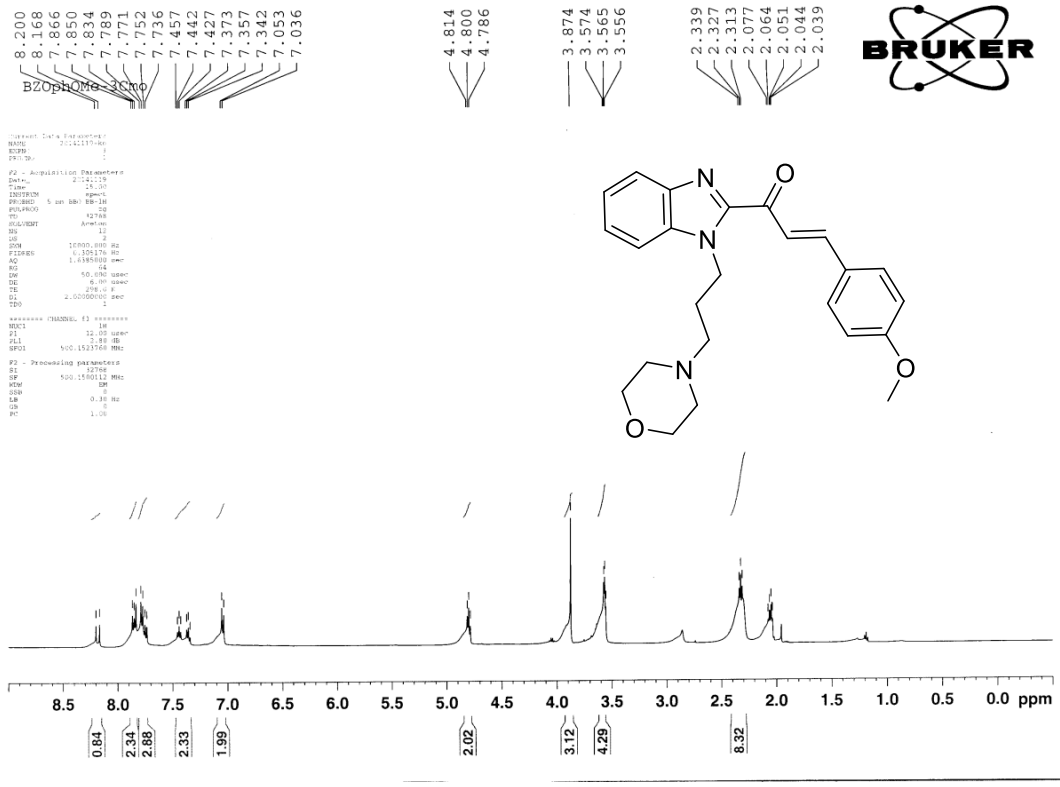
¹H-NMR spectrum of compound 23c

¹³C-NMR chemical shifts (ppm):
183.210

163.112

148.265, 144.357, 142.896, 137.961, 131.565, 128.535, 126.342, 124.242, 122.434, 122.030, 115.512, 112.410

67.431

56.341, 55.938, 54.495

44.262, 30.382, 30.229, 30.075, 29.922, 29.768, 29.614, 29.461, 29.619

BZOphOMe-3Cmo

¹³C-NMR spectrum of compound 23c

IR spectrum of compound **23c**

HPLC spectrum of compound **23c**

Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	11.105	0.1937	513.34729	3.631
2	11.619	0.2083	13623.2	96.369
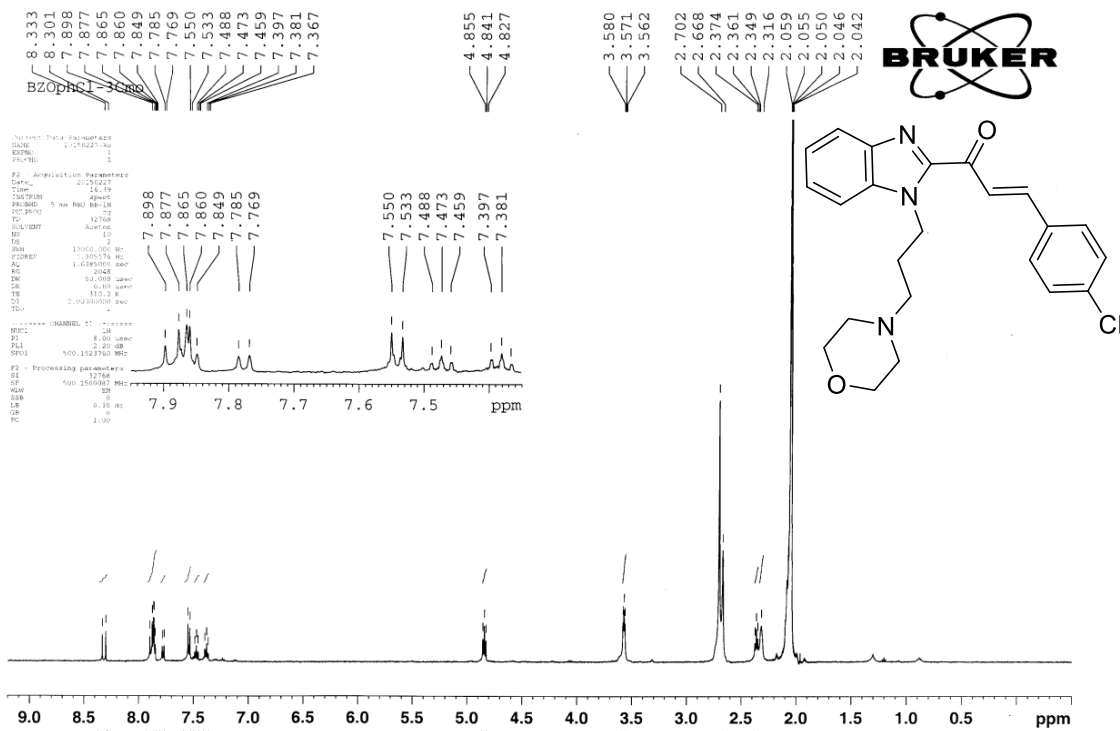
^{1}H-NMR spectrum of compound **23d**
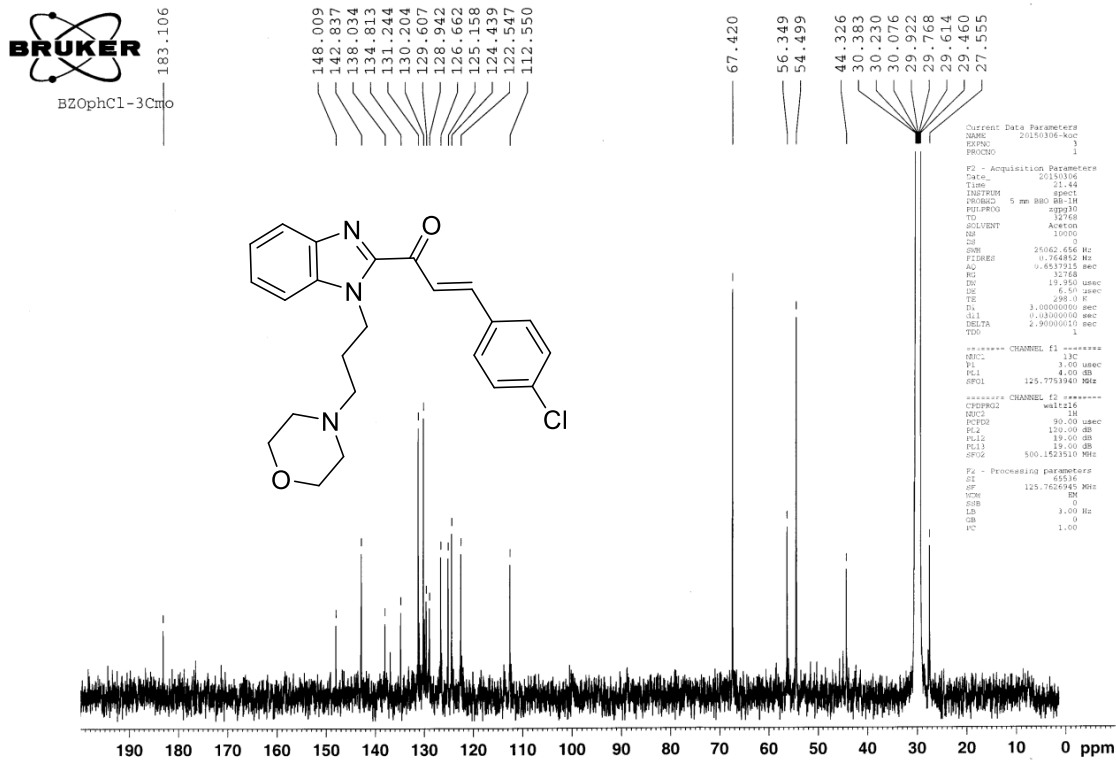
^{13}C-NMR spectrum of compound **23d**
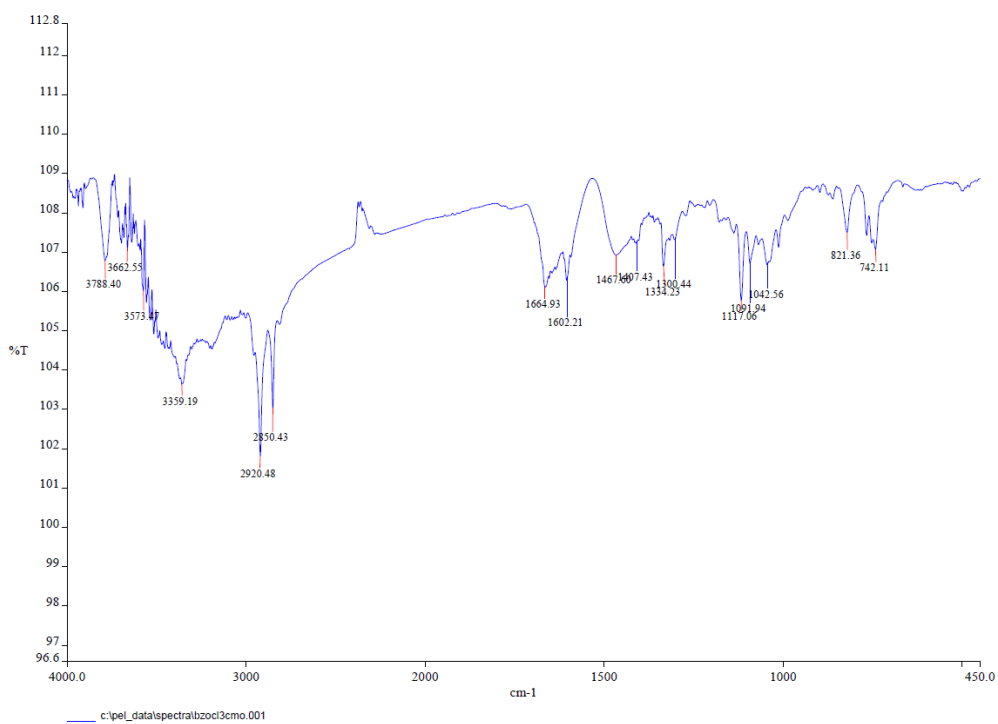
IR spectrum of compound **23d**
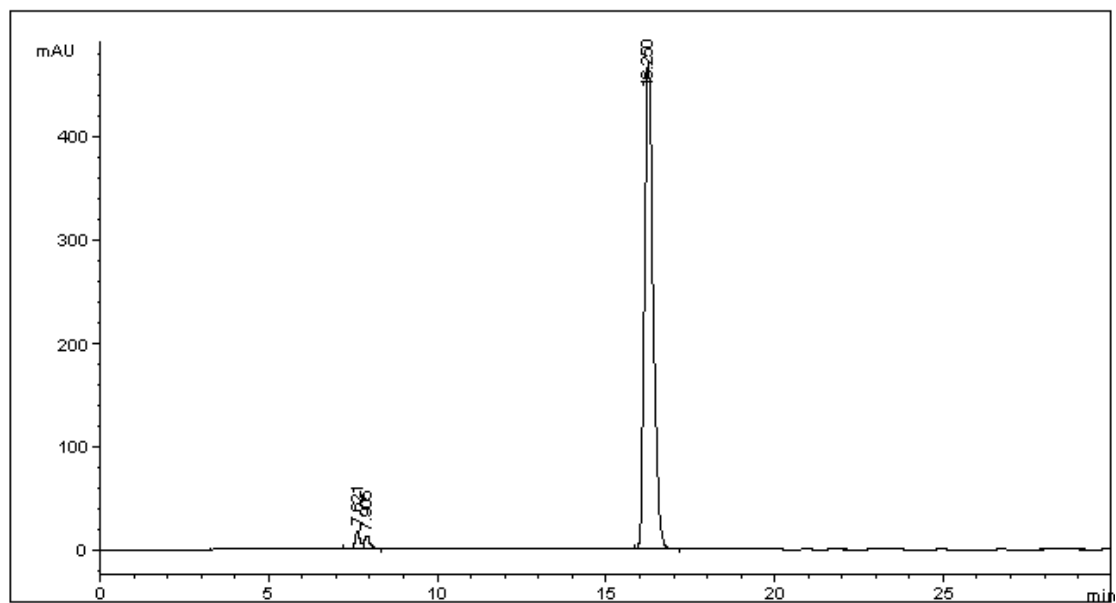
HPLC spectrum of compound **23d**

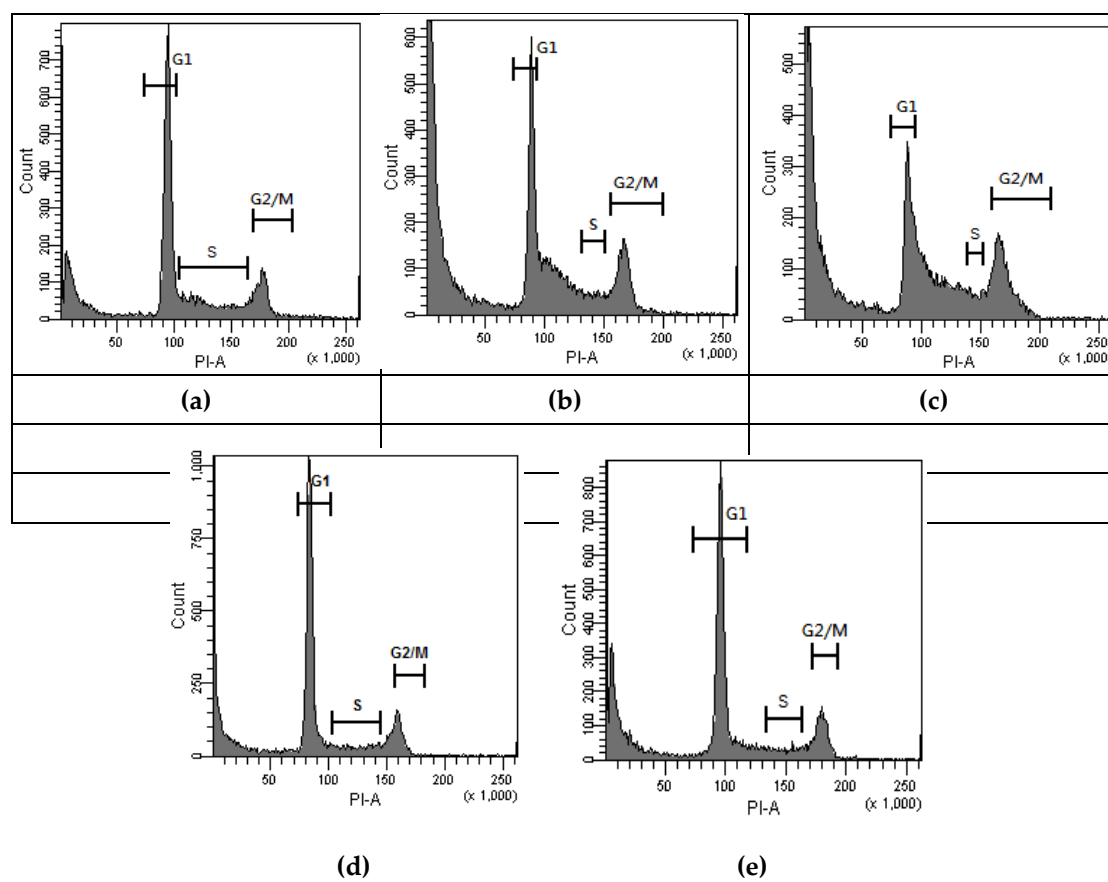| Peak #	RetTime [min]	Width [min]	Area mAU *s	Area %
1	7.621	0.1547	187.74409	2.1252
2	7.905	0.1755	161.00226	1.8225
3	16.250	0.2775	8485.20020	96.052

(2) Flow Cytometry Data

Figure S1. DNA histograms of exponentially growing OVCAR-3 cells with different treatments: (a) cell only; (b) compound **20a**; (c) compound **21a**; (d) compound **22a**; (e) compound **23a**.