

Table S1. Percentage of inhibition of test compounds **2a-2o** against AChE, MAO-A and MAO-B enzymes.

Compound	AChE Inhibition (%)		MAO-A Inhibition (%)		MAO-B Inhibition (%)	
	10 ⁻³ M	10 ⁻⁴ M	10 ⁻³ M	10 ⁻⁴ M	10 ⁻³ M	10 ⁻⁴ M
2a	21.80	21.80	24.29	19.15	25.27	16.63
	±0.95	±0.95	±1.08	±0.87	±0.96	±0.74
2b	5.19	5.19	29.44	24.61	32.44	31.75
	±0.21	±0.21	±0.88	±0.79	±1.06	±0.92
2c	5.48	5.48	31.58	26.17	41.12	33.54
	±0.19	±0.19	±1.12	±1.06	±1.21	±1.07
2d	16.20	16.20	39.79	33.11	45.29	38.96
	±0.74	±0.74	±1.08	±0.89	±1.20	±0.93
2e	17.51	17.51	24.29	17.31	35.47	26.65
	±0.76	±0.76	±0.92	±0.80	±1.30	±1.15
2f	15.75	15.75	32.14	20.65	39.32	31.14
	±0.64	±0.64	±0.90	±0.86	±1.08	±1.00
2g	13.04	13.04	30.85	22.29	38.63	30.87
	±0.52	±0.52	±0.94	±0.97	±1.11	±0.84
2h	10.49	10.49	36.71	23.16	45.58	36.16
	±0.48	±0.48	±1.03	±0.94	±1.27	±1.20
2i	7.54	7.54	26.91	19.20	22.17	14.43
	±0.33	±0.33	±0.92	±0.77	±0.95	±0.60
2j	7.20	7.20	28.47	19.42	41.73	32.44
	±0.28	±0.28	±1.04	±0.85	±1.77	±1.16
2k	20.45	20.45	31.99	26.86	43.22	34.29
	±0.98	±0.98	±1.00	±0.93	±1.08	±1.09
2l	33.88	33.88	38.51	30.16	47.66	38.09
	±1.09	±1.09	±1.20	±1.08	±1.17	±0.95
2m	32.90	32.90	34.29	16.39	25.84	12.43
	±0.99	±0.99	±1.07	±0.72	±0.98	±0.42
2n	12.21	12.21	32.73	24.05	34.75	32.24
	±0.58	±0.58	±1.18	±0.92	±0.85	±0.89
2o	6.33	6.33	31.85	26.19	31.12	23.54
	±0.29	±0.29	±1.05	±0.86	±0.91	±0.87
Ref-1	99.48	99.48	-	-	-	-
	±1.92	±1.92	-	-	-	-
Ref-2	-	-	94.12	82.14	-	-
	-	-	±2.76	±2.69	-	-
Ref-3	-	-	-	-	98.94	94.73
	-	-	-	-	±2.06	±1.97

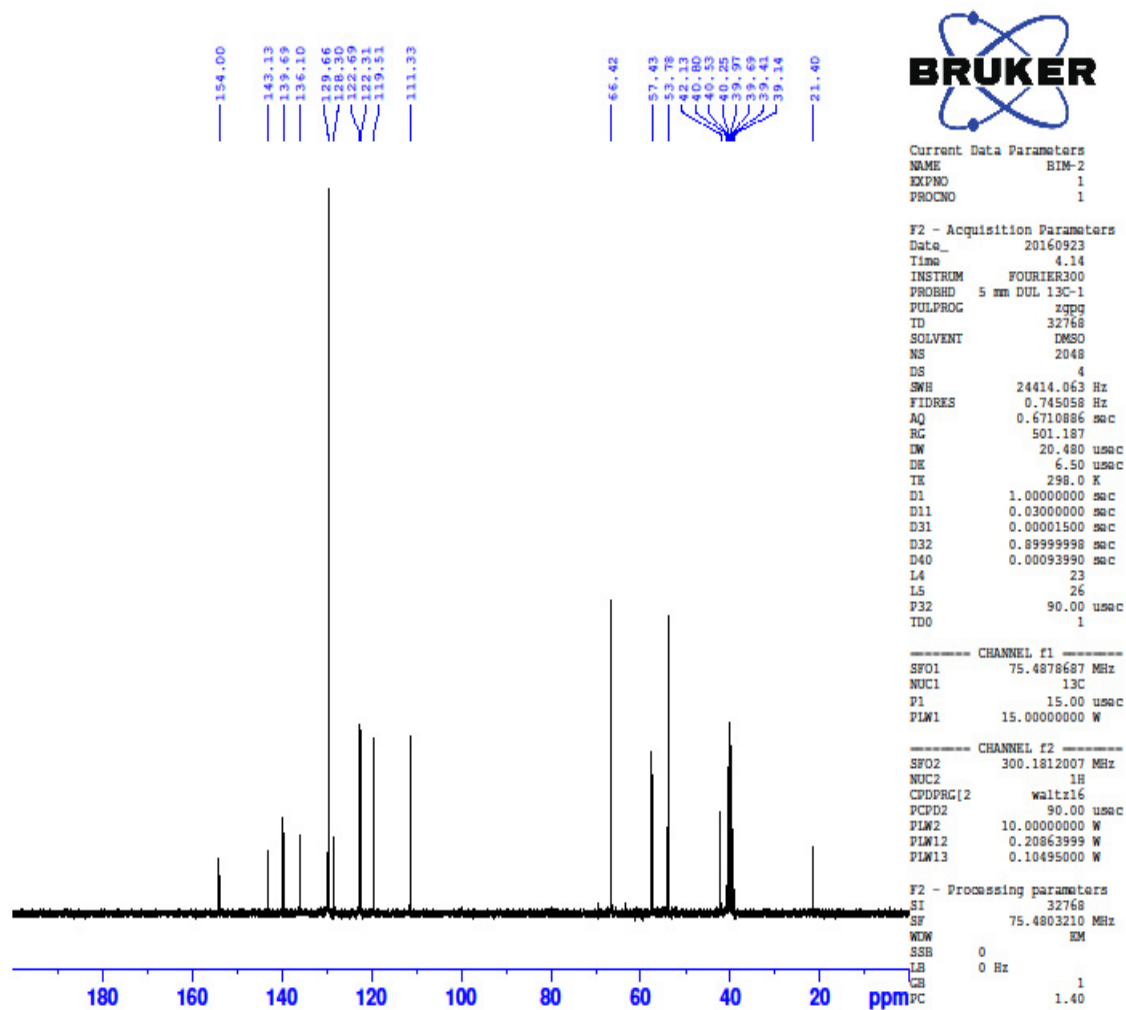
Ref-1: Donepezil; **Ref-2:** Moclobemide; **Ref-3:** Selegiline.

Table S2. Inhibitory potencies of test compounds **2a-2o** at higher concentrations against COX-1 and COX-2 enzymes.

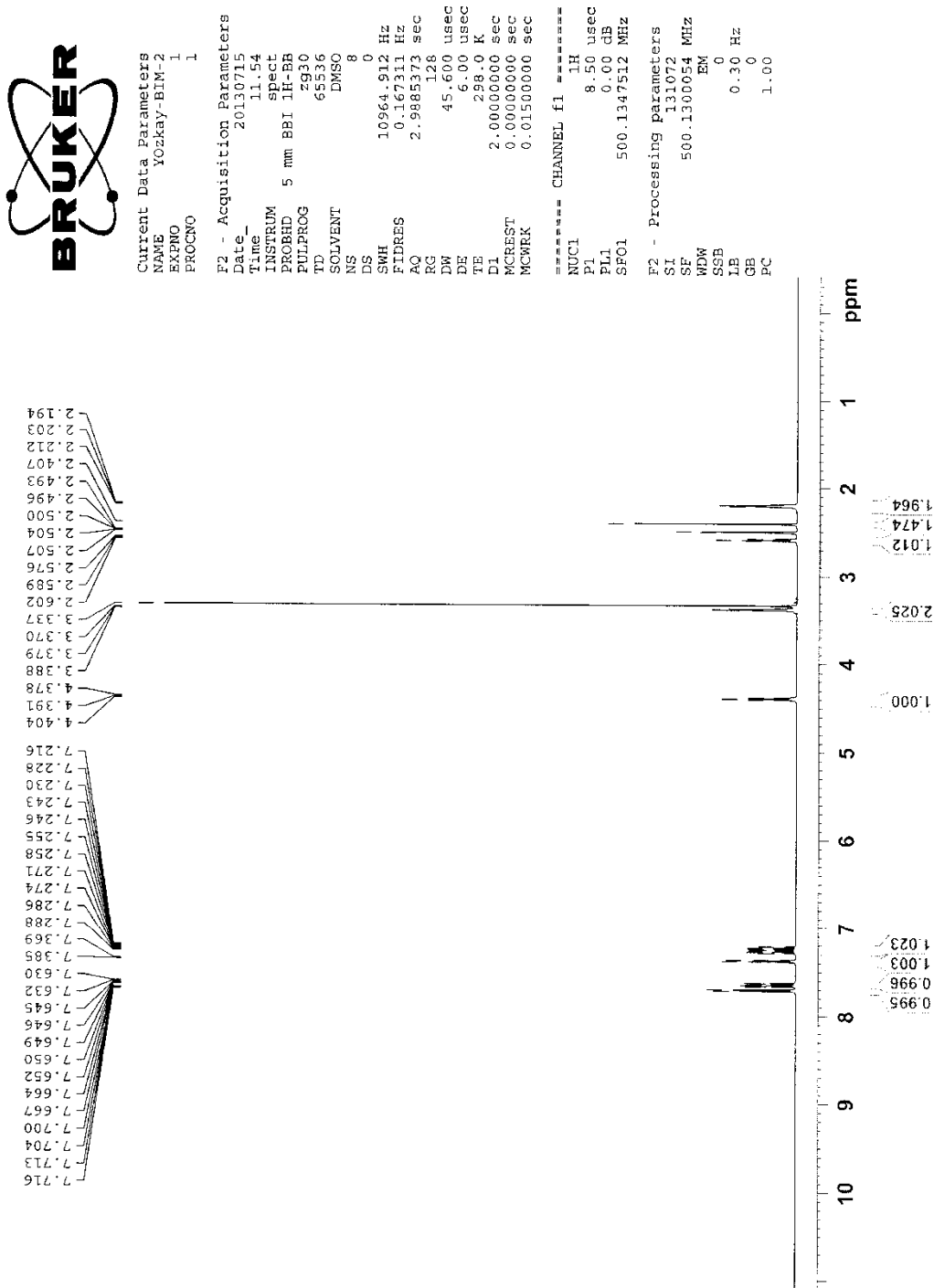
Compound	COX-1 Inhibition (%)		COX-2 Inhibition (%)	
	10 ⁻³ M	10 ⁻⁴ M	10 ⁻³ M	10 ⁻⁴ M
2a	75.08	71.23	58.28	56.23
	±1.28	±1.28	±1.16	±1.25
2b	90.12	87.62	79.41	84.23
	±1.39	±1.19	±1.24	±1.24
2c	24.55	22.15	17.85	20.99
	±0.94	±0.82	±0.67	±0.72
2d	31.87	29.36	21.08	28.46
	±0.82	±0.90	±0.88	±0.69
2e	26.47	19.88	14.26	22.61
	±0.83	±0.82	±0.52	±0.61
2f	75.37	79.08	61.23	60.20
	±1.20	±1.37	±1.25	±1.18
2g	29.47	21.74	16.30	19.03
	±0.86	±0.83	±0.42	±0.74
2h	75.21	78.21	56.20	57.08
	±1.06	±1.27	±1.08	±1.00
2i	30.08	22.62	18.47	25.76
	±1.05	±0.86	±0.51	±1.08
2j	85.07	88.68	80.66	79.23
	±1.49	±1.47	±1.26	±1.37
2k	28.63	28.13	26.39	20.46
	±0.86	±0.86	±0.76	±0.73
2l	36.87	33.46	21.00	34.62
	±0.90	±0.84	±0.71	±0.70
2m	79.15	78.61	64.22	59.67
	±1.20	±1.26	±1.09	±1.24
2n	39.42	32.78	30.08	33.46
	±1.18	±0.86	±0.88	±0.97
2o	27.63	34.00	30.76	21.48
	±0.96	±0.89	±0.62	±0.81
Ref-1	98.15	98.23	88.15	89.36
	±1.56	±1.49	±1.37	±1.43
Ref-2	96.53	97.82	89.57	84.22
	±1.38	±1.32	±1.28	±1.23

Ref-1: Ibuprofen; **Ref-2:** Nimesulide.

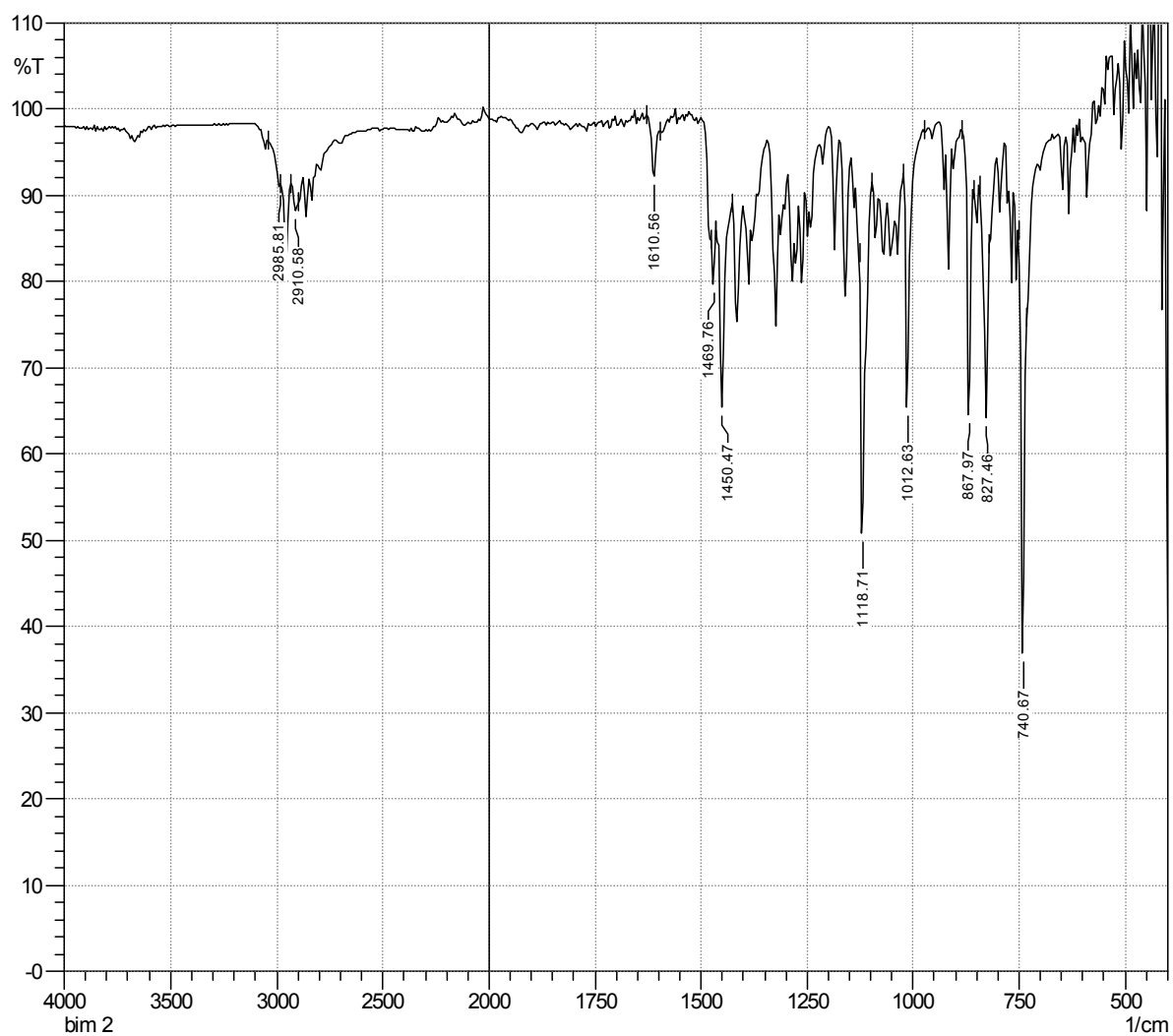
¹³C-NMR spectrum of 2-(4-Methylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2a)



¹H-NMR spectrum of 2-(4-Methylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2a)



FTIR spectrum of 2-(4-Methylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2a**)



HRMS spectrum of 2-(4-Methylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2a)

Formula Predictor Report - Bim-2_09.lcd

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Data File: C:\LabSolutions\Data\Analz\Bim series\Bim-2_09.lcd

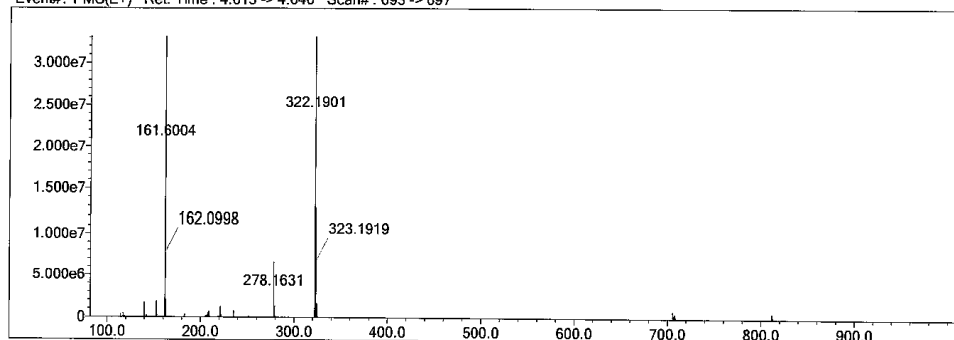
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C	4	12	30	S	2	0	0	
N	3	3	4	Cl	1	0	0	

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

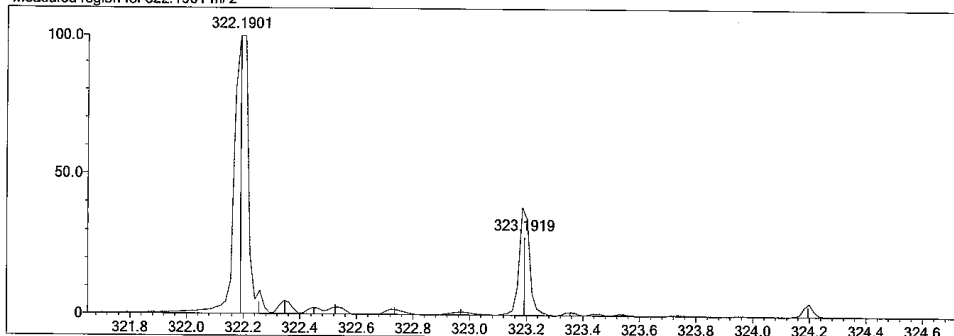
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

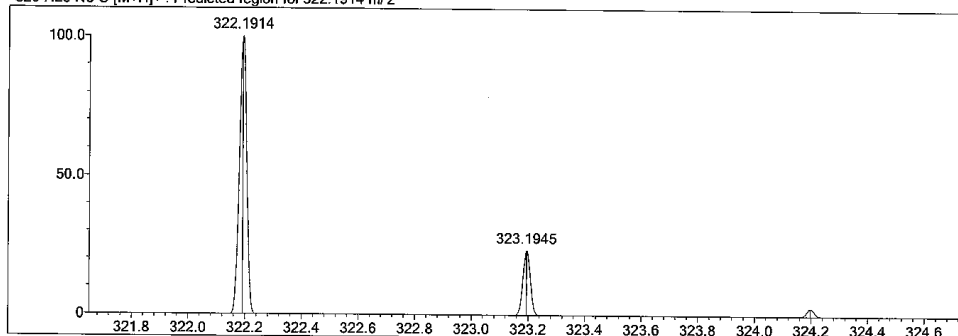
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Measured region for 322.1901 m/z

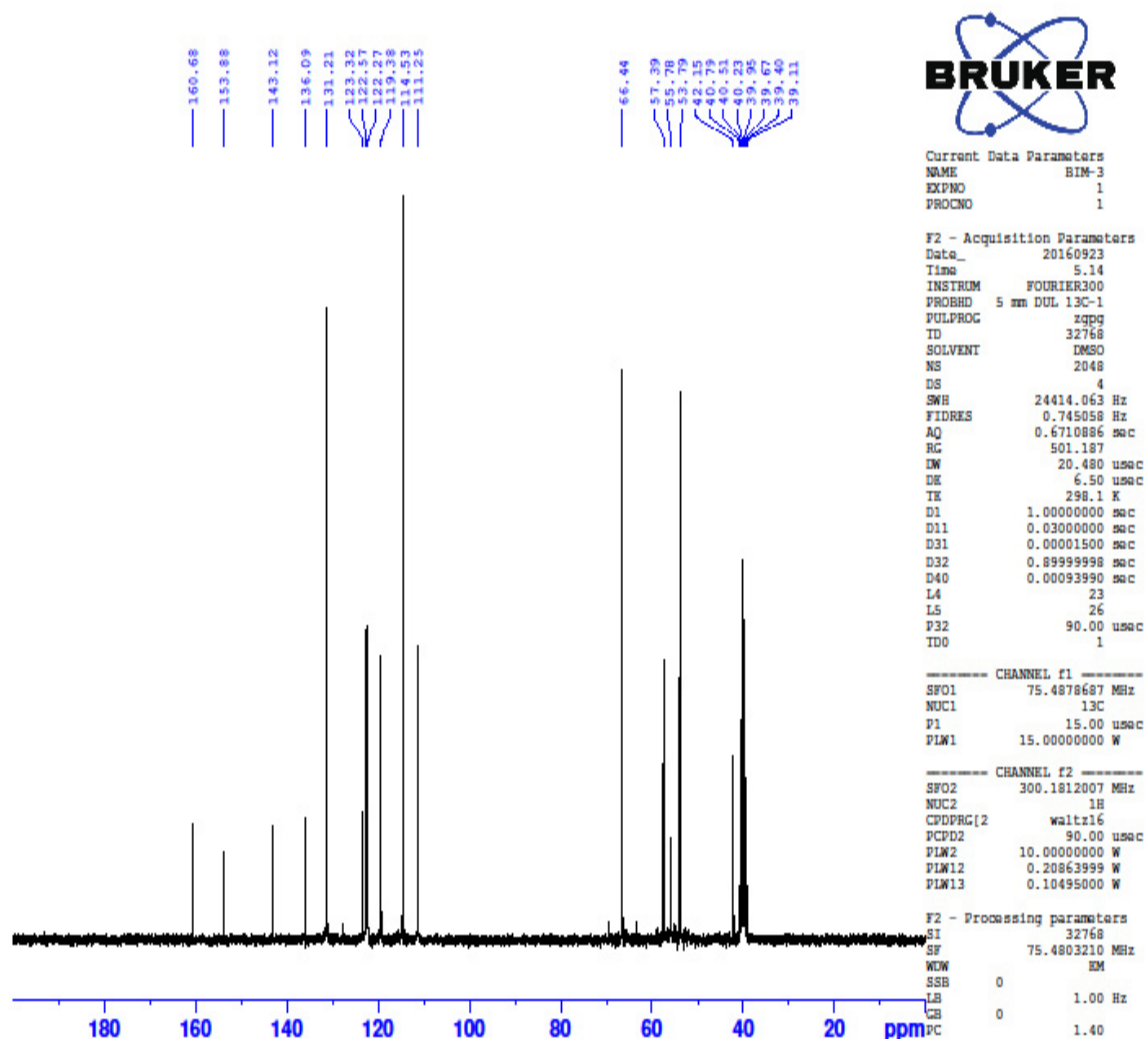


C20 H23 N3 O [M+H]⁺ : Predicted region for 322.1914 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Isol.	DBE
1	65.89	C20 H23 N3 O	[M+H] ⁺	322.1901	322.1914	-1.3	-4.03	71.29	11.0

¹³C-NMR spectrum of 2-(4-Methoxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2b**)



¹H-NMR spectrum of 2-(4-Methoxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2b**)

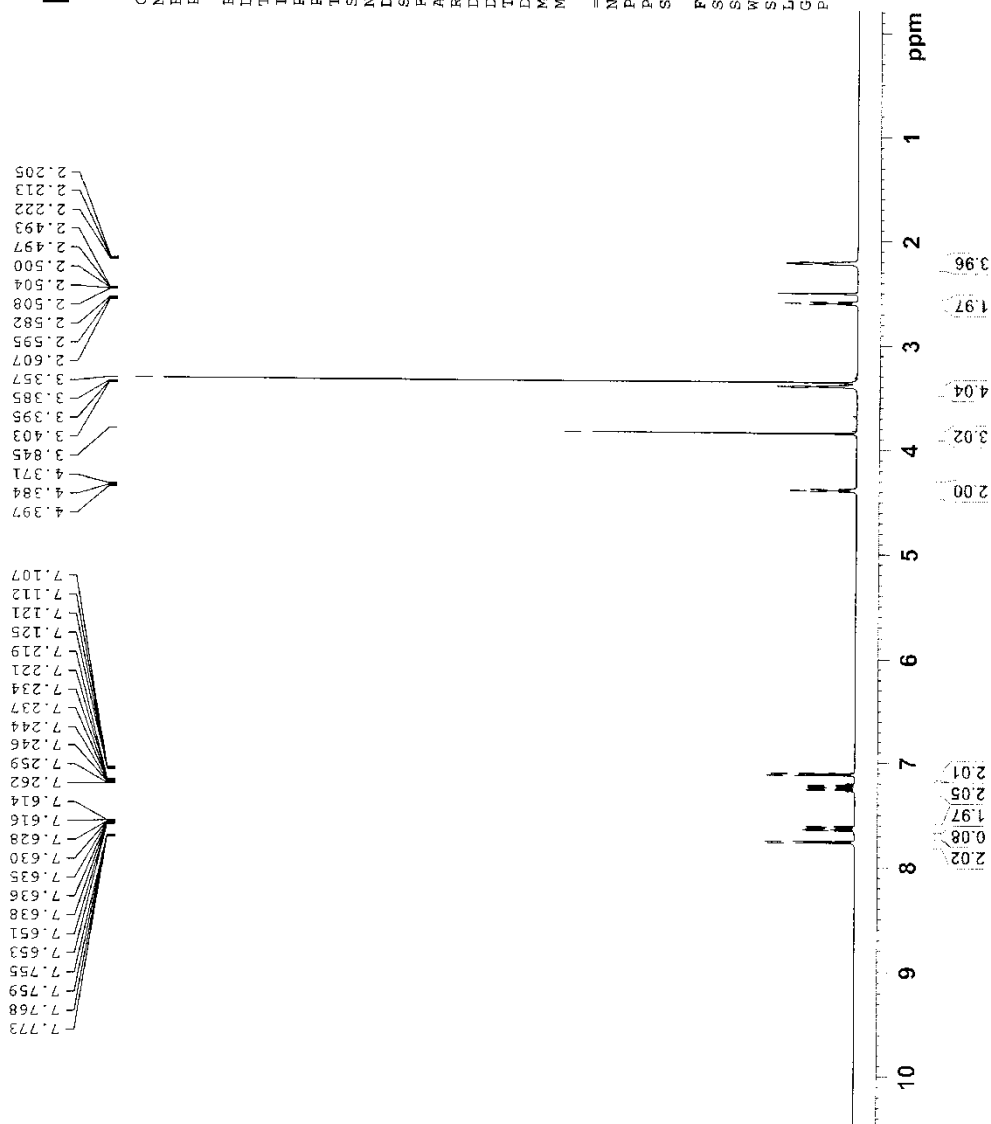


Current Data Parameters
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EXPNO 1
PROCNO 1

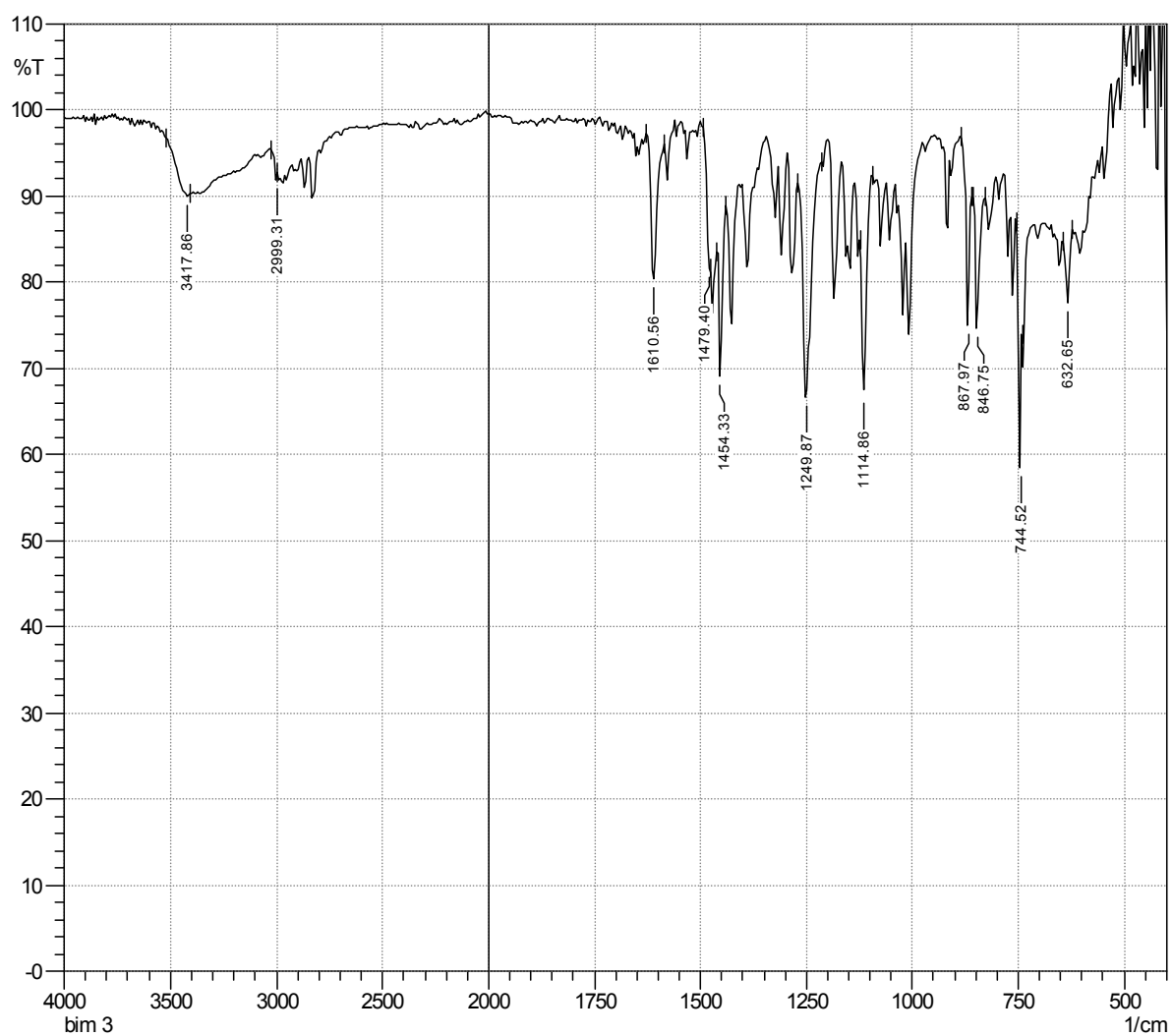
F2 - Acquisition Parameters
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Time 12.06
INSTRUM spect
PROBHD 5 mm BBI 1H-BB
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10964.912 Hz
FIDRES 0.167311 Hz
AQ 2.9885373 sec
RG 71.8
DW 45.600 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.50 usec
PL1 0.00 dB
SFO1 500.1347512 MHz

F2 - Processing parameters
SI 131072
SF 500.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



FTIR spectrum of 2-(4-Methoxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2b**)



HRMS spectrum of 2-(4-Methoxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2b**)

Formula Predictor Report - Bim-3_11.lcd

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Data File: C:\LabSolutions\Data\Analiz\Bim series\Bim-3_11.lcd

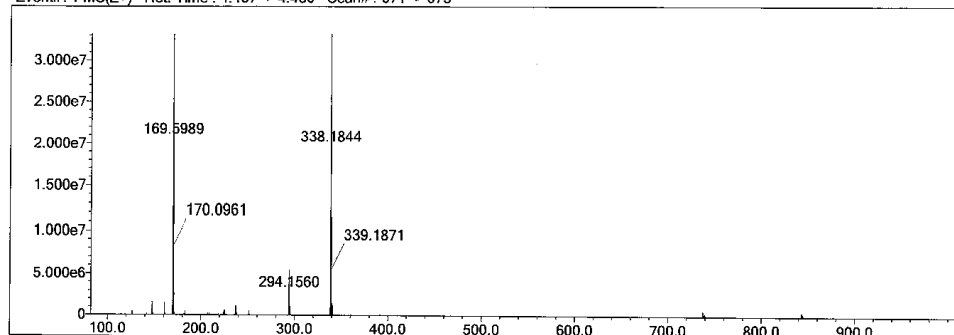
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C	4	12	30	S	2	0	0	
N	3	3	4	Cl	1	0	0	

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

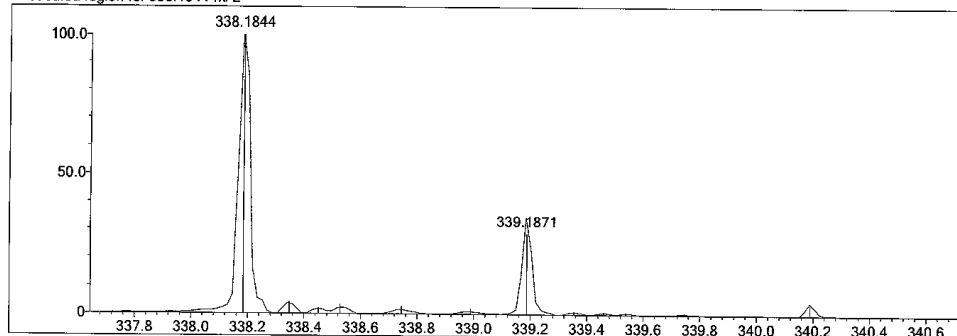
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

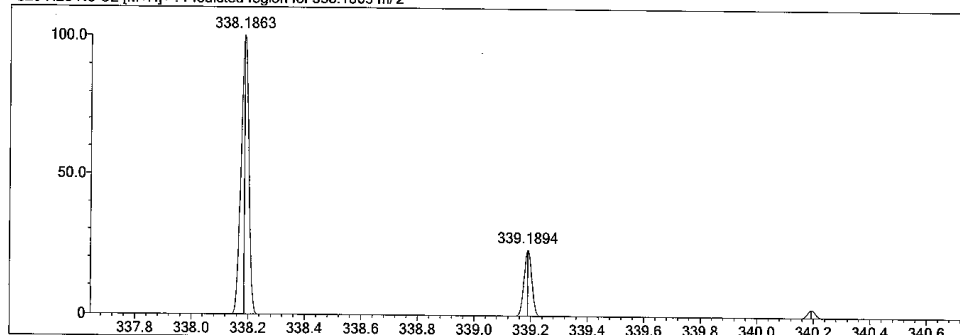
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Measured region for 338.1844 m/z

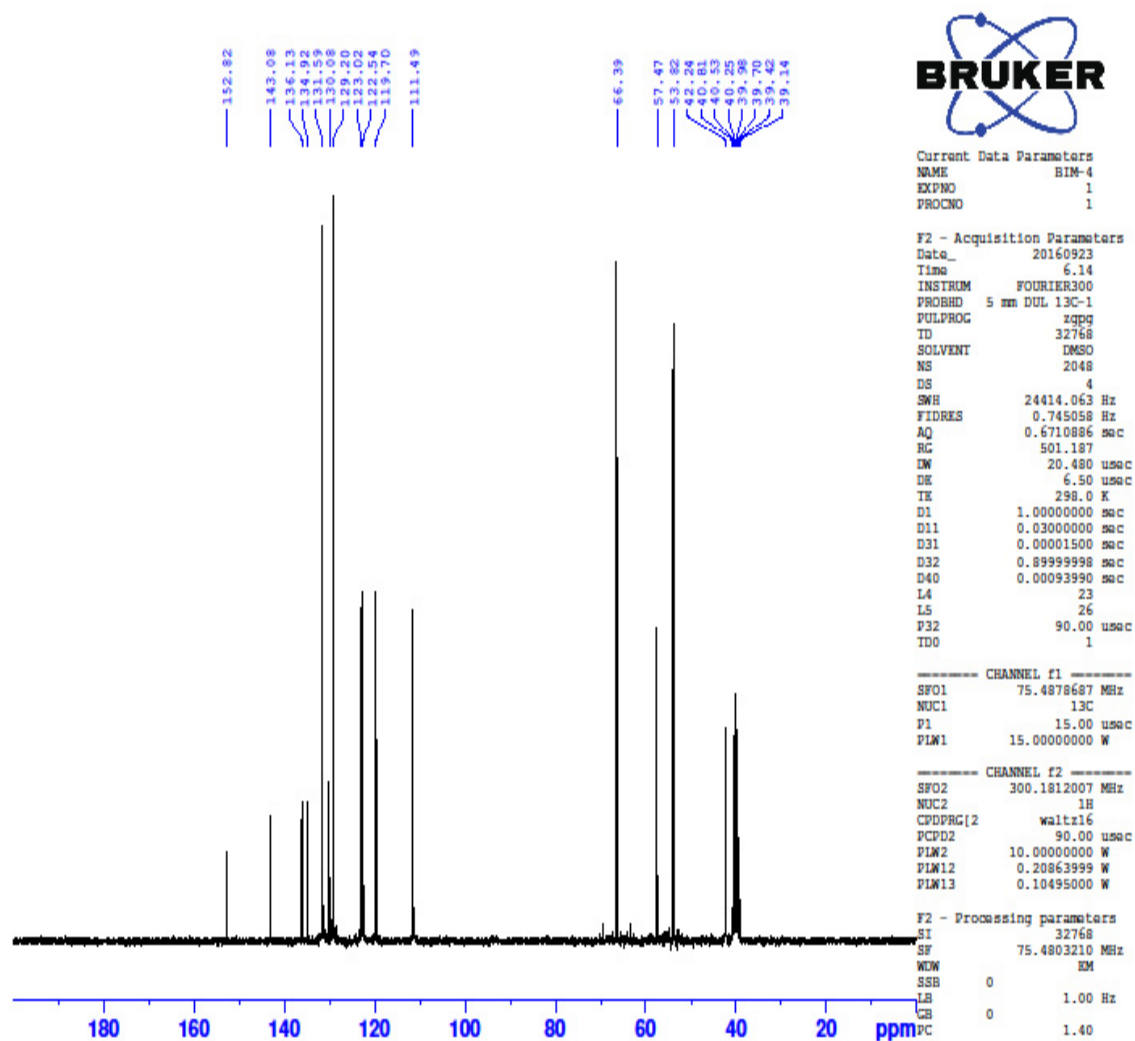


C20 H23 N3 O2 [M+H]⁺ : Predicted region for 338.1863 m/z

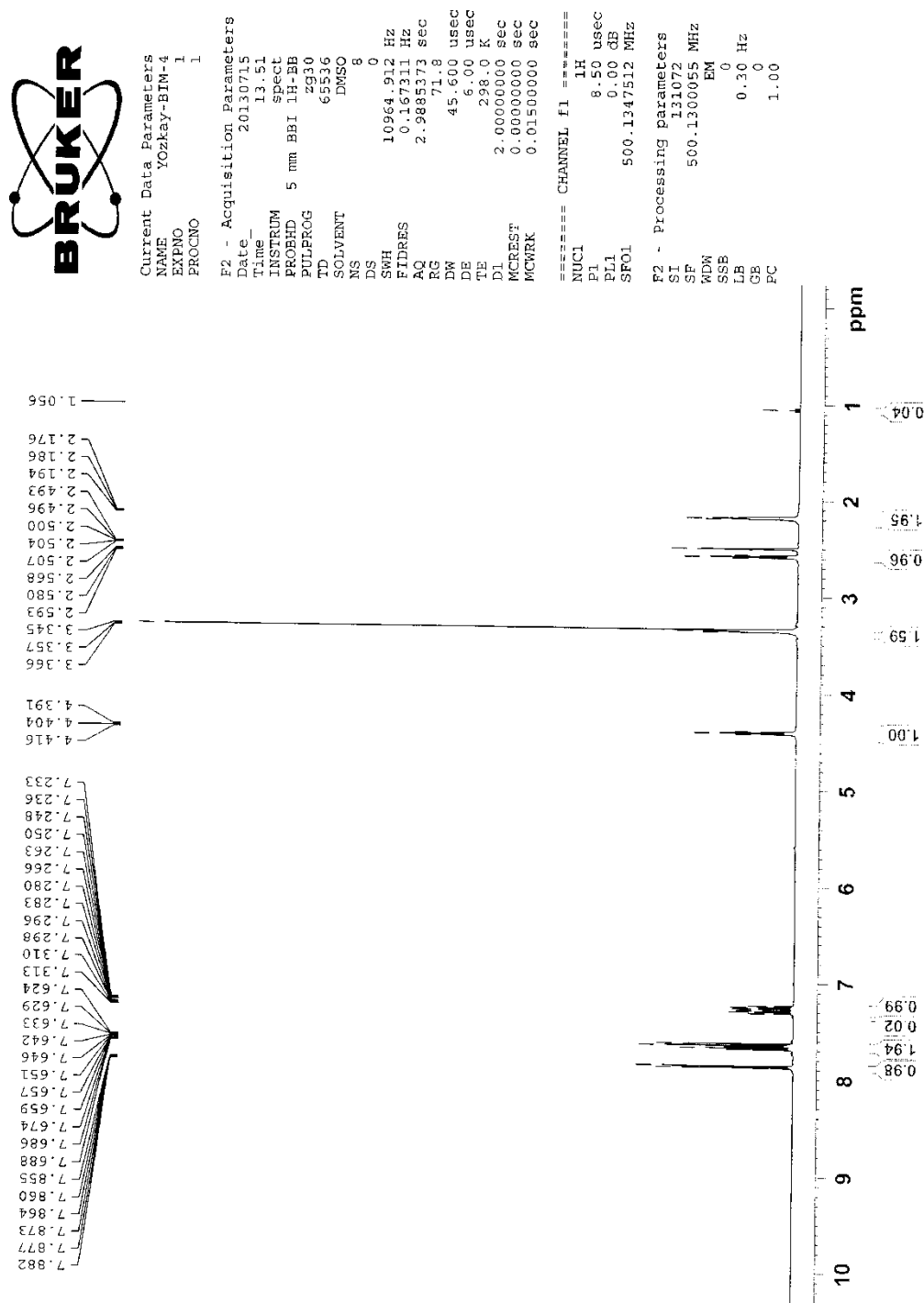


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	63.81	C20 H23 N3 O2	[M+H] ⁺	338.1844	338.1863	-1.9	-5.62	76.15	11.0

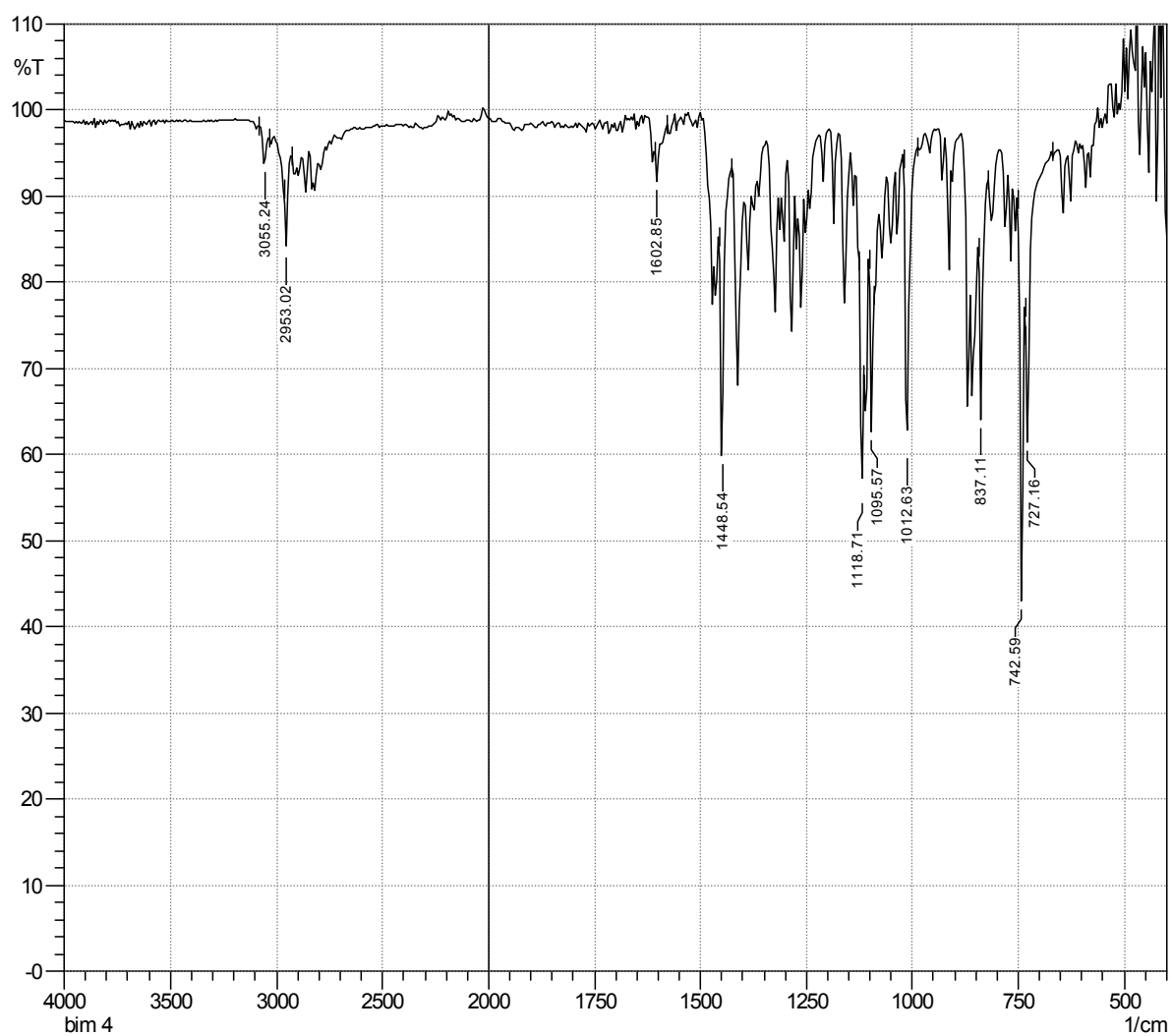
¹³C-NMR spectrum of 2-(4-Chlorophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2c**)



¹H-NMR spectrum of 2-(4-Chlorophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2c)



FTIR spectrum of 2-(4-Chlorophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2c**)



HRMS spectrum of 2-(4-Chlorophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2c)

Formula Predictor Report - Bim-4_12.lcd

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Data File: C:\LabSolutions\Data\Analiz\Bim series\Bim-4_12.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	14	30	O	2	1	5	H
C	4	12	30	S	2	0	0	
N	3	3	4	Cl	1	0	1	

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: -2.0 - 1000.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

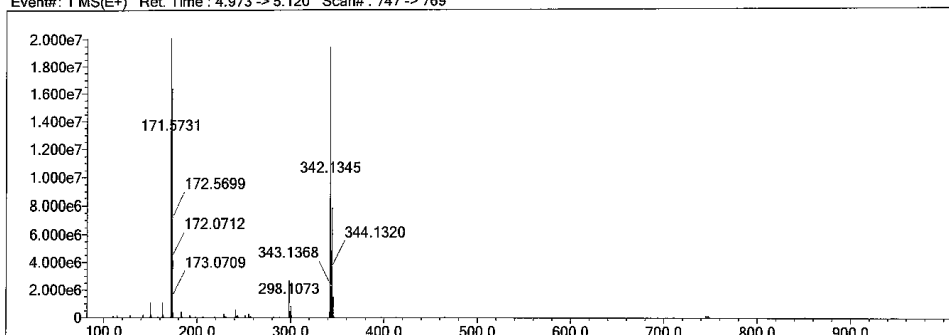
Electron Ions: both

Use MSn Info: no

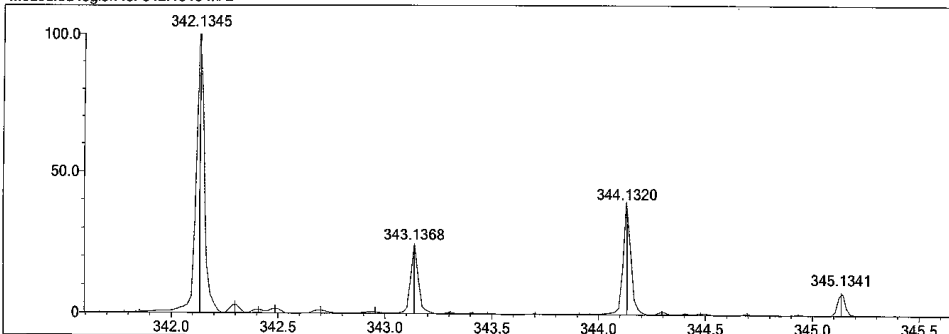
Isotope Res: 10000

Max Results: 500

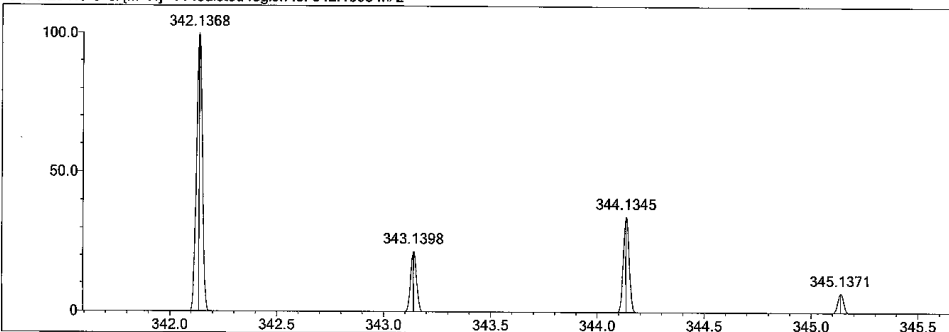
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Measured region for 342.1345 m/z

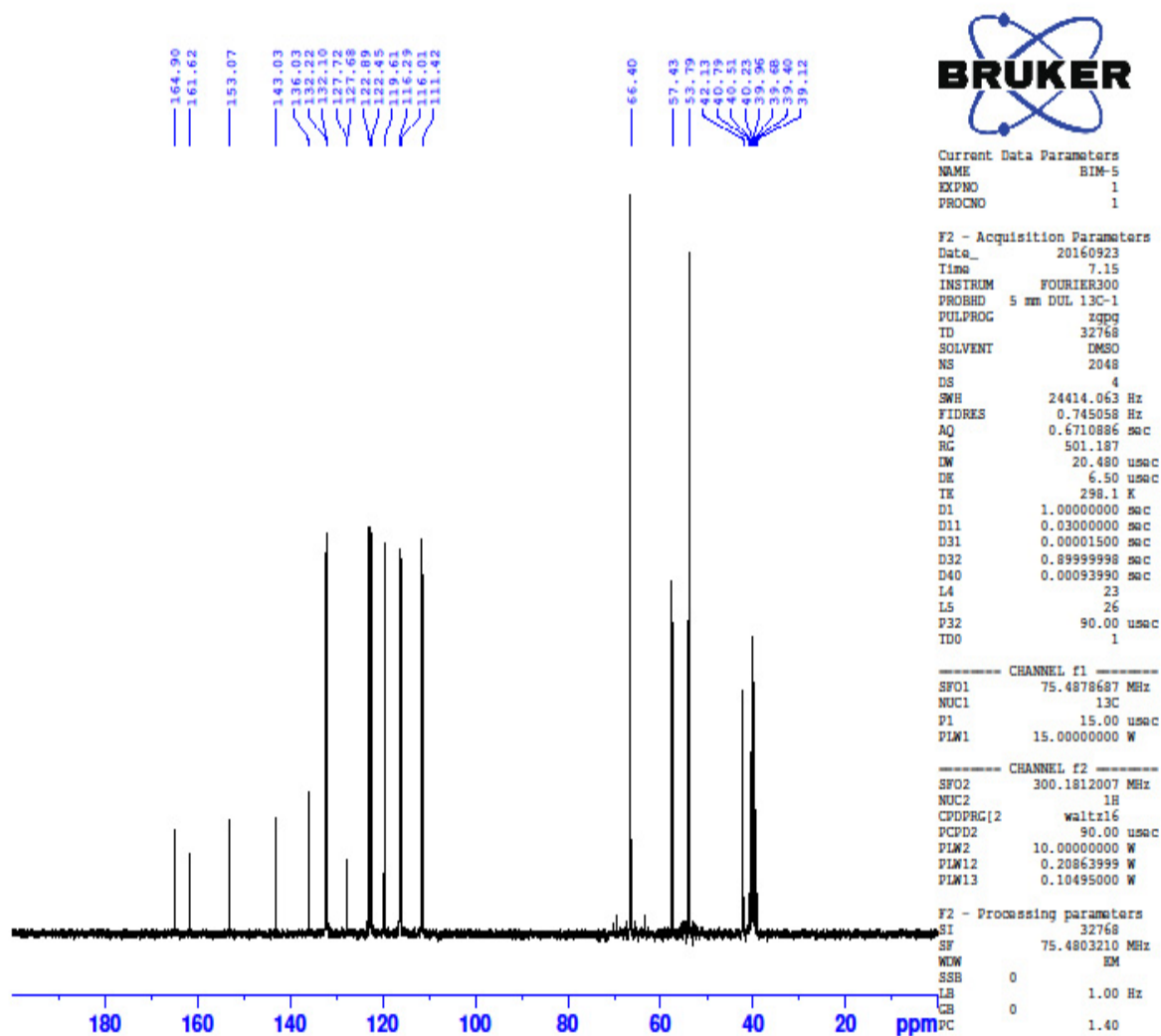


C19 H20 N3 O Cl [M+H]+ : Predicted region for 342.1368 m/z

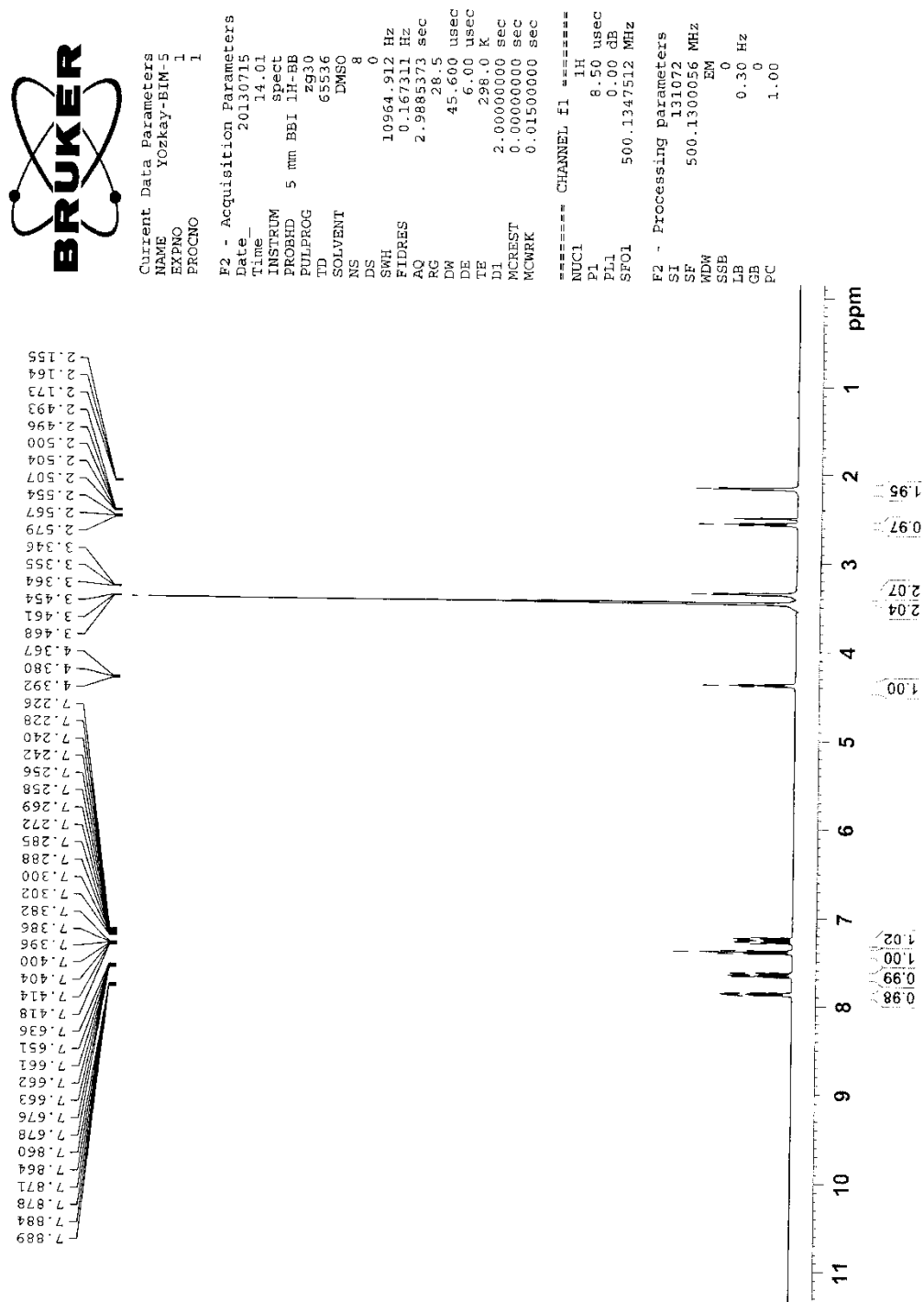


Peak	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Diff. (mDa)	Diff. (ppm)	Iso	DBE
1	56.76	C19 H20 N3 O Cl	[M+H]+	342.1345	342.1368	-2.3	-6.72	77.97	11.0

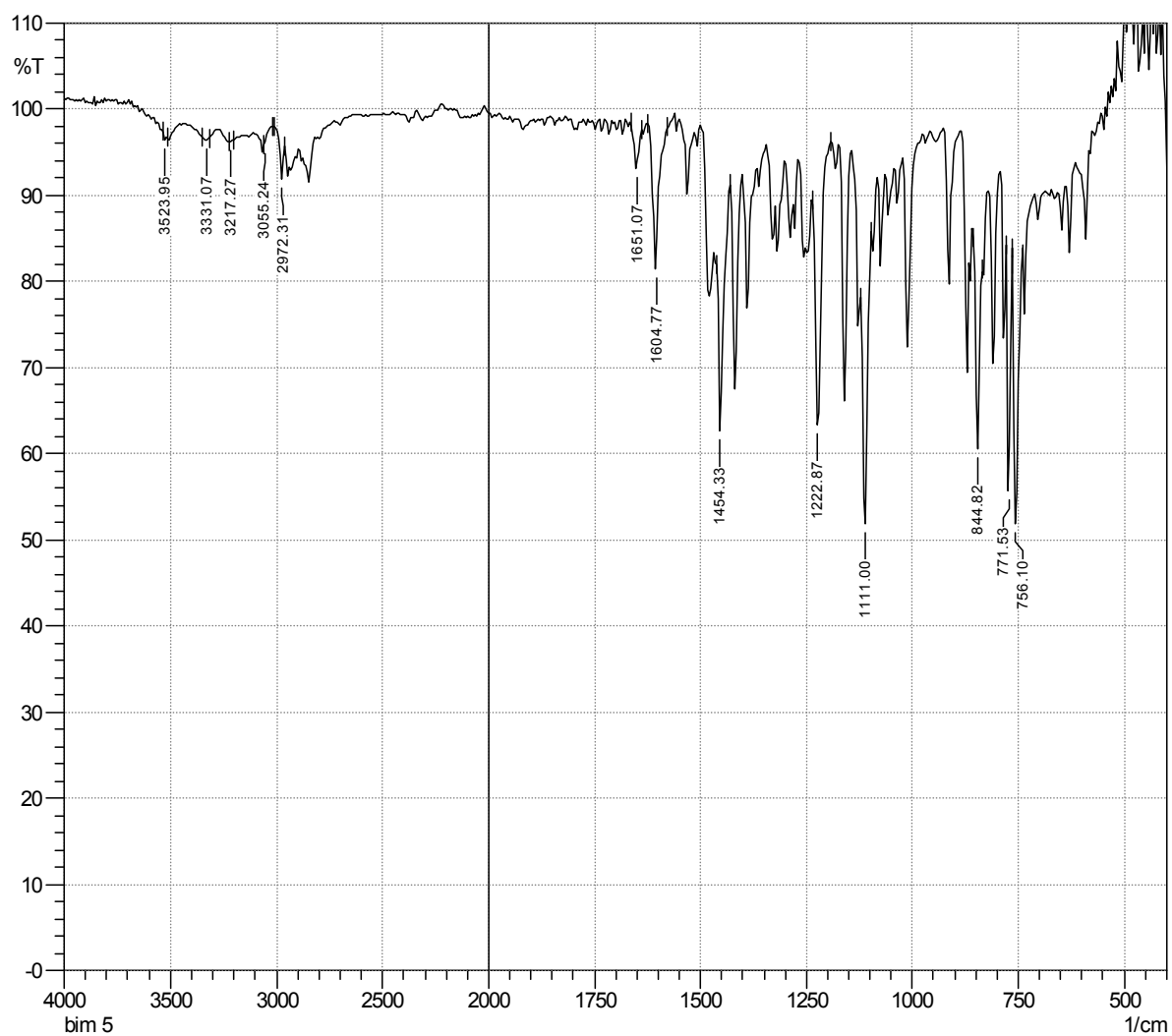
^{13}C -NMR spectrum of 2-(4-Fluorophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2d**)



¹H-NMR spectrum of 2-(4-Fluorophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2d)



FTIR spectrum of 2-(4-Fluorophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2d**)



HRMS spectrum of 2-(4-Fluorophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2d)

Formula Predictor Report - Bim-5_13.lcd

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Data File: C:\LabSolutions\1 Data\Analiz\Bim series\Bim-5_13.lcd

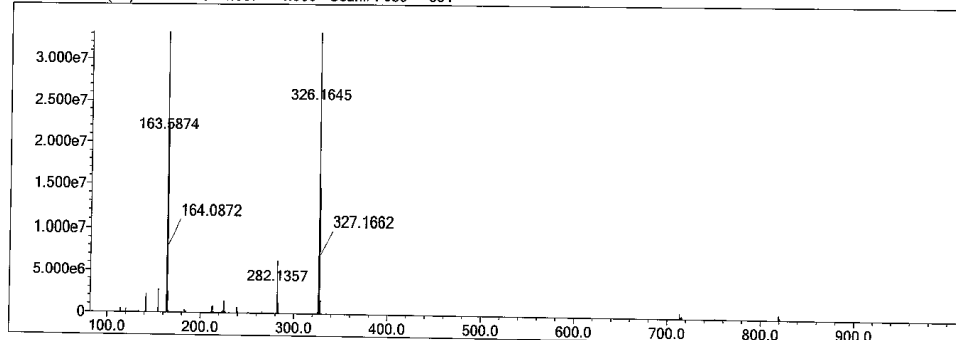
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H	1	14	30	O	2	1	5	Cl	1	0	0		H
C	4	12	30	F	1	0	1						
N	3	3	4	S	2	0	0						

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

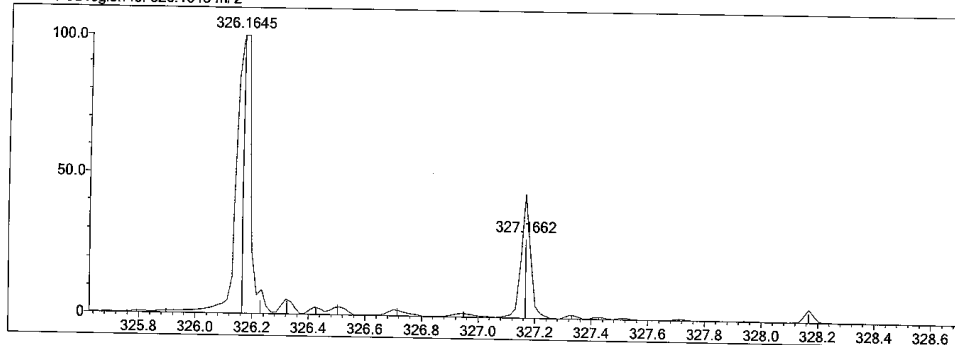
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

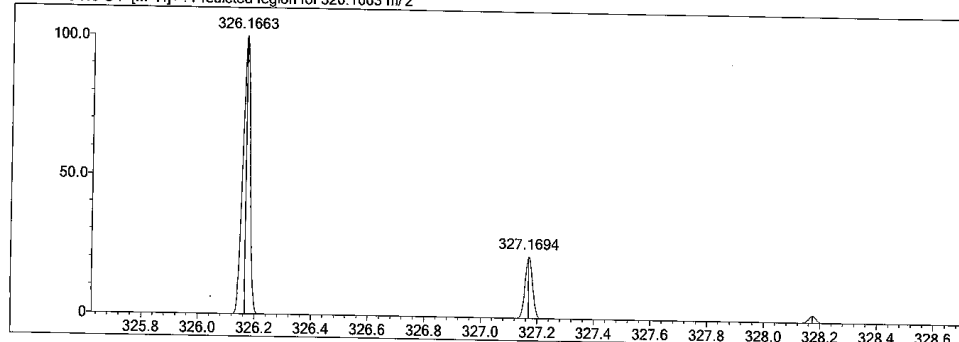
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Measured region for 326.1645 m/z

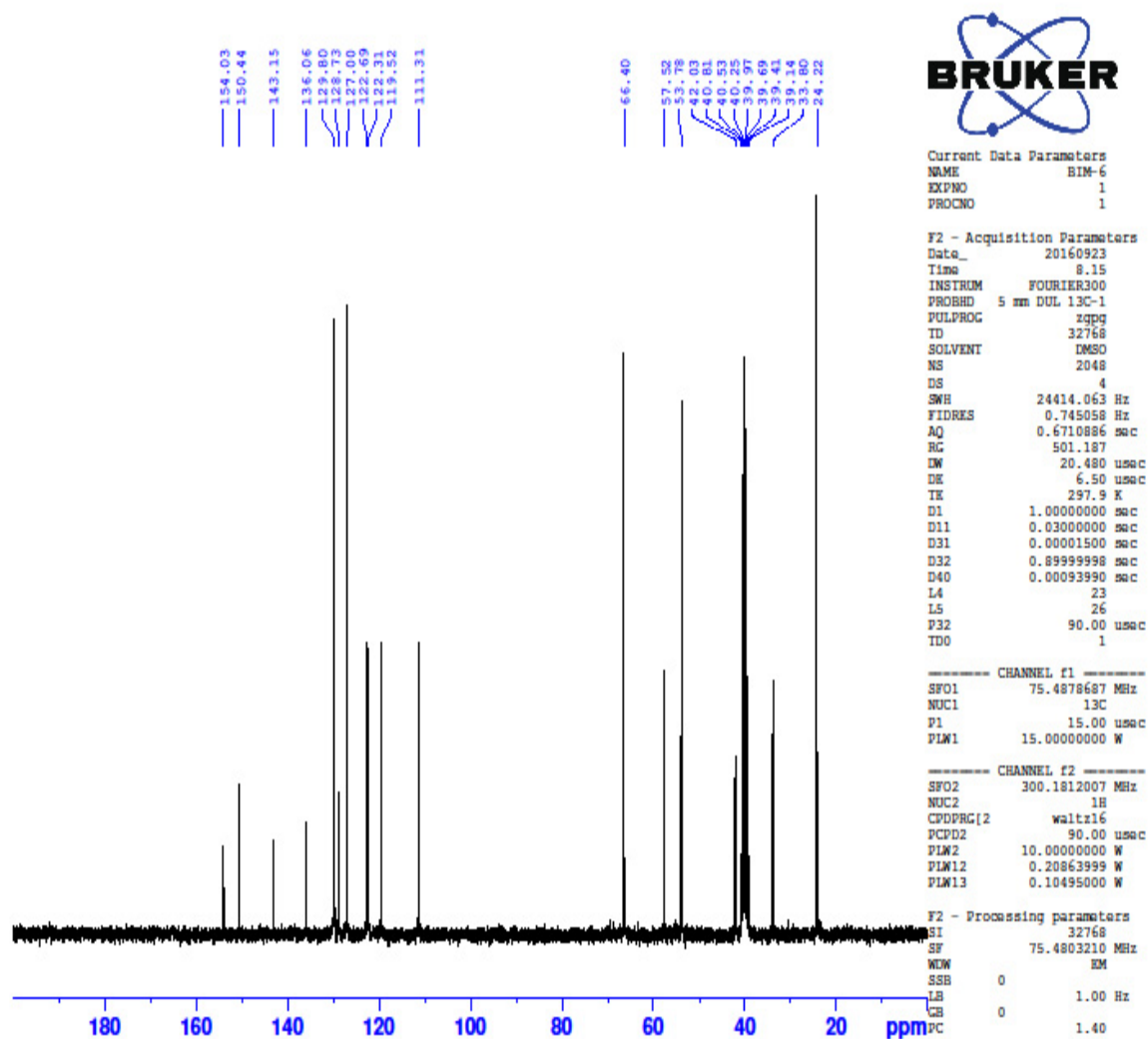


C19 H20 N3 O F [M+H]⁺ : Predicted region for 326.1663 m/z

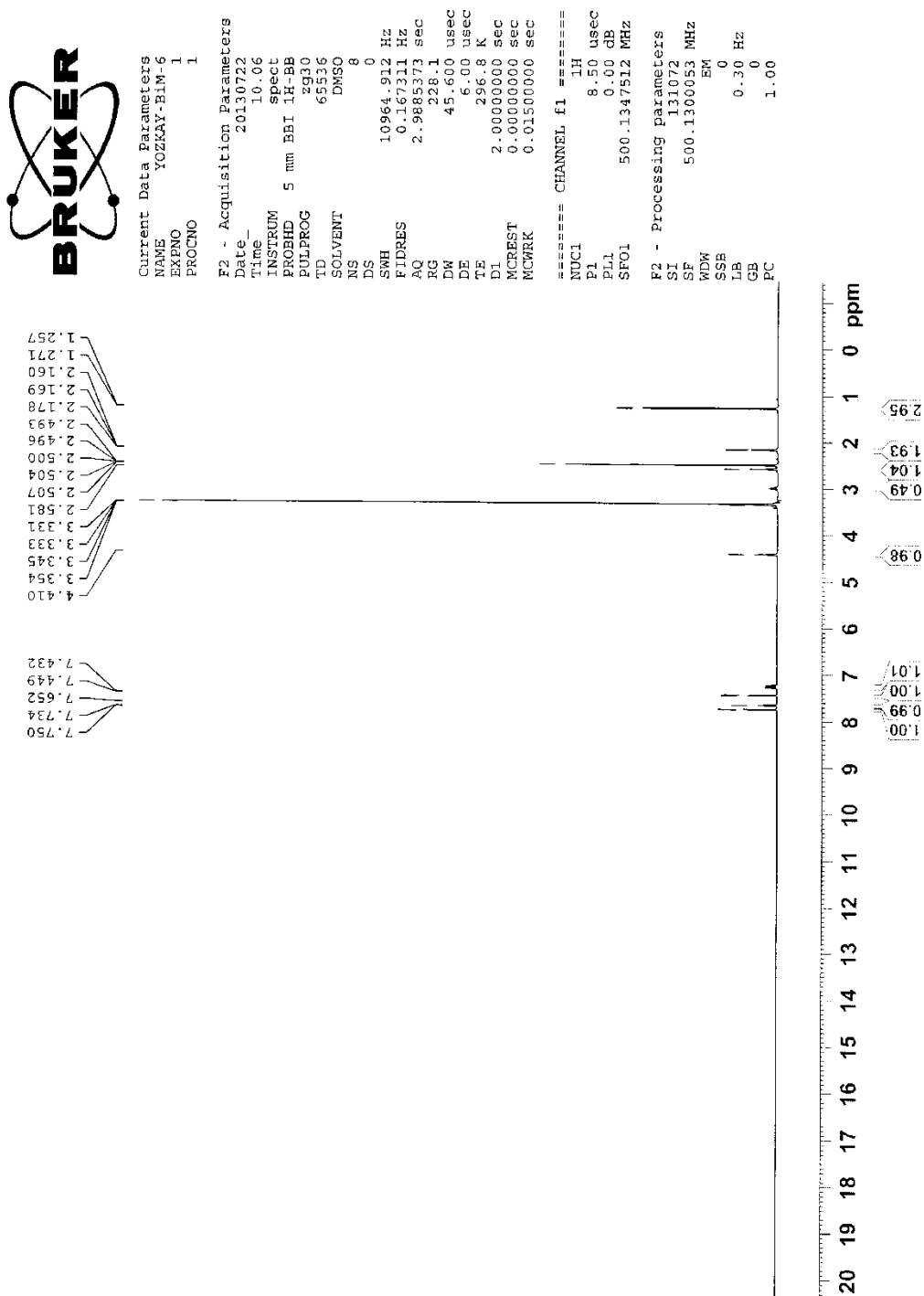


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	51.00	C19 H20 N3 O F	[M+H] ⁺	326.1645	326.1663	-1.8	-5.52	60.14	11.0

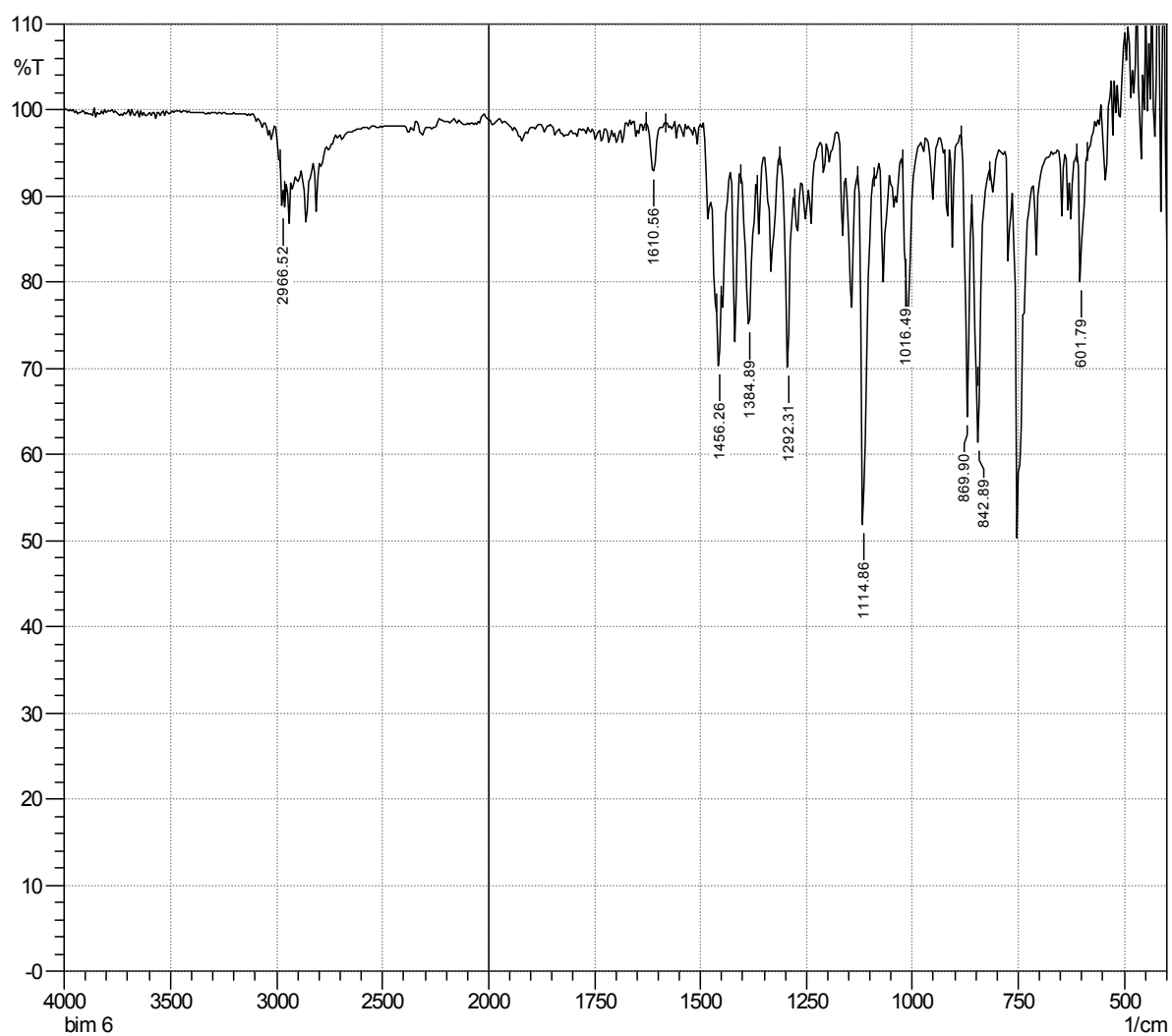
¹³C-NMR spectrum of 2-(4-Isopropylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2e**)



¹H-NMR spectrum of 2-(4-Isopropylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2e)



FTIR spectrum of 2-(4-Isopropylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2e**)



HRMS spectrum of 2-(4-Isopropylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2e)

Formula Predictor Report - Bim-6_14.lcd

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Data File: C:\LabSolutions\1 Data\Analiz\Bim series\Bim-6_14.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
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C	4	12	30	F	1	0	1					
N	3	3	4	S	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: -2.0 - 1000.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

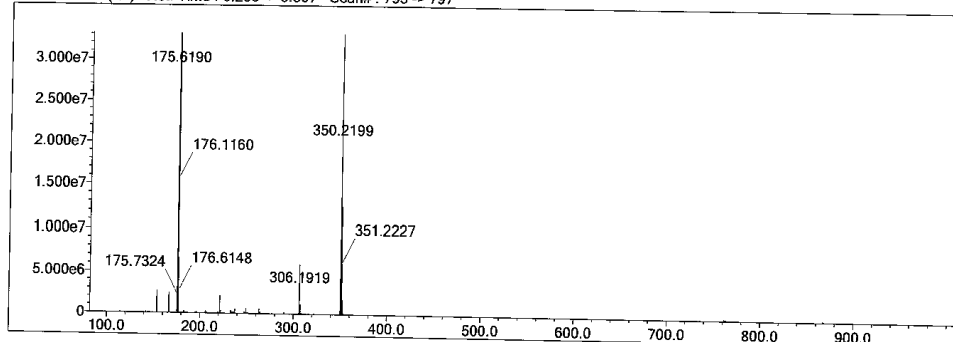
Electron Ions: both

Use MSn Info: no

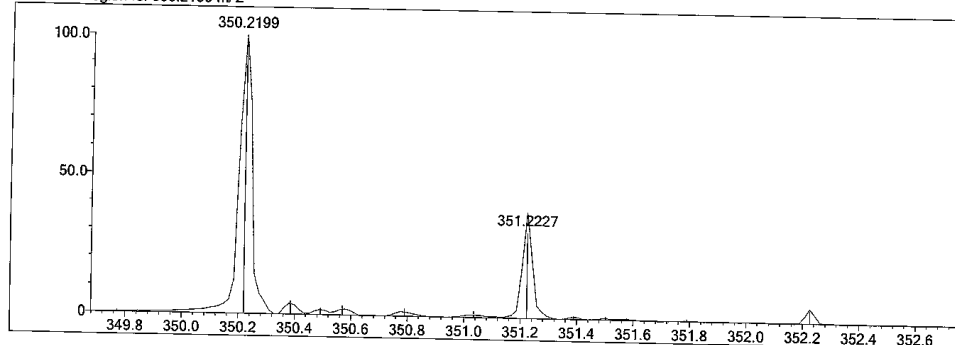
Isotope Res: 10000

Max Results: 500

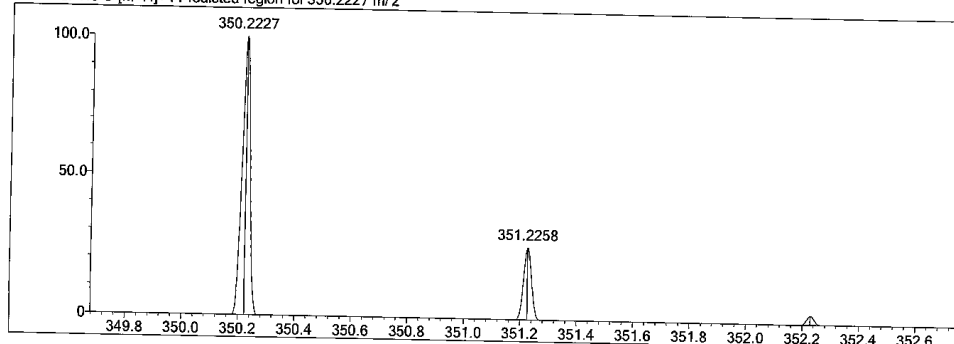
Event#: 1 MS(E+) Ret. Time : 5.280 -> 5.307 Scan#: 793 -> 797



Measured region for 350.2199 m/z

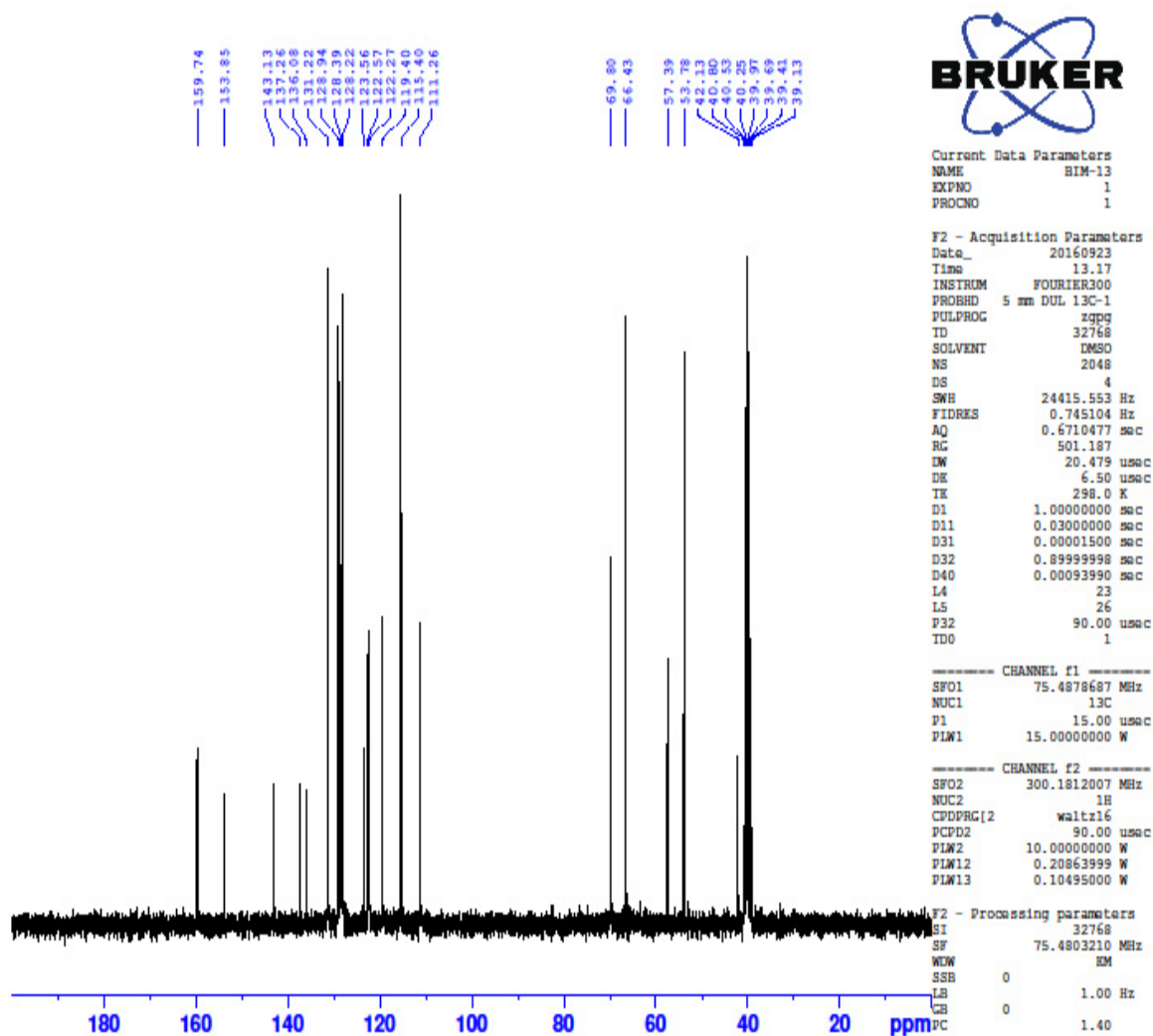


C22 H27 N3 O [M+H]⁺ : Predicted region for 350.2227 m/z

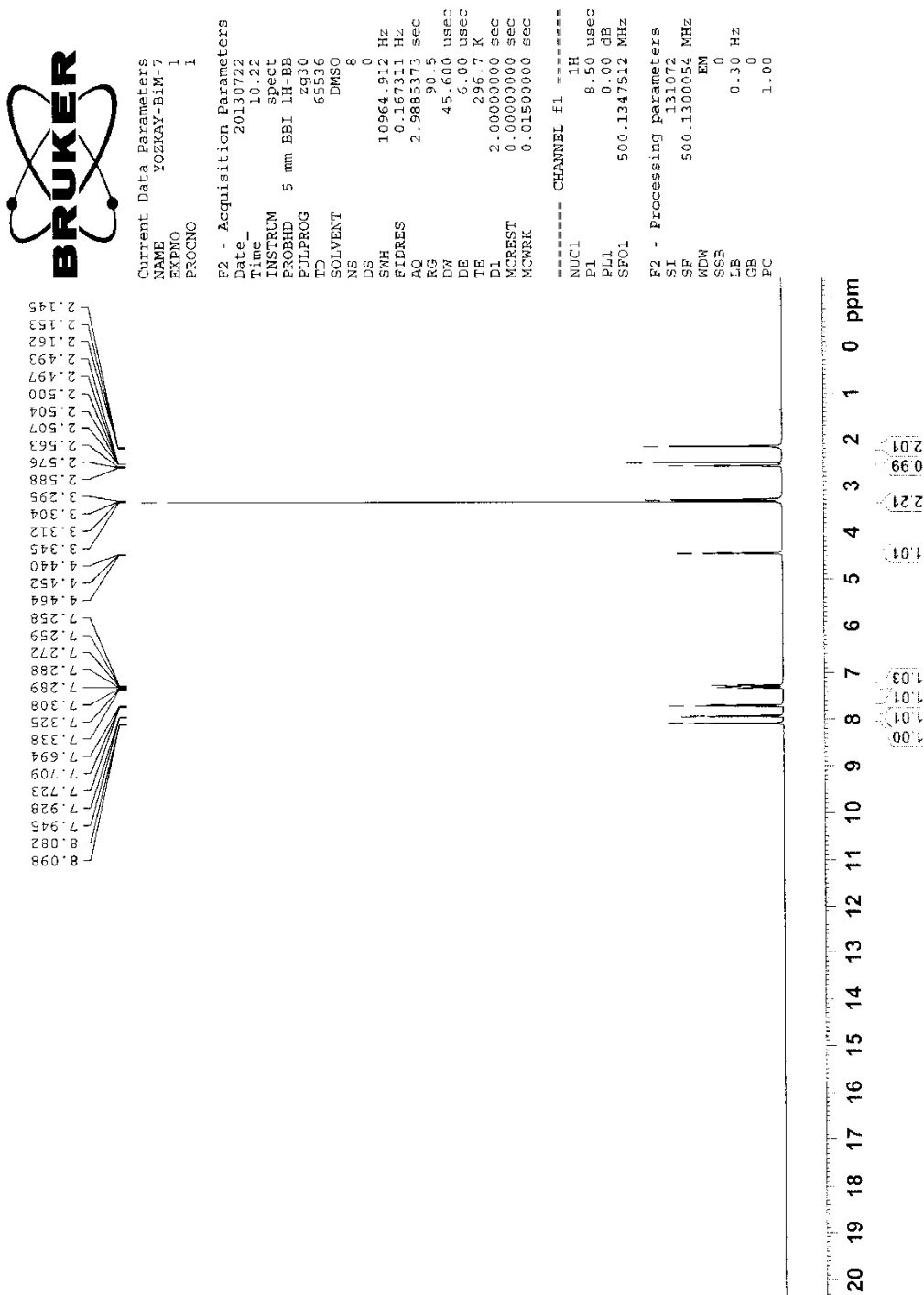


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	46.38	C22 H27 N3 O	[M+H] ⁺	350.2199	350.2227	-2.8	-7.99	77.17	11.0

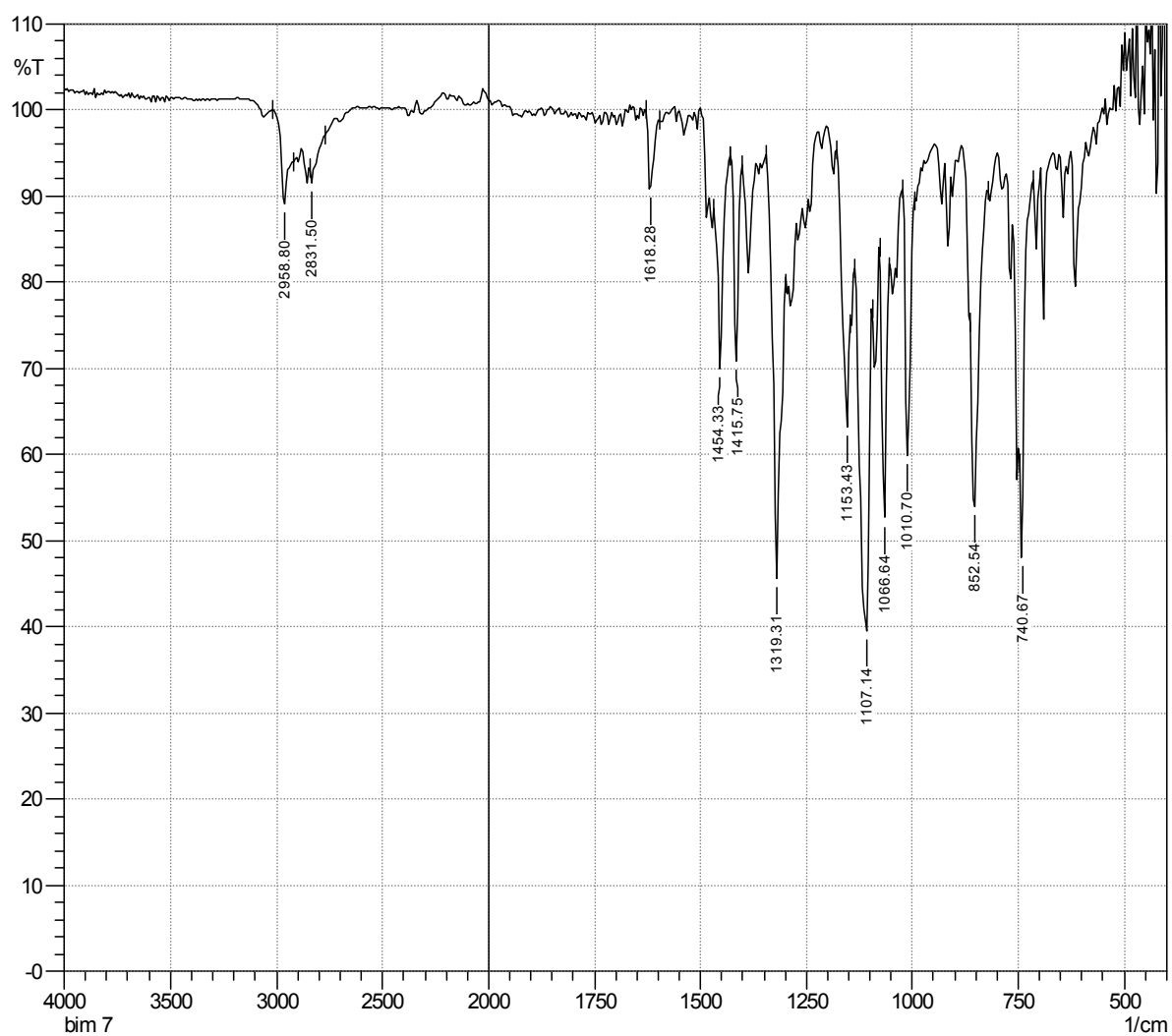
¹³C-NMR spectrum of 2-(4-Benzyloxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2f**)



¹H-NMR spectrum of 2-(4-Benzyloxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2f)



FTIR spectrum of 2-(4-Benzyloxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2f**)



HRMS spectrum of 2-(4-Benzyloxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2f)

Formula Predictor Report - Bim-7_15.lcd

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Data File: C:\LabSolutions\Data\Analiz\Bim series\Bim-7_15.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	14	30	O	2	1	5	Cl	1	0	0	H
C	4	12	30	F	1	0	3					
N	3	3	4	S	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: -2.0 - 1000.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

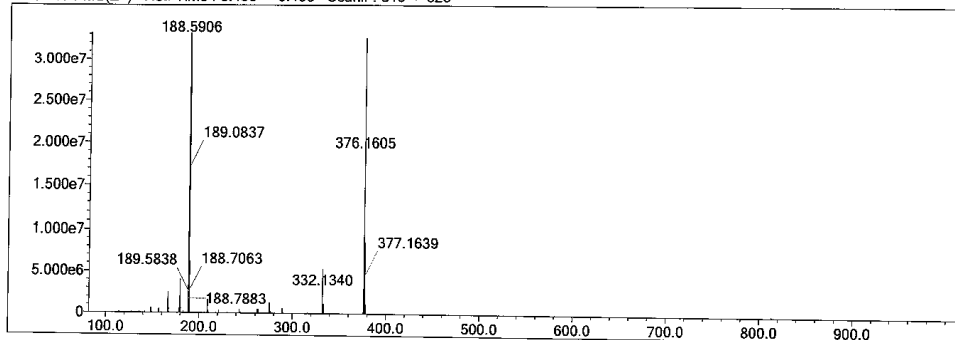
Electron Ions: both

Use MSn Info: no

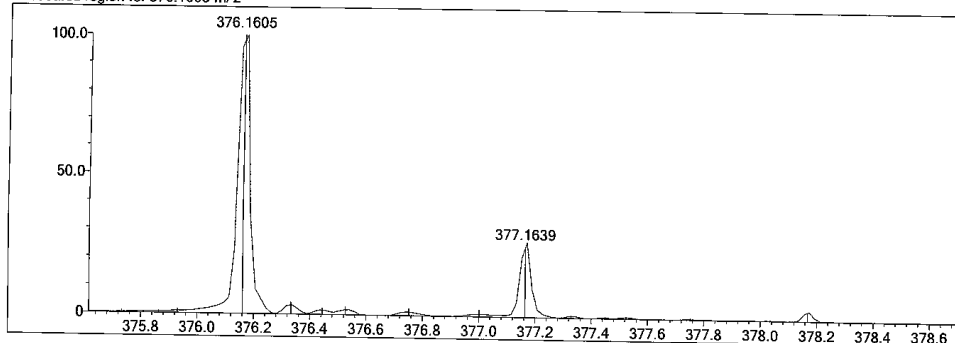
Isotope Res: 10000

Max Results: 500

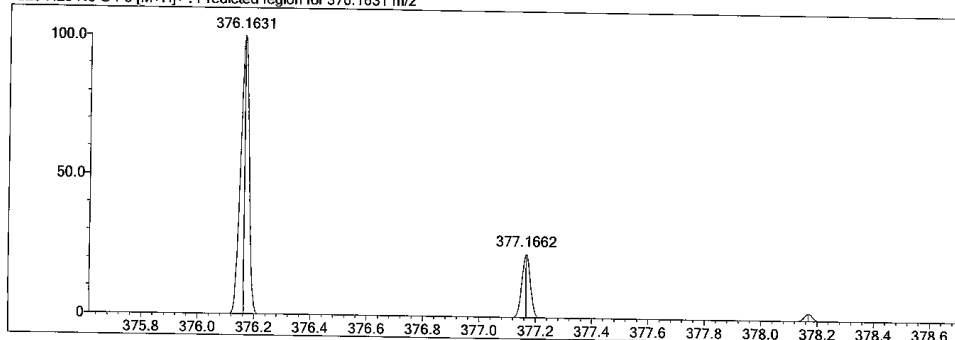
Event#: 1 MS(E+) Ret. Time : 5.453 -> 5.493 Scan#: 819 -> 825



Measured region for 376.1605 m/z

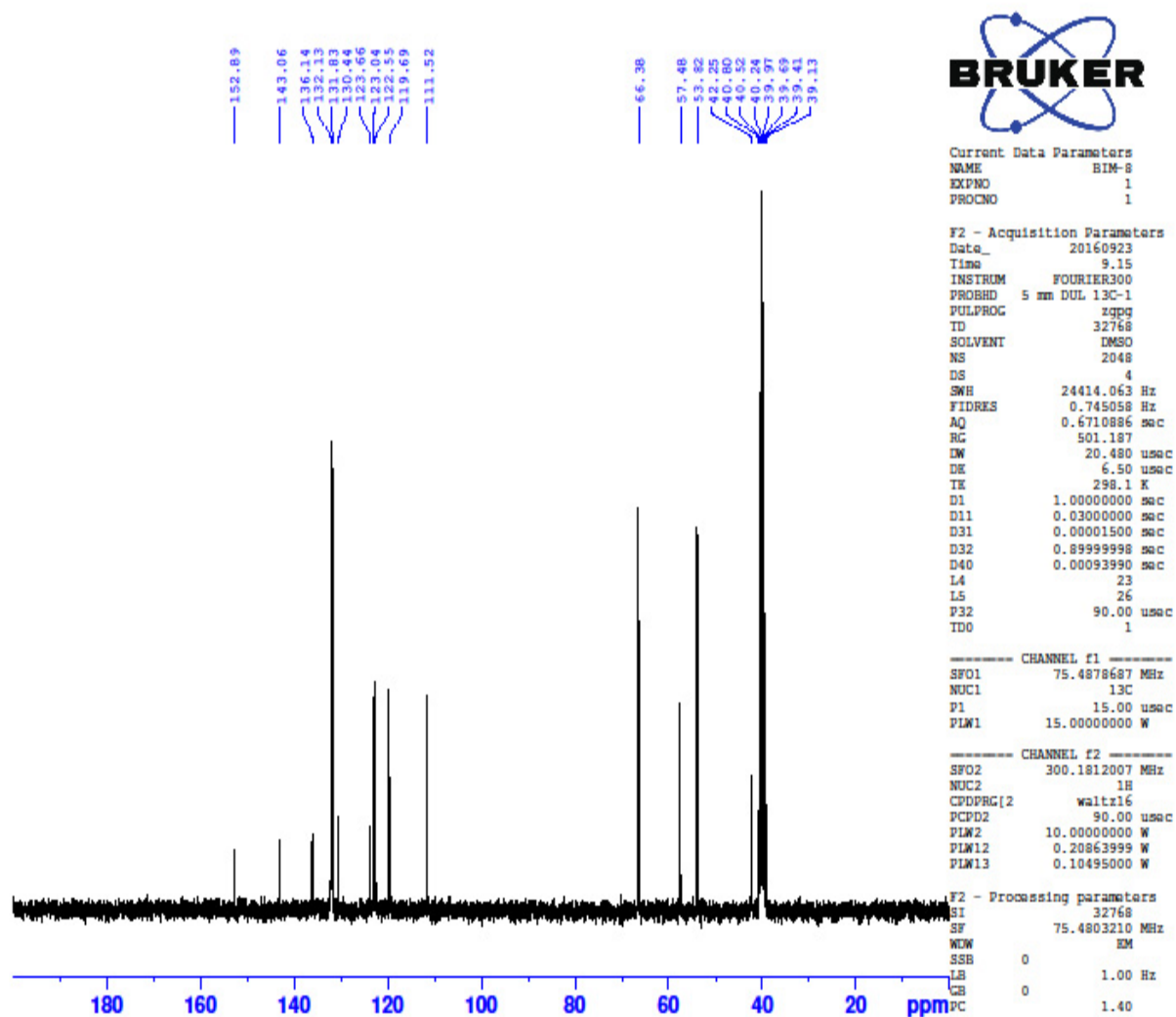


C20 H20 N3 O F3 [M+H]⁺ : Predicted region for 376.1631 m/z

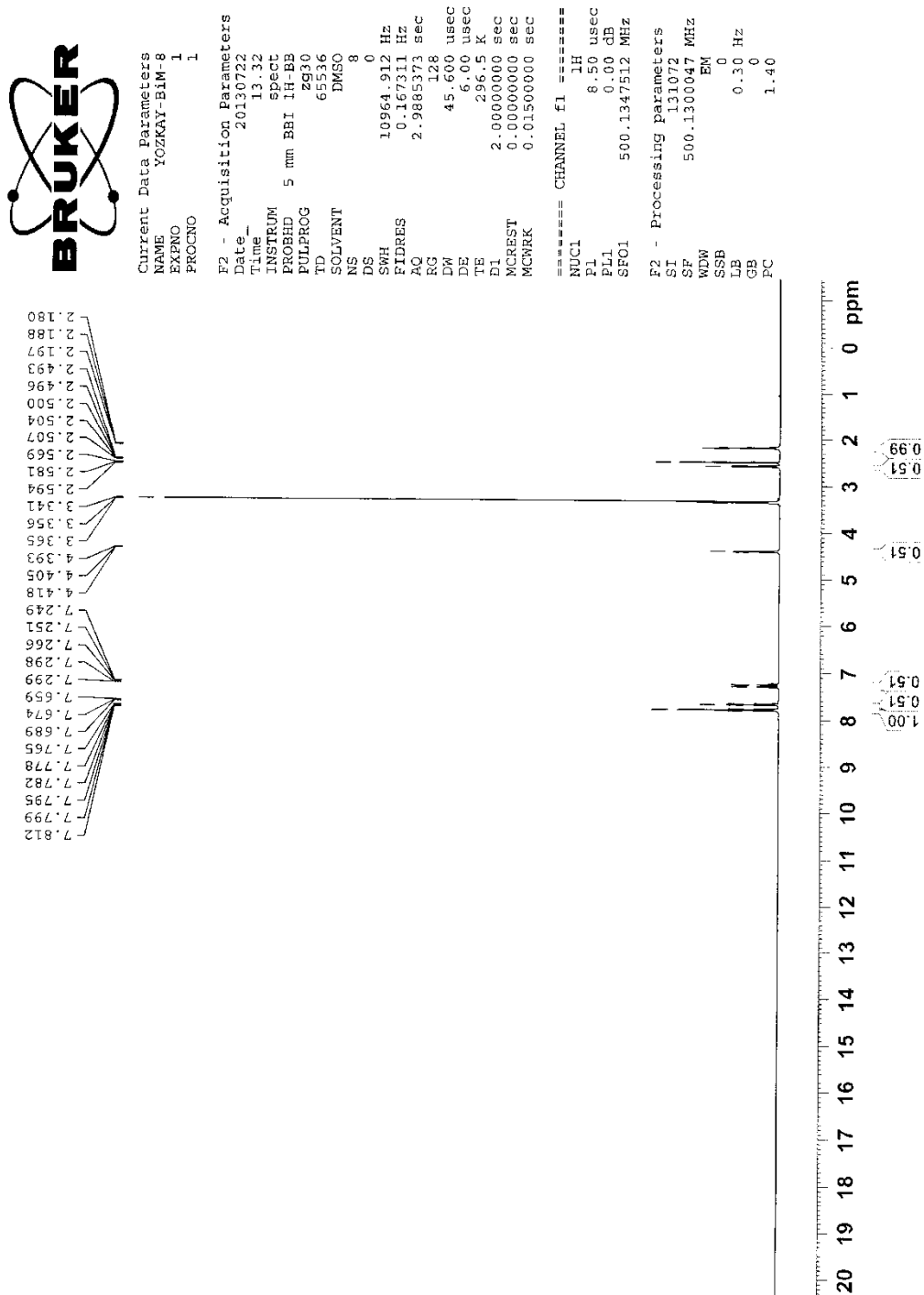


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	70.90	C20 H20 N3 O F3	[M+H] ⁺	376.1605	376.1631	-2.6	-6.91	100.00	11.0

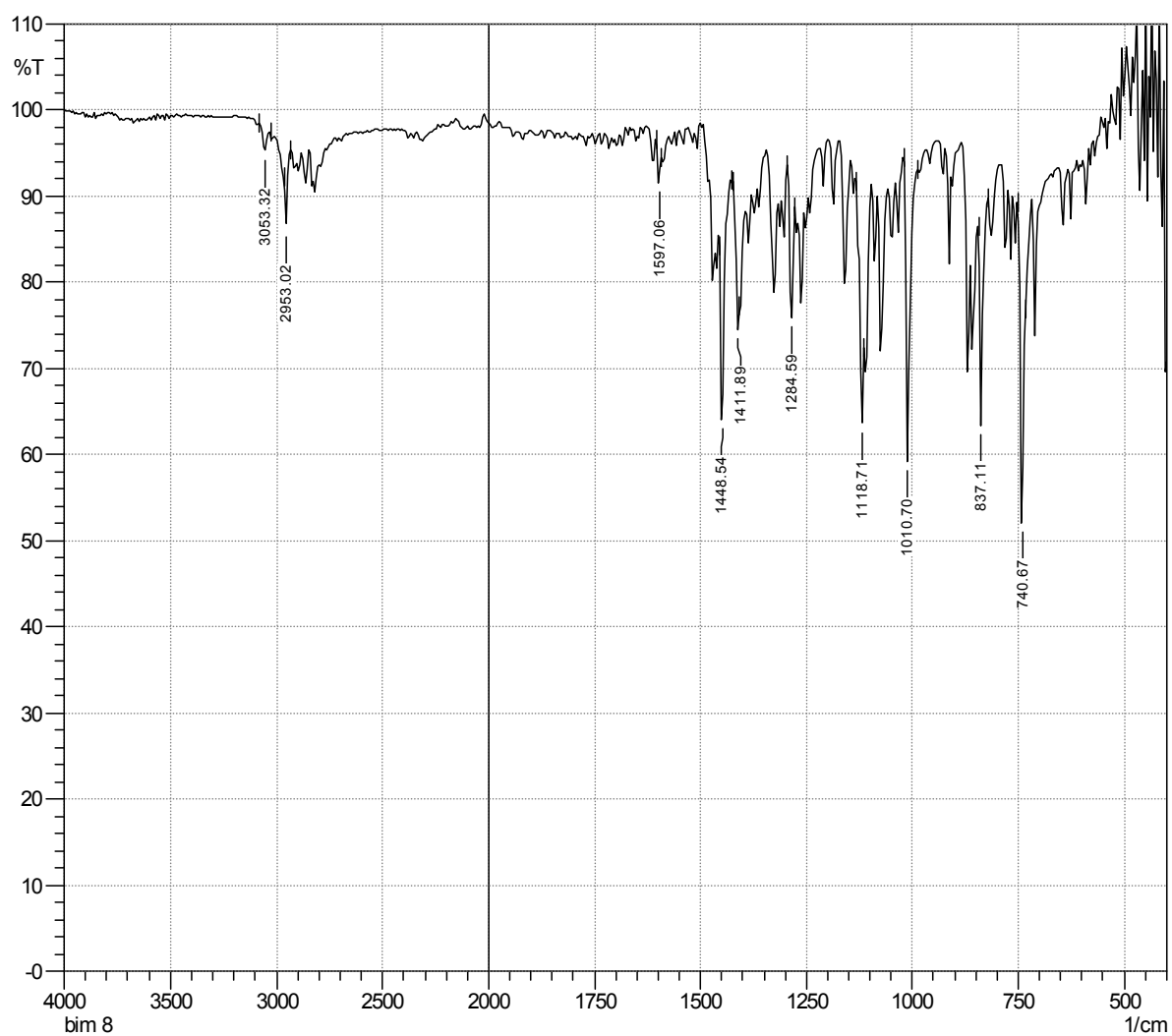
¹³C-NMR spectrum of 2-(4-Bromophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2g)



¹H-NMR spectrum of 2-(4-Bromophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2g)



FTIR spectrum of 2-(4-Bromophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2g**)



HRMS spectrum of 2-(4-Bromophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2g)

Formula Predictor Report - Bim-8_16.lcd

Page 1 of 1

Data File: C:\LabSolutions\Data\Analiz\Bim series\Bim-8_16.lcd

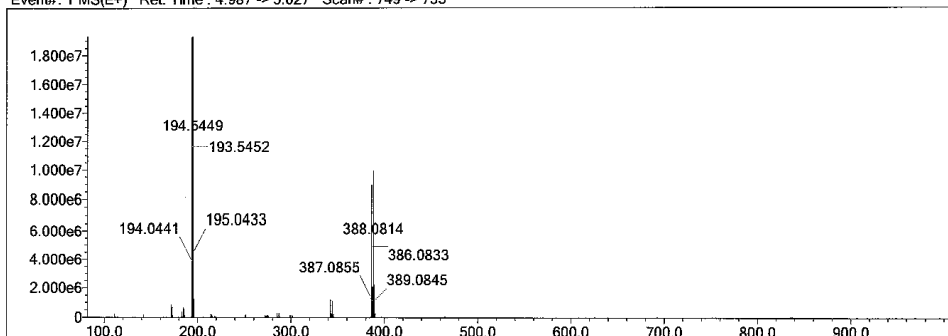
Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	14	30	O	2	1	5	Cl	1	0	0	H
C	4	12	30	F	1	0	3	Br	1	0	1	
N	3	3	4	S	2	0	0					

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

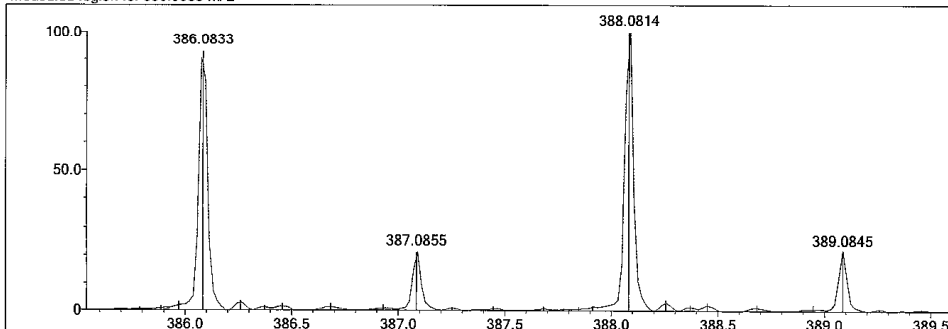
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

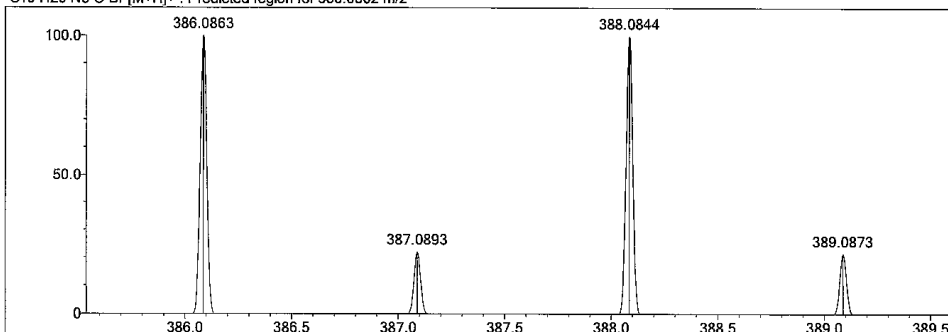
Event#: 1 MS(E+) Ret. Time : 4.987 -> 5.027 Scan# : 749 -> 755



Measured region for 386.0833 m/z

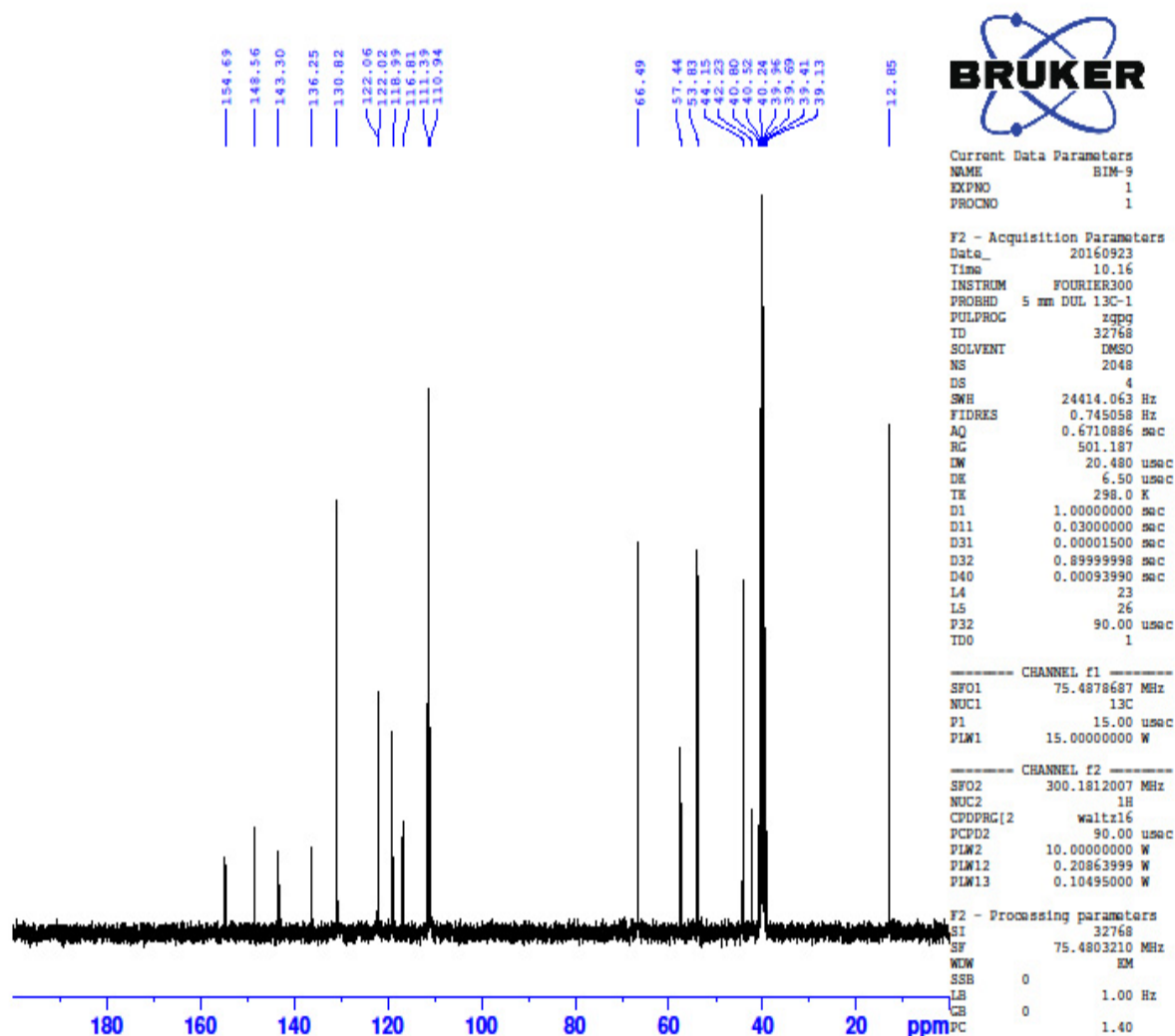


C19 H20 N3 O Br [M+H]⁺ : Predicted region for 386.0862 m/z

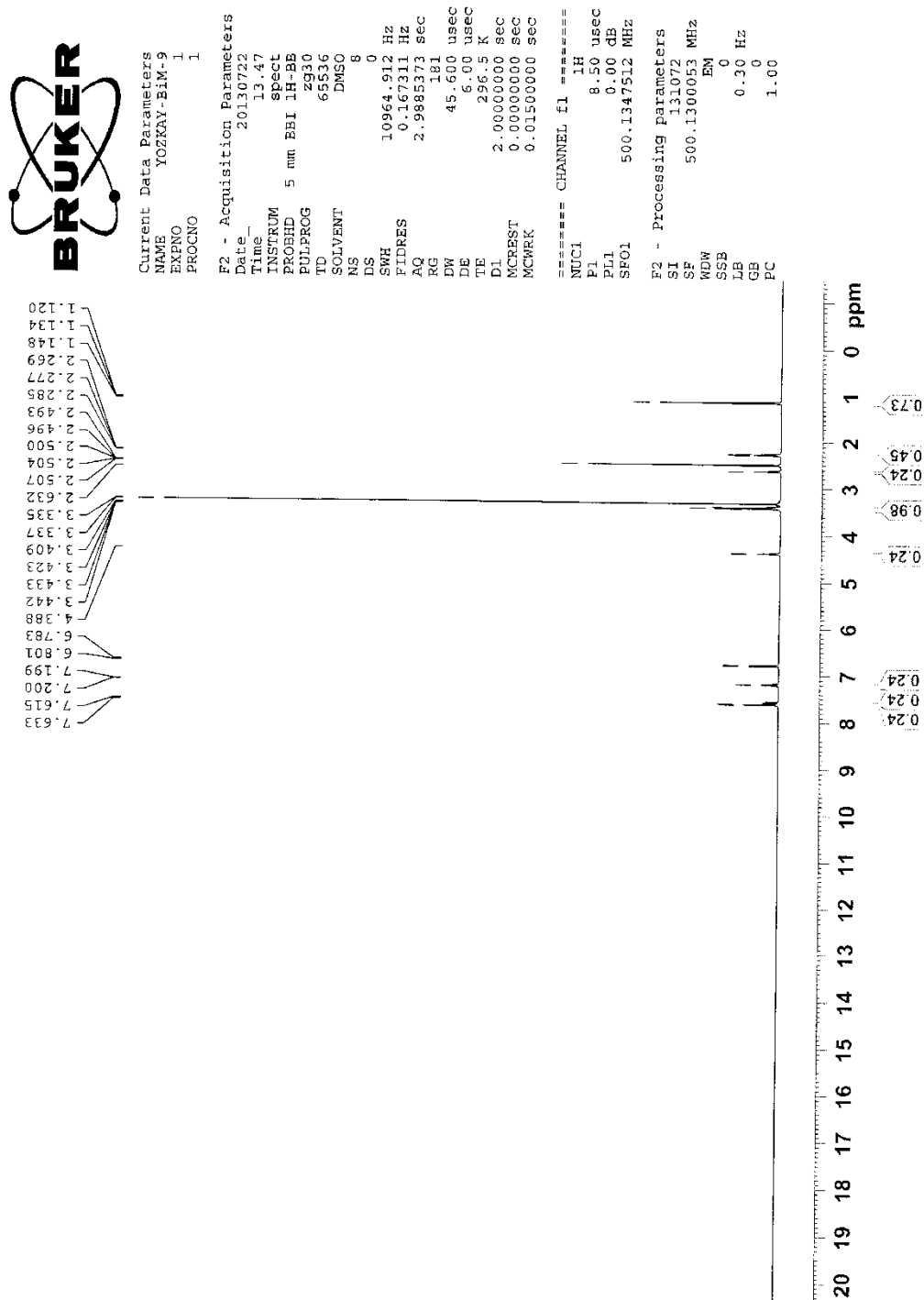


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Is.	DBE
1	45.47	C19 H20 N3 O Br	[M+H] ⁺	386.0833	386.0862	-2.9	-7.51	70.06	11.0

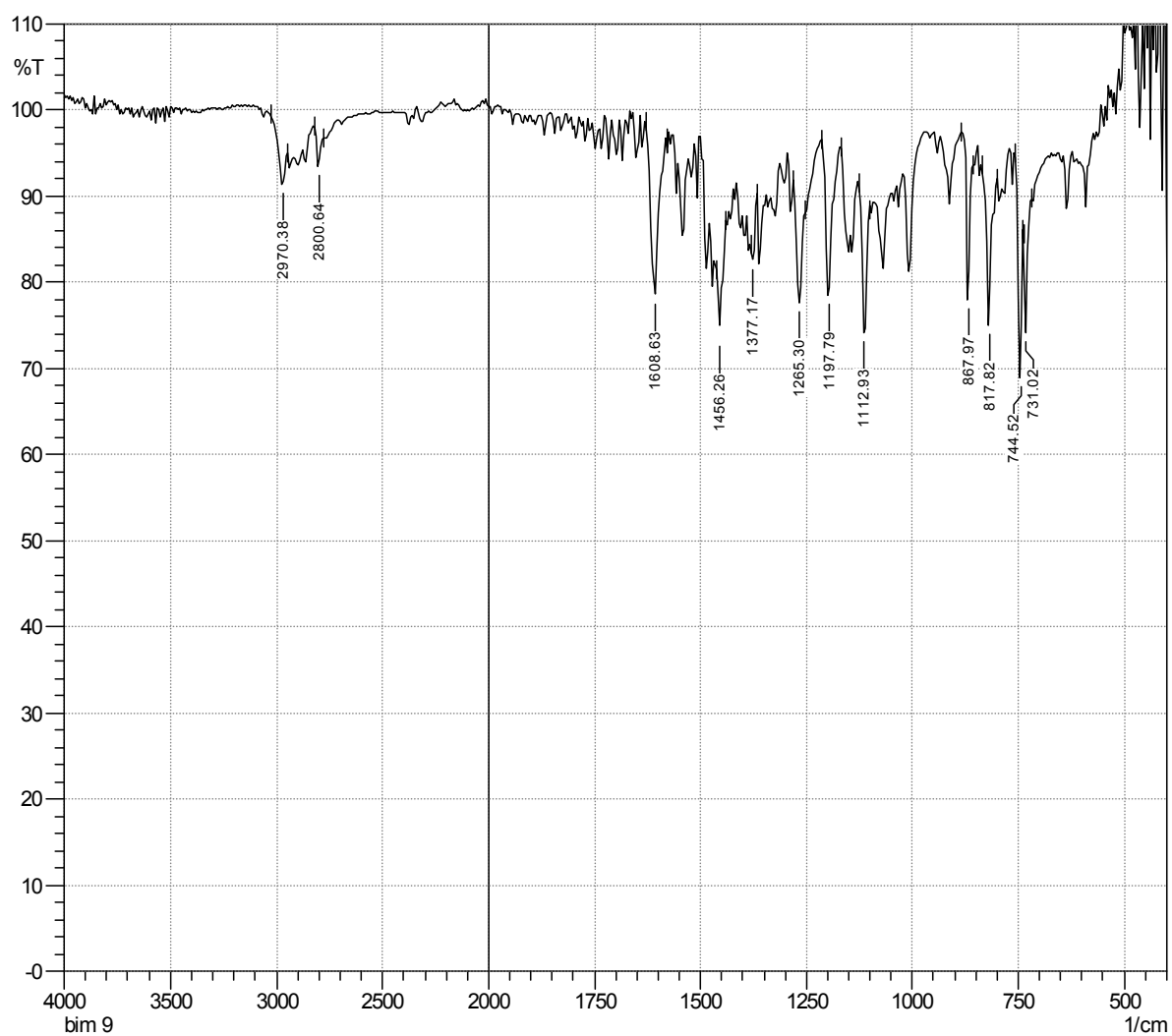
¹³C-NMR spectrum of 2-(4-Diethylaminophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2h**)



¹H-NMR spectrum of 2-(4-Diethylaminophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2h**)



FTIR spectrum of 2-(4-Diethylaminophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2h**)



HRMS spectrum of 2-(4-Diethylaminophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (2h)

Formula Predictor Report - Bim-9_17.lcd

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Data File: C:\LabSolutions\Data\Analiz\Bim series\Bim-9_17.lcd

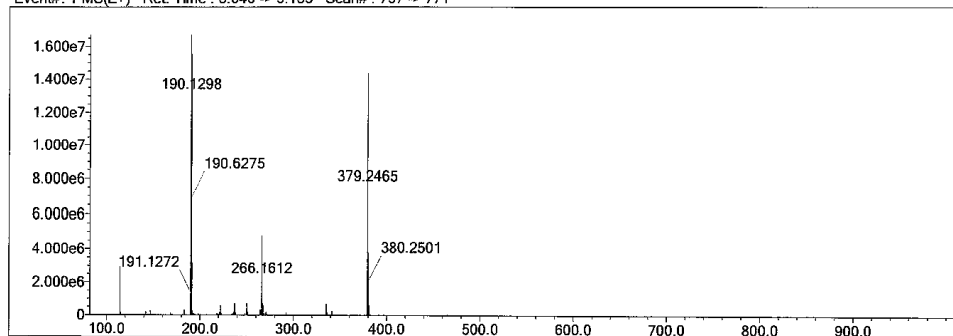
Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use	Adduct
H	1	14	30	O	2	1	5	Cl	1	0	0		H
C	4	12	30	F	1	0	3	Br	1	0	1		
N	3	3	4	S	2	0	0						

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

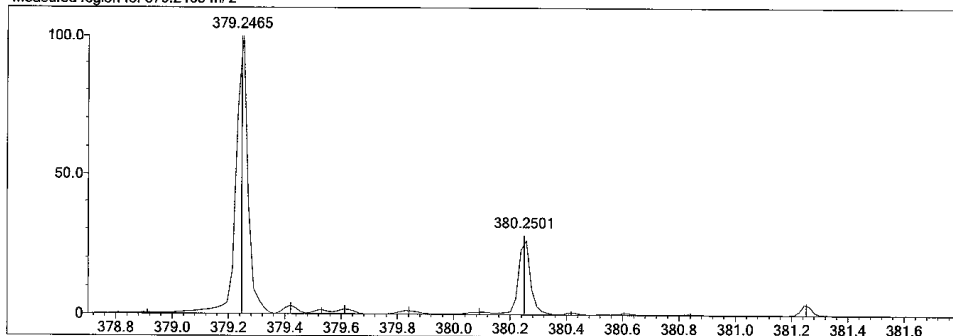
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

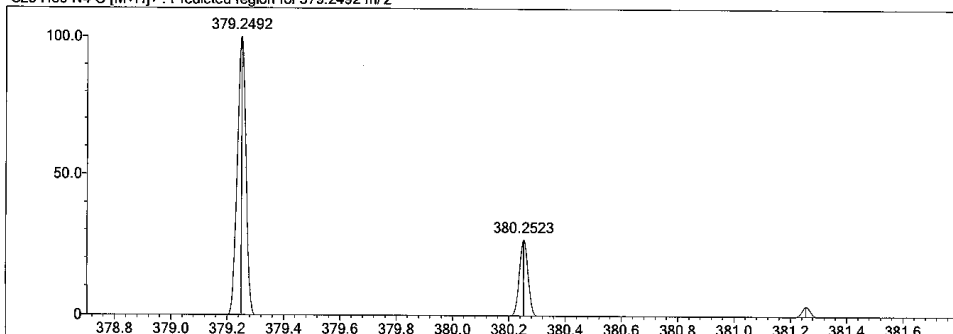
Event#: 1 MS(E+) Ret. Time : 5.040 -> 5.133 Scan# : 757 -> 771



Measured region for 379.2465 m/z

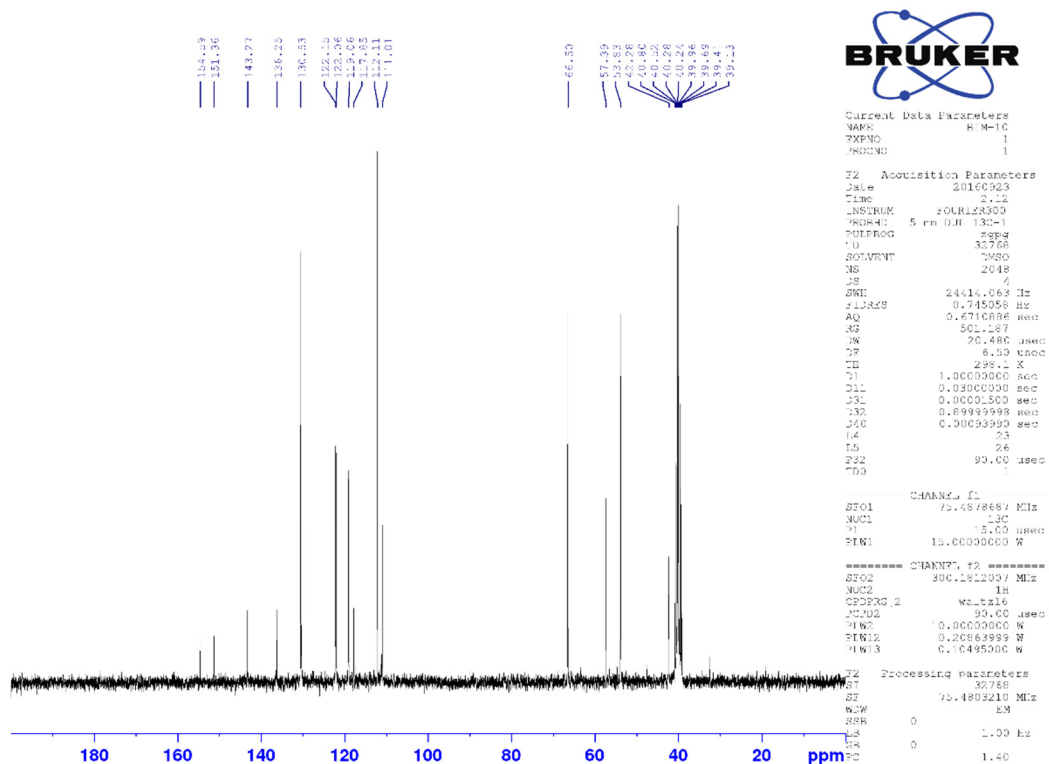


C23 H30 N4 O [M+H]⁺ : Predicted region for 379.2492 m/z

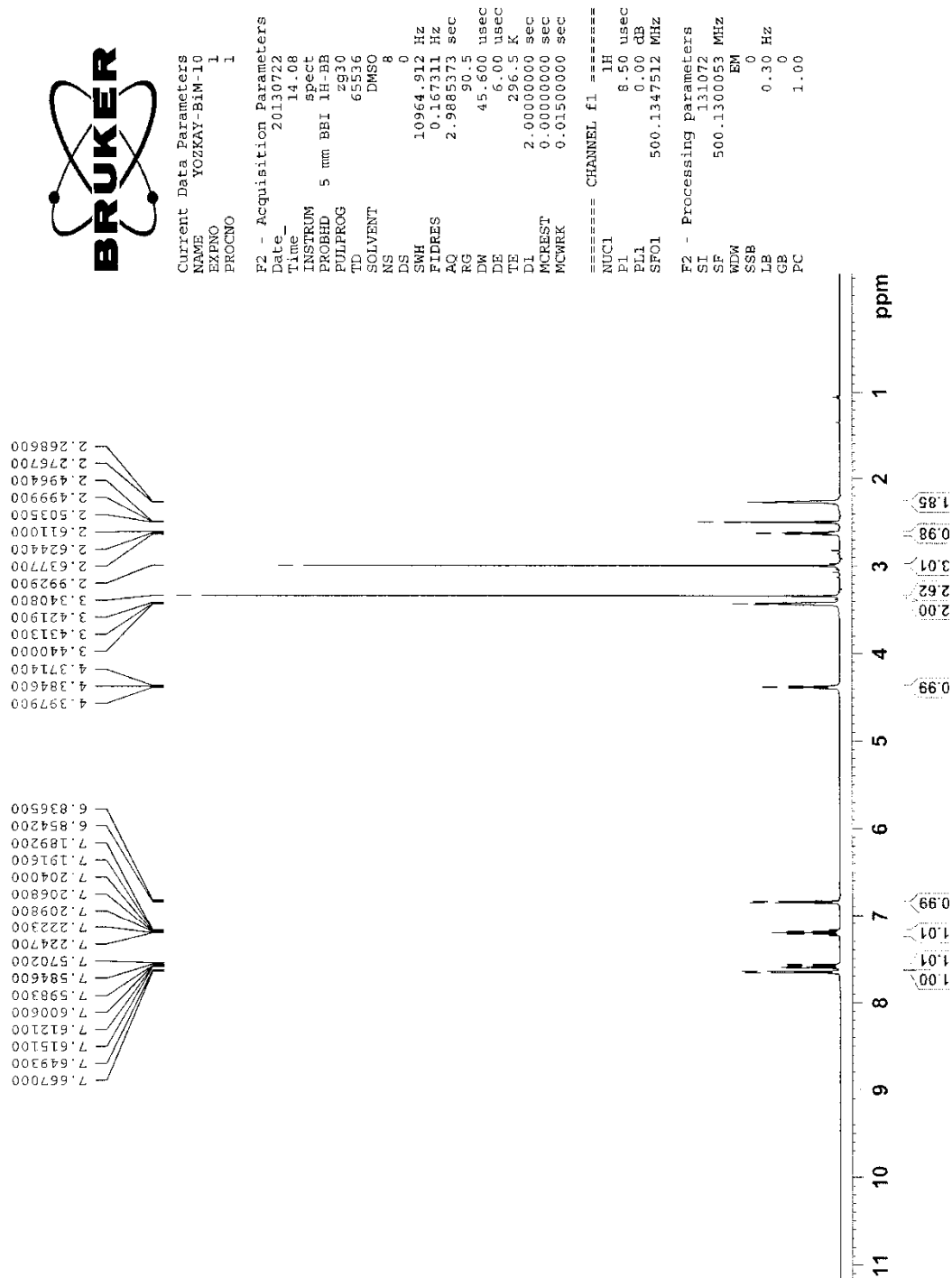


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	68.41	C23 H30 N4 O	[M+H] ⁺	379.2465	379.2492	-2.7	-7.12	99.44	11.0

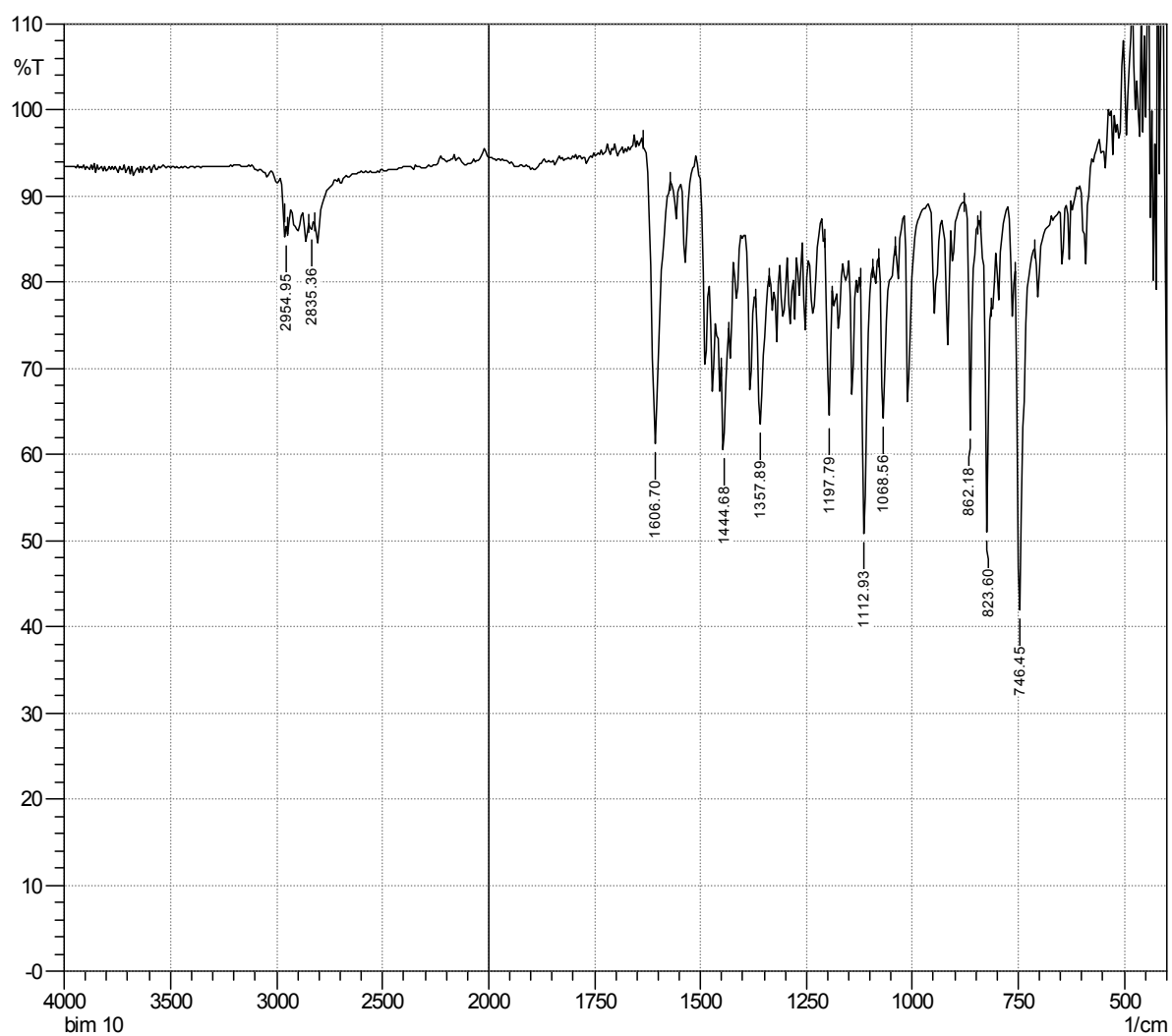
¹³C-NMR spectrum of 2-(4-Dimethylaminophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole
(2i)



¹H-NMR spectrum of 2-(4-Dimethylaminophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (2i)



FTIR spectrum of 2-(4-Dimethylaminophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2i**)



HRMS spectrum of 2-(4-Dimethylaminophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2i**)

Formula Predictor Report - Bim-10_18.lcd

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Data File: C:\LabSolutions\Data\Analiz\Bim series\Bim-10_18.lcd

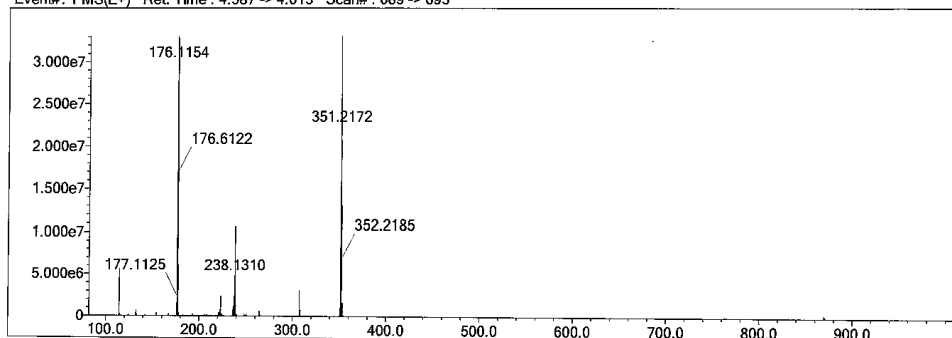
Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use	Adduct
H	1	14	30	O	2	1	5	Cl	1	0	0		H
C	4	12	30	F	1	0	0	Br	1	0	1		
N	3	3	4	S	2	0	0						

Error Margin (ppm): 10
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

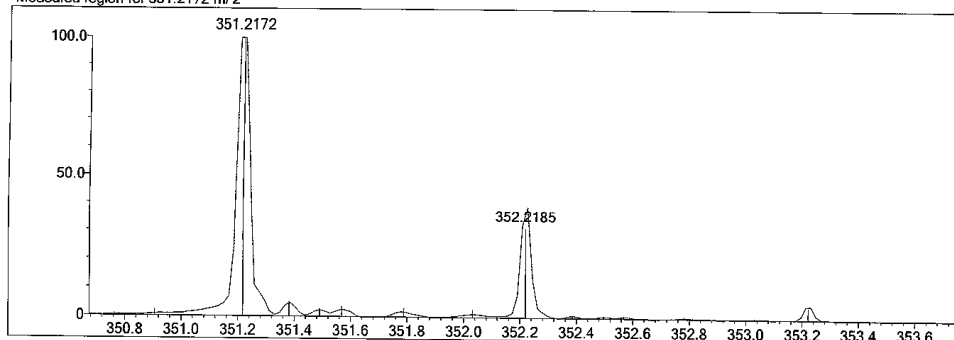
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

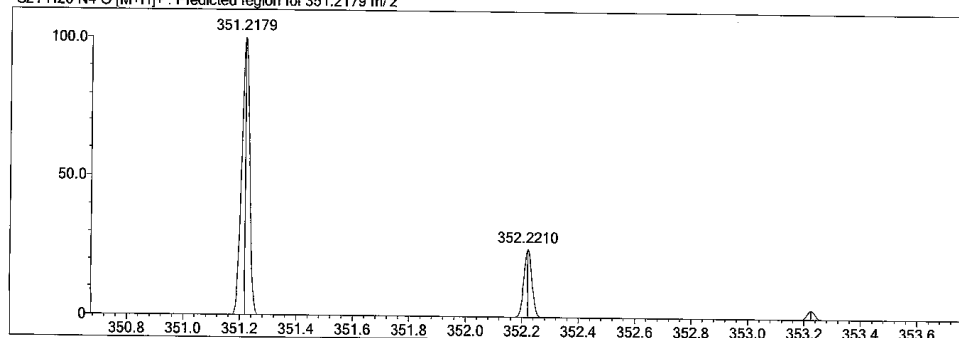
Event#: 1 MS(E+) Ret. Time : 4.587 -> 4.613 Scan#: 689 -> 693



Measured region for 351.2172 m/z

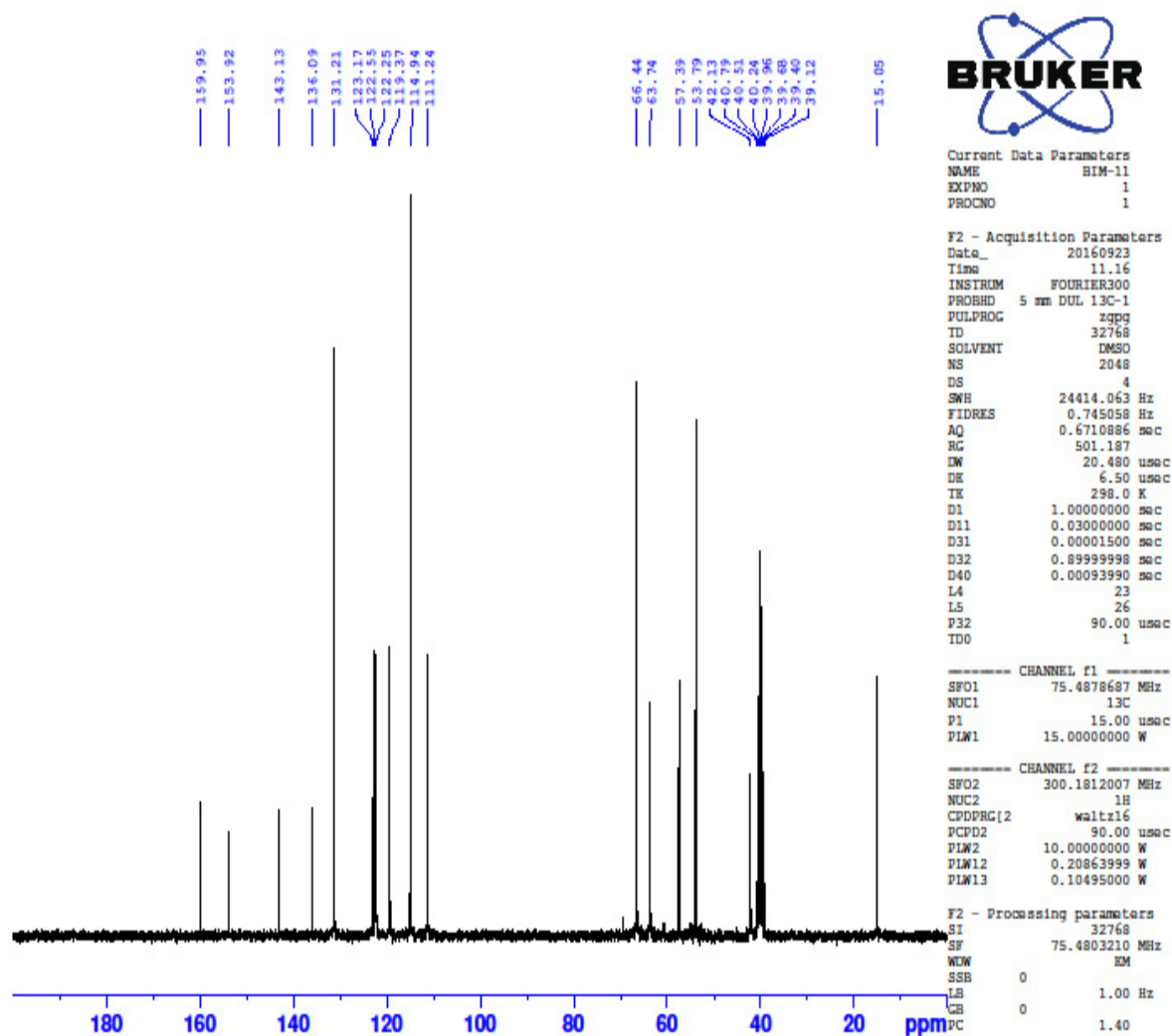


C21 H26 N4 O [M+H]⁺ : Predicted region for 351.2179 m/z

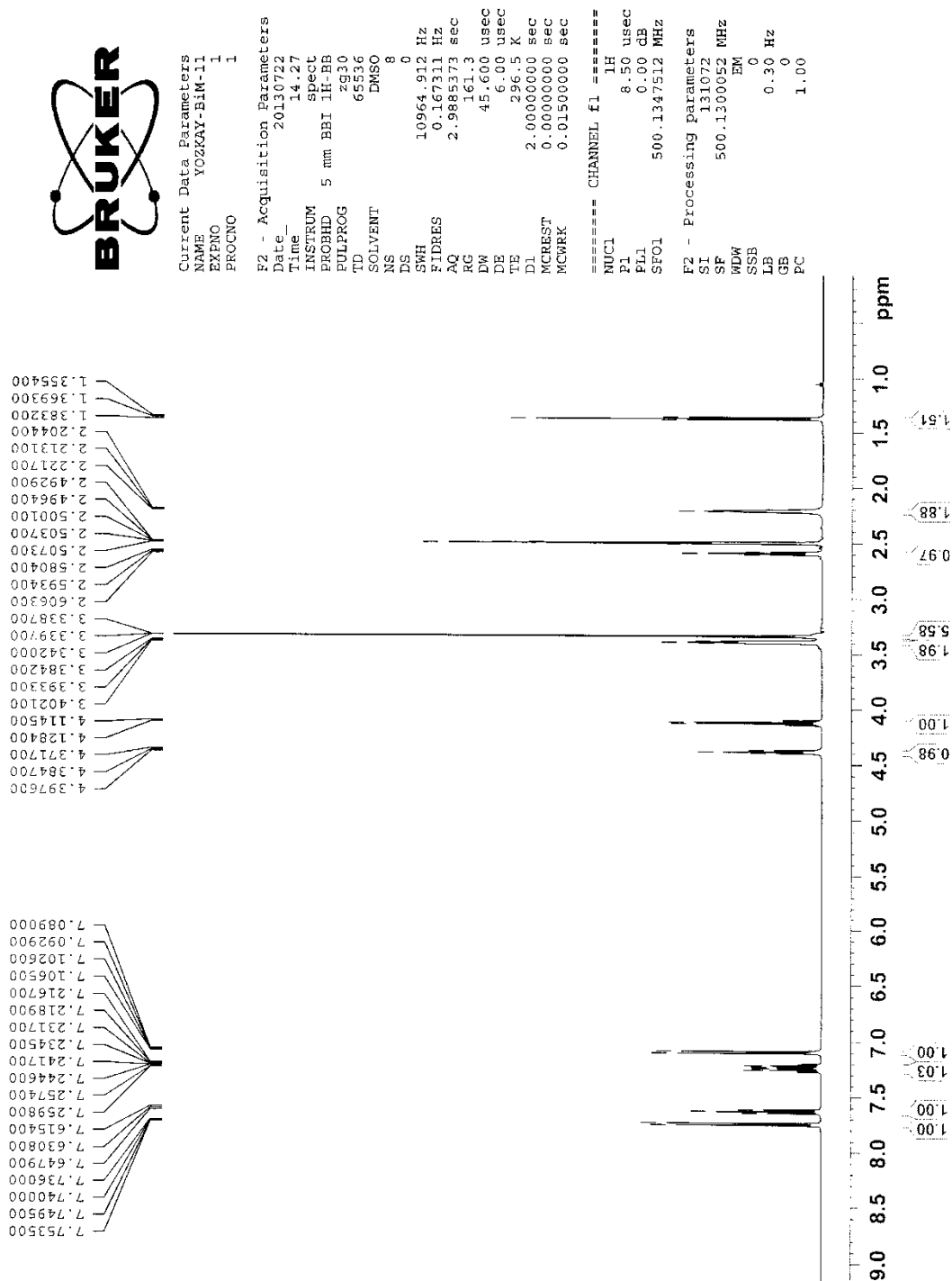


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	70.70	C21 H26 N4 O	[M+H] ⁺	351.2172	351.2179	-0.7	-1.99	72.49	11.0

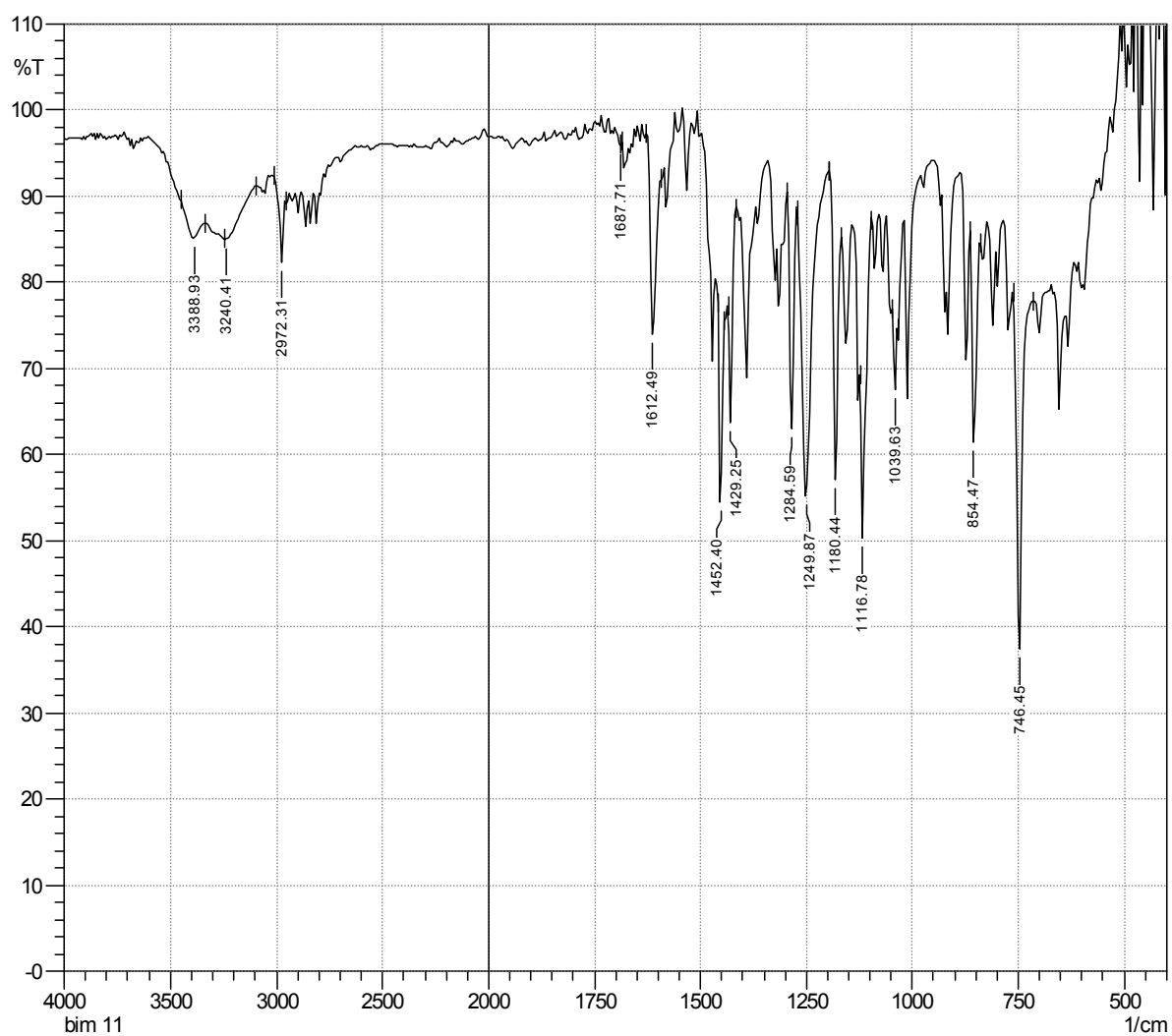
¹³C-NMR spectrum of 2-(4-Ethoxyphenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2j**)



¹H-NMR spectrum of 2-(4-Ethoxyphenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (2j)



FTIR spectrum of 2-(4-Ethoxyphenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2j**)



HRMS spectrum of 2-(4-Ethoxyphenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (2j)

Formula Predictor Report - Bim-11_01.lcd

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Data File: C:\LabSolutions\ Data\Analiz\Bim series\ Bim-11_01.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use	Adduct
H	1	14	30	O	2	1	5	Cl	1	0	0		H
C	4	12	30	F	1	0	0	Br	1	0	1		
N	3	3	4	S	2	0	0						

Error Margin (ppm): 15

DBE Range: -2.0 - 1000.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: no

Max Isotopes: 3

Isotope RI (%): 1.00

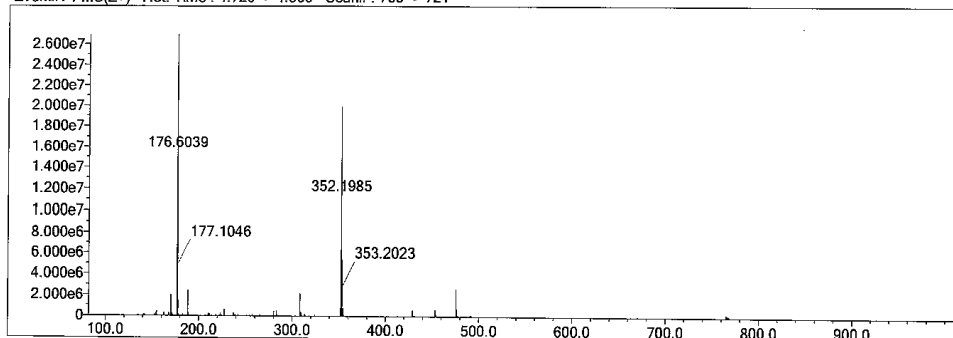
Isotope Res: 10000

MSn Iso RI (%): 10.00

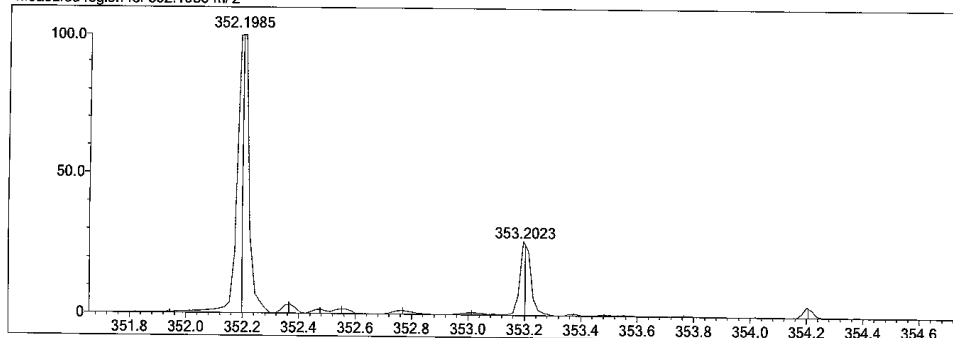
MSn Logic Mode: AND

Max Results: 500

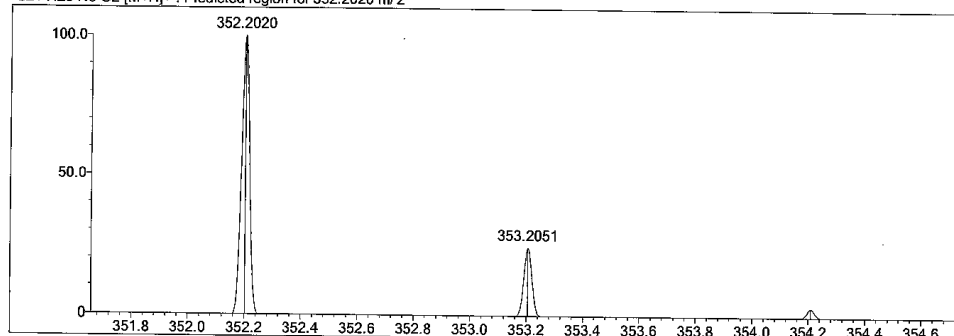
Event#: 1 MS(E+) Ret. Time : 4.720 -> 4.800 Scan#: 709 -> 721



Measured region for 352.1985 m/z

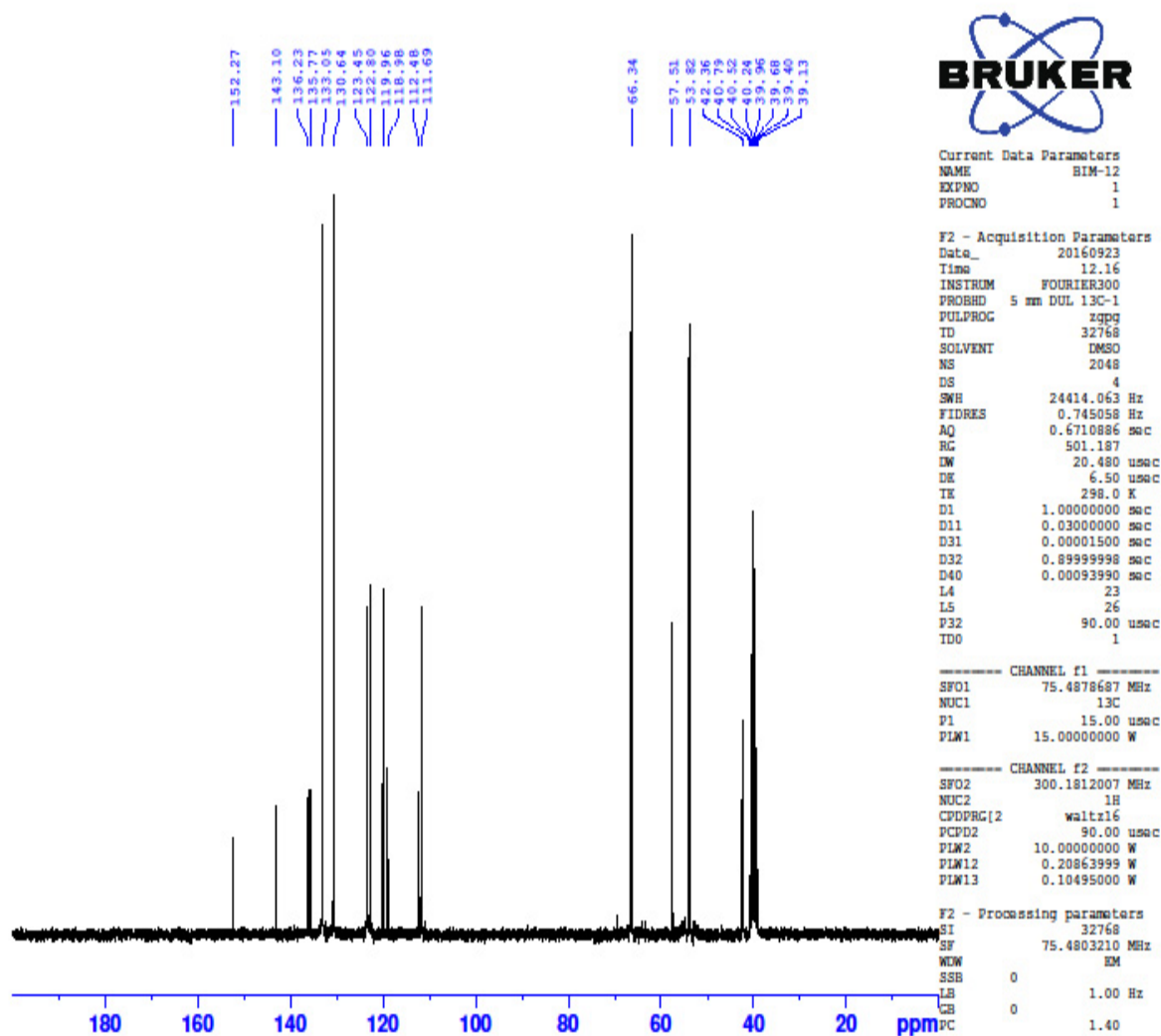


C21 H25 N3 O2 [M+H]⁺ : Predicted region for 352.2020 m/z

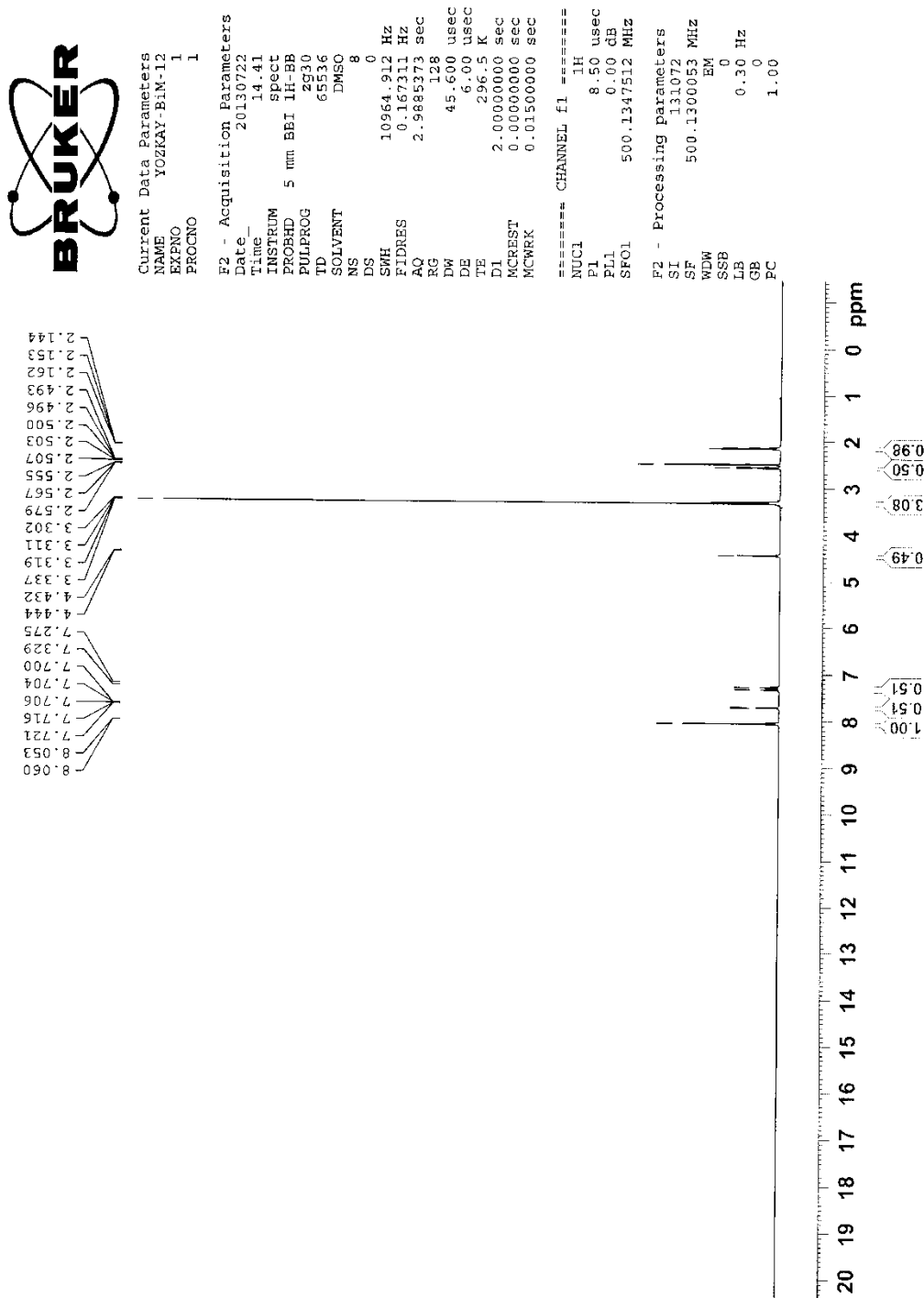


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Is	DBE
1	35.22	C21 H25 N3 O2	[M+H] ⁺	352.1985	352.2020	-3.5	-9.94	86.76	11.0

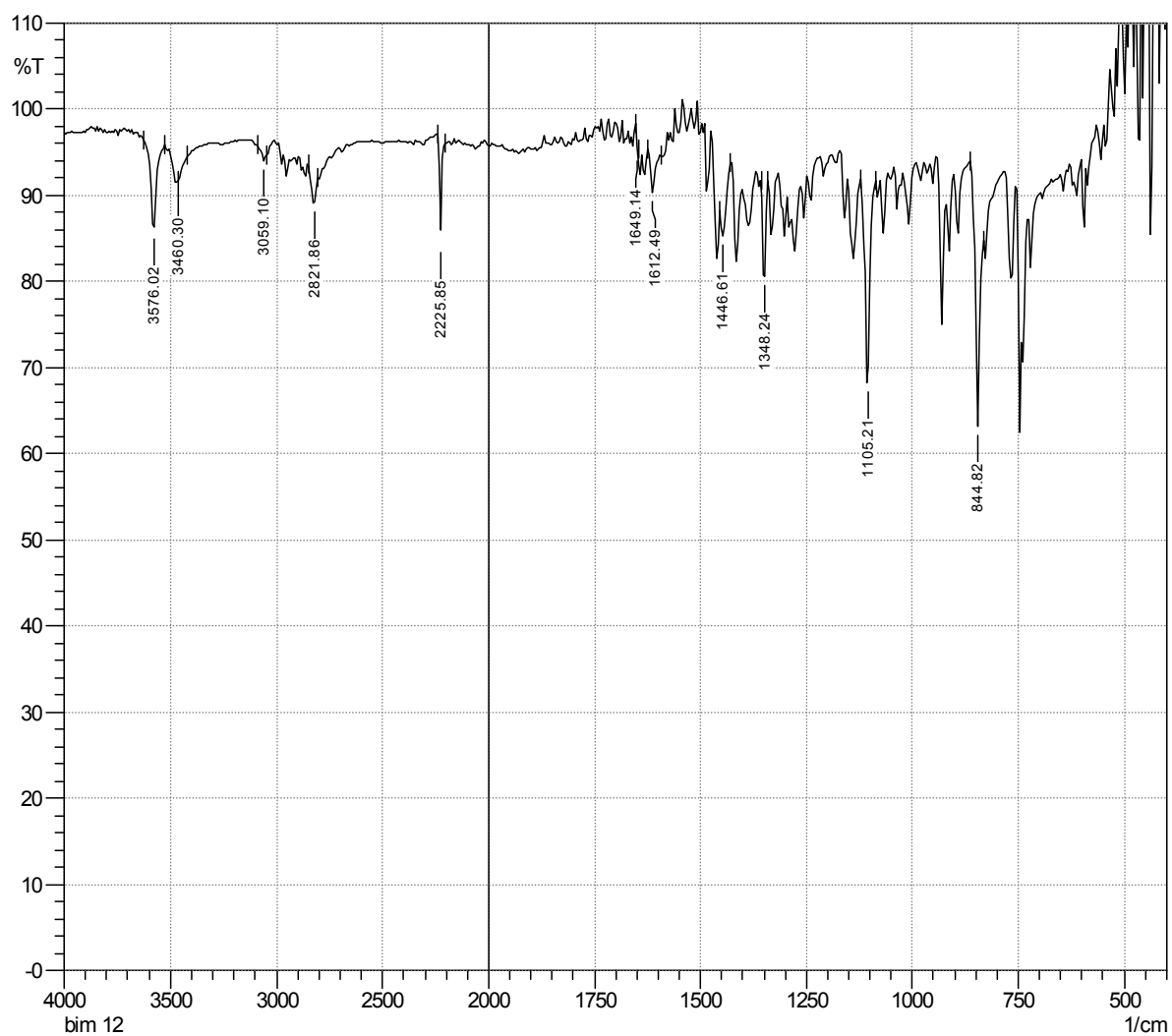
¹³C-NMR of 2-(4-Cyanophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2k**)



¹H-NMR spectrum of 2-(4-Cyanophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2k**)



FTIR spectrum of 2-(4-Cyanophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2k**)



HRMS spectrum of 2-(4-Cyanophenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2k)

Formula Predictor Report - Bim-12_20.lcd

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Data File: C:\LabSolutions\1 Data\Analiz\Bim series\Bim-12_20.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	14	30	O	2	1	5	Cl	1	0	0	H
C	4	12	30	F	1	0	0	Br	1	0	1	
N	3	3	4	S	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: -2.0 - 1000.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

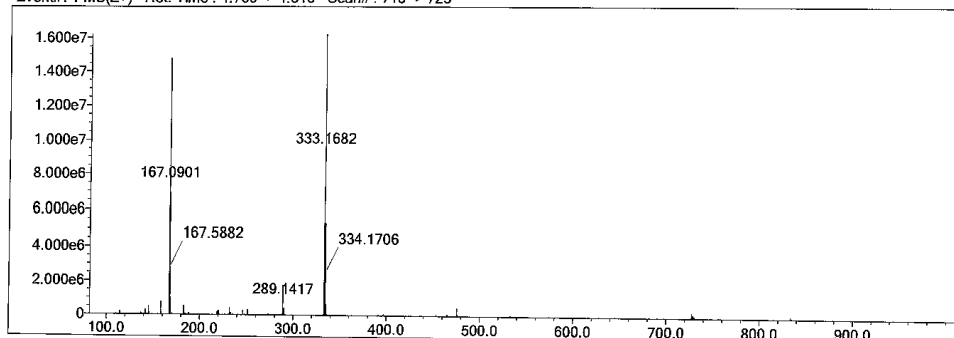
Electron Ions: both

Use MSn Info: no

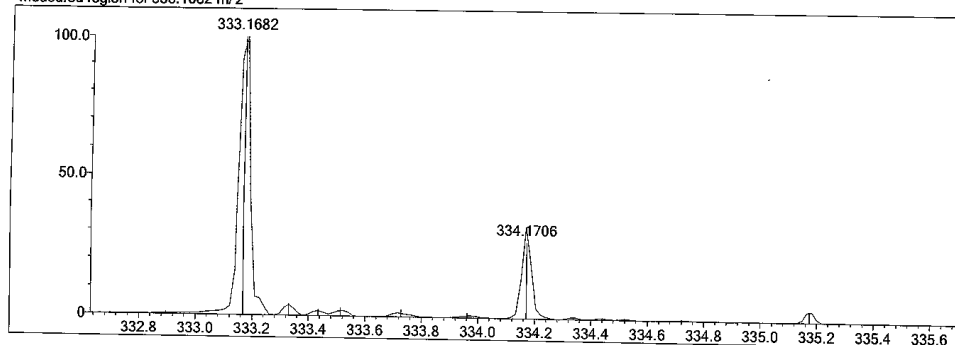
Isotope Res: 10000

Max Results: 500

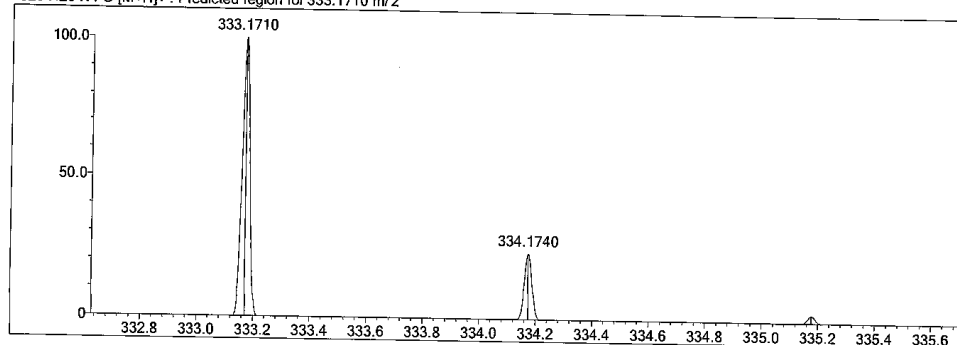
Event#: 1 MS(E+) Rel. Time : 4.760 -> 4.813 Scan#: 715 -> 723



Measured region for 333.1682 m/z

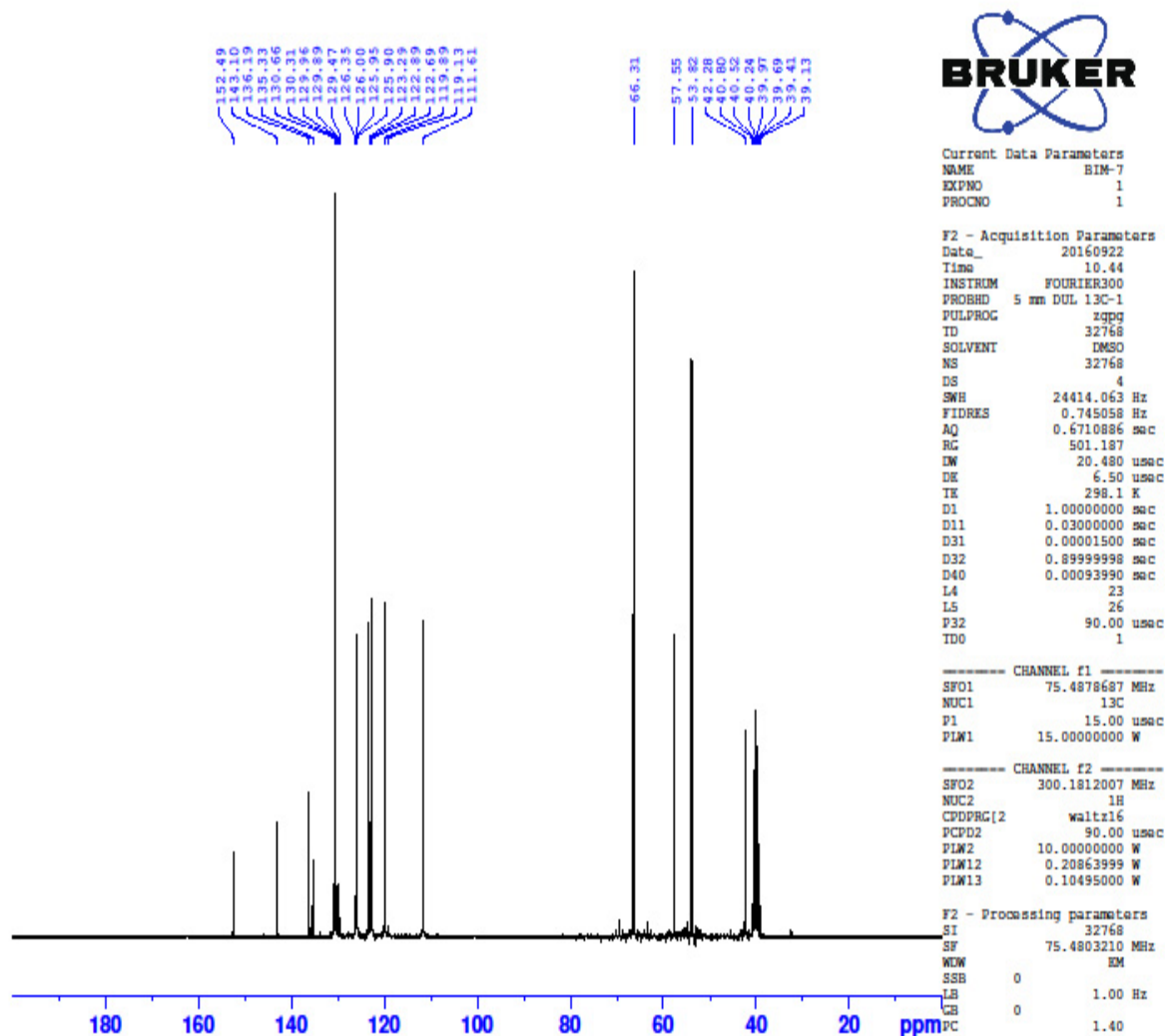


C20 H20 N4 O [M+H]⁺ : Predicted region for 333.1710 m/z

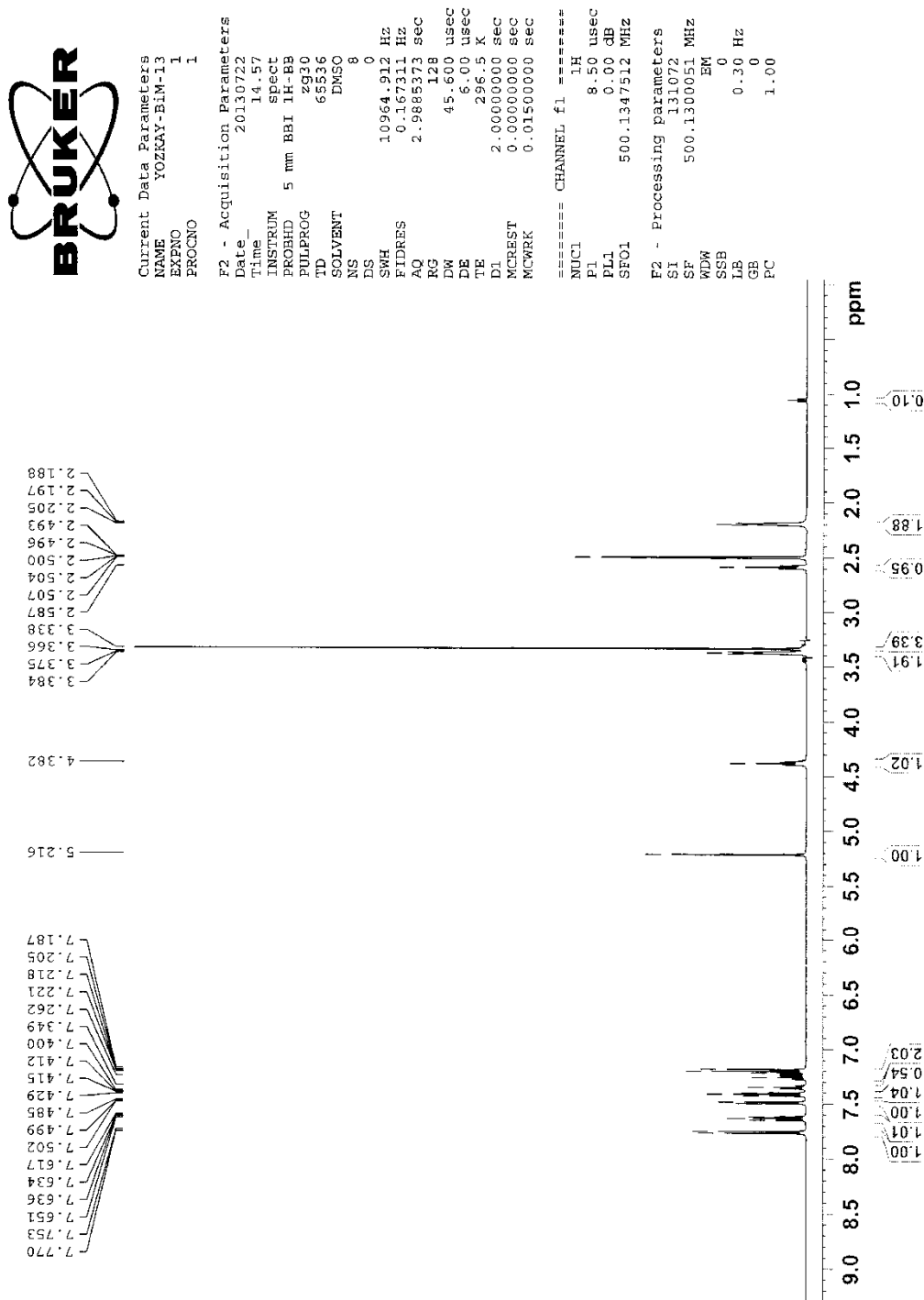


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	49.12	C20 H20 N4 O	[M+H] ⁺	333.1682	333.1710	-2.8	-8.40	87.71	13.0

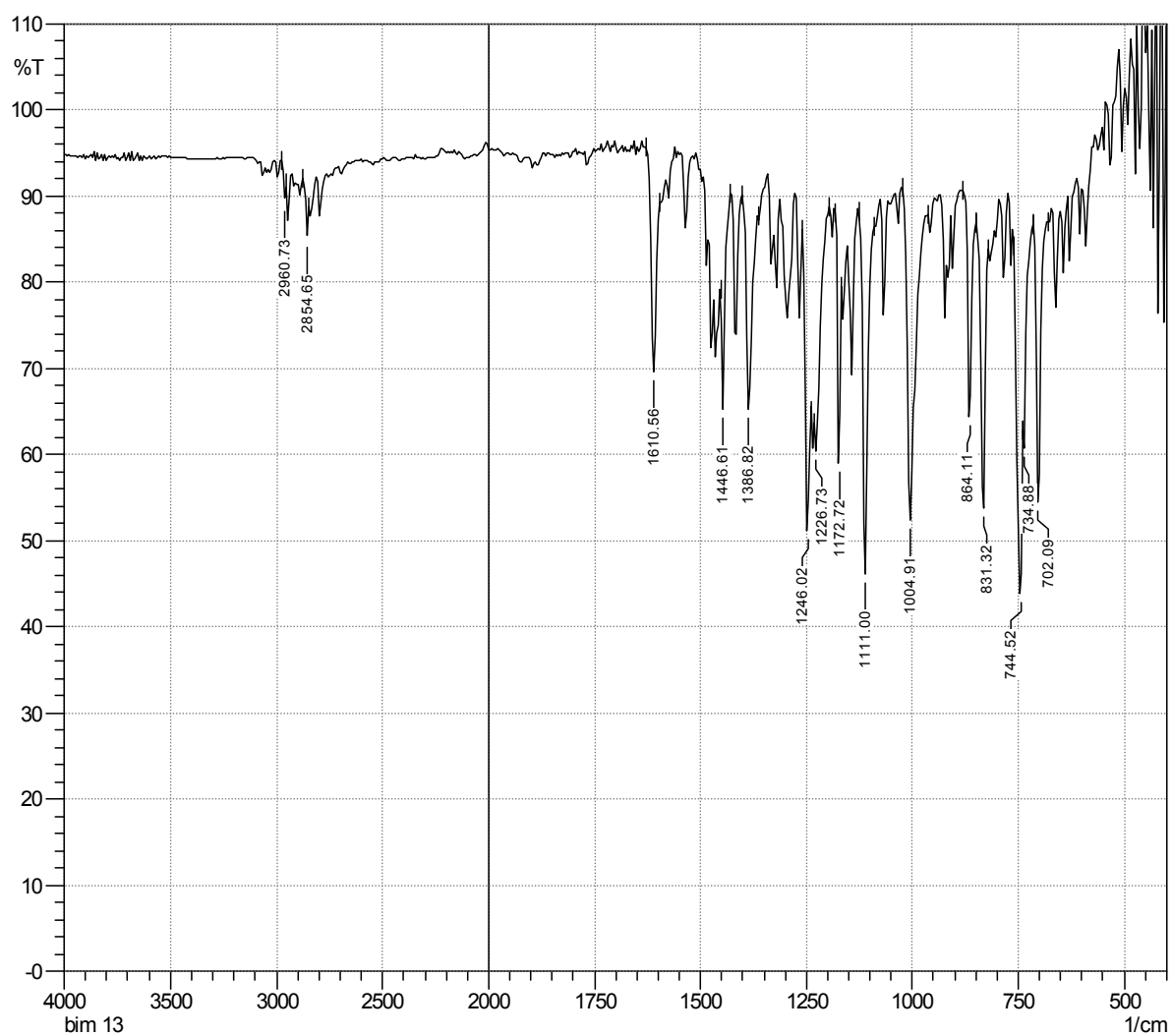
¹³C-NMR spectrum of 2-(4-Trifluoromethylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole
(2I)



¹H-NMR spectrum of 2-(4-Trifluoromethylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2I)



FTIR spectrum of 2-(4-Trifluoromethylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2l**)



HRMS spectrum of 2-(4-Trifluoromethylphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2I)

Formula Predictor Report - Bim-13_21.lcd

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Data File: C:\LabSolutions\Data\Analiz\Bim series\Bim-13_21.lcd

Elm	Val	Min	Max	Elm	Val	Min	Max	Elm	Val	Min	Max	Use Adduct
H	1	14	30	O	2	1	5	Cl	1	0	0	H
C	4	12	30	F	1	0	0	Br	1	0	1	
N	3	3	4	S	2	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: 3

MSn Iso RI (%): 10.00

DBE Range: -2.0 - 1000.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

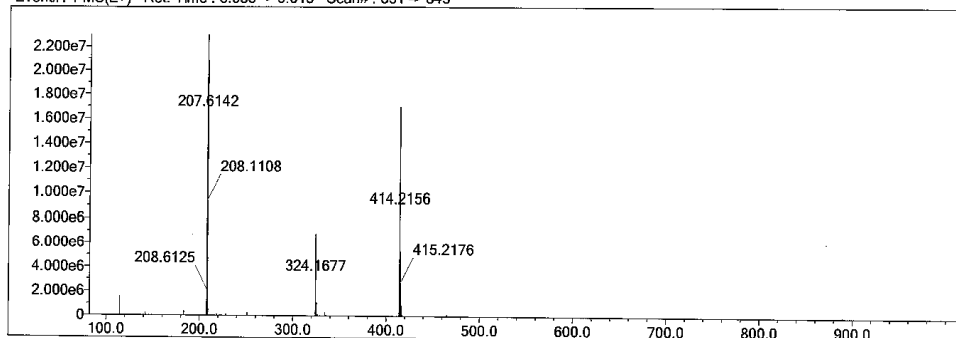
Electron Ions: both

Use MSn Info: no

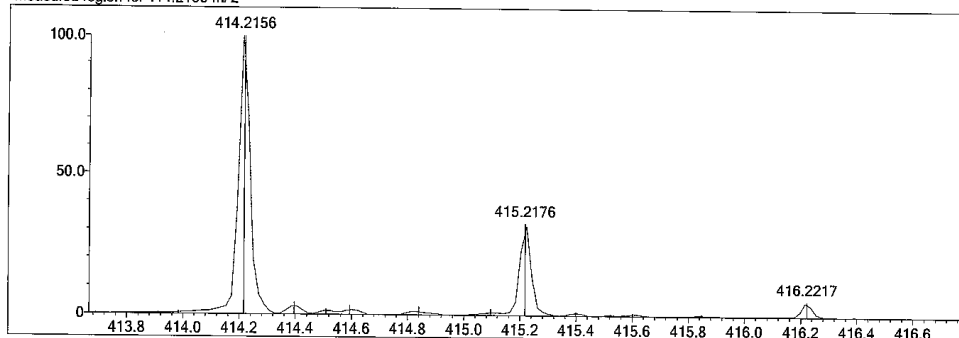
Isotope Res: 10000

Max Results: 500

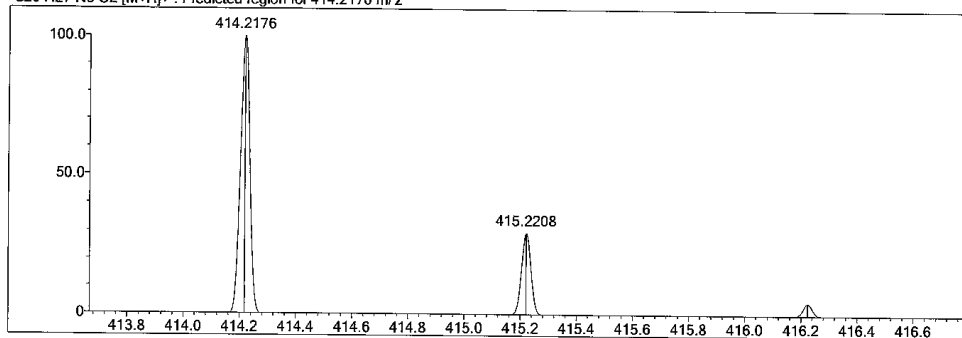
Event#: 1 MS(E+) Ret. Time : 5.533 -> 5.613 Scan#: 831 -> 843



Measured region for 414.2156 m/z



C26 H27 N3 O2 [M+H]⁺ : Predicted region for 414.2176 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	67.55	C26 H27 N3 O2	[M+H] ⁺	414.2156	414.2176	-2.0	-4.83	74.71	15.0

13C NMR Spectrum (DMSO-d₆)

Chemical Shifts (ppm): 152.68, 148.23, 145.21, 143.17, 136.06, 131.85, 130.88, 128.44, 127.25, 125.24, 123.24, 121.42, 119.73, 118.83, 115.43, 111.48, 66.32, 57.53, 53.79, 42.11, 40.79, 40.52, 40.24, 39.96, 39.68, 39.40, 39.12.

Current Data Parameters:

NAME	BIM-14
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters:

Date_	20160923
Time	14.17
INSTRUM	FOURIER300
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg
TD	32768
SOLVENT	DMSO
NS	2048
DS	4
SWH	24414.063 Hz
FIDRES	0.745058 Hz
AQ	0.6710886 sec
RG	501.187
DW	20.480 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
D11	0.03000000 sec
D31	0.00001500 sec
D32	0.89999998 sec
D40	0.00093990 sec
L4	23
L5	26
P32	90.00 usec
TDO	1

Channel f1:

SFO1	75.4878687 MHz
NUC1	13C
P1	15.00 usec
PLW1	15.00000000 W

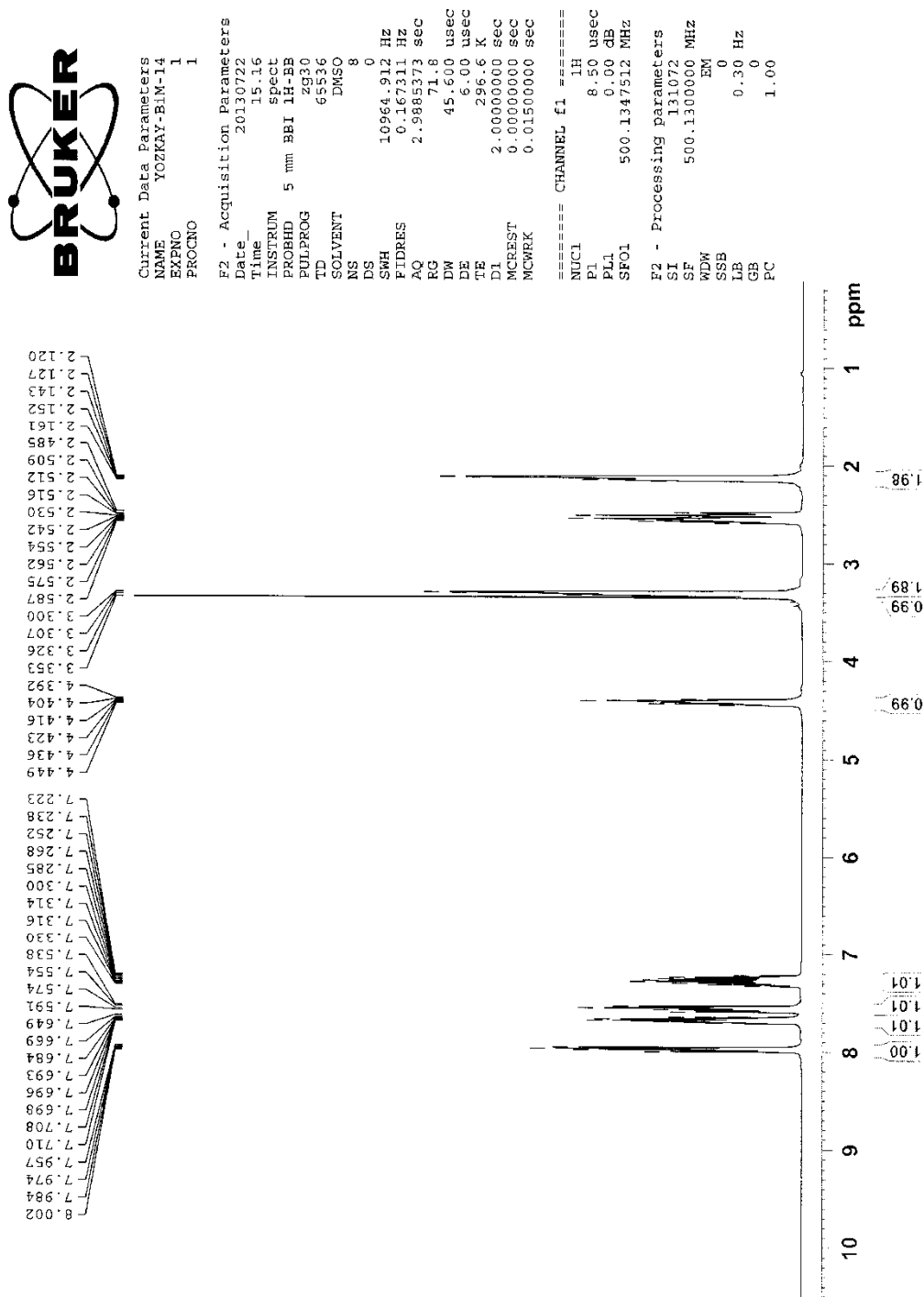
Channel f2:

SFO2	300.1812007 MHz
NUC2	1H
CPDPRG[2]	waltz16
PCPD2	90.00 usec
PLW2	10.00000000 W
PLW12	0.20863999 W
PLW13	0.10495000 W

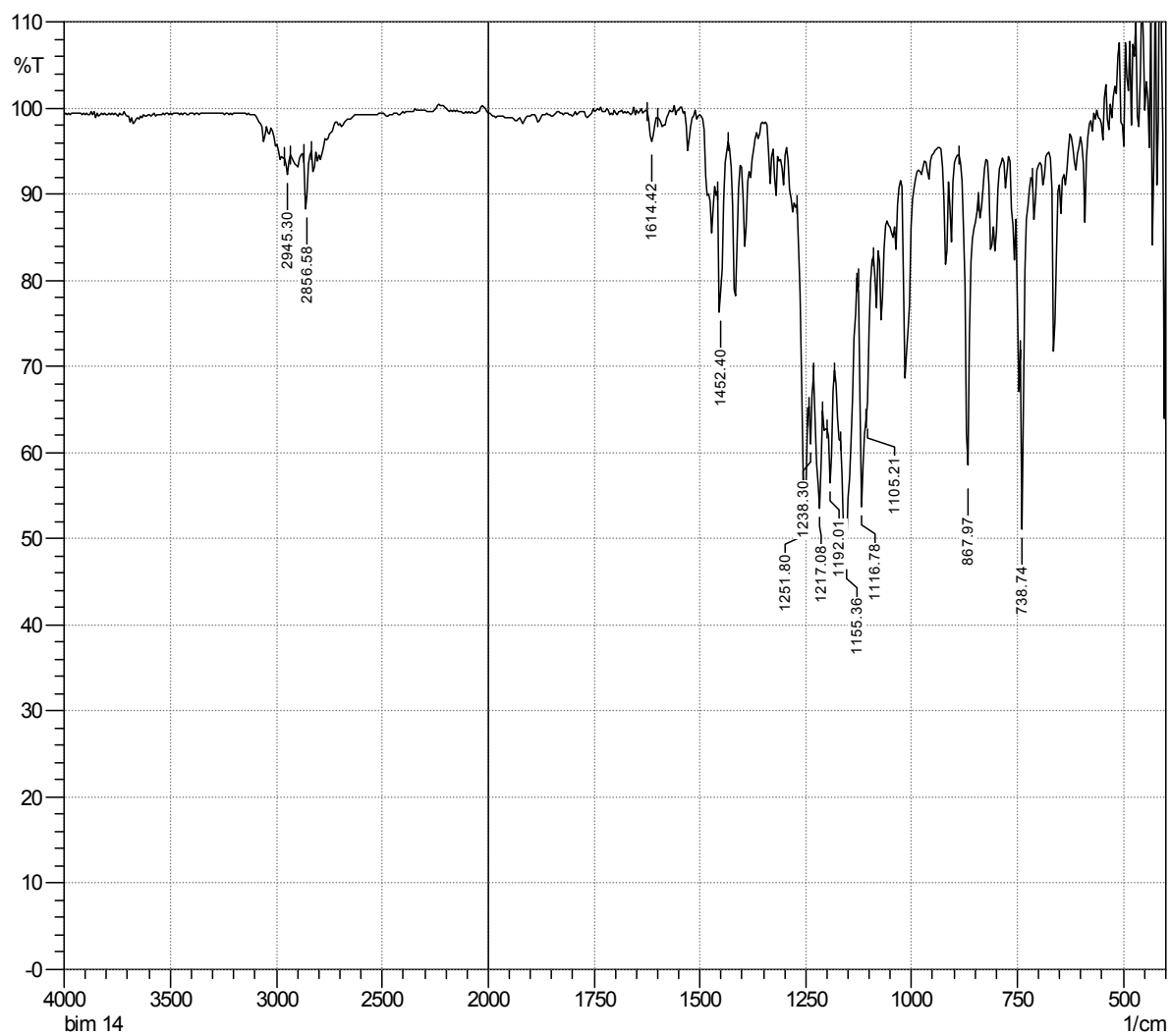
F2 - Processing parameters:

SI	32768
SF	75.4803210 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

¹H-NMR spectrum of 2-(4-Trifluoromethoxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2m)



FTIR spectrum of 2-(4-Trifluoromethoxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole
(2m)



HRMS spectrum of 2-(4-Trifluoromethoxyphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2m)

Formula Predictor Report - Bim-14_22.lcd

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Data File: C:\LabSolutions\Data\Analiz\Bim series\Bim-14_22.lcd

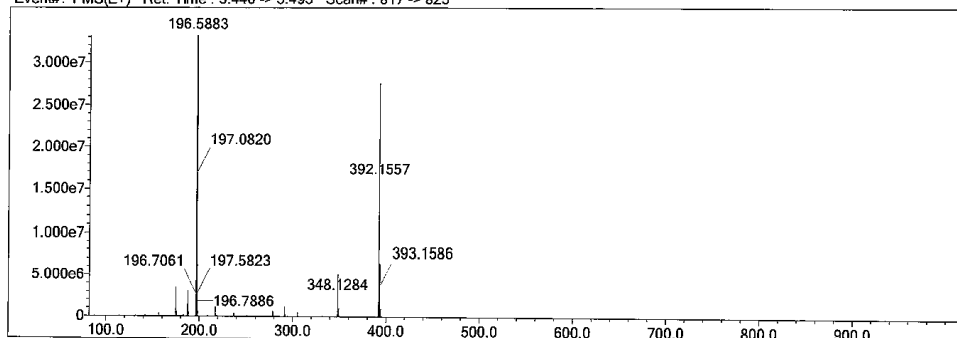
Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	14	30	O	2	2	3	Cl	1	0	0	H
C	4	12	30	F	1	0	3	Br	1	0	0	
N	3	3	4	S	2	0	0					

Error Margin (ppm): 15
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

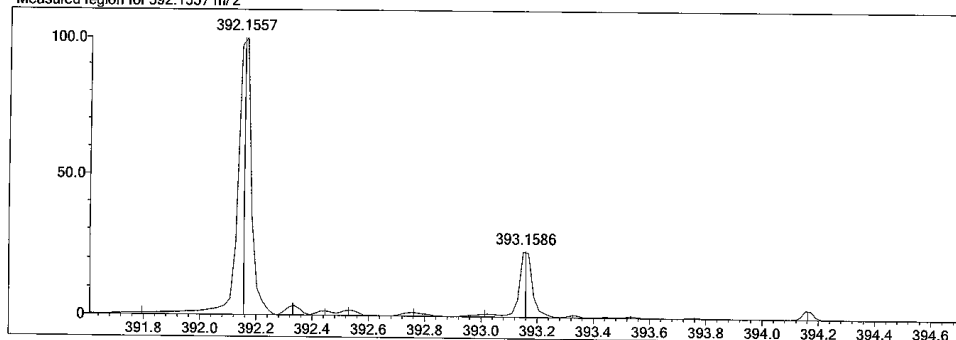
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

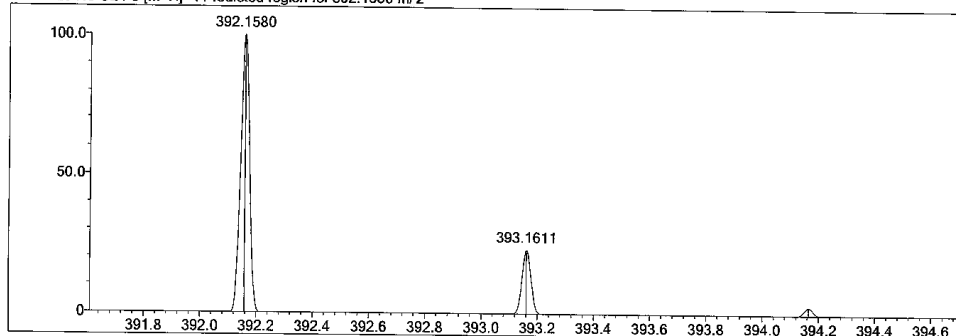
Event#: 1 MS(E+) Ret. Time : 5.440 -> 5.493 Scan#: 817 -> 825



Measured region for 392.1557 m/z

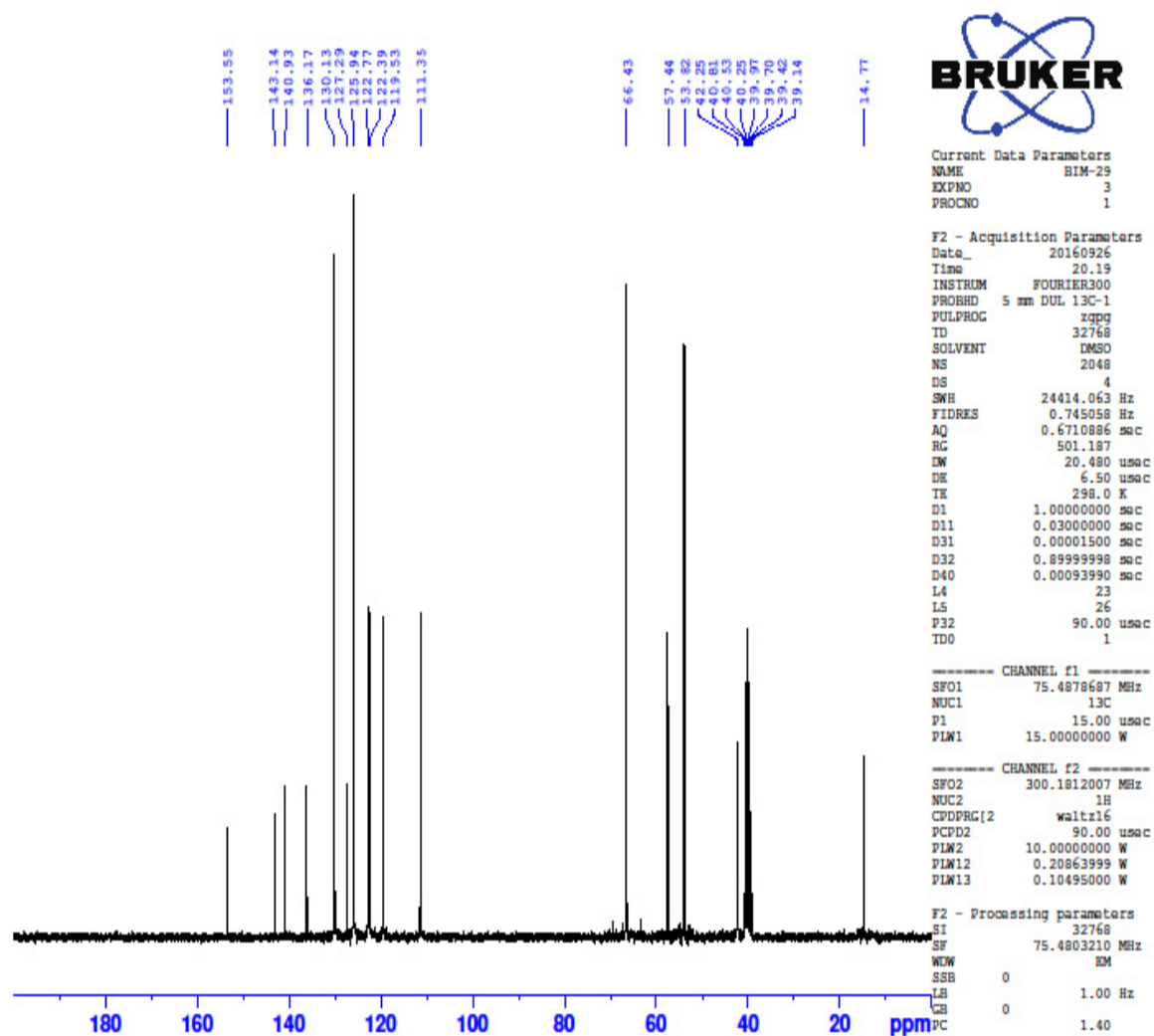


C20 H20 N3 O2 F3 [M+H]⁺ : Predicted region for 392.1580 m/z

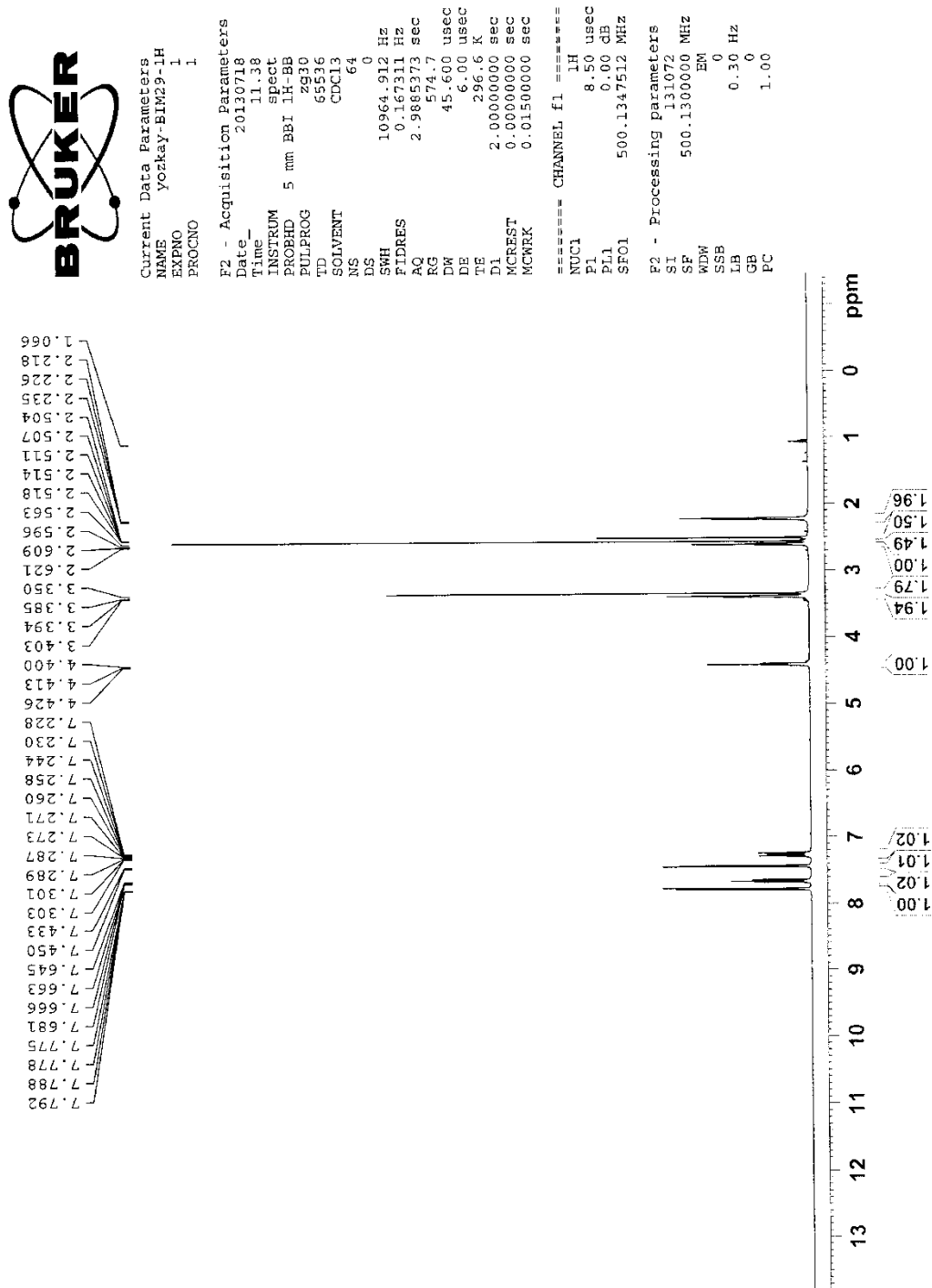


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	81.30	C20 H20 N3 O2 F3	[M+H] ⁺	392.1557	392.1580	-2.3	-5.87	100.00	11.0

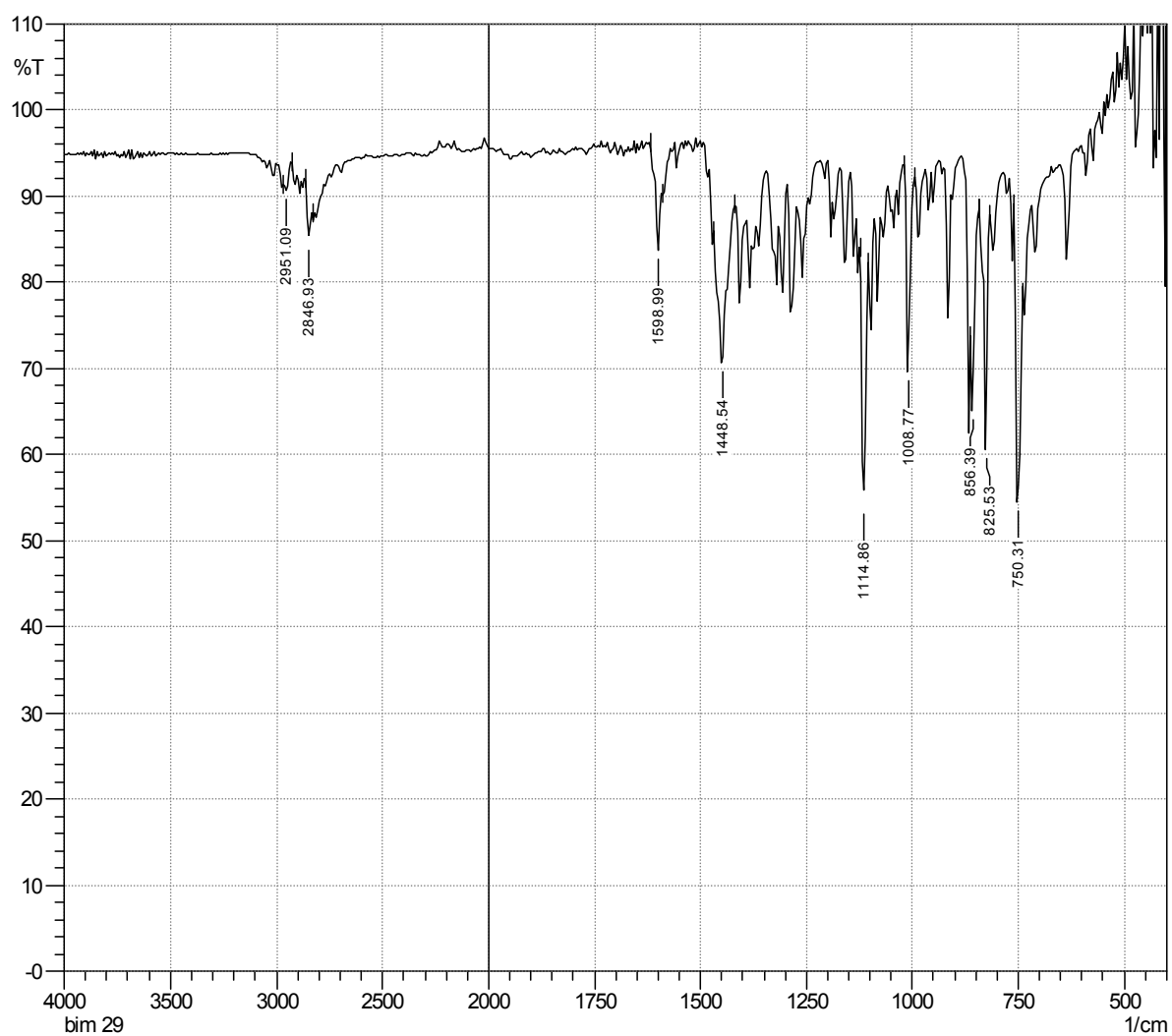
^{13}C -NMR spectrum of 2-(4-Methylthiophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2n**)



¹H-NMR spectrum of 2-(4-Methylthiophenyl)-1- [2-(morpholin-4-yl) ethyl]-1H-benzimidazole (2n)



FTIR spectrum of 2-(4-Methylthiophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (**2n**)



HRMS spectrum of 2-(4-Methylthiophenyl)-1-[2-(morpholin-4-yl) ethyl]-1H-benzimidazole (2n)

Formula Predictor Report - Bim-29_01.lcd

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Data File: C:\LabSolutions\Data\Analyze\Bim series\Bim-29_01.lcd

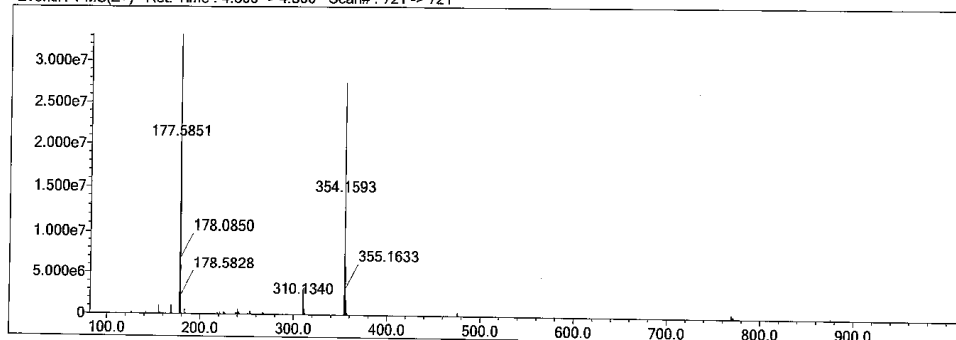
Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	14	30	O	2	1	3	Cl	1	0	0	H
C	4	12	30	F	1	0	0	Br	1	0	0	
N	3	3	4	S	2	1	1					

Error Margin (ppm): 15
 HC Ratio: unlimited
 Max Isotopes: 3
 MSn Iso RI (%): 10.00

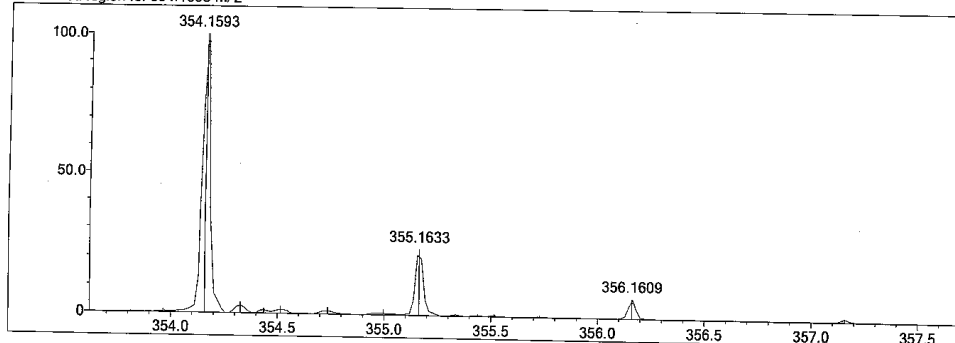
DBE Range: -2.0 - 1000.0
 Apply N Rule: yes
 Isotope RI (%): 1.00
 MSn Logic Mode: AND

Electron Ions: both
 Use MSn Info: no
 Isotope Res: 10000
 Max Results: 500

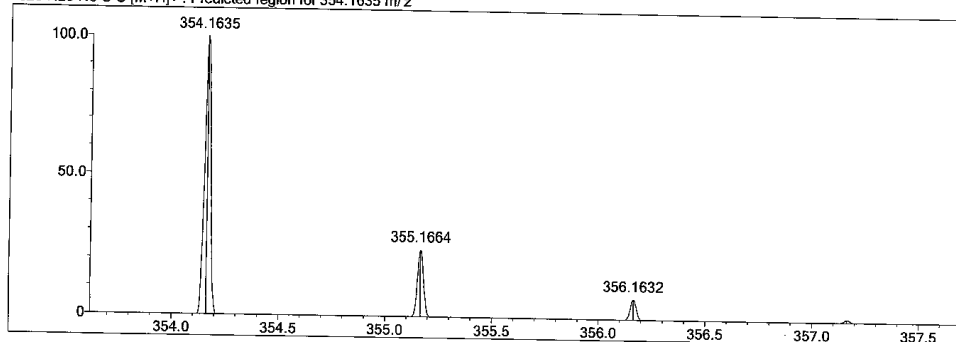
Event#: 1 MS(E+) Ret. Time: 4.800 -> 4.800 Scan#: 721 -> 721



Measured region for 354.1593 m/z

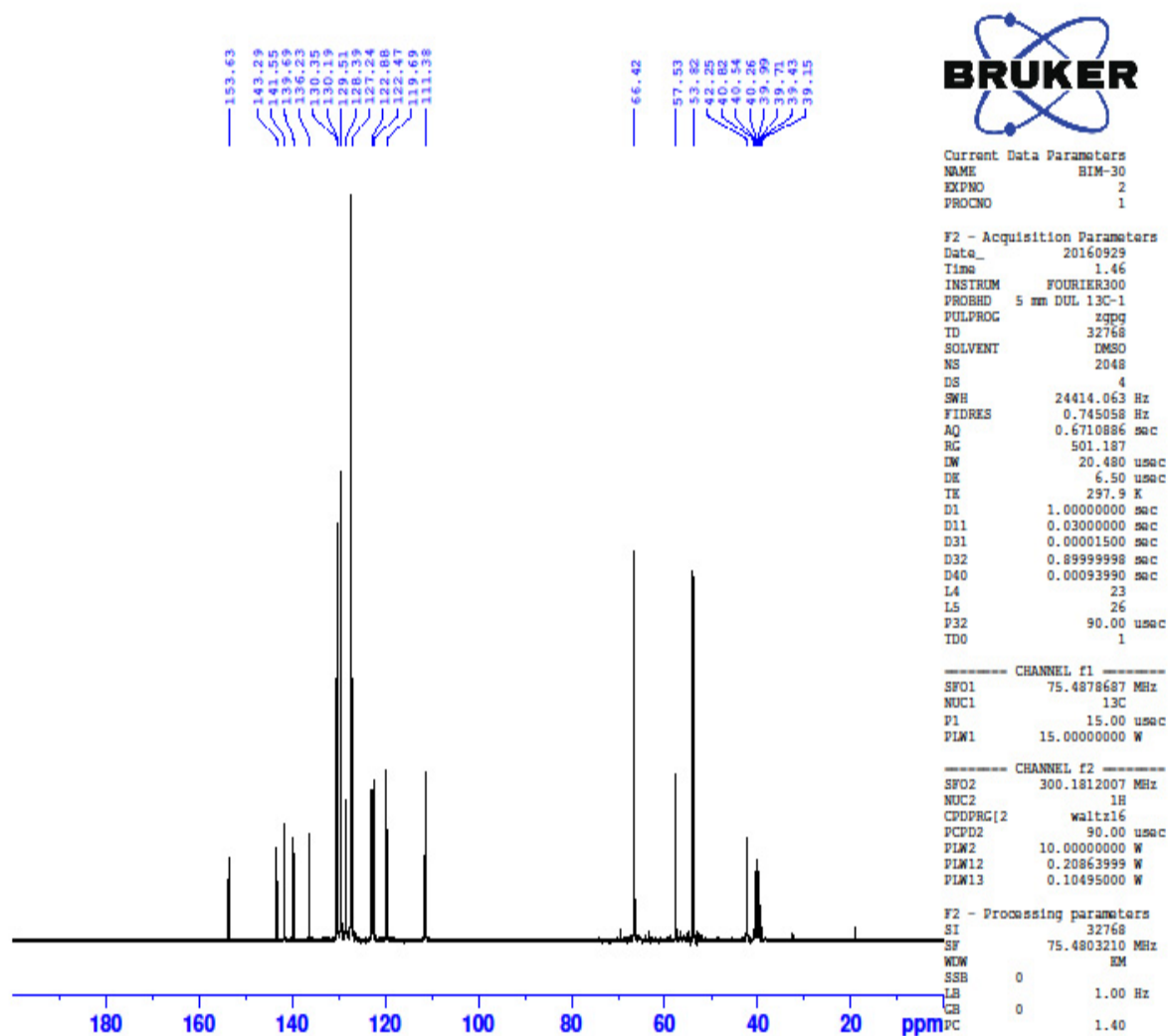


C20 H23 N3 O S [M+H]⁺ : Predicted region for 354.1635 m/z

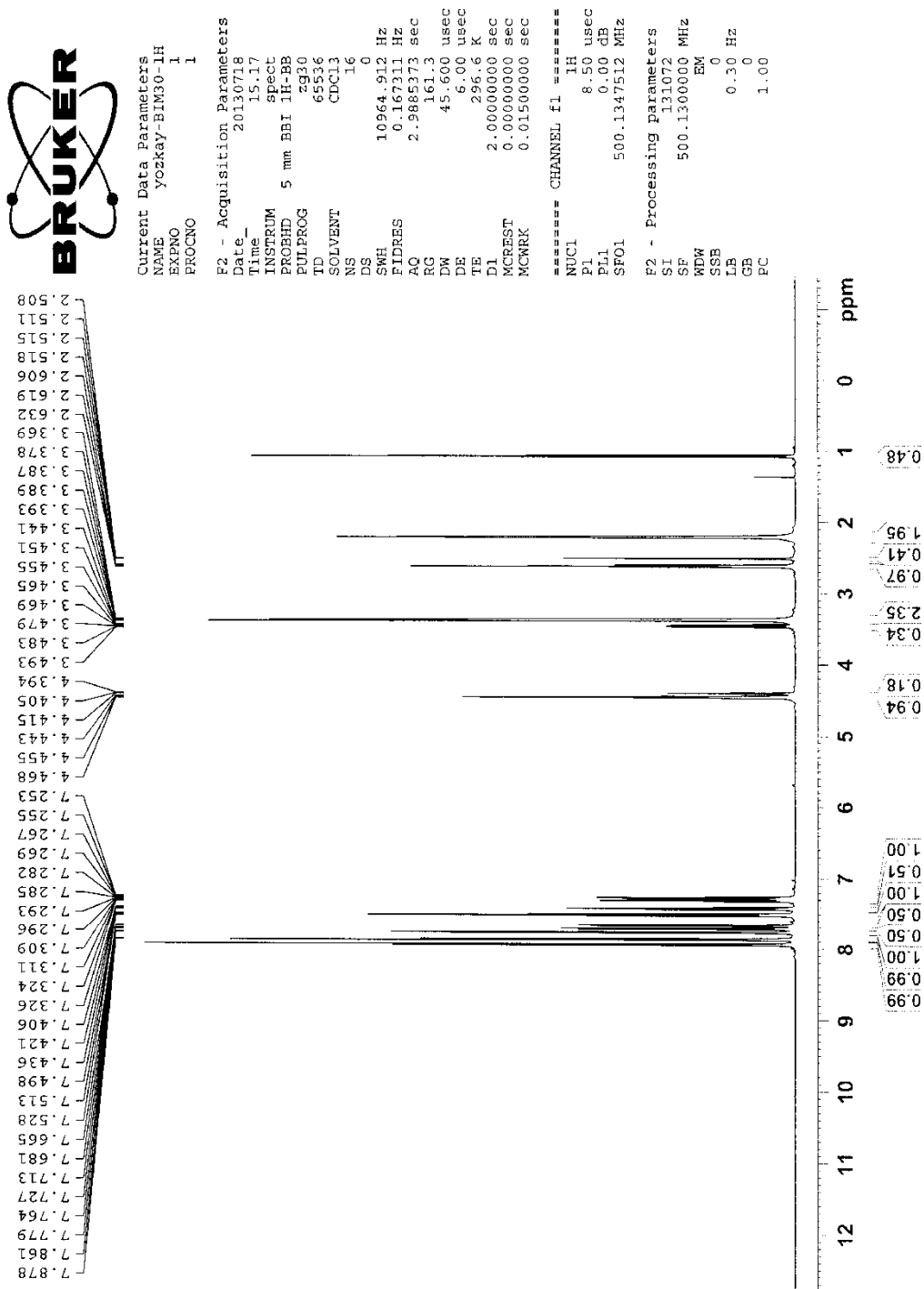


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	29.29	C20 H23 N3 O S	[M+H] ⁺	354.1593	354.1635	-4.2	-11.86	83.58	11.0

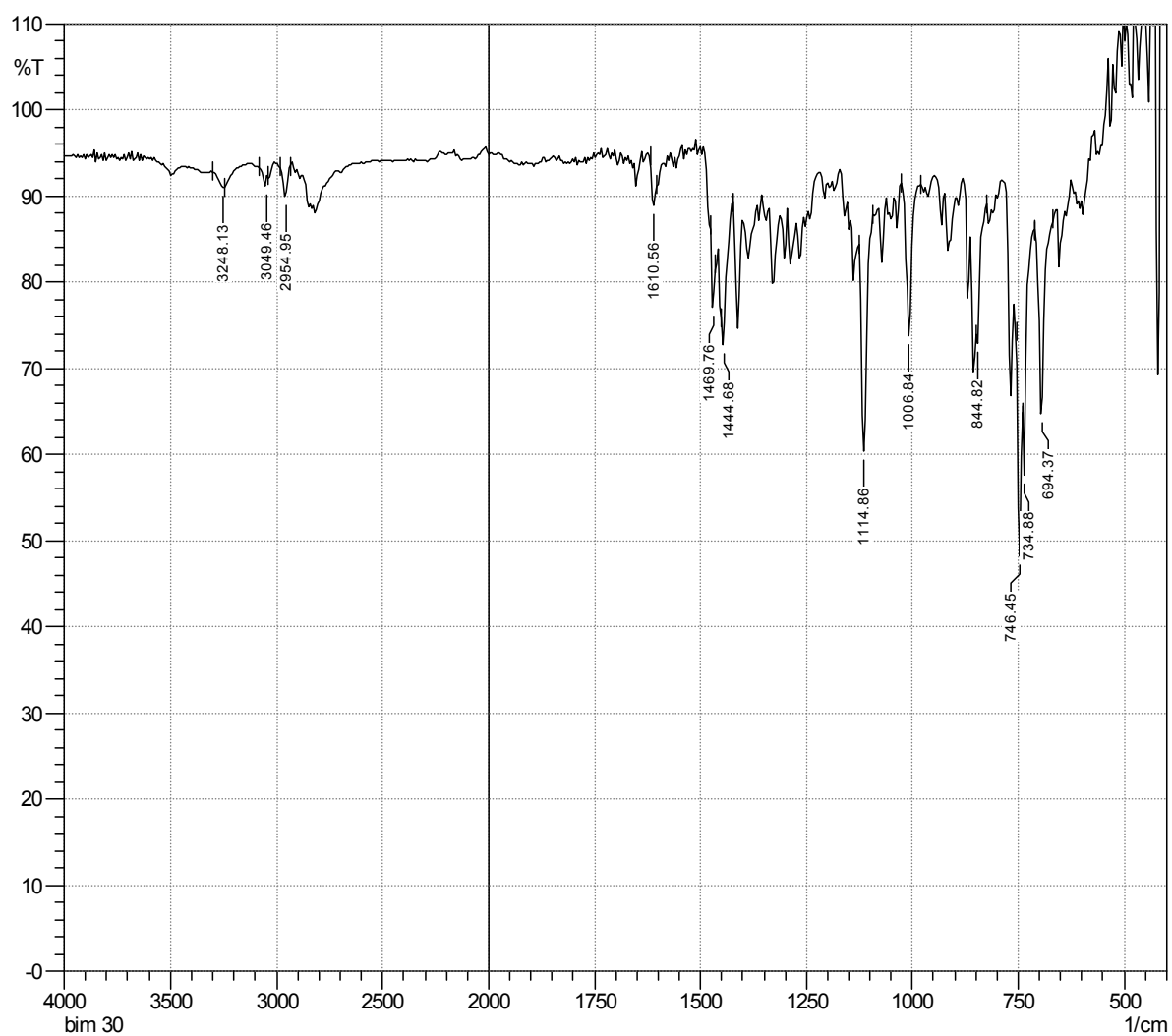
^{13}C -NMR spectrum of 2-(1,1'-Biphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**20**)



¹H-NMR spectrum of 2-(1,1'-Biphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2o)



FTIR spectrum of 2-(1,1'-Biphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (**2o**)



HRMS spectrum of 2-(1,1'-Biphenyl)-1-[2-(morpholin-4-yl)ethyl]-1H-benzimidazole (2o)

Formula Predictor Report - Bim-30_38.lcd

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Data File: C:\LabSolutions\Data\Analz\Bim series\Bim-30_38.lcd

Elmt	Val	Min	Max	Elmt	Val	Min	Max	Elmt	Val	Min	Max	Use Adduct
H	1	14	30	O	2	1	3	Cl	1	0	0	H
C	4	12	30	F	1	0	0	Br	1	0	0	
N	3	3	4	S	2	0	0					

Error Margin (ppm): 15

DBE Range: -2.0 - 1000.0

Electron Ions: both

HC Ratio: unlimited

Apply N Rule: yes

Use MSn Info: no

Max isotopes: 3

Isotope RI (%): 1.00

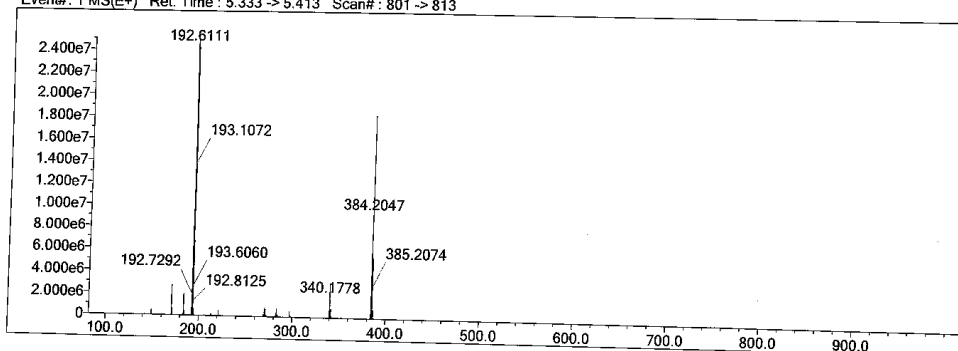
Isotope Res: 10000

MSn Iso RI (%): 10.00

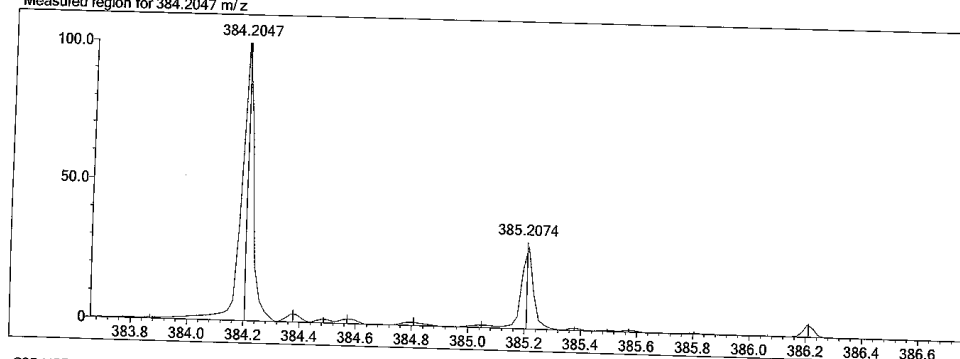
MSn Logic Mode: AND

Max Results: 500

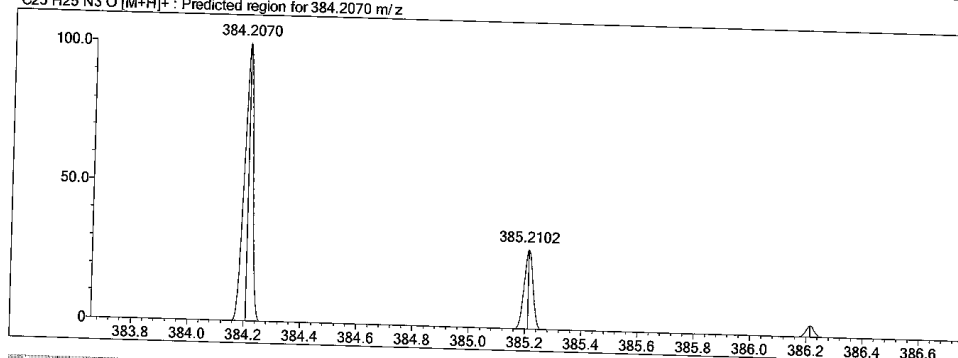
Event#: 1 MS(E+) Ret. Time: 5.333 -> 5.413 Scan#: 801 -> 813



Measured region for 384.2047 m/z



C25 H25 N3 O [M+H]⁺ : Predicted region for 384.2070 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	51.26	C25 H25 N3 O	[M+H] ⁺	384.2047	384.2070	-2.3	-5.99	64.00	15.0