Organoselenocyanates tethered methyl anthranilate hybrids with promising anticancer, antimicrobial, and antioxidant activities

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1.1. The biological assays

1.1.1. The anticancer activity

The breast adenocarcinoma (MCF-7), Hepatocellular carcinoma (HEPG-2), and normal fibroblast (WI-38) cells were obtained from ATCC via Holding company for biological products and vaccines (VACSERA), Cairo, Egypt. The reagents RPMI-1640 medium, MTT, DMSO, and fetal bovine serum was obtained from Sigma Aldrich. Dulbecco's modified Eagle's medium was used as the culture medium for the cells, and the cytotoxicity was evaluated using the reported MTT assay. Doxorubicin was used as the positive reference, and the IC_{50} values were obtained from the corresponding dose-response curve.

MTT assay[1-3]

This colorimetric assay is based on converting the yellow tetrazolium bromide (MTT) to a purple formazan derivative by mitochondrial succinate dehydrogenase in viable cells. Cell lines were cultured in RPMI-1640 medium with 10% fetal bovine serum. Antibiotics added were 100 units/ml penicillin and 100µg/ml streptomycin at 37 C in a 5% Co_2 incubator. The cell lines were seeded in a 96-well plate at a density of $1.0x10^4$ cells/well. at 37 C for 48 h under 5% Co_2. After incubation, the cells were treated with different concentrations of compounds and incubated for 24 h. After 24 h of drug treatment, 20 µl of MTT solution at 5mg/ml was added and incubated for 4 h. Finally, dimethyl sulfoxide (DMSO) in the volume of 100 µl is added to each well to dissolve the purple formazan formed. The colorimetric assay is measured and recorded at an absorbance of 570 nm using a plate reader (EXL 800, USA). The percentage of the relative cell viability was calculated as (A570 of treated samples/A570 of the untreated sample) X 100.

1.1.2. The antimicrobial activity

The antimicrobial activities of the OSe compounds were evaluated against *C. albicans* yeast as well as *E. coli* gram-negative and *S. aureus* gram-positive bacteria employing the agar well diffusion assay [4].

Briefly, a concentration of 1 mM was prepared for each compound by dissolving in DMSO. Paper discs of standard size (5cm) were sterilized in an autoclave and soaked in 20 µL of the test compounds, and placed in the Petri dishes, which in turn contain a nutrient media (agar 20 g, peptone 5 g, and beef extract 3 g) seeded with the dedicated strain. Incubation lasted for 24 h at 36 ^{0}C. Experiments were replicated three times and the antifungal clotrimazole and antibiotic ampicillin were used as standards. The % activity index for the complex was determined and depicted in table 2.

1.1.3. The antioxidant activity

1.1.3.1. The DPPH bioassay

The hydrogen atom or electron donation ability of the corresponding compounds was measured by estimating the bleaching of the purple color of a methanolic solution of DPPH [5]. This spectrophotometric assay uses stable DPPH$^{\cdot}$ reagent. The sample was prepared by adding 200 mL of the OSe compounds (1 mM in methanol) to 400 mL DPPH in methanol. After 30 min of incubation in the dark, the absorbance was read against a blank at 517 nm. Ascorbic acid (vitamin C) and ebselen were used as standard antioxidants (positive control). A blank sample was run without DPPH. A negative control sample was run using methanol instead of the sample. The radical scavenging activity was calculated

using the following equation:

$$\text{Inhibition\%} = (A_{blank}-A_{sample})/(A_{blank})*100.$$

1.1.3.2. The ABTS bioassay

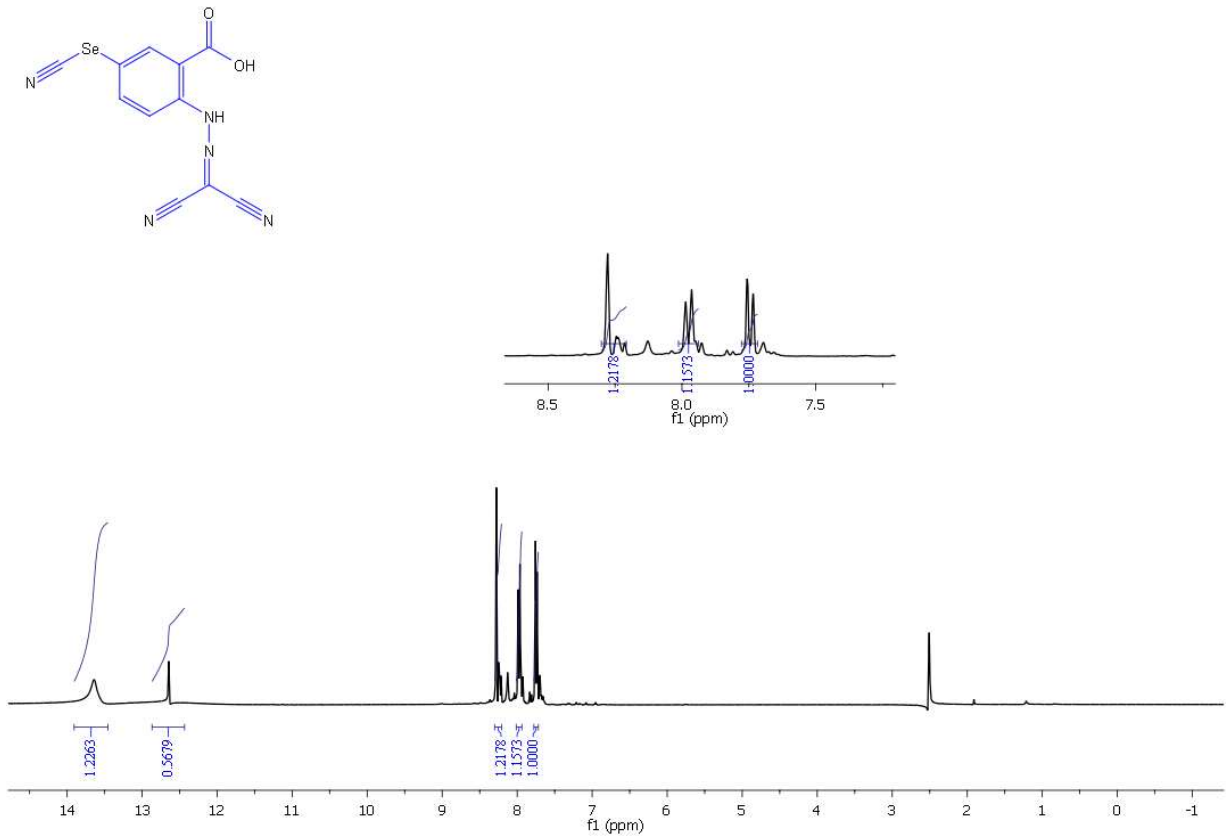
The antioxidant activity of the investigated compounds was assessed using 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid (ABTS) method [6]. The radical cation derived from ABTS was prepared by the reaction of 60 mM ABTS solution with 0.3 M manganese dioxide solution in 0.1M phosphate buffer, pH 7. Then, the mixture was shaken, centrifuged, filtered, and the absorbance ($A_{control}$) of the resulting green-blue solution (ABTS radical solution) was measured at wavelength 734 nm. Then,

50 mL of 1 mg/ml test compound in phosphate-buffered methanol was added. The absorbance (A_{test}) was measured. The reduction in color intensity was expressed as % inhibition. The % inhibition for each compound is calculated from the following equation

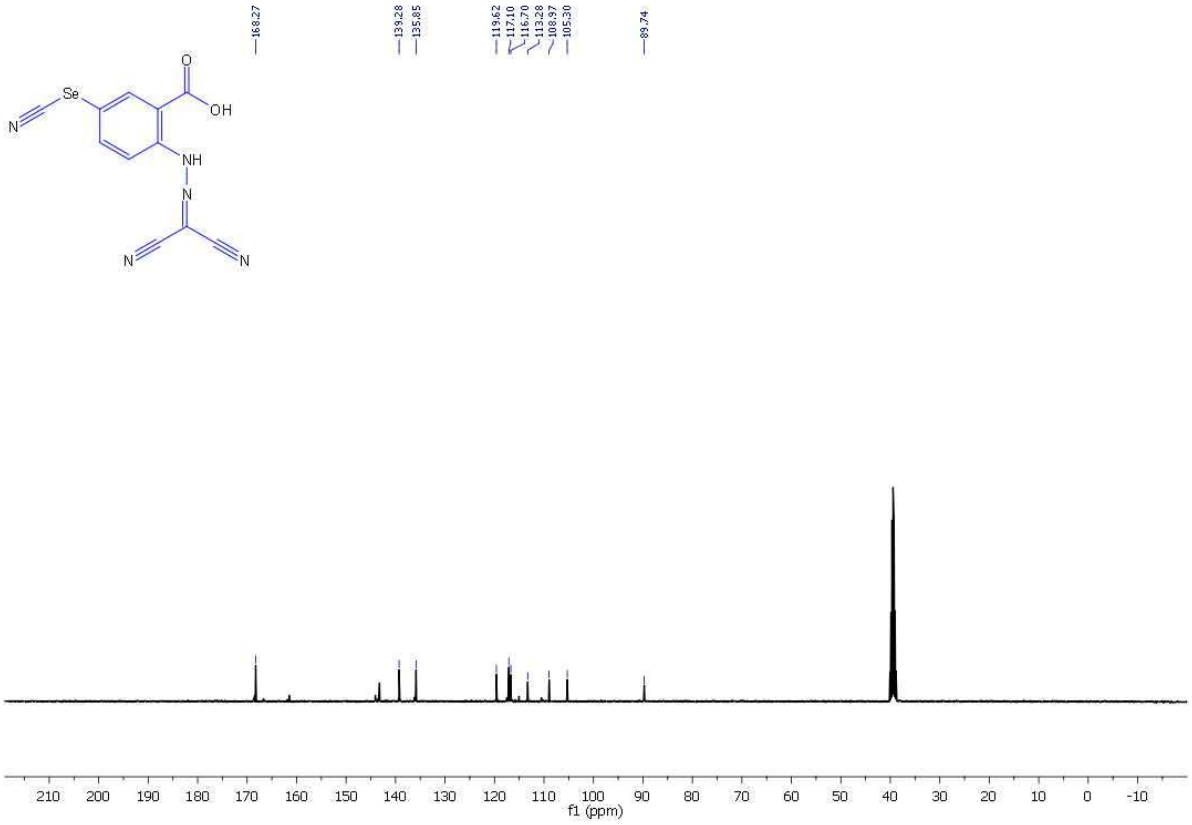
$$\text{Inhibition\%} = (A_{control}-A_{sample})/(A_{control})*100$$

Ascorbic acid (vitamin C) was used as a standard antioxidant (positive control). A blank sample was run without ABTS and using MeOH/phosphate buffer (1:1) instead of the sample. A negative control sample was run with MeOH/phosphate buffer (1:1) instead of a tested compound.

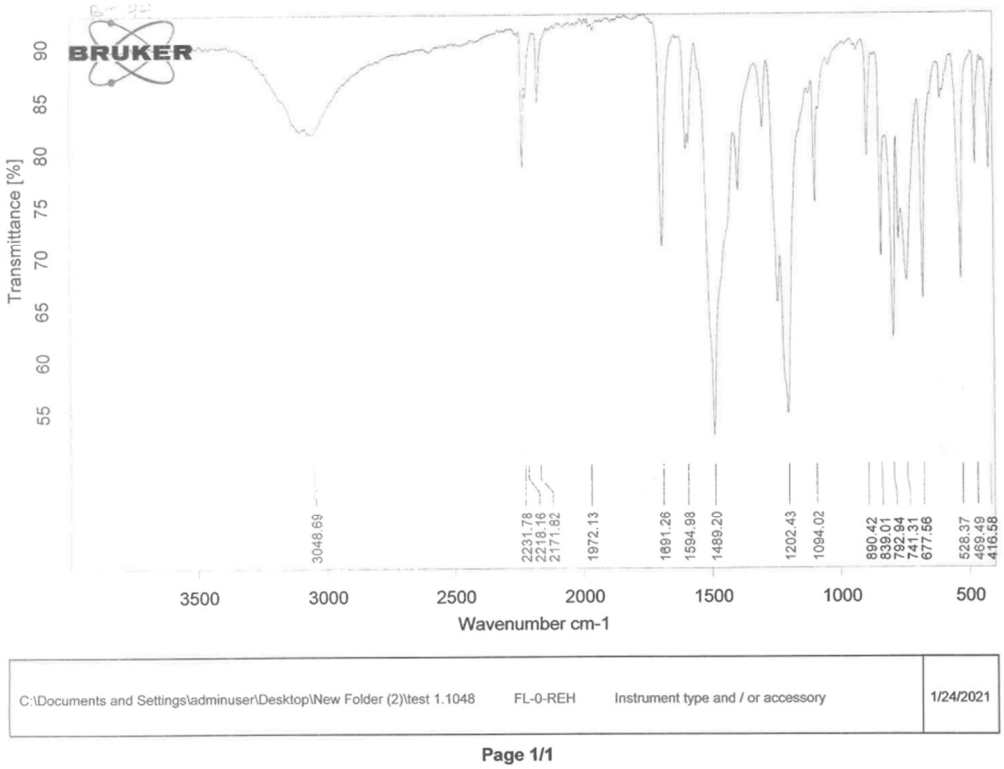
*2-(2-(dicyanomethylene) hydrazinyl)-5-selenocyanatobenzoic acid (**3**).*



[1]HNMR chart of compound **3**



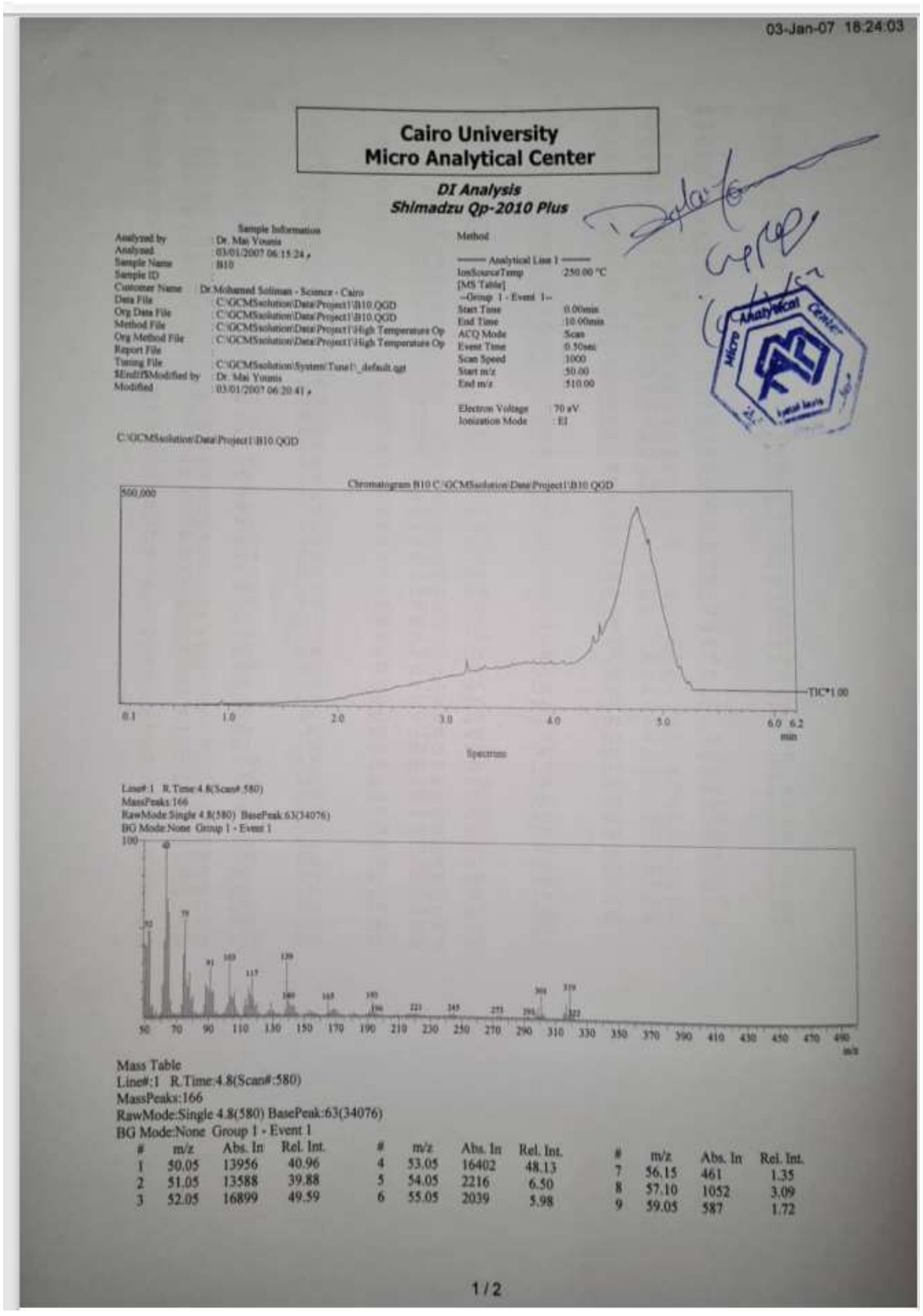
^{13}CNMR chart of compound **3**



C:\Documents and Settings\adminuser\Desktop\New Folder (2)\test 1.1048	FL-0-REH	Instrument type and / or accessory	1/24/2021

Page 1/1

IR chart of compound **3**

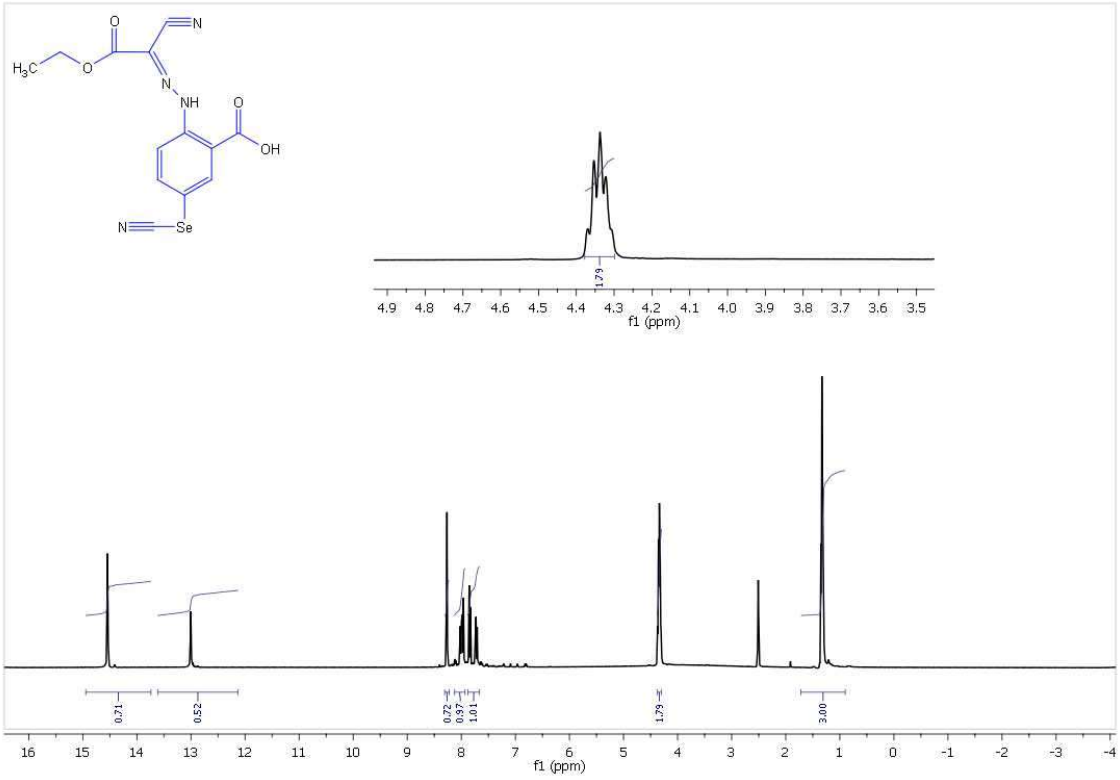


Mass chart of compound **3**

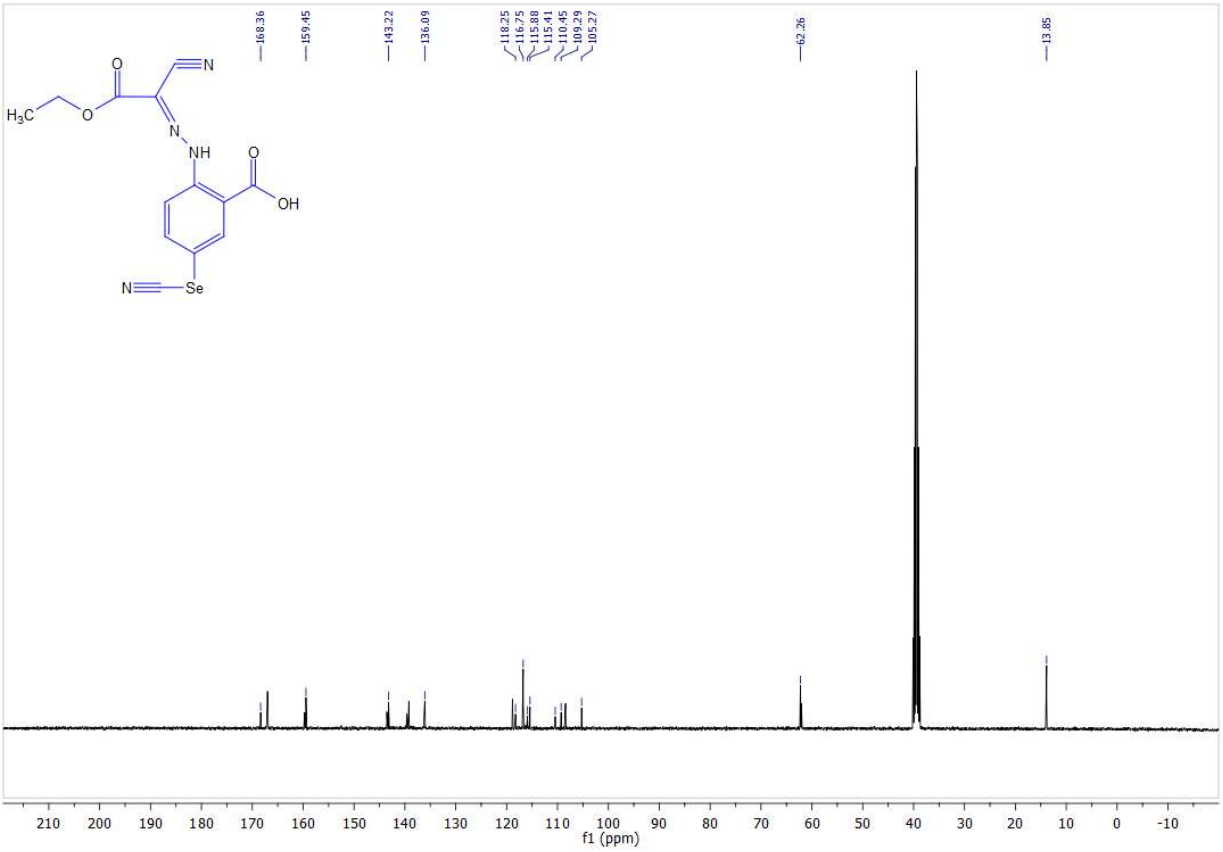
#	m/z	Abs. In	Rel. Int.
10	60.15	961	2.82
11	61.05	6212	18.23
12	62.10	14762	43.32
13	63.05	34076	100.00
14	64.05	22773	66.83
15	65.05	20118	59.04
16	66.05	3100	9.10
17	67.05	977	2.87
18	68.10	566	1.66
19	69.10	750	2.20
20	70.10	359	1.05
21	71.10	762	2.24
22	72.15	534	1.57
23	73.15	2432	7.14
24	74.10	12095	35.49
25	75.05	18860	55.35
26	76.05	6964	20.44
27	77.05	5786	16.98
28	78.05	8451	24.80
29	79.05	3241	9.51
30	79.95	4069	11.94
31	81.05	950	2.79
32	82.00	817	2.40
33	83.10	578	1.70
34	84.15	427	1.25
35	85.15	489	1.44
36	86.10	714	2.10
37	87.10	2108	6.19
38	88.10	6418	18.83
39	89.10	5721	16.79
40	90.10	4969	14.58
41	91.05	9289	27.26
42	92.05	4680	13.73
43	93.00	4826	14.16
44	94.05	634	1.86
45	95.05	1046	3.07
46	96.10	303	0.89
47	97.10	321	0.94
48	98.10	343	1.01
49	99.10	564	1.66
50	100.10	878	2.58
51	101.10	1774	5.21
52	102.15	2318	6.80
53	103.10	10292	30.20
54	104.05	3866	11.35
55	105.05	3418	10.03
56	106.00	4604	13.51
57	107.00	1857	5.45
58	108.00	940	2.76
59	108.95	463	1.36
60	111.15	347	1.02
61	112.15	1703	5.00
62	113.10	3310	9.71
63	114.05	2044	6.00
64	115.05	5425	15.92
65	116.10	4161	12.21
66	117.05	7201	21.13
67	118.05	3355	9.85
68	119.05	1789	5.25
69	120.10	2447	7.18
70	121.00	410	1.20
71	122.05	798	2.34
72	125.00	239	0.70
73	126.05	449	1.32
74	127.10	985	2.89
75	128.10	951	2.79
76	129.10	2607	7.65
77	130.05	1338	3.93
78	131.10	734	2.15
79	132.10	446	1.31
80	133.15	327	0.96
81	134.10	455	1.34
82	135.10	204	0.60
83	137.10	279	0.82
84	138.15	1179	3.46
85	139.10	10457	30.69
86	140.10	2862	8.40
87	141.10	1970	5.78
88	142.05	1871	5.49
89	143.05	1986	5.83
90	144.05	1654	4.85
91	145.05	616	1.81
92	146.05	552	1.62
93	150.10	273	0.80
94	151.05	381	1.12
95	152.15	417	1.22
96	153.10	1052	3.09
97	154.05	674	1.98
98	155.10	790	2.32
99	156.20	486	1.43
100	157.20	295	0.87
101	158.20	265	0.78
102	164.15	478	1.40
103	165.10	2705	7.94
104	166.00	788	2.31
105	167.05	1020	2.99
106	168.05	1213	3.56
107	169.05	1370	4.02
108	170.00	951	2.79
109	171.05	1051	3.08
110	172.00	311	0.91
111	173.00	234	0.69
112	179.00	457	1.34
113	181.05	662	1.94
114	182.10	321	0.94
115	183.10	255	0.75
116	189.10	404	1.19
117	190.10	457	1.34
118	191.05	979	2.87
119	192.15	578	1.70
120	193.05	3024	8.87
121	194.00	558	1.64
122	195.05	647	1.90
123	196.15	449	1.32
124	197.10	218	0.64
125	198.10	238	0.70
126	199.10	350	1.03
127	207.10	236	0.69
128	209.10	329	0.97
129	214.10	233	0.68
130	215.10	358	1.05
131	216.10	378	1.11
132	217.10	319	0.94
133	218.00	628	1.84
134	219.05	446	1.31
135	220.00	322	0.94
136	221.00	817	2.40
137	222.00	273	0.80
138	223.00	212	0.62
139	224.00	252	0.74
140	226.00	316	0.93
141	242.00	273	0.80
142	243.05	380	1.12
143	244.00	287	0.84
144	245.00	814	2.39
145	246.00	210	0.62
146	247.00	215	0.63
147	273.10	498	1.46
148	275.15	468	1.37
149	291.20	207	0.61
150	292.20	238	0.70
151	293.20	295	0.87
152	297.15	941	2.76
153	298.15	975	2.86
154	299.15	2177	6.39
155	300.15	599	1.76
156	301.15	4384	12.87
157	302.10	823	2.42
158	303.10	866	2.54
159	315.15	1153	3.38
160	316.10	1126	3.30
161	317.10	2886	8.47
162	318.15	708	2.08
163	319.15	5256	15.42
164	320.05	1047	3.07
165	321.10	1230	3.61
166	322.10	314	0.92

Mass chart of compound **3**

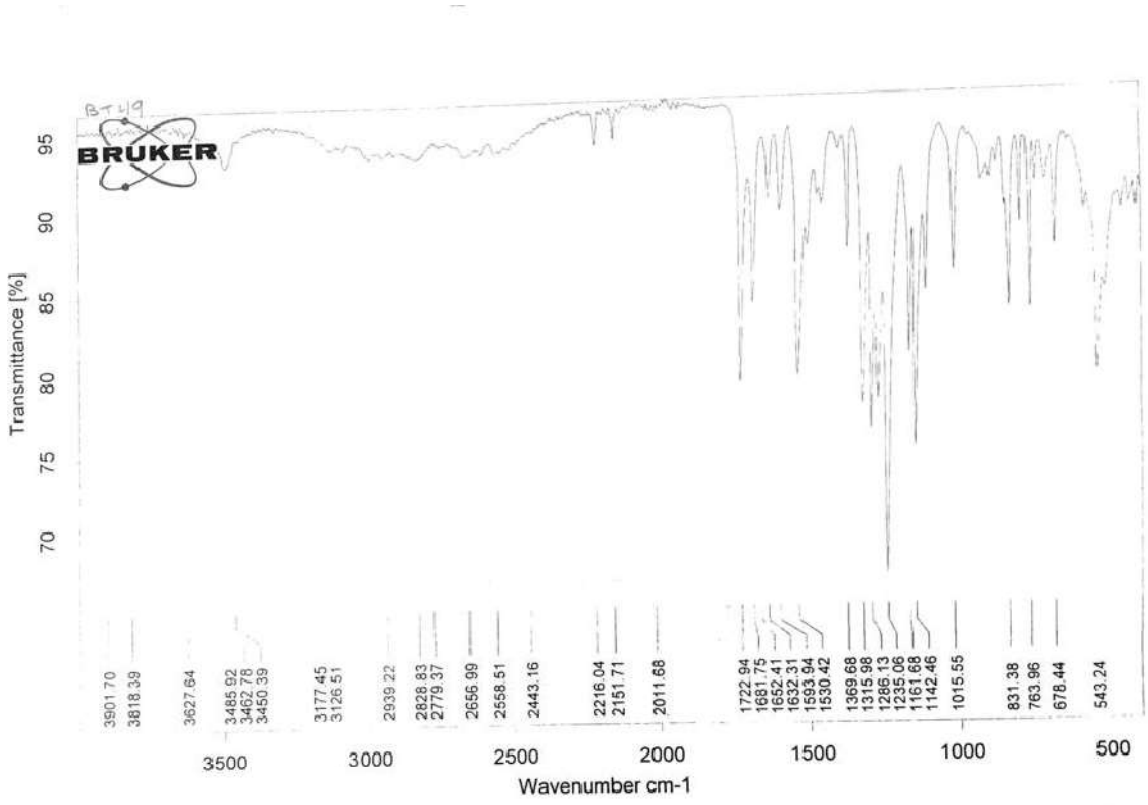
*2-(2-(1-cyano-2-ethoxy-2-oxoethylidene) hydrazinyl)-5-selenocyanatobenzoic acid (**4**).*



^{1}HNMR chart of compound **4**



^{13}CNMR chart of compound **4**



IR chart of compound **4**

06-Jan-07 20:02:36

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

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Analyzed	: 06/01/2007 07:55:34 م
Sample Name	: B11
Sample ID	:
Customer Name	: Dr.Mohamed Soliman - Science - Cairo
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Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op
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Report File	:
Tuning File	: C:\GCMSsolution\System\Tune1_default.qgt
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Modified	: 06/01/2007 08:01:25 م

Method

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End Time	10.00min
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Event Time	0.50sec
Scan Speed	1000
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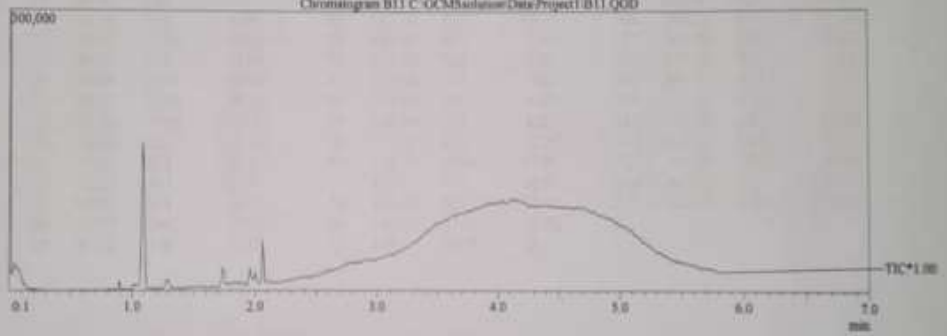
End m/z	510.00
Electron Voltage	70 eV
Ionization Mode	EI

C:\GCMSsolution\Data\Project1\B11.QGD

Chromatogram B11 C:\GCMSsolution\Data\Project1\B11.QGD



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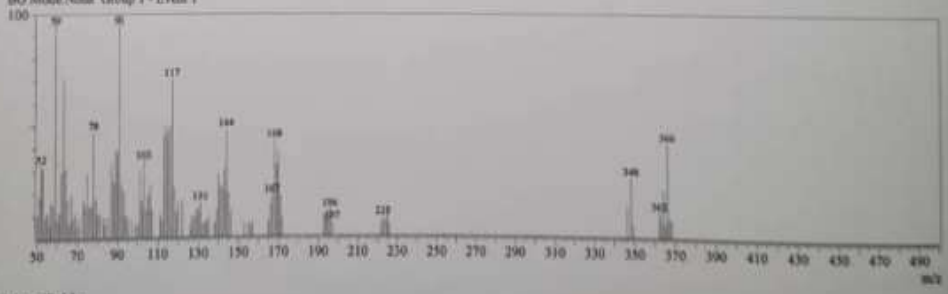

Mass Table
Line#:1 R.Time:3.7(Scan#:447)
MassPeaks:115
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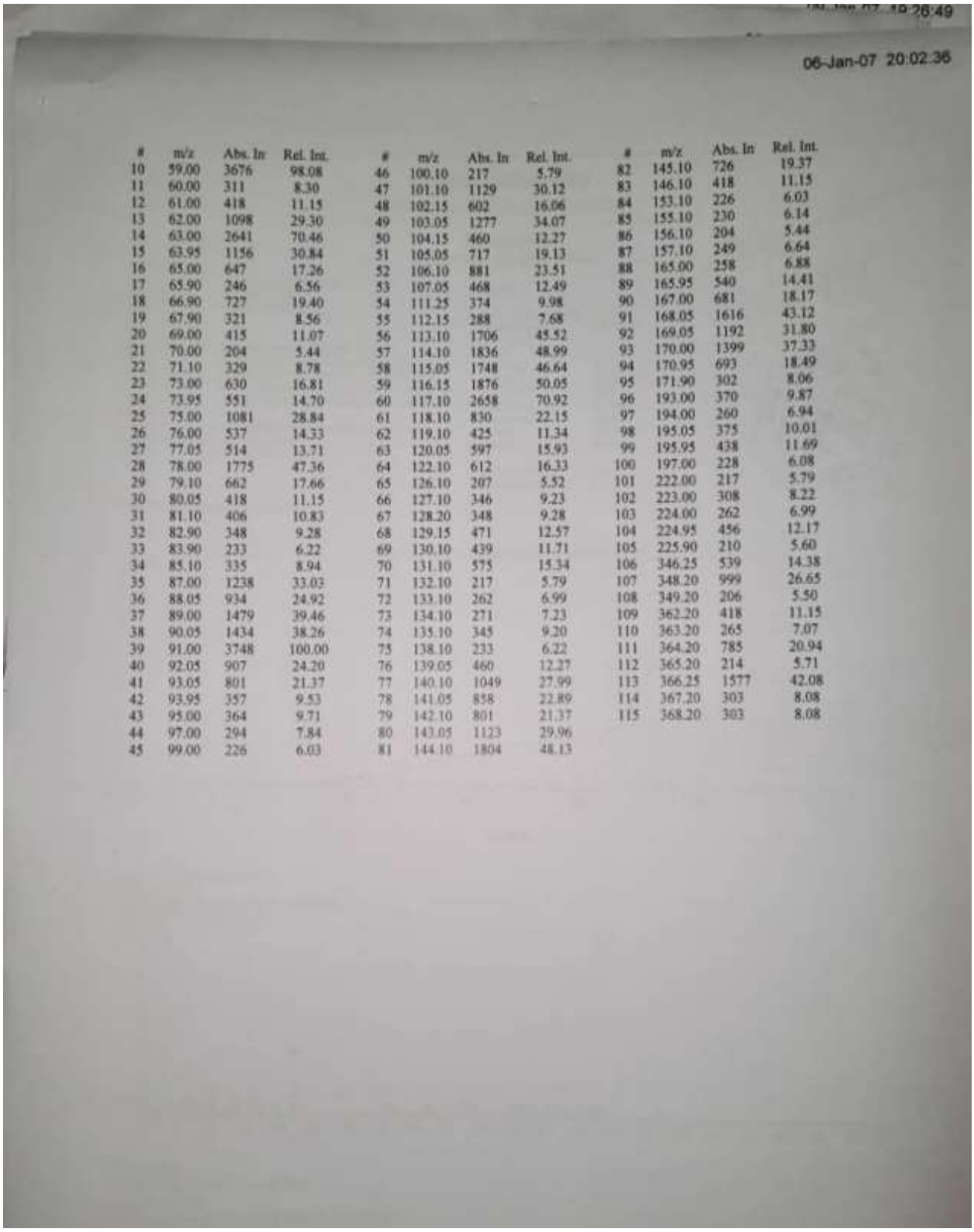
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	49.95	385	10.27	4	52.95	1154	30.79	7	56.00	231	6.16
2	51.00	697	18.60	5	54.00	345	9.20	8	56.90	604	16.12
3	52.00	1220	32.55	6	55.00	431	11.50	9	58.05	552	14.73

Mass chart of compound **4**



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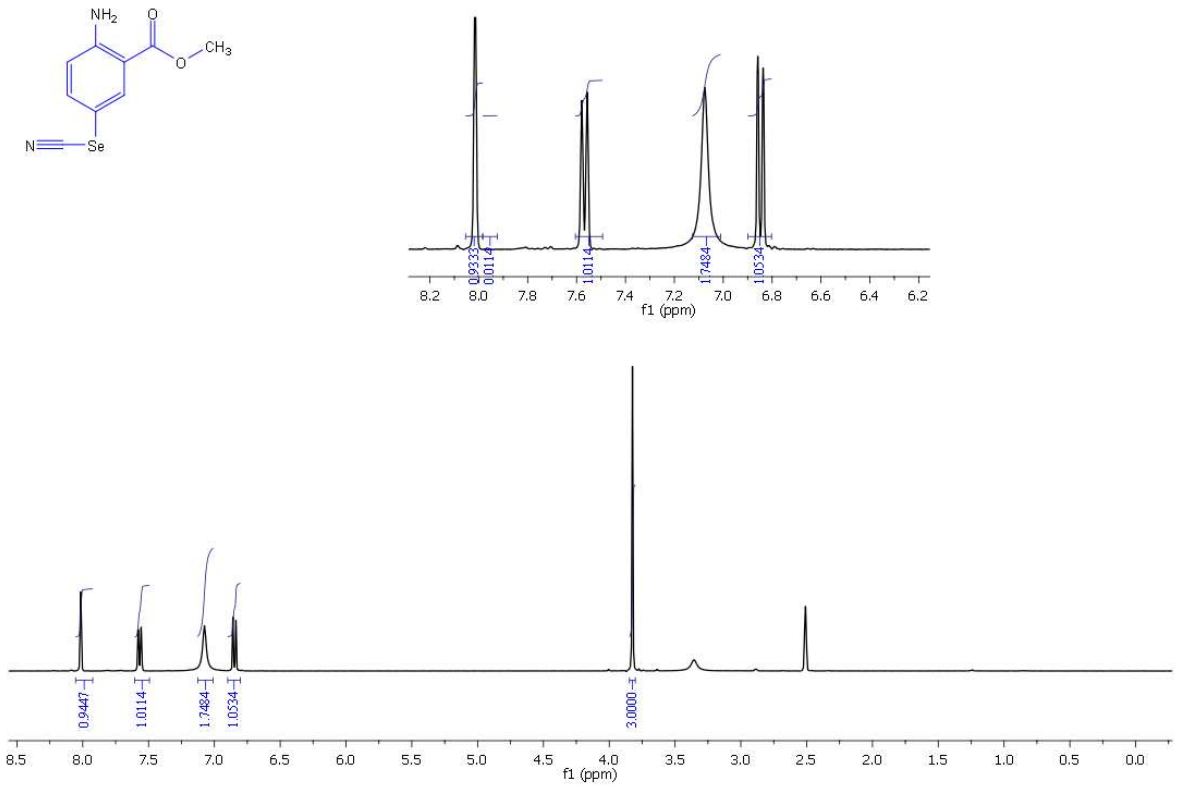
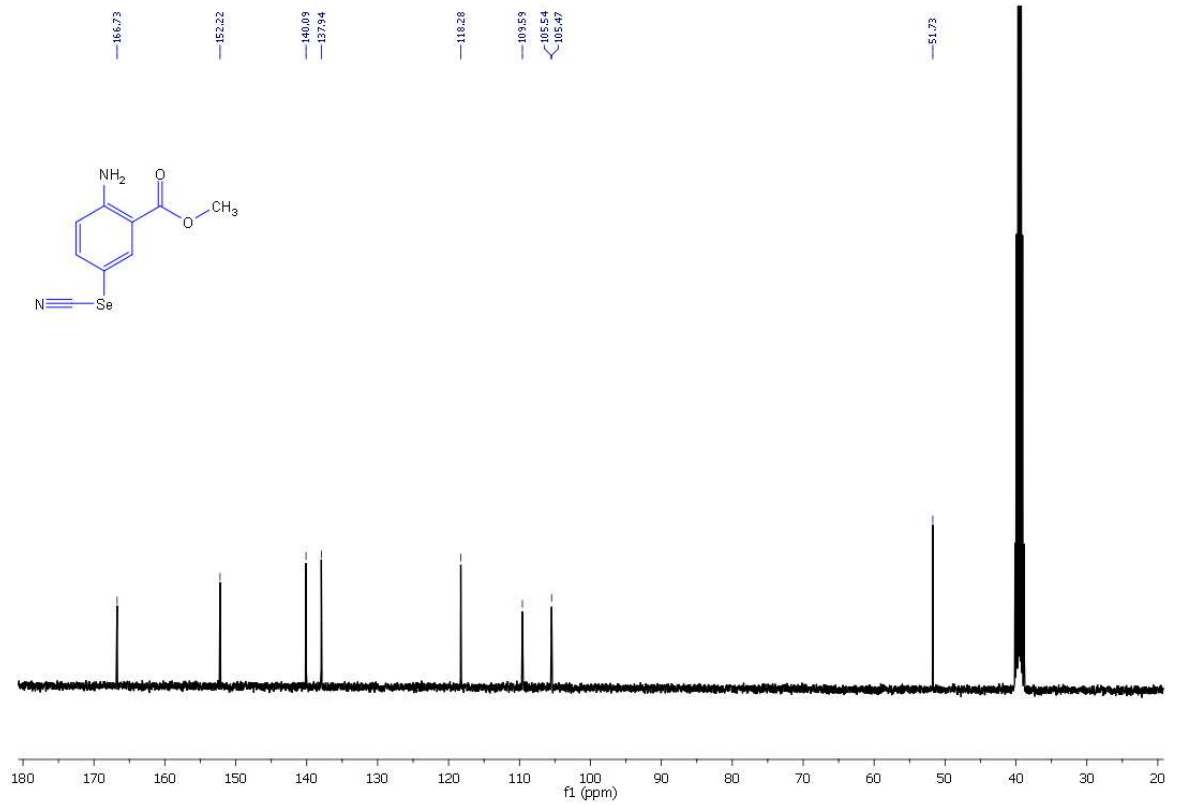
#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	59.00	3676	98.08	46	100.10	217	5.79	82	145.10	726	19.37
11	60.00	311	8.30	47	101.10	1129	30.12	83	146.10	418	11.15
12	61.00	418	11.15	48	102.15	602	16.06	84	153.10	226	6.03
13	62.00	1098	29.30	49	103.05	1277	34.07	85	155.10	230	6.14
14	63.00	2641	70.46	50	104.15	460	12.27	86	156.10	204	5.44
15	63.95	1156	30.84	51	105.05	717	19.13	87	157.10	249	6.64
16	65.00	647	17.26	52	106.10	881	23.51	88	165.00	258	6.88
17	65.90	246	6.56	53	107.05	468	12.49	89	165.95	540	14.41
18	66.90	727	19.40	54	111.25	374	9.98	90	167.00	681	18.17
19	67.90	321	8.56	55	112.15	288	7.68	91	168.05	1616	43.12
20	69.00	415	11.07	56	113.10	1706	45.52	92	169.05	1192	31.80
21	70.00	204	5.44	57	114.10	1836	48.99	93	170.00	1399	37.33
22	71.10	329	8.78	58	115.05	1748	46.64	94	170.95	693	18.49
23	73.00	630	16.81	59	116.15	1876	50.05	95	171.90	302	8.06
24	73.95	551	14.70	60	117.10	2658	70.92	96	193.00	370	9.87
25	75.00	1081	28.84	61	118.10	830	22.15	97	194.00	260	6.94
26	76.00	537	14.33	62	119.10	425	11.34	98	195.05	375	10.01
27	77.05	514	13.71	63	120.05	597	15.93	99	195.95	438	11.69
28	78.00	1775	47.36	64	122.10	612	16.33	100	197.00	228	6.08
29	79.10	662	17.66	65	126.10	207	5.52	101	222.00	217	5.79
30	80.05	418	11.15	66	127.10	346	9.23	102	223.00	308	8.22
31	81.10	406	10.83	67	128.20	348	9.28	103	224.00	262	6.99
32	82.90	348	9.28	68	129.15	471	12.57	104	224.95	456	12.17
33	83.90	233	6.22	69	130.10	439	11.71	105	225.90	210	5.60
34	85.10	335	8.94	70	131.10	575	15.34	106	346.25	539	14.38
35	87.00	1238	33.03	71	132.10	217	5.79	107	348.20	999	26.65
36	88.05	934	24.92	72	133.10	262	6.99	108	349.20	206	5.50
37	89.00	1479	39.46	73	134.10	271	7.23	109	362.20	418	11.15
38	90.05	1434	38.26	74	135.10	345	9.20	110	363.20	265	7.07
39	91.00	3748	100.00	75	138.10	233	6.22	111	364.20	785	20.94
40	92.05	907	24.20	76	139.05	460	12.27	112	365.20	214	5.71
41	93.05	801	21.37	77	140.10	1049	27.99	113	366.25	1577	42.08
42	93.95	357	9.53	78	141.05	858	22.89	114	367.20	303	8.08
43	95.00	364	9.71	79	142.10	801	21.37	115	368.20	303	8.08
44	97.00	294	7.84	80	143.05	1123	29.96				
45	99.00	226	6.03	81	144.10	1804	48.13				

Mass chart of compound **4**

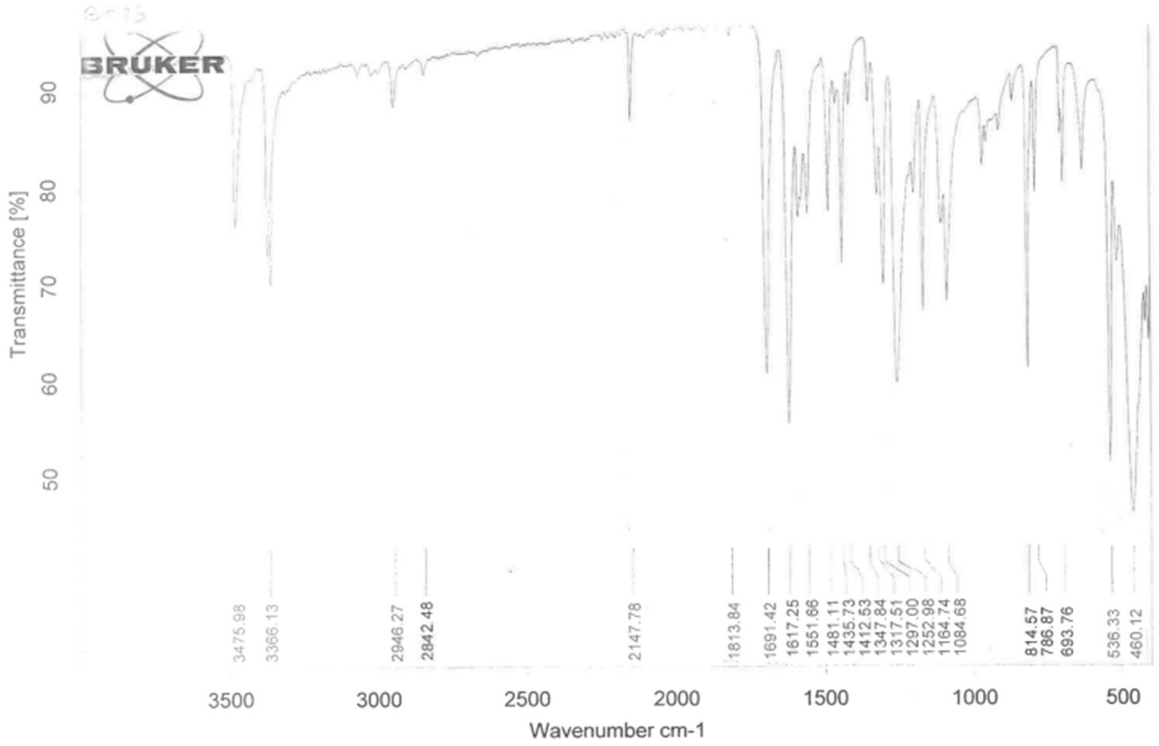
*Methyl 2-amino-5-selenocyanatobnzoate. (**6**).*



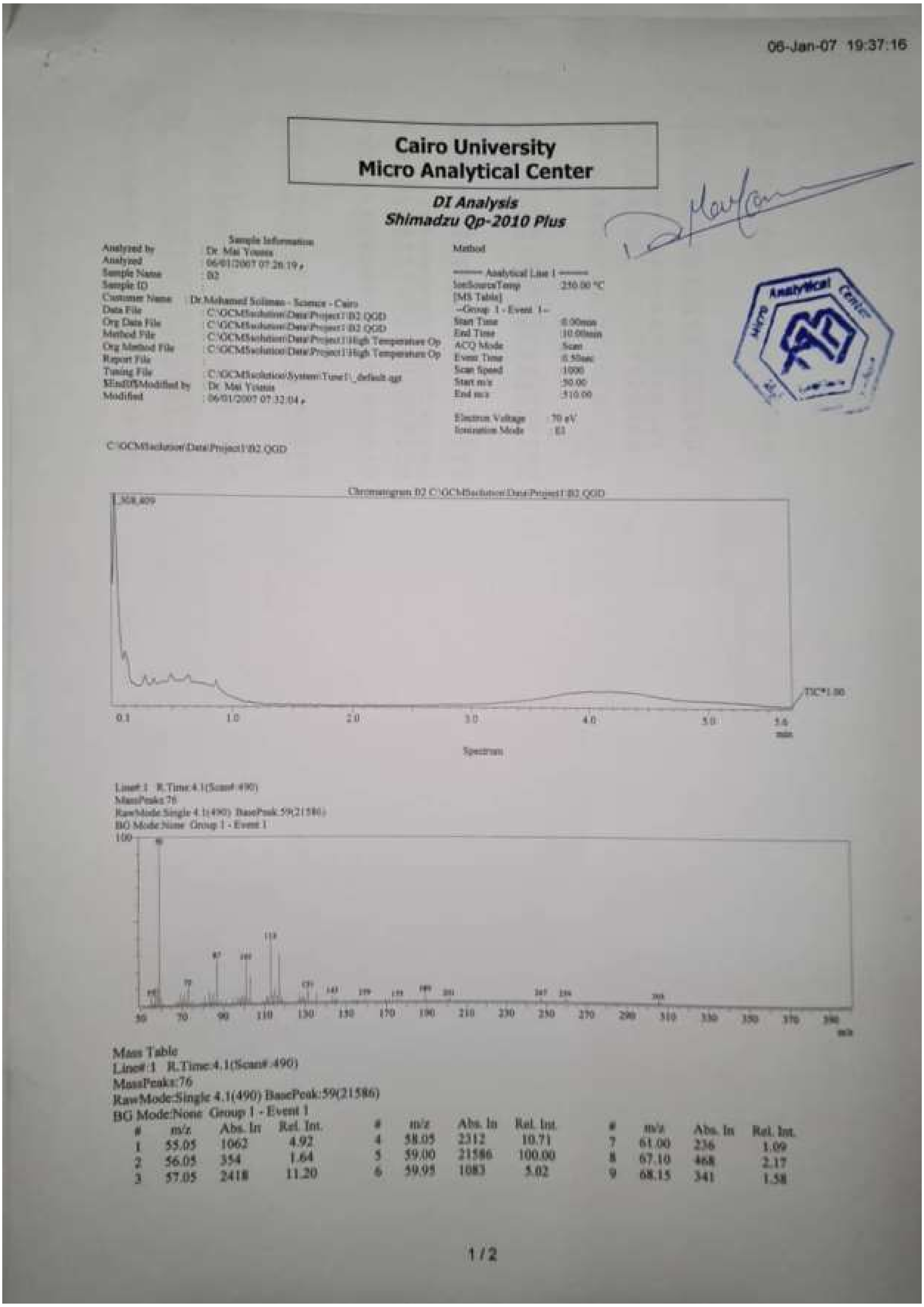
^{1}HNMR chart of compound **6**



^{13}CNMR chart of compound **6**



IR chart of compound **6**



06-Jan-07 19:37:16

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

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Analyzed : 06/01/2007 07:26:19
Sample Name : B2
Sample ID
Customer Name : Dr.Mohamed Soliman - Science - Cairo
Data File : C:\GCMSsolution\Data\Project1\B2.QGD
Org Data File : C:\GCMSsolution\Data\Project1\B2.QGD
Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.qgt
Modified by : Dr. Mai Younis
Modified : 06/01/2007 07:32:04

Method

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End Time :10.00min
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Event Time :0.50sec
Scan Speed :1000
Start m/z :50.00
End m/z :510.00

Electron Voltage :70 eV
Ionization Mode :EI

C:\GCMSsolution\Data\Project1\B2.QGD

Chromatogram B2 C:\GCMSsolution\Data\Project1\B2.QGD

Spectrum

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BG Mode:None Group 1 - Event 1

Mass Table
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MassPeaks:76
RawMode:Single 4.1(490) BasePeak:59(21586)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	55.05	1062	4.92	4	58.05	2312	10.71	7	61.00	236	1.09
2	56.05	354	1.64	5	59.00	21586	100.00	8	67.10	468	2.17
3	57.05	2418	11.20	6	59.95	1083	5.02	9	68.15	341	1.58

1/2

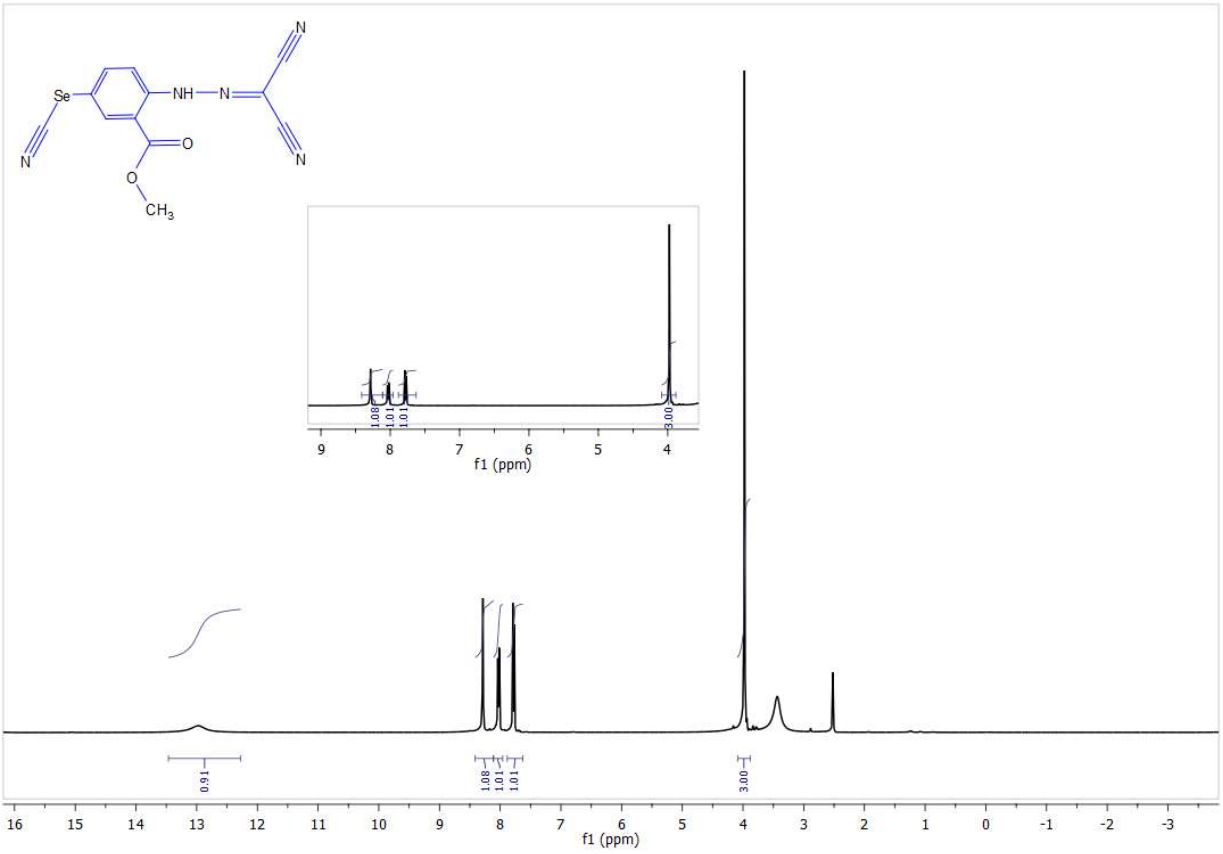
Mass chart of compound **6**

#	m/z	Abs. In	Rel. Int.
10	69.05	1515	7.02
11	70.10	633	2.93
12	71.05	1365	6.32
13	72.05	440	2.04
14	73.00	2258	10.46
15	74.00	302	1.40
16	75.05	583	2.70
17	77.00	268	1.24
18	79.00	223	1.03
19	80.10	324	1.50
20	81.10	954	4.42
21	82.15	315	1.46
22	83.10	1628	7.54
23	84.10	481	2.23
24	85.05	1397	6.47
25	86.05	492	2.28
26	87.05	5752	26.65
27	88.00	314	1.45
28	89.05	560	2.59
29	91.10	327	1.51
30	94.10	202	0.94
31	95.10	807	3.74
32	96.10	278	1.29
33	97.10	945	4.38
34	98.15	599	2.77
35	99.10	1268	5.87
36	100.15	840	3.89
37	101.10	5503	25.49
38	102.15	699	3.24
39	103.10	3649	16.90
40	104.10	322	1.49
41	109.10	401	1.86
42	110.10	220	1.02
43	111.10	969	4.49
44	112.15	807	3.74
45	113.10	8084	37.45
46	114.10	1199	5.55
47	115.10	2001	9.27
48	116.25	936	4.34
49	117.15	6264	29.02
50	118.15	607	2.81
51	119.20	271	1.26
52	126.15	310	1.44
53	127.10	1102	5.11
54	128.15	589	2.73
55	129.10	740	3.43
56	130.15	304	1.41
57	131.10	1722	7.98
58	133.15	432	2.00
59	135.20	1132	5.24
60	143.10	908	4.21
61	144.10	210	0.97
62	145.20	492	2.28
63	153.20	234	1.08
64	155.20	281	1.30
65	159.15	662	3.07
66	169.20	334	1.55
67	171.20	204	0.95
68	173.20	202	0.94
69	175.20	346	1.60
70	189.20	1038	4.81
71	201.15	502	2.33
72	247.20	575	2.66
73	259.35	515	2.39
74	260.40	207	0.96
75	305.40	401	1.86
76	306.40	281	1.30

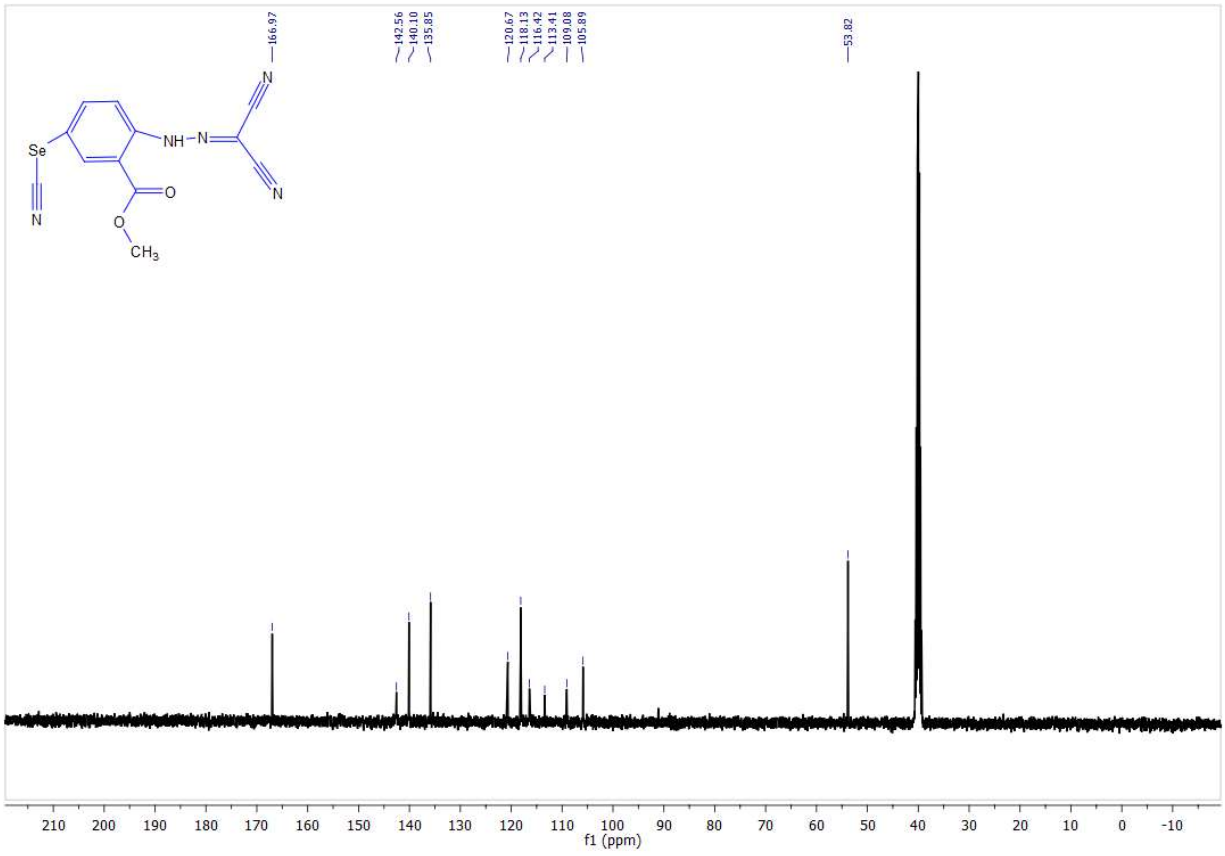
2 / 2

Mass chart of compound **6**

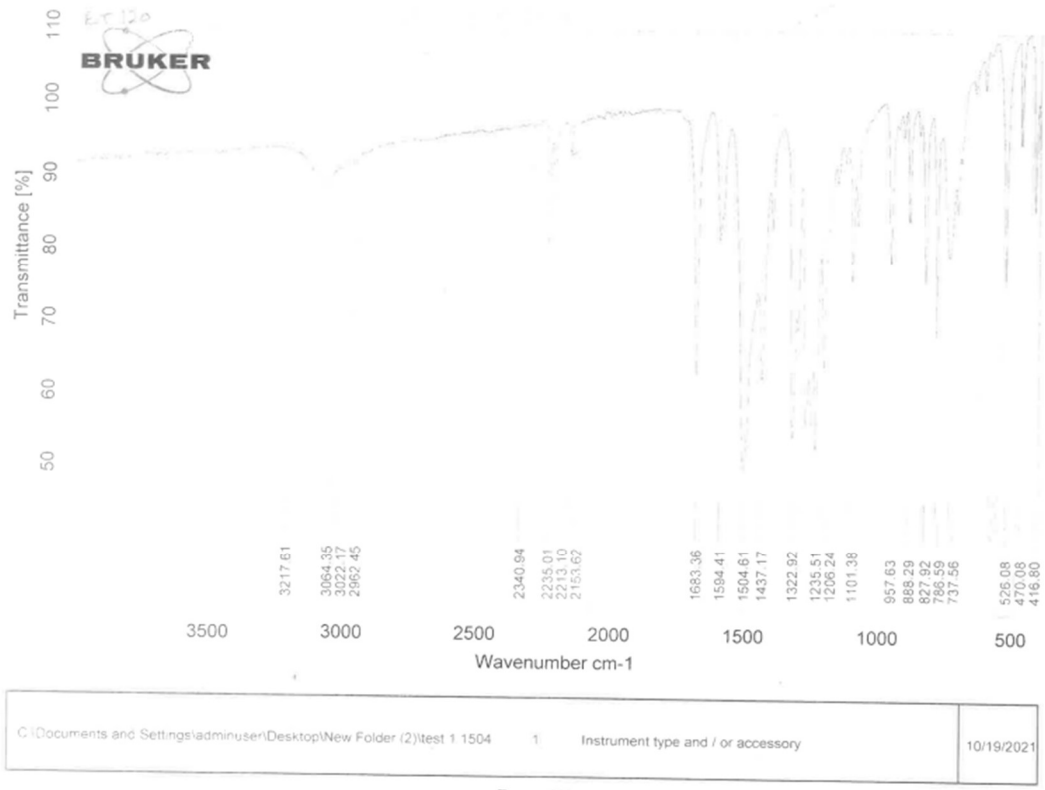
Methyl 2-(2-(dicyanomethylene) hydrazinyl)-5-selenocyanatobenzoate (7).



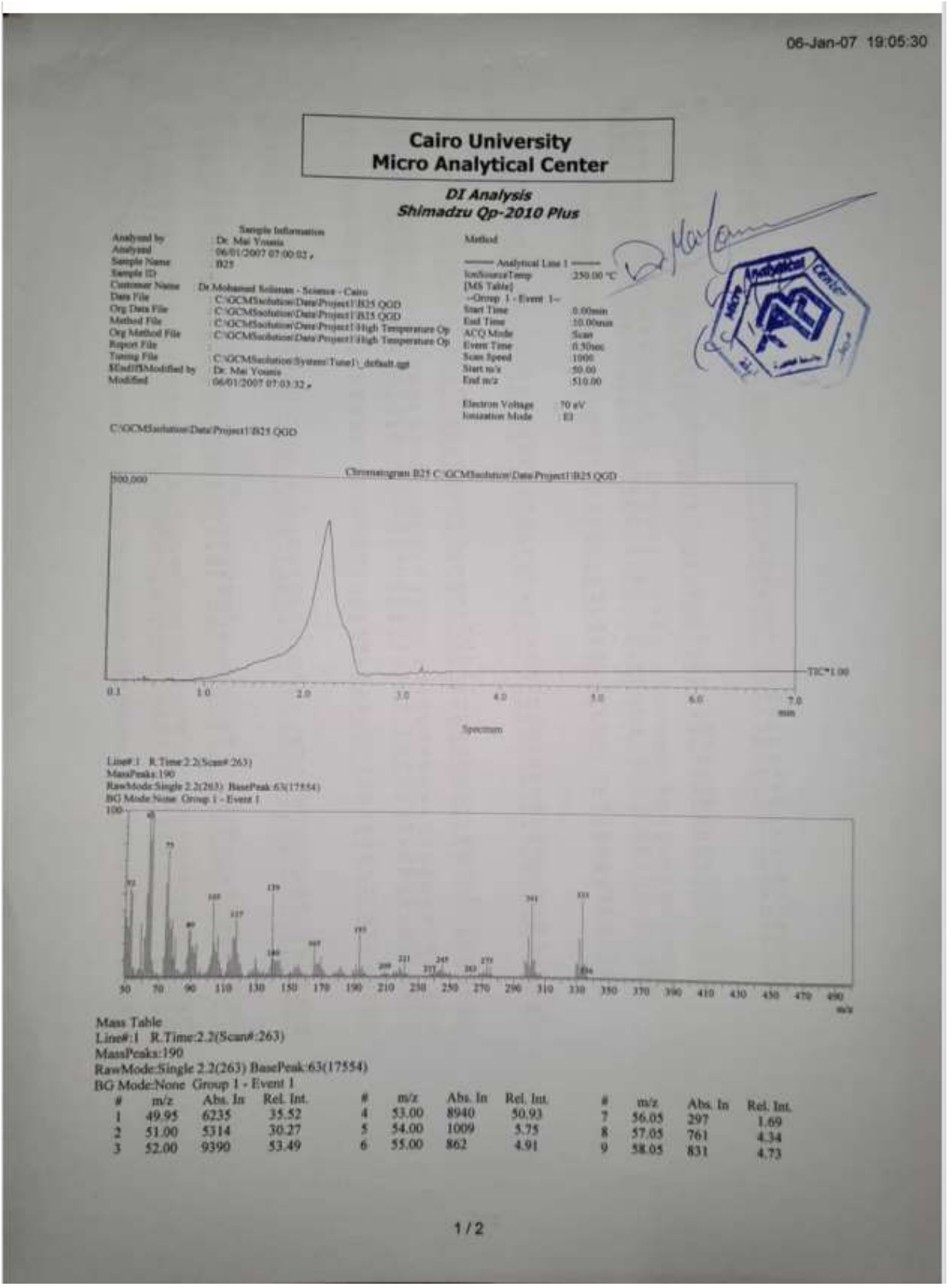
[1]HNMR chart of compound **7**



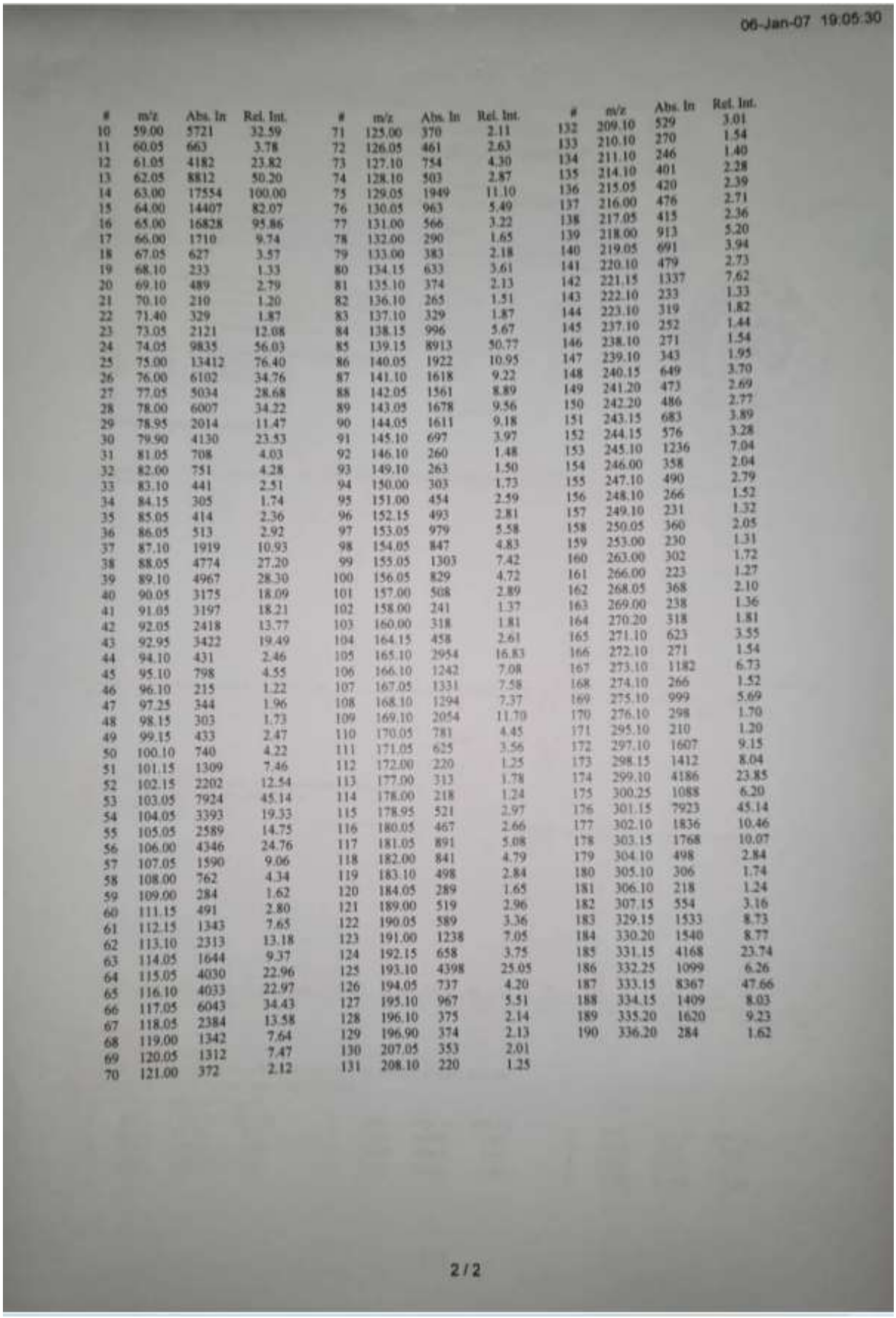
^{13}CNMR chart of compound **7**



IR chart of compound **7**



Mass chart of compound **7**



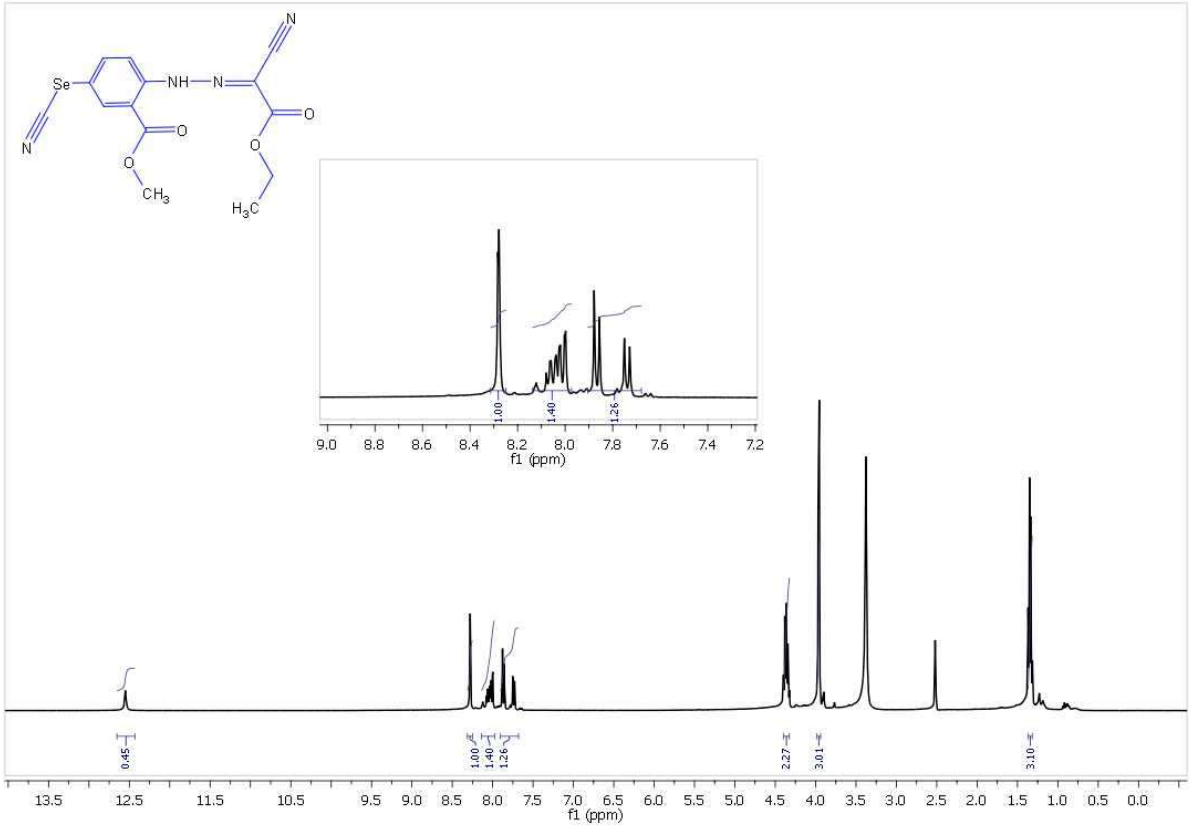
06-Jan-07 19:05:30

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	59.00	5721	32.59	71	125.00	370	2.11	132	209.10	529	3.01
11	60.05	663	3.78	72	126.05	461	2.63	133	210.10	270	1.54
12	61.05	4182	23.82	73	127.10	754	4.30	134	211.10	246	1.40
13	62.05	8812	50.20	74	128.10	503	2.87	135	214.10	401	2.28
14	63.00	17554	100.00	75	129.05	1949	11.10	136	215.05	420	2.39
15	64.00	14407	82.07	76	130.05	963	5.49	137	216.00	476	2.71
16	65.00	16828	95.86	77	131.00	566	3.22	138	217.05	415	2.36
17	66.00	1710	9.74	78	132.00	290	1.65	139	218.00	913	5.20
18	67.05	627	3.57	79	133.00	383	2.18	140	219.05	691	3.94
19	68.10	233	1.33	80	134.15	633	3.61	141	220.10	479	2.73
20	69.10	489	2.79	81	135.10	374	2.13	142	221.15	1337	7.62
21	70.10	210	1.20	82	136.10	265	1.51	143	222.10	233	1.33
22	71.40	329	1.87	83	137.10	329	1.87	144	223.10	319	1.82
23	73.05	2121	12.08	84	138.15	996	5.67	145	237.10	252	1.44
24	74.05	9835	56.03	85	139.15	8913	50.77	146	238.10	271	1.54
25	75.00	13412	76.40	86	140.05	1922	10.95	147	239.10	343	1.95
26	76.00	6102	34.76	87	141.10	1618	9.22	148	240.15	649	3.70
27	77.05	5034	28.68	88	142.05	1561	8.89	149	241.20	473	2.69
28	78.00	6007	34.22	89	143.05	1678	9.56	150	242.20	486	2.77
29	78.95	2014	11.47	90	144.05	1611	9.18	151	243.15	683	3.89
30	79.90	4130	23.53	91	145.10	697	3.97	152	244.15	576	3.28
31	81.05	708	4.03	92	146.10	260	1.48	153	245.10	1236	7.04
32	82.00	751	4.28	93	149.10	263	1.50	154	246.00	358	2.04
33	83.10	441	2.51	94	150.00	303	1.73	155	247.10	490	2.79
34	84.15	305	1.74	95	151.00	454	2.59	156	248.10	266	1.52
35	85.05	414	2.36	96	152.15	493	2.81	157	249.10	231	1.32
36	86.05	513	2.92	97	153.05	979	5.58	158	250.05	360	2.05
37	87.10	1919	10.93	98	154.05	847	4.83	159	253.00	230	1.31
38	88.05	4774	27.20	99	155.05	1303	7.42	160	263.00	302	1.72
39	89.10	4967	28.30	100	156.05	829	4.72	161	266.00	223	1.27
40	90.05	3175	18.09	101	157.00	508	2.89	162	268.05	368	2.10
41	91.05	3197	18.21	102	158.00	241	1.37	163	269.00	238	1.36
42	92.05	2418	13.77	103	160.00	318	1.81	164	270.20	318	1.81
43	92.95	3422	19.49	104	164.15	458	2.61	165	271.10	623	3.55
44	94.10	431	2.46	105	165.10	2954	16.83	166	272.10	271	1.54
45	95.10	798	4.55	106	166.10	1242	7.08	167	273.10	1182	6.73
46	96.10	215	1.22	107	167.05	1331	7.58	168	274.10	266	1.52
47	97.25	344	1.96	108	168.10	1294	7.37	169	275.10	999	5.69
48	98.15	303	1.73	109	169.10	2054	11.70	170	276.10	298	1.70
49	99.15	433	2.47	110	170.05	781	4.45	171	295.10	210	1.20
50	100.10	740	4.22	111	171.05	625	3.56	172	297.10	1607	9.15
51	101.15	1309	7.46	112	172.00	220	1.25	173	298.15	1412	8.04
52	102.15	2202	12.54	113	177.00	313	1.78	174	299.10	4186	23.85
53	103.05	7924	45.14	114	178.00	218	1.24	175	300.25	1088	6.20
54	104.05	3393	19.33	115	178.95	521	2.97	176	301.15	7923	45.14
55	105.05	2589	14.75	116	180.05	467	2.66	177	302.10	1836	10.46
56	106.00	4346	24.76	117	181.05	891	5.08	178	303.15	1768	10.07
57	107.05	1590	9.06	118	182.00	841	4.79	179	304.10	498	2.84
58	108.00	762	4.34	119	183.10	498	2.84	180	305.10	306	1.74
59	109.00	284	1.62	120	184.05	289	1.65	181	306.10	218	1.24
60	111.15	491	2.80	121	189.00	519	2.96	182	307.15	554	3.16
61	112.15	1343	7.65	122	190.05	589	3.36	183	329.15	1533	8.73
62	113.10	2313	13.18	123	191.00	1238	7.05	184	330.20	1540	8.77
63	114.05	1644	9.37	124	192.15	658	3.75	185	331.15	4168	23.74
64	115.05	4030	22.96	125	193.10	4398	25.05	186	332.25	1099	6.26
65	116.10	4033	22.97	126	194.05	737	4.20	187	333.15	8367	47.66
66	117.05	6043	34.43	127	195.10	967	5.51	188	334.15	1409	8.03
67	118.05	2384	13.58	128	196.10	375	2.14	189	335.20	1620	9.23
68	119.00	1342	7.64	129	196.90	374	2.13	190	336.20	284	1.62
69	120.05	1312	7.47	130	207.05	353	2.01				
70	121.00	372	2.12	131	208.10	220	1.25				

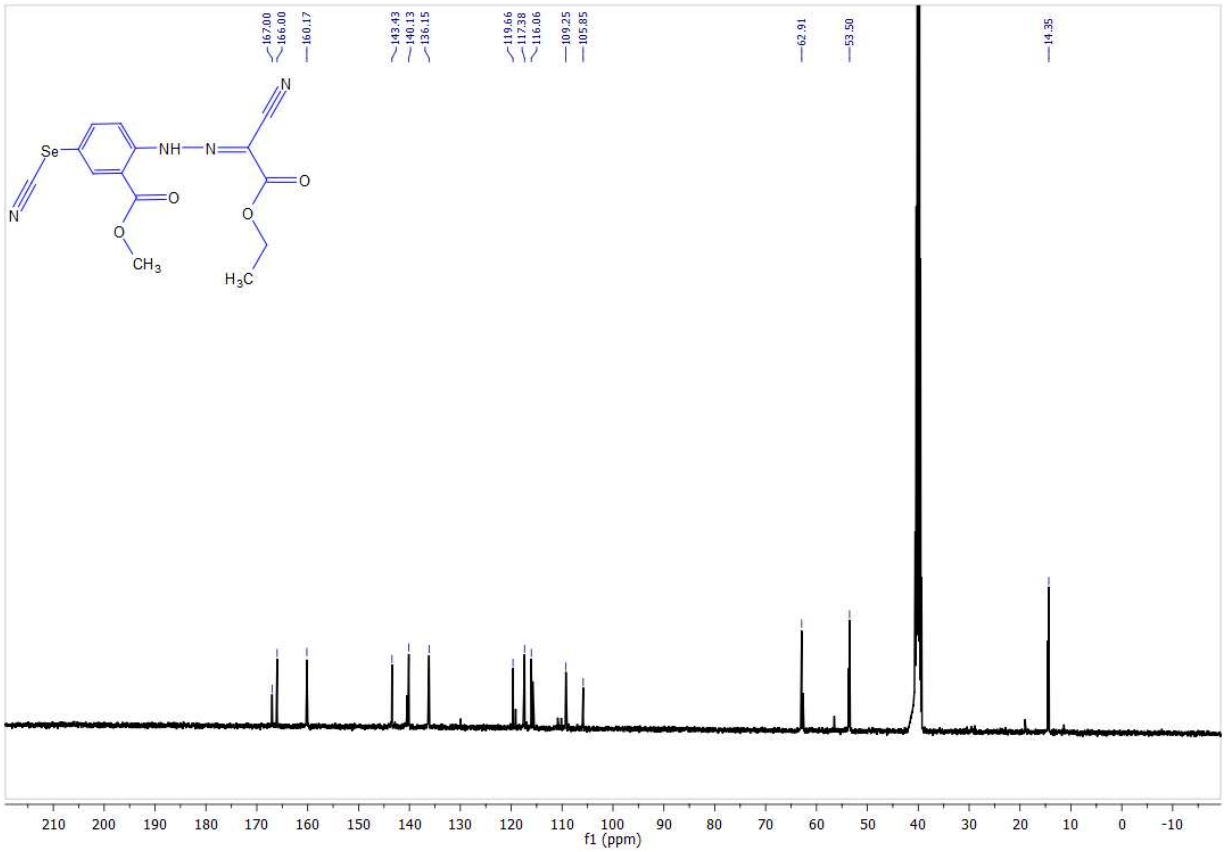
2 / 2

Mass chart of compound **7**

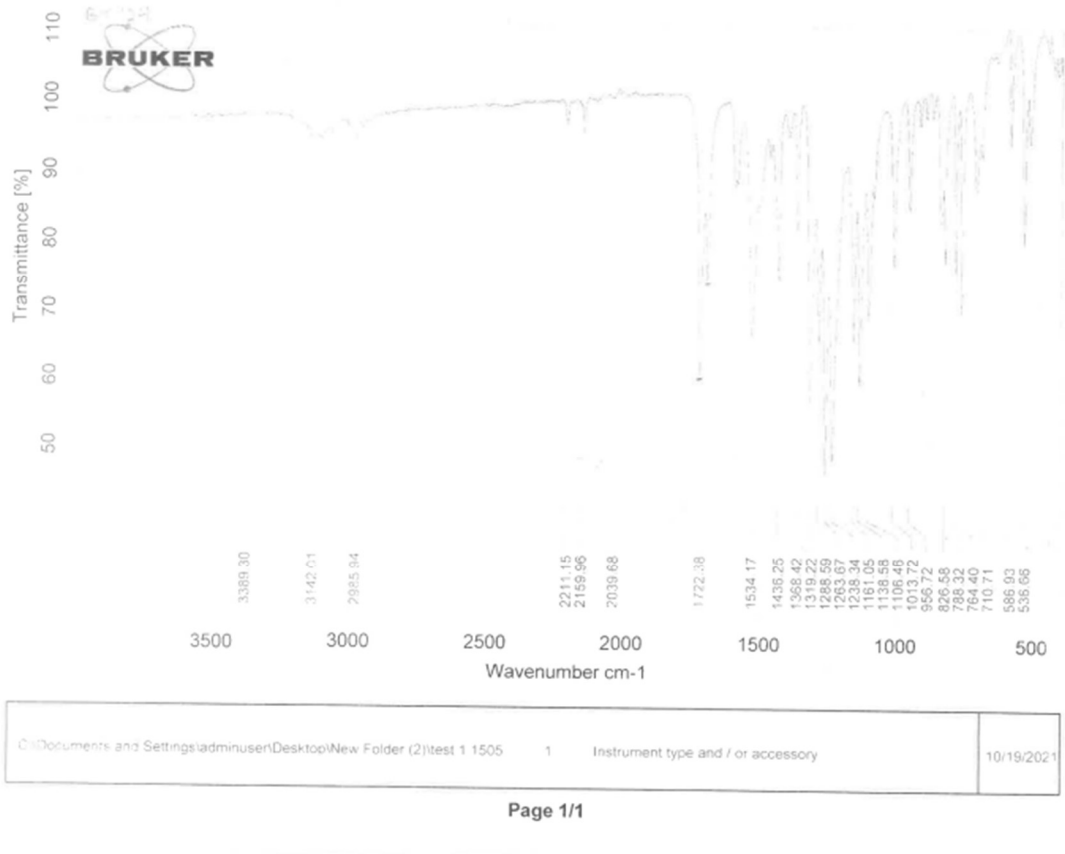
*Methyl 2-(2-(1-cyano-2-ethoxy-2-oxoethylidene) hydrazinyl)-5-selenocyanatobenzoate (**8**).*



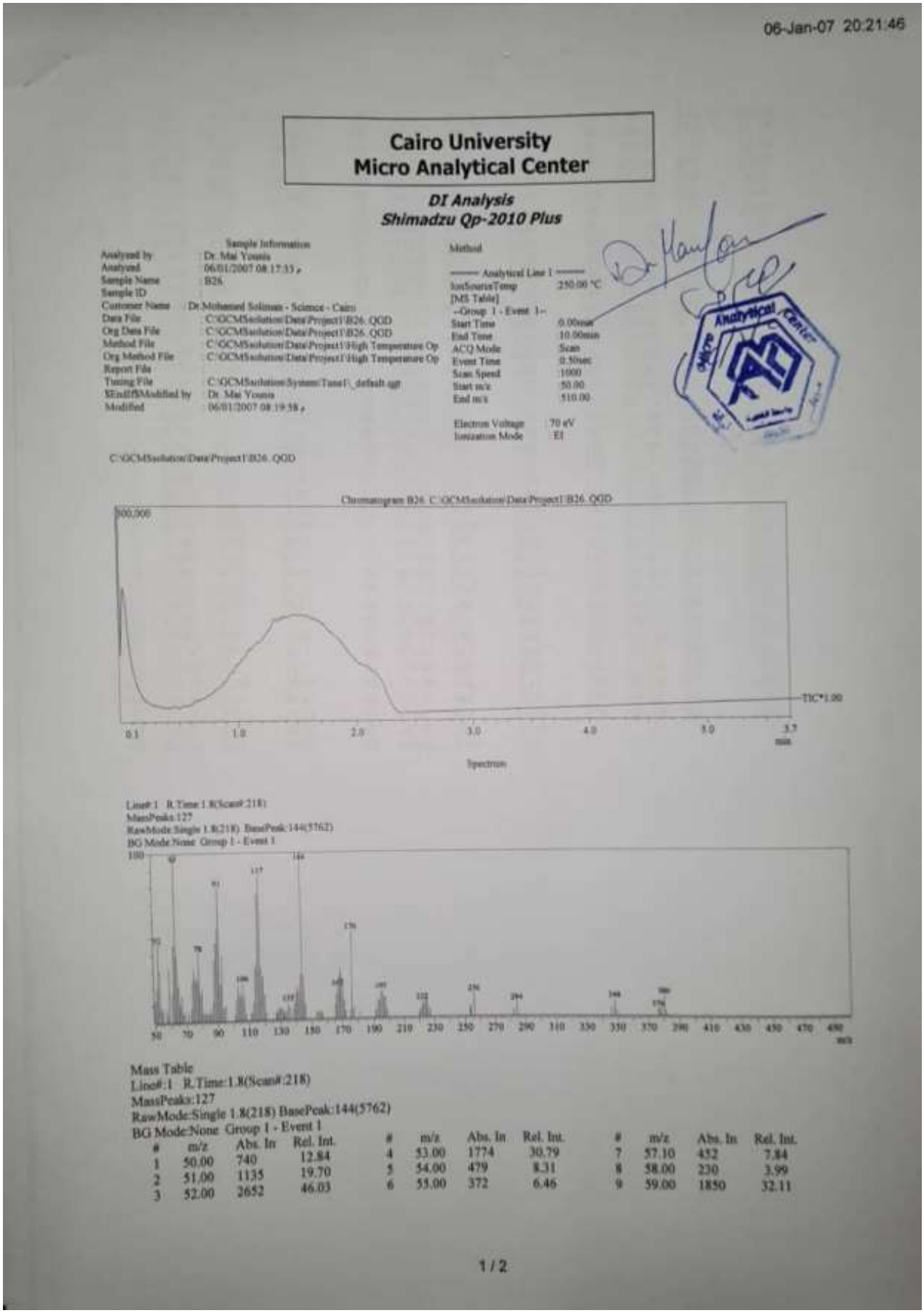
^{1}HNMR chart of compound **8**



^{13}CNMR chart of compound **8**



IR chart of compound **8**



06-Jan-07 20:21:46

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

Analyzed by	Dr. Mai Younis
Analyzed	06/01/2007 08:17:33
Sample Name	B26
Sample ID	
Customer Name	Dr.Mohamed Soliman - Science - Cairo
Data File	C:\GCMSsolution\Data\Project1\B26. QGD
Org Data File	C:\GCMSsolution\Data\Project1\B26. QGD
Method File	C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File	C:\GCMSsolution\Data\Project1\High Temperature Op
Report File	
Tuning File	C:\GCMSsolution\System\Tune1_default.qgt
ReEdit/Modified by	Dr. Mai Younis
Modified	06/01/2007 08:19:58

Method

Analytical Line 1	
IonSourceTemp	250.00 °C
[MS Table]	
--Group 1 - Event 1--	
Start Time	0.00min
End Time	10.00min
ACQ Mode	Scan
Event Time	0.50sec
Scan Speed	1000
Start m/z	50.00
End m/z	510.00
Electron Voltage	70 eV
Ionization Mode	EI

C:\GCMSsolution\Data\Project1\B26. QGD

Chromatogram B26. C:\GCMSsolution\Data\Project1\B26. QGD

Spectrum

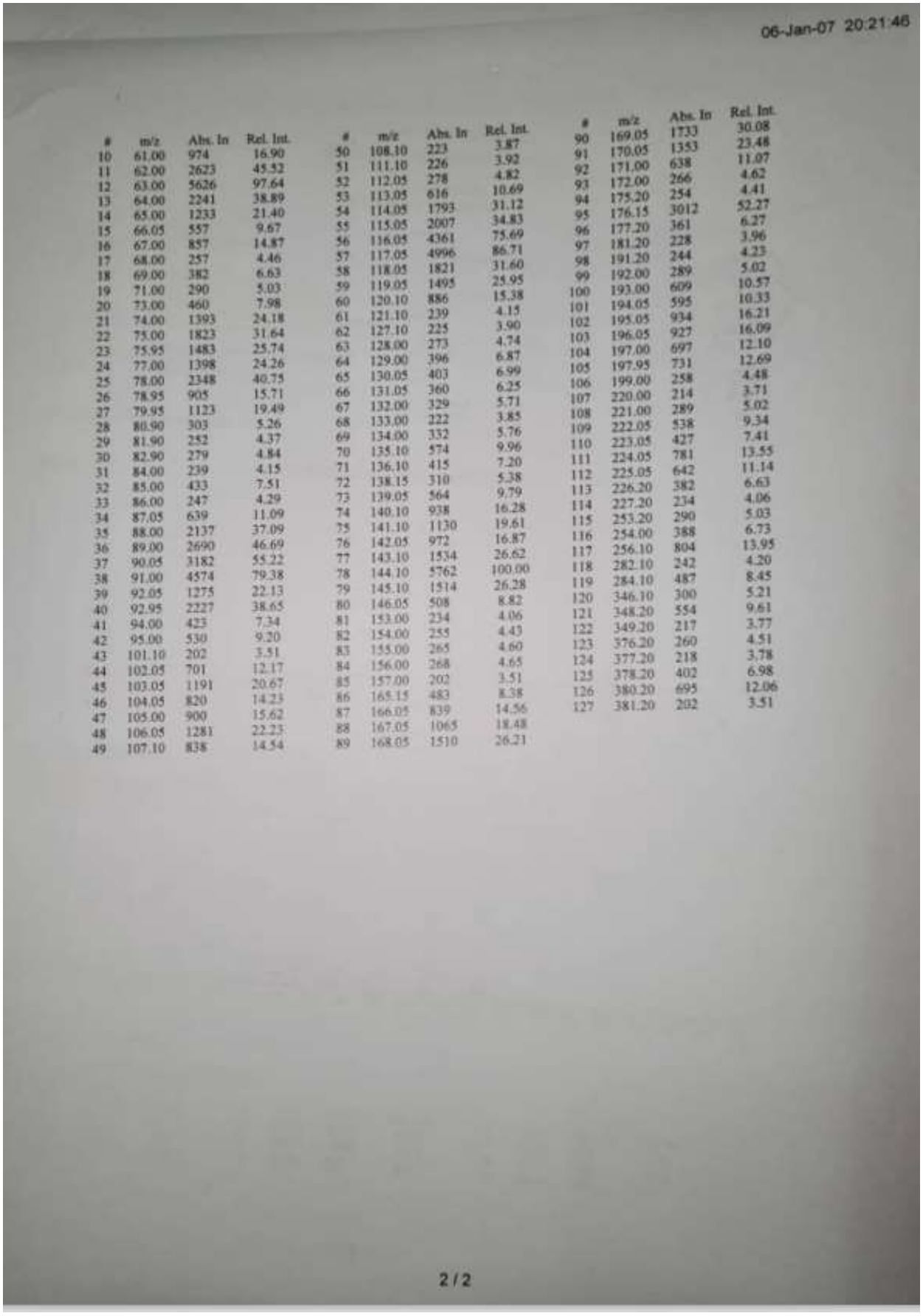
Line#:1 R.Time:1.8(Scan#:218)
MassPeaks:127
RawMode:Single 1.8(218) BasePeak:144(5762)
BG Mode:None Group 1 - Event 1

Mass Table
Line#:1 R.Time:1.8(Scan#:218)
MassPeaks:127
RawMode:Single 1.8(218) BasePeak:144(5762)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	740	12.84	4	53.00	1774	30.79	7	57.10	452	7.84
2	51.00	1135	19.70	5	54.00	479	8.31	8	58.00	230	3.99
3	52.00	2652	46.03	6	55.00	372	6.46	9	59.00	1850	32.11

1 / 2

Mass chart of compound **8**



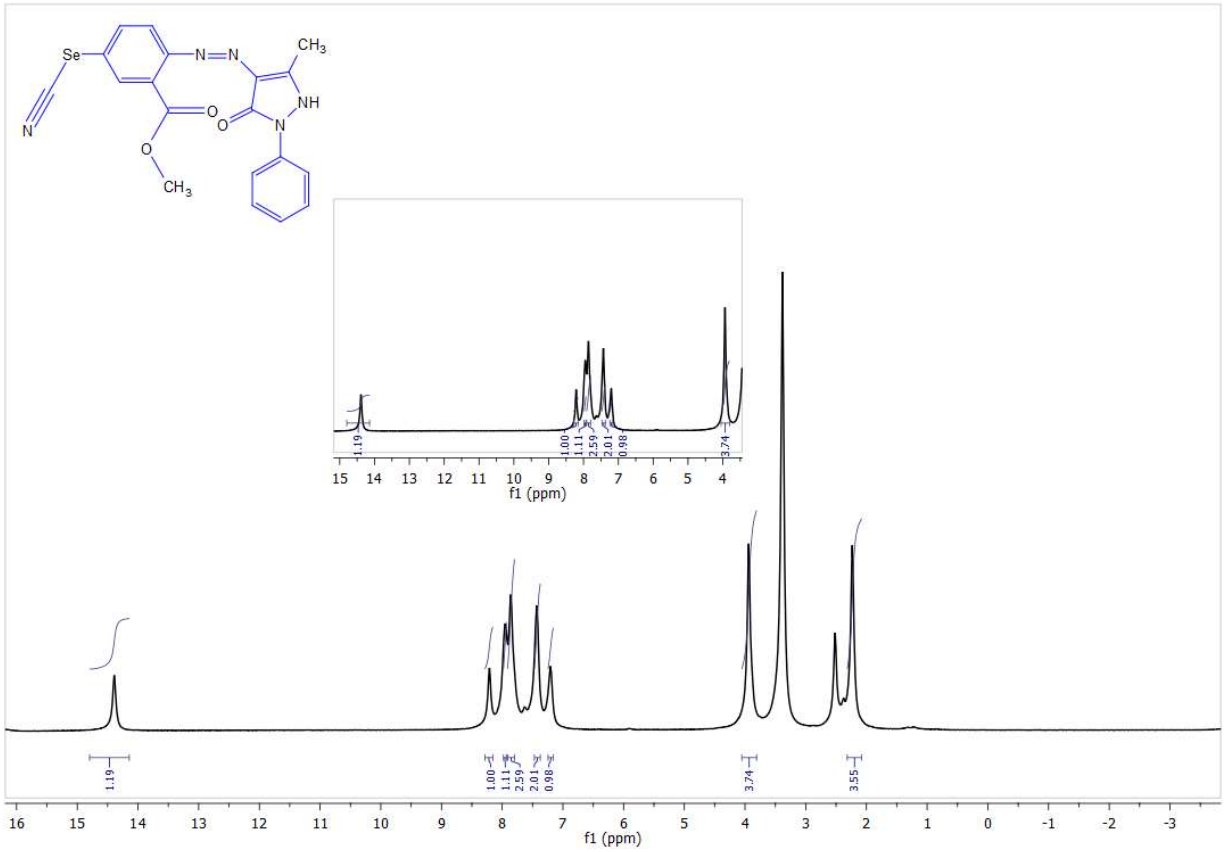
06-Jan-07 20:21:46

#	m/z	Abs. In	Rel. Int.
10	61.00	974	16.90
11	62.00	2623	45.52
12	63.00	5626	97.64
13	64.00	2241	38.89
14	65.00	1233	21.40
15	66.05	557	9.67
16	67.00	857	14.87
17	68.00	257	4.46
18	69.00	382	6.63
19	71.00	290	5.03
20	73.00	460	7.98
21	74.00	1393	24.18
22	75.00	1823	31.64
23	75.95	1483	25.74
24	77.00	1398	24.26
25	78.00	2348	40.75
26	78.95	905	15.71
27	79.95	1123	19.49
28	80.90	303	5.26
29	81.90	252	4.37
30	82.90	279	4.84
31	84.00	239	4.15
32	85.00	433	7.51
33	86.00	247	4.29
34	87.05	639	11.09
35	88.00	2137	37.09
36	89.00	2690	46.69
37	90.05	3182	55.22
38	91.00	4574	79.38
39	92.05	1275	22.13
40	92.95	2227	38.65
41	94.00	423	7.34
42	95.00	530	9.20
43	101.10	202	3.51
44	102.05	701	12.17
45	103.05	1191	20.67
46	104.05	820	14.23
47	105.00	900	15.62
48	106.05	1281	22.23
49	107.10	838	14.54
50	108.10	223	3.87
51	111.10	226	3.92
52	112.05	278	4.82
53	113.05	616	10.69
54	114.05	1793	31.12
55	115.05	2007	34.83
56	116.05	4361	75.69
57	117.05	4996	86.71
58	118.05	1821	31.60
59	119.05	1495	25.95
60	120.10	886	15.38
61	121.10	239	4.15
62	127.10	225	3.90
63	128.00	273	4.74
64	129.00	396	6.87
65	130.05	403	6.99
66	131.05	360	6.25
67	132.00	329	5.71
68	133.00	222	3.85
69	134.00	332	5.76
70	135.10	574	9.96
71	136.10	415	7.20
72	138.15	310	5.38
73	139.05	564	9.79
74	140.10	938	16.28
75	141.10	1130	19.61
76	142.05	972	16.87
77	143.10	1534	26.62
78	144.10	5762	100.00
79	145.10	1514	26.28
80	146.05	508	8.82
81	153.00	234	4.06
82	154.00	255	4.43
83	155.00	265	4.60
84	156.00	268	4.65
85	157.00	202	3.51
86	165.15	483	8.38
87	166.05	839	14.56
88	167.05	1065	18.48
89	168.05	1510	26.21
90	169.05	1733	30.08
91	170.05	1353	23.48
92	171.00	638	11.07
93	172.00	266	4.62
94	175.20	254	4.41
95	176.15	3012	52.27
96	177.20	361	6.27
97	181.20	228	3.96
98	191.20	244	4.23
99	192.00	289	5.02
100	193.00	609	10.57
101	194.05	595	10.33
102	195.05	934	16.21
103	196.05	927	16.09
104	197.00	697	12.10
105	197.95	731	12.69
106	199.00	258	4.48
107	220.00	214	3.71
108	221.00	289	5.02
109	222.05	538	9.34
110	223.05	427	7.41
111	224.05	781	13.55
112	225.05	642	11.14
113	226.20	382	6.63
114	227.20	234	4.06
115	253.20	290	5.03
116	254.00	388	6.73
117	256.10	804	13.95
118	282.10	242	4.20
119	284.10	487	8.45
120	346.10	300	5.21
121	348.20	554	9.61
122	349.20	217	3.77
123	376.20	260	4.51
124	377.20	218	3.78
125	378.20	402	6.98
126	380.20	695	12.06
127	381.20	202	3.51

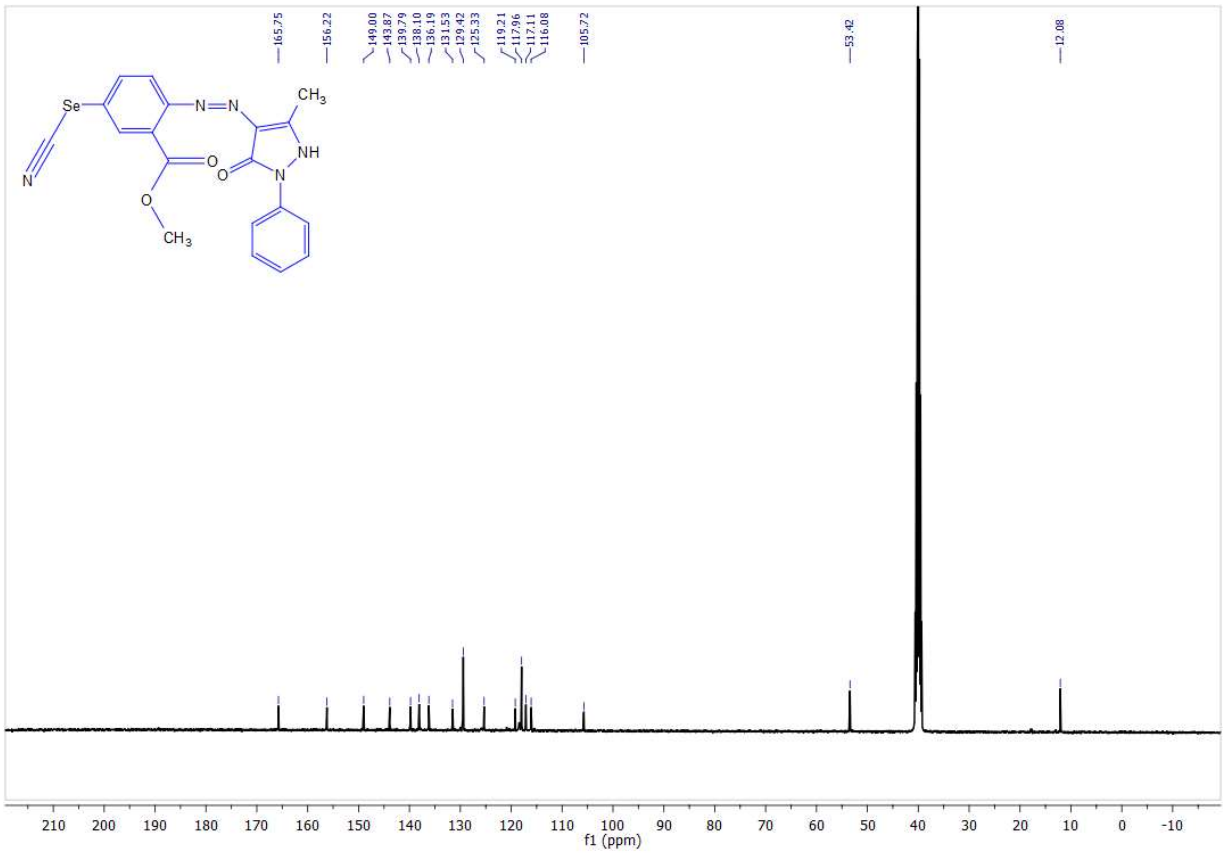
2 / 2

Mass chart of compound **8**

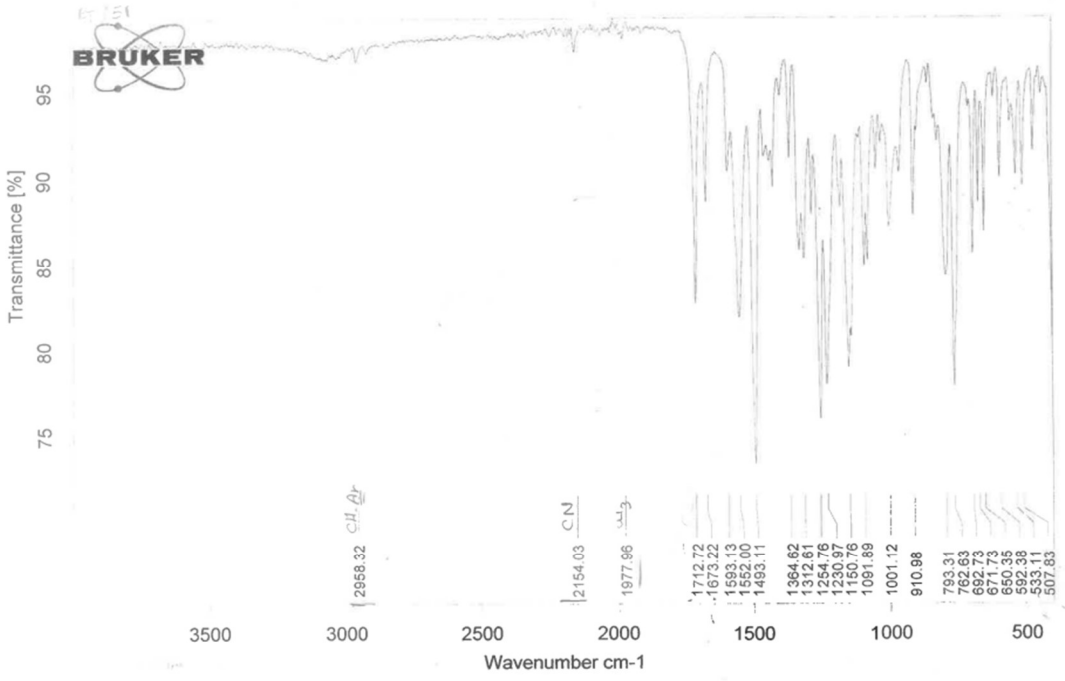
*Methyl2-((5-methyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)diazenyl)-5-selenocyanatobenzoate (**9**).*



^{1}HNMR chart of compound **9**



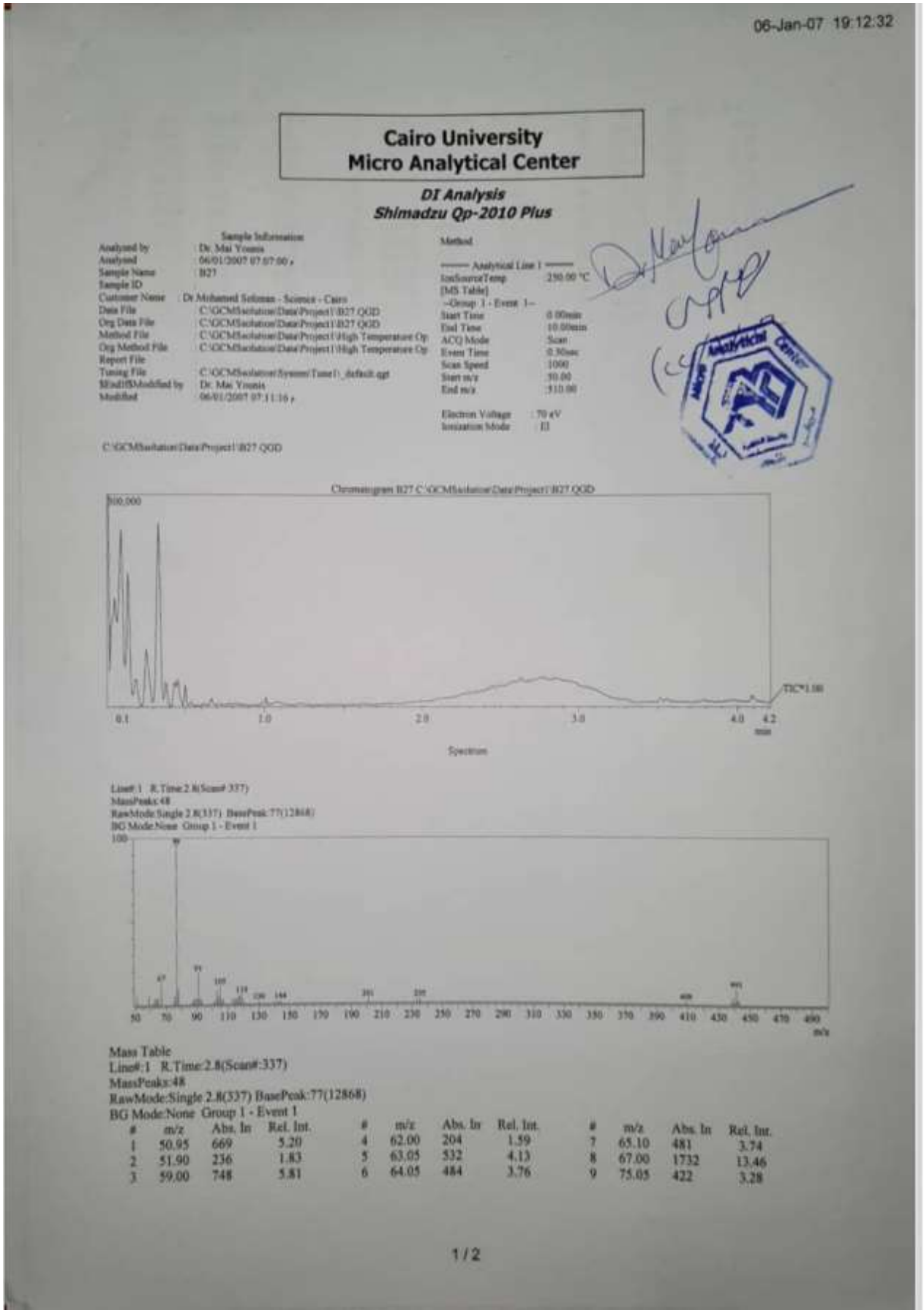
^{13}CNMR chart of compound **9**



C:\Documents and Settings\adminuser\Desktop\New Folder (2)\test 1.1597	1: Instrument type and / or accessory	11/25/2021

Page 1/1

IR chart of compound **9**



06-Jan-07 19:12:32

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

Analyzed by	Dr. Mai Younis
Analyzed	06/01/2007 07:07:00 م
Sample Name	B27
Sample ID	
Customer Name	Dr Mohamed Soliman - Science - Cairo
Data File	C:\GCMSsolution\Data\Project1\B27.QGD
Org Data File	C:\GCMSsolution\Data\Project1\B27.QGD
Method File	C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File	C:\GCMSsolution\Data\Project1\High Temperature Op
Report File	
Tuning File	C:\GCMSsolution\System\Tune1_default.qgt
Modified by	Dr. Mai Younis
Modified	06/01/2007 07:11:16 م

Method

Analytical Line 1	
IonSourceTemp	250.00 °C
[MS Table]	
--Group 1 - Event 1--	
Start Time	0.00min
End Time	10.00min
ACQ Mode	Scan
Event Time	0.30sec
Scan Speed	1000
Start m/z	50.00
End m/z	510.00
Electron Voltage	70 eV
Ionization Mode	EI

C:\GCMSsolution\Data\Project1\B27.QGD

Chromatogram B27 C:\GCMSsolution\Data\Project1\B27.QGD

Spectrum

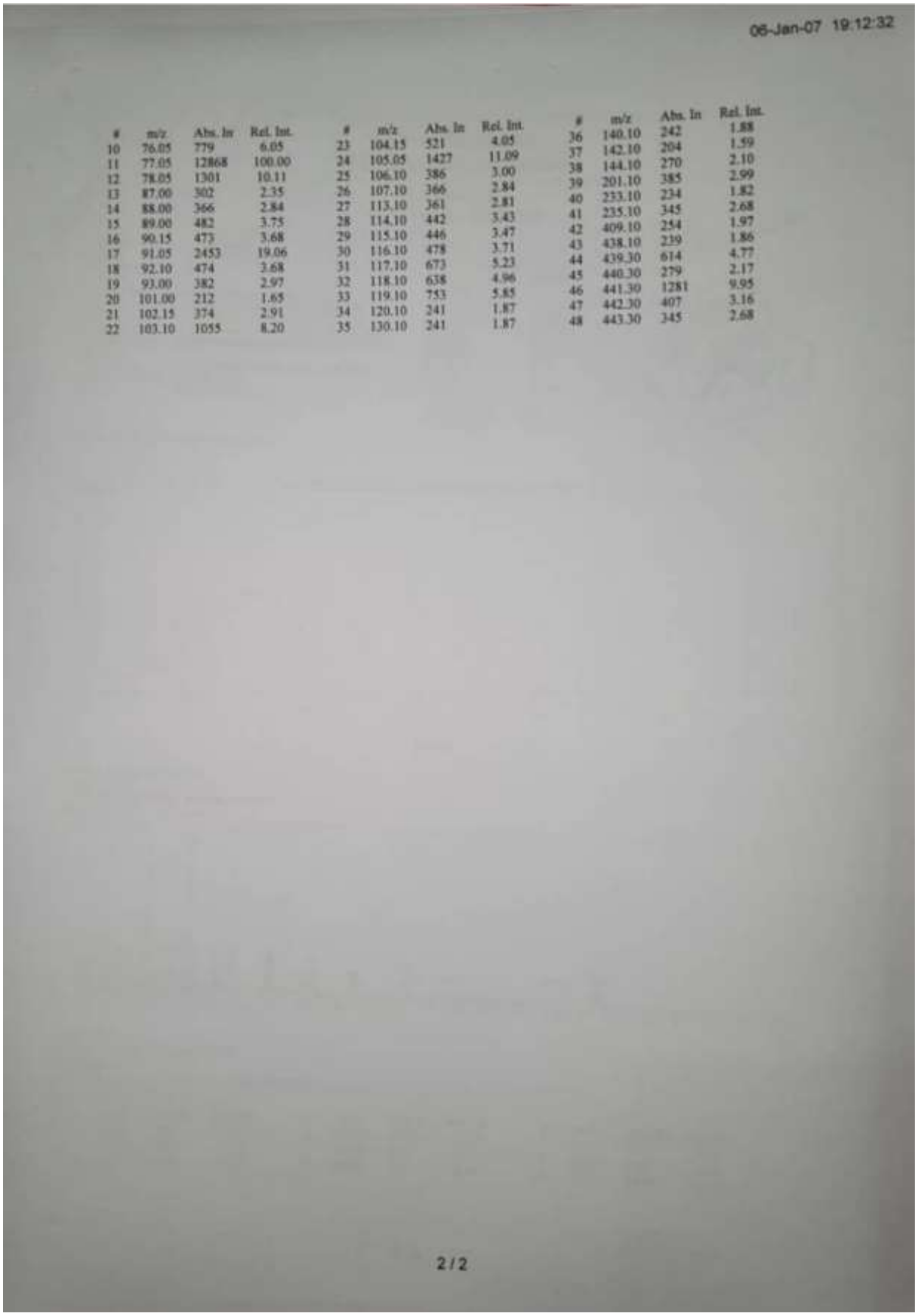
Line#:1 R.Time:2.8(Scan#:337)
MassPeaks:48
RawMode:Single 2.8(337) BasePeak:77(12868)
BG Mode:None Group 1 - Event 1

Mass Table
Line#:1 R.Time:2.8(Scan#:337)
MassPeaks:48
RawMode:Single 2.8(337) BasePeak:77(12868)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.95	669	5.20	4	62.00	204	1.59	7	65.10	481	3.74
2	51.90	236	1.83	5	63.05	532	4.13	8	67.00	1732	13.46
3	59.00	748	5.81	6	64.05	484	3.76	9	75.05	422	3.28

1 / 2

Mass chart of compound **9**



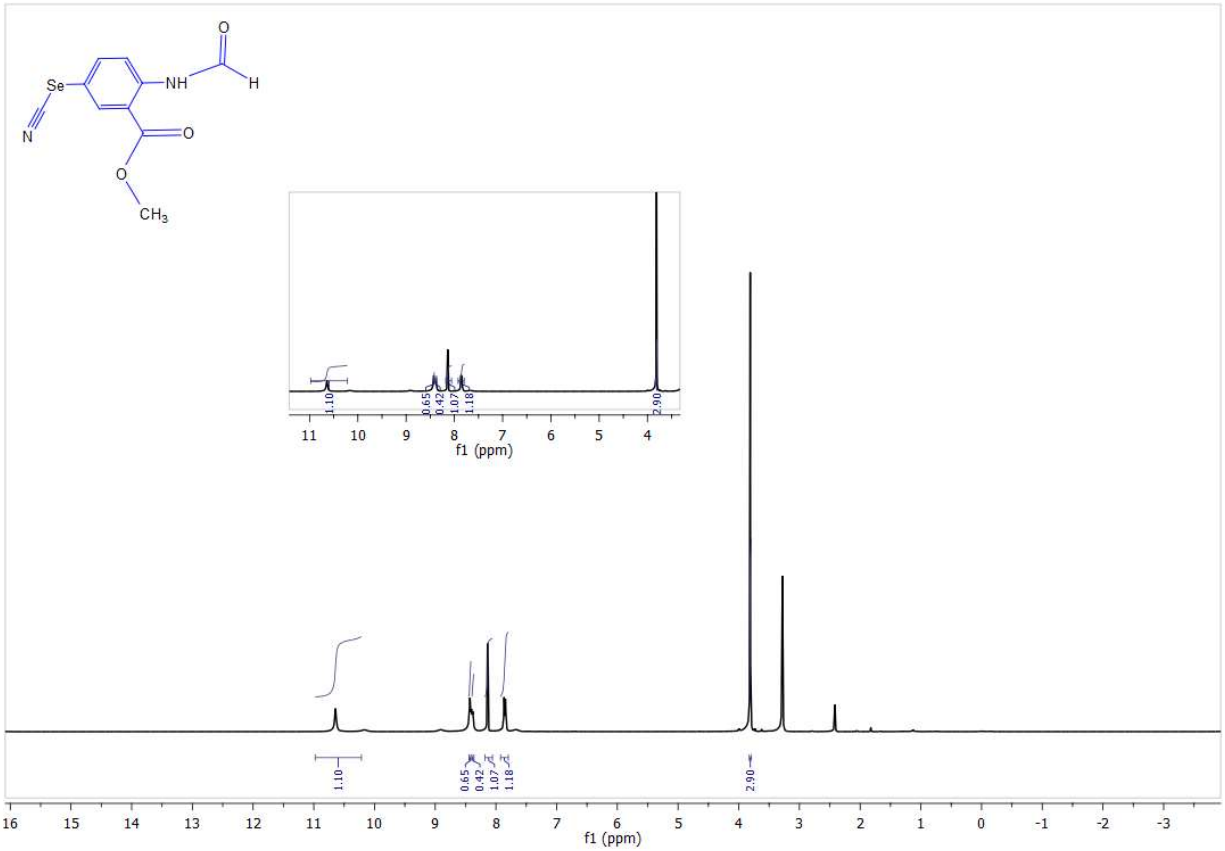
06-Jan-07 19:12:32

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	76.05	779	6.05	23	104.15	521	4.05	36	140.10	242	1.88
11	77.05	12868	100.00	24	105.05	1427	11.09	37	142.10	204	1.59
12	78.05	1301	10.11	25	106.10	386	3.00	38	144.10	270	2.10
13	87.00	302	2.35	26	107.10	366	2.84	39	201.10	385	2.99
14	88.00	366	2.84	27	113.10	361	2.81	40	233.10	234	1.82
15	89.00	482	3.75	28	114.10	442	3.43	41	235.10	345	2.68
16	90.15	473	3.68	29	115.10	446	3.47	42	409.10	254	1.97
17	91.05	2453	19.06	30	116.10	478	3.71	43	438.10	239	1.86
18	92.10	474	3.68	31	117.10	673	5.23	44	439.30	614	4.77
19	93.00	382	2.97	32	118.10	638	4.96	45	440.30	279	2.17
20	101.00	212	1.65	33	119.10	753	5.85	46	441.30	1281	9.95
21	102.15	374	2.91	34	120.10	241	1.87	47	442.30	407	3.16
22	103.10	1055	8.20	35	130.10	241	1.87	48	443.30	345	2.68

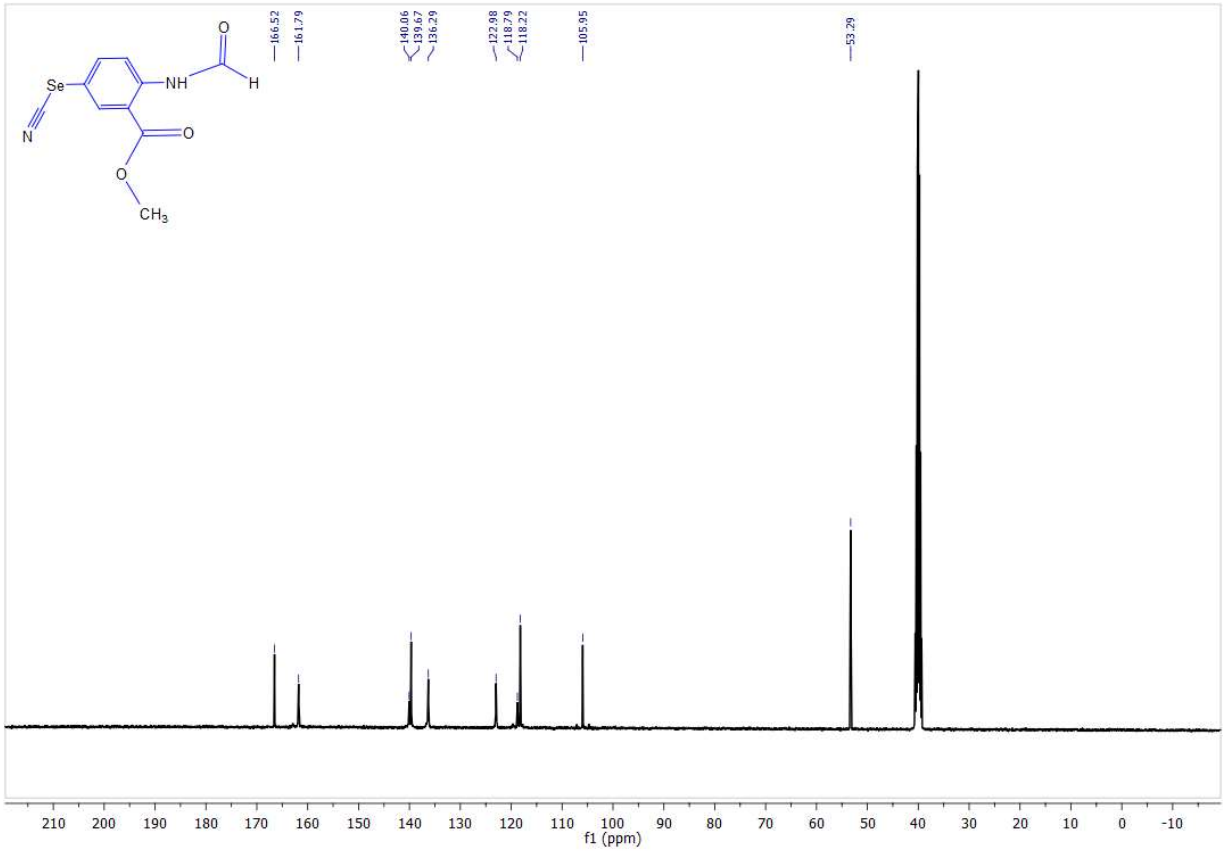
2 / 2

Mass chart of compound **9**

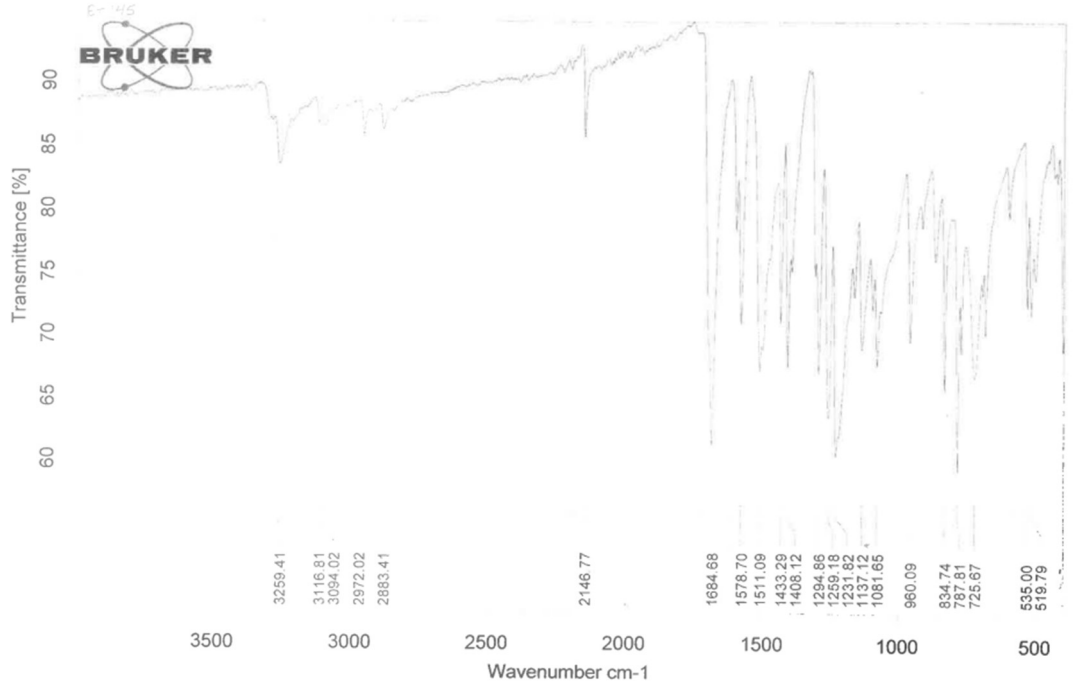
*Methyl 2-formamido-5-selenocyanatobenzoate (**10**).*



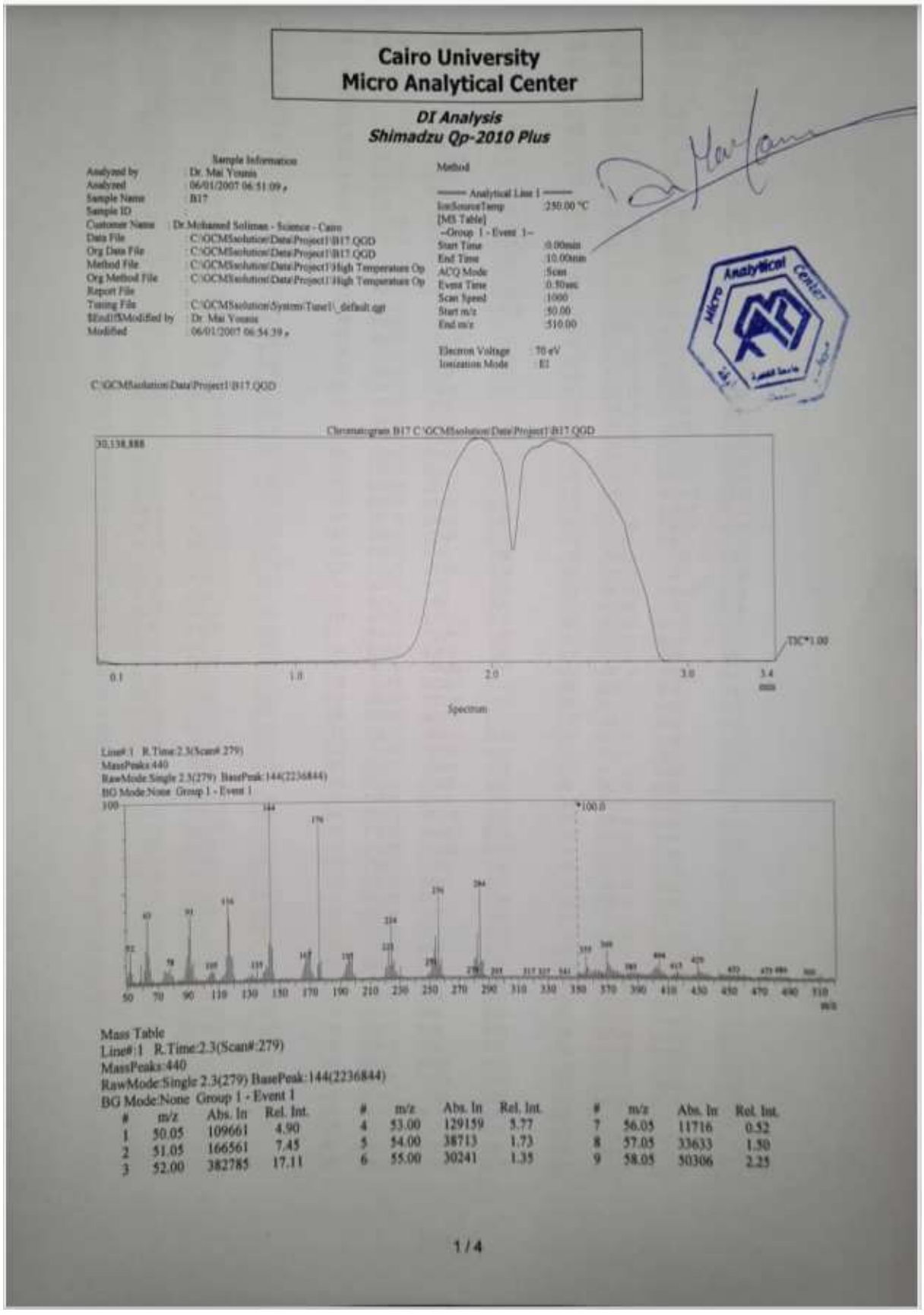
^{1}HNMR chart of compound **10**



^{13}CNMR chart of compound **10**



IR chart of compound **10**



Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

Analyzed by	Dr. Mai Younis
Analyzed	06/01/2007 06:51:09 م
Sample Name	B17
Sample ID	
Customer Name	Dr.Mohamed Soliman - Science - Cairo
Data File	C:\GCMSolution\Data\Project1\B17.QGD
Org Data File	C:\GCMSolution\Data\Project1\B17.QGD
Method File	C:\GCMSolution\Data\Project1\High Temperature Op
Org Method File	C:\GCMSolution\Data\Project1\High Temperature Op
Report File	
Tuning File	C:\GCMSolution\System\Tune1_default.qgt
Modified by	Dr. Mai Younis
Modified	06/01/2007 06:54:39 م

Method

Analytical Line 1	
IonSourceTemp	250.00 °C
[MS Table]	
--Group 1 - Event 1--	
Start Time	0.00min
End Time	10.00min
ACQ Mode	Scan
Event Time	0.50sec
Scan Speed	1000
Start m/z	50.00
End m/z	510.00
Electron Voltage	70 eV
Ionization Mode	EI

C:\GCMSolution\Data\Project1\B17.QGD

Chromatogram B17 C:\GCMSolution\Data\Project1\B17.QGD

30,138,888

TIC*1.00

0.1 1.0 2.0 3.0 3.4 min

Spectrum

Line#:1 R.Time:2.3(Scan#:279)
MassPeaks:440
RawMode:Single 2.3(279) BasePeak:144(2236844)
BG Mode:None Group 1 - Event 1

100 144 176 *100.0

50 70 90 110 130 150 170 190 210 230 250 270 290 310 330 350 370 390 410 430 450 470 490 510 m/z

Mass Table
Line#:1 R.Time:2.3(Scan#:279)
MassPeaks:440
RawMode:Single 2.3(279) BasePeak:144(2236844)
BG Mode:None Group 1 - Event 1

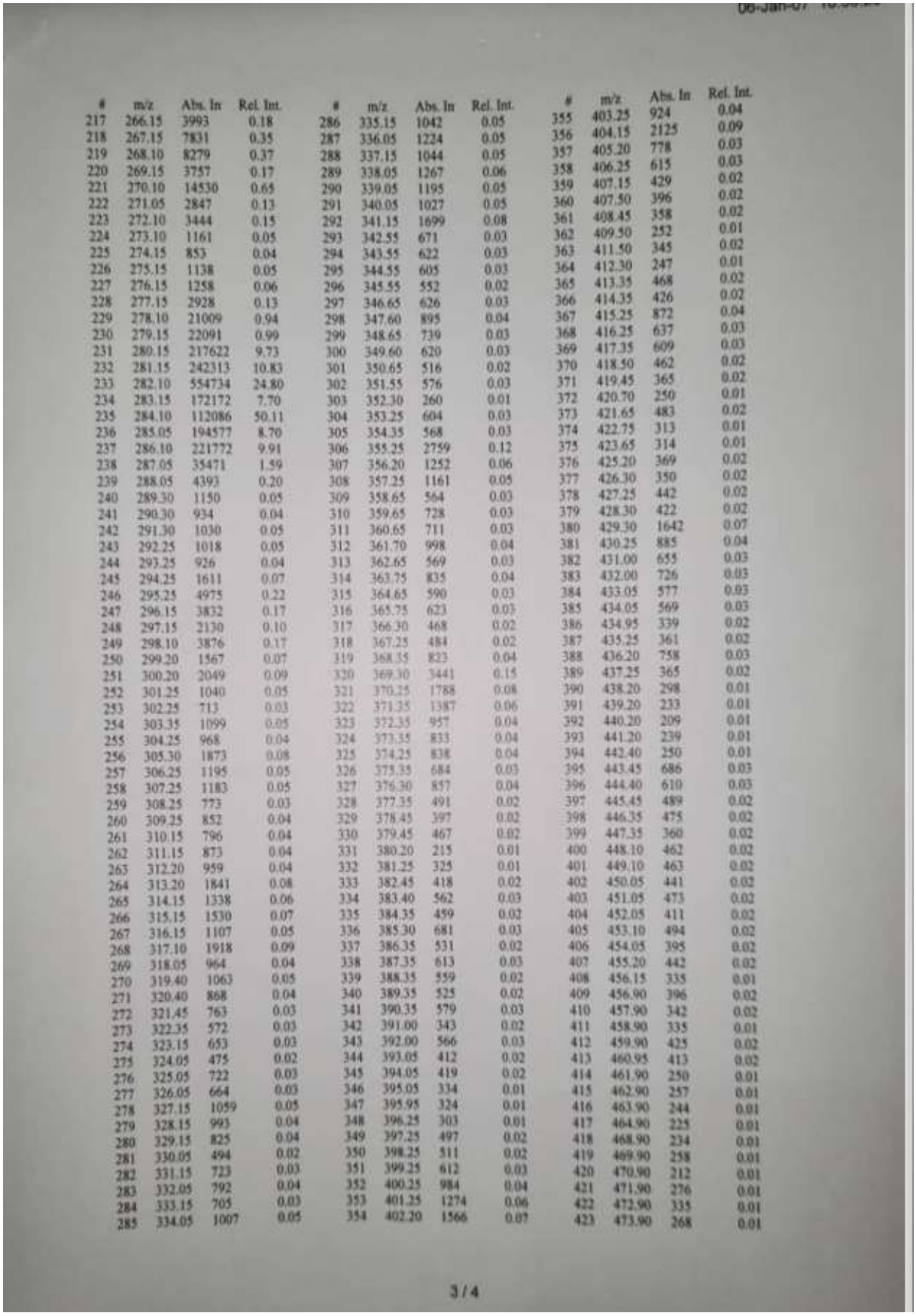
#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	109661	4.90	4	53.00	129159	5.77	7	56.05	11716	0.52
2	51.05	166561	7.45	5	54.00	38713	1.73	8	57.05	33633	1.50
3	52.00	382785	17.11	6	55.00	30241	1.35	9	58.05	50306	2.25

1 / 4

Mass chart of compound **10**

#	m/z	Abs. In	Rel. Int.
10	58.95	248038	11.09
11	60.05	37046	1.66
12	61.05	171368	7.66
13	62.05	405699	18.14
14	63.00	790895	35.36
15	64.00	340220	15.21
16	65.00	175745	7.86
17	66.00	43822	1.96
18	67.00	27620	1.23
19	68.05	17799	0.80
20	69.05	22727	1.02
21	70.15	13106	0.59
22	71.10	23615	1.06
23	72.05	14990	0.67
24	73.05	57567	2.57
25	74.05	155034	6.93
26	75.05	151885	6.79
27	76.05	139269	6.23
28	77.05	124039	5.55
29	78.05	196182	8.77
30	79.10	96289	4.30
31	80.05	79250	3.54
32	81.05	25263	1.13
33	82.05	21681	0.97
34	83.15	33708	1.51
35	84.15	34112	1.53
36	85.10	47278	2.11
37	86.05	30547	1.37
38	87.15	76498	3.42
39	88.15	204197	9.13
40	89.15	323167	14.45
41	90.15	570146	25.49
42	91.05	821014	36.70
43	92.05	187284	8.37
44	93.00	248361	11.10
45	94.05	36015	1.61
46	95.00	62678	2.80
47	96.15	16798	0.75
48	97.15	32440	1.45
49	98.15	26792	1.20
50	99.10	29567	1.32
51	100.05	17202	0.77
52	101.15	28430	1.27
53	102.15	47338	2.12
54	103.10	73967	3.31
55	104.15	92825	4.15
56	105.10	144042	6.44
57	106.05	122516	5.48
58	107.10	121215	5.42
59	108.00	29655	1.33
60	109.10	17502	0.78
61	110.15	17774	0.79
62	111.15	37661	1.68
63	112.15	46156	2.06
64	113.05	76707	3.43
65	114.15	107105	4.79
66	115.15	316300	14.14
67	116.15	943917	42.20
68	117.05	758447	33.91
69	118.10	322599	14.42
70	119.05	289581	12.95
71	120.05	80684	3.61
72	121.10	19041	0.85
73	122.15	12399	0.55
74	123.15	11324	0.51
75	124.15	6748	0.30
76	125.15	16084	0.72
77	126.15	20881	0.93
78	127.10	31537	1.41
79	128.10	38044	1.70
80	129.10	47119	2.11
81	130.10	50866	2.27
82	131.15	59939	2.68
83	132.10	94556	4.23
84	133.15	26411	1.18
85	134.15	44017	1.97
86	135.10	137478	6.15
87	136.10	22551	1.01
88	137.15	22836	1.02
89	138.15	39326	1.76
90	139.05	96165	4.30
91	140.10	117126	5.24
92	141.05	190298	8.51
93	142.10	173746	7.77
94	143.15	461224	20.62
95	144.10	223684	100.00
96	145.05	407435	18.21
97	146.05	116539	5.21
98	147.10	25393	1.14
99	148.10	9620	0.43
100	149.15	10612	0.47
101	150.15	22430	1.00
102	151.10	30009	1.34
103	152.05	14428	0.65
104	153.00	22937	1.03
105	154.05	20315	0.91
106	155.00	25121	1.12
107	156.00	18710	0.84
108	157.05	18190	0.81
109	158.05	17399	0.78
110	159.05	8855	0.40
111	160.05	10300	0.46
112	161.05	3907	0.17
113	162.05	5843	0.26
114	163.05	11311	0.51
115	164.05	27265	1.22
116	165.05	86175	3.85
117	166.05	169438	7.57
118	167.05	242637	10.85
119	168.05	275735	12.33
120	169.05	361299	16.15
121	170.00	399524	17.86
122	171.00	137100	6.13
123	172.00	77889	3.48
124	173.05	20440	0.91
125	174.15	20145	0.90
126	175.15	183799	8.22
127	176.10	195482	87.39
128	177.05	232465	10.39
129	178.05	37231	1.66
130	179.05	10931	0.49
131	180.05	6735	0.30
132	181.00	12223	0.55
133	182.00	7977	0.36
134	183.05	6187	0.28
135	184.00	5886	0.26
136	185.00	3644	0.16
137	186.00	2986	0.13
138	187.05	1991	0.09
139	188.05	1490	0.07
140	189.05	3736	0.17
141	190.05	16283	0.73
142	191.05	21724	0.97
143	192.05	51790	2.32
144	193.05	99157	4.43
145	194.05	174553	7.80
146	195.05	220661	9.86
147	196.05	315843	14.12
148	197.05	221630	9.91
149	198.00	332970	14.89
150	198.95	66888	2.99
151	200.00	55724	2.49
152	200.95	7102	0.32
153	201.95	1209	0.05
154	203.15	1180	0.05
155	204.15	1487	0.07
156	205.10	2825	0.13
157	206.10	3714	0.17
158	207.15	5696	0.25
159	208.05	8627	0.39
160	209.10	9858	0.44
161	210.05	12367	0.55
162	211.15	6149	0.27
163	212.10	19145	0.86
164	213.05	4154	0.19
165	214.05	4873	0.22
166	215.10	1366	0.06
167	216.05	1471	0.07
168	217.15	2322	0.10
169	218.10	11678	0.52
170	219.15	19188	0.86
171	220.10	122052	5.46
172	221.15	153624	6.87
173	222.05	327911	14.66
174	223.15	164908	7.37
175	224.05	664483	29.71
176	225.05	173844	7.77
177	226.05	230824	10.32
178	227.05	72362	3.24
179	228.05	91204	4.08
180	229.15	29097	1.30
181	230.10	145849	6.52
182	231.05	21762	0.97
183	232.10	29526	1.32
184	233.05	4955	0.22
185	234.15	1888	0.08
186	235.10	2953	0.13
187	236.15	1818	0.08
188	237.10	4244	0.19
189	238.15	2684	0.12
190	239.10	4319	0.19
191	240.15	2851	0.13
192	241.10	4428	0.20
193	242.10	3199	0.14
194	243.15	1666	0.07
195	244.10	3049	0.14
196	245.15	1847	0.08
197	246.15	2790	0.12
198	247.10	13729	0.61
199	248.15	16080	0.72
200	249.10	51572	2.31
201	250.15	54456	2.43
202	251.15	130744	5.85
203	252.15	224754	10.05
204	253.15	343150	15.34
205	254.10	517751	23.15
206	255.15	196030	8.76
207	256.10	104249	46.61
208	257.05	153740	6.87
209	258.10	237652	10.62
210	259.05	37170	1.66
211	260.05	11779	0.53
212	260.95	2812	0.13
213	261.95	931	0.04
214	263.15	1654	0.07
215	264.15	2174	0.10
216	265.15	3066	0.14

Mass chart of compound **10**

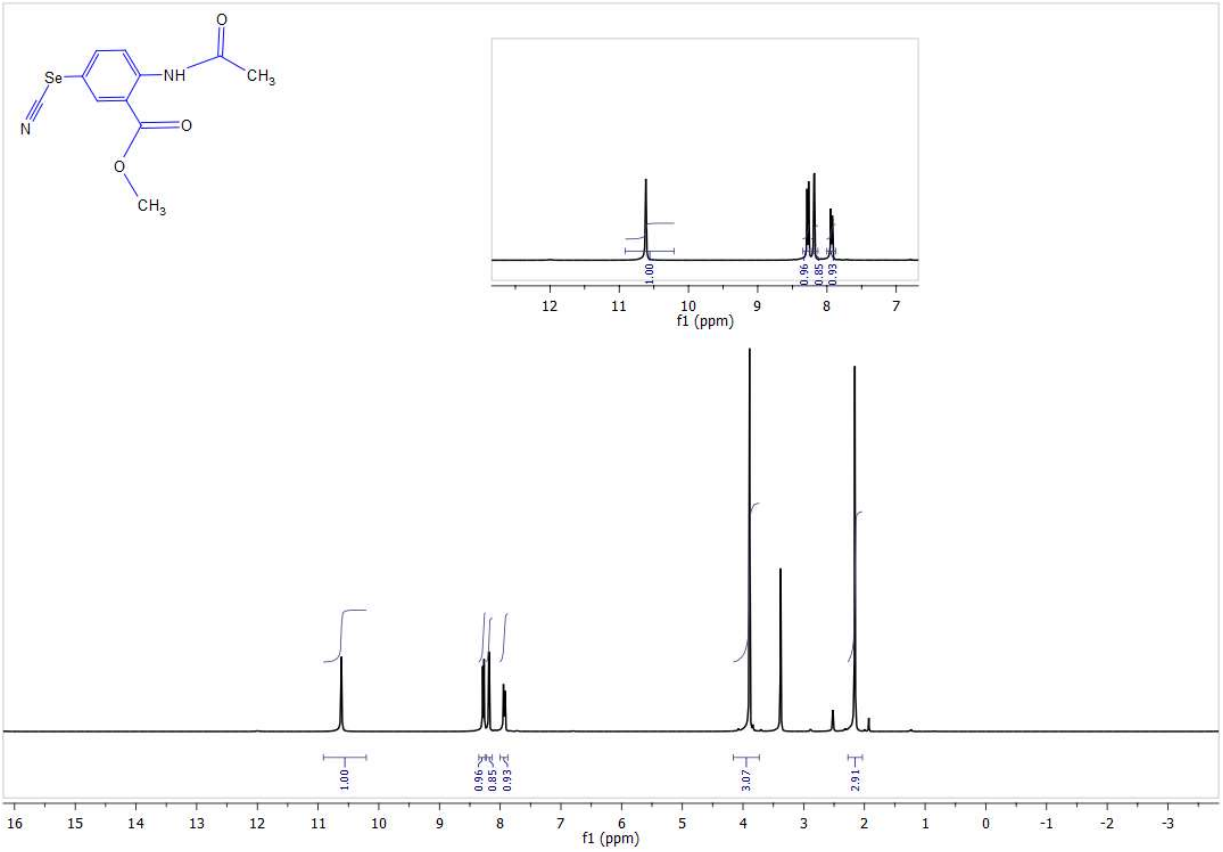


#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
217	266.15	3993	0.18	286	335.15	1042	0.05	355	403.25	924	0.04
218	267.15	7831	0.35	287	336.05	1224	0.05	356	404.15	2125	0.09
219	268.10	8279	0.37	288	337.15	1044	0.05	357	405.20	778	0.03
220	269.15	3757	0.17	289	338.05	1267	0.06	358	406.25	615	0.03
221	270.10	14530	0.65	290	339.05	1195	0.05	359	407.15	429	0.02
222	271.05	2847	0.13	291	340.05	1027	0.05	360	407.50	396	0.02
223	272.10	3444	0.15	292	341.15	1699	0.08	361	408.45	358	0.02
224	273.10	1161	0.05	293	342.55	671	0.03	362	409.50	252	0.01
225	274.15	853	0.04	294	343.55	622	0.03	363	411.50	345	0.02
226	275.15	1138	0.05	295	344.55	605	0.03	364	412.30	247	0.01
227	276.15	1258	0.06	296	345.55	552	0.02	365	413.35	468	0.02
228	277.15	2928	0.13	297	346.65	626	0.03	366	414.35	426	0.02
229	278.10	21009	0.94	298	347.60	895	0.04	367	415.25	872	0.04
230	279.15	22091	0.99	299	348.65	739	0.03	368	416.25	637	0.03
231	280.15	217622	9.73	300	349.60	620	0.03	369	417.35	609	0.03
232	281.15	242313	10.83	301	350.65	516	0.02	370	418.50	462	0.02
233	282.10	554734	24.80	302	351.55	576	0.03	371	419.45	365	0.02
234	283.15	172172	7.70	303	352.30	260	0.01	372	420.70	250	0.01
235	284.10	112086	50.11	304	353.25	604	0.03	373	421.65	483	0.02
236	285.05	194577	8.70	305	354.35	568	0.03	374	422.75	313	0.01
237	286.10	221772	9.91	306	355.25	2759	0.12	375	423.65	314	0.01
238	287.05	35471	1.59	307	356.20	1252	0.06	376	425.20	369	0.02
239	288.05	4393	0.20	308	357.25	1161	0.05	377	426.30	350	0.02
240	289.30	1150	0.05	309	358.65	564	0.03	378	427.25	442	0.02
241	290.30	934	0.04	310	359.65	728	0.03	379	428.30	422	0.02
242	291.30	1030	0.05	311	360.65	711	0.03	380	429.30	1642	0.07
243	292.25	1018	0.05	312	361.70	998	0.04	381	430.25	885	0.04
244	293.25	926	0.04	313	362.65	569	0.03	382	431.00	655	0.03
245	294.25	1611	0.07	314	363.75	835	0.04	383	432.00	726	0.03
246	295.25	4975	0.22	315	364.65	590	0.03	384	433.05	577	0.03
247	296.15	3832	0.17	316	365.75	623	0.03	385	434.05	569	0.03
248	297.15	2130	0.10	317	366.30	468	0.02	386	434.95	339	0.02
249	298.10	3876	0.17	318	367.25	484	0.02	387	435.25	361	0.02
250	299.20	1567	0.07	319	368.35	823	0.04	388	436.20	758	0.03
251	300.20	2049	0.09	320	369.30	3441	0.15	389	437.25	365	0.02
252	301.25	1040	0.05	321	370.25	1788	0.08	390	438.20	298	0.01
253	302.25	713	0.03	322	371.35	1387	0.06	391	439.20	233	0.01
254	303.35	1099	0.05	323	372.35	957	0.04	392	440.20	209	0.01
255	304.25	968	0.04	324	373.35	833	0.04	393	441.20	239	0.01
256	305.30	1873	0.08	325	374.25	838	0.04	394	442.40	250	0.01
257	306.25	1195	0.05	326	375.35	684	0.03	395	443.45	686	0.03
258	307.25	1183	0.05	327	376.30	857	0.04	396	444.40	610	0.03
259	308.25	773	0.03	328	377.35	491	0.02	397	445.45	489	0.02
260	309.25	852	0.04	329	378.45	397	0.02	398	446.35	475	0.02
261	310.15	796	0.04	330	379.45	467	0.02	399	447.35	360	0.02
262	311.15	873	0.04	331	380.20	215	0.01	400	448.10	462	0.02
263	312.20	959	0.04	332	381.25	325	0.01	401	449.10	463	0.02
264	313.20	1841	0.08	333	382.45	418	0.02	402	450.05	441	0.02
265	314.15	1338	0.06	334	383.40	562	0.03	403	451.05	473	0.02
266	315.15	1530	0.07	335	384.35	459	0.02	404	452.05	411	0.02
267	316.15	1107	0.05	336	385.30	681	0.03	405	453.10	494	0.02
268	317.10	1918	0.09	337	386.35	531	0.02	406	454.05	395	0.02
269	318.05	964	0.04	338	387.35	613	0.03	407	455.20	442	0.02
270	319.40	1063	0.05	339	388.35	559	0.02	408	456.15	335	0.01
271	320.40	868	0.04	340	389.35	525	0.02	409	456.90	396	0.02
272	321.45	763	0.03	341	390.35	579	0.03	410	457.90	342	0.02
273	322.35	572	0.03	342	391.00	343	0.02	411	458.90	335	0.01
274	323.15	653	0.03	343	392.00	566	0.03	412	459.90	425	0.02
275	324.05	475	0.02	344	393.05	412	0.02	413	460.95	413	0.02
276	325.05	722	0.03	345	394.05	419	0.02	414	461.90	250	0.01
277	326.05	664	0.03	346	395.05	334	0.01	415	462.90	257	0.01
278	327.15	1059	0.05	347	395.95	324	0.01	416	463.90	244	0.01
279	328.15	993	0.04	348	396.25	303	0.01	417	464.90	225	0.01
280	329.15	825	0.04	349	397.25	497	0.02	418	468.90	234	0.01
281	330.05	494	0.02	350	398.25	511	0.02	419	469.90	258	0.01
282	331.15	723	0.03	351	399.25	612	0.03	420	470.90	212	0.01
283	332.05	792	0.04	352	400.25	984	0.04	421	471.90	276	0.01
284	333.15	705	0.03	353	401.25	1274	0.06	422	472.90	335	0.01
285	334.05	1007	0.05	354	402.20	1566	0.07	423	473.90	268	0.01

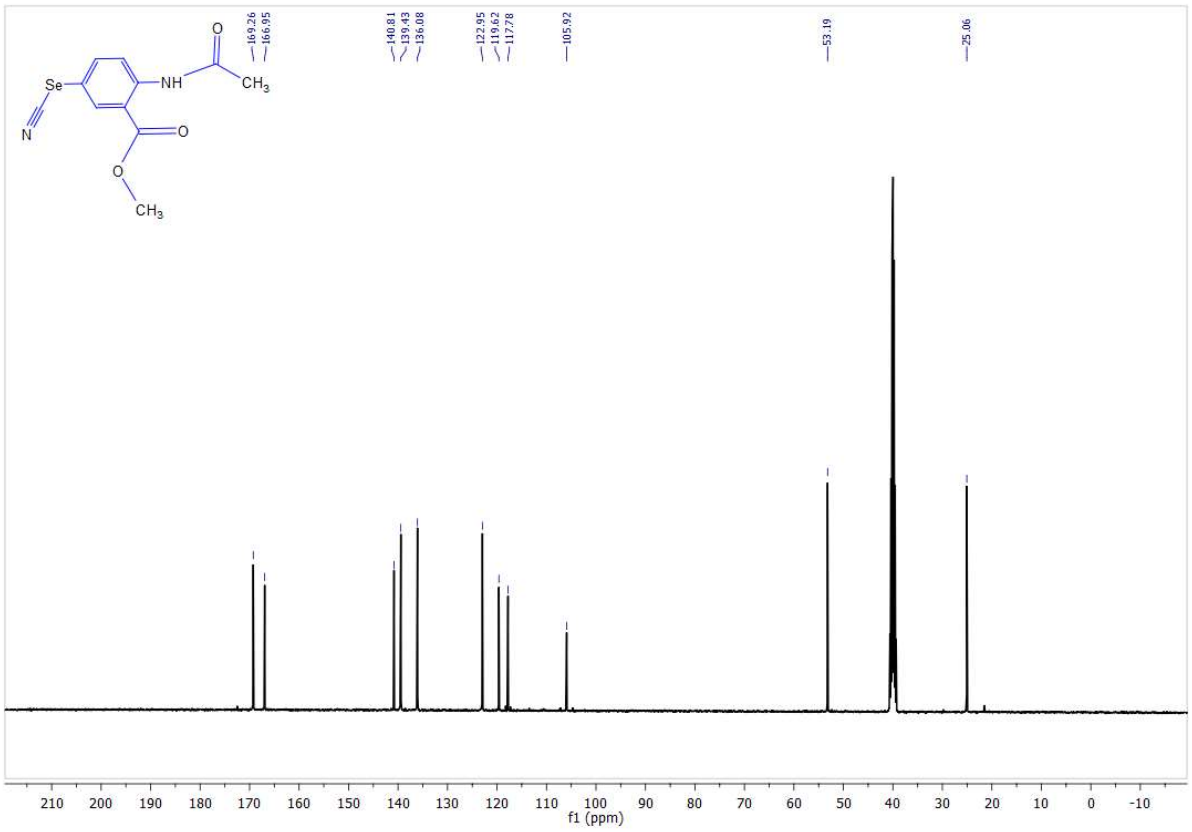
3 / 4

Mass chart of compound **10**

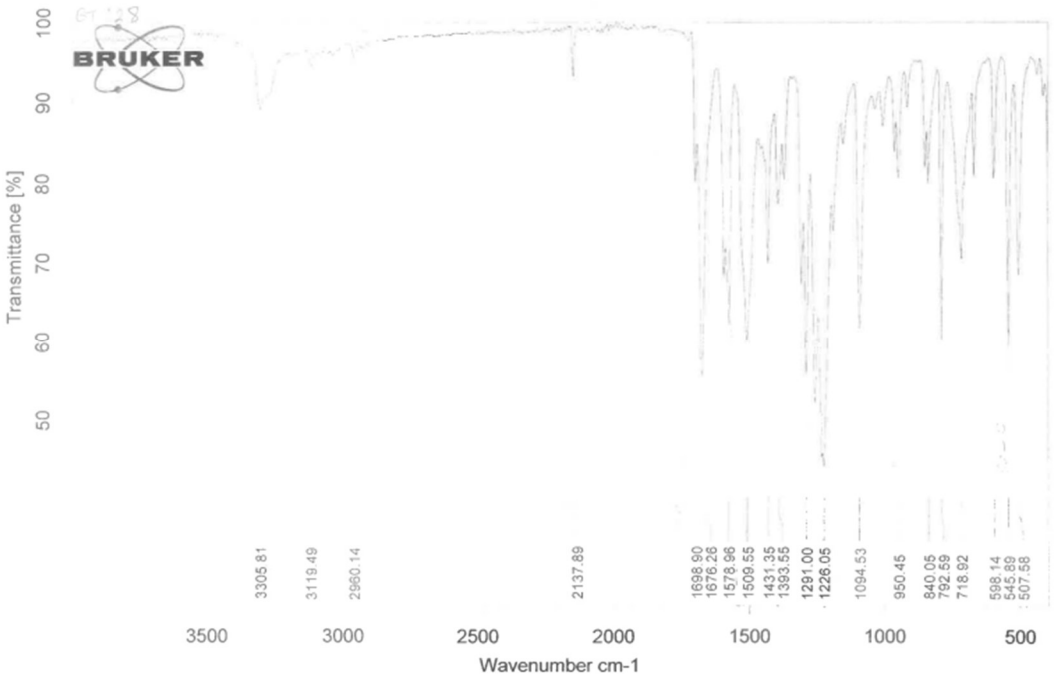
*Methyl 2-acetamido-5-selenocyanatobenzoate (**11**).*



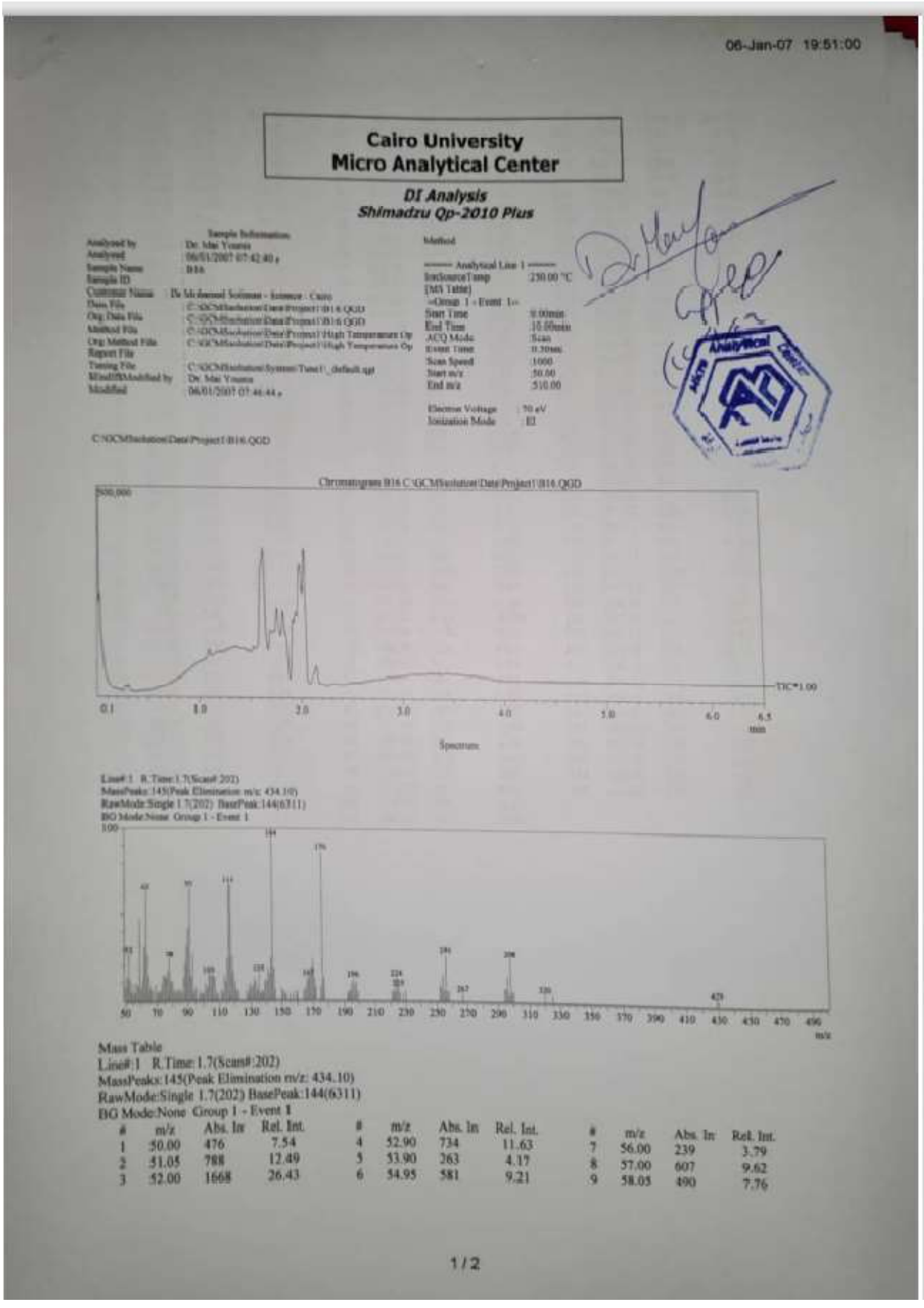
^{1}HNMR chart of compound **11**



^{13}CNMR chart of compound **11**



IR chart of compound **11**



06-Jan-07 19:51:00

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information
Analysed by : Dr. Mai Younes
Analysed : 06/01/2007 07:42:40 م
Sample Name : B16
Sample ID :
Comment Name : Dr Mohamed Soliman - Ismaeia - Cairo
Data File : C:\GCMSsolution\Data\Project1\B16.QGD
Org. Data File : C:\GCMSsolution\Data\Project1\B16.QGD
Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Org. Method File : C:\GCMSsolution\Data\Project1\High Temperature Op
Report File :
Tuning File : C:\GCMSsolution\System\Tune1_default.qpt
Modified/Modified by : Dr. Mai Younes
Modified : 06/01/2007 07:46:44 م

Method
Analytical Line 1
InterfaceTemp : 230.00 °C
[MS Table]
<<Group 1 - Event 1>>
Start Time : 0.00min
End Time : 10.00min
ACQ Mode : Scan
Event Time : 0.30sec
Scan Speed : 1000
Start m/z : 50.00
End m/z : 510.00
Electron Voltage : 70 eV
Ionization Mode : EI

C:\GCMSsolution\Data\Project1\B16.QGD

Chromatogram B16 C:\GCMSsolution\Data\Project1\B16.QGD

Spectrum:

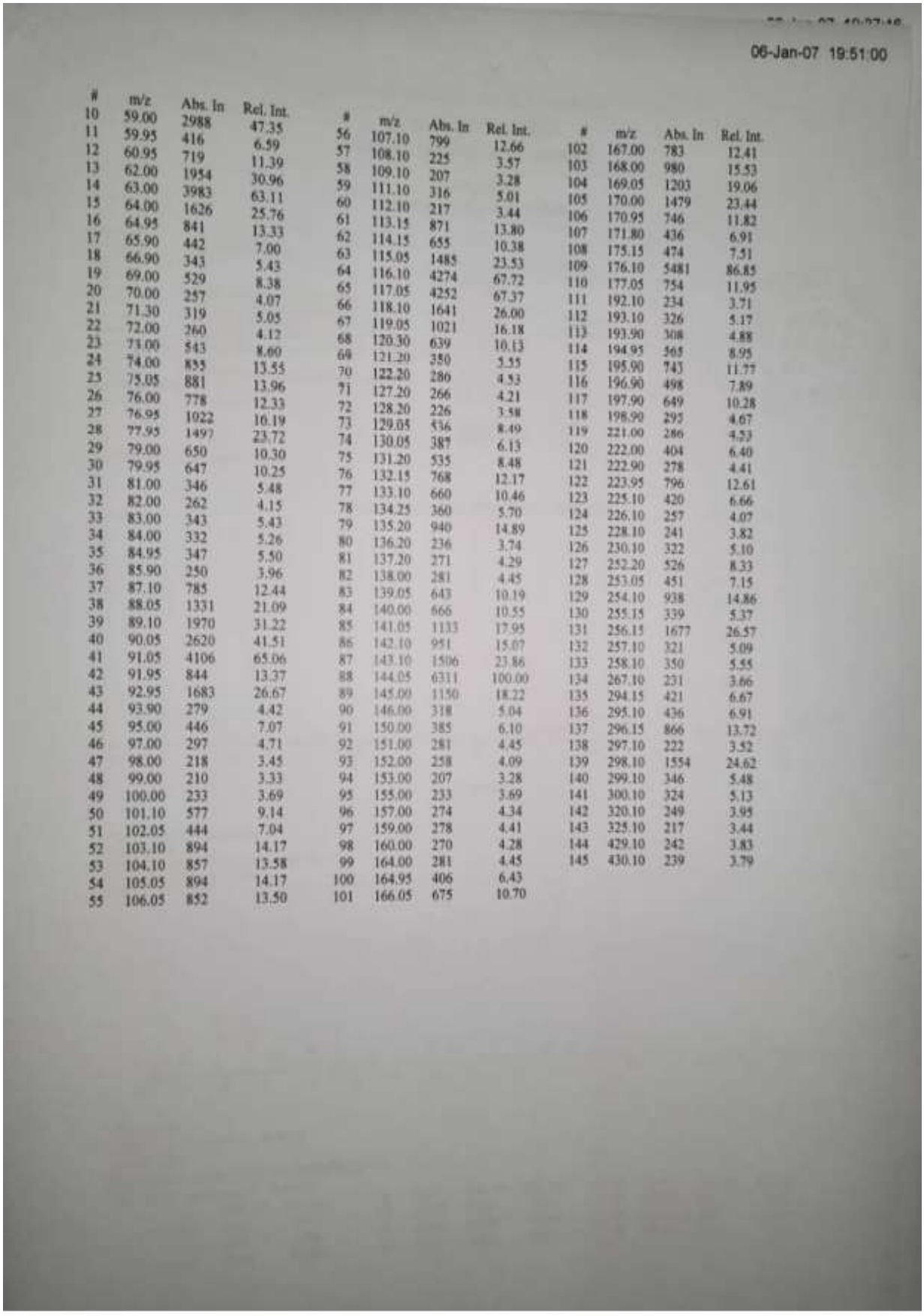
Line#:1 R.Time:1.7(Scan#:202)
MassPeaks:145(Peak Elimination m/z: 434.10)
RawMode:Single 1.7(202) BasePeak:144(6311)
BG Mode:None Group 1 - Event 1

Mass Table
Line#:1 R.Time:1.7(Scan#:202)
MassPeaks:145(Peak Elimination m/z: 434.10)
RawMode:Single 1.7(202) BasePeak:144(6311)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.00	476	7.54	4	52.90	734	11.63	7	56.00	239	3.79
2	51.05	788	12.49	5	53.90	263	4.17	8	57.00	607	9.62
3	52.00	1668	26.43	6	54.95	581	9.21	9	58.05	490	7.76

1 / 2

Mass chart of compound **11**

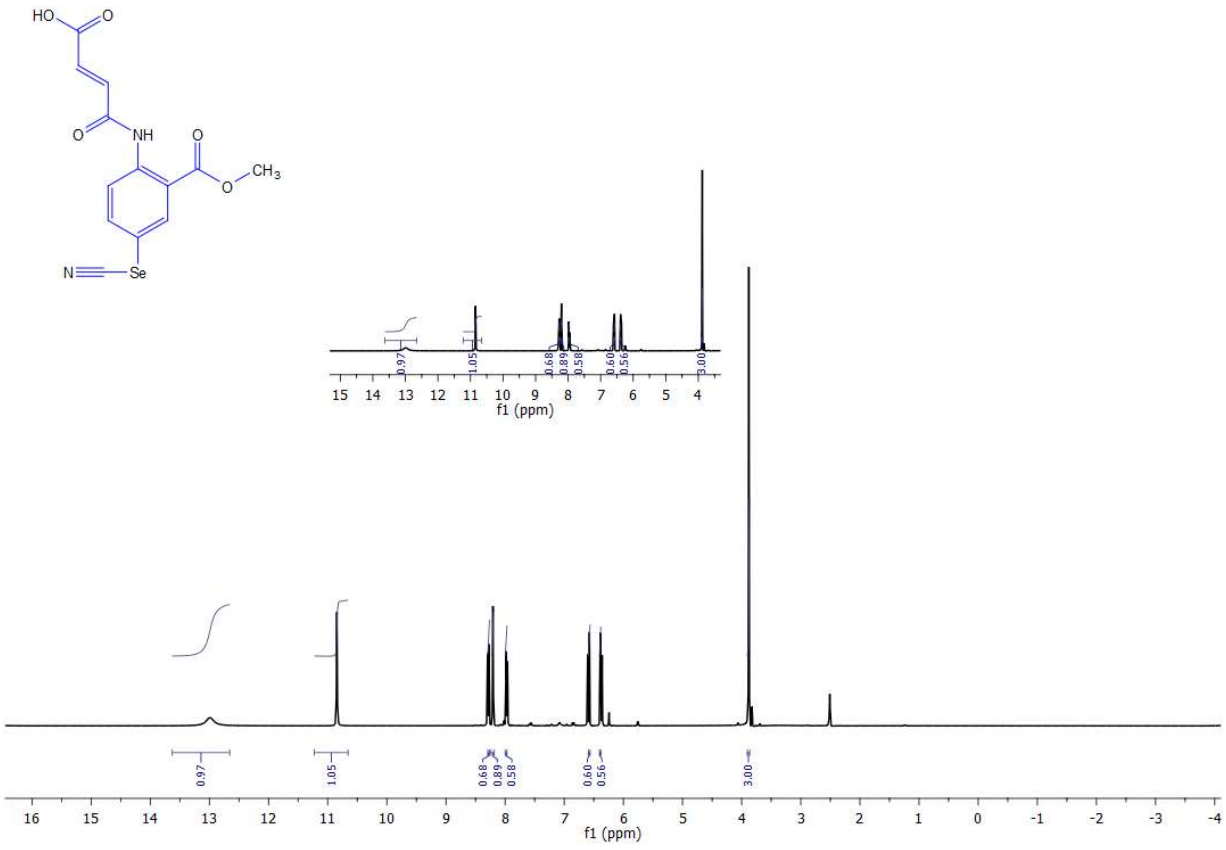


06-Jan-07 19:51:00

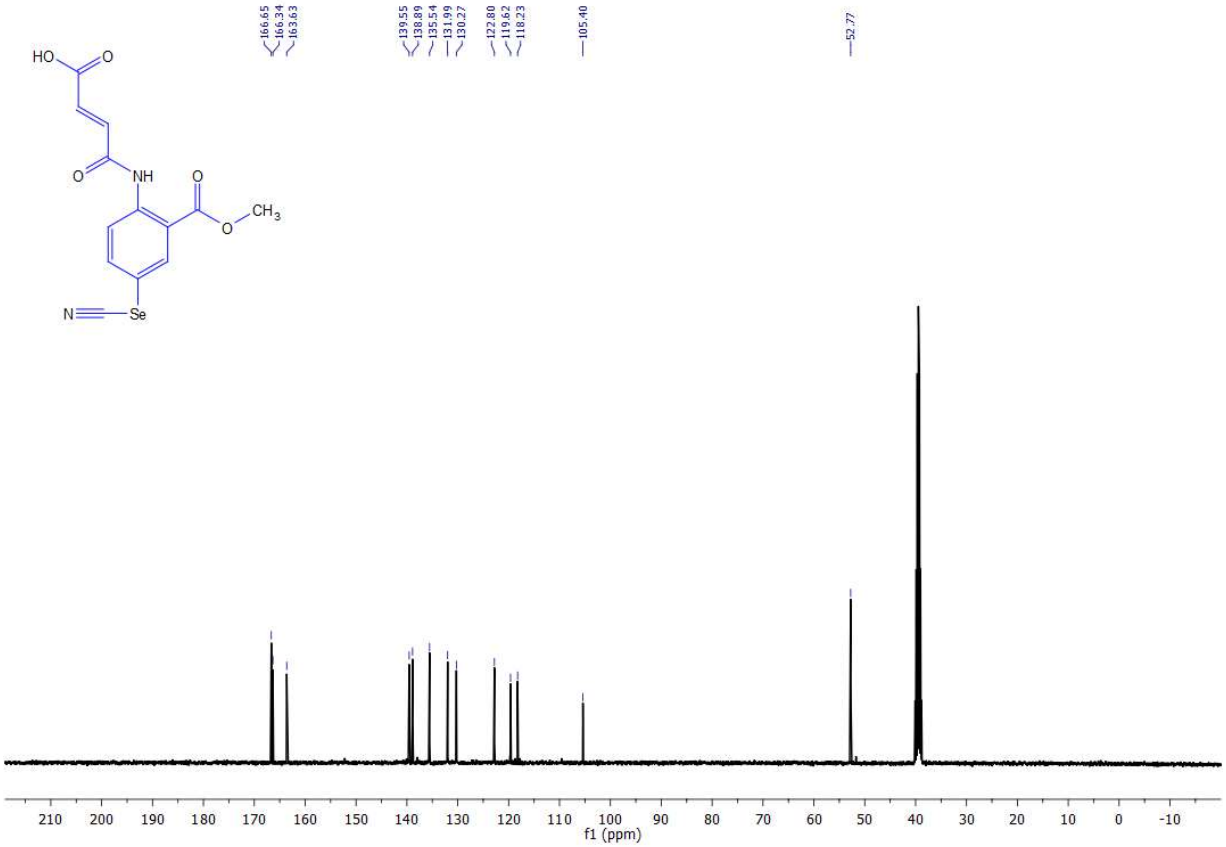
#	m/z	Abs. In	Rel. Int.
10	59.00	2988	47.35
11	59.95	416	6.59
12	60.95	719	11.39
13	62.00	1954	30.96
14	63.00	3983	63.11
15	64.00	1626	25.76
16	64.95	841	13.33
17	65.90	442	7.00
18	66.90	343	5.43
19	69.00	529	8.38
20	70.00	257	4.07
21	71.30	319	5.05
22	72.00	260	4.12
23	73.00	543	8.60
24	74.00	855	13.55
25	75.05	881	13.96
26	76.00	778	12.33
27	76.95	1022	16.19
28	77.95	1497	23.72
29	79.00	650	10.30
30	79.95	647	10.25
31	81.00	346	5.48
32	82.00	262	4.15
33	83.00	343	5.43
34	84.00	332	5.26
35	84.95	347	5.50
36	85.90	250	3.96
37	87.10	785	12.44
38	88.05	1331	21.09
39	89.10	1970	31.22
40	90.05	2620	41.51
41	91.05	4106	65.06
42	91.95	844	13.37
43	92.95	1683	26.67
44	93.90	279	4.42
45	95.00	446	7.07
46	97.00	297	4.71
47	98.00	218	3.45
48	99.00	210	3.33
49	100.00	233	3.69
50	101.10	577	9.14
51	102.05	444	7.04
52	103.10	894	14.17
53	104.10	857	13.58
54	105.05	894	14.17
55	106.05	852	13.50
56	107.10	799	12.66
57	108.10	225	3.57
58	109.10	207	3.28
59	111.10	316	5.01
60	112.10	217	3.44
61	113.15	871	13.80
62	114.15	655	10.38
63	115.05	1485	23.53
64	116.10	4274	67.72
65	117.05	4252	67.37
66	118.10	1641	26.00
67	119.05	1021	16.18
68	120.30	639	10.13
69	121.20	350	5.55
70	122.20	286	4.53
71	127.20	266	4.21
72	128.20	226	3.58
73	129.05	536	8.49
74	130.05	387	6.13
75	131.20	535	8.48
76	132.15	768	12.17
77	133.10	660	10.46
78	134.25	360	5.70
79	135.20	940	14.89
80	136.20	236	3.74
81	137.20	271	4.29
82	138.00	281	4.45
83	139.05	643	10.19
84	140.00	666	10.55
85	141.05	1133	17.95
86	142.10	951	15.07
87	143.10	1506	23.86
88	144.05	6311	100.00
89	145.00	1150	18.22
90	146.00	318	5.04
91	150.00	385	6.10
92	151.00	281	4.45
93	152.00	258	4.09
94	153.00	207	3.28
95	155.00	233	3.69
96	157.00	274	4.34
97	159.00	278	4.41
98	160.00	270	4.28
99	164.00	281	4.45
100	164.95	406	6.43
101	166.05	675	10.70
102	167.00	783	12.41
103	168.00	980	15.53
104	169.05	1203	19.06
105	170.00	1479	23.44
106	170.95	746	11.82
107	171.80	436	6.91
108	175.15	474	7.51
109	176.10	5481	86.85
110	177.05	754	11.95
111	192.10	234	3.71
112	193.10	326	5.17
113	193.90	308	4.88
114	194.95	565	8.95
115	195.90	743	11.77
116	196.90	498	7.89
117	197.90	649	10.28
118	198.90	295	4.67
119	221.00	286	4.53
120	222.00	404	6.40
121	222.90	278	4.41
122	223.95	796	12.61
123	225.10	420	6.66
124	226.10	257	4.07
125	228.10	241	3.82
126	230.10	322	5.10
127	252.20	526	8.33
128	253.05	451	7.15
129	254.10	938	14.86
130	255.15	339	5.37
131	256.15	1677	26.57
132	257.10	321	5.09
133	258.10	350	5.55
134	267.10	231	3.66
135	294.15	421	6.67
136	295.10	436	6.91
137	296.15	866	13.72
138	297.10	222	3.52
139	298.10	1554	24.62
140	299.10	346	5.48
141	300.10	324	5.13
142	320.10	249	3.95
143	325.10	217	3.44
144	429.10	242	3.83
145	430.10	239	3.79

Mass chart of compound **11**

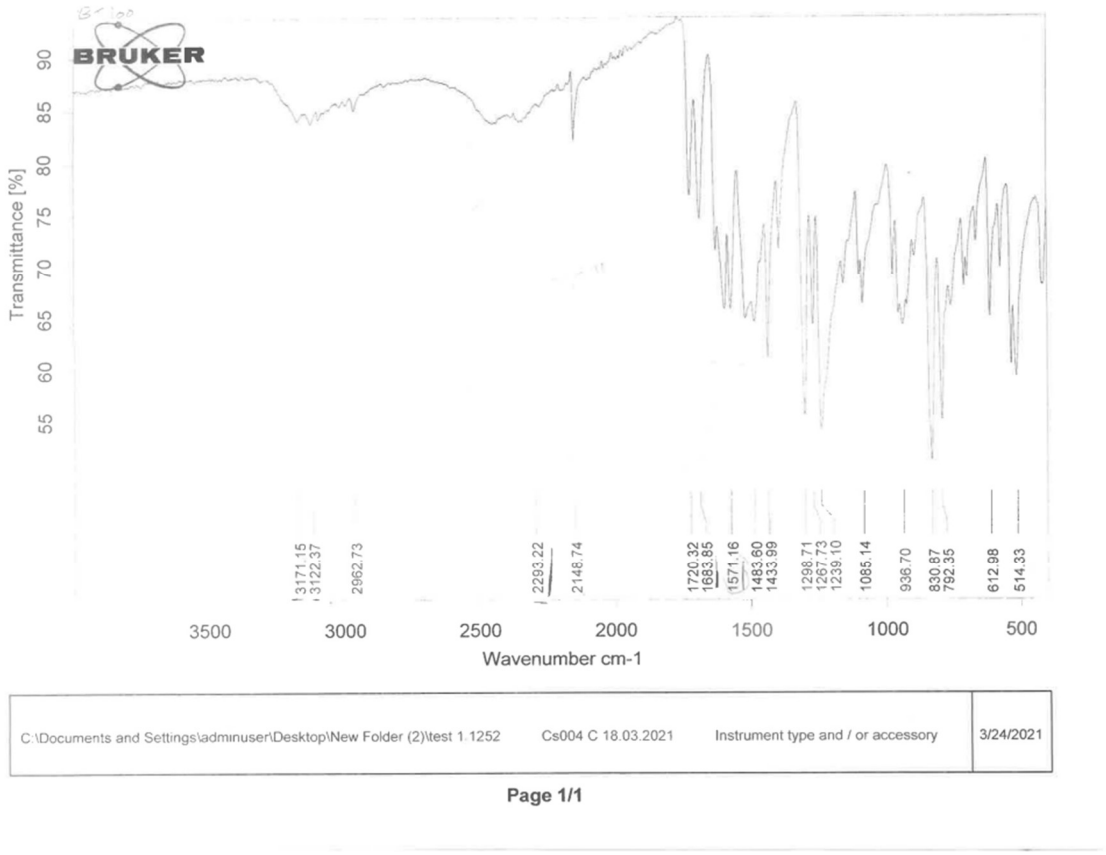
*(Z)-4-((2-(methoxycarbonyl)-4-selenocyanatophenyl) amino)-4-oxobut-2-enoic acid (**12**).*



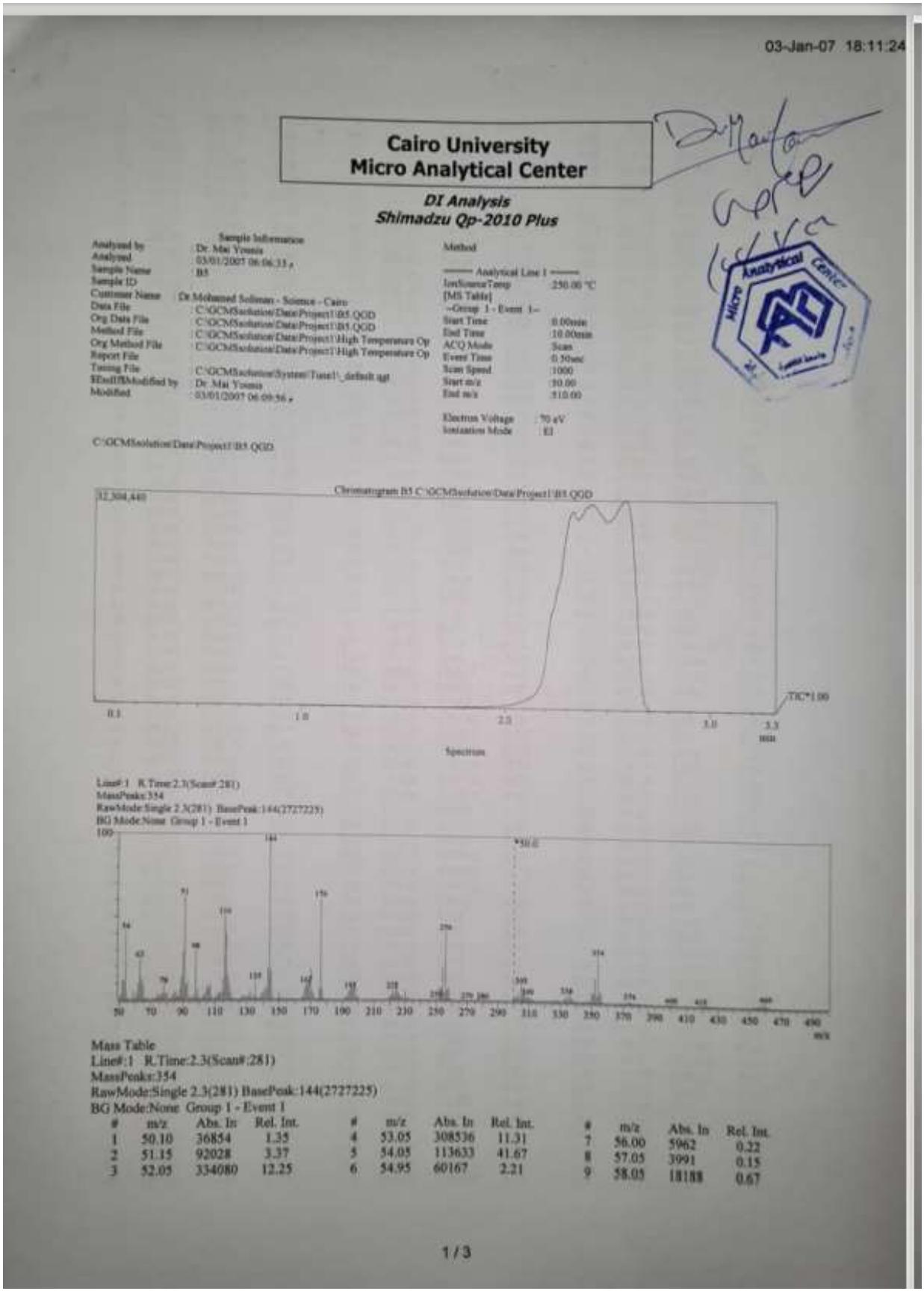
[1]HNMR chart compound of **12**



^{13}CNMR chart compound of **12**



IR chart of compound **12**



03-Jan-07 18:11:24

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

Analyzed by	Dr. Mai Younis
Analyzed	03/01/2007 06:06:33 م
Sample Name	B5
Sample ID	
Customer Name	Dr Mohamed Soliman - Science - Cairo
Data File	C:\GCMSolution\Data\Project1\B5.QGD
Org Data File	C:\GCMSolution\Data\Project1\B5.QGD
Method File	C:\GCMSolution\Data\Project1\High Temperature Op
Org Method File	C:\GCMSolution\Data\Project1\High Temperature Op
Report File	
Tuning File	C:\GCMSolution\System\Tune1_default.qgt
Modified by	Dr. Mai Younis
Modified	03/01/2007 06:09:56 م

Method

Analytical Line 1	
IonSourceTemp	250.00 °C
[MS Table]	
--Group 1 - Event 1--	
Start Time	0.00min
End Time	10.00min
ACQ Mode	Scan
Event Time	0.50sec
Scan Speed	1000
Start m/z	30.00
End m/z	510.00
Electron Voltage	70 eV
Ionization Mode	EI

C:\GCMSolution\Data\Project1\B5.QGD

Chromatogram B5 C:\GCMSolution\Data\Project1\B5.QGD

12,304,440

TIC*1.00

0.1 1.0 2.0 3.0 3.3 min

Spectrum

Line#:1 R.Time:2.3(Scan#:281)
MassPeaks:354
RawMode:Single 2.3(281) BasePeak:144(2727225)
BG Mode:None Group 1 - Event 1

100

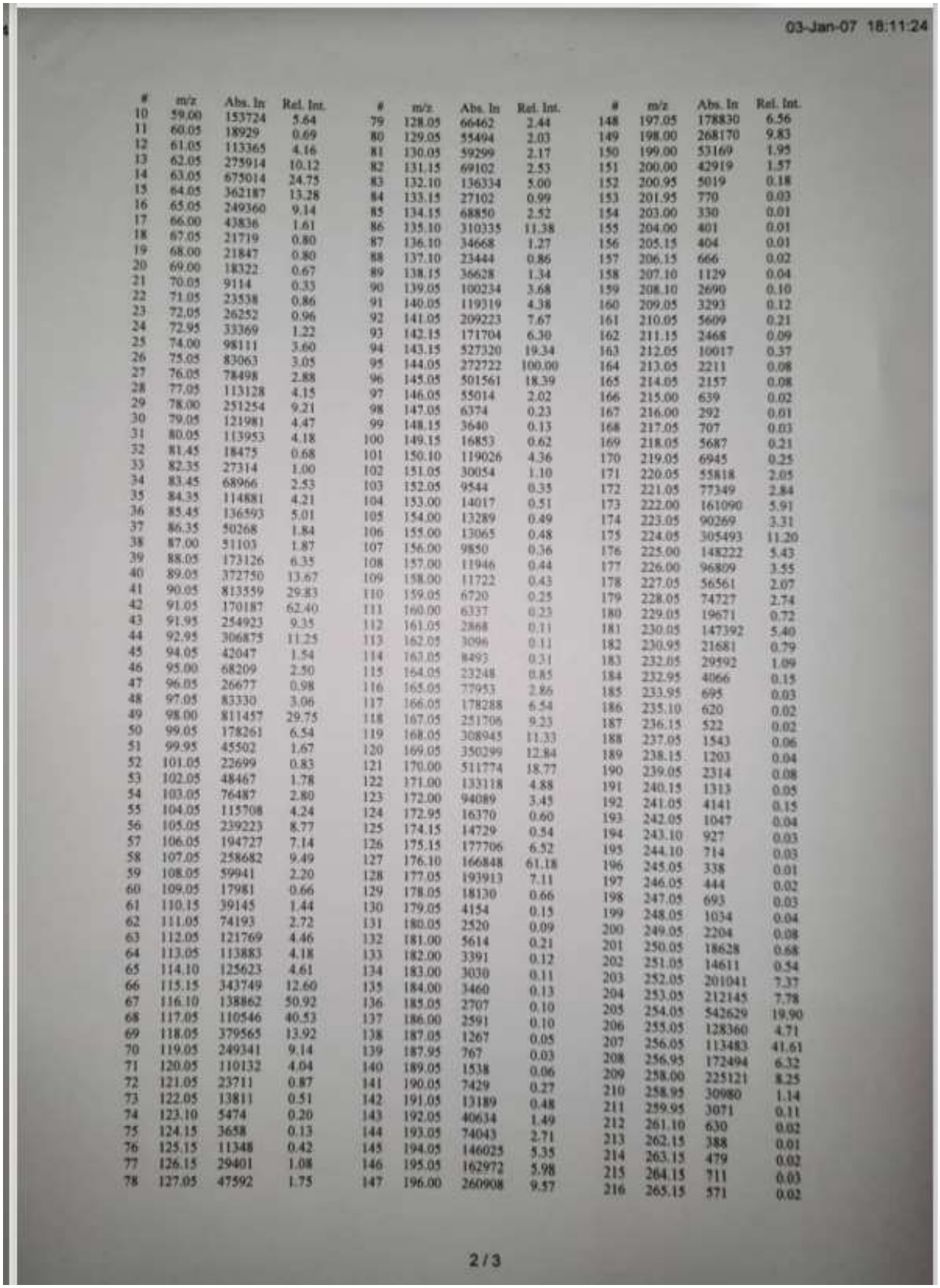
50 70 90 110 130 150 170 190 210 230 250 270 290 310 330 350 370 390 410 430 450 470 490 m/z

Mass Table
Line#:1 R.Time:2.3(Scan#:281)
MassPeaks:354
RawMode:Single 2.3(281) BasePeak:144(2727225)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.10	36854	1.35	4	53.05	308536	11.31	7	56.00	5962	0.22
2	51.15	92028	3.37	5	54.05	113633	41.67	8	57.05	3991	0.15
3	52.05	334080	12.25	6	54.95	60167	2.21	9	58.05	18188	0.67

1 / 3

Mass chart of compound **12**

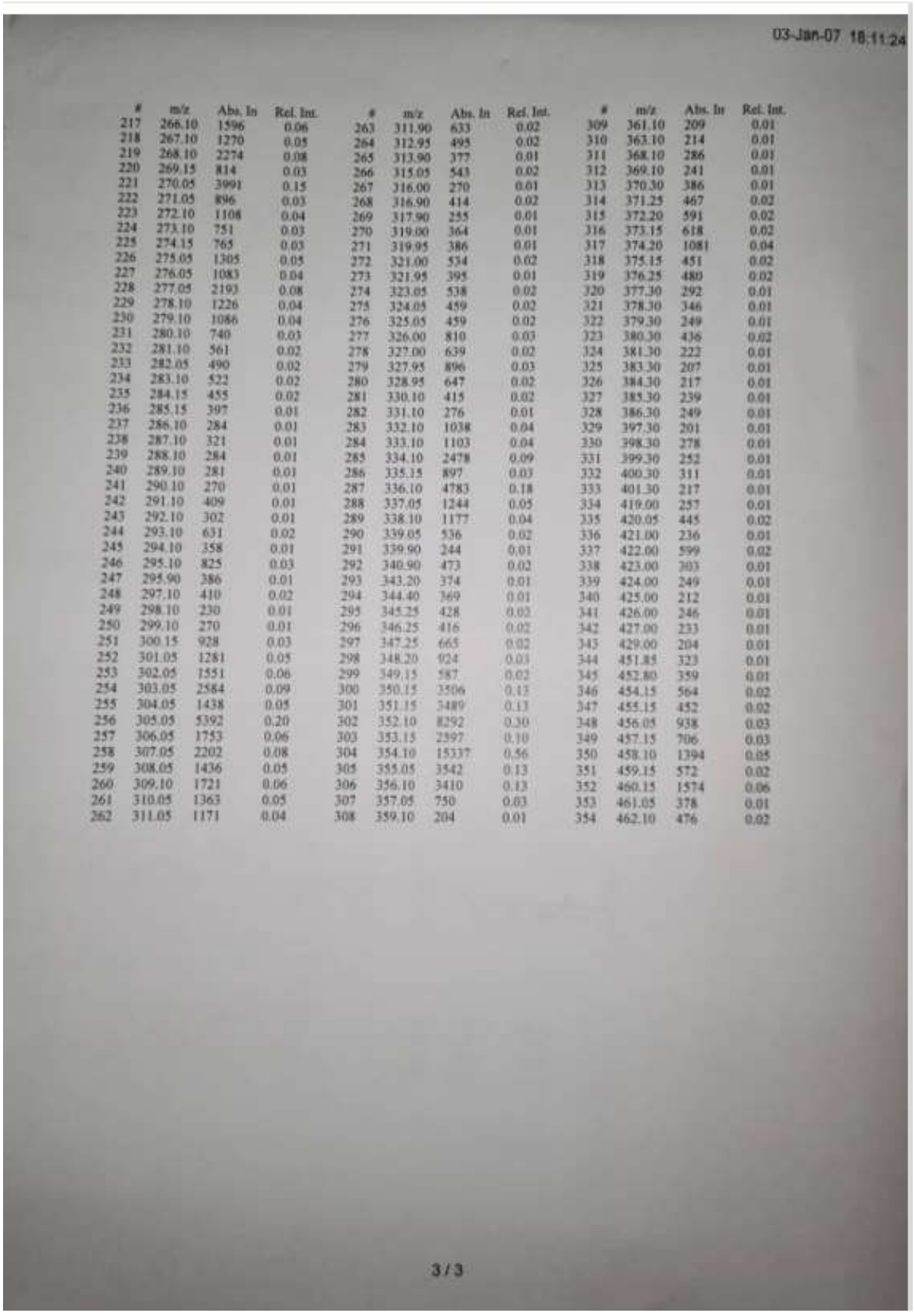


03-Jan-07 18:11:24

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	59.00	153724	5.64	79	128.05	66462	2.44	148	197.05	178830	6.56
11	60.05	18929	0.69	80	129.05	55494	2.03	149	198.00	268170	9.83
12	61.05	113365	4.16	81	130.05	59299	2.17	150	199.00	53169	1.95
13	62.05	275914	10.12	82	131.15	69102	2.53	151	200.00	42919	1.57
14	63.05	675014	24.75	83	132.10	136334	5.00	152	200.95	5019	0.18
15	64.05	362187	13.28	84	133.15	27102	0.99	153	201.95	770	0.03
16	65.05	249360	9.14	85	134.15	68850	2.52	154	203.00	330	0.01
17	66.00	43836	1.61	86	135.10	310335	11.38	155	204.00	401	0.01
18	67.05	21719	0.80	87	136.10	34668	1.27	156	205.15	404	0.01
19	68.00	21847	0.80	88	137.10	23444	0.86	157	206.15	666	0.02
20	69.00	18322	0.67	89	138.15	36628	1.34	158	207.10	1129	0.04
21	70.05	9114	0.33	90	139.05	100234	3.68	159	208.10	2690	0.10
22	71.05	23538	0.86	91	140.05	119319	4.38	160	209.05	3293	0.12
23	72.05	26252	0.96	92	141.05	209223	7.67	161	210.05	5609	0.21
24	72.95	33369	1.22	93	142.15	171704	6.30	162	211.15	2468	0.09
25	74.00	98111	3.60	94	143.15	527320	19.34	163	212.05	10017	0.37
26	75.05	83063	3.05	95	144.05	272722	100.00	164	213.05	2211	0.08
27	76.05	78498	2.88	96	145.05	501561	18.39	165	214.05	2157	0.08
28	77.05	113128	4.15	97	146.05	55014	2.02	166	215.00	639	0.02
29	78.00	251254	9.21	98	147.05	6374	0.23	167	216.00	292	0.01
30	79.05	121981	4.47	99	148.15	3640	0.13	168	217.05	707	0.03
31	80.05	113953	4.18	100	149.15	16853	0.62	169	218.05	5687	0.21
32	81.45	18475	0.68	101	150.10	119026	4.36	170	219.05	6945	0.25
33	82.35	27314	1.00	102	151.05	30054	1.10	171	220.05	55818	2.05
34	83.45	68966	2.53	103	152.05	9544	0.35	172	221.05	77349	2.84
35	84.35	114881	4.21	104	153.00	14017	0.51	173	222.00	161090	5.91
36	85.45	136593	5.01	105	154.00	13289	0.49	174	223.05	90269	3.31
37	86.35	50268	1.84	106	155.00	13065	0.48	175	224.05	305493	11.20
38	87.00	51103	1.87	107	156.00	9850	0.36	176	225.00	148222	5.43
39	88.05	173126	6.35	108	157.00	11946	0.44	177	226.00	96809	3.55
40	89.05	372750	13.67	109	158.00	11722	0.43	178	227.05	56561	2.07
41	90.05	813559	29.83	110	159.05	6720	0.25	179	228.05	74727	2.74
42	91.05	170187	62.40	111	160.00	6337	0.23	180	229.05	19671	0.72
43	91.95	254923	9.35	112	161.05	2868	0.11	181	230.05	147392	5.40
44	92.95	306875	11.25	113	162.05	3096	0.11	182	230.95	21681	0.79
45	94.05	42047	1.54	114	163.05	8493	0.31	183	232.05	29592	1.09
46	95.00	68209	2.50	115	164.05	23248	0.85	184	232.95	4066	0.15
47	96.05	26677	0.98	116	165.05	77953	2.86	185	233.95	695	0.03
48	97.05	83330	3.06	117	166.05	178288	6.54	186	235.10	620	0.02
49	98.00	811457	29.75	118	167.05	251706	9.23	187	236.15	522	0.02
50	99.05	178261	6.54	119	168.05	308945	11.33	188	237.05	1543	0.06
51	99.95	45502	1.67	120	169.05	350299	12.84	189	238.15	1203	0.04
52	101.05	22699	0.83	121	170.00	511774	18.77	190	239.05	2314	0.08
53	102.05	48467	1.78	122	171.00	133118	4.88	191	240.15	1313	0.05
54	103.05	76487	2.80	123	172.00	94089	3.45	192	241.05	4141	0.15
55	104.05	115708	4.24	124	172.95	16370	0.60	193	242.05	1047	0.04
56	105.05	239223	8.77	125	174.15	14729	0.54	194	243.10	927	0.03
57	106.05	194727	7.14	126	175.15	177706	6.52	195	244.10	714	0.03
58	107.05	258682	9.49	127	176.10	166848	61.18	196	245.05	338	0.01
59	108.05	59941	2.20	128	177.05	193913	7.11	197	246.05	444	0.02
60	109.05	17981	0.66	129	178.05	18130	0.66	198	247.05	693	0.03
61	110.15	39145	1.44	130	179.05	4154	0.15	199	248.05	1034	0.04
62	111.05	74193	2.72	131	180.05	2520	0.09	200	249.05	2204	0.08
63	112.05	121769	4.46	132	181.00	5614	0.21	201	250.05	18628	0.68
64	113.05	113883	4.18	133	182.00	3391	0.12	202	251.05	14611	0.54
65	114.10	125623	4.61	134	183.00	3030	0.11	203	252.05	201041	7.37
66	115.15	343749	12.60	135	184.00	3460	0.13	204	253.05	212145	7.78
67	116.10	138862	50.92	136	185.05	2707	0.10	205	254.05	542629	19.90
68	117.05	110546	40.53	137	186.00	2591	0.10	206	255.05	128360	4.71
69	118.05	379565	13.92	138	187.05	1267	0.05	207	256.05	113483	41.61
70	119.05	249341	9.14	139	187.95	767	0.03	208	256.95	172494	6.32
71	120.05	110132	4.04	140	189.05	1538	0.06	209	258.00	225121	8.25
72	121.05	23711	0.87	141	190.05	7429	0.27	210	258.95	30980	1.14
73	122.05	13811	0.51	142	191.05	13189	0.48	211	259.95	3071	0.11
74	123.10	5474	0.20	143	192.05	40634	1.49	212	261.10	630	0.02
75	124.15	3658	0.13	144	193.05	74043	2.71	213	262.15	388	0.01
76	125.15	11348	0.42	145	194.05	146025	5.35	214	263.15	479	0.02
77	126.15	29401	1.08	146	195.05	162972	5.98	215	264.15	711	0.03
78	127.05	47592	1.75	147	196.00	260908	9.57	216	265.15	571	0.02

2 / 3

Mass chart of compound **12**



03-Jan-07 18:11:24

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
217	266.10	1596	0.06	263	311.90	633	0.02	309	361.10	209	0.01
218	267.10	1270	0.05	264	312.95	495	0.02	310	363.10	214	0.01
219	268.10	2274	0.08	265	313.90	377	0.01	311	368.10	286	0.01
220	269.15	814	0.03	266	315.05	543	0.02	312	369.10	241	0.01
221	270.05	3991	0.15	267	316.00	270	0.01	313	370.30	386	0.01
222	271.05	896	0.03	268	316.90	414	0.02	314	371.25	467	0.02
223	272.10	1108	0.04	269	317.90	255	0.01	315	372.20	591	0.02
224	273.10	751	0.03	270	319.00	364	0.01	316	373.15	618	0.02
225	274.15	765	0.03	271	319.95	386	0.01	317	374.20	1081	0.04
226	275.05	1305	0.05	272	321.00	534	0.02	318	375.15	451	0.02
227	276.05	1083	0.04	273	321.95	395	0.01	319	376.25	480	0.02
228	277.05	2193	0.08	274	323.05	538	0.02	320	377.30	292	0.01
229	278.10	1226	0.04	275	324.05	459	0.02	321	378.30	346	0.01
230	279.10	1086	0.04	276	325.05	459	0.02	322	379.30	249	0.01
231	280.10	740	0.03	277	326.00	810	0.03	323	380.30	436	0.02
232	281.10	561	0.02	278	327.00	639	0.02	324	381.30	222	0.01
233	282.05	490	0.02	279	327.95	896	0.03	325	383.30	207	0.01
234	283.10	522	0.02	280	328.95	647	0.02	326	384.30	217	0.01
235	284.15	455	0.02	281	330.10	415	0.02	327	385.30	239	0.01
236	285.15	397	0.01	282	331.10	276	0.01	328	386.30	249	0.01
237	286.10	284	0.01	283	332.10	1038	0.04	329	397.30	201	0.01
238	287.10	321	0.01	284	333.10	1103	0.04	330	398.30	278	0.01
239	288.10	284	0.01	285	334.10	2478	0.09	331	399.30	252	0.01
240	289.10	281	0.01	286	335.15	897	0.03	332	400.30	311	0.01
241	290.10	270	0.01	287	336.10	4783	0.18	333	401.30	217	0.01
242	291.10	409	0.01	288	337.05	1244	0.05	334	419.00	257	0.01
243	292.10	302	0.01	289	338.10	1177	0.04	335	420.05	445	0.02
244	293.10	631	0.02	290	339.05	536	0.02	336	421.00	236	0.01
245	294.10	358	0.01	291	339.90	244	0.01	337	422.00	599	0.02
246	295.10	825	0.03	292	340.90	473	0.02	338	423.00	303	0.01
247	295.90	386	0.01	293	343.20	374	0.01	339	424.00	249	0.01
248	297.10	410	0.02	294	344.40	369	0.01	340	425.00	212	0.01
249	298.10	230	0.01	295	345.25	428	0.02	341	426.00	246	0.01
250	299.10	270	0.01	296	346.25	416	0.02	342	427.00	233	0.01
251	300.15	928	0.03	297	347.25	665	0.02	343	429.00	204	0.01
252	301.05	1281	0.05	298	348.20	924	0.03	344	451.85	323	0.01
253	302.05	1551	0.06	299	349.15	587	0.02	345	452.80	359	0.01
254	303.05	2584	0.09	300	350.15	3506	0.13	346	454.15	564	0.02
255	304.05	1438	0.05	301	351.15	3489	0.13	347	455.15	452	0.02
256	305.05	5392	0.20	302	352.10	8292	0.30	348	456.05	938	0.03
257	306.05	1753	0.06	303	353.15	2597	0.10	349	457.15	706	0.03
258	307.05	2202	0.08	304	354.10	15337	0.56	350	458.10	1394	0.05
259	308.05	1436	0.05	305	355.05	3542	0.13	351	459.15	572	0.02
260	309.10	1721	0.06	306	356.10	3410	0.13	352	460.15	1574	0.06
261	310.05	1363	0.05	307	357.05	750	0.03	353	461.05	378	0.01
262	311.05	1171	0.04	308	359.10	204	0.01	354	462.10	476	0.02

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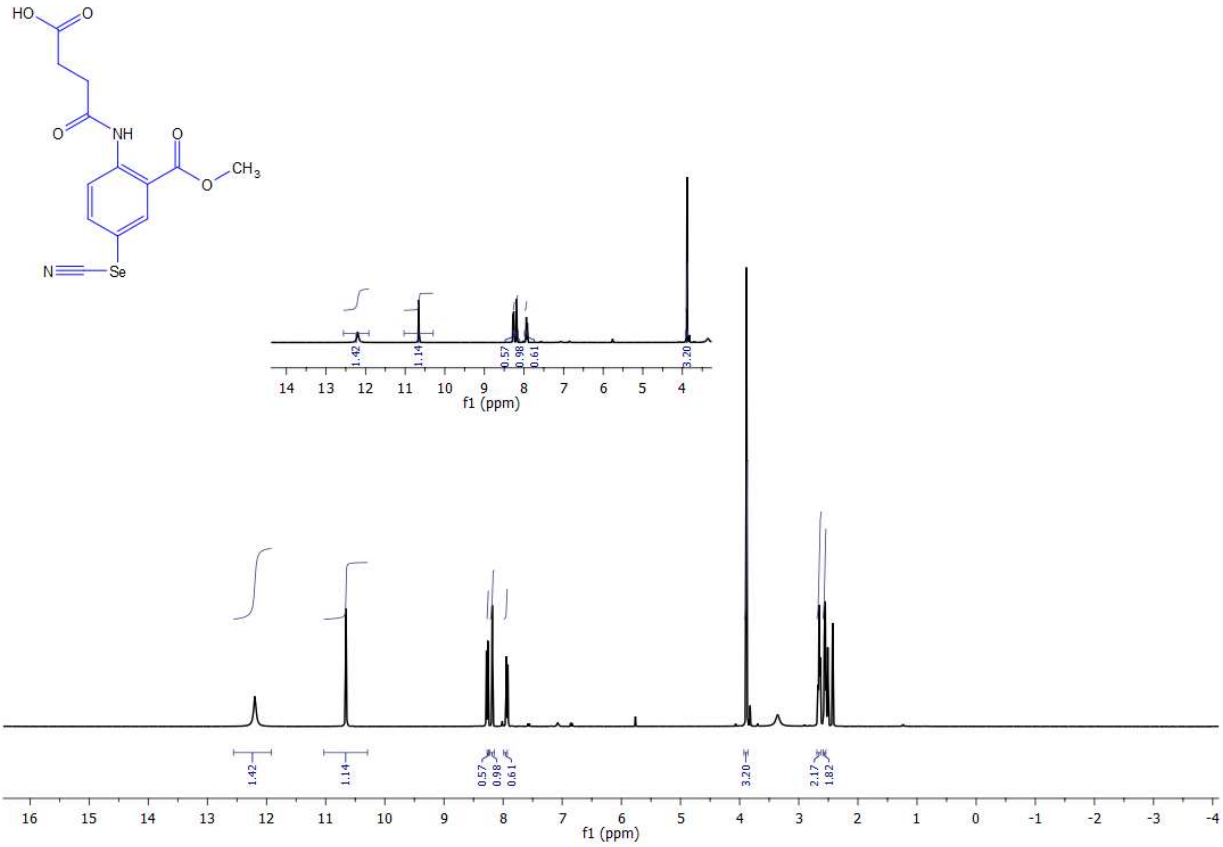
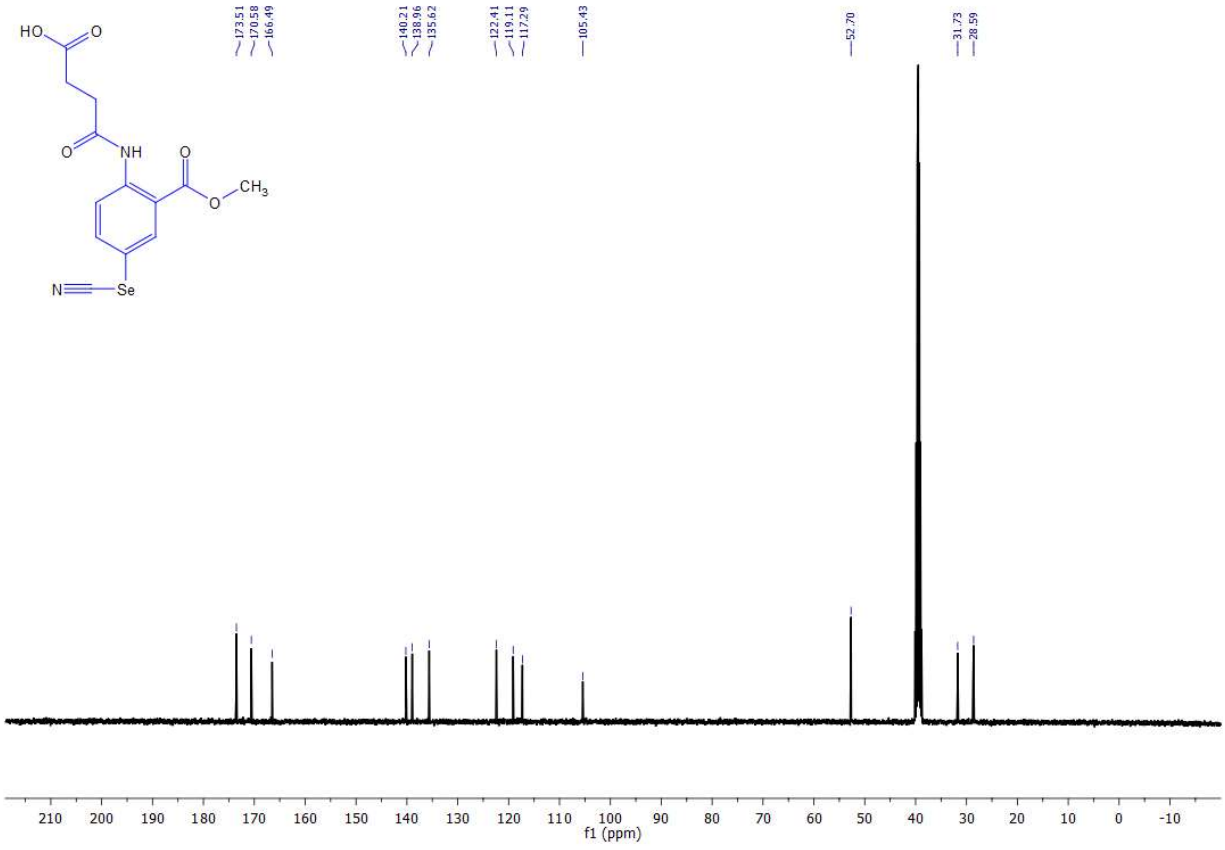
Mass chart of compound **12**

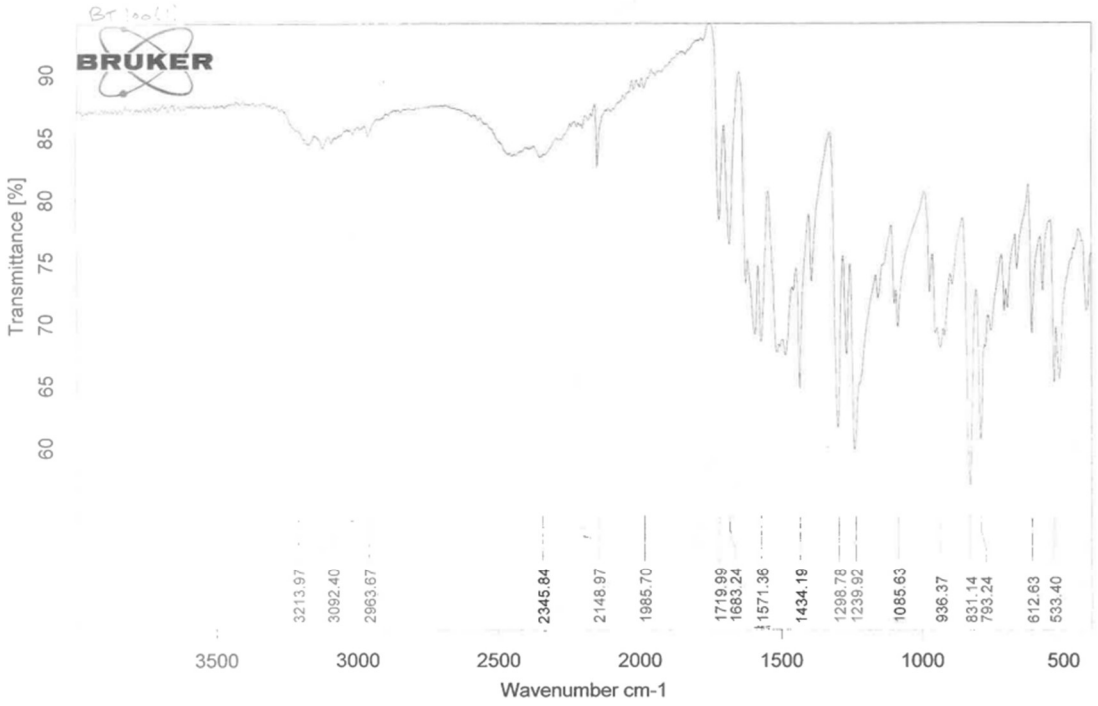
*4-((2-(methoxycarbonyl)-4-selenocyanatophenyl) amino)-4-oxobutanoic acid (**13**).*



[1]HNMR chart of compound **13**



^{13}CNMR chart of compound **13**



C:\Documents and Settings\adminuser\Desktop\New Folder (2)\test 1.1224	FL-HG-TU	Instrument type and / or accessory	3/16/2021

Page 1/1

IR chart of compound **13**

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

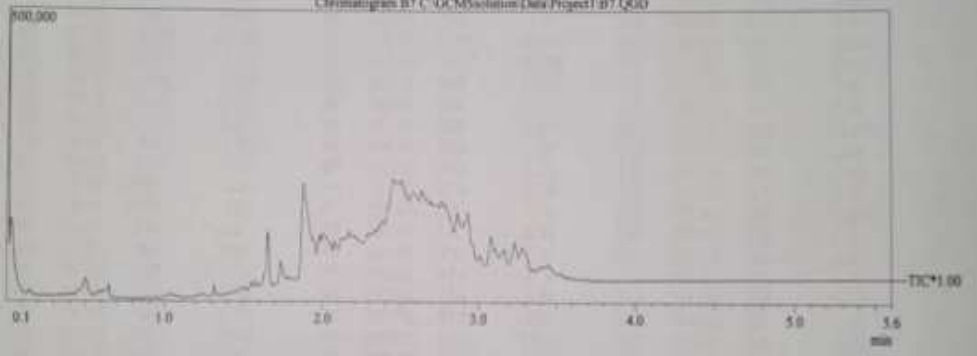
Analyzed by	: Dr. Mai Younis
Analyzed	: 03/01/2007 07:56:32
Sample Name	: B7
Sample ID	
Customer Name	: Dr.Mohamed Soliman - Science - Cairo
Data File	: C:\GCMSsolution\Data\Project1\B7.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\B7.QGD
Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op
Org Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op
Report File	
Tuning File	: C:\GCMSsolution\System\Tune1_default.qgt
EndModified by	: Dr. Mai Younis
Modified	: 03/01/2007 08:00:19

Method

——— Analytical Line 1 ———	
IonSourceTemp	250.00 °C
[MS Table]	
--Group 1 - Event 1--	
Start Time	0.00min
End Time	10.00min
ACQ Mode	Scan
Event Time	0.50sec
Scan Speed	1000
Start m/z	50.00
End m/z	510.00
Electron Voltage	: 70 eV
Ionization Mode	: EI

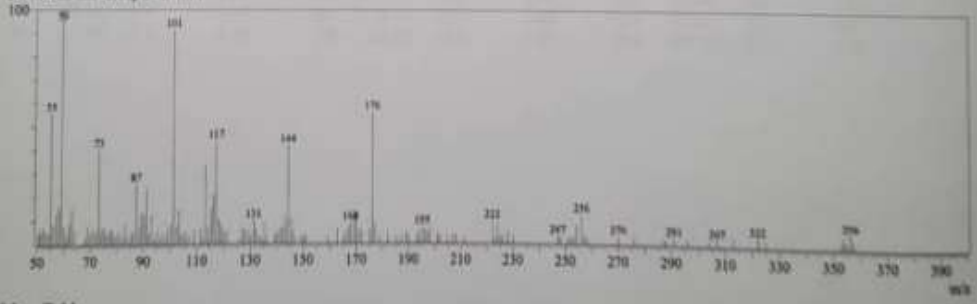
C:\GCMSsolution\Data\Project1\B7.QGD

Chromatogram B7 C:\GCMSsolution\Data\Project1\B7.QGD



Spectrum

Line#:1 R.Time:2.4(Scan#:284)
MassPeaks:153(Peak Elimination m/z: 371.30)
RawMode:Single 2.4(284) BasePeak:59(9121)
BG Mode:None Group 1 - Event 1



Mass Table
Line#:1 R.Time:2.4(Scan#:284)
MassPeaks:153(Peak Elimination m/z: 371.30)
RawMode:Single 2.4(284) BasePeak:59(9121)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.45	479	5.25	4	52.95	503	5.51	7	55.95	774	8.49
2	51.00	418	4.58	5	54.05	456	5.00	8	57.05	1175	12.88
3	52.00	654	7.17	6	55.00	5094	55.85	9	58.05	1464	16.05

1 / 2

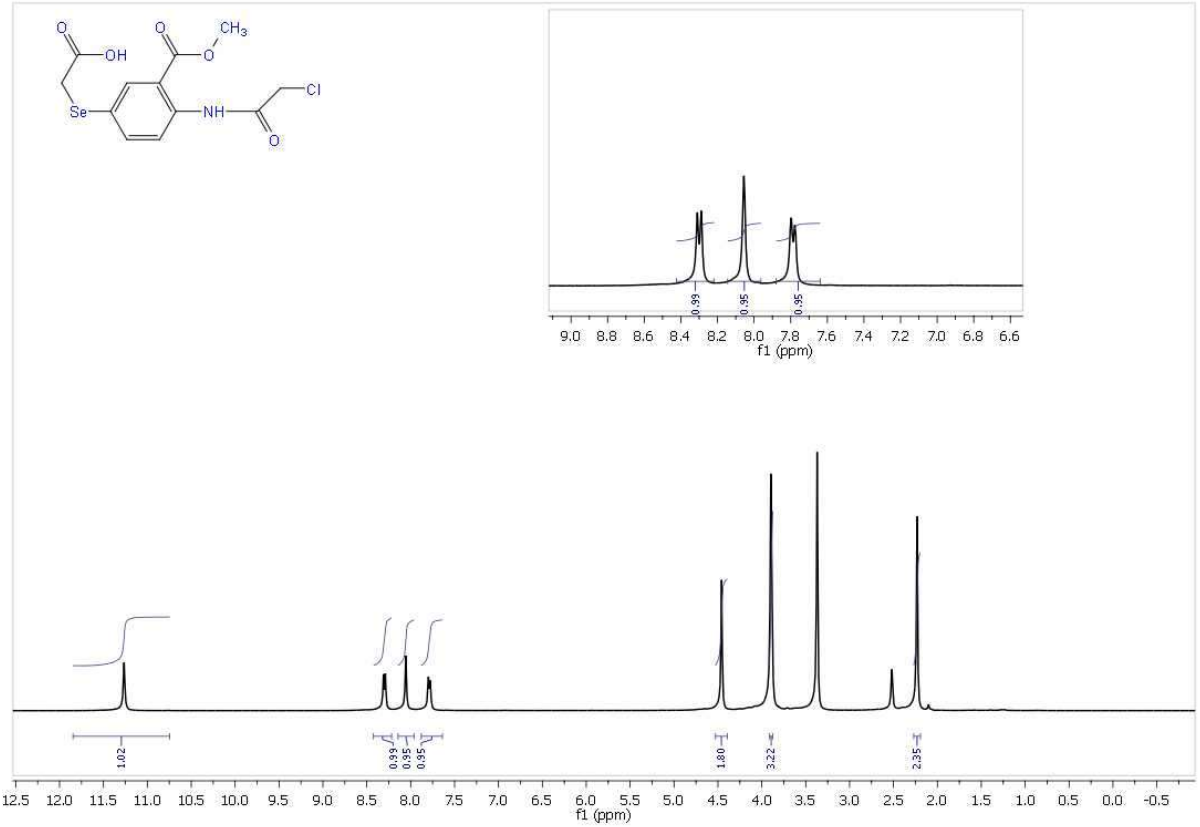
Mass chart of compound **13**

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	59.00	9121	100.00	58	112.20	249	2.73	106	185.10	271	2.97
11	60.10	700	7.67	59	113.15	3079	33.76	107	187.10	295	3.23
12	61.00	313	3.43	60	114.10	686	7.52	108	189.10	401	4.40
13	62.00	793	8.69	61	115.15	1410	15.46	109	190.10	274	3.00
14	63.00	1394	15.28	62	116.10	1900	20.83	110	193.10	250	2.74
15	64.05	587	6.44	63	117.15	4007	43.93	111	193.90	438	4.80
16	68.00	257	2.82	64	118.10	937	10.27	112	195.15	628	6.89
17	69.00	702	7.70	65	119.10	727	7.97	113	196.10	530	5.81
18	70.00	398	4.36	66	120.00	471	5.16	114	197.05	454	4.98
19	71.10	585	6.41	67	121.35	501	5.49	115	198.00	618	6.78
20	72.15	488	5.35	68	126.00	220	2.41	116	201.00	356	3.90
21	73.05	3687	40.42	69	127.00	602	6.60	117	202.00	314	3.44
22	74.10	556	6.10	70	128.10	521	5.71	118	205.00	268	2.94
23	75.10	663	7.27	71	129.10	463	5.08	119	207.00	351	3.85
24	76.00	369	4.05	72	130.10	361	3.96	120	208.15	344	3.77
25	77.05	545	5.98	73	131.15	893	9.79	121	211.20	274	3.00
26	78.00	574	6.29	74	132.10	534	5.85	122	222.00	873	9.57
27	79.00	318	3.49	75	133.10	327	3.59	123	223.00	201	2.20
28	79.90	446	4.89	76	134.10	209	2.29	124	223.95	782	8.57
29	81.05	399	4.37	77	135.20	836	9.17	125	225.00	319	3.50
30	82.00	222	2.43	78	136.20	321	3.52	126	226.00	250	2.74
31	83.15	848	9.30	79	139.20	378	4.14	127	228.00	450	4.93
32	84.10	265	2.91	80	140.00	402	4.41	128	230.00	286	3.14
33	85.30	417	4.57	81	141.00	591	6.48	129	247.00	310	3.40
34	86.15	456	5.00	82	142.00	598	6.56	130	248.00	303	3.32
35	87.10	2335	25.60	83	143.10	1033	11.33	131	251.00	241	2.64
36	88.20	636	6.97	84	144.10	3812	41.79	132	252.00	262	2.87
37	89.15	1264	13.86	85	145.15	968	10.61	133	253.00	295	3.23
38	90.15	1123	12.31	86	146.00	506	5.55	134	254.10	719	7.88
39	91.10	2137	23.43	87	147.00	265	2.91	135	256.05	1146	12.56
40	92.05	408	4.47	88	149.00	260	2.85	136	257.00	314	3.44
41	93.00	1156	12.67	89	150.00	343	3.76	137	258.00	266	2.92
42	94.00	231	2.53	90	151.00	254	2.78	138	270.00	321	3.52
43	95.10	506	5.55	91	159.00	252	2.76	139	276.00	257	2.82
44	96.10	242	2.65	92	162.80	562	6.16	140	287.00	220	2.41
45	97.30	462	5.07	93	165.00	236	2.59	141	288.00	202	2.21
46	98.30	252	2.76	94	166.00	434	4.76	142	291.00	292	3.20
47	99.15	556	6.10	95	167.00	610	6.69	143	296.00	222	2.43
48	100.15	784	8.60	96	167.95	794	8.71	144	304.00	207	2.27
49	101.10	8338	91.42	97	169.00	1034	11.34	145	307.00	246	2.70
50	102.15	677	7.42	98	170.00	1202	13.18	146	313.00	351	3.85
51	103.10	1345	14.75	99	171.10	588	6.45	147	322.00	356	3.90
52	104.10	334	3.66	100	172.10	422	4.63	148	325.00	241	2.64
53	105.20	450	4.93	101	175.15	491	5.38	149	353.00	218	2.39
54	106.20	390	4.28	102	176.10	5108	56.00	150	353.75	429	4.70
55	107.20	313	3.43	103	177.10	766	8.40	151	354.80	233	2.55
56	109.10	554	6.07	104	179.10	263	2.88	152	356.30	585	6.41
57	111.30	574	6.29	105	182.10	412	4.52	153	357.30	222	2.43

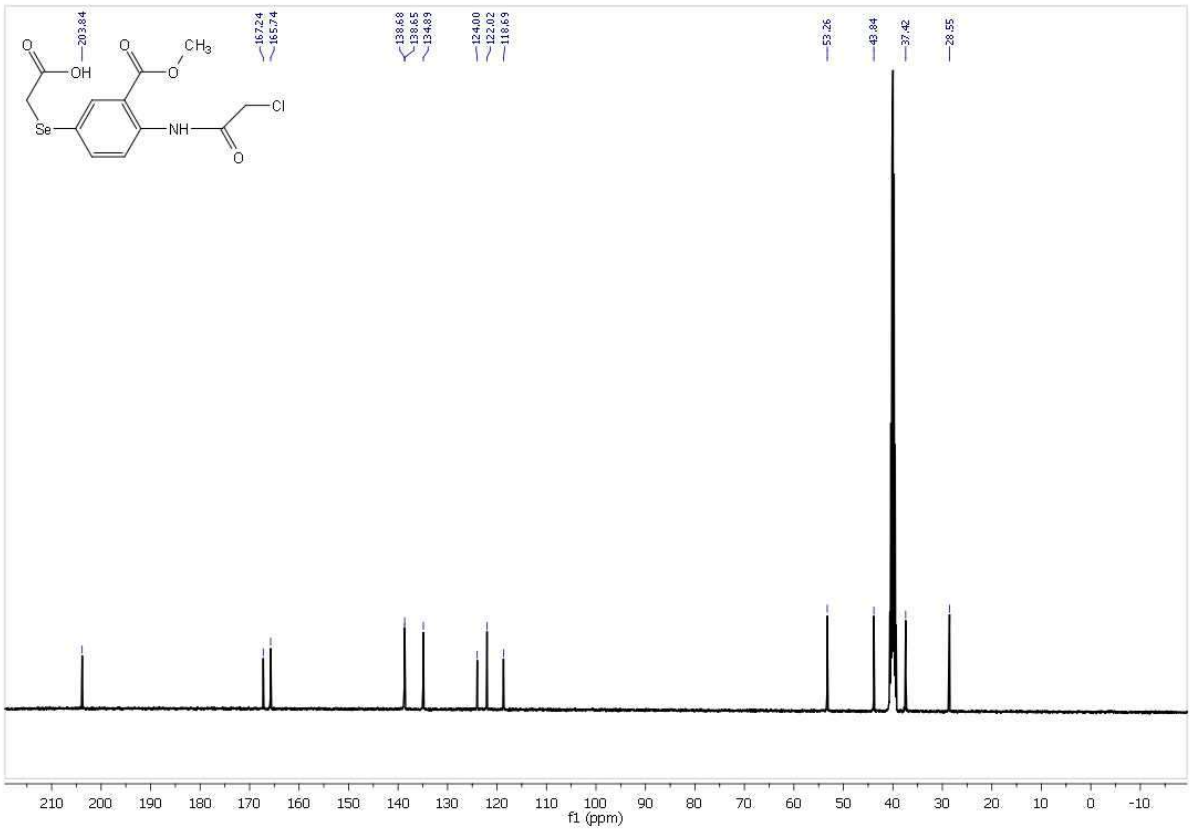
2 / 2

Mass chart of compound **13**

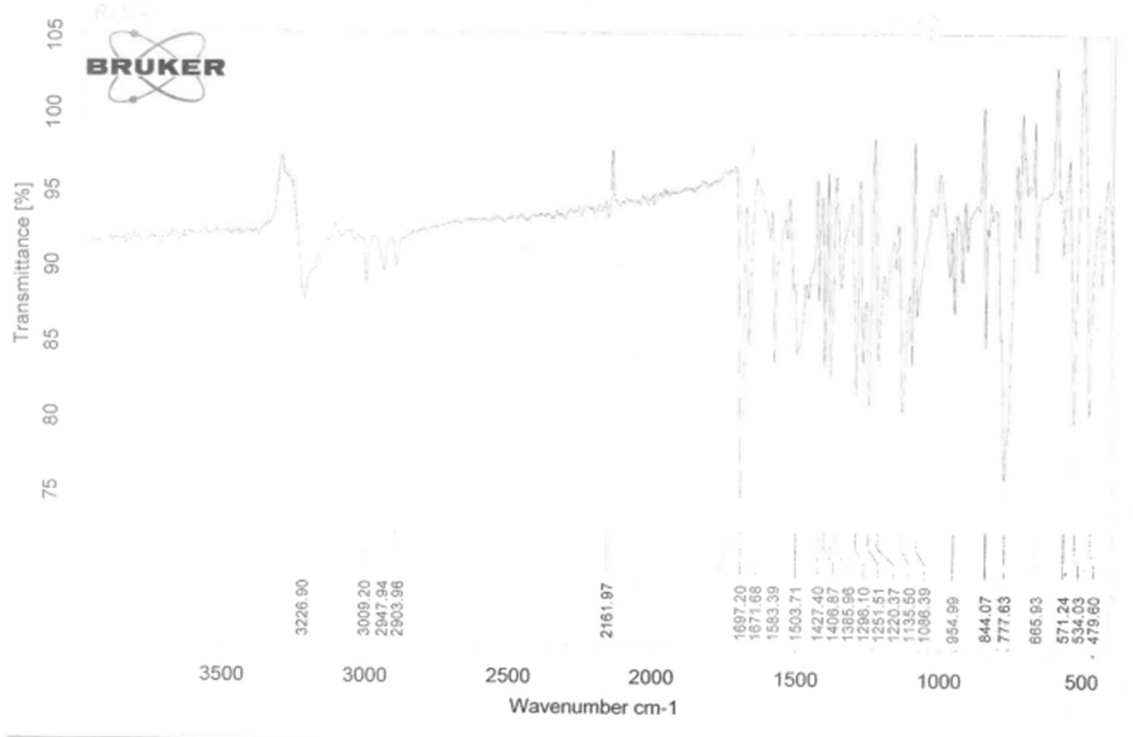
*Methyl 2-(2-chloroacetamido)-5-selenocyanatobenzoate (**14**).*



[1]HNMR chart of compound **14**



^{13}CNMR chart of compound **14**



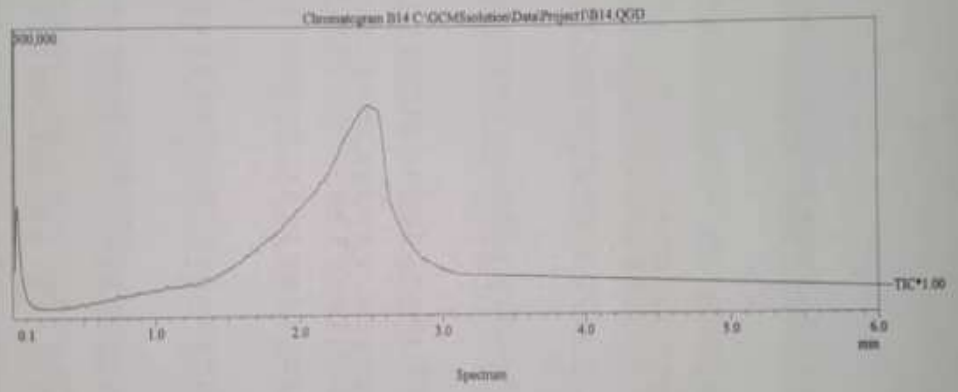
IR chart of compound **14**

Cairo University
Micro Analytical Center

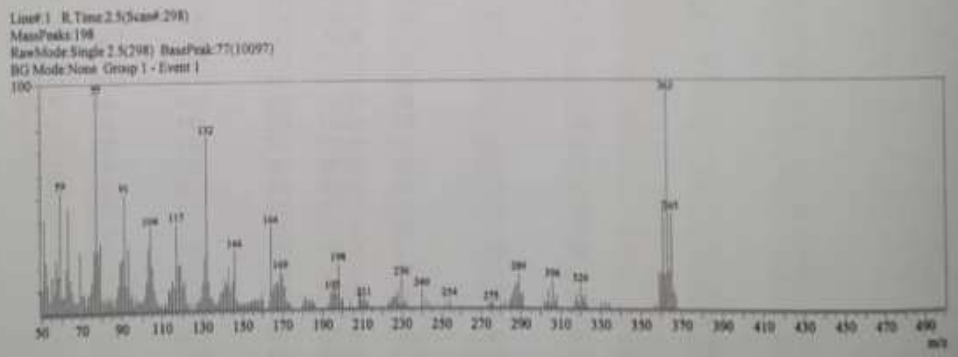
DI Analysis
Shimadzu Qp-2010 Plus

Sample Information		Method	
Analyzed by	: Dr. Mai Younis		
Analyzed	: 03/01/2007 08:07:39	——— Analytical Line 1 ———	
Sample Name	: B14	IonSourceTemp	:250.00 °C
Sample ID		[MS Table]	
Customer Name	: Dr.Mohamed Soliman - Science - Cairo	--Group 1 - Event 1--	
Data File	: C:\GCMSsolution\Data\Project1\B14.QGD	Start Time	:0.00min
Org Data File	: C:\GCMSsolution\Data\Project1\B14.QGD	End Time	:10.00min
Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op	ACQ Mode	:Scan
Org Method File	: C:\GCMSsolution\Data\Project1\High Temperature Op	Event Time	:0.50sec
Report File	:	Scan Speed	:1000
Tuning File	: C:\GCMSsolution\System\Tune1_default.qgt	Start m/z	:50.00
EndModified by	: Dr. Mai Younis	End m/z	:510.00
Modified	: 03/01/2007 08:10:32	Electron Voltage	:70 eV
		Ionization Mode	: EI

C:\GCMSsolution\Data\Project1\B14.QGD



Spectrum

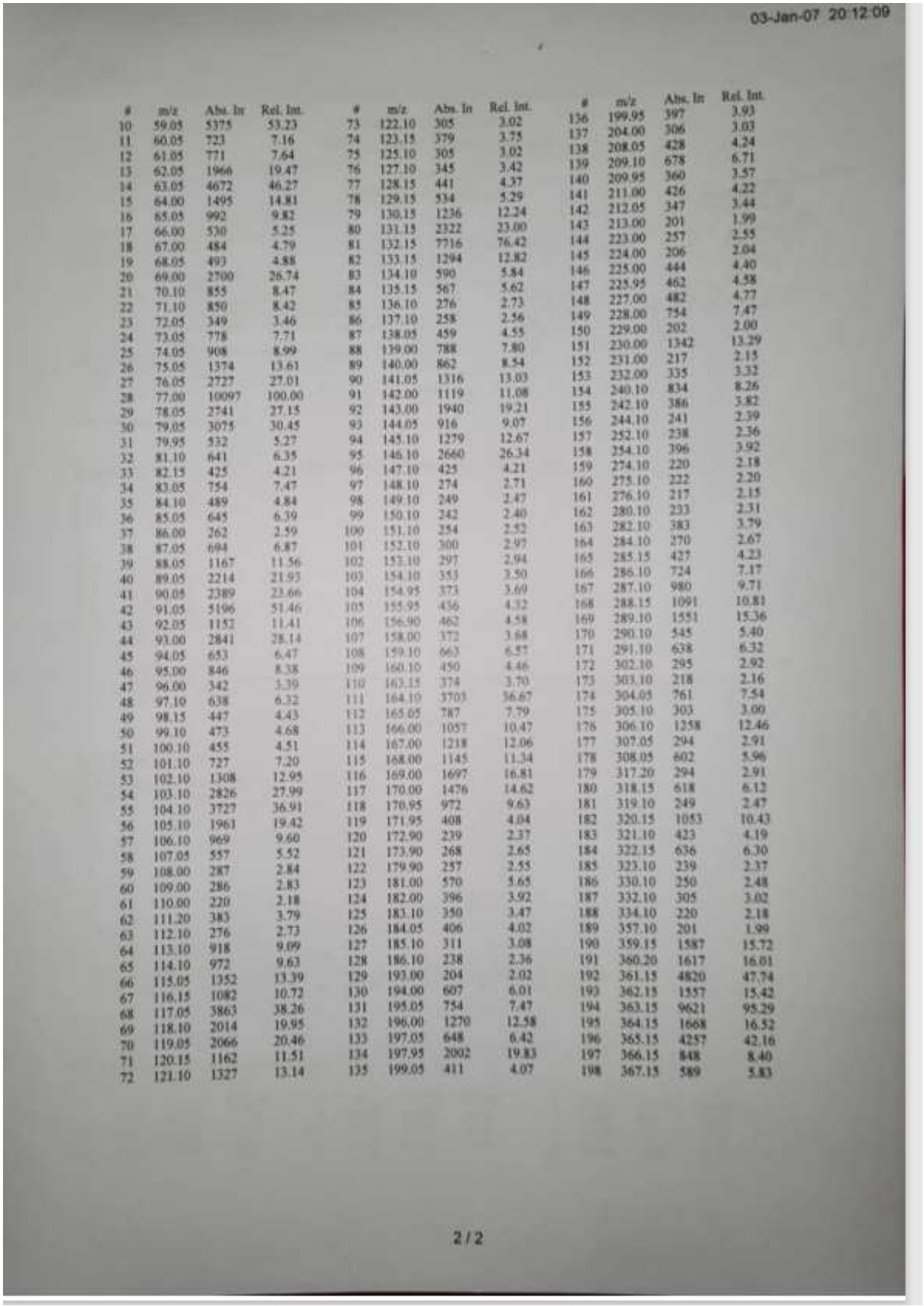


Mass Table
Line#:1 R.Time:2.5(Scan#:298)
MassPeaks:198
RawMode:Single 2.5(298) BasePeak:77(10097)
BG Mode:None Group 1 - Event 1

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
1	50.05	1090	10.80	4	53.00	1297	12.85	7	56.10	962	9.53
2	51.00	4151	41.11	5	54.05	547	5.42	8	57.05	2388	23.65
3	52.00	2271	22.49	6	55.05	1624	16.08	9	58.05	1652	16.36

1 / 2

Mass chart of compound **14**



03-Jan-07 20:12:09

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	59.05	5375	53.23	73	122.10	305	3.02	136	199.95	397	3.93
11	60.05	723	7.16	74	123.15	379	3.75	137	204.00	306	3.03
12	61.05	771	7.64	75	125.10	305	3.02	138	208.05	428	4.24
13	62.05	1966	19.47	76	127.10	345	3.42	139	209.10	678	6.71
14	63.05	4672	46.27	77	128.15	441	4.37	140	209.95	360	3.57
15	64.00	1495	14.81	78	129.15	534	5.29	141	211.00	426	4.22
16	65.05	992	9.82	79	130.15	1236	12.24	142	212.05	347	3.44
17	66.00	530	5.25	80	131.15	2322	23.00	143	213.00	201	1.99
18	67.00	484	4.79	81	132.15	7716	76.42	144	223.00	257	2.55
19	68.05	493	4.88	82	133.15	1294	12.82	145	224.00	206	2.04
20	69.00	2700	26.74	83	134.10	590	5.84	146	225.00	444	4.40
21	70.10	855	8.47	84	135.15	567	5.62	147	225.95	462	4.58
22	71.10	850	8.42	85	136.10	276	2.73	148	227.00	482	4.77
23	72.05	349	3.46	86	137.10	258	2.56	149	228.00	754	7.47
24	73.05	778	7.71	87	138.05	459	4.55	150	229.00	202	2.00
25	74.05	908	8.99	88	139.00	788	7.80	151	230.00	1342	13.29
26	75.05	1374	13.61	89	140.00	862	8.54	152	231.00	217	2.15
27	76.05	2727	27.01	90	141.05	1316	13.03	153	232.00	335	3.32
28	77.00	10097	100.00	91	142.00	1119	11.08	154	240.10	834	8.26
29	78.05	2741	27.15	92	143.00	1940	19.21	155	242.10	386	3.82
30	79.05	3075	30.45	93	144.05	916	9.07	156	244.10	241	2.39
31	79.95	532	5.27	94	145.10	1279	12.67	157	252.10	238	2.36
32	81.10	641	6.35	95	146.10	2660	26.34	158	254.10	396	3.92
33	82.15	425	4.21	96	147.10	425	4.21	159	274.10	220	2.18
34	83.05	754	7.47	97	148.10	274	2.71	160	275.10	222	2.20
35	84.10	489	4.84	98	149.10	249	2.47	161	276.10	217	2.15
36	85.05	645	6.39	99	150.10	242	2.40	162	280.10	233	2.31
37	86.00	262	2.59	100	151.10	254	2.52	163	282.10	383	3.79
38	87.05	694	6.87	101	152.10	300	2.97	164	284.10	270	2.67
39	88.05	1167	11.56	102	153.10	297	2.94	165	285.15	427	4.23
40	89.05	2214	21.93	103	154.10	353	3.50	166	286.10	724	7.17
41	90.05	2389	23.66	104	154.95	373	3.69	167	287.10	980	9.71
42	91.05	5196	51.46	105	155.95	436	4.32	168	288.15	1091	10.81
43	92.05	1152	11.41	106	156.90	462	4.58	169	289.10	1551	15.36
44	93.00	2841	28.14	107	158.00	372	3.68	170	290.10	545	5.40
45	94.05	653	6.47	108	159.10	663	6.57	171	291.10	638	6.32
46	95.00	846	8.38	109	160.10	450	4.46	172	302.10	295	2.92
47	96.00	342	3.39	110	163.15	374	3.70	173	303.10	218	2.16
48	97.10	638	6.32	111	164.10	5703	56.67	174	304.05	761	7.54
49	98.15	447	4.43	112	165.05	787	7.79	175	305.10	303	3.00
50	99.10	473	4.68	113	166.00	1057	10.47	176	306.10	1258	12.46
51	100.10	455	4.51	114	167.00	1218	12.06	177	307.05	294	2.91
52	101.10	727	7.20	115	168.00	1145	11.34	178	308.05	602	5.96
53	102.10	1308	12.95	116	169.00	1697	16.81	179	317.20	294	2.91
54	103.10	2826	27.99	117	170.00	1476	14.62	180	318.15	618	6.12
55	104.10	3727	36.91	118	170.95	972	9.63	181	319.10	249	2.47
56	105.10	1961	19.42	119	171.95	408	4.04	182	320.15	1053	10.43
57	106.10	969	9.60	120	172.90	239	2.37	183	321.10	423	4.19
58	107.05	557	5.52	121	173.90	268	2.65	184	322.15	636	6.30
59	108.00	287	2.84	122	179.90	257	2.55	185	323.10	239	2.37
60	109.00	286	2.83	123	181.00	570	5.65	186	330.10	250	2.48
61	110.00	220	2.18	124	182.00	396	3.92	187	332.10	305	3.02
62	111.20	383	3.79	125	183.10	350	3.47	188	334.10	220	2.18
63	112.10	276	2.73	126	184.05	406	4.02	189	357.10	201	1.99
64	113.10	918	9.09	127	185.10	311	3.08	190	359.15	1587	15.72
65	114.10	972	9.63	128	186.10	238	2.36	191	360.20	1617	16.01
66	115.05	1352	13.39	129	193.00	204	2.02	192	361.15	4820	47.74
67	116.15	1082	10.72	130	194.00	607	6.01	193	362.15	1557	15.42
68	117.05	3863	38.26	131	195.05	754	7.47	194	363.15	9621	95.29
69	118.10	2014	19.95	132	196.00	1270	12.58	195	364.15	1668	16.52
70	119.05	2066	20.46	133	197.05	648	6.42	196	365.15	4257	42.16
71	120.15	1162	11.51	134	197.95	2002	19.83	197	366.15	848	8.40
72	121.10	1327	13.14	135	199.05	411	4.07	198	367.15	589	5.83

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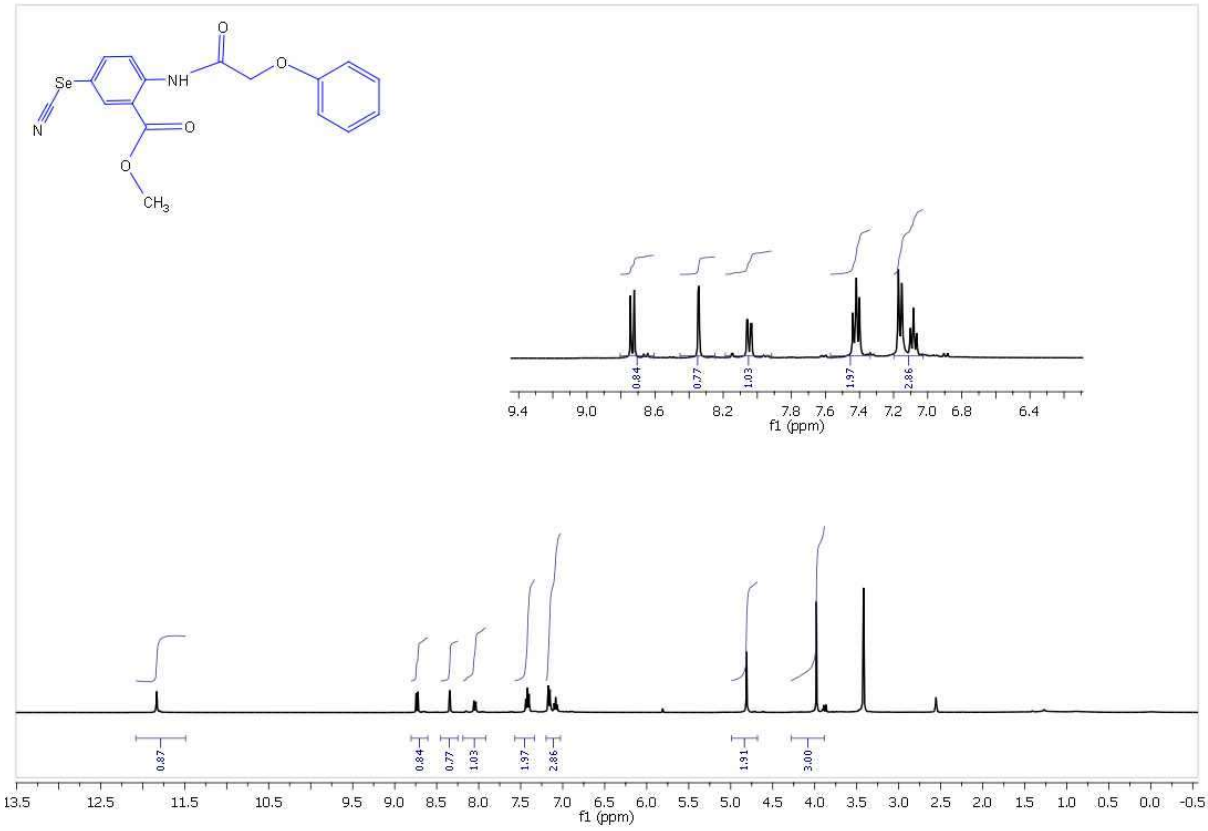
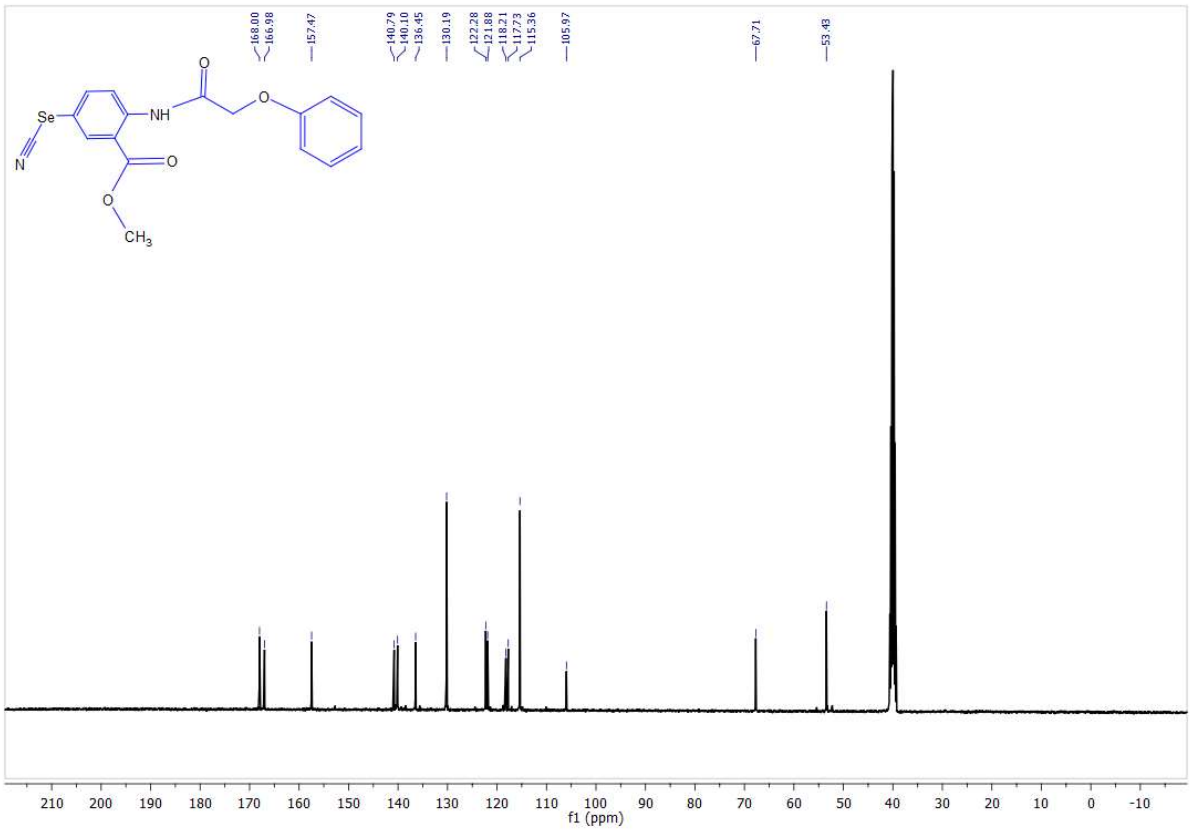
Mass chart of compound **14**

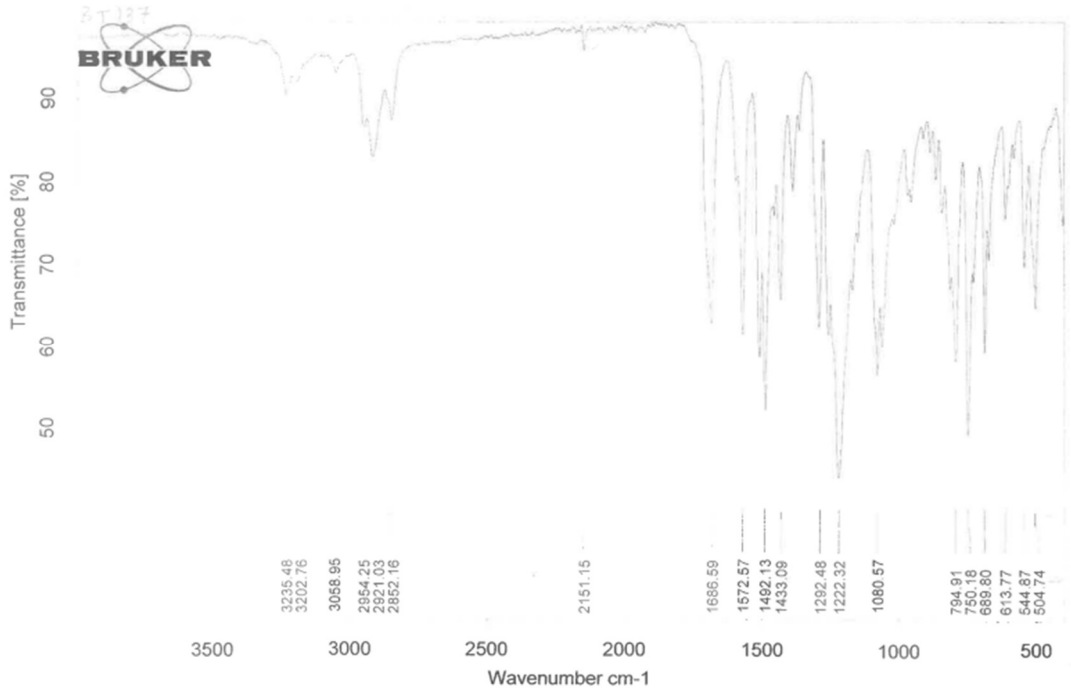
*Methyl 2-(2-phenoxyacetamido)-5-selenocyanatobenzoate (**15**).*



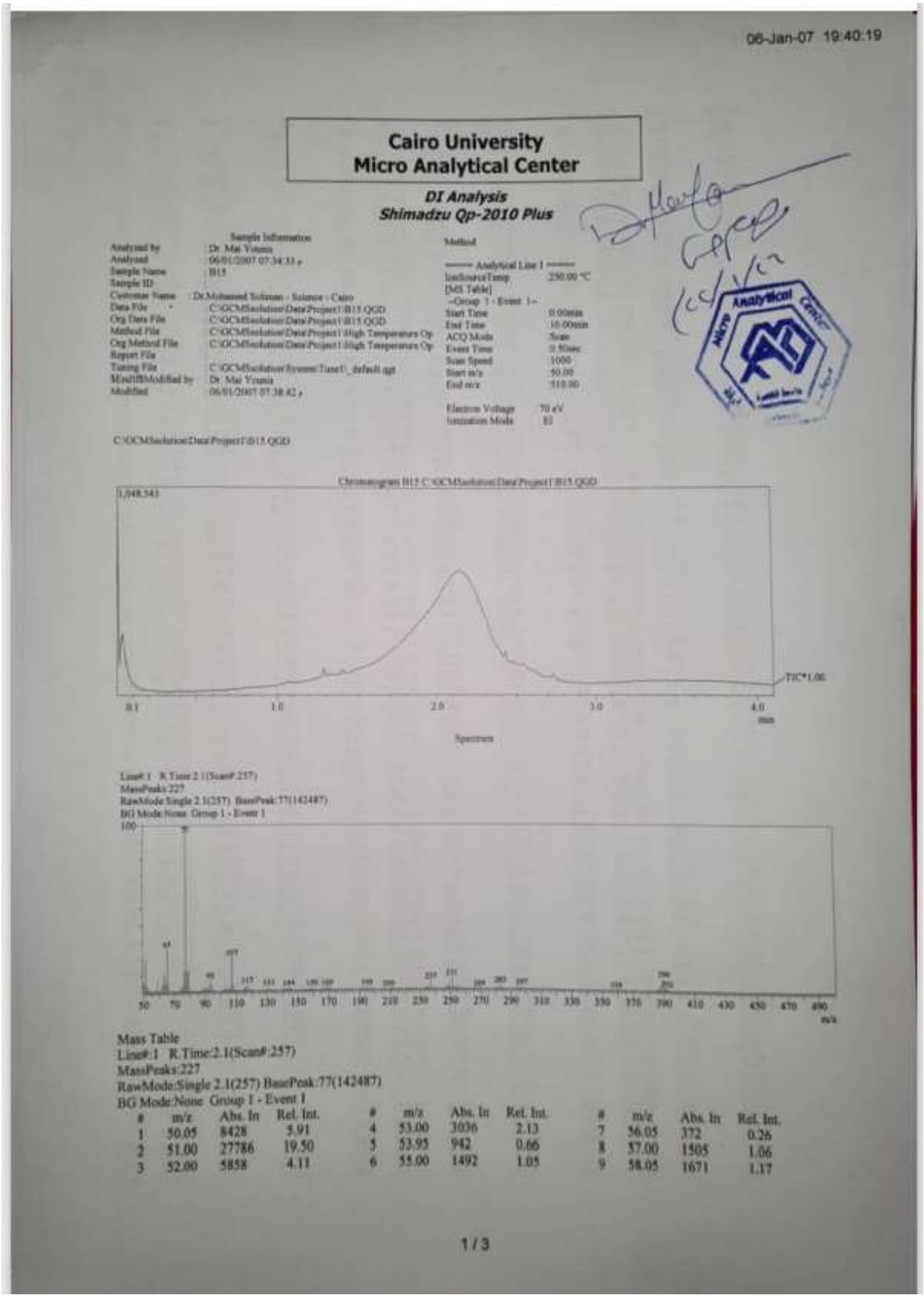
^{1}HNMR chart of compound **15**



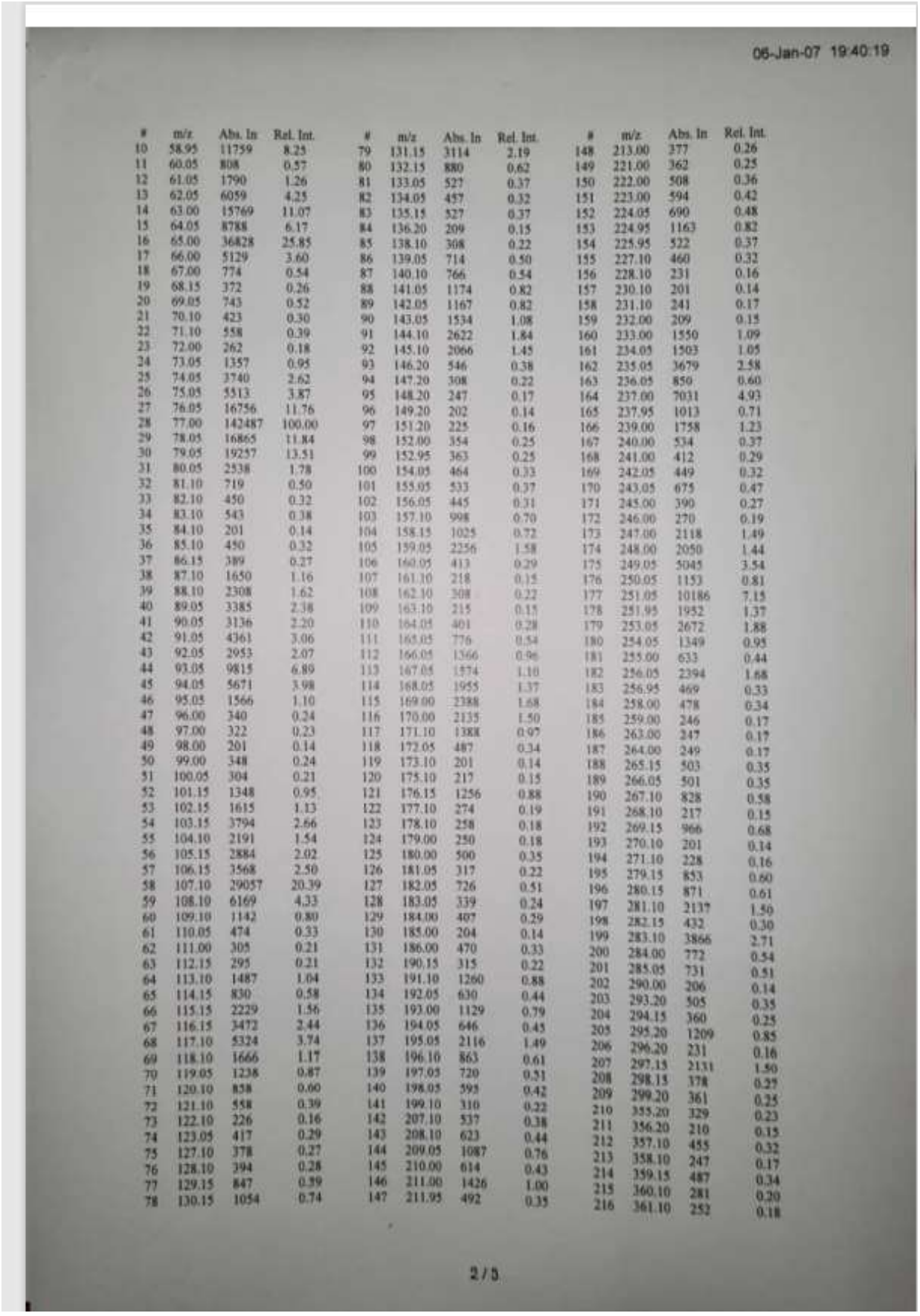
^{13}CNMR chart of compound **15**



IR chart of compound **15**



Mass chart of compound **15**



06-Jan-07 19:40:19

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	58.95	11759	8.25	79	131.15	3114	2.19	148	213.00	377	0.26
11	60.05	808	0.57	80	132.15	880	0.62	149	221.00	362	0.25
12	61.05	1790	1.26	81	133.05	527	0.37	150	222.00	508	0.36
13	62.05	6059	4.25	82	134.05	457	0.32	151	223.00	594	0.42
14	63.00	15769	11.07	83	135.15	527	0.37	152	224.05	690	0.48
15	64.05	8788	6.17	84	136.20	209	0.15	153	224.95	1163	0.82
16	65.00	36828	25.85	85	138.10	308	0.22	154	225.95	522	0.37
17	66.00	5129	3.60	86	139.05	714	0.50	155	227.10	460	0.32
18	67.00	774	0.54	87	140.10	766	0.54	156	228.10	231	0.16
19	68.15	372	0.26	88	141.05	1174	0.82	157	230.10	201	0.14
20	69.05	743	0.52	89	142.05	1167	0.82	158	231.10	241	0.17
21	70.10	423	0.30	90	143.05	1534	1.08	159	232.00	209	0.15
22	71.10	558	0.39	91	144.10	2622	1.84	160	233.00	1550	1.09
23	72.00	262	0.18	92	145.10	2066	1.45	161	234.05	1503	1.05
24	73.05	1357	0.95	93	146.20	546	0.38	162	235.05	3679	2.58
25	74.05	3740	2.62	94	147.20	308	0.22	163	236.05	850	0.60
26	75.05	5513	3.87	95	148.20	247	0.17	164	237.00	7031	4.93
27	76.05	16756	11.76	96	149.20	202	0.14	165	237.95	1013	0.71
28	77.00	142487	100.00	97	151.20	225	0.16	166	239.00	1758	1.23
29	78.05	16865	11.84	98	152.00	354	0.25	167	240.00	534	0.37
30	79.05	19257	13.51	99	152.95	363	0.25	168	241.00	412	0.29
31	80.05	2538	1.78	100	154.05	464	0.33	169	242.05	449	0.32
32	81.10	719	0.50	101	155.05	533	0.37	170	243.05	675	0.47
33	82.10	450	0.32	102	156.05	445	0.31	171	245.00	390	0.27
34	83.10	543	0.38	103	157.10	998	0.70	172	246.00	270	0.19
35	84.10	201	0.14	104	158.15	1025	0.72	173	247.00	2118	1.49
36	85.10	450	0.32	105	159.05	2256	1.58	174	248.00	2050	1.44
37	86.15	389	0.27	106	160.05	413	0.29	175	249.05	5045	3.54
38	87.10	1650	1.16	107	161.10	218	0.15	176	250.05	1153	0.81
39	88.10	2308	1.62	108	162.10	308	0.22	177	251.05	10186	7.15
40	89.05	3385	2.38	109	163.10	215	0.15	178	251.95	1952	1.37
41	90.05	3136	2.20	110	164.05	401	0.28	179	253.05	2672	1.88
42	91.05	4361	3.06	111	165.05	776	0.54	180	254.05	1349	0.95
43	92.05	2953	2.07	112	166.05	1366	0.96	181	255.00	633	0.44
44	93.05	9815	6.89	113	167.05	1574	1.10	182	256.05	2394	1.68
45	94.05	5671	3.98	114	168.05	1955	1.37	183	256.95	469	0.33
46	95.05	1566	1.10	115	169.00	2388	1.68	184	258.00	478	0.34
47	96.00	340	0.24	116	170.00	2135	1.50	185	259.00	246	0.17
48	97.00	322	0.23	117	171.10	1388	0.97	186	263.00	247	0.17
49	98.00	201	0.14	118	172.05	487	0.34	187	264.00	249	0.17
50	99.00	348	0.24	119	173.10	201	0.14	188	265.15	503	0.35
51	100.05	304	0.21	120	175.10	217	0.15	189	266.05	501	0.35
52	101.15	1348	0.95	121	176.15	1256	0.88	190	267.10	828	0.58
53	102.15	1615	1.13	122	177.10	274	0.19	191	268.10	217	0.15
54	103.15	3794	2.66	123	178.10	258	0.18	192	269.15	966	0.68
55	104.10	2191	1.54	124	179.00	250	0.18	193	270.10	201	0.14
56	105.15	2884	2.02	125	180.00	500	0.35	194	271.10	228	0.16
57	106.15	3568	2.50	126	181.05	317	0.22	195	279.15	853	0.60
58	107.10	29057	20.39	127	182.05	726	0.51	196	280.15	871	0.61
59	108.10	6169	4.33	128	183.05	339	0.24	197	281.10	2137	1.50
60	109.10	1142	0.80	129	184.00	407	0.29	198	282.15	432	0.30
61	110.05	474	0.33	130	185.00	204	0.14	199	283.10	3866	2.71
62	111.00	305	0.21	131	186.00	470	0.33	200	284.00	772	0.54
63	112.15	295	0.21	132	190.15	315	0.22	201	285.05	731	0.51
64	113.10	1487	1.04	133	191.10	1260	0.88	202	290.00	206	0.14
65	114.15	830	0.58	134	192.05	630	0.44	203	293.20	505	0.35
66	115.15	2229	1.56	135	193.00	1129	0.79	204	294.15	360	0.25
67	116.15	3472	2.44	136	194.05	646	0.45	205	295.20	1209	0.85
68	117.10	5324	3.74	137	195.05	2116	1.49	206	296.20	231	0.16
69	118.10	1666	1.17	138	196.10	863	0.61	207	297.15	2131	1.50
70	119.05	1238	0.87	139	197.05	720	0.51	208	298.15	378	0.27
71	120.10	858	0.60	140	198.05	595	0.42	209	299.20	361	0.25
72	121.10	558	0.39	141	199.10	310	0.22	210	355.20	329	0.23
73	122.10	226	0.16	142	207.10	537	0.38	211	356.20	210	0.15
74	123.05	417	0.29	143	208.10	623	0.44	212	357.10	455	0.32
75	127.10	378	0.27	144	209.05	1087	0.76	213	358.10	247	0.17
76	128.10	394	0.28	145	210.00	614	0.43	214	359.15	487	0.34
77	129.15	847	0.59	146	211.00	1426	1.00	215	360.10	281	0.20
78	130.15	1054	0.74	147	211.95	492	0.35	216	361.10	252	0.18

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Mass chart of compound **15**

Mass chart of compound **15**