Supplementary Information

Article

Synthesis of new organoselenium-based succinanilic and maleanilic derivatives and in-silico studies as possible SARS-CoV-2 main protease inhibitors

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SI.1. MD simulations

The MD simulations were carried out using Desmond simulation package of Schrödinger LLC [1]. The NPT ensemble with the temperature 300 K and a pressure 1 bar was applied in all runs. The simulation length was 200 ns with a relaxation time 1 ps for the ligands. The OPLS3 force field parameters were used in all simulations [2]. The cutoff radius in Coulomb interactions was 9.0 Å. The orthorhombic periodic box boundaries were set 10 Å away from the protein atoms. The water molecules were explicitly described using the transferable intermolecular potential with three points (TIP3P) model [3]. Salt concentration set to 0.15 M NaCl and was built using the System Builder utility of Desmond [4]. The Martyna−Tuckerman−Klein chain coupling scheme with a coupling constant of 2.0 ps was used for the pressure control and the Nosé−Hoover chain coupling scheme for the temperature control [5]. Nonbonded forces were calculated using a RESPA integrator where the short-range forces were updated every step and the long-range forces were updated every three steps. The trajectories were saved at 20 ns intervals for analysis. The behavior and interactions between the ligands and protein were analyzed using the Simulation Interaction Diagram tool implemented in Desmond MD package. The stability of MD simulations was monitored by looking on the RMSD of the ligand and protein atom positions in time.

SI.2. MM-GBSA calculations and MD trajectory analysis

Simulation interactions diagram panel of Maestro software was used to monitoring interactions contribution in the ligand-protein stability. The molecular mechanics generalized born/solvent accessibility (MM – GBSA) was performed to calculate the ligand binding free energies and ligand strain energies for docked compounds over the last 50 ns with thermal_mmgbsa.py python script provided by Schrodinger which takes a Desmond trajectory file, splits it into individual snapshots, runs the MM-GBSA calculations on each frame, and outputs the average computed binding energy.

SI.3. Molecular docking against 6lu7

Also, the titled compounds were used as ligands (substrates) for investigation of their binding ability towards SARS-CoV-2 protease (PDB ID: 6LU7).

The 6LU7protein serves as the target receptor, while the chemicals that have been mentioned serve as the substrate. Figure (S3.a) displays the three-dimensional structure of the SARS-CoV-2 protease (PDB ID: 6LU7)that was developed before. Figure (S3.b) illustrates the active site pocket inside the Dummy atoms where molecular docking occurred. The amino acids of active site pocket are THR24, THR25, THR26, LEU27, HIS41, CYS44, THR45, SER46, MET49, PRO52, TYR54, PHE140, LEU141, ASN142, GLY143, SER144, CYS145, HIS163, HIS164, MET165, GLU166, LEU167, PRO168, HIS172, ASP187, ARG188, GLN189, THR190, and GLN192. The molecular docking results are shown in Table (S3), and Figure (S3.c) illustrates the location of the optimal conformation of the substrates under study inside the binding pocket. Table (S3) shows a presentation of the outcomes of the molecular docking.

As can be shown in Table (S3), and Figure (S3.c); the docking scores (S) for the subject substrates are significantly on the negative side. They connect to the 6LU7pocket in several different ways, including via hydrogen bonds and interactions that are hydrophobic. This suggests that the docked substrates are engaging in a robust interaction with the active region of the receptor. According to Table (S3), the compounds in issue have low RMSD values and high docking scores (regarding S and Kcal/mol) regarding the 6LU7. These values varied from -8.96 kcal/mol and 1.40 for compound 10and -8.93 kcal/mol and 1.43 for compound 12to -6.79 kcal/mol and 1.69 for compound 7. Therefore, compounds10and 12 seem to be the most energetic candidate because it has a high docking score (-8.96and -8.93Kcal/mol) and a low RMSD value (1.40 and 1.43). The following is a list of the levels of inhibitory activity in the order that they were reached: 10≈ 12 >11 > 9 >8>7, Table (S3). The docking results showed that the compounds with the highest activity level were compounds 10, 12, and 11.

Compound 10 creates two hydrogen bond donors: between SE11, and O17 with HIS164, and THR45, with distances of 3.29, and 2.93 angstroms, respectively, Table (S3) and Figure (S3.c). While, compound 12 creates two hydrogen bond donors: between N13, and O19 with GLN189, and THR190, with distances of 3.06, and 3.03 angstroms, respectively, Table (S3) and Figure (S3.c).In addition to two hydrogen bond acceptors, between SE11, and O16with GLY143, and GLU166, with distances of 3.13, and 2.94angstroms, respectively, Table (S3) and Fig. (S3.c).In

the case of compound 11 creates two hydrogen bond donors: between SE11-MET165, and SE11-THR190, with distances of 3.19, and 3.10angstroms. In addition to one hydrogen bond acceptor, between O20 with GLY143, with distances of 3.11 angstroms, Table (S3) and Fig. (S3.c).

The inhibition constant, sometimes referred to as the Ki value, is a critical component that is taken into consideration when deciding whether a molecule has the potential to be a hit, lead, or therapeutic candidate. For a molecule to be considered a hit or a lead chemical, the Ki value of the molecule must fall within the micromolar (μM) range. This is because, in most cases, a low Ki number indicates a high potency. The 6LU7domain Ki values of the discovered compounds varied from 0.27 μM (in the case of compound 10) and 0.29μM (in the case of compound 12) to 8.27 μM (in the case of compound 8) and 10.77μM (in the case of compound 7), which shows that every single one of them has the potential to be a hit and a lead. Accordingly, therapeutic applications are a viable option for the compounds produced and shown to have the lowest Ki value (Table (S3)).

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Figure S1. Various possible conformers of the title compounds

Figure S2. The plot of Natural charges distribution of the compounds 7-12 using the B3LYP/6-311G(d,p) in the gas phase

Figure S3. (a): The 3D structure of the 6lu7of novel coronavirus (COVID–19); (b): Active site pocket in which molecular docking occurred; and (c) 3D and 2D interactions of the titled compounds inside the active site of the target receptor.

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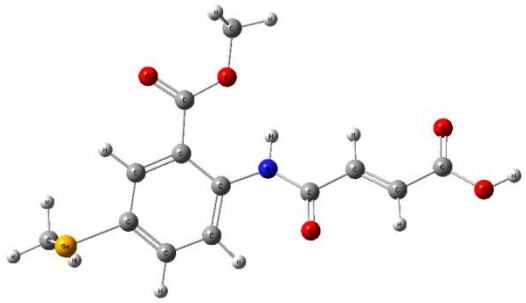
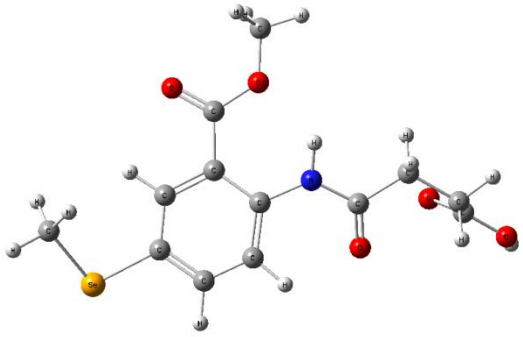
C1		
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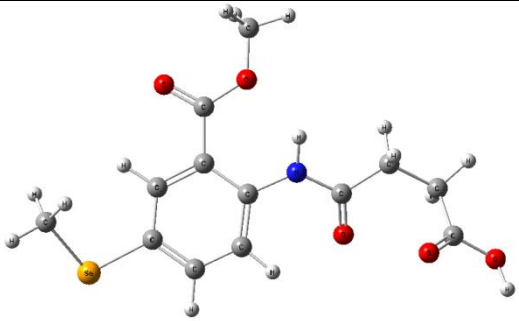
C2		
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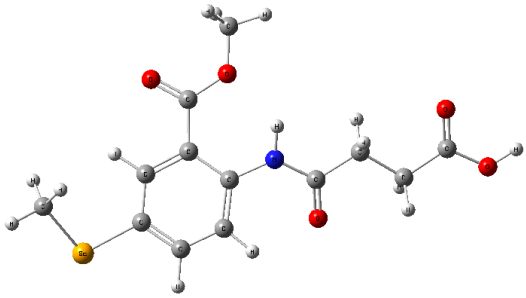
C3		
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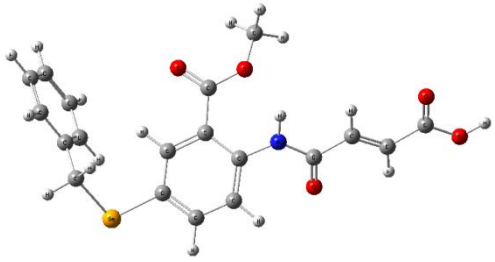
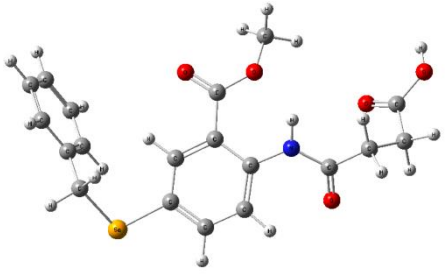
C1		
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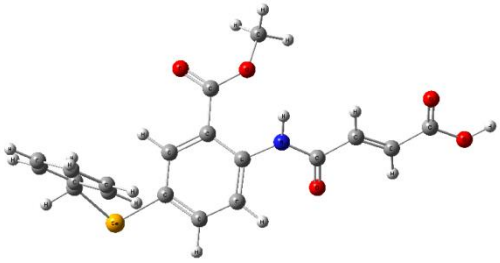
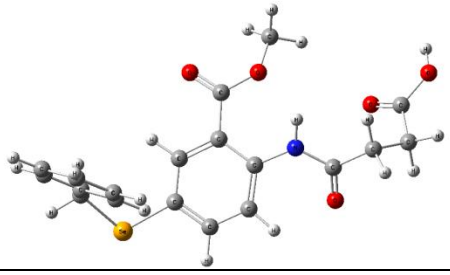
C2		
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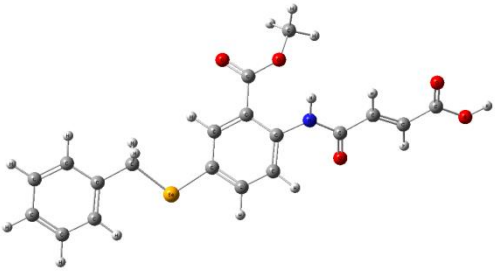
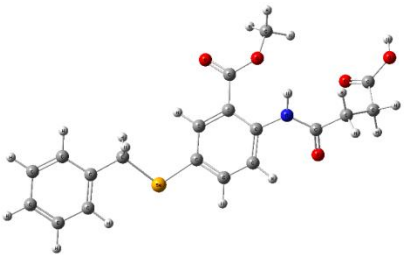
C3		
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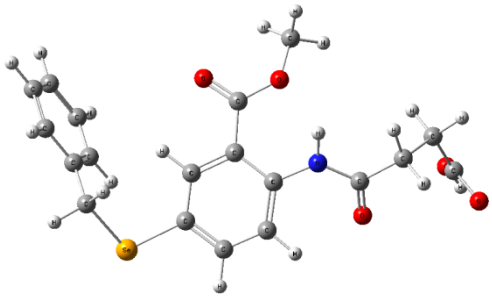
C4		
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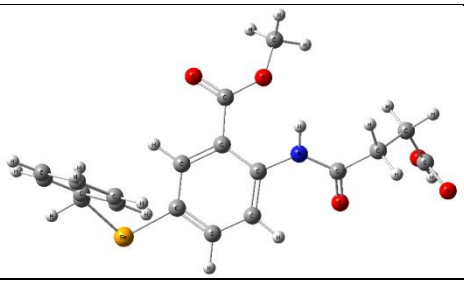
C5		
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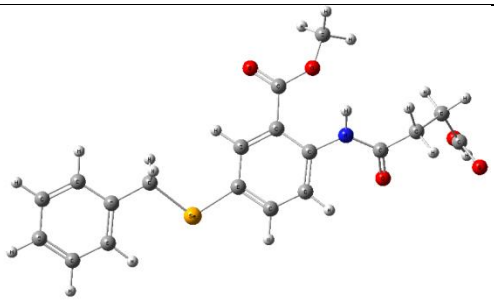
C6		
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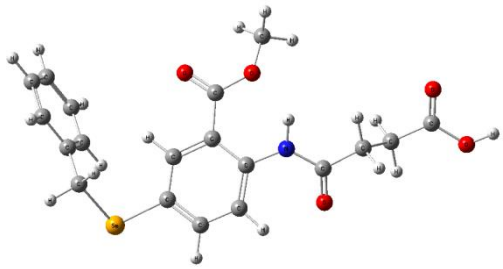
C7		
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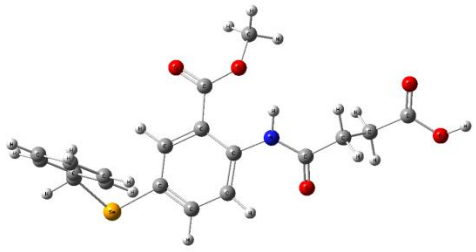
C8		
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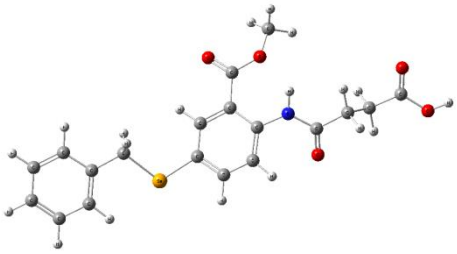
C9		
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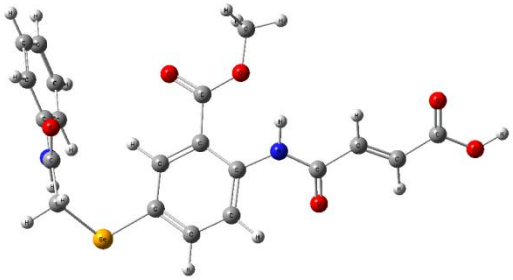
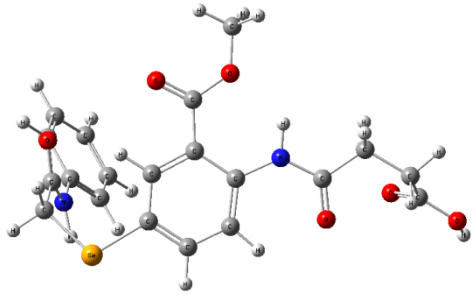
C1		
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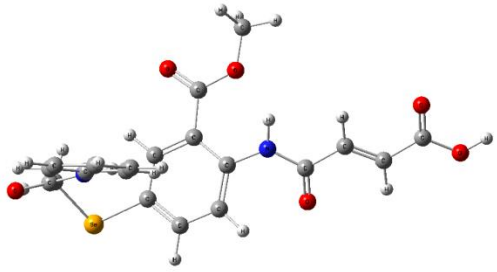
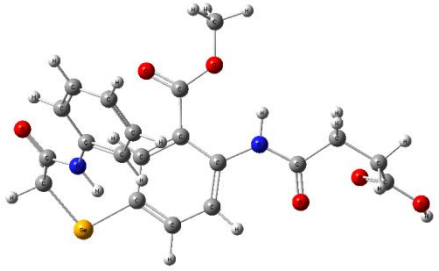
C2		
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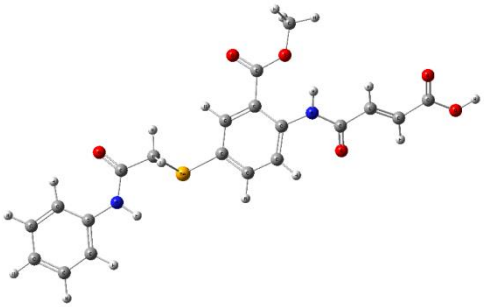
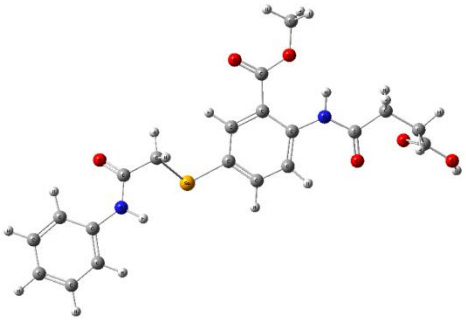
C3		
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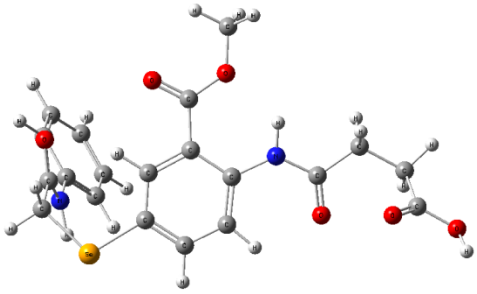
C4		
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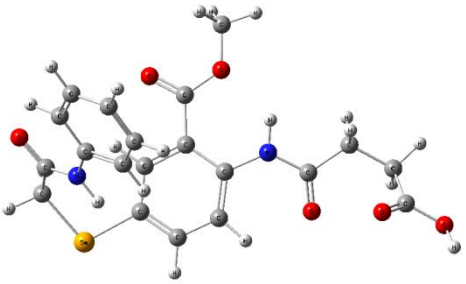
C5		
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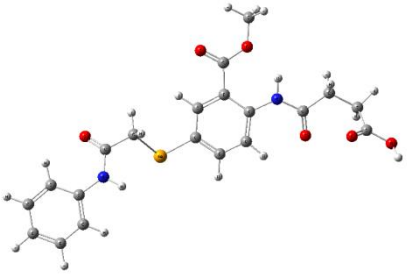
C6		
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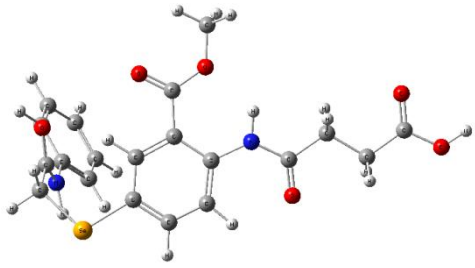
C7		

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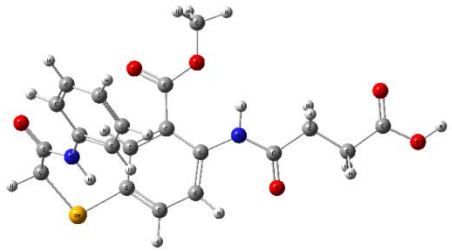
C8		
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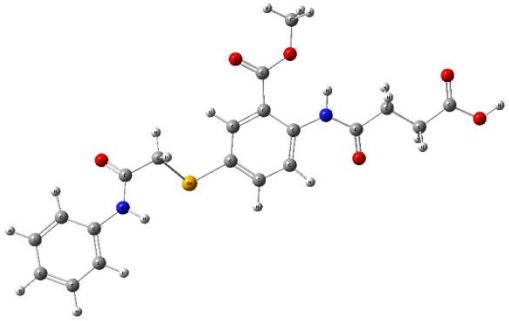
C9		
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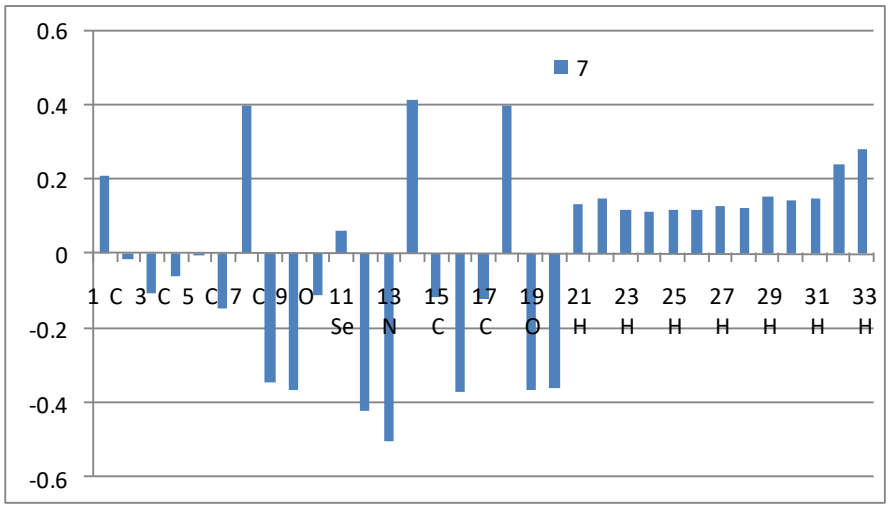
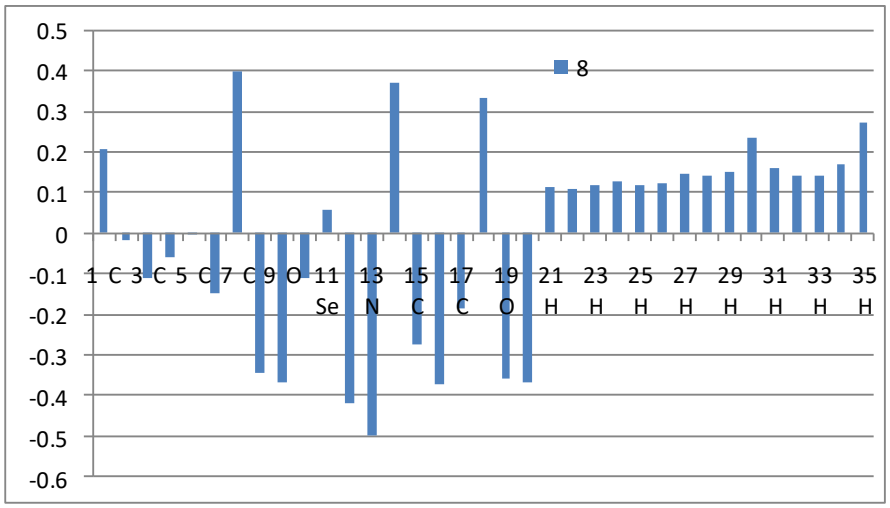
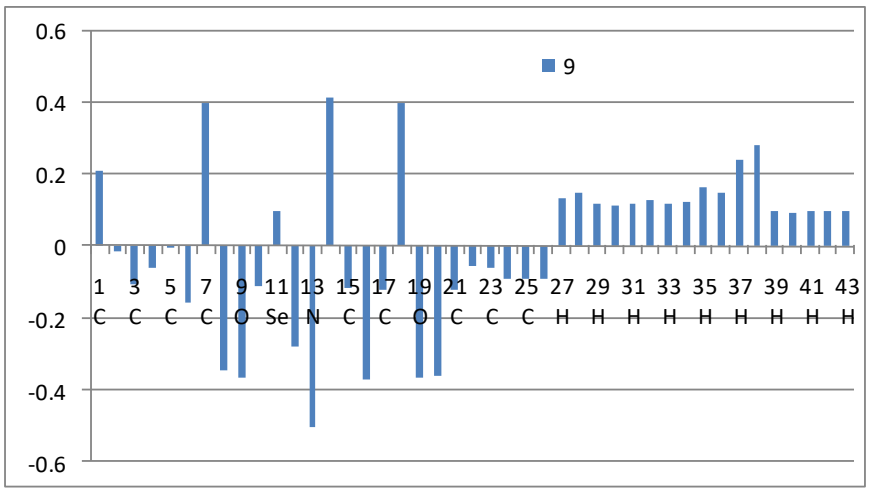
Figure S1. Various possible conformers of the title compounds.		

7	 7 0.6 0.4 0.2 0 -0.2 -0.4 -0.6 1 C 3 C 5 C 7 C 9 O 11 Se 13 N 15 C 17 C 19 O 21 H 23 H 25 H 27 H 29 H 31 H 33 H
8	 8 0.5 0.4 0.3 0.2 0.1 0 -0.1 -0.2 -0.3 -0.4 -0.5 -0.6 1 C 3 C 5 C 7 C 9 O 11 Se 13 N 15 C 17 C 19 O 21 H 23 H 25 H 27 H 29 H 31 H 33 H 35 H
9	 9 0.6 0.4 0.2 0 -0.2 -0.4 -0.6 1 C 3 C 5 C 7 C 9 O 11 Se 13 N 15 C 17 C 19 O 21 C 23 C 25 C 27 H 29 H 31 H 33 H 35 H 37 H 39 H 41 H 43 H

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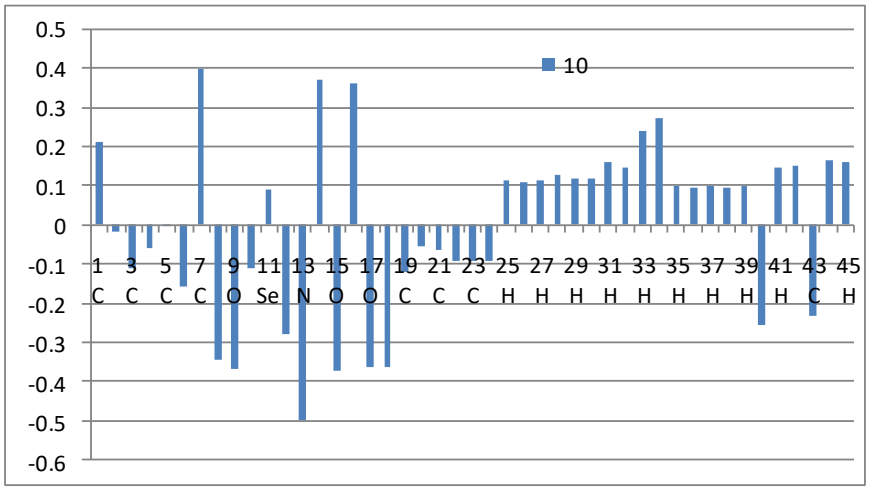

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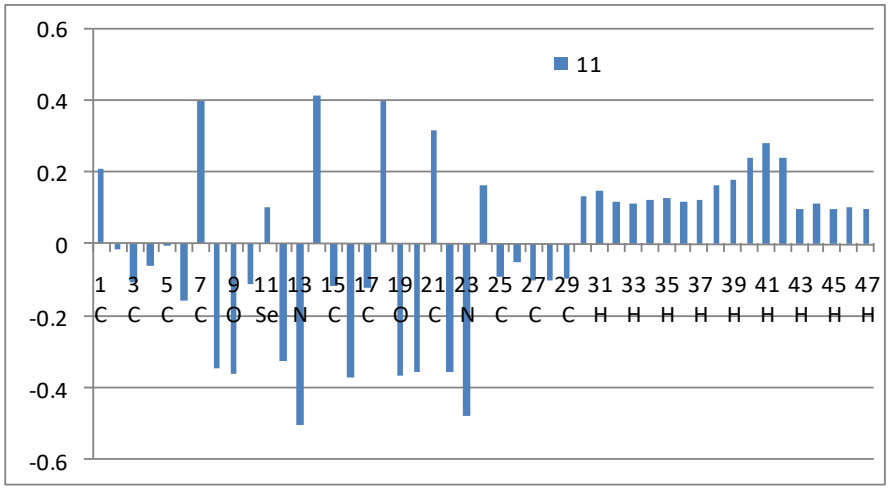

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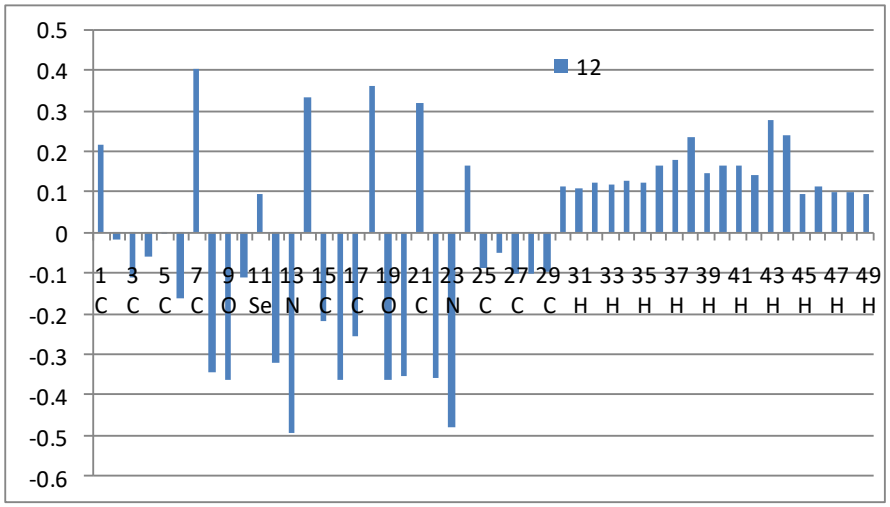

Figure S2. The plot of Natural charges distribution of the compounds 7-12 using the B3LYP/6-311G(d,p) in the gas phase

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	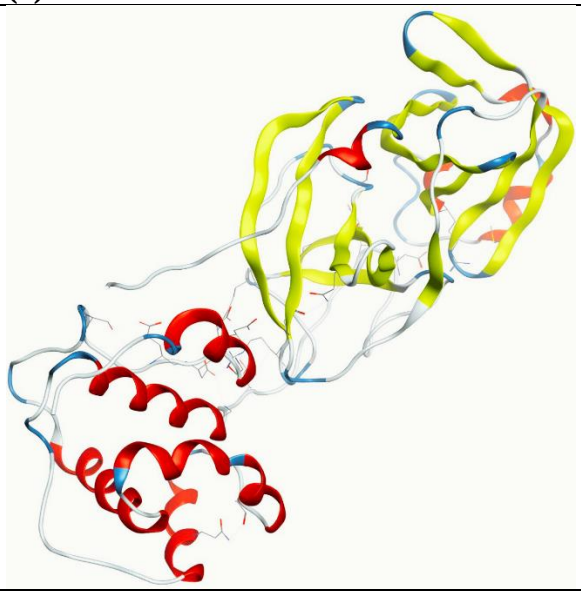	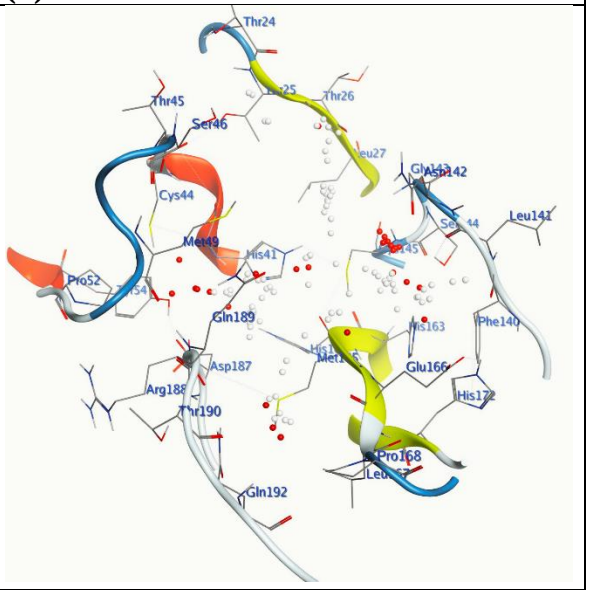
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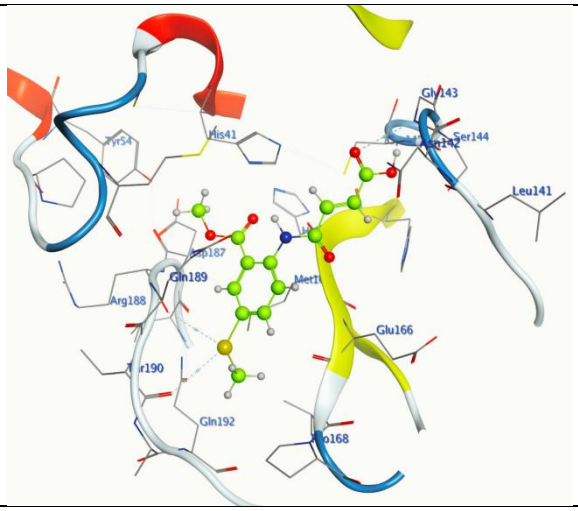
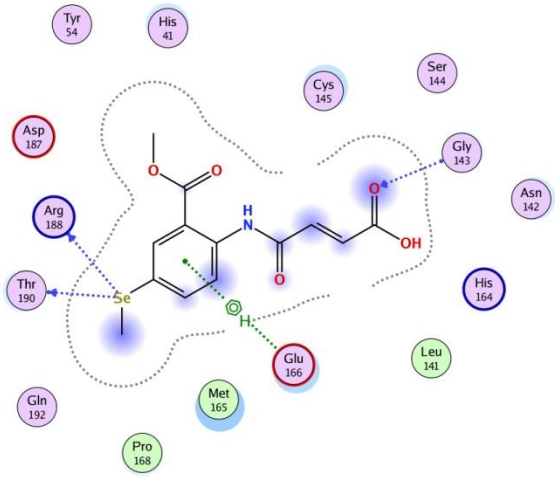
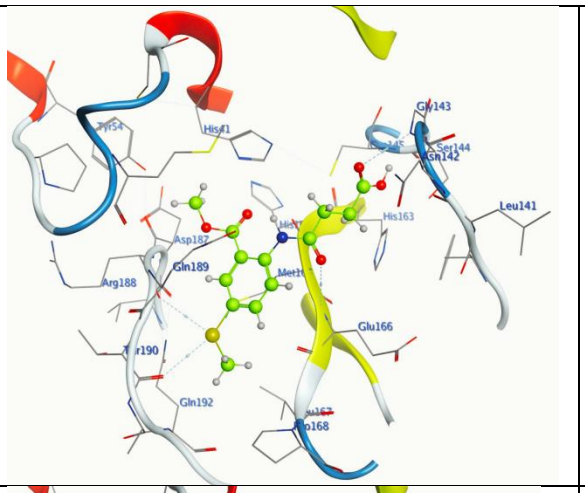
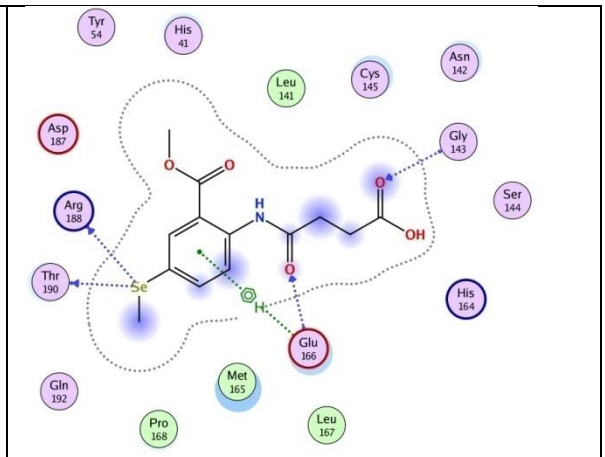
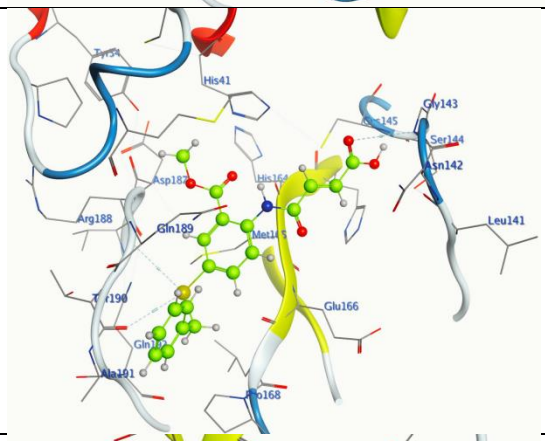
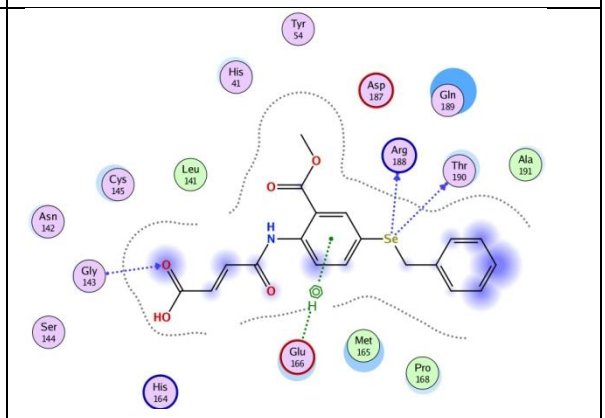
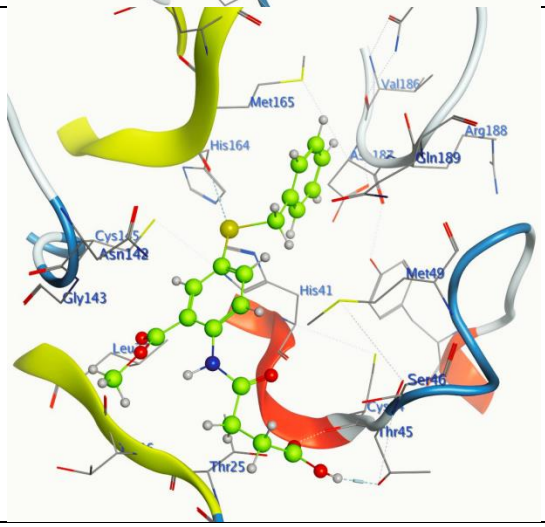
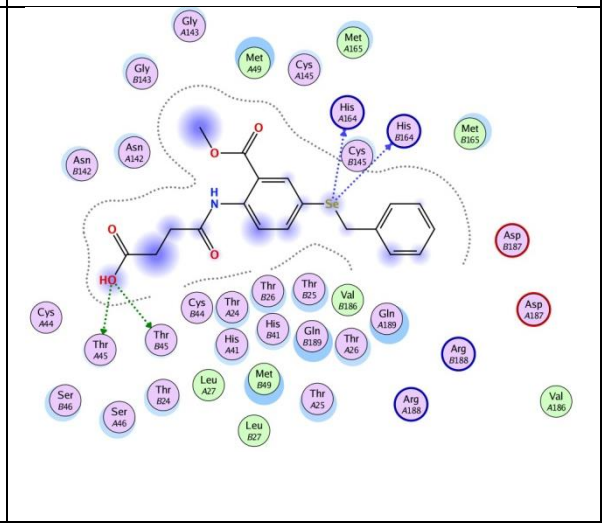
7		

8		
9		
10		

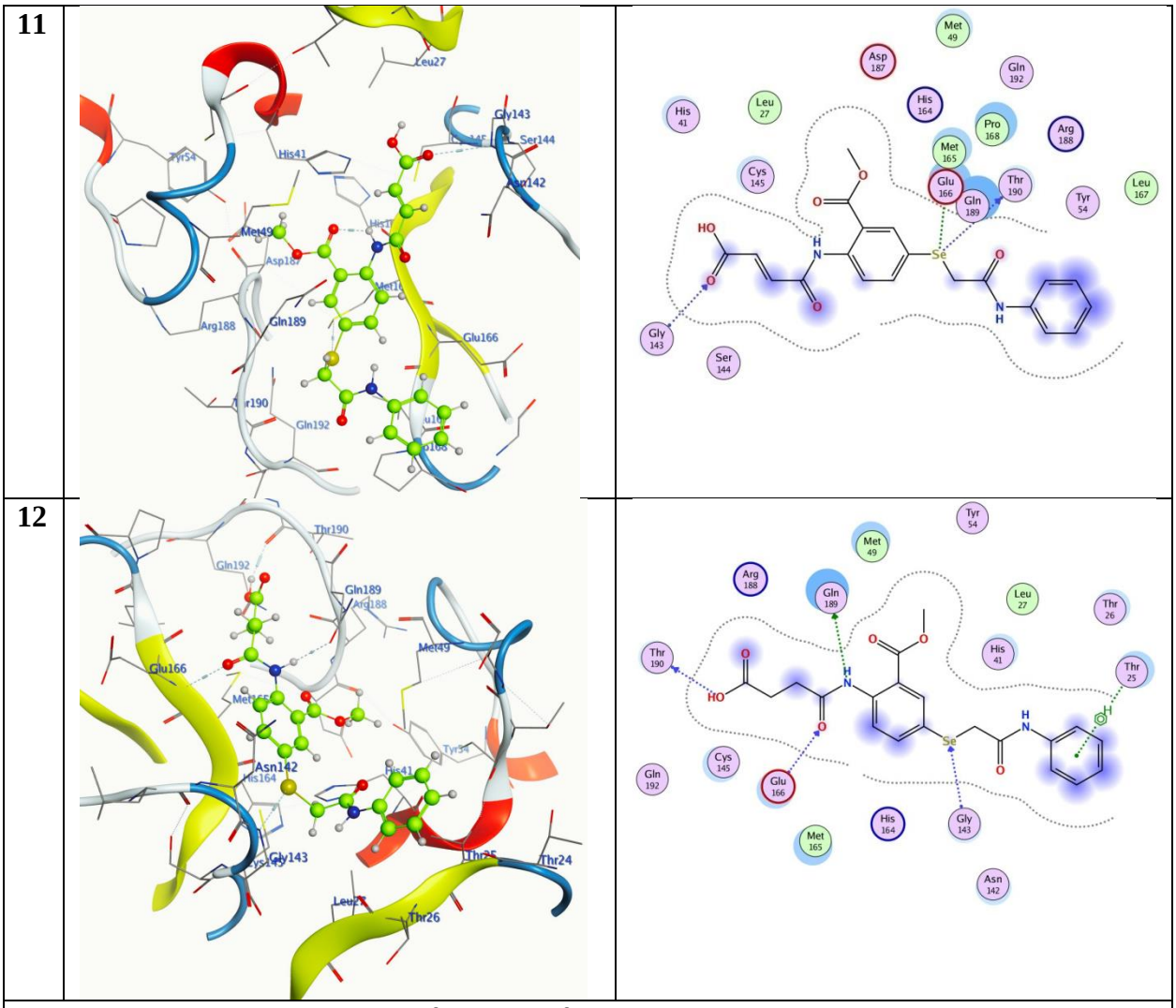


Figure S3: (a): The 3D structure of the 6lu7of novel coronavirus (COVID–19); (b): Active site pocket in which molecular docking occurred; and (c) 3D and 2D interactions of the titled compounds inside the active site of the target receptor.

List f SI Tables

Table S1. Drug Likeness parameters

Table S2. Pharmacokinetics, toxicities and receptor binding properties of potential bioactive compounds from medicinal plants using pkCSM web server

Table (S3): Molecular Docking data; Interaction type, and distance between ligand and receptor of the title compounds

Table S1. Drug Likeness parameters

	7	**8**	**9**	**10**	**11**	**12**
MW	342.209	344.225	418.307	420.323	461.332	463.348
log *P*	0.4301	0.6541	1.5822	1.8062	1.439	1.663
n_{Rot}	5	6	7	8	8	9
nHBA	4	4	4	4	5	5
nHBD	2	2	2	2	3	3
Lipinski rule	Yes; 0 violation	Yes; 0 violation	Yes; 0 violation	Yes; 0 violation	Yes; 0 violation	Yes; 0 violation
ABS	0.56	0.56	0.56	0.56	0.56	0.56
Log S	-2.84	-2.58	-4.19	-3.93	-2.84	-3.30
GI	High	High	High	High	High	High
Pgp	No	No	No	No	No	No
BBB	No	No	No	No	No	No
TPSA	121.519	122.209	156.576	157.266	172.653	173.342
LogKp	-7.13	-7.38	-6.59	-6.83	-7.13	-7.91
SA	2.70	2.56	3.26	3.15	2.70	3.36

MW: molecular weight; n_{Rot}: number of rotatable bonds; HBA: number of hydrogen bond acceptors; nHBD: number of hydrogen bond donors; log *P:* n–octanol/water partition coefficient; TPSA: topological polar surface area; S.A.: synthetic accessibility; G.I.: gastrointestinal absorption; BBB: blood-brain barrier; Pgp: P-glycoprotein substrate; **LogKp:**skin permeation (cm/s);**ABS**: Abbot Bioavailability Score.

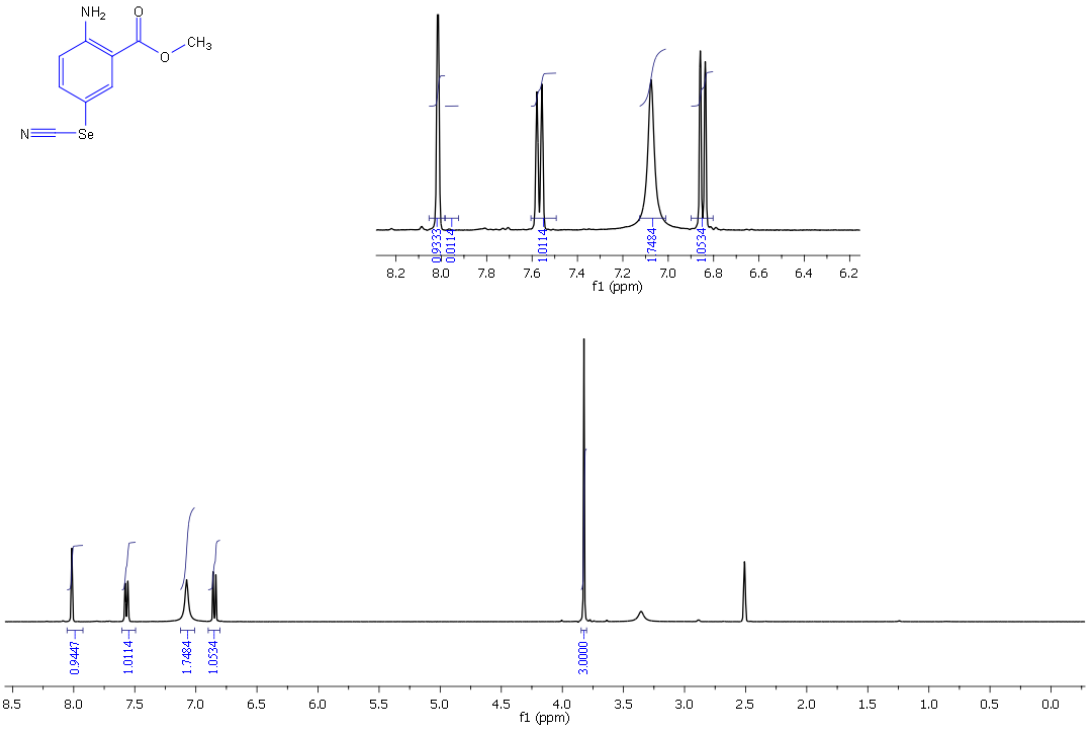
Table S2. Pharmacokinetics, toxicities and receptor binding properties of potential bioactive compounds from medicinal plants using pkCSM web server.

		7	**8**	**9**	**10**	**11**	**12**
Absorption	Water solubility	-2.323	-2.353	-3.99	-4.045	-3.878	-3.898
	Caco2 permeability	0.18	0.159	0.005	0.367	-0.031	-0.033
	Intestinal absorption (human)	44.025	44.803	49.294	50.072	45.608	46.385
	Skin Permeability	-2.735	-2.735	-2.735	-2.735	-2.735	-2.735
	P-glycoprotein substrate	Yes	Yes	Yes	Yes	Yes	Yes
	P-glycoprotein I inhibitor	No	No	No	No	No	No
	P-glycoprotein II inhibitor	No	No	No	No	No	No
Distribution	VDss (human)	-1.053	-1.021	-1.201	-1.152	-1.041	-0.998
	Fraction unbound (human)	0.395	0.391	0.074	0.074	0.062	0.062
	BBB permeability	-0.47	-0.506	-0.272	-0.308	-0.936	-0.997
	CNS permeability	-3.04	-3.053	-2.863	-2.915	-3.336	-3.355
Metabolism	CYP2D6 substrate	No	No	No	No	No	No
	CYP3A4 substrate	No	No	No	No	No	No
	CYP1A2 inhibitior	No	No	No	No	No	No
	CYP2C19 inhibitior	No	No	No	No	No	No
	CYP2C9 inhibitior	No	No	No	No	No	No
	CYP2D6 inhibitior	No	No	No	No	No	No
	CYP3A4 inhibitior	No	No	No	No	No	No
Excretion	Total Clearance	1.83	1.822	2.133	2.129	2.212	2.209
	Renal OCT2 substrate	No	No	No	No	No	No
Toxicity	AMES toxicity	No	No	No	No	No	No
	Max. tolerated dose (human)	1.566	1.535	0.305	0.289	0.396	0.372
	hERG I inhibitor	No	No	No	No	No	No
	hERG II inhibitor	No	No	No	No	No	No
	Oral Rat Acute Toxicity (LD50)	2.294	2.302	2.631	2.638	2.549	2.559
	Oral Rat Chronic Toxicity (LOAEL)	2.115	2.093	2.088	2.067	2.138	2.117
	Hepatotoxicity	No	No	No	Yes	No	No
	Skin Sensitisation	No	No	No	No	No	No
	T.Pyriformis toxicity	0.283	0.283	0.285	0.285	0.285	0.285
	Minnow toxicity	0.834	0.706	-0.765	-0.892	-0.11	-0.237

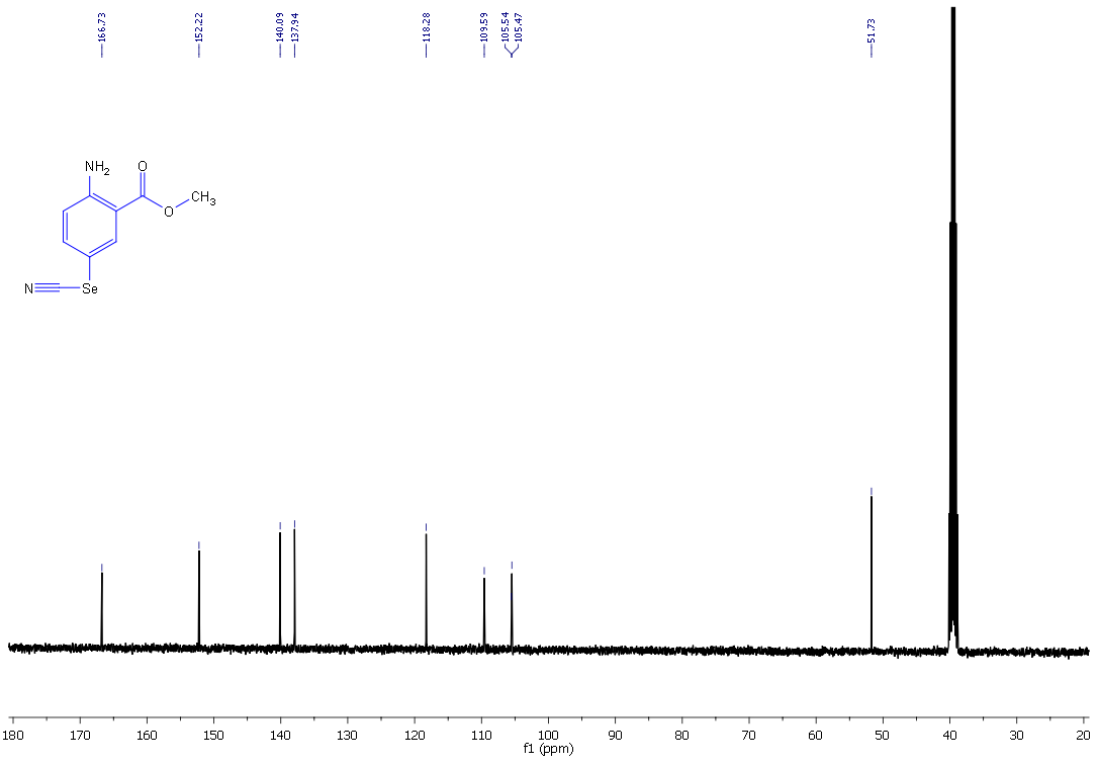
Table (S3): Molecular Docking data; Interaction type, and distance between ligand and receptor of the title compounds.								
6lu7	Ligand	Receptor	Interaction	Distance	E (kcal/mol)	S (kcal/mol)	RMSD	Ki (μM)
7	SE11	ARG 188	H-donor	3.43	-0.80	-6.79	1.69	10.77
	SE11	THR 190	H-donor	3.33	-1.00			
	O20	GLY 143	H-acceptor	3.30	-1.20			
	6-ring	GLU 166	pi-H	4.50	-0.90			
8	SE11	ARG 188	H-donor	3.37	-1.00	-6.94	1.27	8.27
	SE11	THR 190	H-donor	3.38	-0.90			
	O16	GLU 166	H-acceptor	3.25	-0.70			
	O20	GLY 143	H-acceptor	3.07	-2.80			
	6-ring	GLU 166	pi-H	4.48	-0.90			
9	SE11	ARG 188	H-donor	3.48	-1.00	-7.68	1.33	2.39
	SE11	THR 190	H-donor	3.41	-1.70			
	O20	GLY 143	H-acceptor	3.30	-1.20			
	6-ring	GLU 166	pi-H	4.47	-1.00			
10	SE11	HIS 164	H-donor	3.29	-1.10	-8.96	1.40	0.27
	O17	THR 45	H-donor	2.93	-2.70			
11	SE11	MET 165	H-donor	3.19	-1.60	-7.99	1.33	1.41
	SE11	THR 190	H-donor	3.10	-0.50			
	O20	GLY 143	H-acceptor	3.11	-2.50			
12	N13	GLN 189	H-donor	3.06	-1.00	-8.93	1.43	0.29
	O19	THR 190	H-donor	3.03	-4.00			
	SE11	GLY 143	H-acceptor	3.13	-2.20			
	O16	GLU 166	H-acceptor	2.94	-2.60			
	6-ring	THR 25	pi-H	4.04	-0.70			

*Synthesis of methyl 2-amino-5-selenocyanatobnzoate (**2**)[6]*

Methyl 2-amino-5-selenocyanatobenzoate (**2**) was synthesized from methyl 2-aminobenzoate (12.5 mmol,1.80 g) with triselenium dicyanide prepared *in situ* from malononitrile (15 mmol,1.00 g) and selenium dioxide (30 mmol,3.30 g). It was isolated as reddish solid; yield:3.07 g (96%); m.p. =118–119°C; Rf =0.4(petroleum ether/ ethyl acetate 4:2, *v*/*v*). IR(KBr): ν3475 (N-H), 3366 (N-H), 2946 (C_{aliph}-H), 2842 (C_{aliph}-H), 2148 (CN), 1691 (C=O), 1551 (C=C), 1253 (C_{Ar}–N), 1085 (C–O), 910, 815 (C-H bending), 556 (C-Se), 536 (C-H rocking), 460;^{1}HNMR (400 MHz, DMSO-d_6) δ8.02(s, 1H, Ar-H), 7.57(d, J = 8.8 Hz, 1H, Ar-H), 7.08(s, br, 2H, NH_2), 6.84(d, J= 8.8 Hz, 1H, Ar-H), 3.82(s, 3H, OCH_3). ^{13}C NMR (101 MHz, DMSO- d_6) δ166.73, 152.22, 140.09, 137.94, 118.28, 109.59, 105.54, 105.47, 51.73. MS (EI, 70 ev) m/z (%) = 259.35(M+3H, 2.39), 117(29.02), 87(26.6), 75(2.70), 59(100.0, base peak).



^{1}HNMR chart of compound **2**



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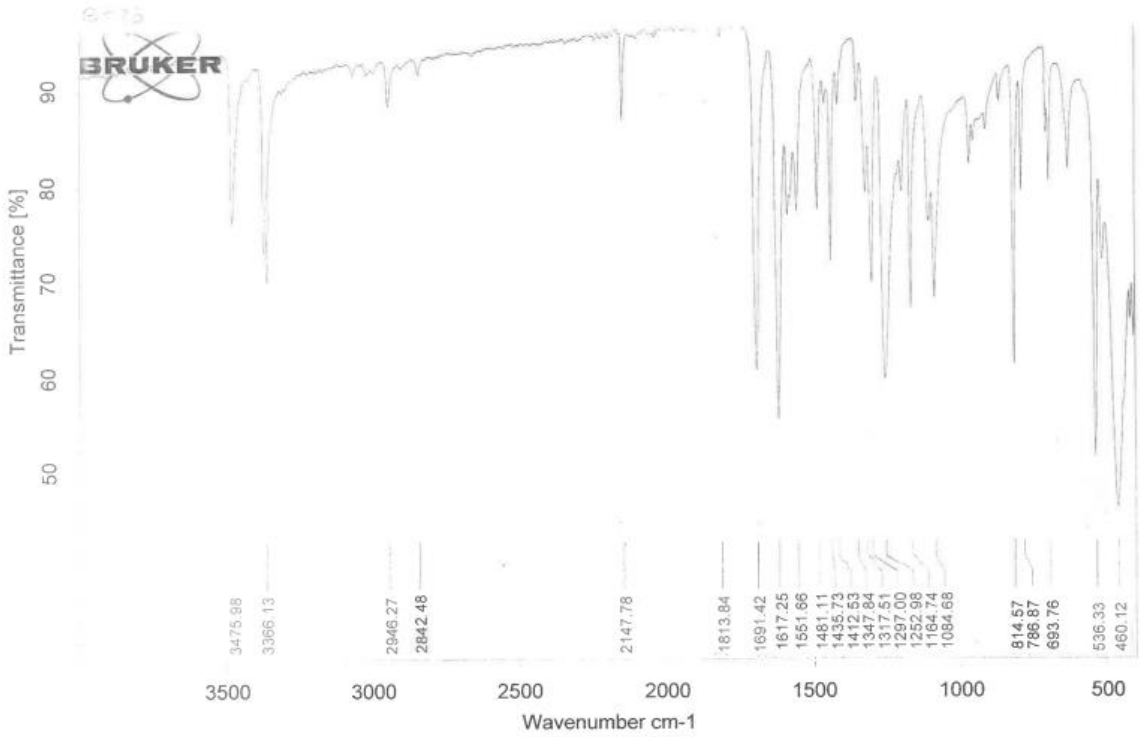
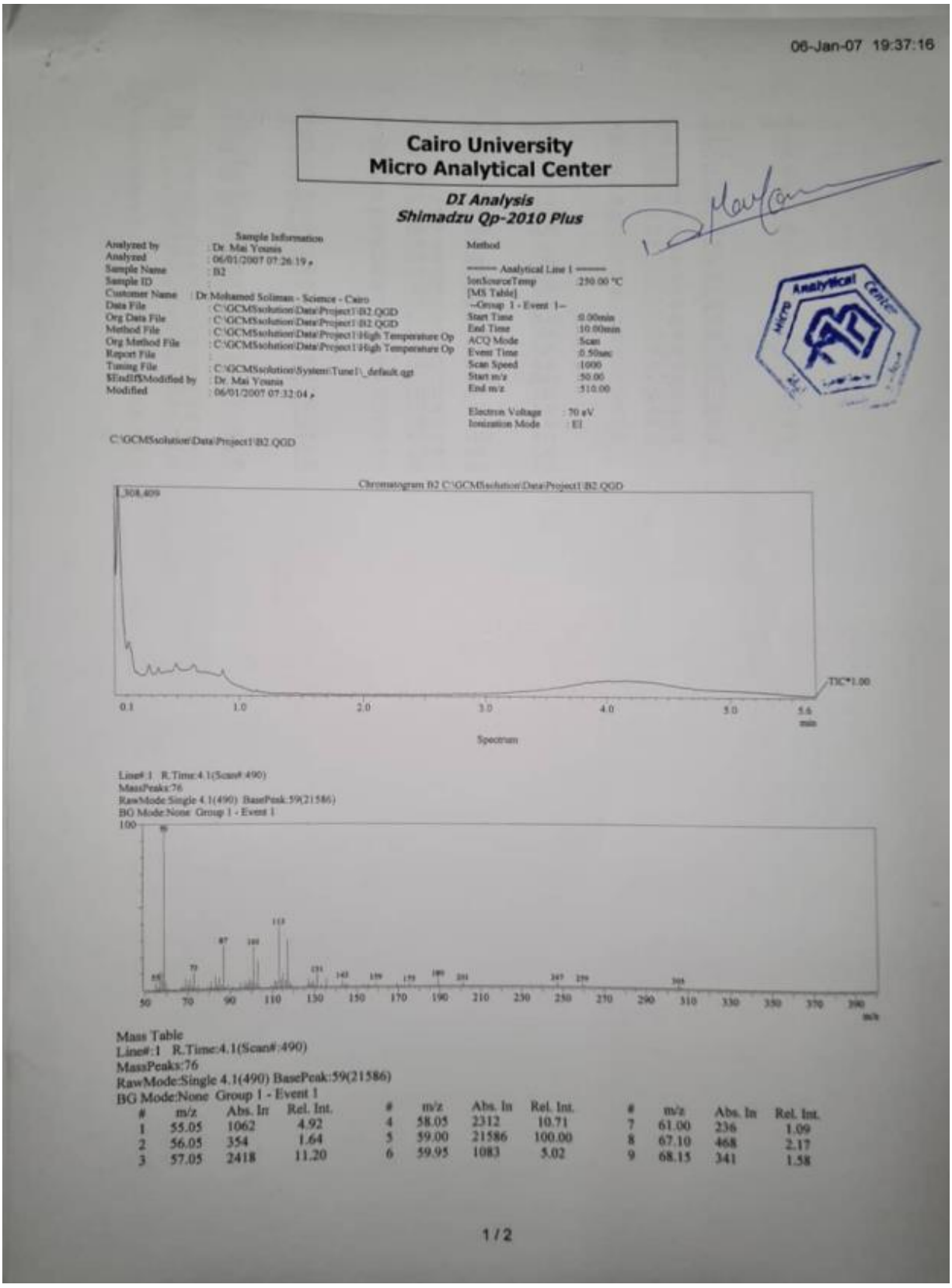


IR chart of compound **2**



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
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Sample ID	:
Customer Name	: Dr.Mohamed Soliman - Science - Cairo
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Modified	: 06/01/2007 07:32:04

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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 **2**

#	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

#	m/z	Abs. In	Rel. Int.
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

#	m/z	Abs. In	Rel. Int.
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

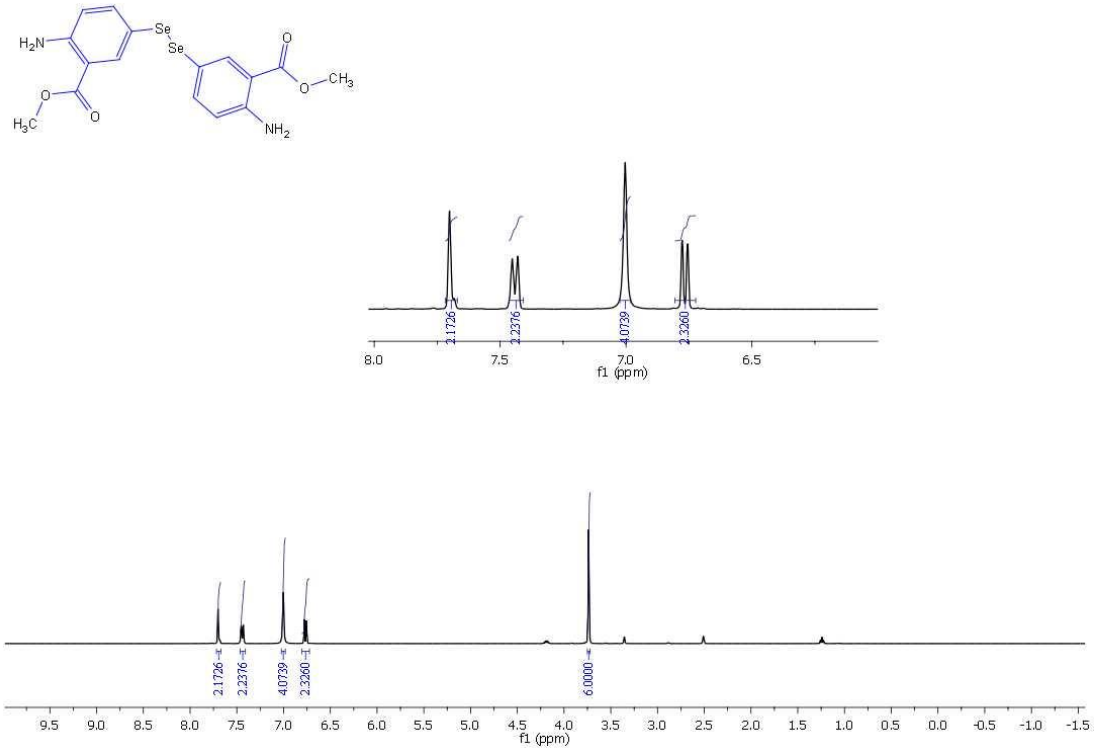
2 / 2

Mass chart of compound **2**

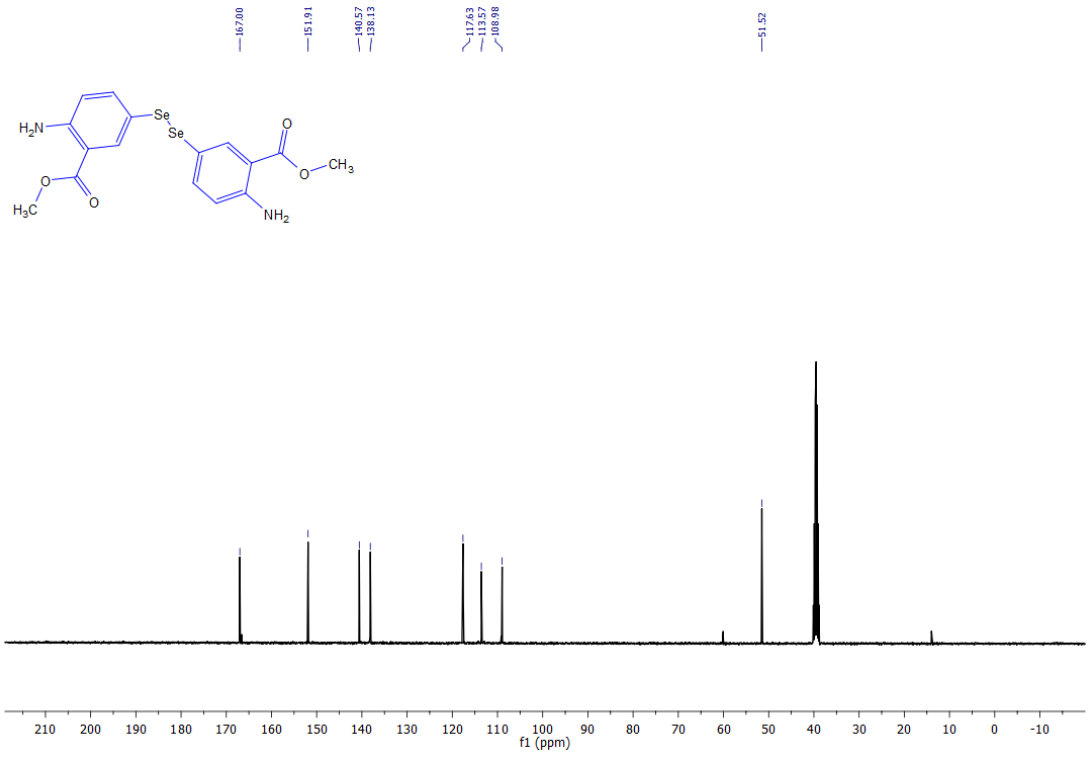
Synthesis of dimethyl 5,5'-diselanediylbis(2-aminobenzoate) (***3***)*[6]*

Compound dimethyl 5,5-diselanediylbis(2-aminobenzoate) (**3**) was synthesized from methyl 2-amino-5-selenocyanatobenzoate (4 mmol,1.00 g) and sodium hydroxide (4 mmol,1.60 g) in anhydrous ethanol (20 mL). Dimethyl 5,5'-diselanediylbis(2-aminobenzoate) (**3**) appeared as a single compound on TLC and was isolated as a yellow solid; yield: 1.69g (92%); m.p. =138–139°C; Rf =0.5(petroleum ether/ ethyl acetate 4:3, *v*/*v*). IR(KBr): ν3455 (N-H), 3344 (N-H), 2931 (C_{aliph}-H), 2890 (C_{aliph}-H), 2168 (CN), 1684 (C=O), 1560 (C=C), 1603, 1238 (C_{Ar}–N), 1079 (C–O), 811, 784 (C-H bending), 699 (C-H rocking), 533 (C-Se);

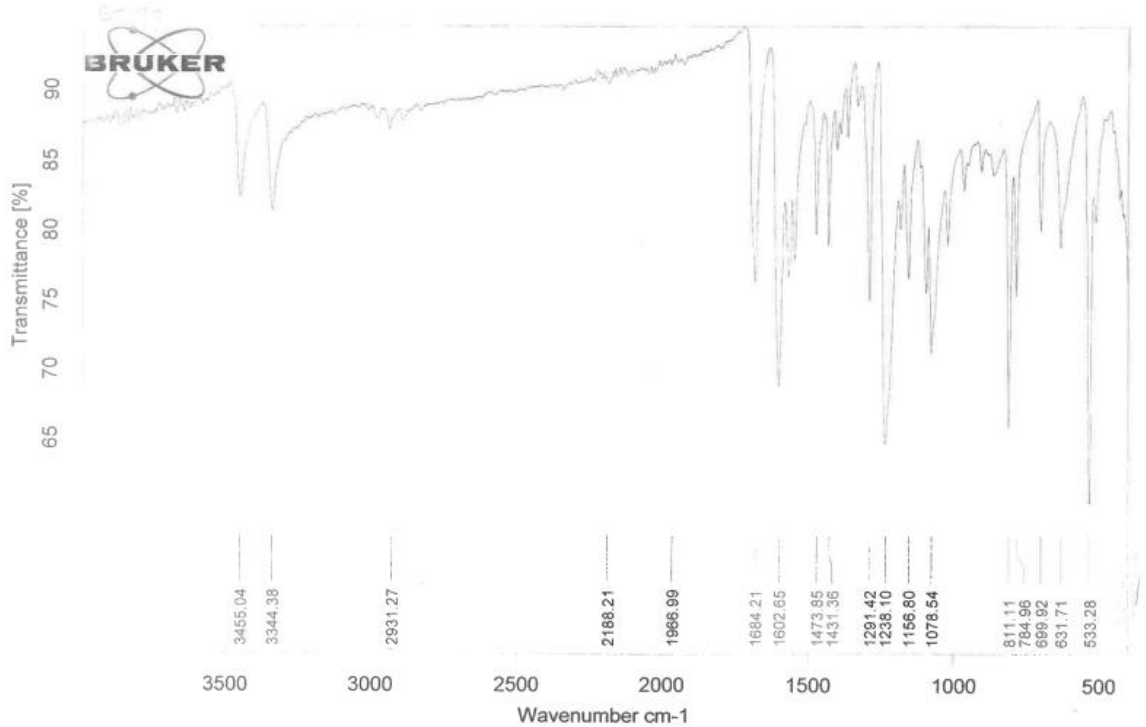
^{1}HNMR (400 MHz, DMSO- d_6) δ7.70(s,2H, Ar-H), 7.44(d, J = 8.6 Hz, 2H, Ar-H), 7.00(s, 4H,2NH_2), 6.77(d, J = 8.6 Hz, 2H, Ar-H), 3.74(s, 6H,2OCH_3). ^{13}CNMR (101 MHz, DMSO- d_6) δ167.00, 151.91, 140.57, 138.13, 117.63, 113.57, 108.98, 51.52. MS (EI, 70 ev) *m/z* (%) = 460.15(M+H, 20.76), 459.15(M, 5.20) or 230(24.42), 119(9.45), 91 (100.0, base peak),65(8.88).



^{1}HNMR chart of compound **3**



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



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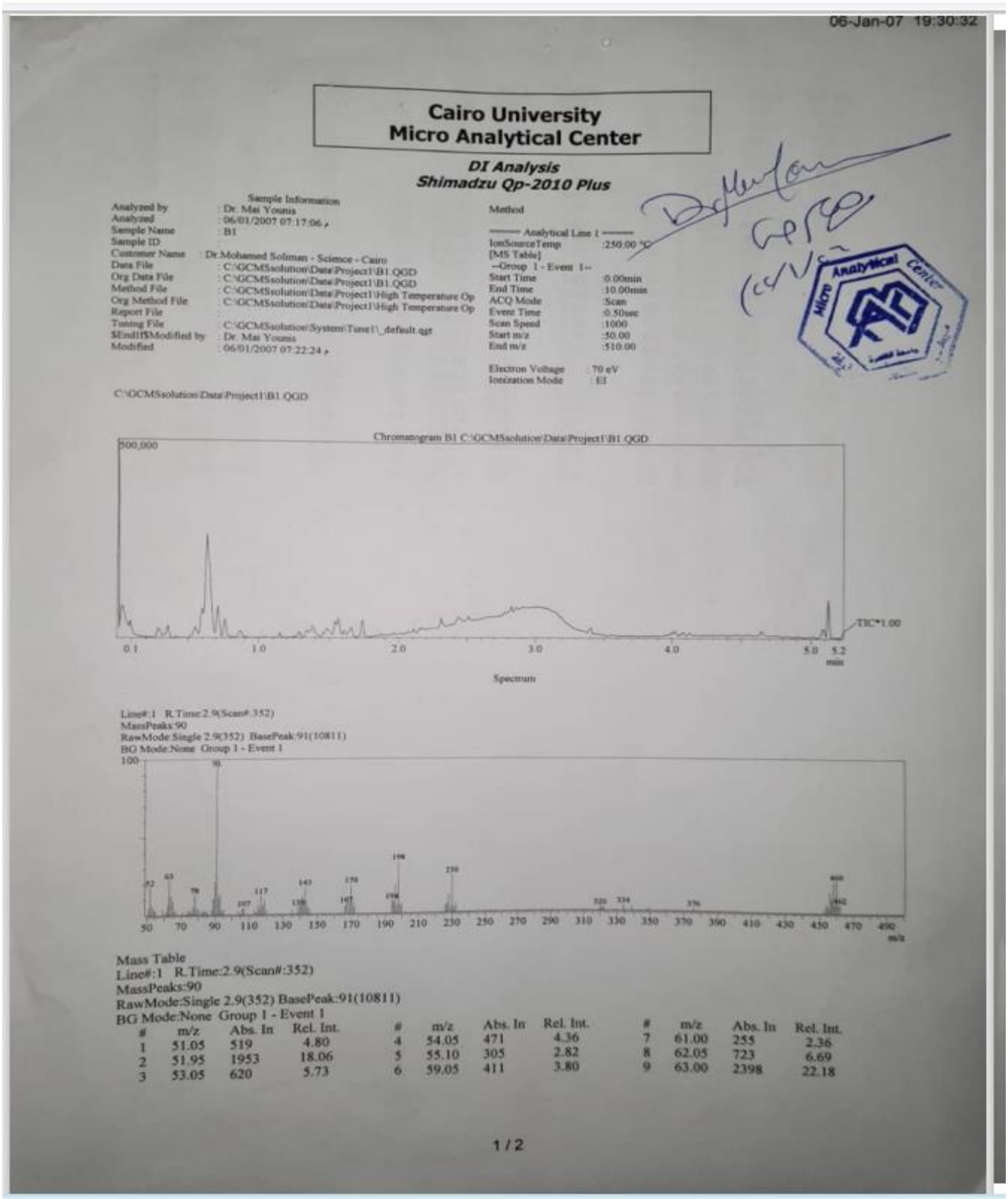

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Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

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Analyzed	: 06/01/2007 07:17:06 م
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Customer Name	: Dr.Mohamed Soliman - Science - Cairo
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Modified	: 06/01/2007 07:22:24 م

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2	51.95	1953	18.06	5	55.10	305	2.82	8	62.05	723	6.69
3	53.05	620	5.73	6	59.05	411	3.80	9	63.00	2398	22.18

1 / 2

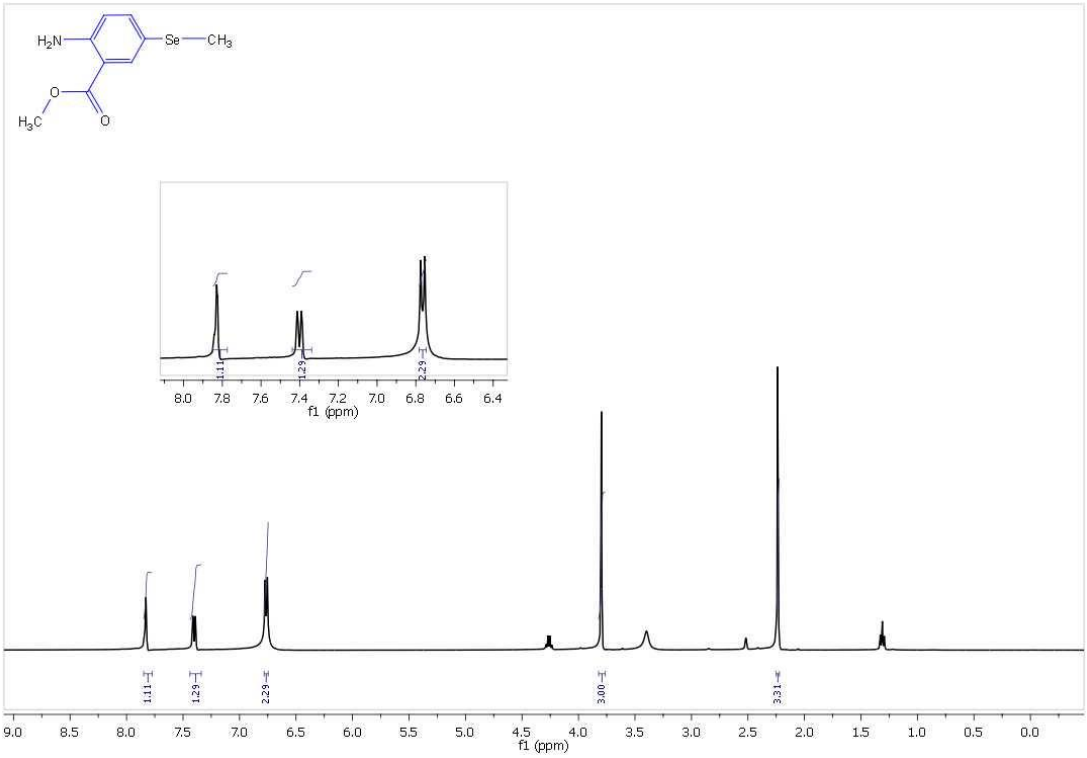
Mass chart of compound **3**

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	64.05	1311	12.13	37	113.00	308	2.85	64	198.00	3602	33.32
11	65.05	960	8.88	38	113.90	222	2.05	65	199.00	591	5.47
12	66.00	278	2.57	39	114.90	636	5.88	66	200.05	690	6.38
13	67.00	247	2.28	40	116.05	385	3.56	67	226.05	505	4.67
14	71.00	202	1.87	41	117.00	1319	12.20	68	227.05	655	6.06
15	74.00	313	2.90	42	118.05	599	5.54	69	228.00	1222	11.30
16	75.00	255	2.36	43	119.10	1022	9.45	70	229.15	316	2.92
17	76.00	214	1.98	44	120.10	310	2.87	71	230.05	2640	24.42
18	77.05	571	5.28	45	135.10	289	2.67	72	231.05	347	3.21
19	78.05	1366	12.64	46	139.00	482	4.46	73	232.05	594	5.49
20	79.10	466	4.31	47	140.00	614	5.68	74	320.00	290	2.68
21	80.10	388	3.59	48	141.05	1196	11.06	75	321.00	222	2.05
22	82.10	233	2.16	49	142.05	619	5.73	76	322.00	228	2.11
23	83.10	260	2.40	50	143.00	1894	17.52	77	334.00	398	3.68
24	84.10	220	2.03	51	144.00	850	7.86	78	339.00	318	2.94
25	85.10	278	2.57	52	144.95	409	3.78	79	349.00	230	2.13
26	88.05	377	3.49	53	166.05	493	4.56	80	376.00	215	1.99
27	89.05	1081	10.00	54	167.05	639	5.91	81	453.00	263	2.43
28	90.05	2287	21.15	55	168.05	1148	10.62	82	454.20	604	5.59
29	91.05	10811	100.00	56	169.15	688	6.36	83	455.20	425	3.93
30	92.05	1150	10.64	57	170.05	2031	18.79	84	456.25	1479	13.68
31	92.95	1429	13.22	58	171.10	802	7.42	85	457.20	1015	9.39
32	94.00	254	2.35	59	172.10	420	3.88	86	458.20	2169	20.06
33	95.00	354	3.27	60	194.05	863	7.98	87	459.15	562	5.20
34	104.00	249	2.30	61	195.05	858	7.94	88	460.15	2244	20.76
35	106.10	398	3.68	62	196.00	1993	18.43	89	461.15	521	4.82
36	107.00	444	4.11	63	197.05	575	5.32	90	462.10	618	5.72

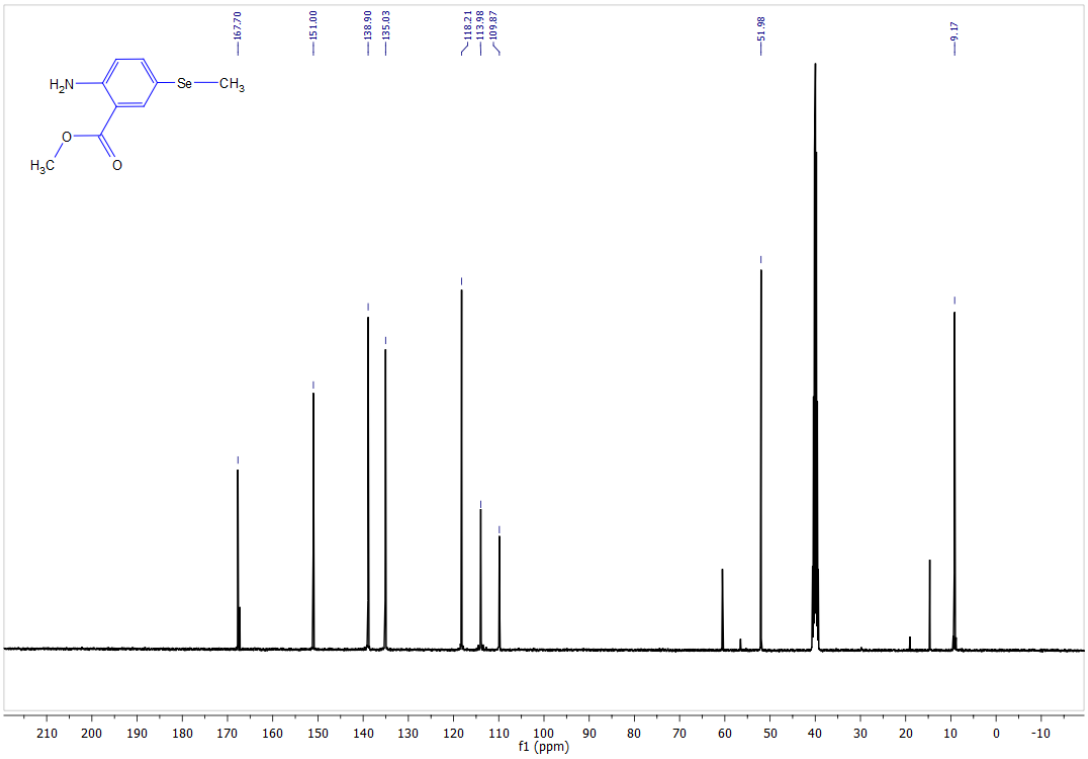
Mass chart of compound **3**

*Synthesis of methyl 2-amino-5-(methylselanyl) benzoate (**4**)[6]*

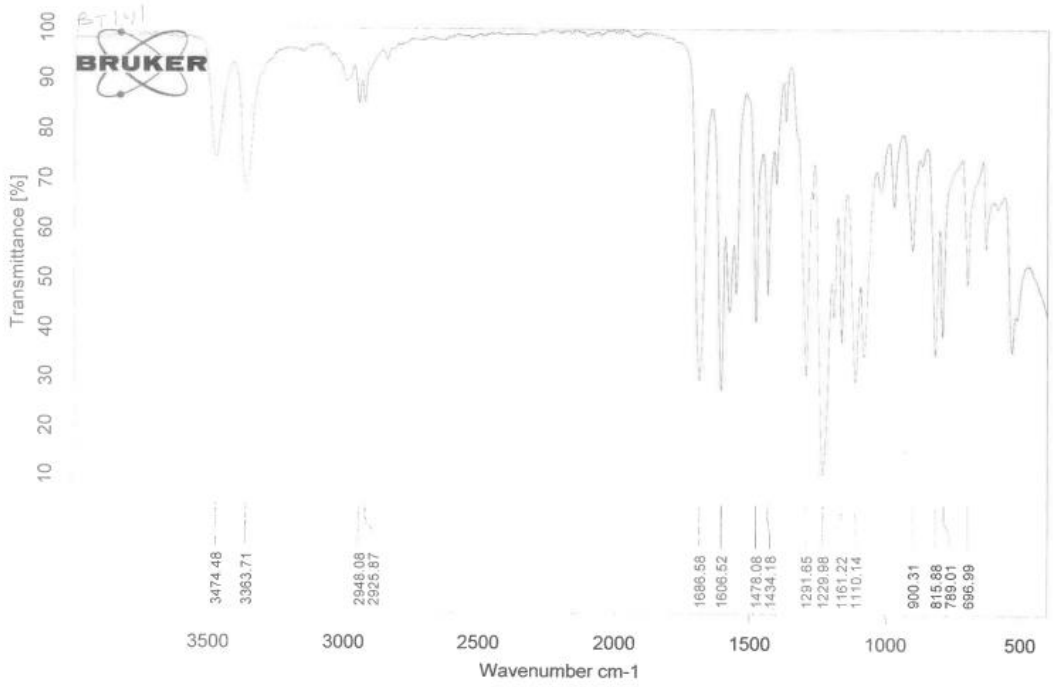
Compound **4** was synthesized from dimethyl 5,5'-diselanediylbis (2-aminobenzoate) (**3**)(2 mmol,916 mg) and methyl iodide (4.4 mmol,0.27 mL). It was isolated as brown oil; yield: 402 mg (82%); Rf=0.6(petroleum ether/ ethyl acetate 4:2, *v*/*v*). IR(KBr): ν3474 (N-H), 3364 (N-H), 2948 (C_{aliph}-H), 2926 (C_{aliph}-H),1686 (C=O), 1607, 1292 (C_{Ar}–N), 1110 (C–O), 815, 789, 696 (C-H bending), 559 (C-Se);^{1}HNMR (400 MHz, DMSO- d_6) δ7.82(s,1H, Ar-H), 7.40(d, J = 8.6 Hz, 1H, Ar-H), 6.77(d, J = 8.6 Hz, 1H, Ar-H), 6.75(s, 2H, NH_2), 3.62(s, 3H, OCH_3), 2.22 (s, 3H, CH_3). ^{13}CNMR (101 MHz, DMSO- d_6) δ167.70, 151.00, 138.90, 135.03, 118.21, 113.98, 109.87, 51.98, 9.17. MS (EI, 70 ev) *m/z* (%) = 245.10(M, 100.0, base peak), 230(38.06),186(10.46),170(35.08),91(91.10).



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



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



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IR chart of compound **4**

Cairo University
Micro Analytical Center

DI Analysis
Shimadzu Qp-2010 Plus

Sample Information

Analyzed by	: Dr. Mai Younis
Analyzed	: 16/01/2007 03:02:11 ص
Sample Name	: B35
Sample ID	:
Customer Name	: Dr.Mohamed Soliman - Science - Cairo
Data File	: C:\GCMSsolution\Data\Project1\B35.QGD
Org Data File	: C:\GCMSsolution\Data\Project1\B35.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
IndModified by	: Dr. Mai Younis
Modified	: 16/01/2007 03:12:11 ص

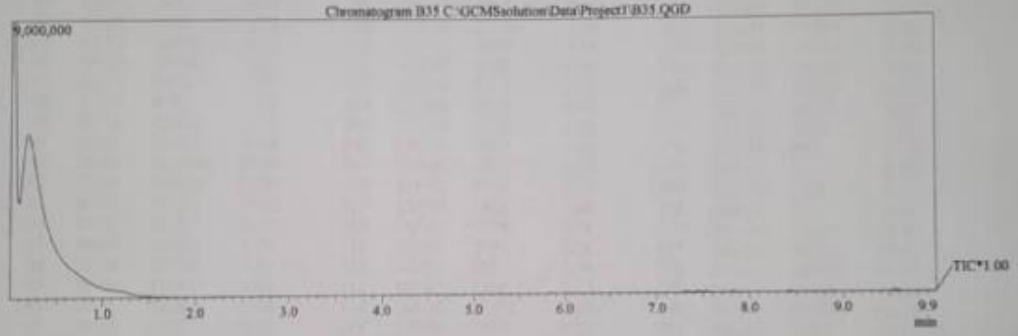
Method

——— 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\B35.QGD

Chromatogram B35 C:\GCMSsolution\Data\Project1\B35.QGD



Spectrum

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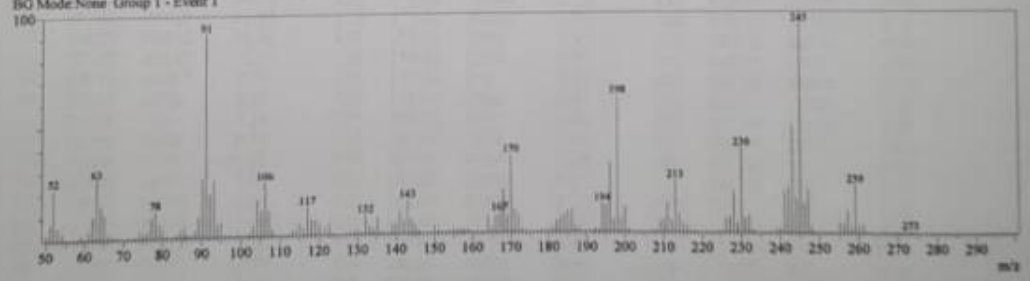
RawMode:Single 0.2(26) BasePeak:245(391154)
BG Mode:None Group 1 - Event 1



Mass Table
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MassPeaks:205
RawMode:Single 0.2(26) BasePeak:245(391154)
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	10411	2.66	4	53.00	21482	5.49	7	56.05	488	0.12
2	51.05	26260	6.71	5	54.05	11184	2.86	8	57.05	709	0.18
3	52.00	89298	22.83	6	55.00	2246	0.57	9	58.05	1164	0.30

1 / 2

Mass chart of compound **4**

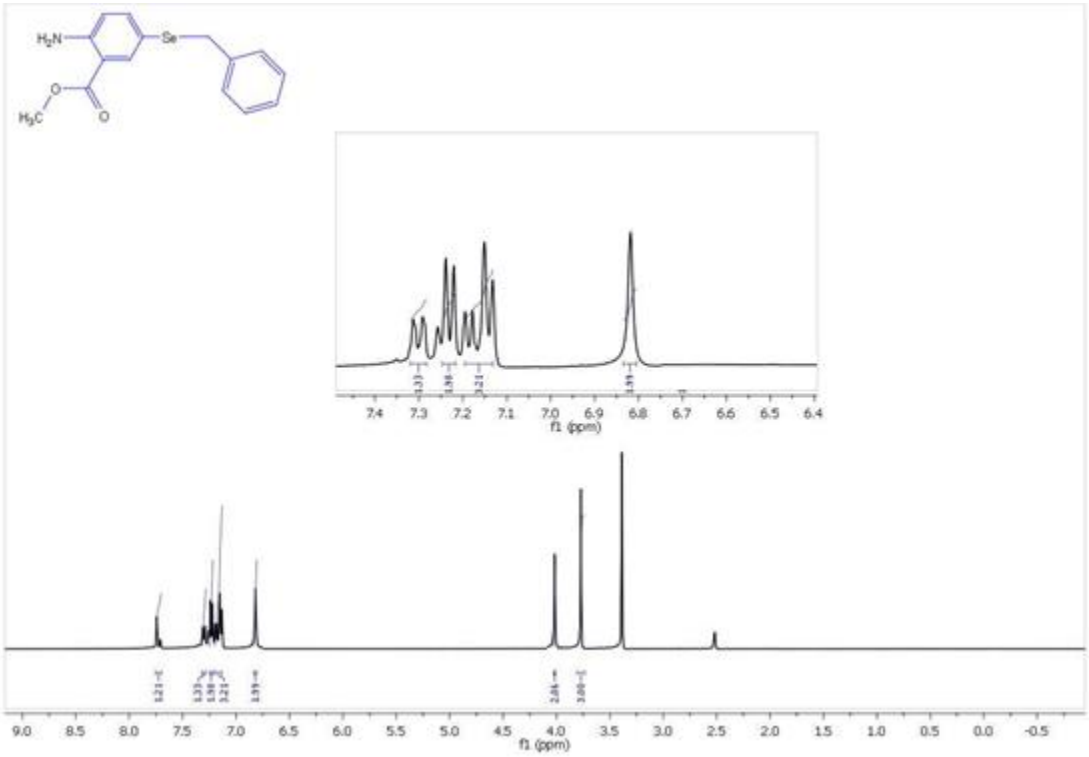
16-Jan-07 03:18:00

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	59.00	6150	1.57	76	126.05	2179	0.56	142	195.00	47017	12.02
11	60.05	1575	0.40	77	127.05	3204	0.82	143	196.00	122146	31.23
12	61.05	14415	3.69	78	128.00	4023	1.03	144	197.05	22307	5.70
13	62.05	39733	10.16	79	129.05	5617	1.44	145	198.00	241660	61.78
14	63.05	103836	26.55	80	130.00	7762	1.98	146	198.95	25629	6.55
15	64.05	57318	14.65	81	131.15	4478	1.14	147	200.00	43719	11.18
16	65.05	43819	11.20	82	132.10	33902	8.67	148	200.95	4204	1.07
17	66.10	9838	2.52	83	133.10	15628	4.00	149	201.95	533	0.14
18	67.05	4572	1.17	84	134.15	8746	2.24	150	207.00	2228	0.57
19	68.05	2933	0.75	85	135.10	31116	7.95	151	208.05	2526	0.65
20	69.10	1041	0.27	86	136.15	5476	1.40	152	209.05	20084	5.13
21	70.05	837	0.21	87	137.00	2783	0.71	153	210.05	23473	6.00
22	71.05	1646	0.42	88	138.05	3352	0.86	154	211.00	50268	12.85
23	72.05	1669	0.43	89	139.00	15473	3.96	155	212.05	22070	5.64
24	72.95	2952	0.75	90	140.00	17660	4.51	156	213.00	91327	23.35
25	74.05	12141	3.10	91	141.00	39022	9.98	157	214.00	31220	7.98
26	75.10	10198	2.61	92	142.05	21311	5.45	158	215.00	18164	4.64
27	76.10	12385	3.17	93	143.00	58711	15.01	159	216.00	12508	3.20
28	77.10	36498	9.33	94	144.00	25175	6.44	160	216.95	1191	0.30
29	78.05	47310	12.09	95	145.00	13801	3.53	161	218.00	1618	0.41
30	79.10	24441	6.25	96	146.00	5042	1.29	162	224.00	2599	0.66
31	80.00	15313	3.91	97	147.00	1039	0.27	163	225.05	1510	0.39
32	81.00	4794	1.23	98	148.10	804	0.21	164	226.05	26426	6.76
33	82.55	1873	0.48	99	149.15	1515	0.39	165	227.05	28172	7.20
34	83.55	6981	1.78	100	150.10	13154	3.36	166	228.05	72774	18.60
35	84.55	13095	3.35	101	151.10	4439	1.13	167	229.05	16399	4.19
36	85.50	19868	5.08	102	151.95	1797	0.46	168	230.05	148867	38.06
37	86.10	5970	1.53	103	153.00	3161	0.81	169	231.00	25292	6.47
38	87.05	4792	1.23	104	154.00	3514	0.90	170	232.05	29923	7.65
39	88.10	12948	3.31	105	155.00	5122	1.31	171	233.00	4730	1.21
40	89.10	37161	9.50	106	156.00	4514	1.15	172	233.95	605	0.15
41	90.15	101589	25.97	107	157.05	6492	1.66	173	238.15	734	0.19
42	91.10	358905	91.76	108	158.00	3975	1.02	174	239.10	6298	1.61
43	92.05	75198	19.22	109	159.00	5625	1.44	175	240.15	7887	2.02
44	93.00	97377	24.89	110	160.00	1470	0.38	176	241.10	72847	18.62
45	94.00	22561	5.77	111	161.00	1084	0.28	177	242.10	80234	20.51
46	95.00	26670	6.82	112	162.00	380	0.10	178	243.10	187193	47.86
47	96.00	4114	1.05	113	163.15	1307	0.33	179	244.15	60066	15.36
48	97.05	4225	1.08	114	164.10	28951	7.40	180	245.10	391154	100.00
49	98.35	2449	0.63	115	165.05	9689	2.48	181	246.05	51306	13.12
50	99.30	3386	0.87	116	166.00	30183	7.72	182	247.05	74480	19.04
51	100.25	1374	0.35	117	167.05	33926	8.67	183	248.05	8926	2.28
52	101.05	1757	0.45	118	168.00	75583	19.32	184	249.05	953	0.24
53	102.10	5450	1.39	119	169.05	30276	7.74	185	253.10	1460	0.37
54	103.15	15671	4.01	120	170.00	137220	35.08	186	254.15	1011	0.26
55	104.15	62814	16.06	121	171.00	40180	10.27	187	255.10	15329	3.92
56	105.25	45718	11.69	122	172.00	30348	7.76	188	256.15	16105	4.12
57	106.20	94842	24.25	123	173.00	7290	1.86	189	257.10	40538	10.36
58	107.15	45188	11.55	124	174.00	1239	0.32	190	258.15	9549	2.44
59	108.15	10687	2.73	125	177.20	238	0.06	191	259.10	84319	21.56
60	109.05	2089	0.53	126	178.15	3162	0.81	192	260.05	12047	3.08
61	110.05	710	0.18	127	179.05	1817	0.46	193	261.10	15478	3.96
62	111.05	1314	0.34	128	180.00	3514	0.90	194	262.05	2350	0.60
63	112.05	1199	0.31	129	181.05	9794	2.50	195	263.05	335	0.09
64	113.00	7610	1.95	130	182.00	19970	5.11	196	264.10	220	0.06
65	114.00	10354	2.65	131	183.00	25158	6.43	197	269.15	730	0.19
66	115.00	21430	5.48	132	184.00	31201	7.98	198	270.15	629	0.16
67	116.05	12818	3.28	133	185.00	38050	9.73	199	271.15	1493	0.38
68	117.05	50031	12.79	134	186.00	40924	10.46	200	272.25	533	0.14
69	118.05	27671	7.07	135	187.00	10028	2.56	201	273.15	2823	0.72
70	119.10	26692	6.82	136	188.00	6714	1.72	202	274.20	558	0.14
71	120.10	18391	4.70	137	189.00	868	0.22	203	275.20	654	0.17
72	121.55	12099	3.09	138	191.05	296	0.08	204	276.20	290	0.07
73	122.60	19750	5.05	139	192.00	4826	1.23	205	277.10	369	0.09
74	123.55	4338	1.11	140	193.05	2875	0.74				
75	125.05	1061	0.27	141	194.00	49812	12.73				

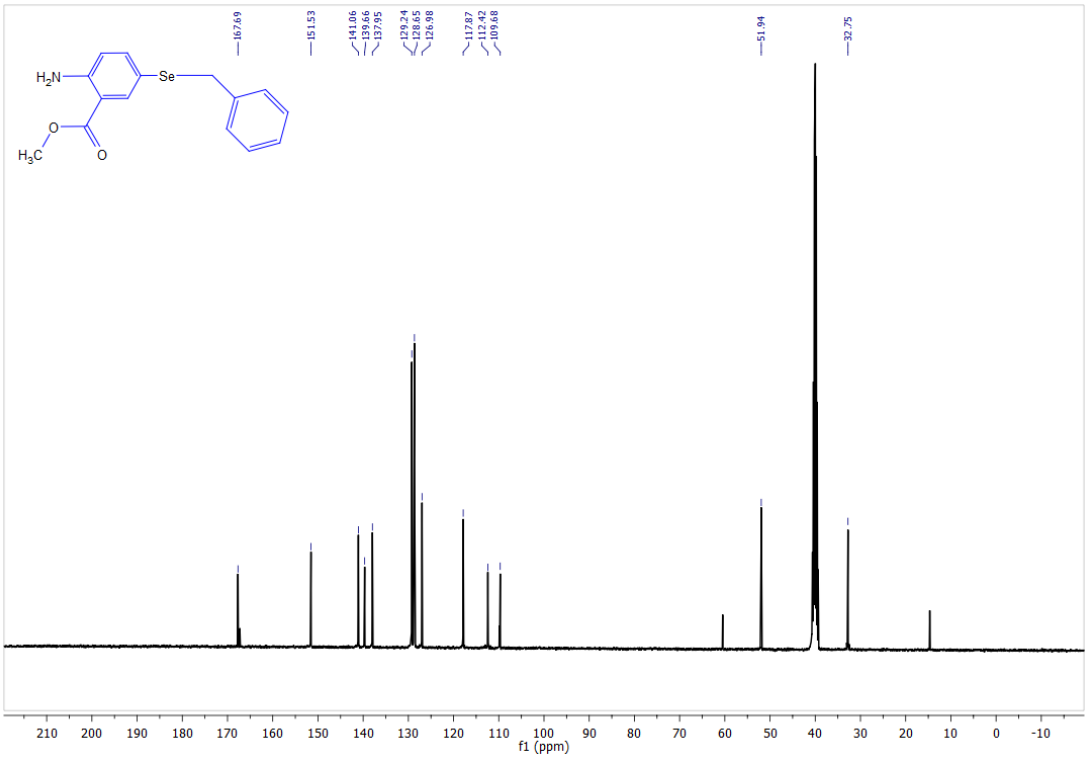
Mass chart of compound **4**

*Synthesis of methyl 2-amino-5-(benzylselanyl) benzoate (**5**)[6]*

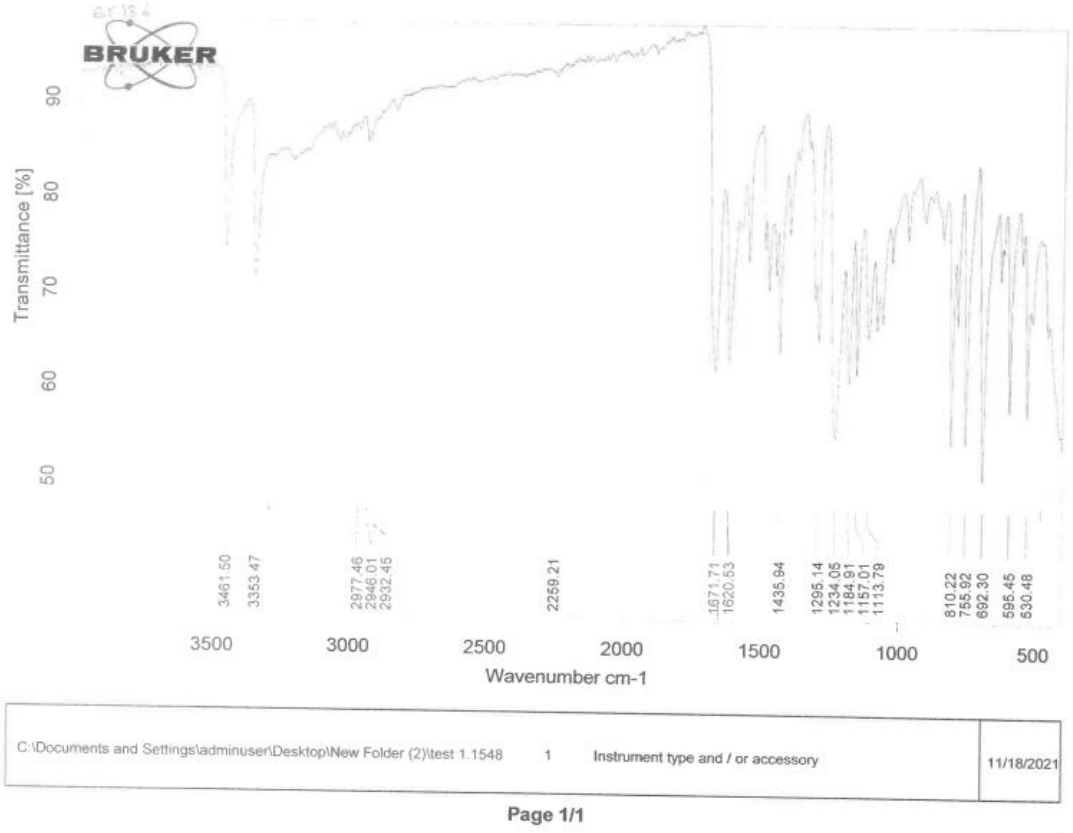
Compound **5** was synthesized from dimethyl 5,5'-diselanediylbis(2-aminobenzoate) (**3**) (2mmol,916 mg) and benzyl chloride (4.4 mmol,0.50 mL). It was isolated as light brown solid; yield: 597 mg (93%); m.p. =78ºC; Rf =0.6(petroleum ether/ ethyl acetate 4:3, *v*/*v*).IR(KBr): ν3462 (N-H), 3353 (N-H), 2977 (C_{aliph}-H), 2946 (C_{aliph}-H), 1672 (C=O), 1621, 1436, 1234 (C_{Ar}-N), 1114 (C-O), 810 (C-H bending), 692 (C-H rocking), 595 (C-Se);^{1}HNMR (400 MHz, DMSO- d_6) δ7.70(s,1H, Ar-H), 7.30(d,J = 8.6 Hz, 1H, Ar-H), 7.23(dd, J = 8.6 Hz, J = 2.1 Hz,2H, Ar-H), 7.19(d, J = 8.7 Hz, 2H, Ar-H), 7.14(d, J = 8.6 Hz, 2H, Ar-H), 6.82(s, 2H, NH_2), 4.00 (s, 2H, $SeCH_2$), 3.77(s, 3H, OCH_3); ^{13}CNMR (101 MHz, DMSO- d_6) δ167.69, 151.53, 141.06, 139.66, 137.95, 129.24, 128.65, 126.98, 117.87, 112.42, 109.68, 51.94, 32.75. MS (EI, 70 ev) *m/z* (%) = 321.20(M, 46.87), 244.10(2.77), 230(34.88), 150.15(1.02), 91.05(100.0, base peak).



^{1}HNMR chart of compound **5**



^{13}CNMR chart of compound **5**



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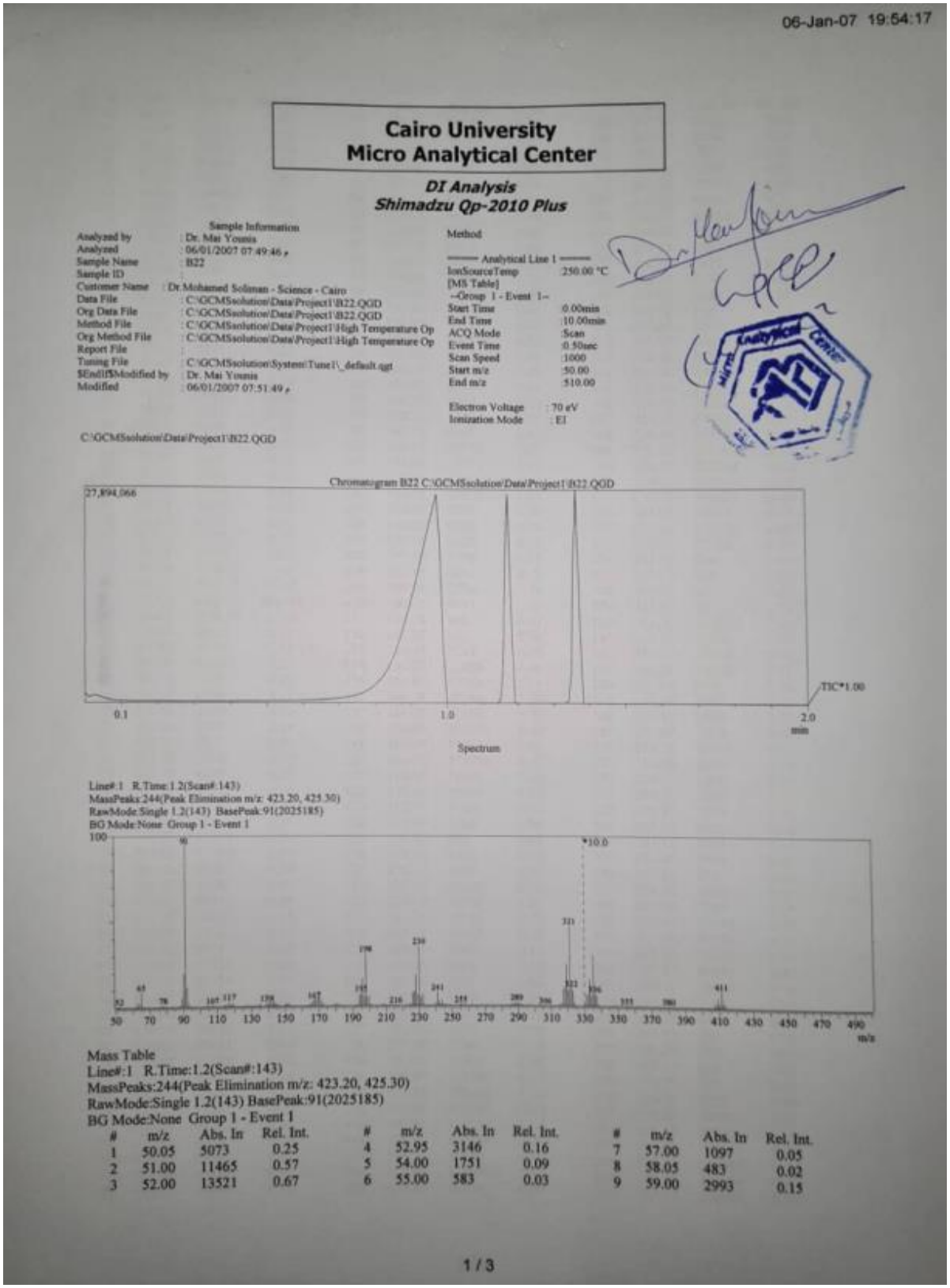
IR chart of compound **5**



Mass Table

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MassPeaks:244(Peak Elimination m/z: 423.20, 425.30)
RawMode:Single 1.2(143) BasePeak:91(2025185)
BG Mode:None Group 1 - Event 1

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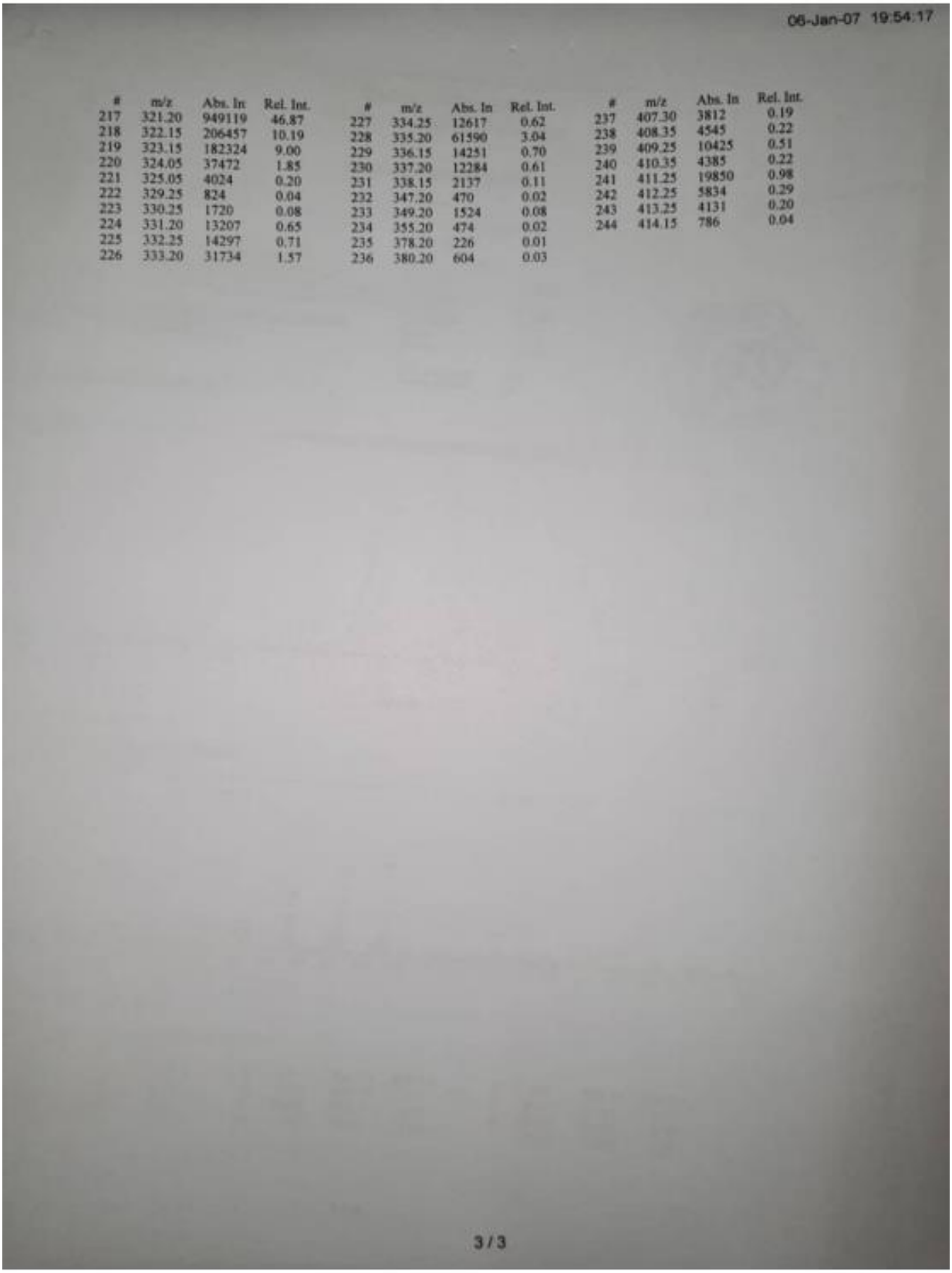
1	50.05	5073	0.25	4	52.95	3146	0.16	7	57.00	1097	0.05
2	51.00	11465	0.57	5	54.00	1751	0.09	8	58.05	483	0.02
3	52.00	13521	0.67	6	55.00	583	0.03	9	59.00	2993	0.15

1 / 3

Mass chart of compound **5**

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	60.05	391	0.02	79	129.05	9313	0.46	148	201.95	1028	0.05
11	61.05	3772	0.19	80	130.05	11086	0.55	149	204.25	5464	0.27
12	62.05	17107	0.84	81	131.10	5054	0.25	150	205.15	701	0.03
13	63.00	56926	2.81	82	132.05	10987	0.54	151	206.20	1020	0.05
14	64.05	36812	1.82	83	133.10	3684	0.18	152	207.25	2877	0.14
15	65.00	176463	8.71	84	134.15	9264	0.46	153	208.20	14284	0.71
16	65.95	12878	0.64	85	135.05	30121	1.49	154	209.15	17645	0.87
17	67.00	1580	0.08	86	136.05	4109	0.20	155	210.05	5896	0.29
18	68.05	483	0.02	87	137.05	5343	0.26	156	211.15	1898	0.09
19	69.10	985	0.05	88	138.05	7879	0.39	157	212.05	5471	0.27
20	70.10	1497	0.07	89	139.00	35607	1.76	158	213.10	2154	0.11
21	71.10	1663	0.08	90	140.05	41787	2.06	159	214.05	4336	0.21
22	72.05	379	0.02	91	141.00	77244	3.81	160	215.15	994	0.05
23	73.05	2080	0.10	92	142.05	47101	2.33	161	216.10	6855	0.34
24	74.05	4921	0.24	93	142.95	126529	6.25	162	217.05	395	0.02
25	75.05	5212	0.26	94	143.95	48735	2.41	163	218.10	921	0.05
26	76.05	6114	0.30	95	144.95	28945	1.43	164	221.20	846	0.04
27	77.05	10886	0.54	96	146.05	23129	1.14	165	223.15	1595	0.08
28	78.05	20811	1.03	97	146.95	4067	0.20	166	224.10	14468	0.71
29	79.05	8101	0.40	98	148.15	1843	0.09	167	225.15	19403	0.96
30	80.00	5090	0.25	99	149.15	8597	0.42	168	226.10	153471	7.58
31	81.05	1605	0.08	100	150.15	20578	1.02	169	227.15	166163	8.20
32	82.15	1045	0.05	101	151.05	33271	1.64	170	228.10	368934	18.22
33	83.10	2590	0.13	102	152.05	32505	1.61	171	229.15	120571	5.95
34	84.15	2599	0.13	103	153.05	20872	1.03	172	230.10	706377	34.88
35	85.15	4470	0.22	104	154.05	7855	0.39	173	231.05	94541	4.67
36	86.05	4174	0.21	105	155.00	4855	0.24	174	232.10	132870	6.56
37	87.15	6312	0.31	106	155.95	3585	0.18	175	233.05	15116	0.75
38	88.15	20787	1.03	107	157.00	3398	0.17	176	234.05	960	0.05
39	89.15	110480	5.46	108	157.95	2693	0.13	177	238.15	969	0.05
40	90.15	391518	19.33	109	159.05	2274	0.11	178	239.25	4131	0.20
41	91.05	202518	100.00	110	160.05	4165	0.21	179	240.25	35113	1.73
42	92.05	228419	11.28	111	161.00	602	0.03	180	241.25	155831	7.69
43	93.05	46032	2.27	112	162.05	482	0.02	181	242.10	54386	2.69
44	94.00	4180	0.21	113	163.05	3714	0.18	182	243.15	12588	0.62
45	95.00	8522	0.42	114	164.05	12889	0.64	183	244.10	56178	2.77
46	96.15	1388	0.07	115	165.05	22436	1.11	184	245.05	8044	0.40
47	97.10	2596	0.13	116	166.05	47284	2.33	185	246.10	9770	0.48
48	98.10	2490	0.12	117	167.05	66556	3.29	186	247.10	1503	0.07
49	99.10	2721	0.13	118	168.00	102111	5.04	187	254.35	1823	0.09
50	100.15	911	0.04	119	169.05	77098	3.81	188	255.25	10721	0.53
51	101.10	2750	0.14	120	169.95	174770	8.63	189	256.15	3888	0.19
52	102.10	4402	0.22	121	170.95	74461	3.68	190	257.15	1891	0.09
53	103.10	7242	0.36	122	172.00	39018	1.93	191	258.15	4289	0.21
54	104.05	11796	0.58	123	172.95	11808	0.58	192	259.15	3074	0.15
55	105.05	7012	0.35	124	173.95	1305	0.06	193	260.15	2910	0.14
56	106.10	11636	0.57	125	176.15	889	0.04	194	261.15	2231	0.11
57	107.05	13258	0.65	126	177.15	2401	0.12	195	262.20	1594	0.08
58	108.00	3873	0.19	127	178.15	5969	0.29	196	283.25	376	0.02
59	109.15	1378	0.07	128	179.15	10187	0.50	197	284.25	1803	0.09
60	110.05	979	0.05	129	180.15	36701	1.81	198	285.20	7185	0.35
61	111.05	2440	0.12	130	181.10	18865	0.93	199	286.20	14742	0.73
62	112.05	2793	0.14	131	182.15	14965	0.74	200	287.15	23239	1.15
63	113.05	9979	0.49	132	183.05	3441	0.17	201	288.20	24534	1.21
64	114.05	12822	0.63	133	184.00	2350	0.12	202	289.15	36611	1.81
65	115.00	27724	1.37	134	185.10	1281	0.06	203	290.15	36028	1.78
66	116.05	18052	0.89	135	186.05	1167	0.06	204	291.10	11612	0.57
67	117.00	53988	2.67	136	190.05	602	0.03	205	292.15	6462	0.32
68	118.05	26835	1.33	137	191.05	1736	0.09	206	293.15	552	0.03
69	119.05	43451	2.15	138	192.05	12467	0.62	207	306.20	302	0.01
70	120.05	15785	0.78	139	193.05	17901	0.88	208	308.10	636	0.03
71	121.10	4878	0.24	140	194.05	131489	6.49	209	310.05	707	0.03
72	122.05	2063	0.10	141	195.05	146464	7.23	210	314.25	1728	0.09
73	123.10	1527	0.08	142	196.00	323593	15.98	211	315.20	18481	0.91
74	124.05	682	0.03	143	197.05	113333	5.60	212	316.25	23945	1.18
75	125.05	4002	0.20	144	198.00	620129	30.62	213	317.20	196281	9.69
76	126.05	5459	0.27	145	198.95	99120	4.89	214	318.25	227987	11.26
77	127.05	10480	0.52	146	200.00	113441	5.60	215	319.20	494574	24.42
78	128.05	10844	0.54	147	200.95	16159	0.80	216	320.25	188395	9.30

Mass chart of compound **5**

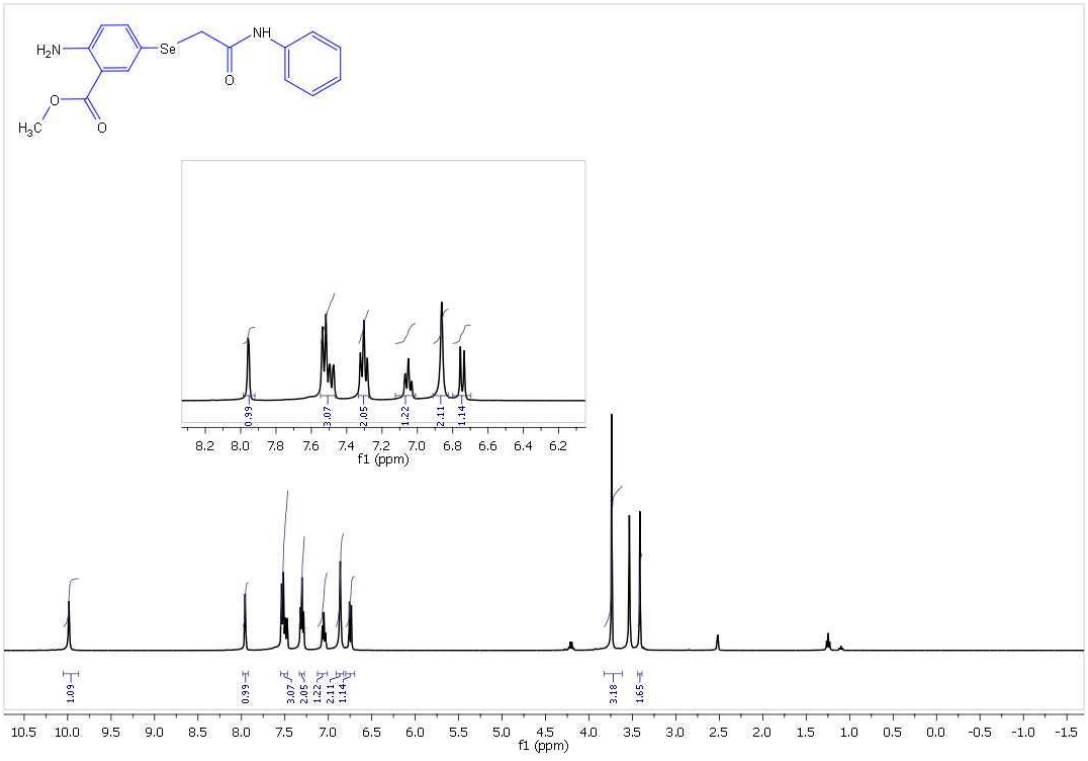


#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
217	321.20	949119	46.87	227	334.25	12617	0.62	237	407.30	3812	0.19
218	322.15	206457	10.19	228	335.20	61590	3.04	238	408.35	4545	0.22
219	323.15	182324	9.00	229	336.15	14251	0.70	239	409.25	10425	0.51
220	324.05	37472	1.85	230	337.20	12284	0.61	240	410.35	4385	0.22
221	325.05	4024	0.20	231	338.15	2137	0.11	241	411.25	19850	0.98
222	329.25	824	0.04	232	347.20	470	0.02	242	412.25	5834	0.29
223	330.25	1720	0.08	233	349.20	1524	0.08	243	413.25	4131	0.20
224	331.20	13207	0.65	234	355.20	474	0.02	244	414.15	786	0.04
225	332.25	14297	0.71	235	378.20	226	0.01				
226	333.20	31734	1.57	236	380.20	604	0.03				

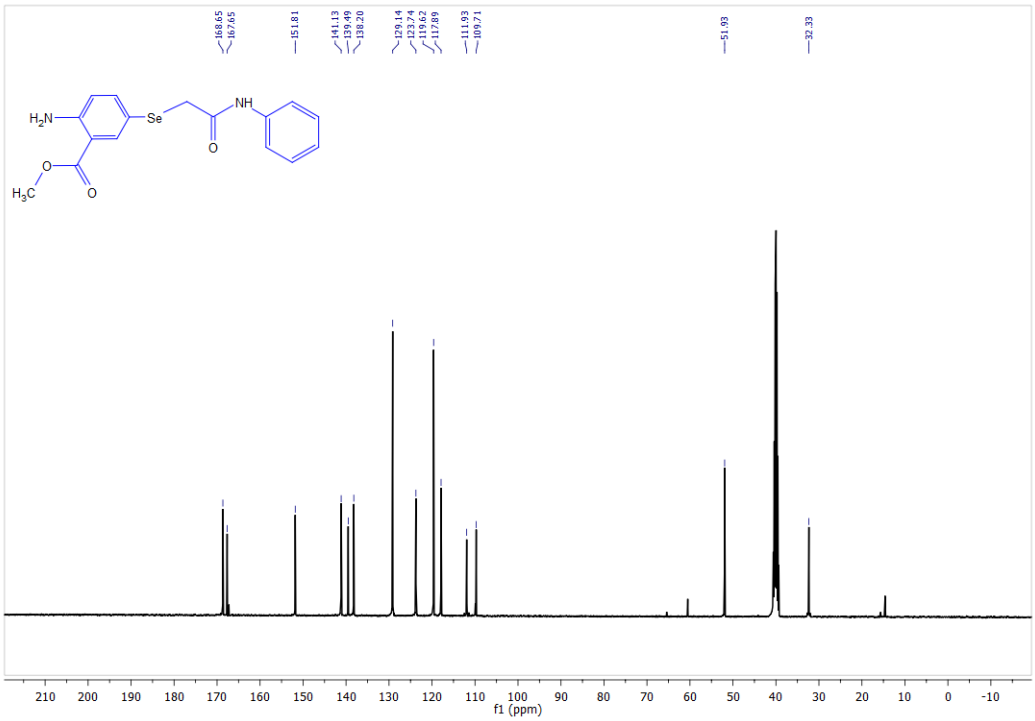
Mass chart of compound **5**

*Synthesis of methyl 2-amino-5-((2-oxo-2-(phenylamino) ethyl) selanyl) benzoate (**6**)[6]*

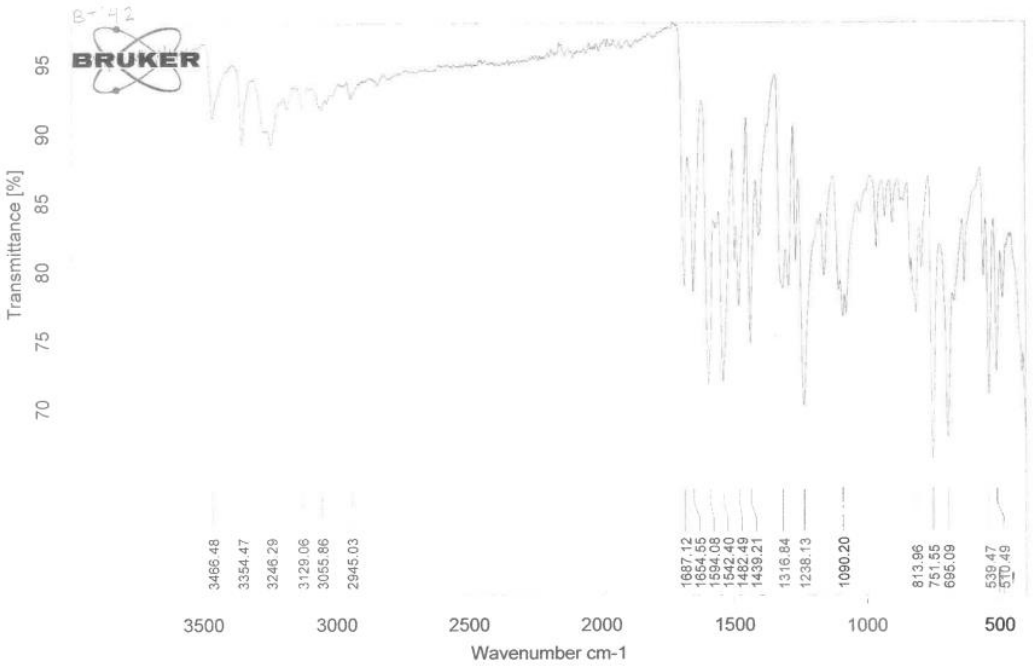
Compound **6** was synthesized from dimethyl 5,5'-diselanediylbis (2-aminobenzoate) (**3**)(2.0 mmol,916 mg) and 2-chloro-*N*-phenylacetamide (4.4 mmol,744 mg). It was isolated as violet solid; yield: 699 mg (96%); m.p. =126–128°C; Rf =0.50(petroleum ether/ ethyl acetate 4:2, *v*/*v*).IR(KBr): ν3466 (N-H), 3354 (N-H), 3246 (N-H), 2945 (C_{aliph}-H), 1678, 1594 (C=O), 1542 (C=C), 1439, 1238 (C_{Ar}-N), 1090 (C-O), 752 (C-H bending), 695, 552 (C-Se), 539 (C-H rocking);^{1}H NMR (400 MHz, DMSO- d_6) δ9.99(s, 1H, NH), 7.96(s, 1H, Ar-H),7.53 (d, J = 8.6 Hz, 2H, ArH), 7.48 (d, J = 8.6 Hz, 1H, ArH), 7.30 (dd, J = 8.6 Hz, J = 2.1 Hz, 2H, Ar-H), 7.04(t, 1H, J = 8.6 Hz, Ar-H), 6.86(s, 2H, NH_2), 6.75(d, J = 8.6 Hz, 1H, Ar-H), 3.74 (s, 3H, OCH_3), 3.42(s, 2H, $SeCH_2$); ^{13}CNMR (101 MHz, DMSO- d_6) δ168.65, 167.65, 151.81, 141.13, 139.49, 138.20, 129.14, 123.74, 119.62, 117.89, 111, 109.71, 51.93, 32.33. MS (EI,70 ev) *m/z* (%) = 364.20(M, 100.0, base peak), 230(40.48), 91.10(31), 77.05(24.13), 59(14.56).



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



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



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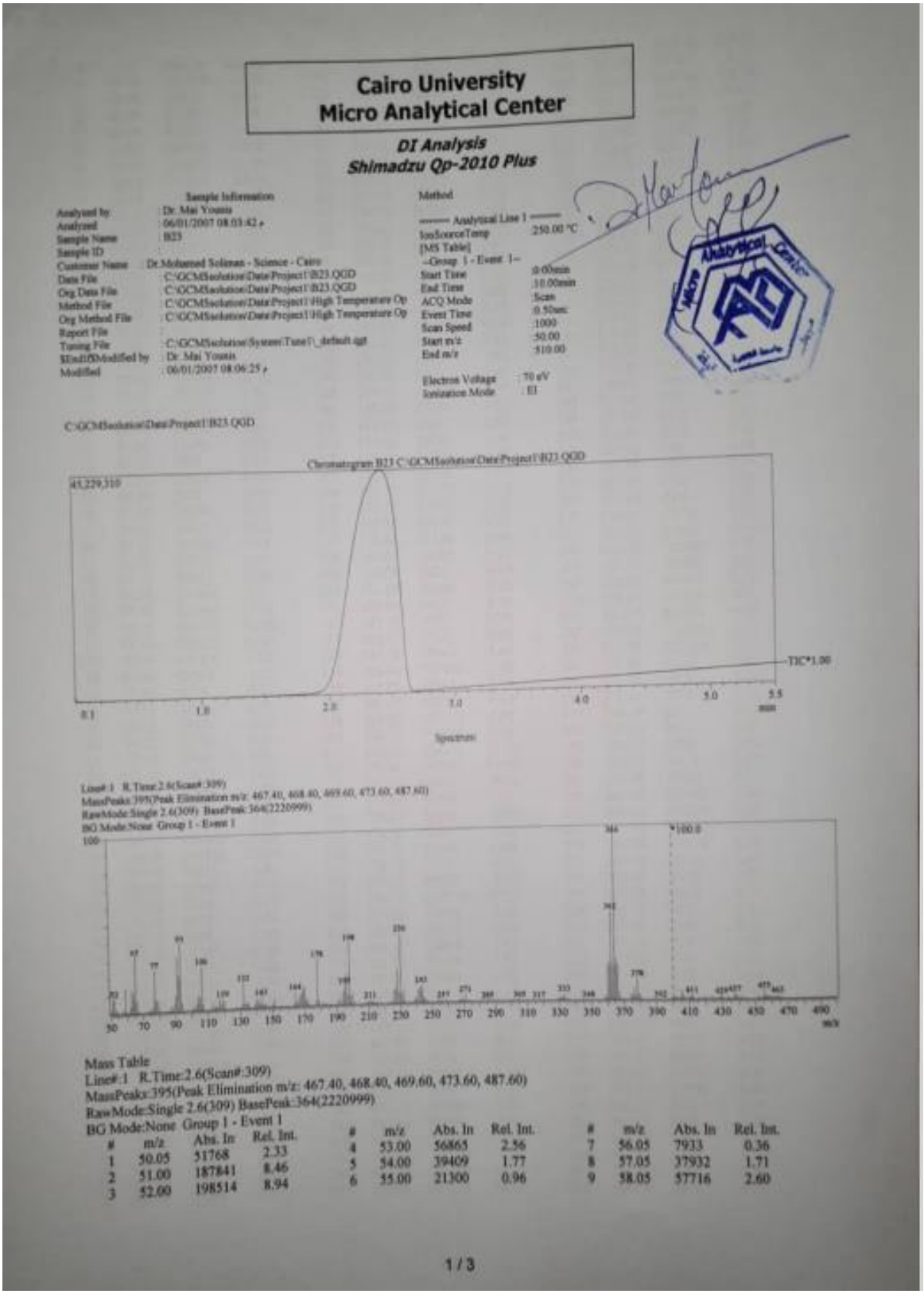
IR chart of compound **6**



Mass chart of compound **6**

#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
10	59.00	323380	14.56	79	128.15	17920	0.81	148	197.05	127657	5.75
11	60.00	19518	0.88	80	129.15	16582	0.75	149	198.00	802486	36.13
12	61.05	25294	1.14	81	130.15	23991	1.08	150	198.95	111117	5.00
13	62.05	85663	3.86	82	131.15	62358	2.81	151	200.00	147049	6.62
14	63.05	284974	12.83	83	132.10	333977	15.04	152	201.00	27327	1.23
15	64.05	250676	11.29	84	133.15	66067	2.97	153	202.05	6591	0.30
16	65.00	718538	32.35	85	134.15	78340	3.53	154	203.15	3651	0.16
17	66.00	152620	6.87	86	135.15	69517	3.13	155	204.15	2634	0.12
18	66.95	28433	1.28	87	136.15	11769	0.53	156	205.10	8610	0.39
19	68.05	8877	0.40	88	137.10	7681	0.35	157	206.05	3512	0.16
20	69.05	15359	0.69	89	138.15	13090	0.59	158	207.05	11680	0.53
21	70.05	8547	0.38	90	139.15	52322	2.36	159	208.05	15928	0.72
22	71.05	14796	0.67	91	140.10	117575	5.29	160	209.05	33769	1.52
23	72.05	7256	0.33	92	141.05	90195	4.06	161	210.05	30291	1.36
24	73.05	29968	1.35	93	142.05	52676	2.37	162	211.05	55042	2.48
25	74.05	26922	1.21	94	143.00	141599	6.38	163	212.05	30408	1.37
26	75.05	38018	1.71	95	144.00	54009	2.43	164	213.05	31320	1.41
27	76.05	89648	4.04	96	145.05	43425	1.96	165	214.05	18869	0.85
28	77.05	535908	24.13	97	146.05	54032	2.43	166	215.05	9367	0.42
29	78.05	171575	7.73	98	147.10	12569	0.57	167	216.05	19840	0.89
30	79.05	144276	6.50	99	148.10	17756	0.80	168	217.05	4333	0.20
31	80.05	37639	1.69	100	149.15	8208	0.37	169	218.05	4479	0.20
32	81.05	11176	0.50	101	150.15	38743	1.74	170	219.10	2612	0.12
33	82.15	5419	0.24	102	151.10	102964	4.64	171	220.10	778	0.04
34	83.10	15562	0.70	103	152.05	16710	0.75	172	221.15	1397	0.06
35	84.15	7935	0.36	104	153.10	11177	0.50	173	222.15	1142	0.05
36	85.10	16374	0.74	105	154.10	14711	0.66	174	223.15	4881	0.22
37	86.15	16002	0.72	106	155.05	15641	0.70	175	224.05	17976	0.81
38	87.10	69636	3.14	107	156.05	11100	0.50	176	225.15	20916	0.94
39	88.15	32733	1.47	108	157.05	15214	0.69	177	226.10	174902	7.87
40	89.15	88448	3.98	109	158.05	8233	0.37	178	227.15	189200	8.52
41	90.15	210874	9.49	110	159.10	16986	0.76	179	228.05	447454	20.15
42	91.10	688561	31.00	111	160.05	4503	0.20	180	229.15	133404	6.01
43	92.15	463765	20.88	112	161.15	4537	0.20	181	230.05	899020	40.48
44	93.10	862055	38.81	113	162.15	5173	0.23	182	231.05	114924	5.17
45	94.05	112159	5.05	114	163.15	35647	1.60	183	232.05	173318	7.80
46	95.00	27708	1.25	115	164.10	195450	8.80	184	233.05	21637	0.97
47	96.10	5274	0.24	116	165.05	50811	2.29	185	234.05	3484	0.16
48	97.10	9146	0.41	117	166.05	92270	4.15	186	235.15	3179	0.14
49	98.15	5237	0.24	118	167.05	149172	6.72	187	236.15	3807	0.17
50	99.10	12962	0.58	119	168.05	172761	7.78	188	237.05	8985	0.40
51	100.15	13487	0.61	120	169.05	226041	10.18	189	238.15	10887	0.49
52	101.10	60012	2.70	121	170.00	257615	11.60	190	239.10	48174	2.17
53	102.15	30642	1.38	122	171.00	96798	4.36	191	240.10	75681	3.41
54	103.15	88585	3.99	123	172.00	69998	3.15	192	241.10	157647	7.10
55	104.10	204116	9.19	124	173.00	21033	0.95	193	242.15	186228	8.38
56	105.15	159966	7.20	125	174.10	7897	0.36	194	243.10	230793	10.39
57	106.10	568420	25.59	126	175.15	17735	0.80	195	244.05	179124	8.07
58	107.10	76871	3.46	127	176.15	7737	0.35	196	245.05	65413	2.95
59	108.05	12580	0.57	128	177.15	62536	2.82	197	246.05	36727	1.65
60	109.10	3719	0.17	129	178.10	605762	27.27	198	247.20	22822	1.03
61	110.15	3039	0.14	130	179.05	72024	3.24	199	248.15	7827	0.35
62	111.15	9856	0.44	131	180.05	20815	0.94	200	249.15	2124	0.10
63	112.15	15347	0.69	132	181.10	26969	1.21	201	250.25	1855	0.08
64	113.10	93678	4.22	133	182.05	36544	1.65	202	251.20	7351	0.33
65	114.15	34219	1.54	134	183.10	28086	1.26	203	252.15	3123	0.14
66	115.10	49390	2.22	135	184.05	26423	1.19	204	253.15	6626	0.30
67	116.15	38664	1.74	136	185.00	19938	0.90	205	254.15	7024	0.32
68	117.10	130407	5.87	137	186.00	10751	0.48	206	255.10	19212	0.87
69	118.15	63644	2.87	138	187.05	6516	0.29	207	256.15	19273	0.87
70	119.10	142945	6.44	139	188.25	4750	0.21	208	257.10	29007	1.31
71	120.10	98100	4.42	140	189.15	25047	1.13	209	258.15	10175	0.46
72	121.05	14291	0.64	141	190.15	9994	0.45	210	259.20	21718	0.98
73	122.10	5969	0.27	142	191.15	57570	2.59	211	260.15	6061	0.27
74	123.05	3081	0.14	143	192.10	82754	3.73	212	261.15	4356	0.20
75	124.15	1538	0.07	144	193.05	33585	1.51	213	262.15	3391	0.15
76	125.15	3955	0.18	145	194.05	172249	7.76	214	263.15	3353	0.15
77	126.15	7068	0.32	146	195.05	249002	11.21	215	264.10	1687	0.08
78	127.15	19469	0.88	147	196.00	413670	18.63	216	265.15	3515	0.16

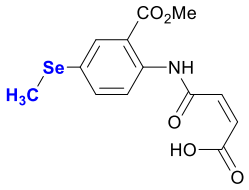
Mass chart of compound **6**

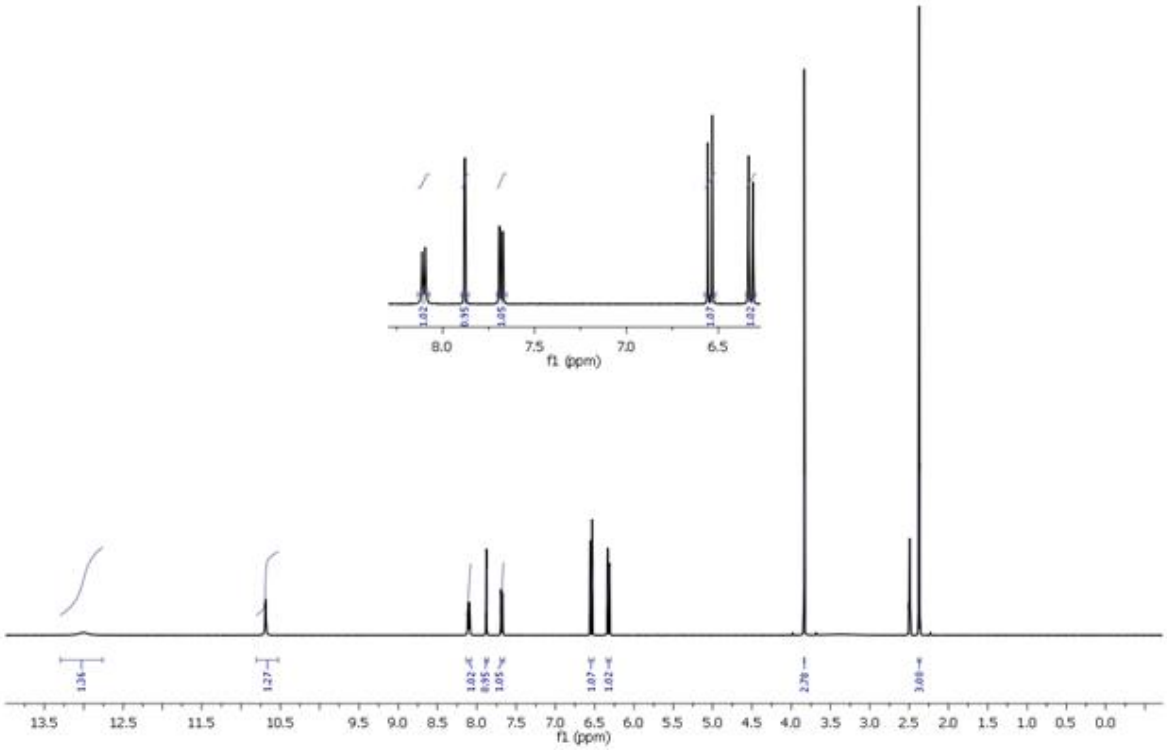
#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.	#	m/z	Abs. In	Rel. Int.
217	266.15	2637	0.12	277	326.15	836	0.04	337	387.30	279	0.01
218	267.10	18146	0.82	278	327.15	2834	0.13	338	388.25	396	0.02
219	268.15	20158	0.91	279	328.15	6050	0.27	339	389.35	651	0.03
220	269.10	46786	2.11	280	329.15	23275	1.05	340	390.25	1290	0.06
221	270.15	15694	0.71	281	330.15	29151	1.31	341	391.35	1022	0.05
222	271.10	96137	4.33	282	331.15	50733	2.28	342	392.30	1966	0.09
223	272.05	16070	0.72	283	332.15	33893	1.53	343	393.35	1297	0.06
224	273.10	21305	0.96	284	333.15	88344	3.98	344	394.30	940	0.04
225	274.05	3890	0.18	285	334.05	24078	1.08	345	395.30	473	0.02
226	275.15	1899	0.09	286	335.15	19856	0.89	346	396.45	384	0.02
227	276.25	1345	0.06	287	336.15	4538	0.20	347	397.50	1070	0.05
228	277.20	2796	0.13	288	337.15	1006	0.05	348	398.45	585	0.03
229	278.15	1435	0.06	289	338.25	662	0.03	349	399.45	317	0.01
230	279.15	898	0.04	290	339.30	1508	0.07	350	400.20	370	0.02
231	280.15	727	0.03	291	340.25	578	0.03	351	401.20	289	0.01
232	281.15	2478	0.11	292	341.25	684	0.03	352	402.20	250	0.01
233	282.15	2409	0.11	293	342.25	584	0.03	353	403.20	257	0.01
234	283.10	5790	0.26	294	343.25	805	0.04	354	404.45	336	0.02
235	284.15	3531	0.16	295	344.20	1958	0.09	355	405.40	1146	0.05
236	285.10	12303	0.55	296	345.25	2706	0.12	356	406.35	447	0.02
237	286.15	5148	0.23	297	346.20	3890	0.18	357	407.40	271	0.01
238	287.10	5833	0.26	298	347.25	4640	0.21	358	409.45	410	0.02
239	288.25	2633	0.12	299	348.20	7434	0.33	359	410.50	282	0.01
240	289.15	7201	0.32	300	349.15	2578	0.12	360	411.50	583	0.03
241	290.15	2596	0.12	301	350.15	2611	0.12	361	412.50	284	0.01
242	291.20	2186	0.10	302	351.20	977	0.04	362	415.50	254	0.01
243	292.15	1131	0.05	303	352.15	764	0.03	363	417.50	207	0.01
244	293.25	1594	0.07	304	353.25	847	0.04	364	418.50	257	0.01
245	294.25	1118	0.05	305	354.15	553	0.02	365	419.50	354	0.02
246	295.20	5345	0.24	306	355.25	657	0.03	366	421.50	326	0.01
247	296.15	1761	0.08	307	356.25	704	0.03	367	423.50	396	0.02
248	297.25	811	0.04	308	357.25	3443	0.16	368	425.50	250	0.01
249	298.35	617	0.03	309	358.20	42783	1.93	369	426.50	212	0.01
250	299.30	823	0.04	310	359.25	41697	1.88	370	428.35	430	0.02
251	300.25	1273	0.06	311	360.20	448651	20.20	371	429.30	458	0.02
252	301.25	1429	0.06	312	361.25	490508	22.09	372	430.30	231	0.01
253	302.25	2061	0.09	313	362.20	113024	50.89	373	432.30	222	0.01
254	303.30	3346	0.15	314	363.25	433043	19.50	374	433.30	212	0.01
255	304.35	3895	0.18	315	364.20	222099	100.00	375	434.30	201	0.01
256	305.30	14001	0.63	316	365.15	516139	23.24	376	436.40	250	0.01
257	306.20	5601	0.25	317	366.15	453240	20.41	377	437.45	688	0.03
258	307.15	2298	0.10	318	367.15	94607	4.26	378	438.35	497	0.02
259	308.15	902	0.04	319	368.15	13453	0.61	379	439.50	431	0.02
260	309.30	892	0.04	320	369.15	2332	0.10	380	441.50	303	0.01
261	310.25	583	0.03	321	370.30	4468	0.20	381	442.50	233	0.01
262	311.35	721	0.03	322	371.25	1831	0.08	382	444.50	210	0.01
263	312.35	712	0.03	323	372.20	5146	0.23	383	451.50	289	0.01
264	313.35	1160	0.05	324	373.25	5093	0.23	384	452.50	233	0.01
265	314.35	803	0.04	325	374.25	54806	2.47	385	454.45	304	0.01
266	315.35	918	0.04	326	375.25	61887	2.79	386	455.40	1105	0.05
267	316.35	904	0.04	327	376.20	144442	6.50	387	456.35	499	0.02
268	317.30	4386	0.20	328	377.25	48025	2.16	388	457.10	265	0.01
269	318.25	2391	0.11	329	378.20	271025	12.20	389	458.15	443	0.02
270	319.25	2801	0.13	330	379.15	67760	3.05	390	459.10	218	0.01
271	320.25	1770	0.08	331	380.20	56982	2.57	391	460.20	433	0.02
272	321.20	4260	0.19	332	381.15	13270	0.60	392	462.20	287	0.01
273	322.25	2058	0.09	333	382.15	2182	0.10	393	463.40	473	0.02
274	323.25	2501	0.11	334	383.20	484	0.02	394	464.40	252	0.01
275	324.25	848	0.04	335	384.20	236	0.01	395	466.40	212	0.01
276	325.15	508	0.02	336	386.20	215	0.01				

3 / 3

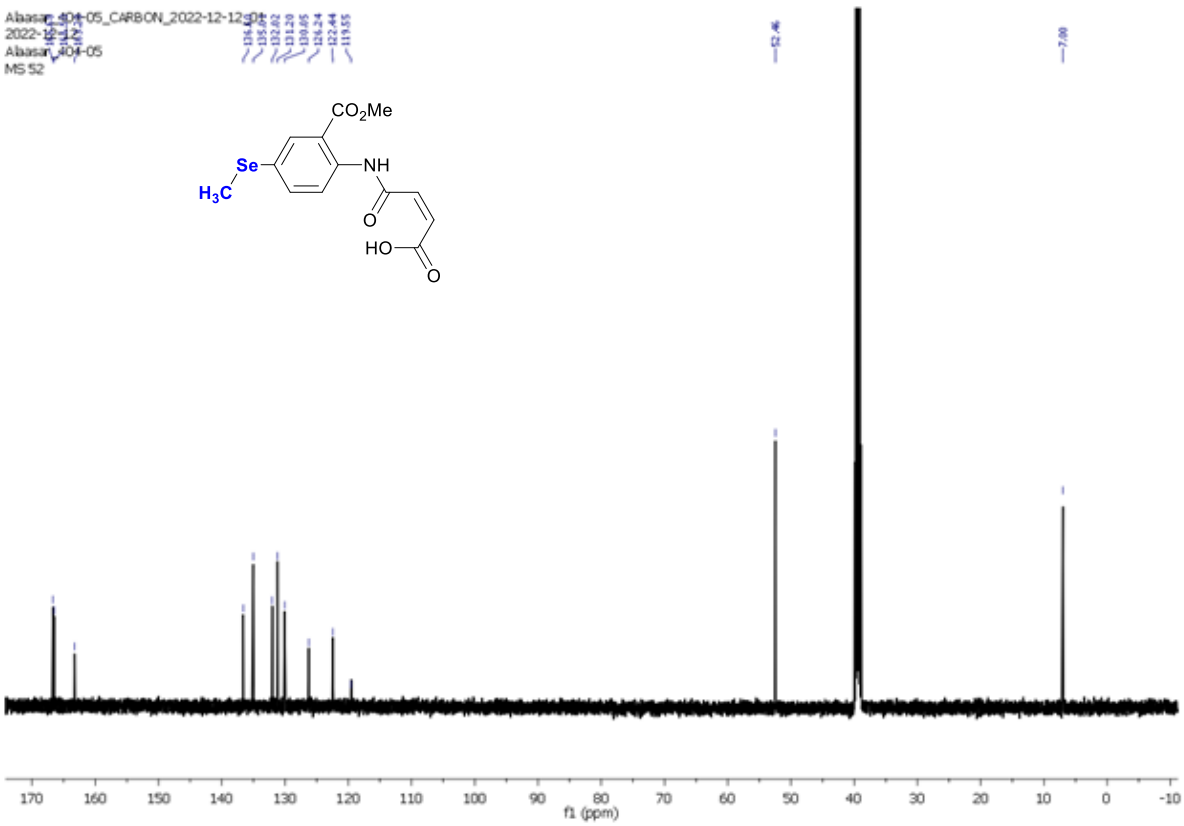
Mass chart of compound **6**

*4-((2-(methoxycarbonyl)-4-(methylselanyl)phenyl)amino)-4-oxobut-2-enoic acid (**7**)*

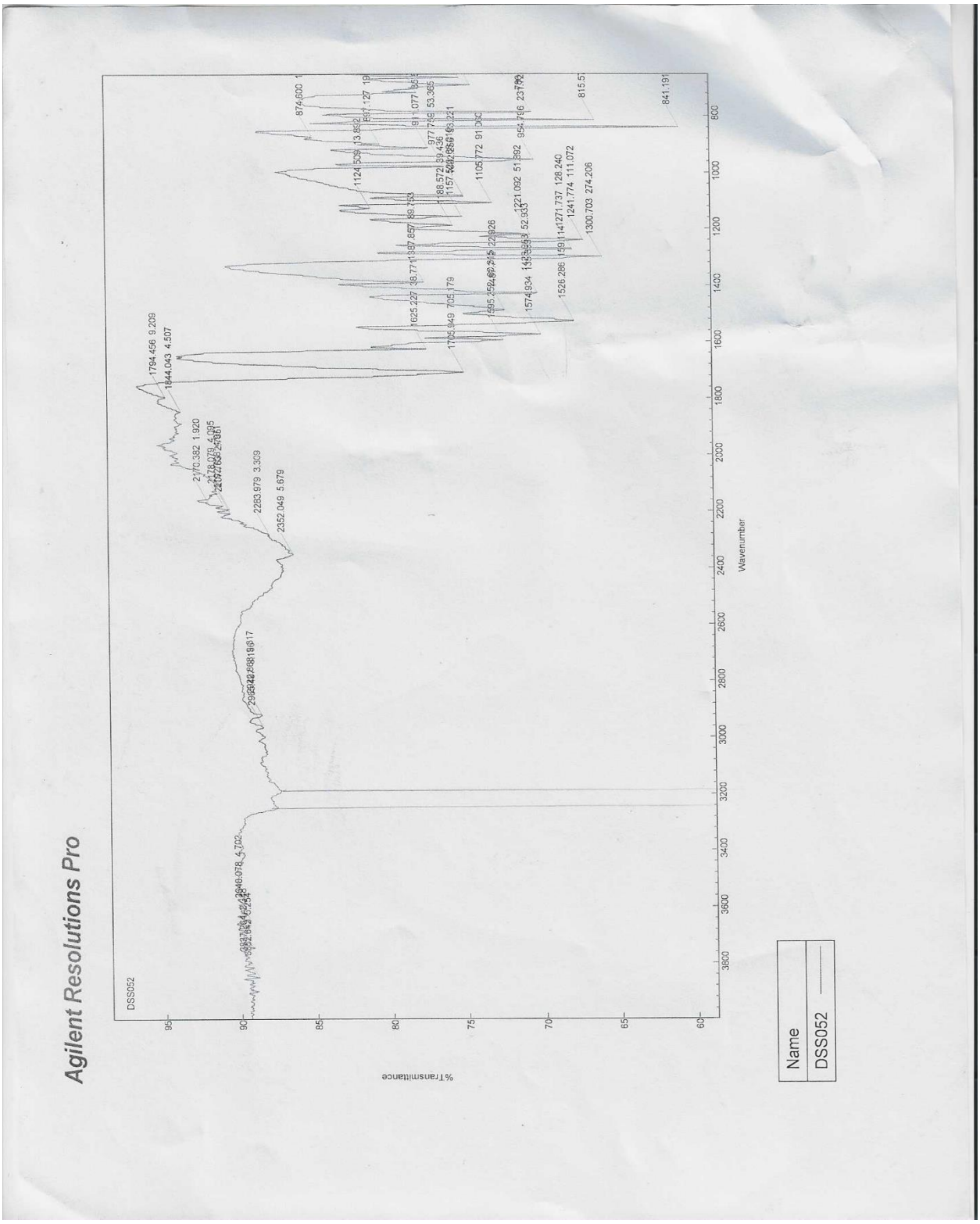




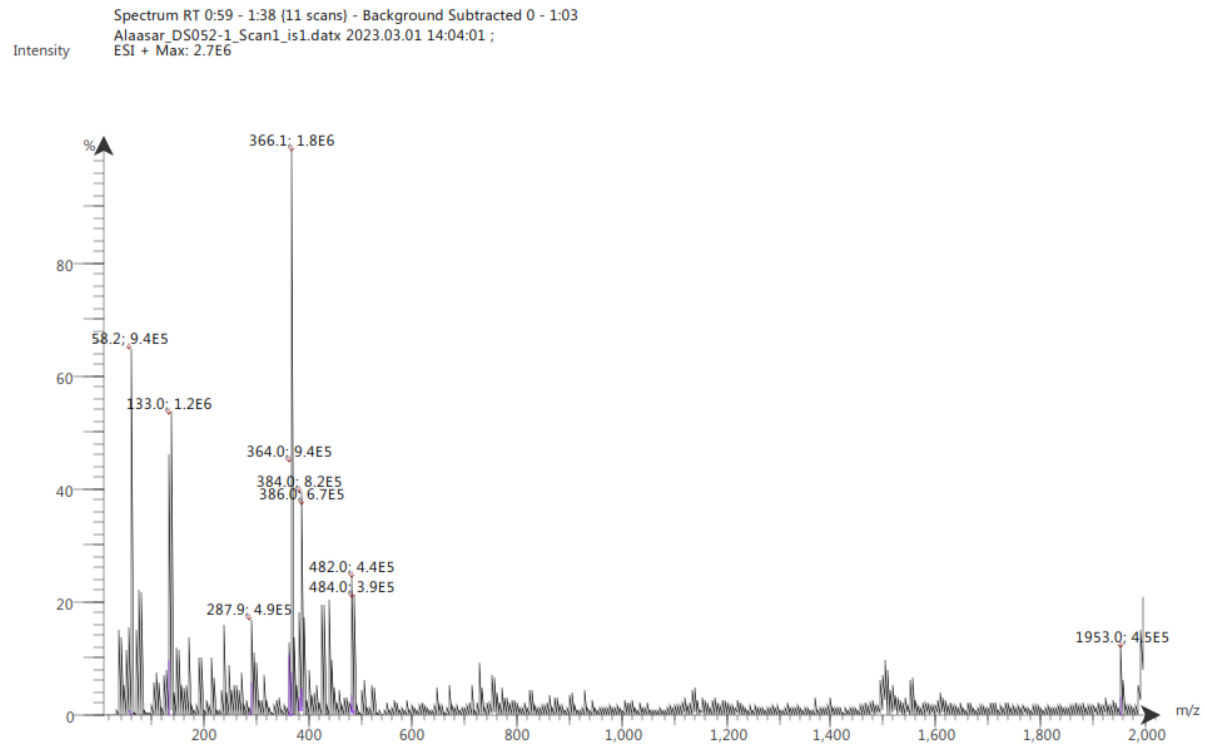
^{1}HNMR chart of compound **7**



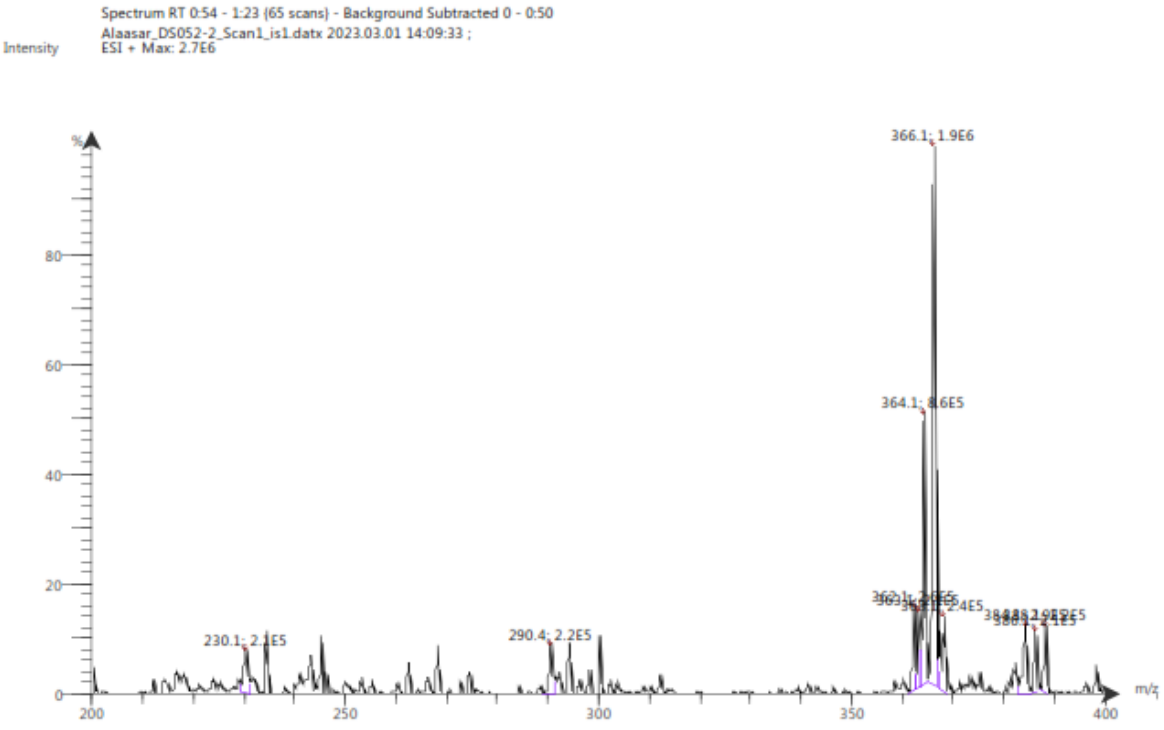
^{13}CNMR chart of compound **7**



IR chart of compound **7**

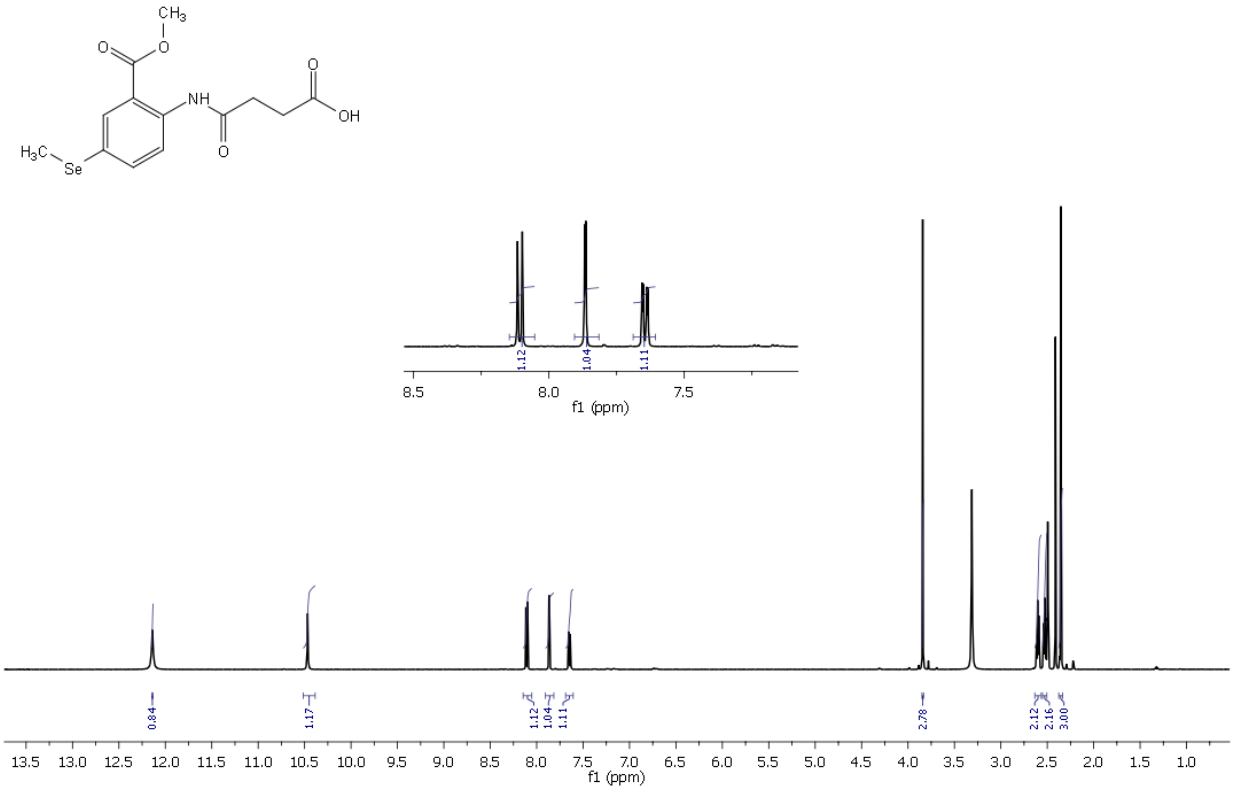


MS chart of compound **7**

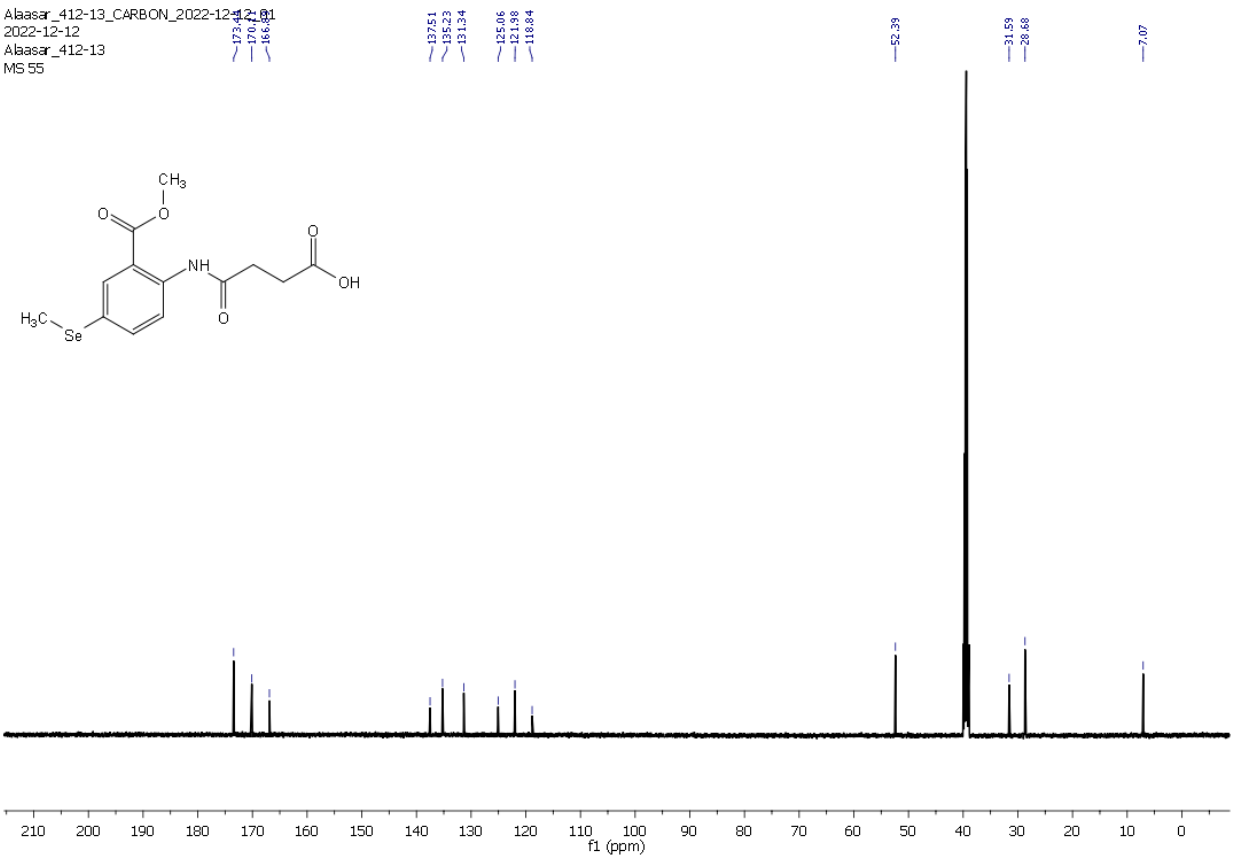


MS chart of compound **7**

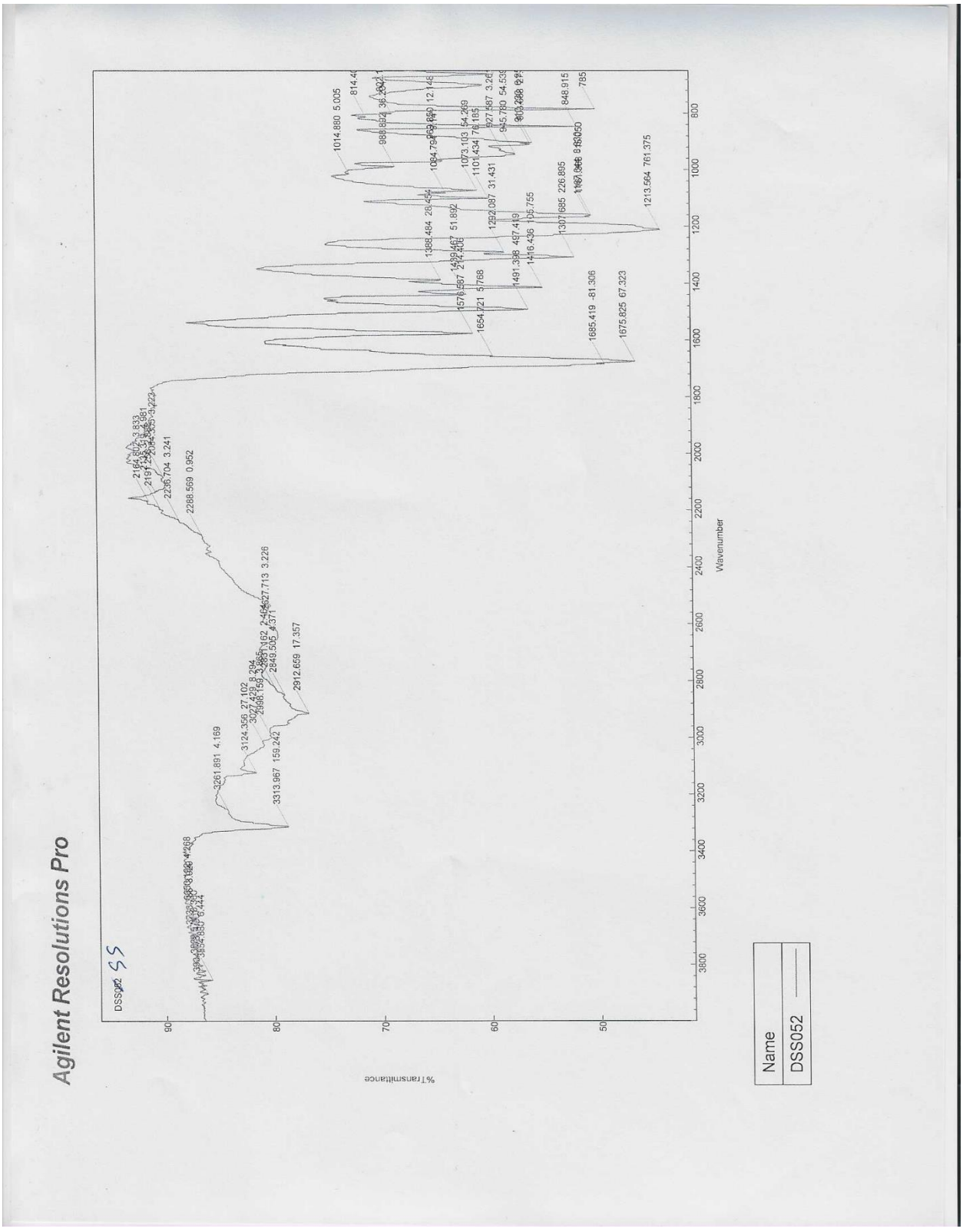
*4-((2-(methoxycarbonyl)-4-(methylselanyl)phenyl)amino)-4-oxobut-2-enoic acid (**8**)*



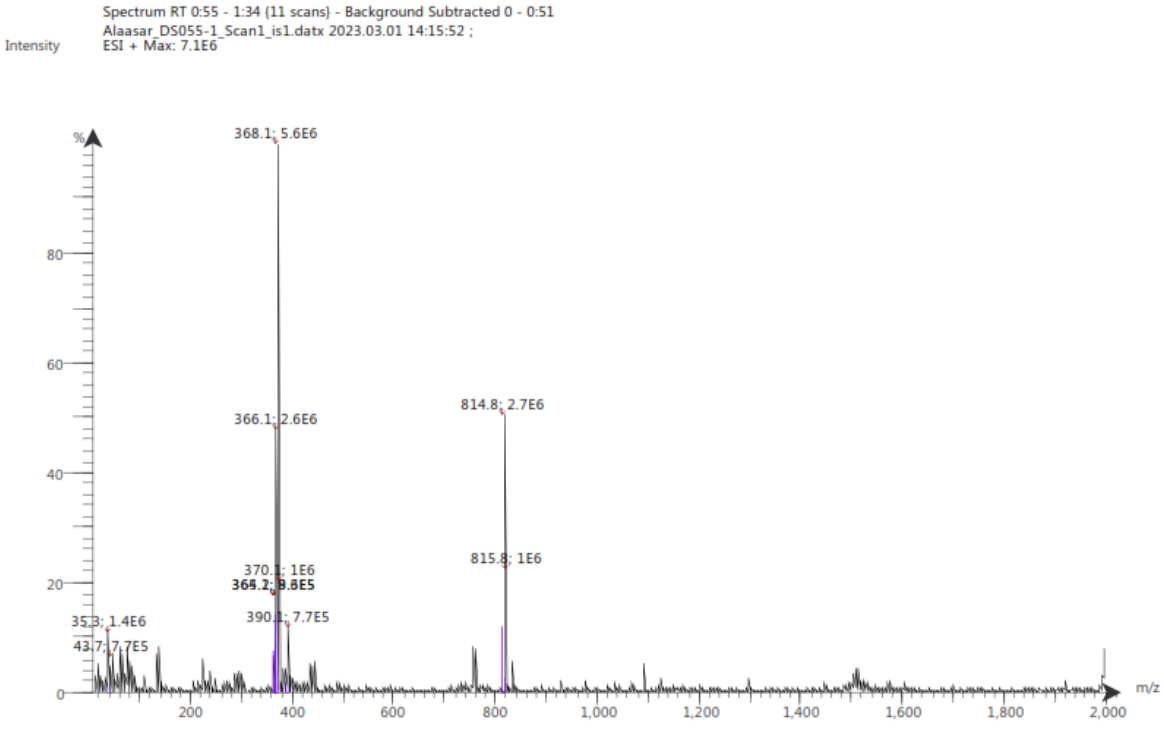
^{1}HNMR chart of compound **8**



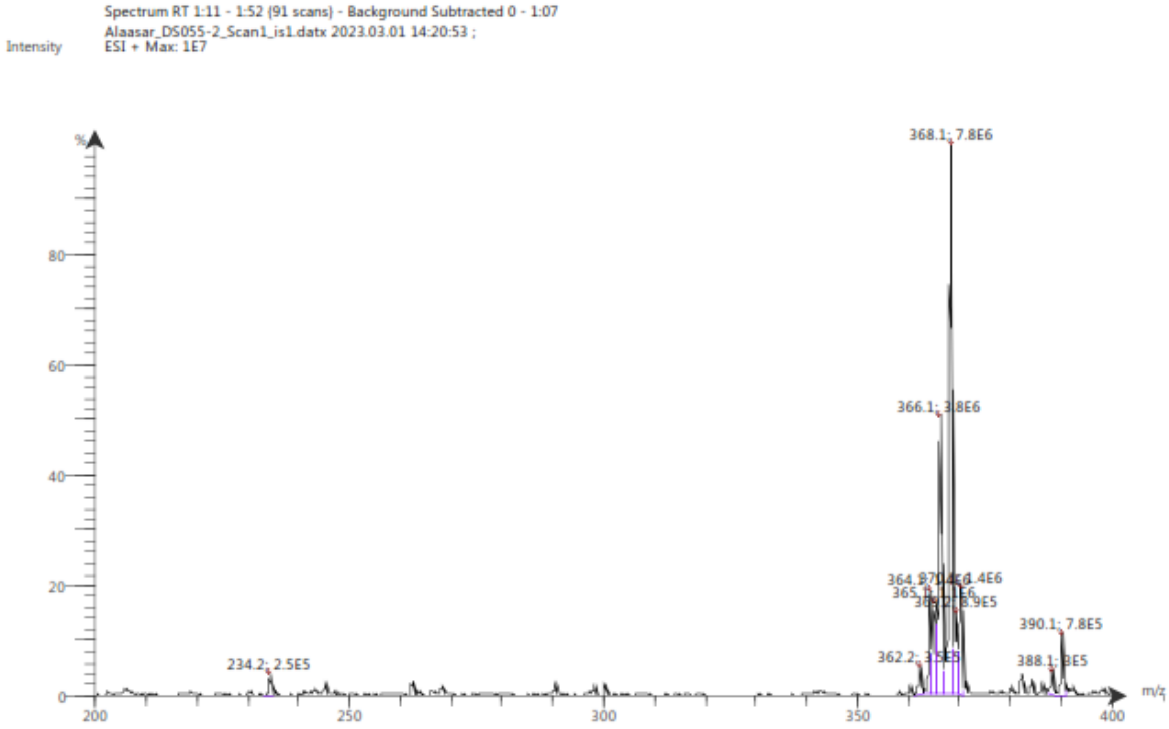
^{13}CNMR chart of compound **8**



IR chart of compound **8**

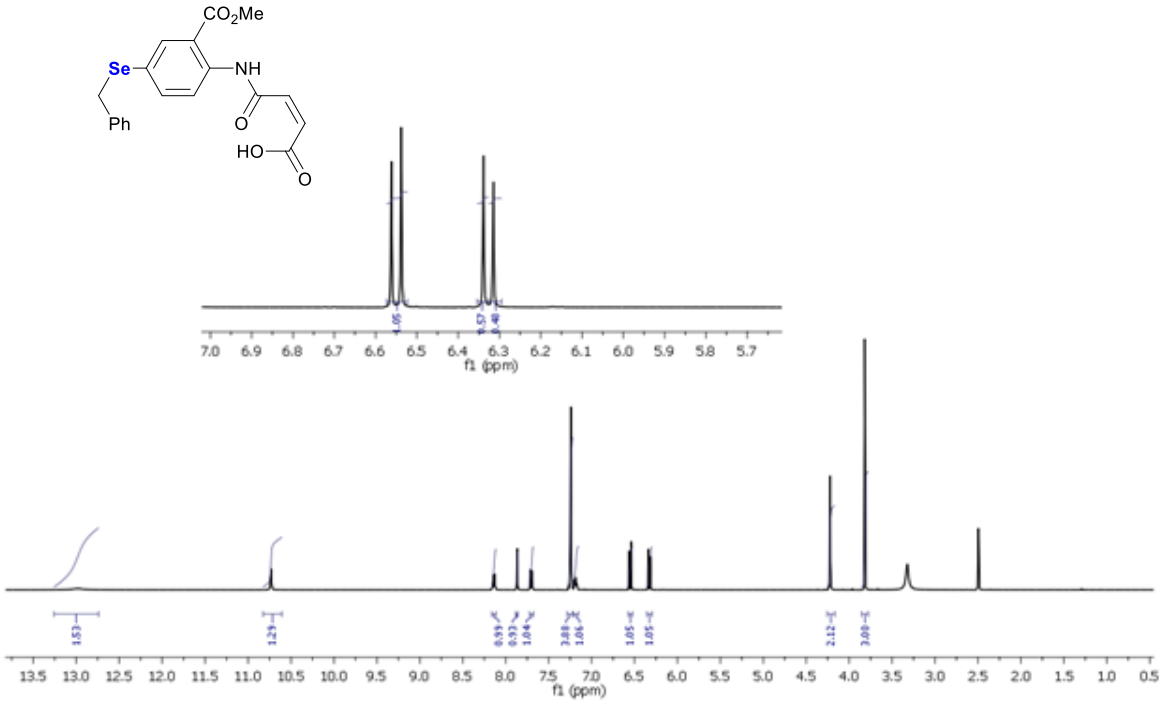


MS chart of compound **8**

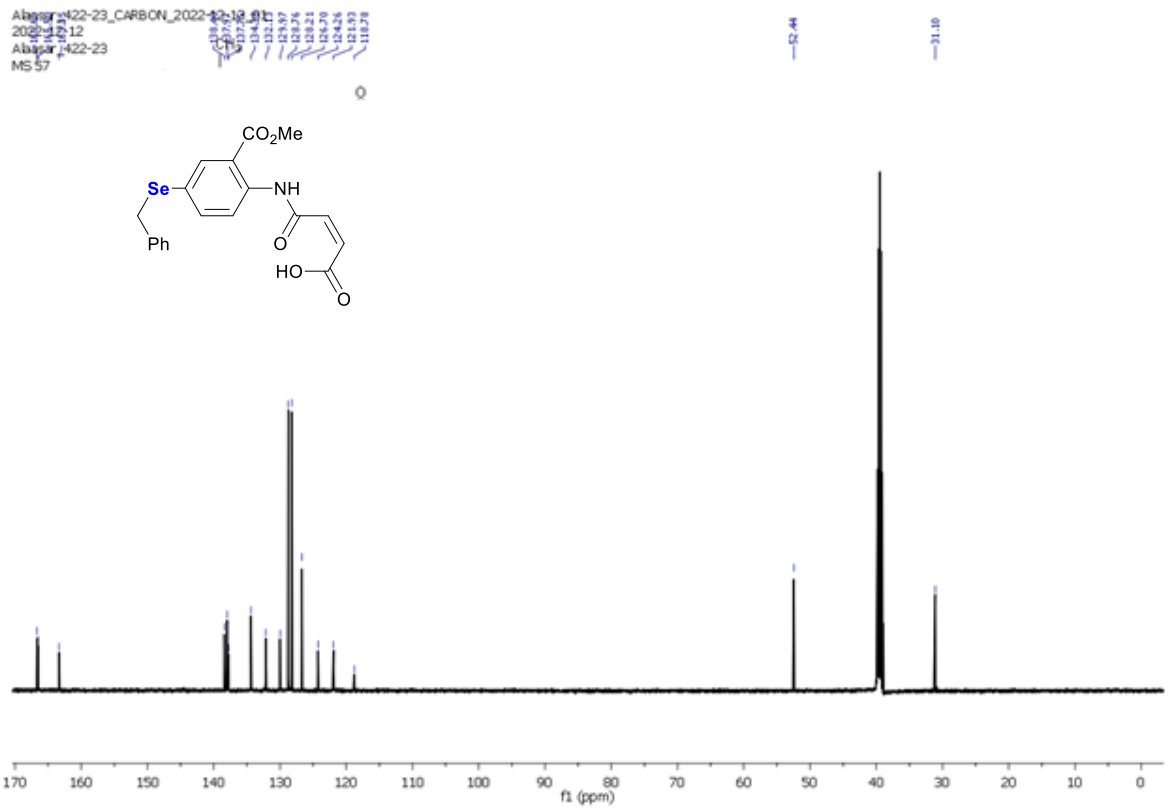


MS chart of compound **8**

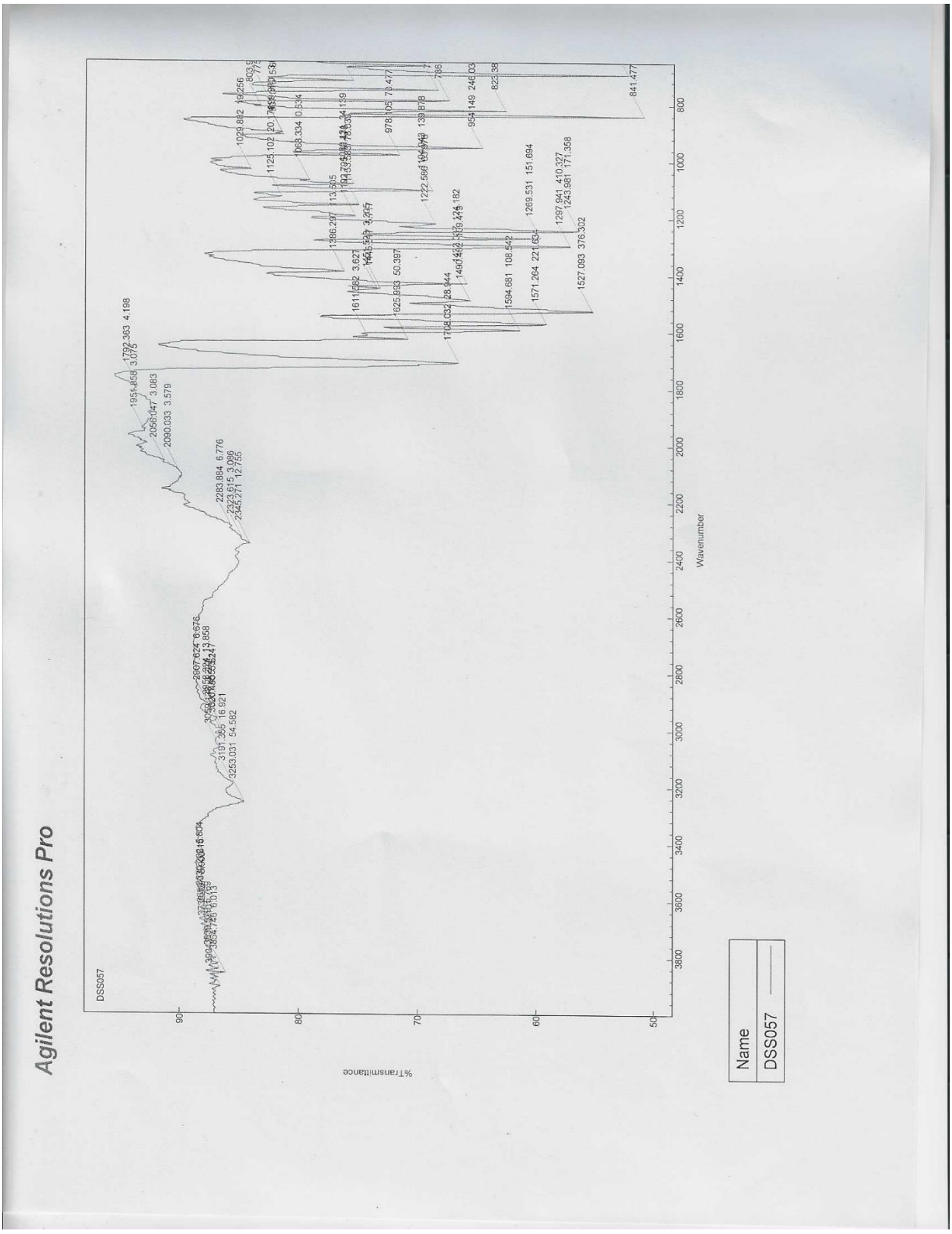
*4-((2-(methoxycarbonyl)-4-(methylselanyl)phenyl)amino)-4-oxobut-2-enoic acid (**9**)*



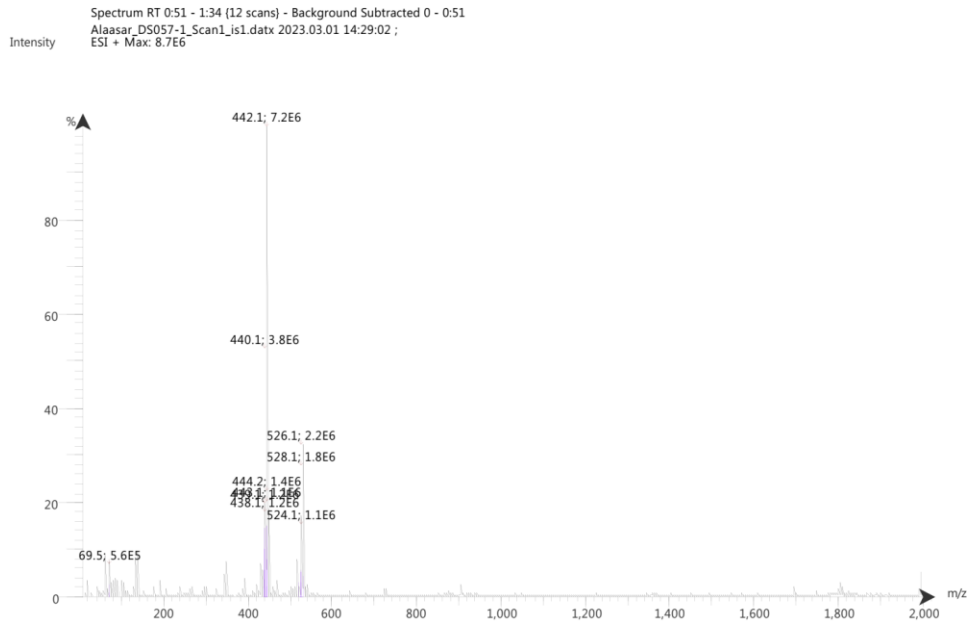
^{1}HNMR chart of compound **9**



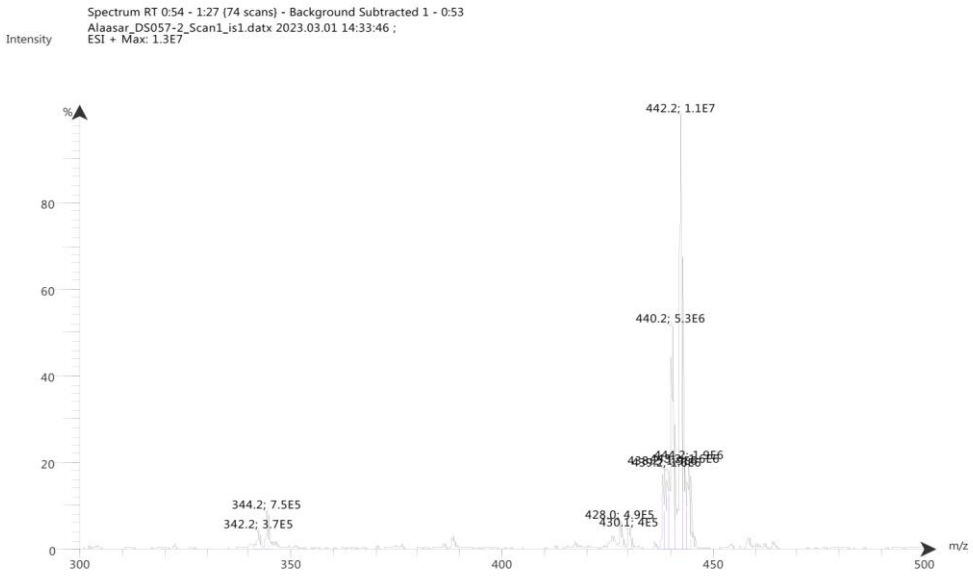
^{13}CNMR chart of compound **9**



IR chart of compound **9**

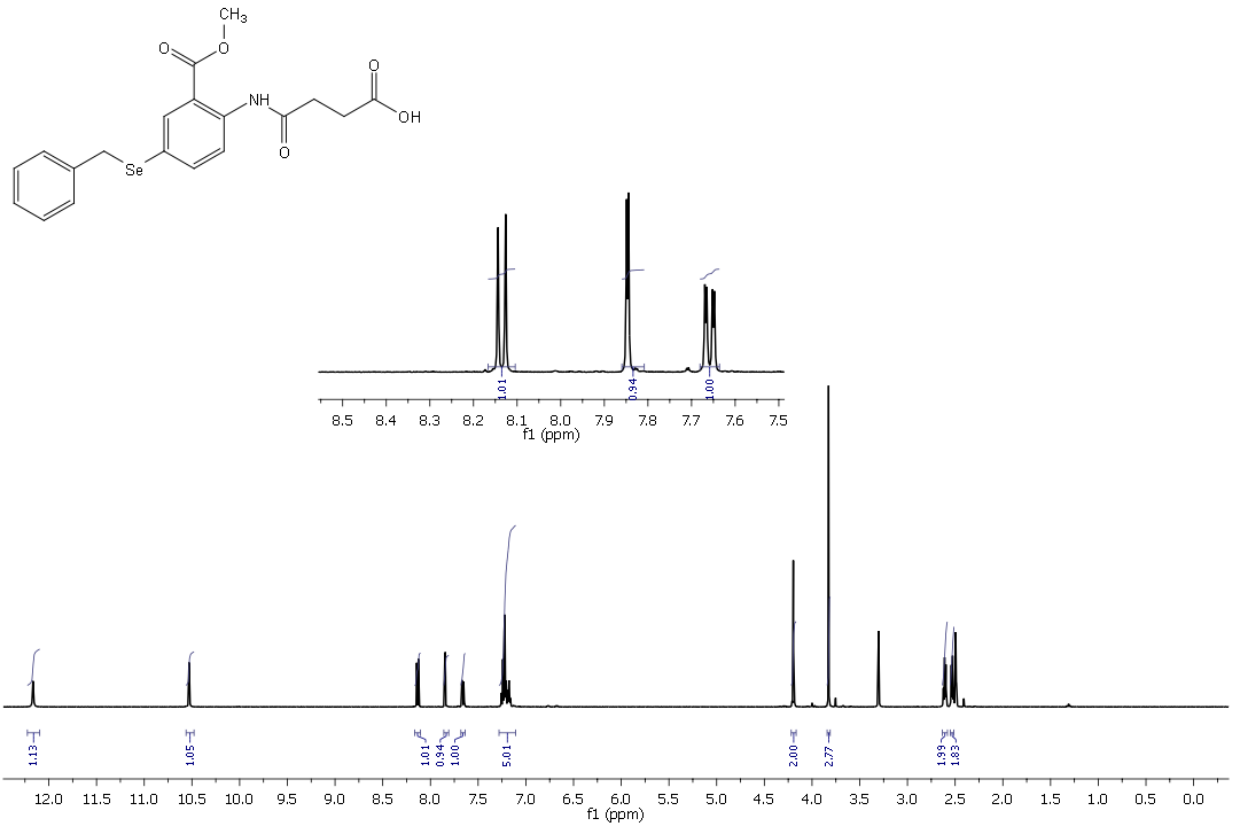


MS chart of compound **9**

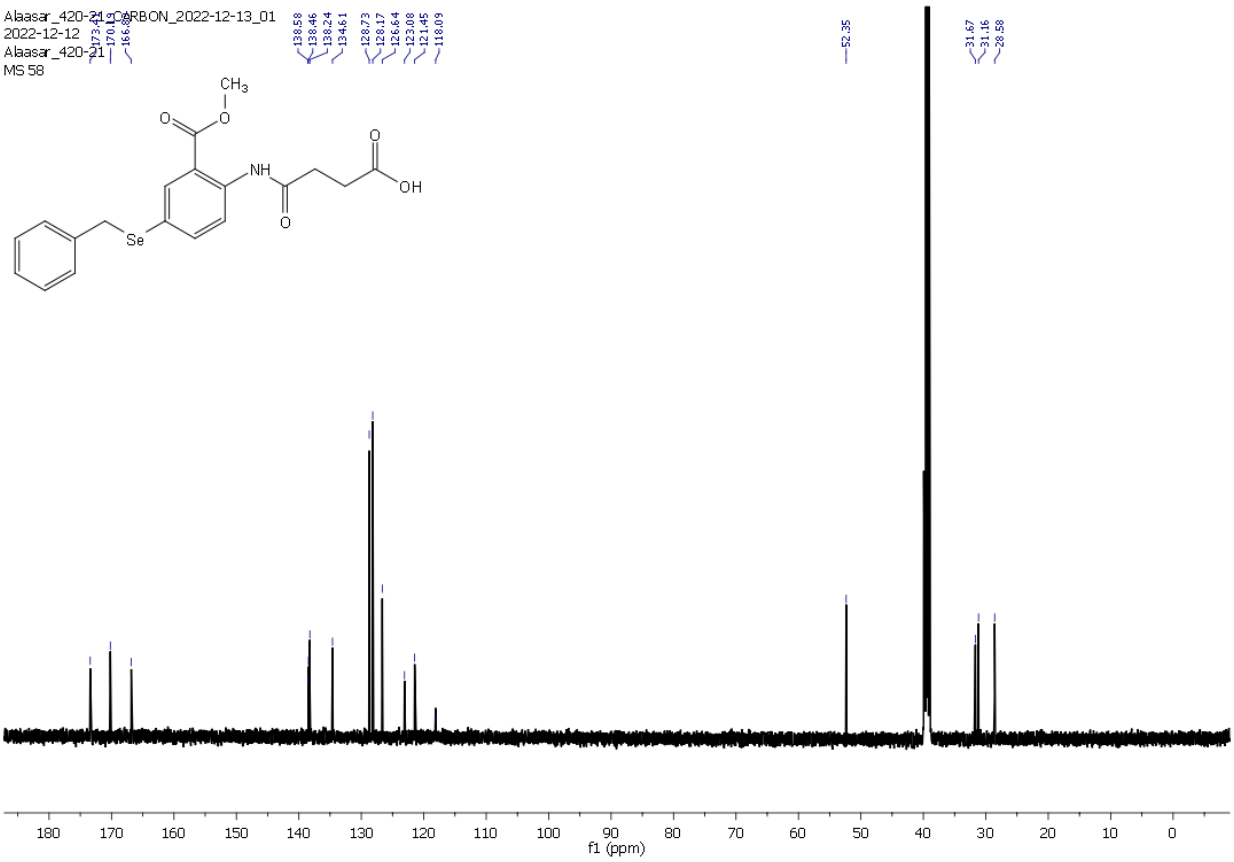


MS chart of compound **9**

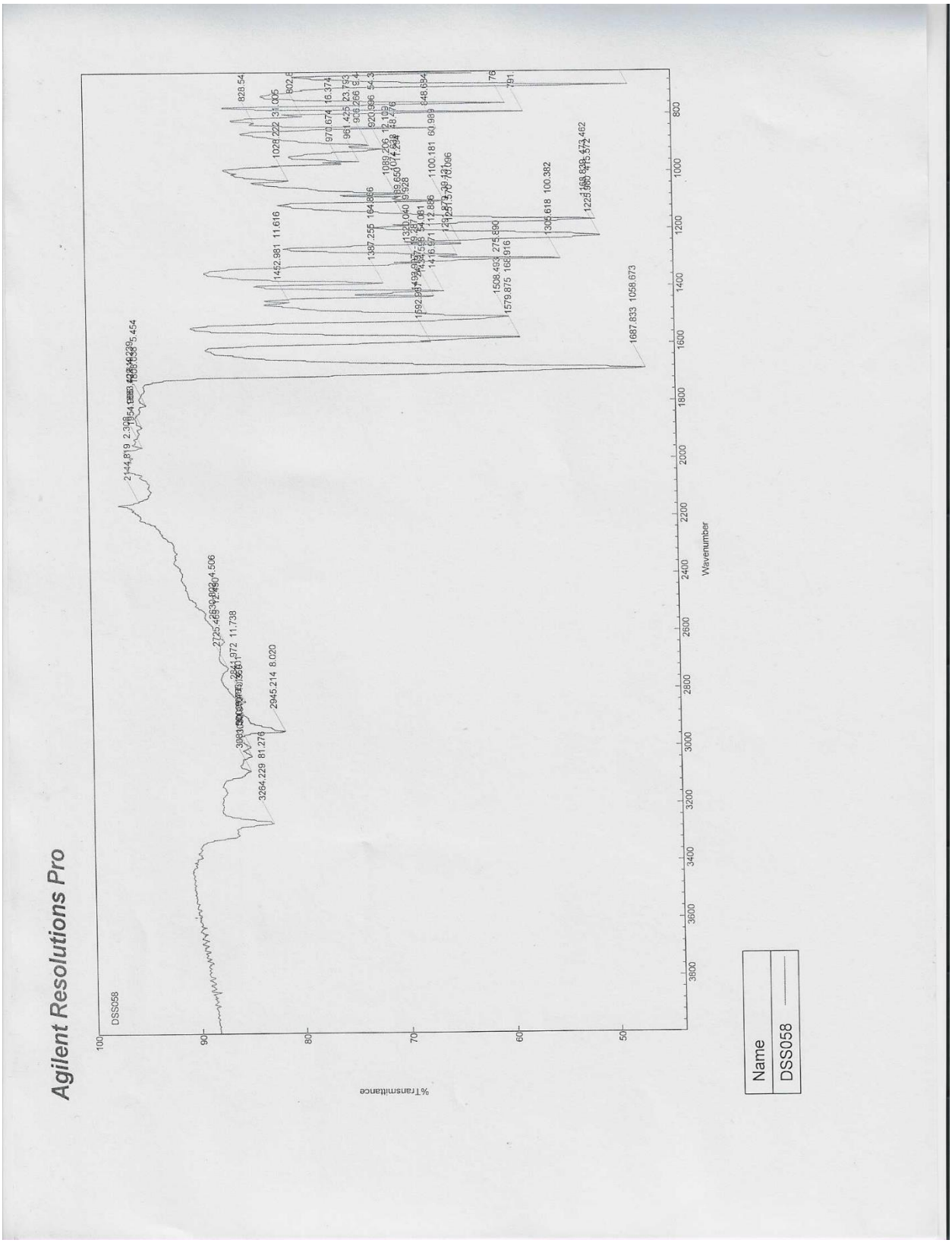
*4-((2-(methoxycarbonyl)-4-(methylselanyl)phenyl)amino)-4-oxobut-2-enoic acid (**10**)*



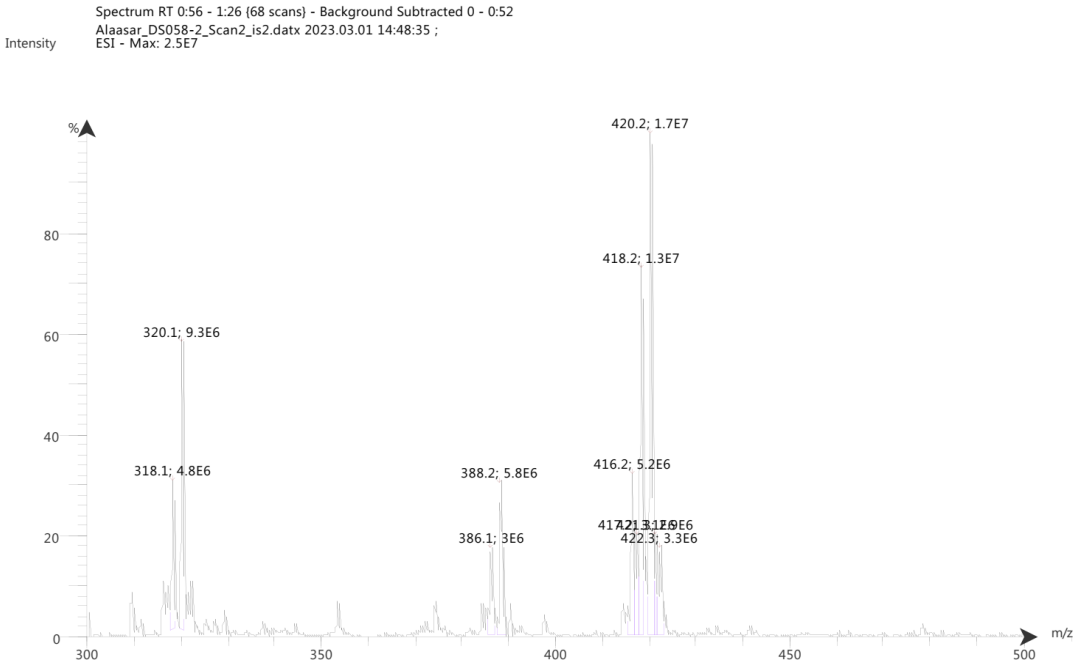
^{1}HNMR chart of compound **10**



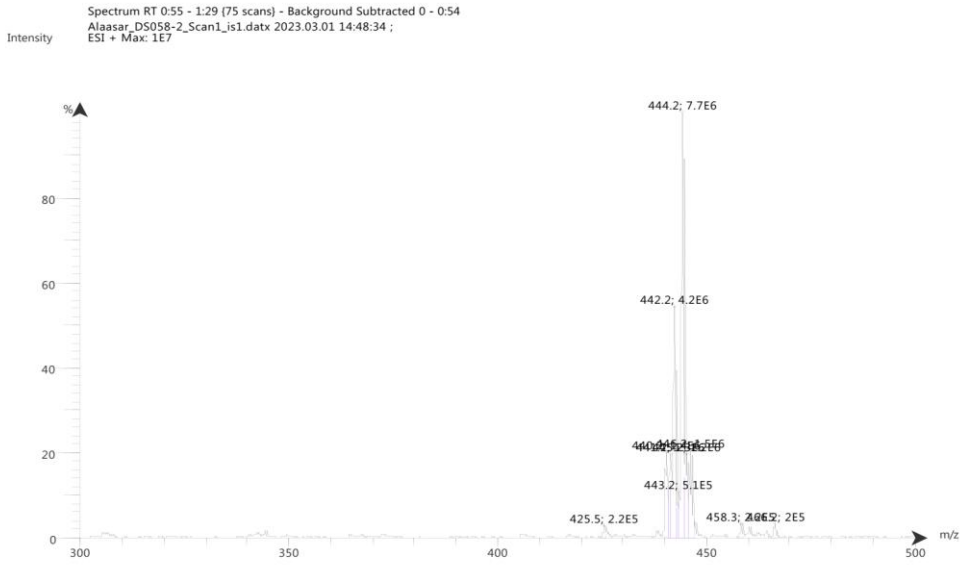
^{13}CNMR chart of compound **10**



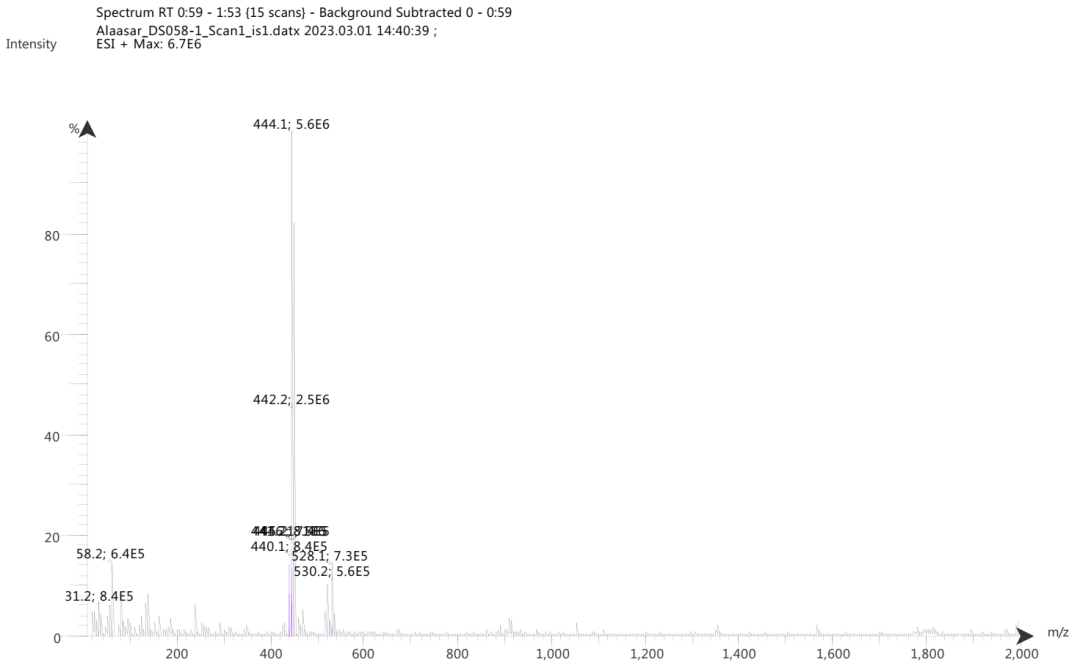
IR chart of compound **10**



MS chart of compound **10**

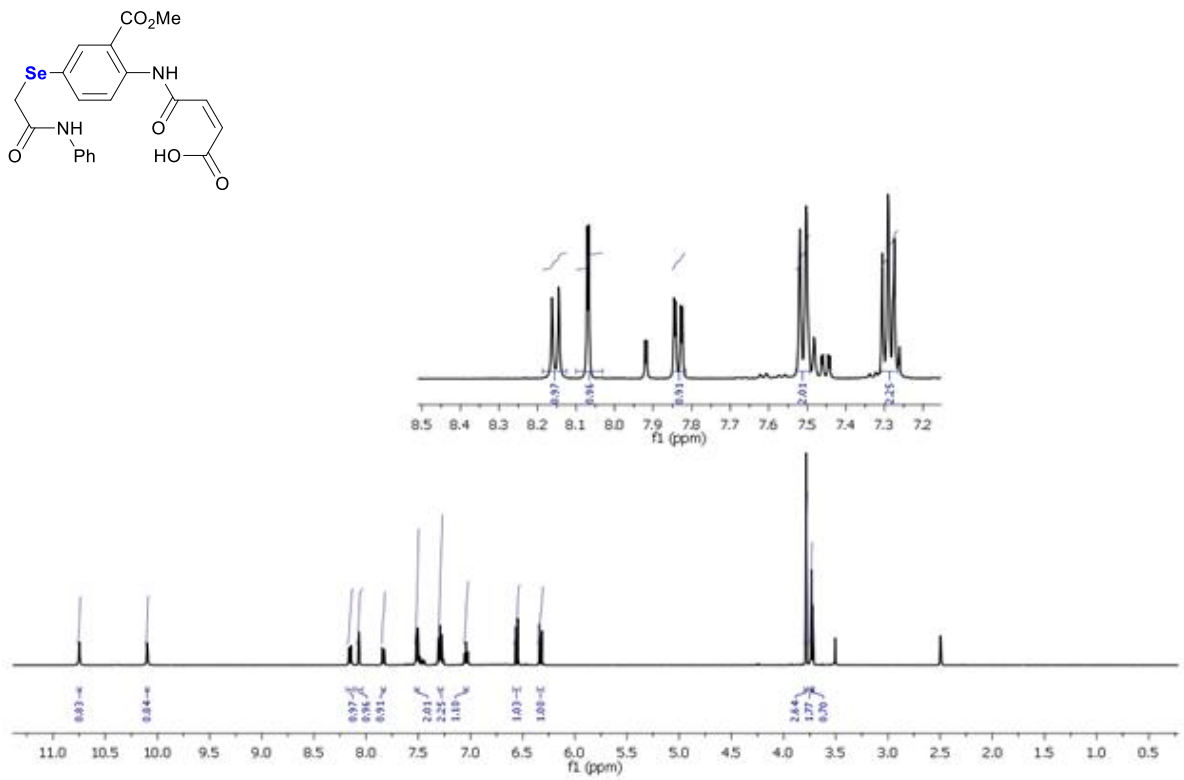


MS chart of compound **10**

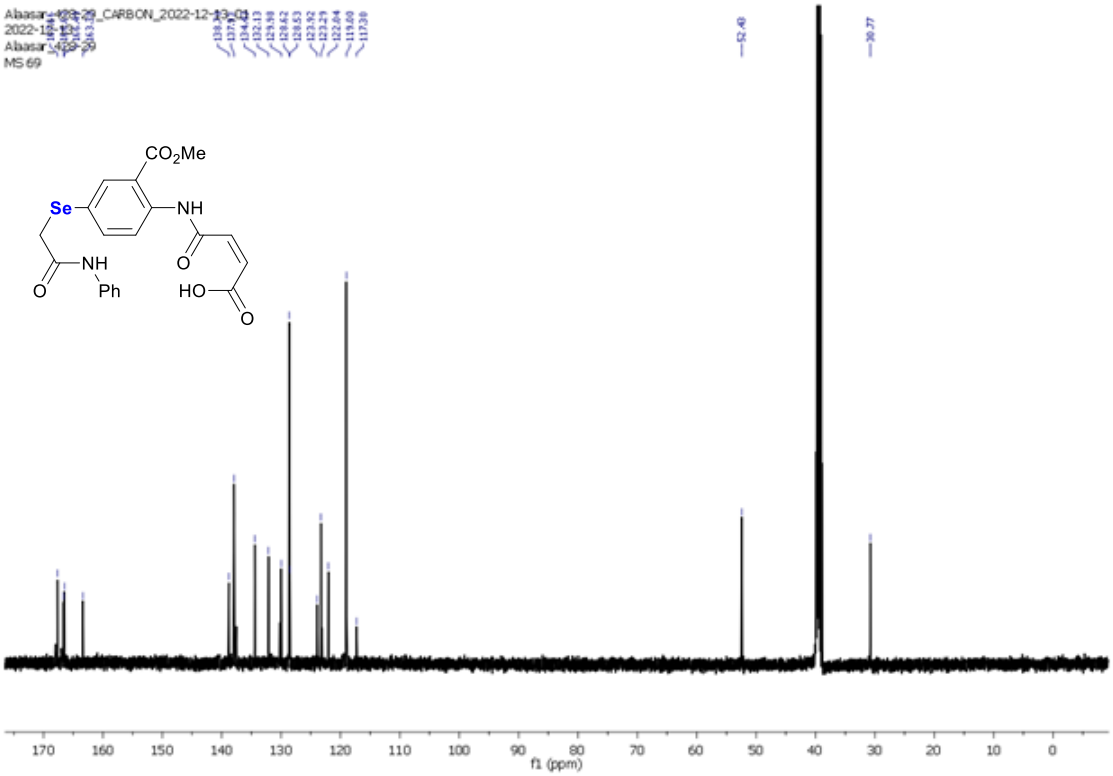


MS chart of compound **10**

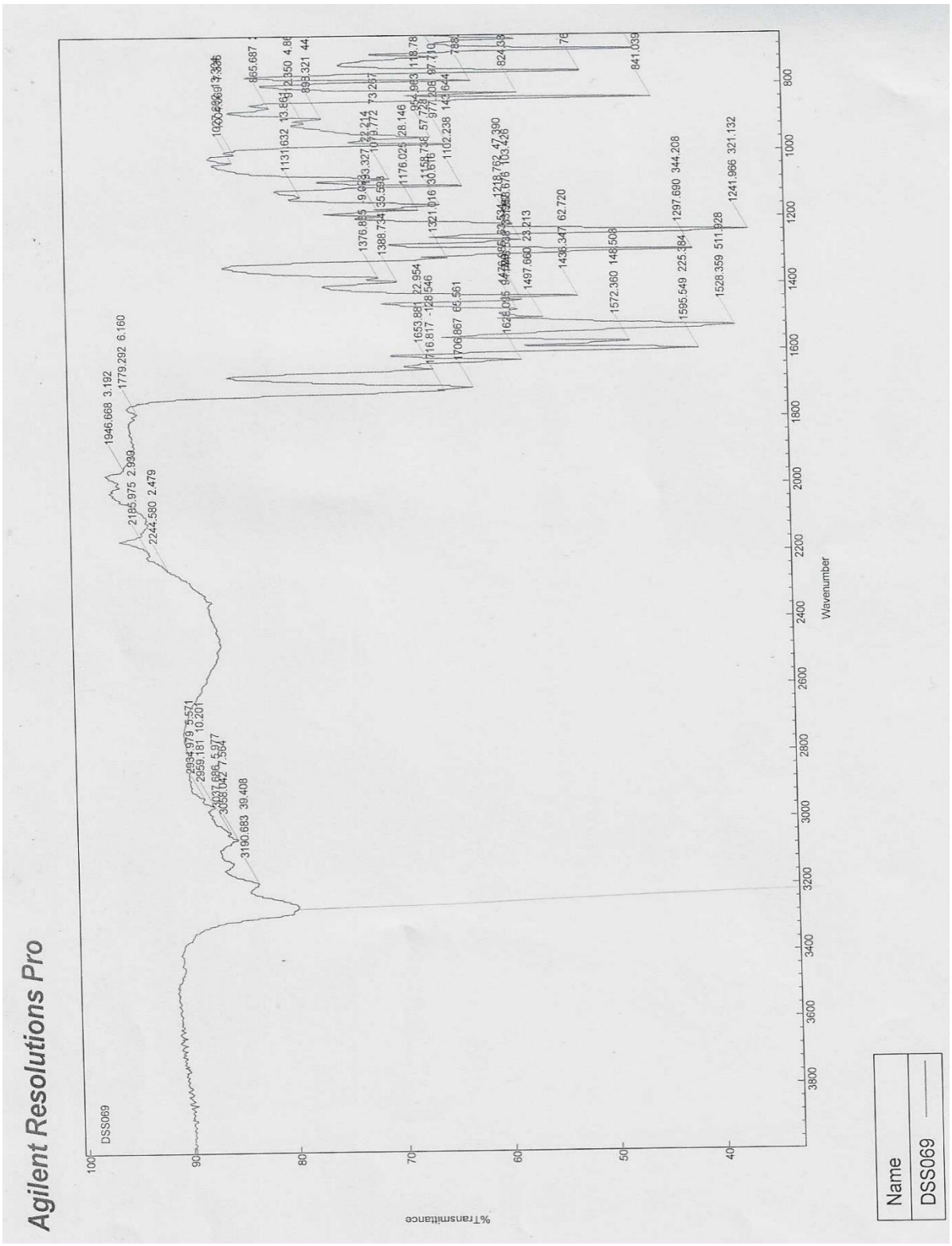
*4-((2-(methoxycarbonyl)-4-(methylselanyl)phenyl)amino)-4-oxobut-2-enoic acid (**11**)*



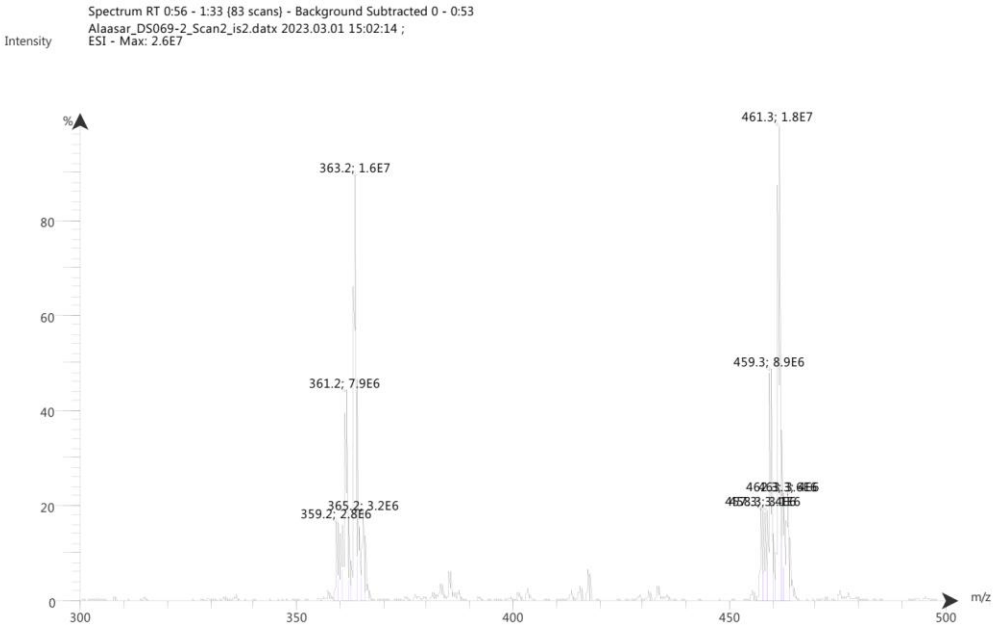
[1]HNMR chart of compound **11**



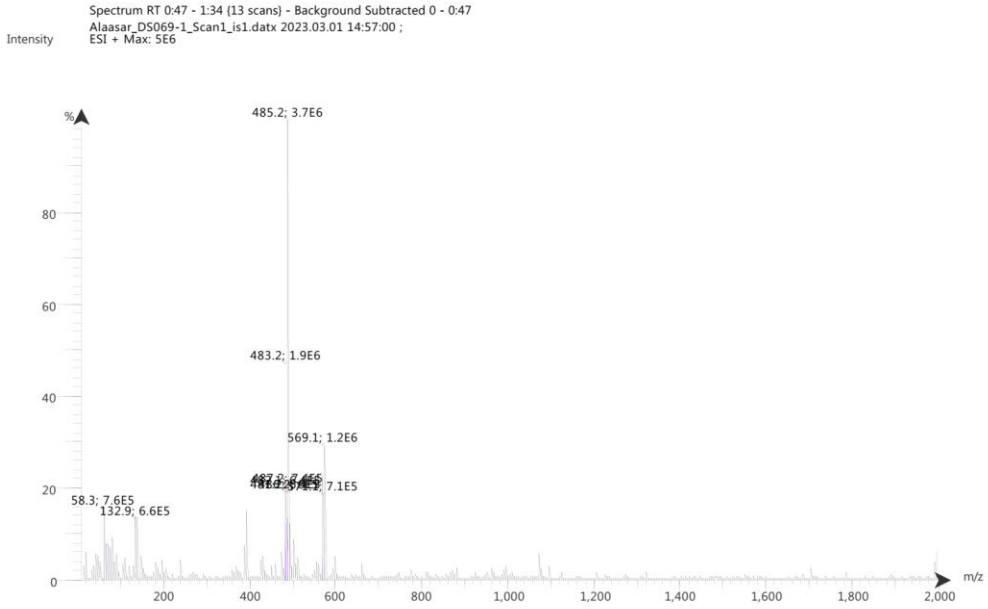
^{13}CNMR chart of compound **11**



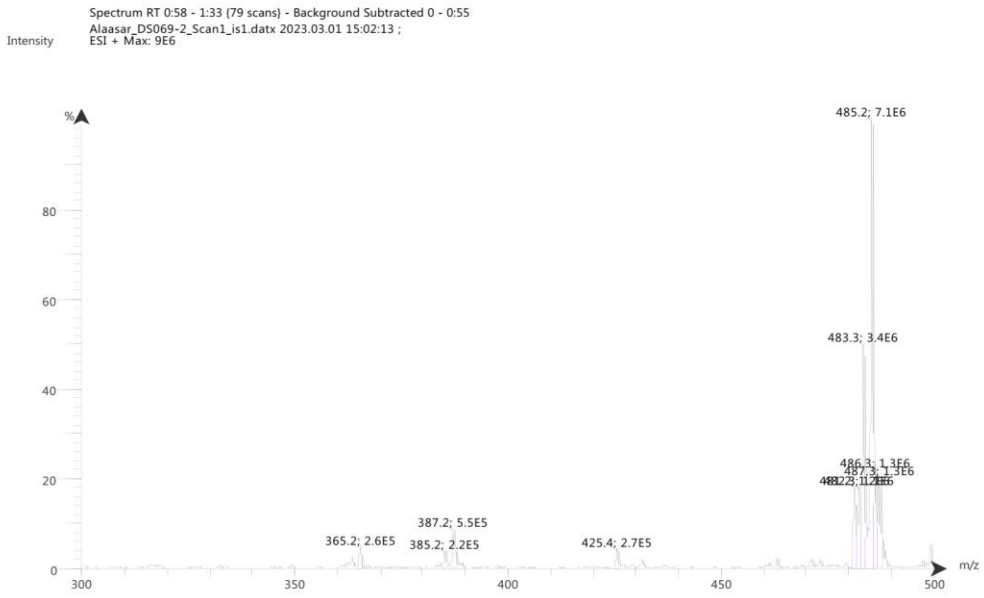
IR chart of compound **11**



MS chart of compound **11**

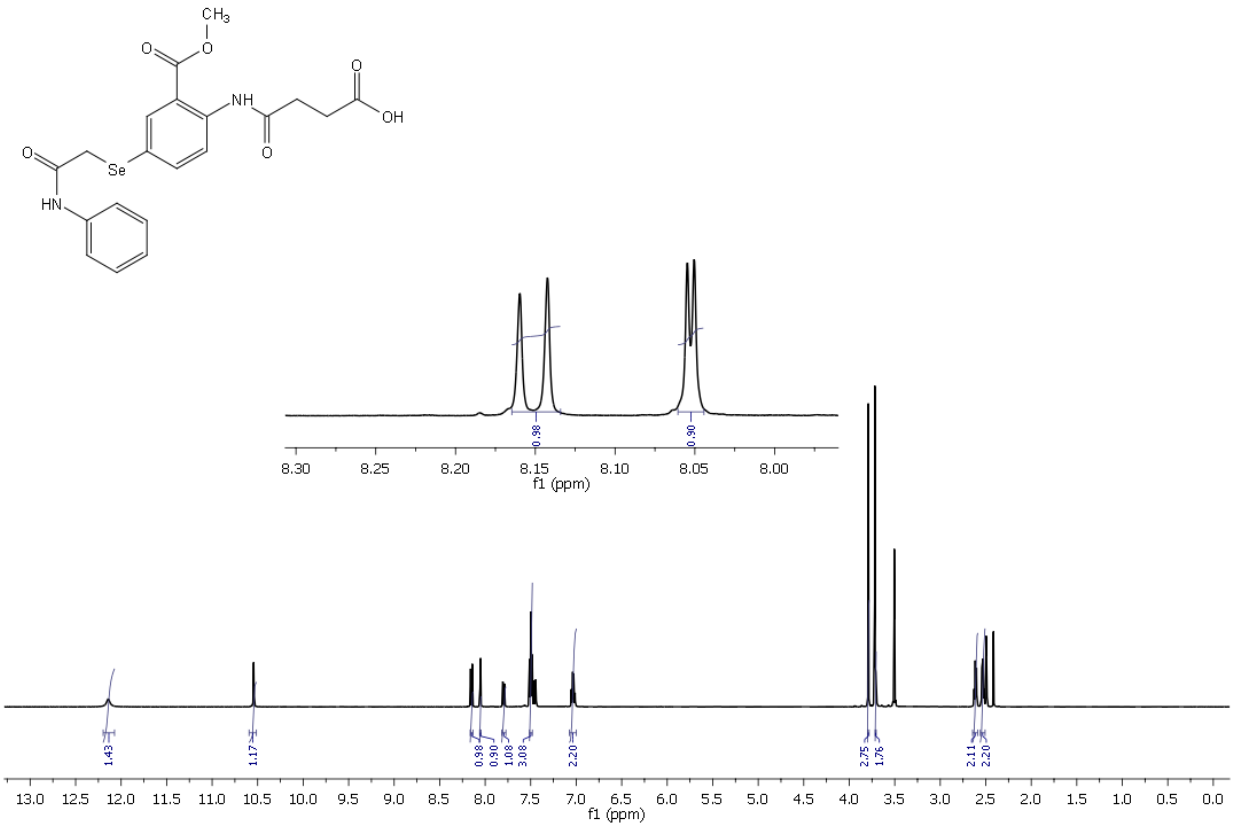


MS chart of compound **11**

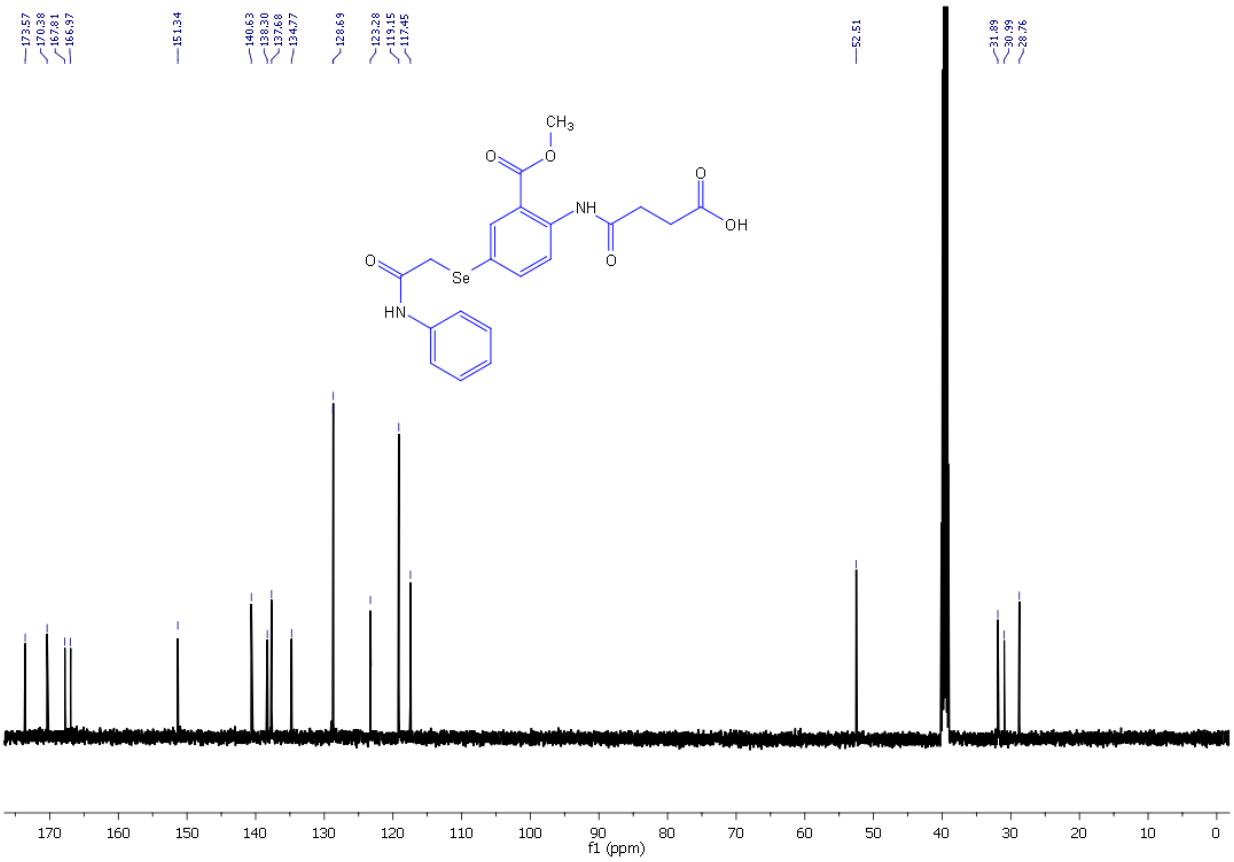


MS chart of compound **11**

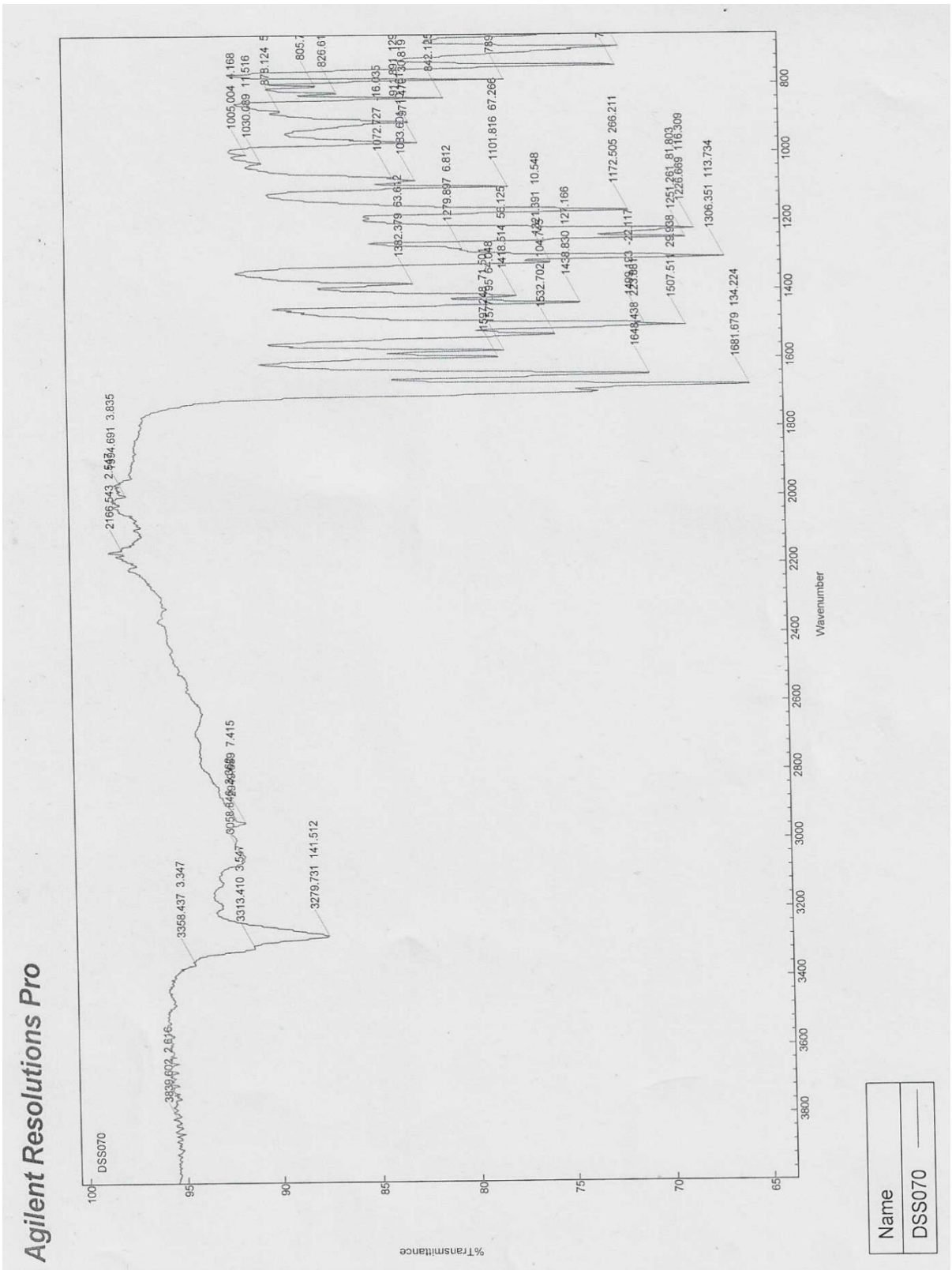
*4-((2-(methoxycarbonyl)-4-(methylselanyl)phenyl)amino)-4-oxobut-2-enoic acid (**12**)*



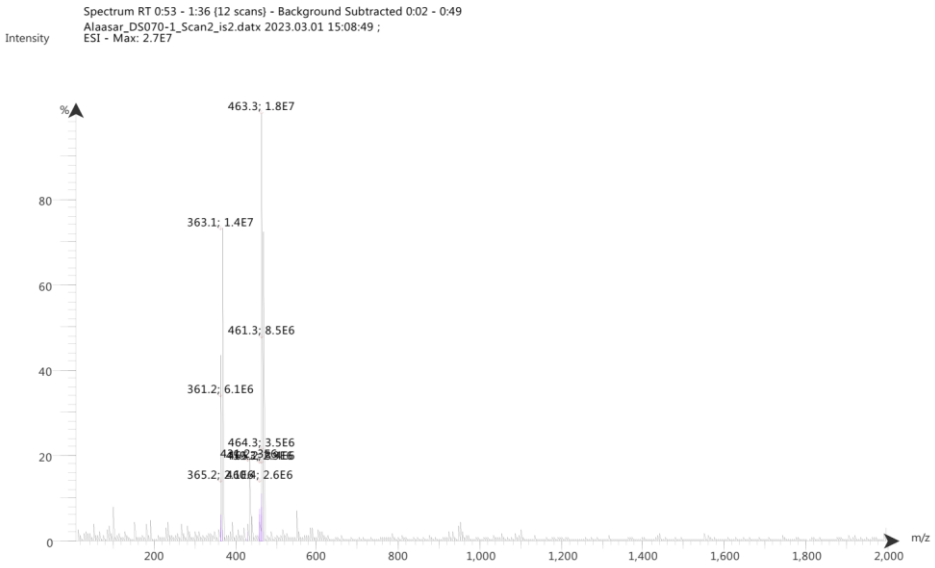
^{1}HNMR chart of compound **12**



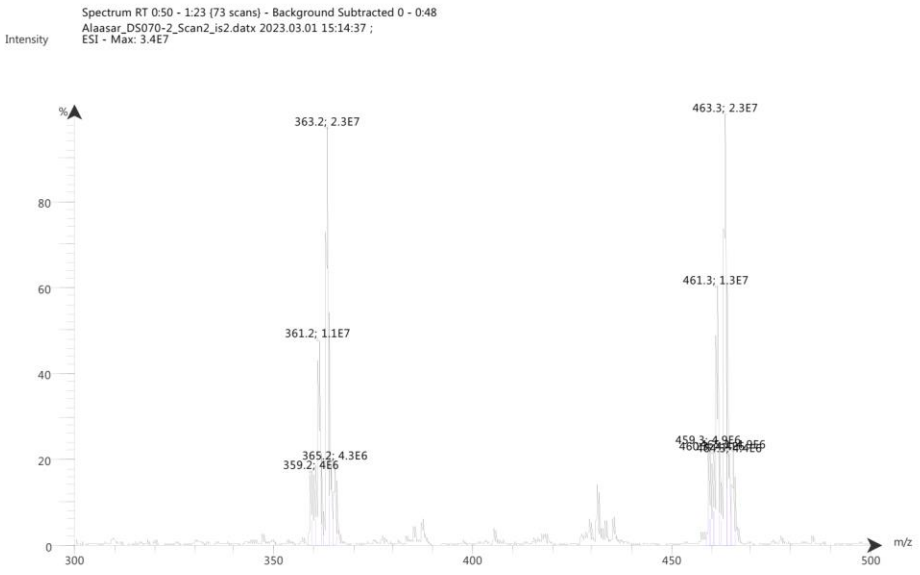
^{13}CNMR chart of compound **12**



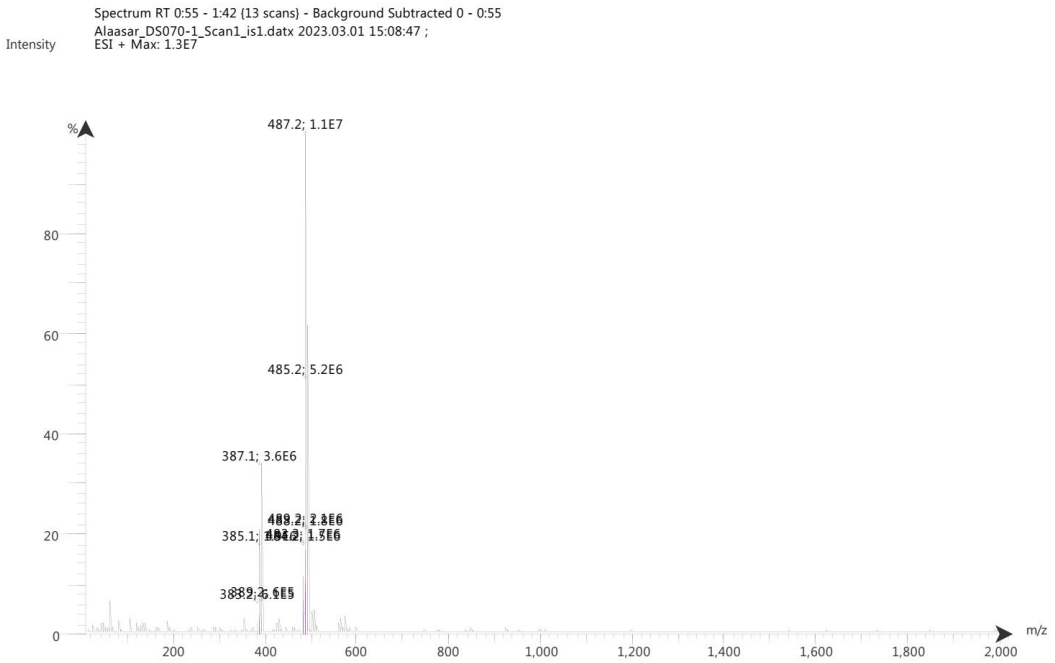
IR chart of compound **12**



MS chart of compound **12**



MS chart of compound **12**



MS chart of compound **12**

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compound 7
Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 2	/113. RY*(1) C 3	0.81	2.48	0.040
1. BD (1) C 1 - C 2	/114. RY*(2) C 3	0.66	1.95	0.032
1. BD (1) C 1 - C 2	/127. RY*(2) C 4	2.14	1.82	0.056
1. BD (1) C 1 - C 2	/256. RY*(1) N 13	0.90	1.52	0.033
1. BD (1) C 1 - C 2	/426. BD*(1) C 1 - C 3	4.27	1.27	0.066
1. BD (1) C 1 - C 2	/428. BD*(1) C 1 - N 13	0.57	1.02	0.022
1. BD (1) C 1 - C 2	/429. BD*(1) C 2 - C 4	2.92	1.31	0.055
1. BD (1) C 1 - C 2	/431. BD*(1) C 2 - H 23	0.61	1.10	0.023
1. BD (1) C 1 - C 2	/433. BD*(1) C 3 - C 7	4.39	1.07	0.062
1. BD (1) C 1 - C 2	/435. BD*(1) C 4 - H 24	2.81	1.10	0.050
1. BD (1) C 1 - C 2	/452. BD*(1) N 13 - H 32	1.59	1.00	0.036
2. BD (1) C 1 - C 3	/100. RY*(1) C 2	0.75	2.02	0.035
2. BD (1) C 1 - C 3	/139. RY*(1) C 5	0.55	1.87	0.029
2. BD (1) C 1 - C 3	/168. RY*(4) C 7	0.58	2.78	0.036
2. BD (1) C 1 - C 3	/256. RY*(1) N 13	0.69	1.62	0.030
2. BD (1) C 1 - C 3	/425. BD*(1) C 1 - C 2	3.49	1.20	0.058
2. BD (1) C 1 - C 3	/428. BD*(1) C 1 - N 13	2.09	1.12	0.043
2. BD (1) C 1 - C 3	/431. BD*(1) C 2 - H 23	1.30	1.20	0.035
2. BD (1) C 1 - C 3	/432. BD*(1) C 3 - C 5	4.24	1.20	0.064
2. BD (1) C 1 - C 3	/433. BD*(1) C 3 - C 7	2.93	1.17	0.053
2. BD (1) C 1 - C 3	/438. BD*(1) C 5 - H 25	1.31	1.21	0.036
2. BD (1) C 1 - C 3	/441. BD*(1) C 7 - O 9	1.16	1.26	0.034
2. BD (1) C 1 - C 3	/451. BD*(1) N 13 - C 14	2.09	1.11	0.044
3. BD (2) C 1 - C 3	/102. RY*(3) C 2	1.13	1.01	0.032
3. BD (2) C 1 - C 3	/141. RY*(3) C 5	0.86	0.86	0.026
3. BD (2) C 1 - C 3	/169. RY*(5) C 7	0.60	1.47	0.029
3. BD (2) C 1 - C 3	/430. BD*(2) C 2 - C 4	10.76	0.33	0.054
3. BD (2) C 1 - C 3	/437. BD*(2) C 5 - C 6	13.48	0.32	0.059
3. BD (2) C 1 - C 3	/440. BD*(1) C 7 - O 8	1.11	0.57	0.023
3. BD (2) C 1 - C 3	/442. BD*(2) C 7 - O 9	18.86	0.27	0.064
3. BD (2) C 1 - C 3	/451. BD*(1) N 13 - C 14	1.51	0.65	0.029
3. BD (2) C 1 - C 3	/452. BD*(1) N 13 - H 32	1.50	0.63	0.029
4. BD (1) C 1 - N 13	/100. RY*(1) C 2	0.53	2.06	0.030
4. BD (1) C 1 - N 13	/113. RY*(1) C 3	1.35	2.62	0.053
4. BD (1) C 1 - N 13	/269. RY*(1) C 14	1.52	1.68	0.045
4. BD (1) C 1 - N 13	/425. BD*(1) C 1 - C 2	0.64	1.24	0.025
4. BD (1) C 1 - N 13	/426. BD*(1) C 1 - C 3	2.16	1.41	0.049
4. BD (1) C 1 - N 13	/429. BD*(1) C 2 - C 4	0.86	1.45	0.031
4. BD (1) C 1 - N 13	/432. BD*(1) C 3 - C 5	2.68	1.24	0.052
4. BD (1) C 1 - N 13	/451. BD*(1) N 13 - C 14	0.86	1.15	0.029
4. BD (1) C 1 - N 13	/453. BD*(1) C 14 - C 15	1.69	1.22	0.041
5. BD (1) C 2 - C 4	/ 87. RY*(1) C 1	1.41	1.94	0.047
5. BD (1) C 2 - C 4	/ 89. RY*(3) C 1	0.92	2.00	0.039
5. BD (1) C 2 - C 4	/152. RY*(1) C 6	1.02	1.81	0.039
5. BD (1) C 2 - C 4	/425. BD*(1) C 1 - C 2	2.72	1.19	0.051

5.	BD (	1) C	2 - C	4	/428.	BD*(	1) C	1 - N	13	2.80	1.12	0.050
5.	BD (	1) C	2 - C	4	/431.	BD*(	1) C	2 - H	23	1.69	1.20	0.040
5.	BD (	1) C	2 - C	4	/434.	BD*(	1) C	4 - C	6	3.64	1.21	0.059
5.	BD (	1) C	2 - C	4	/435.	BD*(	1) C	4 - H	24	1.58	1.19	0.039
5.	BD (	1) C	2 - C	4	/439.	BD*(	1) C	6 -Se	11	3.11	0.88	0.047
6.	BD (	2) C	2 - C	4	/ 92.	RY*(	6) C	1		0.62	1.81	0.032
6.	BD (	2) C	2 - C	4	/427.	BD*(	2) C	1 - C	3	14.29	0.31	0.060
6.	BD (	2) C	2 - C	4	/437.	BD*(	2) C	5 - C	6	12.96	0.31	0.057
7.	BD (	1) C	2 - H	23	/ 87.	RY*(	1) C	1		0.64	1.71	0.030
7.	BD (	1) C	2 - H	23	/ 88.	RY*(	2) C	1		0.88	1.83	0.036
7.	BD (	1) C	2 - H	23	/126.	RY*(	1) C	4		1.44	1.68	0.044
7.	BD (	1) C	2 - H	23	/426.	BD*(	1) C	1 - C	3	3.22	1.14	0.054
7.	BD (	1) C	2 - H	23	/428.	BD*(	1) C	1 - N	13	0.61	0.89	0.021
7.	BD (	1) C	2 - H	23	/429.	BD*(	1) C	2 - C	4	1.59	1.18	0.039
7.	BD (	1) C	2 - H	23	/434.	BD*(	1) C	4 - C	6	5.69	0.98	0.067
7.	BD (	1) C	2 - H	23	/435.	BD*(	1) C	4 - H	24	0.95	0.96	0.027
8.	BD (	1) C	3 - C	5	/ 88.	RY*(	2) C	1		1.22	1.95	0.044
8.	BD (	1) C	3 - C	5	/153.	RY*(	2) C	6		1.32	1.47	0.040
8.	BD (	1) C	3 - C	5	/165.	RY*(	1) C	7		0.99	1.58	0.036
8.	BD (	1) C	3 - C	5	/426.	BD*(	1) C	1 - C	3	4.59	1.26	0.068
8.	BD (	1) C	3 - C	5	/428.	BD*(	1) C	1 - N	13	5.36	1.01	0.066
8.	BD (	1) C	3 - C	5	/433.	BD*(	1) C	3 - C	7	1.67	1.06	0.038
8.	BD (	1) C	3 - C	5	/436.	BD*(	1) C	5 - C	6	3.91	1.29	0.064
8.	BD (	1) C	3 - C	5	/438.	BD*(	1) C	5 - H	25	0.63	1.10	0.024
8.	BD (	1) C	3 - C	5	/439.	BD*(	1) C	6 -Se	11	5.50	0.78	0.058
8.	BD (	1) C	3 - C	5	/440.	BD*(	1) C	7 - O	8	2.84	0.92	0.046
8.	BD (	1) C	3 - C	5	/442.	BD*(	2) C	7 - O	9	0.55	0.63	0.017
9.	BD (	1) C	3 - C	7	/ 87.	RY*(	1) C	1		0.84	1.88	0.036
9.	BD (	1) C	3 - C	7	/ 88.	RY*(	2) C	1		1.04	2.00	0.041
9.	BD (	1) C	3 - C	7	/139.	RY*(	1) C	5		1.02	1.80	0.038
9.	BD (	1) C	3 - C	7	/191.	RY*(	1) O	9		0.72	1.81	0.032
9.	BD (	1) C	3 - C	7	/425.	BD*(	1) C	1 - C	2	3.77	1.13	0.058
9.	BD (	1) C	3 - C	7	/426.	BD*(	1) C	1 - C	3	3.96	1.30	0.064
9.	BD (	1) C	3 - C	7	/432.	BD*(	1) C	3 - C	5	1.28	1.13	0.034
9.	BD (	1) C	3 - C	7	/436.	BD*(	1) C	5 - C	6	1.47	1.33	0.040
9.	BD (	1) C	3 - C	7	/441.	BD*(	1) C	7 - O	9	0.95	1.19	0.030
9.	BD (	1) C	3 - C	7	/443.	BD*(	1) O	8 - C	10	2.85	0.96	0.047
10.	BD (	1) C	4 - C	6	/100.	RY*(	1) C	2		0.75	1.93	0.034
10.	BD (	1) C	4 - C	6	/101.	RY*(	2) C	2		1.59	2.01	0.051
10.	BD (	1) C	4 - C	6	/139.	RY*(	1) C	5		0.92	1.79	0.036
10.	BD (	1) C	4 - C	6	/140.	RY*(	2) C	5		0.86	1.61	0.033
10.	BD (	1) C	4 - C	6	/429.	BD*(	1) C	2 - C	4	3.19	1.32	0.058
10.	BD (	1) C	4 - C	6	/431.	BD*(	1) C	2 - H	23	2.66	1.12	0.049
10.	BD (	1) C	4 - C	6	/435.	BD*(	1) C	4 - H	24	0.87	1.11	0.028
10.	BD (	1) C	4 - C	6	/436.	BD*(	1) C	5 - C	6	3.48	1.32	0.060
10.	BD (	1) C	4 - C	6	/438.	BD*(	1) C	5 - H	25	3.43	1.12	0.055
11.	BD (	1) C	4 - H	24	/100.	RY*(	1) C	2		1.53	1.79	0.047
11.	BD (	1) C	4 - H	24	/152.	RY*(	1) C	6		1.14	1.59	0.038
11.	BD (	1) C	4 - H	24	/425.	BD*(	1) C	1 - C	2	5.69	0.97	0.066
11.	BD (	1) C	4 - H	24	/429.	BD*(	1) C	2 - C	4	1.50	1.18	0.038
11.	BD (	1) C	4 - H	24	/431.	BD*(	1) C	2 - H	23	0.96	0.97	0.027
11.	BD (	1) C	4 - H	24	/436.	BD*(	1) C	5 - C	6	3.19	1.17	0.055
12.	BD (	1) C	5 - C	6	/113.	RY*(	1) C	3		1.43	2.59	0.055
12.	BD (	1) C	5 - C	6	/114.	RY*(	2) C	3		0.71	2.05	0.034
12.	BD (	1) C	5 - C	6	/126.	RY*(	1) C	4		1.05	1.92	0.040

12. BD (1) C 5 - C 6	/432. BD*(1) C 3 - C 5	3.31	1.21	0.057
12. BD (1) C 5 - C 6	/433. BD*(1) C 3 - C 7	2.02	1.18	0.044
12. BD (1) C 5 - C 6	/434. BD*(1) C 4 - C 6	3.12	1.23	0.055
12. BD (1) C 5 - C 6	/435. BD*(1) C 4 - H 24	1.64	1.21	0.040
12. BD (1) C 5 - C 6	/438. BD*(1) C 5 - H 25	2.32	1.22	0.047
13. BD (2) C 5 - C 6	/116. RY*(4) C 3	0.59	1.06	0.024
13. BD (2) C 5 - C 6	/128. RY*(3) C 4	1.69	1.12	0.041
13. BD (2) C 5 - C 6	/217. RY*(1)Se 11	0.99	0.77	0.026
13. BD (2) C 5 - C 6	/427. BD*(2) C 1 - C 3	11.95	0.31	0.056
13. BD (2) C 5 - C 6	/430. BD*(2) C 2 - C 4	13.06	0.32	0.059
14. BD (1) C 5 - H 25	/113. RY*(1) C 3	1.80	2.35	0.058
14. BD (1) C 5 - H 25	/152. RY*(1) C 6	1.74	1.58	0.047
14. BD (1) C 5 - H 25	/426. BD*(1) C 1 - C 3	3.09	1.14	0.053
14. BD (1) C 5 - H 25	/434. BD*(1) C 4 - C 6	5.98	0.98	0.069
14. BD (1) C 5 - H 25	/436. BD*(1) C 5 - C 6	2.17	1.17	0.045
15. BD (1) C 6 -Se 11	/126. RY*(1) C 4	1.99	1.74	0.053
15. BD (1) C 6 -Se 11	/139. RY*(1) C 5	1.60	1.70	0.047
15. BD (1) C 6 -Se 11	/243. RY*(1) C 12	0.59	1.58	0.027
15. BD (1) C 6 -Se 11	/429. BD*(1) C 2 - C 4	2.65	1.24	0.051
15. BD (1) C 6 -Se 11	/432. BD*(1) C 3 - C 5	5.23	1.03	0.066
15. BD (1) C 6 -Se 11	/436. BD*(1) C 5 - C 6	0.95	1.23	0.031
15. BD (1) C 6 -Se 11	/438. BD*(1) C 5 - H 25	0.95	1.04	0.028
15. BD (1) C 6 -Se 11	/447. BD*(1)Se 11 - C 12	0.51	0.69	0.017
15. BD (1) C 6 -Se 11	/449. BD*(1) C 12 - H 30	0.94	0.97	0.027
16. BD (1) C 7 - O 8	/114. RY*(2) C 3	1.04	2.16	0.042
16. BD (1) C 7 - O 8	/206. RY*(3) C 10	1.07	1.84	0.040
16. BD (1) C 7 - O 8	/432. BD*(1) C 3 - C 5	1.27	1.31	0.037
16. BD (1) C 7 - O 8	/446. BD*(1) C 10 - H 28	0.66	1.24	0.025
17. BD (1) C 7 - O 9	/114. RY*(2) C 3	1.32	2.29	0.049
17. BD (1) C 7 - O 9	/165. RY*(1) C 7	1.64	1.94	0.050
17. BD (1) C 7 - O 9	/426. BD*(1) C 1 - C 3	1.54	1.62	0.045
17. BD (1) C 7 - O 9	/433. BD*(1) C 3 - C 7	1.77	1.42	0.045
18. BD (2) C 7 - O 9	/427. BD*(2) C 1 - C 3	4.53	0.40	0.041
18. BD (2) C 7 - O 9	/442. BD*(2) C 7 - O 9	0.65	0.36	0.014
19. BD (1) O 8 - C 10	/165. RY*(1) C 7	1.27	1.77	0.042
19. BD (1) O 8 - C 10	/433. BD*(1) C 3 - C 7	2.61	1.26	0.052
20. BD (1) C 10 - H 26	/179. RY*(2) O 8	0.58	1.51	0.026
20. BD (1) C 10 - H 26	/443. BD*(1) O 8 - C 10	0.58	0.79	0.019
21. BD (1) C 10 - H 27	/179. RY*(2) O 8	0.53	1.51	0.025
22. BD (1) C 10 - H 28	/440. BD*(1) C 7 - O 8	3.93	0.80	0.051
23. BD (1)Se 11 - C 12	/152. RY*(1) C 6	0.64	1.63	0.029
23. BD (1)Se 11 - C 12	/434. BD*(1) C 4 - C 6	1.79	1.03	0.038
23. BD (1)Se 11 - C 12	/437. BD*(2) C 5 - C 6	0.81	0.60	0.021
25. BD (1) C 12 - H 30	/439. BD*(1) C 6 -Se 11	1.01	0.65	0.023
27. BD (1) N 13 - C 14	/ 87. RY*(1) C 1	0.74	1.99	0.034
27. BD (1) N 13 - C 14	/ 88. RY*(2) C 1	0.77	2.10	0.036
27. BD (1) N 13 - C 14	/283. RY*(2) C 15	1.00	1.89	0.039
27. BD (1) N 13 - C 14	/426. BD*(1) C 1 - C 3	1.62	1.41	0.043
27. BD (1) N 13 - C 14	/428. BD*(1) C 1 - N 13	1.06	1.16	0.031
27. BD (1) N 13 - C 14	/456. BD*(1) C 15 - C 17	1.10	1.42	0.035
28. BD (1) N 13 - H 32	/ 87. RY*(1) C 1	1.08	1.85	0.040
28. BD (1) N 13 - H 32	/270. RY*(2) C 14	0.83	2.04	0.037
28. BD (1) N 13 - H 32	/272. RY*(4) C 14	0.92	3.07	0.048
28. BD (1) N 13 - H 32	/425. BD*(1) C 1 - C 2	2.10	1.10	0.043
28. BD (1) N 13 - H 32	/427. BD*(2) C 1 - C 3	1.54	0.69	0.031

28. BD (1) N 13 - H 32	/454. BD*(1) C 14 - O 16	2.95	1.18	0.053
29. BD (1) C 14 - C 15	/257. RY*(2) N 13	1.35	1.77	0.044
29. BD (1) C 14 - C 15	/295. RY*(1) O 16	0.63	1.86	0.031
29. BD (1) C 14 - C 15	/308. RY*(1) C 17	2.27	1.82	0.058
29. BD (1) C 14 - C 15	/428. BD*(1) C 1 - N 13	2.92	1.07	0.050
29. BD (1) C 14 - C 15	/454. BD*(1) C 14 - O 16	0.96	1.21	0.031
29. BD (1) C 14 - C 15	/456. BD*(1) C 15 - C 17	2.75	1.32	0.054
29. BD (1) C 14 - C 15	/459. BD*(1) C 17 - C 18	3.42	1.11	0.055
30. BD (1) C 14 - O 16	/269. RY*(1) C 14	1.66	1.88	0.050
30. BD (1) C 14 - O 16	/451. BD*(1) N 13 - C 14	0.54	1.36	0.025
30. BD (1) C 14 - O 16	/452. BD*(1) N 13 - H 32	1.15	1.34	0.035
30. BD (1) C 14 - O 16	/453. BD*(1) C 14 - C 15	1.56	1.43	0.043
30. BD (1) C 14 - O 16	/458. BD*(1) C 15 - H 21	0.86	1.42	0.031
31. BD (2) C 14 - O 16	/285. RY*(4) C 15	0.64	1.03	0.023
31. BD (2) C 14 - O 16	/455. BD*(2) C 14 - O 16	0.75	0.35	0.016
31. BD (2) C 14 - O 16	/457. BD*(2) C 15 - C 17	5.17	0.38	0.040
32. BD (1) C 15 - C 17	/269. RY*(1) C 14	2.16	1.66	0.053
32. BD (1) C 15 - C 17	/321. RY*(1) C 18	2.20	1.66	0.054
32. BD (1) C 15 - C 17	/451. BD*(1) N 13 - C 14	2.46	1.14	0.048
32. BD (1) C 15 - C 17	/453. BD*(1) C 14 - C 15	2.35	1.20	0.048
32. BD (1) C 15 - C 17	/458. BD*(1) C 15 - H 21	1.64	1.20	0.040
32. BD (1) C 15 - C 17	/459. BD*(1) C 17 - C 18	2.01	1.19	0.044
32. BD (1) C 15 - C 17	/460. BD*(1) C 17 - H 22	1.69	1.21	0.040
32. BD (1) C 15 - C 17	/461. BD*(1) C 18 - O 19	2.33	1.06	0.045
33. BD (2) C 15 - C 17	/273. RY*(5) C 14	0.76	1.57	0.032
33. BD (2) C 15 - C 17	/325. RY*(5) C 18	0.96	1.63	0.037
33. BD (2) C 15 - C 17	/455. BD*(2) C 14 - O 16	17.55	0.29	0.066
33. BD (2) C 15 - C 17	/463. BD*(2) C 18 - O 20	19.28	0.28	0.067
34. BD (1) C 15 - H 21	/270. RY*(2) C 14	0.64	1.93	0.031
34. BD (1) C 15 - H 21	/272. RY*(4) C 14	0.73	2.96	0.042
34. BD (1) C 15 - H 21	/308. RY*(1) C 17	1.01	1.67	0.037
34. BD (1) C 15 - H 21	/309. RY*(2) C 17	0.64	1.60	0.029
34. BD (1) C 15 - H 21	/454. BD*(1) C 14 - O 16	3.45	1.06	0.054
34. BD (1) C 15 - H 21	/456. BD*(1) C 15 - C 17	1.48	1.17	0.037
34. BD (1) C 15 - H 21	/460. BD*(1) C 17 - H 22	4.53	0.98	0.059
35. BD (1) C 17 - C 18	/282. RY*(1) C 15	2.14	1.74	0.055
35. BD (1) C 17 - C 18	/347. RY*(1) O 20	0.75	1.78	0.033
35. BD (1) C 17 - C 18	/453. BD*(1) C 14 - C 15	3.38	1.13	0.056
35. BD (1) C 17 - C 18	/456. BD*(1) C 15 - C 17	2.34	1.33	0.050
35. BD (1) C 17 - C 18	/462. BD*(1) C 18 - O 20	0.75	1.22	0.027
35. BD (1) C 17 - C 18	/464. BD*(1) O 19 - H 33	1.70	1.01	0.037
36. BD (1) C 17 - H 22	/282. RY*(1) C 15	1.05	1.57	0.036
36. BD (1) C 17 - H 22	/283. RY*(2) C 15	0.66	1.63	0.029
36. BD (1) C 17 - H 22	/324. RY*(4) C 18	0.69	2.81	0.040
36. BD (1) C 17 - H 22	/456. BD*(1) C 15 - C 17	1.67	1.16	0.039
36. BD (1) C 17 - H 22	/458. BD*(1) C 15 - H 21	4.95	0.96	0.062
36. BD (1) C 17 - H 22	/461. BD*(1) C 18 - O 19	0.50	0.82	0.018
36. BD (1) C 17 - H 22	/462. BD*(1) C 18 - O 20	3.24	1.05	0.052
37. BD (1) C 18 - O 19	/309. RY*(2) C 17	0.72	1.97	0.034
37. BD (1) C 18 - O 19	/456. BD*(1) C 15 - C 17	1.02	1.53	0.035
38. BD (1) C 18 - O 20	/309. RY*(2) C 17	0.58	2.06	0.031
38. BD (1) C 18 - O 20	/321. RY*(1) C 18	1.59	1.90	0.049
38. BD (1) C 18 - O 20	/459. BD*(1) C 17 - C 18	1.40	1.42	0.040
38. BD (1) C 18 - O 20	/460. BD*(1) C 17 - H 22	0.88	1.44	0.032
39. BD (2) C 18 - O 20	/311. RY*(4) C 17	0.64	0.96	0.022

39. BD (2) C 18 - O 20	/457. BD*(2) C 15 - C 17	5.11	0.39	0.040
39. BD (2) C 18 - O 20	/463. BD*(2) C 18 - O 20	0.73	0.35	0.015
40. BD (1) O 19 - H 33	/321. RY*(1) C 18	0.95	1.62	0.035
40. BD (1) O 19 - H 33	/322. RY*(2) C 18	0.73	2.05	0.035
40. BD (1) O 19 - H 33	/327. RY*(7) C 18	0.69	2.04	0.034
40. BD (1) O 19 - H 33	/459. BD*(1) C 17 - C 18	3.64	1.15	0.058
40. BD (1) O 19 - H 33	/462. BD*(1) C 18 - O 20	1.29	1.24	0.036
41. CR (1) C 1	/101. RY*(2) C 2	0.95	11.45	0.093
41. CR (1) C 1	/113. RY*(1) C 3	0.51	11.94	0.070
41. CR (1) C 1	/114. RY*(2) C 3	1.71	11.41	0.125
41. CR (1) C 1	/426. BD*(1) C 1 - C 3	1.37	10.73	0.109
41. CR (1) C 1	/429. BD*(1) C 2 - C 4	0.57	10.77	0.070
41. CR (1) C 1	/432. BD*(1) C 3 - C 5	1.03	10.56	0.094
41. CR (1) C 1	/433. BD*(1) C 3 - C 7	1.11	10.53	0.098
41. CR (1) C 1	/451. BD*(1) N 13 - C 14	1.03	10.47	0.094
42. CR (1) C 2	/ 88. RY*(2) C 1	1.36	11.36	0.111
42. CR (1) C 2	/126. RY*(1) C 4	0.59	11.21	0.073
42. CR (1) C 2	/127. RY*(2) C 4	1.74	11.21	0.125
42. CR (1) C 2	/426. BD*(1) C 1 - C 3	0.83	10.67	0.085
42. CR (1) C 2	/428. BD*(1) C 1 - N 13	0.54	10.42	0.067
42. CR (1) C 2	/429. BD*(1) C 2 - C 4	0.83	10.70	0.084
42. CR (1) C 2	/434. BD*(1) C 4 - C 6	1.31	10.51	0.105
43. CR (1) C 3	/ 87. RY*(1) C 1	1.15	11.27	0.102
43. CR (1) C 3	/ 89. RY*(3) C 1	1.00	11.32	0.095
43. CR (1) C 3	/140. RY*(2) C 5	0.69	11.02	0.078
43. CR (1) C 3	/166. RY*(2) C 7	0.60	11.51	0.074
43. CR (1) C 3	/171. RY*(7) C 7	0.84	11.19	0.086
43. CR (1) C 3	/425. BD*(1) C 1 - C 2	1.09	10.52	0.096
43. CR (1) C 3	/426. BD*(1) C 1 - C 3	1.23	10.69	0.103
43. CR (1) C 3	/428. BD*(1) C 1 - N 13	1.03	10.44	0.093
43. CR (1) C 3	/436. BD*(1) C 5 - C 6	0.72	10.72	0.079
43. CR (1) C 3	/440. BD*(1) C 7 - O 8	0.61	10.35	0.073
44. CR (1) C 4	/101. RY*(2) C 2	1.34	11.39	0.110
44. CR (1) C 4	/103. RY*(4) C 2	0.66	11.07	0.076
44. CR (1) C 4	/153. RY*(2) C 6	1.13	10.87	0.099
44. CR (1) C 4	/155. RY*(4) C 6	0.75	11.11	0.081
44. CR (1) C 4	/425. BD*(1) C 1 - C 2	1.21	10.49	0.101
44. CR (1) C 4	/429. BD*(1) C 2 - C 4	0.67	10.70	0.076
44. CR (1) C 4	/436. BD*(1) C 5 - C 6	0.82	10.69	0.084
44. CR (1) C 4	/439. BD*(1) C 6 -Se 11	0.81	10.18	0.082
45. CR (1) C 5	/114. RY*(2) C 3	0.77	11.34	0.083
45. CR (1) C 5	/152. RY*(1) C 6	0.98	11.11	0.093
45. CR (1) C 5	/153. RY*(2) C 6	1.93	10.87	0.130
45. CR (1) C 5	/154. RY*(3) C 6	0.66	10.94	0.076
45. CR (1) C 5	/426. BD*(1) C 1 - C 3	0.76	10.66	0.081
45. CR (1) C 5	/433. BD*(1) C 3 - C 7	0.65	10.46	0.075
45. CR (1) C 5	/434. BD*(1) C 4 - C 6	1.23	10.51	0.102
45. CR (1) C 5	/436. BD*(1) C 5 - C 6	1.20	10.70	0.102
45. CR (1) C 5	/439. BD*(1) C 6 -Se 11	1.24	10.18	0.101
46. CR (1) C 6	/127. RY*(2) C 4	1.04	11.25	0.096
46. CR (1) C 6	/129. RY*(4) C 4	0.50	11.05	0.066
46. CR (1) C 6	/140. RY*(2) C 5	2.16	11.03	0.138
46. CR (1) C 6	/142. RY*(4) C 5	0.62	11.15	0.074
46. CR (1) C 6	/429. BD*(1) C 2 - C 4	0.63	10.74	0.073
46. CR (1) C 6	/432. BD*(1) C 3 - C 5	1.17	10.53	0.100

46. CR (1) C 6	/436. BD*(1) C 5 - C 6	1.22	10.73	0.103
46. CR (1) C 6	/438. BD*(1) C 5 - H 25	0.56	10.54	0.069
46. CR (1) C 6	/439. BD*(1) C 6 -Se 11	1.35	10.22	0.105
47. CR (1) C 7	/113. RY*(1) C 3	1.20	12.04	0.107
47. CR (1) C 7	/426. BD*(1) C 1 - C 3	0.87	10.83	0.087
47. CR (1) C 7	/432. BD*(1) C 3 - C 5	0.54	10.66	0.068
47. CR (1) C 7	/433. BD*(1) C 3 - C 7	0.56	10.63	0.069
47. CR (1) C 7	/440. BD*(1) C 7 - O 8	0.67	10.49	0.077
47. CR (1) C 7	/443. BD*(1) O 8 - C 10	1.11	10.48	0.096
48. CR (1) O 8	/165. RY*(1) C 7	1.01	19.92	0.127
48. CR (1) O 8	/166. RY*(2) C 7	1.11	20.42	0.135
48. CR (1) O 8	/206. RY*(3) C 10	0.91	19.96	0.121
49. CR (1) O 9	/165. RY*(1) C 7	5.27	19.81	0.290
49. CR (1) O 9	/433. BD*(1) C 3 - C 7	0.78	19.29	0.111
50. CR (1) C 10	/396. RY*(2) H 28	0.60	12.19	0.076
50. CR (1) C 10	/440. BD*(1) C 7 - O 8	1.10	10.40	0.098
50. CR (1) C 10	/443. BD*(1) O 8 - C 10	1.49	10.39	0.111
53. CR (3)Se 11	/152. RY*(1) C 6	1.00	11.34	0.095
53. CR (3)Se 11	/246. RY*(4) C 12	0.60	11.19	0.073
53. CR (3)Se 11	/434. BD*(1) C 4 - C 6	0.74	10.74	0.080
53. CR (3)Se 11	/436. BD*(1) C 5 - C 6	1.24	10.92	0.105
65. CR (1) C 12	/447. BD*(1)Se 11 - C 12	1.46	10.19	0.109
66. CR (1) N 13	/ 87. RY*(1) C 1	1.11	15.41	0.117
66. CR (1) N 13	/ 88. RY*(2) C 1	0.54	15.52	0.082
66. CR (1) N 13	/270. RY*(2) C 14	1.43	15.60	0.133
66. CR (1) N 13	/426. BD*(1) C 1 - C 3	0.59	14.83	0.084
67. CR (1) C 14	/283. RY*(2) C 15	0.56	11.28	0.071
67. CR (1) C 14	/428. BD*(1) C 1 - N 13	1.14	10.56	0.099
67. CR (1) C 14	/456. BD*(1) C 15 - C 17	0.65	10.81	0.075
68. CR (1) C 15	/270. RY*(2) C 14	1.07	11.46	0.099
68. CR (1) C 15	/309. RY*(2) C 17	1.86	11.14	0.129
68. CR (1) C 15	/310. RY*(3) C 17	0.53	11.25	0.069
68. CR (1) C 15	/451. BD*(1) N 13 - C 14	0.51	10.44	0.067
68. CR (1) C 15	/456. BD*(1) C 15 - C 17	0.66	10.70	0.075
68. CR (1) C 15	/459. BD*(1) C 17 - C 18	1.06	10.50	0.095
69. CR (1) O 16	/269. RY*(1) C 14	5.52	19.74	0.296
69. CR (1) O 16	/453. BD*(1) C 14 - C 15	0.75	19.28	0.109
70. CR (1) C 17	/283. RY*(2) C 15	1.59	11.17	0.119
70. CR (1) C 17	/284. RY*(3) C 15	0.70	11.38	0.080
70. CR (1) C 17	/322. RY*(2) C 18	0.78	11.39	0.084
70. CR (1) C 17	/327. RY*(7) C 18	0.58	11.39	0.073
70. CR (1) C 17	/453. BD*(1) C 14 - C 15	1.08	10.50	0.096
70. CR (1) C 17	/456. BD*(1) C 15 - C 17	0.72	10.70	0.079
70. CR (1) C 17	/458. BD*(1) C 15 - H 21	0.53	10.50	0.067
71. CR (1) C 18	/309. RY*(2) C 17	0.55	11.28	0.071
71. CR (1) C 18	/456. BD*(1) C 15 - C 17	0.63	10.84	0.074
71. CR (1) C 18	/461. BD*(1) C 18 - O 19	0.63	10.51	0.075
72. CR (1) O 19	/321. RY*(1) C 18	0.80	19.88	0.113
72. CR (1) O 19	/322. RY*(2) C 18	1.53	20.30	0.158
72. CR (1) O 19	/324. RY*(4) C 18	0.63	21.26	0.104
72. CR (1) O 19	/423. RY*(4) H 33	0.56	20.96	0.097
73. CR (1) O 20	/321. RY*(1) C 18	5.57	19.77	0.298
73. CR (1) O 20	/459. BD*(1) C 17 - C 18	0.75	19.29	0.109
74. LP (1) O 8	/165. RY*(1) C 7	1.66	1.51	0.045
74. LP (1) O 8	/168. RY*(4) C 7	1.61	2.60	0.058

74. LP (1) O 8	/204. RY*(1) C 10	1.64	1.65	0.047
74. LP (1) O 8	/206. RY*(3) C 10	0.79	1.55	0.032
74. LP (1) O 8	/441. BD*(1) C 7 - O 9	5.70	1.08	0.070
74. LP (1) O 8	/445. BD*(1) C 10 - H 27	0.63	0.95	0.022
74. LP (1) O 8	/446. BD*(1) C 10 - H 28	2.37	0.95	0.043
75. LP (2) O 8	/167. RY*(3) C 7	1.80	1.84	0.054
75. LP (2) O 8	/205. RY*(2) C 10	1.51	1.51	0.045
75. LP (2) O 8	/442. BD*(2) C 7 - O 9	38.58	0.31	0.100
75. LP (2) O 8	/444. BD*(1) C 10 - H 26	5.04	0.70	0.055
75. LP (2) O 8	/445. BD*(1) C 10 - H 27	5.05	0.70	0.056
76. LP (1) O 9	/165. RY*(1) C 7	12.34	1.64	0.127
76. LP (1) O 9	/175. RY*(11) C 7	0.76	4.78	0.054
76. LP (1) O 9	/433. BD*(1) C 3 - C 7	2.24	1.13	0.045
76. LP (1) O 9	/440. BD*(1) C 7 - O 8	0.99	0.99	0.029
77. LP (2) O 9	/166. RY*(2) C 7	1.93	1.70	0.053
77. LP (2) O 9	/168. RY*(4) C 7	1.71	2.29	0.058
77. LP (2) O 9	/433. BD*(1) C 3 - C 7	12.43	0.68	0.084
77. LP (2) O 9	/440. BD*(1) C 7 - O 8	28.85	0.55	0.113
77. LP (2) O 9	/446. BD*(1) C 10 - H 28	0.80	0.64	0.021
78. LP (1)Se 11	/152. RY*(1) C 6	1.18	1.76	0.041
78. LP (1)Se 11	/436. BD*(1) C 5 - C 6	3.35	1.34	0.060
79. LP (2)Se 11	/434. BD*(1) C 4 - C 6	1.55	0.69	0.030
79. LP (2)Se 11	/436. BD*(1) C 5 - C 6	1.05	0.87	0.028
79. LP (2)Se 11	/437. BD*(2) C 5 - C 6	9.55	0.26	0.046
79. LP (2)Se 11	/448. BD*(1) C 12 - H 29	2.48	0.61	0.036
79. LP (2)Se 11	/450. BD*(1) C 12 - H 31	4.10	0.61	0.046
80. LP (1) N 13	/ 89. RY*(3) C 1	1.10	1.52	0.040
80. LP (1) N 13	/ 90. RY*(4) C 1	0.73	1.59	0.033
80. LP (1) N 13	/271. RY*(3) C 14	1.60	1.73	0.051
80. LP (1) N 13	/416. RY*(2) H 32	0.75	1.95	0.037
80. LP (1) N 13	/425. BD*(1) C 1 - C 2	3.68	0.71	0.049
80. LP (1) N 13	/426. BD*(1) C 1 - C 3	2.74	0.89	0.047
80. LP (1) N 13	/427. BD*(2) C 1 - C 3	17.38	0.30	0.064
80. LP (1) N 13	/455. BD*(2) C 14 - O 16	50.75	0.26	0.102
81. LP (1) O 16	/269. RY*(1) C 14	13.16	1.58	0.129
81. LP (1) O 16	/451. BD*(1) N 13 - C 14	1.20	1.06	0.032
81. LP (1) O 16	/453. BD*(1) C 14 - C 15	2.17	1.13	0.044
82. LP (2) O 16	/270. RY*(2) C 14	1.39	1.64	0.044
82. LP (2) O 16	/272. RY*(4) C 14	1.82	2.67	0.064
82. LP (2) O 16	/451. BD*(1) N 13 - C 14	23.94	0.62	0.110
82. LP (2) O 16	/453. BD*(1) C 14 - C 15	14.74	0.68	0.091
83. LP (1) O 19	/321. RY*(1) C 18	2.39	1.52	0.054
83. LP (1) O 19	/324. RY*(4) C 18	1.67	2.90	0.062
83. LP (1) O 19	/422. RY*(3) H 33	1.30	2.29	0.049
83. LP (1) O 19	/462. BD*(1) C 18 - O 20	5.36	1.14	0.070
84. LP (2) O 19	/323. RY*(3) C 18	2.03	1.86	0.057
84. LP (2) O 19	/421. RY*(2) H 33	1.57	1.81	0.050
84. LP (2) O 19	/463. BD*(2) C 18 - O 20	40.52	0.32	0.103
85. LP (1) O 20	/321. RY*(1) C 18	13.29	1.61	0.131
85. LP (1) O 20	/459. BD*(1) C 17 - C 18	2.18	1.14	0.045
85. LP (1) O 20	/461. BD*(1) C 18 - O 19	0.84	1.00	0.026
86. LP (2) O 20	/322. RY*(2) C 18	2.68	1.59	0.060
86. LP (2) O 20	/324. RY*(4) C 18	1.04	2.54	0.048
86. LP (2) O 20	/459. BD*(1) C 17 - C 18	13.34	0.69	0.087
86. LP (2) O 20	/461. BD*(1) C 18 - O 19	27.87	0.56	0.112

427. BD*(2) C 1 - C 3	/ 91. RY*(5) C 1	1.03	1.34	0.084
427. BD*(2) C 1 - C 3	/116. RY*(4) C 3	0.95	0.75	0.060
427. BD*(2) C 1 - C 3	/430. BD*(2) C 2 - C 4	121.26	0.01	0.072
427. BD*(2) C 1 - C 3	/440. BD*(1) C 7 - O 8	0.83	0.25	0.028
427. BD*(2) C 1 - C 3	/451. BD*(1) N 13 - C 14	0.71	0.33	0.031
427. BD*(2) C 1 - C 3	/452. BD*(1) N 13 - H 32	0.97	0.31	0.038
430. BD*(2) C 2 - C 4	/102. RY*(3) C 2	0.75	0.68	0.067
430. BD*(2) C 2 - C 4	/130. RY*(5) C 4	0.84	1.38	0.101
437. BD*(2) C 5 - C 6	/141. RY*(3) C 5	2.62	0.54	0.094
437. BD*(2) C 5 - C 6	/154. RY*(3) C 6	0.59	0.86	0.057
437. BD*(2) C 5 - C 6	/447. BD*(1)Se 11 - C 12	1.05	0.08	0.022
440. BD*(1) C 7 - O 8	/166. RY*(2) C 7	1.61	1.15	0.163
440. BD*(1) C 7 - O 8	/178. RY*(1) O 8	0.56	1.05	0.094
440. BD*(1) C 7 - O 8	/432. BD*(1) C 3 - C 5	1.05	0.17	0.046
440. BD*(1) C 7 - O 8	/433. BD*(1) C 3 - C 7	0.80	0.14	0.034
440. BD*(1) C 7 - O 8	/441. BD*(1) C 7 - O 9	0.53	0.22	0.039
442. BD*(2) C 7 - O 9	/167. RY*(3) C 7	1.51	1.53	0.119
442. BD*(2) C 7 - O 9	/192. RY*(2) O 9	1.10	0.98	0.082
442. BD*(2) C 7 - O 9	/427. BD*(2) C 1 - C 3	34.70	0.05	0.068
455. BD*(2) C 14 - O 16	/271. RY*(3) C 14	1.52	1.47	0.108
455. BD*(2) C 14 - O 16	/275. RY*(7) C 14	1.45	1.05	0.089
455. BD*(2) C 14 - O 16	/296. RY*(2) O 16	1.41	1.02	0.087
455. BD*(2) C 14 - O 16	/457. BD*(2) C 15 - C 17	47.23	0.03	0.076
463. BD*(2) C 18 - O 20	/323. RY*(3) C 18	1.60	1.54	0.123
463. BD*(2) C 18 - O 20	/329. RY*(9) C 18	1.00	0.75	0.069
463. BD*(2) C 18 - O 20	/348. RY*(2) O 20	1.01	1.02	0.080
463. BD*(2) C 18 - O 20	/457. BD*(2) C 15 - C 17	29.43	0.04	0.075

NATURAL BOND ORBITAL ANALYSIS:

	Occ.	Occupancies		Lewis Structure				Low occ	High occ	
Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	(L)	(NL)	Dev
1(1)	1.90	165.09987	6.90013	33	40	0	13	17	11	0.81
2(2)	1.90	165.09987	6.90013	33	40	0	13	17	11	0.81
3(1)	1.80	166.98957	5.01043	33	37	0	16	4	7	0.64
4(2)	1.80	166.98957	5.01043	33	37	0	16	4	7	0.64
5(1)	1.70	168.60172	3.39828	33	40	0	13	1	7	0.49
6(2)	1.70	169.18413	2.81587	33	40	0	13	1	7	0.21
7(3)	1.70	169.18413	2.81587	33	40	0	13	1	7	0.21
8(1)	1.60	169.18985	2.81015	33	40	0	13	0	7	0.21
9(2)	1.60	169.18985	2.81015	33	40	0	13	0	7	0.21
10(1)	1.50	168.68293	3.31707	33	39	0	14	0	9	0.74
11(2)	1.50	168.68293	3.31707	33	39	0	14	0	9	0.74
12(1)	1.60	169.18985	2.81015	33	40	0	13	0	7	0.21

Core	65.98323 (99.975% of 66)
Valence Lewis	103.20662 (97.365% of 106)

Total Lewis	169.18985 (98.366% of 172)
Valence non-Lewis	2.50959 (1.459% of 172)
Rydberg non-Lewis	0.30057 (0.175% of 172)
Total non-Lewis	2.81015 (1.634% of 172)

Compound 8

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 2	/114. RY*(1) C 3	0.79	2.49	0.040
1. BD (1) C 1 - C 2	/115. RY*(2) C 3	0.69	1.95	0.033
1. BD (1) C 1 - C 2	/128. RY*(2) C 4	2.14	1.81	0.056
1. BD (1) C 1 - C 2	/257. RY*(1) N 13	0.89	1.52	0.033
1. BD (1) C 1 - C 2	/437. BD*(1) C 1 - C 3	4.23	1.27	0.066
1. BD (1) C 1 - C 2	/439. BD*(1) C 1 - N 13	0.58	1.03	0.022
1. BD (1) C 1 - C 2	/440. BD*(1) C 2 - C 4	2.94	1.31	0.056
1. BD (1) C 1 - C 2	/442. BD*(1) C 2 - H 21	0.62	1.10	0.023
1. BD (1) C 1 - C 2	/444. BD*(1) C 3 - C 7	4.39	1.07	0.062
1. BD (1) C 1 - C 2	/446. BD*(1) C 4 - H 22	2.83	1.10	0.050
1. BD (1) C 1 - C 2	/463. BD*(1) N 13 - H 30	1.59	1.00	0.036
2. BD (1) C 1 - C 3	/101. RY*(1) C 2	0.75	2.02	0.035
2. BD (1) C 1 - C 3	/140. RY*(1) C 5	0.55	1.87	0.029
2. BD (1) C 1 - C 3	/169. RY*(4) C 7	0.58	2.78	0.036
2. BD (1) C 1 - C 3	/257. RY*(1) N 13	0.68	1.62	0.030
2. BD (1) C 1 - C 3	/436. BD*(1) C 1 - C 2	3.46	1.20	0.057
2. BD (1) C 1 - C 3	/439. BD*(1) C 1 - N 13	2.10	1.12	0.043
2. BD (1) C 1 - C 3	/442. BD*(1) C 2 - H 21	1.30	1.20	0.035
2. BD (1) C 1 - C 3	/443. BD*(1) C 3 - C 5	4.27	1.20	0.064
2. BD (1) C 1 - C 3	/444. BD*(1) C 3 - C 7	2.94	1.17	0.053
2. BD (1) C 1 - C 3	/449. BD*(1) C 5 - H 23	1.32	1.20	0.036
2. BD (1) C 1 - C 3	/452. BD*(1) C 7 - O 9	1.16	1.25	0.034
2. BD (1) C 1 - C 3	/462. BD*(1) N 13 - C 14	2.09	1.12	0.044
3. BD (2) C 1 - C 3	/103. RY*(3) C 2	1.09	1.02	0.032
3. BD (2) C 1 - C 3	/142. RY*(3) C 5	0.85	0.86	0.026
3. BD (2) C 1 - C 3	/170. RY*(5) C 7	0.62	1.48	0.029
3. BD (2) C 1 - C 3	/441. BD*(2) C 2 - C 4	10.73	0.33	0.054
3. BD (2) C 1 - C 3	/448. BD*(2) C 5 - C 6	13.63	0.32	0.059
3. BD (2) C 1 - C 3	/451. BD*(1) C 7 - O 8	1.09	0.56	0.023
3. BD (2) C 1 - C 3	/453. BD*(2) C 7 - O 9	19.15	0.27	0.064
3. BD (2) C 1 - C 3	/462. BD*(1) N 13 - C 14	1.53	0.65	0.029
3. BD (2) C 1 - C 3	/463. BD*(1) N 13 - H 30	1.52	0.63	0.029
4. BD (1) C 1 - N 13	/101. RY*(1) C 2	0.53	2.05	0.030

4. BD (1) C 1 - N 13	/114. RY*(1) C 3	1.35	2.62	0.053
4. BD (1) C 1 - N 13	/270. RY*(1) C 14	1.72	1.60	0.047
4. BD (1) C 1 - N 13	/436. BD*(1) C 1 - C 2	0.64	1.23	0.025
4. BD (1) C 1 - N 13	/437. BD*(1) C 1 - C 3	2.16	1.41	0.049
4. BD (1) C 1 - N 13	/440. BD*(1) C 2 - C 4	0.87	1.44	0.032
4. BD (1) C 1 - N 13	/443. BD*(1) C 3 - C 5	2.71	1.23	0.052
4. BD (1) C 1 - N 13	/462. BD*(1) N 13 - C 14	0.95	1.16	0.030
4. BD (1) C 1 - N 13	/464. BD*(1) C 14 - C 15	1.78	1.18	0.041
5. BD (1) C 2 - C 4	/ 88. RY*(1) C 1	1.41	1.93	0.047
5. BD (1) C 2 - C 4	/ 90. RY*(3) C 1	0.94	2.02	0.039
5. BD (1) C 2 - C 4	/153. RY*(1) C 6	1.02	1.81	0.039
5. BD (1) C 2 - C 4	/436. BD*(1) C 1 - C 2	2.73	1.19	0.051
5. BD (1) C 2 - C 4	/439. BD*(1) C 1 - N 13	2.79	1.12	0.050
5. BD (1) C 2 - C 4	/442. BD*(1) C 2 - H 21	1.68	1.20	0.040
5. BD (1) C 2 - C 4	/445. BD*(1) C 4 - C 6	3.65	1.21	0.060
5. BD (1) C 2 - C 4	/446. BD*(1) C 4 - H 22	1.58	1.19	0.039
5. BD (1) C 2 - C 4	/450. BD*(1) C 6 -Se 11	3.11	0.88	0.047
6. BD (2) C 2 - C 4	/ 93. RY*(6) C 1	0.62	1.82	0.032
6. BD (2) C 2 - C 4	/438. BD*(2) C 1 - C 3	14.34	0.31	0.061
6. BD (2) C 2 - C 4	/448. BD*(2) C 5 - C 6	12.91	0.31	0.057
7. BD (1) C 2 - H 21	/ 88. RY*(1) C 1	0.63	1.70	0.029
7. BD (1) C 2 - H 21	/ 89. RY*(2) C 1	0.89	1.83	0.036
7. BD (1) C 2 - H 21	/127. RY*(1) C 4	1.44	1.68	0.044
7. BD (1) C 2 - H 21	/437. BD*(1) C 1 - C 3	3.22	1.14	0.054
7. BD (1) C 2 - H 21	/439. BD*(1) C 1 - N 13	0.60	0.89	0.021
7. BD (1) C 2 - H 21	/440. BD*(1) C 2 - C 4	1.59	1.18	0.039
7. BD (1) C 2 - H 21	/445. BD*(1) C 4 - C 6	5.68	0.98	0.067
7. BD (1) C 2 - H 21	/446. BD*(1) C 4 - H 22	0.94	0.96	0.027
8. BD (1) C 3 - C 5	/ 89. RY*(2) C 1	1.21	1.95	0.044
8. BD (1) C 3 - C 5	/154. RY*(2) C 6	1.34	1.47	0.040
8. BD (1) C 3 - C 5	/166. RY*(1) C 7	1.00	1.58	0.036
8. BD (1) C 3 - C 5	/437. BD*(1) C 1 - C 3	4.59	1.26	0.068
8. BD (1) C 3 - C 5	/439. BD*(1) C 1 - N 13	5.33	1.02	0.066
8. BD (1) C 3 - C 5	/444. BD*(1) C 3 - C 7	1.67	1.06	0.038
8. BD (1) C 3 - C 5	/447. BD*(1) C 5 - C 6	3.92	1.29	0.064
8. BD (1) C 3 - C 5	/449. BD*(1) C 5 - H 23	0.63	1.10	0.024
8. BD (1) C 3 - C 5	/450. BD*(1) C 6 -Se 11	5.51	0.78	0.059
8. BD (1) C 3 - C 5	/451. BD*(1) C 7 - O 8	2.85	0.92	0.046
8. BD (1) C 3 - C 5	/453. BD*(2) C 7 - O 9	0.54	0.63	0.017
9. BD (1) C 3 - C 7	/ 88. RY*(1) C 1	0.84	1.87	0.036
9. BD (1) C 3 - C 7	/ 89. RY*(2) C 1	1.06	1.99	0.041
9. BD (1) C 3 - C 7	/140. RY*(1) C 5	1.01	1.80	0.038
9. BD (1) C 3 - C 7	/192. RY*(1) O 9	0.72	1.80	0.032
9. BD (1) C 3 - C 7	/436. BD*(1) C 1 - C 2	3.77	1.13	0.058
9. BD (1) C 3 - C 7	/437. BD*(1) C 1 - C 3	3.98	1.30	0.064
9. BD (1) C 3 - C 7	/443. BD*(1) C 3 - C 5	1.28	1.13	0.034
9. BD (1) C 3 - C 7	/447. BD*(1) C 5 - C 6	1.46	1.33	0.039
9. BD (1) C 3 - C 7	/452. BD*(1) C 7 - O 9	0.95	1.19	0.030
9. BD (1) C 3 - C 7	/454. BD*(1) O 8 - C 10	2.86	0.95	0.047
10. BD (1) C 4 - C 6	/101. RY*(1) C 2	0.75	1.93	0.034
10. BD (1) C 4 - C 6	/102. RY*(2) C 2	1.57	2.00	0.050
10. BD (1) C 4 - C 6	/140. RY*(1) C 5	0.93	1.78	0.037
10. BD (1) C 4 - C 6	/141. RY*(2) C 5	0.84	1.61	0.033
10. BD (1) C 4 - C 6	/440. BD*(1) C 2 - C 4	3.20	1.32	0.058
10. BD (1) C 4 - C 6	/442. BD*(1) C 2 - H 21	2.67	1.12	0.049

10. BD (1) C 4 - C 6	/446. BD*(1) C 4 - H 22	0.87	1.11	0.028
10. BD (1) C 4 - C 6	/447. BD*(1) C 5 - C 6	3.50	1.32	0.061
10. BD (1) C 4 - C 6	/449. BD*(1) C 5 - H 23	3.42	1.12	0.055
11. BD (1) C 4 - H 22	/101. RY*(1) C 2	1.53	1.79	0.047
11. BD (1) C 4 - H 22	/153. RY*(1) C 6	1.15	1.59	0.038
11. BD (1) C 4 - H 22	/436. BD*(1) C 1 - C 2	5.67	0.97	0.066
11. BD (1) C 4 - H 22	/440. BD*(1) C 2 - C 4	1.49	1.18	0.038
11. BD (1) C 4 - H 22	/442. BD*(1) C 2 - H 21	0.96	0.97	0.027
11. BD (1) C 4 - H 22	/447. BD*(1) C 5 - C 6	3.19	1.17	0.055
12. BD (1) C 5 - C 6	/114. RY*(1) C 3	1.45	2.60	0.055
12. BD (1) C 5 - C 6	/115. RY*(2) C 3	0.69	2.06	0.034
12. BD (1) C 5 - C 6	/127. RY*(1) C 4	1.05	1.92	0.040
12. BD (1) C 5 - C 6	/443. BD*(1) C 3 - C 5	3.31	1.21	0.057
12. BD (1) C 5 - C 6	/444. BD*(1) C 3 - C 7	2.03	1.18	0.044
12. BD (1) C 5 - C 6	/445. BD*(1) C 4 - C 6	3.14	1.23	0.056
12. BD (1) C 5 - C 6	/446. BD*(1) C 4 - H 22	1.65	1.21	0.040
12. BD (1) C 5 - C 6	/449. BD*(1) C 5 - H 23	2.31	1.22	0.047
13. BD (2) C 5 - C 6	/117. RY*(4) C 3	0.63	1.05	0.024
13. BD (2) C 5 - C 6	/129. RY*(3) C 4	1.70	1.12	0.041
13. BD (2) C 5 - C 6	/218. RY*(1)Se 11	1.00	0.78	0.026
13. BD (2) C 5 - C 6	/438. BD*(2) C 1 - C 3	11.79	0.31	0.056
13. BD (2) C 5 - C 6	/441. BD*(2) C 2 - C 4	13.15	0.32	0.059
13. BD (2) C 5 - C 6	/458. BD*(1)Se 11 - C 12	0.51	0.39	0.013
14. BD (1) C 5 - H 23	/114. RY*(1) C 3	1.79	2.35	0.058
14. BD (1) C 5 - H 23	/153. RY*(1) C 6	1.74	1.58	0.047
14. BD (1) C 5 - H 23	/437. BD*(1) C 1 - C 3	3.07	1.14	0.053
14. BD (1) C 5 - H 23	/445. BD*(1) C 4 - C 6	6.00	0.98	0.069
14. BD (1) C 5 - H 23	/447. BD*(1) C 5 - C 6	2.16	1.17	0.045
15. BD (1) C 6 -Se 11	/127. RY*(1) C 4	1.99	1.74	0.053
15. BD (1) C 6 -Se 11	/140. RY*(1) C 5	1.61	1.70	0.047
15. BD (1) C 6 -Se 11	/244. RY*(1) C 12	0.60	1.58	0.028
15. BD (1) C 6 -Se 11	/440. BD*(1) C 2 - C 4	2.65	1.24	0.051
15. BD (1) C 6 -Se 11	/443. BD*(1) C 3 - C 5	5.23	1.03	0.066
15. BD (1) C 6 -Se 11	/447. BD*(1) C 5 - C 6	0.95	1.23	0.031
15. BD (1) C 6 -Se 11	/449. BD*(1) C 5 - H 23	0.94	1.04	0.028
15. BD (1) C 6 -Se 11	/458. BD*(1)Se 11 - C 12	0.51	0.69	0.017
15. BD (1) C 6 -Se 11	/460. BD*(1) C 12 - H 28	0.94	0.97	0.027
16. BD (1) C 7 - O 8	/115. RY*(2) C 3	1.04	2.17	0.042
16. BD (1) C 7 - O 8	/207. RY*(3) C 10	1.04	1.84	0.039
16. BD (1) C 7 - O 8	/443. BD*(1) C 3 - C 5	1.27	1.32	0.037
16. BD (1) C 7 - O 8	/457. BD*(1) C 10 - H 26	0.66	1.24	0.025
17. BD (1) C 7 - O 9	/115. RY*(2) C 3	1.31	2.30	0.049
17. BD (1) C 7 - O 9	/166. RY*(1) C 7	1.64	1.93	0.050
17. BD (1) C 7 - O 9	/437. BD*(1) C 1 - C 3	1.53	1.62	0.045
17. BD (1) C 7 - O 9	/444. BD*(1) C 3 - C 7	1.77	1.42	0.045
18. BD (2) C 7 - O 9	/438. BD*(2) C 1 - C 3	4.52	0.40	0.041
18. BD (2) C 7 - O 9	/453. BD*(2) C 7 - O 9	0.65	0.36	0.014
19. BD (1) O 8 - C 10	/166. RY*(1) C 7	1.27	1.77	0.042
19. BD (1) O 8 - C 10	/444. BD*(1) C 3 - C 7	2.60	1.26	0.052
20. BD (1) C 10 - H 24	/180. RY*(2) O 8	0.52	1.51	0.025
21. BD (1) C 10 - H 25	/180. RY*(2) O 8	0.57	1.51	0.026
21. BD (1) C 10 - H 25	/454. BD*(1) O 8 - C 10	0.58	0.79	0.019
22. BD (1) C 10 - H 26	/451. BD*(1) C 7 - O 8	3.93	0.80	0.051
23. BD (1)Se 11 - C 12	/153. RY*(1) C 6	0.64	1.63	0.029
23. BD (1)Se 11 - C 12	/445. BD*(1) C 4 - C 6	1.77	1.03	0.038

23. BD (1)Se 11 - C 12	/448. BD*(2) C 5 - C 6	0.85	0.60	0.021
25. BD (1) C 12 - H 28	/450. BD*(1) C 6 -Se 11	1.00	0.65	0.023
27. BD (1) N 13 - C 14	/ 88. RY*(1) C 1	0.76	1.98	0.035
27. BD (1) N 13 - C 14	/ 89. RY*(2) C 1	0.77	2.10	0.036
27. BD (1) N 13 - C 14	/284. RY*(2) C 15	0.87	1.57	0.033
27. BD (1) N 13 - C 14	/437. BD*(1) C 1 - C 3	1.60	1.41	0.043
27. BD (1) N 13 - C 14	/439. BD*(1) C 1 - N 13	1.12	1.17	0.032
27. BD (1) N 13 - C 14	/467. BD*(1) C 15 - C 17	1.06	1.15	0.031
28. BD (1) N 13 - H 30	/ 88. RY*(1) C 1	1.09	1.84	0.040
28. BD (1) N 13 - H 30	/271. RY*(2) C 14	0.80	2.01	0.036
28. BD (1) N 13 - H 30	/273. RY*(4) C 14	0.91	2.92	0.046
28. BD (1) N 13 - H 30	/436. BD*(1) C 1 - C 2	2.09	1.10	0.043
28. BD (1) N 13 - H 30	/438. BD*(2) C 1 - C 3	1.57	0.68	0.032
28. BD (1) N 13 - H 30	/465. BD*(1) C 14 - O 16	3.04	1.17	0.053
29. BD (1) C 14 - C 15	/258. RY*(2) N 13	1.56	1.74	0.047
29. BD (1) C 14 - C 15	/296. RY*(1) O 16	0.58	1.85	0.029
29. BD (1) C 14 - C 15	/310. RY*(2) C 17	1.03	1.45	0.035
29. BD (1) C 14 - C 15	/439. BD*(1) C 1 - N 13	3.05	1.04	0.050
29. BD (1) C 14 - C 15	/465. BD*(1) C 14 - O 16	0.75	1.19	0.027
29. BD (1) C 14 - C 15	/467. BD*(1) C 15 - C 17	0.75	1.03	0.025
29. BD (1) C 14 - C 15	/468. BD*(1) C 15 - H 31	0.51	1.04	0.020
29. BD (1) C 14 - C 15	/469. BD*(1) C 15 - H 32	0.52	1.03	0.021
29. BD (1) C 14 - C 15	/470. BD*(1) C 17 - C 18	1.67	1.06	0.038
30. BD (1) C 14 - O 16	/270. RY*(1) C 14	1.67	1.81	0.049
30. BD (1) C 14 - O 16	/463. BD*(1) N 13 - H 30	1.20	1.35	0.036
30. BD (1) C 14 - O 16	/464. BD*(1) C 14 - C 15	1.23	1.39	0.037
31. BD (2) C 14 - O 16	/466. BD*(2) C 14 - O 16	0.68	0.35	0.015
31. BD (2) C 14 - O 16	/468. BD*(1) C 15 - H 31	1.73	0.73	0.032
31. BD (2) C 14 - O 16	/469. BD*(1) C 15 - H 32	1.83	0.72	0.032
32. BD (1) C 15 - C 17	/270. RY*(1) C 14	1.36	1.44	0.040
32. BD (1) C 15 - C 17	/322. RY*(1) C 18	0.55	1.40	0.025
32. BD (1) C 15 - C 17	/325. RY*(4) C 18	1.00	1.74	0.038
32. BD (1) C 15 - C 17	/462. BD*(1) N 13 - C 14	3.85	1.00	0.056
32. BD (1) C 15 - C 17	/464. BD*(1) C 14 - C 15	1.02	1.02	0.029
32. BD (1) C 15 - C 17	/468. BD*(1) C 15 - H 31	0.54	1.00	0.021
32. BD (1) C 15 - C 17	/470. BD*(1) C 17 - C 18	0.69	1.02	0.024
32. BD (1) C 15 - C 17	/472. BD*(1) C 17 - H 34	0.54	1.01	0.021
32. BD (1) C 15 - C 17	/473. BD*(1) C 18 - O 19	1.92	0.92	0.038
32. BD (1) C 15 - C 17	/475. BD*(2) C 18 - O 20	2.72	0.64	0.039
33. BD (1) C 15 - H 31	/309. RY*(1) C 17	0.58	1.28	0.025
33. BD (1) C 15 - H 31	/465. BD*(1) C 14 - O 16	1.86	1.03	0.039
33. BD (1) C 15 - H 31	/466. BD*(2) C 14 - O 16	5.68	0.50	0.051
33. BD (1) C 15 - H 31	/471. BD*(1) C 17 - H 33	2.63	0.89	0.043
34. BD (1) C 15 - H 32	/309. RY*(1) C 17	0.53	1.29	0.024
34. BD (1) C 15 - H 32	/465. BD*(1) C 14 - O 16	2.11	1.03	0.042
34. BD (1) C 15 - H 32	/466. BD*(2) C 14 - O 16	4.65	0.51	0.046
34. BD (1) C 15 - H 32	/472. BD*(1) C 17 - H 34	2.68	0.89	0.044
35. BD (1) C 17 - C 18	/283. RY*(1) C 15	1.19	1.46	0.037
35. BD (1) C 17 - C 18	/348. RY*(1) O 20	1.16	1.70	0.040
35. BD (1) C 17 - C 18	/464. BD*(1) C 14 - C 15	2.15	1.07	0.043
35. BD (1) C 17 - C 18	/467. BD*(1) C 15 - C 17	0.75	1.03	0.025
35. BD (1) C 17 - C 18	/474. BD*(1) C 18 - O 20	0.57	1.17	0.023
35. BD (1) C 17 - C 18	/476. BD*(1) O 19 - H 35	1.85	0.98	0.038
36. BD (1) C 17 - H 33	/468. BD*(1) C 15 - H 31	2.94	0.87	0.045
36. BD (1) C 17 - H 33	/473. BD*(1) C 18 - O 19	0.90	0.79	0.024

36. BD (1) C 17 - H 33	/474. BD*(1) C 18 - O 20	4.46	0.99	0.060
37. BD (1) C 17 - H 34	/285. RY*(3) C 15	0.51	1.32	0.023
37. BD (1) C 17 - H 34	/469. BD*(1) C 15 - H 32	2.83	0.86	0.044
37. BD (1) C 17 - H 34	/473. BD*(1) C 18 - O 19	2.65	0.79	0.042
37. BD (1) C 17 - H 34	/475. BD*(2) C 18 - O 20	5.19	0.51	0.048
38. BD (1) C 18 - O 19	/309. RY*(1) C 17	0.64	1.68	0.029
39. BD (1) C 18 - O 20	/309. RY*(1) C 17	0.75	1.75	0.032
39. BD (1) C 18 - O 20	/322. RY*(1) C 18	1.62	1.75	0.048
39. BD (1) C 18 - O 20	/470. BD*(1) C 17 - C 18	1.09	1.37	0.035
39. BD (1) C 18 - O 20	/471. BD*(1) C 17 - H 33	0.66	1.36	0.027
40. BD (2) C 18 - O 20	/467. BD*(1) C 15 - C 17	1.17	0.75	0.026
40. BD (2) C 18 - O 20	/472. BD*(1) C 17 - H 34	1.10	0.77	0.026
40. BD (2) C 18 - O 20	/475. BD*(2) C 18 - O 20	0.81	0.40	0.017
41. BD (1) O 19 - H 35	/322. RY*(1) C 18	0.97	1.49	0.034
41. BD (1) O 19 - H 35	/323. RY*(2) C 18	1.15	2.01	0.043
41. BD (1) O 19 - H 35	/470. BD*(1) C 17 - C 18	3.73	1.11	0.058
41. BD (1) O 19 - H 35	/474. BD*(1) C 18 - O 20	1.22	1.22	0.035
42. CR (1) C 1	/102. RY*(2) C 2	0.96	11.45	0.093
42. CR (1) C 1	/114. RY*(1) C 3	0.53	11.95	0.071
42. CR (1) C 1	/115. RY*(2) C 3	1.69	11.41	0.124
42. CR (1) C 1	/437. BD*(1) C 1 - C 3	1.36	10.73	0.109
42. CR (1) C 1	/440. BD*(1) C 2 - C 4	0.57	10.77	0.070
42. CR (1) C 1	/443. BD*(1) C 3 - C 5	1.03	10.56	0.094
42. CR (1) C 1	/444. BD*(1) C 3 - C 7	1.11	10.53	0.098
42. CR (1) C 1	/462. BD*(1) N 13 - C 14	1.04	10.48	0.095
43. CR (1) C 2	/ 89. RY*(2) C 1	1.36	11.36	0.111
43. CR (1) C 2	/127. RY*(1) C 4	0.60	11.21	0.073
43. CR (1) C 2	/128. RY*(2) C 4	1.74	11.21	0.125
43. CR (1) C 2	/437. BD*(1) C 1 - C 3	0.83	10.67	0.085
43. CR (1) C 2	/439. BD*(1) C 1 - N 13	0.54	10.42	0.067
43. CR (1) C 2	/440. BD*(1) C 2 - C 4	0.83	10.70	0.084
43. CR (1) C 2	/445. BD*(1) C 4 - C 6	1.31	10.51	0.105
44. CR (1) C 3	/ 88. RY*(1) C 1	1.13	11.25	0.101
44. CR (1) C 3	/ 90. RY*(3) C 1	1.03	11.34	0.097
44. CR (1) C 3	/141. RY*(2) C 5	0.69	11.02	0.078
44. CR (1) C 3	/167. RY*(2) C 7	0.60	11.50	0.074
44. CR (1) C 3	/172. RY*(7) C 7	0.83	11.19	0.086
44. CR (1) C 3	/436. BD*(1) C 1 - C 2	1.09	10.52	0.096
44. CR (1) C 3	/437. BD*(1) C 1 - C 3	1.24	10.69	0.104
44. CR (1) C 3	/439. BD*(1) C 1 - N 13	1.02	10.45	0.093
44. CR (1) C 3	/447. BD*(1) C 5 - C 6	0.72	10.72	0.079
44. CR (1) C 3	/451. BD*(1) C 7 - O 8	0.61	10.35	0.073
45. CR (1) C 4	/102. RY*(2) C 2	1.30	11.38	0.109
45. CR (1) C 4	/104. RY*(4) C 2	0.69	11.04	0.078
45. CR (1) C 4	/154. RY*(2) C 6	1.15	10.87	0.100
45. CR (1) C 4	/156. RY*(4) C 6	0.75	11.11	0.082
45. CR (1) C 4	/436. BD*(1) C 1 - C 2	1.20	10.49	0.101
45. CR (1) C 4	/440. BD*(1) C 2 - C 4	0.67	10.70	0.076
45. CR (1) C 4	/447. BD*(1) C 5 - C 6	0.82	10.70	0.084
45. CR (1) C 4	/450. BD*(1) C 6 -Se 11	0.82	10.18	0.082
46. CR (1) C 5	/115. RY*(2) C 3	0.78	11.34	0.084
46. CR (1) C 5	/153. RY*(1) C 6	0.98	11.11	0.093
46. CR (1) C 5	/154. RY*(2) C 6	1.96	10.87	0.130
46. CR (1) C 5	/155. RY*(3) C 6	0.64	10.94	0.074
46. CR (1) C 5	/437. BD*(1) C 1 - C 3	0.76	10.67	0.081

46. CR (1) C 5	/444. BD*(1) C 3 - C 7	0.66	10.46	0.075
46. CR (1) C 5	/445. BD*(1) C 4 - C 6	1.23	10.51	0.102
46. CR (1) C 5	/447. BD*(1) C 5 - C 6	1.20	10.70	0.102
46. CR (1) C 5	/450. BD*(1) C 6 -Se 11	1.25	10.18	0.101
47. CR (1) C 6	/128. RY*(2) C 4	1.03	11.25	0.096
47. CR (1) C 6	/141. RY*(2) C 5	2.17	11.03	0.138
47. CR (1) C 6	/143. RY*(4) C 5	0.63	11.15	0.075
47. CR (1) C 6	/440. BD*(1) C 2 - C 4	0.63	10.74	0.074
47. CR (1) C 6	/443. BD*(1) C 3 - C 5	1.17	10.53	0.100
47. CR (1) C 6	/447. BD*(1) C 5 - C 6	1.22	10.73	0.103
47. CR (1) C 6	/449. BD*(1) C 5 - H 23	0.56	10.54	0.069
47. CR (1) C 6	/450. BD*(1) C 6 -Se 11	1.34	10.22	0.105
48. CR (1) C 7	/114. RY*(1) C 3	1.19	12.04	0.107
48. CR (1) C 7	/437. BD*(1) C 1 - C 3	0.87	10.83	0.087
48. CR (1) C 7	/443. BD*(1) C 3 - C 5	0.54	10.66	0.068
48. CR (1) C 7	/444. BD*(1) C 3 - C 7	0.56	10.63	0.070
48. CR (1) C 7	/451. BD*(1) C 7 - O 8	0.67	10.49	0.077
48. CR (1) C 7	/454. BD*(1) O 8 - C 10	1.11	10.48	0.097
49. CR (1) O 8	/166. RY*(1) C 7	1.01	19.92	0.127
49. CR (1) O 8	/167. RY*(2) C 7	1.12	20.42	0.135
49. CR (1) O 8	/207. RY*(3) C 10	0.87	19.95	0.118
50. CR (1) O 9	/166. RY*(1) C 7	5.28	19.80	0.290
50. CR (1) O 9	/444. BD*(1) C 3 - C 7	0.78	19.29	0.111
51. CR (1) C 10	/387. RY*(2) H 26	0.55	12.16	0.073
51. CR (1) C 10	/451. BD*(1) C 7 - O 8	1.10	10.40	0.098
51. CR (1) C 10	/454. BD*(1) O 8 - C 10	1.48	10.39	0.111
54. CR (3)Se 11	/153. RY*(1) C 6	1.00	11.34	0.095
54. CR (3)Se 11	/247. RY*(4) C 12	0.60	11.19	0.073
54. CR (3)Se 11	/445. BD*(1) C 4 - C 6	0.75	10.74	0.081
54. CR (3)Se 11	/447. BD*(1) C 5 - C 6	1.24	10.92	0.104
66. CR (1) C 12	/458. BD*(1)Se 11 - C 12	1.46	10.19	0.109
67. CR (1) N 13	/ 88. RY*(1) C 1	1.10	15.39	0.116
67. CR (1) N 13	/ 89. RY*(2) C 1	0.55	15.52	0.082
67. CR (1) N 13	/271. RY*(2) C 14	1.51	15.56	0.137
67. CR (1) N 13	/275. RY*(6) C 14	0.68	15.24	0.091
67. CR (1) N 13	/408. RY*(3) H 30	0.51	16.46	0.082
67. CR (1) N 13	/437. BD*(1) C 1 - C 3	0.59	14.83	0.084
68. CR (1) C 14	/283. RY*(1) C 15	0.59	10.96	0.072
68. CR (1) C 14	/286. RY*(4) C 15	0.53	11.38	0.069
68. CR (1) C 14	/439. BD*(1) C 1 - N 13	1.16	10.56	0.099
69. CR (1) C 15	/271. RY*(2) C 14	1.00	11.43	0.096
69. CR (1) C 15	/312. RY*(4) C 17	0.66	10.90	0.076
70. CR (1) O 16	/270. RY*(1) C 14	5.82	19.67	0.303
70. CR (1) O 16	/464. BD*(1) C 14 - C 15	0.72	19.25	0.107
71. CR (1) C 17	/284. RY*(2) C 15	0.52	10.85	0.067
71. CR (1) C 17	/323. RY*(2) C 18	0.67	11.35	0.078
71. CR (1) C 17	/328. RY*(7) C 18	0.64	11.16	0.075
71. CR (1) C 17	/473. BD*(1) C 18 - O 19	0.56	10.36	0.070
72. CR (1) C 18	/310. RY*(2) C 17	0.84	10.99	0.086
72. CR (1) C 18	/311. RY*(3) C 17	0.55	11.38	0.070
72. CR (1) C 18	/473. BD*(1) C 18 - O 19	0.71	10.50	0.079
73. CR (1) O 19	/322. RY*(1) C 18	0.71	19.75	0.106
73. CR (1) O 19	/323. RY*(2) C 18	1.94	20.26	0.177
74. CR (1) O 20	/322. RY*(1) C 18	6.17	19.64	0.312
74. CR (1) O 20	/470. BD*(1) C 17 - C 18	0.72	19.26	0.106

75. LP (1) O 8	/166. RY*(1) C 7	1.66	1.51	0.045
75. LP (1) O 8	/169. RY*(4) C 7	1.61	2.61	0.058
75. LP (1) O 8	/205. RY*(1) C 10	1.66	1.65	0.047
75. LP (1) O 8	/207. RY*(3) C 10	0.74	1.54	0.030
75. LP (1) O 8	/452. BD*(1) C 7 - O 9	5.70	1.08	0.070
75. LP (1) O 8	/455. BD*(1) C 10 - H 24	0.64	0.95	0.022
75. LP (1) O 8	/457. BD*(1) C 10 - H 26	2.38	0.95	0.043
76. LP (2) O 8	/168. RY*(3) C 7	1.80	1.84	0.054
76. LP (2) O 8	/206. RY*(2) C 10	1.47	1.50	0.044
76. LP (2) O 8	/453. BD*(2) C 7 - O 9	38.54	0.31	0.100
76. LP (2) O 8	/455. BD*(1) C 10 - H 24	5.05	0.70	0.056
76. LP (2) O 8	/456. BD*(1) C 10 - H 25	5.06	0.69	0.055
77. LP (1) O 9	/166. RY*(1) C 7	12.36	1.64	0.127
77. LP (1) O 9	/176. RY*(11) C 7	0.75	4.91	0.055
77. LP (1) O 9	/444. BD*(1) C 3 - C 7	2.25	1.13	0.045
77. LP (1) O 9	/451. BD*(1) C 7 - O 8	0.98	0.99	0.028
78. LP (2) O 9	/167. RY*(2) C 7	1.92	1.70	0.053
78. LP (2) O 9	/169. RY*(4) C 7	1.72	2.30	0.058
78. LP (2) O 9	/444. BD*(1) C 3 - C 7	12.40	0.68	0.084
78. LP (2) O 9	/451. BD*(1) C 7 - O 8	28.89	0.55	0.113
78. LP (2) O 9	/457. BD*(1) C 10 - H 26	0.81	0.64	0.021
79. LP (1)Se 11	/153. RY*(1) C 6	1.18	1.76	0.041
79. LP (1)Se 11	/447. BD*(1) C 5 - C 6	3.33	1.34	0.060
80. LP (2)Se 11	/445. BD*(1) C 4 - C 6	1.62	0.69	0.030
80. LP (2)Se 11	/447. BD*(1) C 5 - C 6	1.11	0.87	0.028
80. LP (2)Se 11	/448. BD*(2) C 5 - C 6	9.24	0.26	0.045
80. LP (2)Se 11	/459. BD*(1) C 12 - H 27	4.11	0.61	0.046
80. LP (2)Se 11	/461. BD*(1) C 12 - H 29	2.49	0.61	0.036
81. LP (1) N 13	/ 90. RY*(3) C 1	1.09	1.54	0.039
81. LP (1) N 13	/ 91. RY*(4) C 1	0.76	1.61	0.034
81. LP (1) N 13	/272. RY*(3) C 14	1.66	1.71	0.051
81. LP (1) N 13	/277. RY*(8) C 14	0.51	1.71	0.029
81. LP (1) N 13	/407. RY*(2) H 30	0.75	1.95	0.037
81. LP (1) N 13	/436. BD*(1) C 1 - C 2	3.79	0.71	0.050
81. LP (1) N 13	/437. BD*(1) C 1 - C 3	2.86	0.89	0.048
81. LP (1) N 13	/438. BD*(2) C 1 - C 3	17.14	0.30	0.064
81. LP (1) N 13	/466. BD*(2) C 14 - O 16	50.70	0.26	0.103
82. LP (1) O 16	/270. RY*(1) C 14	13.70	1.51	0.128
82. LP (1) O 16	/462. BD*(1) N 13 - C 14	1.21	1.06	0.032
82. LP (1) O 16	/464. BD*(1) C 14 - C 15	2.20	1.09	0.044
83. LP (2) O 16	/271. RY*(2) C 14	1.50	1.61	0.045
83. LP (2) O 16	/273. RY*(4) C 14	1.84	2.52	0.063
83. LP (2) O 16	/462. BD*(1) N 13 - C 14	23.71	0.62	0.110
83. LP (2) O 16	/464. BD*(1) C 14 - C 15	15.30	0.64	0.090
83. LP (2) O 16	/470. BD*(1) C 17 - C 18	0.76	0.64	0.020
84. LP (1) O 19	/322. RY*(1) C 18	2.36	1.39	0.051
84. LP (1) O 19	/323. RY*(2) C 18	0.66	1.90	0.032
84. LP (1) O 19	/325. RY*(4) C 18	0.87	1.74	0.035
84. LP (1) O 19	/326. RY*(5) C 18	1.40	2.47	0.053
84. LP (1) O 19	/433. RY*(3) H 35	1.38	2.33	0.051
84. LP (1) O 19	/474. BD*(1) C 18 - O 20	5.37	1.12	0.069
85. LP (2) O 19	/324. RY*(3) C 18	2.07	1.87	0.058
85. LP (2) O 19	/432. RY*(2) H 35	1.48	1.82	0.049
85. LP (2) O 19	/474. BD*(1) C 18 - O 20	0.52	0.83	0.019
85. LP (2) O 19	/475. BD*(2) C 18 - O 20	37.54	0.34	0.102

86. LP (1) O 20	/322. RY*(1) C 18	14.63	1.48	0.131
86. LP (1) O 20	/333. RY*(12) C 18	0.71	5.48	0.056
86. LP (1) O 20	/470. BD*(1) C 17 - C 18	2.22	1.10	0.044
86. LP (1) O 20	/473. BD*(1) C 18 - O 19	0.90	1.00	0.027
87. LP (2) O 20	/323. RY*(2) C 18	2.66	1.54	0.059
87. LP (2) O 20	/325. RY*(4) C 18	0.70	1.38	0.029
87. LP (2) O 20	/326. RY*(5) C 18	1.02	2.11	0.043
87. LP (2) O 20	/470. BD*(1) C 17 - C 18	12.78	0.65	0.083
87. LP (2) O 20	/471. BD*(1) C 17 - H 33	0.69	0.64	0.019
87. LP (2) O 20	/473. BD*(1) C 18 - O 19	28.42	0.55	0.113
438. BD*(2) C 1 - C 3	/ 92. RY*(5) C 1	1.07	1.29	0.084
438. BD*(2) C 1 - C 3	/117. RY*(4) C 3	0.92	0.74	0.059
438. BD*(2) C 1 - C 3	/441. BD*(2) C 2 - C 4	129.94	0.01	0.072
438. BD*(2) C 1 - C 3	/451. BD*(1) C 7 - O 8	0.80	0.25	0.028
438. BD*(2) C 1 - C 3	/462. BD*(1) N 13 - C 14	0.71	0.34	0.031
438. BD*(2) C 1 - C 3	/463. BD*(1) N 13 - H 30	0.99	0.31	0.039
441. BD*(2) C 2 - C 4	/103. RY*(3) C 2	0.75	0.69	0.067
441. BD*(2) C 2 - C 4	/131. RY*(5) C 4	0.85	1.38	0.101
448. BD*(2) C 5 - C 6	/142. RY*(3) C 5	2.55	0.54	0.094
448. BD*(2) C 5 - C 6	/155. RY*(3) C 6	0.55	0.86	0.055
448. BD*(2) C 5 - C 6	/458. BD*(1)Se 11 - C 12	1.09	0.08	0.023
451. BD*(1) C 7 - O 8	/167. RY*(2) C 7	1.61	1.15	0.162
451. BD*(1) C 7 - O 8	/179. RY*(1) O 8	0.55	1.04	0.093
451. BD*(1) C 7 - O 8	/443. BD*(1) C 3 - C 5	1.05	0.17	0.046
451. BD*(1) C 7 - O 8	/444. BD*(1) C 3 - C 7	0.80	0.14	0.034
451. BD*(1) C 7 - O 8	/452. BD*(1) C 7 - O 9	0.53	0.22	0.039
453. BD*(2) C 7 - O 9	/168. RY*(3) C 7	1.52	1.52	0.119
453. BD*(2) C 7 - O 9	/193. RY*(2) O 9	1.10	0.98	0.082
453. BD*(2) C 7 - O 9	/438. BD*(2) C 1 - C 3	33.68	0.05	0.068
466. BD*(2) C 14 - O 16	/272. RY*(3) C 14	1.29	1.45	0.106
466. BD*(2) C 14 - O 16	/277. RY*(8) C 14	0.77	1.45	0.083
466. BD*(2) C 14 - O 16	/297. RY*(2) O 16	1.21	1.00	0.086
466. BD*(2) C 14 - O 16	/468. BD*(1) C 15 - H 31	1.13	0.37	0.050
466. BD*(2) C 14 - O 16	/469. BD*(1) C 15 - H 32	1.10	0.37	0.048
475. BD*(2) C 18 - O 20	/324. RY*(3) C 18	1.20	1.53	0.119
475. BD*(2) C 18 - O 20	/467. BD*(1) C 15 - C 17	0.91	0.35	0.049
475. BD*(2) C 18 - O 20	/472. BD*(1) C 17 - H 34	1.17	0.37	0.057
475. BD*(2) C 18 - O 20	/474. BD*(1) C 18 - O 20	3.30	0.49	0.105

NATURAL BOND ORBITAL ANALYSIS:

		Occupancies		Lewis Structure				Low	High	
	Occ.							occ	occ	
Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	(L)	(NL)	Dev
1(1)	1.90	168.02397	5.97603	33	42	0	12	18	10	0.64
2(2)	1.90	168.02397	5.97603	33	42	0	12	18	10	0.64
3(1)	1.80	169.18403	4.81597	33	39	0	15	3	7	0.64
4(2)	1.80	169.18403	4.81597	33	39	0	15	3	7	0.64
5(1)	1.70	171.29753	2.70247	33	41	0	13	0	7	0.21
6(2)	1.70	171.29753	2.70247	33	41	0	13	0	7	0.21
7(1)	1.60	171.29753	2.70247	33	41	0	13	0	7	0.21
8(2)	1.60	171.29753	2.70247	33	41	0	13	0	7	0.21
9(1)	1.50	170.78598	3.21402	33	40	0	14	0	9	0.74

10(2)	1.50	170.33265	3.66735	33	40	0	14	1	9	1.04
11(3)	1.50	170.78598	3.21402	33	40	0	14	0	9	0.74
12(1)	1.70	171.29753	2.70247	33	41	0	13	0	7	0.21

Core	65.98363 (99.975% of 66)
Valence Lewis	105.31390 (97.513% of 108)
==========	==========
Total Lewis	171.29753 (98.447% of 174)
Valence non-Lewis	2.39409 (1.376% of 174)
Rydberg non-Lewis	0.30839 (0.177% of 174)
==========	==========
Total non-Lewis	2.70247 (1.553% of 174)

Compound 9

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 2	/133. RY*(1) C 3	0.81	2.49	0.040
1. BD (1) C 1 - C 2	/134. RY*(2) C 3	0.65	1.95	0.032
1. BD (1) C 1 - C 2	/147. RY*(2) C 4	2.14	1.82	0.056
1. BD (1) C 1 - C 2	/276. RY*(1) N 13	0.90	1.52	0.033
1. BD (1) C 1 - C 2	/544. BD*(1) C 1 - C 3	4.26	1.27	0.066
1. BD (1) C 1 - C 2	/546. BD*(1) C 1 - N 13	0.57	1.02	0.022
1. BD (1) C 1 - C 2	/547. BD*(1) C 2 - C 4	2.92	1.31	0.055
1. BD (1) C 1 - C 2	/549. BD*(1) C 2 - H 29	0.61	1.10	0.023
1. BD (1) C 1 - C 2	/551. BD*(1) C 3 - C 7	4.39	1.07	0.062
1. BD (1) C 1 - C 2	/553. BD*(1) C 4 - H 30	2.81	1.10	0.050
1. BD (1) C 1 - C 2	/570. BD*(1) N 13 - H 37	1.59	1.00	0.036
2. BD (1) C 1 - C 3	/120. RY*(1) C 2	0.74	2.02	0.035
2. BD (1) C 1 - C 3	/159. RY*(1) C 5	0.60	1.90	0.030
2. BD (1) C 1 - C 3	/188. RY*(4) C 7	0.58	2.78	0.036
2. BD (1) C 1 - C 3	/276. RY*(1) N 13	0.68	1.62	0.030
2. BD (1) C 1 - C 3	/543. BD*(1) C 1 - C 2	3.48	1.20	0.058
2. BD (1) C 1 - C 3	/546. BD*(1) C 1 - N 13	2.08	1.12	0.043
2. BD (1) C 1 - C 3	/549. BD*(1) C 2 - H 29	1.30	1.20	0.035
2. BD (1) C 1 - C 3	/550. BD*(1) C 3 - C 5	4.25	1.20	0.064
2. BD (1) C 1 - C 3	/551. BD*(1) C 3 - C 7	2.93	1.17	0.053
2. BD (1) C 1 - C 3	/556. BD*(1) C 5 - H 31	1.32	1.21	0.036
2. BD (1) C 1 - C 3	/559. BD*(1) C 7 - O 9	1.16	1.26	0.034
2. BD (1) C 1 - C 3	/569. BD*(1) N 13 - C 14	2.11	1.11	0.044
3. BD (2) C 1 - C 3	/122. RY*(3) C 2	1.13	1.01	0.032
3. BD (2) C 1 - C 3	/161. RY*(3) C 5	0.88	0.86	0.026

3. BD (2) C 1 - C 3	/189. RY*(5) C 7	0.60	1.47	0.029
3. BD (2) C 1 - C 3	/548. BD*(2) C 2 - C 4	10.74	0.33	0.054
3. BD (2) C 1 - C 3	/555. BD*(2) C 5 - C 6	13.48	0.32	0.059
3. BD (2) C 1 - C 3	/558. BD*(1) C 7 - O 8	1.11	0.57	0.023
3. BD (2) C 1 - C 3	/560. BD*(2) C 7 - O 9	18.85	0.27	0.064
3. BD (2) C 1 - C 3	/569. BD*(1) N 13 - C 14	1.49	0.65	0.029
3. BD (2) C 1 - C 3	/570. BD*(1) N 13 - H 37	1.48	0.63	0.029
4. BD (1) C 1 - N 13	/120. RY*(1) C 2	0.52	2.06	0.029
4. BD (1) C 1 - N 13	/133. RY*(1) C 3	1.36	2.63	0.053
4. BD (1) C 1 - N 13	/289. RY*(1) C 14	1.52	1.68	0.045
4. BD (1) C 1 - N 13	/543. BD*(1) C 1 - C 2	0.64	1.24	0.025
4. BD (1) C 1 - N 13	/544. BD*(1) C 1 - C 3	2.15	1.41	0.049
4. BD (1) C 1 - N 13	/547. BD*(1) C 2 - C 4	0.86	1.45	0.031
4. BD (1) C 1 - N 13	/550. BD*(1) C 3 - C 5	2.69	1.24	0.052
4. BD (1) C 1 - N 13	/569. BD*(1) N 13 - C 14	0.86	1.15	0.029
4. BD (1) C 1 - N 13	/571. BD*(1) C 14 - C 15	1.69	1.22	0.041
5. BD (1) C 2 - C 4	/107. RY*(1) C 1	1.41	1.95	0.047
5. BD (1) C 2 - C 4	/109. RY*(3) C 1	0.91	1.99	0.038
5. BD (1) C 2 - C 4	/172. RY*(1) C 6	1.10	1.82	0.040
5. BD (1) C 2 - C 4	/543. BD*(1) C 1 - C 2	2.72	1.19	0.051
5. BD (1) C 2 - C 4	/546. BD*(1) C 1 - N 13	2.80	1.12	0.050
5. BD (1) C 2 - C 4	/549. BD*(1) C 2 - H 29	1.69	1.20	0.040
5. BD (1) C 2 - C 4	/552. BD*(1) C 4 - C 6	3.64	1.21	0.059
5. BD (1) C 2 - C 4	/553. BD*(1) C 4 - H 30	1.57	1.19	0.039
5. BD (1) C 2 - C 4	/557. BD*(1) C 6 -Se 11	3.10	0.88	0.047
6. BD (2) C 2 - C 4	/112. RY*(6) C 1	0.63	1.80	0.032
6. BD (2) C 2 - C 4	/545. BD*(2) C 1 - C 3	14.31	0.31	0.060
6. BD (2) C 2 - C 4	/555. BD*(2) C 5 - C 6	13.00	0.31	0.057
7. BD (1) C 2 - H 29	/107. RY*(1) C 1	0.64	1.72	0.030
7. BD (1) C 2 - H 29	/108. RY*(2) C 1	0.87	1.83	0.036
7. BD (1) C 2 - H 29	/146. RY*(1) C 4	1.44	1.68	0.044
7. BD (1) C 2 - H 29	/544. BD*(1) C 1 - C 3	3.22	1.14	0.054
7. BD (1) C 2 - H 29	/546. BD*(1) C 1 - N 13	0.61	0.89	0.021
7. BD (1) C 2 - H 29	/547. BD*(1) C 2 - C 4	1.59	1.18	0.039
7. BD (1) C 2 - H 29	/552. BD*(1) C 4 - C 6	5.68	0.98	0.067
7. BD (1) C 2 - H 29	/553. BD*(1) C 4 - H 30	0.94	0.96	0.027
8. BD (1) C 3 - C 5	/108. RY*(2) C 1	1.22	1.95	0.044
8. BD (1) C 3 - C 5	/173. RY*(2) C 6	1.44	1.48	0.042
8. BD (1) C 3 - C 5	/185. RY*(1) C 7	0.99	1.58	0.036
8. BD (1) C 3 - C 5	/544. BD*(1) C 1 - C 3	4.60	1.26	0.068
8. BD (1) C 3 - C 5	/546. BD*(1) C 1 - N 13	5.34	1.01	0.066
8. BD (1) C 3 - C 5	/551. BD*(1) C 3 - C 7	1.68	1.06	0.038
8. BD (1) C 3 - C 5	/554. BD*(1) C 5 - C 6	3.91	1.29	0.064
8. BD (1) C 3 - C 5	/556. BD*(1) C 5 - H 31	0.62	1.10	0.023
8. BD (1) C 3 - C 5	/557. BD*(1) C 6 -Se 11	5.49	0.78	0.059
8. BD (1) C 3 - C 5	/558. BD*(1) C 7 - O 8	2.84	0.92	0.046
8. BD (1) C 3 - C 5	/560. BD*(2) C 7 - O 9	0.55	0.63	0.018
9. BD (1) C 3 - C 7	/107. RY*(1) C 1	0.84	1.88	0.036
9. BD (1) C 3 - C 7	/108. RY*(2) C 1	1.03	2.00	0.041
9. BD (1) C 3 - C 7	/159. RY*(1) C 5	1.05	1.84	0.039
9. BD (1) C 3 - C 7	/211. RY*(1) O 9	0.72	1.81	0.032
9. BD (1) C 3 - C 7	/543. BD*(1) C 1 - C 2	3.77	1.13	0.058
9. BD (1) C 3 - C 7	/544. BD*(1) C 1 - C 3	3.96	1.30	0.064
9. BD (1) C 3 - C 7	/550. BD*(1) C 3 - C 5	1.29	1.13	0.034
9. BD (1) C 3 - C 7	/554. BD*(1) C 5 - C 6	1.47	1.33	0.040

9. BD (1) C 3 - C 7	/559. BD*(1) C 7 - O 9	0.95	1.19	0.030
9. BD (1) C 3 - C 7	/561. BD*(1) O 8 - C 10	2.85	0.96	0.047
10. BD (1) C 4 - C 6	/120. RY*(1) C 2	0.74	1.93	0.034
10. BD (1) C 4 - C 6	/121. RY*(2) C 2	1.59	2.01	0.051
10. BD (1) C 4 - C 6	/159. RY*(1) C 5	0.84	1.82	0.035
10. BD (1) C 4 - C 6	/160. RY*(2) C 5	0.95	1.63	0.035
10. BD (1) C 4 - C 6	/547. BD*(1) C 2 - C 4	3.20	1.32	0.058
10. BD (1) C 4 - C 6	/549. BD*(1) C 2 - H 29	2.66	1.12	0.049
10. BD (1) C 4 - C 6	/553. BD*(1) C 4 - H 30	0.87	1.11	0.028
10. BD (1) C 4 - C 6	/554. BD*(1) C 5 - C 6	3.49	1.32	0.061
10. BD (1) C 4 - C 6	/556. BD*(1) C 5 - H 31	3.42	1.12	0.055
11. BD (1) C 4 - H 30	/120. RY*(1) C 2	1.53	1.79	0.047
11. BD (1) C 4 - H 30	/172. RY*(1) C 6	1.12	1.60	0.038
11. BD (1) C 4 - H 30	/543. BD*(1) C 1 - C 2	5.68	0.97	0.066
11. BD (1) C 4 - H 30	/547. BD*(1) C 2 - C 4	1.50	1.18	0.038
11. BD (1) C 4 - H 30	/549. BD*(1) C 2 - H 29	0.96	0.97	0.027
11. BD (1) C 4 - H 30	/554. BD*(1) C 5 - C 6	3.20	1.17	0.055
12. BD (1) C 5 - C 6	/133. RY*(1) C 3	1.41	2.60	0.054
12. BD (1) C 5 - C 6	/134. RY*(2) C 3	0.71	2.06	0.034
12. BD (1) C 5 - C 6	/146. RY*(1) C 4	1.04	1.92	0.040
12. BD (1) C 5 - C 6	/550. BD*(1) C 3 - C 5	3.34	1.21	0.057
12. BD (1) C 5 - C 6	/551. BD*(1) C 3 - C 7	2.03	1.18	0.044
12. BD (1) C 5 - C 6	/552. BD*(1) C 4 - C 6	3.14	1.23	0.056
12. BD (1) C 5 - C 6	/553. BD*(1) C 4 - H 30	1.64	1.21	0.040
12. BD (1) C 5 - C 6	/556. BD*(1) C 5 - H 31	2.31	1.22	0.047
13. BD (2) C 5 - C 6	/136. RY*(4) C 3	0.61	1.06	0.024
13. BD (2) C 5 - C 6	/148. RY*(3) C 4	1.68	1.13	0.041
13. BD (2) C 5 - C 6	/237. RY*(1)Se 11	0.93	0.82	0.026
13. BD (2) C 5 - C 6	/545. BD*(2) C 1 - C 3	11.98	0.31	0.056
13. BD (2) C 5 - C 6	/548. BD*(2) C 2 - C 4	13.07	0.32	0.059
14. BD (1) C 5 - H 31	/133. RY*(1) C 3	1.81	2.36	0.059
14. BD (1) C 5 - H 31	/172. RY*(1) C 6	1.79	1.59	0.048
14. BD (1) C 5 - H 31	/544. BD*(1) C 1 - C 3	3.08	1.14	0.053
14. BD (1) C 5 - H 31	/552. BD*(1) C 4 - C 6	6.01	0.98	0.069
14. BD (1) C 5 - H 31	/554. BD*(1) C 5 - C 6	2.18	1.17	0.045
15. BD (1) C 6 -Se 11	/146. RY*(1) C 4	2.10	1.74	0.054
15. BD (1) C 6 -Se 11	/159. RY*(1) C 5	1.68	1.73	0.048
15. BD (1) C 6 -Se 11	/264. RY*(2) C 12	0.66	1.57	0.029
15. BD (1) C 6 -Se 11	/547. BD*(1) C 2 - C 4	2.68	1.24	0.052
15. BD (1) C 6 -Se 11	/550. BD*(1) C 3 - C 5	5.32	1.03	0.066
15. BD (1) C 6 -Se 11	/554. BD*(1) C 5 - C 6	1.01	1.23	0.032
15. BD (1) C 6 -Se 11	/556. BD*(1) C 5 - H 31	0.95	1.04	0.028
15. BD (1) C 6 -Se 11	/566. BD*(1) C 12 - C 21	0.89	1.01	0.027
16. BD (1) C 7 - O 8	/134. RY*(2) C 3	1.04	2.16	0.042
16. BD (1) C 7 - O 8	/226. RY*(3) C 10	1.07	1.84	0.040
16. BD (1) C 7 - O 8	/550. BD*(1) C 3 - C 5	1.27	1.32	0.037
16. BD (1) C 7 - O 8	/564. BD*(1) C 10 - H 34	0.66	1.24	0.025
17. BD (1) C 7 - O 9	/134. RY*(2) C 3	1.33	2.30	0.049
17. BD (1) C 7 - O 9	/185. RY*(1) C 7	1.64	1.94	0.050
17. BD (1) C 7 - O 9	/544. BD*(1) C 1 - C 3	1.54	1.62	0.045
17. BD (1) C 7 - O 9	/551. BD*(1) C 3 - C 7	1.77	1.42	0.045
18. BD (2) C 7 - O 9	/545. BD*(2) C 1 - C 3	4.53	0.40	0.041
18. BD (2) C 7 - O 9	/560. BD*(2) C 7 - O 9	0.65	0.36	0.014
19. BD (1) O 8 - C 10	/185. RY*(1) C 7	1.27	1.77	0.042
19. BD (1) O 8 - C 10	/551. BD*(1) C 3 - C 7	2.61	1.26	0.052

20. BD (1) C 10 - H 32	/199. RY*(2) O 8	0.53	1.51	0.025
21. BD (1) C 10 - H 33	/199. RY*(2) O 8	0.58	1.51	0.026
21. BD (1) C 10 - H 33	/561. BD*(1) O 8 - C 10	0.58	0.79	0.019
22. BD (1) C 10 - H 34	/558. BD*(1) C 7 - O 8	3.93	0.80	0.051
23. BD (1)Se 11 - C 12	/382. RY*(3) C 21	0.87	1.27	0.030
23. BD (1)Se 11 - C 12	/552. BD*(1) C 4 - C 6	1.79	1.02	0.038
23. BD (1)Se 11 - C 12	/555. BD*(2) C 5 - C 6	1.00	0.59	0.023
23. BD (1)Se 11 - C 12	/584. BD*(1) C 21 - C 23	1.64	1.21	0.040
23. BD (1)Se 11 - C 12	/585. BD*(2) C 21 - C 23	4.19	0.61	0.048
24. BD (1) C 12 - C 21	/393. RY*(1) C 22	1.63	1.81	0.049
24. BD (1) C 12 - C 21	/406. RY*(1) C 23	1.83	1.82	0.052
24. BD (1) C 12 - C 21	/567. BD*(1) C 12 - H 35	0.66	1.04	0.023
24. BD (1) C 12 - C 21	/568. BD*(1) C 12 - H 36	0.54	1.04	0.021
24. BD (1) C 12 - C 21	/583. BD*(1) C 21 - C 22	1.52	1.12	0.037
24. BD (1) C 12 - C 21	/584. BD*(1) C 21 - C 23	3.69	1.31	0.062
24. BD (1) C 12 - C 21	/586. BD*(1) C 22 - C 24	1.40	1.32	0.038
24. BD (1) C 12 - C 21	/589. BD*(1) C 23 - C 25	3.28	1.13	0.054
25. BD (1) C 12 - H 35	/382. RY*(3) C 21	0.82	1.23	0.028
25. BD (1) C 12 - H 35	/566. BD*(1) C 12 - C 21	0.58	0.93	0.021
25. BD (1) C 12 - H 35	/584. BD*(1) C 21 - C 23	2.62	1.17	0.049
25. BD (1) C 12 - H 35	/585. BD*(2) C 21 - C 23	3.18	0.56	0.040
26. BD (1) C 12 - H 36	/381. RY*(2) C 21	0.67	1.65	0.030
26. BD (1) C 12 - H 36	/566. BD*(1) C 12 - C 21	0.52	0.94	0.020
26. BD (1) C 12 - H 36	/583. BD*(1) C 21 - C 22	4.83	0.98	0.062
27. BD (1) N 13 - C 14	/107. RY*(1) C 1	0.75	1.99	0.034
27. BD (1) N 13 - C 14	/108. RY*(2) C 1	0.77	2.10	0.036
27. BD (1) N 13 - C 14	/303. RY*(2) C 15	1.00	1.89	0.039
27. BD (1) N 13 - C 14	/544. BD*(1) C 1 - C 3	1.62	1.41	0.043
27. BD (1) N 13 - C 14	/546. BD*(1) C 1 - N 13	1.06	1.16	0.031
27. BD (1) N 13 - C 14	/574. BD*(1) C 15 - C 17	1.10	1.42	0.035
28. BD (1) N 13 - H 37	/107. RY*(1) C 1	1.09	1.85	0.040
28. BD (1) N 13 - H 37	/290. RY*(2) C 14	0.83	2.04	0.037
28. BD (1) N 13 - H 37	/292. RY*(4) C 14	0.91	3.07	0.047
28. BD (1) N 13 - H 37	/543. BD*(1) C 1 - C 2	2.11	1.10	0.043
28. BD (1) N 13 - H 37	/545. BD*(2) C 1 - C 3	1.53	0.69	0.031
28. BD (1) N 13 - H 37	/572. BD*(1) C 14 - O 16	2.95	1.18	0.053
29. BD (1) C 14 - C 15	/277. RY*(2) N 13	1.36	1.77	0.044
29. BD (1) C 14 - C 15	/315. RY*(1) O 16	0.63	1.86	0.031
29. BD (1) C 14 - C 15	/328. RY*(1) C 17	2.27	1.82	0.058
29. BD (1) C 14 - C 15	/546. BD*(1) C 1 - N 13	2.92	1.07	0.050
29. BD (1) C 14 - C 15	/572. BD*(1) C 14 - O 16	0.96	1.21	0.031
29. BD (1) C 14 - C 15	/574. BD*(1) C 15 - C 17	2.76	1.32	0.054
29. BD (1) C 14 - C 15	/577. BD*(1) C 17 - C 18	3.42	1.11	0.055
30. BD (1) C 14 - O 16	/289. RY*(1) C 14	1.66	1.88	0.050
30. BD (1) C 14 - O 16	/569. BD*(1) N 13 - C 14	0.54	1.36	0.025
30. BD (1) C 14 - O 16	/570. BD*(1) N 13 - H 37	1.15	1.34	0.035
30. BD (1) C 14 - O 16	/571. BD*(1) C 14 - C 15	1.56	1.43	0.043
30. BD (1) C 14 - O 16	/576. BD*(1) C 15 - H 27	0.86	1.42	0.031
31. BD (2) C 14 - O 16	/305. RY*(4) C 15	0.64	1.03	0.023
31. BD (2) C 14 - O 16	/573. BD*(2) C 14 - O 16	0.75	0.35	0.016
31. BD (2) C 14 - O 16	/575. BD*(2) C 15 - C 17	5.17	0.38	0.040
32. BD (1) C 15 - C 17	/289. RY*(1) C 14	2.15	1.66	0.053
32. BD (1) C 15 - C 17	/341. RY*(1) C 18	2.20	1.66	0.054
32. BD (1) C 15 - C 17	/569. BD*(1) N 13 - C 14	2.46	1.14	0.048
32. BD (1) C 15 - C 17	/571. BD*(1) C 14 - C 15	2.35	1.20	0.048

32. BD (1) C 15 - C 17	/576. BD*(1) C 15 - H 27	1.64	1.20	0.040
32. BD (1) C 15 - C 17	/577. BD*(1) C 17 - C 18	2.00	1.19	0.044
32. BD (1) C 15 - C 17	/578. BD*(1) C 17 - H 28	1.69	1.21	0.040
32. BD (1) C 15 - C 17	/579. BD*(1) C 18 - O 19	2.33	1.06	0.045
33. BD (2) C 15 - C 17	/293. RY*(5) C 14	0.76	1.57	0.032
33. BD (2) C 15 - C 17	/345. RY*(5) C 18	0.96	1.63	0.037
33. BD (2) C 15 - C 17	/573. BD*(2) C 14 - O 16	17.56	0.29	0.066
33. BD (2) C 15 - C 17	/581. BD*(2) C 18 - O 20	19.27	0.28	0.067
34. BD (1) C 15 - H 27	/290. RY*(2) C 14	0.64	1.93	0.031
34. BD (1) C 15 - H 27	/292. RY*(4) C 14	0.73	2.96	0.042
34. BD (1) C 15 - H 27	/328. RY*(1) C 17	1.01	1.67	0.037
34. BD (1) C 15 - H 27	/329. RY*(2) C 17	0.63	1.60	0.029
34. BD (1) C 15 - H 27	/572. BD*(1) C 14 - O 16	3.46	1.06	0.054
34. BD (1) C 15 - H 27	/574. BD*(1) C 15 - C 17	1.48	1.17	0.037
34. BD (1) C 15 - H 27	/578. BD*(1) C 17 - H 28	4.54	0.98	0.060
35. BD (1) C 17 - C 18	/302. RY*(1) C 15	2.14	1.74	0.055
35. BD (1) C 17 - C 18	/367. RY*(1) O 20	0.75	1.78	0.033
35. BD (1) C 17 - C 18	/571. BD*(1) C 14 - C 15	3.39	1.13	0.056
35. BD (1) C 17 - C 18	/574. BD*(1) C 15 - C 17	2.34	1.33	0.050
35. BD (1) C 17 - C 18	/580. BD*(1) C 18 - O 20	0.75	1.22	0.027
35. BD (1) C 17 - C 18	/582. BD*(1) O 19 - H 38	1.70	1.01	0.037
36. BD (1) C 17 - H 28	/302. RY*(1) C 15	1.05	1.57	0.036
36. BD (1) C 17 - H 28	/303. RY*(2) C 15	0.66	1.63	0.029
36. BD (1) C 17 - H 28	/344. RY*(4) C 18	0.69	2.81	0.040
36. BD (1) C 17 - H 28	/574. BD*(1) C 15 - C 17	1.67	1.16	0.039
36. BD (1) C 17 - H 28	/576. BD*(1) C 15 - H 27	4.95	0.96	0.062
36. BD (1) C 17 - H 28	/580. BD*(1) C 18 - O 20	3.24	1.05	0.052
37. BD (1) C 18 - O 19	/329. RY*(2) C 17	0.72	1.97	0.034
37. BD (1) C 18 - O 19	/574. BD*(1) C 15 - C 17	1.02	1.53	0.035
38. BD (1) C 18 - O 20	/329. RY*(2) C 17	0.58	2.06	0.031
38. BD (1) C 18 - O 20	/341. RY*(1) C 18	1.59	1.90	0.049
38. BD (1) C 18 - O 20	/577. BD*(1) C 17 - C 18	1.40	1.42	0.040
38. BD (1) C 18 - O 20	/578. BD*(1) C 17 - H 28	0.88	1.44	0.032
39. BD (2) C 18 - O 20	/331. RY*(4) C 17	0.64	0.96	0.022
39. BD (2) C 18 - O 20	/575. BD*(2) C 15 - C 17	5.11	0.39	0.040
39. BD (2) C 18 - O 20	/581. BD*(2) C 18 - O 20	0.73	0.35	0.015
40. BD (1) O 19 - H 38	/341. RY*(1) C 18	0.95	1.62	0.035
40. BD (1) O 19 - H 38	/342. RY*(2) C 18	0.73	2.04	0.035
40. BD (1) O 19 - H 38	/347. RY*(7) C 18	0.69	2.04	0.034
40. BD (1) O 19 - H 38	/577. BD*(1) C 17 - C 18	3.64	1.15	0.058
40. BD (1) O 19 - H 38	/580. BD*(1) C 18 - O 20	1.29	1.24	0.036
41. BD (1) C 21 - C 22	/263. RY*(1) C 12	1.25	1.30	0.036
41. BD (1) C 21 - C 22	/406. RY*(1) C 23	0.93	1.80	0.037
41. BD (1) C 21 - C 22	/419. RY*(1) C 24	0.90	1.92	0.037
41. BD (1) C 21 - C 22	/420. RY*(2) C 24	1.68	2.10	0.053
41. BD (1) C 21 - C 22	/566. BD*(1) C 12 - C 21	1.52	1.06	0.036
41. BD (1) C 21 - C 22	/568. BD*(1) C 12 - H 36	1.12	1.02	0.030
41. BD (1) C 21 - C 22	/584. BD*(1) C 21 - C 23	3.67	1.29	0.062
41. BD (1) C 21 - C 22	/586. BD*(1) C 22 - C 24	3.17	1.30	0.058
41. BD (1) C 21 - C 22	/588. BD*(1) C 22 - H 39	0.61	1.09	0.023
41. BD (1) C 21 - C 22	/590. BD*(1) C 23 - H 40	3.34	1.08	0.054
41. BD (1) C 21 - C 22	/592. BD*(1) C 24 - H 41	2.98	1.09	0.051
42. BD (1) C 21 - C 23	/263. RY*(1) C 12	0.91	1.40	0.032
42. BD (1) C 21 - C 23	/393. RY*(1) C 22	0.81	1.89	0.035
42. BD (1) C 21 - C 23	/432. RY*(1) C 25	0.99	2.03	0.040

42. BD (1) C 21 - C 23	/433. RY*(2) C 25	1.06	2.19	0.043
42. BD (1) C 21 - C 23	/565. BD*(1)Se 11 - C 12	0.83	0.84	0.023
42. BD (1) C 21 - C 23	/566. BD*(1) C 12 - C 21	3.53	1.16	0.057
42. BD (1) C 21 - C 23	/583. BD*(1) C 21 - C 22	3.50	1.20	0.058
42. BD (1) C 21 - C 23	/588. BD*(1) C 22 - H 39	1.56	1.19	0.039
42. BD (1) C 21 - C 23	/589. BD*(1) C 23 - C 25	2.95	1.21	0.053
42. BD (1) C 21 - C 23	/590. BD*(1) C 23 - H 40	1.81	1.18	0.041
42. BD (1) C 21 - C 23	/595. BD*(1) C 25 - H 42	1.39	1.19	0.036
43. BD (2) C 21 - C 23	/395. RY*(3) C 22	1.46	0.99	0.036
43. BD (2) C 21 - C 23	/434. RY*(3) C 25	1.38	1.12	0.037
43. BD (2) C 21 - C 23	/565. BD*(1)Se 11 - C 12	4.56	0.37	0.039
43. BD (2) C 21 - C 23	/567. BD*(1) C 12 - H 35	2.66	0.65	0.039
43. BD (2) C 21 - C 23	/587. BD*(2) C 22 - C 24	12.42	0.32	0.056
43. BD (2) C 21 - C 23	/594. BD*(2) C 25 - C 26	13.26	0.32	0.058
44. BD (1) C 22 - C 24	/380. RY*(1) C 21	1.41	2.04	0.048
44. BD (1) C 22 - C 24	/381. RY*(2) C 21	0.78	1.87	0.034
44. BD (1) C 22 - C 24	/445. RY*(1) C 26	0.87	2.03	0.038
44. BD (1) C 22 - C 24	/446. RY*(2) C 26	0.96	2.18	0.041
44. BD (1) C 22 - C 24	/566. BD*(1) C 12 - C 21	2.68	1.16	0.050
44. BD (1) C 22 - C 24	/583. BD*(1) C 21 - C 22	3.18	1.20	0.055
44. BD (1) C 22 - C 24	/588. BD*(1) C 22 - H 39	1.63	1.19	0.039
44. BD (1) C 22 - C 24	/591. BD*(1) C 24 - C 26	2.54	1.21	0.050
44. BD (1) C 22 - C 24	/592. BD*(1) C 24 - H 41	1.62	1.19	0.039
44. BD (1) C 22 - C 24	/596. BD*(1) C 26 - H 43	1.56	1.19	0.038
45. BD (2) C 22 - C 24	/447. RY*(3) C 26	1.43	0.96	0.035
45. BD (2) C 22 - C 24	/585. BD*(2) C 21 - C 23	13.88	0.32	0.059
45. BD (2) C 22 - C 24	/594. BD*(2) C 25 - C 26	13.17	0.31	0.058
46. BD (1) C 22 - H 39	/380. RY*(1) C 21	1.57	1.82	0.048
46. BD (1) C 22 - H 39	/419. RY*(1) C 24	1.60	1.80	0.048
46. BD (1) C 22 - H 39	/584. BD*(1) C 21 - C 23	3.18	1.17	0.054
46. BD (1) C 22 - H 39	/586. BD*(1) C 22 - C 24	1.45	1.18	0.037
46. BD (1) C 22 - H 39	/591. BD*(1) C 24 - C 26	5.18	0.99	0.064
46. BD (1) C 22 - H 39	/592. BD*(1) C 24 - H 41	0.86	0.97	0.026
47. BD (1) C 23 - C 25	/381. RY*(2) C 21	1.77	1.77	0.050
47. BD (1) C 23 - C 25	/445. RY*(1) C 26	0.70	1.93	0.033
47. BD (1) C 23 - C 25	/446. RY*(2) C 26	1.60	2.08	0.052
47. BD (1) C 23 - C 25	/566. BD*(1) C 12 - C 21	5.18	1.06	0.066
47. BD (1) C 23 - C 25	/584. BD*(1) C 21 - C 23	3.49	1.29	0.060
47. BD (1) C 23 - C 25	/593. BD*(1) C 25 - C 26	2.80	1.30	0.054
47. BD (1) C 23 - C 25	/595. BD*(1) C 25 - H 42	0.52	1.09	0.021
47. BD (1) C 23 - C 25	/596. BD*(1) C 26 - H 43	3.22	1.09	0.053
48. BD (1) C 23 - H 40	/380. RY*(1) C 21	2.22	1.82	0.057
48. BD (1) C 23 - H 40	/432. RY*(1) C 25	1.24	1.81	0.043
48. BD (1) C 23 - H 40	/583. BD*(1) C 21 - C 22	6.02	0.98	0.069
48. BD (1) C 23 - H 40	/584. BD*(1) C 21 - C 23	1.80	1.17	0.041
48. BD (1) C 23 - H 40	/593. BD*(1) C 25 - C 26	2.42	1.18	0.048
49. BD (1) C 24 - C 26	/394. RY*(2) C 22	2.07	1.74	0.054
49. BD (1) C 24 - C 26	/432. RY*(1) C 25	0.71	1.93	0.033
49. BD (1) C 24 - C 26	/433. RY*(2) C 25	1.63	2.09	0.052
49. BD (1) C 24 - C 26	/586. BD*(1) C 22 - C 24	2.86	1.30	0.055
49. BD (1) C 24 - C 26	/588. BD*(1) C 22 - H 39	3.27	1.09	0.053
49. BD (1) C 24 - C 26	/592. BD*(1) C 24 - H 41	0.52	1.09	0.021
49. BD (1) C 24 - C 26	/593. BD*(1) C 25 - C 26	2.81	1.30	0.054
49. BD (1) C 24 - C 26	/595. BD*(1) C 25 - H 42	3.26	1.09	0.053
49. BD (1) C 24 - C 26	/596. BD*(1) C 26 - H 43	0.53	1.09	0.021

50. BD (1) C 24 - H 41	/393. RY*(1) C 22	1.45	1.67	0.044
50. BD (1) C 24 - H 41	/445. RY*(1) C 26	1.26	1.81	0.043
50. BD (1) C 24 - H 41	/583. BD*(1) C 21 - C 22	5.51	0.98	0.066
50. BD (1) C 24 - H 41	/586. BD*(1) C 22 - C 24	1.35	1.18	0.036
50. BD (1) C 24 - H 41	/588. BD*(1) C 22 - H 39	0.85	0.97	0.026
50. BD (1) C 24 - H 41	/593. BD*(1) C 25 - C 26	2.52	1.18	0.049
51. BD (1) C 25 - C 26	/406. RY*(1) C 23	0.59	1.91	0.030
51. BD (1) C 25 - C 26	/407. RY*(2) C 23	1.45	1.97	0.048
51. BD (1) C 25 - C 26	/419. RY*(1) C 24	0.88	2.03	0.038
51. BD (1) C 25 - C 26	/420. RY*(2) C 24	1.00	2.21	0.042
51. BD (1) C 25 - C 26	/589. BD*(1) C 23 - C 25	2.52	1.21	0.049
51. BD (1) C 25 - C 26	/590. BD*(1) C 23 - H 40	1.55	1.18	0.038
51. BD (1) C 25 - C 26	/591. BD*(1) C 24 - C 26	2.51	1.21	0.049
51. BD (1) C 25 - C 26	/592. BD*(1) C 24 - H 41	1.59	1.19	0.039
51. BD (1) C 25 - C 26	/595. BD*(1) C 25 - H 42	1.61	1.19	0.039
51. BD (1) C 25 - C 26	/596. BD*(1) C 26 - H 43	1.62	1.19	0.039
52. BD (2) C 25 - C 26	/408. RY*(3) C 23	1.11	0.82	0.028
52. BD (2) C 25 - C 26	/421. RY*(3) C 24	1.36	1.08	0.036
52. BD (2) C 25 - C 26	/585. BD*(2) C 21 - C 23	12.94	0.31	0.057
52. BD (2) C 25 - C 26	/587. BD*(2) C 22 - C 24	13.29	0.31	0.058
53. BD (1) C 25 - H 42	/406. RY*(1) C 23	1.14	1.68	0.039
53. BD (1) C 25 - H 42	/445. RY*(1) C 26	1.63	1.81	0.049
53. BD (1) C 25 - H 42	/584. BD*(1) C 21 - C 23	2.63	1.17	0.049
53. BD (1) C 25 - H 42	/591. BD*(1) C 24 - C 26	5.29	0.99	0.065
53. BD (1) C 25 - H 42	/593. BD*(1) C 25 - C 26	1.33	1.18	0.035
53. BD (1) C 25 - H 42	/596. BD*(1) C 26 - H 43	0.86	0.97	0.026
54. BD (1) C 26 - H 43	/419. RY*(1) C 24	1.32	1.80	0.044
54. BD (1) C 26 - H 43	/432. RY*(1) C 25	1.71	1.81	0.050
54. BD (1) C 26 - H 43	/586. BD*(1) C 22 - C 24	2.55	1.18	0.049
54. BD (1) C 26 - H 43	/589. BD*(1) C 23 - C 25	5.33	0.99	0.065
54. BD (1) C 26 - H 43	/593. BD*(1) C 25 - C 26	1.33	1.18	0.035
54. BD (1) C 26 - H 43	/595. BD*(1) C 25 - H 42	0.86	0.97	0.026
55. CR (1) C 1	/121. RY*(2) C 2	0.95	11.45	0.093
55. CR (1) C 1	/134. RY*(2) C 3	1.71	11.41	0.125
55. CR (1) C 1	/135. RY*(3) C 3	0.51	11.03	0.067
55. CR (1) C 1	/544. BD*(1) C 1 - C 3	1.37	10.73	0.109
55. CR (1) C 1	/547. BD*(1) C 2 - C 4	0.57	10.77	0.070
55. CR (1) C 1	/550. BD*(1) C 3 - C 5	1.03	10.56	0.094
55. CR (1) C 1	/551. BD*(1) C 3 - C 7	1.11	10.53	0.098
55. CR (1) C 1	/569. BD*(1) N 13 - C 14	1.03	10.47	0.095
56. CR (1) C 2	/108. RY*(2) C 1	1.36	11.36	0.111
56. CR (1) C 2	/146. RY*(1) C 4	0.60	11.21	0.073
56. CR (1) C 2	/147. RY*(2) C 4	1.75	11.21	0.125
56. CR (1) C 2	/544. BD*(1) C 1 - C 3	0.83	10.67	0.084
56. CR (1) C 2	/546. BD*(1) C 1 - N 13	0.54	10.42	0.068
56. CR (1) C 2	/547. BD*(1) C 2 - C 4	0.83	10.71	0.084
56. CR (1) C 2	/552. BD*(1) C 4 - C 6	1.30	10.51	0.105
57. CR (1) C 3	/107. RY*(1) C 1	1.16	11.27	0.102
57. CR (1) C 3	/109. RY*(3) C 1	0.98	11.32	0.094
57. CR (1) C 3	/160. RY*(2) C 5	0.74	11.04	0.081
57. CR (1) C 3	/186. RY*(2) C 7	0.60	11.51	0.074
57. CR (1) C 3	/191. RY*(7) C 7	0.83	11.19	0.086
57. CR (1) C 3	/543. BD*(1) C 1 - C 2	1.09	10.52	0.096
57. CR (1) C 3	/544. BD*(1) C 1 - C 3	1.23	10.69	0.103
57. CR (1) C 3	/546. BD*(1) C 1 - N 13	1.03	10.44	0.093

57. CR (1) C 3	/554. BD*(1) C 5 - C 6	0.72	10.72	0.079
57. CR (1) C 3	/558. BD*(1) C 7 - O 8	0.61	10.35	0.073
58. CR (1) C 4	/121. RY*(2) C 2	1.34	11.39	0.110
58. CR (1) C 4	/123. RY*(4) C 2	0.65	11.08	0.076
58. CR (1) C 4	/173. RY*(2) C 6	1.28	10.88	0.106
58. CR (1) C 4	/175. RY*(4) C 6	0.67	11.13	0.077
58. CR (1) C 4	/543. BD*(1) C 1 - C 2	1.21	10.49	0.101
58. CR (1) C 4	/547. BD*(1) C 2 - C 4	0.67	10.70	0.076
58. CR (1) C 4	/554. BD*(1) C 5 - C 6	0.82	10.70	0.084
58. CR (1) C 4	/557. BD*(1) C 6 -Se 11	0.82	10.18	0.082
59. CR (1) C 5	/134. RY*(2) C 3	0.76	11.34	0.083
59. CR (1) C 5	/172. RY*(1) C 6	1.14	11.12	0.101
59. CR (1) C 5	/173. RY*(2) C 6	1.84	10.88	0.126
59. CR (1) C 5	/174. RY*(3) C 6	0.55	10.93	0.069
59. CR (1) C 5	/544. BD*(1) C 1 - C 3	0.77	10.66	0.081
59. CR (1) C 5	/551. BD*(1) C 3 - C 7	0.66	10.46	0.075
59. CR (1) C 5	/552. BD*(1) C 4 - C 6	1.23	10.51	0.102
59. CR (1) C 5	/554. BD*(1) C 5 - C 6	1.21	10.70	0.102
59. CR (1) C 5	/557. BD*(1) C 6 -Se 11	1.25	10.18	0.102
60. CR (1) C 6	/147. RY*(2) C 4	1.02	11.25	0.096
60. CR (1) C 6	/160. RY*(2) C 5	2.08	11.05	0.136
60. CR (1) C 6	/162. RY*(4) C 5	0.65	11.16	0.076
60. CR (1) C 6	/547. BD*(1) C 2 - C 4	0.63	10.74	0.074
60. CR (1) C 6	/550. BD*(1) C 3 - C 5	1.18	10.53	0.100
60. CR (1) C 6	/554. BD*(1) C 5 - C 6	1.21	10.73	0.102
60. CR (1) C 6	/556. BD*(1) C 5 - H 31	0.55	10.54	0.068
60. CR (1) C 6	/557. BD*(1) C 6 -Se 11	1.28	10.22	0.103
61. CR (1) C 7	/133. RY*(1) C 3	1.20	12.05	0.108
61. CR (1) C 7	/544. BD*(1) C 1 - C 3	0.87	10.83	0.087
61. CR (1) C 7	/550. BD*(1) C 3 - C 5	0.54	10.66	0.068
61. CR (1) C 7	/551. BD*(1) C 3 - C 7	0.56	10.63	0.069
61. CR (1) C 7	/558. BD*(1) C 7 - O 8	0.67	10.49	0.077
61. CR (1) C 7	/561. BD*(1) O 8 - C 10	1.11	10.48	0.096
62. CR (1) O 8	/185. RY*(1) C 7	1.01	19.92	0.127
62. CR (1) O 8	/186. RY*(2) C 7	1.11	20.42	0.135
62. CR (1) O 8	/226. RY*(3) C 10	0.91	19.96	0.121
63. CR (1) O 9	/185. RY*(1) C 7	5.27	19.81	0.290
63. CR (1) O 9	/551. BD*(1) C 3 - C 7	0.79	19.29	0.111
64. CR (1) C 10	/494. RY*(2) H 34	0.60	12.19	0.076
64. CR (1) C 10	/558. BD*(1) C 7 - O 8	1.10	10.40	0.098
64. CR (1) C 10	/561. BD*(1) O 8 - C 10	1.49	10.39	0.111
67. CR (3)Se 11	/172. RY*(1) C 6	0.96	11.34	0.093
67. CR (3)Se 11	/552. BD*(1) C 4 - C 6	0.76	10.73	0.081
67. CR (3)Se 11	/554. BD*(1) C 5 - C 6	1.24	10.91	0.104
79. CR (1) C 12	/380. RY*(1) C 21	0.92	11.39	0.091
79. CR (1) C 12	/384. RY*(5) C 21	0.61	11.17	0.074
79. CR (1) C 12	/565. BD*(1)Se 11 - C 12	1.23	10.19	0.100
79. CR (1) C 12	/583. BD*(1) C 21 - C 22	0.71	10.55	0.078
79. CR (1) C 12	/584. BD*(1) C 21 - C 23	0.79	10.74	0.083
80. CR (1) N 13	/107. RY*(1) C 1	1.10	15.41	0.117
80. CR (1) N 13	/108. RY*(2) C 1	0.54	15.52	0.082
80. CR (1) N 13	/290. RY*(2) C 14	1.43	15.60	0.133
80. CR (1) N 13	/544. BD*(1) C 1 - C 3	0.59	14.83	0.084
81. CR (1) C 14	/303. RY*(2) C 15	0.56	11.28	0.071
81. CR (1) C 14	/546. BD*(1) C 1 - N 13	1.15	10.56	0.099

81. CR (1) C 14	/574. BD*(1) C 15 - C 17	0.65	10.81	0.075
82. CR (1) C 15	/290. RY*(2) C 14	1.07	11.46	0.099
82. CR (1) C 15	/329. RY*(2) C 17	1.86	11.14	0.129
82. CR (1) C 15	/330. RY*(3) C 17	0.53	11.25	0.069
82. CR (1) C 15	/569. BD*(1) N 13 - C 14	0.51	10.44	0.066
82. CR (1) C 15	/574. BD*(1) C 15 - C 17	0.66	10.70	0.075
82. CR (1) C 15	/577. BD*(1) C 17 - C 18	1.06	10.50	0.095
83. CR (1) O 16	/289. RY*(1) C 14	5.52	19.74	0.296
83. CR (1) O 16	/571. BD*(1) C 14 - C 15	0.75	19.28	0.109
84. CR (1) C 17	/303. RY*(2) C 15	1.59	11.17	0.119
84. CR (1) C 17	/304. RY*(3) C 15	0.70	11.38	0.080
84. CR (1) C 17	/342. RY*(2) C 18	0.78	11.39	0.084
84. CR (1) C 17	/347. RY*(7) C 18	0.58	11.39	0.072
84. CR (1) C 17	/571. BD*(1) C 14 - C 15	1.08	10.50	0.096
84. CR (1) C 17	/574. BD*(1) C 15 - C 17	0.72	10.70	0.079
84. CR (1) C 17	/576. BD*(1) C 15 - H 27	0.53	10.50	0.067
85. CR (1) C 18	/329. RY*(2) C 17	0.55	11.28	0.070
85. CR (1) C 18	/574. BD*(1) C 15 - C 17	0.63	10.84	0.074
85. CR (1) C 18	/579. BD*(1) C 18 - O 19	0.63	10.51	0.075
86. CR (1) O 19	/341. RY*(1) C 18	0.80	19.88	0.113
86. CR (1) O 19	/342. RY*(2) C 18	1.53	20.30	0.158
86. CR (1) O 19	/344. RY*(4) C 18	0.63	21.26	0.104
86. CR (1) O 19	/516. RY*(4) H 38	0.56	20.96	0.097
87. CR (1) O 20	/341. RY*(1) C 18	5.57	19.77	0.298
87. CR (1) O 20	/577. BD*(1) C 17 - C 18	0.75	19.29	0.109
88. CR (1) C 21	/265. RY*(3) C 12	0.71	11.16	0.080
88. CR (1) C 21	/394. RY*(2) C 22	1.10	11.15	0.099
88. CR (1) C 21	/407. RY*(2) C 23	2.19	11.28	0.141
88. CR (1) C 21	/584. BD*(1) C 21 - C 23	1.01	10.71	0.093
88. CR (1) C 21	/586. BD*(1) C 22 - C 24	0.58	10.71	0.071
88. CR (1) C 21	/589. BD*(1) C 23 - C 25	1.02	10.52	0.093
88. CR (1) C 21	/590. BD*(1) C 23 - H 40	0.54	10.50	0.068
89. CR (1) C 22	/381. RY*(2) C 21	1.31	11.17	0.108
89. CR (1) C 22	/420. RY*(2) C 24	2.12	11.50	0.140
89. CR (1) C 22	/566. BD*(1) C 12 - C 21	0.75	10.46	0.079
89. CR (1) C 22	/584. BD*(1) C 21 - C 23	0.76	10.69	0.081
89. CR (1) C 22	/586. BD*(1) C 22 - C 24	0.76	10.70	0.080
89. CR (1) C 22	/591. BD*(1) C 24 - C 26	1.06	10.51	0.095
90. CR (1) C 23	/380. RY*(1) C 21	1.31	11.34	0.109
90. CR (1) C 23	/381. RY*(2) C 21	1.68	11.17	0.122
90. CR (1) C 23	/433. RY*(2) C 25	0.79	11.49	0.085
90. CR (1) C 23	/524. RY*(2) H 40	0.51	12.36	0.071
90. CR (1) C 23	/566. BD*(1) C 12 - C 21	1.39	10.46	0.108
90. CR (1) C 23	/583. BD*(1) C 21 - C 22	1.21	10.50	0.101
90. CR (1) C 23	/584. BD*(1) C 21 - C 23	0.93	10.69	0.090
90. CR (1) C 23	/593. BD*(1) C 25 - C 26	0.62	10.70	0.073
91. CR (1) C 24	/393. RY*(1) C 22	0.62	11.20	0.074
91. CR (1) C 24	/394. RY*(2) C 22	0.85	11.14	0.087
91. CR (1) C 24	/396. RY*(4) C 22	1.12	11.28	0.101
91. CR (1) C 24	/446. RY*(2) C 26	0.80	11.48	0.086
91. CR (1) C 24	/529. RY*(2) H 41	0.56	12.29	0.074
91. CR (1) C 24	/583. BD*(1) C 21 - C 22	1.19	10.50	0.101
91. CR (1) C 24	/586. BD*(1) C 22 - C 24	0.79	10.70	0.082
91. CR (1) C 24	/588. BD*(1) C 22 - H 39	0.51	10.49	0.066
91. CR (1) C 24	/593. BD*(1) C 25 - C 26	0.63	10.70	0.073

92. CR (1) C 25	/410. RY*(5) C 23	0.65	11.15	0.076
92. CR (1) C 25	/446. RY*(2) C 26	2.11	11.48	0.139
92. CR (1) C 25	/534. RY*(2) H 42	0.55	12.28	0.073
92. CR (1) C 25	/584. BD*(1) C 21 - C 23	0.70	10.69	0.077
92. CR (1) C 25	/591. BD*(1) C 24 - C 26	1.07	10.51	0.095
92. CR (1) C 25	/593. BD*(1) C 25 - C 26	0.80	10.70	0.083
92. CR (1) C 25	/596. BD*(1) C 26 - H 43	0.50	10.49	0.065
93. CR (1) C 26	/420. RY*(2) C 24	0.76	11.51	0.084
93. CR (1) C 26	/423. RY*(5) C 24	0.50	10.97	0.066
93. CR (1) C 26	/433. RY*(2) C 25	2.09	11.49	0.139
93. CR (1) C 26	/539. RY*(2) H 43	0.55	12.28	0.074
93. CR (1) C 26	/586. BD*(1) C 22 - C 24	0.63	10.70	0.074
93. CR (1) C 26	/589. BD*(1) C 23 - C 25	1.07	10.51	0.095
93. CR (1) C 26	/593. BD*(1) C 25 - C 26	0.79	10.70	0.082
93. CR (1) C 26	/595. BD*(1) C 25 - H 42	0.50	10.49	0.065
94. LP (1) O 8	/185. RY*(1) C 7	1.66	1.51	0.045
94. LP (1) O 8	/188. RY*(4) C 7	1.61	2.61	0.058
94. LP (1) O 8	/224. RY*(1) C 10	1.64	1.65	0.047
94. LP (1) O 8	/226. RY*(3) C 10	0.79	1.55	0.031
94. LP (1) O 8	/559. BD*(1) C 7 - O 9	5.70	1.08	0.070
94. LP (1) O 8	/562. BD*(1) C 10 - H 32	0.63	0.95	0.022
94. LP (1) O 8	/564. BD*(1) C 10 - H 34	2.37	0.95	0.043
95. LP (2) O 8	/187. RY*(3) C 7	1.80	1.84	0.054
95. LP (2) O 8	/225. RY*(2) C 10	1.51	1.50	0.045
95. LP (2) O 8	/560. BD*(2) C 7 - O 9	38.57	0.31	0.100
95. LP (2) O 8	/562. BD*(1) C 10 - H 32	5.05	0.70	0.056
95. LP (2) O 8	/563. BD*(1) C 10 - H 33	5.04	0.70	0.055
96. LP (1) O 9	/185. RY*(1) C 7	12.35	1.65	0.127
96. LP (1) O 9	/195. RY*(11) C 7	0.75	5.01	0.055
96. LP (1) O 9	/551. BD*(1) C 3 - C 7	2.25	1.13	0.045
96. LP (1) O 9	/558. BD*(1) C 7 - O 8	0.99	0.99	0.029
97. LP (2) O 9	/186. RY*(2) C 7	1.93	1.70	0.053
97. LP (2) O 9	/188. RY*(4) C 7	1.71	2.29	0.058
97. LP (2) O 9	/551. BD*(1) C 3 - C 7	12.44	0.68	0.084
97. LP (2) O 9	/558. BD*(1) C 7 - O 8	28.86	0.55	0.113
97. LP (2) O 9	/564. BD*(1) C 10 - H 34	0.80	0.64	0.021
98. LP (1)Se 11	/172. RY*(1) C 6	1.18	1.78	0.041
98. LP (1)Se 11	/554. BD*(1) C 5 - C 6	3.32	1.35	0.060
99. LP (2)Se 11	/552. BD*(1) C 4 - C 6	1.69	0.69	0.031
99. LP (2)Se 11	/554. BD*(1) C 5 - C 6	1.16	0.87	0.029
99. LP (2)Se 11	/555. BD*(2) C 5 - C 6	9.14	0.26	0.045
99. LP (2)Se 11	/567. BD*(1) C 12 - H 35	2.40	0.61	0.035
99. LP (2)Se 11	/568. BD*(1) C 12 - H 36	3.93	0.61	0.045
100. LP (1) N 13	/109. RY*(3) C 1	1.10	1.51	0.040
100. LP (1) N 13	/110. RY*(4) C 1	0.73	1.59	0.033
100. LP (1) N 13	/291. RY*(3) C 14	1.60	1.73	0.051
100. LP (1) N 13	/509. RY*(2) H 37	0.75	1.95	0.037
100. LP (1) N 13	/543. BD*(1) C 1 - C 2	3.65	0.71	0.049
100. LP (1) N 13	/544. BD*(1) C 1 - C 3	2.68	0.89	0.047
100. LP (1) N 13	/545. BD*(2) C 1 - C 3	17.63	0.30	0.065
100. LP (1) N 13	/573. BD*(2) C 14 - O 16	50.66	0.26	0.102
101. LP (1) O 16	/289. RY*(1) C 14	13.16	1.58	0.129
101. LP (1) O 16	/569. BD*(1) N 13 - C 14	1.20	1.06	0.032
101. LP (1) O 16	/571. BD*(1) C 14 - C 15	2.18	1.13	0.045
102. LP (2) O 16	/290. RY*(2) C 14	1.39	1.64	0.044

102. LP (2) O 16	/292. RY*(4) C 14	1.82	2.67	0.064
102. LP (2) O 16	/569. BD*(1) N 13 - C 14	23.94	0.62	0.110
102. LP (2) O 16	/571. BD*(1) C 14 - C 15	14.74	0.68	0.091
103. LP (1) O 19	/341. RY*(1) C 18	2.39	1.52	0.054
103. LP (1) O 19	/344. RY*(4) C 18	1.67	2.90	0.062
103. LP (1) O 19	/515. RY*(3) H 38	1.30	2.29	0.049
103. LP (1) O 19	/580. BD*(1) C 18 - O 20	5.36	1.14	0.070
104. LP (2) O 19	/343. RY*(3) C 18	2.03	1.86	0.057
104. LP (2) O 19	/514. RY*(2) H 38	1.57	1.81	0.050
104. LP (2) O 19	/581. BD*(2) C 18 - O 20	40.53	0.32	0.103
105. LP (1) O 20	/341. RY*(1) C 18	13.29	1.61	0.131
105. LP (1) O 20	/352. RY*(12) C 18	0.51	4.87	0.045
105. LP (1) O 20	/577. BD*(1) C 17 - C 18	2.18	1.14	0.045
105. LP (1) O 20	/579. BD*(1) C 18 - O 19	0.84	1.01	0.026
106. LP (2) O 20	/342. RY*(2) C 18	2.68	1.59	0.060
106. LP (2) O 20	/344. RY*(4) C 18	1.04	2.54	0.048
106. LP (2) O 20	/577. BD*(1) C 17 - C 18	13.34	0.69	0.087
106. LP (2) O 20	/579. BD*(1) C 18 - O 19	27.86	0.56	0.112
545. BD*(2) C 1 - C 3	/111. RY*(5) C 1	1.03	1.34	0.084
545. BD*(2) C 1 - C 3	/136. RY*(4) C 3	0.91	0.75	0.059
545. BD*(2) C 1 - C 3	/548. BD*(2) C 2 - C 4	119.88	0.01	0.072
545. BD*(2) C 1 - C 3	/558. BD*(1) C 7 - O 8	0.83	0.25	0.028
545. BD*(2) C 1 - C 3	/569. BD*(1) N 13 - C 14	0.69	0.33	0.031
545. BD*(2) C 1 - C 3	/570. BD*(1) N 13 - H 37	0.96	0.31	0.038
548. BD*(2) C 2 - C 4	/122. RY*(3) C 2	0.77	0.68	0.068
548. BD*(2) C 2 - C 4	/150. RY*(5) C 4	0.85	1.36	0.101
555. BD*(2) C 5 - C 6	/161. RY*(3) C 5	2.57	0.54	0.094
555. BD*(2) C 5 - C 6	/174. RY*(3) C 6	0.55	0.85	0.055
555. BD*(2) C 5 - C 6	/565. BD*(1)Se 11 - C 12	1.23	0.07	0.023
558. BD*(1) C 7 - O 8	/186. RY*(2) C 7	1.61	1.15	0.163
558. BD*(1) C 7 - O 8	/198. RY*(1) O 8	0.56	1.05	0.094
558. BD*(1) C 7 - O 8	/550. BD*(1) C 3 - C 5	1.05	0.17	0.046
558. BD*(1) C 7 - O 8	/551. BD*(1) C 3 - C 7	0.80	0.14	0.034
558. BD*(1) C 7 - O 8	/559. BD*(1) C 7 - O 9	0.53	0.22	0.039
560. BD*(2) C 7 - O 9	/187. RY*(3) C 7	1.51	1.53	0.119
560. BD*(2) C 7 - O 9	/212. RY*(2) O 9	1.10	0.98	0.082
560. BD*(2) C 7 - O 9	/545. BD*(2) C 1 - C 3	34.78	0.05	0.068
573. BD*(2) C 14 - O 16	/291. RY*(3) C 14	1.52	1.47	0.107
573. BD*(2) C 14 - O 16	/295. RY*(7) C 14	1.46	1.04	0.089
573. BD*(2) C 14 - O 16	/316. RY*(2) O 16	1.41	1.02	0.087
573. BD*(2) C 14 - O 16	/575. BD*(2) C 15 - C 17	47.13	0.03	0.076
581. BD*(2) C 18 - O 20	/343. RY*(3) C 18	1.60	1.54	0.123
581. BD*(2) C 18 - O 20	/349. RY*(9) C 18	1.00	0.75	0.069
581. BD*(2) C 18 - O 20	/368. RY*(2) O 20	1.01	1.02	0.080
581. BD*(2) C 18 - O 20	/575. BD*(2) C 15 - C 17	29.42	0.04	0.075
585. BD*(2) C 21 - C 23	/383. RY*(4) C 21	0.61	1.47	0.077
585. BD*(2) C 21 - C 23	/408. RY*(3) C 23	2.45	0.50	0.090
585. BD*(2) C 21 - C 23	/557. BD*(1) C 6 -Se 11	0.52	0.08	0.016
585. BD*(2) C 21 - C 23	/565. BD*(1)Se 11 - C 12	4.81	0.05	0.039
585. BD*(2) C 21 - C 23	/567. BD*(1) C 12 - H 35	0.69	0.33	0.037
587. BD*(2) C 22 - C 24	/395. RY*(3) C 22	0.81	0.67	0.065
587. BD*(2) C 22 - C 24	/397. RY*(5) C 22	0.54	1.52	0.081
587. BD*(2) C 22 - C 24	/422. RY*(4) C 24	0.71	1.42	0.090
594. BD*(2) C 25 - C 26	/435. RY*(4) C 25	0.83	1.38	0.094
594. BD*(2) C 25 - C 26	/447. RY*(3) C 26	0.88	0.65	0.066

594. BD*(2) C 25 - C 26 /448. RY*(4) C 26 0.57 1.52 0.081

NATURAL BOND ORBITAL ANALYSIS:

Cycle	Occ. Thresh.	Occupancies Lewis	Occupancies Non-Lewis	Lewis Structure CR	BD	3C	LP	Low occ (L)	High occ (NL)	Dev
1(1)	1.90	201.80567	10.19433	39	51	0	16	20	14	0.81
2(2)	1.90	201.80567	10.19433	39	51	0	16	20	14	0.81
3(1)	1.80	203.68901	8.31099	39	48	0	19	7	10	0.64
4(2)	1.80	203.68901	8.31099	39	48	0	19	7	10	0.64
5(1)	1.70	207.62517	4.37483	39	54	0	13	1	10	0.49
6(2)	1.70	208.20560	3.79440	39	54	0	13	1	10	0.25
7(3)	1.70	208.20560	3.79440	39	54	0	13	1	10	0.25
8(1)	1.60	208.21104	3.78896	39	54	0	13	0	10	0.25
9(2)	1.60	208.21104	3.78896	39	54	0	13	0	10	0.25
10(1)	1.50	206.90575	5.09425	39	53	0	14	0	12	0.74
11(2)	1.50	206.90575	5.09425	39	53	0	14	0	12	0.74
12(1)	1.60	208.21104	3.78896	39	54	0	13	0	10	0.25

Core	77.97695 (99.970% of 78)
Valence Lewis	130.23409 (97.190% of 134)
Total Lewis	208.21104 (98.213% of 212)
Valence non-Lewis	3.40183 (1.605% of 212)
Rydberg non-Lewis	0.38713 (0.183% of 212)
Total non-Lewis	3.78896 (1.787% of 212)

Compound 10

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 2	/134. RY*(1) C 3	0.80	2.50	0.040
1. BD (1) C 1 - C 2	/135. RY*(2) C 3	0.67	1.95	0.033
1. BD (1) C 1 - C 2	/148. RY*(2) C 4	2.14	1.82	0.056
1. BD (1) C 1 - C 2	/277. RY*(1) N 13	0.89	1.52	0.033

1. BD (1) C 1 - C 2	/555. BD*(1) C 1 - C 3	4.22	1.27	0.065
1. BD (1) C 1 - C 2	/557. BD*(1) C 1 - N 13	0.58	1.03	0.022
1. BD (1) C 1 - C 2	/558. BD*(1) C 2 - C 4	2.95	1.31	0.056
1. BD (1) C 1 - C 2	/560. BD*(1) C 2 - H 25	0.62	1.10	0.023
1. BD (1) C 1 - C 2	/562. BD*(1) C 3 - C 7	4.39	1.07	0.062
1. BD (1) C 1 - C 2	/564. BD*(1) C 4 - H 26	2.83	1.10	0.050
1. BD (1) C 1 - C 2	/581. BD*(1) N 13 - H 33	1.59	1.00	0.036
2. BD (1) C 1 - C 3	/121. RY*(1) C 2	0.74	2.01	0.035
2. BD (1) C 1 - C 3	/160. RY*(1) C 5	0.59	1.90	0.030
2. BD (1) C 1 - C 3	/189. RY*(4) C 7	0.58	2.79	0.036
2. BD (1) C 1 - C 3	/277. RY*(1) N 13	0.67	1.62	0.029
2. BD (1) C 1 - C 3	/554. BD*(1) C 1 - C 2	3.45	1.20	0.057
2. BD (1) C 1 - C 3	/557. BD*(1) C 1 - N 13	2.09	1.12	0.043
2. BD (1) C 1 - C 3	/560. BD*(1) C 2 - H 25	1.31	1.20	0.035
2. BD (1) C 1 - C 3	/561. BD*(1) C 3 - C 5	4.28	1.20	0.064
2. BD (1) C 1 - C 3	/562. BD*(1) C 3 - C 7	2.94	1.17	0.053
2. BD (1) C 1 - C 3	/567. BD*(1) C 5 - H 27	1.33	1.20	0.036
2. BD (1) C 1 - C 3	/570. BD*(1) C 7 - O 9	1.16	1.25	0.034
2. BD (1) C 1 - C 3	/580. BD*(1) N 13 - C 14	2.11	1.12	0.044
3. BD (2) C 1 - C 3	/123. RY*(3) C 2	1.07	1.02	0.032
3. BD (2) C 1 - C 3	/162. RY*(3) C 5	0.87	0.86	0.026
3. BD (2) C 1 - C 3	/190. RY*(5) C 7	0.62	1.48	0.029
3. BD (2) C 1 - C 3	/559. BD*(2) C 2 - C 4	10.69	0.33	0.054
3. BD (2) C 1 - C 3	/566. BD*(2) C 5 - C 6	13.67	0.32	0.059
3. BD (2) C 1 - C 3	/569. BD*(1) C 7 - O 8	1.09	0.56	0.023
3. BD (2) C 1 - C 3	/571. BD*(2) C 7 - O 9	19.22	0.27	0.064
3. BD (2) C 1 - C 3	/580. BD*(1) N 13 - C 14	1.47	0.65	0.029
3. BD (2) C 1 - C 3	/581. BD*(1) N 13 - H 33	1.51	0.63	0.029
4. BD (1) C 1 - N 13	/121. RY*(1) C 2	0.53	2.05	0.029
4. BD (1) C 1 - N 13	/134. RY*(1) C 3	1.36	2.63	0.054
4. BD (1) C 1 - N 13	/290. RY*(1) C 14	1.71	1.60	0.047
4. BD (1) C 1 - N 13	/554. BD*(1) C 1 - C 2	0.64	1.23	0.025
4. BD (1) C 1 - N 13	/555. BD*(1) C 1 - C 3	2.16	1.41	0.049
4. BD (1) C 1 - N 13	/558. BD*(1) C 2 - C 4	0.87	1.44	0.032
4. BD (1) C 1 - N 13	/561. BD*(1) C 3 - C 5	2.72	1.23	0.052
4. BD (1) C 1 - N 13	/580. BD*(1) N 13 - C 14	0.94	1.16	0.030
4. BD (1) C 1 - N 13	/584. BD*(1) C 14 - C 40	1.77	1.18	0.041
5. BD (1) C 2 - C 4	/108. RY*(1) C 1	1.41	1.93	0.047
5. BD (1) C 2 - C 4	/110. RY*(3) C 1	0.92	2.02	0.039
5. BD (1) C 2 - C 4	/173. RY*(1) C 6	1.10	1.82	0.040
5. BD (1) C 2 - C 4	/554. BD*(1) C 1 - C 2	2.73	1.19	0.051
5. BD (1) C 2 - C 4	/557. BD*(1) C 1 - N 13	2.78	1.12	0.050
5. BD (1) C 2 - C 4	/560. BD*(1) C 2 - H 25	1.69	1.20	0.040
5. BD (1) C 2 - C 4	/563. BD*(1) C 4 - C 6	3.65	1.21	0.060
5. BD (1) C 2 - C 4	/564. BD*(1) C 4 - H 26	1.57	1.19	0.039
5. BD (1) C 2 - C 4	/568. BD*(1) C 6 -Se 11	3.12	0.88	0.047
6. BD (2) C 2 - C 4	/113. RY*(6) C 1	0.63	1.82	0.032
6. BD (2) C 2 - C 4	/556. BD*(2) C 1 - C 3	14.35	0.31	0.061
6. BD (2) C 2 - C 4	/566. BD*(2) C 5 - C 6	12.94	0.31	0.057
7. BD (1) C 2 - H 25	/108. RY*(1) C 1	0.63	1.70	0.029
7. BD (1) C 2 - H 25	/109. RY*(2) C 1	0.89	1.83	0.036
7. BD (1) C 2 - H 25	/147. RY*(1) C 4	1.44	1.68	0.044
7. BD (1) C 2 - H 25	/555. BD*(1) C 1 - C 3	3.21	1.14	0.054
7. BD (1) C 2 - H 25	/557. BD*(1) C 1 - N 13	0.60	0.89	0.021
7. BD (1) C 2 - H 25	/558. BD*(1) C 2 - C 4	1.58	1.18	0.039

7. BD (1) C 2 - H 25	/563. BD*(1) C 4 - C 6	5.67	0.98	0.067
7. BD (1) C 2 - H 25	/564. BD*(1) C 4 - H 26	0.94	0.96	0.027
8. BD (1) C 3 - C 5	/109. RY*(2) C 1	1.21	1.95	0.044
8. BD (1) C 3 - C 5	/174. RY*(2) C 6	1.45	1.48	0.042
8. BD (1) C 3 - C 5	/186. RY*(1) C 7	0.99	1.58	0.036
8. BD (1) C 3 - C 5	/555. BD*(1) C 1 - C 3	4.61	1.26	0.068
8. BD (1) C 3 - C 5	/557. BD*(1) C 1 - N 13	5.31	1.02	0.066
8. BD (1) C 3 - C 5	/562. BD*(1) C 3 - C 7	1.68	1.06	0.038
8. BD (1) C 3 - C 5	/565. BD*(1) C 5 - C 6	3.92	1.29	0.064
8. BD (1) C 3 - C 5	/567. BD*(1) C 5 - H 27	0.62	1.10	0.023
8. BD (1) C 3 - C 5	/568. BD*(1) C 6 -Se 11	5.50	0.78	0.059
8. BD (1) C 3 - C 5	/569. BD*(1) C 7 - O 8	2.85	0.92	0.047
8. BD (1) C 3 - C 5	/571. BD*(2) C 7 - O 9	0.54	0.63	0.017
9. BD (1) C 3 - C 7	/108. RY*(1) C 1	0.83	1.87	0.035
9. BD (1) C 3 - C 7	/109. RY*(2) C 1	1.05	1.99	0.041
9. BD (1) C 3 - C 7	/160. RY*(1) C 5	1.05	1.83	0.039
9. BD (1) C 3 - C 7	/212. RY*(1) O 9	0.72	1.81	0.032
9. BD (1) C 3 - C 7	/554. BD*(1) C 1 - C 2	3.77	1.13	0.058
9. BD (1) C 3 - C 7	/555. BD*(1) C 1 - C 3	3.98	1.30	0.064
9. BD (1) C 3 - C 7	/561. BD*(1) C 3 - C 5	1.28	1.13	0.034
9. BD (1) C 3 - C 7	/565. BD*(1) C 5 - C 6	1.47	1.33	0.040
9. BD (1) C 3 - C 7	/570. BD*(1) C 7 - O 9	0.95	1.19	0.030
9. BD (1) C 3 - C 7	/572. BD*(1) O 8 - C 10	2.86	0.95	0.047
10. BD (1) C 4 - C 6	/121. RY*(1) C 2	0.74	1.93	0.034
10. BD (1) C 4 - C 6	/122. RY*(2) C 2	1.56	2.00	0.050
10. BD (1) C 4 - C 6	/160. RY*(1) C 5	0.85	1.82	0.035
10. BD (1) C 4 - C 6	/161. RY*(2) C 5	0.94	1.63	0.035
10. BD (1) C 4 - C 6	/558. BD*(1) C 2 - C 4	3.21	1.32	0.058
10. BD (1) C 4 - C 6	/560. BD*(1) C 2 - H 25	2.68	1.12	0.049
10. BD (1) C 4 - C 6	/564. BD*(1) C 4 - H 26	0.88	1.11	0.028
10. BD (1) C 4 - C 6	/565. BD*(1) C 5 - C 6	3.51	1.32	0.061
10. BD (1) C 4 - C 6	/567. BD*(1) C 5 - H 27	3.42	1.12	0.055
11. BD (1) C 4 - H 26	/121. RY*(1) C 2	1.52	1.79	0.047
11. BD (1) C 4 - H 26	/173. RY*(1) C 6	1.13	1.60	0.038
11. BD (1) C 4 - H 26	/554. BD*(1) C 1 - C 2	5.67	0.97	0.066
11. BD (1) C 4 - H 26	/558. BD*(1) C 2 - C 4	1.49	1.18	0.038
11. BD (1) C 4 - H 26	/560. BD*(1) C 2 - H 25	0.95	0.97	0.027
11. BD (1) C 4 - H 26	/565. BD*(1) C 5 - C 6	3.20	1.17	0.055
12. BD (1) C 5 - C 6	/134. RY*(1) C 3	1.42	2.60	0.054
12. BD (1) C 5 - C 6	/135. RY*(2) C 3	0.69	2.06	0.034
12. BD (1) C 5 - C 6	/147. RY*(1) C 4	1.03	1.92	0.040
12. BD (1) C 5 - C 6	/561. BD*(1) C 3 - C 5	3.35	1.21	0.057
12. BD (1) C 5 - C 6	/562. BD*(1) C 3 - C 7	2.04	1.18	0.044
12. BD (1) C 5 - C 6	/563. BD*(1) C 4 - C 6	3.16	1.23	0.056
12. BD (1) C 5 - C 6	/564. BD*(1) C 4 - H 26	1.65	1.20	0.040
12. BD (1) C 5 - C 6	/567. BD*(1) C 5 - H 27	2.30	1.22	0.047
13. BD (2) C 5 - C 6	/137. RY*(4) C 3	0.65	1.06	0.025
13. BD (2) C 5 - C 6	/149. RY*(3) C 4	1.69	1.13	0.041
13. BD (2) C 5 - C 6	/238. RY*(1)Se 11	0.94	0.82	0.026
13. BD (2) C 5 - C 6	/556. BD*(2) C 1 - C 3	11.77	0.31	0.055
13. BD (2) C 5 - C 6	/559. BD*(2) C 2 - C 4	13.16	0.32	0.059
13. BD (2) C 5 - C 6	/576. BD*(1)Se 11 - C 12	0.52	0.39	0.013
14. BD (1) C 5 - H 27	/134. RY*(1) C 3	1.81	2.36	0.059
14. BD (1) C 5 - H 27	/173. RY*(1) C 6	1.80	1.59	0.048
14. BD (1) C 5 - H 27	/555. BD*(1) C 1 - C 3	3.07	1.14	0.053

14. BD (1) C 5 - H 27	/563. BD*(1) C 4 - C 6	6.02	0.98	0.069
14. BD (1) C 5 - H 27	/565. BD*(1) C 5 - C 6	2.17	1.17	0.045
15. BD (1) C 6 -Se 11	/147. RY*(1) C 4	2.10	1.74	0.054
15. BD (1) C 6 -Se 11	/160. RY*(1) C 5	1.69	1.73	0.049
15. BD (1) C 6 -Se 11	/265. RY*(2) C 12	0.65	1.57	0.029
15. BD (1) C 6 -Se 11	/558. BD*(1) C 2 - C 4	2.67	1.24	0.052
15. BD (1) C 6 -Se 11	/561. BD*(1) C 3 - C 5	5.31	1.03	0.066
15. BD (1) C 6 -Se 11	/565. BD*(1) C 5 - C 6	1.01	1.23	0.032
15. BD (1) C 6 -Se 11	/567. BD*(1) C 5 - H 27	0.94	1.04	0.028
15. BD (1) C 6 -Se 11	/577. BD*(1) C 12 - C 19	0.89	1.01	0.027
16. BD (1) C 7 - O 8	/135. RY*(2) C 3	1.04	2.17	0.042
16. BD (1) C 7 - O 8	/227. RY*(3) C 10	1.05	1.83	0.039
16. BD (1) C 7 - O 8	/561. BD*(1) C 3 - C 5	1.27	1.32	0.037
16. BD (1) C 7 - O 8	/575. BD*(1) C 10 - H 30	0.66	1.24	0.026
17. BD (1) C 7 - O 9	/135. RY*(2) C 3	1.32	2.30	0.049
17. BD (1) C 7 - O 9	/186. RY*(1) C 7	1.65	1.94	0.051
17. BD (1) C 7 - O 9	/555. BD*(1) C 1 - C 3	1.54	1.62	0.045
17. BD (1) C 7 - O 9	/562. BD*(1) C 3 - C 7	1.77	1.42	0.045
18. BD (2) C 7 - O 9	/556. BD*(2) C 1 - C 3	4.51	0.41	0.041
18. BD (2) C 7 - O 9	/571. BD*(2) C 7 - O 9	0.65	0.36	0.014
19. BD (1) O 8 - C 10	/186. RY*(1) C 7	1.27	1.77	0.042
19. BD (1) O 8 - C 10	/562. BD*(1) C 3 - C 7	2.60	1.26	0.052
20. BD (1) C 10 - H 28	/200. RY*(2) O 8	0.52	1.51	0.025
21. BD (1) C 10 - H 29	/200. RY*(2) O 8	0.57	1.51	0.026
21. BD (1) C 10 - H 29	/572. BD*(1) O 8 - C 10	0.57	0.79	0.019
22. BD (1) C 10 - H 30	/569. BD*(1) C 7 - O 8	3.92	0.81	0.051
23. BD (1)Se 11 - C 12	/357. RY*(3) C 19	0.86	1.28	0.030
23. BD (1)Se 11 - C 12	/563. BD*(1) C 4 - C 6	1.77	1.02	0.038
23. BD (1)Se 11 - C 12	/566. BD*(2) C 5 - C 6	1.03	0.59	0.023
23. BD (1)Se 11 - C 12	/591. BD*(1) C 19 - C 21	1.67	1.21	0.040
23. BD (1)Se 11 - C 12	/592. BD*(2) C 19 - C 21	4.17	0.61	0.047
24. BD (1) C 12 - C 19	/368. RY*(1) C 20	1.62	1.81	0.049
24. BD (1) C 12 - C 19	/381. RY*(1) C 21	1.82	1.82	0.052
24. BD (1) C 12 - C 19	/578. BD*(1) C 12 - H 31	0.66	1.04	0.023
24. BD (1) C 12 - C 19	/579. BD*(1) C 12 - H 32	0.54	1.04	0.021
24. BD (1) C 12 - C 19	/590. BD*(1) C 19 - C 20	1.52	1.12	0.037
24. BD (1) C 12 - C 19	/591. BD*(1) C 19 - C 21	3.69	1.31	0.062
24. BD (1) C 12 - C 19	/593. BD*(1) C 20 - C 22	1.41	1.32	0.039
24. BD (1) C 12 - C 19	/596. BD*(1) C 21 - C 23	3.29	1.13	0.054
25. BD (1) C 12 - H 31	/357. RY*(3) C 19	0.82	1.23	0.029
25. BD (1) C 12 - H 31	/577. BD*(1) C 12 - C 19	0.58	0.93	0.021
25. BD (1) C 12 - H 31	/591. BD*(1) C 19 - C 21	2.60	1.17	0.049
25. BD (1) C 12 - H 31	/592. BD*(2) C 19 - C 21	3.22	0.56	0.040
26. BD (1) C 12 - H 32	/356. RY*(2) C 19	0.67	1.65	0.030
26. BD (1) C 12 - H 32	/577. BD*(1) C 12 - C 19	0.51	0.94	0.020
26. BD (1) C 12 - H 32	/590. BD*(1) C 19 - C 20	4.84	0.98	0.062
27. BD (1) N 13 - C 14	/108. RY*(1) C 1	0.78	1.97	0.035
27. BD (1) N 13 - C 14	/109. RY*(2) C 1	0.78	2.10	0.036
27. BD (1) N 13 - C 14	/509. RY*(2) C 40	0.91	1.58	0.034
27. BD (1) N 13 - C 14	/555. BD*(1) C 1 - C 3	1.62	1.41	0.043
27. BD (1) N 13 - C 14	/557. BD*(1) C 1 - N 13	1.13	1.17	0.032
27. BD (1) N 13 - C 14	/606. BD*(1) C 40 - C 43	1.10	1.15	0.032
28. BD (1) N 13 - H 33	/108. RY*(1) C 1	1.10	1.84	0.040
28. BD (1) N 13 - H 33	/291. RY*(2) C 14	0.77	2.02	0.035
28. BD (1) N 13 - H 33	/293. RY*(4) C 14	0.94	2.90	0.047

28. BD (1) N 13 - H 33	/554. BD*(1) C 1 - C 2	2.09	1.10	0.043
28. BD (1) N 13 - H 33	/556. BD*(2) C 1 - C 3	1.58	0.68	0.032
28. BD (1) N 13 - H 33	/582. BD*(1) C 14 - O 15	3.03	1.17	0.053
29. BD (1) C 14 - O 15	/290. RY*(1) C 14	1.69	1.81	0.050
29. BD (1) C 14 - O 15	/581. BD*(1) N 13 - H 33	1.20	1.35	0.036
29. BD (1) C 14 - O 15	/584. BD*(1) C 14 - C 40	1.22	1.40	0.037
30. BD (2) C 14 - O 15	/583. BD*(2) C 14 - O 15	0.68	0.35	0.015
30. BD (2) C 14 - O 15	/604. BD*(1) C 40 - H 41	1.76	0.73	0.032
30. BD (2) C 14 - O 15	/605. BD*(1) C 40 - H 42	1.77	0.73	0.032
31. BD (1) C 14 - C 40	/278. RY*(2) N 13	1.56	1.74	0.047
31. BD (1) C 14 - C 40	/303. RY*(1) O 15	0.59	1.84	0.030
31. BD (1) C 14 - C 40	/531. RY*(1) C 43	1.06	1.48	0.036
31. BD (1) C 14 - C 40	/557. BD*(1) C 1 - N 13	3.05	1.04	0.050
31. BD (1) C 14 - C 40	/582. BD*(1) C 14 - O 15	0.76	1.19	0.027
31. BD (1) C 14 - C 40	/588. BD*(1) C 16 - C 43	1.80	1.05	0.039
31. BD (1) C 14 - C 40	/606. BD*(1) C 40 - C 43	0.75	1.03	0.025
32. BD (1) C 16 - O 17	/532. RY*(2) C 43	0.62	1.64	0.028
32. BD (1) C 16 - O 17	/606. BD*(1) C 40 - C 43	0.99	1.27	0.032
33. BD (1) C 16 - O 18	/316. RY*(1) C 16	1.59	1.80	0.048
33. BD (1) C 16 - O 18	/588. BD*(1) C 16 - C 43	1.08	1.39	0.035
34. BD (2) C 16 - O 18	/587. BD*(2) C 16 - O 18	0.75	0.36	0.015
34. BD (2) C 16 - O 18	/607. BD*(1) C 43 - H 44	1.73	0.75	0.032
34. BD (2) C 16 - O 18	/608. BD*(1) C 43 - H 45	1.75	0.75	0.032
35. BD (1) C 16 - C 43	/342. RY*(1) O 18	0.76	1.78	0.033
35. BD (1) C 16 - C 43	/508. RY*(1) C 40	1.13	1.43	0.036
35. BD (1) C 16 - C 43	/584. BD*(1) C 14 - C 40	1.76	1.07	0.039
35. BD (1) C 16 - C 43	/586. BD*(1) C 16 - O 18	0.57	1.19	0.023
35. BD (1) C 16 - C 43	/589. BD*(1) O 17 - H 34	1.84	0.98	0.038
35. BD (1) C 16 - C 43	/606. BD*(1) C 40 - C 43	0.53	1.04	0.021
36. BD (1) O 17 - H 34	/316. RY*(1) C 16	1.04	1.52	0.036
36. BD (1) O 17 - H 34	/317. RY*(2) C 16	1.01	1.96	0.040
36. BD (1) O 17 - H 34	/322. RY*(7) C 16	0.59	2.42	0.034
36. BD (1) O 17 - H 34	/586. BD*(1) C 16 - O 18	1.30	1.24	0.036
36. BD (1) O 17 - H 34	/588. BD*(1) C 16 - C 43	3.73	1.11	0.058
37. BD (1) C 19 - C 20	/264. RY*(1) C 12	1.25	1.31	0.036
37. BD (1) C 19 - C 20	/381. RY*(1) C 21	0.93	1.81	0.037
37. BD (1) C 19 - C 20	/394. RY*(1) C 22	0.90	1.92	0.037
37. BD (1) C 19 - C 20	/395. RY*(2) C 22	1.68	2.10	0.053
37. BD (1) C 19 - C 20	/577. BD*(1) C 12 - C 19	1.52	1.06	0.036
37. BD (1) C 19 - C 20	/579. BD*(1) C 12 - H 32	1.12	1.02	0.030
37. BD (1) C 19 - C 20	/591. BD*(1) C 19 - C 21	3.66	1.29	0.061
37. BD (1) C 19 - C 20	/593. BD*(1) C 20 - C 22	3.18	1.30	0.058
37. BD (1) C 19 - C 20	/595. BD*(1) C 20 - H 35	0.61	1.09	0.023
37. BD (1) C 19 - C 20	/597. BD*(1) C 21 - H 36	3.35	1.08	0.054
37. BD (1) C 19 - C 20	/599. BD*(1) C 22 - H 37	2.99	1.09	0.051
38. BD (1) C 19 - C 21	/264. RY*(1) C 12	0.91	1.40	0.032
38. BD (1) C 19 - C 21	/368. RY*(1) C 20	0.81	1.89	0.035
38. BD (1) C 19 - C 21	/407. RY*(1) C 23	0.98	2.03	0.040
38. BD (1) C 19 - C 21	/408. RY*(2) C 23	1.06	2.19	0.043
38. BD (1) C 19 - C 21	/576. BD*(1)Se 11 - C 12	0.84	0.84	0.024
38. BD (1) C 19 - C 21	/577. BD*(1) C 12 - C 19	3.53	1.16	0.057
38. BD (1) C 19 - C 21	/590. BD*(1) C 19 - C 20	3.49	1.20	0.058
38. BD (1) C 19 - C 21	/595. BD*(1) C 20 - H 35	1.56	1.19	0.039
38. BD (1) C 19 - C 21	/596. BD*(1) C 21 - C 23	2.95	1.21	0.053
38. BD (1) C 19 - C 21	/597. BD*(1) C 21 - H 36	1.81	1.18	0.041

38. BD (1) C 19 - C 21	/602. BD*(1) C 23 - H 38	1.39	1.19	0.036
39. BD (2) C 19 - C 21	/370. RY*(3) C 20	1.47	0.98	0.036
39. BD (2) C 19 - C 21	/409. RY*(3) C 23	1.38	1.12	0.037
39. BD (2) C 19 - C 21	/576. BD*(1)Se 11 - C 12	4.52	0.37	0.038
39. BD (2) C 19 - C 21	/578. BD*(1) C 12 - H 31	2.68	0.65	0.039
39. BD (2) C 19 - C 21	/594. BD*(2) C 20 - C 22	12.42	0.32	0.056
39. BD (2) C 19 - C 21	/601. BD*(2) C 23 - C 24	13.29	0.32	0.058
40. BD (1) C 20 - C 22	/355. RY*(1) C 19	1.41	2.04	0.048
40. BD (1) C 20 - C 22	/356. RY*(2) C 19	0.78	1.88	0.034
40. BD (1) C 20 - C 22	/420. RY*(1) C 24	0.87	2.03	0.038
40. BD (1) C 20 - C 22	/421. RY*(2) C 24	0.96	2.18	0.041
40. BD (1) C 20 - C 22	/577. BD*(1) C 12 - C 19	2.68	1.16	0.050
40. BD (1) C 20 - C 22	/590. BD*(1) C 19 - C 20	3.18	1.20	0.055
40. BD (1) C 20 - C 22	/595. BD*(1) C 20 - H 35	1.63	1.19	0.039
40. BD (1) C 20 - C 22	/598. BD*(1) C 22 - C 24	2.55	1.21	0.050
40. BD (1) C 20 - C 22	/599. BD*(1) C 22 - H 37	1.62	1.19	0.039
40. BD (1) C 20 - C 22	/603. BD*(1) C 24 - H 39	1.56	1.19	0.038
41. BD (2) C 20 - C 22	/422. RY*(3) C 24	1.43	0.96	0.035
41. BD (2) C 20 - C 22	/592. BD*(2) C 19 - C 21	13.87	0.32	0.059
41. BD (2) C 20 - C 22	/601. BD*(2) C 23 - C 24	13.18	0.31	0.058
42. BD (1) C 20 - H 35	/355. RY*(1) C 19	1.57	1.82	0.048
42. BD (1) C 20 - H 35	/394. RY*(1) C 22	1.59	1.80	0.048
42. BD (1) C 20 - H 35	/591. BD*(1) C 19 - C 21	3.17	1.17	0.054
42. BD (1) C 20 - H 35	/593. BD*(1) C 20 - C 22	1.45	1.18	0.037
42. BD (1) C 20 - H 35	/598. BD*(1) C 22 - C 24	5.18	0.99	0.064
42. BD (1) C 20 - H 35	/599. BD*(1) C 22 - H 37	0.86	0.97	0.026
43. BD (1) C 21 - C 23	/356. RY*(2) C 19	1.77	1.77	0.050
43. BD (1) C 21 - C 23	/420. RY*(1) C 24	0.70	1.93	0.033
43. BD (1) C 21 - C 23	/421. RY*(2) C 24	1.60	2.08	0.052
43. BD (1) C 21 - C 23	/577. BD*(1) C 12 - C 19	5.17	1.06	0.066
43. BD (1) C 21 - C 23	/591. BD*(1) C 19 - C 21	3.49	1.29	0.060
43. BD (1) C 21 - C 23	/600. BD*(1) C 23 - C 24	2.81	1.30	0.054
43. BD (1) C 21 - C 23	/602. BD*(1) C 23 - H 38	0.52	1.09	0.021
43. BD (1) C 21 - C 23	/603. BD*(1) C 24 - H 39	3.22	1.09	0.053
44. BD (1) C 21 - H 36	/355. RY*(1) C 19	2.22	1.82	0.057
44. BD (1) C 21 - H 36	/407. RY*(1) C 23	1.24	1.81	0.042
44. BD (1) C 21 - H 36	/590. BD*(1) C 19 - C 20	6.01	0.98	0.069
44. BD (1) C 21 - H 36	/591. BD*(1) C 19 - C 21	1.80	1.17	0.041
44. BD (1) C 21 - H 36	/600. BD*(1) C 23 - C 24	2.42	1.18	0.048
45. BD (1) C 22 - C 24	/369. RY*(2) C 20	2.07	1.73	0.054
45. BD (1) C 22 - C 24	/407. RY*(1) C 23	0.71	1.93	0.033
45. BD (1) C 22 - C 24	/408. RY*(2) C 23	1.63	2.09	0.052
45. BD (1) C 22 - C 24	/593. BD*(1) C 20 - C 22	2.86	1.30	0.055
45. BD (1) C 22 - C 24	/595. BD*(1) C 20 - H 35	3.27	1.09	0.053
45. BD (1) C 22 - C 24	/599. BD*(1) C 22 - H 37	0.52	1.09	0.021
45. BD (1) C 22 - C 24	/600. BD*(1) C 23 - C 24	2.81	1.30	0.054
45. BD (1) C 22 - C 24	/602. BD*(1) C 23 - H 38	3.26	1.09	0.053
45. BD (1) C 22 - C 24	/603. BD*(1) C 24 - H 39	0.53	1.09	0.021
46. BD (1) C 22 - H 37	/368. RY*(1) C 20	1.45	1.67	0.044
46. BD (1) C 22 - H 37	/420. RY*(1) C 24	1.26	1.81	0.043
46. BD (1) C 22 - H 37	/590. BD*(1) C 19 - C 20	5.51	0.98	0.066
46. BD (1) C 22 - H 37	/593. BD*(1) C 20 - C 22	1.35	1.18	0.036
46. BD (1) C 22 - H 37	/595. BD*(1) C 20 - H 35	0.85	0.97	0.026
46. BD (1) C 22 - H 37	/600. BD*(1) C 23 - C 24	2.52	1.18	0.049
47. BD (1) C 23 - C 24	/381. RY*(1) C 21	0.59	1.91	0.030

47. BD (1) C 23 - C 24	/382. RY*(2) C 21	1.45	1.97	0.048
47. BD (1) C 23 - C 24	/394. RY*(1) C 22	0.88	2.03	0.038
47. BD (1) C 23 - C 24	/395. RY*(2) C 22	1.00	2.21	0.042
47. BD (1) C 23 - C 24	/596. BD*(1) C 21 - C 23	2.52	1.21	0.049
47. BD (1) C 23 - C 24	/597. BD*(1) C 21 - H 36	1.55	1.18	0.038
47. BD (1) C 23 - C 24	/598. BD*(1) C 22 - C 24	2.52	1.21	0.049
47. BD (1) C 23 - C 24	/599. BD*(1) C 22 - H 37	1.59	1.19	0.039
47. BD (1) C 23 - C 24	/602. BD*(1) C 23 - H 38	1.61	1.19	0.039
47. BD (1) C 23 - C 24	/603. BD*(1) C 24 - H 39	1.62	1.19	0.039
48. BD (2) C 23 - C 24	/383. RY*(3) C 21	1.12	0.82	0.029
48. BD (2) C 23 - C 24	/396. RY*(3) C 22	1.36	1.08	0.036
48. BD (2) C 23 - C 24	/592. BD*(2) C 19 - C 21	12.91	0.31	0.057
48. BD (2) C 23 - C 24	/594. BD*(2) C 20 - C 22	13.29	0.31	0.058
49. BD (1) C 23 - H 38	/381. RY*(1) C 21	1.15	1.69	0.039
49. BD (1) C 23 - H 38	/420. RY*(1) C 24	1.63	1.81	0.049
49. BD (1) C 23 - H 38	/591. BD*(1) C 19 - C 21	2.63	1.17	0.049
49. BD (1) C 23 - H 38	/598. BD*(1) C 22 - C 24	5.29	0.99	0.065
49. BD (1) C 23 - H 38	/600. BD*(1) C 23 - C 24	1.33	1.18	0.035
49. BD (1) C 23 - H 38	/603. BD*(1) C 24 - H 39	0.86	0.97	0.026
50. BD (1) C 24 - H 39	/394. RY*(1) C 22	1.32	1.80	0.044
50. BD (1) C 24 - H 39	/407. RY*(1) C 23	1.71	1.81	0.050
50. BD (1) C 24 - H 39	/593. BD*(1) C 20 - C 22	2.54	1.18	0.049
50. BD (1) C 24 - H 39	/596. BD*(1) C 21 - C 23	5.32	0.99	0.065
50. BD (1) C 24 - H 39	/600. BD*(1) C 23 - C 24	1.33	1.18	0.035
50. BD (1) C 24 - H 39	/602. BD*(1) C 23 - H 38	0.86	0.97	0.026
51. BD (1) C 40 - H 41	/533. RY*(3) C 43	0.52	1.23	0.023
51. BD (1) C 40 - H 41	/582. BD*(1) C 14 - O 15	2.24	1.03	0.043
51. BD (1) C 40 - H 41	/583. BD*(2) C 14 - O 15	4.74	0.50	0.046
51. BD (1) C 40 - H 41	/607. BD*(1) C 43 - H 44	2.69	0.88	0.044
52. BD (1) C 40 - H 42	/533. RY*(3) C 43	0.51	1.23	0.022
52. BD (1) C 40 - H 42	/582. BD*(1) C 14 - O 15	1.82	1.03	0.039
52. BD (1) C 40 - H 42	/583. BD*(2) C 14 - O 15	5.76	0.50	0.051
52. BD (1) C 40 - H 42	/608. BD*(1) C 43 - H 45	2.67	0.88	0.043
53. BD (1) C 40 - C 43	/290. RY*(1) C 14	1.35	1.44	0.039
53. BD (1) C 40 - C 43	/316. RY*(1) C 16	1.40	1.42	0.040
53. BD (1) C 40 - C 43	/580. BD*(1) N 13 - C 14	3.80	1.00	0.056
53. BD (1) C 40 - C 43	/584. BD*(1) C 14 - C 40	0.97	1.02	0.028
53. BD (1) C 40 - C 43	/585. BD*(1) C 16 - O 17	3.86	0.92	0.054
53. BD (1) C 40 - C 43	/588. BD*(1) C 16 - C 43	0.72	1.01	0.024
53. BD (1) C 40 - C 43	/604. BD*(1) C 40 - H 41	0.52	1.00	0.020
53. BD (1) C 40 - C 43	/605. BD*(1) C 40 - H 42	0.53	1.00	0.020
53. BD (1) C 40 - C 43	/607. BD*(1) C 43 - H 44	0.52	1.00	0.020
53. BD (1) C 40 - C 43	/608. BD*(1) C 43 - H 45	0.51	1.00	0.020
54. BD (1) C 43 - H 44	/320. RY*(5) C 16	0.54	1.59	0.026
54. BD (1) C 43 - H 44	/510. RY*(3) C 40	0.51	1.26	0.023
54. BD (1) C 43 - H 44	/586. BD*(1) C 16 - O 18	1.88	1.02	0.039
54. BD (1) C 43 - H 44	/587. BD*(2) C 16 - O 18	5.49	0.49	0.048
54. BD (1) C 43 - H 44	/604. BD*(1) C 40 - H 41	2.81	0.87	0.044
55. BD (1) C 43 - H 45	/510. RY*(3) C 40	0.50	1.26	0.023
55. BD (1) C 43 - H 45	/586. BD*(1) C 16 - O 18	1.86	1.02	0.039
55. BD (1) C 43 - H 45	/587. BD*(2) C 16 - O 18	5.48	0.49	0.048
55. BD (1) C 43 - H 45	/605. BD*(1) C 40 - H 42	2.81	0.87	0.044
56. CR (1) C 1	/122. RY*(2) C 2	0.95	11.44	0.093
56. CR (1) C 1	/134. RY*(1) C 3	0.52	11.95	0.070
56. CR (1) C 1	/135. RY*(2) C 3	1.70	11.41	0.125

56. CR (1) C 1	/136. RY*(3) C 3	0.50	11.02	0.066
56. CR (1) C 1	/555. BD*(1) C 1 - C 3	1.36	10.73	0.109
56. CR (1) C 1	/558. BD*(1) C 2 - C 4	0.57	10.77	0.070
56. CR (1) C 1	/561. BD*(1) C 3 - C 5	1.03	10.56	0.094
56. CR (1) C 1	/562. BD*(1) C 3 - C 7	1.11	10.53	0.098
56. CR (1) C 1	/580. BD*(1) N 13 - C 14	1.04	10.48	0.095
57. CR (1) C 2	/109. RY*(2) C 1	1.36	11.36	0.111
57. CR (1) C 2	/147. RY*(1) C 4	0.60	11.21	0.073
57. CR (1) C 2	/148. RY*(2) C 4	1.75	11.21	0.125
57. CR (1) C 2	/555. BD*(1) C 1 - C 3	0.83	10.67	0.084
57. CR (1) C 2	/557. BD*(1) C 1 - N 13	0.54	10.42	0.067
57. CR (1) C 2	/558. BD*(1) C 2 - C 4	0.83	10.70	0.084
57. CR (1) C 2	/563. BD*(1) C 4 - C 6	1.30	10.51	0.105
58. CR (1) C 3	/108. RY*(1) C 1	1.14	11.25	0.101
58. CR (1) C 3	/110. RY*(3) C 1	1.02	11.34	0.096
58. CR (1) C 3	/161. RY*(2) C 5	0.74	11.04	0.081
58. CR (1) C 3	/187. RY*(2) C 7	0.60	11.50	0.074
58. CR (1) C 3	/192. RY*(7) C 7	0.83	11.19	0.086
58. CR (1) C 3	/554. BD*(1) C 1 - C 2	1.09	10.52	0.096
58. CR (1) C 3	/555. BD*(1) C 1 - C 3	1.24	10.69	0.103
58. CR (1) C 3	/557. BD*(1) C 1 - N 13	1.02	10.45	0.093
58. CR (1) C 3	/565. BD*(1) C 5 - C 6	0.72	10.72	0.079
58. CR (1) C 3	/569. BD*(1) C 7 - O 8	0.61	10.35	0.073
59. CR (1) C 4	/122. RY*(2) C 2	1.29	11.37	0.108
59. CR (1) C 4	/124. RY*(4) C 2	0.68	11.05	0.078
59. CR (1) C 4	/174. RY*(2) C 6	1.29	10.88	0.106
59. CR (1) C 4	/176. RY*(4) C 6	0.66	11.13	0.076
59. CR (1) C 4	/554. BD*(1) C 1 - C 2	1.20	10.49	0.101
59. CR (1) C 4	/558. BD*(1) C 2 - C 4	0.67	10.70	0.076
59. CR (1) C 4	/565. BD*(1) C 5 - C 6	0.83	10.70	0.084
59. CR (1) C 4	/568. BD*(1) C 6 -Se 11	0.82	10.18	0.082
60. CR (1) C 5	/135. RY*(2) C 3	0.78	11.35	0.084
60. CR (1) C 5	/173. RY*(1) C 6	1.14	11.12	0.101
60. CR (1) C 5	/174. RY*(2) C 6	1.85	10.88	0.127
60. CR (1) C 5	/175. RY*(3) C 6	0.54	10.93	0.069
60. CR (1) C 5	/555. BD*(1) C 1 - C 3	0.76	10.67	0.081
60. CR (1) C 5	/562. BD*(1) C 3 - C 7	0.66	10.46	0.075
60. CR (1) C 5	/563. BD*(1) C 4 - C 6	1.23	10.51	0.102
60. CR (1) C 5	/565. BD*(1) C 5 - C 6	1.21	10.70	0.102
60. CR (1) C 5	/568. BD*(1) C 6 -Se 11	1.26	10.18	0.102
61. CR (1) C 6	/148. RY*(2) C 4	1.02	11.25	0.096
61. CR (1) C 6	/161. RY*(2) C 5	2.09	11.05	0.136
61. CR (1) C 6	/163. RY*(4) C 5	0.65	11.16	0.076
61. CR (1) C 6	/558. BD*(1) C 2 - C 4	0.63	10.74	0.074
61. CR (1) C 6	/561. BD*(1) C 3 - C 5	1.18	10.53	0.100
61. CR (1) C 6	/565. BD*(1) C 5 - C 6	1.22	10.73	0.103
61. CR (1) C 6	/567. BD*(1) C 5 - H 27	0.56	10.54	0.069
61. CR (1) C 6	/568. BD*(1) C 6 -Se 11	1.29	10.22	0.103
62. CR (1) C 7	/134. RY*(1) C 3	1.20	12.05	0.107
62. CR (1) C 7	/555. BD*(1) C 1 - C 3	0.87	10.83	0.087
62. CR (1) C 7	/561. BD*(1) C 3 - C 5	0.54	10.66	0.068
62. CR (1) C 7	/562. BD*(1) C 3 - C 7	0.56	10.63	0.070
62. CR (1) C 7	/569. BD*(1) C 7 - O 8	0.68	10.49	0.077
62. CR (1) C 7	/572. BD*(1) O 8 - C 10	1.11	10.48	0.097
63. CR (1) O 8	/186. RY*(1) C 7	1.01	19.92	0.127

63. CR (1) O 8	/187. RY*(2) C 7	1.12	20.41	0.135
63. CR (1) O 8	/227. RY*(3) C 10	0.88	19.95	0.118
64. CR (1) O 9	/186. RY*(1) C 7	5.28	19.81	0.290
64. CR (1) O 9	/562. BD*(1) C 3 - C 7	0.78	19.29	0.111
65. CR (1) C 10	/459. RY*(2) H 30	0.53	12.15	0.072
65. CR (1) C 10	/569. BD*(1) C 7 - O 8	1.10	10.40	0.098
65. CR (1) C 10	/572. BD*(1) O 8 - C 10	1.48	10.39	0.111
68. CR (3)Se 11	/173. RY*(1) C 6	0.96	11.34	0.093
68. CR (3)Se 11	/563. BD*(1) C 4 - C 6	0.76	10.73	0.081
68. CR (3)Se 11	/565. BD*(1) C 5 - C 6	1.23	10.91	0.104
80. CR (1) C 12	/355. RY*(1) C 19	0.92	11.39	0.091
80. CR (1) C 12	/359. RY*(5) C 19	0.60	11.18	0.073
80. CR (1) C 12	/576. BD*(1)Se 11 - C 12	1.22	10.19	0.100
80. CR (1) C 12	/590. BD*(1) C 19 - C 20	0.71	10.55	0.078
80. CR (1) C 12	/591. BD*(1) C 19 - C 21	0.79	10.74	0.083
81. CR (1) N 13	/108. RY*(1) C 1	1.10	15.39	0.117
81. CR (1) N 13	/109. RY*(2) C 1	0.55	15.52	0.083
81. CR (1) N 13	/291. RY*(2) C 14	1.54	15.57	0.139
81. CR (1) N 13	/295. RY*(6) C 14	0.67	15.24	0.090
81. CR (1) N 13	/475. RY*(3) H 33	0.51	16.46	0.082
81. CR (1) N 13	/555. BD*(1) C 1 - C 3	0.59	14.83	0.084
82. CR (1) C 14	/508. RY*(1) C 40	0.75	10.94	0.081
82. CR (1) C 14	/557. BD*(1) C 1 - N 13	1.16	10.56	0.100
83. CR (1) O 15	/290. RY*(1) C 14	5.85	19.67	0.304
83. CR (1) O 15	/584. BD*(1) C 14 - C 40	0.71	19.25	0.106
84. CR (1) C 16	/531. RY*(1) C 43	0.83	11.03	0.086
84. CR (1) C 16	/585. BD*(1) C 16 - O 17	0.67	10.51	0.077
85. CR (1) O 17	/316. RY*(1) C 16	0.67	19.77	0.103
85. CR (1) O 17	/317. RY*(2) C 16	1.88	20.21	0.174
85. CR (1) O 17	/319. RY*(4) C 16	0.69	21.12	0.108
85. CR (1) O 17	/481. RY*(4) H 34	0.55	20.96	0.096
86. CR (1) O 18	/316. RY*(1) C 16	6.05	19.66	0.309
86. CR (1) O 18	/588. BD*(1) C 16 - C 43	0.71	19.25	0.105
87. CR (1) C 19	/266. RY*(3) C 12	0.72	11.16	0.080
87. CR (1) C 19	/369. RY*(2) C 20	1.10	11.15	0.099
87. CR (1) C 19	/382. RY*(2) C 21	2.19	11.29	0.140
87. CR (1) C 19	/591. BD*(1) C 19 - C 21	1.01	10.71	0.093
87. CR (1) C 19	/593. BD*(1) C 20 - C 22	0.58	10.71	0.071
87. CR (1) C 19	/596. BD*(1) C 21 - C 23	1.02	10.52	0.093
87. CR (1) C 19	/597. BD*(1) C 21 - H 36	0.54	10.50	0.068
88. CR (1) C 20	/356. RY*(2) C 19	1.31	11.17	0.108
88. CR (1) C 20	/395. RY*(2) C 22	2.12	11.50	0.139
88. CR (1) C 20	/577. BD*(1) C 12 - C 19	0.75	10.46	0.079
88. CR (1) C 20	/591. BD*(1) C 19 - C 21	0.76	10.69	0.081
88. CR (1) C 20	/593. BD*(1) C 20 - C 22	0.76	10.70	0.080
88. CR (1) C 20	/598. BD*(1) C 22 - C 24	1.07	10.51	0.095
89. CR (1) C 21	/355. RY*(1) C 19	1.31	11.34	0.109
89. CR (1) C 21	/356. RY*(2) C 19	1.68	11.18	0.122
89. CR (1) C 21	/408. RY*(2) C 23	0.79	11.49	0.085
89. CR (1) C 21	/489. RY*(2) H 36	0.51	12.36	0.071
89. CR (1) C 21	/577. BD*(1) C 12 - C 19	1.38	10.46	0.108
89. CR (1) C 21	/590. BD*(1) C 19 - C 20	1.21	10.50	0.101
89. CR (1) C 21	/591. BD*(1) C 19 - C 21	0.93	10.69	0.090
89. CR (1) C 21	/600. BD*(1) C 23 - C 24	0.62	10.70	0.073
90. CR (1) C 22	/368. RY*(1) C 20	0.62	11.20	0.074

90. CR (1) C 22	/369. RY*(2) C 20	0.85	11.13	0.087
90. CR (1) C 22	/371. RY*(4) C 20	1.13	11.28	0.101
90. CR (1) C 22	/421. RY*(2) C 24	0.80	11.48	0.086
90. CR (1) C 22	/494. RY*(2) H 37	0.56	12.29	0.074
90. CR (1) C 22	/590. BD*(1) C 19 - C 20	1.19	10.51	0.101
90. CR (1) C 22	/593. BD*(1) C 20 - C 22	0.79	10.70	0.082
90. CR (1) C 22	/595. BD*(1) C 20 - H 35	0.51	10.49	0.066
90. CR (1) C 22	/600. BD*(1) C 23 - C 24	0.63	10.70	0.073
91. CR (1) C 23	/385. RY*(5) C 21	0.65	11.15	0.076
91. CR (1) C 23	/421. RY*(2) C 24	2.11	11.48	0.139
91. CR (1) C 23	/499. RY*(2) H 38	0.55	12.28	0.073
91. CR (1) C 23	/591. BD*(1) C 19 - C 21	0.70	10.69	0.077
91. CR (1) C 23	/598. BD*(1) C 22 - C 24	1.07	10.51	0.095
91. CR (1) C 23	/600. BD*(1) C 23 - C 24	0.80	10.70	0.083
91. CR (1) C 23	/603. BD*(1) C 24 - H 39	0.50	10.49	0.065
92. CR (1) C 24	/395. RY*(2) C 22	0.76	11.51	0.084
92. CR (1) C 24	/398. RY*(5) C 22	0.50	10.97	0.066
92. CR (1) C 24	/408. RY*(2) C 23	2.10	11.49	0.139
92. CR (1) C 24	/504. RY*(2) H 39	0.55	12.28	0.074
92. CR (1) C 24	/593. BD*(1) C 20 - C 22	0.63	10.70	0.074
92. CR (1) C 24	/596. BD*(1) C 21 - C 23	1.07	10.51	0.095
92. CR (1) C 24	/600. BD*(1) C 23 - C 24	0.79	10.70	0.082
92. CR (1) C 24	/602. BD*(1) C 23 - H 38	0.50	10.49	0.065
93. CR (1) C 40	/291. RY*(2) C 14	0.96	11.44	0.094
93. CR (1) C 40	/532. RY*(2) C 43	0.57	10.80	0.070
94. CR (1) C 43	/317. RY*(2) C 16	0.73	11.31	0.081
94. CR (1) C 43	/509. RY*(2) C 40	0.55	10.86	0.069
95. LP (1) O 8	/186. RY*(1) C 7	1.66	1.51	0.045
95. LP (1) O 8	/189. RY*(4) C 7	1.60	2.61	0.058
95. LP (1) O 8	/225. RY*(1) C 10	1.65	1.65	0.047
95. LP (1) O 8	/227. RY*(3) C 10	0.74	1.54	0.030
95. LP (1) O 8	/570. BD*(1) C 7 - O 9	5.69	1.08	0.070
95. LP (1) O 8	/573. BD*(1) C 10 - H 28	0.64	0.95	0.022
95. LP (1) O 8	/575. BD*(1) C 10 - H 30	2.38	0.95	0.043
96. LP (2) O 8	/188. RY*(3) C 7	1.79	1.84	0.054
96. LP (2) O 8	/226. RY*(2) C 10	1.48	1.50	0.044
96. LP (2) O 8	/571. BD*(2) C 7 - O 9	38.51	0.31	0.100
96. LP (2) O 8	/573. BD*(1) C 10 - H 28	5.06	0.70	0.056
96. LP (2) O 8	/574. BD*(1) C 10 - H 29	5.06	0.69	0.055
97. LP (1) O 9	/186. RY*(1) C 7	12.37	1.64	0.127
97. LP (1) O 9	/196. RY*(11) C 7	0.75	4.97	0.055
97. LP (1) O 9	/562. BD*(1) C 3 - C 7	2.24	1.13	0.045
97. LP (1) O 9	/569. BD*(1) C 7 - O 8	0.98	0.99	0.028
98. LP (2) O 9	/187. RY*(2) C 7	1.92	1.69	0.053
98. LP (2) O 9	/189. RY*(4) C 7	1.73	2.30	0.058
98. LP (2) O 9	/562. BD*(1) C 3 - C 7	12.39	0.68	0.084
98. LP (2) O 9	/569. BD*(1) C 7 - O 8	28.91	0.55	0.113
98. LP (2) O 9	/575. BD*(1) C 10 - H 30	0.81	0.64	0.021
99. LP (1)Se 11	/173. RY*(1) C 6	1.17	1.78	0.041
99. LP (1)Se 11	/565. BD*(1) C 5 - C 6	3.29	1.35	0.060
100. LP (2)Se 11	/563. BD*(1) C 4 - C 6	1.73	0.69	0.031
100. LP (2)Se 11	/565. BD*(1) C 5 - C 6	1.20	0.87	0.030
100. LP (2)Se 11	/566. BD*(2) C 5 - C 6	8.94	0.26	0.045
100. LP (2)Se 11	/578. BD*(1) C 12 - H 31	2.37	0.61	0.035
100. LP (2)Se 11	/579. BD*(1) C 12 - H 32	3.94	0.61	0.045

101. LP (1) N 13	/110. RY*(3) C 1	1.08	1.53	0.039
101. LP (1) N 13	/111. RY*(4) C 1	0.78	1.62	0.034
101. LP (1) N 13	/292. RY*(3) C 14	1.64	1.72	0.051
101. LP (1) N 13	/297. RY*(8) C 14	0.52	1.68	0.029
101. LP (1) N 13	/474. RY*(2) H 33	0.74	1.95	0.037
101. LP (1) N 13	/554. BD*(1) C 1 - C 2	3.77	0.71	0.050
101. LP (1) N 13	/555. BD*(1) C 1 - C 3	2.77	0.88	0.047
101. LP (1) N 13	/556. BD*(2) C 1 - C 3	17.55	0.30	0.065
101. LP (1) N 13	/583. BD*(2) C 14 - O 15	50.40	0.26	0.103
102. LP (1) O 15	/290. RY*(1) C 14	13.76	1.51	0.129
102. LP (1) O 15	/580. BD*(1) N 13 - C 14	1.20	1.06	0.032
102. LP (1) O 15	/584. BD*(1) C 14 - C 40	2.18	1.09	0.044
103. LP (2) O 15	/291. RY*(2) C 14	1.53	1.62	0.046
103. LP (2) O 15	/293. RY*(4) C 14	1.81	2.51	0.062
103. LP (2) O 15	/580. BD*(1) N 13 - C 14	23.79	0.62	0.110
103. LP (2) O 15	/584. BD*(1) C 14 - C 40	15.11	0.65	0.090
103. LP (2) O 15	/588. BD*(1) C 16 - C 43	0.75	0.64	0.020
104. LP (1) O 17	/316. RY*(1) C 16	2.24	1.41	0.050
104. LP (1) O 17	/319. RY*(4) C 16	1.90	2.76	0.065
104. LP (1) O 17	/480. RY*(3) H 34	1.29	2.28	0.049
104. LP (1) O 17	/586. BD*(1) C 16 - O 18	5.42	1.14	0.070
105. LP (2) O 17	/318. RY*(3) C 16	1.99	1.87	0.057
105. LP (2) O 17	/479. RY*(2) H 34	1.57	1.81	0.050
105. LP (2) O 17	/587. BD*(2) C 16 - O 18	41.20	0.32	0.103
106. LP (1) O 18	/316. RY*(1) C 16	14.35	1.51	0.131
106. LP (1) O 18	/585. BD*(1) C 16 - O 17	0.86	1.00	0.027
106. LP (1) O 18	/588. BD*(1) C 16 - C 43	2.14	1.10	0.044
107. LP (2) O 18	/317. RY*(2) C 16	2.58	1.50	0.057
107. LP (2) O 18	/319. RY*(4) C 16	1.18	2.41	0.049
107. LP (2) O 18	/584. BD*(1) C 14 - C 40	0.74	0.66	0.020
107. LP (2) O 18	/585. BD*(1) C 16 - O 17	27.87	0.56	0.112
107. LP (2) O 18	/588. BD*(1) C 16 - C 43	13.64	0.65	0.086
556. BD*(2) C 1 - C 3	/112. RY*(5) C 1	1.08	1.28	0.084
556. BD*(2) C 1 - C 3	/137. RY*(4) C 3	0.88	0.75	0.058
556. BD*(2) C 1 - C 3	/559. BD*(2) C 2 - C 4	130.35	0.01	0.072
556. BD*(2) C 1 - C 3	/569. BD*(1) C 7 - O 8	0.80	0.25	0.028
556. BD*(2) C 1 - C 3	/580. BD*(1) N 13 - C 14	0.68	0.34	0.031
556. BD*(2) C 1 - C 3	/581. BD*(1) N 13 - H 33	0.99	0.31	0.039
559. BD*(2) C 2 - C 4	/123. RY*(3) C 2	0.76	0.69	0.068
559. BD*(2) C 2 - C 4	/151. RY*(5) C 4	0.86	1.36	0.101
566. BD*(2) C 5 - C 6	/162. RY*(3) C 5	2.54	0.54	0.094
566. BD*(2) C 5 - C 6	/175. RY*(3) C 6	0.52	0.85	0.053
566. BD*(2) C 5 - C 6	/576. BD*(1)Se 11 - C 12	1.27	0.07	0.023
569. BD*(1) C 7 - O 8	/187. RY*(2) C 7	1.61	1.15	0.162
569. BD*(1) C 7 - O 8	/199. RY*(1) O 8	0.56	1.05	0.093
569. BD*(1) C 7 - O 8	/561. BD*(1) C 3 - C 5	1.05	0.17	0.046
569. BD*(1) C 7 - O 8	/562. BD*(1) C 3 - C 7	0.80	0.14	0.034
569. BD*(1) C 7 - O 8	/570. BD*(1) C 7 - O 9	0.53	0.22	0.039
569. BD*(1) C 7 - O 8	/575. BD*(1) C 10 - H 30	0.50	0.09	0.025
571. BD*(2) C 7 - O 9	/188. RY*(3) C 7	1.52	1.52	0.119
571. BD*(2) C 7 - O 9	/213. RY*(2) O 9	1.10	0.98	0.082
571. BD*(2) C 7 - O 9	/556. BD*(2) C 1 - C 3	33.53	0.05	0.068
583. BD*(2) C 14 - O 15	/292. RY*(3) C 14	1.29	1.46	0.107
583. BD*(2) C 14 - O 15	/297. RY*(8) C 14	0.79	1.42	0.083
583. BD*(2) C 14 - O 15	/304. RY*(2) O 15	1.20	1.00	0.086

583. BD*(2) C 14 - O 15	/604. BD*(1) C 40 - H 41	1.04	0.37	0.048
583. BD*(2) C 14 - O 15	/605. BD*(1) C 40 - H 42	1.15	0.37	0.050
587. BD*(2) C 16 - O 18	/318. RY*(3) C 16	1.41	1.55	0.126
587. BD*(2) C 16 - O 18	/324. RY*(9) C 16	0.52	1.17	0.067
587. BD*(2) C 16 - O 18	/343. RY*(2) O 18	0.81	0.95	0.076
587. BD*(2) C 16 - O 18	/607. BD*(1) C 43 - H 44	0.88	0.39	0.049
587. BD*(2) C 16 - O 18	/608. BD*(1) C 43 - H 45	0.89	0.39	0.049
592. BD*(2) C 19 - C 21	/358. RY*(4) C 19	0.62	1.46	0.077
592. BD*(2) C 19 - C 21	/383. RY*(3) C 21	2.45	0.50	0.090
592. BD*(2) C 19 - C 21	/568. BD*(1) C 6 -Se 11	0.50	0.08	0.016
592. BD*(2) C 19 - C 21	/576. BD*(1)Se 11 - C 12	4.72	0.05	0.039
592. BD*(2) C 19 - C 21	/578. BD*(1) C 12 - H 31	0.70	0.33	0.038
594. BD*(2) C 20 - C 22	/370. RY*(3) C 20	0.82	0.67	0.066
594. BD*(2) C 20 - C 22	/372. RY*(5) C 20	0.54	1.53	0.081
594. BD*(2) C 20 - C 22	/397. RY*(4) C 22	0.72	1.42	0.090
601. BD*(2) C 23 - C 24	/410. RY*(4) C 23	0.83	1.38	0.094
601. BD*(2) C 23 - C 24	/422. RY*(3) C 24	0.89	0.65	0.066
601. BD*(2) C 23 - C 24	/423. RY*(4) C 24	0.57	1.52	0.081

NATURAL BOND ORBITAL ANALYSIS:

		Occupancies		Lewis Structure				Low	High	
	Occ.							occ	occ	
Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	(L)	(NL)	Dev
1(1)	1.90	204.74027	9.25973	39	53	0	15	21	13	0.64
2(2)	1.90	204.74027	9.25973	39	53	0	15	21	13	0.64
3(1)	1.80	205.89211	8.10789	39	50	0	18	6	10	0.64
4(2)	1.80	205.89211	8.10789	39	50	0	18	6	10	0.64
5(1)	1.70	210.32619	3.67381	39	55	0	13	0	10	0.25
6(2)	1.70	210.32619	3.67381	39	55	0	13	0	10	0.25
7(1)	1.60	210.32619	3.67381	39	55	0	13	0	10	0.25
8(2)	1.60	210.32619	3.67381	39	55	0	13	0	10	0.25
9(1)	1.50	209.81510	4.18490	39	54	0	14	1	12	0.74
10(2)	1.50	209.35626	4.64374	39	54	0	14	1	12	1.04
11(3)	1.50	209.81510	4.18490	39	54	0	14	1	12	0.74
12(1)	1.70	210.32619	3.67381	39	55	0	13	0	10	0.25

Core	77.97738	(99.971% of 78)
Valence Lewis	132.34881	(97.315% of 136)
Total Lewis	210.32619	(98.283% of 214)
Valence non-Lewis	3.28120	(1.533% of 214)
Rydberg non-Lewis	0.39261	(0.183% of 214)
Total non-Lewis	3.67381	(1.717% of 214)

Compound 11

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 2	/144. RY*(1) C 3	0.78	2.49	0.040
1. BD (1) C 1 - C 2	/145. RY*(2) C 3	0.70	1.95	0.033
1. BD (1) C 1 - C 2	/158. RY*(2) C 4	2.14	1.83	0.056
1. BD (1) C 1 - C 2	/287. RY*(1) N 13	0.89	1.52	0.033
1. BD (1) C 1 - C 2	/599. BD*(1) C 1 - C 3	4.22	1.27	0.065
1. BD (1) C 1 - C 2	/601. BD*(1) C 1 - N 13	0.57	1.03	0.022
1. BD (1) C 1 - C 2	/602. BD*(1) C 2 - C 4	2.90	1.31	0.055
1. BD (1) C 1 - C 2	/604. BD*(1) C 2 - H 32	0.61	1.10	0.023
1. BD (1) C 1 - C 2	/606. BD*(1) C 3 - C 7	4.37	1.07	0.061
1. BD (1) C 1 - C 2	/608. BD*(1) C 4 - H 33	2.83	1.10	0.050
1. BD (1) C 1 - C 2	/625. BD*(1) N 13 - H 40	1.58	1.00	0.036
2. BD (1) C 1 - C 3	/131. RY*(1) C 2	0.75	2.02	0.035
2. BD (1) C 1 - C 3	/170. RY*(1) C 5	0.59	1.88	0.030
2. BD (1) C 1 - C 3	/199. RY*(4) C 7	0.59	2.77	0.036
2. BD (1) C 1 - C 3	/287. RY*(1) N 13	0.70	1.62	0.030
2. BD (1) C 1 - C 3	/598. BD*(1) C 1 - C 2	3.46	1.20	0.057
2. BD (1) C 1 - C 3	/601. BD*(1) C 1 - N 13	2.09	1.12	0.043
2. BD (1) C 1 - C 3	/604. BD*(1) C 2 - H 32	1.29	1.20	0.035
2. BD (1) C 1 - C 3	/605. BD*(1) C 3 - C 5	4.21	1.20	0.063
2. BD (1) C 1 - C 3	/606. BD*(1) C 3 - C 7	2.94	1.17	0.053
2. BD (1) C 1 - C 3	/611. BD*(1) C 5 - H 34	1.32	1.20	0.036
2. BD (1) C 1 - C 3	/614. BD*(1) C 7 - O 9	1.15	1.26	0.034
2. BD (1) C 1 - C 3	/624. BD*(1) N 13 - C 14	2.08	1.12	0.044
3. BD (2) C 1 - C 3	/133. RY*(3) C 2	1.10	1.01	0.032
3. BD (2) C 1 - C 3	/172. RY*(3) C 5	0.87	0.85	0.026
3. BD (2) C 1 - C 3	/200. RY*(5) C 7	0.61	1.46	0.029
3. BD (2) C 1 - C 3	/603. BD*(2) C 2 - C 4	10.81	0.33	0.054
3. BD (2) C 1 - C 3	/610. BD*(2) C 5 - C 6	13.76	0.32	0.059
3. BD (2) C 1 - C 3	/613. BD*(1) C 7 - O 8	1.11	0.57	0.023
3. BD (2) C 1 - C 3	/615. BD*(2) C 7 - O 9	18.62	0.27	0.063
3. BD (2) C 1 - C 3	/624. BD*(1) N 13 - C 14	1.51	0.65	0.029
3. BD (2) C 1 - C 3	/625. BD*(1) N 13 - H 40	1.48	0.63	0.029
4. BD (1) C 1 - N 13	/131. RY*(1) C 2	0.53	2.06	0.030
4. BD (1) C 1 - N 13	/144. RY*(1) C 3	1.33	2.63	0.053
4. BD (1) C 1 - N 13	/300. RY*(1) C 14	1.53	1.68	0.045
4. BD (1) C 1 - N 13	/598. BD*(1) C 1 - C 2	0.64	1.24	0.025
4. BD (1) C 1 - N 13	/599. BD*(1) C 1 - C 3	2.16	1.41	0.049
4. BD (1) C 1 - N 13	/602. BD*(1) C 2 - C 4	0.86	1.45	0.032
4. BD (1) C 1 - N 13	/605. BD*(1) C 3 - C 5	2.70	1.24	0.052
4. BD (1) C 1 - N 13	/624. BD*(1) N 13 - C 14	0.85	1.15	0.029
4. BD (1) C 1 - N 13	/626. BD*(1) C 14 - C 15	1.68	1.22	0.041
5. BD (1) C 2 - C 4	/118. RY*(1) C 1	1.42	1.95	0.047
5. BD (1) C 2 - C 4	/120. RY*(3) C 1	0.91	2.01	0.038
5. BD (1) C 2 - C 4	/183. RY*(1) C 6	1.07	1.82	0.040
5. BD (1) C 2 - C 4	/598. BD*(1) C 1 - C 2	2.70	1.19	0.051

5. BD (1) C 2 - C 4	/601. BD*(1) C 1 - N 13	2.79	1.12	0.050
5. BD (1) C 2 - C 4	/604. BD*(1) C 2 - H 32	1.68	1.20	0.040
5. BD (1) C 2 - C 4	/607. BD*(1) C 4 - C 6	3.67	1.21	0.060
5. BD (1) C 2 - C 4	/608. BD*(1) C 4 - H 33	1.59	1.19	0.039
5. BD (1) C 2 - C 4	/612. BD*(1) C 6 -Se 11	3.17	0.88	0.047
6. BD (2) C 2 - C 4	/123. RY*(6) C 1	0.62	1.83	0.032
6. BD (2) C 2 - C 4	/185. RY*(3) C 6	0.54	1.12	0.023
6. BD (2) C 2 - C 4	/600. BD*(2) C 1 - C 3	14.23	0.31	0.060
6. BD (2) C 2 - C 4	/610. BD*(2) C 5 - C 6	13.05	0.31	0.057
7. BD (1) C 2 - H 32	/118. RY*(1) C 1	0.65	1.72	0.030
7. BD (1) C 2 - H 32	/119. RY*(2) C 1	0.88	1.83	0.036
7. BD (1) C 2 - H 32	/157. RY*(1) C 4	1.44	1.68	0.044
7. BD (1) C 2 - H 32	/599. BD*(1) C 1 - C 3	3.22	1.14	0.054
7. BD (1) C 2 - H 32	/601. BD*(1) C 1 - N 13	0.61	0.89	0.021
7. BD (1) C 2 - H 32	/602. BD*(1) C 2 - C 4	1.59	1.17	0.039
7. BD (1) C 2 - H 32	/607. BD*(1) C 4 - C 6	5.73	0.98	0.067
7. BD (1) C 2 - H 32	/608. BD*(1) C 4 - H 33	0.95	0.96	0.027
8. BD (1) C 3 - C 5	/119. RY*(2) C 1	1.22	1.95	0.044
8. BD (1) C 3 - C 5	/184. RY*(2) C 6	1.45	1.48	0.042
8. BD (1) C 3 - C 5	/196. RY*(1) C 7	0.99	1.58	0.036
8. BD (1) C 3 - C 5	/599. BD*(1) C 1 - C 3	4.55	1.26	0.068
8. BD (1) C 3 - C 5	/601. BD*(1) C 1 - N 13	5.32	1.02	0.066
8. BD (1) C 3 - C 5	/606. BD*(1) C 3 - C 7	1.66	1.06	0.038
8. BD (1) C 3 - C 5	/609. BD*(1) C 5 - C 6	3.94	1.29	0.064
8. BD (1) C 3 - C 5	/611. BD*(1) C 5 - H 34	0.63	1.10	0.024
8. BD (1) C 3 - C 5	/612. BD*(1) C 6 -Se 11	5.62	0.77	0.059
8. BD (1) C 3 - C 5	/613. BD*(1) C 7 - O 8	2.80	0.93	0.046
8. BD (1) C 3 - C 5	/615. BD*(2) C 7 - O 9	0.54	0.63	0.017
9. BD (1) C 3 - C 7	/118. RY*(1) C 1	0.85	1.88	0.036
9. BD (1) C 3 - C 7	/119. RY*(2) C 1	1.03	1.99	0.041
9. BD (1) C 3 - C 7	/170. RY*(1) C 5	1.04	1.82	0.039
9. BD (1) C 3 - C 7	/222. RY*(1) O 9	0.72	1.81	0.032
9. BD (1) C 3 - C 7	/598. BD*(1) C 1 - C 2	3.78	1.13	0.058
9. BD (1) C 3 - C 7	/599. BD*(1) C 1 - C 3	3.98	1.30	0.064
9. BD (1) C 3 - C 7	/605. BD*(1) C 3 - C 5	1.29	1.13	0.034
9. BD (1) C 3 - C 7	/609. BD*(1) C 5 - C 6	1.49	1.33	0.040
9. BD (1) C 3 - C 7	/614. BD*(1) C 7 - O 9	0.94	1.19	0.030
9. BD (1) C 3 - C 7	/616. BD*(1) O 8 - C 10	2.83	0.96	0.047
10. BD (1) C 4 - C 6	/131. RY*(1) C 2	0.75	1.94	0.034
10. BD (1) C 4 - C 6	/132. RY*(2) C 2	1.59	2.00	0.051
10. BD (1) C 4 - C 6	/170. RY*(1) C 5	0.87	1.80	0.035
10. BD (1) C 4 - C 6	/171. RY*(2) C 5	0.95	1.64	0.035
10. BD (1) C 4 - C 6	/602. BD*(1) C 2 - C 4	3.18	1.32	0.058
10. BD (1) C 4 - C 6	/604. BD*(1) C 2 - H 32	2.63	1.12	0.049
10. BD (1) C 4 - C 6	/608. BD*(1) C 4 - H 33	0.87	1.11	0.028
10. BD (1) C 4 - C 6	/609. BD*(1) C 5 - C 6	3.54	1.32	0.061
10. BD (1) C 4 - C 6	/611. BD*(1) C 5 - H 34	3.40	1.12	0.055
11. BD (1) C 4 - H 33	/131. RY*(1) C 2	1.54	1.79	0.047
11. BD (1) C 4 - H 33	/183. RY*(1) C 6	1.12	1.60	0.038
11. BD (1) C 4 - H 33	/598. BD*(1) C 1 - C 2	5.65	0.97	0.066
11. BD (1) C 4 - H 33	/602. BD*(1) C 2 - C 4	1.52	1.18	0.038
11. BD (1) C 4 - H 33	/604. BD*(1) C 2 - H 32	0.95	0.97	0.027
11. BD (1) C 4 - H 33	/609. BD*(1) C 5 - C 6	3.20	1.17	0.055
12. BD (1) C 5 - C 6	/144. RY*(1) C 3	1.48	2.60	0.056
12. BD (1) C 5 - C 6	/145. RY*(2) C 3	0.65	2.05	0.033

12. BD (1) C 5 - C 6	/157. RY*(1) C 4	1.03	1.92	0.040
12. BD (1) C 5 - C 6	/605. BD*(1) C 3 - C 5	3.32	1.21	0.057
12. BD (1) C 5 - C 6	/606. BD*(1) C 3 - C 7	2.01	1.18	0.044
12. BD (1) C 5 - C 6	/607. BD*(1) C 4 - C 6	3.19	1.23	0.056
12. BD (1) C 5 - C 6	/608. BD*(1) C 4 - H 33	1.64	1.21	0.040
12. BD (1) C 5 - C 6	/611. BD*(1) C 5 - H 34	2.30	1.22	0.047
13. BD (2) C 5 - C 6	/147. RY*(4) C 3	0.64	1.07	0.025
13. BD (2) C 5 - C 6	/159. RY*(3) C 4	1.74	1.11	0.042
13. BD (2) C 5 - C 6	/248. RY*(1)Se 11	0.91	0.84	0.026
13. BD (2) C 5 - C 6	/600. BD*(2) C 1 - C 3	11.67	0.31	0.055
13. BD (2) C 5 - C 6	/603. BD*(2) C 2 - C 4	13.05	0.33	0.059
13. BD (2) C 5 - C 6	/620. BD*(1)Se 11 - C 12	0.51	0.38	0.013
14. BD (1) C 5 - H 34	/144. RY*(1) C 3	1.80	2.36	0.058
14. BD (1) C 5 - H 34	/183. RY*(1) C 6	1.77	1.59	0.048
14. BD (1) C 5 - H 34	/599. BD*(1) C 1 - C 3	3.07	1.14	0.053
14. BD (1) C 5 - H 34	/607. BD*(1) C 4 - C 6	6.02	0.98	0.069
14. BD (1) C 5 - H 34	/609. BD*(1) C 5 - C 6	2.13	1.17	0.045
15. BD (1) C 6 -Se 11	/157. RY*(1) C 4	2.06	1.74	0.054
15. BD (1) C 6 -Se 11	/170. RY*(1) C 5	1.65	1.72	0.048
15. BD (1) C 6 -Se 11	/274. RY*(1) C 12	0.59	1.34	0.025
15. BD (1) C 6 -Se 11	/602. BD*(1) C 2 - C 4	2.63	1.24	0.051
15. BD (1) C 6 -Se 11	/605. BD*(1) C 3 - C 5	5.19	1.03	0.065
15. BD (1) C 6 -Se 11	/609. BD*(1) C 5 - C 6	0.96	1.23	0.031
15. BD (1) C 6 -Se 11	/611. BD*(1) C 5 - H 34	0.92	1.04	0.028
15. BD (1) C 6 -Se 11	/621. BD*(1) C 12 - C 21	0.92	0.99	0.027
16. BD (1) C 7 - O 8	/145. RY*(2) C 3	1.04	2.16	0.042
16. BD (1) C 7 - O 8	/237. RY*(3) C 10	1.07	1.84	0.040
16. BD (1) C 7 - O 8	/605. BD*(1) C 3 - C 5	1.28	1.31	0.037
16. BD (1) C 7 - O 8	/619. BD*(1) C 10 - H 37	0.65	1.24	0.025
17. BD (1) C 7 - O 9	/145. RY*(2) C 3	1.28	2.29	0.048
17. BD (1) C 7 - O 9	/196. RY*(1) C 7	1.64	1.94	0.050
17. BD (1) C 7 - O 9	/599. BD*(1) C 1 - C 3	1.55	1.62	0.045
17. BD (1) C 7 - O 9	/606. BD*(1) C 3 - C 7	1.77	1.42	0.045
18. BD (2) C 7 - O 9	/600. BD*(2) C 1 - C 3	4.57	0.40	0.041
18. BD (2) C 7 - O 9	/615. BD*(2) C 7 - O 9	0.64	0.36	0.014
19. BD (1) O 8 - C 10	/196. RY*(1) C 7	1.27	1.77	0.042
19. BD (1) O 8 - C 10	/606. BD*(1) C 3 - C 7	2.63	1.25	0.052
20. BD (1) C 10 - H 35	/210. RY*(2) O 8	0.53	1.51	0.025
20. BD (1) C 10 - H 35	/616. BD*(1) O 8 - C 10	0.50	0.79	0.018
21. BD (1) C 10 - H 36	/210. RY*(2) O 8	0.58	1.51	0.026
21. BD (1) C 10 - H 36	/616. BD*(1) O 8 - C 10	0.59	0.79	0.019
22. BD (1) C 10 - H 37	/613. BD*(1) C 7 - O 8	3.95	0.80	0.051
23. BD (1)Se 11 - C 12	/395. RY*(5) C 21	0.65	2.07	0.033
23. BD (1)Se 11 - C 12	/607. BD*(1) C 4 - C 6	1.77	1.03	0.038
23. BD (1)Se 11 - C 12	/610. BD*(2) C 5 - C 6	0.88	0.59	0.022
23. BD (1)Se 11 - C 12	/638. BD*(1) C 21 - O 22	0.71	1.09	0.025
23. BD (1)Se 11 - C 12	/639. BD*(2) C 21 - O 22	6.56	0.58	0.058
24. BD (1) C 12 - C 21	/404. RY*(1) O 22	0.80	1.81	0.034
24. BD (1) C 12 - C 21	/417. RY*(1) N 23	1.84	1.70	0.050
24. BD (1) C 12 - C 21	/622. BD*(1) C 12 - H 38	0.59	1.06	0.022
24. BD (1) C 12 - C 21	/638. BD*(1) C 21 - O 22	0.80	1.21	0.028
24. BD (1) C 12 - C 21	/641. BD*(1) N 23 - C 24	2.90	1.08	0.050
25. BD (1) C 12 - H 38	/394. RY*(4) C 21	0.66	2.40	0.036
25. BD (1) C 12 - H 38	/638. BD*(1) C 21 - O 22	3.19	1.04	0.052
25. BD (1) C 12 - H 38	/639. BD*(2) C 21 - O 22	2.65	0.54	0.036

26. BD (1) C 12 - H 39	/391. RY*(1) C 21	0.55	1.29	0.024
26. BD (1) C 12 - H 39	/621. BD*(1) C 12 - C 21	0.54	0.92	0.020
26. BD (1) C 12 - H 39	/638. BD*(1) C 21 - O 22	1.04	1.04	0.029
26. BD (1) C 12 - H 39	/640. BD*(1) C 21 - N 23	5.68	0.89	0.065
27. BD (1) N 13 - C 14	/118. RY*(1) C 1	0.72	1.99	0.034
27. BD (1) N 13 - C 14	/119. RY*(2) C 1	0.76	2.10	0.036
27. BD (1) N 13 - C 14	/314. RY*(2) C 15	1.00	1.89	0.039
27. BD (1) N 13 - C 14	/599. BD*(1) C 1 - C 3	1.62	1.41	0.043
27. BD (1) N 13 - C 14	/601. BD*(1) C 1 - N 13	1.05	1.16	0.031
27. BD (1) N 13 - C 14	/629. BD*(1) C 15 - C 17	1.10	1.42	0.035
28. BD (1) N 13 - H 40	/118. RY*(1) C 1	1.08	1.85	0.040
28. BD (1) N 13 - H 40	/301. RY*(2) C 14	0.83	2.04	0.037
28. BD (1) N 13 - H 40	/303. RY*(4) C 14	0.92	3.07	0.048
28. BD (1) N 13 - H 40	/598. BD*(1) C 1 - C 2	2.12	1.10	0.043
28. BD (1) N 13 - H 40	/600. BD*(2) C 1 - C 3	1.54	0.69	0.031
28. BD (1) N 13 - H 40	/627. BD*(1) C 14 - O 16	2.95	1.18	0.053
29. BD (1) C 14 - C 15	/288. RY*(2) N 13	1.34	1.76	0.044
29. BD (1) C 14 - C 15	/326. RY*(1) O 16	0.63	1.86	0.031
29. BD (1) C 14 - C 15	/339. RY*(1) C 17	2.27	1.82	0.058
29. BD (1) C 14 - C 15	/601. BD*(1) C 1 - N 13	2.94	1.06	0.050
29. BD (1) C 14 - C 15	/627. BD*(1) C 14 - O 16	0.97	1.21	0.031
29. BD (1) C 14 - C 15	/629. BD*(1) C 15 - C 17	2.75	1.32	0.054
29. BD (1) C 14 - C 15	/632. BD*(1) C 17 - C 18	3.41	1.11	0.055
30. BD (1) C 14 - O 16	/300. RY*(1) C 14	1.66	1.88	0.050
30. BD (1) C 14 - O 16	/624. BD*(1) N 13 - C 14	0.53	1.36	0.024
30. BD (1) C 14 - O 16	/625. BD*(1) N 13 - H 40	1.15	1.34	0.035
30. BD (1) C 14 - O 16	/626. BD*(1) C 14 - C 15	1.57	1.43	0.043
30. BD (1) C 14 - O 16	/631. BD*(1) C 15 - H 30	0.86	1.42	0.031
31. BD (2) C 14 - O 16	/316. RY*(4) C 15	0.63	1.03	0.023
31. BD (2) C 14 - O 16	/628. BD*(2) C 14 - O 16	0.75	0.35	0.016
31. BD (2) C 14 - O 16	/630. BD*(2) C 15 - C 17	5.13	0.38	0.040
32. BD (1) C 15 - C 17	/300. RY*(1) C 14	2.15	1.66	0.053
32. BD (1) C 15 - C 17	/352. RY*(1) C 18	2.20	1.67	0.054
32. BD (1) C 15 - C 17	/624. BD*(1) N 13 - C 14	2.47	1.13	0.048
32. BD (1) C 15 - C 17	/626. BD*(1) C 14 - C 15	2.35	1.20	0.048
32. BD (1) C 15 - C 17	/631. BD*(1) C 15 - H 30	1.65	1.20	0.040
32. BD (1) C 15 - C 17	/632. BD*(1) C 17 - C 18	2.00	1.19	0.044
32. BD (1) C 15 - C 17	/633. BD*(1) C 17 - H 31	1.68	1.21	0.040
32. BD (1) C 15 - C 17	/634. BD*(1) C 18 - O 19	2.32	1.06	0.045
33. BD (2) C 15 - C 17	/304. RY*(5) C 14	0.76	1.59	0.032
33. BD (2) C 15 - C 17	/356. RY*(5) C 18	0.96	1.63	0.037
33. BD (2) C 15 - C 17	/628. BD*(2) C 14 - O 16	17.70	0.29	0.066
33. BD (2) C 15 - C 17	/636. BD*(2) C 18 - O 20	19.14	0.28	0.067
34. BD (1) C 15 - H 30	/301. RY*(2) C 14	0.64	1.93	0.031
34. BD (1) C 15 - H 30	/303. RY*(4) C 14	0.73	2.96	0.042
34. BD (1) C 15 - H 30	/339. RY*(1) C 17	1.01	1.67	0.037
34. BD (1) C 15 - H 30	/340. RY*(2) C 17	0.64	1.60	0.029
34. BD (1) C 15 - H 30	/627. BD*(1) C 14 - O 16	3.46	1.06	0.054
34. BD (1) C 15 - H 30	/629. BD*(1) C 15 - C 17	1.49	1.17	0.037
34. BD (1) C 15 - H 30	/633. BD*(1) C 17 - H 31	4.53	0.98	0.059
35. BD (1) C 17 - C 18	/313. RY*(1) C 15	2.14	1.74	0.055
35. BD (1) C 17 - C 18	/378. RY*(1) O 20	0.75	1.78	0.033
35. BD (1) C 17 - C 18	/626. BD*(1) C 14 - C 15	3.40	1.13	0.056
35. BD (1) C 17 - C 18	/629. BD*(1) C 15 - C 17	2.34	1.33	0.050
35. BD (1) C 17 - C 18	/635. BD*(1) C 18 - O 20	0.75	1.22	0.027

35. BD (1) C 17 - C 18	/637. BD*(1) O 19 - H 41	1.69	1.01	0.037
36. BD (1) C 17 - H 31	/313. RY*(1) C 15	1.05	1.57	0.036
36. BD (1) C 17 - H 31	/314. RY*(2) C 15	0.66	1.63	0.029
36. BD (1) C 17 - H 31	/355. RY*(4) C 18	0.69	2.81	0.040
36. BD (1) C 17 - H 31	/629. BD*(1) C 15 - C 17	1.66	1.16	0.039
36. BD (1) C 17 - H 31	/631. BD*(1) C 15 - H 30	4.95	0.96	0.062
36. BD (1) C 17 - H 31	/634. BD*(1) C 18 - O 19	0.50	0.82	0.018
36. BD (1) C 17 - H 31	/635. BD*(1) C 18 - O 20	3.24	1.05	0.052
37. BD (1) C 18 - O 19	/340. RY*(2) C 17	0.72	1.97	0.034
37. BD (1) C 18 - O 19	/629. BD*(1) C 15 - C 17	1.02	1.53	0.035
38. BD (1) C 18 - O 20	/340. RY*(2) C 17	0.58	2.06	0.031
38. BD (1) C 18 - O 20	/352. RY*(1) C 18	1.58	1.90	0.049
38. BD (1) C 18 - O 20	/632. BD*(1) C 17 - C 18	1.40	1.42	0.040
38. BD (1) C 18 - O 20	/633. BD*(1) C 17 - H 31	0.88	1.44	0.032
39. BD (2) C 18 - O 20	/342. RY*(4) C 17	0.64	0.97	0.022
39. BD (2) C 18 - O 20	/630. BD*(2) C 15 - C 17	5.15	0.39	0.040
39. BD (2) C 18 - O 20	/636. BD*(2) C 18 - O 20	0.73	0.35	0.015
40. BD (1) O 19 - H 41	/352. RY*(1) C 18	0.95	1.62	0.035
40. BD (1) O 19 - H 41	/353. RY*(2) C 18	0.72	2.05	0.034
40. BD (1) O 19 - H 41	/358. RY*(7) C 18	0.69	2.04	0.034
40. BD (1) O 19 - H 41	/632. BD*(1) C 17 - C 18	3.65	1.15	0.058
40. BD (1) O 19 - H 41	/635. BD*(1) C 18 - O 20	1.29	1.24	0.036
41. BD (1) C 21 - O 22	/391. RY*(1) C 21	1.59	1.75	0.047
41. BD (1) C 21 - O 22	/621. BD*(1) C 12 - C 21	1.44	1.37	0.040
41. BD (1) C 21 - O 22	/622. BD*(1) C 12 - H 38	0.55	1.35	0.024
41. BD (1) C 21 - O 22	/642. BD*(1) N 23 - H 42	1.00	1.33	0.033
42. BD (2) C 21 - O 22	/620. BD*(1)Se 11 - C 12	3.08	0.46	0.034
42. BD (2) C 21 - O 22	/622. BD*(1) C 12 - H 38	1.41	0.74	0.029
42. BD (2) C 21 - O 22	/639. BD*(2) C 21 - O 22	0.74	0.38	0.016
43. BD (1) C 21 - N 23	/274. RY*(1) C 12	0.81	1.53	0.031
43. BD (1) C 21 - N 23	/430. RY*(1) C 24	0.93	2.03	0.039
43. BD (1) C 21 - N 23	/431. RY*(2) C 24	0.74	2.18	0.036
43. BD (1) C 21 - N 23	/623. BD*(1) C 12 - H 39	0.64	1.17	0.024
43. BD (1) C 21 - N 23	/641. BD*(1) N 23 - C 24	1.07	1.17	0.032
43. BD (1) C 21 - N 23	/643. BD*(1) C 24 - C 25	1.67	1.25	0.041
44. BD (1) N 23 - C 24	/391. RY*(1) C 21	1.66	1.54	0.045
44. BD (1) N 23 - C 24	/443. RY*(1) C 25	0.81	2.06	0.037
44. BD (1) N 23 - C 24	/456. RY*(1) C 26	0.64	2.04	0.032
44. BD (1) N 23 - C 24	/621. BD*(1) C 12 - C 21	1.81	1.17	0.041
44. BD (1) N 23 - C 24	/640. BD*(1) C 21 - N 23	0.91	1.15	0.029
44. BD (1) N 23 - C 24	/643. BD*(1) C 24 - C 25	0.62	1.24	0.025
44. BD (1) N 23 - C 24	/644. BD*(1) C 24 - C 26	2.05	1.43	0.048
44. BD (1) N 23 - C 24	/646. BD*(1) C 25 - C 27	0.83	1.44	0.031
44. BD (1) N 23 - C 24	/649. BD*(1) C 26 - C 28	2.10	1.26	0.046
45. BD (1) N 23 - H 42	/392. RY*(2) C 21	0.70	1.90	0.033
45. BD (1) N 23 - H 42	/394. RY*(4) C 21	0.93	2.51	0.043
45. BD (1) N 23 - H 42	/430. RY*(1) C 24	1.36	1.89	0.045
45. BD (1) N 23 - H 42	/638. BD*(1) C 21 - O 22	2.70	1.16	0.050
45. BD (1) N 23 - H 42	/639. BD*(2) C 21 - O 22	0.85	0.65	0.022
45. BD (1) N 23 - H 42	/644. BD*(1) C 24 - C 26	2.64	1.29	0.052
45. BD (1) N 23 - H 42	/645. BD*(2) C 24 - C 26	0.70	0.69	0.021
46. BD (1) C 24 - C 25	/418. RY*(2) N 23	1.03	1.54	0.036
46. BD (1) C 24 - C 25	/456. RY*(1) C 26	0.76	1.90	0.034
46. BD (1) C 24 - C 25	/457. RY*(2) C 26	0.58	1.90	0.030
46. BD (1) C 24 - C 25	/469. RY*(1) C 27	0.81	1.95	0.036

46. BD (1) C 24 - C 25	/470. RY*(2) C 27	1.68	2.11	0.053
46. BD (1) C 24 - C 25	/640. BD*(1) C 21 - N 23	2.62	1.01	0.047
46. BD (1) C 24 - C 25	/641. BD*(1) N 23 - C 24	0.54	1.03	0.021
46. BD (1) C 24 - C 25	/644. BD*(1) C 24 - C 26	4.09	1.29	0.065
46. BD (1) C 24 - C 25	/646. BD*(1) C 25 - C 27	2.97	1.30	0.056
46. BD (1) C 24 - C 25	/648. BD*(1) C 25 - H 43	0.61	1.09	0.023
46. BD (1) C 24 - C 25	/650. BD*(1) C 26 - H 44	3.04	1.11	0.052
46. BD (1) C 24 - C 25	/652. BD*(1) C 27 - H 45	2.90	1.10	0.051
47. BD (1) C 24 - C 26	/418. RY*(2) N 23	0.68	1.63	0.030
47. BD (1) C 24 - C 26	/443. RY*(1) C 25	0.77	2.02	0.035
47. BD (1) C 24 - C 26	/482. RY*(1) C 28	0.85	2.03	0.037
47. BD (1) C 24 - C 26	/483. RY*(2) C 28	1.05	2.18	0.043
47. BD (1) C 24 - C 26	/641. BD*(1) N 23 - C 24	2.02	1.12	0.043
47. BD (1) C 24 - C 26	/642. BD*(1) N 23 - H 42	1.69	1.08	0.038
47. BD (1) C 24 - C 26	/643. BD*(1) C 24 - C 25	3.82	1.19	0.060
47. BD (1) C 24 - C 26	/648. BD*(1) C 25 - H 43	1.49	1.18	0.037
47. BD (1) C 24 - C 26	/649. BD*(1) C 26 - C 28	2.66	1.21	0.051
47. BD (1) C 24 - C 26	/650. BD*(1) C 26 - H 44	1.80	1.20	0.042
47. BD (1) C 24 - C 26	/655. BD*(1) C 28 - H 46	1.35	1.19	0.036
48. BD (2) C 24 - C 26	/445. RY*(3) C 25	1.40	1.07	0.037
48. BD (2) C 24 - C 26	/485. RY*(4) C 28	1.07	0.90	0.030
48. BD (2) C 24 - C 26	/640. BD*(1) C 21 - N 23	0.87	0.63	0.022
48. BD (2) C 24 - C 26	/642. BD*(1) N 23 - H 42	0.91	0.61	0.022
48. BD (2) C 24 - C 26	/647. BD*(2) C 25 - C 27	13.10	0.31	0.057
48. BD (2) C 24 - C 26	/654. BD*(2) C 28 - C 29	13.50	0.32	0.059
49. BD (1) C 25 - C 27	/431. RY*(2) C 24	1.93	2.13	0.057
49. BD (1) C 25 - C 27	/495. RY*(1) C 29	0.92	2.04	0.039
49. BD (1) C 25 - C 27	/496. RY*(2) C 29	0.95	2.18	0.041
49. BD (1) C 25 - C 27	/641. BD*(1) N 23 - C 24	3.00	1.12	0.052
49. BD (1) C 25 - C 27	/643. BD*(1) C 24 - C 25	2.90	1.20	0.053
49. BD (1) C 25 - C 27	/648. BD*(1) C 25 - H 43	1.74	1.18	0.040
49. BD (1) C 25 - C 27	/651. BD*(1) C 27 - C 29	2.54	1.22	0.050
49. BD (1) C 25 - C 27	/652. BD*(1) C 27 - H 45	1.53	1.19	0.038
49. BD (1) C 25 - C 27	/656. BD*(1) C 29 - H 47	1.57	1.19	0.039
50. BD (2) C 25 - C 27	/434. RY*(5) C 24	0.56	1.82	0.030
50. BD (2) C 25 - C 27	/497. RY*(3) C 29	1.38	0.90	0.033
50. BD (2) C 25 - C 27	/645. BD*(2) C 24 - C 26	13.36	0.32	0.059
50. BD (2) C 25 - C 27	/654. BD*(2) C 28 - C 29	12.36	0.32	0.056
51. BD (1) C 25 - H 43	/430. RY*(1) C 24	0.88	1.77	0.035
51. BD (1) C 25 - H 43	/431. RY*(2) C 24	0.78	1.92	0.035
51. BD (1) C 25 - H 43	/469. RY*(1) C 27	1.62	1.83	0.049
51. BD (1) C 25 - H 43	/641. BD*(1) N 23 - C 24	0.59	0.91	0.021
51. BD (1) C 25 - H 43	/644. BD*(1) C 24 - C 26	3.00	1.17	0.053
51. BD (1) C 25 - H 43	/646. BD*(1) C 25 - C 27	1.51	1.18	0.038
51. BD (1) C 25 - H 43	/651. BD*(1) C 27 - C 29	5.11	1.00	0.064
51. BD (1) C 25 - H 43	/652. BD*(1) C 27 - H 45	0.83	0.97	0.025
52. BD (1) C 26 - C 28	/430. RY*(1) C 24	1.90	1.88	0.054
52. BD (1) C 26 - C 28	/495. RY*(1) C 29	0.70	1.93	0.033
52. BD (1) C 26 - C 28	/496. RY*(2) C 29	1.59	2.07	0.052
52. BD (1) C 26 - C 28	/641. BD*(1) N 23 - C 24	5.67	1.02	0.068
52. BD (1) C 26 - C 28	/644. BD*(1) C 24 - C 26	3.18	1.28	0.057
52. BD (1) C 26 - C 28	/650. BD*(1) C 26 - H 44	0.59	1.10	0.023
52. BD (1) C 26 - C 28	/653. BD*(1) C 28 - C 29	2.78	1.30	0.054
52. BD (1) C 26 - C 28	/656. BD*(1) C 29 - H 47	3.29	1.09	0.054
53. BD (1) C 26 - H 44	/431. RY*(2) C 24	1.98	1.90	0.055

53. BD (1) C 26 - H 44	/482. RY*(1) C 28	1.19	1.80	0.042
53. BD (1) C 26 - H 44	/641. BD*(1) N 23 - C 24	0.97	0.89	0.026
53. BD (1) C 26 - H 44	/643. BD*(1) C 24 - C 25	5.75	0.97	0.067
53. BD (1) C 26 - H 44	/644. BD*(1) C 24 - C 26	1.51	1.15	0.037
53. BD (1) C 26 - H 44	/653. BD*(1) C 28 - C 29	2.54	1.17	0.049
54. BD (1) C 27 - C 29	/443. RY*(1) C 25	0.59	1.92	0.030
54. BD (1) C 27 - C 29	/444. RY*(2) C 25	1.80	1.98	0.054
54. BD (1) C 27 - C 29	/482. RY*(1) C 28	0.76	1.94	0.034
54. BD (1) C 27 - C 29	/483. RY*(2) C 28	1.59	2.08	0.052
54. BD (1) C 27 - C 29	/646. BD*(1) C 25 - C 27	2.80	1.29	0.054
54. BD (1) C 27 - C 29	/648. BD*(1) C 25 - H 43	3.35	1.08	0.054
54. BD (1) C 27 - C 29	/652. BD*(1) C 27 - H 45	0.55	1.09	0.022
54. BD (1) C 27 - C 29	/653. BD*(1) C 28 - C 29	2.82	1.30	0.054
54. BD (1) C 27 - C 29	/655. BD*(1) C 28 - H 46	3.23	1.09	0.053
54. BD (1) C 27 - C 29	/656. BD*(1) C 29 - H 47	0.53	1.09	0.022
55. BD (1) C 27 - H 45	/443. RY*(1) C 25	1.63	1.80	0.049
55. BD (1) C 27 - H 45	/495. RY*(1) C 29	1.30	1.82	0.044
55. BD (1) C 27 - H 45	/643. BD*(1) C 24 - C 25	5.60	0.98	0.066
55. BD (1) C 27 - H 45	/646. BD*(1) C 25 - C 27	1.33	1.17	0.035
55. BD (1) C 27 - H 45	/648. BD*(1) C 25 - H 43	0.87	0.96	0.026
55. BD (1) C 27 - H 45	/653. BD*(1) C 28 - C 29	2.50	1.18	0.049
56. BD (1) C 28 - C 29	/456. RY*(1) C 26	0.95	1.99	0.039
56. BD (1) C 28 - C 29	/457. RY*(2) C 26	1.02	1.99	0.040
56. BD (1) C 28 - C 29	/469. RY*(1) C 27	0.88	2.04	0.038
56. BD (1) C 28 - C 29	/470. RY*(2) C 27	1.01	2.20	0.042
56. BD (1) C 28 - C 29	/593. RY*(1) H 47	0.51	1.20	0.022
56. BD (1) C 28 - C 29	/649. BD*(1) C 26 - C 28	2.41	1.21	0.048
56. BD (1) C 28 - C 29	/650. BD*(1) C 26 - H 44	1.44	1.20	0.037
56. BD (1) C 28 - C 29	/651. BD*(1) C 27 - C 29	2.54	1.21	0.050
56. BD (1) C 28 - C 29	/652. BD*(1) C 27 - H 45	1.60	1.19	0.039
56. BD (1) C 28 - C 29	/655. BD*(1) C 28 - H 46	1.60	1.19	0.039
56. BD (1) C 28 - C 29	/656. BD*(1) C 29 - H 47	1.67	1.19	0.040
57. BD (2) C 28 - C 29	/458. RY*(3) C 26	0.92	0.98	0.028
57. BD (2) C 28 - C 29	/471. RY*(3) C 27	1.38	1.08	0.037
57. BD (2) C 28 - C 29	/645. BD*(2) C 24 - C 26	13.01	0.31	0.057
57. BD (2) C 28 - C 29	/647. BD*(2) C 25 - C 27	14.20	0.31	0.059
58. BD (1) C 28 - H 46	/456. RY*(1) C 26	1.28	1.77	0.043
58. BD (1) C 28 - H 46	/495. RY*(1) C 29	1.66	1.81	0.049
58. BD (1) C 28 - H 46	/644. BD*(1) C 24 - C 26	2.72	1.16	0.050
58. BD (1) C 28 - H 46	/651. BD*(1) C 27 - C 29	5.31	0.99	0.065
58. BD (1) C 28 - H 46	/653. BD*(1) C 28 - C 29	1.31	1.18	0.035
58. BD (1) C 28 - H 46	/656. BD*(1) C 29 - H 47	0.85	0.97	0.026
59. BD (1) C 29 - H 47	/469. RY*(1) C 27	1.31	1.82	0.044
59. BD (1) C 29 - H 47	/482. RY*(1) C 28	1.70	1.81	0.050
59. BD (1) C 29 - H 47	/646. BD*(1) C 25 - C 27	2.57	1.17	0.049
59. BD (1) C 29 - H 47	/649. BD*(1) C 26 - C 28	5.28	0.99	0.065
59. BD (1) C 29 - H 47	/653. BD*(1) C 28 - C 29	1.34	1.18	0.036
59. BD (1) C 29 - H 47	/655. BD*(1) C 28 - H 46	0.84	0.97	0.026
60. CR (1) C 1	/132. RY*(2) C 2	0.95	11.44	0.093
60. CR (1) C 1	/144. RY*(1) C 3	0.55	11.95	0.073
60. CR (1) C 1	/145. RY*(2) C 3	1.67	11.40	0.123
60. CR (1) C 1	/599. BD*(1) C 1 - C 3	1.37	10.73	0.109
60. CR (1) C 1	/602. BD*(1) C 2 - C 4	0.57	10.77	0.070
60. CR (1) C 1	/605. BD*(1) C 3 - C 5	1.03	10.56	0.094
60. CR (1) C 1	/606. BD*(1) C 3 - C 7	1.11	10.53	0.098

60. CR (1) C 1	/624. BD*(1) N 13 - C 14	1.02	10.48	0.094
61. CR (1) C 2	/119. RY*(2) C 1	1.36	11.36	0.111
61. CR (1) C 2	/157. RY*(1) C 4	0.60	11.21	0.073
61. CR (1) C 2	/158. RY*(2) C 4	1.71	11.23	0.124
61. CR (1) C 2	/599. BD*(1) C 1 - C 3	0.83	10.67	0.084
61. CR (1) C 2	/601. BD*(1) C 1 - N 13	0.54	10.42	0.067
61. CR (1) C 2	/602. BD*(1) C 2 - C 4	0.82	10.70	0.084
61. CR (1) C 2	/607. BD*(1) C 4 - C 6	1.32	10.51	0.106
62. CR (1) C 3	/118. RY*(1) C 1	1.15	11.27	0.102
62. CR (1) C 3	/120. RY*(3) C 1	0.99	11.33	0.095
62. CR (1) C 3	/171. RY*(2) C 5	0.74	11.04	0.081
62. CR (1) C 3	/197. RY*(2) C 7	0.60	11.52	0.074
62. CR (1) C 3	/202. RY*(7) C 7	0.84	11.20	0.086
62. CR (1) C 3	/598. BD*(1) C 1 - C 2	1.09	10.52	0.096
62. CR (1) C 3	/599. BD*(1) C 1 - C 3	1.23	10.69	0.103
62. CR (1) C 3	/601. BD*(1) C 1 - N 13	1.02	10.44	0.093
62. CR (1) C 3	/609. BD*(1) C 5 - C 6	0.72	10.72	0.079
62. CR (1) C 3	/613. BD*(1) C 7 - O 8	0.61	10.36	0.073
63. CR (1) C 4	/132. RY*(2) C 2	1.34	11.38	0.110
63. CR (1) C 4	/134. RY*(4) C 2	0.65	11.07	0.076
63. CR (1) C 4	/184. RY*(2) C 6	1.29	10.89	0.106
63. CR (1) C 4	/186. RY*(4) C 6	0.62	11.13	0.074
63. CR (1) C 4	/598. BD*(1) C 1 - C 2	1.20	10.49	0.101
63. CR (1) C 4	/602. BD*(1) C 2 - C 4	0.67	10.70	0.076
63. CR (1) C 4	/609. BD*(1) C 5 - C 6	0.83	10.69	0.084
63. CR (1) C 4	/612. BD*(1) C 6 -Se 11	0.84	10.18	0.083
64. CR (1) C 5	/145. RY*(2) C 3	0.79	11.34	0.085
64. CR (1) C 5	/183. RY*(1) C 6	1.13	11.12	0.100
64. CR (1) C 5	/184. RY*(2) C 6	1.86	10.89	0.127
64. CR (1) C 5	/185. RY*(3) C 6	0.52	10.89	0.067
64. CR (1) C 5	/599. BD*(1) C 1 - C 3	0.76	10.67	0.081
64. CR (1) C 5	/606. BD*(1) C 3 - C 7	0.65	10.47	0.075
64. CR (1) C 5	/607. BD*(1) C 4 - C 6	1.23	10.51	0.102
64. CR (1) C 5	/609. BD*(1) C 5 - C 6	1.20	10.69	0.102
64. CR (1) C 5	/612. BD*(1) C 6 -Se 11	1.28	10.18	0.103
65. CR (1) C 6	/158. RY*(2) C 4	1.04	11.27	0.097
65. CR (1) C 6	/171. RY*(2) C 5	2.13	11.06	0.137
65. CR (1) C 6	/173. RY*(4) C 5	0.60	11.16	0.073
65. CR (1) C 6	/602. BD*(1) C 2 - C 4	0.62	10.74	0.073
65. CR (1) C 6	/605. BD*(1) C 3 - C 5	1.16	10.53	0.099
65. CR (1) C 6	/609. BD*(1) C 5 - C 6	1.22	10.73	0.103
65. CR (1) C 6	/611. BD*(1) C 5 - H 34	0.55	10.54	0.068
65. CR (1) C 6	/612. BD*(1) C 6 -Se 11	1.33	10.22	0.105
66. CR (1) C 7	/144. RY*(1) C 3	1.20	12.05	0.108
66. CR (1) C 7	/599. BD*(1) C 1 - C 3	0.88	10.83	0.087
66. CR (1) C 7	/605. BD*(1) C 3 - C 5	0.54	10.65	0.068
66. CR (1) C 7	/606. BD*(1) C 3 - C 7	0.55	10.63	0.069
66. CR (1) C 7	/613. BD*(1) C 7 - O 8	0.67	10.49	0.077
66. CR (1) C 7	/616. BD*(1) O 8 - C 10	1.10	10.48	0.096
67. CR (1) O 8	/196. RY*(1) C 7	1.02	19.92	0.127
67. CR (1) O 8	/197. RY*(2) C 7	1.09	20.43	0.133
67. CR (1) O 8	/237. RY*(3) C 10	0.91	19.96	0.121
68. CR (1) O 9	/196. RY*(1) C 7	5.25	19.81	0.289
68. CR (1) O 9	/606. BD*(1) C 3 - C 7	0.79	19.29	0.111
69. CR (1) C 10	/544. RY*(2) H 37	0.56	12.17	0.074

69. CR (1) C 10	/613. BD*(1) C 7 - O 8	1.11	10.39	0.098
69. CR (1) C 10	/616. BD*(1) O 8 - C 10	1.50	10.39	0.112
72. CR (3)Se 11	/183. RY*(1) C 6	0.96	11.37	0.093
72. CR (3)Se 11	/607. BD*(1) C 4 - C 6	0.74	10.76	0.080
72. CR (3)Se 11	/609. BD*(1) C 5 - C 6	1.23	10.94	0.104
84. CR (1) C 12	/392. RY*(2) C 21	1.09	11.36	0.100
84. CR (1) C 12	/620. BD*(1)Se 11 - C 12	1.05	10.19	0.093
84. CR (1) C 12	/640. BD*(1) C 21 - N 23	0.60	10.47	0.073
85. CR (1) N 13	/118. RY*(1) C 1	1.12	15.41	0.117
85. CR (1) N 13	/119. RY*(2) C 1	0.53	15.52	0.081
85. CR (1) N 13	/301. RY*(2) C 14	1.44	15.60	0.134
85. CR (1) N 13	/599. BD*(1) C 1 - C 3	0.59	14.83	0.084
86. CR (1) C 14	/314. RY*(2) C 15	0.56	11.28	0.071
86. CR (1) C 14	/601. BD*(1) C 1 - N 13	1.15	10.56	0.099
86. CR (1) C 14	/629. BD*(1) C 15 - C 17	0.65	10.81	0.075
87. CR (1) C 15	/301. RY*(2) C 14	1.06	11.46	0.099
87. CR (1) C 15	/340. RY*(2) C 17	1.86	11.14	0.129
87. CR (1) C 15	/341. RY*(3) C 17	0.53	11.25	0.069
87. CR (1) C 15	/624. BD*(1) N 13 - C 14	0.51	10.44	0.067
87. CR (1) C 15	/629. BD*(1) C 15 - C 17	0.66	10.70	0.075
87. CR (1) C 15	/632. BD*(1) C 17 - C 18	1.06	10.50	0.095
88. CR (1) O 16	/300. RY*(1) C 14	5.53	19.74	0.296
88. CR (1) O 16	/626. BD*(1) C 14 - C 15	0.75	19.29	0.109
89. CR (1) C 17	/314. RY*(2) C 15	1.59	11.17	0.119
89. CR (1) C 17	/315. RY*(3) C 15	0.70	11.38	0.080
89. CR (1) C 17	/353. RY*(2) C 18	0.78	11.40	0.085
89. CR (1) C 17	/358. RY*(7) C 18	0.58	11.39	0.073
89. CR (1) C 17	/626. BD*(1) C 14 - C 15	1.08	10.50	0.096
89. CR (1) C 17	/629. BD*(1) C 15 - C 17	0.72	10.70	0.079
89. CR (1) C 17	/631. BD*(1) C 15 - H 30	0.53	10.50	0.067
90. CR (1) C 18	/340. RY*(2) C 17	0.55	11.28	0.071
90. CR (1) C 18	/629. BD*(1) C 15 - C 17	0.63	10.84	0.074
90. CR (1) C 18	/634. BD*(1) C 18 - O 19	0.63	10.51	0.074
91. CR (1) O 19	/352. RY*(1) C 18	0.80	19.88	0.113
91. CR (1) O 19	/353. RY*(2) C 18	1.52	20.31	0.157
91. CR (1) O 19	/355. RY*(4) C 18	0.64	21.26	0.104
91. CR (1) O 19	/566. RY*(4) H 41	0.56	20.96	0.097
92. CR (1) O 20	/352. RY*(1) C 18	5.57	19.77	0.297
92. CR (1) O 20	/632. BD*(1) C 17 - C 18	0.75	19.29	0.109
93. CR (1) C 21	/276. RY*(3) C 12	1.04	10.99	0.096
93. CR (1) C 21	/641. BD*(1) N 23 - C 24	1.15	10.57	0.099
94. CR (1) O 22	/391. RY*(1) C 21	5.94	19.61	0.306
94. CR (1) O 22	/621. BD*(1) C 12 - C 21	0.84	19.24	0.115
95. CR (1) N 23	/392. RY*(2) C 21	1.76	15.46	0.147
95. CR (1) N 23	/430. RY*(1) C 24	0.59	15.45	0.085
95. CR (1) N 23	/431. RY*(2) C 24	0.67	15.60	0.092
95. CR (1) N 23	/433. RY*(4) C 24	0.88	15.39	0.104
95. CR (1) N 23	/570. RY*(3) H 42	0.51	16.47	0.082
95. CR (1) N 23	/644. BD*(1) C 24 - C 26	0.58	14.85	0.083
96. CR (1) C 24	/444. RY*(2) C 25	0.92	11.43	0.092
96. CR (1) C 24	/457. RY*(2) C 26	1.85	11.35	0.130
96. CR (1) C 24	/640. BD*(1) C 21 - N 23	1.08	10.46	0.097
96. CR (1) C 24	/644. BD*(1) C 24 - C 26	1.41	10.74	0.111
96. CR (1) C 24	/646. BD*(1) C 25 - C 27	0.57	10.75	0.070
96. CR (1) C 24	/649. BD*(1) C 26 - C 28	0.92	10.57	0.089

96. CR (1) C 24	/650. BD*(1) C 26 - H 44	0.52	10.56	0.066
97. CR (1) C 25	/430. RY*(1) C 24	1.21	11.29	0.104
97. CR (1) C 25	/470. RY*(2) C 27	2.12	11.50	0.140
97. CR (1) C 25	/574. RY*(2) H 43	0.52	12.32	0.071
97. CR (1) C 25	/641. BD*(1) N 23 - C 24	0.57	10.43	0.069
97. CR (1) C 25	/644. BD*(1) C 24 - C 26	0.75	10.68	0.080
97. CR (1) C 25	/646. BD*(1) C 25 - C 27	0.83	10.70	0.084
97. CR (1) C 25	/651. BD*(1) C 27 - C 29	1.06	10.52	0.095
98. CR (1) C 26	/431. RY*(2) C 24	2.59	11.43	0.154
98. CR (1) C 26	/483. RY*(2) C 28	0.79	11.48	0.085
98. CR (1) C 26	/641. BD*(1) N 23 - C 24	1.03	10.42	0.093
98. CR (1) C 26	/643. BD*(1) C 24 - C 25	1.21	10.49	0.101
98. CR (1) C 26	/644. BD*(1) C 24 - C 26	0.73	10.68	0.079
98. CR (1) C 26	/653. BD*(1) C 28 - C 29	0.64	10.70	0.074
99. CR (1) C 27	/444. RY*(2) C 25	1.57	11.38	0.119
99. CR (1) C 27	/446. RY*(4) C 25	0.51	11.00	0.067
99. CR (1) C 27	/496. RY*(2) C 29	0.81	11.48	0.086
99. CR (1) C 27	/584. RY*(2) H 45	0.58	12.28	0.075
99. CR (1) C 27	/643. BD*(1) C 24 - C 25	1.18	10.50	0.100
99. CR (1) C 27	/646. BD*(1) C 25 - C 27	0.75	10.70	0.080
99. CR (1) C 27	/648. BD*(1) C 25 - H 43	0.53	10.48	0.067
99. CR (1) C 27	/653. BD*(1) C 28 - C 29	0.62	10.70	0.073
100. CR (1) C 28	/496. RY*(2) C 29	2.11	11.48	0.139
100. CR (1) C 28	/589. RY*(2) H 46	0.55	12.28	0.073
100. CR (1) C 28	/644. BD*(1) C 24 - C 26	0.69	10.68	0.077
100. CR (1) C 28	/651. BD*(1) C 27 - C 29	1.07	10.51	0.095
100. CR (1) C 28	/653. BD*(1) C 28 - C 29	0.82	10.70	0.084
100. CR (1) C 28	/656. BD*(1) C 29 - H 47	0.51	10.49	0.066
101. CR (1) C 29	/470. RY*(2) C 27	0.77	11.49	0.084
101. CR (1) C 29	/483. RY*(2) C 28	2.14	11.48	0.140
101. CR (1) C 29	/594. RY*(2) H 47	0.56	12.28	0.074
101. CR (1) C 29	/646. BD*(1) C 25 - C 27	0.63	10.69	0.073
101. CR (1) C 29	/649. BD*(1) C 26 - C 28	1.04	10.51	0.094
101. CR (1) C 29	/653. BD*(1) C 28 - C 29	0.80	10.70	0.083
101. CR (1) C 29	/655. BD*(1) C 28 - H 46	0.50	10.49	0.065
102. LP (1) O 8	/196. RY*(1) C 7	1.66	1.51	0.045
102. LP (1) O 8	/199. RY*(4) C 7	1.63	2.60	0.058
102. LP (1) O 8	/235. RY*(1) C 10	1.64	1.66	0.047
102. LP (1) O 8	/237. RY*(3) C 10	0.79	1.55	0.031
102. LP (1) O 8	/614. BD*(1) C 7 - O 9	5.71	1.08	0.070
102. LP (1) O 8	/617. BD*(1) C 10 - H 35	0.63	0.95	0.022
102. LP (1) O 8	/619. BD*(1) C 10 - H 37	2.36	0.95	0.043
103. LP (2) O 8	/198. RY*(3) C 7	1.81	1.84	0.054
103. LP (2) O 8	/236. RY*(2) C 10	1.51	1.50	0.045
103. LP (2) O 8	/615. BD*(2) C 7 - O 9	38.70	0.31	0.100
103. LP (2) O 8	/617. BD*(1) C 10 - H 35	5.02	0.70	0.056
103. LP (2) O 8	/618. BD*(1) C 10 - H 36	5.02	0.70	0.055
104. LP (1) O 9	/196. RY*(1) C 7	12.30	1.65	0.127
104. LP (1) O 9	/606. BD*(1) C 3 - C 7	2.25	1.13	0.045
104. LP (1) O 9	/613. BD*(1) C 7 - O 8	0.98	0.99	0.028
105. LP (2) O 9	/197. RY*(2) C 7	1.95	1.71	0.053
105. LP (2) O 9	/199. RY*(4) C 7	1.69	2.28	0.057
105. LP (2) O 9	/606. BD*(1) C 3 - C 7	12.51	0.68	0.084
105. LP (2) O 9	/613. BD*(1) C 7 - O 8	28.81	0.55	0.113
105. LP (2) O 9	/619. BD*(1) C 10 - H 37	0.80	0.64	0.021

106. LP (1)Se 11	/183. RY*(1) C 6	1.15	1.78	0.040
106. LP (1)Se 11	/609. BD*(1) C 5 - C 6	3.29	1.36	0.060
107. LP (2)Se 11	/607. BD*(1) C 4 - C 6	1.59	0.70	0.030
107. LP (2)Se 11	/609. BD*(1) C 5 - C 6	1.04	0.88	0.028
107. LP (2)Se 11	/610. BD*(2) C 5 - C 6	9.08	0.27	0.045
107. LP (2)Se 11	/622. BD*(1) C 12 - H 38	2.39	0.61	0.035
107. LP (2)Se 11	/623. BD*(1) C 12 - H 39	3.92	0.62	0.045
108. LP (1) N 13	/120. RY*(3) C 1	1.11	1.52	0.040
108. LP (1) N 13	/121. RY*(4) C 1	0.73	1.59	0.033
108. LP (1) N 13	/302. RY*(3) C 14	1.60	1.72	0.051
108. LP (1) N 13	/559. RY*(2) H 40	0.75	1.95	0.037
108. LP (1) N 13	/598. BD*(1) C 1 - C 2	3.68	0.71	0.049
108. LP (1) N 13	/599. BD*(1) C 1 - C 3	2.77	0.89	0.048
108. LP (1) N 13	/600. BD*(2) C 1 - C 3	17.51	0.30	0.065
108. LP (1) N 13	/628. BD*(2) C 14 - O 16	50.61	0.26	0.102
109. LP (1) O 16	/300. RY*(1) C 14	13.17	1.58	0.129
109. LP (1) O 16	/624. BD*(1) N 13 - C 14	1.20	1.06	0.032
109. LP (1) O 16	/626. BD*(1) C 14 - C 15	2.16	1.13	0.044
110. LP (2) O 16	/301. RY*(2) C 14	1.40	1.64	0.044
110. LP (2) O 16	/303. RY*(4) C 14	1.82	2.67	0.064
110. LP (2) O 16	/624. BD*(1) N 13 - C 14	23.97	0.62	0.110
110. LP (2) O 16	/626. BD*(1) C 14 - C 15	14.70	0.68	0.091
111. LP (1) O 19	/352. RY*(1) C 18	2.40	1.52	0.054
111. LP (1) O 19	/355. RY*(4) C 18	1.67	2.90	0.062
111. LP (1) O 19	/565. RY*(3) H 41	1.30	2.29	0.049
111. LP (1) O 19	/635. BD*(1) C 18 - O 20	5.36	1.14	0.070
112. LP (2) O 19	/354. RY*(3) C 18	2.04	1.85	0.057
112. LP (2) O 19	/564. RY*(2) H 41	1.56	1.81	0.050
112. LP (2) O 19	/636. BD*(2) C 18 - O 20	40.59	0.32	0.103
113. LP (1) O 20	/352. RY*(1) C 18	13.28	1.61	0.131
113. LP (1) O 20	/632. BD*(1) C 17 - C 18	2.18	1.14	0.045
113. LP (1) O 20	/634. BD*(1) C 18 - O 19	0.84	1.01	0.026
114. LP (2) O 20	/353. RY*(2) C 18	2.69	1.59	0.060
114. LP (2) O 20	/355. RY*(4) C 18	1.04	2.54	0.047
114. LP (2) O 20	/632. BD*(1) C 17 - C 18	13.36	0.69	0.087
114. LP (2) O 20	/634. BD*(1) C 18 - O 19	27.85	0.56	0.112
115. LP (1) O 22	/391. RY*(1) C 21	14.07	1.45	0.128
115. LP (1) O 22	/621. BD*(1) C 12 - C 21	2.48	1.08	0.047
115. LP (1) O 22	/640. BD*(1) C 21 - N 23	1.37	1.06	0.034
116. LP (2) O 22	/392. RY*(2) C 21	1.82	1.51	0.048
116. LP (2) O 22	/394. RY*(4) C 21	1.52	2.12	0.052
116. LP (2) O 22	/395. RY*(5) C 21	0.73	1.74	0.033
116. LP (2) O 22	/621. BD*(1) C 12 - C 21	14.51	0.64	0.088
116. LP (2) O 22	/640. BD*(1) C 21 - N 23	24.14	0.62	0.110
117. LP (1) N 23	/393. RY*(3) C 21	1.47	1.65	0.048
117. LP (1) N 23	/398. RY*(8) C 21	0.57	1.81	0.031
117. LP (1) N 23	/432. RY*(3) C 24	1.80	1.48	0.050
117. LP (1) N 23	/569. RY*(2) H 42	0.92	1.87	0.040
117. LP (1) N 23	/638. BD*(1) C 21 - O 22	1.75	0.78	0.035
117. LP (1) N 23	/639. BD*(2) C 21 - O 22	42.53	0.27	0.096
117. LP (1) N 23	/643. BD*(1) C 24 - C 25	2.00	0.72	0.036
117. LP (1) N 23	/644. BD*(1) C 24 - C 26	1.50	0.91	0.036
117. LP (1) N 23	/645. BD*(2) C 24 - C 26	20.75	0.31	0.073
600. BD*(2) C 1 - C 3	/122. RY*(5) C 1	1.04	1.30	0.084
600. BD*(2) C 1 - C 3	/147. RY*(4) C 3	0.86	0.75	0.058

600. BD*(2) C 1 - C 3	/603. BD*(2) C 2 - C 4	130.80	0.01 0.072
600. BD*(2) C 1 - C 3	/613. BD*(1) C 7 - O 8	0.82	0.25 0.028
600. BD*(2) C 1 - C 3	/624. BD*(1) N 13 - C 14	0.70	0.33 0.031
600. BD*(2) C 1 - C 3	/625. BD*(1) N 13 - H 40	0.95	0.31 0.038
603. BD*(2) C 2 - C 4	/133. RY*(3) C 2	0.79	0.69 0.069
603. BD*(2) C 2 - C 4	/161. RY*(5) C 4	0.84	1.38 0.101
610. BD*(2) C 5 - C 6	/172. RY*(3) C 5	2.89	0.53 0.099
610. BD*(2) C 5 - C 6	/185. RY*(3) C 6	0.71	0.81 0.060
610. BD*(2) C 5 - C 6	/603. BD*(2) C 2 - C 4	123.76	0.01 0.071
610. BD*(2) C 5 - C 6	/620. BD*(1)Se 11 - C 12	1.27	0.07 0.022
613. BD*(1) C 7 - O 8	/197. RY*(2) C 7	1.59	1.16 0.163
613. BD*(1) C 7 - O 8	/209. RY*(1) O 8	0.57	1.05 0.094
613. BD*(1) C 7 - O 8	/605. BD*(1) C 3 - C 5	1.07	0.16 0.046
613. BD*(1) C 7 - O 8	/606. BD*(1) C 3 - C 7	0.81	0.14 0.034
613. BD*(1) C 7 - O 8	/614. BD*(1) C 7 - O 9	0.52	0.22 0.039
615. BD*(2) C 7 - O 9	/198. RY*(3) C 7	1.50	1.53 0.119
615. BD*(2) C 7 - O 9	/223. RY*(2) O 9	1.09	0.98 0.082
615. BD*(2) C 7 - O 9	/600. BD*(2) C 1 - C 3	35.74	0.04 0.068
628. BD*(2) C 14 - O 16	/302. RY*(3) C 14	1.50	1.47 0.107
628. BD*(2) C 14 - O 16	/306. RY*(7) C 14	1.52	1.02 0.091
628. BD*(2) C 14 - O 16	/327. RY*(2) O 16	1.40	1.02 0.087
628. BD*(2) C 14 - O 16	/630. BD*(2) C 15 - C 17	44.98	0.03 0.076
636. BD*(2) C 18 - O 20	/354. RY*(3) C 18	1.59	1.54 0.123
636. BD*(2) C 18 - O 20	/360. RY*(9) C 18	1.00	0.76 0.069
636. BD*(2) C 18 - O 20	/379. RY*(2) O 20	1.01	1.02 0.080
636. BD*(2) C 18 - O 20	/630. BD*(2) C 15 - C 17	29.86	0.04 0.075
639. BD*(2) C 21 - O 22	/393. RY*(3) C 21	1.19	1.38 0.099
639. BD*(2) C 21 - O 22	/405. RY*(2) O 22	1.15	0.97 0.083
639. BD*(2) C 21 - O 22	/612. BD*(1) C 6 -Se 11	0.51	0.11 0.018
639. BD*(2) C 21 - O 22	/620. BD*(1)Se 11 - C 12	5.16	0.08 0.049
639. BD*(2) C 21 - O 22	/622. BD*(1) C 12 - H 38	0.69	0.36 0.038
639. BD*(2) C 21 - O 22	/638. BD*(1) C 21 - O 22	2.41	0.51 0.083
645. BD*(2) C 24 - C 26	/435. RY*(6) C 24	0.84	1.29 0.081
645. BD*(2) C 24 - C 26	/458. RY*(3) C 26	1.78	0.67 0.085
645. BD*(2) C 24 - C 26	/640. BD*(1) C 21 - N 23	0.57	0.31 0.029
647. BD*(2) C 25 - C 27	/445. RY*(3) C 25	0.54	0.76 0.054
647. BD*(2) C 25 - C 27	/447. RY*(5) C 25	0.73	1.45 0.087
647. BD*(2) C 25 - C 27	/471. RY*(3) C 27	0.56	0.77 0.056
647. BD*(2) C 25 - C 27	/472. RY*(4) C 27	0.78	1.43 0.090
654. BD*(2) C 28 - C 29	/485. RY*(4) C 28	1.75	0.58 0.086
654. BD*(2) C 28 - C 29	/497. RY*(3) C 29	1.37	0.58 0.075

NATURAL BOND ORBITAL ANALYSIS:

	Occ.	Occupancies		Lewis Structure				Low occ	High occ	
Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	(L)	(NL)	Dev
1(1)	1.90	222.98911	11.01089	42	57	0	18	23	16	0.81
2(2)	1.90	222.98911	11.01089	42	57	0	18	23	16	0.81
3(1)	1.80	226.07281	7.92719	42	55	0	20	6	11	0.64
4(2)	1.80	226.07281	7.92719	42	55	0	20	6	11	0.64
5(1)	1.70	229.10645	4.89355	42	59	0	16	1	11	0.49
6(2)	1.70	229.68741	4.31259	42	59	0	16	1	11	0.26

7(3)	1.70	229.68741	4.31259	42	59	0	16	1	11	0.26
8(1)	1.60	229.69356	4.30644	42	59	0	16	0	11	0.26
9(2)	1.60	229.69356	4.30644	42	59	0	16	0	11	0.26
10(1)	1.50	228.43709	5.56291	42	58	0	17	0	13	0.74
11(2)	1.50	228.43709	5.56291	42	58	0	17	0	13	0.74
12(1)	1.60	229.69356	4.30644	42	59	0	16	0	11	0.26

Core	83.97523 (99.971% of 84)
Valence Lewis	145.71833 (97.146% of 150)
Total Lewis	229.69356 (98.160% of 234)
Valence non-Lewis	3.86669 (1.652% of 234)
Rydberg non-Lewis	0.43975 (0.188% of 234)
Total non-Lewis	4.30644 (1.840% of 234)

Compound 12

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 2	/145. RY*(1) C 3	0.69	2.49	0.037
1. BD (1) C 1 - C 2	/146. RY*(2) C 3	0.84	1.95	0.036
1. BD (1) C 1 - C 2	/159. RY*(2) C 4	2.16	1.83	0.056
1. BD (1) C 1 - C 2	/288. RY*(1) N 13	0.89	1.52	0.033
1. BD (1) C 1 - C 2	/610. BD*(1) C 1 - C 3	4.20	1.27	0.065
1. BD (1) C 1 - C 2	/612. BD*(1) C 1 - N 13	0.59	1.03	0.022
1. BD (1) C 1 - C 2	/613. BD*(1) C 2 - C 4	2.94	1.31	0.056
1. BD (1) C 1 - C 2	/615. BD*(1) C 2 - H 30	0.62	1.10	0.023
1. BD (1) C 1 - C 2	/617. BD*(1) C 3 - C 7	4.36	1.07	0.061
1. BD (1) C 1 - C 2	/619. BD*(1) C 4 - H 31	2.83	1.10	0.050
1. BD (1) C 1 - C 2	/636. BD*(1) N 13 - H 38	1.65	1.00	0.036
2. BD (1) C 1 - C 3	/132. RY*(1) C 2	0.73	2.02	0.035
2. BD (1) C 1 - C 3	/171. RY*(1) C 5	0.56	1.88	0.029
2. BD (1) C 1 - C 3	/200. RY*(4) C 7	0.59	2.77	0.036
2. BD (1) C 1 - C 3	/288. RY*(1) N 13	0.55	1.62	0.027
2. BD (1) C 1 - C 3	/609. BD*(1) C 1 - C 2	3.43	1.20	0.057
2. BD (1) C 1 - C 3	/612. BD*(1) C 1 - N 13	2.10	1.12	0.043
2. BD (1) C 1 - C 3	/615. BD*(1) C 2 - H 30	1.30	1.20	0.035
2. BD (1) C 1 - C 3	/616. BD*(1) C 3 - C 5	4.24	1.20	0.064
2. BD (1) C 1 - C 3	/617. BD*(1) C 3 - C 7	2.95	1.17	0.053
2. BD (1) C 1 - C 3	/622. BD*(1) C 5 - H 32	1.33	1.20	0.036

2. BD (1) C 1 - C 3	/625. BD*(1) C 7 - O 9	1.16	1.26	0.034
2. BD (1) C 1 - C 3	/635. BD*(1) N 13 - C 14	2.09	1.12	0.044
3. BD (2) C 1 - C 3	/134. RY*(3) C 2	1.11	1.00	0.032
3. BD (2) C 1 - C 3	/173. RY*(3) C 5	0.87	0.88	0.026
3. BD (2) C 1 - C 3	/201. RY*(5) C 7	0.60	1.46	0.028
3. BD (2) C 1 - C 3	/614. BD*(2) C 2 - C 4	10.75	0.33	0.054
3. BD (2) C 1 - C 3	/621. BD*(2) C 5 - C 6	13.97	0.32	0.059
3. BD (2) C 1 - C 3	/624. BD*(1) C 7 - O 8	1.19	0.57	0.024
3. BD (2) C 1 - C 3	/626. BD*(2) C 7 - O 9	18.73	0.27	0.064
3. BD (2) C 1 - C 3	/635. BD*(1) N 13 - C 14	1.41	0.66	0.028
3. BD (2) C 1 - C 3	/636. BD*(1) N 13 - H 38	1.43	0.63	0.029
4. BD (1) C 1 - N 13	/132. RY*(1) C 2	0.52	2.06	0.029
4. BD (1) C 1 - N 13	/145. RY*(1) C 3	1.26	2.62	0.051
4. BD (1) C 1 - N 13	/301. RY*(1) C 14	1.81	1.57	0.048
4. BD (1) C 1 - N 13	/609. BD*(1) C 1 - C 2	0.64	1.23	0.025
4. BD (1) C 1 - N 13	/610. BD*(1) C 1 - C 3	2.19	1.41	0.050
4. BD (1) C 1 - N 13	/613. BD*(1) C 2 - C 4	0.87	1.44	0.032
4. BD (1) C 1 - N 13	/616. BD*(1) C 3 - C 5	2.73	1.23	0.052
4. BD (1) C 1 - N 13	/635. BD*(1) N 13 - C 14	0.95	1.16	0.030
4. BD (1) C 1 - N 13	/637. BD*(1) C 14 - C 15	1.75	1.19	0.041
5. BD (1) C 2 - C 4	/119. RY*(1) C 1	1.38	1.91	0.046
5. BD (1) C 2 - C 4	/121. RY*(3) C 1	0.95	2.03	0.040
5. BD (1) C 2 - C 4	/184. RY*(1) C 6	1.07	1.82	0.040
5. BD (1) C 2 - C 4	/609. BD*(1) C 1 - C 2	2.72	1.20	0.051
5. BD (1) C 2 - C 4	/612. BD*(1) C 1 - N 13	2.77	1.12	0.050
5. BD (1) C 2 - C 4	/615. BD*(1) C 2 - H 30	1.68	1.20	0.040
5. BD (1) C 2 - C 4	/618. BD*(1) C 4 - C 6	3.68	1.21	0.060
5. BD (1) C 2 - C 4	/619. BD*(1) C 4 - H 31	1.59	1.19	0.039
5. BD (1) C 2 - C 4	/623. BD*(1) C 6 -Se 11	3.18	0.88	0.047
6. BD (2) C 2 - C 4	/124. RY*(6) C 1	0.63	1.82	0.032
6. BD (2) C 2 - C 4	/611. BD*(2) C 1 - C 3	14.30	0.31	0.061
6. BD (2) C 2 - C 4	/621. BD*(2) C 5 - C 6	12.98	0.31	0.057
7. BD (1) C 2 - H 30	/119. RY*(1) C 1	0.58	1.68	0.028
7. BD (1) C 2 - H 30	/120. RY*(2) C 1	0.89	1.83	0.036
7. BD (1) C 2 - H 30	/158. RY*(1) C 4	1.43	1.68	0.044
7. BD (1) C 2 - H 30	/610. BD*(1) C 1 - C 3	3.22	1.14	0.054
7. BD (1) C 2 - H 30	/612. BD*(1) C 1 - N 13	0.60	0.89	0.021
7. BD (1) C 2 - H 30	/613. BD*(1) C 2 - C 4	1.59	1.18	0.039
7. BD (1) C 2 - H 30	/618. BD*(1) C 4 - C 6	5.70	0.98	0.067
7. BD (1) C 2 - H 30	/619. BD*(1) C 4 - H 31	0.94	0.96	0.027
8. BD (1) C 3 - C 5	/120. RY*(2) C 1	1.22	1.95	0.044
8. BD (1) C 3 - C 5	/185. RY*(2) C 6	1.46	1.48	0.042
8. BD (1) C 3 - C 5	/197. RY*(1) C 7	0.97	1.59	0.035
8. BD (1) C 3 - C 5	/610. BD*(1) C 1 - C 3	4.57	1.26	0.068
8. BD (1) C 3 - C 5	/612. BD*(1) C 1 - N 13	5.31	1.02	0.066
8. BD (1) C 3 - C 5	/617. BD*(1) C 3 - C 7	1.67	1.06	0.038
8. BD (1) C 3 - C 5	/620. BD*(1) C 5 - C 6	3.92	1.29	0.064
8. BD (1) C 3 - C 5	/622. BD*(1) C 5 - H 32	0.64	1.10	0.024
8. BD (1) C 3 - C 5	/623. BD*(1) C 6 -Se 11	5.63	0.77	0.059
8. BD (1) C 3 - C 5	/624. BD*(1) C 7 - O 8	2.78	0.93	0.046
8. BD (1) C 3 - C 5	/626. BD*(2) C 7 - O 9	0.59	0.63	0.018
9. BD (1) C 3 - C 7	/119. RY*(1) C 1	0.80	1.85	0.035
9. BD (1) C 3 - C 7	/120. RY*(2) C 1	1.07	2.00	0.041
9. BD (1) C 3 - C 7	/171. RY*(1) C 5	1.04	1.82	0.039
9. BD (1) C 3 - C 7	/223. RY*(1) O 9	0.73	1.81	0.033

9. BD (1) C 3 - C 7	/609. BD*(1) C 1 - C 2	3.79	1.13	0.058
9. BD (1) C 3 - C 7	/610. BD*(1) C 1 - C 3	4.01	1.30	0.065
9. BD (1) C 3 - C 7	/616. BD*(1) C 3 - C 5	1.29	1.13	0.034
9. BD (1) C 3 - C 7	/620. BD*(1) C 5 - C 6	1.47	1.33	0.040
9. BD (1) C 3 - C 7	/625. BD*(1) C 7 - O 9	0.95	1.19	0.030
9. BD (1) C 3 - C 7	/627. BD*(1) O 8 - C 10	2.85	0.96	0.047
10. BD (1) C 4 - C 6	/132. RY*(1) C 2	0.76	1.94	0.034
10. BD (1) C 4 - C 6	/133. RY*(2) C 2	1.55	2.01	0.050
10. BD (1) C 4 - C 6	/171. RY*(1) C 5	0.90	1.80	0.036
10. BD (1) C 4 - C 6	/172. RY*(2) C 5	0.89	1.63	0.034
10. BD (1) C 4 - C 6	/613. BD*(1) C 2 - C 4	3.21	1.33	0.058
10. BD (1) C 4 - C 6	/615. BD*(1) C 2 - H 30	2.66	1.12	0.049
10. BD (1) C 4 - C 6	/619. BD*(1) C 4 - H 31	0.87	1.11	0.028
10. BD (1) C 4 - C 6	/620. BD*(1) C 5 - C 6	3.55	1.32	0.061
10. BD (1) C 4 - C 6	/622. BD*(1) C 5 - H 32	3.39	1.12	0.055
11. BD (1) C 4 - H 31	/132. RY*(1) C 2	1.54	1.79	0.047
11. BD (1) C 4 - H 31	/184. RY*(1) C 6	1.12	1.60	0.038
11. BD (1) C 4 - H 31	/609. BD*(1) C 1 - C 2	5.65	0.97	0.066
11. BD (1) C 4 - H 31	/613. BD*(1) C 2 - C 4	1.52	1.18	0.038
11. BD (1) C 4 - H 31	/615. BD*(1) C 2 - H 30	0.95	0.97	0.027
11. BD (1) C 4 - H 31	/620. BD*(1) C 5 - C 6	3.20	1.17	0.055
12. BD (1) C 5 - C 6	/145. RY*(1) C 3	1.61	2.60	0.058
12. BD (1) C 5 - C 6	/146. RY*(2) C 3	0.57	2.06	0.031
12. BD (1) C 5 - C 6	/158. RY*(1) C 4	1.04	1.92	0.040
12. BD (1) C 5 - C 6	/616. BD*(1) C 3 - C 5	3.32	1.21	0.057
12. BD (1) C 5 - C 6	/617. BD*(1) C 3 - C 7	2.01	1.18	0.044
12. BD (1) C 5 - C 6	/618. BD*(1) C 4 - C 6	3.21	1.23	0.056
12. BD (1) C 5 - C 6	/619. BD*(1) C 4 - H 31	1.64	1.21	0.040
12. BD (1) C 5 - C 6	/622. BD*(1) C 5 - H 32	2.29	1.22	0.047
13. BD (2) C 5 - C 6	/148. RY*(4) C 3	0.69	1.08	0.026
13. BD (2) C 5 - C 6	/160. RY*(3) C 4	1.78	1.11	0.042
13. BD (2) C 5 - C 6	/249. RY*(1)Se 11	0.92	0.84	0.026
13. BD (2) C 5 - C 6	/611. BD*(2) C 1 - C 3	11.40	0.32	0.055
13. BD (2) C 5 - C 6	/614. BD*(2) C 2 - C 4	13.21	0.33	0.059
13. BD (2) C 5 - C 6	/631. BD*(1)Se 11 - C 12	0.54	0.38	0.014
14. BD (1) C 5 - H 32	/145. RY*(1) C 3	1.79	2.35	0.058
14. BD (1) C 5 - H 32	/184. RY*(1) C 6	1.78	1.59	0.048
14. BD (1) C 5 - H 32	/610. BD*(1) C 1 - C 3	3.07	1.14	0.053
14. BD (1) C 5 - H 32	/618. BD*(1) C 4 - C 6	6.04	0.98	0.069
14. BD (1) C 5 - H 32	/620. BD*(1) C 5 - C 6	2.13	1.17	0.045
15. BD (1) C 6 -Se 11	/158. RY*(1) C 4	2.06	1.74	0.054
15. BD (1) C 6 -Se 11	/171. RY*(1) C 5	1.67	1.72	0.048
15. BD (1) C 6 -Se 11	/275. RY*(1) C 12	0.60	1.35	0.026
15. BD (1) C 6 -Se 11	/613. BD*(1) C 2 - C 4	2.64	1.24	0.051
15. BD (1) C 6 -Se 11	/616. BD*(1) C 3 - C 5	5.19	1.03	0.065
15. BD (1) C 6 -Se 11	/620. BD*(1) C 5 - C 6	0.96	1.23	0.031
15. BD (1) C 6 -Se 11	/622. BD*(1) C 5 - H 32	0.91	1.04	0.028
15. BD (1) C 6 -Se 11	/632. BD*(1) C 12 - C 21	0.93	0.99	0.027
16. BD (1) C 7 - O 8	/146. RY*(2) C 3	1.07	2.17	0.043
16. BD (1) C 7 - O 8	/238. RY*(3) C 10	1.01	1.84	0.039
16. BD (1) C 7 - O 8	/616. BD*(1) C 3 - C 5	1.27	1.31	0.037
16. BD (1) C 7 - O 8	/630. BD*(1) C 10 - H 35	0.65	1.24	0.025
17. BD (1) C 7 - O 9	/146. RY*(2) C 3	1.18	2.30	0.046
17. BD (1) C 7 - O 9	/197. RY*(1) C 7	1.65	1.94	0.051
17. BD (1) C 7 - O 9	/610. BD*(1) C 1 - C 3	1.54	1.62	0.045

17. BD (1) C 7 - O 9	/617. BD*(1) C 3 - C 7	1.76	1.42	0.045
18. BD (2) C 7 - O 9	/611. BD*(2) C 1 - C 3	4.49	0.40	0.041
18. BD (2) C 7 - O 9	/626. BD*(2) C 7 - O 9	0.65	0.36	0.014
19. BD (1) O 8 - C 10	/197. RY*(1) C 7	1.27	1.78	0.042
19. BD (1) O 8 - C 10	/617. BD*(1) C 3 - C 7	2.61	1.26	0.052
20. BD (1) C 10 - H 33	/211. RY*(2) O 8	0.57	1.51	0.026
20. BD (1) C 10 - H 33	/627. BD*(1) O 8 - C 10	0.59	0.79	0.019
21. BD (1) C 10 - H 34	/211. RY*(2) O 8	0.53	1.51	0.025
22. BD (1) C 10 - H 35	/624. BD*(1) C 7 - O 8	3.94	0.80	0.051
23. BD (1)Se 11 - C 12	/396. RY*(5) C 21	0.64	2.07	0.033
23. BD (1)Se 11 - C 12	/618. BD*(1) C 4 - C 6	1.74	1.03	0.038
23. BD (1)Se 11 - C 12	/621. BD*(2) C 5 - C 6	0.93	0.59	0.022
23. BD (1)Se 11 - C 12	/650. BD*(1) C 21 - O 22	0.70	1.09	0.025
23. BD (1)Se 11 - C 12	/651. BD*(2) C 21 - O 22	6.60	0.58	0.059
24. BD (1) C 12 - C 21	/405. RY*(1) O 22	0.80	1.81	0.034
24. BD (1) C 12 - C 21	/418. RY*(1) N 23	1.89	1.70	0.051
24. BD (1) C 12 - C 21	/633. BD*(1) C 12 - H 36	0.59	1.06	0.022
24. BD (1) C 12 - C 21	/650. BD*(1) C 21 - O 22	0.80	1.21	0.028
24. BD (1) C 12 - C 21	/653. BD*(1) N 23 - C 24	2.90	1.08	0.050
25. BD (1) C 12 - H 36	/395. RY*(4) C 21	0.67	2.40	0.036
25. BD (1) C 12 - H 36	/650. BD*(1) C 21 - O 22	3.21	1.05	0.052
25. BD (1) C 12 - H 36	/651. BD*(2) C 21 - O 22	2.61	0.54	0.036
26. BD (1) C 12 - H 37	/392. RY*(1) C 21	0.55	1.29	0.024
26. BD (1) C 12 - H 37	/632. BD*(1) C 12 - C 21	0.54	0.92	0.020
26. BD (1) C 12 - H 37	/650. BD*(1) C 21 - O 22	1.04	1.04	0.029
26. BD (1) C 12 - H 37	/652. BD*(1) C 21 - N 23	5.67	0.89	0.065
27. BD (1) N 13 - C 14	/119. RY*(1) C 1	0.80	1.95	0.035
27. BD (1) N 13 - C 14	/120. RY*(2) C 1	0.83	2.10	0.037
27. BD (1) N 13 - C 14	/314. RY*(1) C 15	0.99	1.60	0.036
27. BD (1) N 13 - C 14	/610. BD*(1) C 1 - C 3	1.67	1.41	0.043
27. BD (1) N 13 - C 14	/612. BD*(1) C 1 - N 13	1.19	1.16	0.033
27. BD (1) N 13 - C 14	/642. BD*(1) C 15 - H 40	0.60	1.18	0.024
28. BD (1) N 13 - H 38	/119. RY*(1) C 1	1.10	1.82	0.040
28. BD (1) N 13 - H 38	/302. RY*(2) C 14	0.64	2.01	0.032
28. BD (1) N 13 - H 38	/305. RY*(5) C 14	1.16	2.54	0.049
28. BD (1) N 13 - H 38	/609. BD*(1) C 1 - C 2	2.15	1.10	0.044
28. BD (1) N 13 - H 38	/611. BD*(2) C 1 - C 3	1.48	0.68	0.031
28. BD (1) N 13 - H 38	/638. BD*(1) C 14 - O 16	2.97	1.18	0.053
29. BD (1) C 14 - C 15	/289. RY*(2) N 13	1.51	1.73	0.046
29. BD (1) C 14 - C 15	/327. RY*(1) O 16	0.89	1.79	0.036
29. BD (1) C 14 - C 15	/340. RY*(1) C 17	1.02	1.46	0.035
29. BD (1) C 14 - C 15	/612. BD*(1) C 1 - N 13	3.08	1.04	0.051
29. BD (1) C 14 - C 15	/638. BD*(1) C 14 - O 16	0.71	1.19	0.026
29. BD (1) C 14 - C 15	/640. BD*(1) C 15 - C 17	1.00	1.02	0.029
29. BD (1) C 14 - C 15	/641. BD*(1) C 15 - H 39	0.51	1.04	0.020
29. BD (1) C 14 - C 15	/643. BD*(1) C 17 - C 18	2.35	1.04	0.044
30. BD (1) C 14 - O 16	/301. RY*(1) C 14	1.74	1.78	0.050
30. BD (1) C 14 - O 16	/636. BD*(1) N 13 - H 38	1.22	1.34	0.036
30. BD (1) C 14 - O 16	/637. BD*(1) C 14 - C 15	1.28	1.40	0.038
31. BD (2) C 14 - O 16	/639. BD*(2) C 14 - O 16	0.60	0.36	0.014
31. BD (2) C 14 - O 16	/640. BD*(1) C 15 - C 17	1.89	0.71	0.033
31. BD (2) C 14 - O 16	/641. BD*(1) C 15 - H 39	1.75	0.73	0.032
32. BD (1) C 15 - C 17	/303. RY*(3) C 14	0.61	1.87	0.030
32. BD (1) C 15 - C 17	/304. RY*(4) C 14	0.84	2.22	0.039
32. BD (1) C 15 - C 17	/353. RY*(1) C 18	1.40	1.43	0.040

32. BD (1) C 15 - C 17	/637. BD*(1) C 14 - C 15	0.55	1.03	0.021
32. BD (1) C 15 - C 17	/638. BD*(1) C 14 - O 16	1.28	1.16	0.035
32. BD (1) C 15 - C 17	/639. BD*(2) C 14 - O 16	2.67	0.63	0.039
32. BD (1) C 15 - C 17	/643. BD*(1) C 17 - C 18	0.89	1.00	0.027
32. BD (1) C 15 - C 17	/645. BD*(1) C 17 - H 42	0.52	0.99	0.020
32. BD (1) C 15 - C 17	/646. BD*(1) C 18 - O 19	3.99	0.92	0.055
33. BD (1) C 15 - H 39	/342. RY*(3) C 17	0.55	1.43	0.025
33. BD (1) C 15 - H 39	/638. BD*(1) C 14 - O 16	1.98	1.03	0.041
33. BD (1) C 15 - H 39	/639. BD*(2) C 14 - O 16	5.17	0.50	0.048
33. BD (1) C 15 - H 39	/644. BD*(1) C 17 - H 41	2.84	0.86	0.044
34. BD (1) C 15 - H 40	/635. BD*(1) N 13 - C 14	5.67	0.87	0.064
34. BD (1) C 15 - H 40	/638. BD*(1) C 14 - O 16	1.15	1.02	0.031
34. BD (1) C 15 - H 40	/645. BD*(1) C 17 - H 42	2.97	0.85	0.045
35. BD (1) C 17 - C 18	/315. RY*(2) C 15	0.70	1.41	0.028
35. BD (1) C 17 - C 18	/379. RY*(1) O 20	0.75	1.78	0.033
35. BD (1) C 17 - C 18	/637. BD*(1) C 14 - C 15	1.61	1.08	0.038
35. BD (1) C 17 - C 18	/640. BD*(1) C 15 - C 17	0.59	1.04	0.022
35. BD (1) C 17 - C 18	/647. BD*(1) C 18 - O 20	0.56	1.20	0.023
35. BD (1) C 17 - C 18	/649. BD*(1) O 19 - H 43	1.82	0.98	0.038
36. BD (1) C 17 - H 41	/314. RY*(1) C 15	0.89	1.33	0.031
36. BD (1) C 17 - H 41	/641. BD*(1) C 15 - H 39	2.85	0.89	0.045
36. BD (1) C 17 - H 41	/647. BD*(1) C 18 - O 20	1.83	1.03	0.039
36. BD (1) C 17 - H 41	/648. BD*(2) C 18 - O 20	5.19	0.50	0.047
37. BD (1) C 17 - H 42	/315. RY*(2) C 15	0.69	1.25	0.026
37. BD (1) C 17 - H 42	/357. RY*(5) C 18	0.57	1.55	0.027
37. BD (1) C 17 - H 42	/642. BD*(1) C 15 - H 40	2.58	0.91	0.043
37. BD (1) C 17 - H 42	/647. BD*(1) C 18 - O 20	1.77	1.03	0.038
37. BD (1) C 17 - H 42	/648. BD*(2) C 18 - O 20	5.22	0.50	0.048
38. BD (1) C 18 - O 19	/341. RY*(2) C 17	0.56	1.63	0.027
38. BD (1) C 18 - O 19	/640. BD*(1) C 15 - C 17	0.93	1.27	0.031
39. BD (1) C 18 - O 20	/353. RY*(1) C 18	1.55	1.81	0.047
39. BD (1) C 18 - O 20	/643. BD*(1) C 17 - C 18	1.13	1.38	0.036
40. BD (2) C 18 - O 20	/644. BD*(1) C 17 - H 41	1.79	0.74	0.032
40. BD (2) C 18 - O 20	/645. BD*(1) C 17 - H 42	1.83	0.73	0.033
40. BD (2) C 18 - O 20	/648. BD*(2) C 18 - O 20	0.71	0.36	0.015
41. BD (1) O 19 - H 43	/353. RY*(1) C 18	1.12	1.53	0.037
41. BD (1) O 19 - H 43	/354. RY*(2) C 18	0.92	1.97	0.038
41. BD (1) O 19 - H 43	/359. RY*(7) C 18	0.61	2.47	0.035
41. BD (1) O 19 - H 43	/643. BD*(1) C 17 - C 18	3.77	1.10	0.058
41. BD (1) O 19 - H 43	/647. BD*(1) C 18 - O 20	1.29	1.24	0.036
42. BD (1) C 21 - O 22	/392. RY*(1) C 21	1.60	1.75	0.047
42. BD (1) C 21 - O 22	/632. BD*(1) C 12 - C 21	1.44	1.38	0.040
42. BD (1) C 21 - O 22	/633. BD*(1) C 12 - H 36	0.55	1.35	0.024
42. BD (1) C 21 - O 22	/654. BD*(1) N 23 - H 44	1.00	1.34	0.033
43. BD (2) C 21 - O 22	/631. BD*(1)Se 11 - C 12	3.07	0.46	0.034
43. BD (2) C 21 - O 22	/633. BD*(1) C 12 - H 36	1.41	0.74	0.029
43. BD (2) C 21 - O 22	/651. BD*(2) C 21 - O 22	0.74	0.38	0.016
44. BD (1) C 21 - N 23	/275. RY*(1) C 12	0.80	1.54	0.031
44. BD (1) C 21 - N 23	/431. RY*(1) C 24	0.94	2.04	0.039
44. BD (1) C 21 - N 23	/432. RY*(2) C 24	0.74	2.18	0.036
44. BD (1) C 21 - N 23	/634. BD*(1) C 12 - H 37	0.64	1.17	0.024
44. BD (1) C 21 - N 23	/653. BD*(1) N 23 - C 24	1.07	1.17	0.032
44. BD (1) C 21 - N 23	/655. BD*(1) C 24 - C 25	1.67	1.25	0.041
45. BD (1) N 23 - C 24	/392. RY*(1) C 21	1.66	1.54	0.045
45. BD (1) N 23 - C 24	/444. RY*(1) C 25	0.81	2.06	0.037

45. BD (1) N 23 - C 24	/457. RY*(1) C 26	0.64	2.04	0.032
45. BD (1) N 23 - C 24	/632. BD*(1) C 12 - C 21	1.81	1.17	0.041
45. BD (1) N 23 - C 24	/652. BD*(1) C 21 - N 23	0.91	1.15	0.029
45. BD (1) N 23 - C 24	/655. BD*(1) C 24 - C 25	0.61	1.24	0.025
45. BD (1) N 23 - C 24	/656. BD*(1) C 24 - C 26	2.05	1.43	0.048
45. BD (1) N 23 - C 24	/658. BD*(1) C 25 - C 27	0.83	1.44	0.031
45. BD (1) N 23 - C 24	/661. BD*(1) C 26 - C 28	2.10	1.26	0.046
46. BD (1) N 23 - H 44	/393. RY*(2) C 21	0.70	1.90	0.033
46. BD (1) N 23 - H 44	/395. RY*(4) C 21	0.93	2.51	0.043
46. BD (1) N 23 - H 44	/431. RY*(1) C 24	1.37	1.89	0.046
46. BD (1) N 23 - H 44	/650. BD*(1) C 21 - O 22	2.71	1.16	0.050
46. BD (1) N 23 - H 44	/651. BD*(2) C 21 - O 22	0.84	0.65	0.022
46. BD (1) N 23 - H 44	/656. BD*(1) C 24 - C 26	2.66	1.29	0.052
46. BD (1) N 23 - H 44	/657. BD*(2) C 24 - C 26	0.69	0.69	0.021
47. BD (1) C 24 - C 25	/419. RY*(2) N 23	1.01	1.53	0.035
47. BD (1) C 24 - C 25	/457. RY*(1) C 26	0.76	1.90	0.034
47. BD (1) C 24 - C 25	/458. RY*(2) C 26	0.58	1.90	0.030
47. BD (1) C 24 - C 25	/470. RY*(1) C 27	0.81	1.95	0.036
47. BD (1) C 24 - C 25	/471. RY*(2) C 27	1.68	2.11	0.053
47. BD (1) C 24 - C 25	/652. BD*(1) C 21 - N 23	2.63	1.01	0.047
47. BD (1) C 24 - C 25	/653. BD*(1) N 23 - C 24	0.54	1.03	0.021
47. BD (1) C 24 - C 25	/656. BD*(1) C 24 - C 26	4.08	1.29	0.065
47. BD (1) C 24 - C 25	/658. BD*(1) C 25 - C 27	2.97	1.30	0.056
47. BD (1) C 24 - C 25	/660. BD*(1) C 25 - H 45	0.61	1.09	0.023
47. BD (1) C 24 - C 25	/662. BD*(1) C 26 - H 46	3.04	1.11	0.052
47. BD (1) C 24 - C 25	/664. BD*(1) C 27 - H 47	2.90	1.10	0.051
48. BD (1) C 24 - C 26	/419. RY*(2) N 23	0.70	1.62	0.030
48. BD (1) C 24 - C 26	/444. RY*(1) C 25	0.77	2.02	0.035
48. BD (1) C 24 - C 26	/483. RY*(1) C 28	0.84	2.03	0.037
48. BD (1) C 24 - C 26	/484. RY*(2) C 28	1.05	2.18	0.043
48. BD (1) C 24 - C 26	/653. BD*(1) N 23 - C 24	2.02	1.12	0.043
48. BD (1) C 24 - C 26	/654. BD*(1) N 23 - H 44	1.69	1.08	0.038
48. BD (1) C 24 - C 26	/655. BD*(1) C 24 - C 25	3.82	1.19	0.060
48. BD (1) C 24 - C 26	/660. BD*(1) C 25 - H 45	1.49	1.18	0.037
48. BD (1) C 24 - C 26	/661. BD*(1) C 26 - C 28	2.66	1.21	0.051
48. BD (1) C 24 - C 26	/662. BD*(1) C 26 - H 46	1.80	1.20	0.042
48. BD (1) C 24 - C 26	/667. BD*(1) C 28 - H 48	1.35	1.19	0.036
49. BD (2) C 24 - C 26	/446. RY*(3) C 25	1.40	1.07	0.037
49. BD (2) C 24 - C 26	/486. RY*(4) C 28	1.10	0.90	0.030
49. BD (2) C 24 - C 26	/652. BD*(1) C 21 - N 23	0.85	0.63	0.022
49. BD (2) C 24 - C 26	/654. BD*(1) N 23 - H 44	0.89	0.61	0.022
49. BD (2) C 24 - C 26	/659. BD*(2) C 25 - C 27	13.10	0.31	0.057
49. BD (2) C 24 - C 26	/666. BD*(2) C 28 - C 29	13.52	0.32	0.059
50. BD (1) C 25 - C 27	/432. RY*(2) C 24	1.93	2.13	0.057
50. BD (1) C 25 - C 27	/496. RY*(1) C 29	0.92	2.04	0.039
50. BD (1) C 25 - C 27	/497. RY*(2) C 29	0.95	2.18	0.041
50. BD (1) C 25 - C 27	/653. BD*(1) N 23 - C 24	3.00	1.12	0.052
50. BD (1) C 25 - C 27	/655. BD*(1) C 24 - C 25	2.90	1.20	0.053
50. BD (1) C 25 - C 27	/660. BD*(1) C 25 - H 45	1.74	1.18	0.040
50. BD (1) C 25 - C 27	/663. BD*(1) C 27 - C 29	2.54	1.22	0.050
50. BD (1) C 25 - C 27	/664. BD*(1) C 27 - H 47	1.53	1.19	0.038
50. BD (1) C 25 - C 27	/668. BD*(1) C 29 - H 49	1.57	1.19	0.039
51. BD (2) C 25 - C 27	/435. RY*(5) C 24	0.56	1.82	0.030
51. BD (2) C 25 - C 27	/498. RY*(3) C 29	1.38	0.90	0.033
51. BD (2) C 25 - C 27	/657. BD*(2) C 24 - C 26	13.35	0.32	0.059

51. BD (2) C 25 - C 27	/666. BD*(2) C 28 - C 29	12.36	0.32	0.056
52. BD (1) C 25 - H 45	/431. RY*(1) C 24	0.88	1.77	0.035
52. BD (1) C 25 - H 45	/432. RY*(2) C 24	0.78	1.92	0.035
52. BD (1) C 25 - H 45	/470. RY*(1) C 27	1.62	1.83	0.049
52. BD (1) C 25 - H 45	/653. BD*(1) N 23 - C 24	0.59	0.91	0.021
52. BD (1) C 25 - H 45	/656. BD*(1) C 24 - C 26	3.00	1.16	0.053
52. BD (1) C 25 - H 45	/658. BD*(1) C 25 - C 27	1.51	1.18	0.038
52. BD (1) C 25 - H 45	/663. BD*(1) C 27 - C 29	5.11	1.00	0.064
52. BD (1) C 25 - H 45	/664. BD*(1) C 27 - H 47	0.83	0.97	0.025
53. BD (1) C 26 - C 28	/431. RY*(1) C 24	1.91	1.88	0.054
53. BD (1) C 26 - C 28	/496. RY*(1) C 29	0.70	1.93	0.033
53. BD (1) C 26 - C 28	/497. RY*(2) C 29	1.59	2.07	0.052
53. BD (1) C 26 - C 28	/653. BD*(1) N 23 - C 24	5.67	1.02	0.068
53. BD (1) C 26 - C 28	/656. BD*(1) C 24 - C 26	3.18	1.28	0.057
53. BD (1) C 26 - C 28	/662. BD*(1) C 26 - H 46	0.59	1.10	0.023
53. BD (1) C 26 - C 28	/665. BD*(1) C 28 - C 29	2.78	1.30	0.054
53. BD (1) C 26 - C 28	/668. BD*(1) C 29 - H 49	3.30	1.09	0.054
54. BD (1) C 26 - H 46	/432. RY*(2) C 24	1.98	1.90	0.055
54. BD (1) C 26 - H 46	/483. RY*(1) C 28	1.19	1.80	0.042
54. BD (1) C 26 - H 46	/653. BD*(1) N 23 - C 24	0.97	0.89	0.026
54. BD (1) C 26 - H 46	/655. BD*(1) C 24 - C 25	5.74	0.97	0.067
54. BD (1) C 26 - H 46	/656. BD*(1) C 24 - C 26	1.51	1.15	0.037
54. BD (1) C 26 - H 46	/665. BD*(1) C 28 - C 29	2.54	1.17	0.049
55. BD (1) C 27 - C 29	/444. RY*(1) C 25	0.59	1.92	0.030
55. BD (1) C 27 - C 29	/445. RY*(2) C 25	1.80	1.98	0.054
55. BD (1) C 27 - C 29	/483. RY*(1) C 28	0.76	1.94	0.034
55. BD (1) C 27 - C 29	/484. RY*(2) C 28	1.59	2.08	0.052
55. BD (1) C 27 - C 29	/658. BD*(1) C 25 - C 27	2.80	1.29	0.054
55. BD (1) C 27 - C 29	/660. BD*(1) C 25 - H 45	3.35	1.08	0.054
55. BD (1) C 27 - C 29	/664. BD*(1) C 27 - H 47	0.55	1.09	0.022
55. BD (1) C 27 - C 29	/665. BD*(1) C 28 - C 29	2.82	1.30	0.054
55. BD (1) C 27 - C 29	/667. BD*(1) C 28 - H 48	3.23	1.09	0.053
55. BD (1) C 27 - C 29	/668. BD*(1) C 29 - H 49	0.53	1.09	0.022
56. BD (1) C 27 - H 47	/444. RY*(1) C 25	1.63	1.80	0.049
56. BD (1) C 27 - H 47	/496. RY*(1) C 29	1.30	1.82	0.044
56. BD (1) C 27 - H 47	/655. BD*(1) C 24 - C 25	5.60	0.98	0.066
56. BD (1) C 27 - H 47	/658. BD*(1) C 25 - C 27	1.33	1.17	0.035
56. BD (1) C 27 - H 47	/660. BD*(1) C 25 - H 45	0.87	0.96	0.026
56. BD (1) C 27 - H 47	/665. BD*(1) C 28 - C 29	2.50	1.18	0.049
57. BD (1) C 28 - C 29	/457. RY*(1) C 26	0.95	1.99	0.039
57. BD (1) C 28 - C 29	/458. RY*(2) C 26	1.02	1.99	0.040
57. BD (1) C 28 - C 29	/470. RY*(1) C 27	0.88	2.04	0.038
57. BD (1) C 28 - C 29	/471. RY*(2) C 27	1.01	2.20	0.042
57. BD (1) C 28 - C 29	/604. RY*(1) H 49	0.51	1.20	0.022
57. BD (1) C 28 - C 29	/661. BD*(1) C 26 - C 28	2.41	1.21	0.048
57. BD (1) C 28 - C 29	/662. BD*(1) C 26 - H 46	1.44	1.20	0.037
57. BD (1) C 28 - C 29	/663. BD*(1) C 27 - C 29	2.54	1.21	0.050
57. BD (1) C 28 - C 29	/664. BD*(1) C 27 - H 47	1.60	1.19	0.039
57. BD (1) C 28 - C 29	/667. BD*(1) C 28 - H 48	1.60	1.19	0.039
57. BD (1) C 28 - C 29	/668. BD*(1) C 29 - H 49	1.67	1.19	0.040
58. BD (2) C 28 - C 29	/459. RY*(3) C 26	0.92	0.98	0.028
58. BD (2) C 28 - C 29	/472. RY*(3) C 27	1.38	1.09	0.037
58. BD (2) C 28 - C 29	/657. BD*(2) C 24 - C 26	12.99	0.31	0.057
58. BD (2) C 28 - C 29	/659. BD*(2) C 25 - C 27	14.18	0.31	0.059
59. BD (1) C 28 - H 48	/457. RY*(1) C 26	1.28	1.77	0.043

59. BD (1) C 28 - H 48	/496. RY*(1) C 29	1.66	1.82	0.049
59. BD (1) C 28 - H 48	/656. BD*(1) C 24 - C 26	2.72	1.16	0.050
59. BD (1) C 28 - H 48	/663. BD*(1) C 27 - C 29	5.31	0.99	0.065
59. BD (1) C 28 - H 48	/665. BD*(1) C 28 - C 29	1.31	1.18	0.035
59. BD (1) C 28 - H 48	/668. BD*(1) C 29 - H 49	0.85	0.97	0.026
60. BD (1) C 29 - H 49	/470. RY*(1) C 27	1.31	1.82	0.044
60. BD (1) C 29 - H 49	/483. RY*(1) C 28	1.70	1.81	0.050
60. BD (1) C 29 - H 49	/658. BD*(1) C 25 - C 27	2.57	1.17	0.049
60. BD (1) C 29 - H 49	/661. BD*(1) C 26 - C 28	5.28	0.99	0.065
60. BD (1) C 29 - H 49	/665. BD*(1) C 28 - C 29	1.34	1.18	0.036
60. BD (1) C 29 - H 49	/667. BD*(1) C 28 - H 48	0.84	0.97	0.026
61. CR (1) C 1	/133. RY*(2) C 2	0.95	11.45	0.093
61. CR (1) C 1	/145. RY*(1) C 3	0.67	11.95	0.080
61. CR (1) C 1	/146. RY*(2) C 3	1.48	11.41	0.116
61. CR (1) C 1	/147. RY*(3) C 3	0.51	11.04	0.067
61. CR (1) C 1	/610. BD*(1) C 1 - C 3	1.35	10.73	0.108
61. CR (1) C 1	/613. BD*(1) C 2 - C 4	0.57	10.77	0.070
61. CR (1) C 1	/616. BD*(1) C 3 - C 5	1.03	10.56	0.094
61. CR (1) C 1	/617. BD*(1) C 3 - C 7	1.11	10.53	0.098
61. CR (1) C 1	/635. BD*(1) N 13 - C 14	1.03	10.48	0.095
62. CR (1) C 2	/120. RY*(2) C 1	1.36	11.36	0.111
62. CR (1) C 2	/158. RY*(1) C 4	0.60	11.21	0.074
62. CR (1) C 2	/159. RY*(2) C 4	1.71	11.22	0.124
62. CR (1) C 2	/610. BD*(1) C 1 - C 3	0.83	10.67	0.084
62. CR (1) C 2	/612. BD*(1) C 1 - N 13	0.54	10.42	0.067
62. CR (1) C 2	/613. BD*(1) C 2 - C 4	0.83	10.70	0.084
62. CR (1) C 2	/618. BD*(1) C 4 - C 6	1.31	10.51	0.106
63. CR (1) C 3	/119. RY*(1) C 1	1.12	11.23	0.100
63. CR (1) C 3	/121. RY*(3) C 1	1.05	11.36	0.097
63. CR (1) C 3	/172. RY*(2) C 5	0.70	11.03	0.079
63. CR (1) C 3	/198. RY*(2) C 7	0.60	11.51	0.074
63. CR (1) C 3	/203. RY*(7) C 7	0.83	11.19	0.086
63. CR (1) C 3	/609. BD*(1) C 1 - C 2	1.09	10.52	0.096
63. CR (1) C 3	/610. BD*(1) C 1 - C 3	1.24	10.69	0.104
63. CR (1) C 3	/612. BD*(1) C 1 - N 13	1.02	10.45	0.093
63. CR (1) C 3	/620. BD*(1) C 5 - C 6	0.72	10.72	0.079
63. CR (1) C 3	/624. BD*(1) C 7 - O 8	0.61	10.35	0.073
64. CR (1) C 4	/133. RY*(2) C 2	1.29	11.38	0.108
64. CR (1) C 4	/135. RY*(4) C 2	0.74	11.07	0.081
64. CR (1) C 4	/185. RY*(2) C 6	1.29	10.88	0.106
64. CR (1) C 4	/187. RY*(4) C 6	0.62	11.14	0.074
64. CR (1) C 4	/609. BD*(1) C 1 - C 2	1.20	10.49	0.101
64. CR (1) C 4	/613. BD*(1) C 2 - C 4	0.68	10.70	0.076
64. CR (1) C 4	/620. BD*(1) C 5 - C 6	0.83	10.69	0.084
64. CR (1) C 4	/623. BD*(1) C 6 -Se 11	0.83	10.18	0.083
65. CR (1) C 5	/146. RY*(2) C 3	0.86	11.35	0.088
65. CR (1) C 5	/184. RY*(1) C 6	1.12	11.12	0.100
65. CR (1) C 5	/185. RY*(2) C 6	1.88	10.88	0.128
65. CR (1) C 5	/186. RY*(3) C 6	0.52	10.91	0.067
65. CR (1) C 5	/610. BD*(1) C 1 - C 3	0.76	10.67	0.081
65. CR (1) C 5	/617. BD*(1) C 3 - C 7	0.65	10.47	0.075
65. CR (1) C 5	/618. BD*(1) C 4 - C 6	1.23	10.51	0.102
65. CR (1) C 5	/620. BD*(1) C 5 - C 6	1.21	10.69	0.102
65. CR (1) C 5	/623. BD*(1) C 6 -Se 11	1.28	10.18	0.103
66. CR (1) C 6	/159. RY*(2) C 4	1.03	11.26	0.096

66. CR (1) C 6	/161. RY*(4) C 4	0.50	11.05	0.067
66. CR (1) C 6	/172. RY*(2) C 5	2.10	11.04	0.136
66. CR (1) C 6	/174. RY*(4) C 5	0.53	11.20	0.069
66. CR (1) C 6	/613. BD*(1) C 2 - C 4	0.62	10.74	0.073
66. CR (1) C 6	/616. BD*(1) C 3 - C 5	1.16	10.53	0.099
66. CR (1) C 6	/620. BD*(1) C 5 - C 6	1.22	10.73	0.103
66. CR (1) C 6	/622. BD*(1) C 5 - H 32	0.55	10.54	0.068
66. CR (1) C 6	/623. BD*(1) C 6 -Se 11	1.33	10.22	0.105
67. CR (1) C 7	/145. RY*(1) C 3	1.19	12.04	0.107
67. CR (1) C 7	/610. BD*(1) C 1 - C 3	0.87	10.83	0.087
67. CR (1) C 7	/616. BD*(1) C 3 - C 5	0.54	10.65	0.068
67. CR (1) C 7	/617. BD*(1) C 3 - C 7	0.55	10.63	0.069
67. CR (1) C 7	/624. BD*(1) C 7 - O 8	0.67	10.49	0.077
67. CR (1) C 7	/627. BD*(1) O 8 - C 10	1.11	10.48	0.096
68. CR (1) O 8	/197. RY*(1) C 7	1.01	19.93	0.127
68. CR (1) O 8	/198. RY*(2) C 7	1.10	20.42	0.134
68. CR (1) O 8	/238. RY*(3) C 10	0.86	19.96	0.117
69. CR (1) O 9	/197. RY*(1) C 7	5.26	19.81	0.289
69. CR (1) O 9	/617. BD*(1) C 3 - C 7	0.79	19.29	0.111
70. CR (1) C 10	/535. RY*(2) H 35	0.54	12.16	0.072
70. CR (1) C 10	/624. BD*(1) C 7 - O 8	1.11	10.40	0.098
70. CR (1) C 10	/627. BD*(1) O 8 - C 10	1.49	10.39	0.111
73. CR (3)Se 11	/184. RY*(1) C 6	0.96	11.37	0.093
73. CR (3)Se 11	/618. BD*(1) C 4 - C 6	0.75	10.76	0.081
73. CR (3)Se 11	/620. BD*(1) C 5 - C 6	1.22	10.94	0.104
85. CR (1) C 12	/393. RY*(2) C 21	1.09	11.36	0.100
85. CR (1) C 12	/631. BD*(1)Se 11 - C 12	1.05	10.19	0.093
85. CR (1) C 12	/652. BD*(1) C 21 - N 23	0.60	10.47	0.073
86. CR (1) N 13	/119. RY*(1) C 1	1.08	15.37	0.115
86. CR (1) N 13	/120. RY*(2) C 1	0.58	15.52	0.085
86. CR (1) N 13	/302. RY*(2) C 14	1.75	15.56	0.148
86. CR (1) N 13	/610. BD*(1) C 1 - C 3	0.59	14.83	0.084
87. CR (1) C 14	/316. RY*(3) C 15	0.52	11.40	0.069
87. CR (1) C 14	/612. BD*(1) C 1 - N 13	1.18	10.55	0.100
88. CR (1) C 15	/302. RY*(2) C 14	0.85	11.42	0.088
88. CR (1) C 15	/305. RY*(5) C 14	0.53	11.95	0.071
88. CR (1) C 15	/635. BD*(1) N 13 - C 14	0.59	10.44	0.071
89. CR (1) O 16	/301. RY*(1) C 14	5.93	19.63	0.306
89. CR (1) O 16	/637. BD*(1) C 14 - C 15	0.76	19.25	0.109
90. CR (1) C 17	/317. RY*(4) C 15	0.72	11.15	0.080
90. CR (1) C 17	/354. RY*(2) C 18	0.78	11.33	0.084
91. CR (1) C 18	/340. RY*(1) C 17	0.66	11.01	0.076
91. CR (1) C 18	/343. RY*(4) C 17	0.54	11.34	0.070
91. CR (1) C 18	/646. BD*(1) C 18 - O 19	0.66	10.51	0.076
92. CR (1) O 19	/353. RY*(1) C 18	0.74	19.78	0.108
92. CR (1) O 19	/354. RY*(2) C 18	1.77	20.23	0.169
92. CR (1) O 19	/356. RY*(4) C 18	0.71	21.10	0.110
92. CR (1) O 19	/577. RY*(4) H 43	0.55	20.96	0.096
93. CR (1) O 20	/353. RY*(1) C 18	5.96	19.67	0.307
93. CR (1) O 20	/643. BD*(1) C 17 - C 18	0.74	19.25	0.108
94. CR (1) C 21	/277. RY*(3) C 12	1.09	10.99	0.098
94. CR (1) C 21	/653. BD*(1) N 23 - C 24	1.15	10.57	0.099
95. CR (1) O 22	/392. RY*(1) C 21	5.95	19.61	0.306
95. CR (1) O 22	/632. BD*(1) C 12 - C 21	0.84	19.24	0.115
96. CR (1) N 23	/393. RY*(2) C 21	1.76	15.46	0.147

96. CR (1) N 23	/431. RY*(1) C 24	0.58	15.45	0.085	
96. CR (1) N 23	/432. RY*(2) C 24	0.68	15.60	0.092	
96. CR (1) N 23	/434. RY*(4) C 24	0.88	15.38	0.104	
96. CR (1) N 23	/581. RY*(3) H 44	0.51	16.47	0.082	
96. CR (1) N 23	/656. BD*(1) C 24 - C 26	0.58	14.85	0.083	
97. CR (1) C 24	/445. RY*(2) C 25	0.92	11.43	0.092	
97. CR (1) C 24	/458. RY*(2) C 26	1.85	11.35	0.129	
97. CR (1) C 24	/652. BD*(1) C 21 - N 23	1.08	10.46	0.097	
97. CR (1) C 24	/656. BD*(1) C 24 - C 26	1.41	10.74	0.110	
97. CR (1) C 24	/658. BD*(1) C 25 - C 27	0.57	10.75	0.070	
97. CR (1) C 24	/661. BD*(1) C 26 - C 28	0.92	10.57	0.089	
97. CR (1) C 24	/662. BD*(1) C 26 - H 46	0.52	10.56	0.066	
98. CR (1) C 25	/431. RY*(1) C 24	1.22	11.29	0.105	
98. CR (1) C 25	/471. RY*(2) C 27	2.12	11.50	0.140	
98. CR (1) C 25	/585. RY*(2) H 45	0.52	12.32	0.071	
98. CR (1) C 25	/653. BD*(1) N 23 - C 24	0.57	10.43	0.069	
98. CR (1) C 25	/656. BD*(1) C 24 - C 26	0.75	10.68	0.080	
98. CR (1) C 25	/658. BD*(1) C 25 - C 27	0.83	10.70	0.084	
98. CR (1) C 25	/663. BD*(1) C 27 - C 29	1.06	10.52	0.095	
99. CR (1) C 26	/432. RY*(2) C 24	2.58	11.43	0.153	
99. CR (1) C 26	/484. RY*(2) C 28	0.79	11.48	0.085	
99. CR (1) C 26	/653. BD*(1) N 23 - C 24	1.03	10.42	0.093	
99. CR (1) C 26	/655. BD*(1) C 24 - C 25	1.20	10.49	0.101	
99. CR (1) C 26	/656. BD*(1) C 24 - C 26	0.73	10.68	0.079	
99. CR (1) C 26	/665. BD*(1) C 28 - C 29	0.64	10.70	0.074	
100. CR (1) C 27	/445. RY*(2) C 25	1.57	11.38	0.119	
100. CR (1) C 27	/447. RY*(4) C 25	0.51	11.00	0.067	
100. CR (1) C 27	/497. RY*(2) C 29	0.81	11.48	0.086	
100. CR (1) C 27	/595. RY*(2) H 47	0.58	12.28	0.075	
100. CR (1) C 27	/655. BD*(1) C 24 - C 25	1.18	10.50	0.100	
100. CR (1) C 27	/658. BD*(1) C 25 - C 27	0.75	10.70	0.080	
100. CR (1) C 27	/660. BD*(1) C 25 - H 45	0.53	10.48	0.067	
100. CR (1) C 27	/665. BD*(1) C 28 - C 29	0.62	10.71	0.073	
101. CR (1) C 28	/497. RY*(2) C 29	2.11	11.48	0.139	
101. CR (1) C 28	/600. RY*(2) H 48	0.55	12.28	0.073	
101. CR (1) C 28	/656. BD*(1) C 24 - C 26	0.69	10.68	0.077	
101. CR (1) C 28	/663. BD*(1) C 27 - C 29	1.07	10.51	0.095	
101. CR (1) C 28	/665. BD*(1) C 28 - C 29	0.82	10.70	0.084	
101. CR (1) C 28	/668. BD*(1) C 29 - H 49	0.51	10.49	0.066	
102. CR (1) C 29	/471. RY*(2) C 27	0.78	11.49	0.084	
102. CR (1) C 29	/484. RY*(2) C 28	2.15	11.48	0.140	
102. CR (1) C 29	/605. RY*(2) H 49	0.56	12.28	0.074	
102. CR (1) C 29	/658. BD*(1) C 25 - C 27	0.63	10.69	0.073	
102. CR (1) C 29	/661. BD*(1) C 26 - C 28	1.04	10.51	0.094	
102. CR (1) C 29	/665. BD*(1) C 28 - C 29	0.80	10.70	0.083	
102. CR (1) C 29	/667. BD*(1) C 28 - H 48	0.50	10.49	0.065	
103. LP (1) O 8	/197. RY*(1) C 7	1.65	1.52	0.045	
103. LP (1) O 8	/200. RY*(4) C 7	1.62	2.60	0.058	
103. LP (1) O 8	/236. RY*(1) C 10	1.66	1.66	0.047	
103. LP (1) O 8	/238. RY*(3) C 10	0.72	1.55	0.030	
103. LP (1) O 8	/625. BD*(1) C 7 - O 9	5.70	1.08	0.070	
103. LP (1) O 8	/629. BD*(1) C 10 - H 34	0.64	0.95	0.022	
103. LP (1) O 8	/630. BD*(1) C 10 - H 35	2.37	0.95	0.043	
104. LP (2) O 8	/199. RY*(3) C 7	1.80	1.84	0.054	
104. LP (2) O 8	/237. RY*(2) C 10	1.44	1.49	0.044	

104. LP (2) O 8	/626. BD*(2) C 7 - O 9	38.61	0.31	0.100
104. LP (2) O 8	/628. BD*(1) C 10 - H 33	5.04	0.70	0.055
104. LP (2) O 8	/629. BD*(1) C 10 - H 34	5.03	0.70	0.056
105. LP (1) O 9	/197. RY*(1) C 7	12.33	1.65	0.127
105. LP (1) O 9	/208. RY*(12) C 7	0.51	10.74	0.067
105. LP (1) O 9	/617. BD*(1) C 3 - C 7	2.26	1.13	0.045
105. LP (1) O 9	/624. BD*(1) C 7 - O 8	0.98	0.99	0.028
106. LP (2) O 9	/198. RY*(2) C 7	1.95	1.70	0.053
106. LP (2) O 9	/200. RY*(4) C 7	1.70	2.28	0.058
106. LP (2) O 9	/617. BD*(1) C 3 - C 7	12.44	0.68	0.084
106. LP (2) O 9	/624. BD*(1) C 7 - O 8	28.87	0.55	0.113
106. LP (2) O 9	/630. BD*(1) C 10 - H 35	0.80	0.64	0.021
107. LP (1)Se 11	/184. RY*(1) C 6	1.15	1.78	0.040
107. LP (1)Se 11	/620. BD*(1) C 5 - C 6	3.27	1.36	0.060
108. LP (2)Se 11	/618. BD*(1) C 4 - C 6	1.72	0.70	0.031
108. LP (2)Se 11	/620. BD*(1) C 5 - C 6	1.11	0.88	0.028
108. LP (2)Se 11	/621. BD*(2) C 5 - C 6	8.58	0.27	0.044
108. LP (2)Se 11	/633. BD*(1) C 12 - H 36	2.40	0.61	0.035
108. LP (2)Se 11	/634. BD*(1) C 12 - H 37	3.92	0.62	0.045
109. LP (1) N 13	/121. RY*(3) C 1	1.06	1.55	0.039
109. LP (1) N 13	/122. RY*(4) C 1	0.78	1.63	0.034
109. LP (1) N 13	/303. RY*(3) C 14	1.62	1.51	0.048
109. LP (1) N 13	/550. RY*(2) H 38	0.74	1.97	0.037
109. LP (1) N 13	/609. BD*(1) C 1 - C 2	3.61	0.71	0.048
109. LP (1) N 13	/610. BD*(1) C 1 - C 3	2.69	0.88	0.047
109. LP (1) N 13	/611. BD*(2) C 1 - C 3	18.13	0.30	0.066
109. LP (1) N 13	/639. BD*(2) C 14 - O 16	48.43	0.26	0.102
110. LP (1) O 16	/301. RY*(1) C 14	13.88	1.47	0.128
110. LP (1) O 16	/635. BD*(1) N 13 - C 14	1.33	1.06	0.034
110. LP (1) O 16	/637. BD*(1) C 14 - C 15	2.25	1.09	0.044
111. LP (2) O 16	/302. RY*(2) C 14	1.87	1.60	0.050
111. LP (2) O 16	/304. RY*(4) C 14	1.01	1.83	0.040
111. LP (2) O 16	/305. RY*(5) C 14	1.10	2.14	0.045
111. LP (2) O 16	/635. BD*(1) N 13 - C 14	24.49	0.62	0.111
111. LP (2) O 16	/637. BD*(1) C 14 - C 15	14.00	0.65	0.087
112. LP (1) O 19	/353. RY*(1) C 18	2.31	1.42	0.051
112. LP (1) O 19	/356. RY*(4) C 18	1.92	2.74	0.065
112. LP (1) O 19	/576. RY*(3) H 43	1.29	2.27	0.049
112. LP (1) O 19	/647. BD*(1) C 18 - O 20	5.42	1.14	0.070
113. LP (2) O 19	/355. RY*(3) C 18	2.01	1.87	0.057
113. LP (2) O 19	/575. RY*(2) H 43	1.55	1.81	0.049
113. LP (2) O 19	/648. BD*(2) C 18 - O 20	41.24	0.32	0.103
114. LP (1) O 20	/353. RY*(1) C 18	14.14	1.52	0.131
114. LP (1) O 20	/365. RY*(13) C 18	0.76	3.79	0.048
114. LP (1) O 20	/643. BD*(1) C 17 - C 18	2.20	1.09	0.044
114. LP (1) O 20	/646. BD*(1) C 18 - O 19	0.88	1.00	0.027
115. LP (2) O 20	/354. RY*(2) C 18	2.62	1.51	0.058
115. LP (2) O 20	/356. RY*(4) C 18	1.17	2.38	0.049
115. LP (2) O 20	/637. BD*(1) C 14 - C 15	0.74	0.67	0.020
115. LP (2) O 20	/643. BD*(1) C 17 - C 18	13.96	0.64	0.086
115. LP (2) O 20	/646. BD*(1) C 18 - O 19	27.80	0.56	0.112
116. LP (1) O 22	/392. RY*(1) C 21	14.07	1.45	0.128
116. LP (1) O 22	/632. BD*(1) C 12 - C 21	2.48	1.08	0.047
116. LP (1) O 22	/652. BD*(1) C 21 - N 23	1.37	1.06	0.034
117. LP (2) O 22	/393. RY*(2) C 21	1.82	1.51	0.048

117. LP (2) O 22	/395. RY*(4) C 21	1.52	2.11	0.052
117. LP (2) O 22	/396. RY*(5) C 21	0.73	1.75	0.033
117. LP (2) O 22	/632. BD*(1) C 12 - C 21	14.50	0.64	0.088
117. LP (2) O 22	/652. BD*(1) C 21 - N 23	24.13	0.62	0.110
118. LP (1) N 23	/394. RY*(3) C 21	1.47	1.65	0.048
118. LP (1) N 23	/399. RY*(8) C 21	0.57	1.80	0.031
118. LP (1) N 23	/433. RY*(3) C 24	1.81	1.48	0.050
118. LP (1) N 23	/580. RY*(2) H 44	0.92	1.87	0.040
118. LP (1) N 23	/650. BD*(1) C 21 - O 22	1.74	0.78	0.035
118. LP (1) N 23	/651. BD*(2) C 21 - O 22	42.73	0.27	0.097
118. LP (1) N 23	/655. BD*(1) C 24 - C 25	1.97	0.72	0.036
118. LP (1) N 23	/656. BD*(1) C 24 - C 26	1.48	0.91	0.035
118. LP (1) N 23	/657. BD*(2) C 24 - C 26	20.90	0.31	0.073
611. BD*(2) C 1 - C 3	/123. RY*(5) C 1	1.08	1.27	0.085
611. BD*(2) C 1 - C 3	/148. RY*(4) C 3	0.73	0.76	0.054
611. BD*(2) C 1 - C 3	/149. RY*(5) C 3	0.55	1.61	0.068
611. BD*(2) C 1 - C 3	/614. BD*(2) C 2 - C 4	150.66	0.01	0.072
611. BD*(2) C 1 - C 3	/624. BD*(1) C 7 - O 8	0.84	0.25	0.029
611. BD*(2) C 1 - C 3	/635. BD*(1) N 13 - C 14	0.66	0.34	0.030
611. BD*(2) C 1 - C 3	/636. BD*(1) N 13 - H 38	0.96	0.31	0.038
614. BD*(2) C 2 - C 4	/134. RY*(3) C 2	0.88	0.67	0.072
614. BD*(2) C 2 - C 4	/162. RY*(5) C 4	0.81	1.39	0.100
621. BD*(2) C 5 - C 6	/173. RY*(3) C 5	2.58	0.56	0.096
621. BD*(2) C 5 - C 6	/186. RY*(3) C 6	0.63	0.83	0.058
621. BD*(2) C 5 - C 6	/614. BD*(2) C 2 - C 4	130.87	0.01	0.071
621. BD*(2) C 5 - C 6	/631. BD*(1)Se 11 - C 12	1.35	0.07	0.023
624. BD*(1) C 7 - O 8	/198. RY*(2) C 7	1.61	1.16	0.163
624. BD*(1) C 7 - O 8	/210. RY*(1) O 8	0.57	1.05	0.094
624. BD*(1) C 7 - O 8	/616. BD*(1) C 3 - C 5	1.05	0.16	0.045
624. BD*(1) C 7 - O 8	/617. BD*(1) C 3 - C 7	0.80	0.14	0.034
624. BD*(1) C 7 - O 8	/625. BD*(1) C 7 - O 9	0.53	0.22	0.039
626. BD*(2) C 7 - O 9	/199. RY*(3) C 7	1.50	1.53	0.119
626. BD*(2) C 7 - O 9	/224. RY*(2) O 9	1.09	0.98	0.082
626. BD*(2) C 7 - O 9	/611. BD*(2) C 1 - C 3	34.06	0.05	0.067
639. BD*(2) C 14 - O 16	/303. RY*(3) C 14	0.91	1.24	0.085
639. BD*(2) C 14 - O 16	/328. RY*(2) O 16	1.21	1.04	0.090
639. BD*(2) C 14 - O 16	/640. BD*(1) C 15 - C 17	1.04	0.36	0.048
639. BD*(2) C 14 - O 16	/641. BD*(1) C 15 - H 39	0.91	0.37	0.046
648. BD*(2) C 18 - O 20	/355. RY*(3) C 18	1.38	1.55	0.125
648. BD*(2) C 18 - O 20	/361. RY*(9) C 18	0.66	1.22	0.078
648. BD*(2) C 18 - O 20	/380. RY*(2) O 20	0.79	0.96	0.075
648. BD*(2) C 18 - O 20	/644. BD*(1) C 17 - H 41	0.90	0.38	0.049
648. BD*(2) C 18 - O 20	/645. BD*(1) C 17 - H 42	0.92	0.38	0.049
651. BD*(2) C 21 - O 22	/394. RY*(3) C 21	1.19	1.38	0.099
651. BD*(2) C 21 - O 22	/406. RY*(2) O 22	1.15	0.97	0.083
651. BD*(2) C 21 - O 22	/623. BD*(1) C 6 -Se 11	0.51	0.11	0.018
651. BD*(2) C 21 - O 22	/631. BD*(1)Se 11 - C 12	5.14	0.08	0.049
651. BD*(2) C 21 - O 22	/633. BD*(1) C 12 - H 36	0.69	0.36	0.038
651. BD*(2) C 21 - O 22	/650. BD*(1) C 21 - O 22	2.33	0.51	0.081
657. BD*(2) C 24 - C 26	/436. RY*(6) C 24	0.84	1.28	0.081
657. BD*(2) C 24 - C 26	/459. RY*(3) C 26	1.77	0.67	0.085
657. BD*(2) C 24 - C 26	/652. BD*(1) C 21 - N 23	0.56	0.31	0.029
659. BD*(2) C 25 - C 27	/446. RY*(3) C 25	0.54	0.76	0.055
659. BD*(2) C 25 - C 27	/448. RY*(5) C 25	0.73	1.45	0.087
659. BD*(2) C 25 - C 27	/472. RY*(3) C 27	0.54	0.78	0.055

659. BD*(2) C 25 - C 27	/473. RY*(4) C 27	0.79	1.43	0.090
666. BD*(2) C 28 - C 29	/486. RY*(4) C 28	1.69	0.59	0.084
666. BD*(2) C 28 - C 29	/498. RY*(3) C 29	1.38	0.58	0.076

NATURAL BOND ORBITAL ANALYSIS:

Cycle	Occ. Thresh.	Occupancies Lewis	Occupancies Non-Lewis	Lewis Structure CR	BD	3C	LP	Low occ (L)	High occ (NL)	Dev
1(1)	1.90	225.92376	10.07624	42	59	0	17	24	15	0.64
2(2)	1.90	225.92376	10.07624	42	59	0	17	24	15	0.64
3(1)	1.80	228.28308	7.71692	42	57	0	19	5	11	0.64
4(2)	1.80	228.28308	7.71692	42	57	0	19	5	11	0.64
5(1)	1.70	231.81065	4.18935	42	60	0	16	0	11	0.26
6(2)	1.70	231.81065	4.18935	42	60	0	16	0	11	0.26
7(1)	1.60	231.81065	4.18935	42	60	0	16	0	11	0.26
8(2)	1.60	231.81065	4.18935	42	60	0	16	0	11	0.26
9(1)	1.50	231.30265	4.69735	42	59	0	17	0	13	0.74
10(2)	1.50	230.83781	5.16219	42	59	0	17	0	13	1.04
11(3)	1.50	231.30265	4.69735	42	59	0	17	0	13	0.74
12(1)	1.70	231.81065	4.18935	42	60	0	16	0	11	0.26

Core	83.97564 (99.971% of 84)
Valence Lewis	147.83501 (97.260% of 152)
Total Lewis	231.81065 (98.225% of 236)
Valence non-Lewis	3.74241 (1.586% of 236)
Rydberg non-Lewis	0.44693 (0.189% of 236)
Total non-Lewis	4.18935 (1.775% of 236)