Biological evaluation of novel amidino substituted coumarin-benzazole hybrids as promising therapeutic agents

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SUPPORTING INFORMATION

Biology

Cell culture and reference compounds

Human cancer cells used in this manuscript, namely Capan-1, HCT-116, NCI-H460, LN-229, HL-60, K-562 and Z-138 were acquired from the American Type Culture Collection (ATCC, Manassas, VA, USA), while the DND-41 cell line was purchased from the Deutsche Sammlung von Mikroorganismen und Zellkulturen (DSMZ Leibniz-Institut, Germany). Culture media were purchased from Gibco Life Technologies, USA, and supplemented with 10% fetal bovine serum (HyClone, GE Healthcare Life Sciences, USA). *Vincristine* and *docetaxel*, which were used as reference inhibitors, were purchased from Selleckchem (Munich, Germany). Stock solutions were prepared in DMSO.

Proliferation assays

Adherent cell lines LN-229, HCT-116, NCI-H460 and Capan-1 cells were seeded at a density between 500 and 1500 cells per well, in 384-well tissue culture plates (Greiner). After overnight incubation, cells were treated with seven different concentrations of the test compounds, ranging from 100 to 0.006 µM. Suspension cell lines HL-60, K-562, Z-138 and DND-41 were seeded at densities ranging from 2500 to 5500 cells per well in 384-well culture plates containing the test compounds at the same concentration points. Cells were incubated for 72 hours with compounds and were then analysed using the CellTiter 96® AQueous One Solution Cell Proliferation Assay (MTS) reagent (Promega) according to the manufacturer's instructions. Absorbance of the samples was measured at 490 nm using a SpectraMax Plus 384 (Molecular Devices), and OD values were used to calculate the 50% inhibitory concentration (IC_{50}). Compounds were tested in at least two independent experiments.

Subcellular distribution of compounds 13 and 18

Fluorescence microscopy was performed on Hep-2 cells treated with 10 µM of compound **13** or **18** for 3h. The samples were imaged by confocal microscopy on a Leica TCS SP5 confocal microscope (Leica Microsystems), employing a HCX PL APO 63x (NA 1.2) water immersion objective.

Toxicity of compounds 13 and 18 to normal cells

Buffy coat preparations from healthy donors were obtained from the Blood Transfusion Center in Leuven, Belgium. Peripheral blood mononuclear cells (PBMC) were isolated by density gradient centrifugation over Lymphoprep (d=1.077 g/ml) (Nycomed) and cultured in cell culture medium (DMEM/F12, Gibco Life Technologies, USA) containing 8% FBS. Freshly prepared PBMC were

seeded at 28000 cells per well in 384-well plates containing the test compounds at seven different concentrations ranging from 100 µM to 6 nM. For determining the viability of the normal cells after 72 hour treatment, the CellTiter 96® AQueous One Solution Cell Proliferation Assay was employed according to the manufacturer's instructions. Absorbance of the samples was measured at 490 nm using a SpectraMax Plus 384 (Molecular Devices), and OD values were used to calculate the 50% inhibitory concentration (IC_{50}). Compounds **13** and **18** were tested in two independent experiments, implying PBMC originated from two different healthy donors.

Antiviral activity

Host cell lines

HEL 299 (ATCC CCL-137; human lung fibroblast), Huh-7 (CLS – 300156; human hepatoblastoma), and MDCK (Madin-Darby canine kidney cells; a kind gift from M. Matrosovich, Marburg, Germany) were maintained in Dulbecco's Modified Eagle Medium (DMEM, Gibco Life Technologies) supplemented with 8% heat-inactivated fetal bovine serum (HyClone, GE Healthcare Life Sciences), 0.075% sodium bicarbonate (Gibco Life Technologies) and 1mM sodium pyruvate (Gibco Life Technologies), and maintained at 37°C under 5% CO_2.

Antiviral CPE reduction assays

Antiviral assays towards herpes simplex virus-1 (HSV-1 KOS), human coronavirus (HCoV-229E and -OC43) and respiratory syncytial virus A in HEL cell cultures, sindbis virus, yellow fever virus, Zika virus and human coronavirus (HCoV-NL63) in Huh-7 cell cultures and influenza A/H1N1 (A/Ned/378/05), influenza A/H3N2 (A/HK/7/87), influenza B (B/Ned/537/05) in MDCK cell cultures were performed.

On the day of the infection, growth medium was aspirated and replaced by serial dilutions of the test compounds. The virus was then added to each well, diluted to obtain a viral input of 100 $CCID_{50}$ ($CCID_{50}$ being the virus dose that is able to infect 50% of the cell cultures). Mock-treated cultures receiving solely the test compounds were included, to determine the cytotoxicity. After 3 to 7 days of incubation, the virus-induced cytopathogenic effect was measured colorimetrically by the formazan-based MTS cell viability assay (CellTiter 96 AQueous One Solution Cell Proliferation Assay from Promega, Madison, WI), and the antiviral activity was expressed as the 50% effective concentration (EC_{50}). In parallel, the 50% cytotoxic concentration (CC_{50}) was derived from the mock-

infected cells. The activities were compared with the activities of reference antiviral drugs: remdesivir, ribavirin, zanamivir, rimantadine and brivudine (BVDU).

Antioxidative activity

Determination of the reducing activity of the stable radical 1,1-diphenyl-picrylhydrazyl (DPPH)

The determination of reducing activity was measured according to the previously reported procedure[32] with modification for the use in a 96-well microplate. Briefly, to solution of DPPH (final concentration 50 μM) in absolute ethanol was added equal volume of various concentrations of tested compounds dissolved in DMSO. The assay was carried out in a 96 well microtiter plate. Ethanol and DMSO were used as control solutions according to the previously published experimental procedure.

Determination of Ferric Reducing/Antioxidant Power (FRAP assay).

The FRAP method was performed according to previously reported procedure with minor modifications for an assay on a 96-well microplate.[32] All results were then expressed as Fe^{2+} equivalents (Fe^{2+} μmol). All tests were done in triplicate and the results were averaged and presented in Table 3.

Free radical scavenging ability by the use of a stable ABTS radical cation (2,20 azinobis-(3-ethylbenzthiazoline-6-sulphonic acid)

The total antioxidant activity (TEAC) method (Gųlcin et al. 2014) was adjusted for microplate reader. The working solution of $ABTS^{\bullet+}$ for standard TEAC assay, was prepared by mixing an ABTS stock solution (7 mM in water) with 2.45 mM potassium persulfate. The mixture was left for 12-16 h at room temperature in the dark to reach a stable oxidative state. Prior to analysis the $ABTS^{\bullet+}$ solution was diluted with PBS (pH 7.4) to an absorbance of 0.700 at 734 nm. The mixture of standards and solutions of tested compounds (10μL) with working $ABTS^{\bullet+}$ radical cation solution (200 μL) were put into each well of the microplate, shake and incubate at room temperature for 5 min. The absorbance at 734 nm was recorded by μQuant (Biotec Inc.). Final concentration of tested compounds was 150μg/ml. Aqueous phosphate buffer solution was used as a control and main calibrating standard. The results of the $ABTS^{\bullet+}$ scavenging activity was calculated according to following equation:

ABTS (%)=[(Acontrol – Acompound) / Acontrol] X 100.

Computational details

As a good compromise between accuracy and feasibility, all geometries were optimized with the density functional theory (DFT) using the B3LYP functional (unrestricted UB3LYP for the radicals), and the 6–31+G(d) basis set followed by the harmonic frequency calculations. Thermal corrections were extracted from the corresponding frequency calculations without scaling factors, while the obtained structures were confirmed as true minima by the absence of imaginary vibrational frequencies. In this way, all reported values correspond to differences in Gibbs free energies obtained at a room temperature (298 K) and a normal pressure (1 atm). To account for the solvation effects, we included the SMD polarizable continuum model with all parameters corresponding to pure ethanol (ε = 24.852), in accordance with presented experiments, giving rise to the (SMD)/B3LYP/6–31+G(d) model employed here. The choice of this computational setup was prompted by its success in modeling mechanisms of various antioxidants,[1,2,3,4,5] and in reproducing kinetic and thermodynamic parameters of a variety of organic[6,7]and enzymatic reactions.[8,9] All calculations were performed using the Gaussian 16 software.[10]

According to the literature, there are multiple mechanisms that describe the antioxidative properties of molecules.[11,12,13] Here we evaluated the three most frequent, and usually thermodynamically most preferred antioxidant mechanisms, namely hydrogen atom transfer (HAT), related with the capacity to transfer the hydrogen atom ($H^{\bullet}$) to a free radical as governed by the M–H bond dissociation energy (BDE), and single electron transfer (SET) related with either ejecting or adding an electron to the system.

All these mechanisms have the same net result, i.e. the formation of corresponding antioxidant radical and are calculated as Gibbs free energies for the following processes:

$\mathbf{M}\text{–H} \rightarrow \mathbf{M}^{\bullet} + H^{\bullet}$ bond dissociation energy, BDE = $G(\mathbf{M}^{\bullet}) + G(H^{\bullet}) - G(\mathbf{M}\text{–H})$

$\mathbf{M} \rightarrow \mathbf{M}^{\bullet+} + e^{-}$ ionization energy, IE = $G(\mathbf{M}^{\bullet+}) + G(e^{-}) - G(\mathbf{M})$

$\mathbf{M} + e^{-} \rightarrow \mathbf{M}^{\bullet-}$ electron affinity, EA = $G(\mathbf{M}^{\bullet-}) - G(\mathbf{M}) - G(e^{-})$

where the Gibbs free energy of an electron in the ethanol solution, $G(e^{-})$, is taken from the literature.[14]

Figure S1. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of **2-(2-(4-chloro-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-4,5-dihydro-1H-imidazol-3-ium chloride 7**

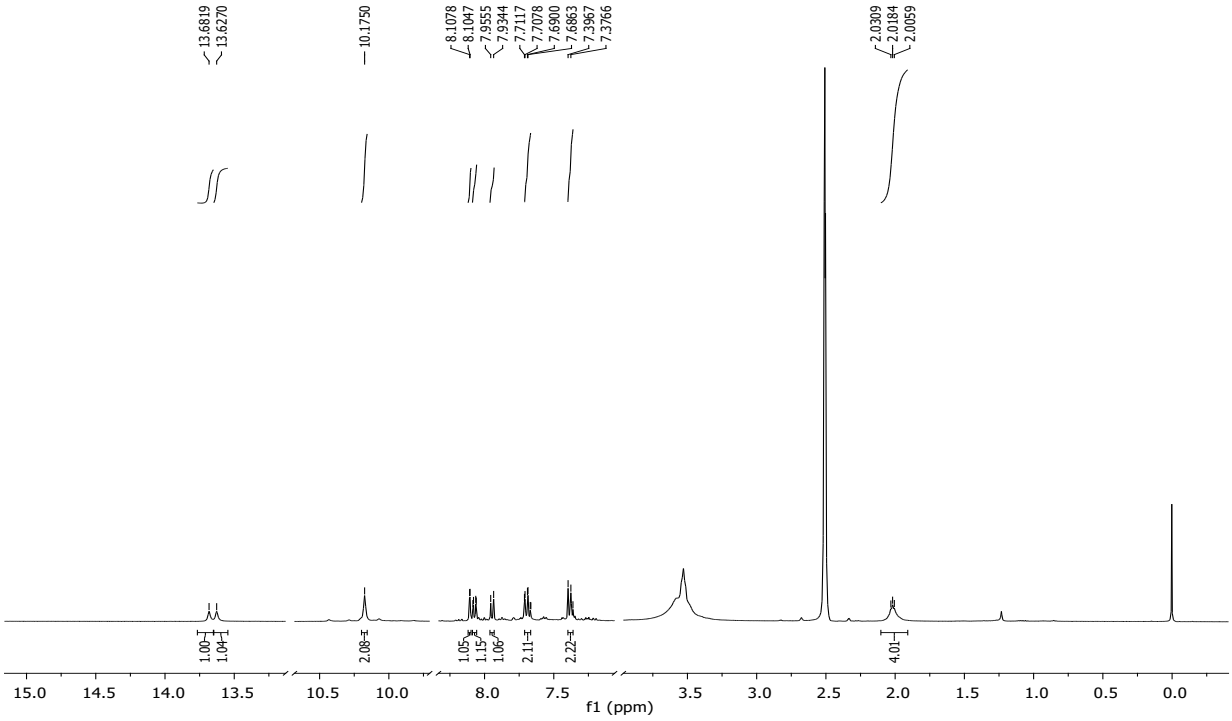


Figure S2. ^{13}C NMR spectrum (DMSO-d_6, 151 MHz) of **2-(2-(4-chloro-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-4,5-dihydro-1H-imidazol-3-ium chloride 7**

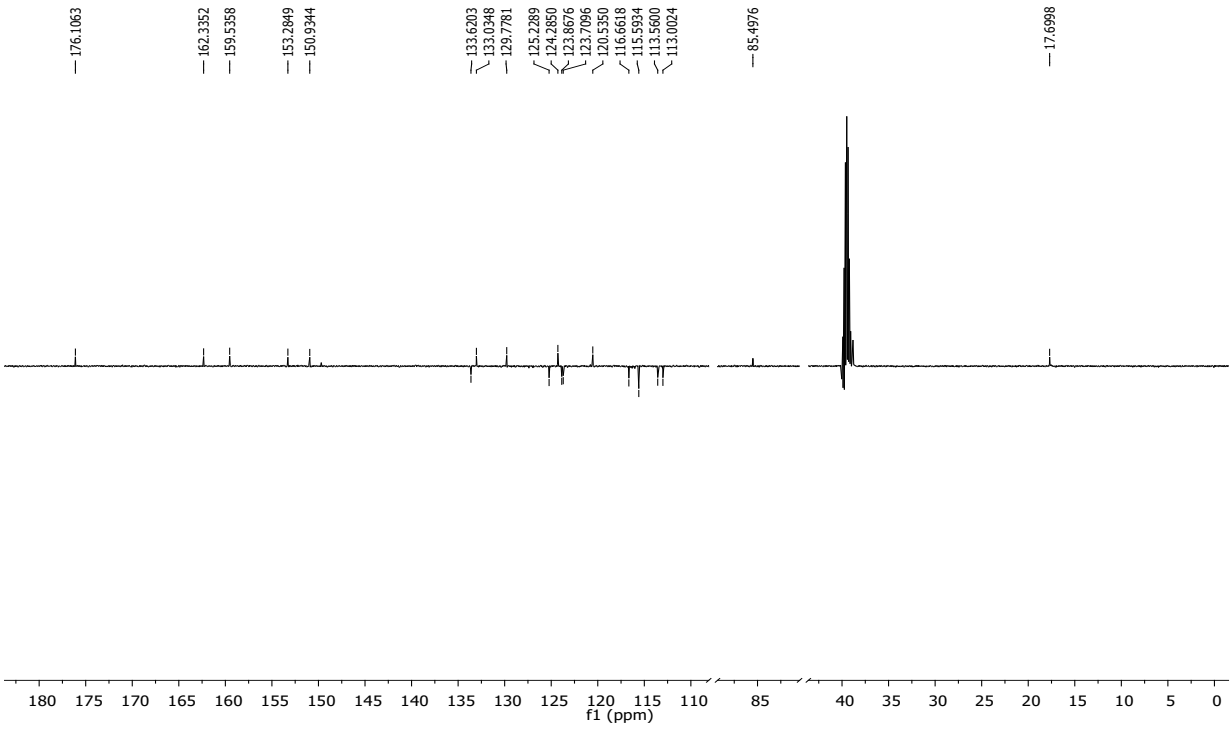


Figure S3. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of **2-(2-(4-chloro-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-3,4,5,6-tetrahydropyrimidin-1-ium chloride 8**

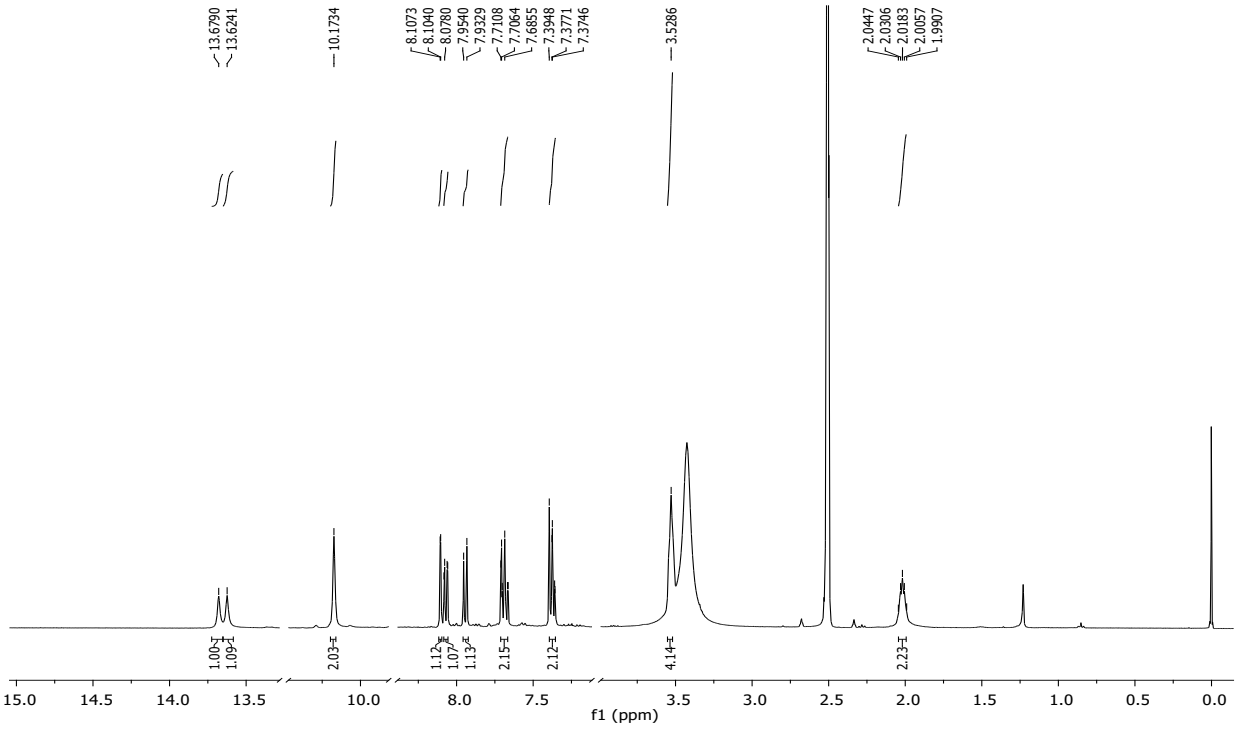


Figure S4. ^{13}C NMR spectrum (DMSO-d_6, 101 MHz) of **2-(2-(4-chloro-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-3,4,5,6-tetrahydropyrimidin-1-ium chloride 8**

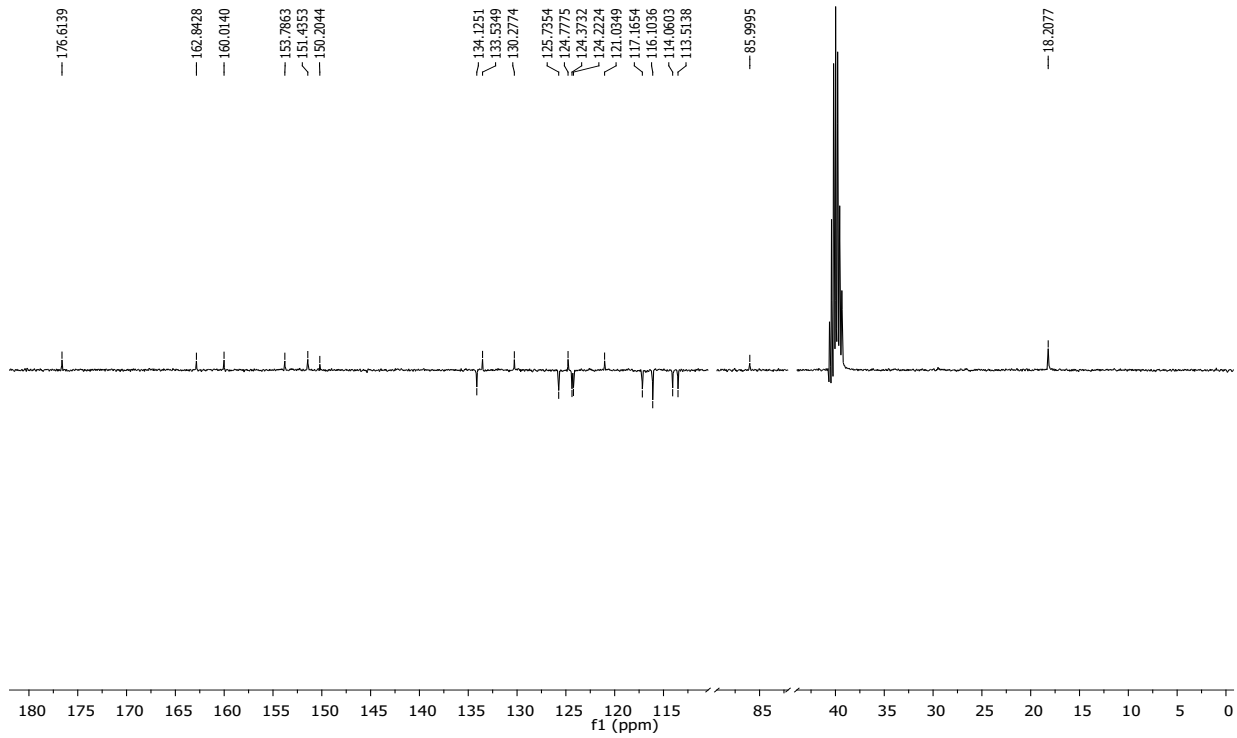


Figure S5. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of **2-(2-(6-bromo-4-chloro-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-4,5-dihydro-1H-imidazol-3-ium chloride 9**

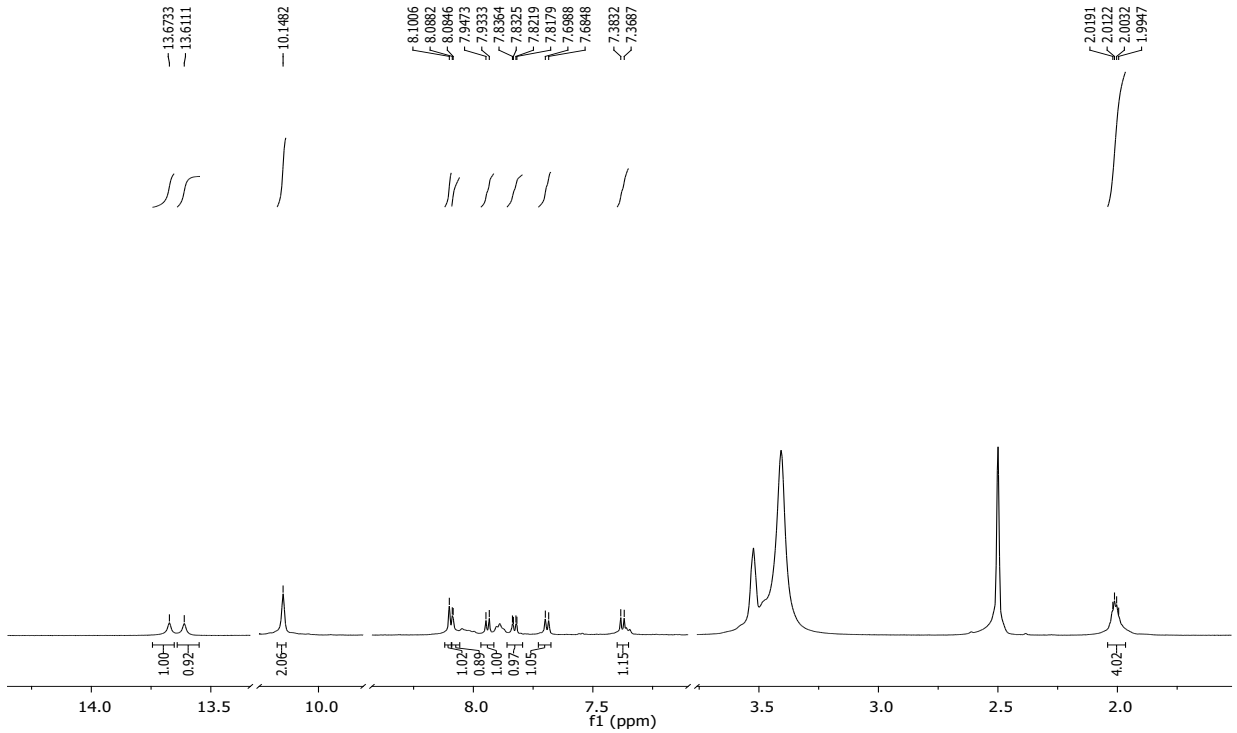


Figure S6. ^{13}C NMR spectrum (DMSO-d_6, 151 MHz) of **2-(2-(6-bromo-4-chloro-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-4,5-dihydro-1H-imidazol-3-ium chloride 9**

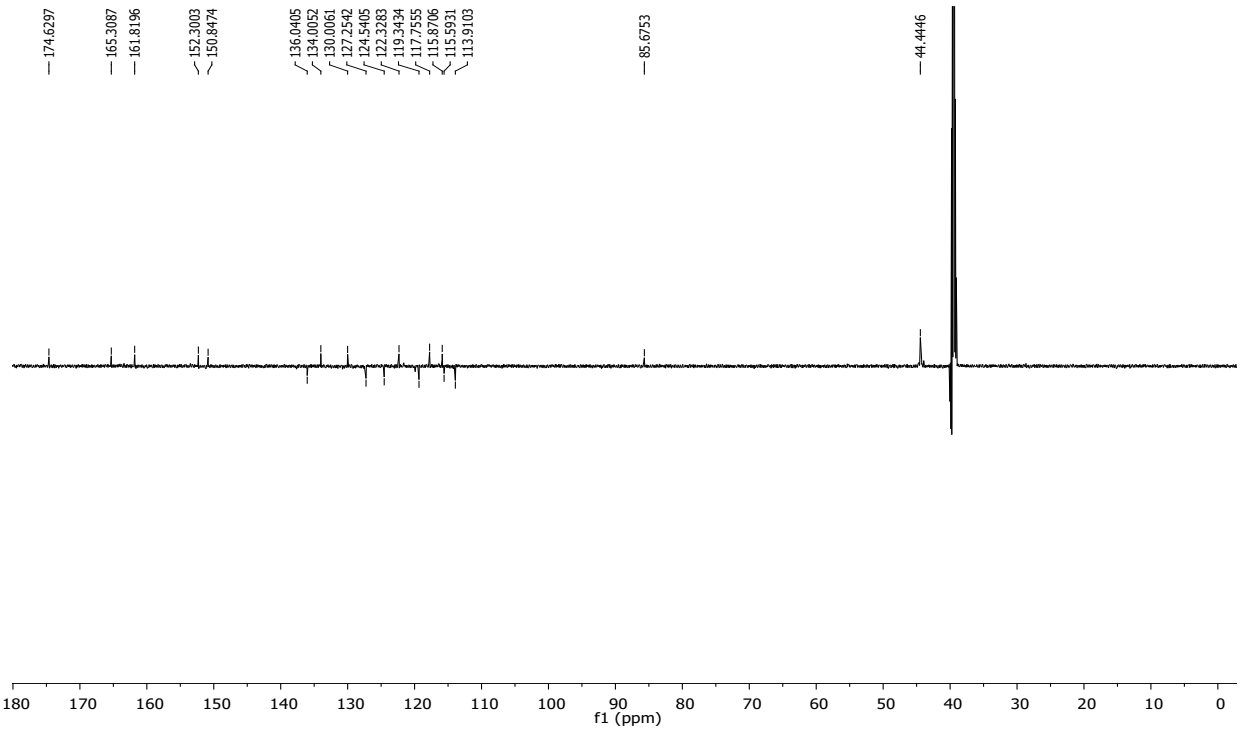


Figure S7. ^{1}H NMR spectrum (DMSO-d_6, 600 MHz) of **2-(2-(6-bromo-4-chloro-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-3,4,5,6-tetrahydropyrimidin-1-ium chloride 10**

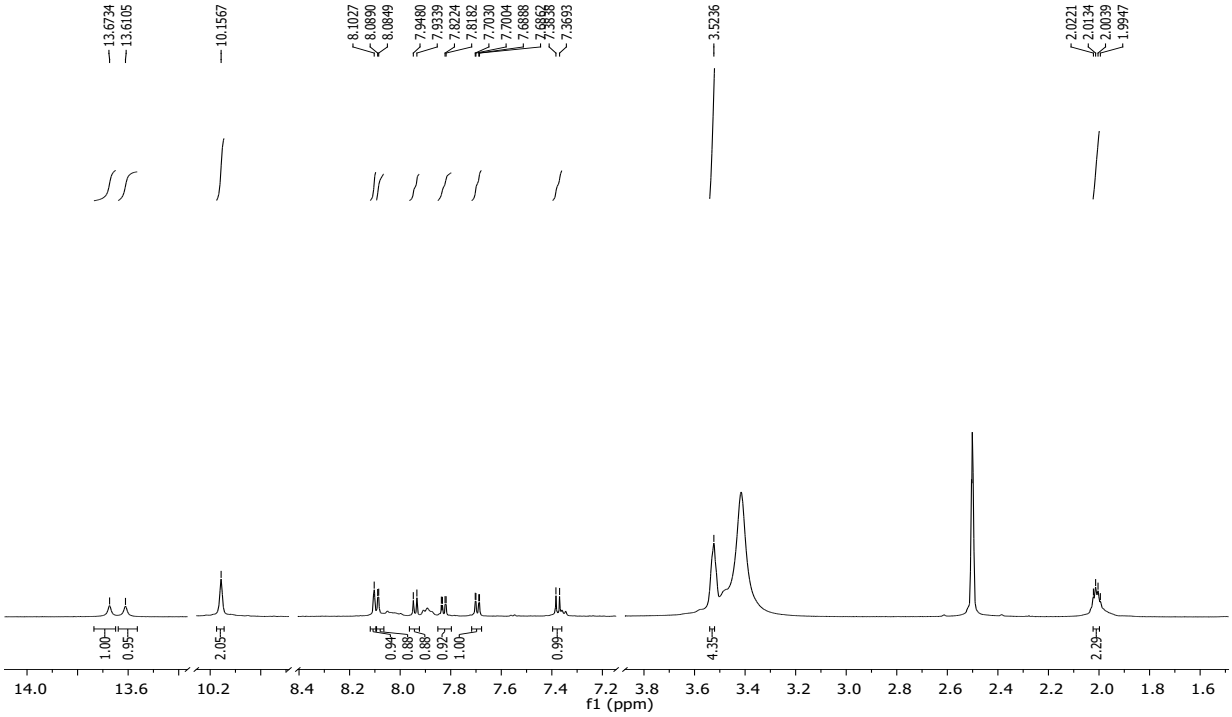


Figure S8. ^{13}C NMR spectrum (DMSO-d_6, 151 MHz) of **2-(2-(6-bromo-4-chloro-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-3,4,5,6-tetrahydropyrimidin-1-ium chloride 10**

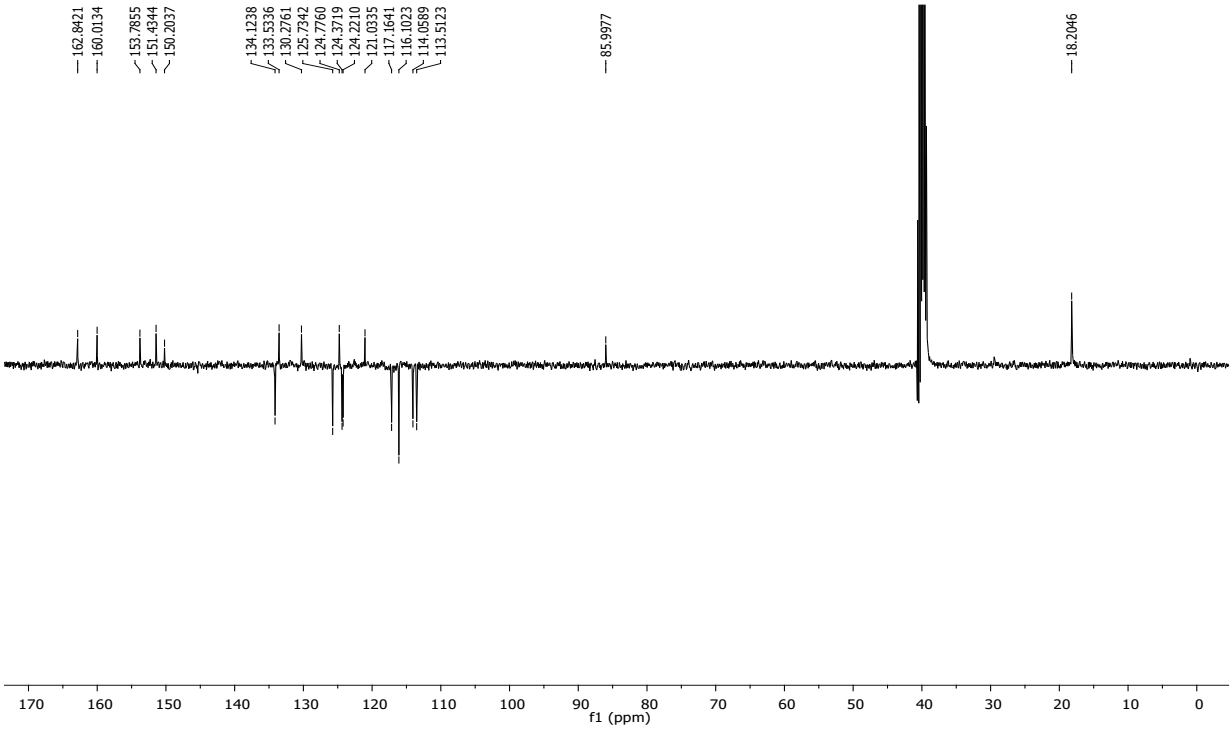
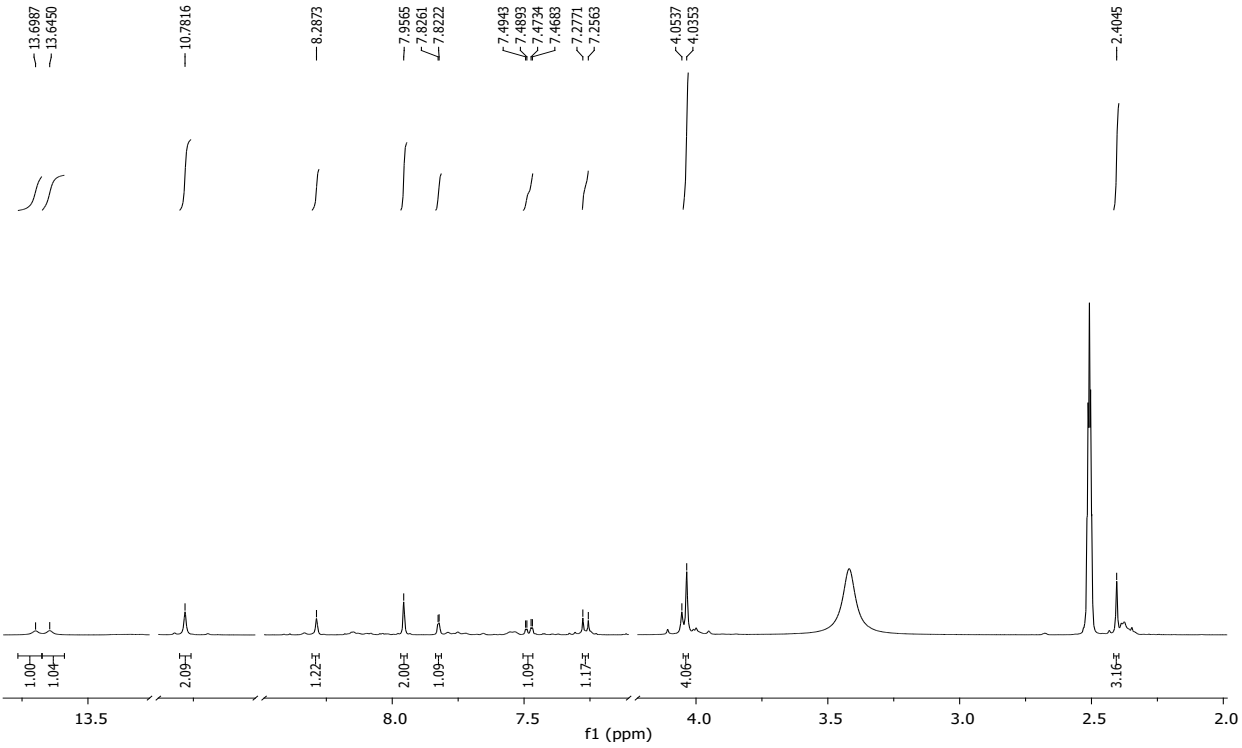


Figure S9. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of **2-(2-(4-chloro-6-methyl-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-4,5-dihydro-1H-imidazol-3-ium chloride 11**



11

Figure S10. ^{13}C NMR spectrum (DMSO-d_6, 101 MHz) of **2-(2-(4-chloro-6-methyl-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-4,5-dihydro-1H-imidazol-3-ium chloride 11**

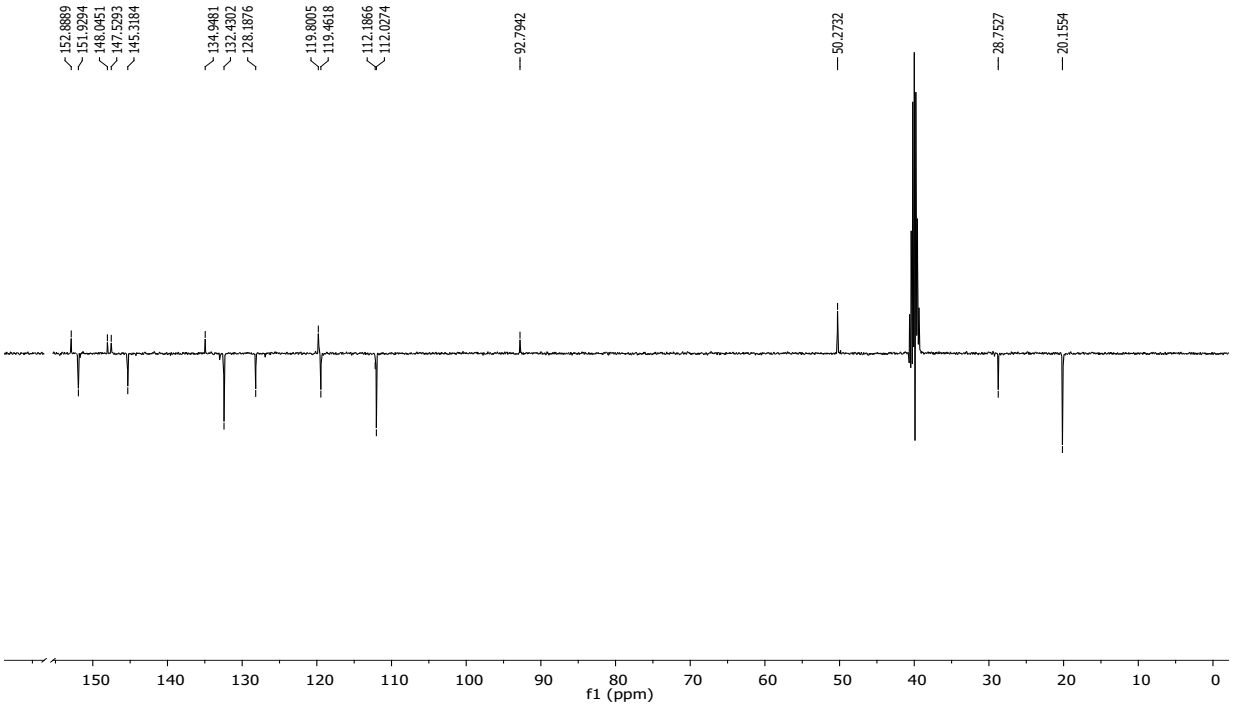


Figure S11. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of **2-(2-(4-chloro-6-methyl-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-3,4,5,6-tetrahydropyrimidin-1-ium chloride 12**

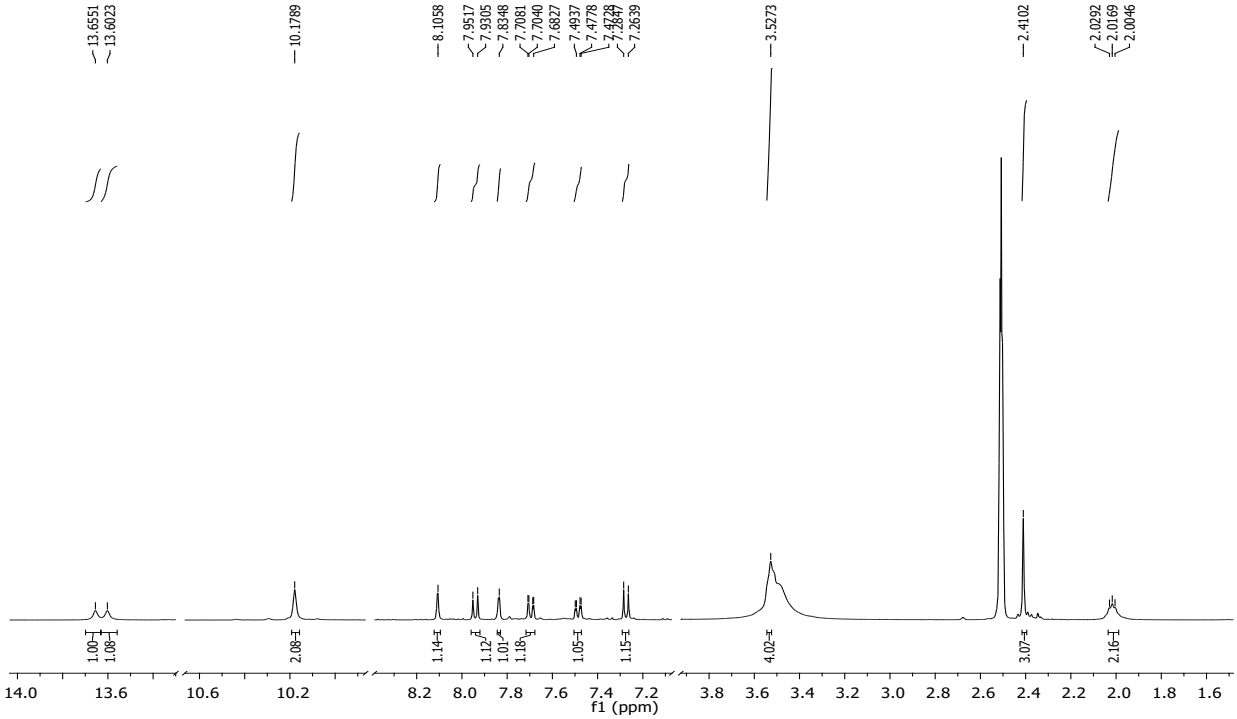


Figure S12. ^{13}C NMR spectrum (DMSO-d_6, 101 MHz) of **2-(2-(4-chloro-6-methyl-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-3,4,5,6-tetrahydropyrimidin-1-ium chloride 12**

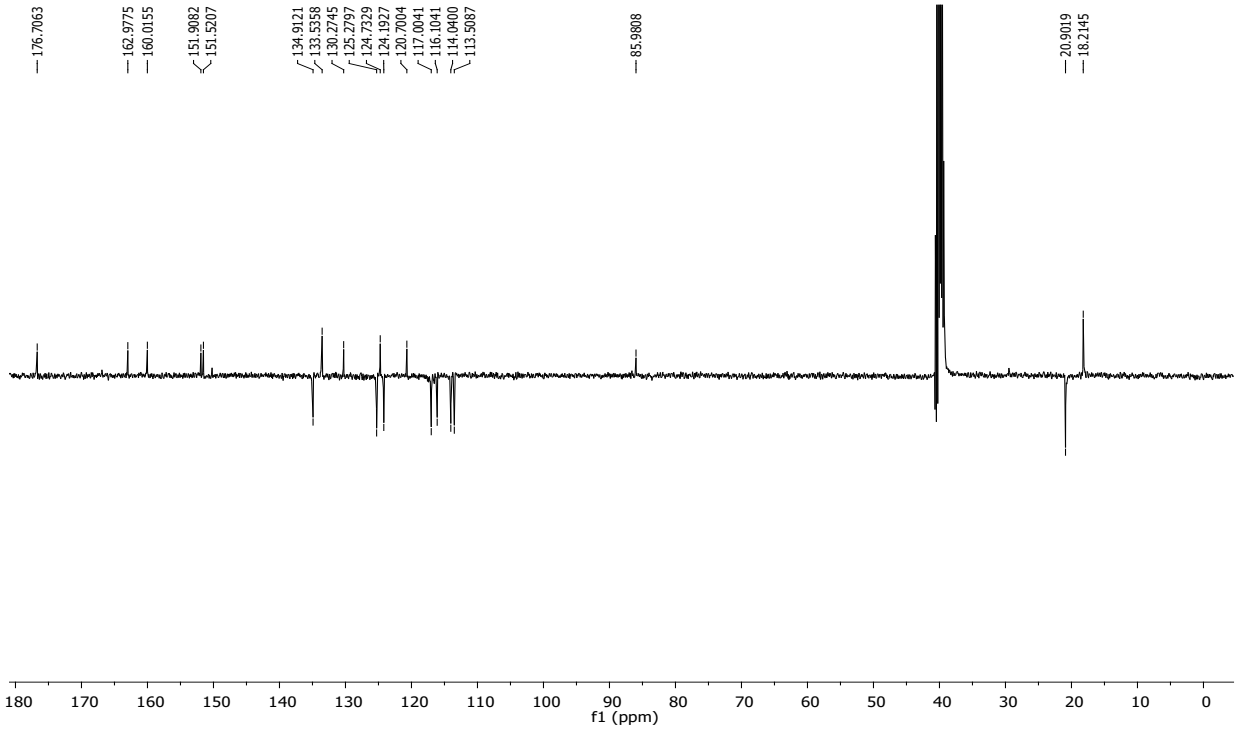


Figure S13. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of **2-(2-(7-(diethylamino)-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-4,5-dihydro-1H-imidazol-3-ium chloride 13**

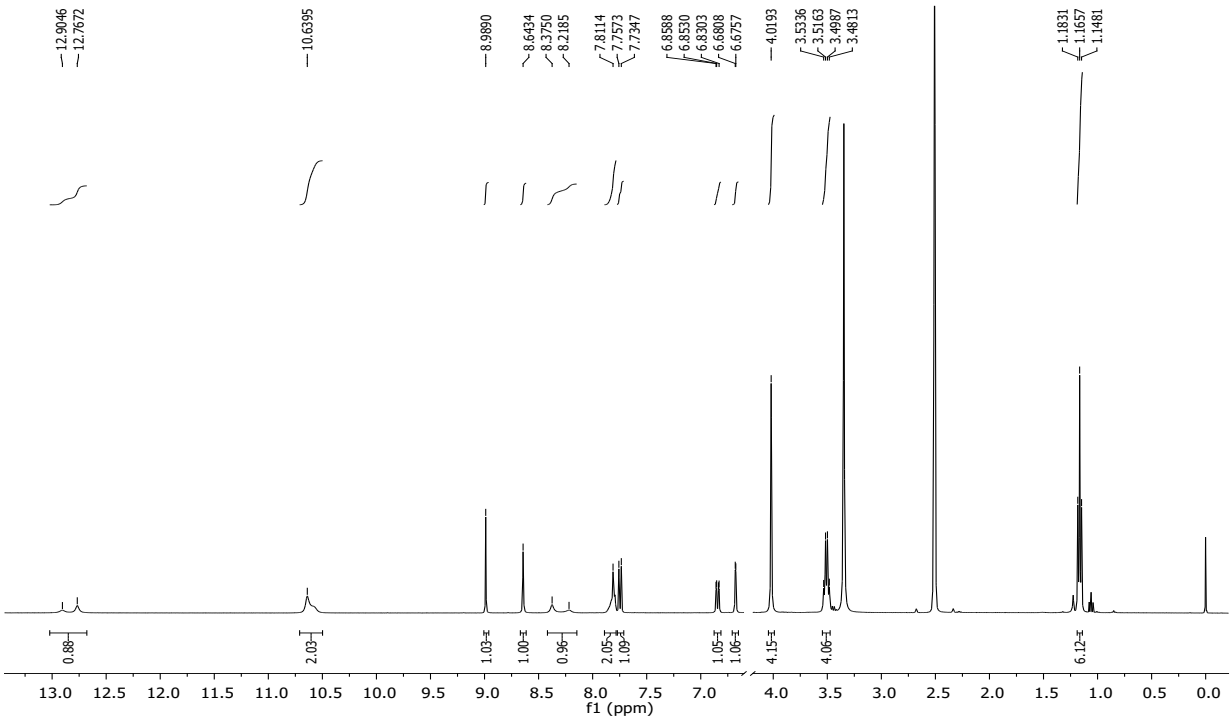


Figure S14. ^{13}C NMR spectrum (DMSO-d_6, 101 MHz) of **2-(2-(7-(diethylamino)-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-4,5-dihydro-1H-imidazol-3-ium chloride 13**

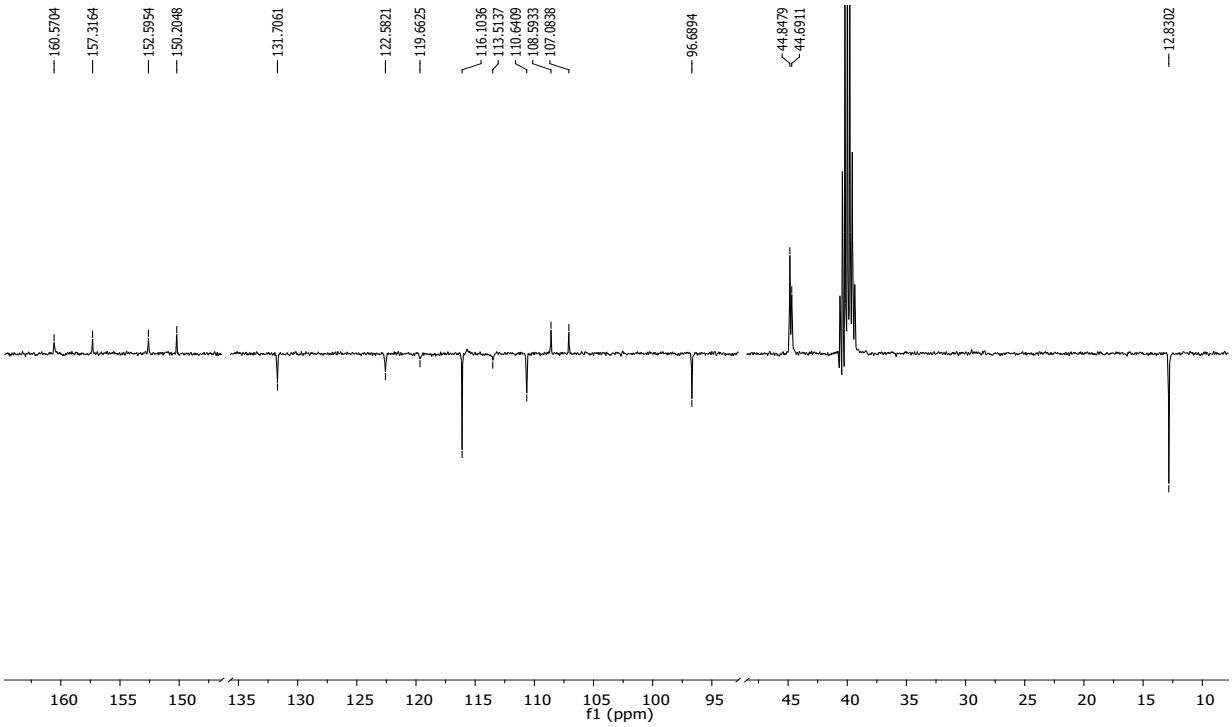


Figure S15. ^{1}H NMR spectrum (DMSO-d_6, 400 MHz) of **2-(2-(7-(diethylamino)-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-3,4,5,6-tetrahydropyrimidin-1-ium chloride 14**

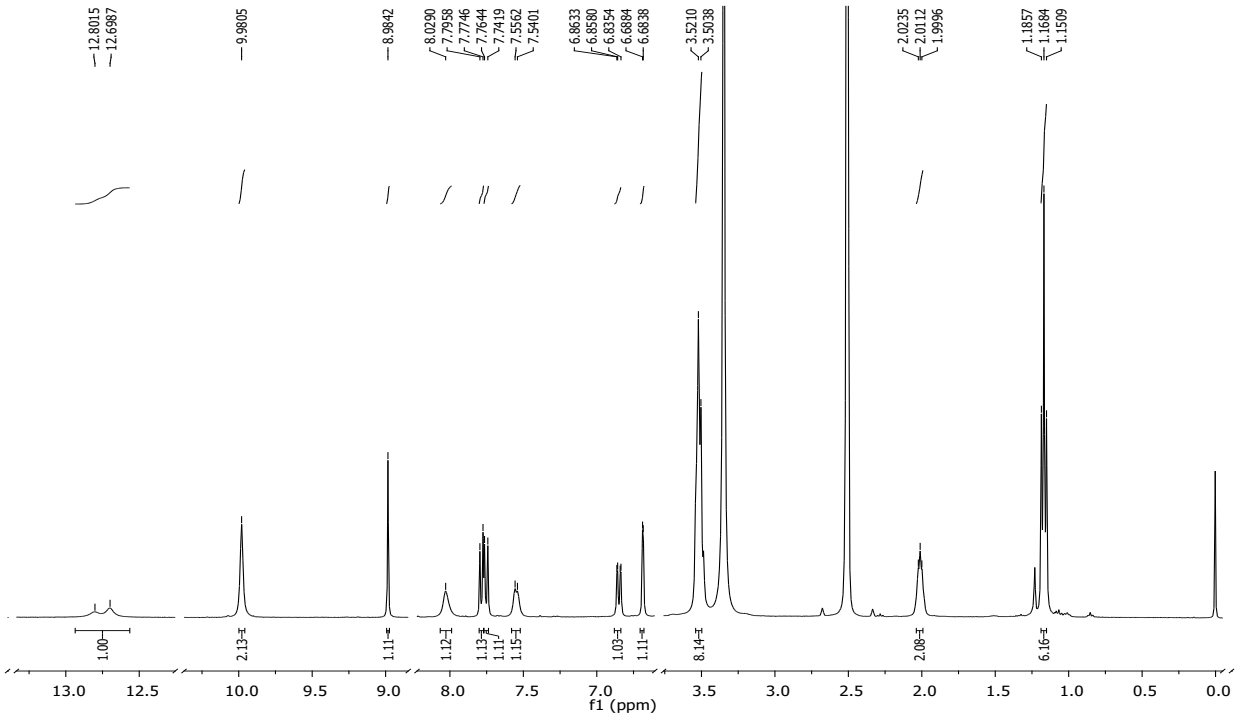


Figure S16. ^{13}C NMR spectrum (DMSO-d_6, 101 MHz) of **2-(2-(7-(diethylamino)-2-oxo-2H-chromen-3-yl)-1H-benzo[d]imidazol-5-yl)-3,4,5,6-tetrahydropyrimidin-1-ium chloride 14**

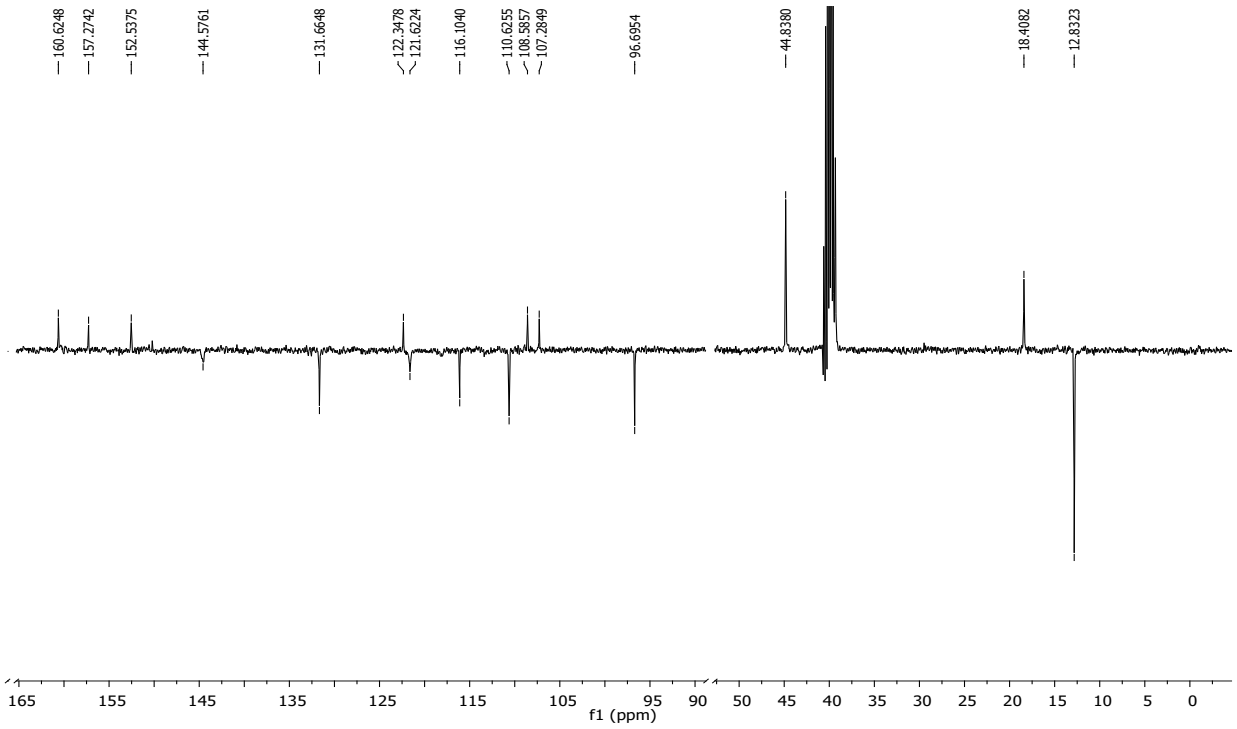


Figure S17. ^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of **2-[2-(7-(*N*,*N*-diethylamino)-2-oxo-2*H*-chromen-3-yl)benzo[*d*]thiazol-6-yl]-4,5-dihydro-1*H*-imidazol-3-ium chloride 17**

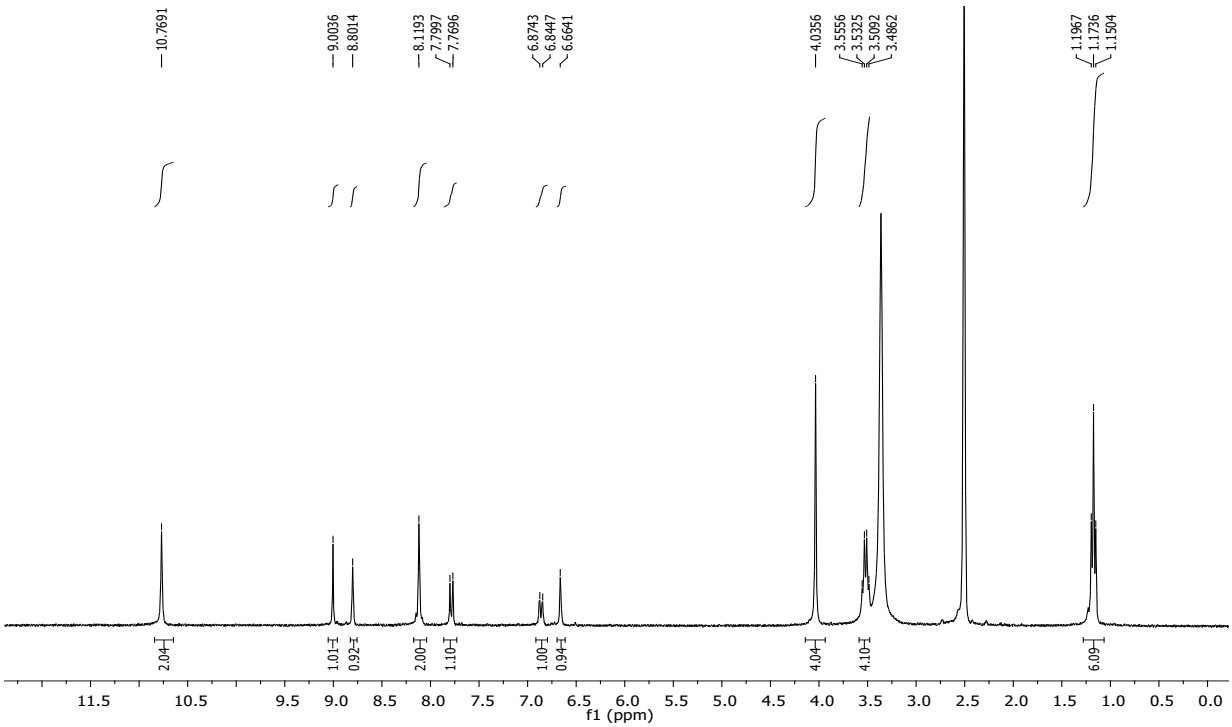


Figure S18. ^{13}C NMR spectrum (DMSO-d_6, 151 MHz) of **2-[2-(7-(*N*,*N*-diethylamino)-2-oxo-2*H*-chromen-3-yl)benzo[*d*]thiazol-6-yl]-4,5-dihydro-1*H*-imidazol-3-ium chloride 17**

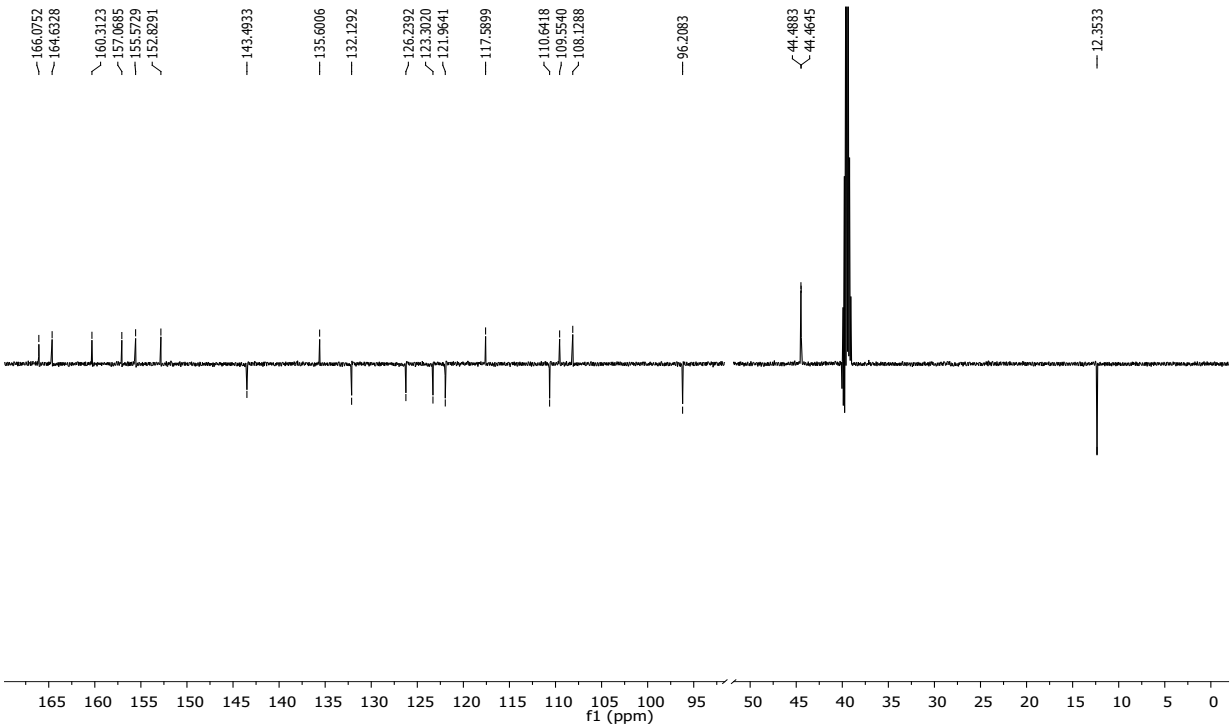


Figure S19. ^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of **2-[2-(7-(*N*,*N*-diethylamino)-2-oxo-2*H*-chromen-3-yl)benzo[*d*]thiazol-6-yl]-3,4,5,6 tetrahydropyrimidin-1-ium chloride 18**

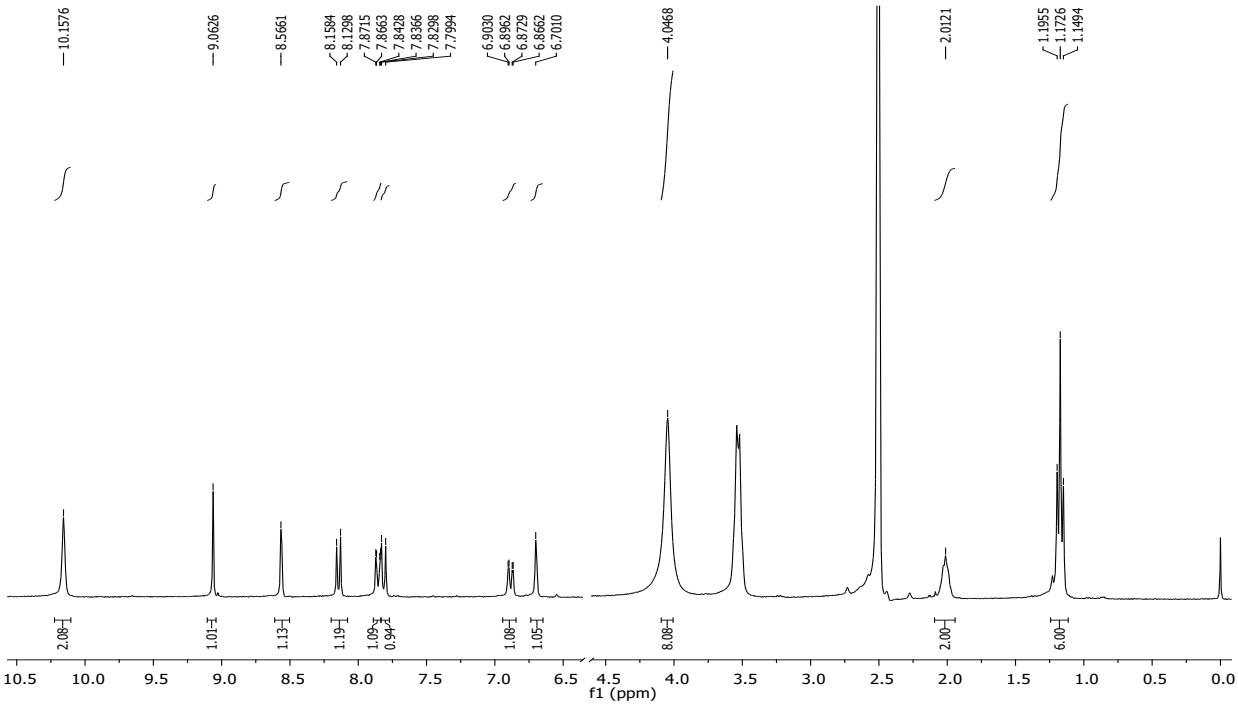
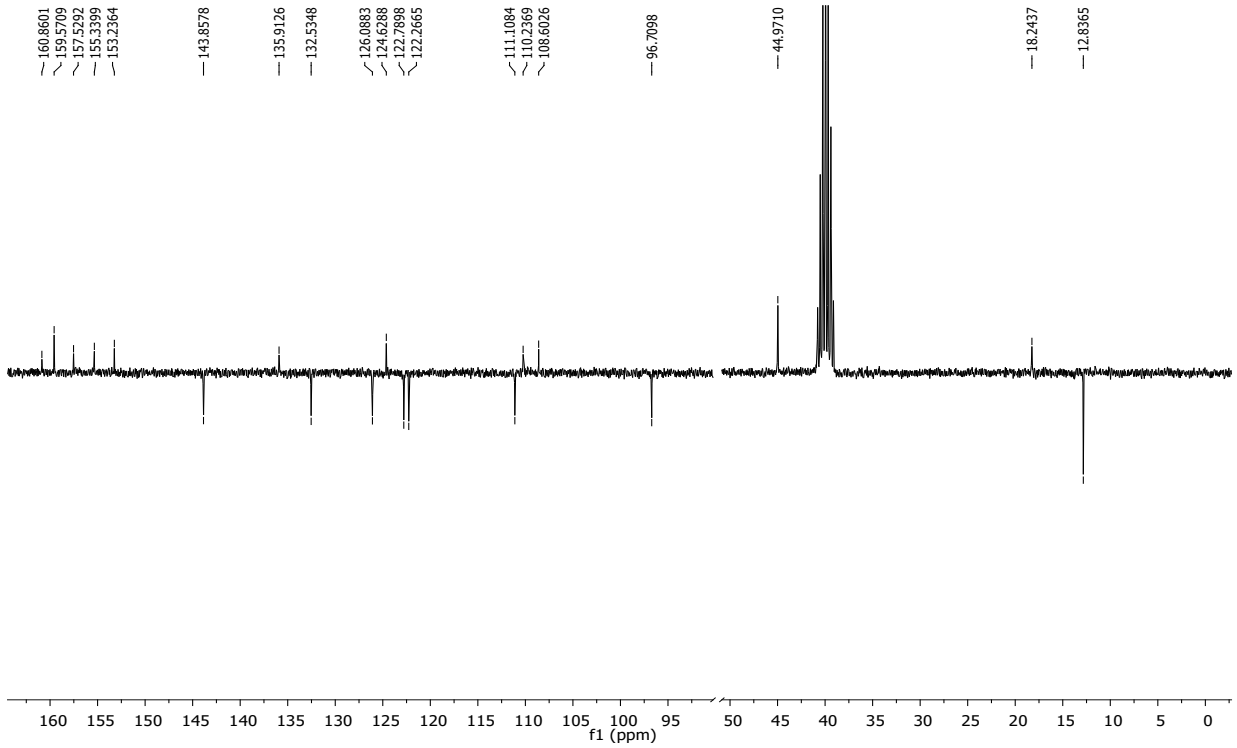
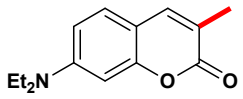


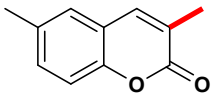
Figure S20. ^{13}C NMR spectrum (DMSO-d_6, 75 MHz) of **2-[2-(7-(*N*,*N*-diethylamino)-2-oxo-2*H*-chromen-3-yl)benzo[*d*]thiazol-6-yl]-3,4,5,6 tetrahydropyrimidin-1-ium chloride 18**





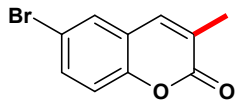
m2

Initial molecule **m2** E_{EL} = -670.359596237 a.u.						Radical cation **m2•+** with 1 e⁻ less E_{EL} = -670.173124412 a.u.						Radical anion **m2•−** with 1 e⁻ more E_{EL} = -670.439599870 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	1.003055	-0.814738	-0.022925	1	6	0	0.992329	-0.830836	0.000066	1	6	0	1.000897	-0.784675	-0.108402
2	1	0	1.175550	-1.883805	-0.020471	2	1	0	1.176979	-1.897174	0.000012	2	1	0	1.161131	-1.856284	-0.138407
3	6	0	2.071712	0.116748	-0.034594	3	6	0	2.057992	0.119151	0.000069	3	6	0	2.087688	0.129784	-0.120919
4	6	0	1.743185	1.510090	-0.019710	4	6	0	1.741936	1.523814	0.000045	4	6	0	1.767852	1.505631	-0.060582
5	6	0	0.428399	1.932159	-0.010110	5	6	0	0.435256	1.937919	0.000054	5	6	0	0.441526	1.940637	-0.018042
6	6	0	-0.644797	1.012210	-0.008796	6	6	0	-0.634711	1.002211	0.000068	6	6	0	-0.655595	1.043912	-0.018859
7	6	0	-0.304768	-0.354187	-0.014338	7	6	0	-0.305581	-0.378161	0.000072	7	6	0	-0.310097	-0.332839	-0.064088
8	7	0	3.375162	-0.302529	-0.062745	8	7	0	3.343801	-0.299056	-0.000003	8	7	0	3.417751	-0.325502	-0.232002
9	1	0	2.530626	2.254020	-0.017251	9	1	0	2.533893	2.261812	0.000002	9	1	0	2.551390	2.254942	-0.052107
10	1	0	0.206099	2.996813	-0.000755	10	1	0	0.199595	2.998042	0.000037	10	1	0	0.240535	3.009915	0.026975
11	6	0	-2.027836	1.362511	0.002692	11	6	0	-2.008433	1.373875	0.000031	11	6	0	-2.034420	1.396379	0.030767
12	8	0	-1.302706	-1.303022	-0.007385	12	8	0	-1.298838	-1.321427	0.000050	12	8	0	-1.298065	-1.303145	-0.057110
13	6	0	-2.647256	-0.981691	0.003340	13	6	0	-2.636696	-0.991638	0.000001	13	6	0	-2.686844	-0.961233	-0.003220
14	6	0	-3.018893	0.418590	0.008271	14	6	0	-3.001168	0.431681	-0.000013	14	6	0	-3.037090	0.387502	0.037478
15	8	0	-3.426985	-1.935893	0.008191	15	8	0	-3.430876	-1.917477	-0.000049	15	8	0	-3.439427	-1.983776	0.001283
16	6	0	-4.486168	0.748052	0.020191	16	6	0	-4.459111	0.760397	-0.000098	16	6	0	-4.505493	0.741341	0.091017
17	1	0	-2.293598	2.418254	0.007292	17	1	0	-2.263502	2.430598	0.000012	17	1	0	-2.320472	2.445465	0.066021
18	1	0	-4.997087	0.334745	-0.859344	18	1	0	-4.954483	0.332004	-0.881120	18	1	0	-5.057621	0.367232	-0.783915
19	1	0	-4.983986	0.329044	0.904512	19	1	0	-4.954610	0.331912	0.880806	19	1	0	-5.004403	0.321302	0.977006
20	1	0	-4.633672	1.832781	0.024811	20	1	0	-4.610730	1.843007	-0.000057	20	1	0	-4.637225	1.829604	0.123241
21	6	0	4.464331	0.663328	0.056438	21	6	0	4.455166	0.662737	-0.000143	21	6	0	4.475747	0.612972	0.131948
22	6	0	3.684941	-1.726248	0.022745	22	6	0	3.668997	-1.732017	-0.000006	22	6	0	3.690523	-1.704227	0.168953
23	1	0	5.414264	0.130101	0.004609	23	1	0	5.393815	0.113518	-0.000272	23	1	0	5.443491	0.130469	-0.026699
24	1	0	4.442473	1.392790	-0.762278	24	1	0	4.407742	1.293682	-0.893276	24	1	0	4.445695	1.503299	-0.503045
25	1	0	4.426733	1.209497	1.009935	25	1	0	4.407981	1.293654	0.893026	25	1	0	4.416051	0.936460	1.186616
26	1	0	4.764513	-1.860198	-0.055584	26	1	0	4.750180	-1.849375	0.000024	26	1	0	4.753240	-1.910106	0.018611
27	1	0	3.349130	-2.162784	0.974988	27	1	0	3.254172	-2.210943	0.892786	27	1	0	3.444546	-1.896618	1.228476
28	1	0	3.214915	-2.283180	-0.796920	28	1	0	3.254220	-2.210915	-0.892843	28	1	0	3.131156	-2.412901	-0.448452



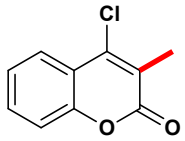
m3

Initial molecule **m3** E_{EL} = -575.699976269 a.u.						Radical cation **m3**$^{\bullet+}$ with 1 e$^-$ less E_{EL} = -575.475814661 a.u.						Radical anion **m3**$^{\bullet-}$ with 1 e$^-$ more E_{EL} = -575.787880132 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	-1.306375	1.681811	-0.000118	1	6	0	-1.309224	1.700074	-0.000808	1	6	0	-1.304164	1.670436	0.000047
2	1	0	-1.164913	2.758771	-0.000172	2	1	0	-1.168170	2.775663	-0.001125	2	1	0	-1.152428	2.747763	0.000076
3	6	0	-2.576802	1.114473	-0.000061	3	6	0	-2.556505	1.121031	-0.000379	3	6	0	-2.602384	1.126536	0.000093
4	6	0	-2.766290	-0.286299	0.000020	4	6	0	-2.741787	-0.314810	0.000157	4	6	0	-2.787732	-0.270369	0.000033
5	6	0	-1.638996	-1.104096	0.000010	5	6	0	-1.622182	-1.135477	0.000034	5	6	0	-1.663663	-1.099082	-0.000049
6	6	0	-0.336066	-0.560561	-0.000056	6	6	0	-0.327969	-0.587175	-0.000329	6	6	0	-0.334160	-0.585721	-0.000075
7	6	0	-0.197980	0.835167	-0.000094	7	6	0	-0.190694	0.853433	-0.000588	7	6	0	-0.200153	0.830538	-0.000048
8	1	0	-3.446046	1.768525	-0.000067	8	1	0	-3.439819	1.753854	-0.000363	8	1	0	-3.463331	1.791779	0.000160
9	6	0	-4.160474	-0.866453	0.000157	9	6	0	-4.129492	-0.862143	0.000910	9	6	0	-4.183092	-0.856489	0.000031
10	1	0	-1.749492	-2.186336	0.000046	10	1	0	-1.732253	-2.215730	0.000334	10	1	0	-1.794881	-2.180577	-0.000058
11	6	0	0.865049	-1.351647	-0.000076	11	6	0	0.855056	-1.369534	-0.000397	11	6	0	0.846753	-1.369664	-0.000082
12	8	0	1.052059	1.411051	-0.000123	12	8	0	1.018769	1.423020	-0.000451	12	8	0	1.058028	1.418656	-0.000138
13	6	0	2.212389	0.671904	0.000086	13	6	0	2.203301	0.677678	0.000531	13	6	0	2.246723	0.636369	-0.000041
14	6	0	2.102478	-0.783059	-0.000035	14	6	0	2.100164	-0.789607	-0.000133	14	6	0	2.128390	-0.756522	-0.000030
15	8	0	3.264883	1.305681	0.000290	15	8	0	3.231216	1.316932	0.001542	15	8	0	3.299298	1.338110	0.000068
16	6	0	3.383578	-1.567160	-0.000066	16	6	0	3.375590	-1.558447	-0.000429	16	6	0	3.394530	-1.580101	0.000114
17	1	0	0.769135	-2.435564	-0.000119	17	1	0	0.764061	-2.452289	-0.000563	17	1	0	0.769096	-2.455010	-0.000072
18	1	0	3.992577	-1.330655	-0.881978	18	1	0	3.979070	-1.302395	-0.881466	18	1	0	4.022279	-1.379979	-0.880787
19	1	0	3.992606	-1.330715	0.881839	19	1	0	3.980002	-1.301912	0.879795	19	1	0	4.021867	-1.380311	0.881388
20	1	0	3.174313	-2.641314	-0.000101	20	1	0	3.177720	-2.632974	-0.000097	20	1	0	3.156114	-2.650361	-0.000136
21	1	0	-4.135582	-1.961184	0.000046	21	1	0	-4.136042	-1.954902	0.001582	21	1	0	-4.156496	-1.952015	-0.000222
22	1	0	-4.725470	-0.540040	0.882976	22	1	0	-4.680708	-0.499005	0.880209	22	1	0	-4.753504	-0.535677	0.882301
23	1	0	-4.725739	-0.539829	-0.882406	23	1	0	-4.681284	-0.500060	-0.878455	23	1	0	-4.753616	-0.535327	-0.882050



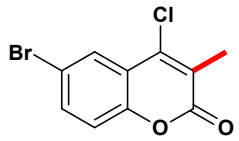
m4

Initial molecule **m4** E_{EL} = -3107.50998155 a.u.						Radical cation **m4**$^{\bullet+}$ with 1 e$^-$ less E_{EL} = -3107.27736216 a.u.						Radical anion **m4**$^{\bullet-}$ with 1 e$^-$ more E_{EL} = -3107.60376727 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	0.078381	1.934973	-0.000015	1	6	0	0.088312	1.949047	0.000092	1	6	0	0.073473	1.920581	-0.000009
2	1	0	-0.185426	2.988083	-0.000018	2	1	0	-0.173849	3.001601	0.000092	2	1	0	-0.199165	2.973023	-0.000009
3	6	0	1.409290	1.529178	-0.000024	3	6	0	1.396941	1.527605	0.000138	3	6	0	1.431349	1.537583	-0.000011
4	6	0	1.716836	0.160818	-0.000035	4	6	0	1.710060	0.126457	0.000192	4	6	0	1.726007	0.173028	-0.000011
5	6	0	0.724982	-0.807455	0.000003	5	6	0	0.726037	-0.839048	0.000056	5	6	0	0.743395	-0.808125	-0.000005
6	6	0	-0.626112	-0.408419	0.000025	6	6	0	-0.624559	-0.434670	-0.000061	6	6	0	-0.632957	-0.437556	0.000005
7	6	0	-0.921863	0.964062	0.000017	7	6	0	-0.925334	0.977626	-0.000026	7	6	0	-0.922837	0.958840	-0.000000
8	1	0	2.198073	2.274571	-0.000034	8	1	0	2.198100	2.259924	0.000148	8	1	0	2.214007	2.288337	-0.000012
9	35	0	3.553449	-0.374847	-0.000001	9	35	0	3.525617	-0.367791	-0.000034	9	35	0	3.573196	-0.371775	0.000002
10	1	0	0.965203	-1.866136	0.000010	10	1	0	0.956489	-1.899250	0.000011	10	1	0	1.005954	-1.861863	-0.000002
11	6	0	-1.727944	-1.335261	0.000018	11	6	0	-1.704160	-1.350119	-0.000054	11	6	0	-1.717118	-1.345454	0.000004
12	8	0	-2.225347	1.391900	0.000046	12	8	0	-2.188669	1.404922	-0.000133	12	8	0	-2.234713	1.396943	0.000014
13	6	0	-3.295423	0.524311	0.000113	13	6	0	-3.281969	0.529413	-0.000414	13	6	0	-3.331264	0.490165	0.000037
14	6	0	-3.019966	-0.910389	0.000023	14	6	0	-3.011142	-0.917153	-0.000083	14	6	0	-3.057784	-0.882228	0.000010
15	8	0	-4.410812	1.033328	-0.000087	15	8	0	-4.374706	1.046847	0.000178	15	8	0	-4.451435	1.069363	-0.000018
16	6	0	-4.205187	-1.831557	-0.000035	16	6	0	-4.186998	-1.826286	0.000145	16	6	0	-4.223880	-1.840852	-0.000012
17	1	0	-1.506589	-2.400282	-0.000011	17	1	0	-1.489294	-2.415351	0.000056	17	1	0	-1.517810	-2.414865	-0.000012
18	1	0	-4.835914	-1.662155	0.881926	18	1	0	-4.817109	-1.636937	0.879963	18	1	0	-4.868864	-1.710550	0.881295
19	1	0	-4.835910	-1.662054	-0.881978	19	1	0	-4.817140	-1.637329	-0.879735	19	1	0	-4.868884	-1.710489	-0.881296
20	1	0	-3.878847	-2.875766	-0.000092	20	1	0	-3.869926	-2.871350	0.000367	20	1	0	-3.868230	-2.877817	-0.000052



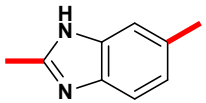
m5

Initial molecule **m5** E_{EL} = -995.971544042 a.u.						Radical cation **m5**$^{\bullet+}$ with 1 e$^-$ less E_{EL} = -995.735777746 a.u.						Radical anion **m5**$^{\bullet-}$ with 1 e$^-$ more E_{EL} = -996.068538166 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	2.340569	-1.432191	0.000032	1	6	0	2.361276	-1.407648	0.000314	1	6	0	2.350243	-1.413067	-0.000001
2	1	0	2.525062	-2.502294	0.000051	2	1	0	2.575898	-2.470966	0.000592	2	1	0	2.536046	-2.484477	-0.000043
3	6	0	3.380434	-0.507929	0.000033	3	6	0	3.365161	-0.453257	0.000126	3	6	0	3.413753	-0.490214	0.000077
4	6	0	3.104704	0.869473	0.000002	4	6	0	3.062817	0.943498	-0.000300	4	6	0	3.128033	0.880209	0.000107
5	6	0	1.791651	1.322253	-0.000028	5	6	0	1.760359	1.375010	-0.000424	5	6	0	1.808711	1.335815	0.000063
6	6	0	0.717527	0.407299	-0.000028	6	6	0	0.696444	0.428415	-0.000135	6	6	0	0.713530	0.427067	-0.000015
7	6	0	1.026365	-0.965062	0.000002	7	6	0	1.037569	-0.975910	0.000103	7	6	0	1.039220	-0.960932	-0.000050
8	1	0	4.408893	-0.858112	0.000050	8	1	0	4.403575	-0.770463	0.000290	8	1	0	4.440686	-0.845776	0.000108
9	1	0	3.920192	1.587087	0.000006	9	1	0	3.875829	1.662324	-0.000527	9	1	0	3.939484	1.605059	0.000169
10	1	0	1.588703	2.387459	-0.000067	10	1	0	1.532687	2.434113	-0.000787	10	1	0	1.607804	2.402610	0.000091
11	6	0	-0.688661	0.754650	-0.000019	11	6	0	-0.677314	0.762261	0.000016	11	6	0	-0.666690	0.749306	-0.000034
12	8	0	0.033684	-1.912057	0.000014	12	8	0	0.086746	-1.927546	0.000213	12	8	0	0.044565	-1.920516	-0.000197
13	6	0	-1.298293	-1.590366	-0.000016	13	6	0	-1.259832	-1.633975	-0.000023	13	6	0	-1.334240	-1.588499	-0.000023
14	6	0	-1.682516	-0.178873	0.000018	14	6	0	-1.674533	-0.217644	0.000027	14	6	0	-1.695718	-0.233950	0.000074
15	8	0	-2.090826	-2.524888	-0.000092	15	8	0	-2.025701	-2.572985	-0.000337	15	8	0	-2.078279	-2.605647	-0.000009
16	6	0	-3.159804	0.085711	0.000092	16	6	0	-3.126690	0.082161	-0.000069	16	6	0	-3.159257	0.129625	0.000230
17	17	0	-1.090404	2.463336	-0.000018	17	17	0	-1.155738	2.423277	0.000237	17	17	0	-1.128914	2.461491	-0.000122
18	1	0	-3.627928	-0.368922	-0.881668	18	1	0	-3.719232	-0.832175	0.000129	18	1	0	-3.775156	-0.773576	0.000905
19	1	0	-3.627810	-0.368793	0.882001	19	1	0	-3.390601	0.684373	0.880927	19	1	0	-3.436316	0.724488	0.882156
20	1	0	-3.384971	1.152652	0.000017	20	1	0	-3.390519	0.683858	-0.881467	20	1	0	-3.436802	0.723470	-0.882238



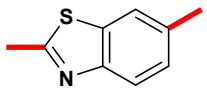
m6

Initial molecule **m6** E_{EL} = -3567.09969719 a.u.						Radical cation **m6**$^{\bullet+}$ with 1 e$^-$ less E_{EL} = -3566.86118978 a.u.						Radical anion **m6**$^{\bullet-}$ with 1 e$^-$ more E_{EL} = -3567.20142320 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	0.424804	-2.260573	0.000068	1	6	0	0.457827	-2.275714	-0.000125	1	6	0	0.426387	-2.252568	0.000005
2	1	0	0.231411	-3.328777	0.000109	2	1	0	0.268214	-3.343766	-0.000159	2	1	0	0.232816	-3.322035	0.000018
3	6	0	1.722280	-1.763975	0.000052	3	6	0	1.729057	-1.762343	-0.000076	3	6	0	1.749276	-1.767034	-0.000076
4	6	0	1.924413	-0.377483	0.000009	4	6	0	1.920894	-0.342748	-0.000022	4	6	0	1.936778	-0.386414	-0.000023
5	6	0	0.865167	0.515761	-0.000034	5	6	0	0.858414	0.546249	-0.000040	5	6	0	0.881264	0.518446	0.000055
6	6	0	-0.455348	0.024575	-0.000005	6	6	0	-0.452020	0.046199	-0.000085	6	6	0	-0.459884	0.041624	0.000126
7	6	0	-0.646071	-1.367681	0.000024	7	6	0	-0.633948	-1.385430	-0.000099	7	6	0	-0.642600	-1.372928	0.000152
8	1	0	2.562925	-2.450116	0.000085	8	1	0	2.585709	-2.428686	-0.000067	8	1	0	2.587014	-2.455697	-0.000158
9	35	0	3.711357	0.299885	-0.000024	9	35	0	3.677918	0.312013	0.000084	9	35	0	3.731765	0.303357	-0.000090
10	1	0	1.045339	1.583600	-0.000066	10	1	0	1.033158	1.614709	-0.000003	10	1	0	1.070657	1.585015	0.000072
11	6	0	-1.650390	0.845672	-0.000000	11	6	0	-1.633695	0.850872	-0.000089	11	6	0	-1.635002	0.828969	0.000148
12	8	0	-1.902411	-1.909689	0.000042	12	8	0	-1.845609	-1.931923	-0.000066	12	8	0	-1.908467	-1.920173	0.000504
13	6	0	-3.039410	-1.142707	-0.000014	13	6	0	-3.016290	-1.170233	0.000029	13	6	0	-3.082073	-1.124705	-0.000023
14	6	0	-2.905649	0.315724	-0.000025	14	6	0	-2.898046	0.296269	0.000056	14	6	0	-2.942501	0.271967	-0.000099
15	8	0	-4.106657	-1.740893	-0.000105	15	8	0	-4.050612	-1.795049	0.000075	15	8	0	-4.135287	-1.810922	-0.000211
16	6	0	-4.198678	1.076037	0.000002	16	6	0	-4.158949	1.088727	0.000277	16	6	0	-4.184092	1.126748	-0.000480
17	17	0	-1.428388	2.584488	0.000043	17	17	0	-1.473656	2.575519	-0.000167	17	17	0	-1.464236	2.591837	0.000229
18	1	0	-4.794558	0.810247	-0.881763	18	1	0	-5.032370	0.436639	0.000193	18	1	0	-5.077974	0.497890	-0.000939
19	1	0	-4.794317	0.810573	0.882037	19	1	0	-4.199638	1.740527	0.883142	19	1	0	-4.234130	1.779979	0.882065
20	1	0	-4.039888	2.154765	-0.000258	20	1	0	-4.199749	1.740993	-0.882215	20	1	0	-4.233404	1.780267	-0.882850



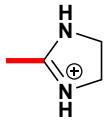
m7

Initial molecule **m7** E_{EL} = -458.545081936 a.u. **Cartesian Coordinates**						Radical cation **m7**$^{\bullet+}$ with 1 e$^-$ less E_{EL} = -458.337326490 a.u. **Cartesian Coordinates**						Radical anion **m7**$^{\bullet-}$ with 1 e$^-$ more E_{EL} = -458.582624795 a.u. **Cartesian Coordinates**					
1	6	0	3.784547	-0.328484	-0.000099	1	6	0	3.761592	-0.282234	-0.000250	1	6	0	3.771912	-0.330722	0.201348
2	6	0	2.313792	-0.080496	-0.000004	2	6	0	2.296227	-0.108442	0.000118	2	6	0	2.360019	-0.097126	-0.240927
3	7	0	1.403613	-1.110146	0.000039	3	7	0	1.415111	-1.129459	0.000089	3	7	0	1.397679	-1.126800	-0.065145
4	6	0	0.136027	-0.555787	0.000107	4	6	0	0.137213	-0.593260	0.000162	4	6	0	0.143103	-0.559957	-0.018296
5	6	0	0.359456	0.839863	0.000092	5	6	0	0.360676	0.834430	0.000131	5	6	0	0.384688	0.852075	-0.013268
6	7	0	1.727271	1.104043	0.000056	6	7	0	1.671494	1.106993	0.000098	6	7	0	1.726563	1.109866	-0.094229
7	1	0	1.632988	-2.097834	0.000018	7	1	0	1.657817	-2.117161	0.000705	7	1	0	1.575079	-2.105833	-0.253101
8	6	0	-0.738487	1.712283	0.000011	8	6	0	-0.756705	1.727726	0.000043	8	6	0	-0.732891	1.727915	0.005711
9	6	0	-1.145700	-1.115746	0.000047	9	6	0	-1.115820	-1.149723	0.000044	9	6	0	-1.140688	-1.114176	-0.017240
10	6	0	-2.017255	1.158644	-0.000058	10	6	0	-2.009346	1.175205	-0.000065	10	6	0	-2.032851	1.159303	0.040827
11	6	0	-2.238719	-0.242872	-0.000030	11	6	0	-2.219349	-0.251635	-0.000073	11	6	0	-2.260247	-0.219288	0.028924
12	1	0	-0.593612	2.790202	0.000038	12	1	0	-0.596183	2.801330	0.000047	12	1	0	-0.595970	2.807819	0.012814
13	1	0	-1.291737	-2.193373	0.000106	13	1	0	-1.278937	-2.222804	0.000045	13	1	0	-1.291418	-2.192830	-0.015583
14	1	0	-2.880913	1.821055	-0.000135	14	1	0	-2.886540	1.815770	-0.000139	14	1	0	-2.892998	1.829315	0.064795
15	6	0	-3.652819	-0.779116	-0.000065	15	6	0	-3.614155	-0.775563	-0.000145	15	6	0	-3.660973	-0.787740	0.044892
16	1	0	4.319575	0.624553	-0.000432	16	1	0	4.187602	0.211649	-0.883181	16	1	0	4.420226	0.483573	-0.141357
17	1	0	4.088337	-0.901311	0.885235	17	1	0	4.188474	0.213776	0.881007	17	1	0	3.865139	-0.381120	1.308851
18	1	0	4.088083	-0.901634	-0.885348	18	1	0	4.043542	-1.337288	0.000696	18	1	0	4.174272	-1.269990	-0.198097
19	1	0	-4.210014	-0.437289	0.882434	19	1	0	-4.159154	-0.400144	0.878451	19	1	0	-4.414763	0.007657	0.096364
20	1	0	-4.210168	-0.436844	-0.882281	20	1	0	-4.159548	-0.399193	-0.878054	20	1	0	-3.874526	-1.385925	-0.855495
21	1	0	-3.663781	-1.874548	-0.000308	21	1	0	-3.645314	-1.867695	-0.000678	21	1	0	-3.827170	-1.455826	0.904595



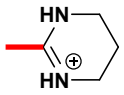
m8

Initial molecule **m8** E_{EL} = -801.368351678 a.u.						Radical cation **m8**$^{\bullet+}$ with 1 e$^-$ less E_{EL} = -801.146227736 a.u.						Radical anion **m8**$^{\bullet-}$ with 1 e$^-$ more E_{EL} = -801.425389124 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	-3.784722	0.270522	0.000141	1	6	0	-3.743002	0.323336	-0.000218	1	6	0	-3.763487	0.270038	0.229217
2	6	0	-2.291849	0.212784	-0.000005	2	6	0	-2.268501	0.193781	-0.000033	2	6	0	-2.347575	0.218003	-0.267223
3	16	0	-1.457768	-1.362549	-0.000072	3	16	0	-1.482058	-1.371540	0.000094	3	16	0	-1.456592	-1.394367	-0.052879
4	6	0	0.080029	-0.515599	-0.000010	4	6	0	0.071643	-0.551696	0.000219	4	6	0	0.078220	-0.510568	-0.032939
5	6	0	-0.164319	0.875930	0.000008	5	6	0	-0.162624	0.871364	0.000159	5	6	0	-0.193953	0.902159	-0.037499
6	7	0	-1.506625	1.245745	-0.000004	6	7	0	-1.452206	1.248848	0.000034	6	7	0	-1.499888	1.271346	-0.068087
7	6	0	0.925410	1.760532	-0.000044	7	6	0	0.952166	1.773409	0.000103	7	6	0	0.929779	1.770125	-0.025230
8	6	0	1.379343	-1.034855	-0.000092	8	6	0	1.341775	-1.067406	-0.000069	8	6	0	1.370694	-1.016308	0.006048
9	6	0	2.215927	1.242370	-0.000088	9	6	0	2.219460	1.256731	-0.000057	9	6	0	2.226924	1.245038	0.017833
10	6	0	2.463293	-0.150591	-0.000080	10	6	0	2.449238	-0.158368	-0.000125	10	6	0	2.482393	-0.136778	0.036619
11	1	0	0.751544	2.833608	-0.000081	11	1	0	0.764419	2.842578	0.000164	11	1	0	0.773282	2.847348	-0.041815
12	1	0	1.551094	-2.108319	-0.000146	12	1	0	1.533568	-2.136124	-0.000201	12	1	0	1.539406	-2.092575	0.019057
13	1	0	3.062582	1.925779	-0.000137	13	1	0	3.080225	1.918764	-0.000111	13	1	0	3.070047	1.935570	0.031145
14	6	0	3.882848	-0.667378	0.000177	14	6	0	3.841077	-0.677476	-0.000114	14	6	0	3.891343	-0.685370	0.071674
15	1	0	-4.107801	1.315420	0.000282	15	1	0	-4.051966	0.898336	-0.883841	15	1	0	-4.231755	1.212539	-0.083183
16	1	0	-4.199021	-0.227699	-0.884965	16	1	0	-4.249976	-0.643727	-0.000563	16	1	0	-4.369810	-0.552050	-0.171778
17	1	0	-4.198806	-0.227846	0.885272	17	1	0	-4.052310	0.897856	0.883591	17	1	0	-3.834429	0.221345	1.336197
18	1	0	4.433969	-0.313223	-0.880918	18	1	0	4.384596	-0.293174	-0.876516	18	1	0	4.127479	-1.276351	-0.826110
19	1	0	4.432119	-0.317288	0.884079	19	1	0	4.383741	-0.294962	0.877636	19	1	0	4.628922	0.123856	0.133552
20	1	0	3.909214	-1.762159	-0.002243	20	1	0	3.878679	-1.768886	-0.001096	20	1	0	4.055512	-1.347268	0.934602



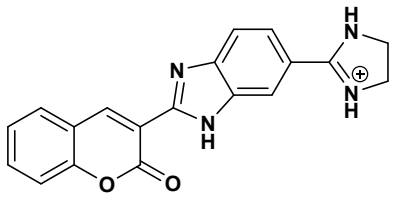
m9

Initial molecule **m9**$^{+}$ E_{EL} = -267.235001920 a.u. **Cartesian Coordinates**						Radical dication **m9**$^{\bullet 2+}$ with 1 e^{-} less E_{EL} = -266.972537089 a.u. **Cartesian Coordinates**						Radical **m9**$^{\bullet}$ with 1 e^{-} more E_{EL} = -267.307796040 a.u. **Cartesian Coordinates**					
1	6	0	-2.202039	0.000625	0.007254	1	6	0	-2.212460	0.002464	0.004069	1	6	0	-2.173246	0.010377	0.114488
2	6	0	-0.715670	0.001315	-0.013827	2	6	0	-0.739145	0.005082	-0.010444	2	6	0	-0.739847	0.065866	-0.309061
3	7	0	0.036438	1.089146	0.053463	3	7	0	0.054885	-1.075990	-0.006947	3	7	0	0.084289	1.130225	0.169876
4	6	0	1.472899	0.771397	-0.052884	4	6	0	1.457572	-0.761037	0.004495	4	6	0	1.474644	0.715803	-0.080981
5	6	0	1.469756	-0.773556	0.066556	5	6	0	1.461506	0.757561	0.005358	5	6	0	1.396126	-0.785550	0.207276
6	7	0	0.035455	-1.087888	-0.072776	6	7	0	0.058089	1.077740	-0.007638	6	7	0	0.038318	-1.126246	-0.271604
7	1	0	-0.347244	-2.025726	-0.027084	7	1	0	-0.308408	2.036396	-0.012506	7	1	0	-0.396049	-1.888196	0.249174
8	1	0	2.048407	-1.258759	-0.721465	8	1	0	1.933326	1.209435	0.893978	8	1	0	2.166129	-1.356674	-0.320926
9	1	0	1.854771	1.113253	-1.019613	9	1	0	1.930049	-1.218399	0.890606	9	1	0	1.772882	0.893545	-1.126336
10	1	0	-0.343153	2.027281	-0.006655	10	1	0	-0.315885	-2.033259	-0.011401	10	1	0	-0.146741	2.035709	-0.233378
11	1	0	1.828767	-1.114908	1.042169	11	1	0	1.952300	1.211639	-0.871365	11	1	0	1.495856	-0.976868	1.284993
12	1	0	2.034885	1.254219	0.748529	12	1	0	1.946009	-1.217710	-0.873039	12	1	0	2.172263	1.240036	0.578111
13	1	0	-2.590886	-0.868401	-0.529910	13	1	0	-2.595742	0.989822	-0.260171	13	1	0	-2.716599	-0.768874	-0.433422
14	1	0	-2.545583	-0.052232	1.047725	14	1	0	-2.587624	-0.755193	-0.690713	14	1	0	-2.274057	-0.210867	1.197331
15	1	0	-2.592896	0.917784	-0.441100	15	1	0	-2.549682	-0.259399	1.015844	15	1	0	-2.677999	0.965357	-0.073787



m10

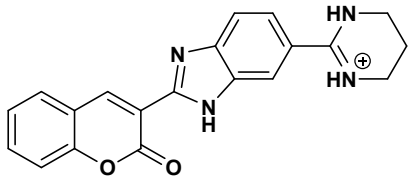
Initial molecule **m10⁺** E_{EL} = -306.561651290 a.u.						Radical dication **m10•²⁺** with 1 e⁻ less E_{EL} = -306.290438118 a.u.						Radical **m10•** with 1 e⁻ more E_{EL} = -306.620749155 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	-2.451778	0.000353	0.126927	1	6	0	-2.474598	0.002417	0.108438	1	6	0	-2.425739	-0.026452	0.162752
2	6	0	-0.963554	0.000715	-0.034453	2	6	0	-0.993248	0.015274	0.006619	2	6	0	-1.003373	-0.121446	-0.310329
3	7	0	-0.307279	1.150402	-0.089681	3	7	0	-0.287678	1.143356	-0.056349	3	7	0	-0.273549	1.083636	-0.509489
4	6	0	1.158067	1.252729	-0.182283	4	6	0	1.161294	1.243245	-0.178433	4	6	0	0.917390	1.254854	0.343923
5	6	0	1.794657	-0.000479	0.414429	5	6	0	1.830313	-0.004815	0.376633	5	6	0	1.912847	0.111927	0.082682
6	7	0	-0.308184	-1.149681	-0.090184	6	7	0	-0.295506	-1.134619	-0.069695	6	7	0	-0.208769	-1.134225	0.285902
7	1	0	-0.853505	-2.004356	-0.047777	7	1	0	-0.846023	-2.002482	-0.116578	7	1	0	-0.673909	-2.037695	0.250164
8	1	0	2.868453	-0.000779	0.205532	8	1	0	2.881735	-0.013700	0.082224	8	1	0	2.564969	0.363341	-0.762327
9	1	0	1.439486	1.376460	-1.234548	9	1	0	1.358097	1.394163	-1.256441	9	1	0	1.368524	2.224848	0.113319
10	1	0	-0.851748	2.005575	-0.047396	10	1	0	-0.823959	2.019976	-0.072887	10	1	0	-0.880206	1.899506	-0.488136
11	1	0	1.660867	-0.000284	1.502680	11	1	0	1.778279	0.001259	1.470534	11	1	0	2.553571	-0.004847	0.965185
12	1	0	1.459809	2.151177	0.361413	12	1	0	1.459195	2.163735	0.332805	12	1	0	0.637795	1.264159	1.409938
13	6	0	1.157201	-1.253356	-0.182043	13	6	0	1.146259	-1.252194	-0.160265	13	6	0	1.166095	-1.204765	-0.230068
14	1	0	1.457999	-2.151755	0.362266	14	1	0	1.425576	-2.174866	0.361028	14	1	0	1.661777	-2.060916	0.236834
15	1	0	1.439187	-1.377834	-1.234068	15	1	0	1.357267	-1.430031	-1.235187	15	1	0	1.159543	-1.379480	-1.319606
16	1	0	-2.892326	-0.872141	-0.363269	16	1	0	-2.891025	-0.522994	-0.759151	16	1	0	-2.924351	-1.002820	0.116863
17	1	0	-2.700001	-0.040486	1.194481	17	1	0	-2.769953	-0.540153	1.013817	17	1	0	-2.494758	0.333818	1.209981
18	1	0	-2.887531	0.909598	-0.295712	18	1	0	-2.867017	1.020382	0.144184	18	1	0	-3.000045	0.669494	-0.460862



m11

Initial molecule **m11**$^{+}$ E_{EL} = -1102.48498369 a.u. **Cartesian Coordinates**						Radical dication **m11**$^{\bullet 2+}$ with 1 e^{-} less E_{EL} = -1102.26104723 a.u. **Cartesian Coordinates**						Radical **m11**$^{\bullet}$ with 1 e^{-} more E_{EL} = -1102.59899385 a.u. **Cartesian Coordinates**					
1	6	0	-6.250587	-1.075472	-0.052036	1	6	0	6.227857	-1.039628	0.075785	1	6	0	6.239671	-1.091351	0.046421
2	1	0	-6.523023	-2.125375	-0.101230	2	1	0	6.528189	-2.081040	0.128351	2	1	0	6.482483	-2.150297	0.086131
3	6	0	-7.213098	-0.069040	-0.002015	3	6	0	7.166146	-0.007074	0.032557	3	6	0	7.247350	-0.113879	0.008853
4	6	0	-6.841429	1.287492	0.060999	4	6	0	6.775623	1.349874	-0.035220	4	6	0	6.894034	1.245659	-0.042021
5	6	0	-5.500129	1.641003	0.074430	5	6	0	5.436831	1.678691	-0.060194	5	6	0	5.557500	1.630792	-0.055761
6	6	0	-4.502498	0.641022	0.025081	6	6	0	4.451532	0.650735	-0.017704	6	6	0	4.511633	0.665002	-0.019208
7	6	0	-4.907666	-0.705324	-0.037740	7	6	0	4.882419	-0.703063	0.050376	7	6	0	4.910303	-0.697289	0.032090
8	1	0	-8.265319	-0.339916	-0.012205	8	1	0	8.223118	-0.257208	0.052052	8	1	0	8.291713	-0.413606	0.019517
9	1	0	-7.607706	2.056422	0.099252	9	1	0	7.533390	2.126422	-0.067197	9	1	0	7.671761	2.005627	-0.071035
10	1	0	-5.196148	2.683291	0.123189	10	1	0	5.107297	2.712248	-0.112208	10	1	0	5.289393	2.684488	-0.095200
11	6	0	-3.102188	0.916187	0.037023	11	6	0	3.072486	0.912165	-0.042091	11	6	0	3.131588	0.965431	-0.031278
12	8	0	-3.969016	-1.706972	-0.087698	12	8	0	3.972240	-1.722202	0.094040	12	8	0	3.950249	-1.701707	0.070324
13	6	0	-2.618378	-1.477345	-0.079176	13	6	0	2.619866	-1.521644	0.075305	13	6	0	2.586549	-1.441194	0.059728
14	6	0	-2.172350	-0.089098	-0.011776	14	6	0	2.147447	-0.130032	-0.001123	14	6	0	2.159046	-0.080350	0.008094
15	8	0	-1.894843	-2.468402	-0.129614	15	8	0	1.905698	-2.508784	0.123857	15	8	0	1.872349	-2.462045	0.097591
16	6	0	-0.741033	0.212597	0.003977	16	6	0	0.750428	0.143098	-0.028164	16	6	0	0.755806	0.212517	-0.005816
17	1	0	-2.770883	1.949517	0.086732	17	1	0	2.719787	1.937669	-0.094732	17	1	0	2.803326	1.998483	-0.070438
18	7	0	0.232331	-0.750095	-0.033902	18	7	0	-0.234115	-0.804601	0.005956	18	7	0	-0.235366	-0.749840	0.030716
19	6	0	1.449765	-0.107677	0.001726	19	6	0	-1.434359	-0.153360	-0.031606	19	6	0	-1.454832	-0.109896	-0.002123
20	6	0	1.127564	1.275466	0.057338	20	6	0	-1.093355	1.247986	-0.089855	20	6	0	-1.128566	1.279280	-0.054469
21	7	0	-0.237301	1.444193	0.058617	21	7	0	0.237154	1.407488	-0.089124	21	7	0	0.226393	1.454767	-0.056385
22	1	0	0.043121	-1.747820	-0.078972	22	1	0	-0.062729	-1.807697	0.056836	22	1	0	-0.036437	-1.744988	0.067348
23	6	0	2.157678	2.229876	0.098455	23	6	0	-2.124618	2.226440	-0.132791	23	6	0	-2.167853	2.228598	-0.092871
24	6	0	2.757901	-0.576662	-0.014243	24	6	0	-2.747203	-0.605362	-0.013025	24	6	0	-2.757791	-0.575847	0.015125
25	6	0	3.468540	1.778249	0.078337	25	6	0	-3.423755	1.783964	-0.107685	25	6	0	-3.479931	1.776505	-0.072368
26	6	0	3.775939	0.390622	0.022986	26	6	0	-3.737869	0.382609	-0.047155	26	6	0	-3.793214	0.391130	-0.018662

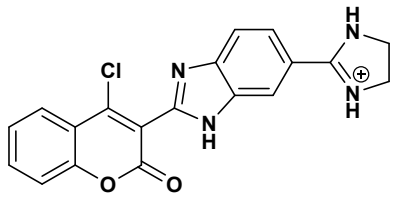
27	1	0	1.932957	3.291314	0.150909	27	1	0	-1.881184	3.282599	-0.186464	27	1	0	-1.947002	3.291325	-0.145040
28	1	0	2.973176	-1.638882	-0.079695	28	1	0	-2.983170	-1.662185	0.052481	28	1	0	-2.968205	-1.639150	0.081767
29	1	0	4.273525	2.504806	0.132342	29	1	0	-4.232044	2.506105	-0.155736	29	1	0	-4.281158	2.507933	-0.126594
30	6	0	5.173444	-0.038854	0.005007	30	6	0	-5.151118	-0.027541	-0.006661	30	6	0	-5.177982	-0.036475	-0.002584
31	7	0	5.598266	-1.254854	0.350035	31	7	0	-5.605387	-1.204771	-0.419298	31	7	0	-5.597865	-1.286341	-0.247424
32	6	0	7.071442	-1.324595	0.365919	32	6	0	-7.080349	-1.254112	-0.362963	32	6	0	-7.068174	-1.347193	-0.327016
33	6	0	7.457756	-0.043511	-0.403125	33	6	0	-7.407776	-0.016845	0.501888	33	6	0	-7.470928	-0.034360	0.368858
34	7	0	6.201613	0.728299	-0.357457	34	7	0	-6.136281	0.732337	0.455657	34	7	0	-6.230139	0.753959	0.259491
35	1	0	6.078416	1.584674	-0.886277	35	1	0	-5.973975	1.567905	1.008677	35	1	0	-6.124089	1.630027	0.758004
36	1	0	8.270280	0.509555	0.071029	36	1	0	-8.222863	0.584445	0.096306	36	1	0	-8.301425	0.472782	-0.125273
37	1	0	7.426067	-1.307486	1.401693	37	1	0	-7.482288	-1.171552	-1.377611	37	1	0	-7.380012	-1.367359	-1.377409
38	1	0	5.025603	-1.893227	0.891340	38	1	0	-5.060399	-1.832999	-1.001216	38	1	0	-5.018941	-1.952630	-0.746041
39	1	0	7.719964	-0.250664	-1.445919	39	1	0	-7.631209	-0.281793	1.540093	39	1	0	-7.717258	-0.188824	1.425573
40	1	0	7.422423	-2.235637	-0.121739	40	1	0	-7.416432	-2.189609	0.086799	40	1	0	-7.451352	-2.234101	0.180649



m12

Initial molecule **m12**$^{+}$ E_{EL} = -1141.80976118 a.u.						Radical dication **m12**$^{\bullet 2+}$ with 1 e^{-} less E_{EL} = -1141.58757662 a.u.						Radical **m12**$^{\bullet}$ with 1 e^{-} more E_{EL} = -1141.92237631 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	-6.561636	-1.139239	-0.090194	1	6	0	-6.536346	-1.103717	-0.116116	1	6	0	-6.550141	-1.155957	-0.087106
2	1	0	-6.814772	-2.192679	-0.162265	2	1	0	-6.817747	-2.149438	-0.186211	2	1	0	-6.772811	-2.217813	-0.157536
3	6	0	-7.542409	-0.152120	-0.015762	3	6	0	-7.493044	-0.088977	-0.058447	3	6	0	-7.577327	-0.199967	-0.016196
4	6	0	-7.195335	1.209213	0.076876	4	6	0	-7.126535	1.272994	0.031154	4	6	0	-7.249871	1.163784	0.074080
5	6	0	-5.860606	1.586918	0.095942	5	6	0	-5.793351	1.624970	0.065027	5	6	0	-5.920679	1.574213	0.094061
6	6	0	-4.844967	0.606872	0.022663	6	6	0	-4.790519	0.615688	0.009076	6	6	0	-4.855697	0.630853	0.024465
7	6	0	-5.225686	-0.744777	-0.069653	7	6	0	-5.196987	-0.743367	-0.082431	7	6	0	-5.228478	-0.737526	-0.066139
8	1	0	-8.589483	-0.442045	-0.030014	8	1	0	-8.545366	-0.357447	-0.084404	8	1	0	-8.615654	-0.519841	-0.031649
9	1	0	-7.975438	1.962925	0.134007	9	1	0	-7.897780	2.035703	0.073093	9	1	0	-8.041817	1.907523	0.129409
10	1	0	-5.575936	2.633334	0.167912	10	1	0	-5.482202	2.663277	0.134230	10	1	0	-5.673086	2.631378	0.164533
11	6	0	-3.449678	0.907053	0.041483	11	6	0	-3.415661	0.900525	0.044619	11	6	0	-3.481911	0.956812	0.041669
12	8	0	-4.268633	-1.727492	-0.142935	12	8	0	-4.268027	-1.745356	-0.142094	12	8	0	-4.249826	-1.722120	-0.138120
13	6	0	-2.922253	-1.473525	-0.128325	13	6	0	-2.919406	-1.521163	-0.117818	13	6	0	-2.888487	-1.434464	-0.119677
14	6	0	-2.501344	-0.079275	-0.029222	14	6	0	-2.472301	-0.123462	-0.012783	14	6	0	-2.489660	-0.070972	-0.029113
15	8	0	-2.181210	-2.450269	-0.201017	15	8	0	-2.187713	-2.494663	-0.184732	15	8	0	-2.156572	-2.443747	-0.187338
16	6	0	-1.075367	0.248252	0.000917	16	6	0	-1.080406	0.174017	0.032012	16	6	0	-1.090310	0.252685	-0.001506
17	1	0	-3.137531	1.944911	0.115594	17	1	0	-3.081514	1.931019	0.118179	17	1	0	-3.171962	1.993862	0.111795
18	7	0	-0.083753	-0.696445	-0.055041	18	7	0	-0.078380	-0.753816	-0.023331	18	7	0	-0.082303	-0.691650	-0.056619
19	6	0	1.121377	-0.034303	0.011513	19	6	0	1.109942	-0.082934	0.049937	19	6	0	1.124884	-0.032255	0.008210
20	6	0	0.775132	1.340135	0.100647	20	6	0	0.742350	1.309379	0.151464	20	6	0	0.776651	1.347563	0.093273
21	7	0	-0.594557	1.485287	0.093227	21	7	0	-0.590699	1.445015	0.139695	21	7	0	-0.586684	1.499707	0.086711
22	1	0	-0.254310	-1.695699	-0.127544	22	1	0	-0.230569	-1.757573	-0.108207	22	1	0	-0.265169	-1.688574	-0.121967
23	6	0	1.788189	2.308822	0.179639	23	6	0	1.754840	2.304417	0.242795	23	6	0	1.798052	2.309604	0.167177
24	6	0	2.439484	-0.481495	0.000326	24	6	0	2.431381	-0.509847	0.030726	24	6	0	2.438520	-0.477977	-0.003603
25	6	0	3.108012	1.878164	0.166222	25	6	0	3.062622	1.885920	0.217940	25	6	0	3.120891	1.877406	0.152706
26	6	0	3.439204	0.499029	0.080321	26	6	0	3.402745	0.493819	0.110483	26	6	0	3.453088	0.501599	0.070623

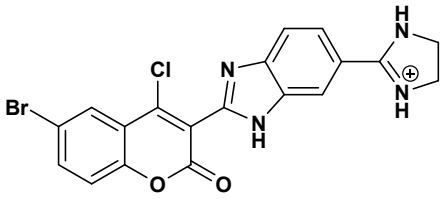
27	1	0	1.546119	3.364845	0.259767	27	1	0	1.491084	3.353145	0.334322	27	1	0	1.561062	3.367297	0.247001
28	1	0	2.674223	-1.537842	-0.092267	28	1	0	2.691055	-1.558674	-0.068384	28	1	0	2.669531	-1.535170	-0.099675
29	1	0	3.902694	2.613322	0.253889	29	1	0	3.861148	2.616244	0.303175	29	1	0	3.913410	2.615039	0.243410
30	6	0	4.860741	0.090962	0.082706	30	6	0	4.838506	0.106617	0.078076	30	6	0	4.865366	0.089646	0.079617
31	7	0	5.228221	-1.026064	0.701955	31	7	0	5.247474	-0.939416	0.781001	31	7	0	5.222018	-1.057095	0.656901
32	6	0	6.598761	-1.562850	0.704346	32	6	0	6.635793	-1.432023	0.779567	32	6	0	6.587978	-1.602507	0.660405
33	6	0	7.380005	-0.999367	-0.478662	33	6	0	7.335720	-0.996657	-0.504240	33	6	0	7.397434	-0.989998	-0.478248
34	7	0	5.770541	0.840332	-0.531928	34	7	0	5.687849	0.808705	-0.658158	34	7	0	5.796091	0.856630	-0.487944
35	1	0	5.448319	1.626256	-1.085120	35	1	0	5.318382	1.550399	-1.244127	35	1	0	5.489377	1.655733	-1.030118
36	1	0	8.439777	-1.245607	-0.364518	36	1	0	8.405938	-1.206772	-0.422412	36	1	0	8.453490	-1.247363	-0.353247
37	1	0	7.077122	-1.297846	1.654461	37	1	0	7.146269	-1.036461	1.664993	37	1	0	7.051183	-1.385888	1.630498
38	1	0	4.527531	-1.514071	1.249160	38	1	0	4.579460	-1.394639	1.394681	38	1	0	4.514546	-1.556049	1.184476
39	1	0	7.024790	-1.451304	-1.412258	39	1	0	6.942135	-1.564727	-1.355096	39	1	0	7.060235	-1.395323	-1.439632
40	1	0	6.524993	-2.652348	0.651177	40	1	0	6.594024	-2.520649	0.864832	40	1	0	6.510676	-2.688254	0.555031
41	6	0	7.205346	0.516148	-0.545094	41	6	0	7.124896	0.496767	-0.742376	41	6	0	7.228675	0.527676	-0.476350
42	1	0	7.624323	0.929646	-1.464706	42	1	0	7.465160	0.798392	-1.734939	42	1	0	7.675164	0.982690	-1.362973
43	1	0	7.691336	1.006814	0.306714	43	1	0	7.657302	1.097142	0.004442	43	1	0	7.695289	0.973246	0.410873



7

Initial molecule **7**$^{+}$ E_{EL} = -1562.06478399 a.u.						Radical dication **7**$^{\bullet 2+}$ with 1 e^{-} less E_{EL} = -1561.83107016 a.u.						Radical **7**$^{\bullet}$ with 1 e^{-} more E_{EL} = -1562.17894092 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	-6.027240	1.274820	-0.264659	1	6	0	-5.822221	1.687409	-0.063453	1	6	0	-6.007592	1.373805	0.308557
2	1	0	-6.316102	2.316205	-0.160854	2	1	0	-5.971637	2.744504	0.131267	2	1	0	-6.240176	2.413866	0.522286
3	6	0	-6.959707	0.276841	-0.529134	3	6	0	-6.869865	0.851593	-0.432819	3	6	0	-7.020935	0.415095	0.163284
4	6	0	-6.555751	-1.063209	-0.657962	4	6	0	-6.650965	-0.521929	-0.679426	4	6	0	-6.676125	-0.909263	-0.141227
5	6	0	-5.218175	-1.406367	-0.523800	5	6	0	-5.385016	-1.056438	-0.561844	5	6	0	-5.342008	-1.282016	-0.287182
6	6	0	-4.251293	-0.414101	-0.254345	6	6	0	-4.290039	-0.231737	-0.183760	6	6	0	-4.292295	-0.337384	-0.126717
7	6	0	-4.685985	0.919955	-0.129530	7	6	0	-4.548385	1.143033	0.061978	7	6	0	-4.679919	0.998495	0.157212
8	1	0	-8.008249	0.540525	-0.635608	8	1	0	-7.870058	1.263428	-0.531380	8	1	0	-8.061771	0.705230	0.277717
9	1	0	-7.291287	-1.835183	-0.863444	9	1	0	-7.482811	-1.158587	-0.963443	9	1	0	-7.454151	-1.658808	-0.265754
10	1	0	-4.911271	-2.441545	-0.625152	10	1	0	-5.222918	-2.110396	-0.753811	10	1	0	-5.094475	-2.312329	-0.521104
11	6	0	-2.835395	-0.645573	-0.100483	11	6	0	-2.942008	-0.674133	-0.068030	11	6	0	-2.898463	-0.594961	-0.228755
12	8	0	-3.802452	1.935505	0.135565	12	8	0	-3.552808	1.993476	0.432857	12	8	0	-3.733631	2.000978	0.262278
13	6	0	-2.457796	1.734332	0.301535	13	6	0	-2.257509	1.597653	0.632842	13	6	0	-2.354499	1.766312	0.207740
14	6	0	-1.959218	0.368228	0.165147	14	6	0	-1.911404	0.198899	0.289891	14	6	0	-1.913122	0.427894	-0.017864
15	8	0	-1.771931	2.713249	0.556779	15	8	0	-1.497648	2.415003	1.107933	15	8	0	-1.673616	2.783801	0.401686
16	6	0	-0.499550	0.179081	0.308133	16	6	0	-0.507642	-0.119181	0.325103	16	6	0	-0.489678	0.157251	0.076840
17	17	0	-2.237482	-2.274418	-0.284578	17	17	0	-2.598872	-2.321352	-0.490004	17	17	0	-2.412571	-2.154598	-0.921174
18	7	0	0.395031	0.523756	-0.594987	18	7	0	0.447755	0.784305	-0.041554	18	7	0	0.507441	0.936938	-0.343678
19	6	0	1.617124	0.177012	-0.036479	19	6	0	1.614300	0.137382	0.077301	19	6	0	1.670625	0.264509	-0.026141
20	6	0	1.422172	-0.387758	1.249945	20	6	0	1.406784	-1.203247	0.554274	20	6	0	1.368450	-0.972174	0.607201
21	7	0	0.061647	-0.370303	1.436713	21	7	0	0.046976	-1.319747	0.675112	21	7	0	0.001496	-1.008913	0.657655
22	6	0	2.486176	-0.823018	2.047938	22	6	0	2.458411	-2.076020	0.793835	22	6	0	2.361461	-1.858823	1.035223
23	6	0	2.904576	0.315227	-0.555647	23	6	0	2.926020	0.612486	-0.191945	23	6	0	2.999150	0.625212	-0.246453
24	6	0	3.763216	-0.674800	1.525879	24	6	0	3.738077	-1.585692	0.536855	24	6	0	3.683650	-1.486000	0.815923
25	6	0	3.977950	-0.112914	0.237735	25	6	0	3.974832	-0.255483	0.047308	25	6	0	4.008724	-0.260380	0.177474
26	1	0	2.325725	-1.262406	3.027685	26	1	0	2.306729	-3.089569	1.149114	26	1	0	2.117776	-2.803645	1.512236

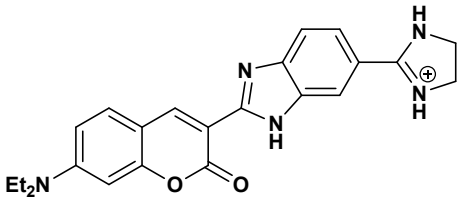
27	1	0	3.059025	0.767650	-1.530899	27	1	0	3.069548	1.630106	-0.540606	27	1	0	3.234852	1.578705	-0.709781
28	1	0	4.609904	-1.021662	2.110319	28	1	0	4.581653	-2.250953	0.693839	28	1	0	4.473750	-2.167390	1.116528
29	6	0	5.343955	0.026466	-0.267825	29	6	0	5.355928	0.189430	-0.199378	29	6	0	5.406744	0.085974	-0.052137
30	7	0	5.669807	0.111321	-1.556673	30	7	0	5.689718	1.154336	-1.047200	30	7	0	5.830448	0.984149	-0.944920
31	6	0	7.133252	0.099391	-1.740978	31	6	0	7.156138	1.284708	-1.159118	31	6	0	7.301358	0.987791	-1.044224
32	6	0	7.634607	0.381891	-0.308840	32	6	0	7.644836	0.441226	0.039544	32	6	0	7.704502	0.234237	0.239109
33	7	0	6.433735	0.087730	0.496540	33	7	0	6.428701	-0.315959	0.397312	33	7	0	6.446301	-0.447594	0.595608
34	1	0	6.386301	0.299163	1.487520	34	1	0	6.376043	-0.894584	1.229230	34	1	0	6.336086	-0.929817	1.480491
35	1	0	8.466608	-0.259809	-0.014255	35	1	0	8.458024	-0.238342	-0.219766	35	1	0	8.506184	-0.487901	0.075447
36	1	0	7.446435	-0.885827	-2.102046	36	1	0	7.482685	0.872052	-2.118602	36	1	0	7.607878	0.453179	-1.949904
37	1	0	5.031153	-0.165031	-2.294573	37	1	0	5.055533	1.508984	-1.755400	37	1	0	5.243909	1.301973	-1.708472
38	1	0	7.917645	1.430501	-0.169872	38	1	0	7.945770	1.061596	0.889445	38	1	0	7.991074	0.917765	1.045584
39	1	0	7.440916	0.862289	-2.457925	39	1	0	7.455516	2.331803	-1.092833	39	1	0	7.687255	2.007991	-1.078374
40	1	0	-0.443591	-0.690355	2.257241	40	1	0	-0.433285	-2.115208	1.086063	40	1	0	-0.556449	-1.734383	1.091510



9

Initial molecule **9**$^{+}$ E_{EL} = -4133.19239989 a.u.						Radical dication **9**$^{\bullet 2+}$ with 1 e^{-} less E_{EL} = -4132.96152522 a.u.						Radical **9**$^{\bullet}$ with 1 e^{-} more E_{EL} = -4133.31649939 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	4.516689	2.233430	-0.303955	1	6	0	4.454576	2.283952	-0.177301	1	6	0	4.444775	2.275372	-0.260273
2	1	0	4.608747	3.300690	-0.478867	2	1	0	4.523157	3.363533	-0.259982	2	1	0	4.485848	3.355809	-0.366297
3	6	0	5.637575	1.431214	-0.136174	3	6	0	5.589127	1.488087	-0.148424	3	6	0	5.618769	1.509153	-0.273466
4	6	0	5.473900	0.056899	0.090744	4	6	0	5.463625	0.087289	-0.035768	4	6	0	5.502679	0.126665	-0.112425
5	6	0	4.220500	-0.527392	0.151326	5	6	0	4.230963	-0.521735	0.042313	5	6	0	4.280363	-0.509046	0.051112
6	6	0	3.072851	0.275396	-0.019214	6	6	0	3.054964	0.273442	0.011229	6	6	0	3.078582	0.252137	0.054074
7	6	0	3.251898	1.651717	-0.241633	7	6	0	3.204818	1.676349	-0.095981	7	6	0	3.217259	1.655712	-0.095647
8	1	0	6.627094	1.873914	-0.181628	8	1	0	6.568510	1.951002	-0.211064	8	1	0	6.584062	1.987110	-0.399098
9	35	0	7.023514	-1.035063	0.320461	9	35	0	7.042431	-0.973555	0.005361	9	35	0	7.098588	-0.940039	-0.120308
10	1	0	4.116459	-1.591295	0.323631	10	1	0	4.152630	-1.597936	0.124014	10	1	0	4.233646	-1.584038	0.170671
11	6	0	1.712234	-0.215310	0.011560	11	6	0	1.728210	-0.255833	0.069513	11	6	0	1.765400	-0.270591	0.196564
12	8	0	2.181423	2.487174	-0.395407	12	8	0	2.126764	2.500168	-0.112824	12	8	0	2.108688	2.474638	-0.047147
13	6	0	0.885239	2.056255	-0.357294	13	6	0	0.843228	2.055337	-0.037887	13	6	0	0.815702	1.990444	0.055724
14	6	0	0.639628	0.618536	-0.189721	14	6	0	0.604851	0.591654	0.023674	14	6	0	0.601274	0.573550	0.128260
15	8	0	0.018463	2.911337	-0.464457	15	8	0	-0.023027	2.912037	-0.031481	15	8	0	-0.045524	2.888438	0.065126
16	6	0	-0.762746	0.178608	-0.251966	16	6	0	-0.762727	0.157561	0.028409	16	6	0	-0.767485	0.108941	0.089309
17	17	0	1.491931	-1.904771	0.355218	17	17	0	1.584608	-1.964440	0.208238	17	17	0	1.639716	-1.977239	0.591316
18	7	0	-1.787589	0.920848	0.277128	18	7	0	-1.829226	1.020505	0.040660	18	7	0	-1.843538	0.975403	0.183656
19	6	0	-2.957312	0.240625	0.031224	19	6	0	-2.970721	0.277573	0.029229	19	6	0	-2.999638	0.238946	0.080886
20	6	0	-2.557187	-0.927206	-0.669369	20	6	0	-2.517270	-1.093927	-0.000473	20	6	0	-2.553968	-1.105941	-0.070055
21	7	0	-1.189626	-0.938186	-0.828620	21	7	0	-1.183808	-1.145208	0.002297	21	7	0	-1.188500	-1.162795	-0.062797
22	1	0	-1.693925	1.836960	0.702067	22	1	0	-1.740970	2.035581	0.054806	22	1	0	-1.732391	1.983250	0.248275
23	6	0	-3.523220	-1.855202	-1.092123	23	6	0	-3.465755	-2.157945	-0.030894	23	6	0	-3.503526	-2.136181	-0.208386
24	6	0	-4.286624	0.520589	0.332562	24	6	0	-4.315263	0.623282	0.034190	24	6	0	-4.339193	0.591749	0.089489
25	6	0	-4.853023	-1.587918	-0.806030	25	6	0	-4.793975	-1.820964	-0.032701	25	6	0	-4.849752	-1.799055	-0.204238

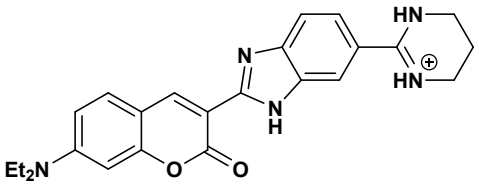
26	6	0	-5.238812	-0.415116	-0.098664	26	6	0	-5.219354	-0.445000	0.002525	26	6	0	-5.281309	-0.452242	-0.058384
27	1	0	-3.235366	-2.757922	-1.623165	27	1	0	-3.135330	-3.191197	-0.046798	27	1	0	-3.189568	-3.171297	-0.312140
28	1	0	-4.565725	1.432115	0.852153	28	1	0	-4.638903	1.658664	0.034157	28	1	0	-4.643231	1.630676	0.173387
29	1	0	-5.608802	-2.306396	-1.107946	29	1	0	-5.543816	-2.605502	-0.035841	29	1	0	-5.586014	-2.593094	-0.289198
30	6	0	-6.654858	-0.175183	0.183824	30	6	0	-6.662560	-0.148784	-0.004214	30	6	0	-6.699770	-0.143241	-0.064820
31	7	0	-7.111060	0.613578	1.156676	31	7	0	-7.203814	0.944823	0.516400	31	7	0	-7.236132	1.007823	0.361705
32	6	0	-8.579727	0.529542	1.269742	32	6	0	-8.678350	0.888854	0.455149	32	6	0	-8.708458	0.936560	0.373613
33	6	0	-8.961603	-0.154555	-0.059627	33	6	0	-8.914932	-0.296840	-0.508130	33	6	0	-8.969221	-0.277676	-0.537150
34	7	0	-7.667103	-0.710700	-0.496496	34	7	0	-7.584846	-0.937726	-0.537897	34	7	0	-7.664641	-0.963306	-0.502176
35	1	0	-7.544560	-1.133521	-1.409897	35	1	0	-7.361024	-1.711400	-1.155775	35	1	0	-7.463469	-1.738738	-1.123288
36	1	0	-9.701697	-0.946802	0.064967	36	1	0	-9.668650	-0.997685	-0.145900	36	1	0	-9.762749	-0.927627	-0.164362
37	1	0	-8.843381	-0.080610	2.139934	37	1	0	-9.073485	0.697573	1.457473	37	1	0	-9.059974	0.765765	1.397304
38	1	0	-6.531226	0.899094	1.938037	38	1	0	-6.704378	1.556573	1.154207	38	1	0	-6.735956	1.629505	0.987248
39	1	0	-9.319430	0.562570	-0.805701	39	1	0	-9.178166	0.032115	-1.518103	39	1	0	-9.198943	0.021964	-1.565832
40	1	0	-9.017836	1.523077	1.378369	40	1	0	-9.081768	1.830048	0.078589	40	1	0	-9.147538	1.859112	-0.009927



13

Initial molecule **13**$^{+}$ E_{EL} = -1236.46805587 a.u.						Radical dication **13**$^{\bullet 2+}$ with 1 e^{-} less E_{EL} = -1236.27314012 a.u.						Radical **13**$^{\bullet}$ with 1 e^{-} more E_{EL} = -1236.57090231 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	5.141020	-0.906029	0.038307	1	6	0	5.131591	-0.912142	0.045127	1	6	0	5.139012	-0.883358	-0.041458
2	1	0	5.399909	-1.956490	0.080558	2	1	0	5.408314	-1.957576	0.087916	2	1	0	5.364912	-1.942668	-0.010310
3	6	0	6.134030	0.111404	0.005013	3	6	0	6.110203	0.129706	0.005761	3	6	0	6.162466	0.097883	-0.087295
4	6	0	5.697904	1.478991	-0.051965	4	6	0	5.669759	1.500883	-0.054666	4	6	0	5.753066	1.458498	-0.100670
5	6	0	4.360293	1.796305	-0.069940	5	6	0	4.334163	1.798662	-0.072119	5	6	0	4.409969	1.811594	-0.097819
6	6	0	3.359732	0.789898	-0.033598	6	6	0	3.349471	0.770284	-0.032431	6	6	0	3.372043	0.843113	-0.070027
7	6	0	3.806975	-0.551312	0.019664	7	6	0	3.801191	-0.575210	0.025395	7	6	0	3.807159	-0.503754	-0.040445
8	7	0	7.456975	-0.200720	0.027488	8	7	0	7.425903	-0.169974	0.025554	8	7	0	7.511479	-0.264104	-0.148294
9	1	0	6.426764	2.279287	-0.081813	9	1	0	6.392081	2.306000	-0.083643	9	1	0	6.490572	2.252467	-0.119041
10	1	0	4.051248	2.837715	-0.112865	10	1	0	4.004741	2.832372	-0.115806	10	1	0	4.138543	2.865297	-0.110500
11	6	0	1.972822	1.033393	-0.046441	11	6	0	1.960622	1.018767	-0.047626	11	6	0	1.984326	1.116002	-0.061903
12	8	0	2.884758	-1.571256	0.057205	12	8	0	2.893326	-1.601564	0.064680	12	8	0	2.872099	-1.532608	0.002102
13	6	0	1.523145	-1.365882	0.047598	13	6	0	1.538013	-1.405109	0.053463	13	6	0	1.501728	-1.305106	0.007115
14	6	0	1.051352	0.001450	-0.007875	14	6	0	1.052073	-0.019609	-0.008521	14	6	0	1.036898	0.044301	-0.026342
15	8	0	0.828011	-2.383291	0.087726	15	8	0	0.836529	-2.403763	0.096369	15	8	0	0.815335	-2.345791	0.041605
16	6	0	-0.379243	0.276793	-0.020700	16	6	0	-0.374618	0.242673	-0.023315	16	6	0	-0.371783	0.295027	-0.024311
17	1	0	1.617028	2.059241	-0.087257	17	1	0	1.604137	2.043127	-0.091343	17	1	0	1.632022	2.141625	-0.083374
18	7	0	-1.334814	-0.705903	0.016074	18	7	0	-1.336512	-0.734427	0.007638	18	7	0	-1.339119	-0.694556	0.009444
19	6	0	-2.567078	-0.089594	-0.012683	19	6	0	-2.557055	-0.108293	-0.019698	19	6	0	-2.575869	-0.087750	-0.005745
20	6	0	-2.273182	1.300906	-0.064072	20	6	0	-2.254307	1.282913	-0.065154	20	6	0	-2.286270	1.311161	-0.044677
21	7	0	-0.912962	1.499376	-0.069062	21	7	0	-0.898974	1.471165	-0.068049	21	7	0	-0.939060	1.523896	-0.055743
22	1	0	-1.121216	-1.698844	0.054717	22	1	0	-1.141241	-1.731404	0.045326	22	1	0	-1.113489	-1.684013	0.034260
23	6	0	-3.324105	2.232394	-0.097661	23	6	0	-3.298691	2.226503	-0.095111	23	6	0	-3.352938	2.232651	-0.063563
24	6	0	-3.863806	-0.585004	0.008130	24	6	0	-3.861701	-0.595286	-0.001557	24	6	0	-3.865166	-0.588227	0.016204
25	6	0	-4.626021	1.753695	-0.072796	25	6	0	-4.599150	1.755773	-0.072236	25	6	0	-4.651526	1.745465	-0.038622

26	6	0	-4.905160	0.360891	-0.019746	26	6	0	-4.886090	0.359838	-0.025192	26	6	0	-4.930515	0.351232	0.000799
27	1	0	-3.122418	3.298669	-0.147681	27	1	0	-3.086880	3.290643	-0.139782	27	1	0	-3.161177	3.301561	-0.104645
28	1	0	-4.056208	-1.651837	0.071804	28	1	0	-4.064181	-1.660279	0.056010	28	1	0	-4.045073	-1.657668	0.072022
29	1	0	-5.445439	2.464355	-0.120823	29	1	0	-5.416844	2.468227	-0.115466	29	1	0	-5.470975	2.457542	-0.076906
30	6	0	-6.291480	-0.097354	0.005565	30	6	0	-6.281861	-0.085951	0.002658	30	6	0	-6.299756	-0.111187	0.019444
31	7	0	-6.691712	-1.326381	-0.325713	31	7	0	-6.698507	-1.292761	-0.375776	31	7	0	-6.686684	-1.380413	-0.196413
32	6	0	-8.162825	-1.425922	-0.342169	32	6	0	-8.171141	-1.381145	-0.360937	32	6	0	-8.153862	-1.477251	-0.290553
33	6	0	-8.573997	-0.150595	0.422452	33	6	0	-8.556911	-0.125118	0.450075	33	6	0	-8.593119	-0.168696	0.388445
34	7	0	-7.337412	0.650931	0.361614	34	7	0	-7.307475	0.658584	0.410201	34	7	0	-7.379000	0.655944	0.256168
35	1	0	-7.232281	1.511225	0.887915	35	1	0	-7.183452	1.504412	0.956096	35	1	0	-7.300500	1.539916	0.745353
36	1	0	-9.403978	0.379251	-0.047939	36	1	0	-9.379480	0.435303	0.002762	36	1	0	-9.443658	0.303827	-0.106030
37	1	0	-8.517684	-1.418714	-1.378128	37	1	0	-8.547823	-1.342698	-1.388143	37	1	0	-8.456064	-1.513706	-1.343664
38	1	0	-6.106838	-1.957275	-0.862486	38	1	0	-6.127201	-1.910611	-0.942148	38	1	0	-6.091639	-2.036043	-0.690022
39	1	0	-8.822434	-0.358538	1.468609	39	1	0	-8.802717	-0.363193	1.490051	39	1	0	-8.826569	-0.316447	1.449383
40	1	0	-8.496194	-2.342190	0.148103	40	1	0	-8.498705	-2.309183	0.110593	40	1	0	-8.521627	-2.368124	0.221694
41	6	0	8.473837	0.850972	-0.004720	41	6	0	8.446066	0.887101	-0.035619	41	6	0	8.510655	0.746245	0.191022
42	6	0	7.881882	-1.598719	0.075566	42	6	0	7.881540	-1.564979	0.103105	42	6	0	7.873793	-1.633303	0.207431
43	1	0	9.460314	0.388983	0.038624	43	1	0	9.431220	0.425833	-0.030166	43	1	0	9.504795	0.309966	0.070914
44	1	0	8.410901	1.441488	-0.927500	44	1	0	8.327904	1.472131	-0.952941	44	1	0	8.446269	1.605784	-0.482813
45	1	0	8.374652	1.528748	0.852154	45	1	0	8.354099	1.549813	0.830883	45	1	0	8.411413	1.108722	1.228490
46	1	0	8.971008	-1.639110	0.085051	46	1	0	8.968153	-1.578931	0.146445	46	1	0	8.950793	-1.757819	0.073786
47	1	0	7.509928	-2.096874	0.980064	47	1	0	7.479866	-2.043299	1.001588	47	1	0	7.620428	-1.881780	1.252438
48	1	0	7.523689	-2.153921	-0.800955	48	1	0	7.549133	-2.117730	-0.782022	48	1	0	7.376362	-2.353877	-0.449006



14

Initial molecule **14**$^{+}$ E_{EL} = -1275.79265411 a.u.						qRadical dication **14**$^{\bullet 2+}$ with 1 e^{-} less E_{EL} = -1275.59845285 a.u.						Radical **14**$^{\bullet}$ with 1 e^{-} more E_{EL} = -1275.89388715 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	5.458909	-0.938603	0.076883	1	6	0	5.447020	-0.944627	0.078998	1	6	0	5.457314	-0.916775	-0.011390
2	1	0	5.699234	-1.991922	0.148359	2	1	0	5.705584	-1.993329	0.148794	2	1	0	5.663744	-1.979252	0.041777
3	6	0	6.469499	0.059967	0.022589	3	6	0	6.443878	0.079315	0.030161	3	6	0	6.499645	0.043779	-0.078764
4	6	0	6.057692	1.432689	-0.073946	4	6	0	6.027560	1.456582	-0.061617	4	6	0	6.115476	1.409820	-0.122436
5	6	0	4.725674	1.772800	-0.107305	5	6	0	4.697653	1.776780	-0.098657	5	6	0	4.777919	1.787568	-0.127308
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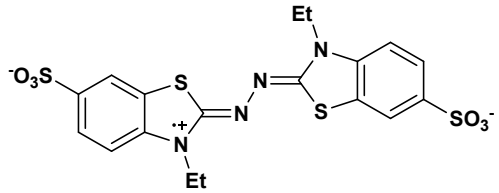
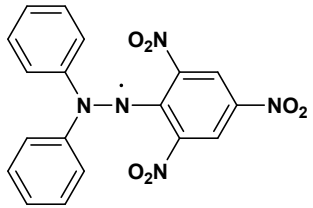
7	6	0	4.131218	-0.561205	0.040539	7	6	0	4.123218	-0.585302	0.041396	7	6	0	4.132238	-0.514350	-0.018120
8	7	0	7.786960	-0.274294	0.061979	8	7	0	7.753332	-0.242946	0.070981	8	7	0	7.843379	-0.346772	-0.133630
9	1	0	6.801081	2.218708	-0.122105	9	1	0	6.765309	2.247187	-0.105053	9	1	0	6.866900	2.190057	-0.158214
10	1	0	4.435418	2.818017	-0.179694	10	1	0	4.386426	2.814734	-0.168905	10	1	0	4.526600	2.845823	-0.163233
11	6	0	2.324571	1.052185	-0.075307	11	6	0	2.311112	1.037702	-0.078956	11	6	0	2.338731	1.138245	-0.076241
12	8	0	3.191174	-1.563632	0.097590	12	8	0	3.197625	-1.595031	0.095463	12	8	0	3.180077	-1.526687	0.047843
13	6	0	1.833302	-1.335326	0.073433	13	6	0	1.846054	-1.376214	0.070363	13	6	0	1.809639	-1.272305	0.043791
14	6	0	1.385117	0.038268	-0.016016	14	6	0	1.383699	0.015608	-0.025256	14	6	0	1.372824	0.079130	-0.019356
15	8	0	1.121286	-2.340267	0.131719	15	8	0	1.128157	-2.362381	0.130190	15	8	0	1.107234	-2.305498	0.098562
16	6	0	-0.041762	0.337411	-0.043540	16	6	0	-0.037560	0.300059	-0.059447	16	6	0	-0.033658	0.359463	-0.030767
17	1	0	1.987147	2.082825	-0.143674	17	1	0	1.972160	2.066720	-0.147342	17	1	0	2.002732	2.168494	-0.120772
18	7	0	-1.012598	-0.631697	-0.004914	18	7	0	-1.015111	-0.662482	-0.016121	18	7	0	-1.014496	-0.615760	0.016412
19	6	0	-2.234950	0.001478	-0.053046	19	6	0	-2.225266	-0.019965	-0.068453	19	6	0	-2.241528	0.007473	-0.026794
20	6	0	-1.922238	1.386019	-0.115425	20	6	0	-1.902818	1.365209	-0.141107	20	6	0	-1.935304	1.399189	-0.091257
21	7	0	-0.556449	1.565396	-0.110435	21	7	0	-0.543798	1.534236	-0.136494	21	7	0	-0.578445	1.593085	-0.093316
22	1	0	-0.814002	-1.626836	0.050160	22	1	0	-0.835283	-1.660944	0.047445	22	1	0	-0.799912	-1.607382	0.061653
23	6	0	-2.960183	2.329647	-0.165017	23	6	0	-2.934212	2.321426	-0.198022	23	6	0	-2.987276	2.330365	-0.139900
24	6	0	-3.540533	-0.477267	-0.039927	24	6	0	-3.538482	-0.488746	-0.049566	24	6	0	-3.540618	-0.477435	-0.009165
25	6	0	-4.270544	1.867484	-0.145174	25	6	0	-4.242416	1.868345	-0.171299	25	6	0	-4.296498	1.858113	-0.119747
26	6	0	-4.566905	0.480160	-0.084941	26	6	0	-4.547356	0.478205	-0.097667	26	6	0	-4.587072	0.472064	-0.056190

27	1	0	-2.745115	3.392941	-0.225273	27	1	0	-2.708115	3.381477	-0.266649	27	1	0	-2.783485	3.396005	-0.205081
28	1	0	-3.749688	-1.540654	0.033064	28	1	0	-3.759579	-1.548884	0.029051	28	1	0	-3.738516	-1.542454	0.073890
29	1	0	-5.082822	2.586034	-0.207132	29	1	0	-5.053389	2.588027	-0.233737	29	1	0	-5.110812	2.573728	-0.192436
30	6	0	-5.975563	0.034618	-0.068908	30	6	0	-5.964461	0.046652	-0.065141	30	6	0	-5.984222	0.016770	-0.055338
31	7	0	-6.327906	-1.073885	-0.712469	31	7	0	-6.342419	-1.027534	-0.747369	31	7	0	-6.309174	-1.142070	-0.628988
32	6	0	-7.683097	-1.647697	-0.698540	32	6	0	-7.707007	-1.580019	-0.729024	32	6	0	-7.657384	-1.729256	-0.623807
33	6	0	-8.449362	-1.142205	0.519989	33	6	0	-8.432937	-1.126815	0.534065	33	6	0	-8.477984	-1.142707	0.520487
34	7	0	-6.890168	0.739098	0.590720	34	7	0	-6.848291	0.732978	0.649552	34	7	0	-6.936027	0.753554	0.519280
35	1	0	-6.573026	1.515960	1.159485	35	1	0	-6.505965	1.488458	1.233155	35	1	0	-6.650336	1.559598	1.062488
36	1	0	-9.504520	-1.414779	0.424260	36	1	0	-9.494094	-1.379812	0.453210	36	1	0	-9.526165	-1.433701	0.402932
37	1	0	-8.192385	-1.367289	-1.628016	37	1	0	-8.232972	-1.242476	-1.629570	37	1	0	-8.134138	-1.526470	-1.590443
38	1	0	-5.627951	-1.523941	-1.292031	38	1	0	-5.658698	-1.466334	-1.354691	38	1	0	-5.591519	-1.616705	-1.164885
39	1	0	-8.058388	-1.611761	1.430336	39	1	0	-8.025157	-1.648247	1.408027	39	1	0	-8.121252	-1.536565	1.479604
40	1	0	-7.579225	-2.735919	-0.681078	40	1	0	-7.620250	-2.668869	-0.771283	40	1	0	-7.546267	-2.812272	-0.519981
41	6	0	-8.314628	0.374996	0.628649	41	6	0	-8.275455	0.380915	0.717843	41	6	0	-8.357315	0.379550	0.516628
42	1	0	-8.721669	0.748622	1.570446	42	1	0	-8.645706	0.708564	1.691352	42	1	0	-8.812705	0.821031	1.405592
43	1	0	-8.835458	0.877000	-0.195579	43	1	0	-8.815706	0.932183	-0.060920	43	1	0	-8.843752	0.809023	-0.367994
44	6	0	8.821532	0.758659	0.007092	44	6	0	8.792347	0.796746	0.037084	44	6	0	8.859934	0.655801	0.175191
45	6	0	8.187472	-1.677066	0.155452	45	6	0	8.182004	-1.646597	0.146804	45	6	0	8.179497	-1.705872	0.282735
46	1	0	9.799598	0.280958	0.066602	46	1	0	9.767891	0.322391	0.119655	46	1	0	9.846649	0.201243	0.060610
47	1	0	8.772475	1.325924	-0.931003	47	1	0	8.740604	1.350582	-0.905944	47	1	0	8.804895	1.498896	-0.519847
48	1	0	8.730859	1.460389	0.845540	48	1	0	8.659731	1.490959	0.872225	48	1	0	8.772694	1.046323	1.203803
49	1	0	9.275702	-1.735543	0.173286	49	1	0	9.268894	-1.683907	0.157529	49	1	0	9.254291	-1.856076	0.157583
50	1	0	7.801731	-2.141072	1.072342	50	1	0	7.797110	-2.108871	1.061483	50	1	0	7.919921	-1.903363	1.337209
51	1	0	7.825113	-2.253257	-0.705706	51	1	0	7.812447	-2.200090	-0.722351	51	1	0	7.670550	-2.445905	-0.342300



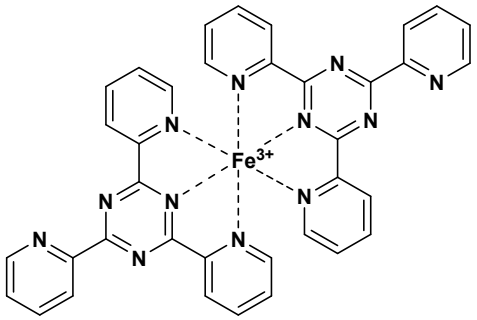
ABTS$^{\bullet+}$ E_{EL} = -2880.16908174 a.u.						**ABTS$^{\bullet\bullet 2+}$** with 1 e$^-$ less E_{EL} = -2879.96703429 a.u.						**ABTS$^{\bullet\bullet}$** with 1 e$^-$ more E_{EL} = -2880.33842044 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	-5.326192	0.752660	0.012284	1	6	0	5.334174	-0.770373	-0.018729	1	6	0	5.328448	-0.732493	-0.017806
2	1	0	-5.494036	1.824222	0.017189	2	1	0	5.511688	-1.840223	-0.031595	2	1	0	5.486274	-1.806202	-0.011641
3	6	0	-6.396049	-0.138842	0.011807	3	6	0	6.387804	0.132537	-0.005936	3	6	0	6.416036	0.150564	-0.012223
4	6	0	-6.194735	-1.532199	0.006578	4	6	0	6.177744	1.533002	0.008955	4	6	0	6.219379	1.536758	-0.023201
5	6	0	-4.911801	-2.064697	0.003773	5	6	0	4.900627	2.061008	0.010584	5	6	0	4.930111	2.072980	-0.045222
6	6	0	-3.828141	-1.175597	0.004763	6	6	0	3.822394	1.158603	-0.001174	6	6	0	3.837982	1.197964	-0.052143
7	6	0	-4.039138	0.215777	0.008820	7	6	0	4.042392	-0.239339	-0.015299	7	6	0	4.047745	-0.194604	-0.039390
8	16	0	-8.093079	0.494354	-0.003985	8	16	0	8.096200	-0.482103	0.009171	8	16	0	8.093542	-0.506849	0.093202
9	1	0	-7.047269	-2.204346	0.007498	9	1	0	7.029935	2.205145	0.017313	9	1	0	7.072847	2.207564	-0.021041
10	1	0	-4.757627	-3.138216	0.001549	10	1	0	4.737376	3.132670	0.020619	10	1	0	4.785522	3.148290	-0.058674
11	7	0	-2.478950	-1.514327	0.002346	11	7	0	2.477531	1.477456	0.000161	11	7	0	2.495829	1.552896	-0.074246
12	16	0	-2.510356	1.088386	0.008943	12	16	0	2.531277	-1.112228	-0.025592	12	16	0	2.506351	-1.070984	-0.056244
13	8	0	-8.661640	0.073352	-1.324117	13	8	0	8.748690	0.176513	-1.162461	13	8	0	8.948746	0.407239	-0.729970
14	8	0	-8.774253	-0.164775	1.154581	14	8	0	8.648808	-0.027755	1.321711	14	8	0	8.462623	-0.476065	1.548634
15	8	0	-7.981024	1.977175	0.141975	15	8	0	7.995630	-1.964545	-0.115991	15	8	0	8.030140	-1.900534	-0.451944
16	6	0	-1.645364	-0.446772	0.003003	16	6	0	1.675926	0.401802	-0.009430	16	6	0	1.619719	0.486696	-0.073074
17	7	0	-0.324077	-0.582350	-0.000429	17	7	0	0.321983	0.550631	-0.006931	17	7	0	0.333883	0.610414	-0.082383
18	7	0	0.324102	0.582407	0.000841	18	7	0	-0.321989	-0.550683	-0.006952	18	7	0	-0.333901	-0.610423	-0.082295
19	6	0	1.645387	0.446837	-0.002650	19	6	0	-1.675926	-0.401837	-0.009458	19	6	0	-1.619735	-0.486706	-0.072918
20	16	0	2.510365	-1.088354	-0.008648	20	16	0	-2.531264	1.112200	-0.025637	20	16	0	-2.506373	1.070963	-0.056072
21	6	0	4.039151	-0.215751	-0.008641	21	6	0	-4.042386	0.239329	-0.015347	21	6	0	-4.047771	0.194581	-0.039257
22	6	0	3.828166	1.175622	-0.004517	22	6	0	-3.822402	-1.158617	-0.001232	22	6	0	-3.837989	-1.198003	-0.052014
23	7	0	2.478978	1.514367	-0.002015	23	7	0	-2.477544	-1.477483	0.000113	23	7	0	-2.495835	-1.552912	-0.073983
24	6	0	5.326199	-0.752644	-0.012192	24	6	0	-5.334162	0.770380	-0.018754	24	6	0	-5.328460	0.732458	-0.017712
25	6	0	4.911839	2.064707	-0.003513	25	6	0	-4.900648	-2.061010	0.010521	25	6	0	-4.930103	-2.073016	-0.045275
26	6	0	6.194762	1.532200	-0.006406	26	6	0	-6.177757	-1.532987	0.008924	26	6	0	-6.219388	-1.536796	-0.023306
27	6	0	6.396057	0.138838	-0.011739	27	6	0	-6.387800	-0.132518	-0.005937	27	6	0	-6.416061	-0.150628	-0.012232

28	1	0	5.494018	-1.824205	-0.017152	28	1	0	-5.511669	1.840231	-0.031610	28	1	0	-5.486305	1.806163	-0.011563
29	16	0	8.093065	-0.494397	0.003480	29	16	0	-8.096191	0.482138	0.009200	29	16	0	-8.093520	0.506878	0.093156
30	1	0	7.047303	2.204325	-0.007289	30	1	0	-7.029958	-2.205119	0.017286	30	1	0	-7.072848	-2.207614	-0.021273
31	1	0	4.757680	3.138222	-0.001234	31	1	0	-4.737414	-3.132675	0.020538	31	1	0	-4.785520	-3.148325	-0.058854
32	8	0	8.773547	0.164122	-1.155844	32	8	0	-8.748619	-0.176174	-1.162643	32	8	0	-8.948916	-0.407625	-0.729337
33	8	0	8.662357	-0.072796	1.323062	33	8	0	-8.648883	0.027455	1.321581	33	8	0	-8.462300	0.476937	1.548692
34	8	0	7.980836	-1.977290	-0.141676	34	8	0	-7.995594	1.964611	-0.115597	34	8	0	-8.030156	1.900278	-0.452773
35	6	0	-2.015674	-2.908111	-0.000481	35	6	0	1.995681	2.872729	0.014903	35	6	0	2.050000	2.944014	-0.083683
36	1	0	-0.928034	-2.917341	-0.002586	36	1	0	0.908904	2.872933	0.011869	36	1	0	0.961737	2.962267	-0.115499
37	1	0	-2.390486	-3.411061	0.894835	37	1	0	2.373708	3.356501	0.918114	37	1	0	2.394093	3.455865	0.821461
38	1	0	-2.393911	-3.408769	-0.895607	38	1	0	2.378851	3.376797	-0.874943	38	1	0	2.445868	3.458482	-0.965549
39	6	0	2.015701	2.908152	0.001074	39	6	0	-1.995712	-2.872763	0.014959	39	6	0	-2.050036	-2.944035	-0.083638
40	1	0	2.394120	3.408703	0.896182	40	1	0	-2.373803	-3.356471	0.918179	40	1	0	-2.395814	-3.456513	0.820495
41	1	0	2.390322	3.411211	-0.894262	41	1	0	-2.378843	-3.376879	-0.874875	41	1	0	-2.444332	-3.457875	-0.966593
42	1	0	0.928062	2.917376	0.003411	42	1	0	-0.908935	-2.872981	0.011995	42	1	0	-0.961718	-2.962307	-0.113438



Initial molecule **DPPH•** E_{EL} = -1417.95271530 a.u.						Radical cation **DPPH$^{\bullet\bullet+}$** with 1 e$^-$ less E_{EL} = -1417.76345342 a.u.						Radical anion **DPPH$^{\bullet\bullet-}$** with 1 e$^-$ more E_{EL} = -1418.12281440 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**						**Cartesian Coordinates**					
1	6	0	2.592565	-0.748387	0.968872	1	6	0	2.711414	0.646761	-1.083335	1	6	0	2.556176	0.752683	-0.714249
2	1	0	2.931042	-1.588263	1.562909	2	1	0	3.140044	1.439510	-1.684506	2	1	0	2.958967	1.647362	-1.172741
3	6	0	3.508677	0.095709	0.347703	3	6	0	3.512858	-0.188849	-0.318056	3	6	0	3.395871	-0.113299	0.000740
4	6	0	3.084256	1.234599	-0.345258	4	6	0	2.985619	-1.238463	0.420194	4	6	0	2.949353	-1.407293	0.362837
5	6	0	1.731246	1.466983	-0.460516	5	6	0	1.608768	-1.416751	0.414269	5	6	0	1.636694	-1.744842	0.166329
6	6	0	0.714036	0.629908	0.111152	6	6	0	0.731396	-0.577551	-0.308511	6	6	0	0.624856	-0.759074	-0.250714
7	6	0	1.236843	-0.468460	0.882108	7	6	0	1.339306	0.431161	-1.092285	7	6	0	1.235222	0.406528	-0.916797
8	7	0	4.920616	-0.190694	0.448024	8	7	0	4.965302	0.035732	-0.304913	8	7	0	4.746323	0.249246	0.224802
9	1	0	3.798963	1.898807	-0.815723	9	1	0	3.619872	-1.897668	1.000111	9	1	0	3.651250	-2.138241	0.743187
10	7	0	1.348854	2.617165	-1.286836	10	7	0	1.070556	-2.519018	1.218113	10	7	0	1.267522	-3.114501	0.428509
11	7	0	-0.564901	1.023271	-0.063372	11	7	0	-0.626761	-0.918641	-0.378741	11	7	0	-0.604820	-0.970970	0.141406
12	7	0	0.386261	-1.249103	1.770863	12	7	0	0.553190	1.263790	-2.014800	12	7	0	0.523269	1.096402	-1.939362
13	8	0	0.720257	-2.410398	2.033220	13	8	0	1.027687	2.344546	-2.352775	13	8	0	0.940805	2.201451	-2.356612
14	8	0	-0.603128	-0.695630	2.263181	14	8	0	-0.522402	0.817370	-2.416233	14	8	0	-0.491767	0.549293	-2.415281
15	8	0	0.443994	2.483166	-2.110556	15	8	0	-0.131869	-2.500737	1.490916	15	8	0	0.327550	-3.612374	-0.207681
16	8	0	1.989374	3.661158	-1.130589	16	8	0	1.848205	-3.401918	1.573292	16	8	0	1.916553	-3.759510	1.273954
17	8	0	5.718692	0.597597	-0.078155	17	8	0	5.658698	-0.736779	0.355416	17	8	0	5.514999	-0.575801	0.767792
18	8	0	5.275319	-1.212060	1.052794	18	8	0	5.404002	0.984966	-0.953226	18	8	0	5.138189	1.388377	-0.113971
19	7	0	-1.573459	0.158150	-0.120522	19	7	0	-1.553409	-0.172833	0.045952	19	7	0	-1.572710	-0.000933	0.058036
20	6	0	-2.849911	0.674799	0.235955	20	6	0	-2.886929	-0.564706	-0.286956	20	6	0	-2.895900	-0.508277	0.055458
21	6	0	-1.441822	-1.140124	-0.732744	21	6	0	-1.354922	1.029294	0.838557	21	6	0	-1.306333	1.342232	0.495887
22	6	0	-2.931119	1.642260	1.251544	22	6	0	-3.111081	-1.260813	-1.487592	22	6	0	-3.157143	-1.730140	-0.593135
23	6	0	-4.173073	2.172940	1.593910	23	6	0	-4.405438	-1.663937	-1.789502	23	6	0	-4.449932	-2.256314	-0.606891
24	6	0	-5.332316	1.746795	0.934269	24	6	0	-5.456038	-1.386704	-0.902444	24	6	0	-5.506158	-1.574698	0.007578
25	6	0	-5.242603	0.784028	-0.077674	25	6	0	-5.215684	-0.699151	0.292900	25	6	0	-5.246956	-0.357420	0.646695
26	6	0	-4.007677	0.243948	-0.433554	26	6	0	-3.929172	-0.275136	0.610937	26	6	0	-3.956114	0.174381	0.679966
27	1	0	-2.032496	1.956255	1.771257	27	1	0	-2.292548	-1.446617	-2.173906	27	1	0	-2.347740	-2.255162	-1.089042

28	1	0	-4.236063	2.914467	2.385879	28	1	0	-4.601125	-2.183659	-2.722637	28	1	0	-4.631269	-3.201237	-1.114112
29	1	0	-6.298787	2.162387	1.206735	29	1	0	-6.465464	-1.705616	-1.146945	29	1	0	-6.513205	-1.983424	-0.012640
30	1	0	-6.136213	0.457832	-0.602955	30	1	0	-6.029512	-0.499112	0.983107	30	1	0	-6.052501	0.183447	1.138171
31	1	0	-3.943615	-0.483593	-1.235443	31	1	0	-3.732613	0.231554	1.549217	31	1	0	-3.777997	1.110374	1.198225
32	6	0	-2.050403	-2.254100	-0.139220	32	6	0	-1.976943	2.209601	0.407669	32	6	0	-1.823795	2.428305	-0.222191
33	6	0	-1.923895	-3.503144	-0.747277	33	6	0	-1.773473	3.372196	1.147621	33	6	0	-1.597916	3.731417	0.225925
34	6	0	-1.198980	-3.640385	-1.936208	34	6	0	-0.992755	3.340390	2.308844	34	6	0	-0.842849	3.960679	1.381490
35	6	0	-0.601639	-2.519912	-2.524093	35	6	0	-0.404811	2.144289	2.736663	35	6	0	-0.323511	2.874906	2.094568
36	6	0	-0.720875	-1.264053	-1.928691	36	6	0	-0.573449	0.974165	1.999292	36	6	0	-0.559502	1.568112	1.661372
37	1	0	-2.600630	-2.146439	0.790069	37	1	0	-2.575783	2.219894	-0.496866	37	1	0	-2.396495	2.249783	-1.127364
38	1	0	-2.386699	-4.370468	-0.284466	38	1	0	-2.228081	4.301139	0.816665	38	1	0	-2.002048	4.568312	-0.338279
39	1	0	-1.102417	-4.616242	-2.404608	39	1	0	-0.848740	4.248664	2.887346	39	1	0	-0.659954	4.976606	1.722455
40	1	0	-0.050669	-2.618348	-3.455477	40	1	0	0.178326	2.116575	3.652296	40	1	0	0.258712	3.041780	2.997578
41	1	0	-0.279948	-0.389006	-2.396117	41	1	0	-0.153084	0.037762	2.348128	41	1	0	-0.167836	0.726885	2.225987



Initial molecule **FRAP** E_{EL} = -3306.72258380 a.u.						Radical anion **FRAP**$^{\bullet-}$ with 1 e^- more E_{EL} = -3306.92783800 a.u.					
Cartesian Coordinates						**Cartesian Coordinates**					
1	26	0	-0.000540	0.079091	0.000185	1	26	0	-0.000045	0.005916	0.016362
2	7	0	1.895039	0.030893	-0.038008	2	7	0	-1.891677	0.000940	0.009560
3	7	0	0.426122	1.511123	1.344768	3	7	0	-0.361507	-1.472497	-1.339129
4	7	0	0.288024	-1.296876	-1.463075	4	7	0	-0.378659	1.481924	1.367450
5	6	0	1.606424	-1.591601	-1.694382	5	7	0	0.369636	1.360556	-1.460868
6	6	0	2.537673	-0.809005	-0.865267	6	7	0	0.370376	-1.344674	1.494845
7	6	0	1.761811	1.696800	1.583116	7	7	0	1.891437	0.008789	0.017614
8	6	0	-0.462262	2.253012	2.017470	8	6	0	-2.589190	0.848692	0.782510
9	1	0	-1.510801	2.089659	1.796417	9	6	0	-2.578234	-0.846219	-0.773278
10	6	0	2.618580	0.830716	0.761332	10	6	0	-1.689093	-1.711987	-1.564342
11	6	0	2.000941	-2.536229	-2.629194	11	6	0	-1.709007	1.715693	1.582421
12	1	0	3.056508	-2.736757	-2.778533	12	6	0	2.584101	-0.771151	0.862806
13	6	0	2.226865	2.621898	2.506701	13	6	0	2.582945	0.782453	-0.834135
14	1	0	3.294314	2.734932	2.663283	14	6	0	1.699520	-1.563805	1.731842
15	6	0	-0.062236	3.201379	2.962843	15	6	0	1.698443	1.579624	-1.699003
16	1	0	-0.819884	3.776815	3.484349	16	6	0	0.533272	-2.208921	-2.012130
17	6	0	-0.649578	-1.942484	-2.167623	17	6	0	0.158004	-3.198159	-2.924773
18	1	0	-1.683317	-1.689632	-1.965521	18	6	0	-1.195143	-3.438511	-3.151743
19	6	0	-0.322399	-2.907536	-3.124381	19	6	0	-2.138486	-2.679702	-2.456563
20	1	0	-1.120485	-3.402422	-3.667580	20	1	0	1.580239	-2.002770	-1.817843
21	6	0	1.014762	-3.209313	-3.358762	21	1	0	0.927464	-3.762492	-3.441903
22	1	0	1.294853	-3.954086	-4.097041	22	1	0	-1.514432	-4.200663	-3.856139
23	6	0	1.294203	3.387241	3.213071	23	1	0	-3.203746	-2.828181	-2.597745

24	1	0	1.628215	4.117791	3.943117	24	6	0	0.507859	2.220923	2.048293
25	7	0	-1.895289	0.032061	0.039069	25	6	0	0.121289	3.207320	2.959385
26	7	0	-0.426416	1.518379	-1.336921	26	6	0	-1.234624	3.441844	3.175989
27	7	0	-0.287213	-1.307359	1.453996	27	6	0	-2.169539	2.680534	2.472080
28	6	0	-1.605870	-1.602742	1.683867	28	1	0	1.556900	2.018286	1.861825
29	6	0	-2.537439	-0.813894	0.860568	29	1	0	0.884274	3.773915	3.483611
30	6	0	-1.762196	1.707774	-1.571911	30	1	0	-1.562585	4.201470	3.879129
31	6	0	0.461980	2.264034	-2.005358	31	1	0	-3.236643	2.823826	2.604558
32	1	0	1.510610	2.097413	-1.787310	32	6	0	2.152929	2.470478	-2.665575
33	6	0	-2.618871	0.836247	-0.755932	33	6	0	1.213523	3.171235	-3.424216
34	6	0	-2.000554	-2.554077	2.611692	34	6	0	-0.140888	2.950509	-3.185224
35	1	0	-3.056157	-2.755366	2.759823	35	6	0	-0.521220	2.038465	-2.197342
36	6	0	-2.227341	2.641036	-2.487194	36	1	0	3.218991	2.606549	-2.813133
37	1	0	-3.294874	2.757099	-2.641000	37	1	0	1.536815	3.874993	-4.185272
38	6	0	0.061859	3.220728	-2.942303	38	1	0	-0.907423	3.472396	-3.749160
39	1	0	0.819502	3.799307	-3.460328	39	1	0	-1.569051	1.848885	-1.991517
40	6	0	0.650156	-1.958049	2.153944	40	6	0	2.155172	-2.451786	2.700510
41	1	0	1.684076	-1.704633	1.953513	41	6	0	1.216468	-3.149516	3.462753
42	6	0	0.322754	-2.929804	3.103914	42	6	0	-0.138217	-2.929012	3.224851
43	1	0	1.120686	-3.428863	3.643509	43	6	0	-0.519873	-2.020054	2.234595
44	6	0	-1.014439	-3.233019	3.336025	44	1	0	3.221554	-2.587383	2.846299
45	1	0	-1.294677	-3.983470	4.068480	45	1	0	1.540566	-3.850746	4.225792
46	6	0	-1.294680	3.410954	-3.188516	46	1	0	-0.904092	-3.448255	3.792135
47	1	0	-1.628767	4.148399	-3.911562	47	1	0	-1.568066	-1.830443	2.030506
48	7	0	-3.939871	0.810831	-0.772937	48	7	0	3.908184	0.804706	-0.870941
49	7	0	-3.854586	-0.900452	0.900620	49	7	0	3.909875	-0.807573	0.891868
50	6	0	-4.526155	-0.076792	0.063349	50	6	0	4.537300	-0.006289	0.007132
51	6	0	-6.006442	-0.141664	0.054018	51	6	0	6.025215	-0.006661	-0.017127
52	7	0	-6.580211	-1.030626	0.890306	52	7	0	6.650231	-0.839991	0.837741
53	6	0	-7.911545	-1.109732	0.895798	53	6	0	7.985772	-0.857897	0.830784
54	6	0	-8.736004	-0.320132	0.081405	54	6	0	8.765248	-0.058577	-0.014210
55	6	0	-8.138115	0.596553	-0.779457	55	6	0	8.114560	0.801838	-0.895859
56	6	0	-6.745795	0.691617	-0.797399	56	6	0	6.719540	0.831271	-0.901156
57	1	0	-8.347973	-1.834710	1.579375	57	1	0	8.460353	-1.541762	1.531457
58	1	0	-9.815225	-0.430905	0.130502	58	1	0	9.849020	-0.116953	0.026011
59	1	0	-8.738910	1.228270	-1.427445	59	1	0	8.678170	1.440867	-1.569983
60	1	0	-6.244076	1.392177	-1.454374	60	1	0	6.179766	1.487469	-1.573591
61	7	0	3.939645	0.806386	0.777486	61	7	0	-3.903289	-0.877545	-0.809067

62	7	0	3.854891	-0.894797	-0.906066	62	7	0	-3.915088	0.882449	0.806119
63	6	0	4.526292	-0.076049	-0.063806	63	6	0	-4.537343	0.002715	-0.004488
64	6	0	6.006673	-0.141010	-0.054273	64	6	0	-6.025086	-0.010491	-0.025771
65	7	0	6.580767	-1.024326	-0.896261	65	7	0	-6.655692	0.879860	0.764971
66	6	0	7.912148	-1.103013	-0.902174	66	6	0	-7.991381	0.884217	0.761901
67	6	0	8.736297	-0.318600	-0.082505	67	6	0	-8.765429	0.015379	-0.016861
68	6	0	8.138044	0.592182	0.784359	68	6	0	-8.108937	-0.903333	-0.832983
69	6	0	6.745690	0.686781	0.802742	69	6	0	-6.713749	-0.920021	-0.840848
70	1	0	8.348830	-1.823329	-1.590498	70	1	0	-8.470546	1.614521	1.410650
71	1	0	9.815554	-0.428705	-0.132258	71	1	0	-9.849603	0.066033	0.023038
72	1	0	8.738574	1.219770	1.436597	72	1	0	-8.668256	-1.597281	-1.454310
73	1	0	6.243731	1.382946	1.464186	73	1	0	-6.169597	-1.621273	-1.462334

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