Supporting Information

Synthesis, Characterization, and Anticancer Potential of Novel NHC Ligands and Their Selenium Complexes: A Combined *In Vitro* and *In Silico* Investigation

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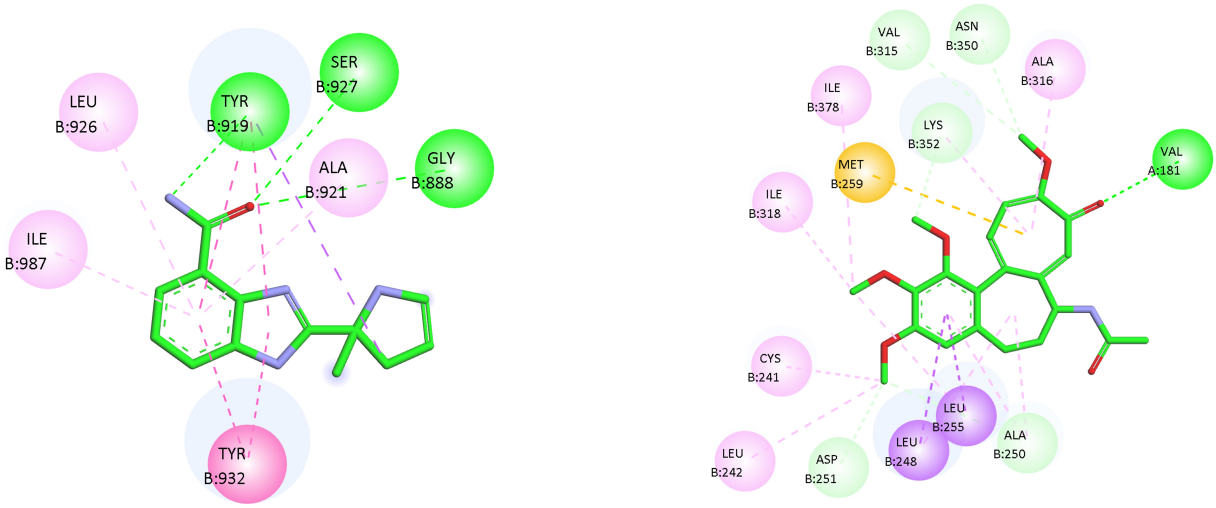


Veliparib-PARP-1
(PDB ID: 5LX6)

Colchicine-Tubulin
(PDB ID: 4O2B)

Figure S1. Binding modes of veliparib and colchicine within the PARP-1 and tubulin binding sites, respectively.

Table S1. Cytotoxic activity of benzimidazolium ligands (**A1–A6**) and their selenium complexes (**B1–B6**) against HCT116, SH-SY5Y, and BEAS-2B cell lines determined by the MTT assay. Data are expressed as IC_{50} values and compared with cisplatin as a reference drug.

Compounds		***Anti-Cancer IC50 (µM)***		
		BEAS-2B[a]	***SHSY5Y[a]***	***HCT116[a]***
Benzimidazolium-Derived NHC Ligands	**A1**	54,11±2,77	87,48±0,21	65,59±2,84
	A2	15,13±0,32	59,51±5,61	40,08±3,42
	A3	19,67±0,58	4,29±0,02	9,54±0,20
	A4	10,71±0,53	3,09±0,03	10,79±0,11
	A5	12,20±0,79	5,14±0,66	26,12±0,29
	A6	413,91±15,63	221,47±15,76	297,13±15,38
Selenium-NHC complexes	**B1**	689,47±17,68	528,34±19,48	692,99±59,63
	B2	NA	NA	NA
	B3	335,14±8,07	651,56±0,68	NA
	B4	NA	231,84±3,46	NA
	B5	455,43±21,76	280,40±28,06	572,64±10,29
	B6	NA	NA	NA
	Cisplatin[b]	118,59 ± 4,90	152,12 ± 4,65	310,12 ± 3,09

IC_{50} values presented as mean ± SD of three independent experiments.
NA: Not Applicable (IC_{50}>800 µM),
[a]: Cell lines,
[b]: Reference Drug.

Table S2: Cartesian coordinates and energies of compound A1 computed at B3LYP/6-311G(d,p) (SMD, Water)

Energies (Hartree)	**Cartesian Coordinates (Å)**
Electronic Energy (EE) = -964.173492	C 0.20928 2.98674 -0.16723
Zero-point Energy Correction = 0.443302	C 0.71309 1.78767 -0.65782
Thermal Correction to Energy = 0.466144	C -0.08762 0.65028 -0.56637
Thermal Correction to Enthalpy = 0.467088	C -1.36266 0.70366 0.00637
Thermal Correction to Free Energy = 0.387711	C -1.87896 1.89871 0.50551
	H 1.70680 1.73995 -1.08291
EE + Zero-point Energy = -963.730190	H -2.86526 1.94528 0.94909
EE + Thermal Energy Correction = -963.707348	C 1.31369 -1.22681 -1.62904
	H 1.06322 -2.25711 -1.89333
EE + Thermal Enthalpy Correction = -963.706404	H 1.45013 -0.67586 -2.56152
	C 2.56824 -1.16518 -0.78445
EE + Thermal Free Energy Correction = -963.785781	C 2.59151 -1.70493 0.50391
	C 3.76138 -1.68761 1.26312
	C 4.91217 -1.12483 0.69781
	C 4.91994 -0.58745 -0.58948
	C 3.72688 -0.60862 -1.32210
	H 1.69383 -2.14503 0.92833
	H 3.71170 -0.19517 -2.32645
	C -1.62704 4.34888 0.94958
	H -1.67347 5.10868 0.16395
	H -2.63002 4.22900 1.35978
	H -0.98603 4.74840 1.74089
	C 1.05290 4.23322 -0.25176
	H 1.23670 4.65766 0.73949
	H 2.01902 4.02441 -0.71142
	H 0.55865 5.00898 -0.84400
	C -3.23171 -0.98929 0.42540
	H -3.34114 -0.51757 1.40616
	C -4.37733 -0.54535 -0.50674
	C -5.57209 -1.44292 -0.08991
	C -4.97244 -2.58720 0.77872
	C -3.44820 -2.49875 0.57797
	H -4.59567 0.52045 -0.43024
	H -4.08312 -0.74324 -1.54168
	H -6.07944 -1.83358 -0.97273
	H -6.31492 -0.87702 0.47377
	H -5.21462 -2.43201 1.83298
	H -5.35922 -3.56914 0.50600
	H -3.17484 -3.01548 -0.34886
	H -2.87521 -2.93691 1.39767
	N 0.11661 -0.67407 -0.95884
	C -0.97508 -1.37353 -0.63392
	N -1.88913 -0.59121 -0.05209
	H -1.09141 -2.42771 -0.81598
	C 6.21151 -1.10090 1.52409
	H 5.97290 -0.98504 2.56070
	H 6.74233 -2.01882 1.38071
	H 6.82209 -0.28220 1.20498

	H 3.77903 -2.09416 2.25272 H 5.81316 -0.17050 -1.00565

Table S3: Cartesian coordinates and energies of compound A2 computed at B3LYP/6-311G(d,p) (SMD, Water)

Energies (Hartree)	**Cartesian Coordinates (Å)**
Electronic Energy (EE) = -1003.501718 Zero-point Energy Correction = 0.470546 Thermal Correction to Energy = 0.495249 Thermal Correction to Enthalpy = 0.496193 Thermal Correction to Free Energy = 0.412417 EE + Zero-point Energy = -1003.031172 EE + Thermal Energy Correction = -1003.006469 EE + Thermal Enthalpy Correction = -1003.005525 EE + Thermal Free Energy Correction = -1003.089301	C -0.46787 3.18359 -0.14248 C 0.25121 2.02827 -0.50126 C -0.35648 0.78710 -0.37450 C -1.67321 0.67219 0.11318 C -2.39434 1.80991 0.45277 H 1.27017 2.11192 -0.86027 H -3.41673 1.73873 0.80531 C 1.28234 -0.79326 -1.43411 H 1.13088 -1.77752 -1.88805 H 1.37147 -0.08247 -2.26627 C 2.57658 -0.79285 -0.63245 C 2.58141 -0.89253 0.75395 C 3.78576 -0.92985 1.46948 C 4.98489 -0.86999 0.76319 C 5.00931 -0.76808 -0.63410 C 3.79605 -0.72670 -1.31654 H 1.63723 -0.92986 1.28643 H 5.92411 -0.89683 1.30877 H 3.79674 -0.64027 -2.39994 C -2.57237 4.30774 0.71115 H -2.67505 5.00087 -0.13109 H -3.57747 4.04489 1.04697 H -2.08889 4.86571 1.52084 C 0.19330 4.53558 -0.27510 H 0.24550 5.05991 0.68552 H 1.21299 4.43695 -0.65241 H -0.35232 5.19159 -0.96269 C -3.36014 -1.17638 0.27991 H -3.85066 -0.51326 0.99942 C -4.19260 -1.22008 -1.02789 C -5.28593 -2.29521 -0.78615 C -4.93978 -2.95749 0.57690 C -3.46386 -2.61166 0.81944 H -4.60302 -0.24071 -1.28112 H -3.52327 -1.51490 -1.84027 H -5.27499 -3.03614 -1.58913 H -6.28956 -1.86459 -0.77176 H -5.55342 -2.52372 1.37327 H -5.12670 -4.03326 0.58160 H -2.82339 -3.27387 0.22812 H -3.15943 -2.69301 1.86547 C 6.32547 -0.70448 -1.37241 H 6.90293 -1.62361 -1.23048 H 6.17481 -0.56809 -2.44513 H 6.94326 0.12372 -1.01215

	C 3.77104 -1.02354 2.97694 H 3.20642 -1.89800 3.31435 H 4.78216 -1.10014 3.38162 H 3.29733 -0.14269 3.42170 N 0.08606 -0.48991 -0.67891 C -0.97141 -1.41311 -0.50503 N -2.00313 -0.67719 0.12550 H -0.71601 -2.38992 -0.09329

Table S4: Cartesian coordinates and energies of compound A3 computed at B3LYP/6-311G(d,p) (SMD, Water)

Energies (Hartree)	**Cartesian Coordinates (Å)**
Electronic Energy (EE) = -1042.821311 Zero-point Energy Correction = 0.500256 Thermal Correction to Energy = 0.525520 Thermal Correction to Enthalpy = 0.526464 Thermal Correction to Free Energy = 0.442773 EE + Zero-point Energy = -1042.321055 EE + Thermal Energy Correction = -1042.295791 EE + Thermal Enthalpy Correction = -1042.294847 EE + Thermal Free Energy Correction = -1042.378538	C -0.68590 3.09338 -0.17120 C -0.10801 1.97553 -0.76174 C -0.77685 0.75677 -0.65961 C -1.99437 0.65112 0.02090 C -2.58347 1.76330 0.62081 H 0.84340 2.05093 -1.27123 H -3.52577 1.68679 1.14802 C 0.70844 -0.91612 -1.92915 H 0.54201 -1.95558 -2.22227 H 0.70398 -0.31633 -2.84125 C 2.02053 -0.75602 -1.19172 C 2.21387 -1.34221 0.06157 C 3.43898 -1.23164 0.71900 C 4.47107 -0.52732 0.08707 C 4.30881 0.05975 -1.16791 C 3.06351 -0.05817 -1.79710 H 1.40742 -1.89203 0.53799 H 2.91646 0.39183 -2.77473 C -2.54470 4.20626 1.16340 H -2.73856 4.98815 0.42332 H -3.48948 3.96396 1.65051 H -1.87977 4.63907 1.91654 C 0.01492 4.42479 -0.26465 H 0.24219 4.82567 0.72740 H 0.95237 4.33862 -0.81422 H -0.60698 5.16712 -0.77358 C -3.63560 -1.24637 0.51176 H -3.70461 -0.82921 1.52053 C -4.89928 -0.88904 -0.29684 C -5.95397 -1.92461 0.17437 C -5.16528 -3.03313 0.93110 C -3.68214 -2.77523 0.60677 H -5.21772 0.14355 -0.14918 H -4.68003 -1.01232 -1.36153 H -6.49556 -2.33071 -0.68070 H -6.69741 -1.46419 0.82636 H -5.32689 -2.94754 2.00849

	H -5.47246 -4.03868 0.64354 H -3.44128 -3.22188 -0.36444 H -2.99642 -3.18304 1.35222 N -0.47418 -0.52133 -1.13339 C -1.45523 -1.34540 -0.75250 N -2.38881 -0.68888 -0.05720 H -1.47898 -2.39769 -0.97631 C 5.82975 -0.39918 0.80062 H 6.32247 0.49202 0.47215 H 3.58644 -1.67393 1.68209 H 5.11395 0.58578 -1.63689 C 5.60576 -0.33066 2.32270 H 5.27228 -1.28350 2.67738 H 6.52393 -0.07121 2.80701 H 4.86545 0.41032 2.54127 C 6.70328 -1.62221 0.46484 H 6.82520 -1.69303 -0.59583 H 7.66192 -1.51367 0.92759 H 6.22966 -2.50969 0.82947

Table S5: Cartesian coordinates and energies of compound A4 computed at B3LYP/6-311G(d,p) (SMD, Water)

Energies (Hartree)	**Cartesian Coordinates (Å)**
Electronic Energy (EE) = -1082.142312 Zero-point Energy Correction = 0.528235 Thermal Correction to Energy = 0.554618 Thermal Correction to Enthalpy = 0.555562 Thermal Correction to Free Energy = 0.470083 EE + Zero-point Energy = -1081.614077 EE + Thermal Energy Correction = -1081.587694 EE + Thermal Enthalpy Correction = -1081.586750 EE + Thermal Free Energy Correction = -1081.672229	C 0.87808 3.07361 0.18894 C 0.33191 1.93922 0.77814 C 1.03099 0.73827 0.66787 C 2.24721 0.66618 -0.01930 C 2.80468 1.79521 -0.61795 H -0.61843 1.98850 1.29281 H 3.74584 1.74467 -1.15029 C -0.40460 -0.97658 1.93860 H -0.21024 -2.01255 2.22685 H -0.41061 -0.38027 2.85297 C -1.72419 -0.84719 1.20856 C -1.90913 -1.43345 -0.04597 C -3.14008 -1.35166 -0.69665 C -4.18642 -0.67619 -0.05670 C -4.03256 -0.08985 1.19968 C -2.78138 -0.17837 1.82198 H -1.09147 -1.96080 -0.52865 H -2.64070 0.27159 2.80057 C 2.70094 4.23840 -1.15092 H 2.87874 5.02221 -0.40885 H 3.64901 4.02204 -1.64382 H 2.02127 4.65694 -1.89896 C 0.14412 4.38640 0.29112 H -0.09848 4.78505 -0.69820 H -0.78794 4.27435 0.84517 H 0.74960 5.14242 0.79970 C 3.93357 -1.18708 -0.52591 H 3.98665 -0.76455 -1.53341

	C 5.19198 -0.80072 0.27754 C 6.27018 -1.80735 -0.20308 C 5.50597 -2.93276 -0.96000 C 4.01848 -2.71390 -0.62704 H 5.48327 0.24019 0.13221 H 4.98153 -0.93349 1.34287 H 6.82640 -2.20270 0.64762 H 6.99824 -1.32573 -0.85711 H 5.65970 -2.83908 -2.03787 H 5.84014 -3.93122 -0.67790 H 3.79416 -3.17014 0.34367 H 3.33945 -3.13626 -1.37051 N 0.76341 -0.54887 1.13828 C 1.76309 -1.34628 0.74918 N 2.67601 -0.66363 0.05160 H 1.81477 -2.39845 0.96881 C -5.55165 -0.58002 -0.76275 H -3.28130 -1.79398 -1.66066 H -4.84835 0.41377 1.67481 C -5.33747 -0.50017 -2.28569 H -4.98172 -1.44288 -2.64575 H -6.26447 -0.26237 -2.76425 H -4.61740 0.26023 -2.50521 C -6.39202 -1.82613 -0.42719 H -6.50653 -1.90397 0.63382 H -7.35552 -1.74030 -0.88457 H -5.89790 -2.69991 -0.79766 C -6.29070 0.68241 -0.28141 H -7.18674 0.81050 -0.85202 H -6.53919 0.57724 0.75401 H -5.65966 1.53663 -0.41178

Table S6: Cartesian coordinates and energies of compound A5 computed at B3LYP/6-311G(d,p) (SMD, Water)

Energies (Hartree)	**Cartesian Coordinates (Å)**
Electronic Energy (EE) = -1239.438396 Zero-point Energy Correction = 0.639794 Thermal Correction to Energy = 0.671888 Thermal Correction to Enthalpy = 0.672832 Thermal Correction to Free Energy = 0.574409 EE + Zero-point Energy = -1238.798602 EE + Thermal Energy Correction = -1238.766508 EE + Thermal Enthalpy Correction = -1238.765564 EE + Thermal Free Energy Correction = -1238.863987	C -1.21463 3.10604 0.83563 C -0.63459 2.20043 -0.04512 C -1.36555 1.06844 -0.40209 C -2.64655 0.83933 0.11089 C -3.23890 1.73738 0.99774 H 0.36395 2.36549 -0.42738 H -4.23013 1.56484 1.39700 C 0.15658 -0.20816 -2.03605 H -0.02850 -1.08051 -2.66759 H 0.26765 0.65384 -2.69659 C 1.39747 -0.39522 -1.18976 C 1.44195 -1.36937 -0.18935 C 2.60178 -1.57063 0.55871 C 3.72129 -0.77892 0.27496 C 3.70792 0.19427 -0.72437 C 2.52494 0.38095 -1.44983

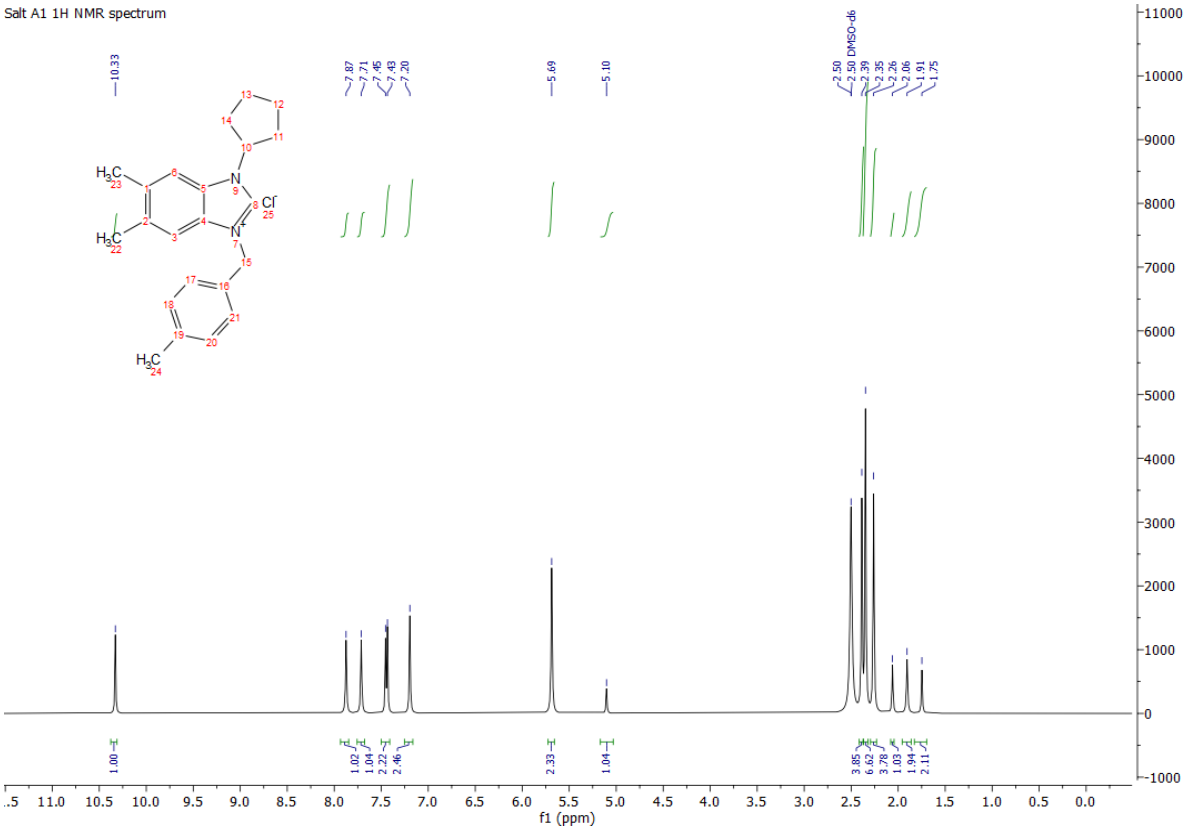
	H 0.56889 -1.98188 0.01619 H 2.49367 1.13371 -2.23230 C -3.14018 3.86158 2.31759 H -3.22562 4.85364 1.86463 H -4.13765 3.54594 2.62421 H -2.53170 3.97514 3.21956 C -0.44752 4.33902 1.24039 H -0.29869 4.37779 2.32338 H 0.53356 4.36580 0.76602 H -0.98264 5.25089 0.95936 C -4.41305 -0.98577 -0.17818 H -4.55967 -0.91483 0.90342 C -5.57512 -0.29139 -0.91697 C -6.71686 -1.34152 -0.89550 C -6.05663 -2.69163 -0.48953 C -4.53885 -2.45457 -0.59698 H -5.85844 0.65814 -0.46136 H -5.26020 -0.07837 -1.94278 H -7.19165 -1.40607 -1.87519 H -7.49769 -1.06328 -0.18651 H -6.31721 -2.94862 0.54016 H -6.38063 -3.52323 -1.11533 H -4.22634 -2.57843 -1.63993 H -3.94766 -3.13263 0.02185 N -1.07779 -0.00549 -1.24678 C -2.12787 -0.83242 -1.23490 N -3.09289 -0.36907 -0.43485 H -2.17835 -1.75009 -1.79463 H 4.61611 -0.92516 0.84312 C 2.64992 -2.63683 1.66889 C 4.95999 1.04019 -1.02158 C 1.85042 -3.87610 1.22546 H 2.20201 -4.73606 1.75626 H 0.81253 -3.72566 1.43767 H 1.98125 -4.02762 0.17436 C 4.11330 -3.03743 1.93277 H 4.63397 -2.21450 2.37616 H 4.13935 -3.87569 2.59727 H 4.58336 -3.30045 1.00823 C 2.03418 -2.06317 2.95861 H 2.39468 -1.06776 3.11384 H 0.96815 -2.04637 2.86807 H 2.31190 -2.67679 3.79001 C 6.14493 0.10925 -1.33922 H 6.89667 0.65666 -1.86848 H 6.55556 -0.26947 -0.42661 H 5.80584 -0.70627 -1.94325 C 4.68687 1.95422 -2.23053 H 4.37548 1.35978 -3.06394 H 3.91517 2.65267 -1.98246 H 5.58020 2.48528 -2.48517 C 5.30026 1.90301 0.20779 H 5.62618 1.27142 1.00764

	H 6.08025 2.59083 -0.04405 H 4.43076 2.44629 0.51394

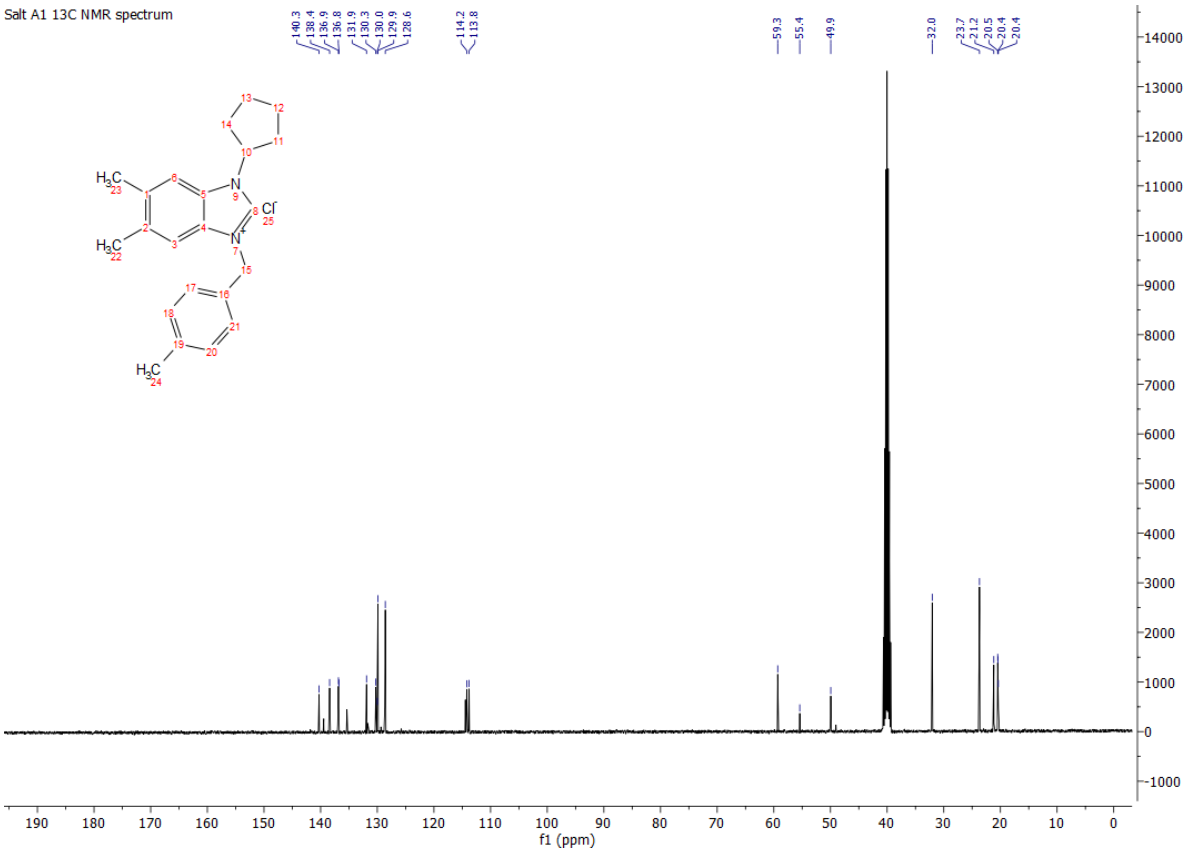
Table S7: Cartesian coordinates and energies of compound A6 computed at B3LYP/6-311G(d,p) (SMD, Water)

Energies (Hartree)	**Cartesian Coordinates (Å)**
Electronic Energy (EE) = -1268.492587 Zero-point Energy Correction = 0.512110 Thermal Correction to Energy = 0.541503 Thermal Correction to Enthalpy = 0.542447 Thermal Correction to Free Energy = 0.448420 EE + Zero-point Energy = -1267.980477 EE + Thermal Energy Correction = -1267.951084 EE + Thermal Enthalpy Correction = -1267.950140 EE + Thermal Free Energy Correction = -1268.044167	C -1.20728 3.15300 0.16806 C -0.58246 2.11801 -0.51799 C -1.24040 0.89196 -0.60210 C -2.49325 0.69784 -0.01110 C -3.12973 1.72601 0.68290 H 0.39539 2.25991 -0.95859 H -4.09947 1.58092 1.14147 C 0.33605 -0.60674 -1.97509 H 0.19988 -1.60416 -2.40019 H 0.37588 0.09875 -2.80719 C 1.60185 -0.52921 -1.14881 C 1.73098 -1.26129 0.03404 C 2.91513 -1.22378 0.77003 C 3.97246 -0.44232 0.28835 C 3.87445 0.29102 -0.89426 C 2.66861 0.24268 -1.60432 H 0.90579 -1.86930 0.39327 H 2.57175 0.80656 -2.52765 C -3.15314 4.08578 1.51652 H -3.31452 4.95016 0.86579 H -4.12096 3.78095 1.91528 H -2.53777 4.42835 2.35356 C -0.51935 4.49001 0.27619 H -0.35409 4.76950 1.32074 H 0.44891 4.47628 -0.22437 H -1.12069 5.28473 -0.17509 C -4.13539 -1.25454 0.15197 H -4.26707 -0.96264 1.19785 C -5.35543 -0.80957 -0.67983 C -6.42192 -1.90058 -0.39857 C -5.66351 -3.08774 0.26396 C -4.16772 -2.78394 0.05967 H -5.69493 0.19577 -0.42787 H -5.07434 -0.80212 -1.73708 H -6.90870 -2.20361 -1.32625 H -7.20712 -1.52658 0.25975 H -5.88730 -3.13379 1.33260 H -5.94093 -4.05298 -0.15973 H -3.86625 -3.10866 -0.94254 H -3.52042 -3.27477 0.78926 N -0.89493 -0.31780 -1.20769 C -1.88546 -1.18752 -0.98624 N -2.86544 -0.62520 -0.27247 H -1.88298 -2.20522 -1.33590 C 2.42587 -1.22486 3.23678

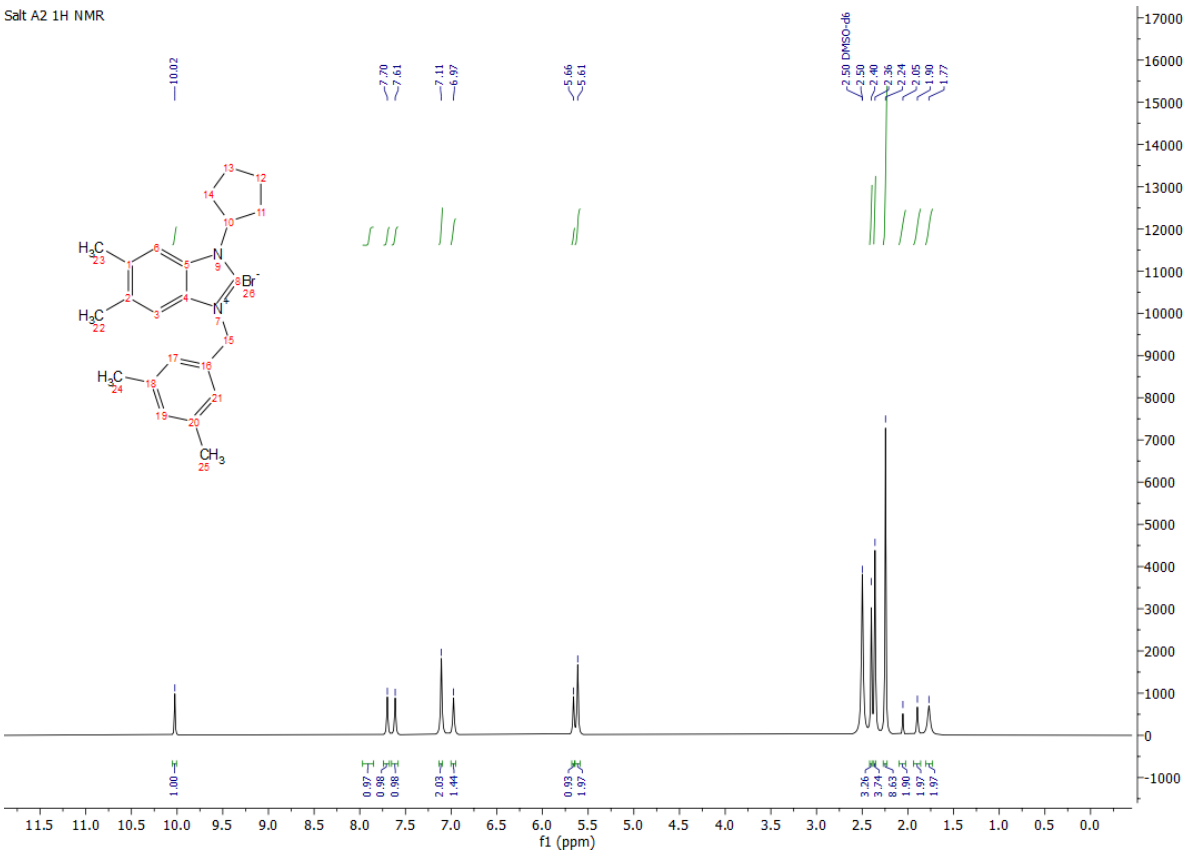
	H 2.72001 -0.19860 3.16490 H 1.35974 -1.29519 3.17915 H 2.75989 -1.62707 4.17035 C 6.30010 0.23008 -1.55512 H 7.00292 0.69754 -2.21271 H 6.75207 0.08263 -0.59653 H 6.00692 -0.71577 -1.96049 O 5.06004 1.13079 -1.40489 O 3.05620 -2.02180 2.07956 O 5.19238 -0.39444 1.03293 C 5.92320 -1.60677 0.83027 H 6.95782 -1.37873 0.68040 H 5.81733 -2.23500 1.68993 H 5.54129 -2.11370 -0.03116



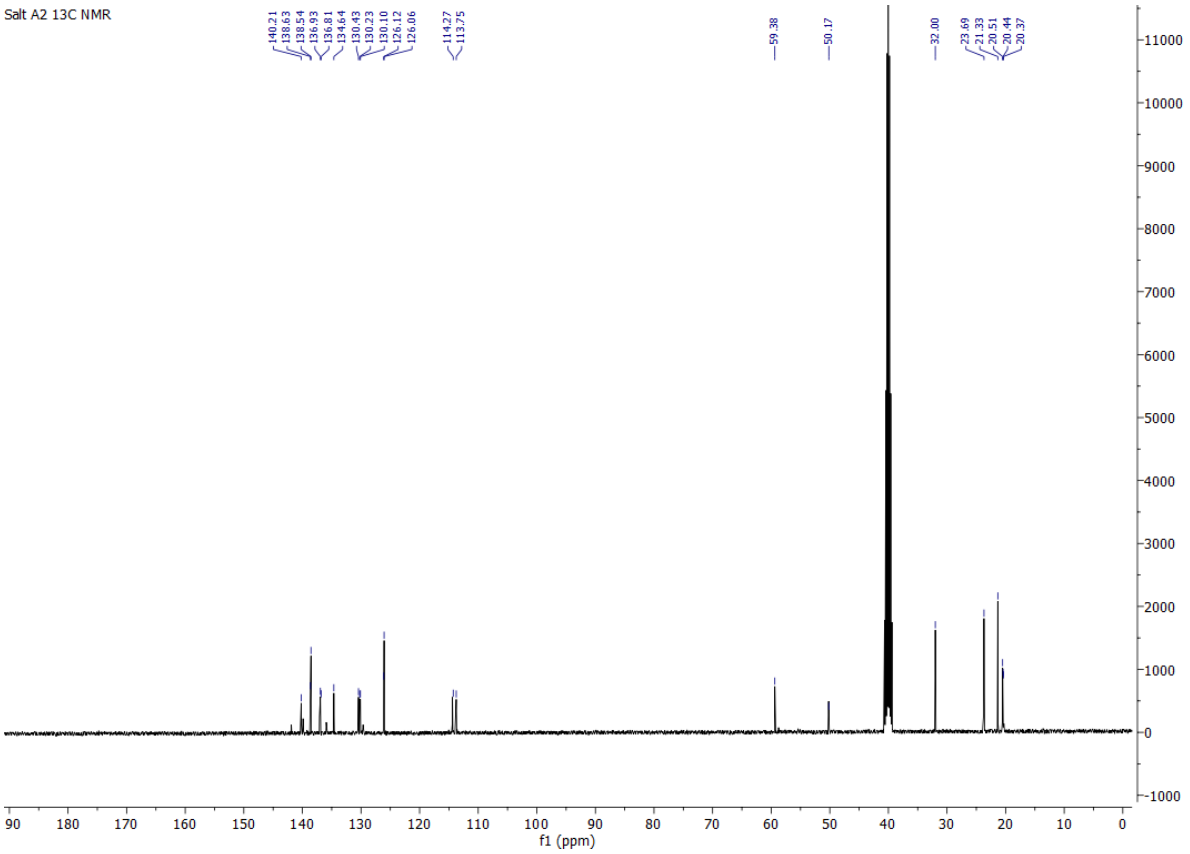
^{1}H NMR Spectrum of compound A1 (DMSO-d^{6})



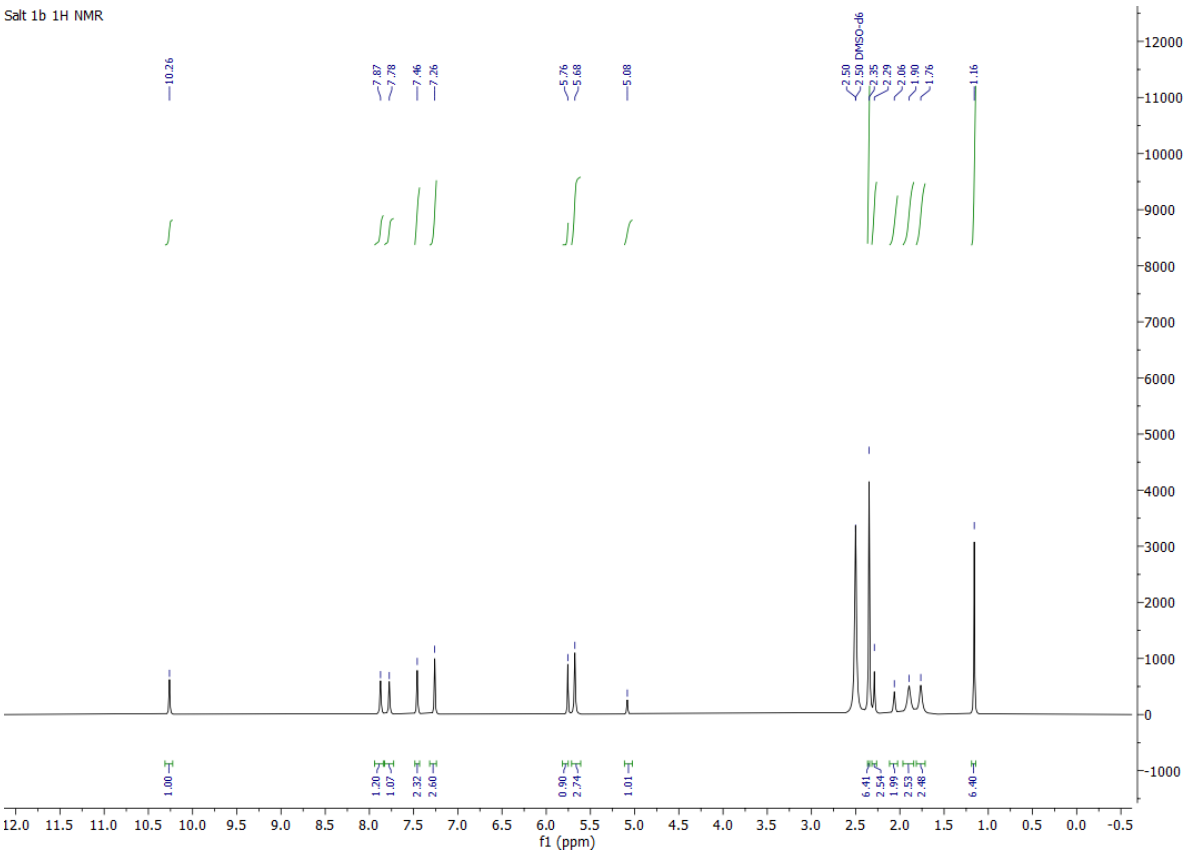
^{13}C NMR Spectrum of compound A1 (DMSO-d^{6})



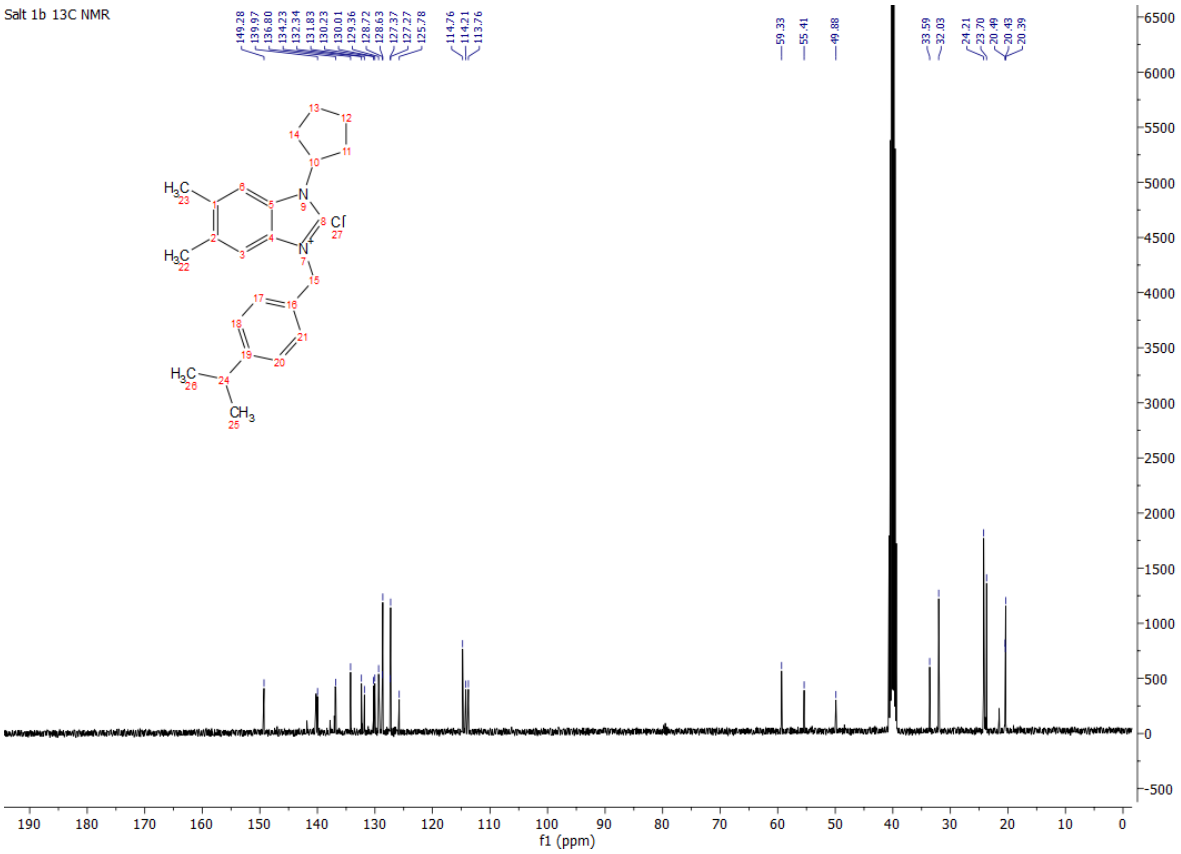
^{1}H NMR Spectrum of compound A2 (DMSO-d^{6})



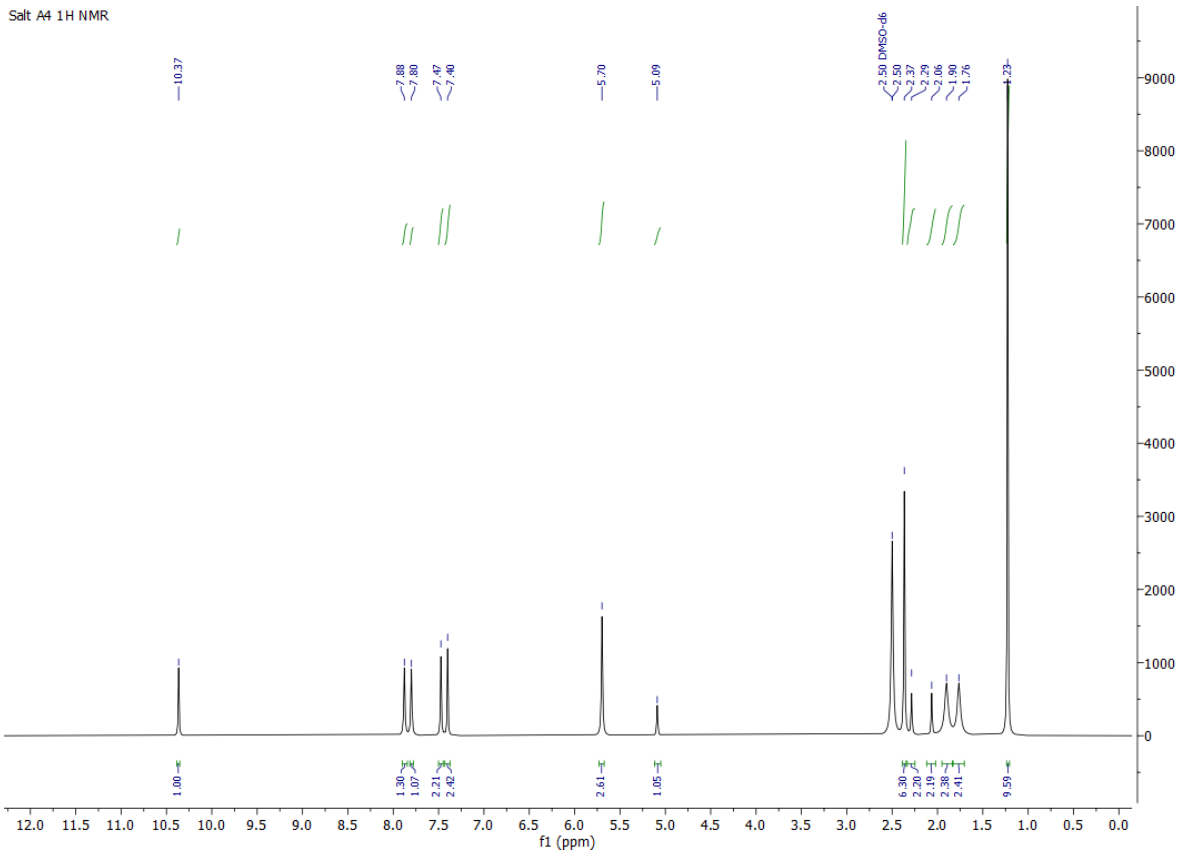
^{13}C NMR Spectrum of compound A2 (DMSO-d^{6})



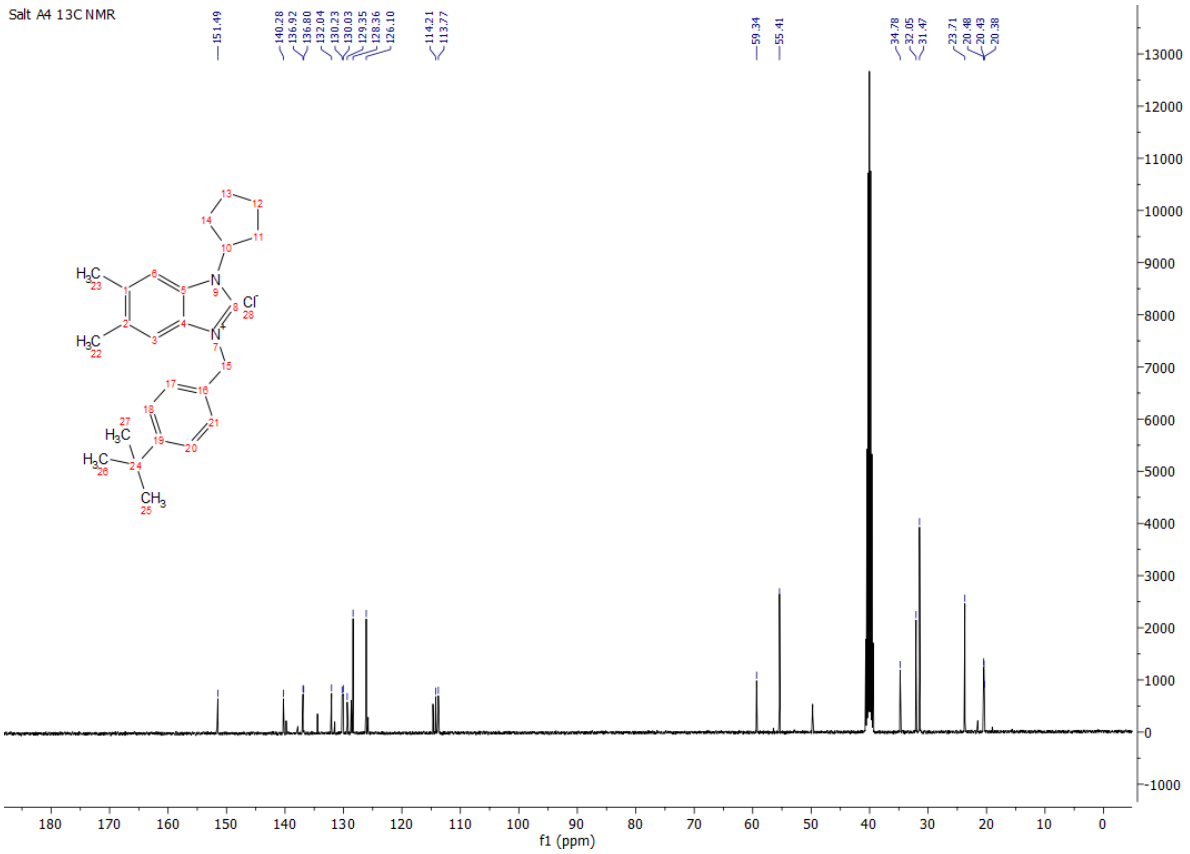
^{1}H NMR Spectrum of compound A3 (DMSO-d^{6})



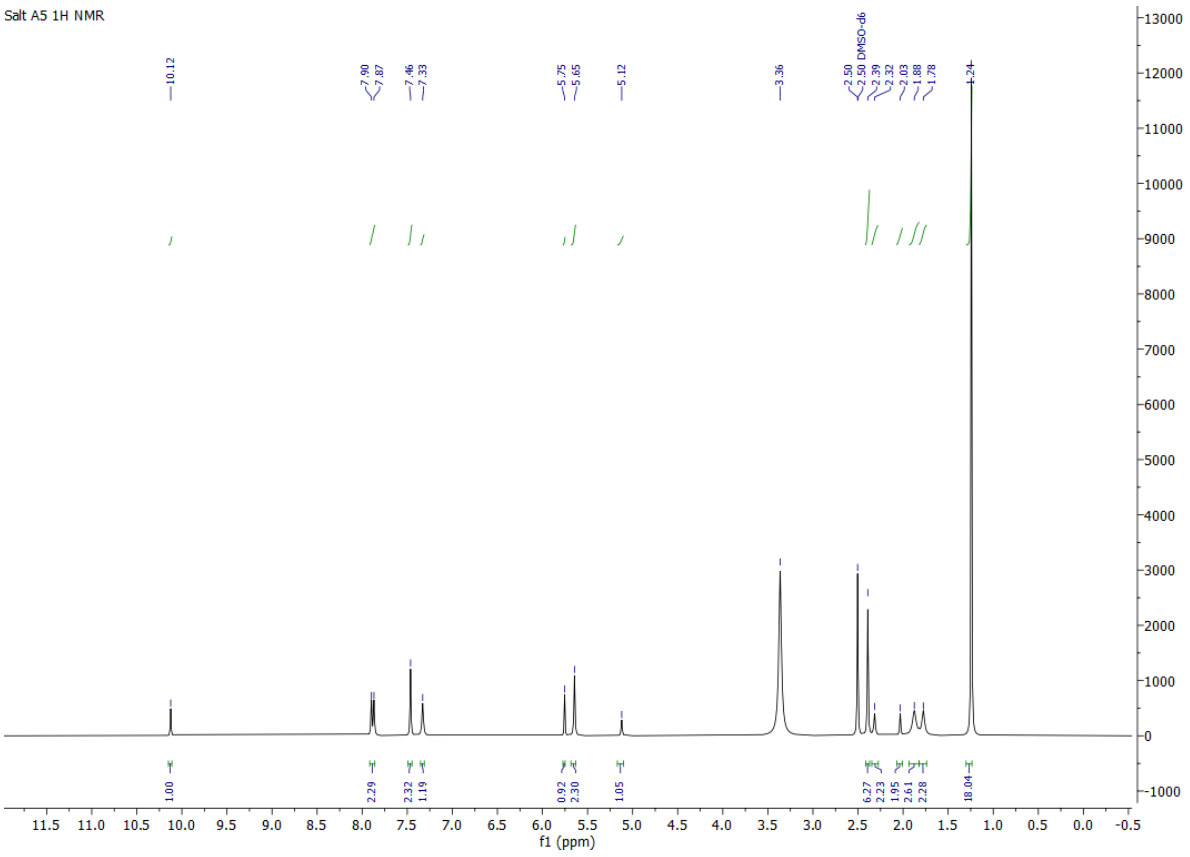
^{13}C NMR Spectrum of compound A3 (DMSO-d^{6})



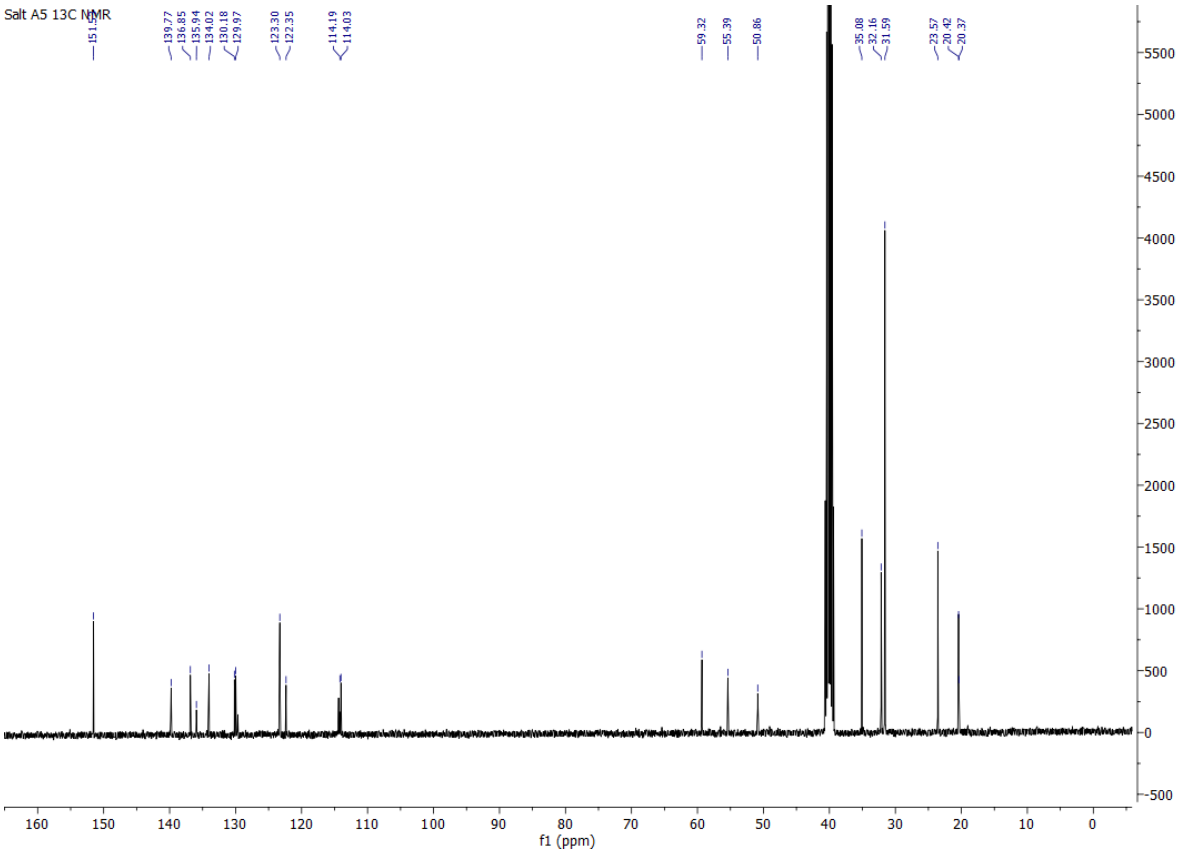
^{13}C NMR Spectrum of compound A4 (DMSO-d^6)



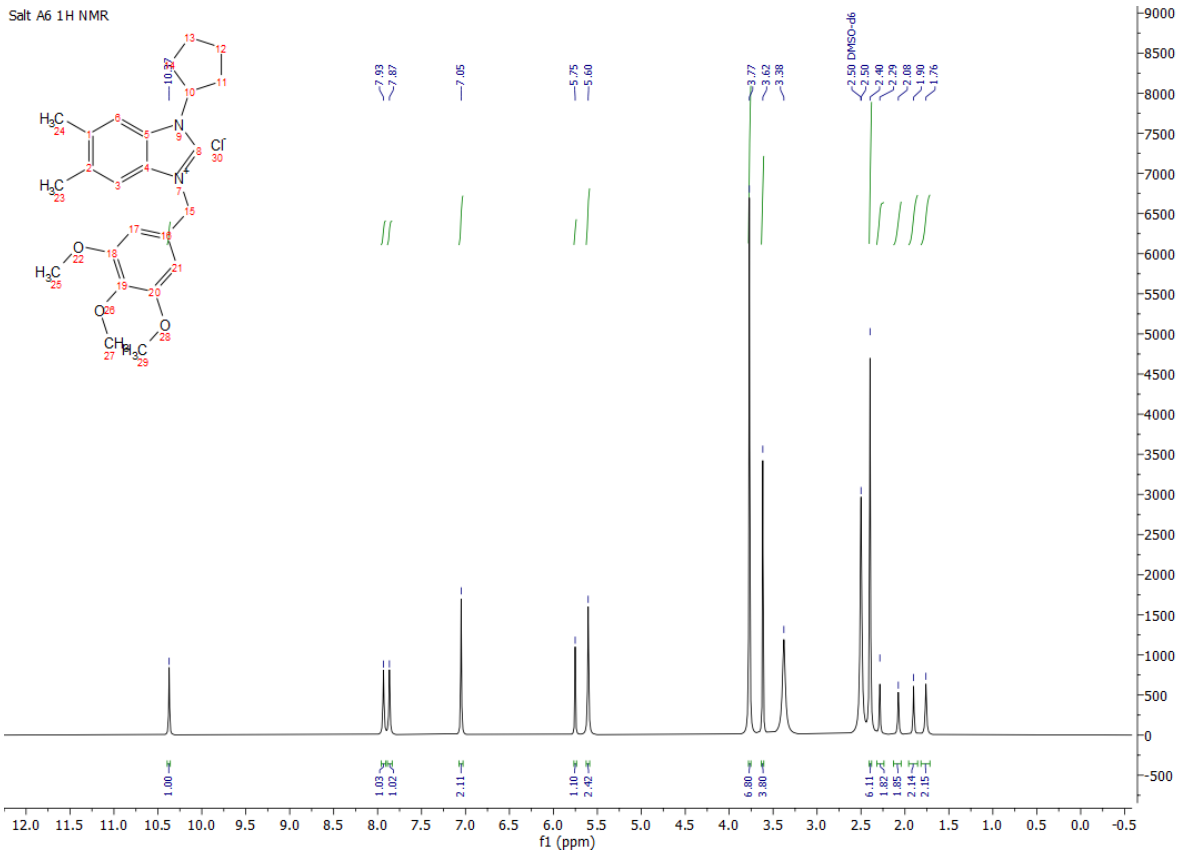
^{13}C NMR Spectrum of compound A4 (DMSO-d^6)



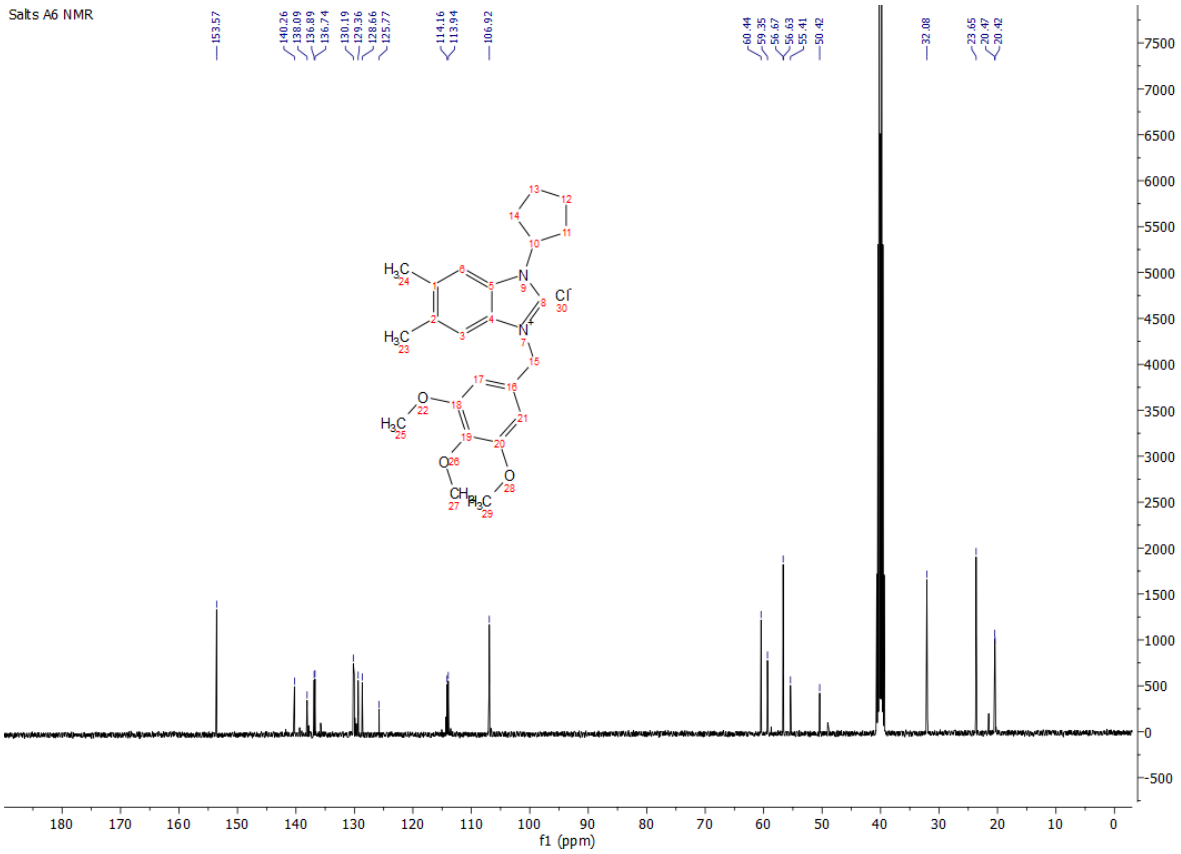
^{1}H NMR Spectrum of compound A5 (DMSO-d^{6})



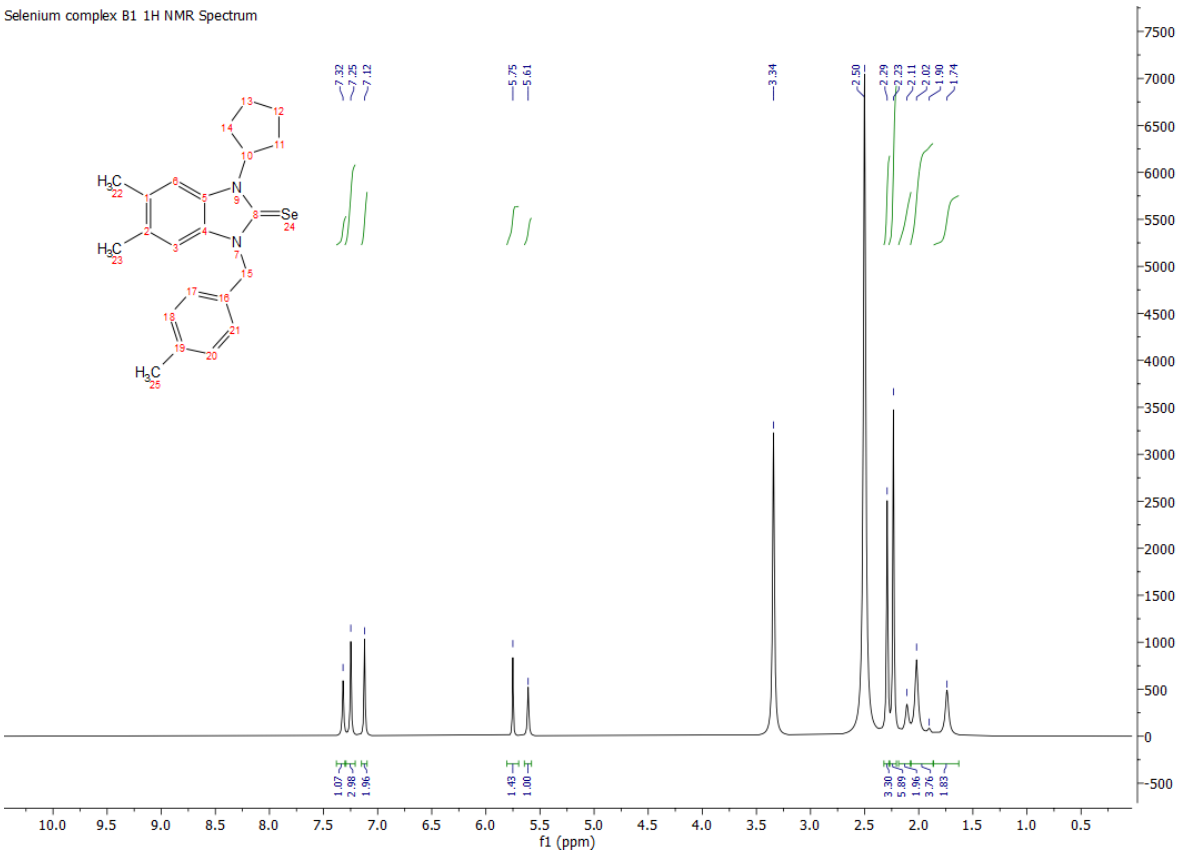
^{13}C NMR Spectrum of compound A5 (DMSO-d^{6})



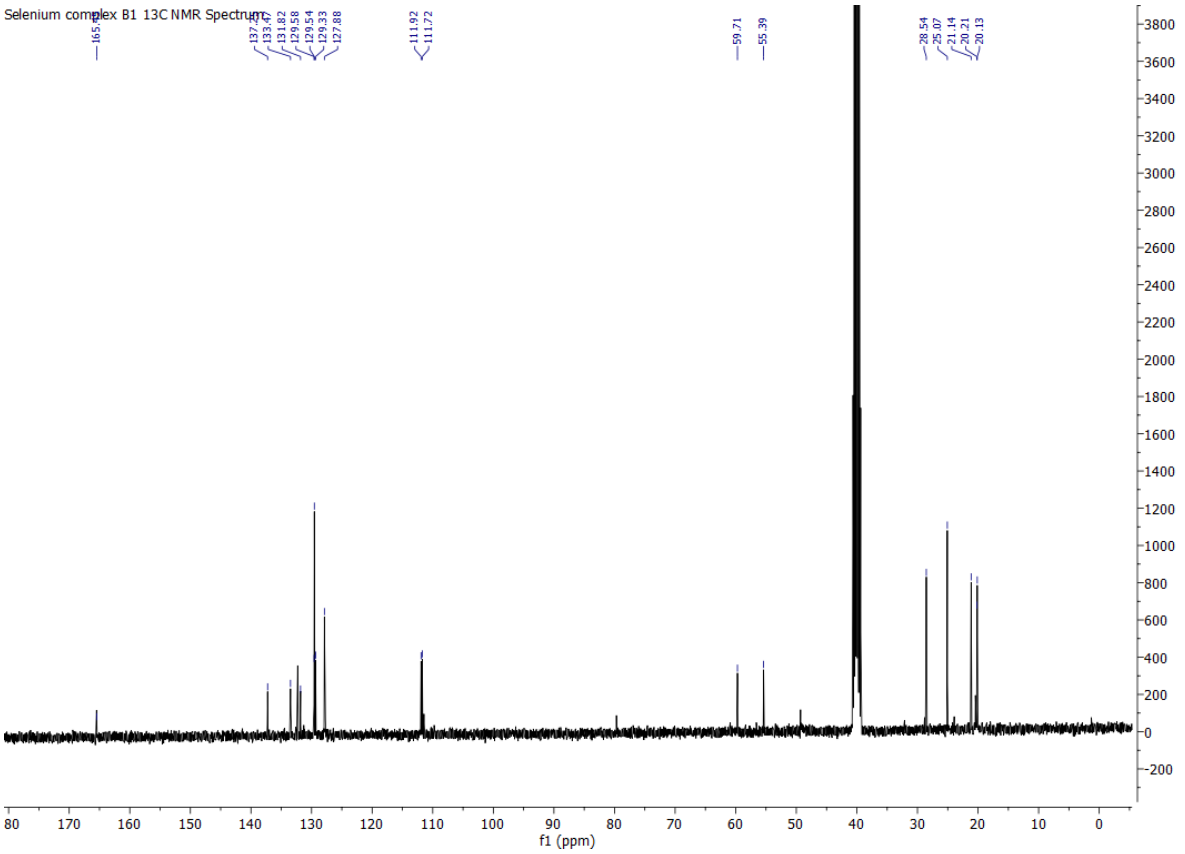
^{1}H NMR Spectrum of compound A6 (DMSO-d^{6})



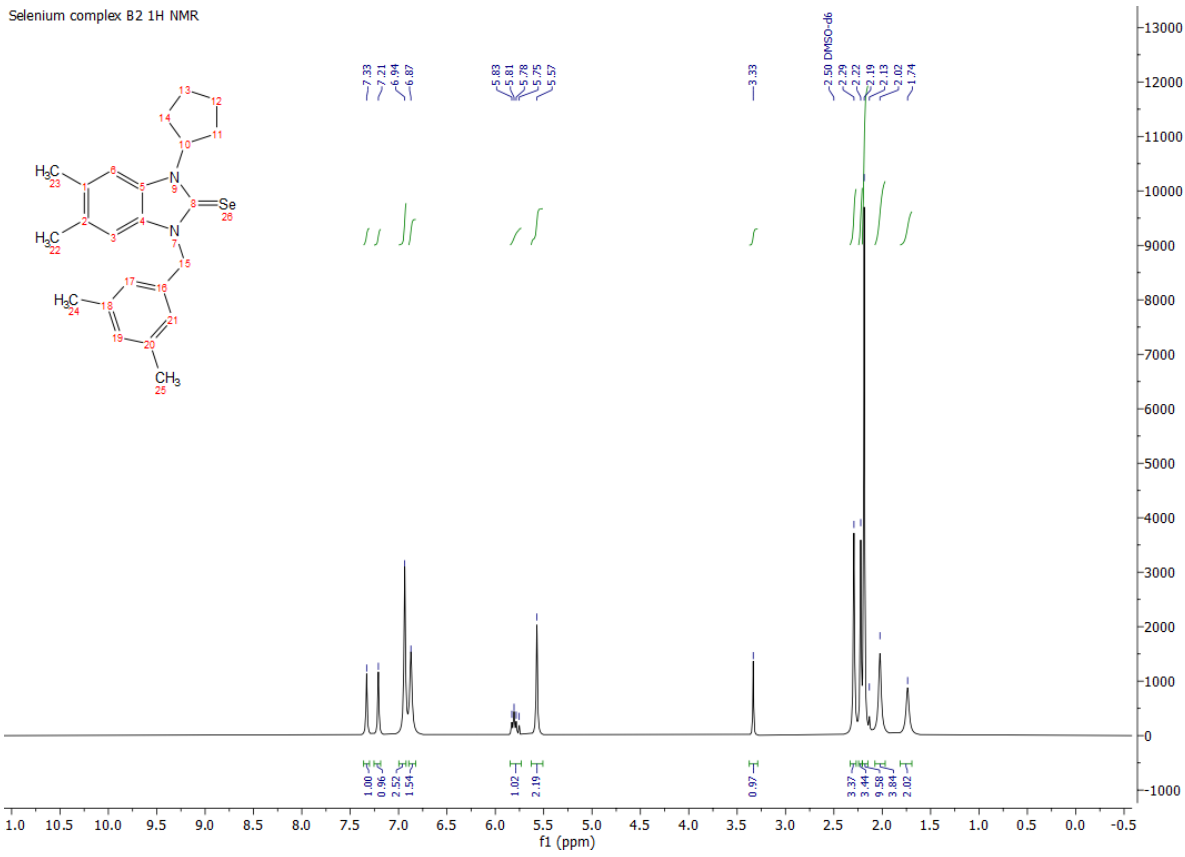
^{13}C NMR Spectrum of compound A6 (DMSO-d^{6})



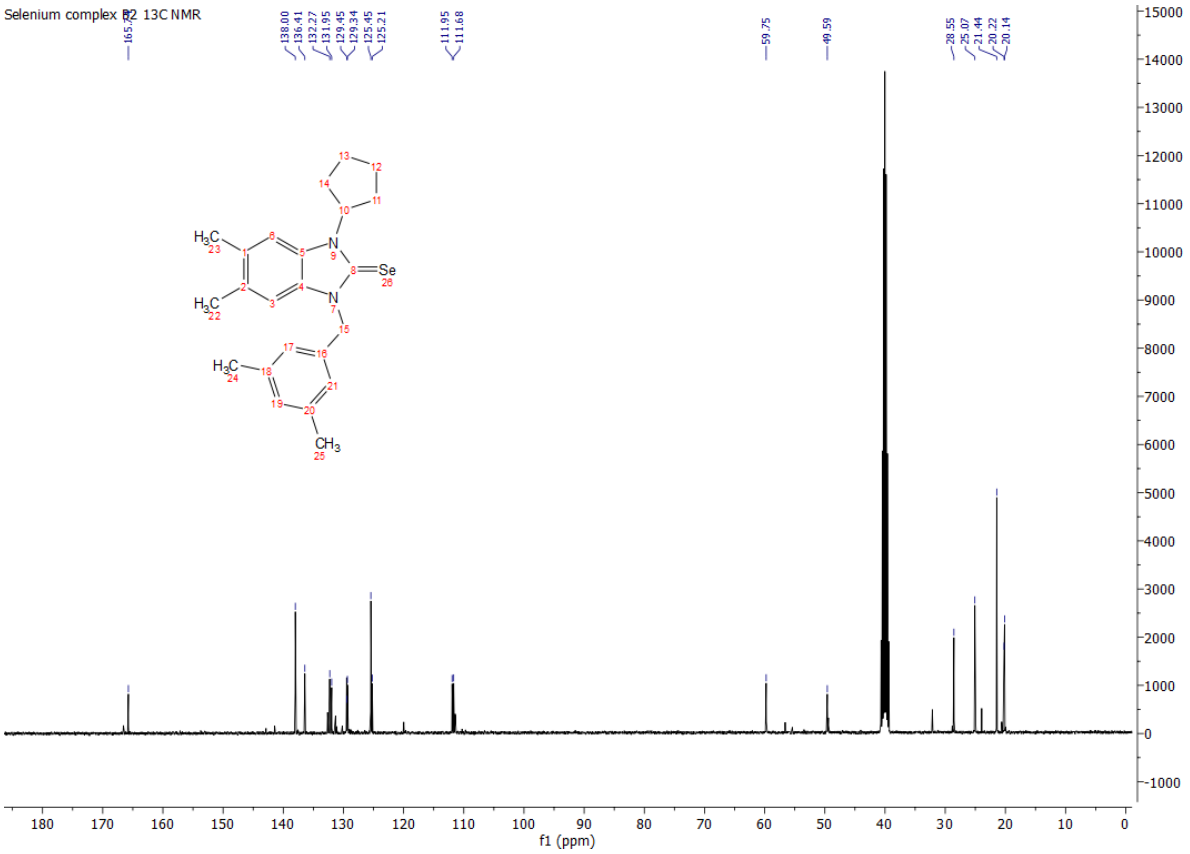
^{1}H NMR Spectrum of compound B1 (DMSO-d^{6})



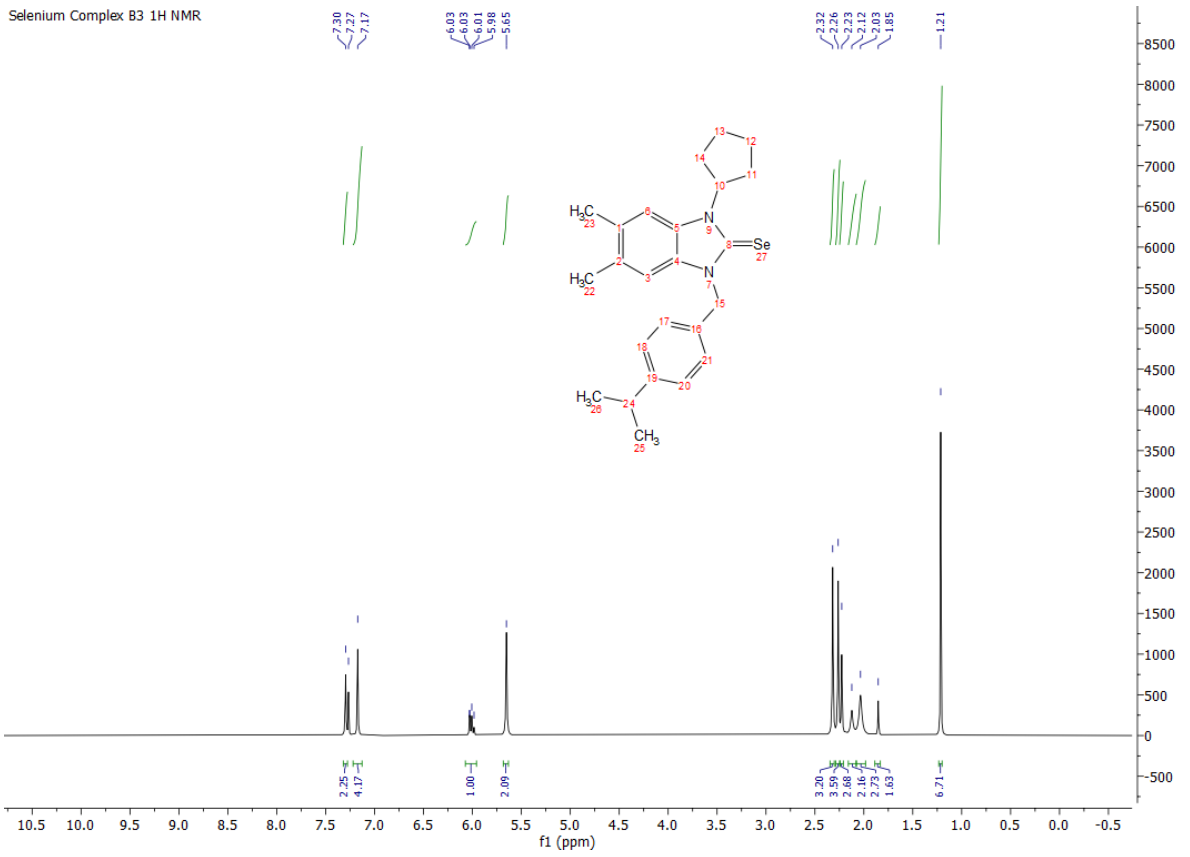
^{13}C NMR Spectrum of compound B1 (DMSO-d^{6})



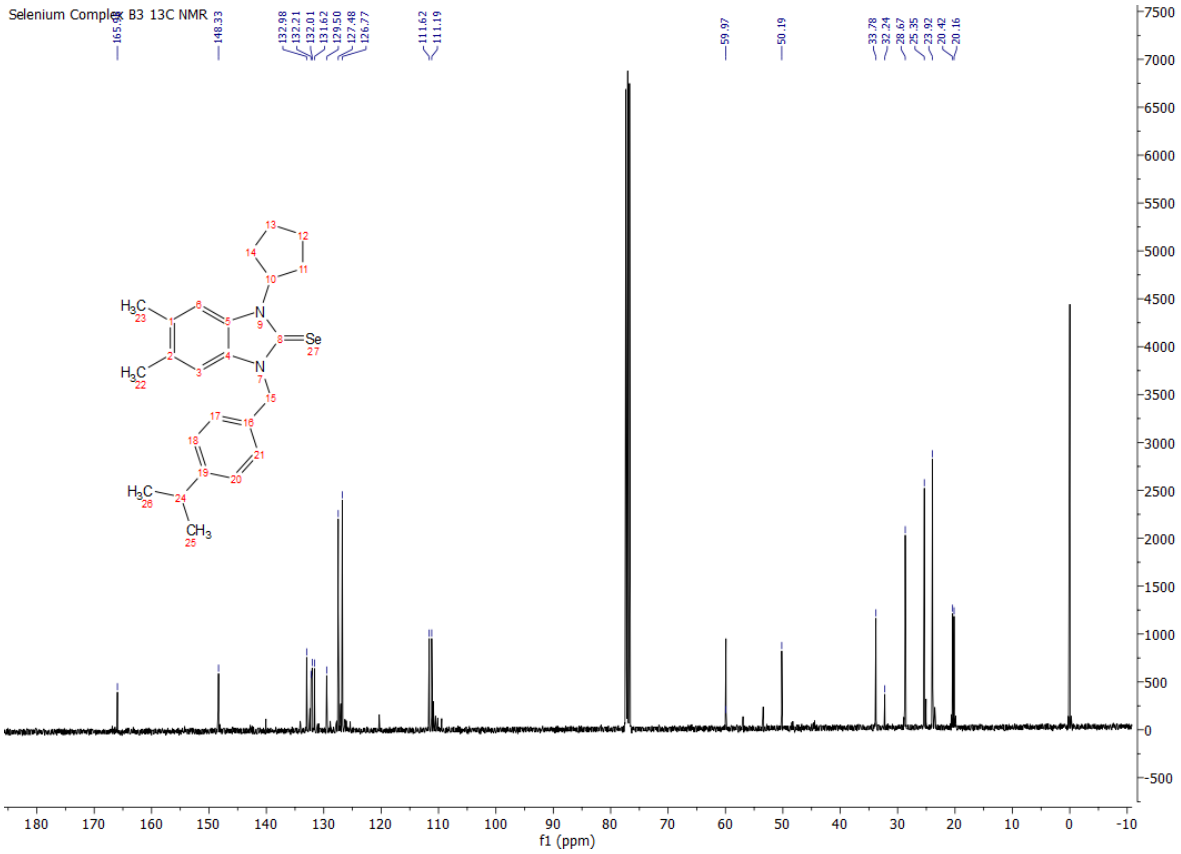
^{1}H NMR Spectrum of compound B2 (DMSO-d^{6})



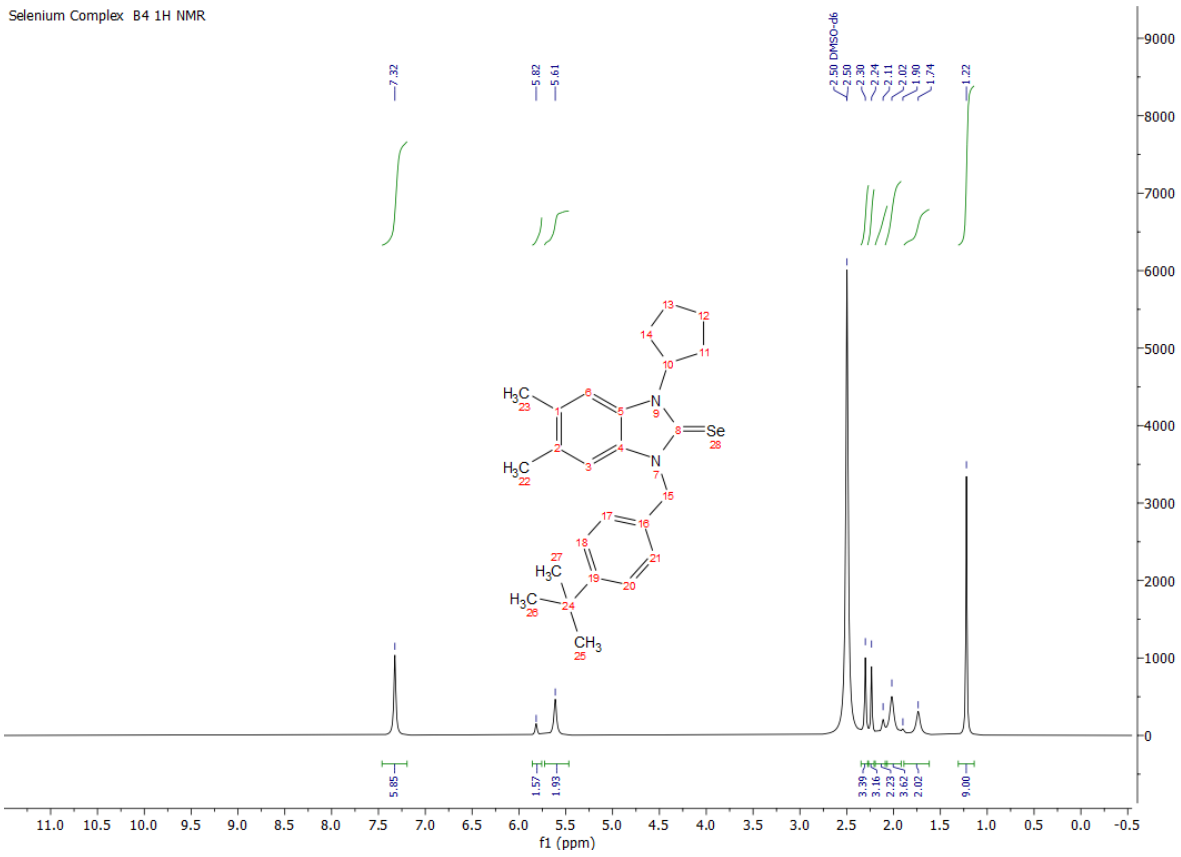
^{13}C NMR Spectrum of compound B2 (DMSO-d^{6})



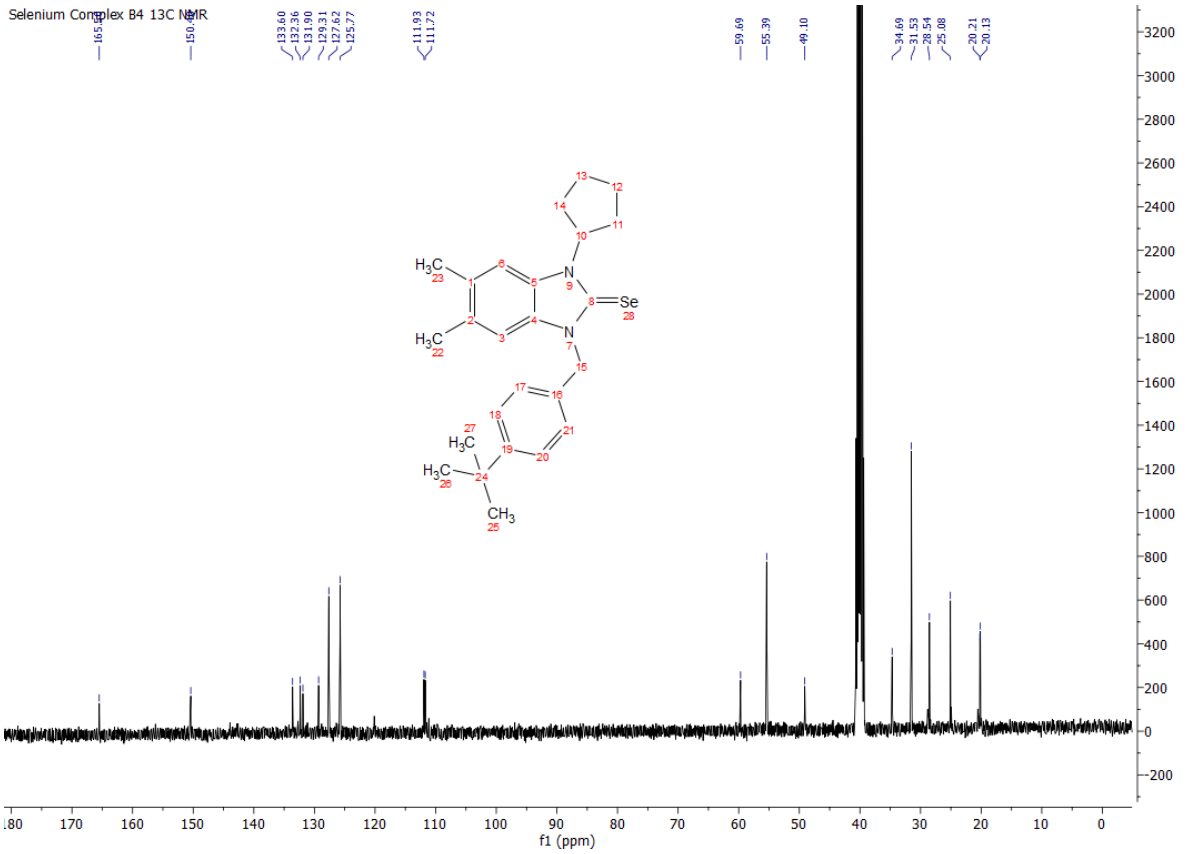
^{1}H NMR Spectrum of compound B3 ($CDCl_3$)



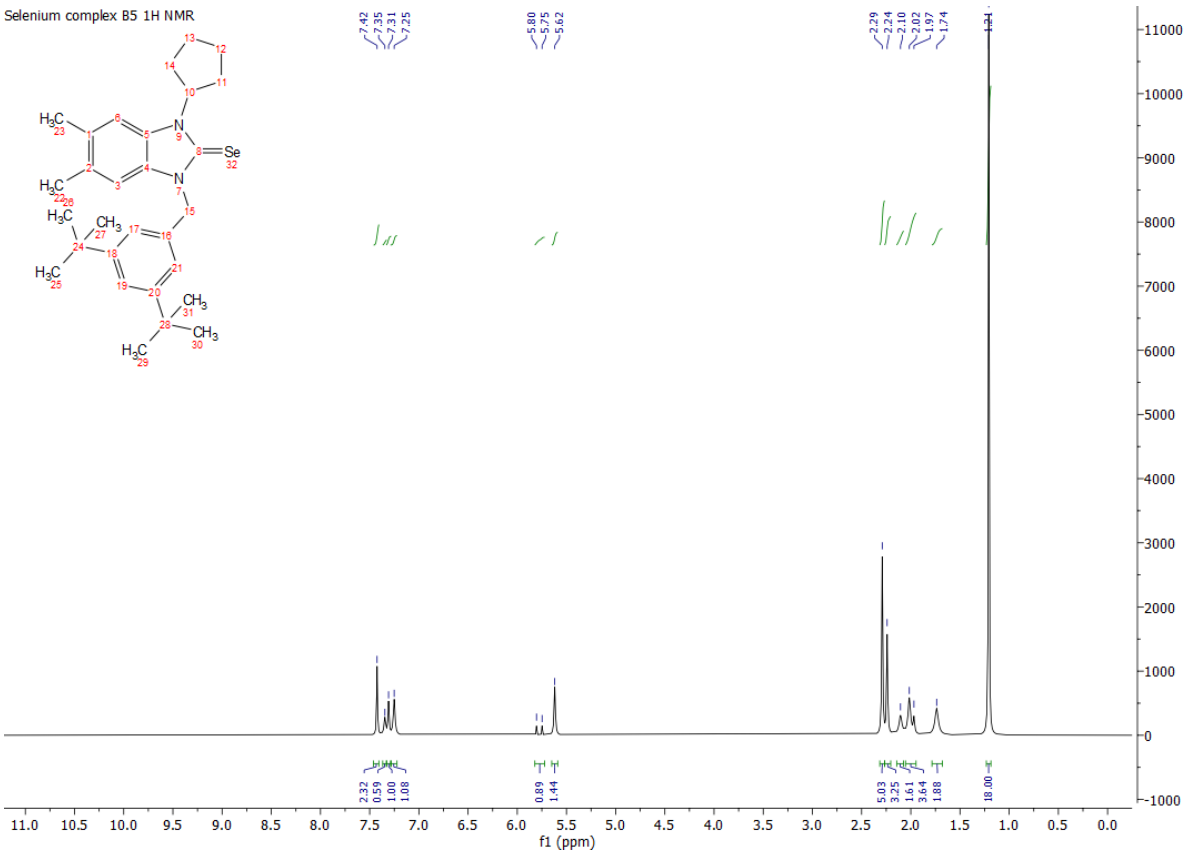
^{13}C NMR Spectrum of compound B3 ($CDCl_3$)



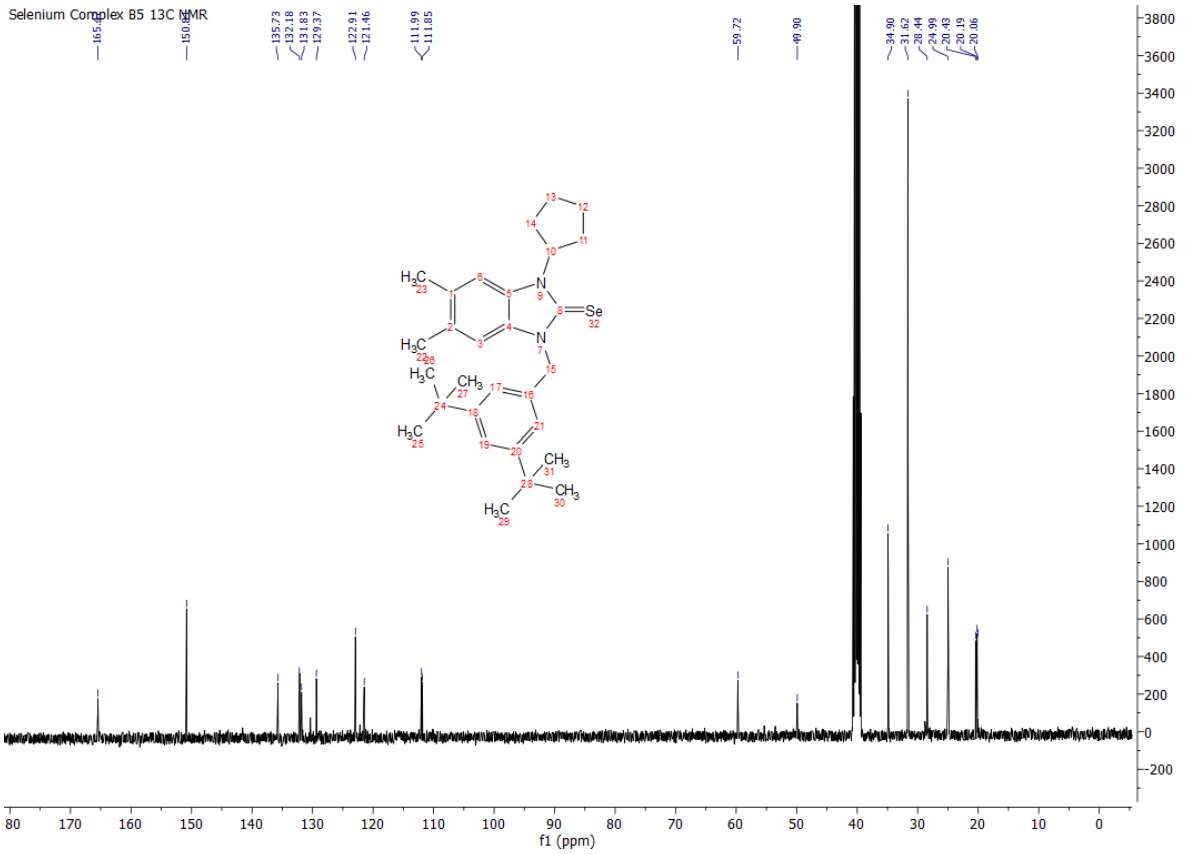
^{1}H NMR Spectrum of compound B4 (DMSO-d^{6})



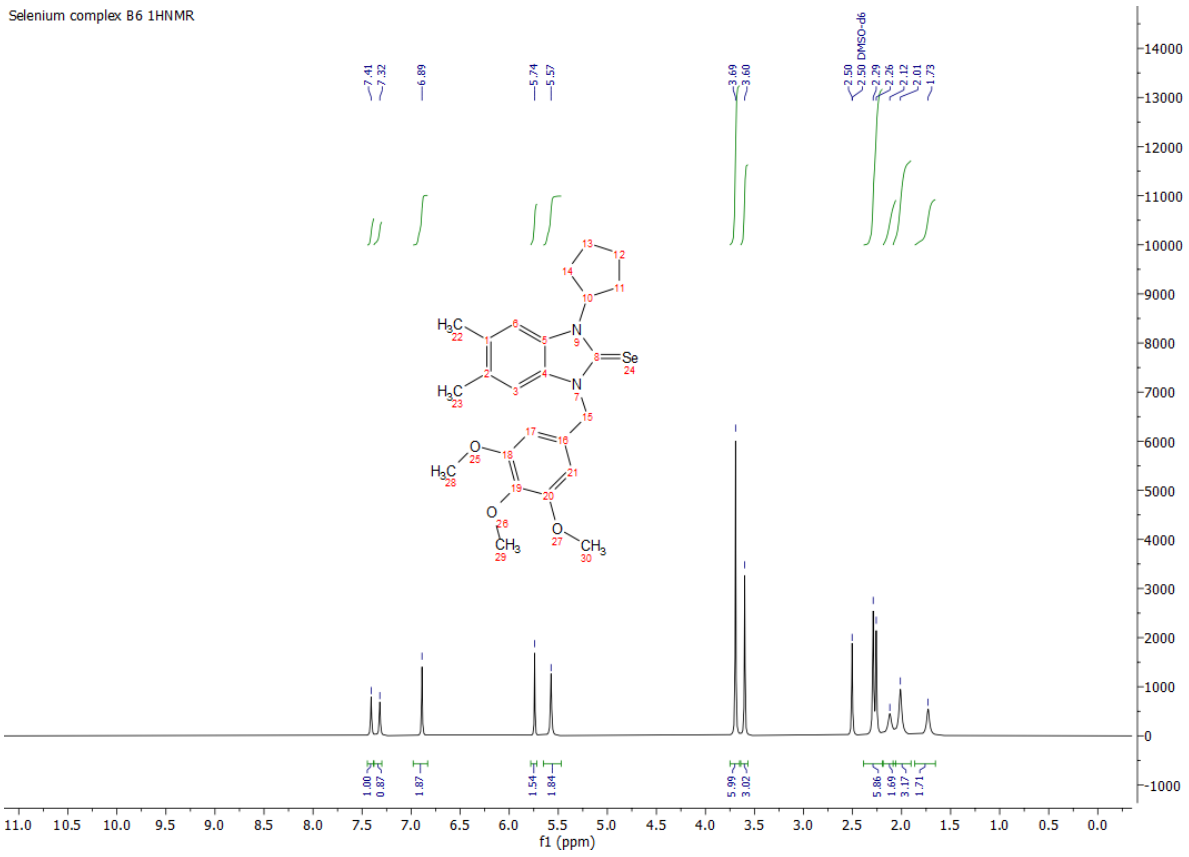
^{13}C NMR Spectrum of compound B4 (DMSO-d^{6})



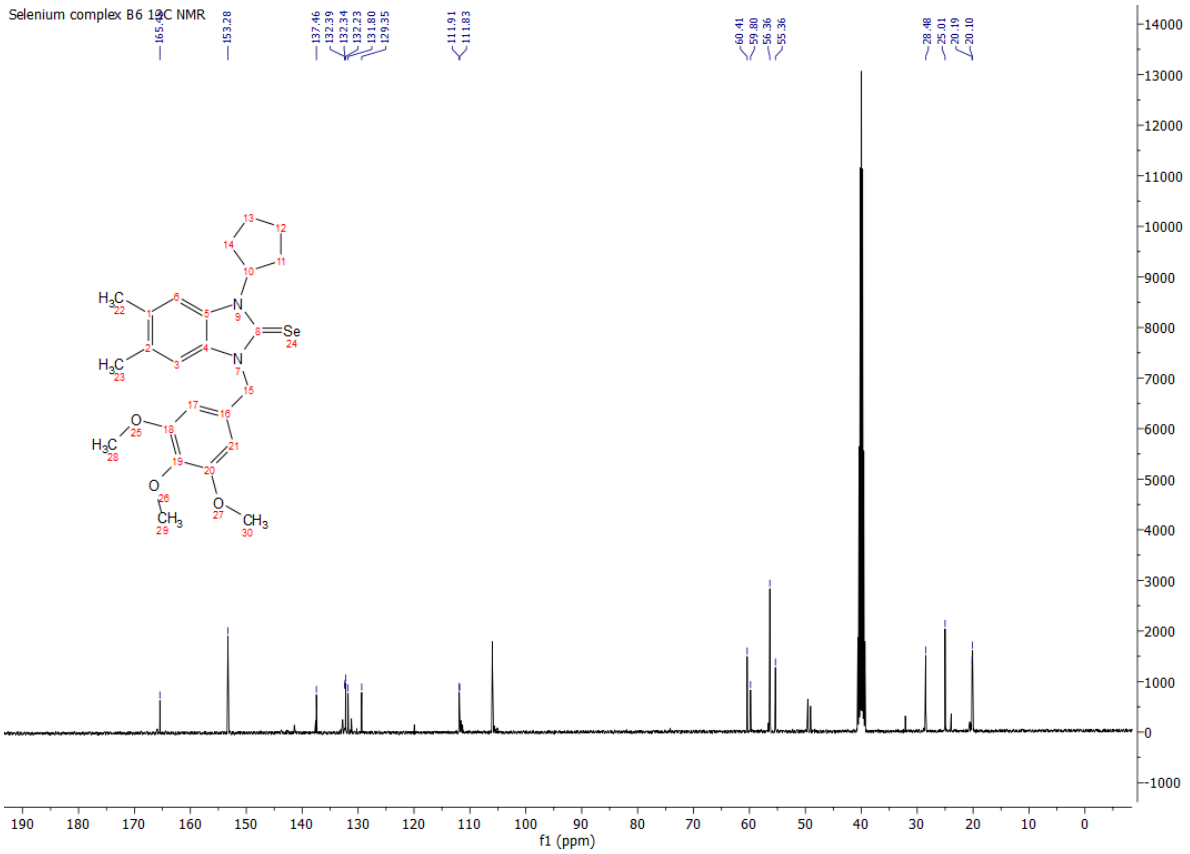
^{1}H NMR Spectrum of compound B5 ($CDCl_3$)



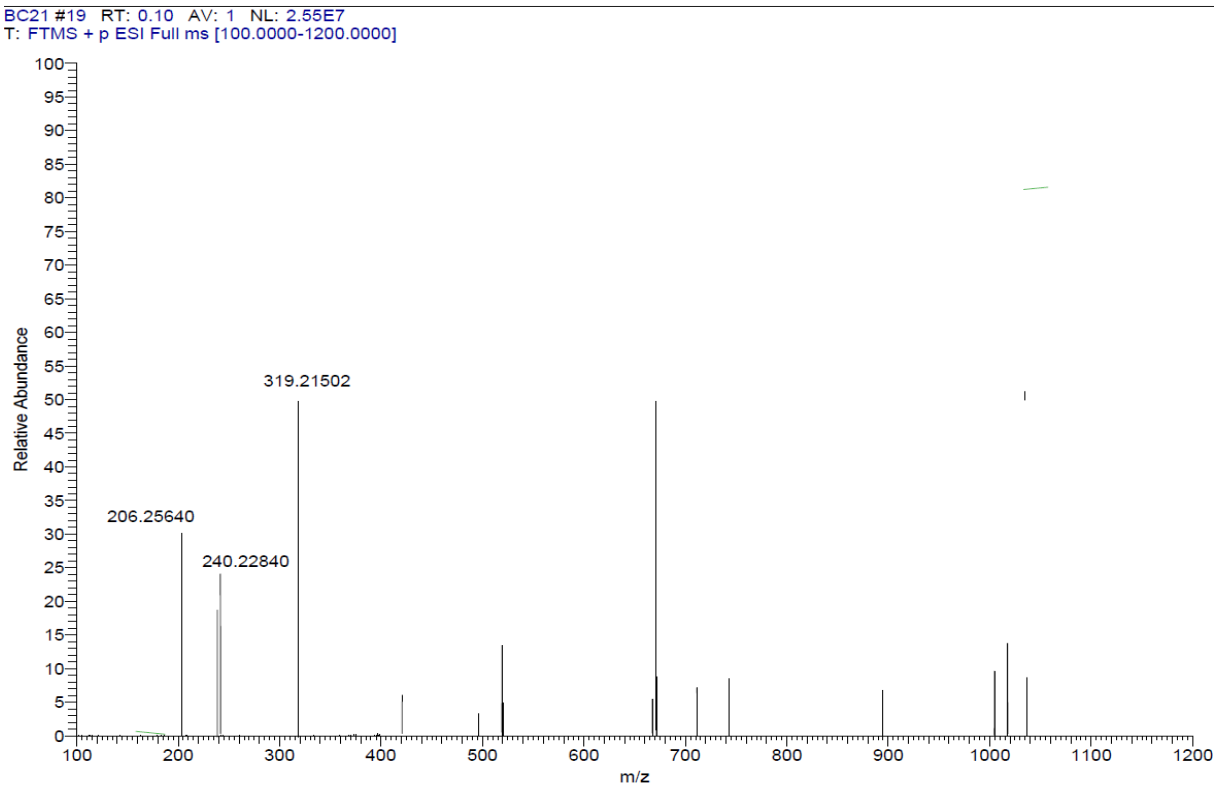
^{13}C NMR Spectrum of compound B5 ($CDCl_3$)



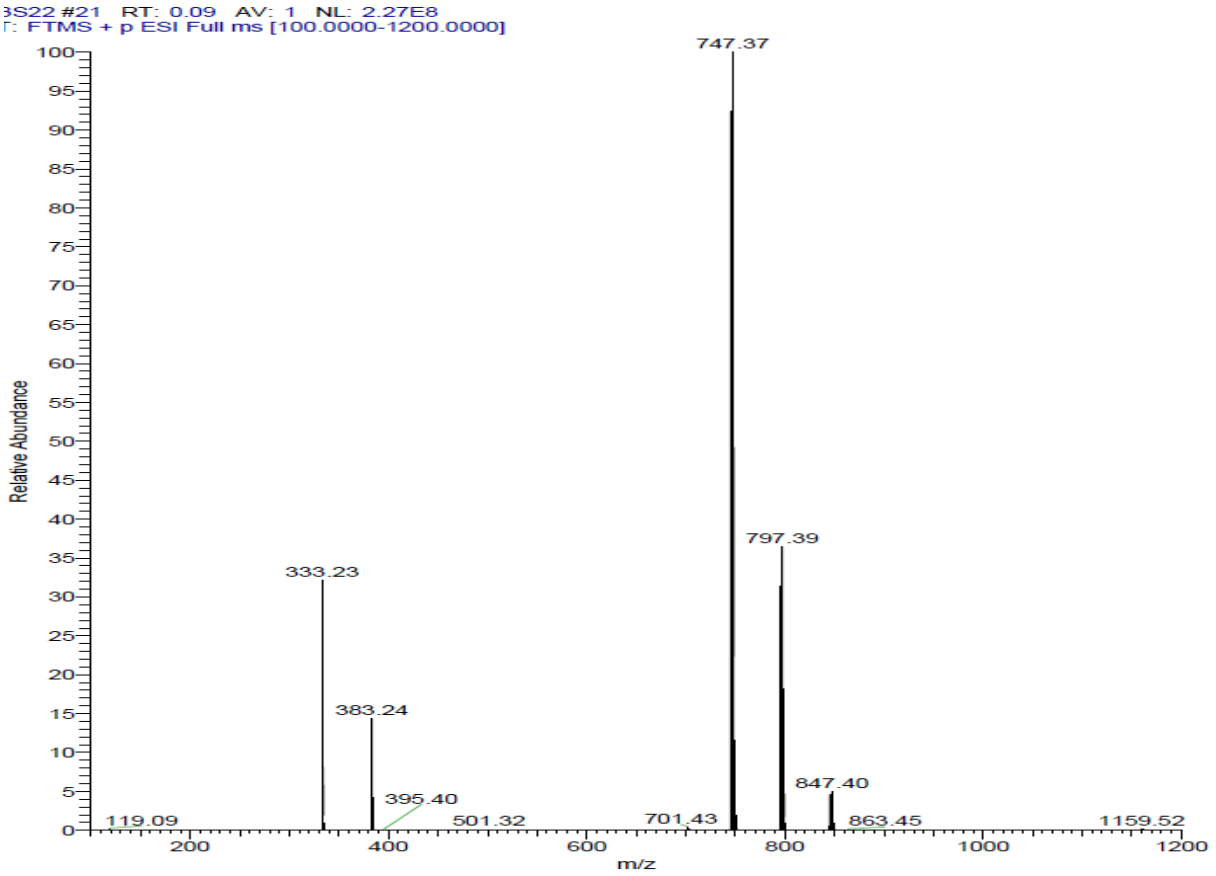
^{1}H NMR Spectrum of compound B6 (DMSO-d^{6})



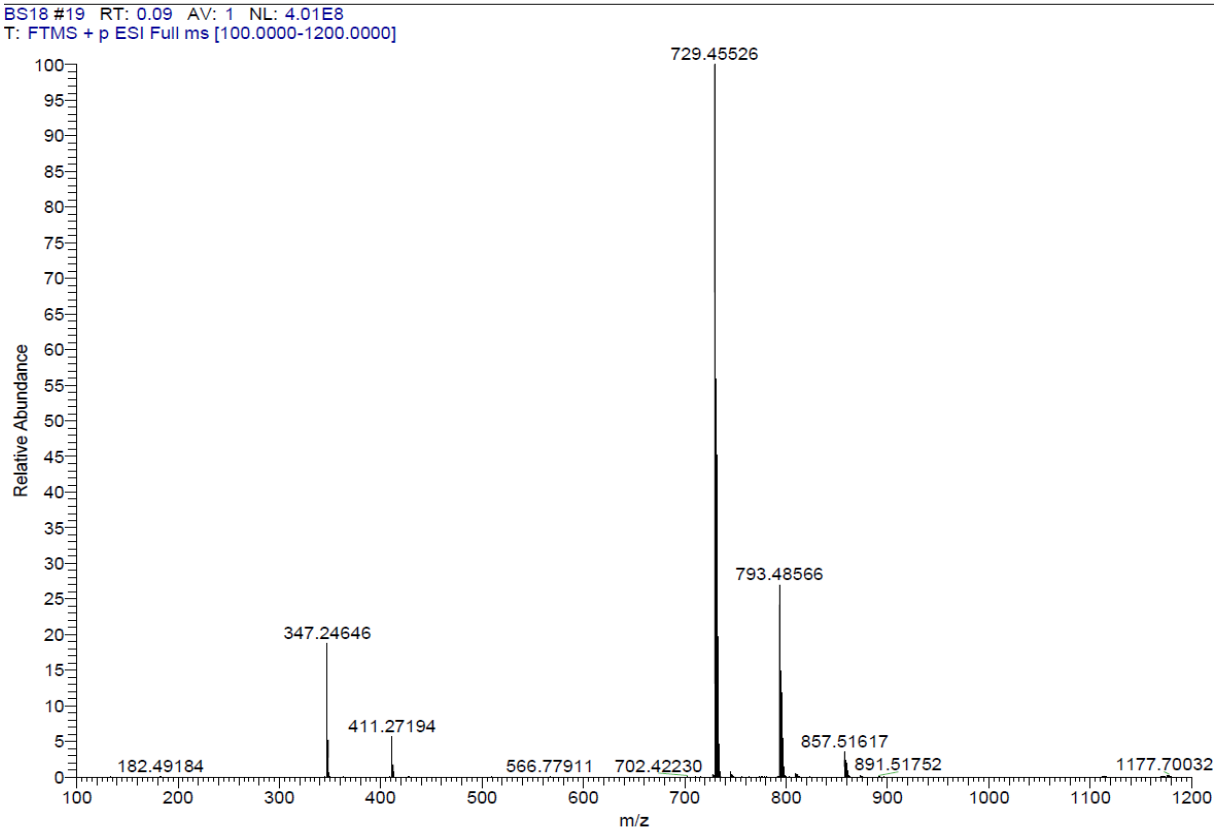
^{13}C NMR Spectrum of compound B4 (DMSO-d^{6})



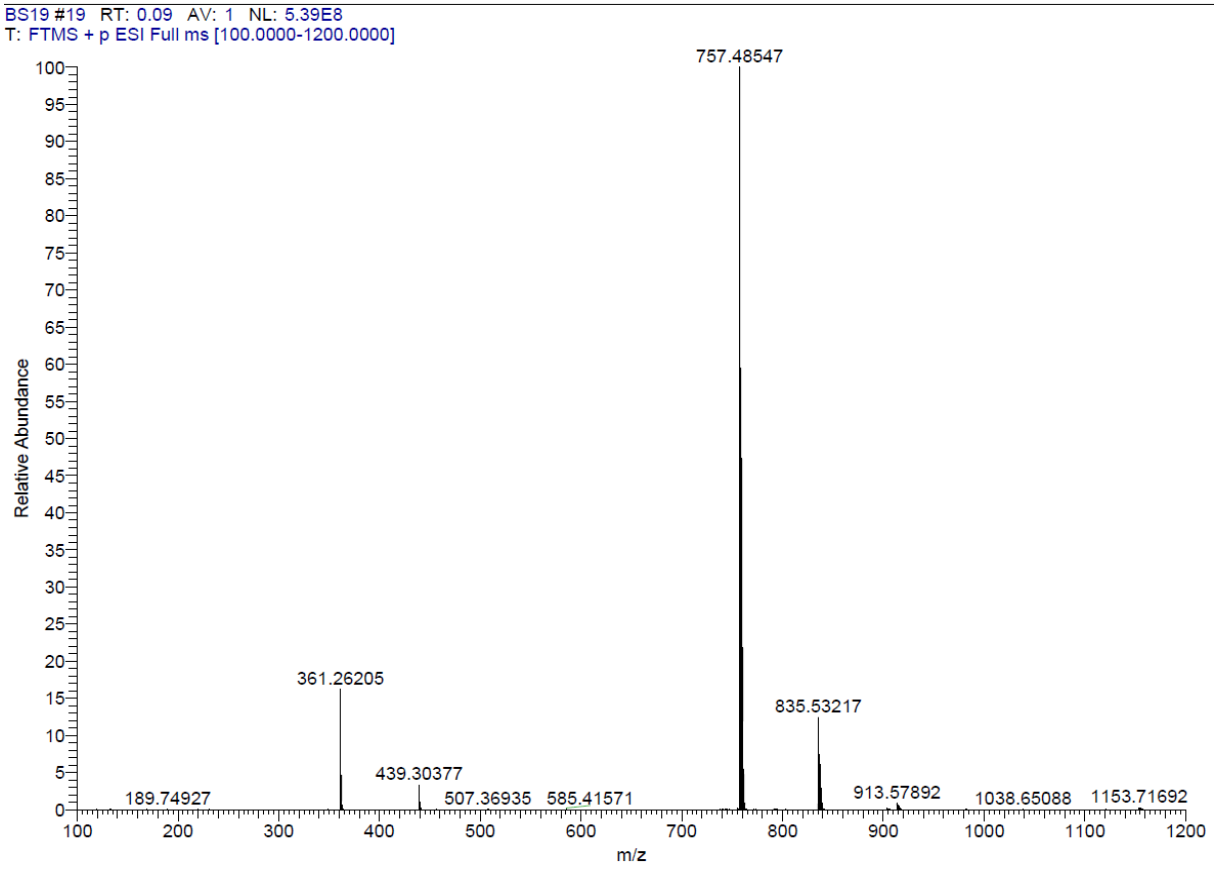
Mass Spectrum of compound A1



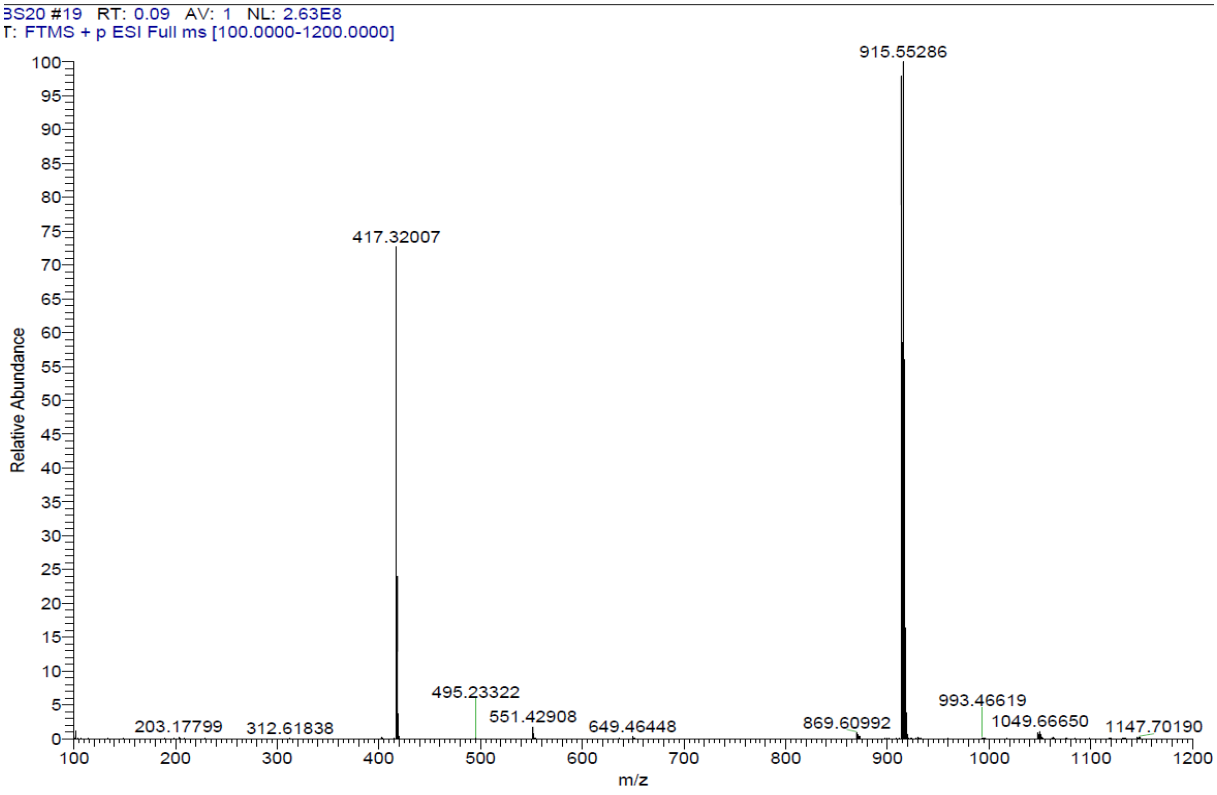
Mass Spectrum of compound A2



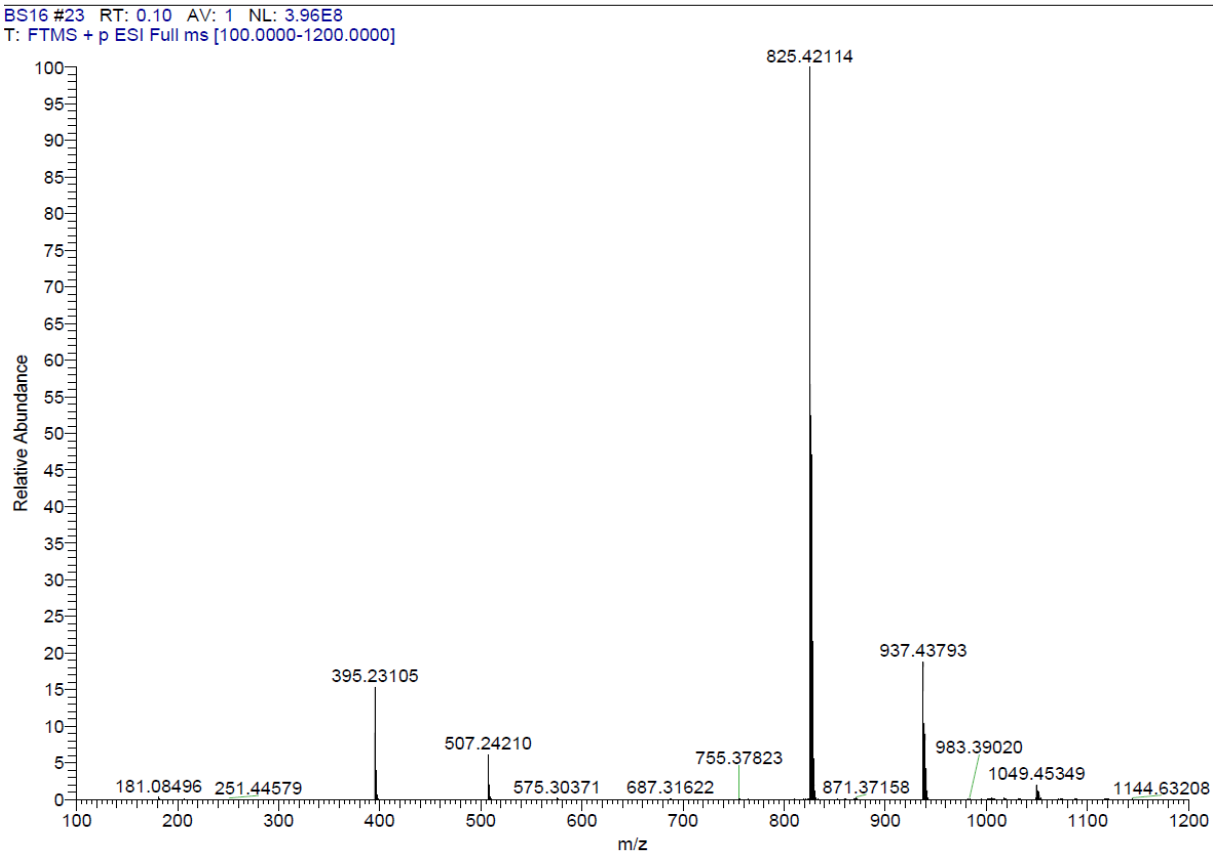
Mass Spectrum of compound A3



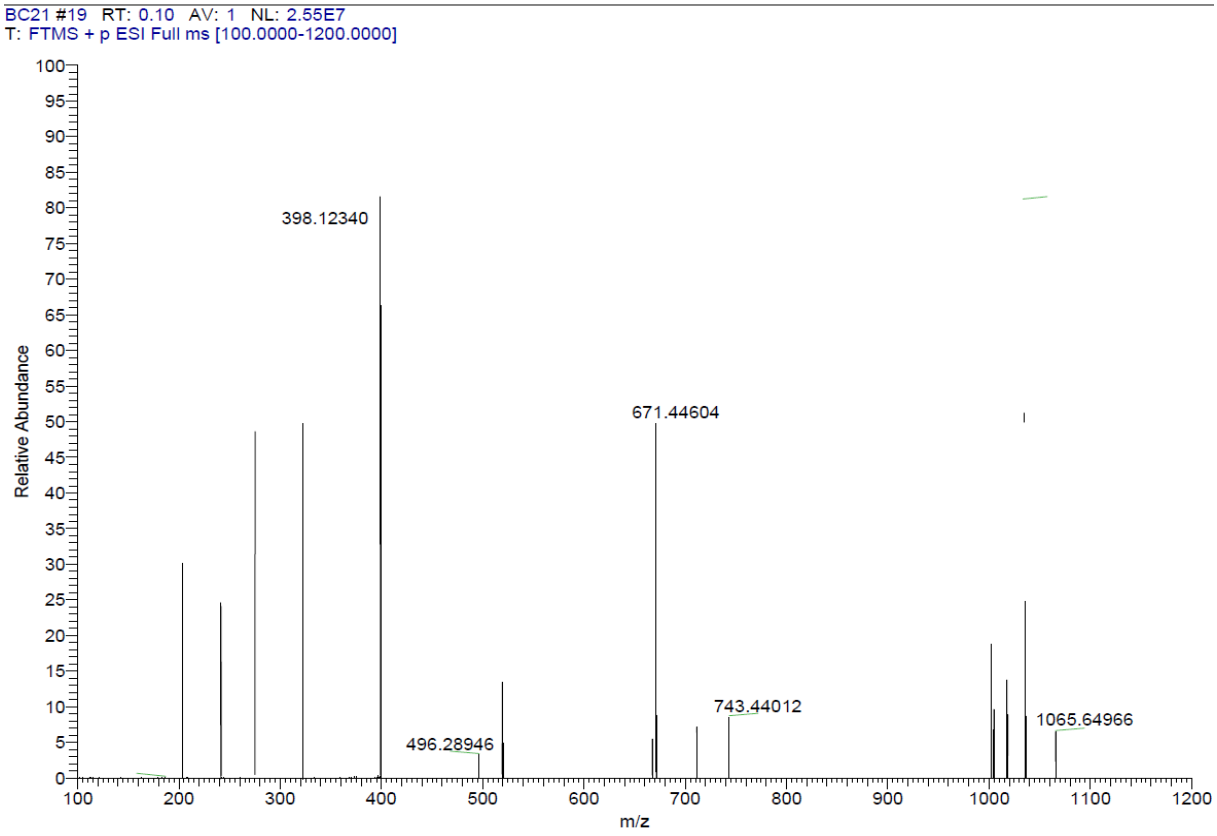
Mass Spectrum of compound A4



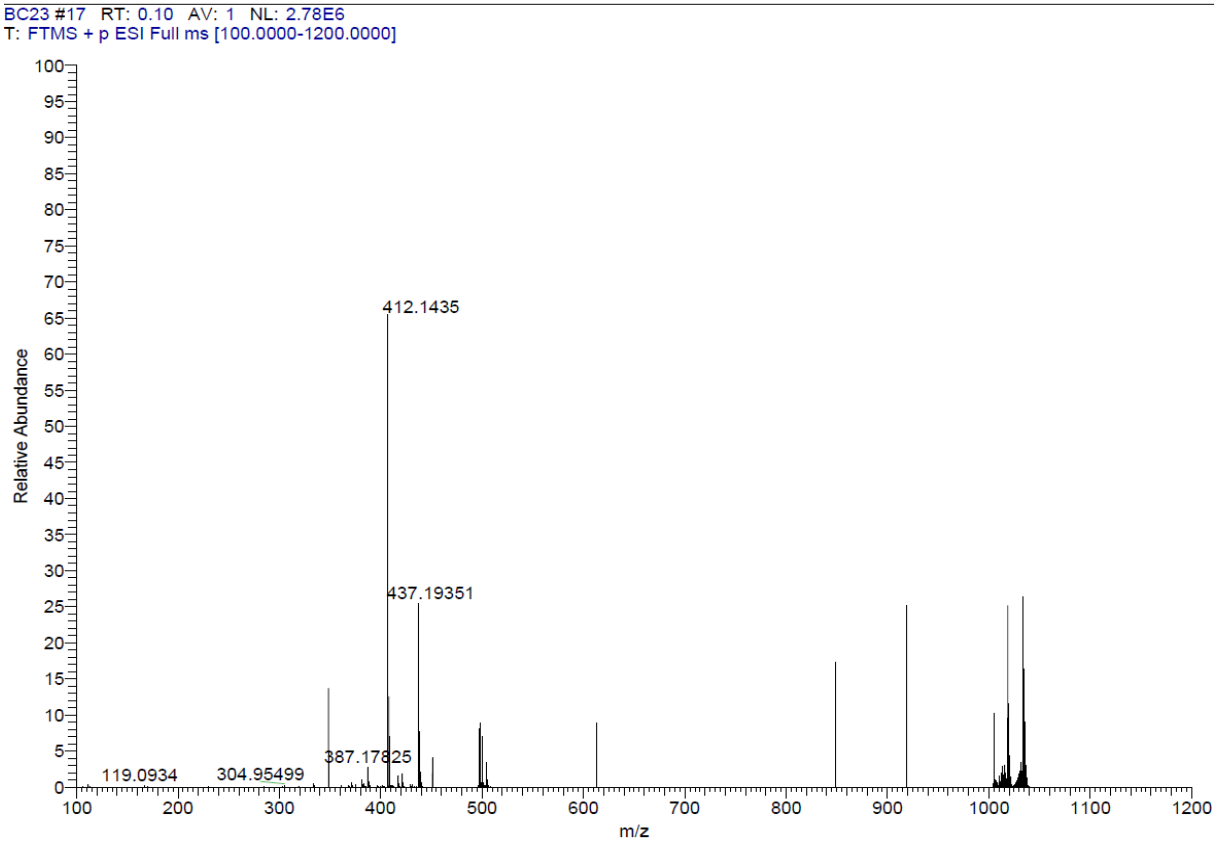
Mass Spectrum of compound A5



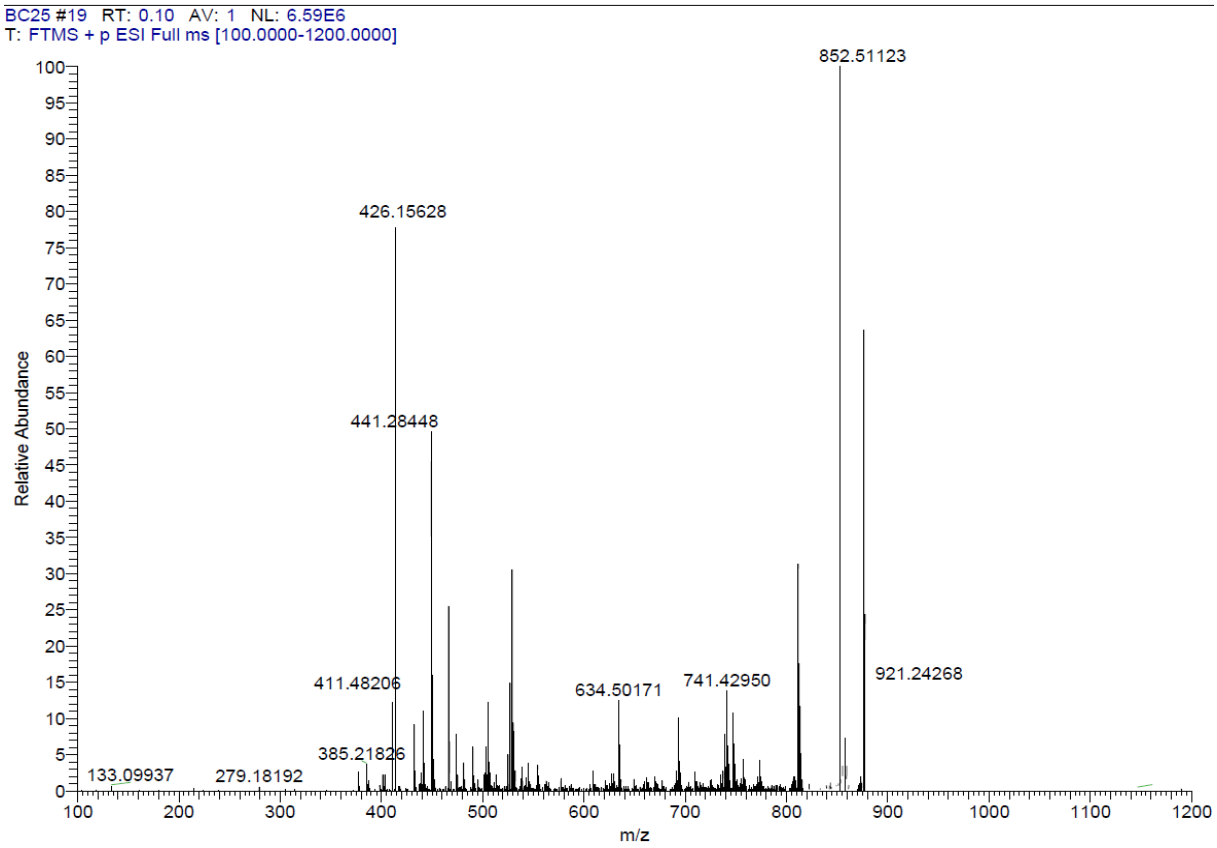
Mass Spectrum of compound A6



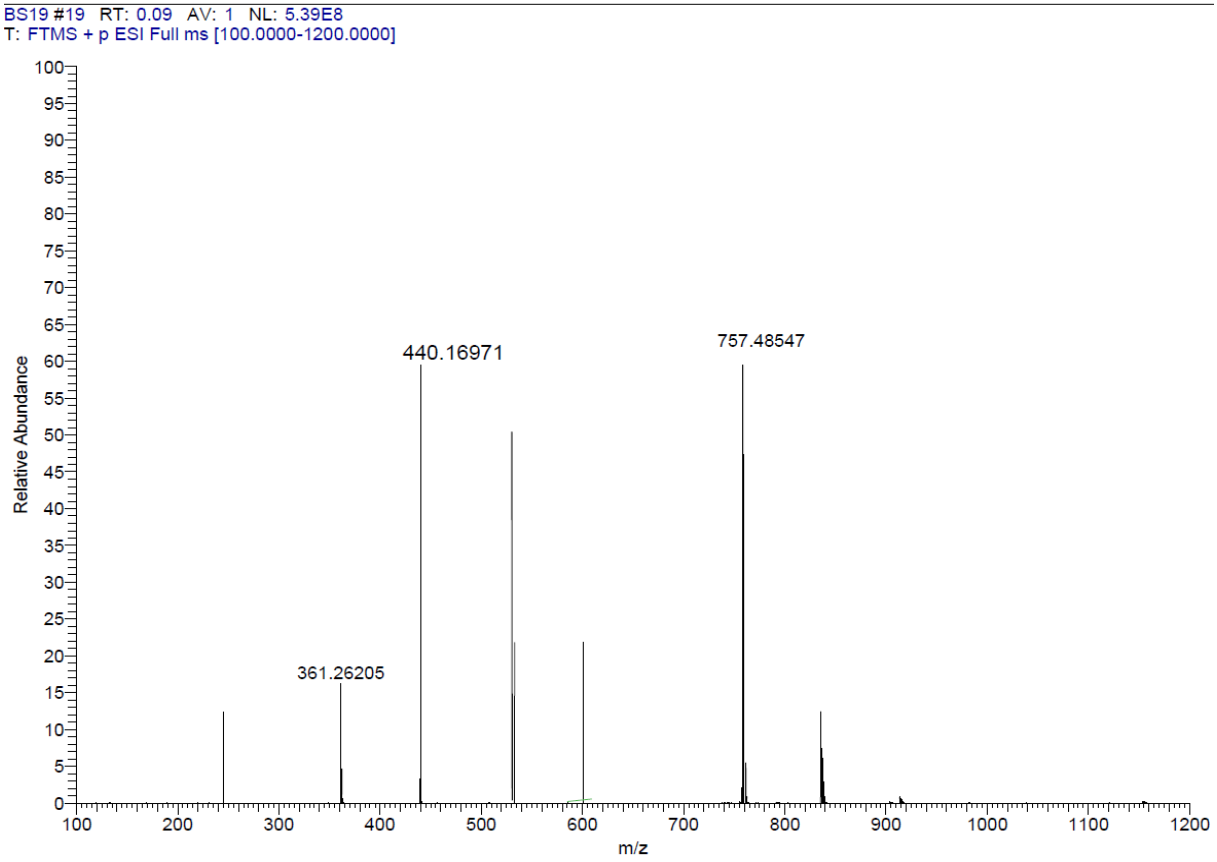
Mass Spectrum of compound B1



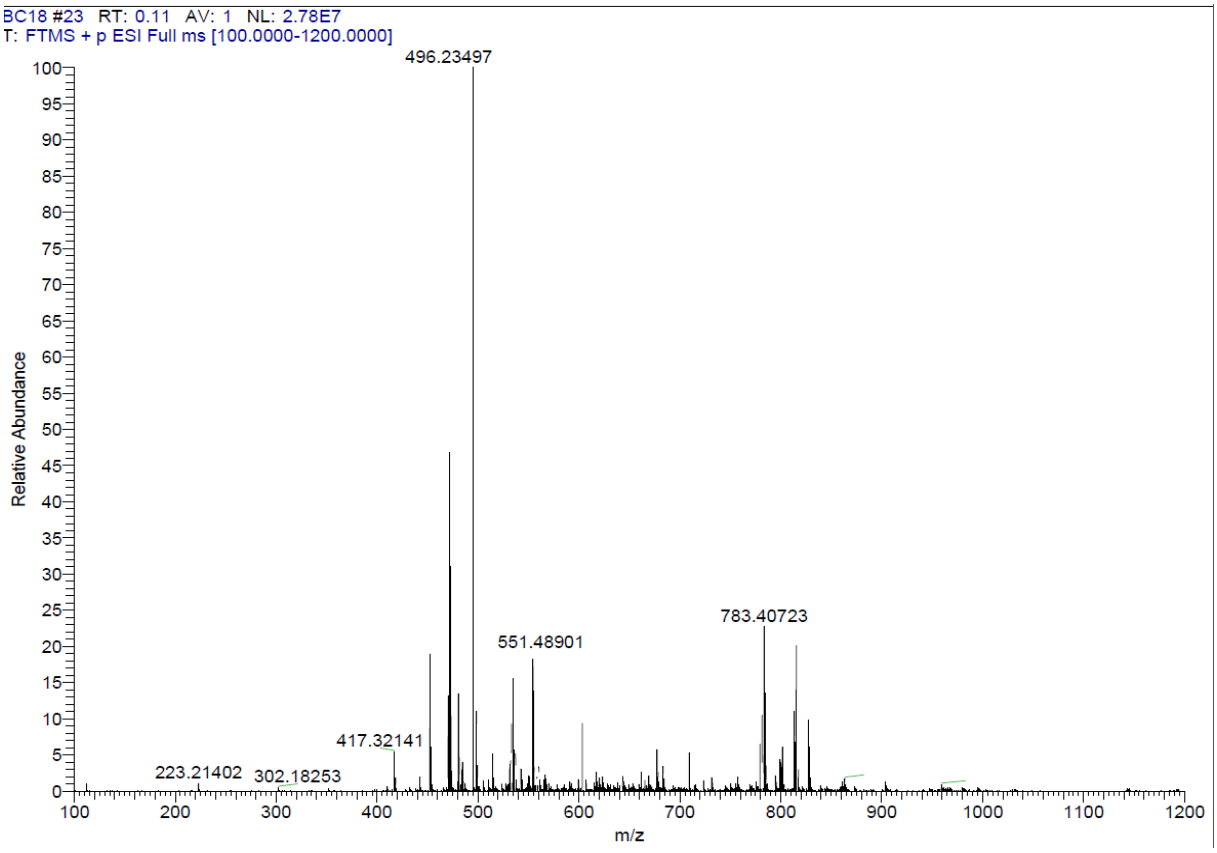
Mass Spectrum of compound B2



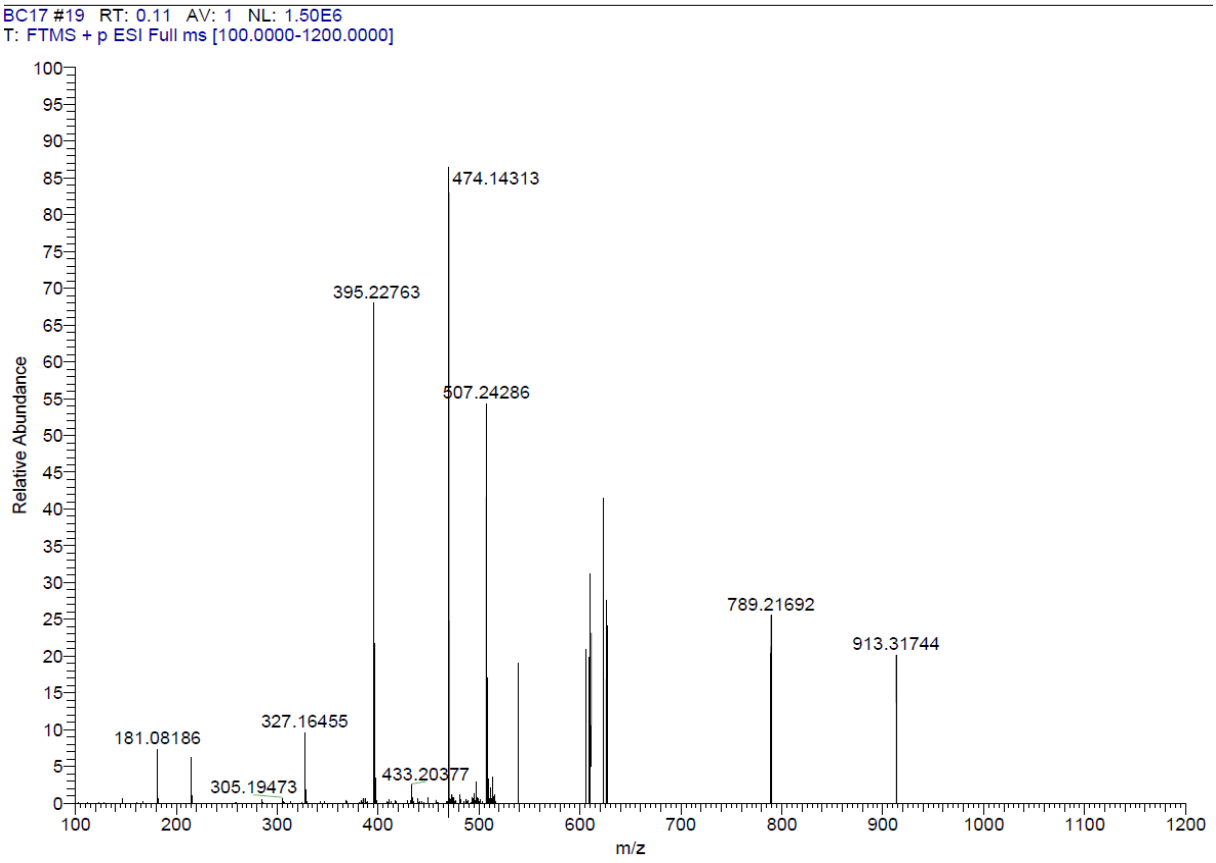
Mass Spectrum of compound B3



Mass Spectrum of compound B4



Mass Spectrum of compound B5



Mass Spectrum of compound B6