

## SUPPORTING INFORMATION

### **Charge transfer facilitated direct electrophilic substitution in phenylaminonaphthoquinones: Experimental, theoretical and electrochemical studies**

A. Satheshkumar, K. Ganesh and Kuppanagounder P. Elango\*

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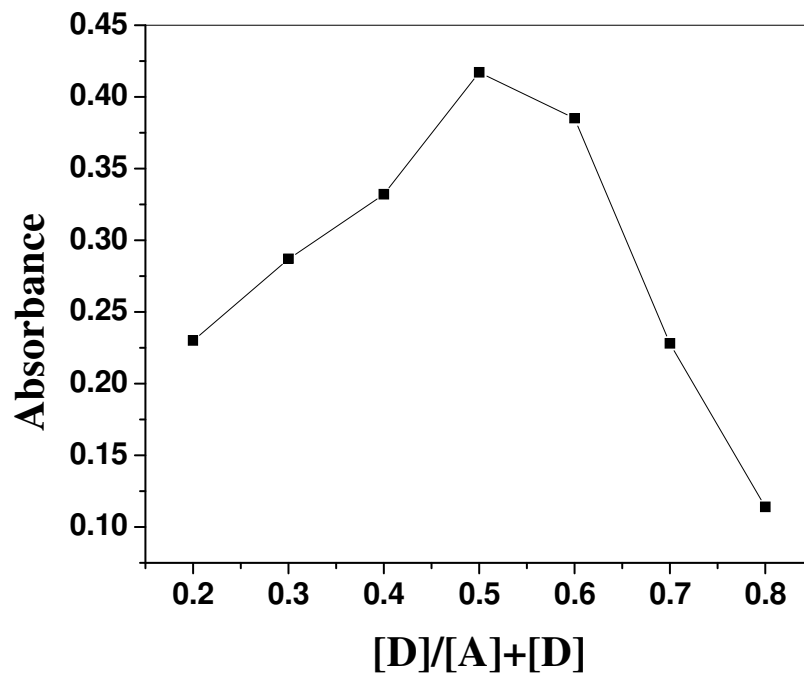


Figure S1 : Job's continuous variation plot for **1a** with HMB

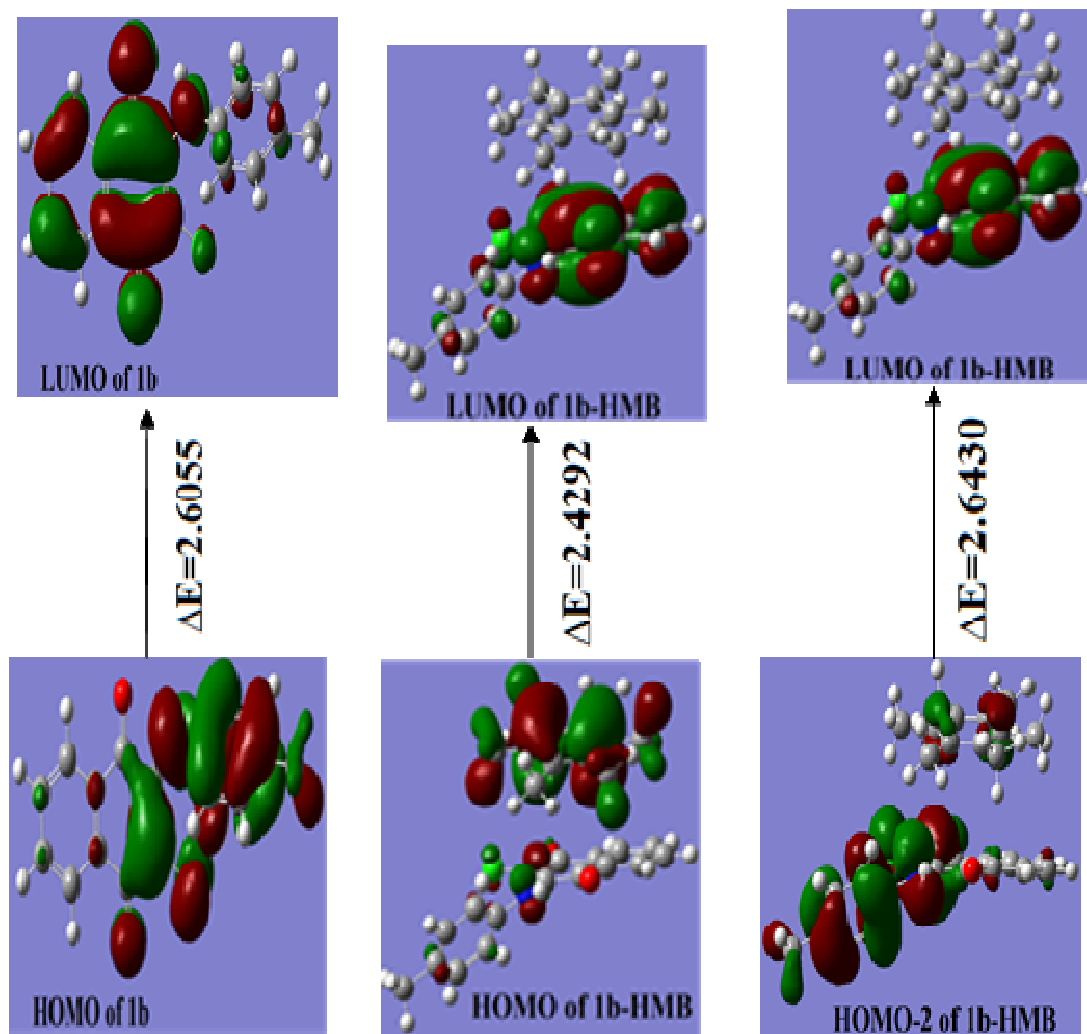


Figure S2 : Frontier molecular orbitals of **1b** and **1b-HMB** and their  $\Delta E$  values.

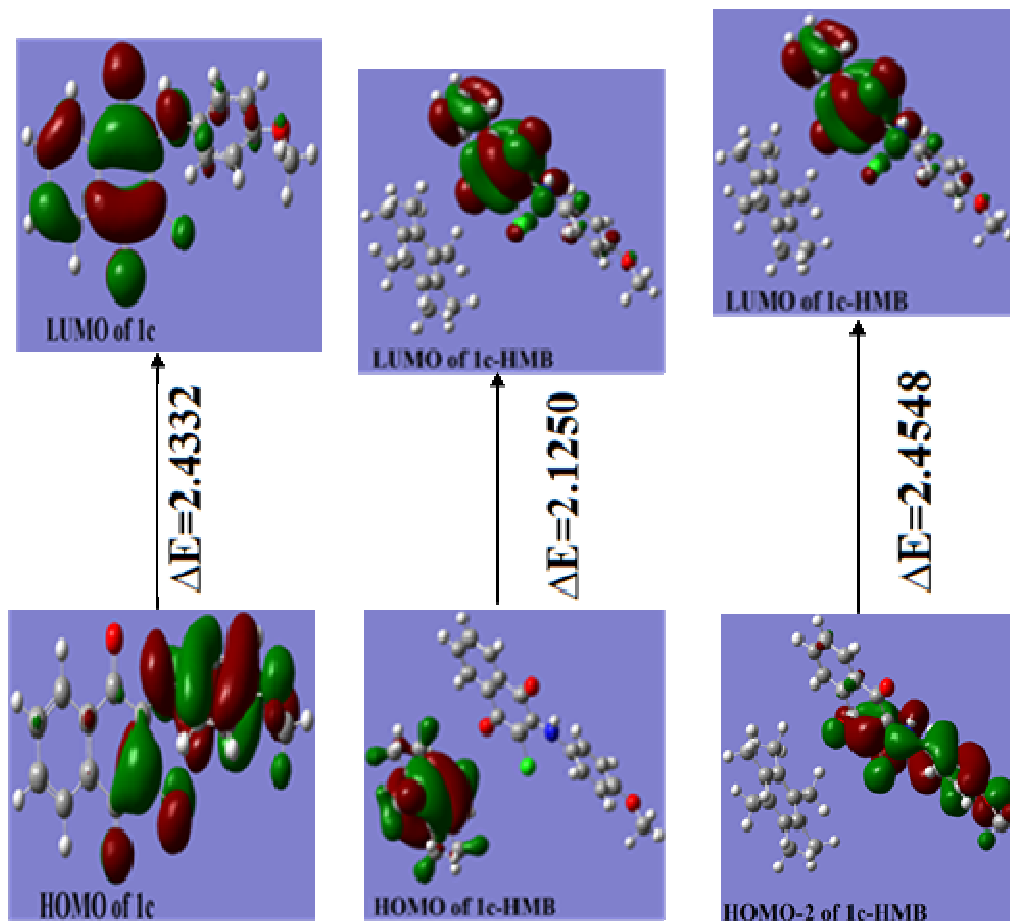


Figure S3 : Frontier molecular orbitals of **1c** and **1c-HMB** and their  $\Delta E$  values.

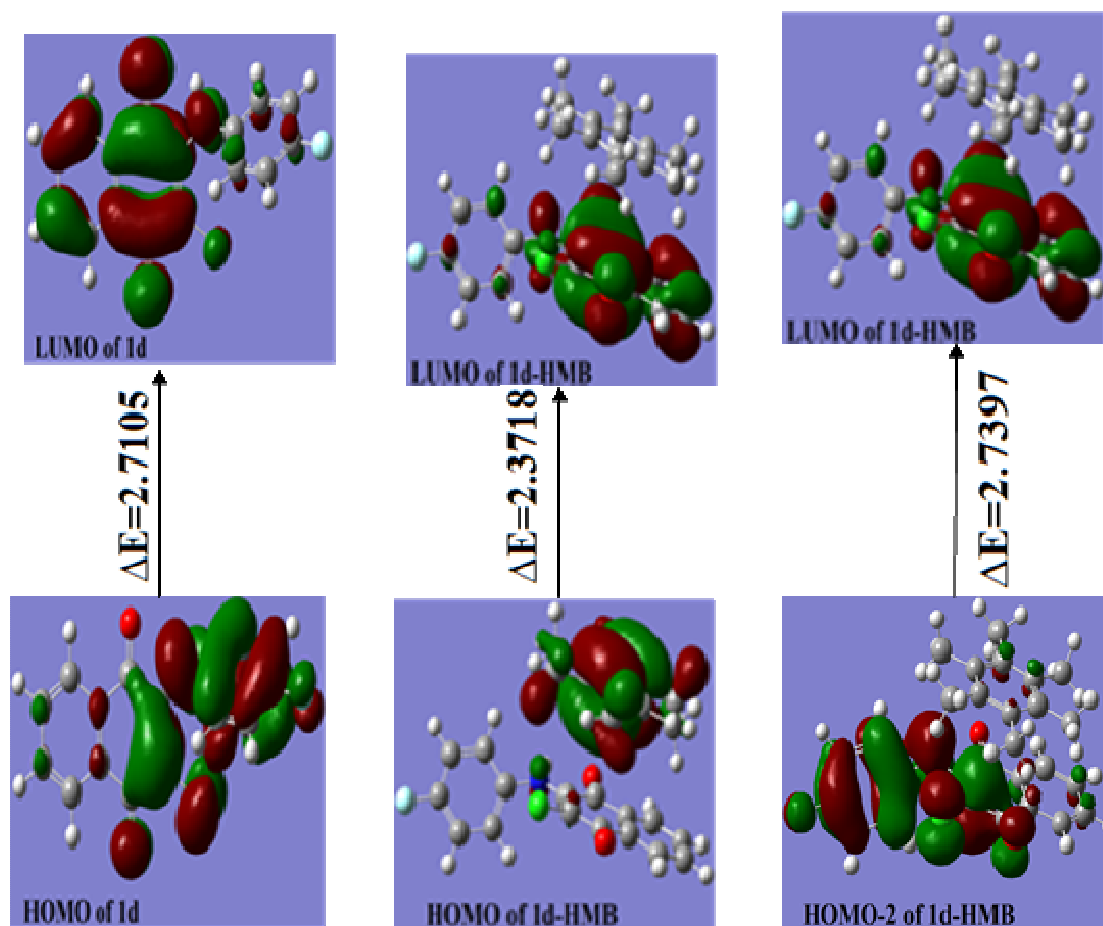


Figure S4 : Frontier molecular orbitals of **1d** and **1d-HMB** and their  $\Delta E$  values.

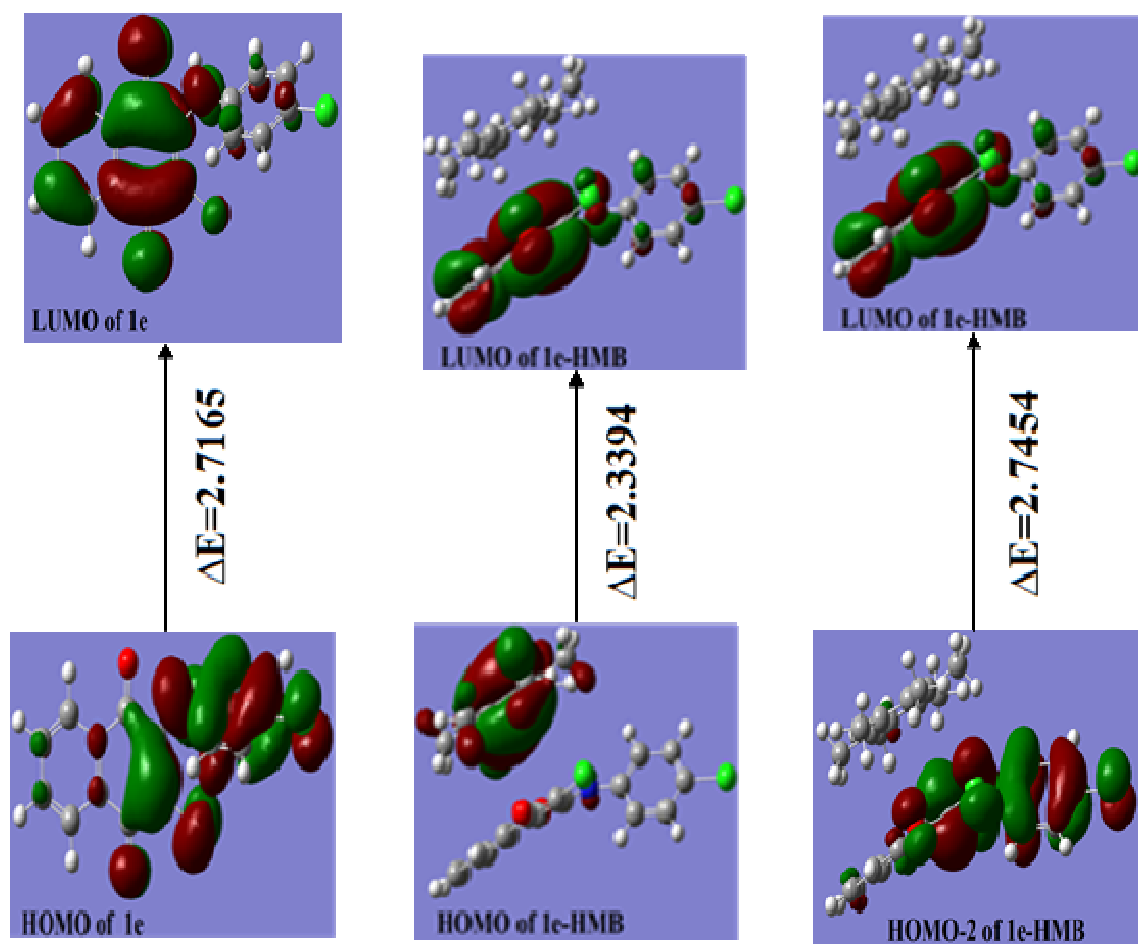


Figure S5 : Frontier molecular orbitals of **1e** and **1e-HMB** and their  $\Delta E$  values.

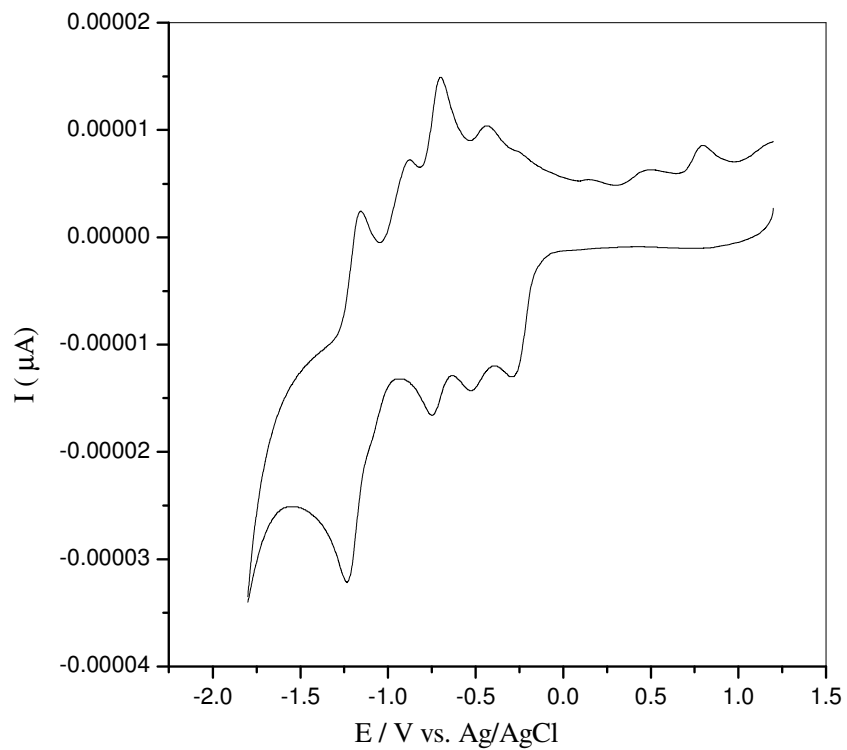


Figure S6. Cyclic voltammogram of 1 mM **3a** in 0.1 M tetrabutyl ammonium perchlorate in ACN obtained in glassy carbon electrode scan rate 100 mV/s.

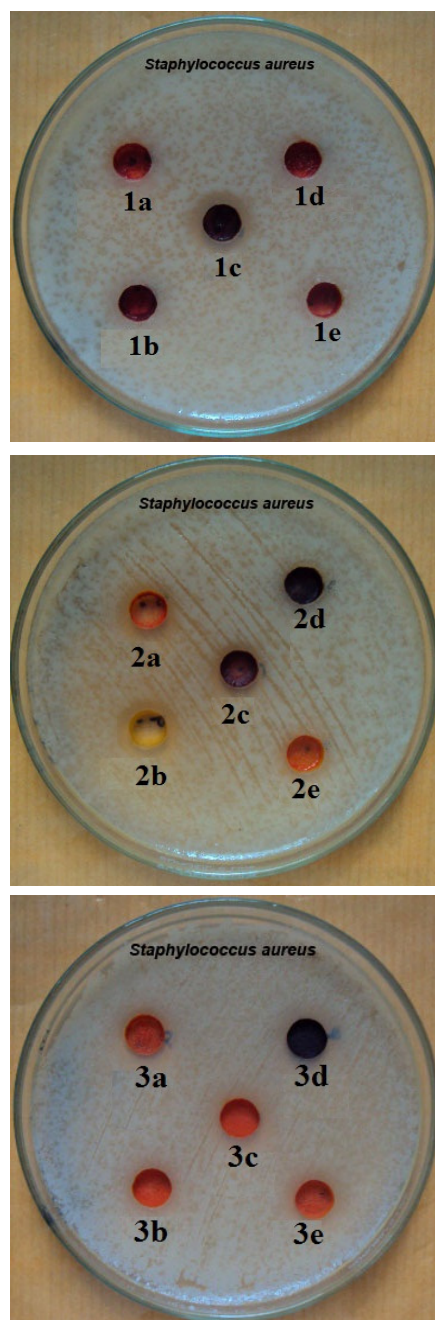
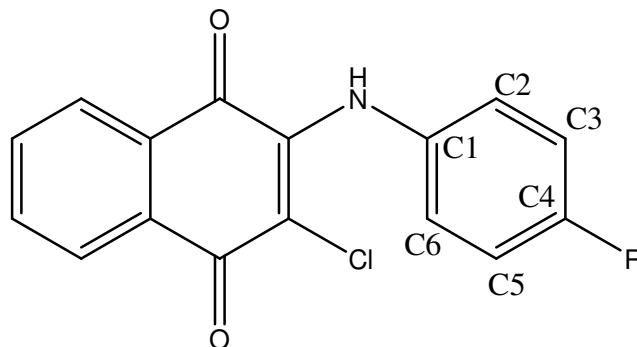


Figure S7: Zone of inhibition for *Staphylococcus aureus* (Compound labeled as Table S3).



**Table S1** Mulliken charges at B3LYP/6-31G Level on the C-atoms of **1a-e**



R	N	C1	C2	C3	C4	C5	C6
Me	-0.831	0.294	-0.135	-0.167	0.126	-0.176	-0.079
OMe	-0.831	0.296	-0.140	-0.135	0.294	-0.154	-0.093
H	-0.83	0.294	-0.136	-0.138	-0.110	-0.148	-0.08
Cl	-0.832	0.301	-0.133	-0.11	-0.225	-0.12	-0.076
F	-0.832	0.296	-0.137	-0.151	0.298	-0.161	-0.081

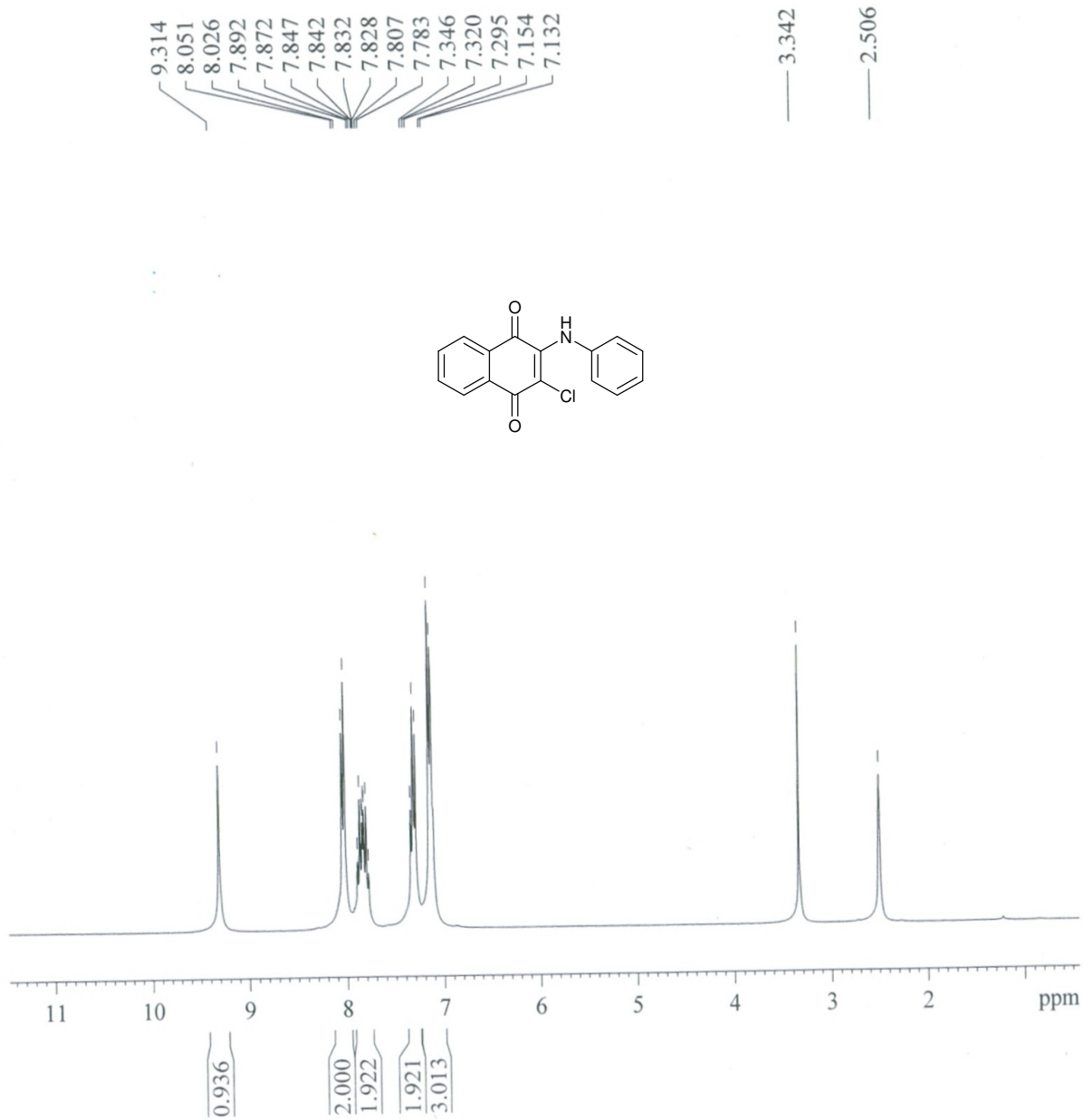
**Table S2** Mulliken charges at B3LYP/6-31G Level on the C-atoms of (**1a-e**) with HMB

CTadduct

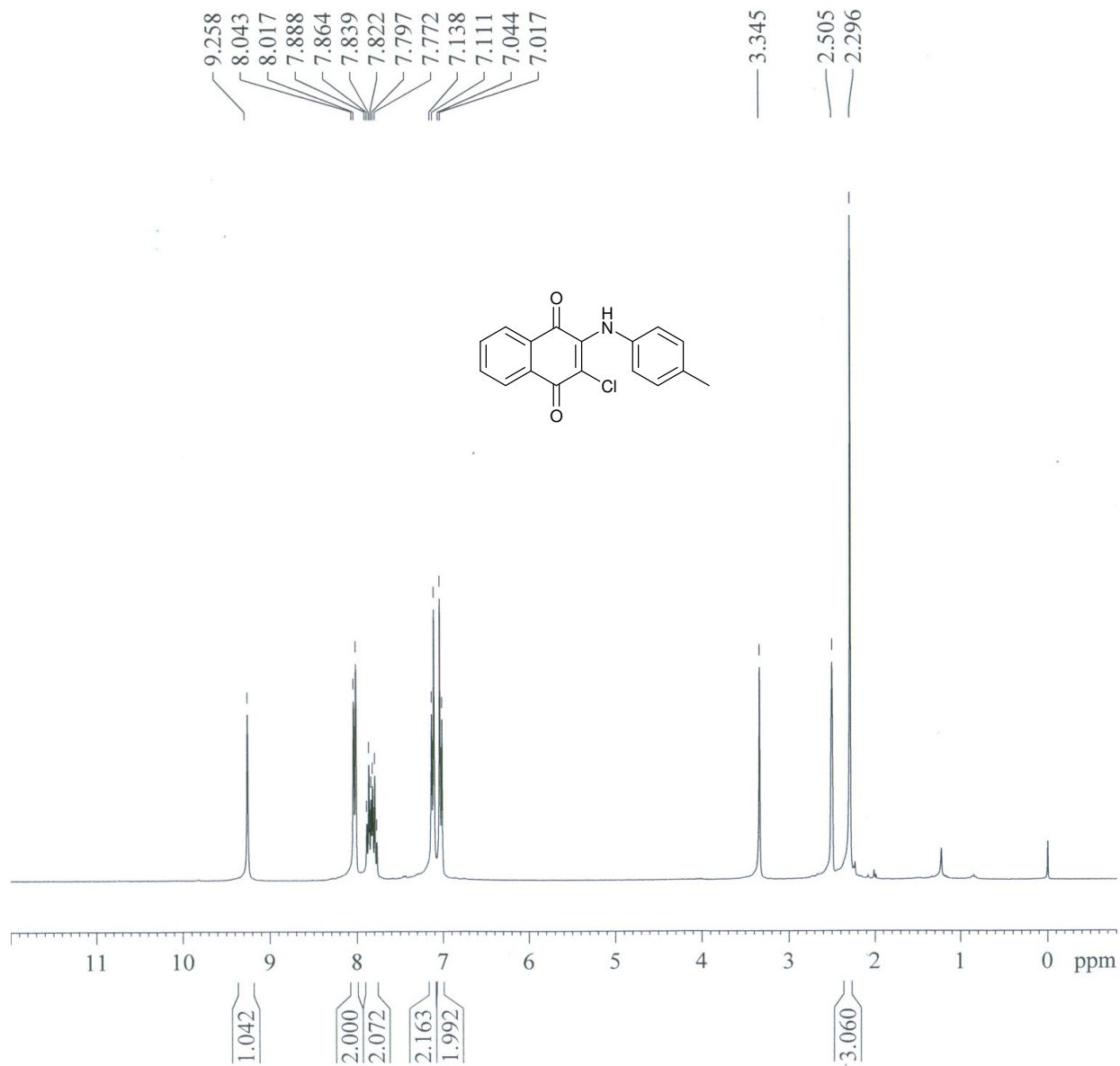
R	N	C1	C2	C3	C4	C5	C6
Me	-0.833	0.292	-0.140	-0.169	0.126	-0.176	-0.080
OMe	-0.830	0.289	-0.144	-0.145	0.299	-0.154	-0.083
H	-0.830	0.289	-0.139	-0.134	-0.114	-0.158	-0.089
Cl	-0.832	0.303	-0.138	-0.110	-0.226	-0.120	-0.077
F	-0.836	0.298	-0.142	-0.151	0.297	-0.161	-0.081

**Table S3** Zones of inhibition (mm) of the compounds at 100µl

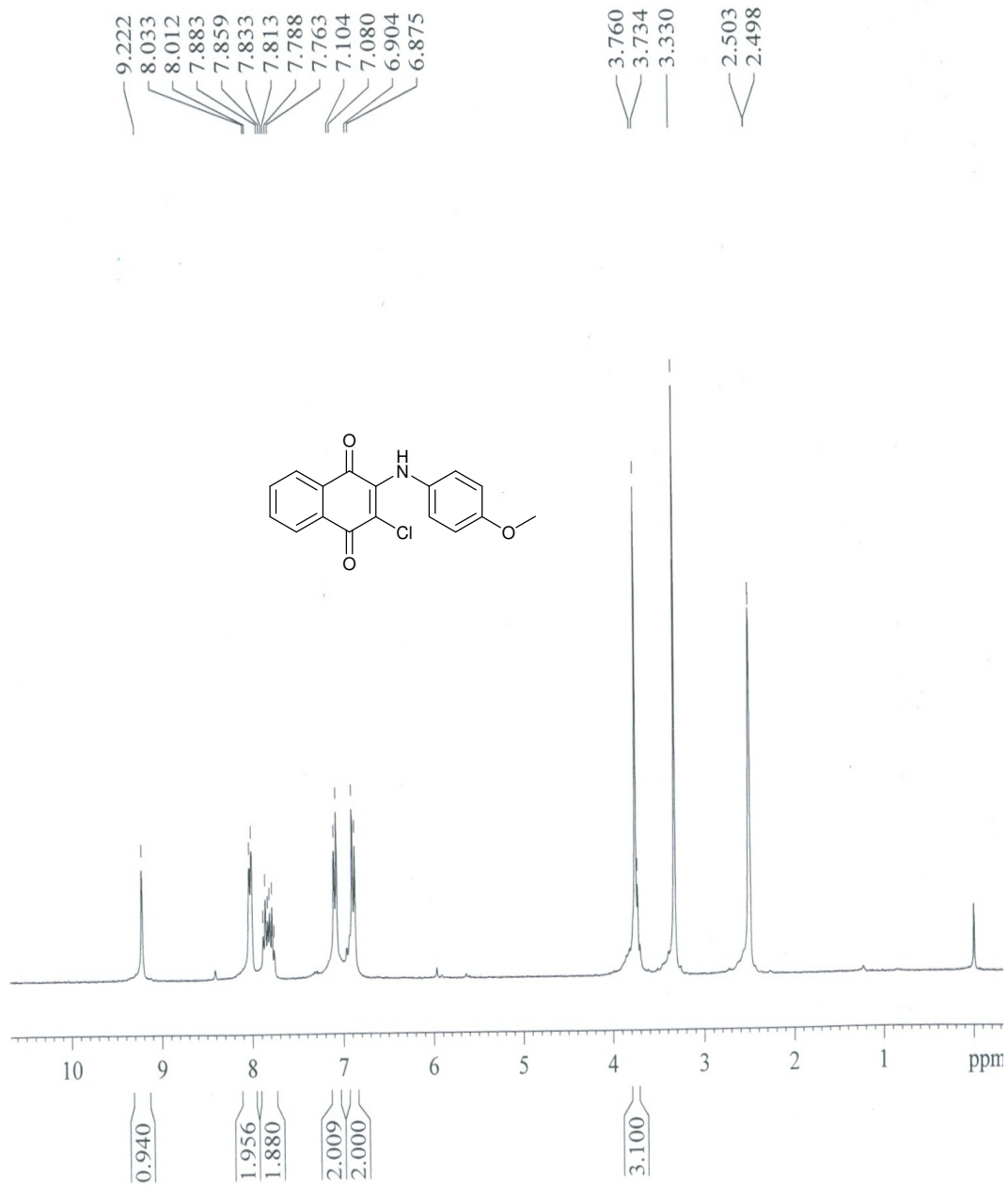
Test Organisms	1a	1b	1c	1d	1e	2a	2b	2c	2d	2e	3a	3b	3c	3d	3e	Contro l (DMS O)
	Zone of Inhibition in mm															-
<i>Staphylococcus aureus</i>	11	-	14	-	-	12	13	11	-	-	13	10	14	13	12	-
<i>Streptococcus mutans</i>	16	18	14	13	-	14	14	15	15	11	18	-	14	-	14	-
<i>Pseudomonas aeruginosa</i>	-	-	-	-	-	-	-	-	-	-	13	-	14	11	16	-
<i>Escherichia coli</i>	-	-	-	-	-	14	16	17	13	14	15	-	-	-	-	-
<i>Klebsiella pneumoniae</i>	-	-	-	-	-	-	-	-	-	-	-	-	13	-	-	-



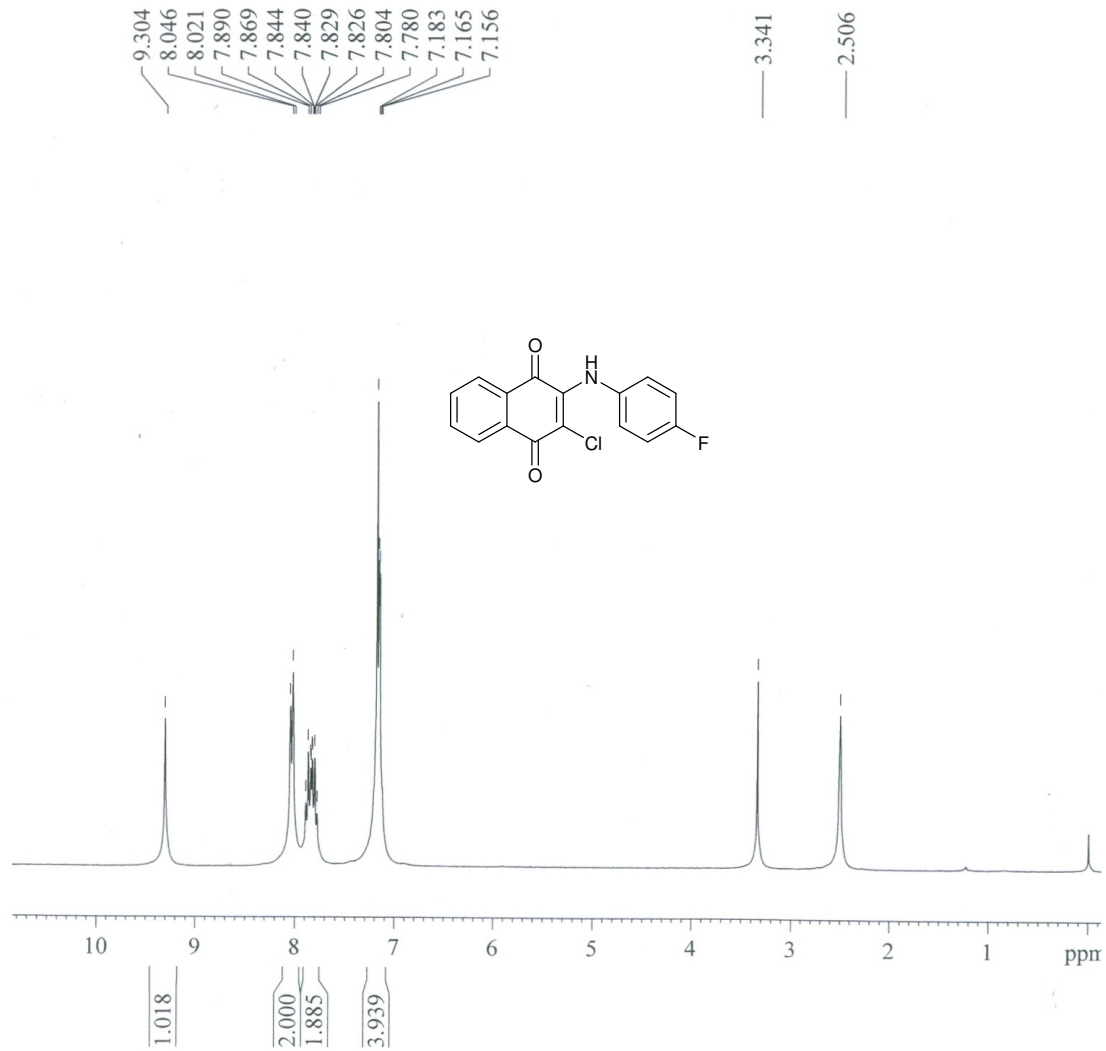
<sup>1</sup>H NMR for **1a**



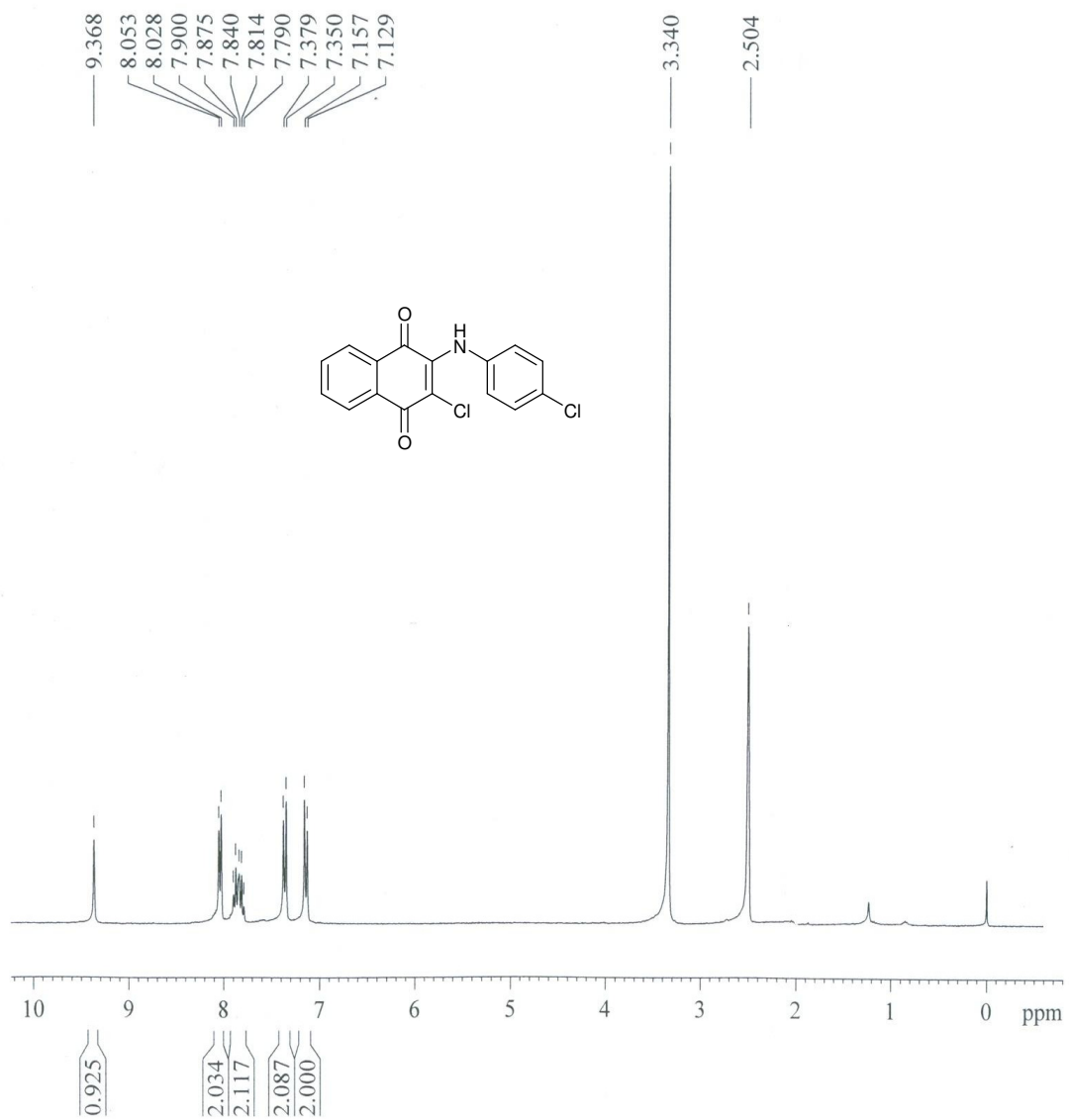
<sup>1</sup>H NMR for **1b**



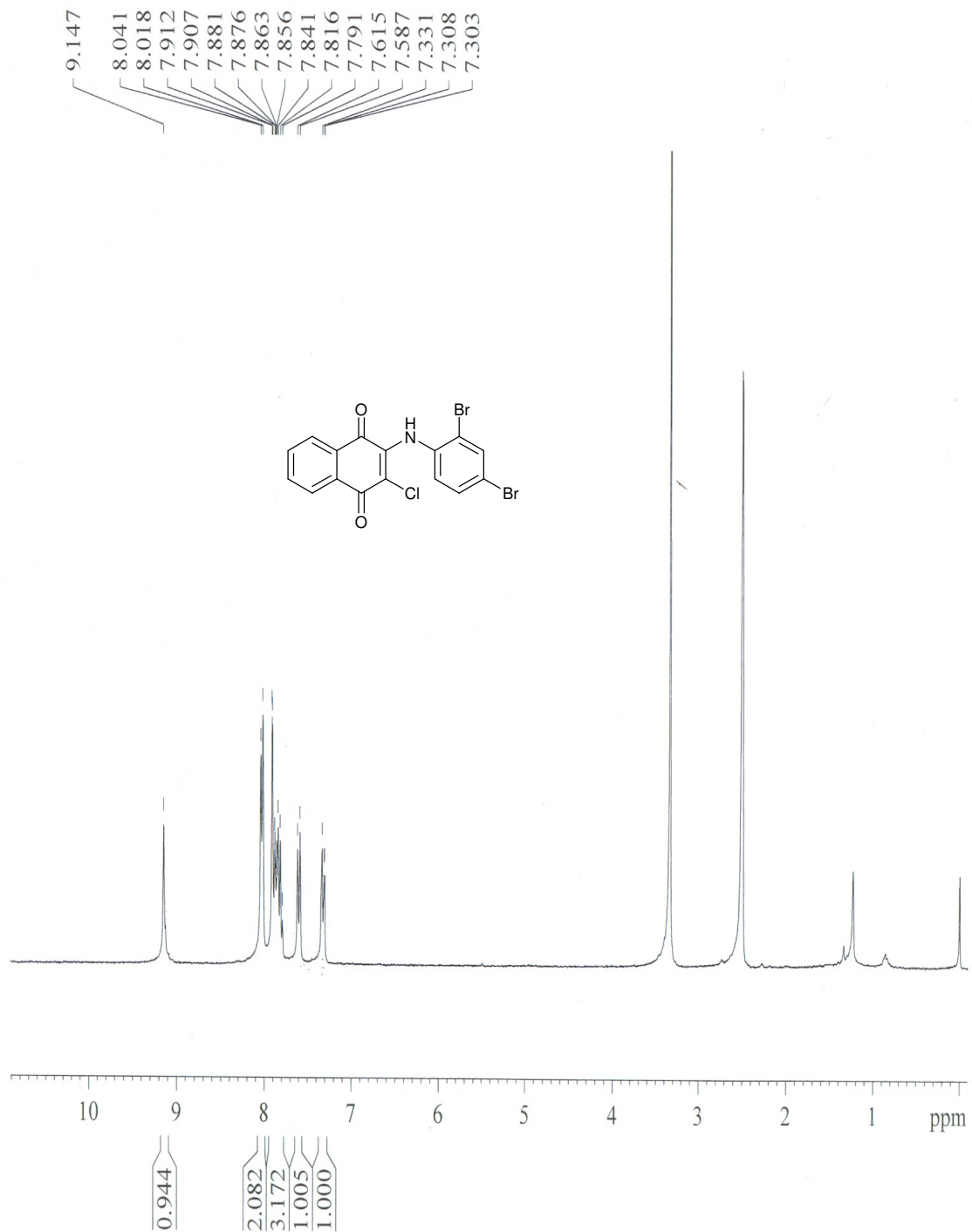
$^1\text{H}$  NMR for **1c**



<sup>1</sup>H NMR for **1d**

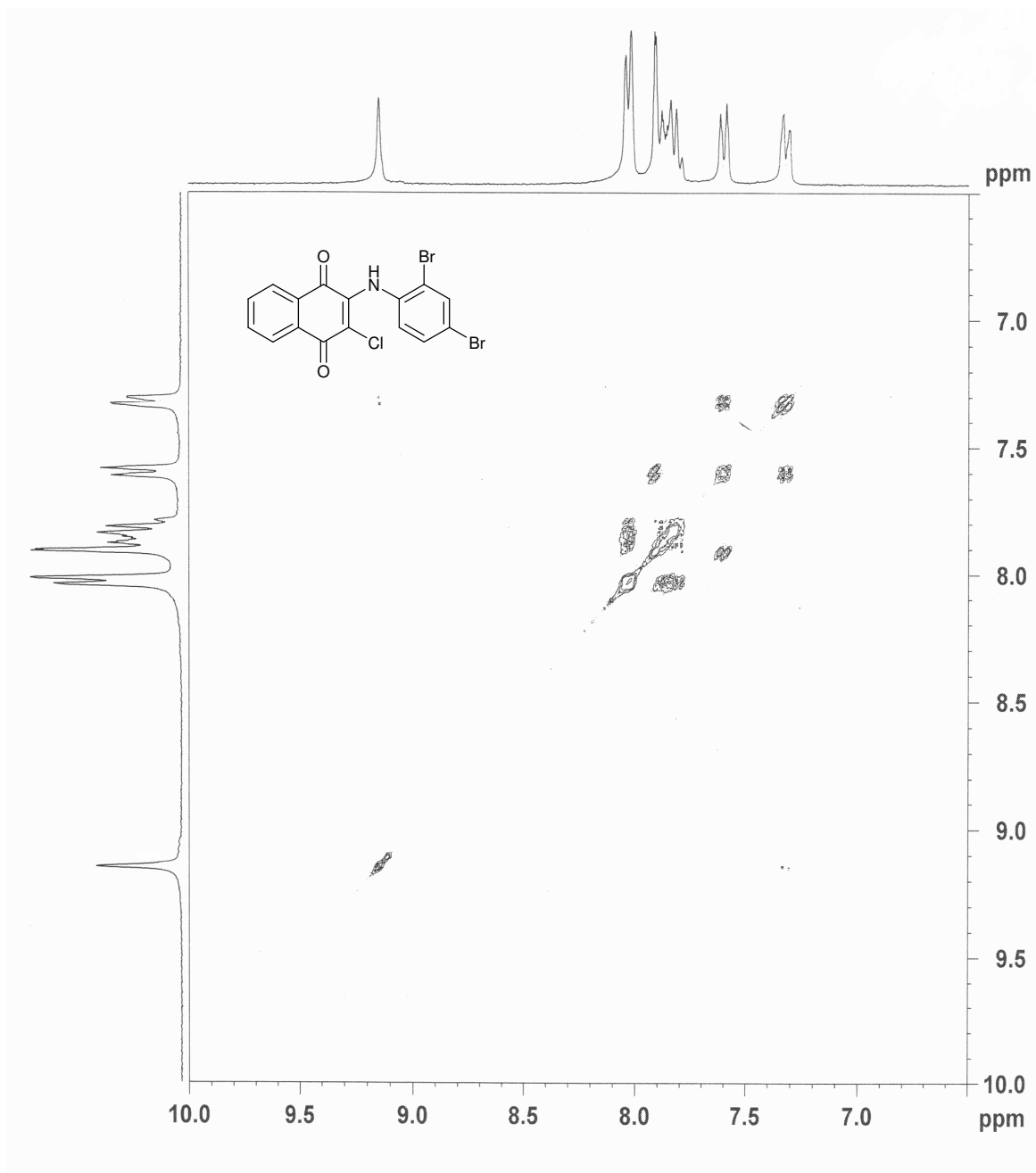


$^1\text{H NMR}$  for **1e**

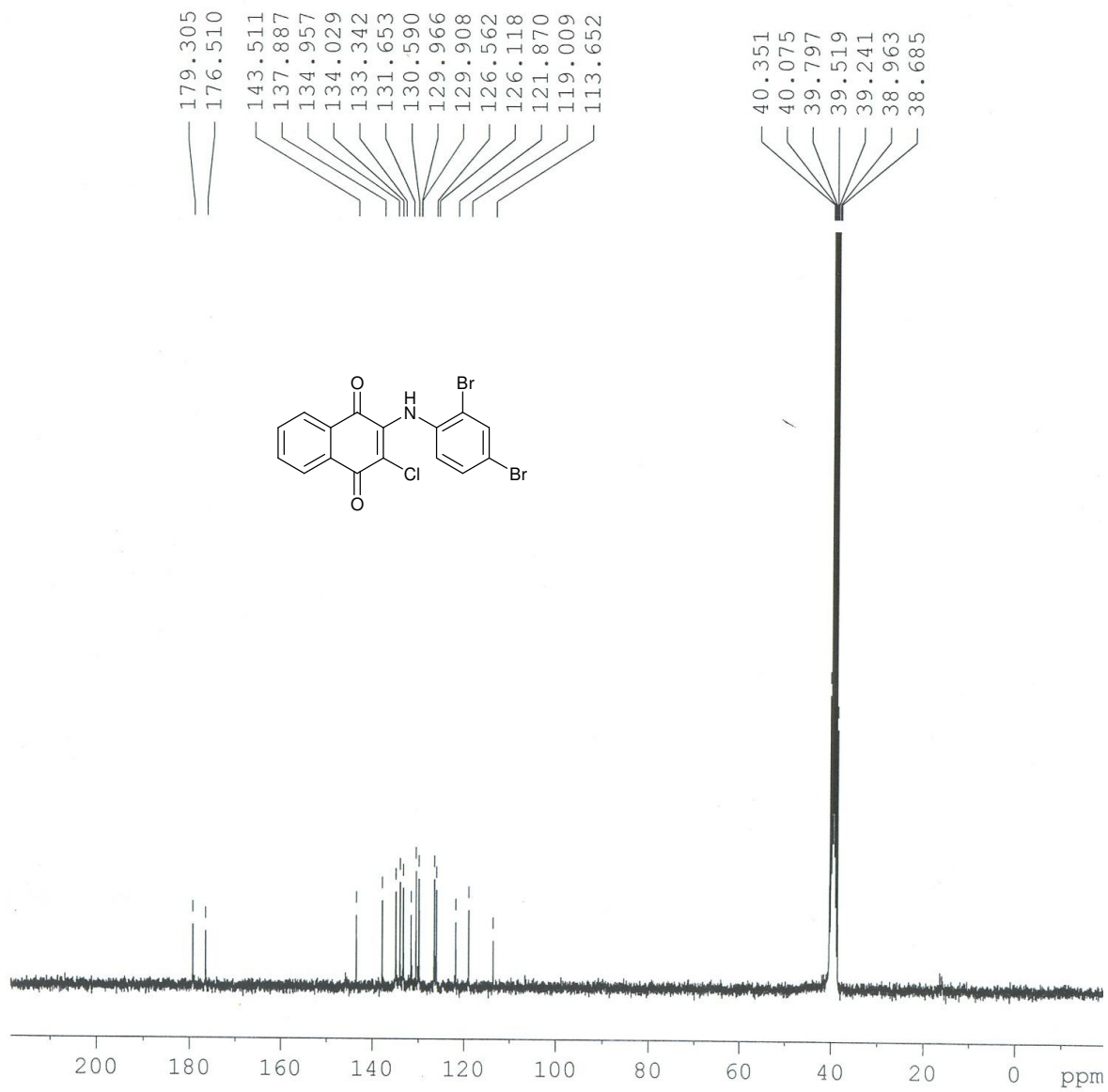


$^1\text{H}$  NMR for **2a**

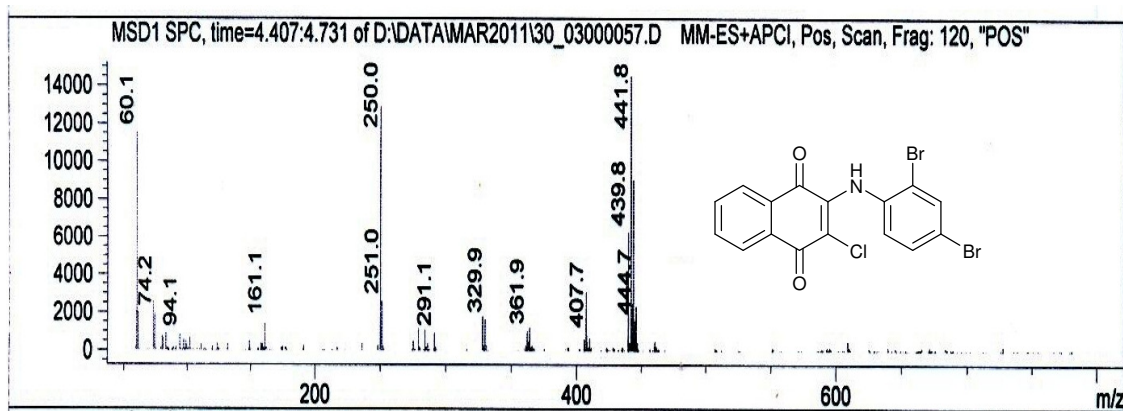




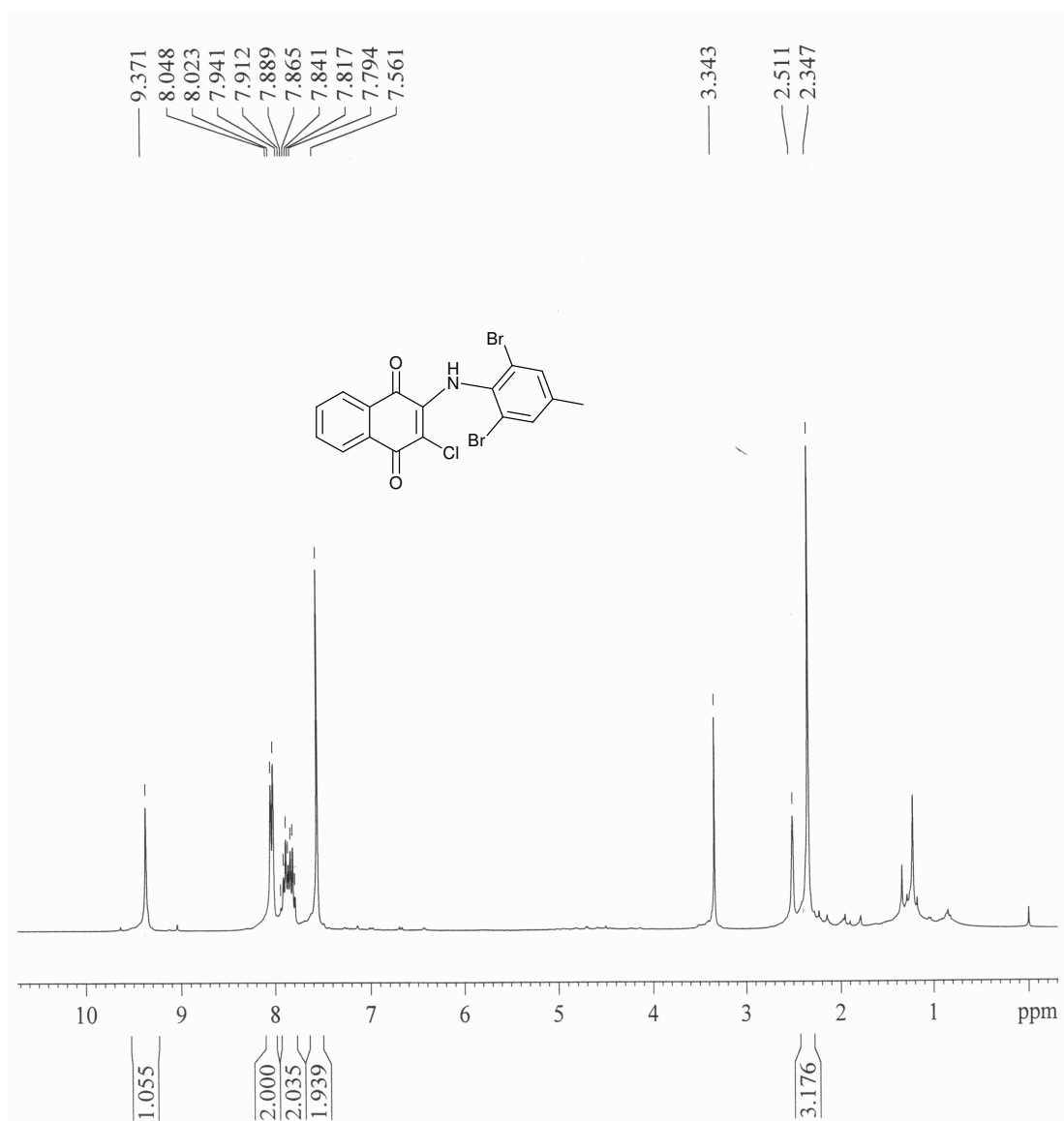
$^1\text{H}$ - $^1\text{H}$  Cosy for **2a**



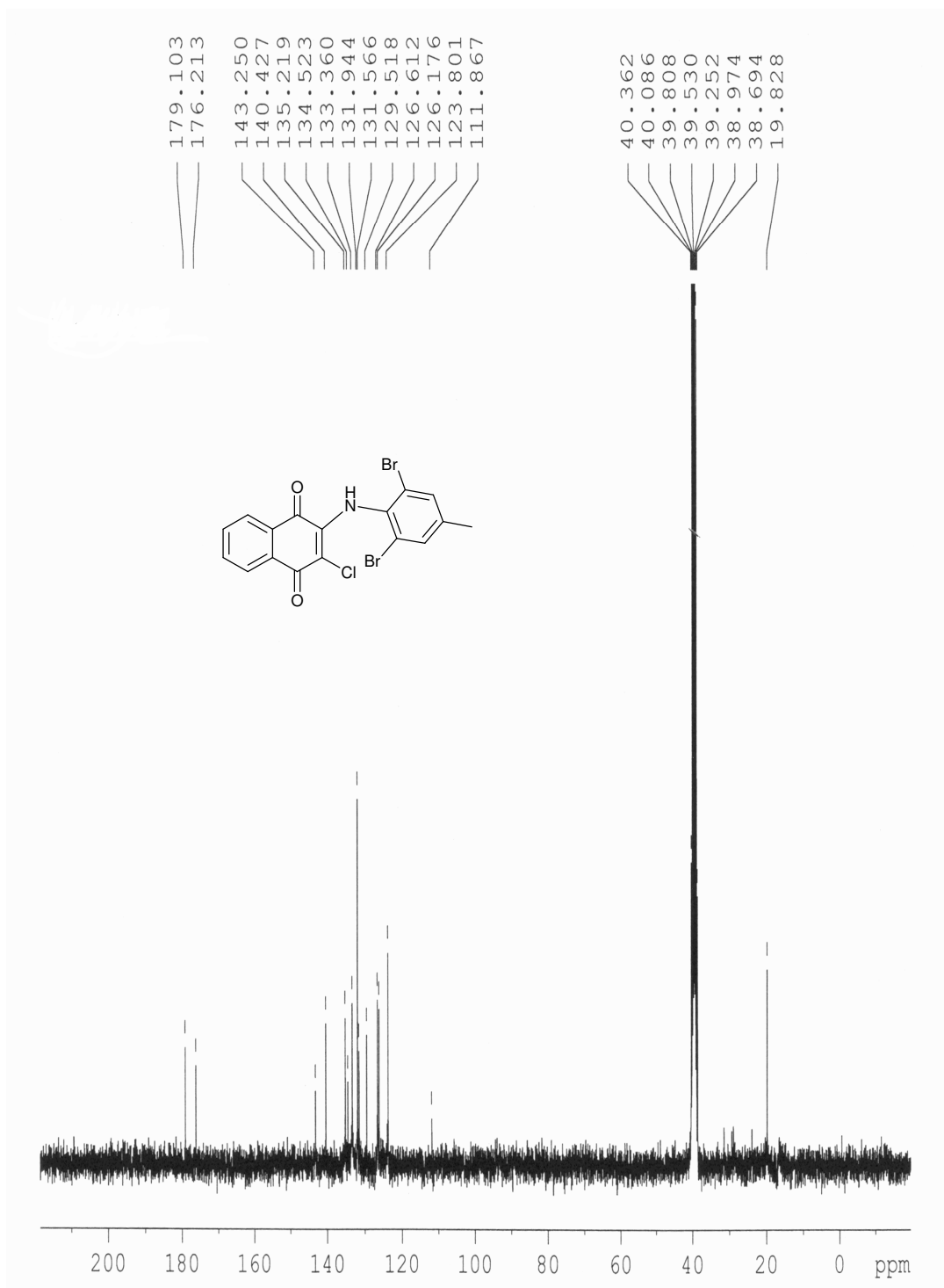
<sup>13</sup>C NMR for **2a**



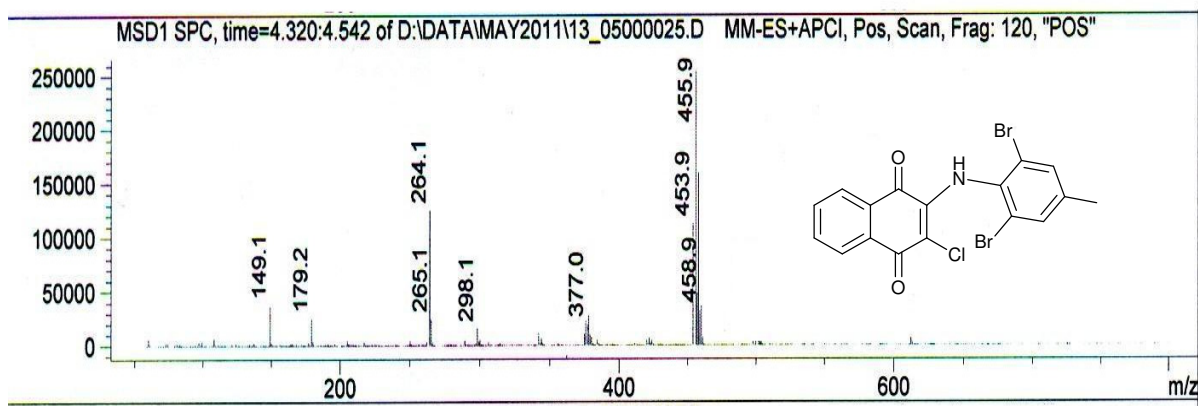
LCMS for **2a**



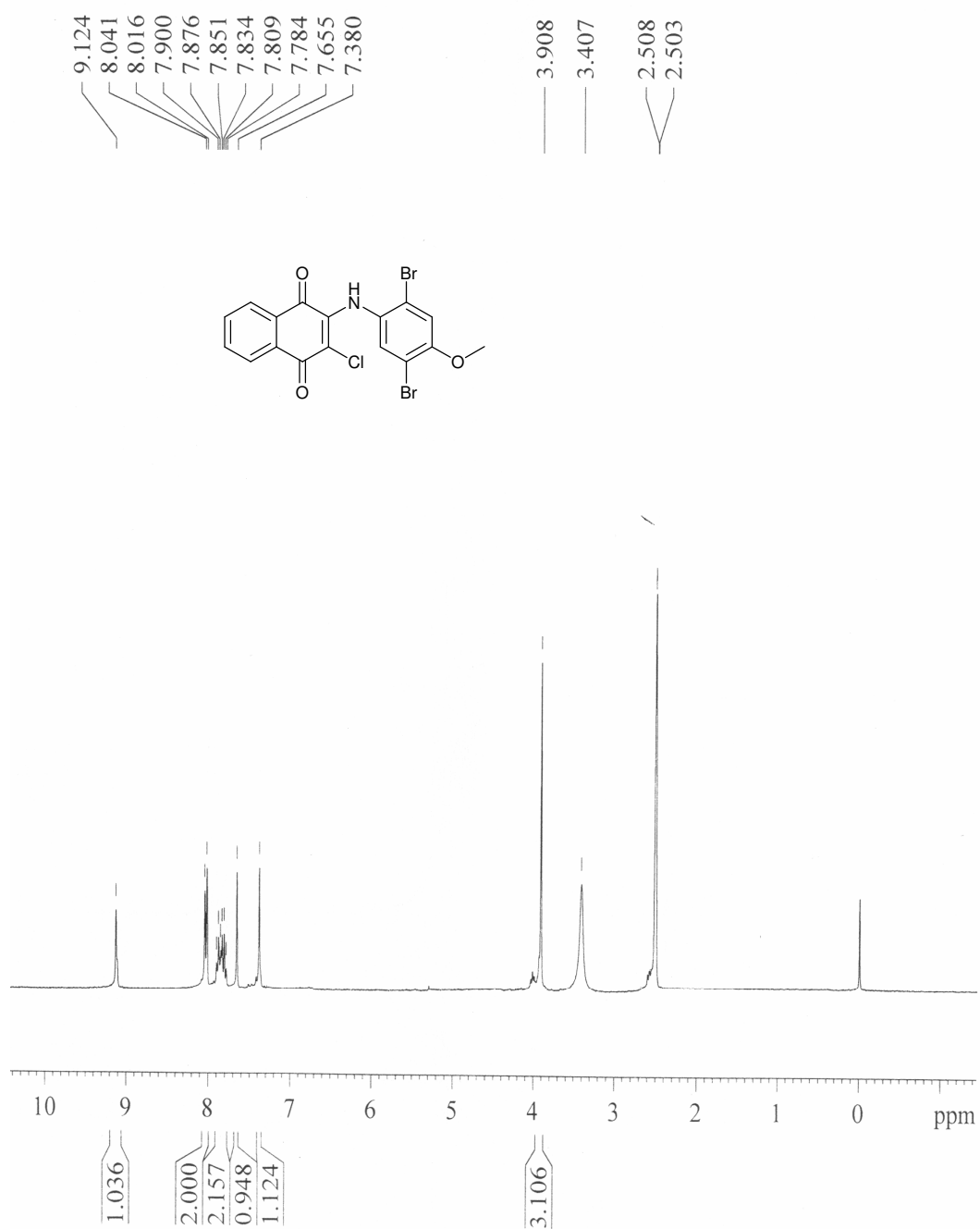
<sup>1</sup>H NMR for **2b**



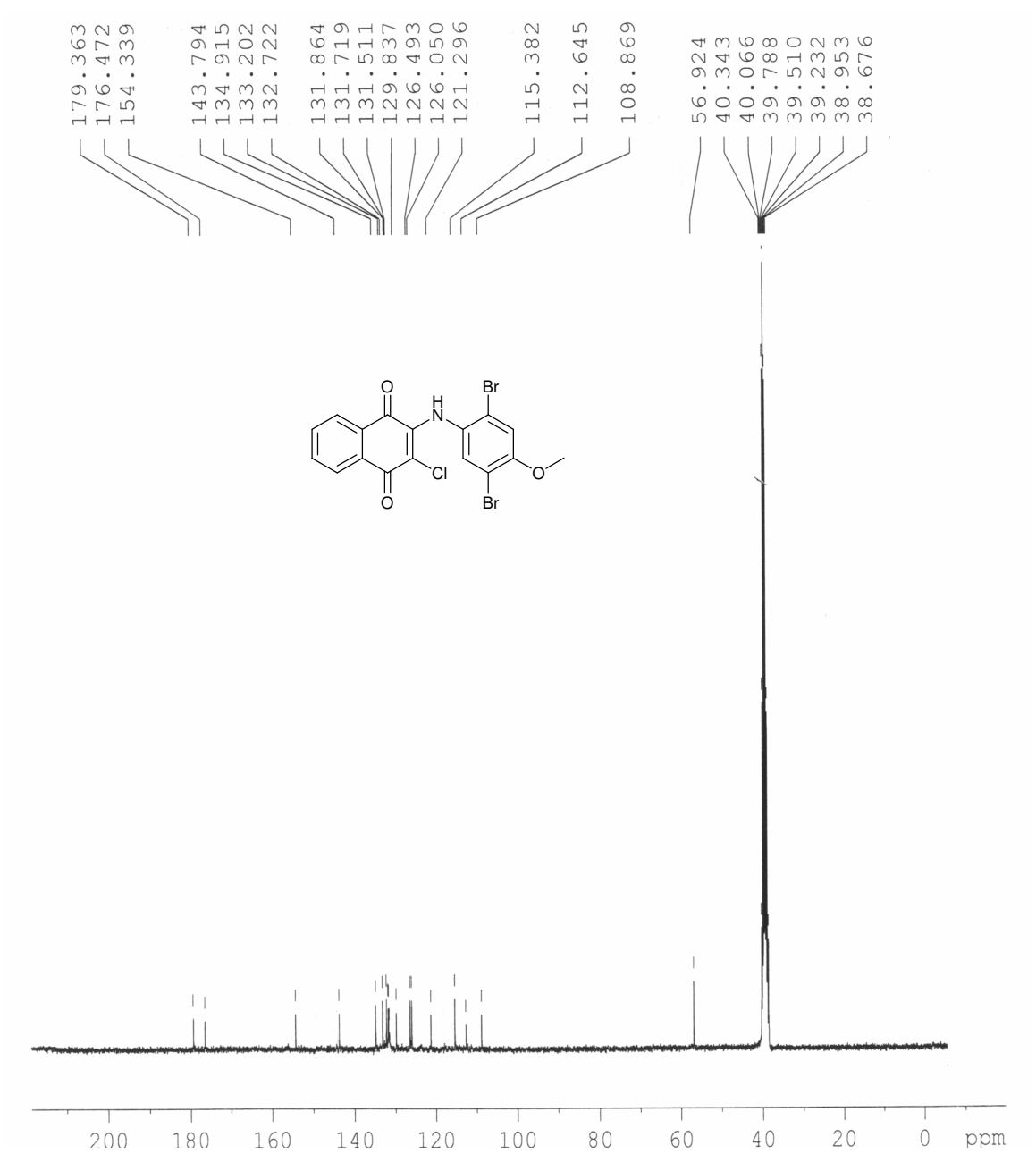
$^{13}\text{C}$  NMR for **2b**



LCMS for **2b**

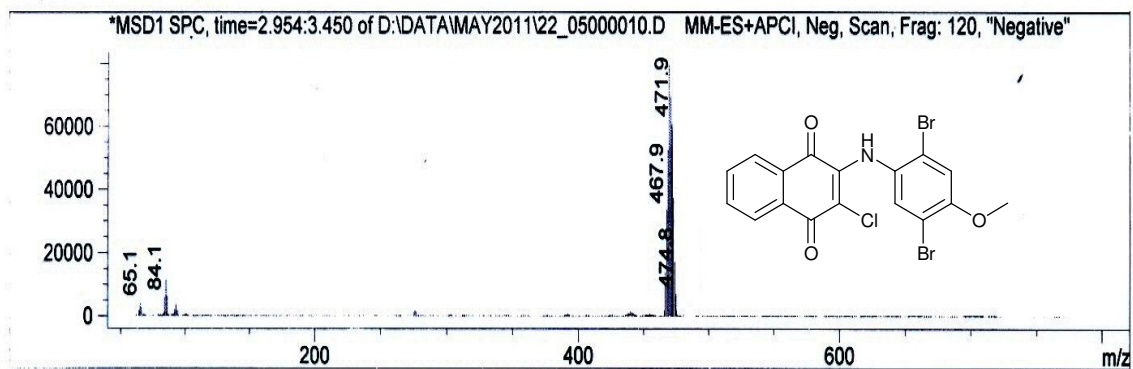


$^1\text{H}$  NMR for **2c**

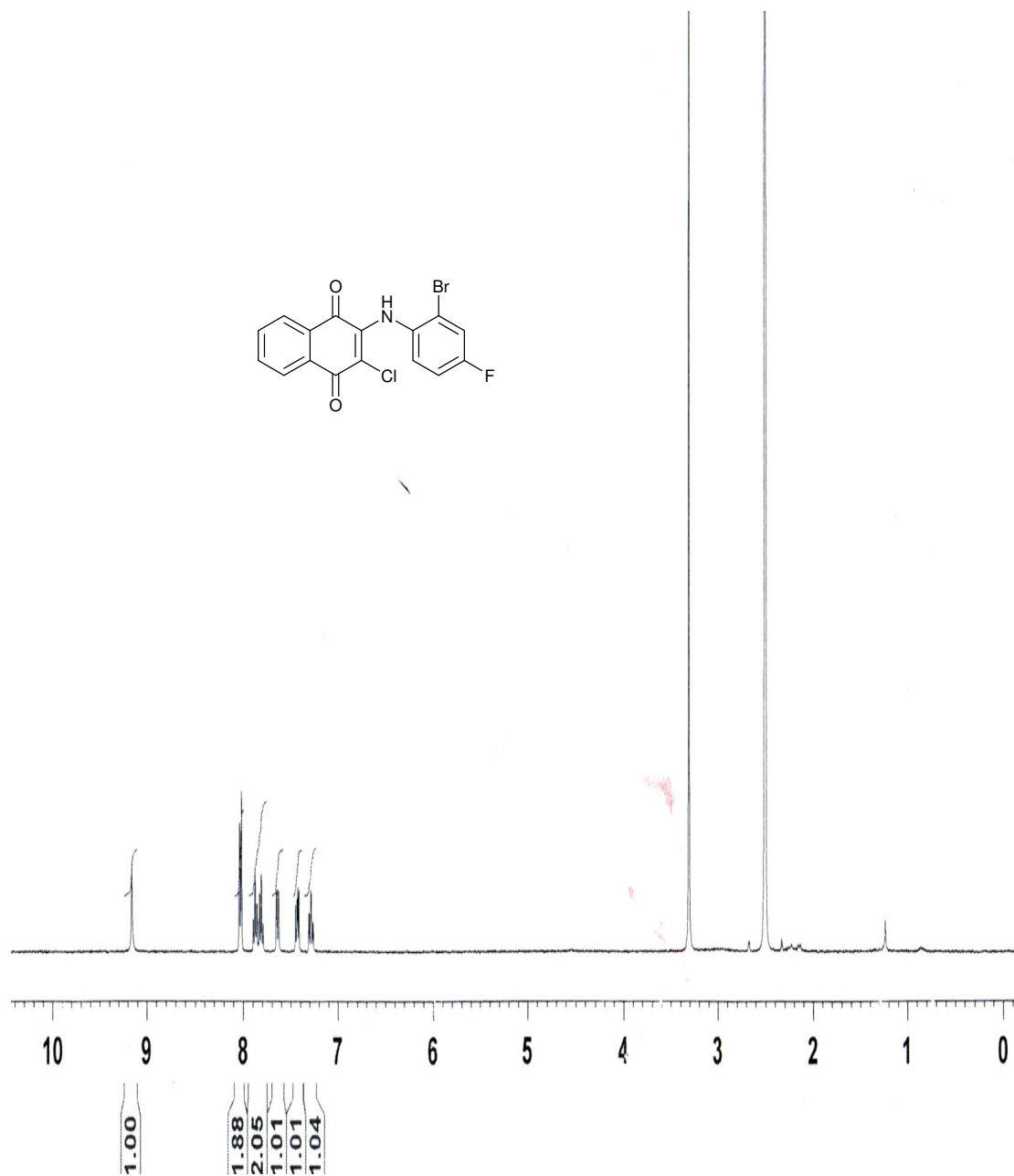


$^{13}\text{C}$  NMR for **2c**

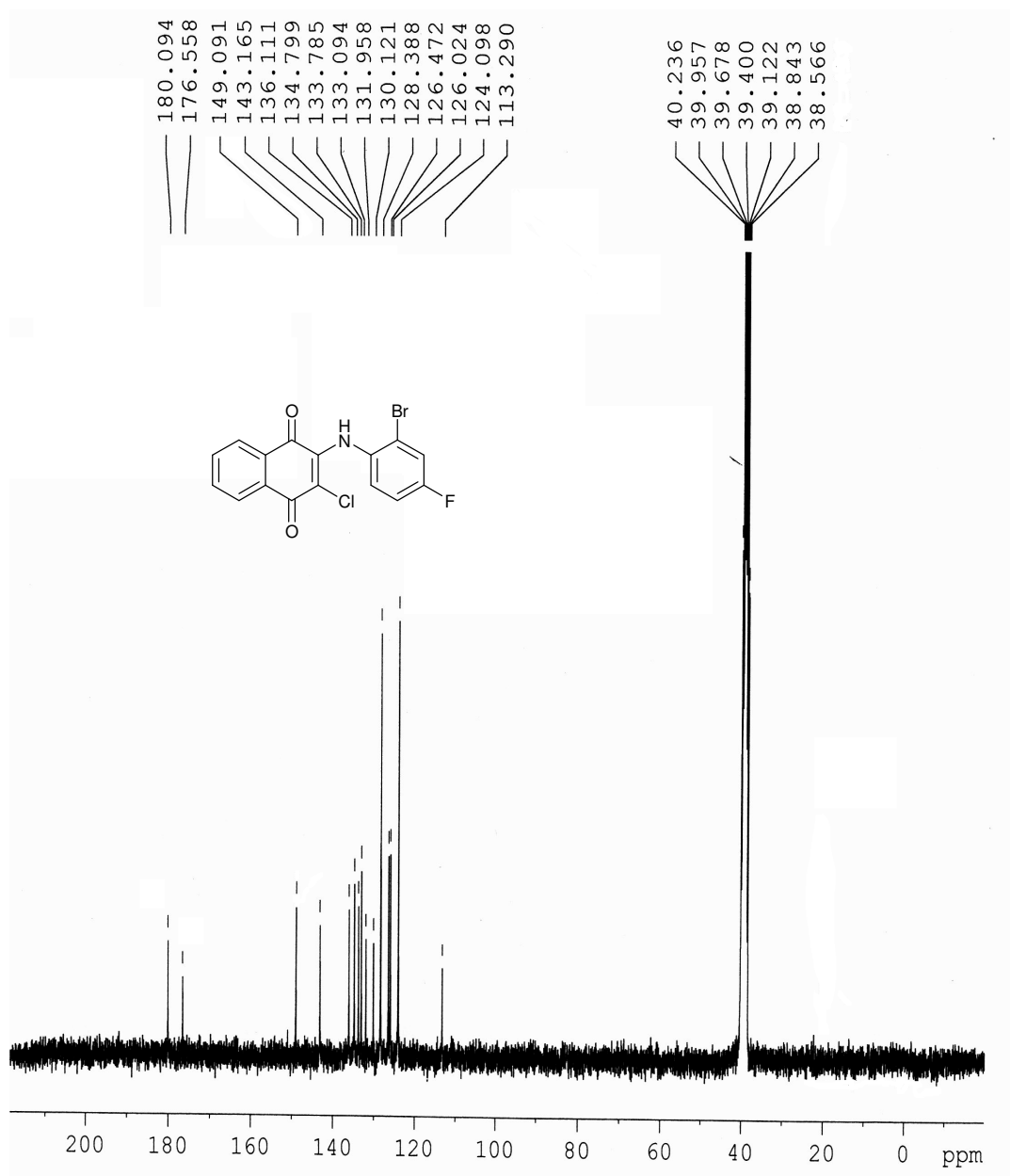




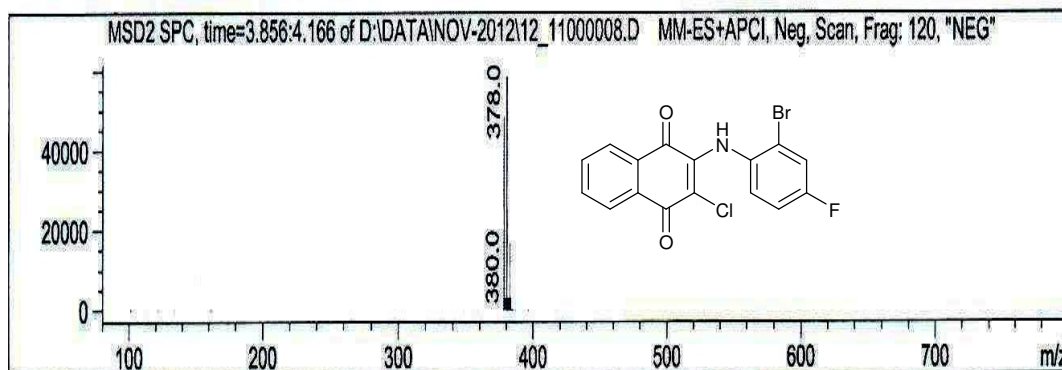
LCMS for 2c



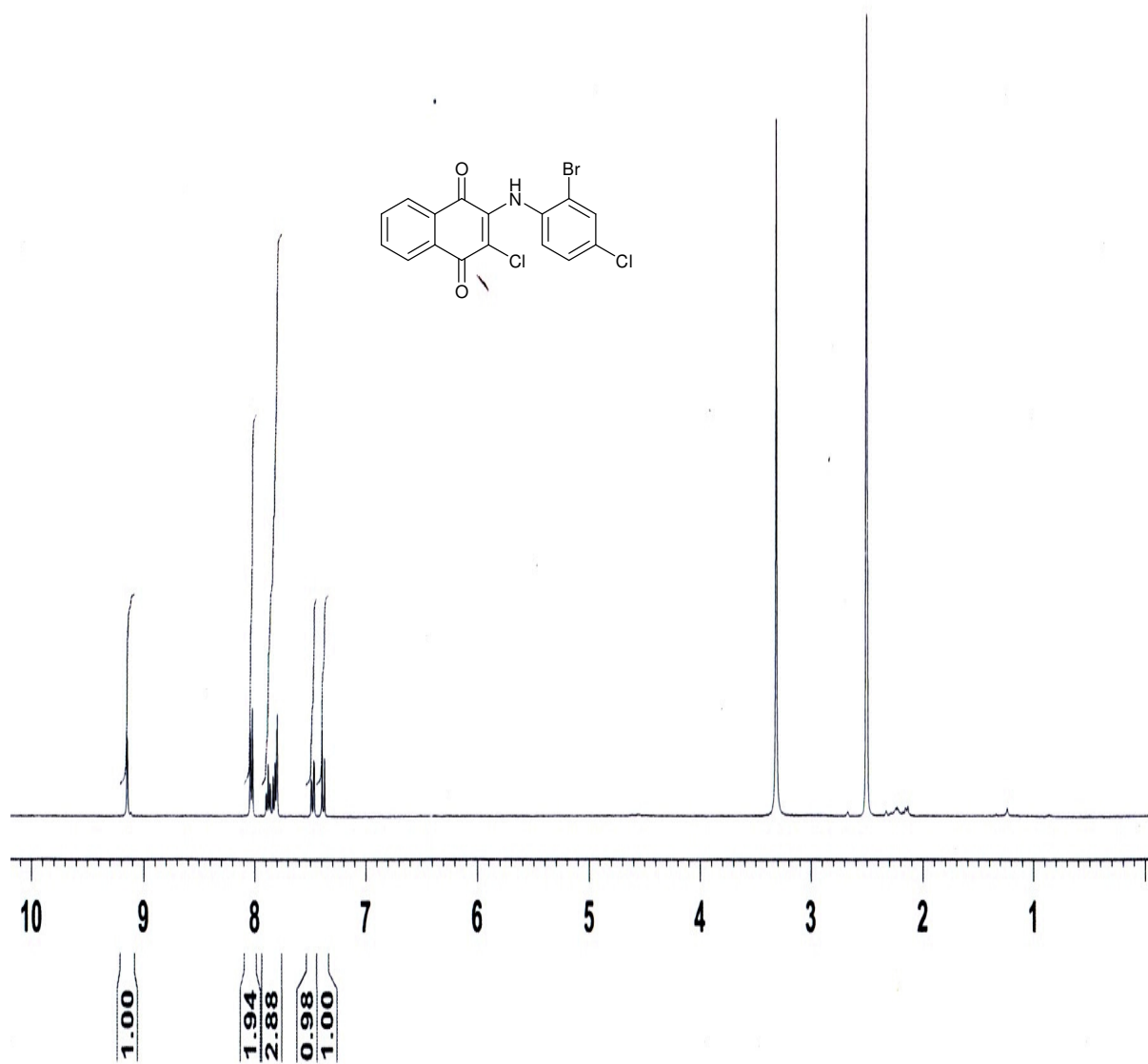
<sup>1</sup>H NMR for 2d



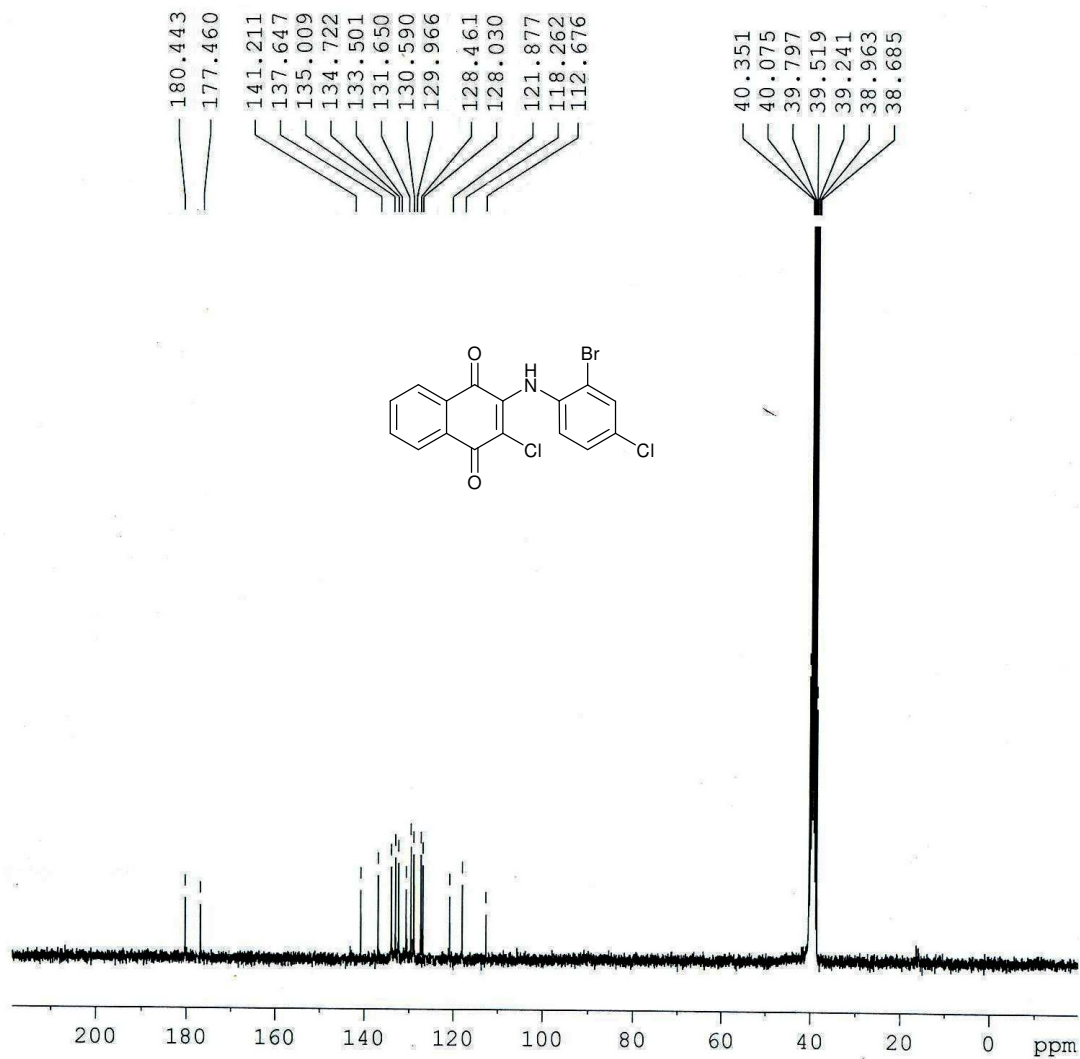
<sup>13</sup>C NMR for **2d**



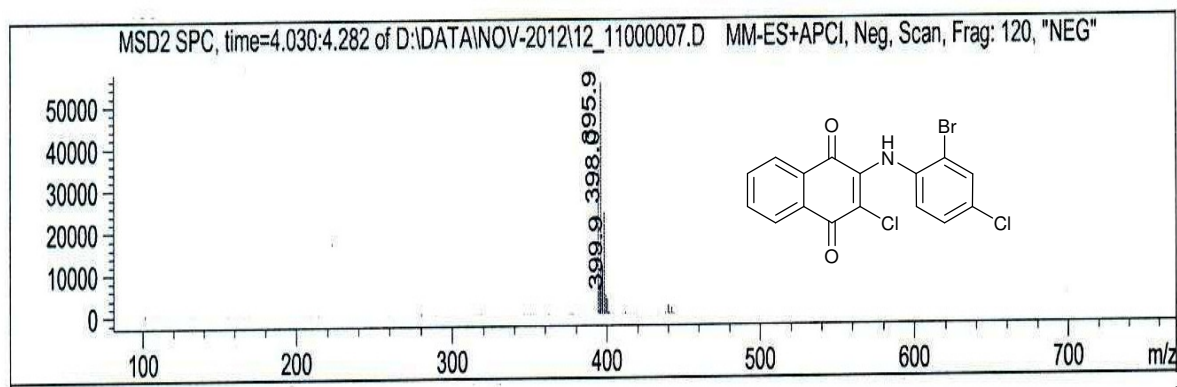
LC- MS for 2d



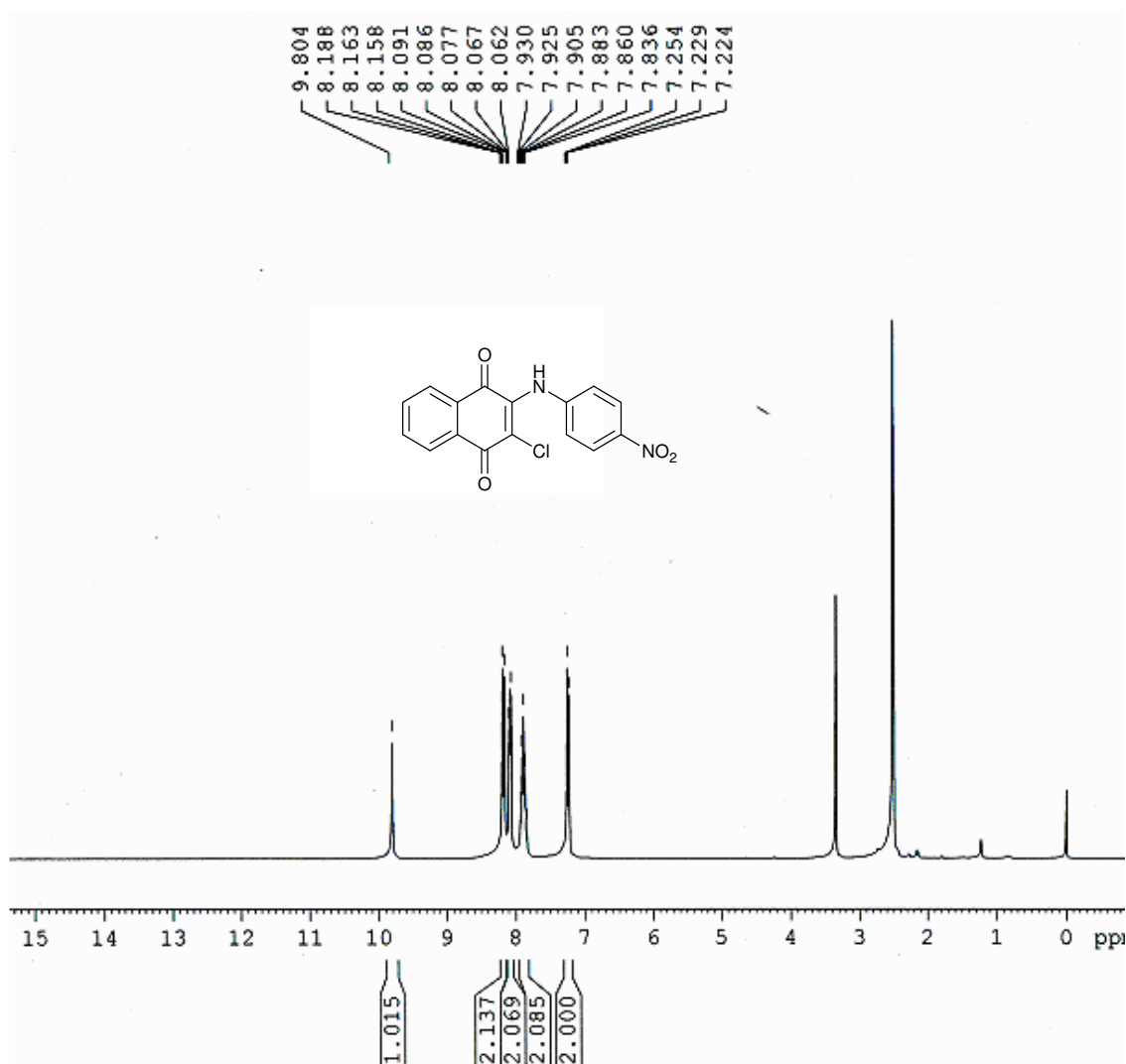
<sup>1</sup>H NMR for 2e



$^{13}\text{C}$  NMR for **2e**

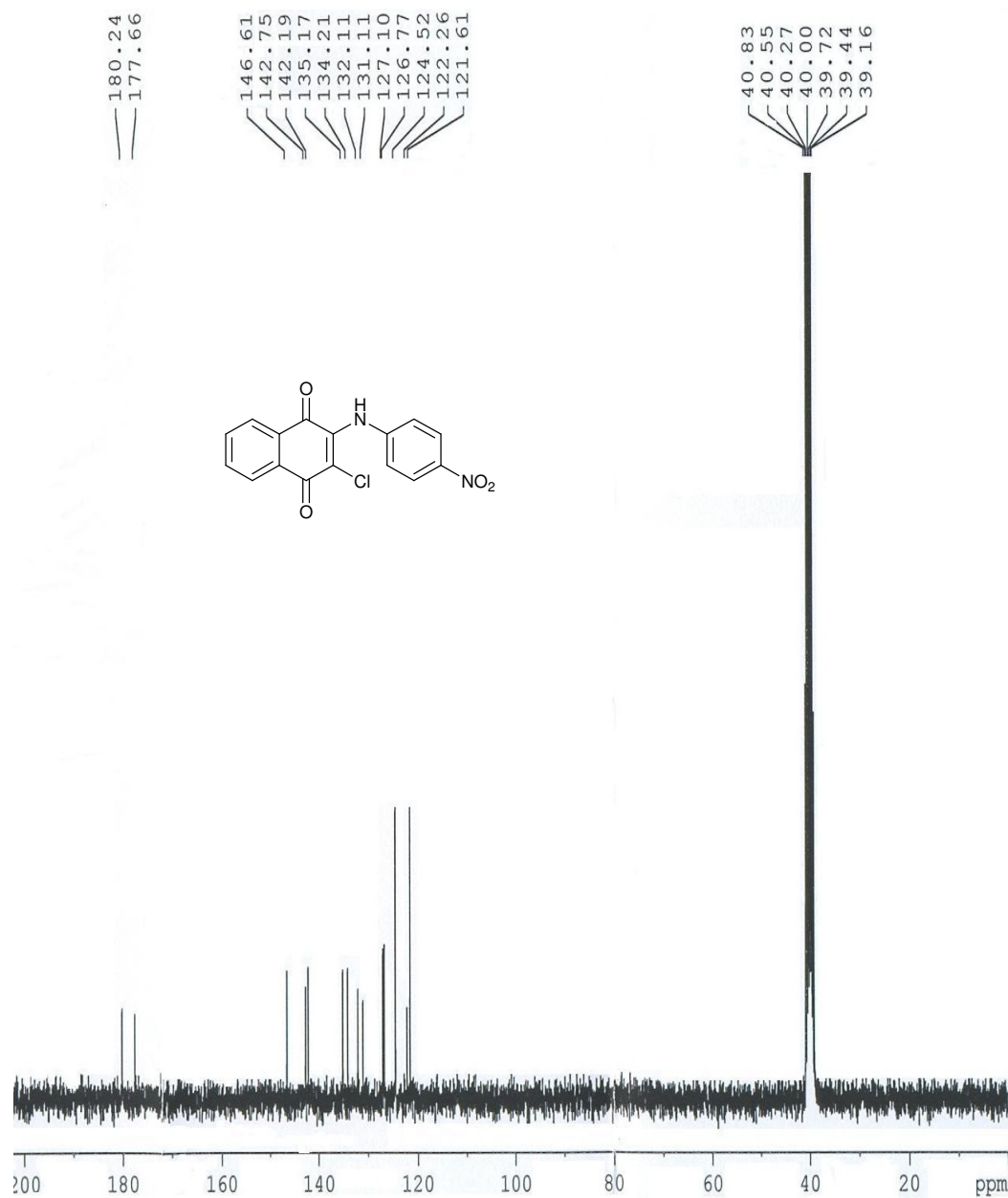


LC- MS for **2e**

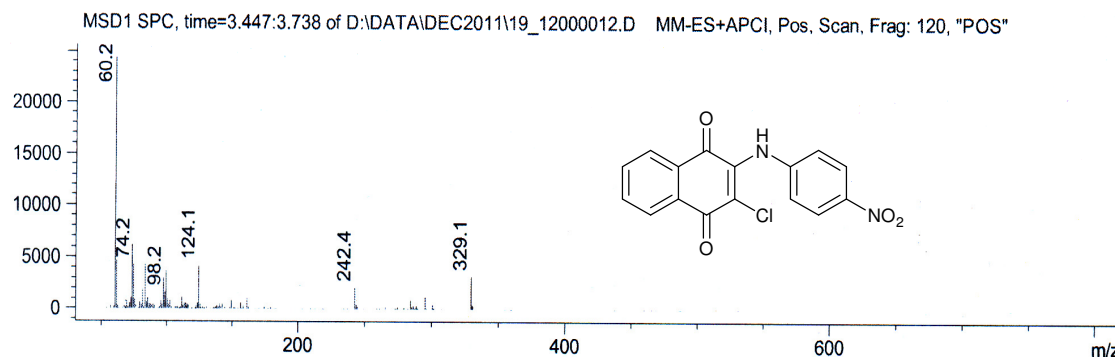


<sup>1</sup>H NMR for **3a**

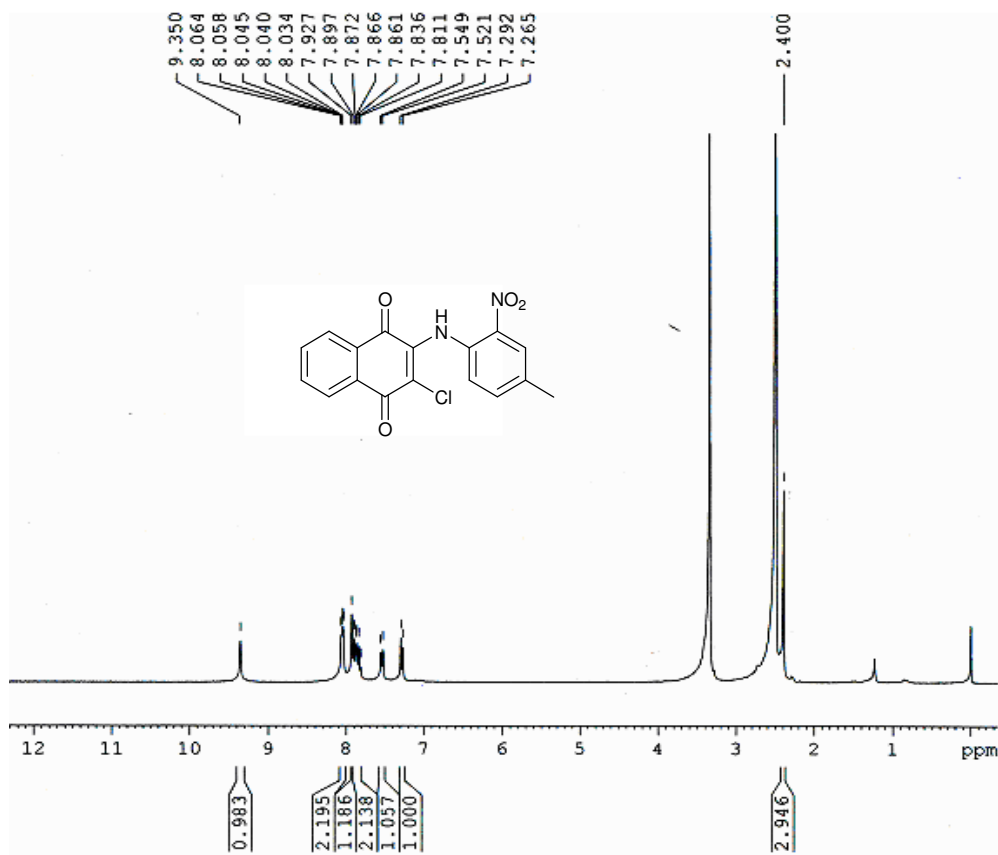




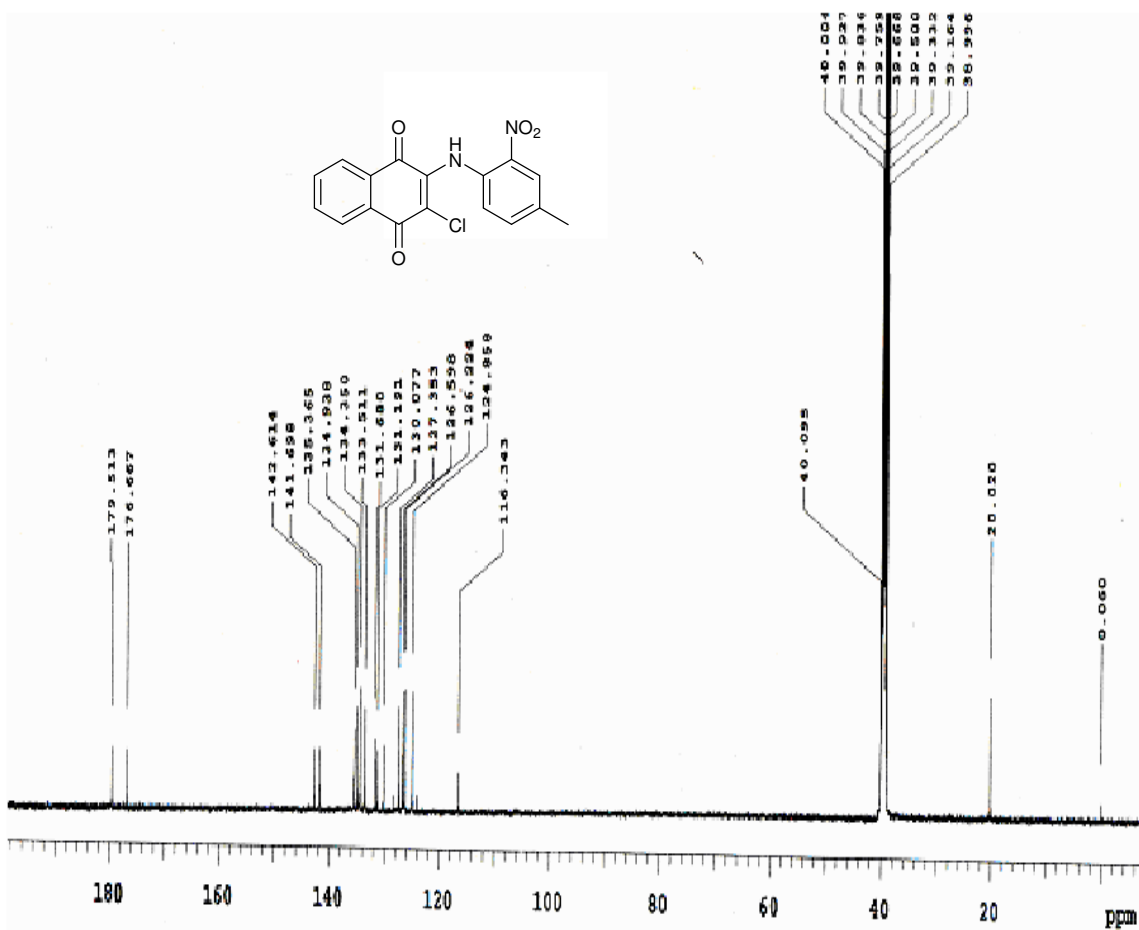
<sup>13</sup>C NMR for **3a**



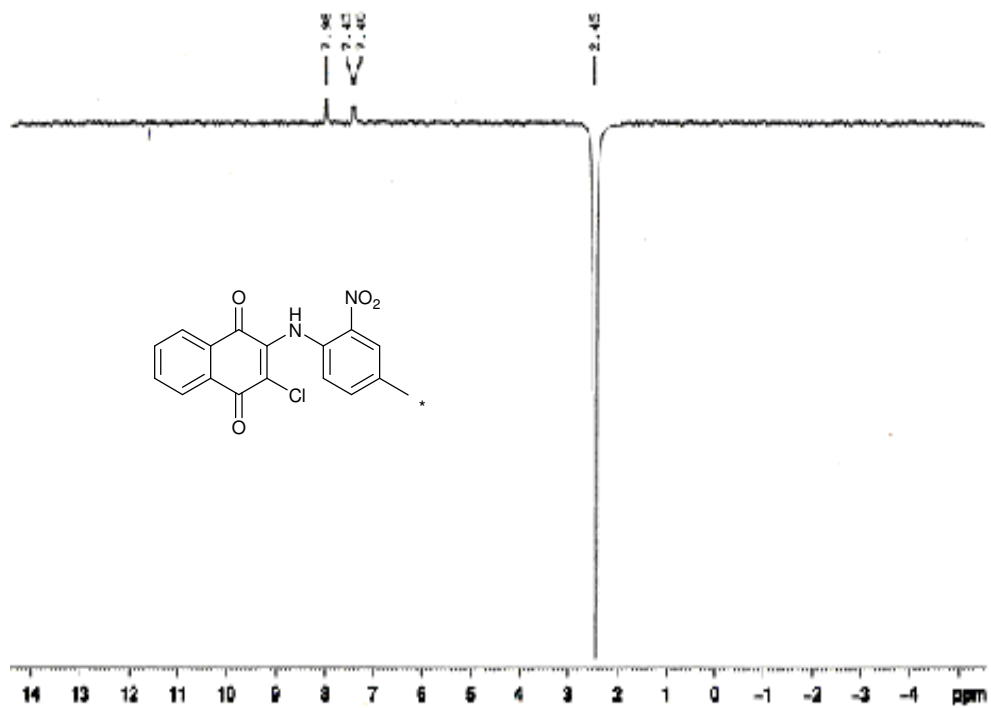
LC-MS for **3a**



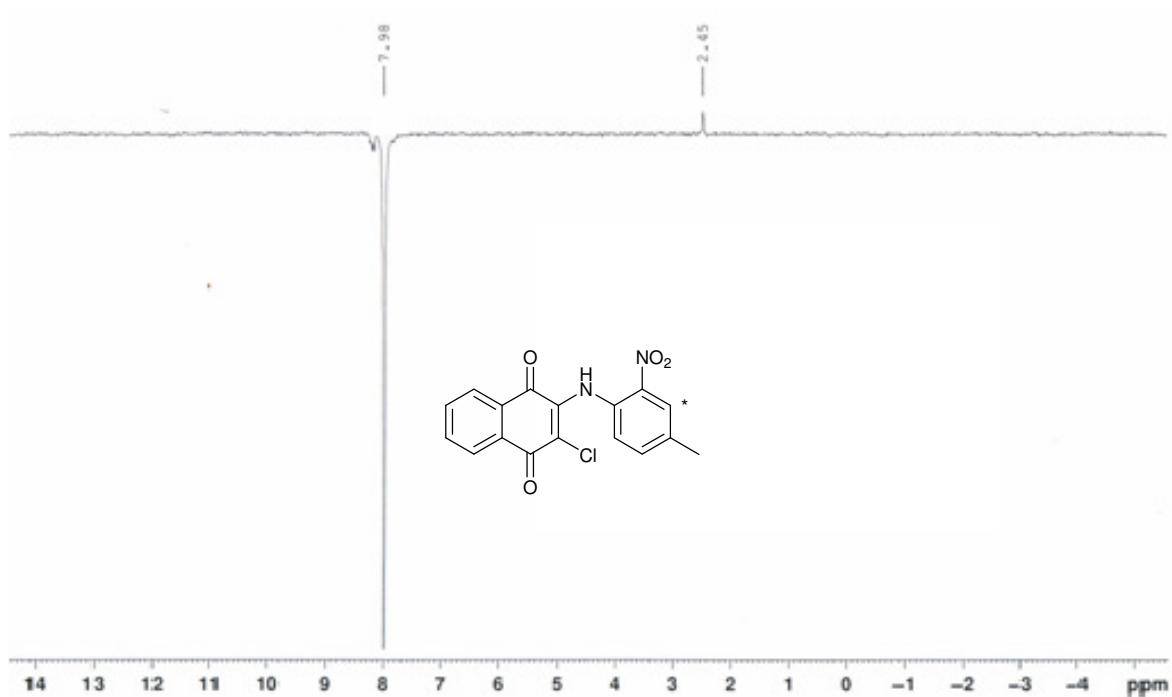
$^1\text{H}$  NMR for **3b**



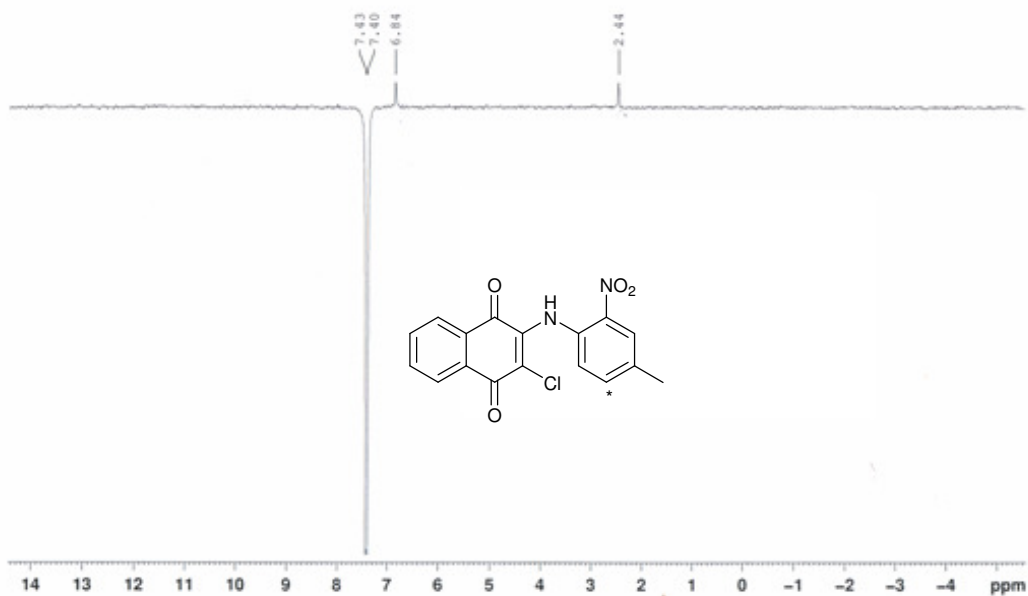
$^{13}\text{C}$  NMR for **3b**



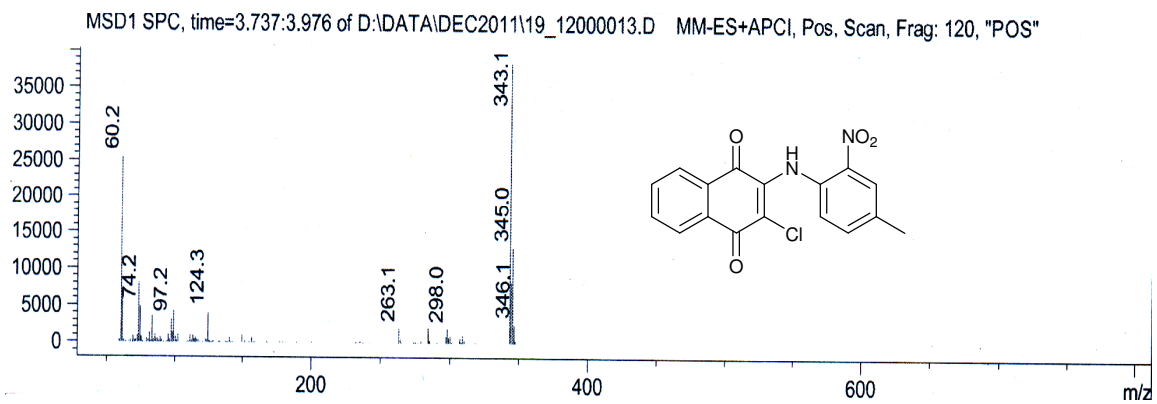
NOSEY for **3b**



NOSEY for **3b**

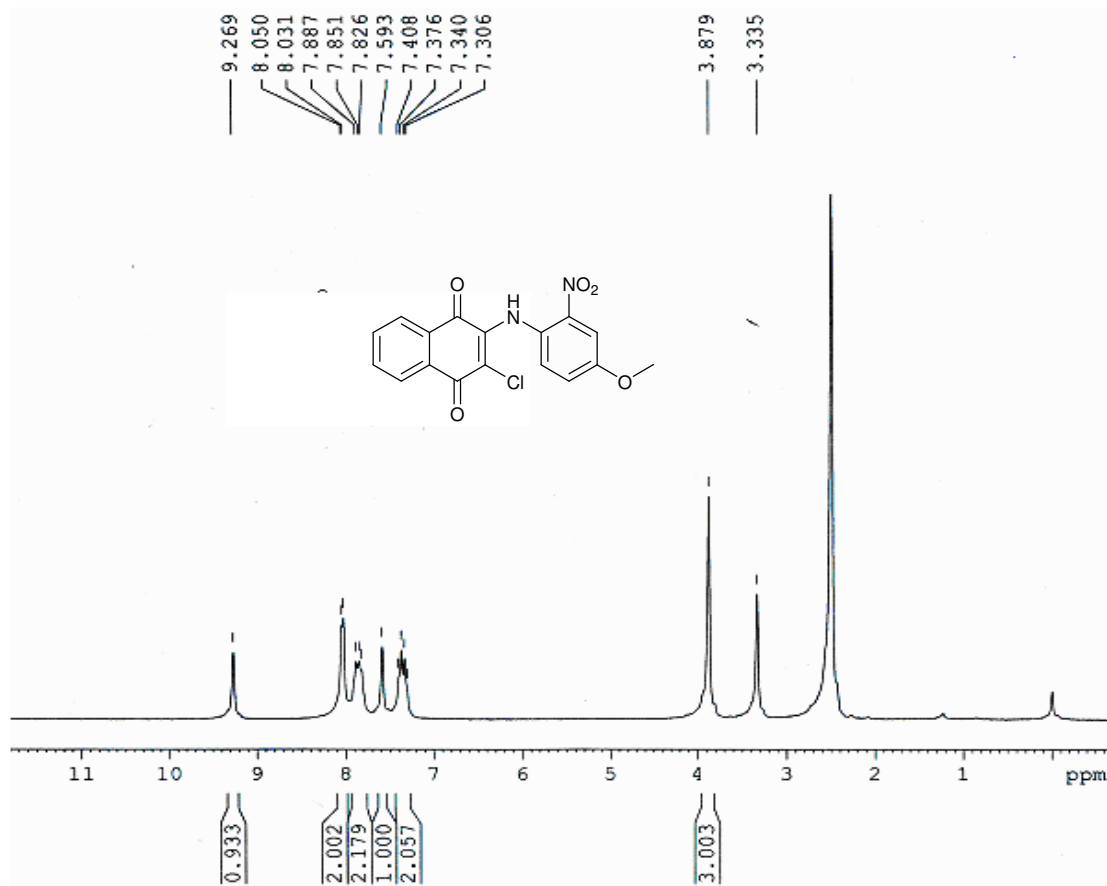


NOSEY for **3b**

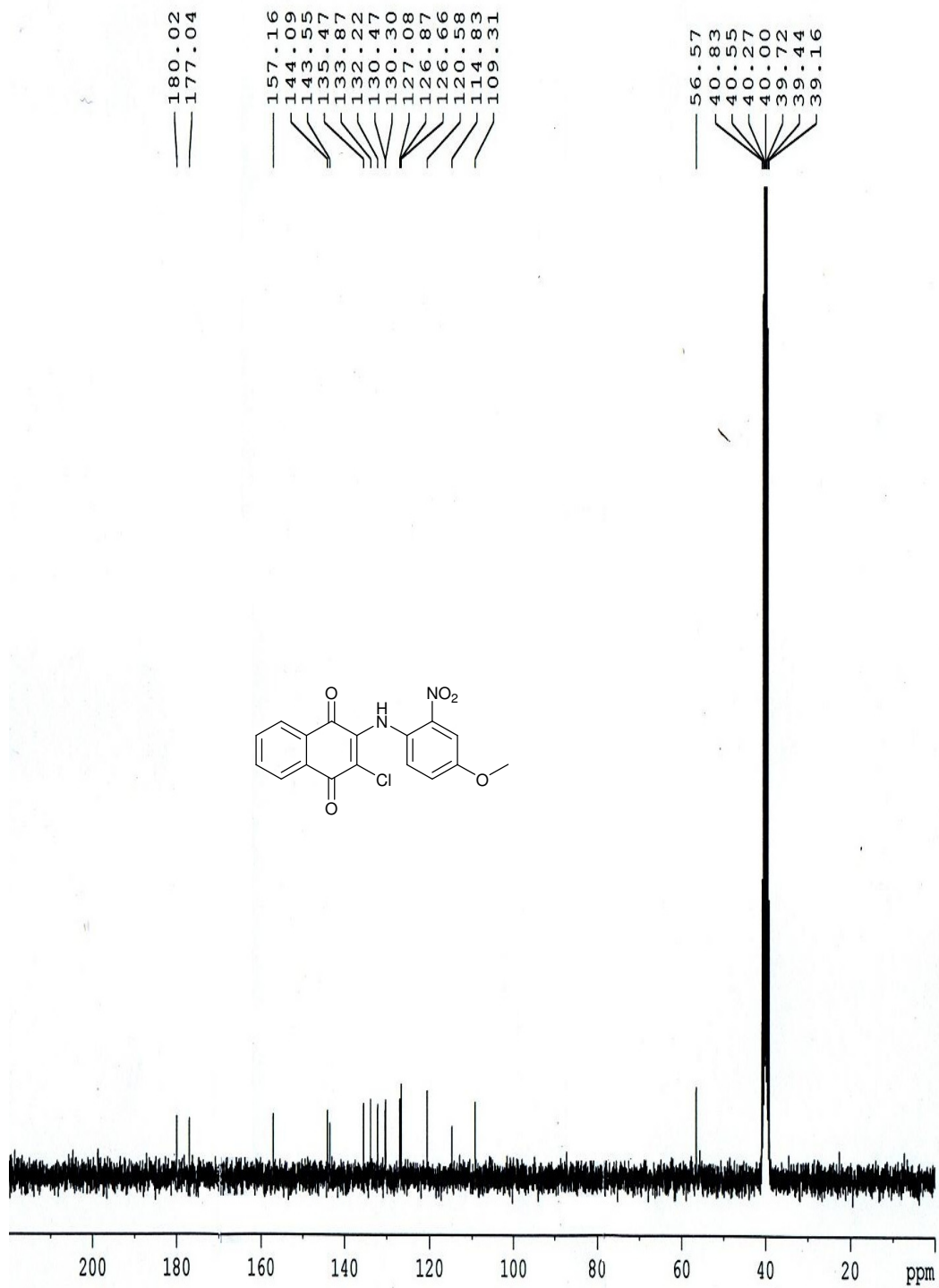


LC-MS for **3b**

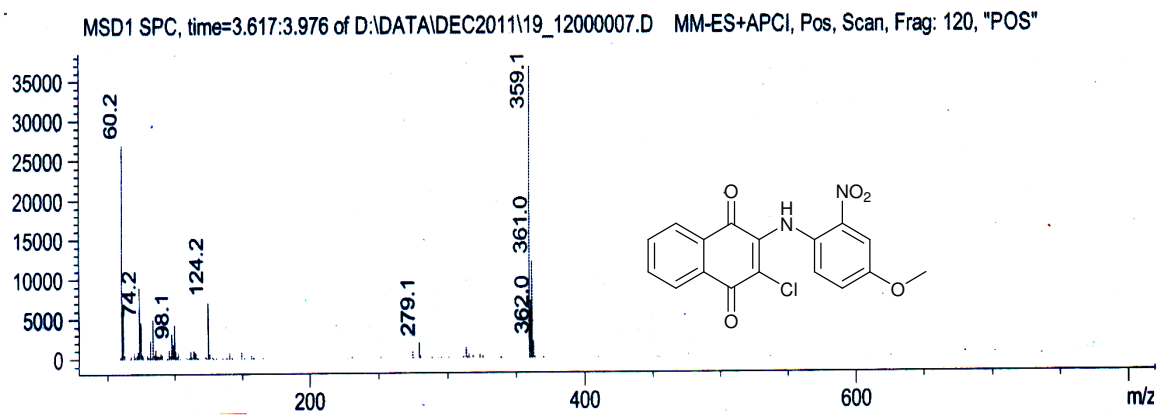




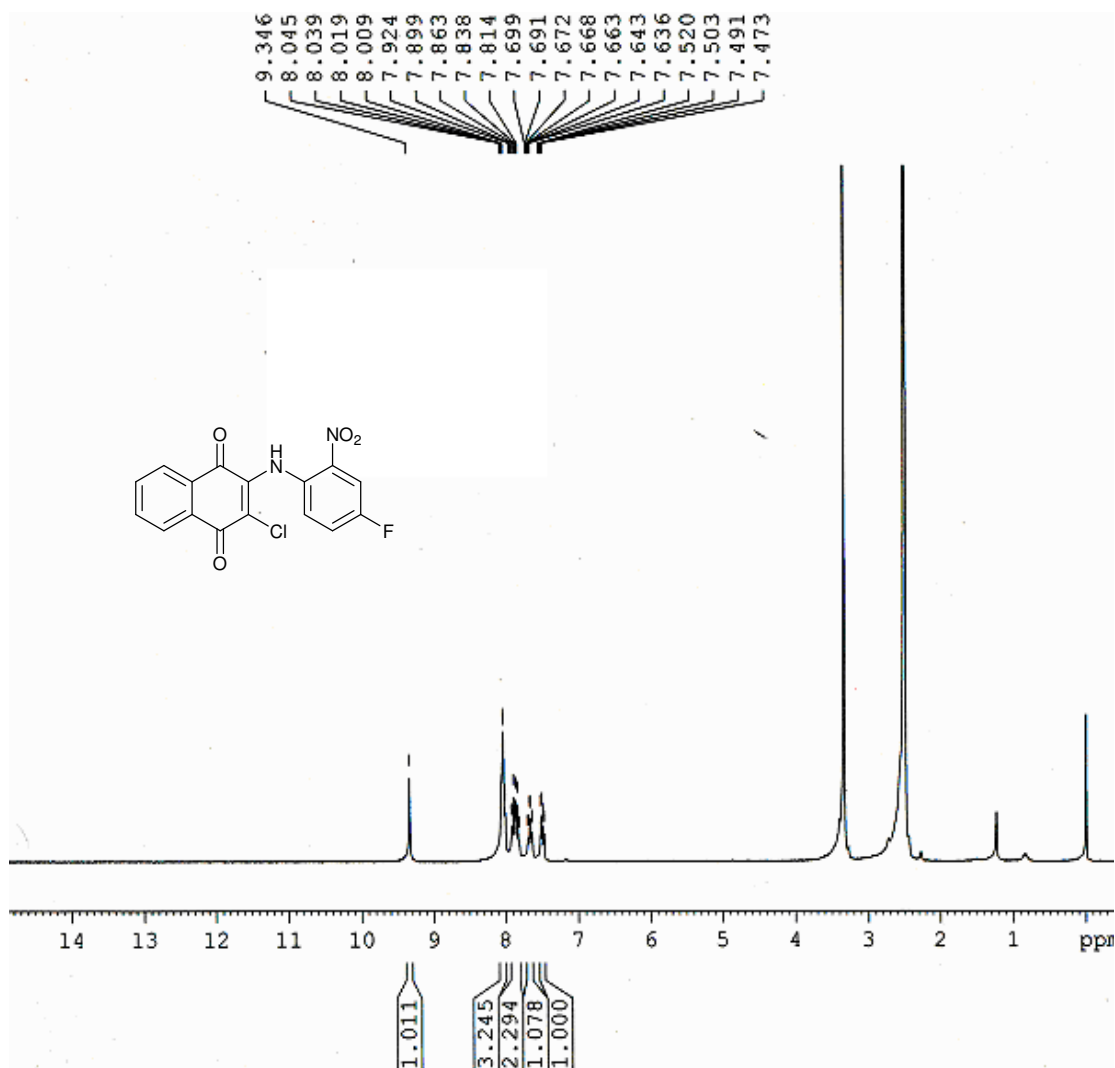
<sup>1</sup>H NMR for **3c**



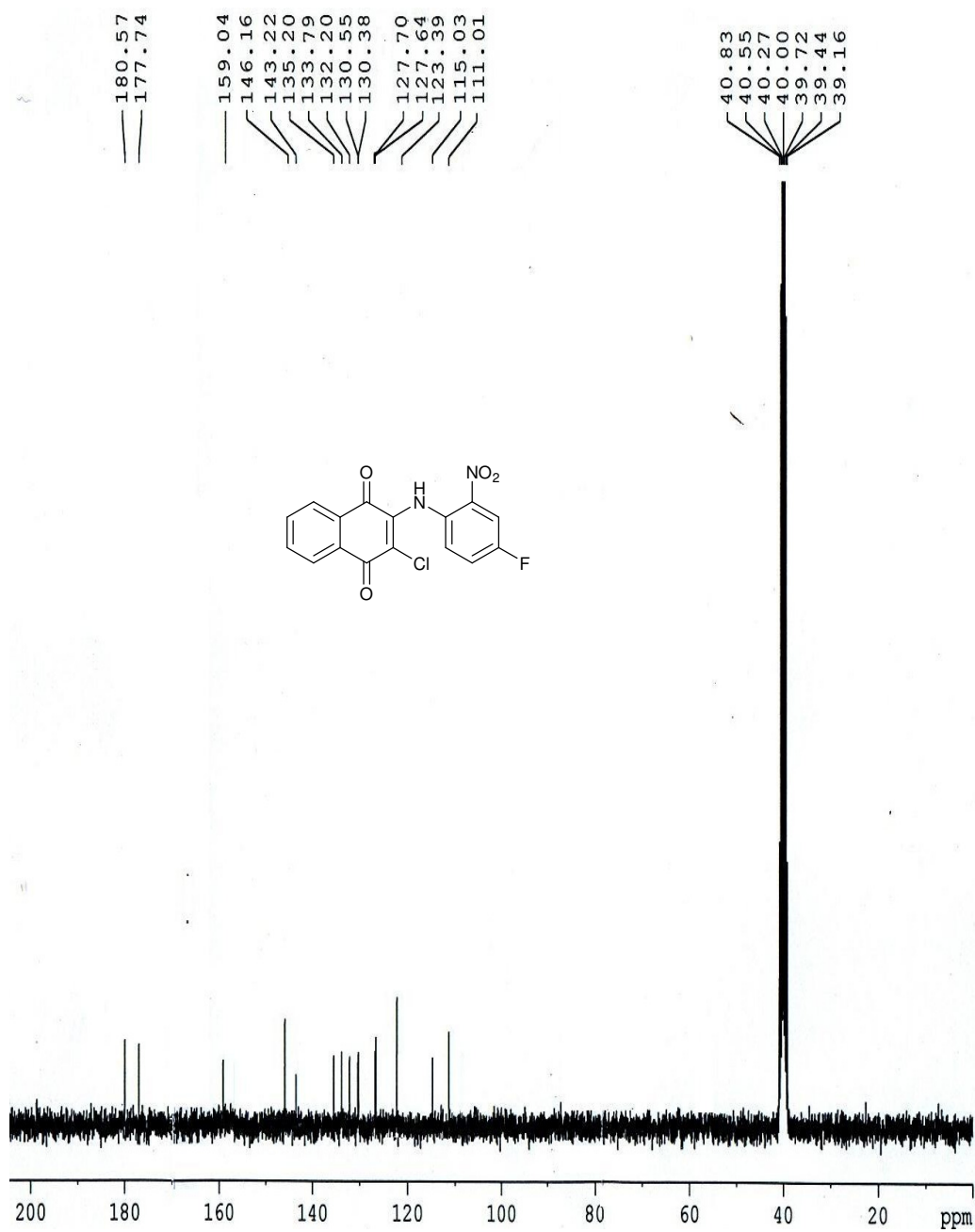
<sup>13</sup>C NMR for 3c



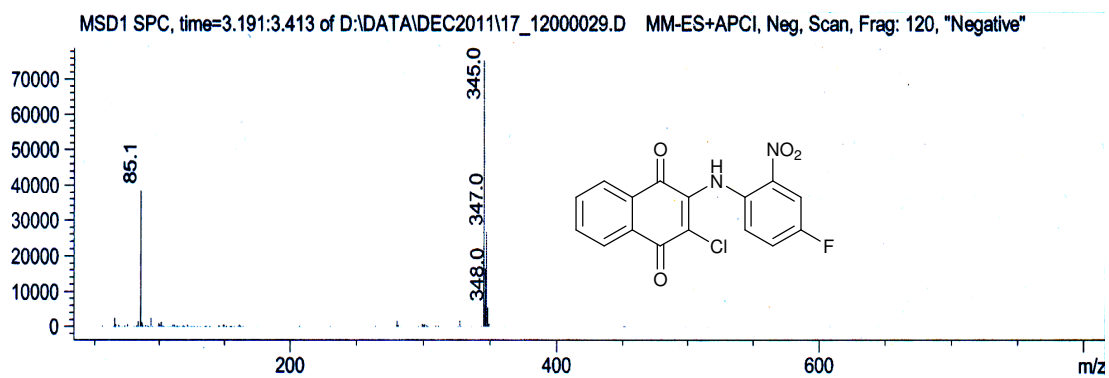
LC-MS for **3c**



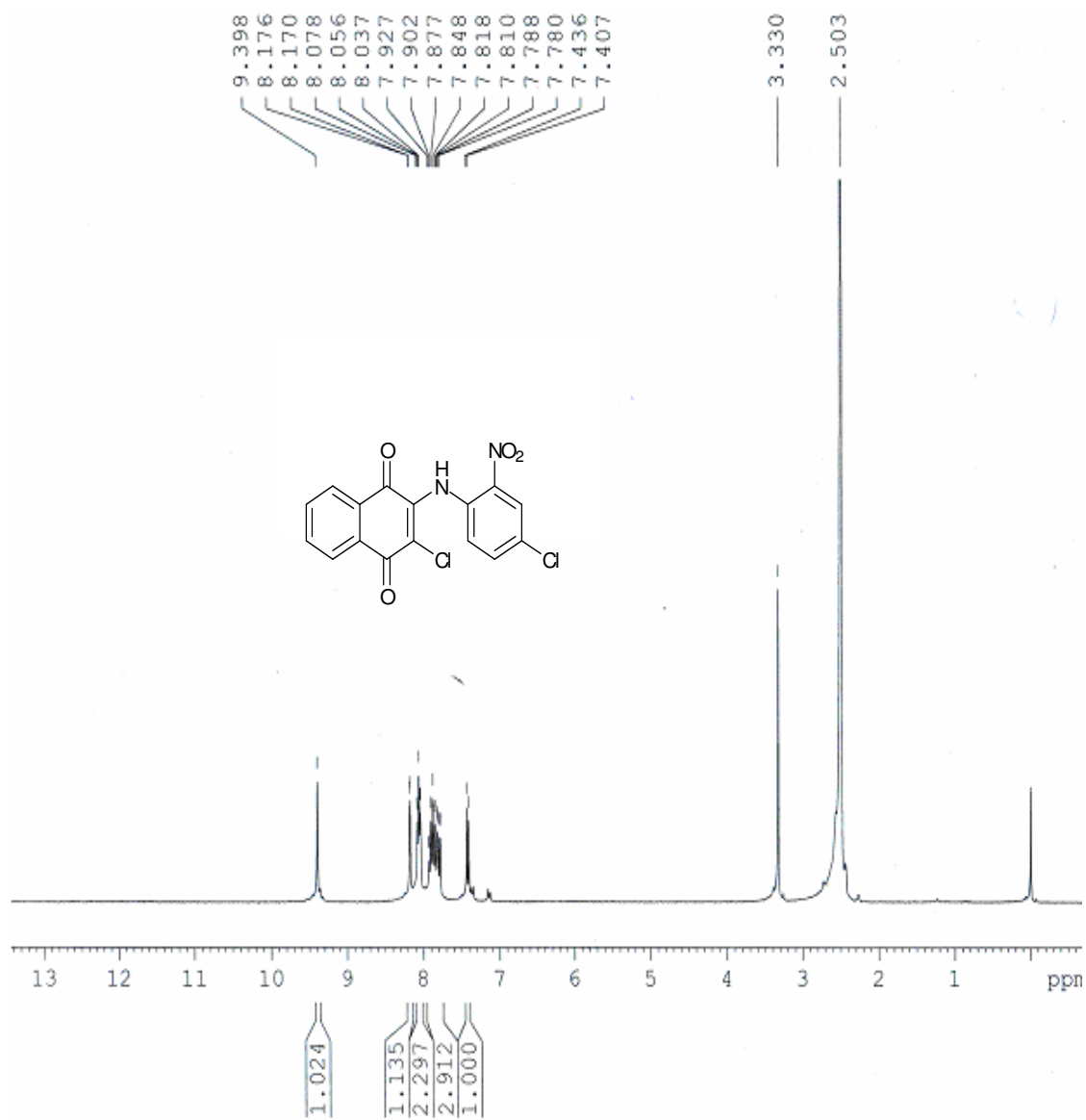
<sup>1</sup>H NMR for **3d**



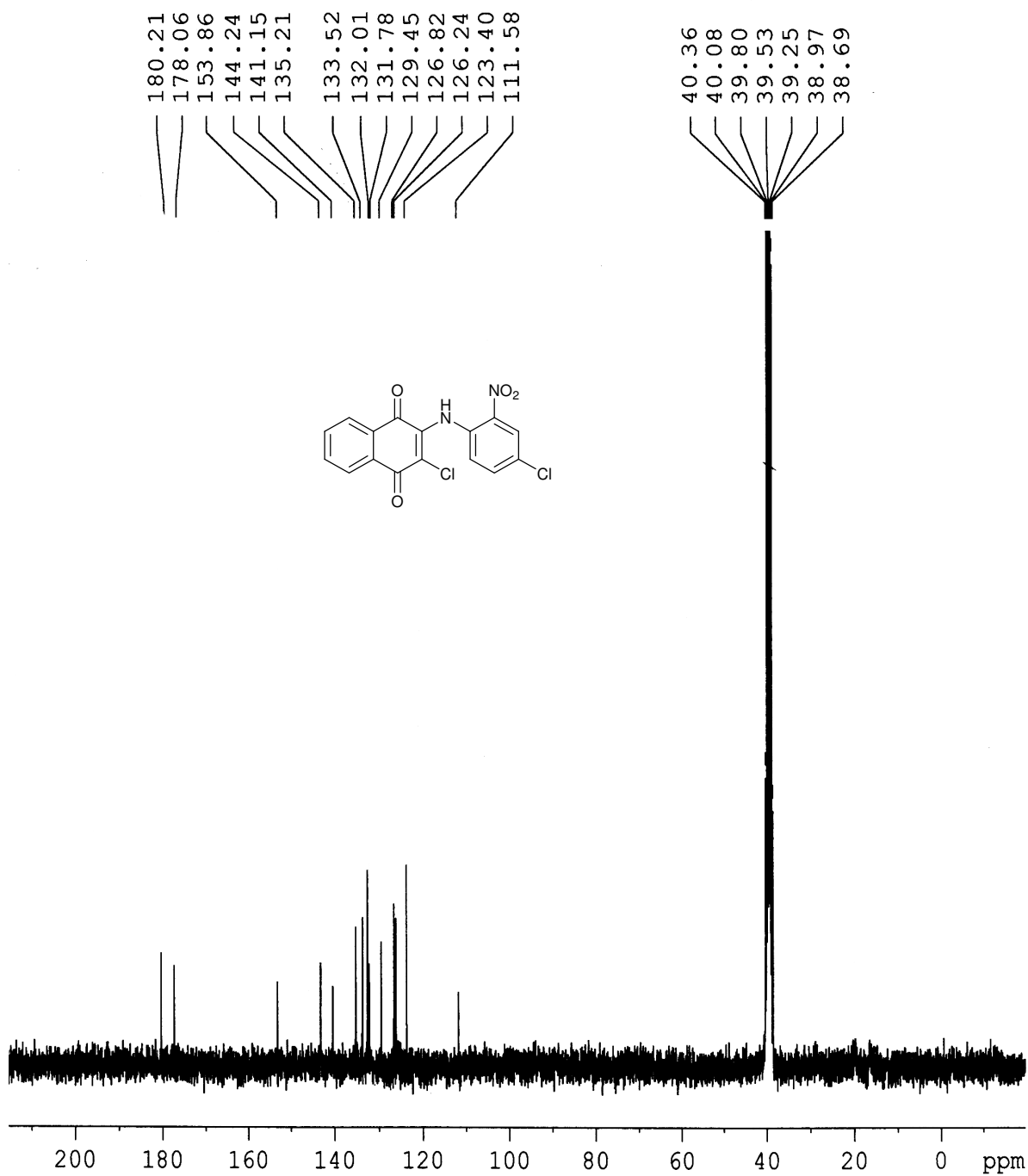
<sup>13</sup>C NMR for **3d**



LC- MS for **3d**

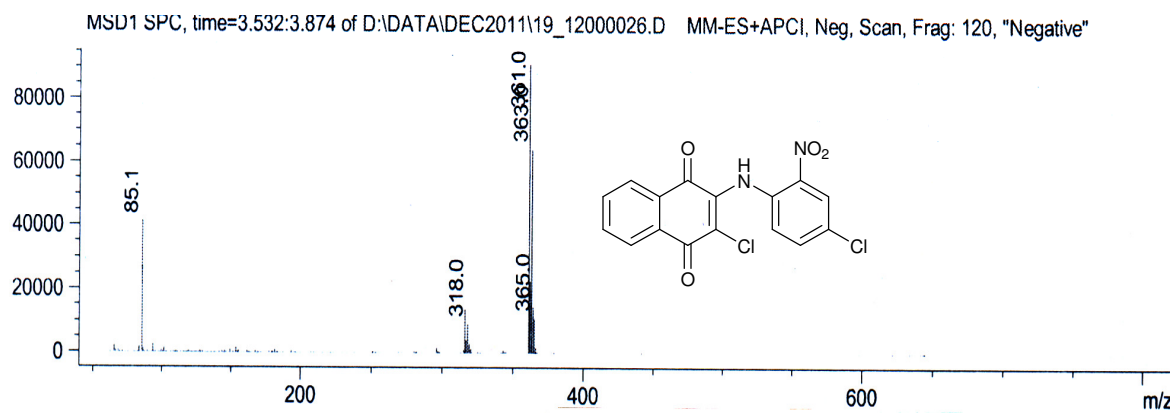


<sup>1</sup>H NMR for **3e**



<sup>13</sup>C NMR for **3e**





LC-MS for **3e**

**Coordinates for 1a**

C	-4.546554000	-2.495627000	-1.283600000
C	-3.303671000	-2.499842000	-0.647346000
C	-2.826684000	-1.328578000	-0.038678000
C	-3.601447000	-0.152425000	-0.061220000
C	-4.846220000	-0.156126000	-0.698912000
C	-5.315928000	-1.323556000	-1.309904000
H	-4.914877000	-3.398997000	-1.757703000
H	-2.689166000	-3.392163000	-0.614472000
C	-1.512118000	-1.324751000	0.613013000
C	-3.127810000	1.093878000	0.613849000
H	-5.427912000	0.758111000	-0.698848000
H	-6.282023000	-1.321018000	-1.803709000
C	-1.817816000	1.055673000	1.255315000
C	-0.987777000	-0.038276000	1.210340000
N	0.276528000	-0.206038000	1.699724000
H	0.544419000	-1.188869000	1.710737000
C	1.318467000	0.724315000	1.965246000
C	1.530074000	1.856760000	1.162409000
C	2.217546000	0.426141000	3.002816000
C	2.618518000	2.694030000	1.419720000
H	0.857296000	2.073037000	0.341703000
C	3.309282000	1.262657000	3.244523000
H	2.046967000	-0.449750000	3.621105000
C	3.511065000	2.403600000	2.458279000
H	2.772844000	3.570406000	0.798934000
H	3.996271000	1.026987000	4.050675000
H	4.355761000	3.056596000	2.650332000
Cl	-1.396517000	2.540520000	2.196400000
O	-3.858203000	2.112074000	0.629413000
O	-0.796428000	-2.351443000	0.693520000

**Coordinates for 1b**

C	-4.414425000	-2.586942000	-1.480998000
C	-3.255811000	-2.562768000	-0.702234000
C	-2.850996000	-1.366753000	-0.089303000
C	-3.614126000	-0.194002000	-0.251181000
C	-4.774452000	-0.226151000	-1.031445000
C	-5.171763000	-1.418317000	-1.645953000
H	-4.726599000	-3.509571000	-1.958331000
H	-2.651943000	-3.451713000	-0.560553000
C	-1.622326000	-1.333590000	0.712051000
C	-3.220594000	1.079808000	0.424542000
H	-5.349334000	0.686260000	-1.137383000
H	-6.072437000	-1.437699000	-2.250646000
C	-1.996565000	1.070335000	1.216862000
C	-1.169125000	-0.022906000	1.315096000
N	0.028756000	-0.167831000	1.953941000
H	0.293405000	-1.148604000	2.030950000
C	1.030955000	0.776045000	2.310264000
C	1.343933000	1.879160000	1.500848000
C	1.801851000	0.522549000	3.455629000
C	2.394393000	2.725946000	1.857190000
H	0.779715000	2.065419000	0.595239000
C	2.857025000	1.370870000	3.793394000
H	1.564306000	-0.332184000	4.081594000
C	3.167673000	2.493987000	3.007715000
H	2.624082000	3.577021000	1.222888000
H	3.443530000	1.161435000	4.683136000
Cl	-1.686066000	2.593556000	2.140685000
O	-3.946230000	2.095768000	0.312023000
O	-0.923138000	-2.354623000	0.916115000

C	4.285380000	3.435010000	3.397257000	Cl	-1.340743000	2.644039000	1.954456000
H	5.059905000	2.920209000	3.975471000	O	-3.498343000	2.264150000	-0.020387000
H	4.760570000	3.879146000	2.515916000	O	-1.161306000	-2.458713000	1.227448000
H	3.911748000	4.262323000	4.016189000	O	4.411701000	2.709660000	3.808040000
<b>Coordinate for 1c</b>				C	4.998822000	3.752292000	2.984981000
C	-4.460507000	-2.471692000	-1.437005000	H	5.823815000	4.149593000	3.574722000
C	-3.372730000	-2.521152000	-0.563230000	H	5.380935000	3.345906000	2.041085000
C	-2.857501000	-1.333317000	-0.021130000	H	4.274479000	4.548439000	2.777006000
C	-3.439215000	-0.093458000	-0.350174000	<b>Coordinates for 1d</b>			
C	-4.529470000	-0.051833000	-1.225308000	C	-4.547094000	-2.496001000	-1.289963000
C	-5.036857000	-1.236903000	-1.768258000	C	-3.302035000	-2.499982000	-0.657945000
H	-4.857825000	-3.388433000	-1.859238000	C	-2.825333000	-1.329829000	-0.046828000
H	-2.908118000	-3.462358000	-0.292629000	C	-3.602488000	-0.154932000	-0.063075000
C	-1.700842000	-1.380920000	0.880158000	C	-4.849249000	-0.158884000	-0.696791000
C	-2.928991000	1.179033000	0.245750000	C	-5.318755000	-1.325358000	-1.309909000
H	-4.964733000	0.912360000	-1.459985000	H	-4.915334000	-3.398524000	-1.765646000
H	-5.882662000	-1.198886000	-2.446828000	H	-2.685877000	-3.391327000	-0.630243000
C	-1.784670000	1.088874000	1.143024000	C	-1.508992000	-1.325730000	0.600202000
C	-1.124761000	-0.087442000	1.411642000	C	-3.128637000	1.090168000	0.613254000
N	-0.012421000	-0.324009000	2.165901000	H	-5.432825000	0.754142000	-0.692367000
H	0.115739000	-1.320217000	2.337222000	H	-6.286434000	-1.323050000	-1.800511000
C	1.067002000	0.519702000	2.549176000	C	-1.816291000	1.051957000	1.252094000
C	1.607517000	1.482114000	1.686730000	C	-0.986674000	-0.041074000	1.203817000
C	1.671705000	0.299950000	3.800960000	N	0.278886000	-0.210944000	1.691667000
C	2.717733000	2.238375000	2.075036000	H	0.549702000	-1.193190000	1.688507000
H	1.169651000	1.640464000	0.708834000	C	1.313769000	0.721806000	1.970981000
C	2.783686000	1.039543000	4.186240000	C	1.533584000	1.854289000	1.168405000
H	1.254484000	-0.443357000	4.472751000	C	2.198333000	0.430825000	3.023677000
C	3.307170000	2.018664000	3.326828000	C	2.611028000	2.701382000	1.433968000
H	3.111770000	2.981196000	1.393004000	H	0.872894000	2.067807000	0.337945000
H	3.257524000	0.886128000	5.148205000	C	3.285498000	1.266585000	3.284646000

H	2.023336000	-0.442215000	3.643394000
C	3.465901000	2.391320000	2.486397000
H	2.794009000	3.581808000	0.830940000
H	3.974878000	1.060178000	4.093611000
Cl	-1.393100000	2.537483000	2.191793000
O	-3.858102000	2.108410000	0.632538000
O	-0.788788000	-2.349826000	0.673193000
F	4.543499000	3.232131000	2.745998000

**Coordinates for 1e**

C	-4.521262000	-2.502537000	-1.317191000
C	-3.288345000	-2.504156000	-0.661683000
C	-2.822717000	-1.331453000	-0.047068000
C	-3.599137000	-0.156357000	-0.083158000
C	-4.833802000	-0.162766000	-0.740187000
C	-5.291979000	-1.331814000	-1.356982000
H	-4.880712000	-3.407022000	-1.795818000
H	-2.673265000	-3.395625000	-0.618442000
C	-1.518762000	-1.324864000	0.624614000
C	-3.138212000	1.090951000	0.597196000
H	-5.417424000	0.750189000	-0.750730000
H	-6.250197000	-1.331414000	-1.865767000
C	-1.836694000	1.055284000	1.260596000
C	-1.006155000	-0.036795000	1.228094000
N	0.252180000	-0.203055000	1.738982000
H	0.517940000	-1.186528000	1.758830000
C	1.288900000	0.726961000	2.007823000
C	1.498196000	1.867101000	1.214388000
C	2.190710000	0.427169000	3.042977000
C	2.581259000	2.711016000	1.471798000
H	0.828257000	2.091164000	0.394217000
C	3.281961000	1.260928000	3.295565000

H	2.027766000	-0.451445000	3.658486000
C	3.457609000	2.396888000	2.508117000
H	2.743138000	3.593105000	0.865034000
H	3.975456000	1.033697000	4.095512000
Cl	-1.433055000	2.540386000	2.207969000
O	-3.866816000	2.109509000	0.600522000
O	-0.801714000	-2.349299000	0.719773000
Cl	4.875912000	3.496853000	2.838629000

**Coordinates for 1a-HMB**

C	4.986937000	-1.503622000	0.064869000
C	3.917048000	-1.165955000	0.900824000
C	2.613513000	-1.536298000	0.553681000
C	2.387528000	-2.250730000	-0.638944000
C	3.463427000	-2.591717000	-1.472947000
C	4.761636000	-2.216516000	-1.121251000
H	5.995945000	-1.214271000	0.339459000
H	4.070972000	-0.625201000	1.826742000
C	1.484154000	-1.196394000	1.470942000
C	1.021152000	-2.630270000	-1.014811000
H	3.262332000	-3.142405000	-2.384662000
H	5.593973000	-2.476844000	-1.766188000
C	-0.131178000	-2.214377000	-0.128035000
C	0.145662000	-1.612570000	1.076235000
O	0.765712000	-3.291797000	-2.048969000
O	1.715735000	-0.587484000	2.544754000
N	-1.324853000	-2.592014000	-0.670606000
Cl	-1.131376000	-1.346084000	2.328985000
C	-2.651074000	-2.121907000	-0.461867000
C	-2.934456000	-0.766471000	-0.227691000
C	-4.264059000	-0.352181000	-0.109517000
C	-5.313507000	-1.269042000	-0.242968000

C	-5.027019000	-2.615632000	-0.497448000	H	-0.110606000	4.137399000	-3.522146000
C	-3.701984000	-3.043317000	-0.604233000	H	0.678206000	2.562312000	-3.625660000
H	-2.129899000	-0.044578000	-0.151590000	H	-1.066628000	2.654869000	-3.480893000
H	-4.477669000	0.694317000	0.080207000	C	-2.525452000	3.373115000	-1.470690000
H	-6.342543000	-0.937417000	-0.153146000	H	-2.419041000	3.924742000	-2.407466000
H	-5.832479000	-3.334732000	-0.604938000	H	-3.066408000	2.443461000	-1.702833000
H	-3.473518000	-4.089533000	-0.782760000	H	-3.174116000	3.973568000	-0.827574000
H	-1.191759000	-3.204270000	-1.474093000	<b>Coordinates for 1b-HMB</b>			
C	1.358534000	2.775718000	0.386658000	C	-0.755618000	1.286175000	0.802077000
C	0.195779000	2.816660000	1.188079000	C	0.382300000	2.092338000	1.226184000
C	-1.074025000	2.970535000	0.585559000	C	1.425802000	2.401441000	0.202156000
C	-1.174964000	3.115085000	-0.818308000	C	1.342888000	1.874392000	-1.101295000
C	-0.011253000	3.051528000	-1.620946000	C	0.198618000	1.037266000	-1.478811000
C	1.259073000	2.919227000	-1.015520000	C	-0.919324000	0.827854000	-0.482569000
C	-2.318708000	2.956948000	1.459512000	H	2.557533000	3.598938000	1.564686000
H	-2.432155000	3.887823000	2.033286000	C	2.511397000	3.210398000	0.554142000
H	-3.231609000	2.826417000	0.876147000	C	2.342838000	2.162333000	-2.042735000
H	-2.282426000	2.136151000	2.183338000	C	3.420735000	2.975127000	-1.686437000
C	0.332721000	2.709610000	2.696617000	C	3.504913000	3.497381000	-0.387597000
H	-0.562847000	3.052733000	3.216738000	H	2.255132000	1.748074000	-3.040436000
H	0.526770000	1.675488000	3.012712000	H	4.191140000	3.202964000	-2.415302000
H	1.168118000	3.317891000	3.060533000	H	4.343438000	4.127916000	-0.110644000
C	2.707452000	2.562714000	1.052032000	N	-1.948172000	0.121815000	-1.038444000
H	3.123063000	3.500441000	1.450876000	Cl	-1.899645000	0.836696000	2.130030000
H	2.625321000	1.863075000	1.888598000	O	0.097076000	0.499359000	-2.608118000
H	3.444118000	2.149678000	0.359288000	O	0.512157000	2.516258000	2.398772000
C	2.521787000	2.961965000	-1.861955000	C	-5.408109000	1.055645000	0.025006000
H	3.336134000	3.465640000	-1.333578000	C	-4.035955000	1.154432000	-0.202478000
H	2.882829000	1.957463000	-2.128759000	C	-3.329074000	0.050159000	-0.706375000
H	2.366350000	3.508349000	-2.794663000	C	-4.023007000	-1.132691000	-1.001380000
C	-0.132832000	3.107099000	-3.136502000	C	-5.399280000	-1.213668000	-0.779488000

C	-6.116687000	-0.127227000	-0.253925000	C	-0.026857000	-3.001792000	1.715555000
H	-5.940940000	1.917438000	0.416601000	H	0.275527000	-3.431801000	2.674597000
H	-3.517719000	2.084218000	-0.001951000	H	-0.786314000	-2.235871000	1.930389000
H	-3.481253000	-1.987057000	-1.395535000	H	-0.518221000	-3.798493000	1.152119000
H	-5.921686000	-2.136912000	-1.011905000	C	0.038941000	-3.088080000	-1.217349000
C	-7.601603000	-0.221693000	0.015968000	H	0.046021000	-4.187589000	-1.253977000
H	-7.811277000	-0.235561000	1.093992000	H	-0.909405000	-2.787151000	-0.761871000
H	-8.141967000	0.634305000	-0.405596000	H	0.026478000	-2.728842000	-2.248624000
H	-8.028173000	-1.133337000	-0.413871000	H	-1.685477000	-0.271509000	-1.940236000
C	1.165879000	-2.436303000	0.962468000	<b>Coordinates for 1c-HMB</b>			
C	2.228701000	-1.835576000	1.673945000	C	-1.624917000	5.298437000	0.678042000
C	3.378563000	-1.391441000	0.982235000	C	-0.541058000	4.618753000	1.237572000
C	3.441598000	-1.492459000	-0.426313000	C	-0.038828000	3.467783000	0.610404000
C	2.372677000	-2.080900000	-1.140294000	C	-0.629022000	2.991940000	-0.576645000
C	1.223660000	-2.527875000	-0.446479000	C	-1.713160000	3.679115000	-1.132187000
C	2.453552000	-2.251303000	-2.648591000	C	-2.208418000	4.828477000	-0.507096000
H	2.017175000	-3.203429000	-2.965228000	H	-2.013137000	6.189037000	1.160283000
H	1.912814000	-1.453506000	-3.178570000	H	-0.070122000	4.961334000	2.151767000
H	3.485491000	-2.245985000	-3.004250000	C	1.111702000	2.762645000	1.185698000
C	4.649469000	-0.945183000	-1.170327000	C	-0.134433000	1.745593000	-1.236796000
H	5.421619000	-1.711922000	-1.332840000	H	-2.153301000	3.296250000	-2.045193000
H	4.373474000	-0.551559000	-2.151865000	H	-3.050656000	5.356181000	-0.942277000
H	5.119090000	-0.123861000	-0.624175000	C	1.010611000	1.075596000	-0.638795000
C	4.555825000	-0.820874000	1.756446000	C	1.674128000	1.556335000	0.466177000
H	5.508466000	-1.075317000	1.283673000	N	2.779445000	1.080122000	1.107259000
H	4.511714000	0.276105000	1.829661000	C	3.832789000	0.228727000	0.666330000
H	4.593408000	-1.210494000	2.776115000	C	4.365472000	-0.699259000	1.569418000
C	2.123549000	-1.643944000	3.177912000	C	5.457227000	-1.497749000	1.213621000
H	2.609902000	-0.718397000	3.497443000	C	6.018588000	-1.368918000	-0.063585000
H	1.082989000	-1.578431000	3.502677000	C	5.494965000	-0.432596000	-0.969534000
H	2.589991000	-2.467994000	3.738382000	C	4.417167000	0.366315000	-0.606538000

H	3.914974000	-0.809245000	2.550702000	H	-5.536412000	0.405194000	1.941349000
H	5.846842000	-2.210877000	1.929036000	H	-5.471723000	1.108523000	0.331702000
H	5.953842000	-0.345518000	-1.946868000	C	-4.303420000	0.338206000	-1.710587000
H	4.029261000	1.099268000	-1.303429000	H	-5.370464000	0.556095000	-1.836449000
H	2.918474000	1.542609000	2.004331000	H	-3.833530000	1.243615000	-1.302322000
Cl	1.453073000	-0.499280000	-1.410697000	H	-3.883701000	0.186248000	-2.704479000
O	7.095248000	-2.113490000	-0.527205000	C	-2.448964000	-1.785176000	-2.516053000
C	7.669368000	-3.129040000	0.337458000	H	-1.683469000	-2.555135000	-2.613459000
H	6.927448000	-3.892678000	0.598934000	H	-3.108644000	-1.870472000	-3.391632000
H	8.081359000	-2.686832000	1.252302000	H	-1.933589000	-0.821059000	-2.586220000
H	8.471369000	-3.579371000	-0.245822000	O	1.658513000	3.124778000	2.254683000
C	-4.771768000	-0.950946000	0.422970000	O	-0.722578000	1.308395000	-2.256608000
C	-4.609408000	-2.086956000	1.246388000	<b>Coordinates for 1d-HMB</b>			
C	-3.727435000	-3.120246000	0.857273000	C	-0.674660000	-1.032455000	-0.419102000
C	-3.058260000	-3.046291000	-0.385959000	C	0.424498000	-1.404062000	-1.388248000
C	-3.220176000	-1.909013000	-1.211625000	C	1.645803000	-2.034190000	-0.875387000
C	-4.087443000	-0.866965000	-0.810322000	C	1.830245000	-2.173811000	0.513713000
C	-3.484095000	-4.298794000	1.787429000	C	0.815192000	-1.654693000	1.479024000
H	-4.087548000	-5.178067000	1.516810000	C	-0.423856000	-1.117866000	0.927698000
H	-2.435942000	-4.611629000	1.771753000	H	2.453061000	-2.390729000	-2.832357000
H	-3.722305000	-4.050656000	2.823724000	C	2.618391000	-2.510476000	-1.767836000
C	-2.178591000	-4.197161000	-0.849776000	C	2.987579000	-2.791254000	0.999594000
H	-1.108105000	-3.966581000	-0.752104000	C	3.951661000	-3.272638000	0.106802000
H	-2.368375000	-5.110833000	-0.284328000	C	3.768145000	-3.132557000	-1.276288000
H	-2.359171000	-4.434387000	-1.903210000	H	3.111255000	-2.883924000	2.072215000
C	-5.397455000	-2.203234000	2.541456000	H	4.844725000	-3.756325000	0.488498000
H	-5.707200000	-3.234798000	2.733166000	H	4.517057000	-3.507897000	-1.965310000
H	-4.815684000	-1.873180000	3.415376000	O	0.238628000	-1.185249000	-2.609882000
H	-6.307469000	-1.599992000	2.515142000	O	1.048106000	-1.690243000	2.710530000
C	-5.673809000	0.185351000	0.877311000	N	-1.783980000	-0.593109000	-1.086401000
H	-6.739005000	-0.049181000	0.733194000	H	-1.586522000	-0.441388000	-2.074058000

Cl	-1.576359000	-0.468292000	2.161486000	H	-1.174841000	2.652653000	1.872608000
C	-5.863223000	-0.373450000	-0.151695000	H	-0.042393000	3.891791000	2.416914000
C	-5.121528000	-1.421593000	0.382967000	H	-0.946615000	4.133171000	0.934837000
C	-3.757368000	-1.497888000	0.096176000	C	-0.596293000	3.180445000	-1.396535000
C	-3.148844000	-0.513983000	-0.702008000	H	-1.499195000	3.028959000	-0.799406000
C	-3.925889000	0.529892000	-1.233539000	H	-0.540488000	4.253206000	-1.634258000
C	-5.293359000	0.602688000	-0.962191000	H	-0.744593000	2.650860000	-2.341526000
H	-5.607182000	-2.166649000	1.000509000	C	1.710405000	2.189025000	-2.925765000
H	-3.452321000	1.289577000	-1.846176000	H	1.279937000	1.266770000	-3.344789000
H	-5.905980000	1.401784000	-1.360361000	H	1.123739000	3.027589000	-3.309129000
H	-3.171341000	-2.321457000	0.483672000	H	2.716532000	2.293322000	-3.339773000
F	-7.224412000	-0.302477000	0.128388000	<b>Coordinates for 1e-HMB</b>			
C	0.642886000	2.682879000	-0.668765000	C	0.410269000	-0.998787000	-0.377600000
C	1.732548000	2.164808000	-1.406250000	C	-0.681465000	-1.456756000	-1.316137000
C	2.856376000	1.639455000	-0.727862000	C	-1.887547000	-2.075752000	-0.756447000
C	2.900597000	1.655398000	0.683809000	C	-2.077932000	-2.098792000	0.638865000
C	1.808140000	2.168114000	1.421621000	C	-1.087794000	-1.461054000	1.557790000
C	0.697044000	2.721832000	0.743635000	C	0.152470000	-0.964848000	0.969523000
C	4.134455000	1.142429000	1.407563000	H	-2.668768000	-2.629075000	-2.678719000
H	4.151749000	0.044683000	1.468971000	C	-2.837942000	-2.658973000	-1.608471000
H	5.052674000	1.451386000	0.897799000	C	-3.218195000	-2.709016000	1.171517000
H	4.192228000	1.521791000	2.429040000	C	-4.158897000	-3.298836000	0.319879000
C	4.009815000	1.048386000	-1.521103000	C	-3.970038000	-3.274093000	-1.069254000
H	4.722288000	1.820075000	-1.849225000	H	-3.349092000	-2.710712000	2.247222000
H	4.571450000	0.316916000	-0.936574000	H	-5.038357000	-3.776995000	0.738318000
H	3.657080000	0.533862000	-2.419337000	H	-4.700787000	-3.733765000	-1.725952000
C	1.828127000	2.086124000	2.939136000	N	1.521896000	-0.607614000	-1.073688000
H	2.140558000	1.090464000	3.271534000	Cl	1.287213000	-0.186000000	2.141898000
H	2.518778000	2.814688000	3.387681000	O	-0.503043000	-1.315413000	-2.550546000
H	0.842726000	2.260937000	3.371512000	O	-1.339085000	-1.366918000	2.782730000
C	-0.425648000	3.379917000	1.530063000	C	5.612378000	-0.363684000	-0.161887000



C	5.052734000	0.522404000	-1.079865000	C	0.522844000	3.494495000	0.301312000
C	3.683767000	0.444715000	-1.344207000	H	1.354757000	2.810204000	0.520984000
C	2.885376000	-0.514986000	-0.698324000	H	0.803294000	4.082860000	-0.575530000
C	3.476792000	-1.410966000	0.208052000	H	0.453296000	4.194901000	1.137504000
C	4.843421000	-1.328451000	0.485170000	C	-3.770534000	1.573981000	2.182814000
H	5.667982000	1.264060000	-1.573763000	H	-3.498091000	0.637899000	2.692377000
H	3.227992000	1.137592000	-2.044037000	H	-3.686236000	2.374175000	2.923970000
H	2.878565000	-2.175000000	0.687825000	H	-4.824315000	1.506956000	1.905532000
H	5.301302000	-2.014500000	1.186715000	C	-1.167326000	2.738393000	2.610415000
H	1.324137000	-0.518855000	-2.068880000	H	-0.090272000	2.893874000	2.676747000
Cl	7.399487000	-0.262539000	0.195807000	H	-1.658004000	3.631204000	3.025719000
C	-0.788240000	2.754849000	0.086465000	H	-1.404617000	1.899834000	3.272664000
C	-1.195279000	2.387195000	-1.216238000	C	-4.626345000	0.789169000	-0.534939000
C	-2.458785000	1.784610000	-1.424741000	H	-4.887990000	0.158341000	0.317660000
C	-3.294700000	1.491788000	-0.322564000	H	-5.452423000	1.501341000	-0.678385000
C	-2.877846000	1.839139000	0.982860000	H	-4.605313000	0.136754000	-1.410663000
C	-1.617626000	2.448173000	1.189268000	C	-2.902292000	1.478909000	-2.845707000
C	-0.282562000	2.610710000	-2.410633000	H	-2.468888000	0.538434000	-3.217870000
H	-0.541057000	3.522059000	-2.970076000	H	-3.987583000	1.398753000	-2.928778000
H	0.764199000	2.701797000	-2.112785000	H	-2.589211000	2.268356000	-3.536282000
H	-0.346917000	1.775400000	-3.115650000				