

# Ultrasound-assisted, one-pot, three-component synthesis and antibacterial activities of novel indole derivatives containing 1,3,4-oxadiazole and 1,2,4-triazole moieties

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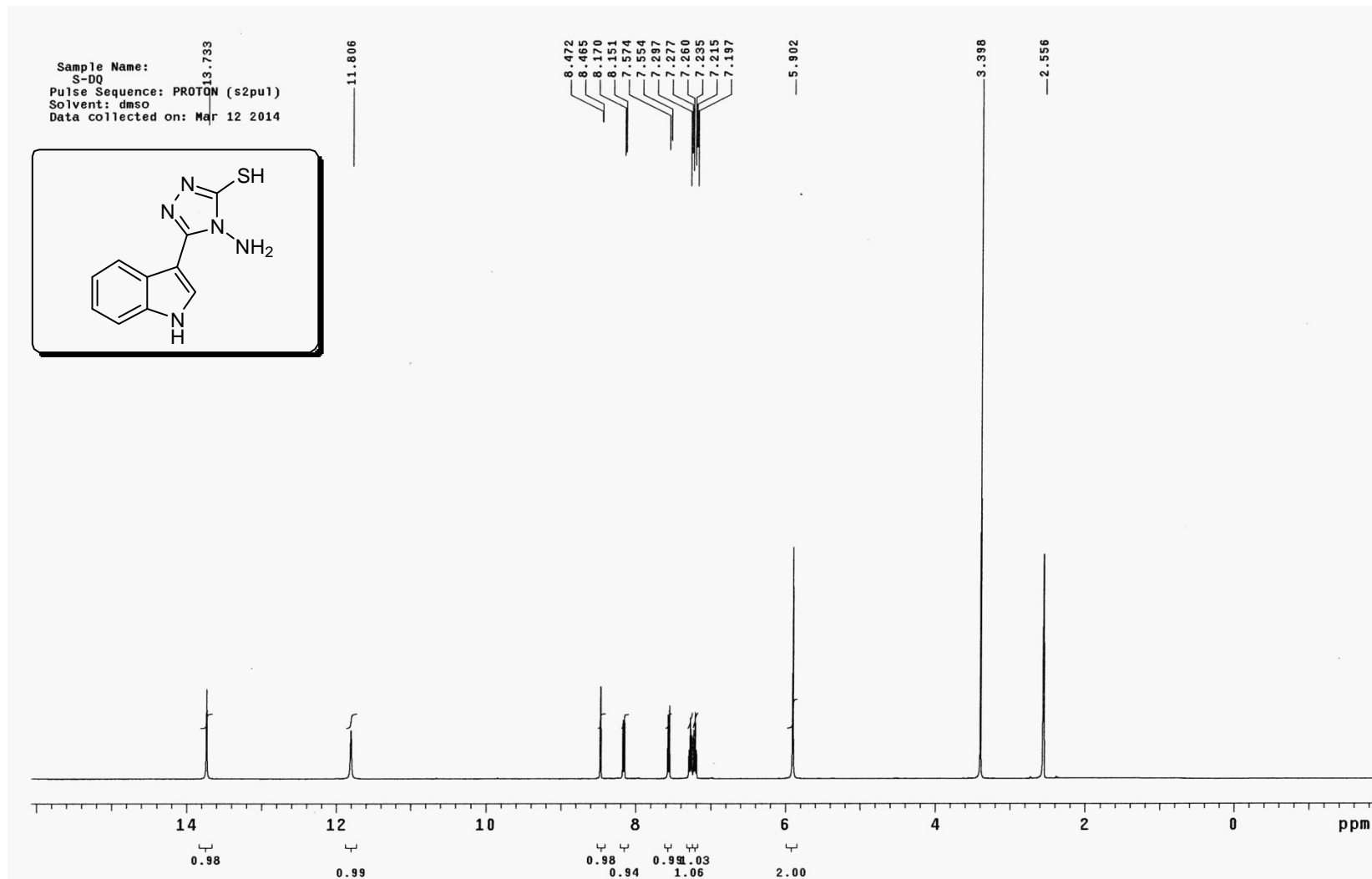
\* Corresponding author. Tel.: +86 028 85522315; fax: +86 028 85524386.

E-mail address: szc169@163.com; zzg63129@163.com

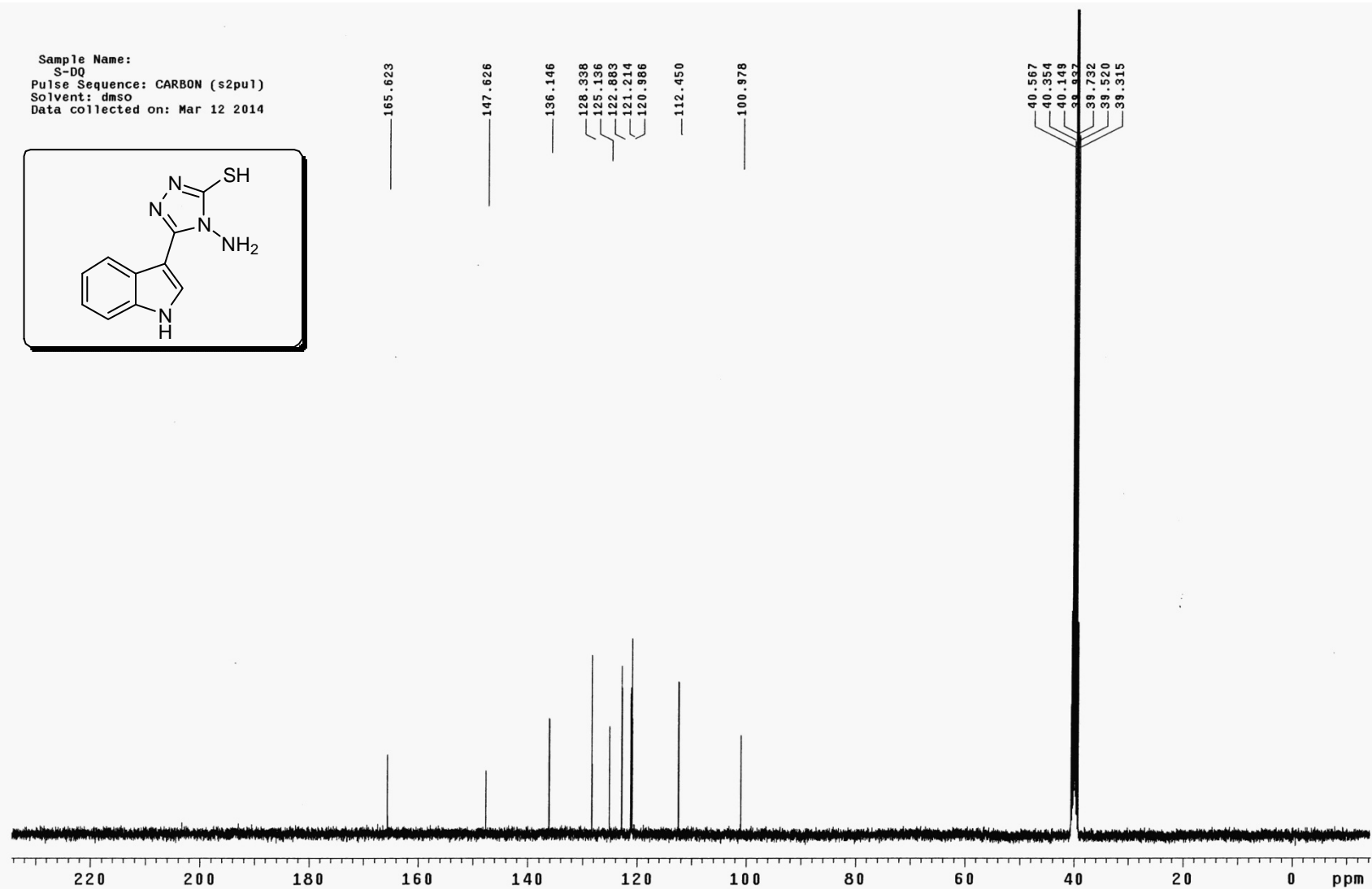
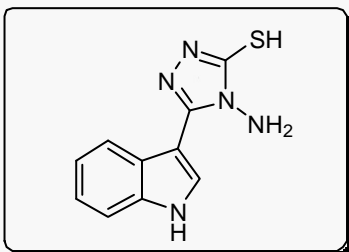
## Supporting information

|   |    |
|---|----|
| Content   | S1 |
| Compound <b>8</b> ( $^1\text{H}$ NMR, $^{13}\text{C}$ NMR)              | S2 |
| Compounds <b>10a-m</b> ( $^1\text{H}$ NMR, $^{13}\text{C}$ NMR, ESI-MS) | S3 |

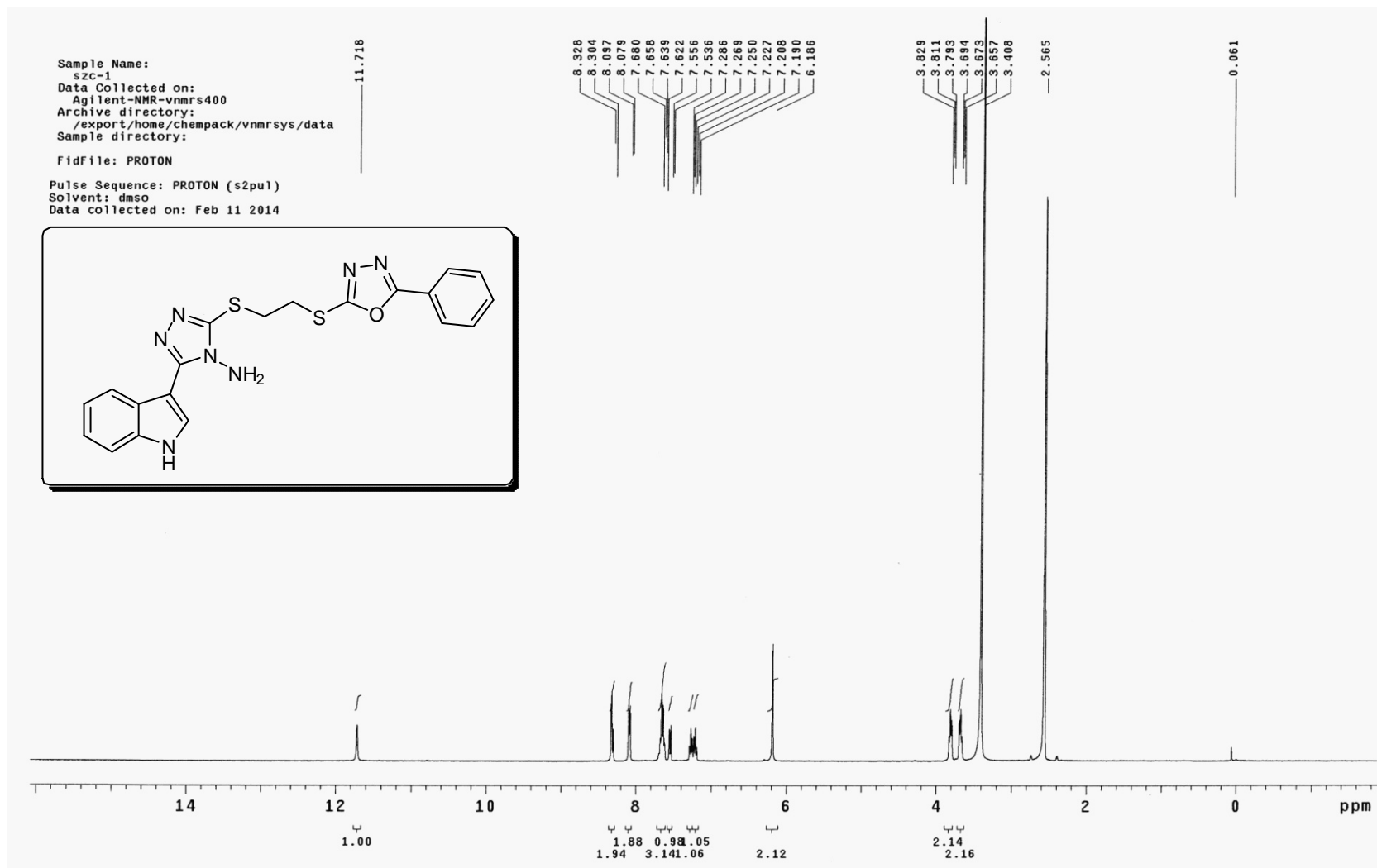
4-amino-5-(1H-indol-3-yl)-4H-[1,2,4]triazole-3-thiol (**8**)



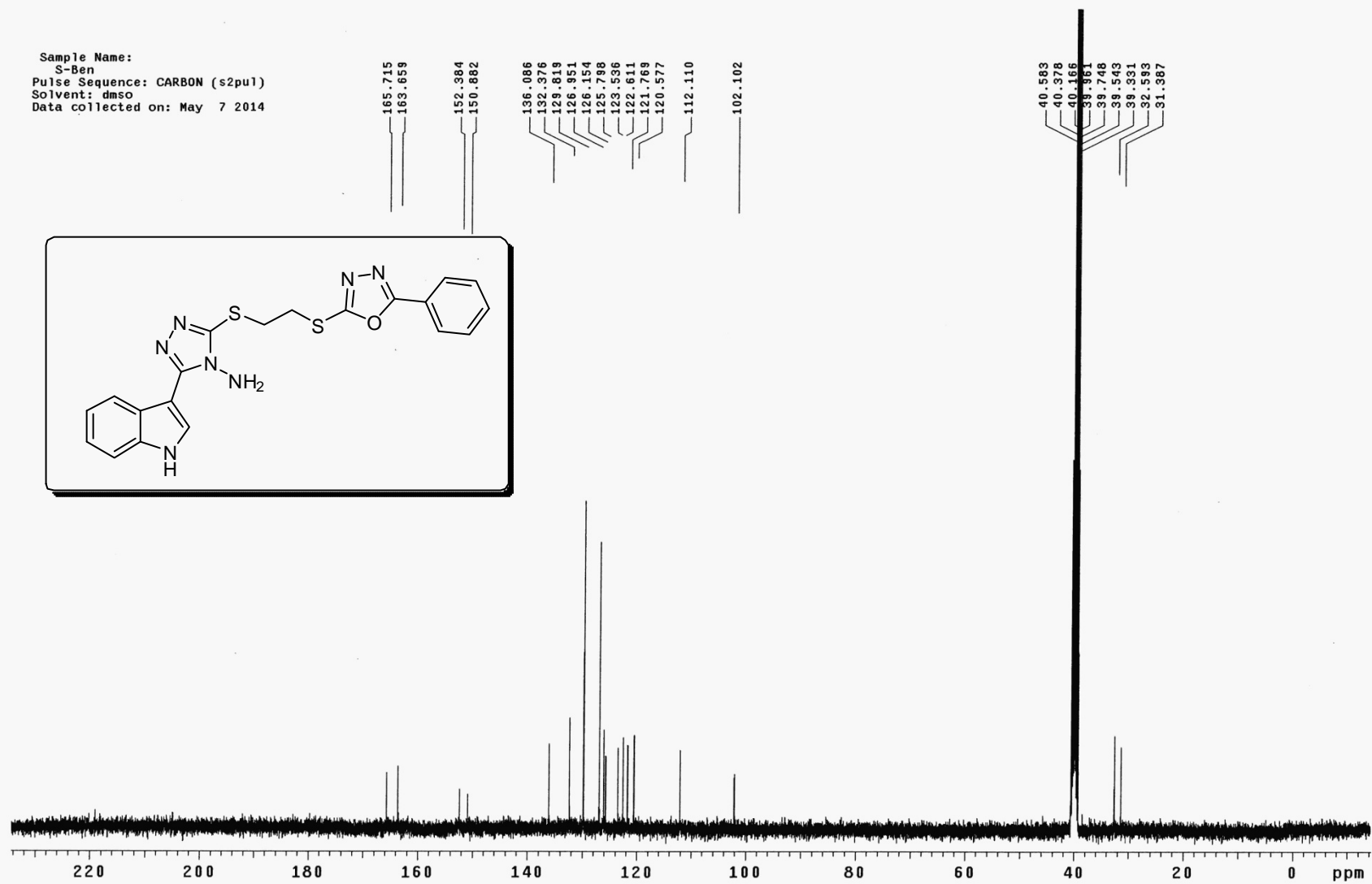
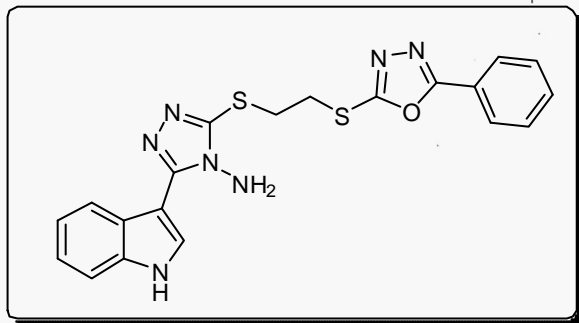
Sample Name:  
S-DQ  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dms0  
Data collected on: Mar 12 2014



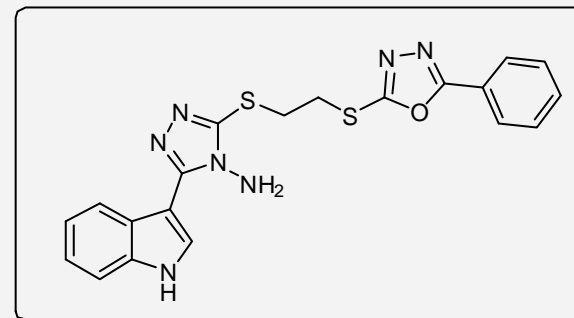
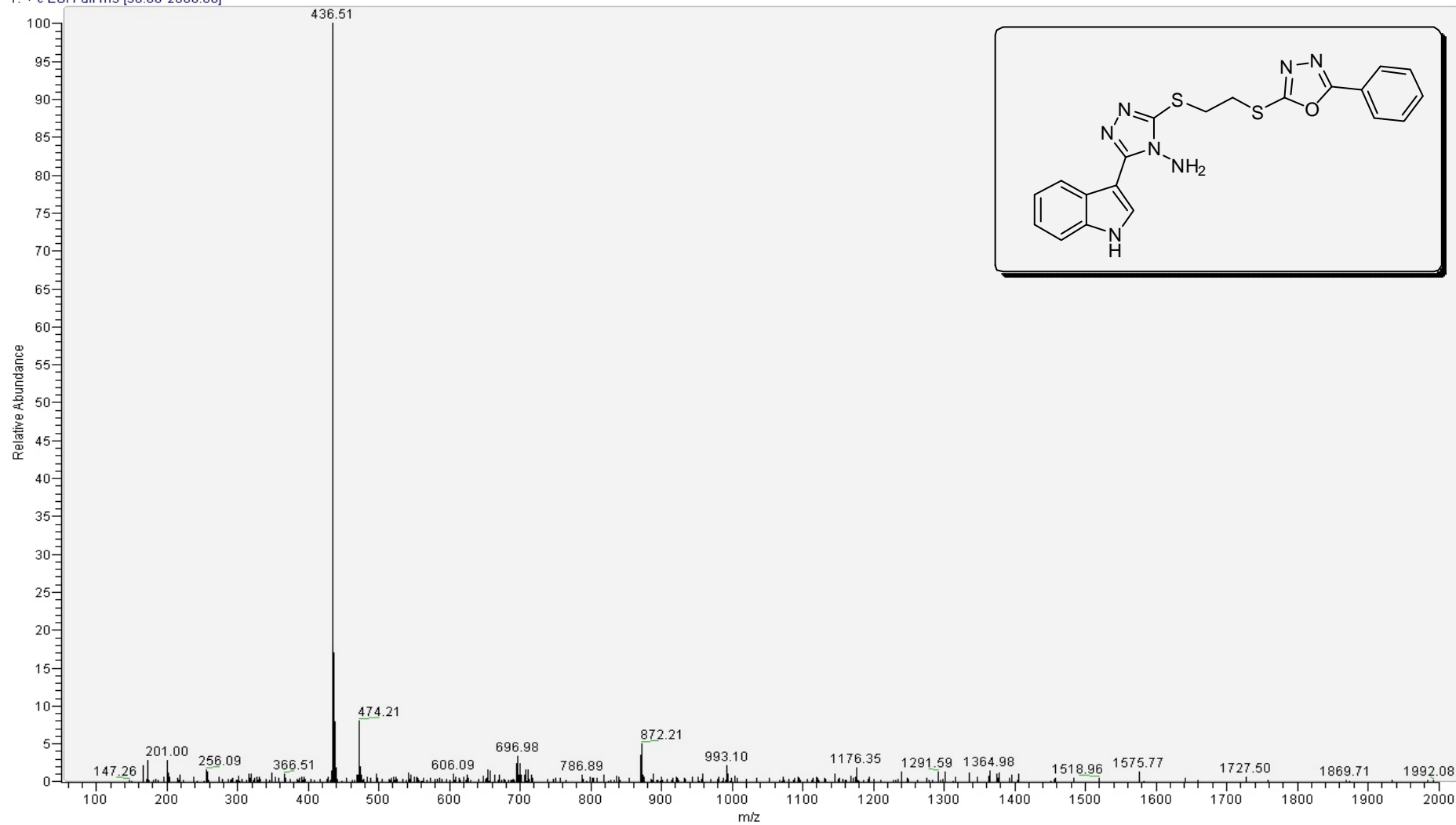
3-(1H-indol-3-yl)-5-[[2-[(5-phenyl-1,3,4-oxadiazol-2-yl)thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10a)



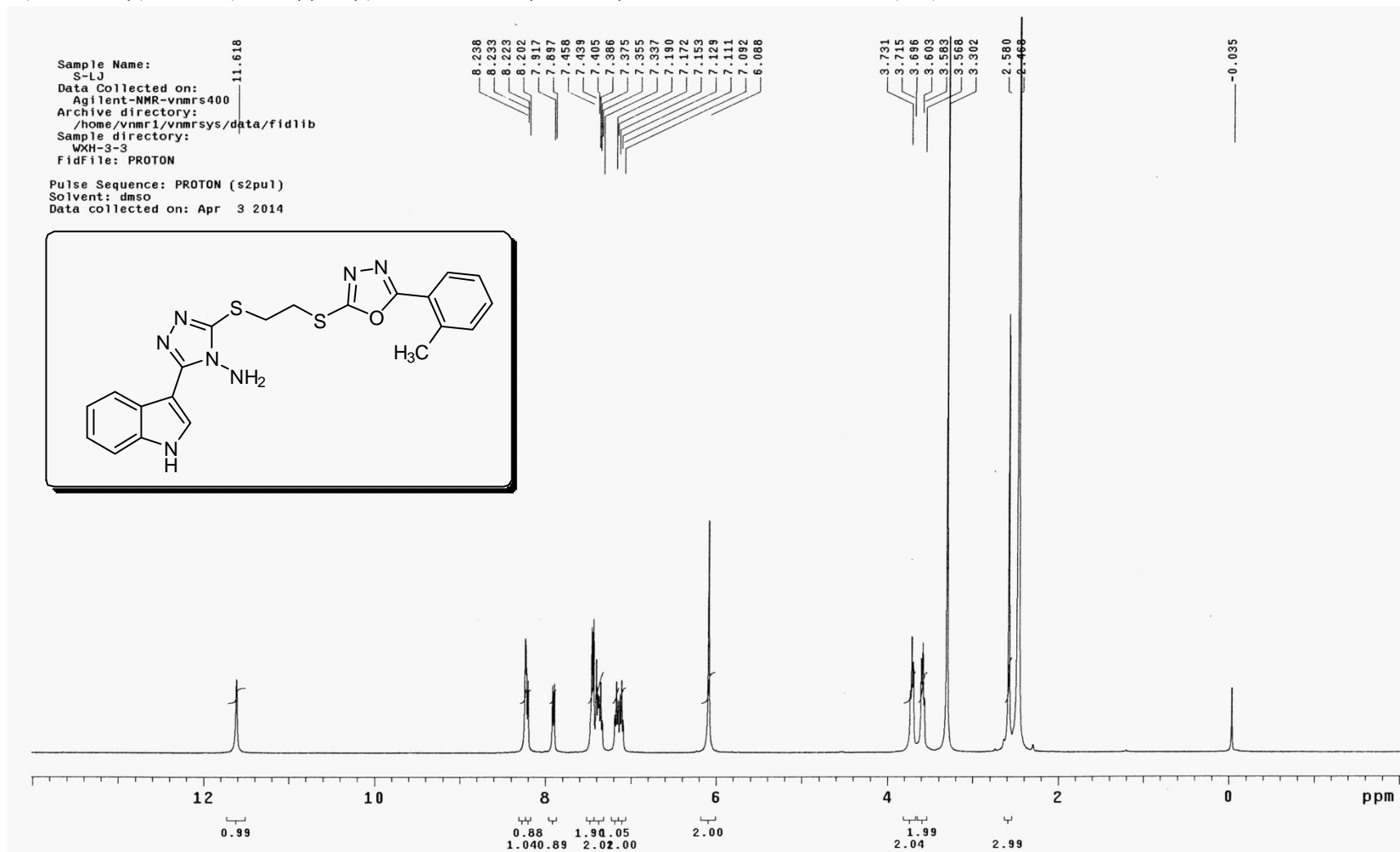
Sample Name:  
S-Ben  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dmsO  
Data collected on: May 7 2014



T: + c ESI Full ms [50.00-2000.00]

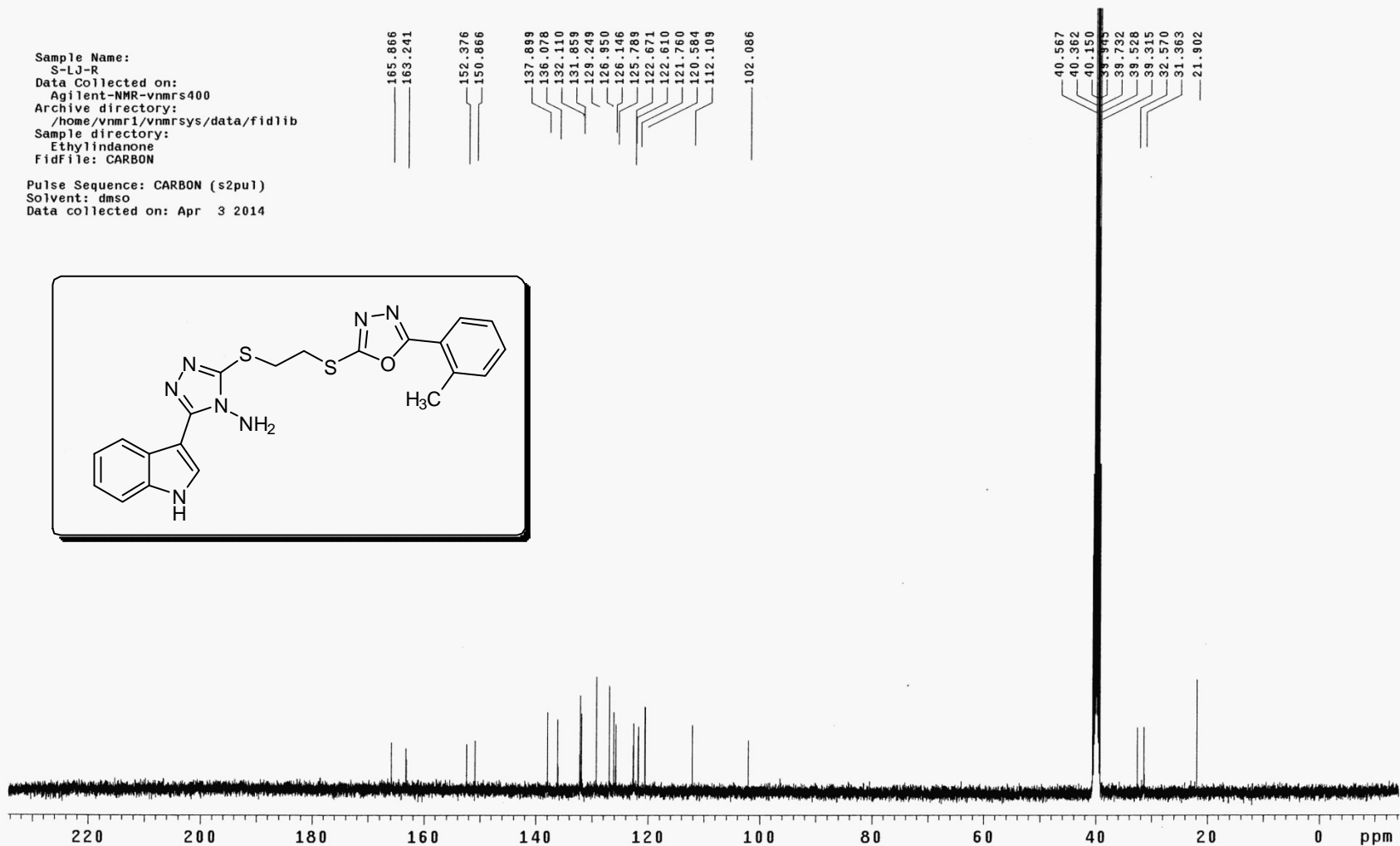
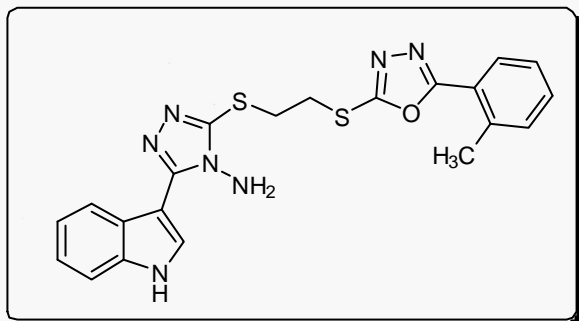


3-(1H-indol-3-yl)-5-[[2-[[5-(2-methylphenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (**10b**)



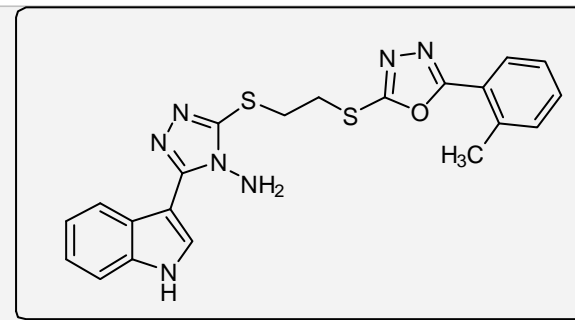
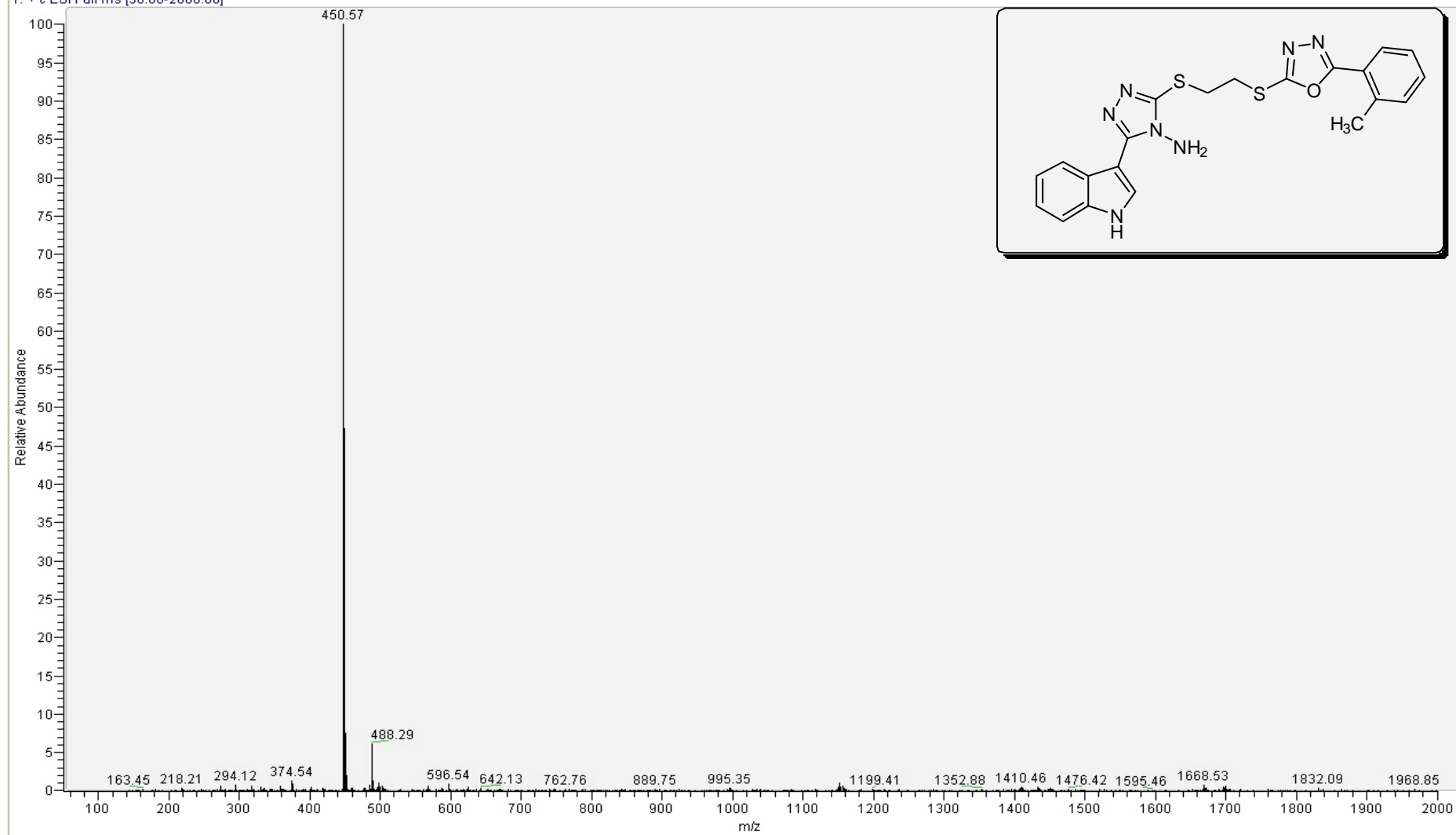
Sample Name:  
S-LJ-R  
Data Collected on:  
Agilent-NMR-vnmrs400  
Archive directory:  
/home/vnmr1/vnmrsys/data/ftdlib  
Sample directory:  
Ethylindanone  
FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)  
Solvent: dms0  
Data collected on: Apr 3 2014

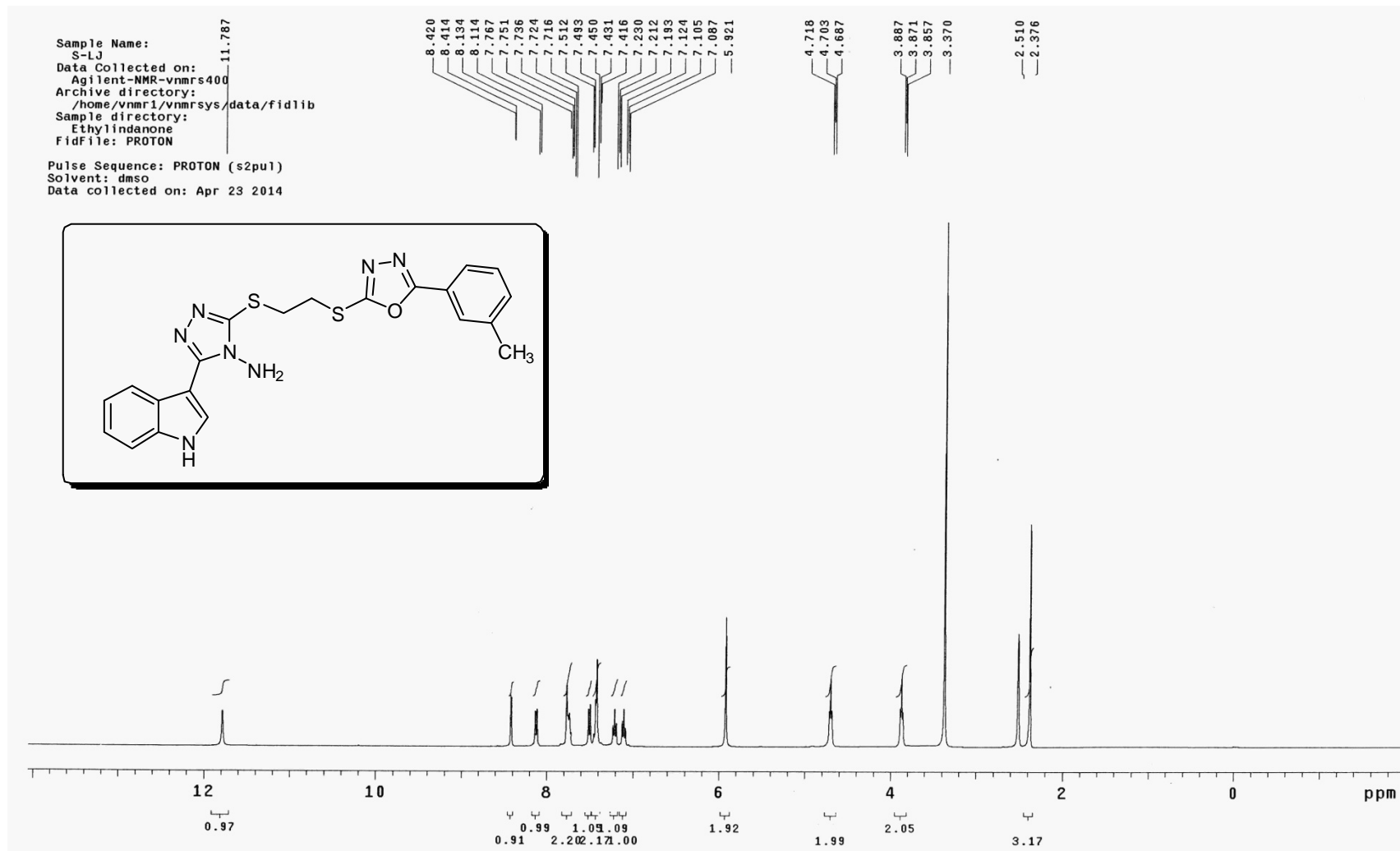




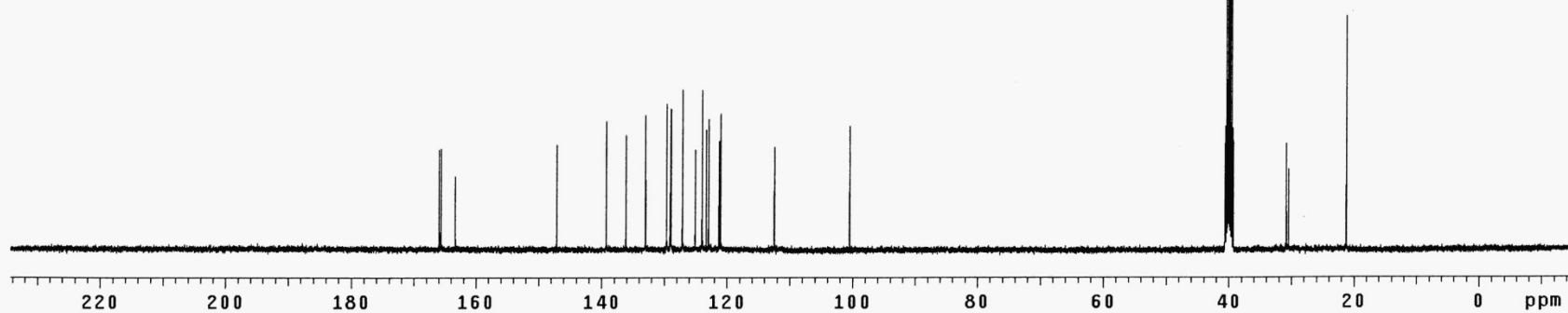
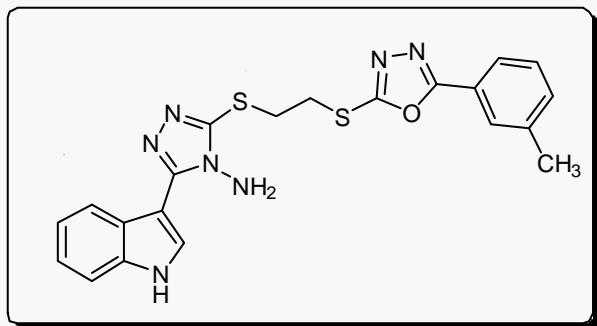
T: + c ESI Full ms [50.00-2000.00]



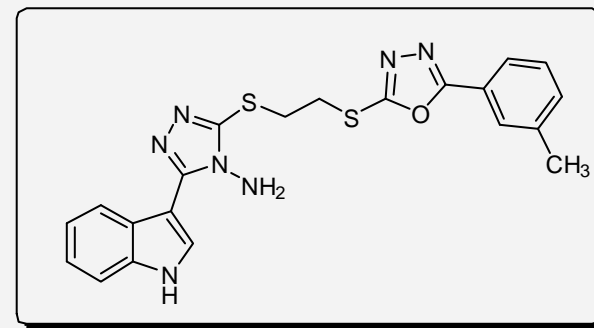
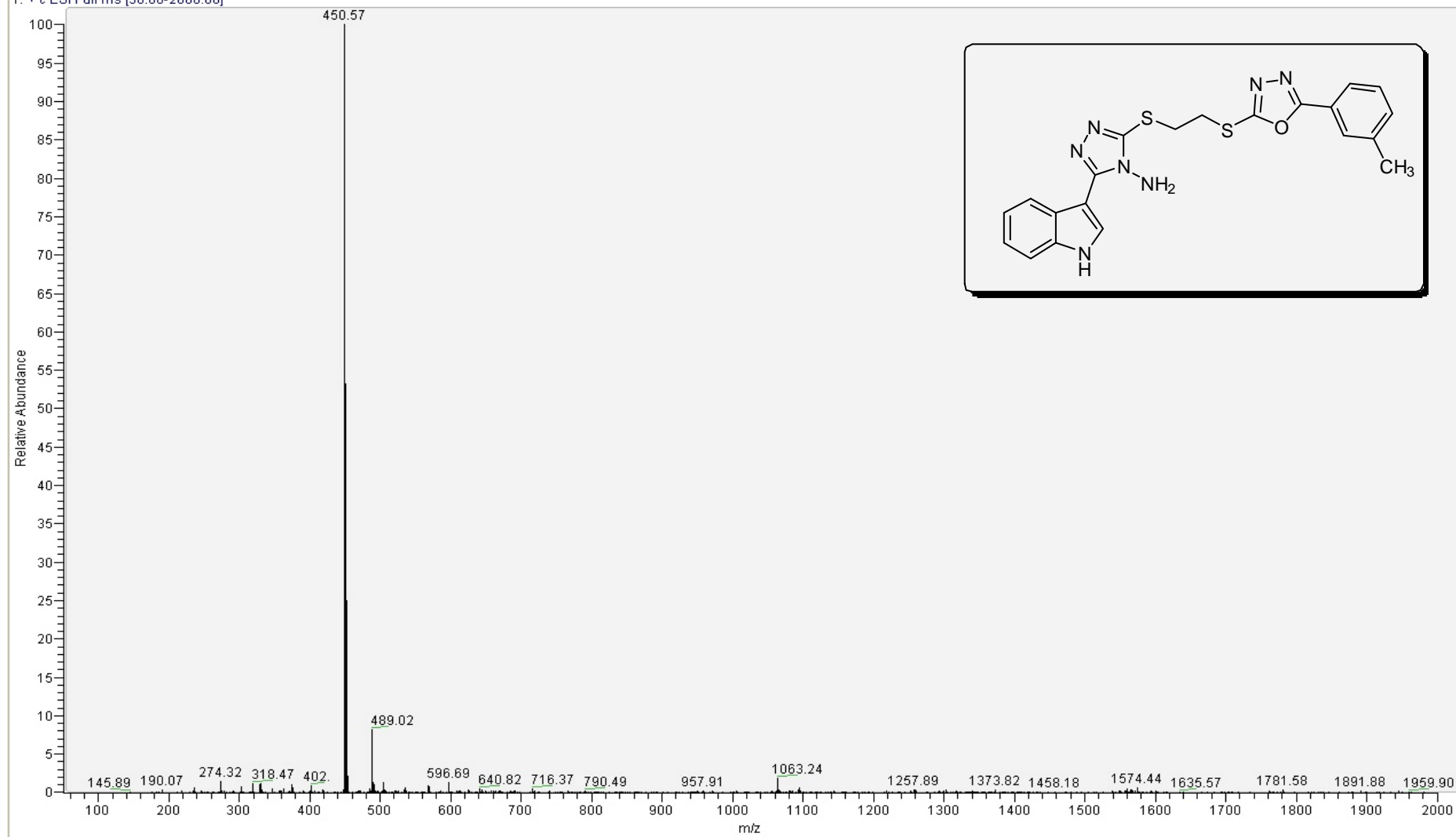
3-(1H-indol-3-yl)-5-[[2-[[5-(3-methylphenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10c)



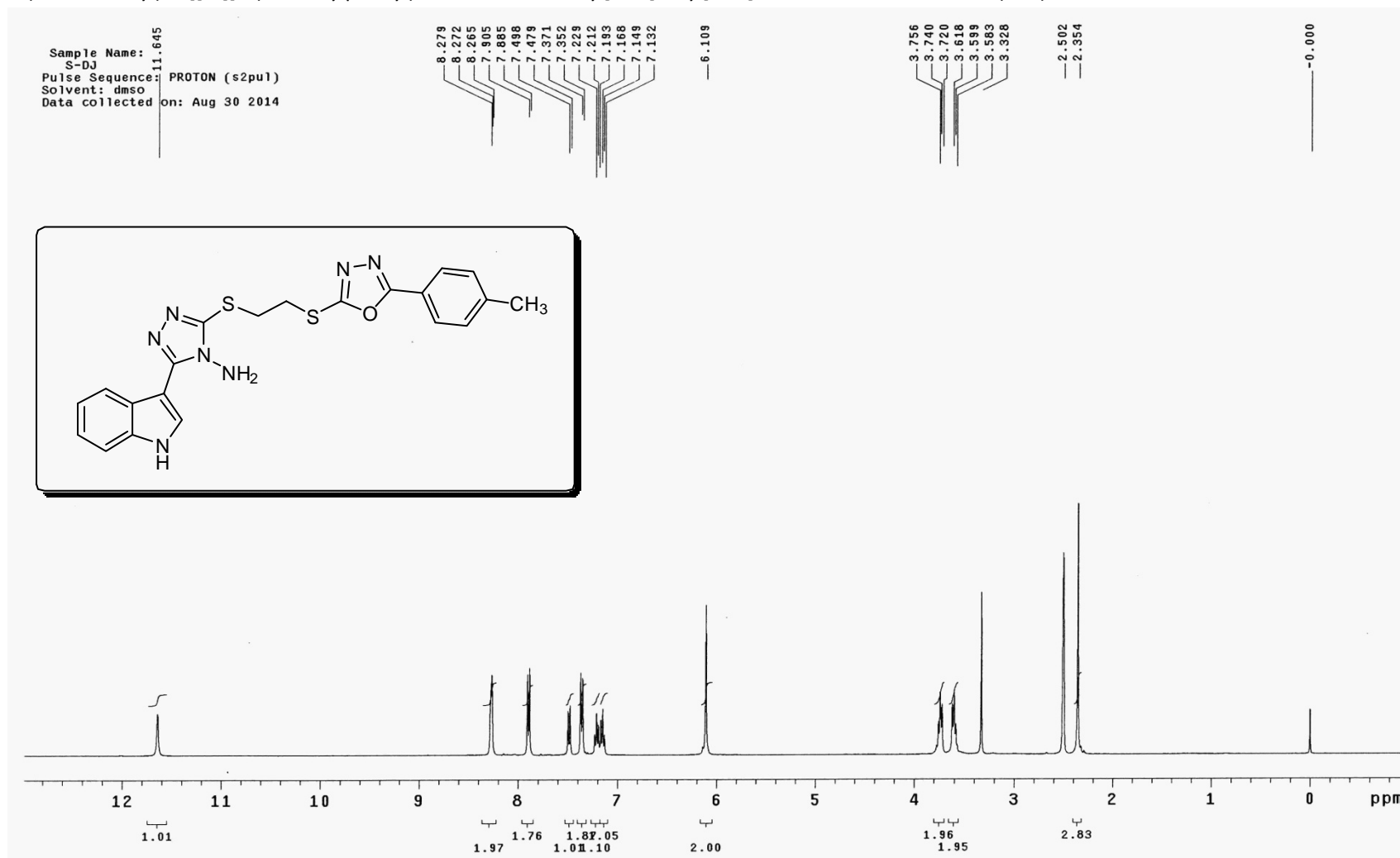
Sample Name:  
S-JJ  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dmsd  
Data collected on: Apr 23 2014



T: + c ESI Full ms [50.00-2000.00]

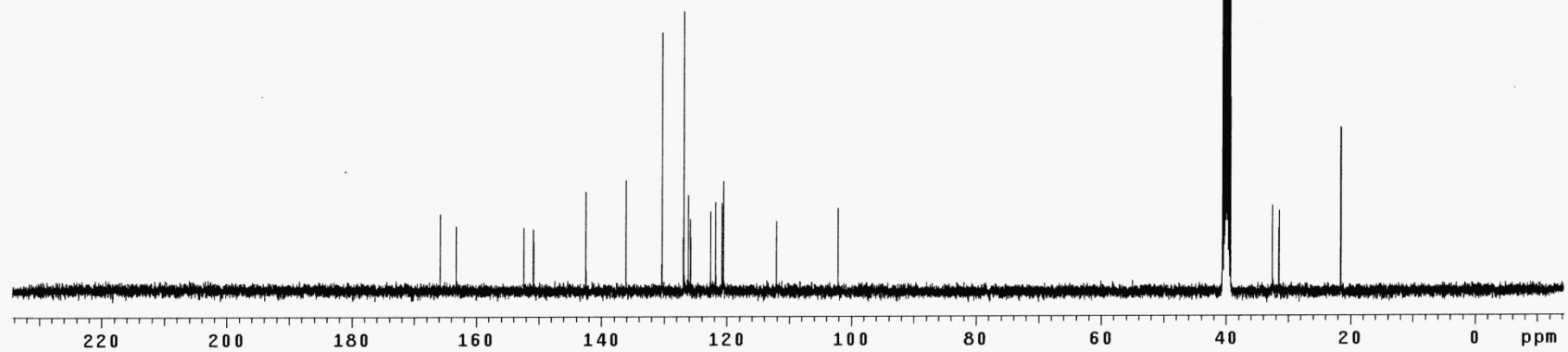
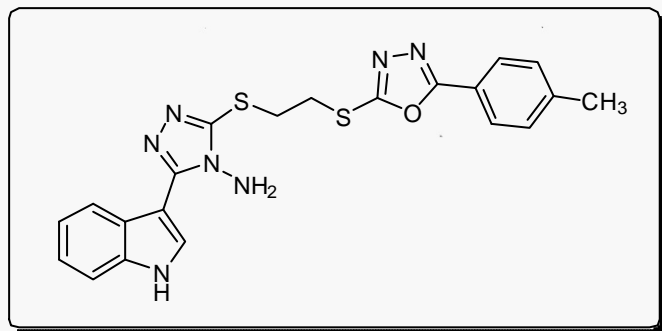


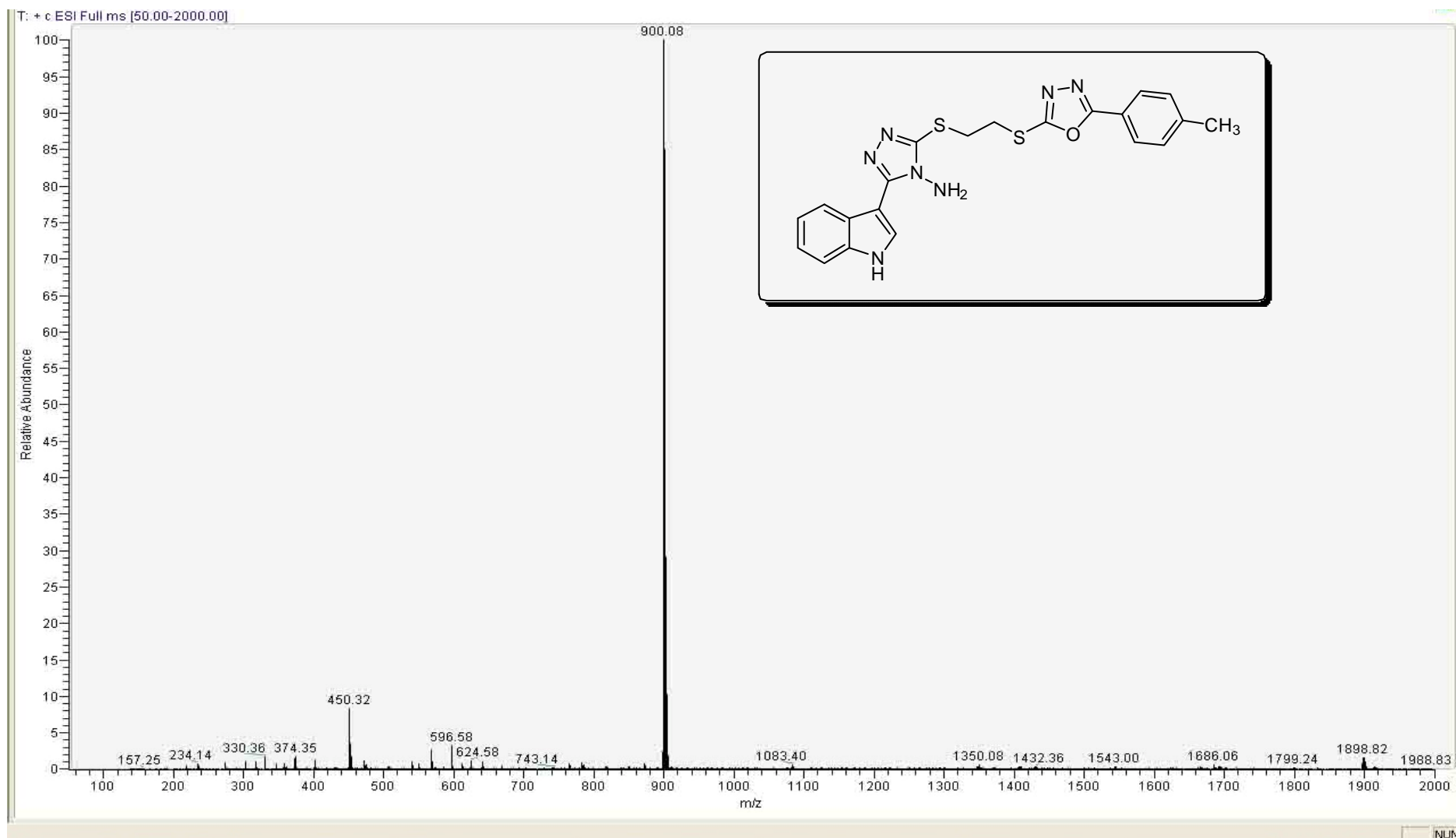
3-(1H-indol-3-yl)-5-[[2-[[5-(4-methylphenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10d)



Sample Name:  
S-DJ  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dms  
Data collected on: Aug 30 2014

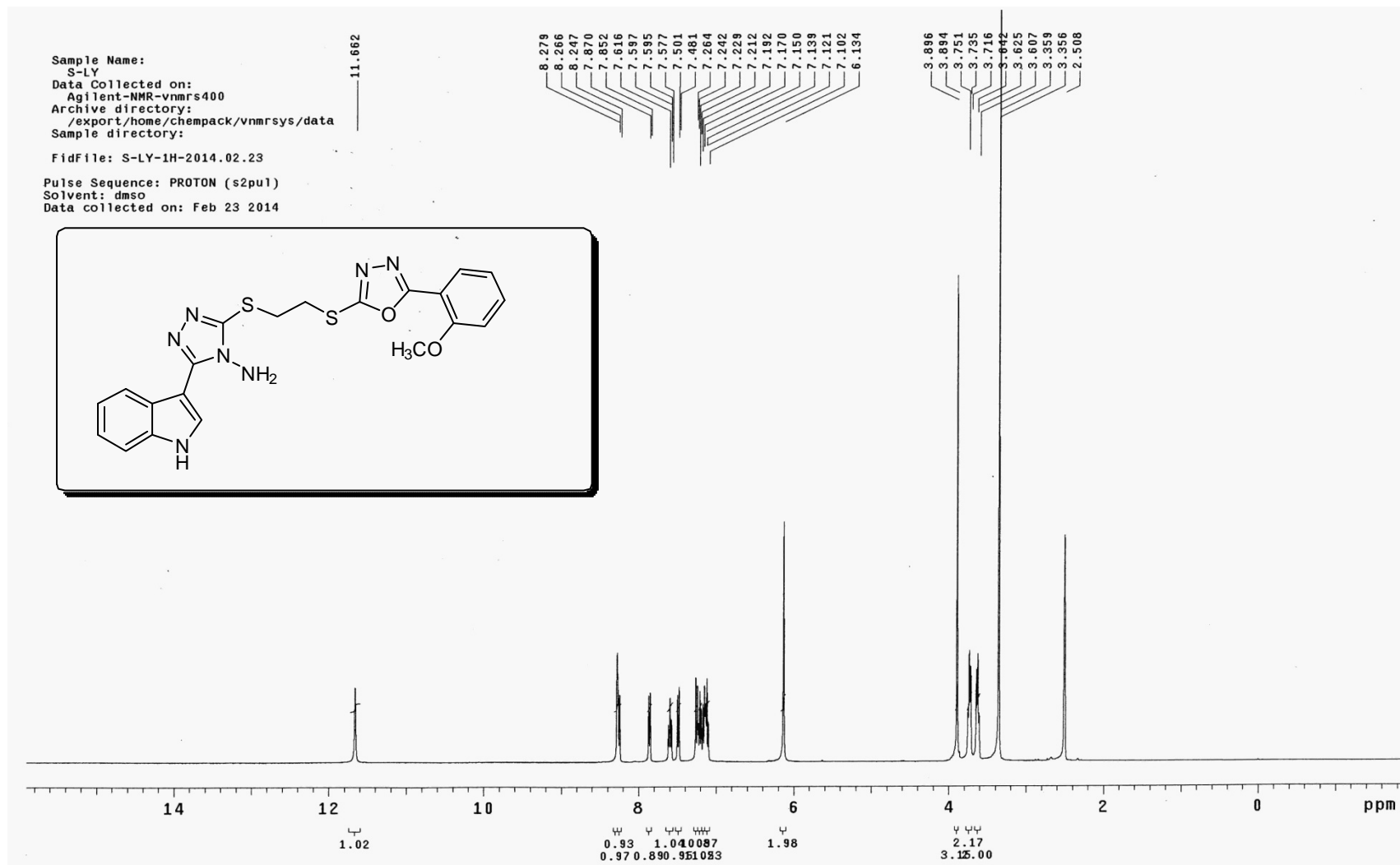
165.783  
163.249  
152.392  
150.844  
142.482  
136.094  
130.358  
126.890  
126.154  
125.805  
122.618  
121.807  
120.767  
120.555  
112.102  
102.132  
40.563  
40.378  
40.166  
39.961  
39.748  
38.543  
38.331  
32.555  
31.493  
21.546





S15

3-(1H-indol-3-yl)-5-[[2-[[5-(2-methoxyphenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10e)

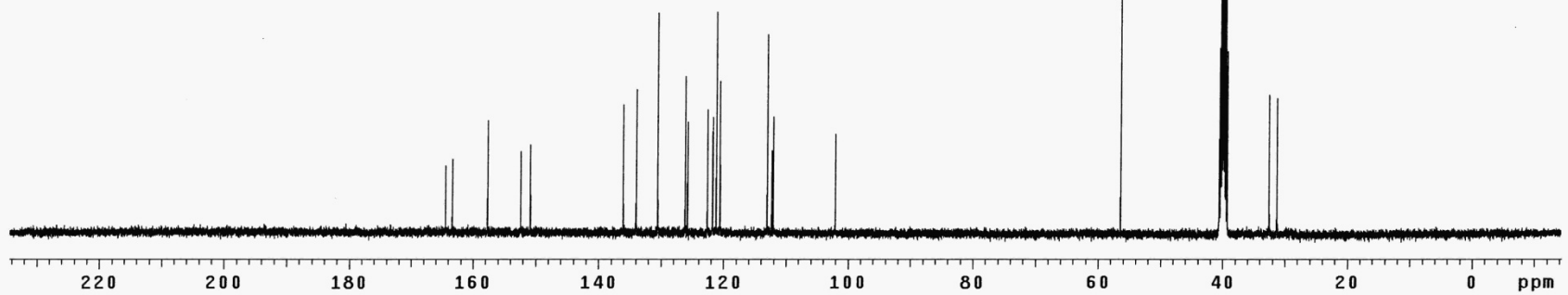
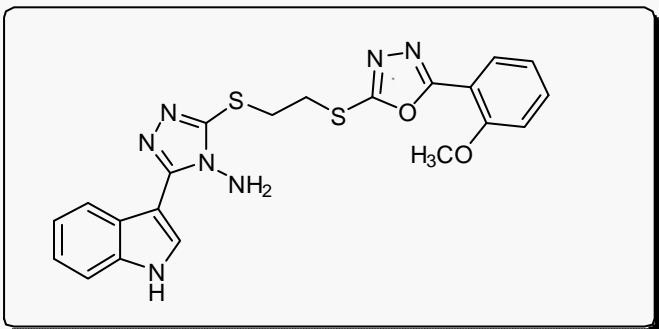




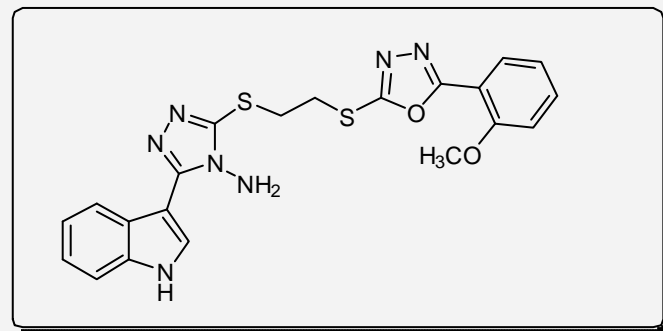
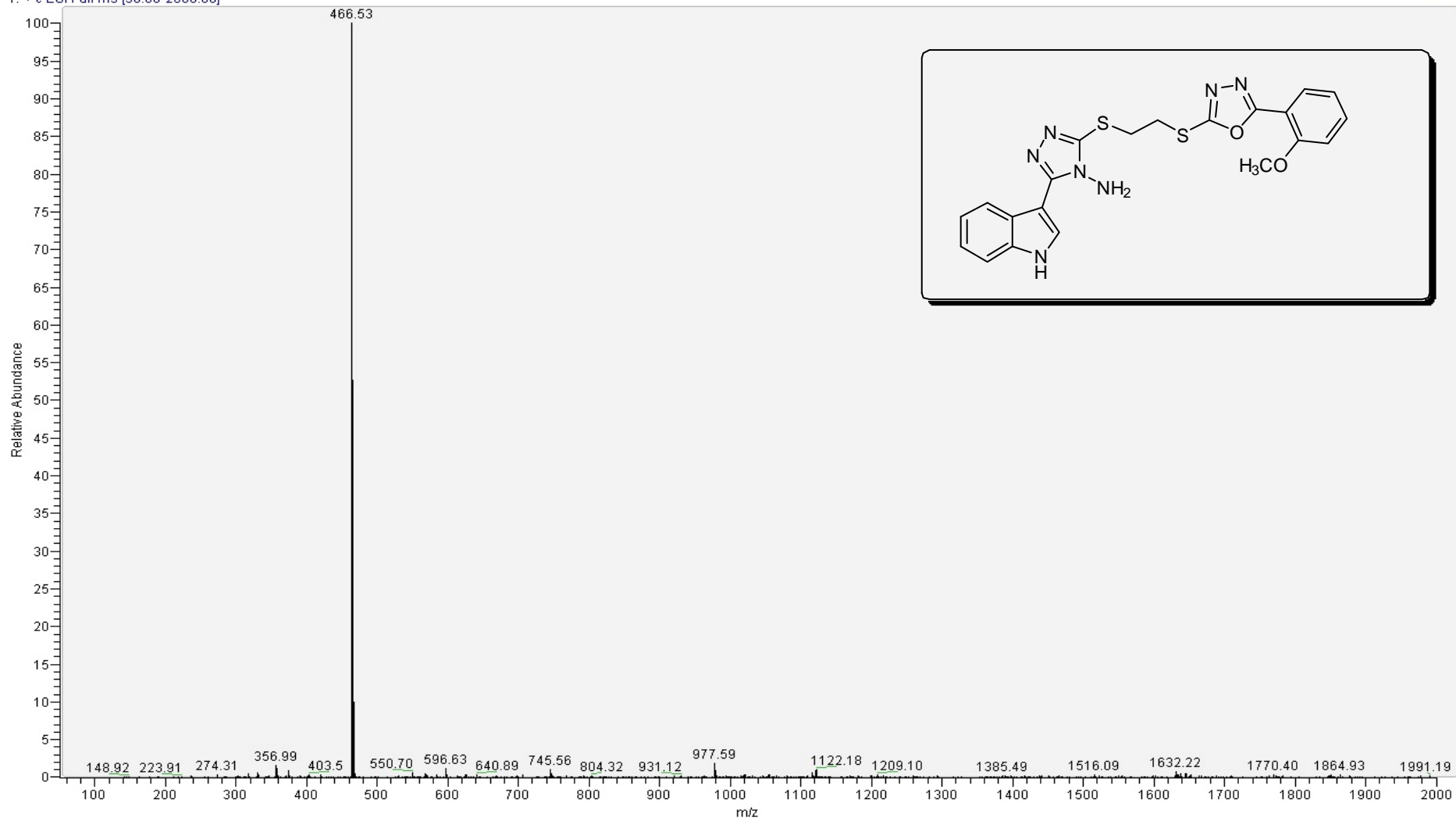
Sample Name:  
S-LY  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dmsd  
Data collected on: Feb 23 2014

164.455  
163.377  
157.702  
152.375  
150.843  
136.085  
133.981  
130.561  
128.168  
125.789  
122.617  
121.760  
121.206  
120.589  
118.065  
112.359  
112.109  
102.086

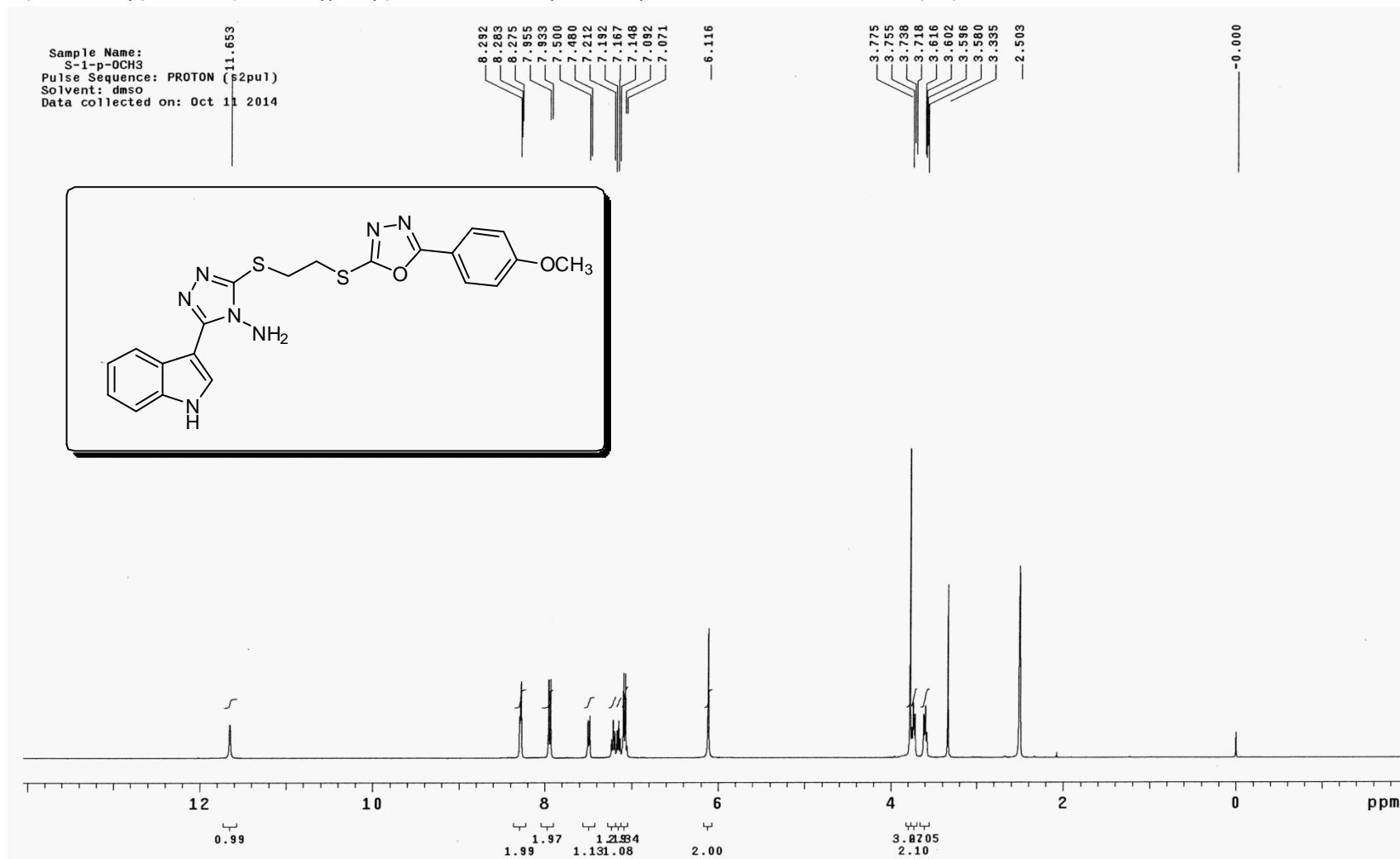
56.432  
40.559  
40.354  
40.142  
39.837  
38.725  
38.520  
38.307  
32.554  
31.802



T: + c ESI Full ms [50.00-2000.00]

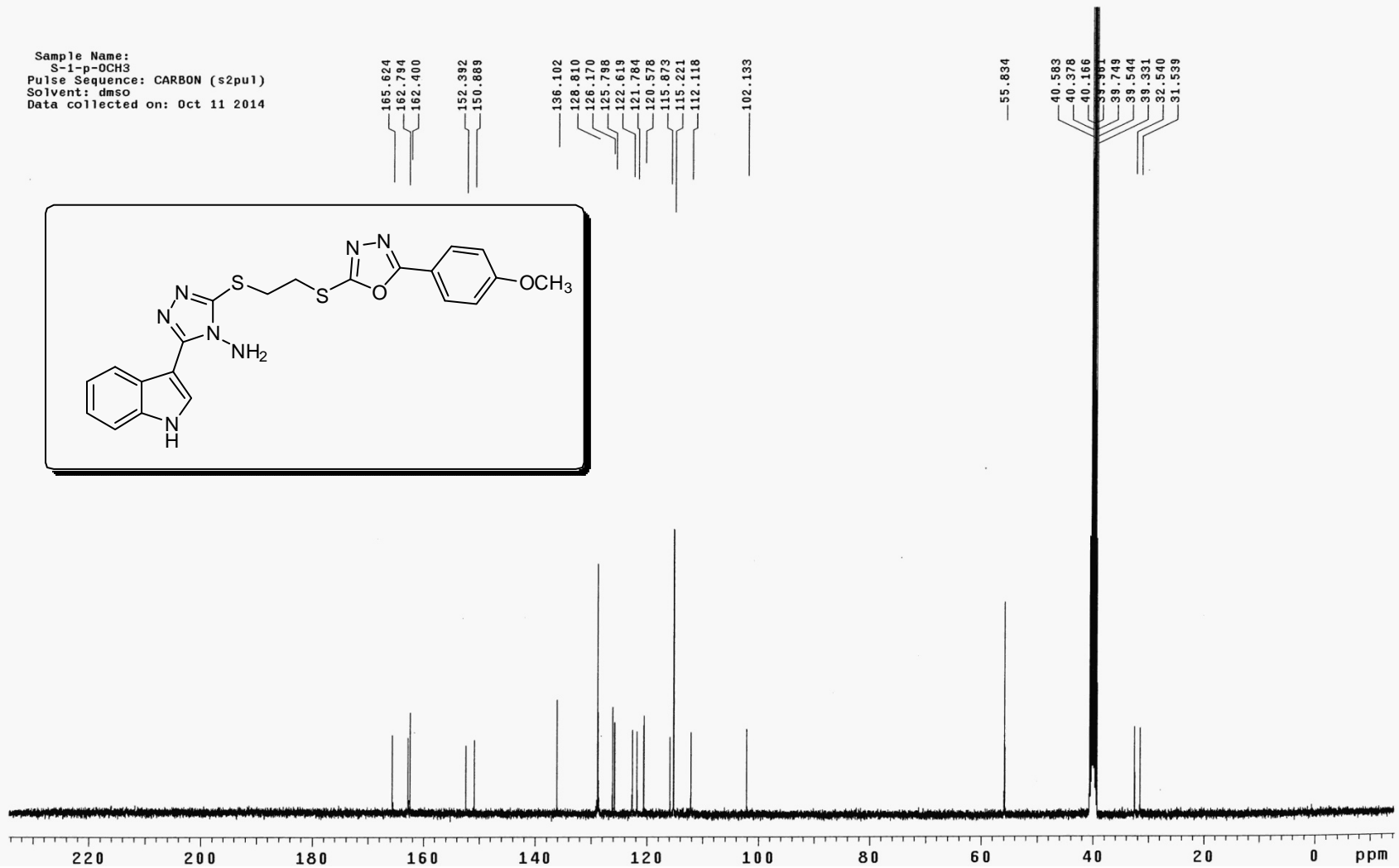
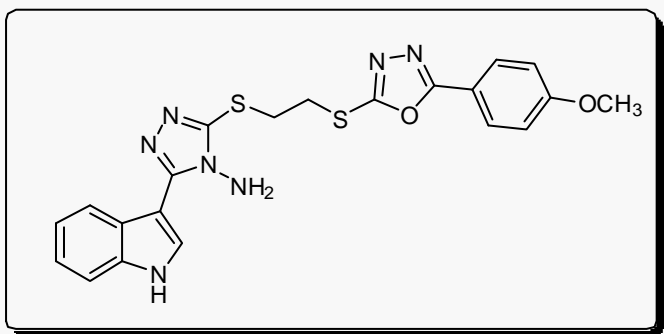


3-(1H-indol-3-yl)-5-[[2-[[5-(4-methoxyphenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10f)

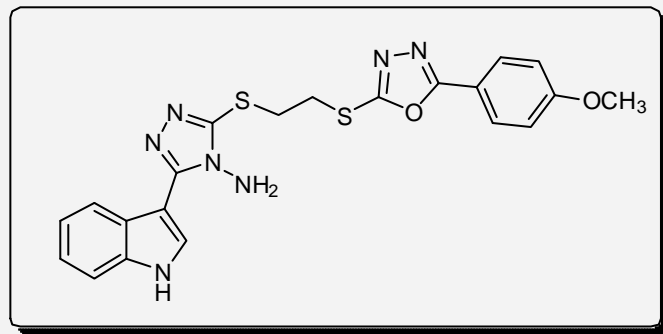
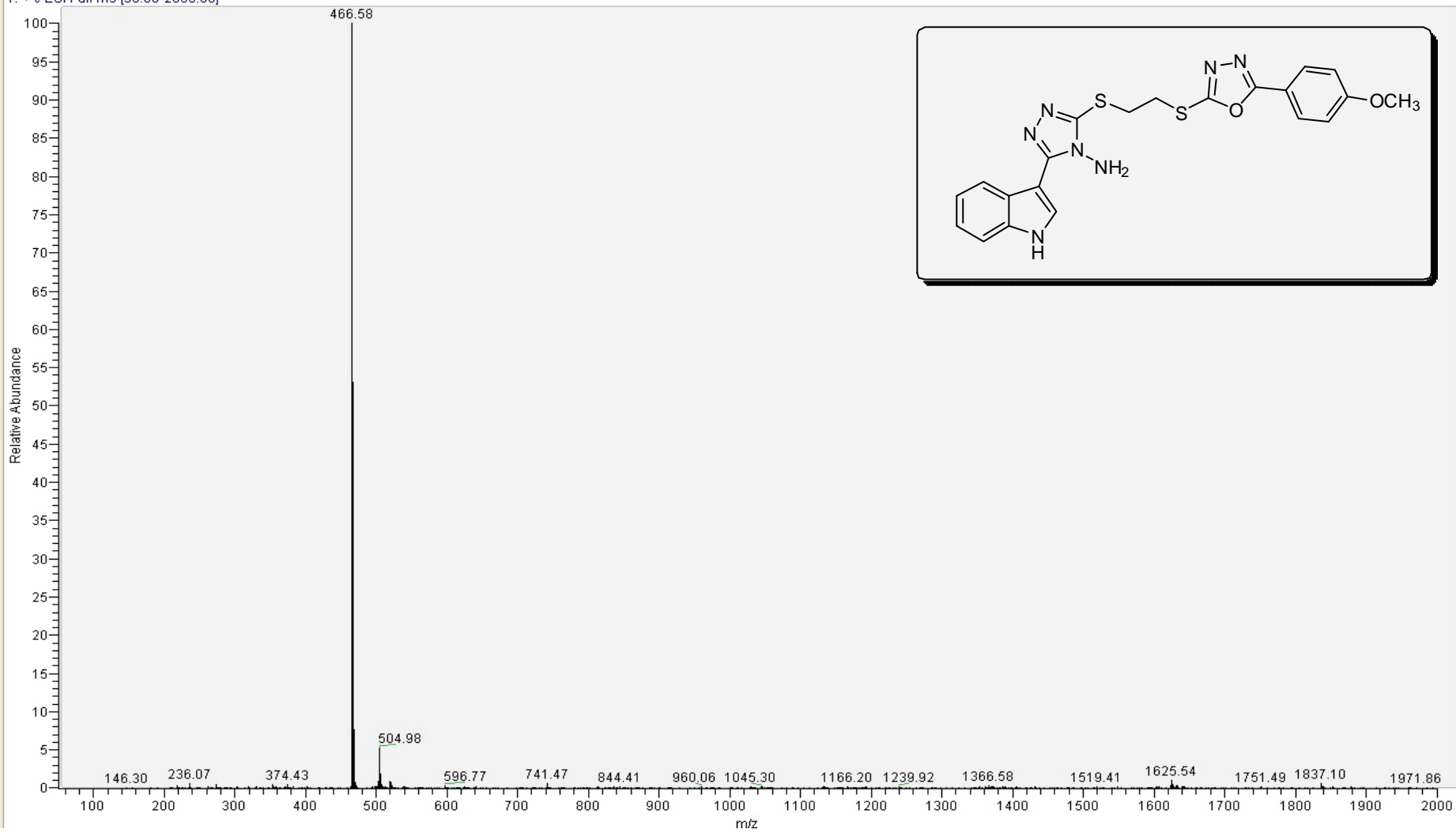


Sample Name:  
S-1-p-OCH3  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dmsd  
Data collected on: Oct 11 2014

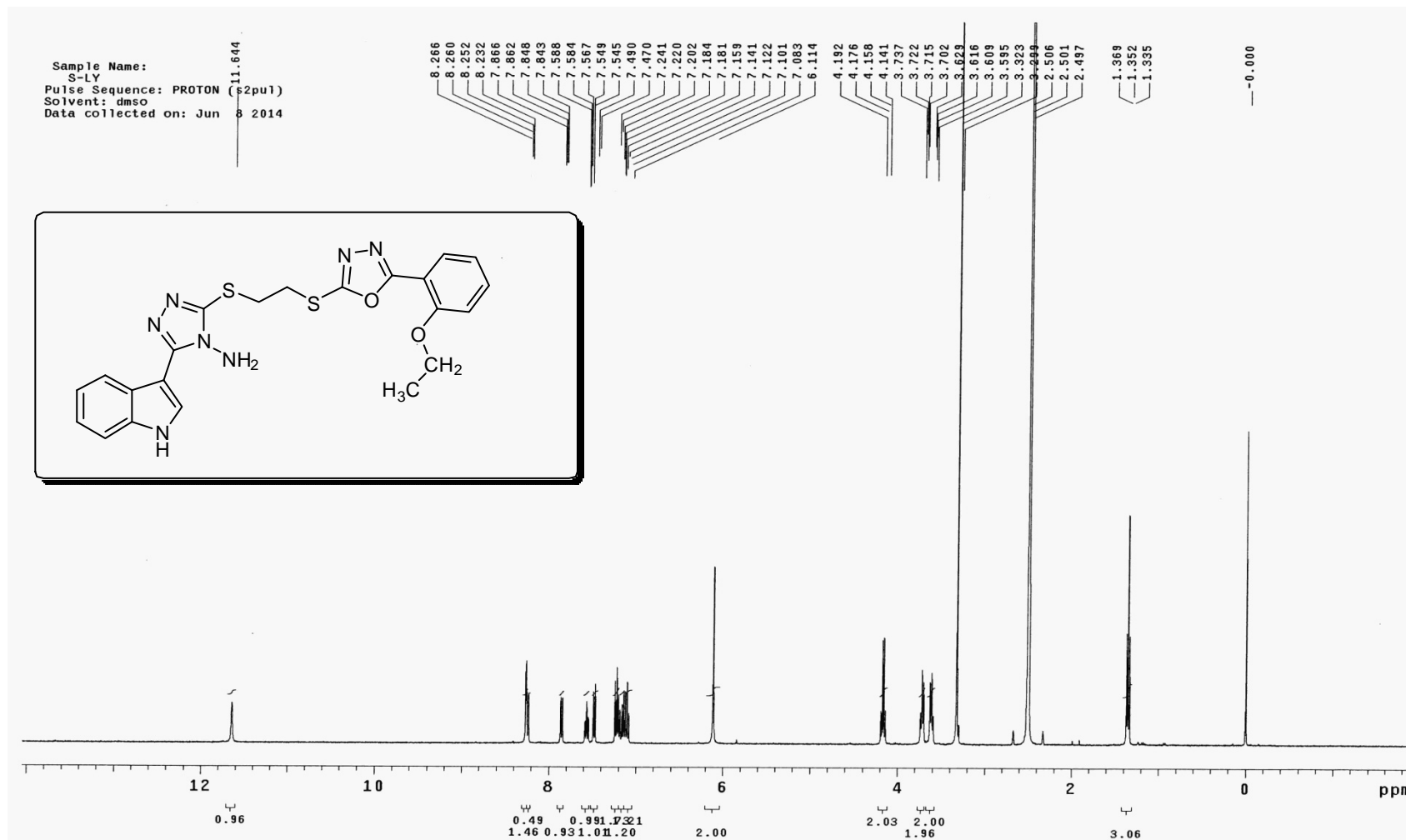
165.624  
162.784  
162.400  
152.382  
150.889  
136.102  
128.810  
126.170  
125.788  
122.619  
121.784  
120.578  
115.873  
115.221  
112.118  
102.133  
55.834  
40.583  
40.378  
40.166  
39.749  
39.544  
39.331  
32.540  
31.539



T: + c ESI Full ms [50.00-2000.00]



3-(1H-indol-3-yl)-5-[[2-[[[5-(2-ethoxyphenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10g)



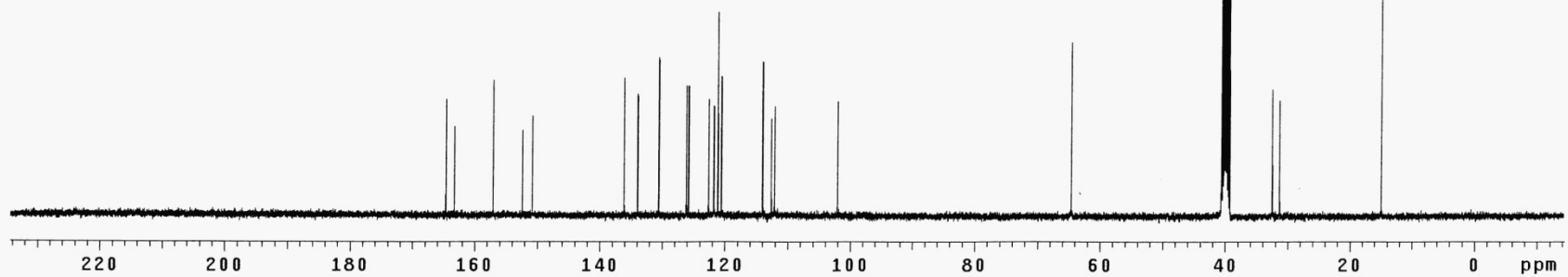
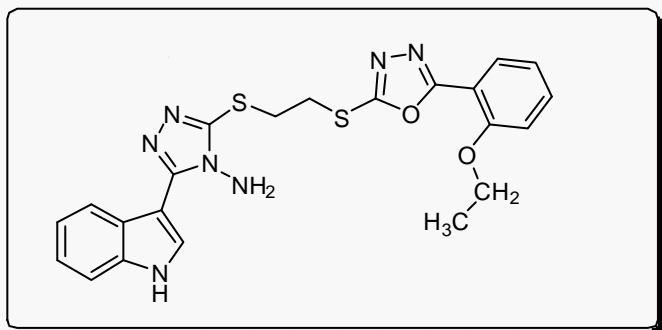
Sample Name:  
S-LEY  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dms  
Data collected on: Jun 9 2014

164.652  
163.294  
157.019  
152.363  
150.805  
136.093  
133.938  
130.547  
126.153  
125.797  
122.610  
121.768  
121.146  
120.584  
114.029  
112.625  
112.101  
102.094

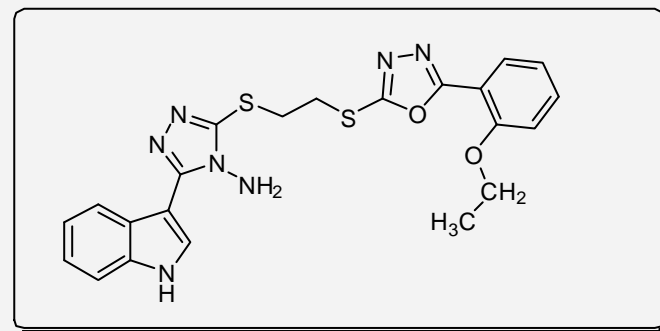
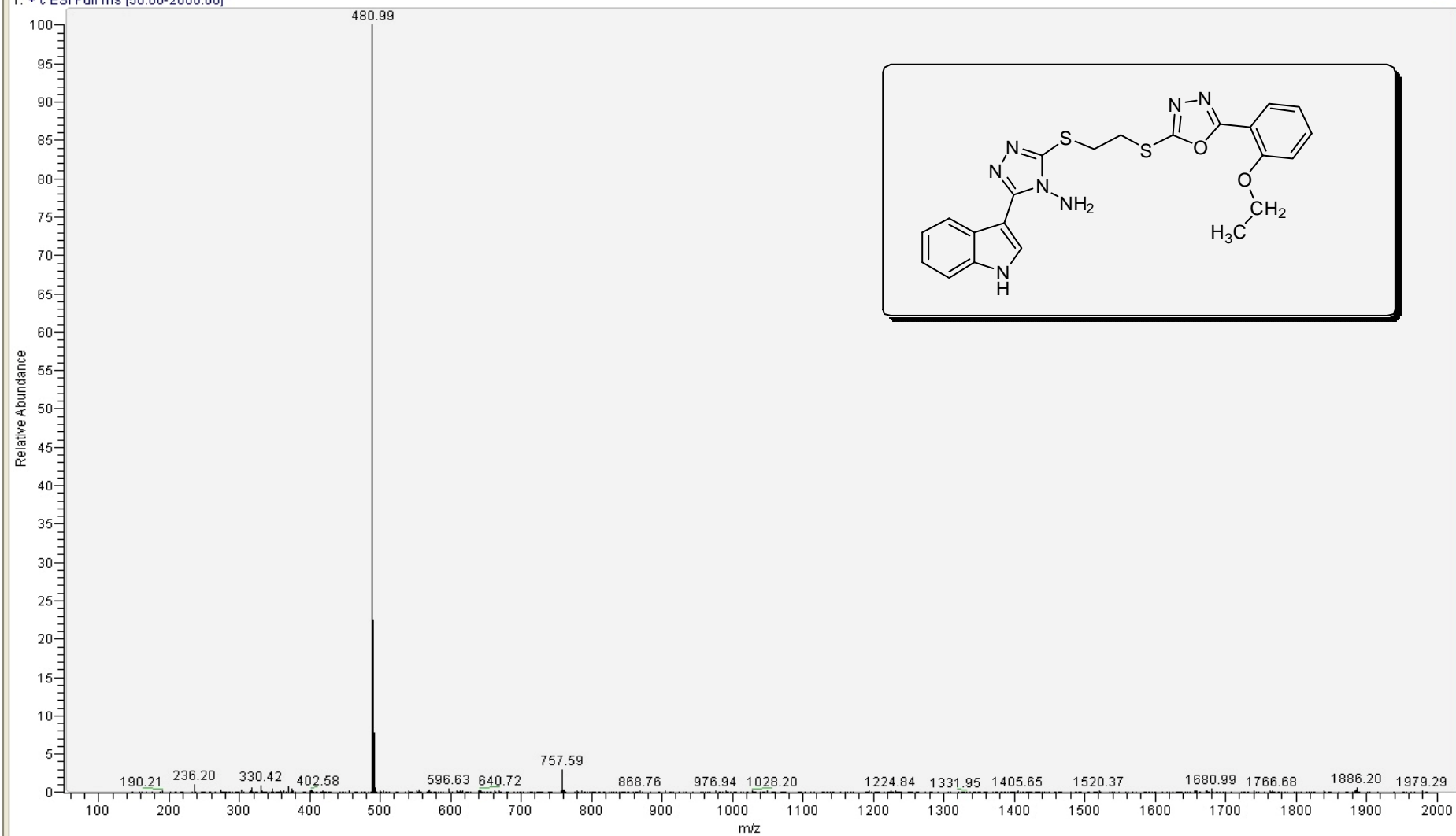
64.634

40.582  
40.377  
40.165  
38.960  
38.748  
39.543  
39.330  
32.539  
31.371

14.944

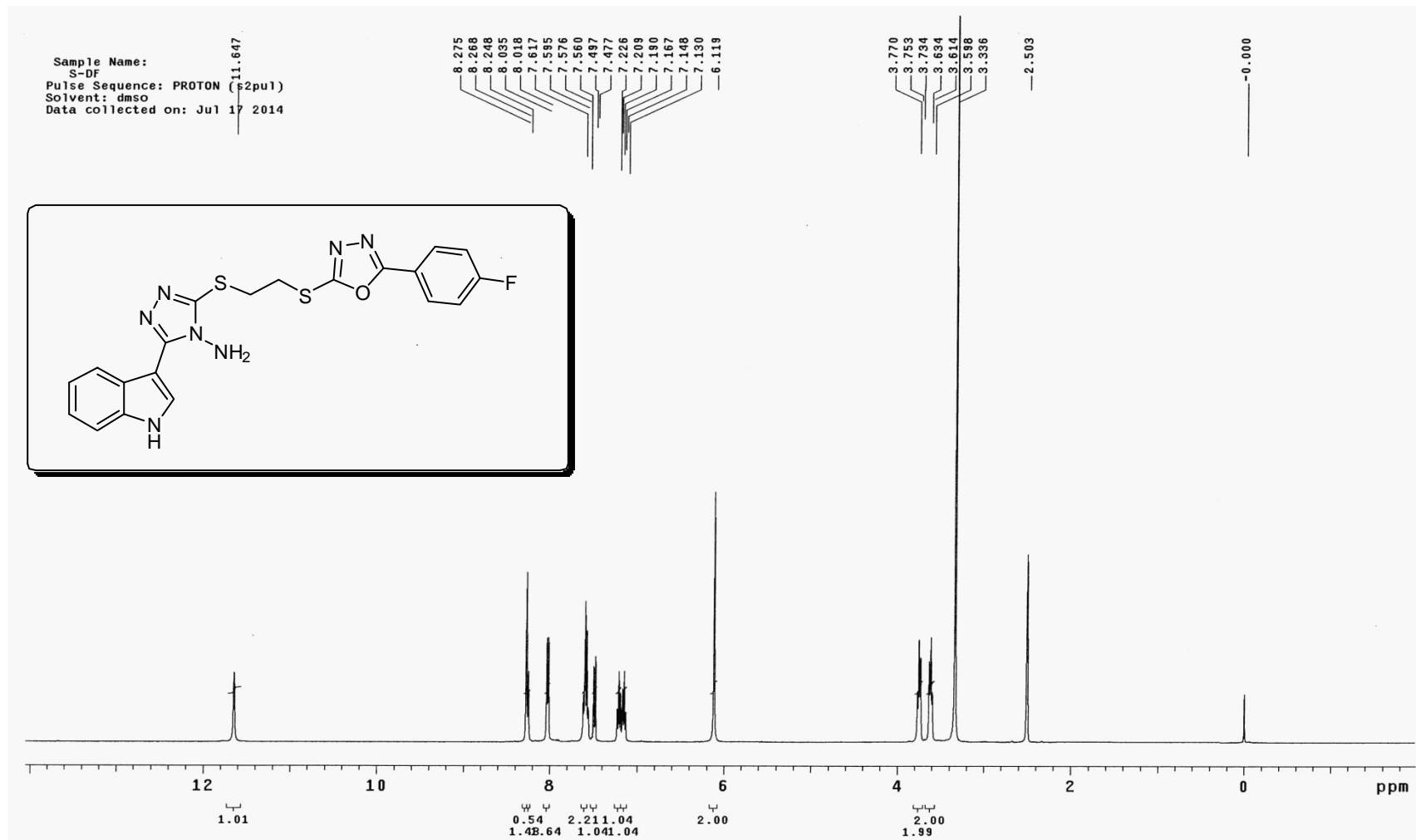


T: + c ESI Full ms [50.00-2000.00]





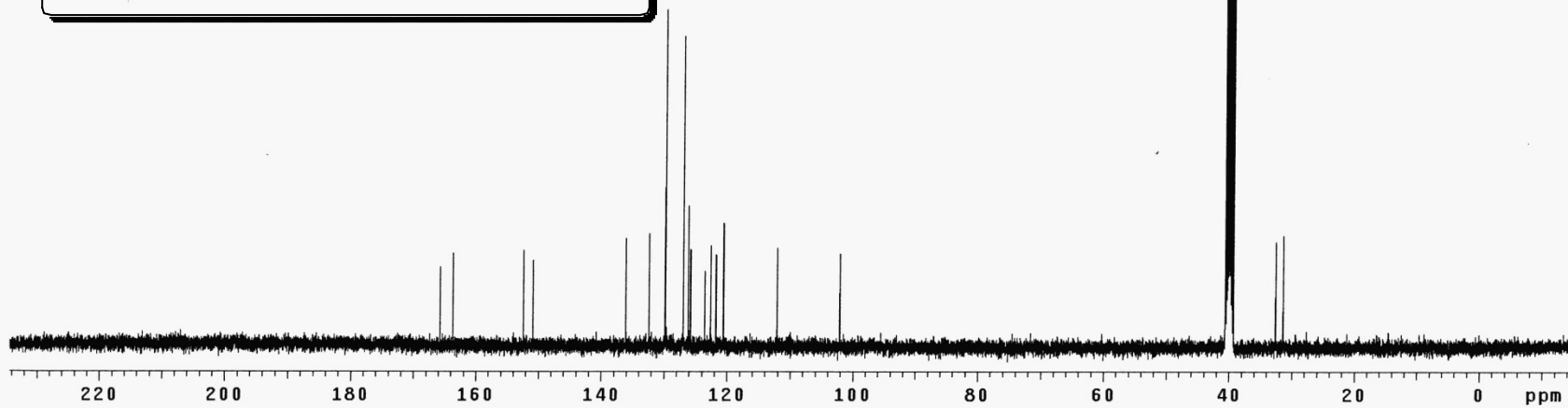
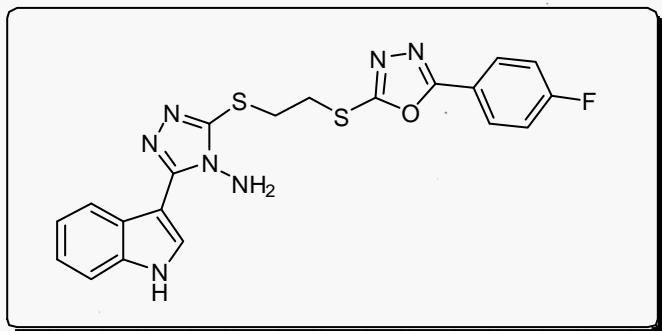
3-(1H-indol-3-yl)-5-[[2-[[5-(4-fluorophenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10h)



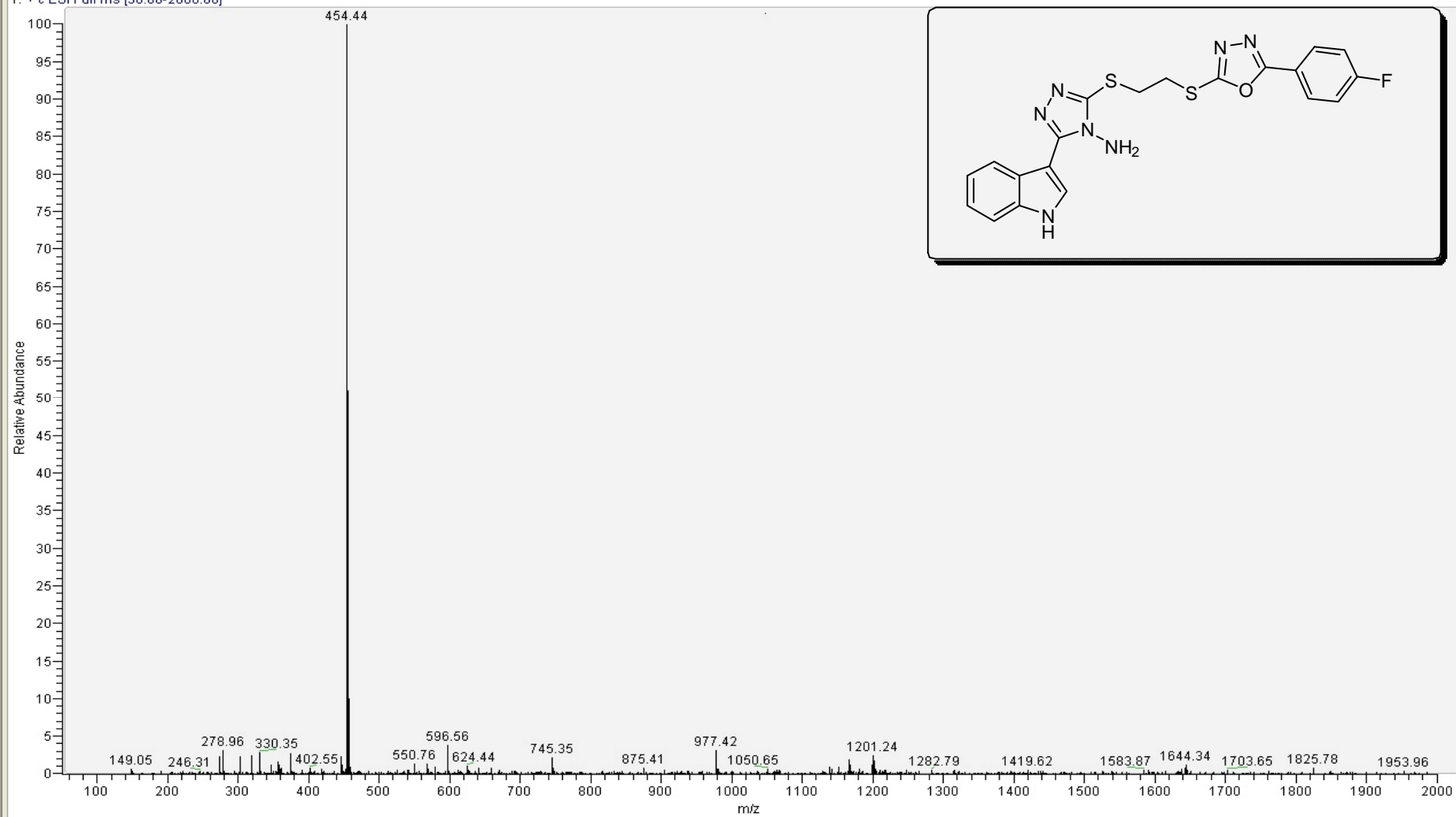
Sample Name:  
S-DF  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dmsO  
Data collected on: Jul 18 2014

165.714  
163.658  
152.383  
150.881  
136.085  
132.375  
129.818  
128.950  
126.153  
125.797  
123.528  
122.610  
121.768  
120.584  
112.109  
102.101

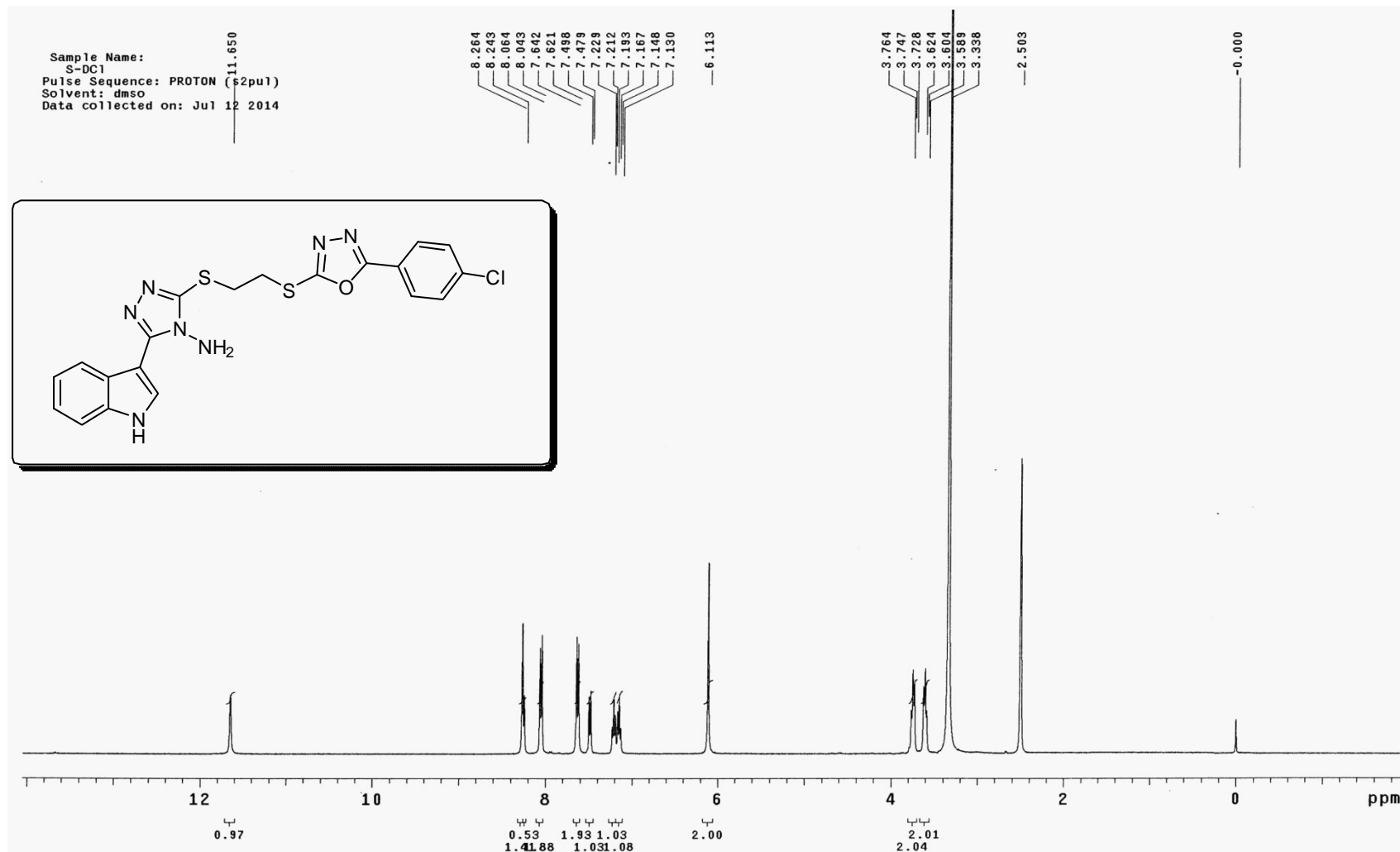
40.575  
40.370  
40.157  
39.952  
39.740  
39.535  
39.323  
32.583  
31.394



4-4F #4 RT: 0.12 AV: 1 NL: 1.33E7  
T: + c ESI Full ms [50.00-2000.00]



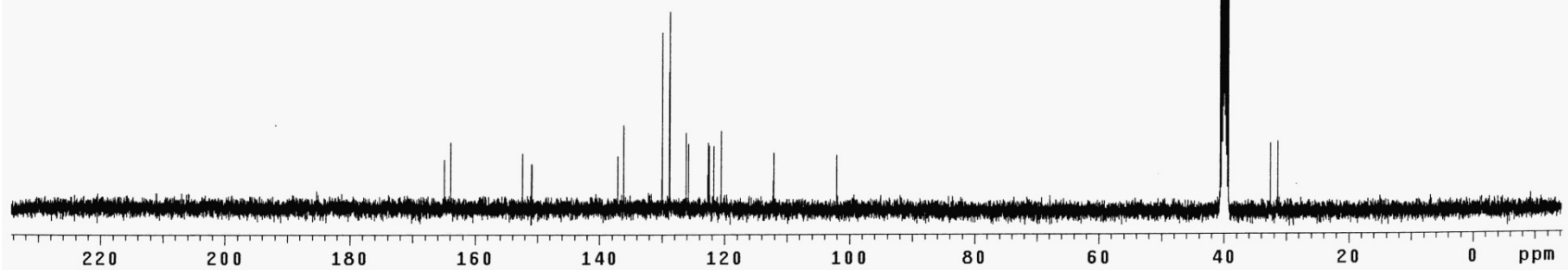
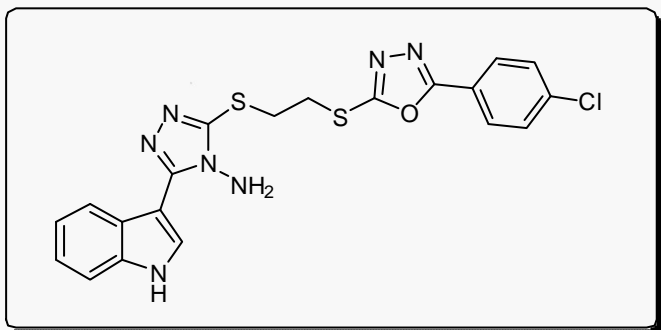
3-(1H-indol-3-yl)-5-[[2-[[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10i)



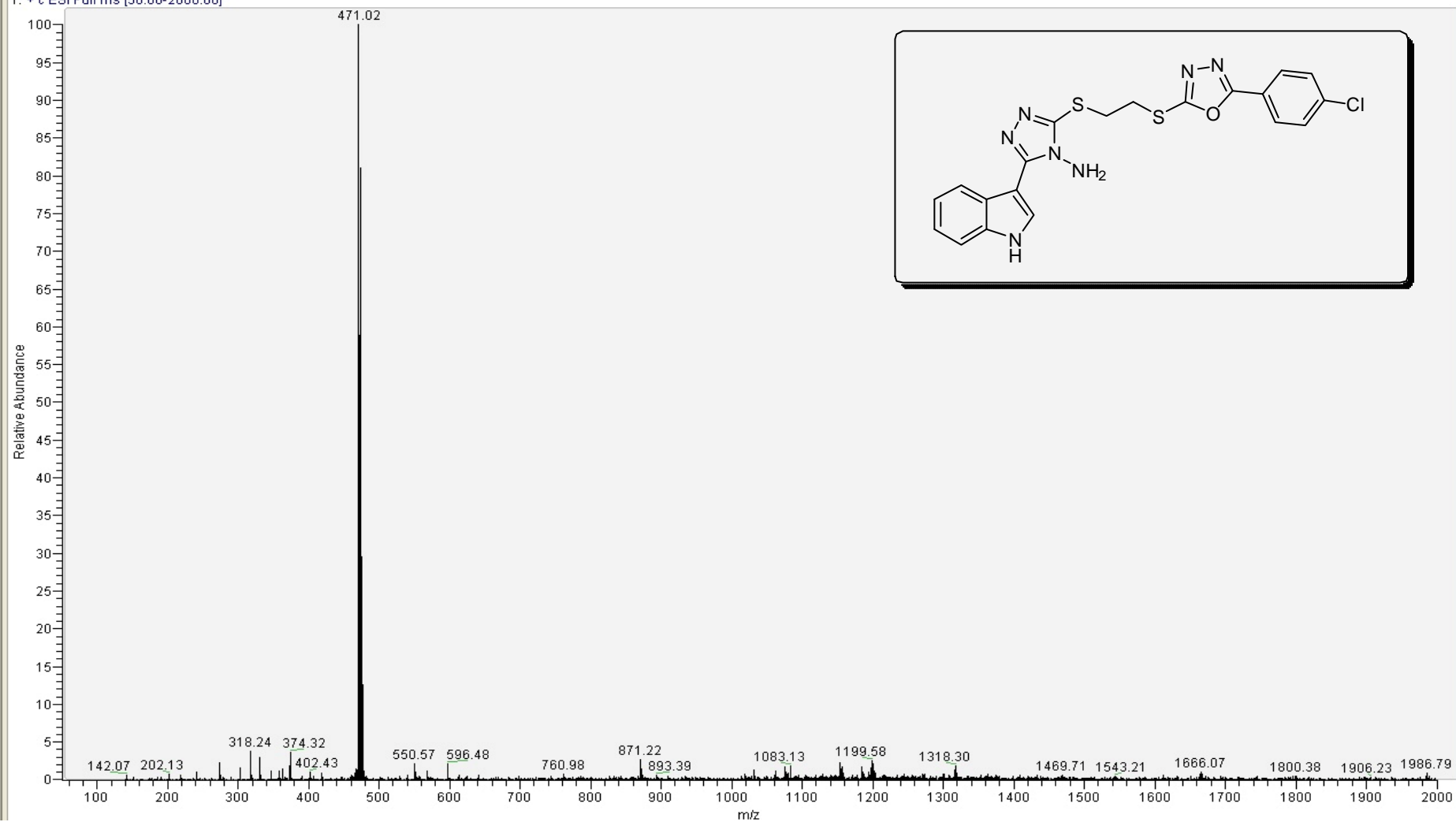
Sample Name:  
S-DC1  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dms0  
Data collected on: Jul 12 2014

164.949  
163.902  
152.399  
150.912  
137.042  
136.094  
129.963  
128.795  
126.147  
125.775  
122.626  
122.421  
121.738  
120.562  
112.125  
102.067

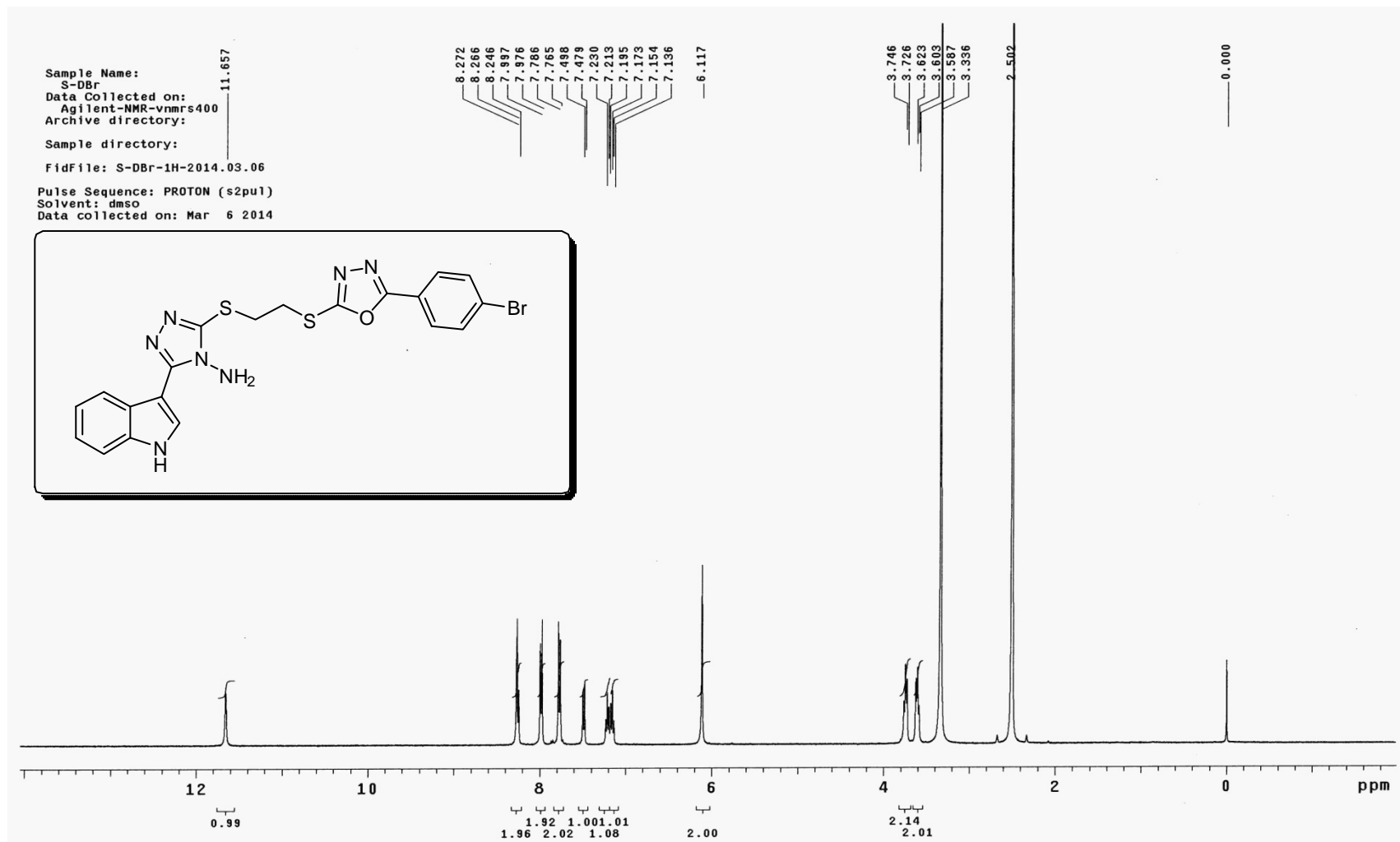
40.575  
40.363  
40.156  
39.646  
39.741  
39.528  
39.316  
32.571  
31.410



4-Cl\_150112163149 #30-60 RT: 0.79-1.59 AV:  
T: + c ESI Full ms [50.00-2000.00]



3-(1H-indol-3-yl)-5-[[2-[[5-(4-bromophenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10)



Sample Name:  
S-DBr  
Data Collected on:  
Agilent-NMR-vnmrs400  
Archive directory:  
/home/vnmr1/vnmrsys/data/fid1ib  
Sample directory:  
Ethylindanone  
FidFile: CARBON

Pulse Sequence: CARBON (s2pu1)  
Solvent: dmsd  
Data collected on: Mar 6 2014

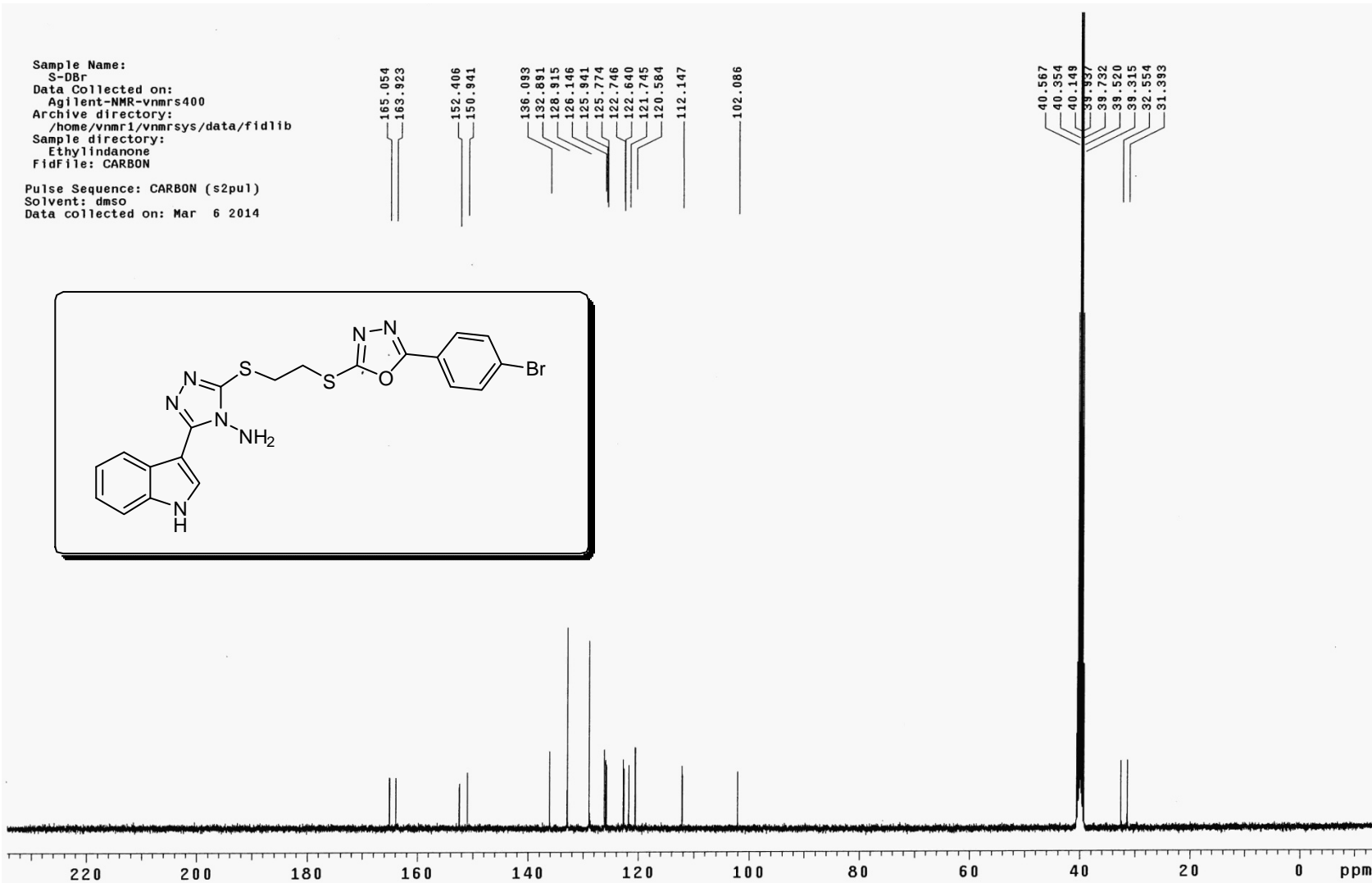
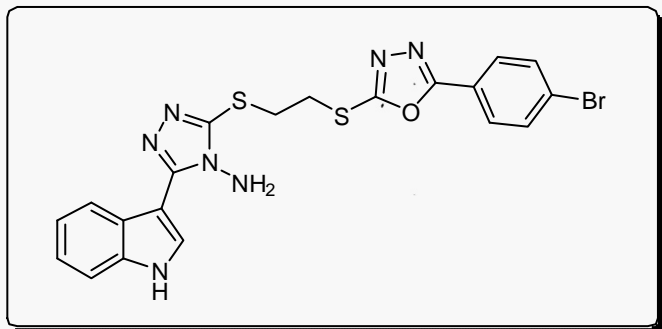
165.054  
163.923

152.406  
150.941

136.093  
132.891  
128.915  
126.146  
125.941  
125.774  
122.746  
122.640  
121.745  
120.584  
112.147

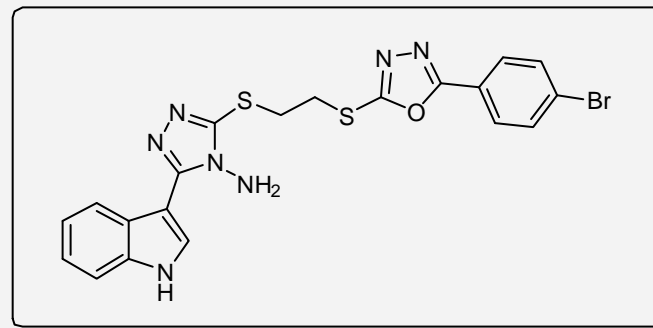
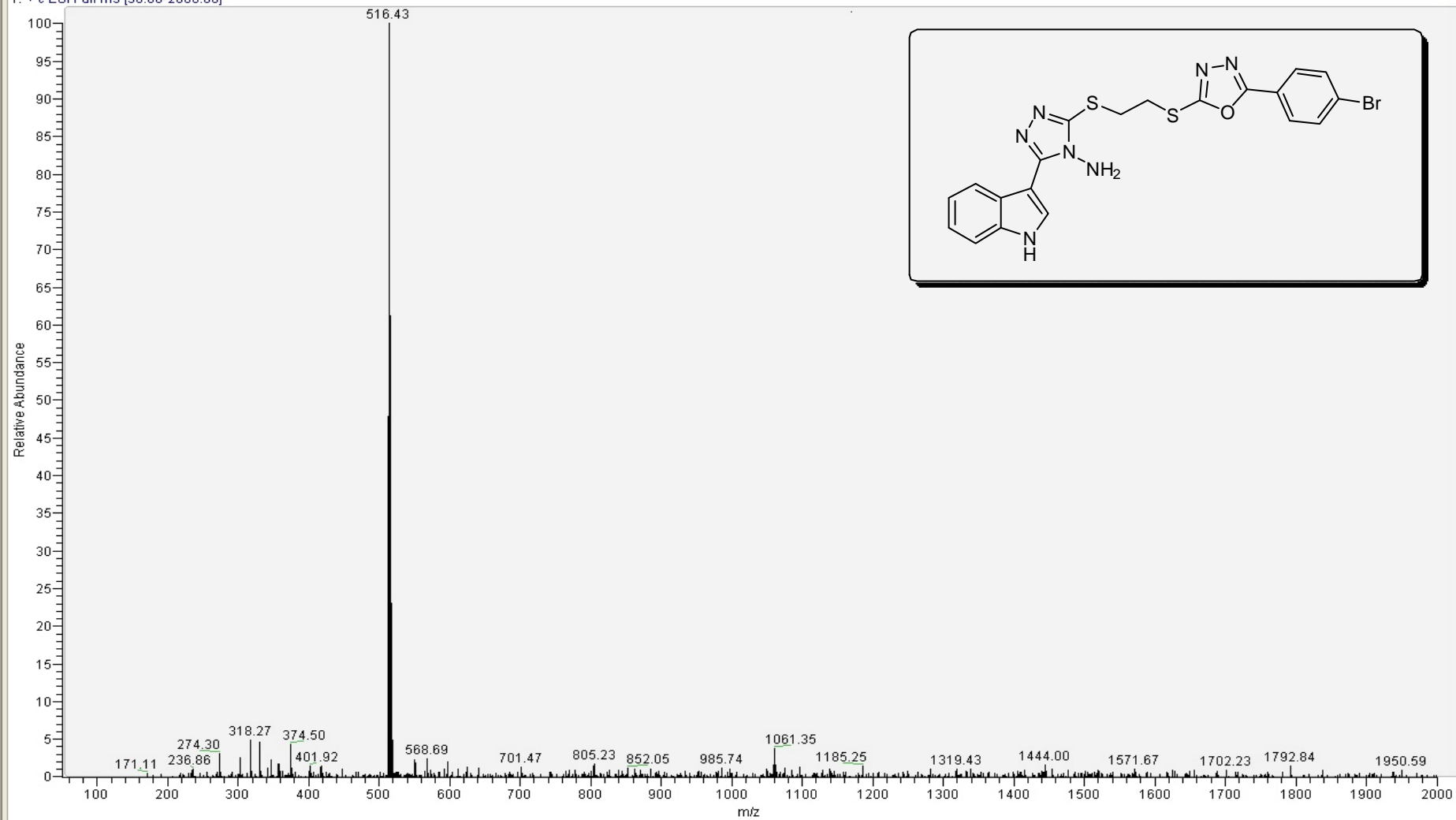
102.086

40.567  
40.354  
40.149  
39.937  
39.732  
39.520  
39.315  
32.554  
31.393

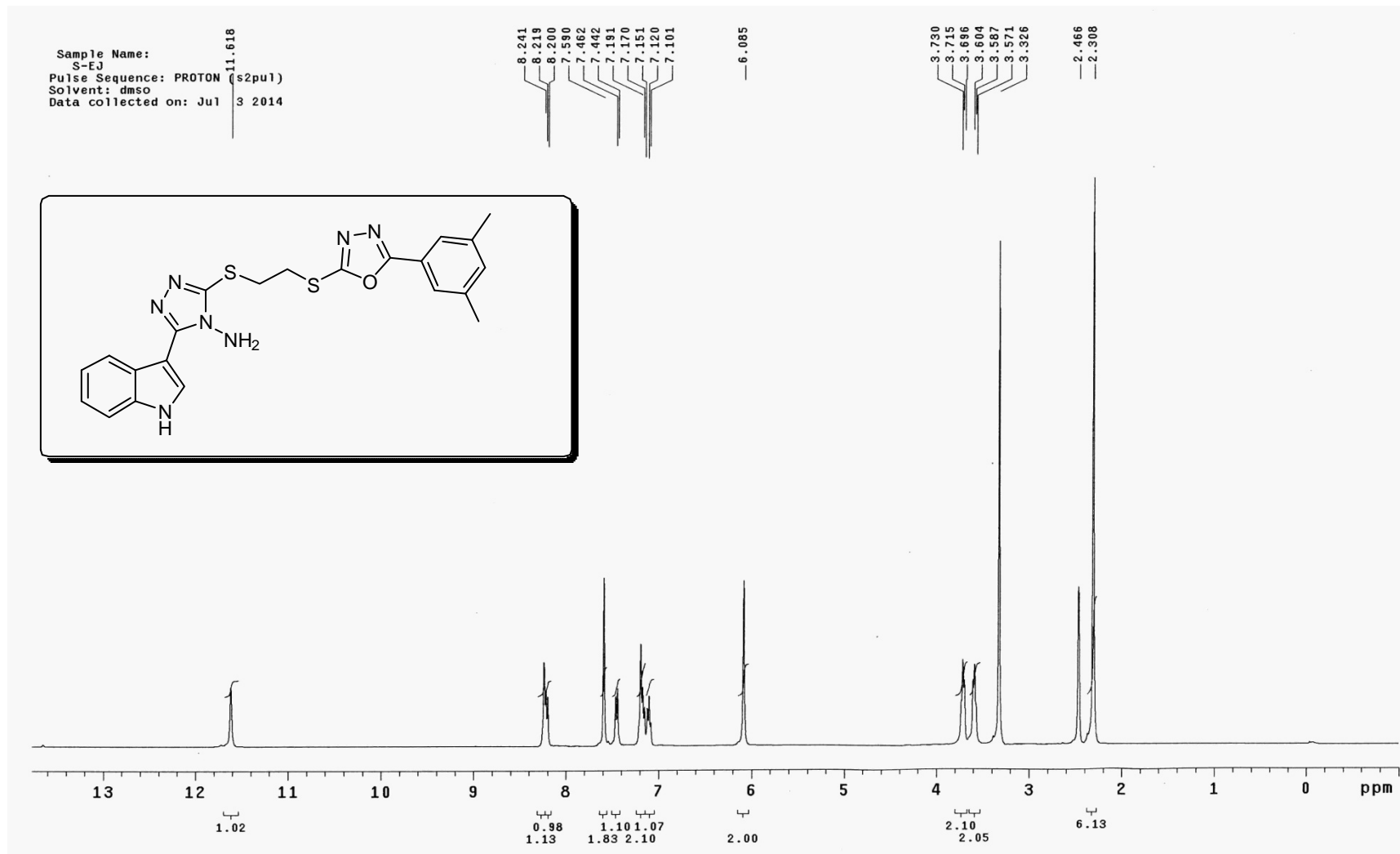




4-Br#15 RT: 0.40 AV: 1 NL: 4.46E6  
T: + c ESI Full ms [50.00-2000.00]



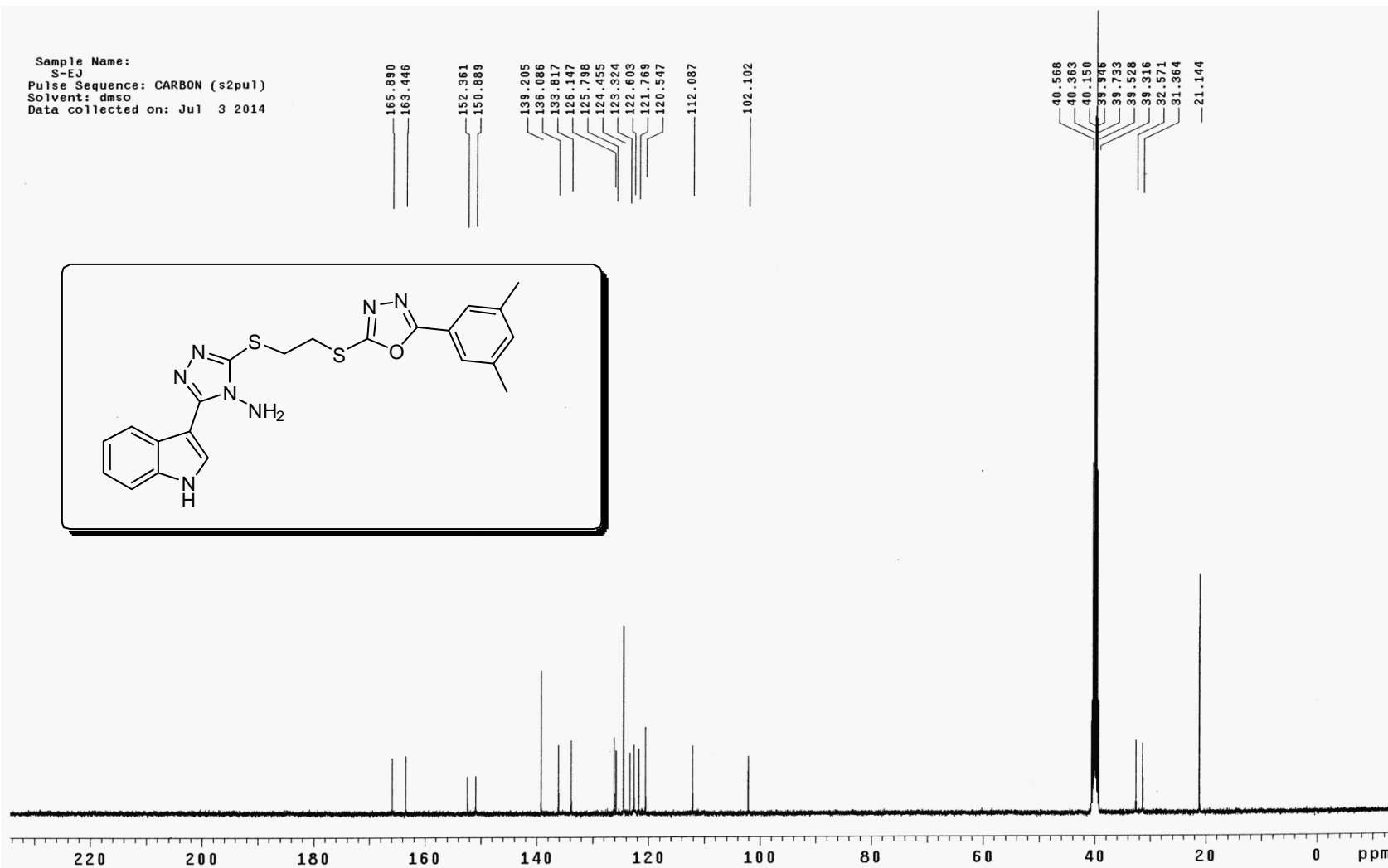
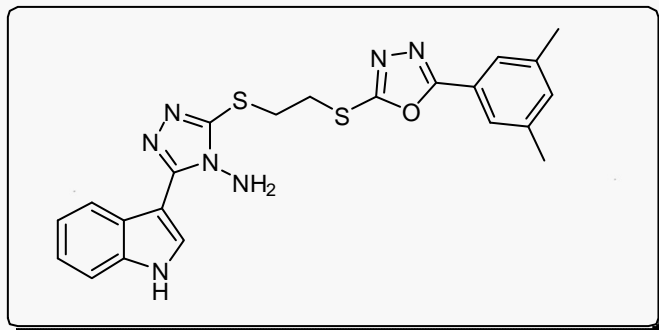
3-(1H-indol-3-yl)-5-[[2-[[[5-(3,5-dimethylphenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10k)



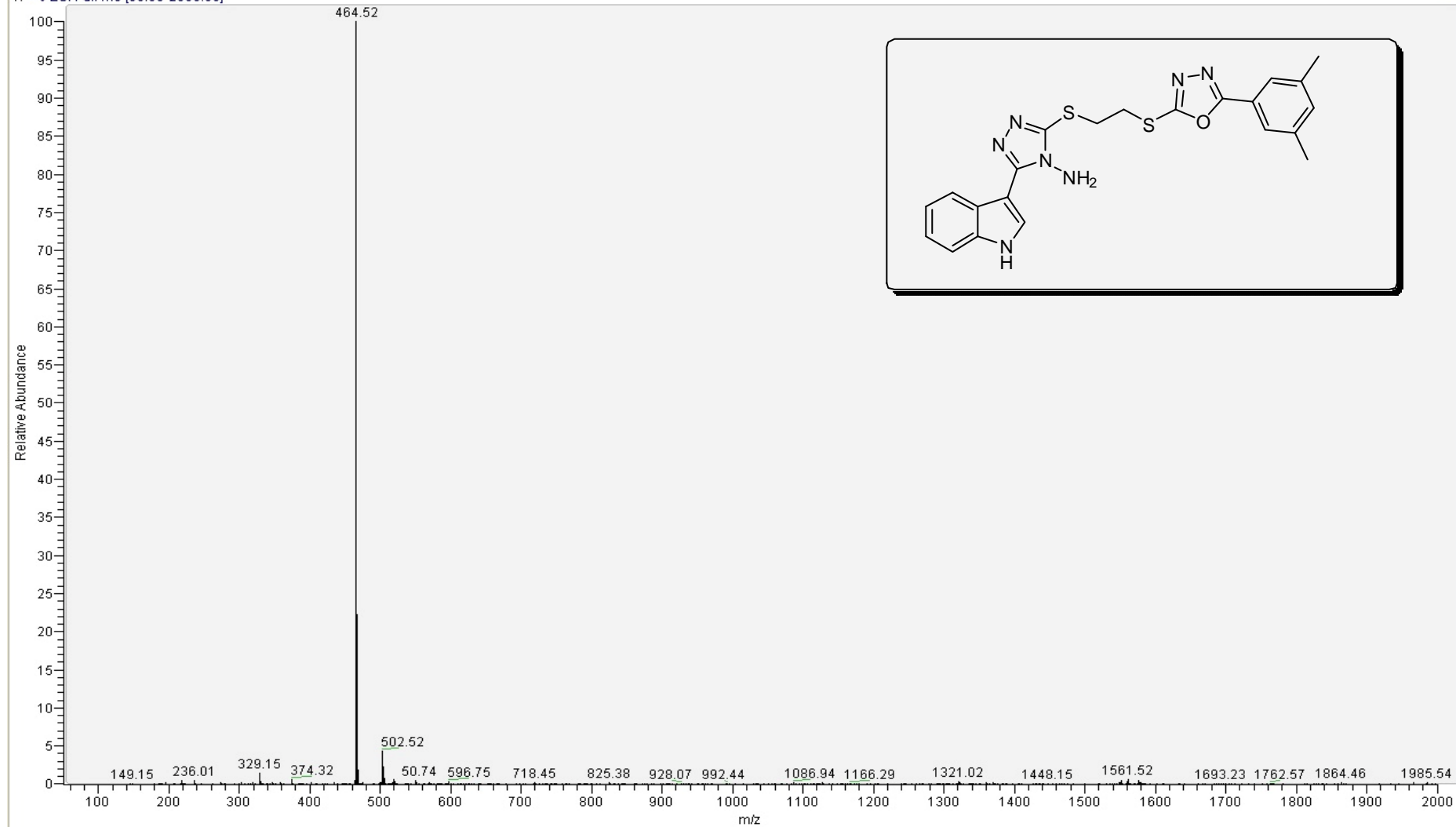
Sample Name:  
S-E3  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dms0  
Data collected on: Jul 3 2014

165.890  
163.446  
152.361  
150.889  
139.205  
136.086  
133.817  
126.147  
125.788  
124.455  
123.324  
122.603  
121.769  
120.547  
112.087  
102.102

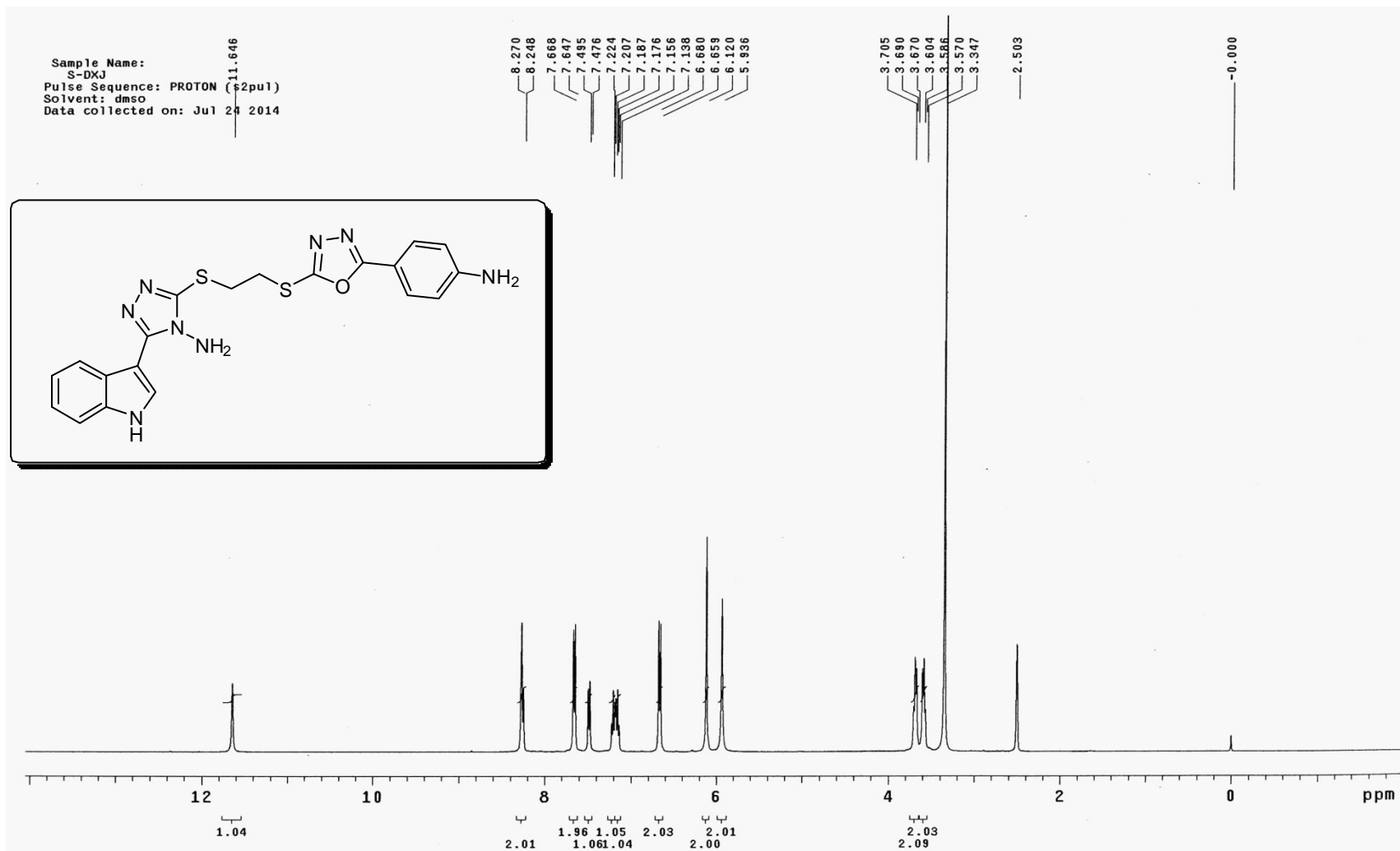
40.568  
40.363  
40.150  
39.946  
39.733  
39.528  
39.316  
32.571  
31.364  
21.144



T: + c ESI Full ms [50.00-2000.00]



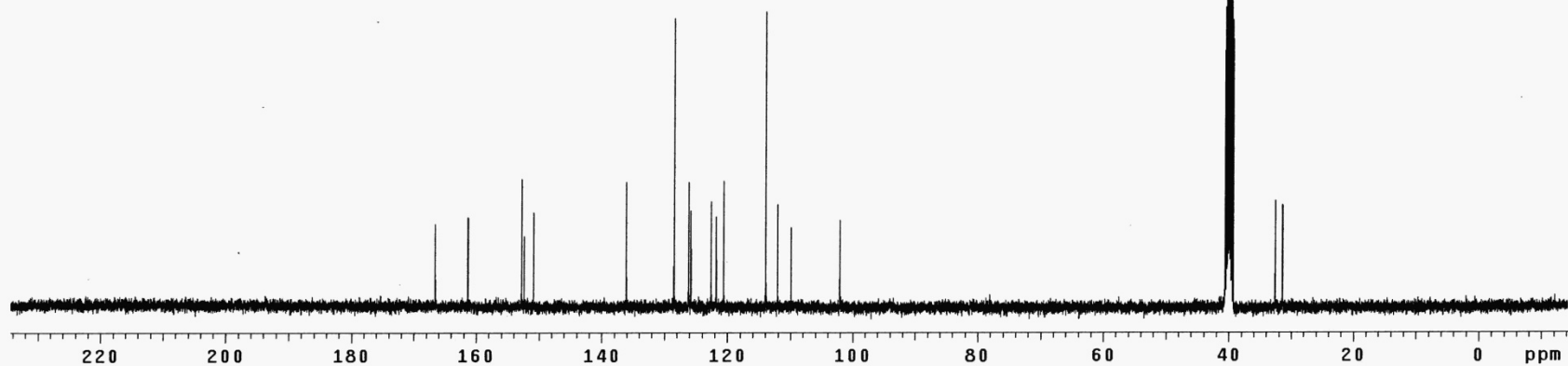
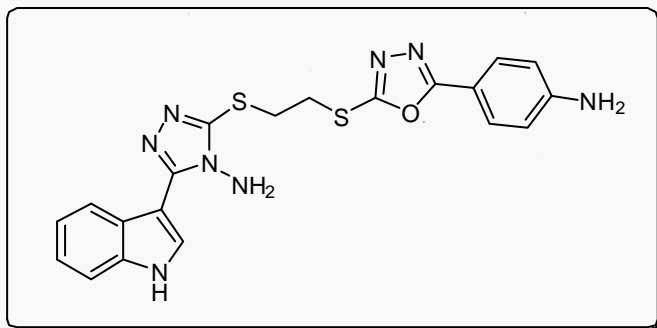
3-(1H-indol-3-yl)-5-[[2-[[5-(4-aminophenyl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10I)



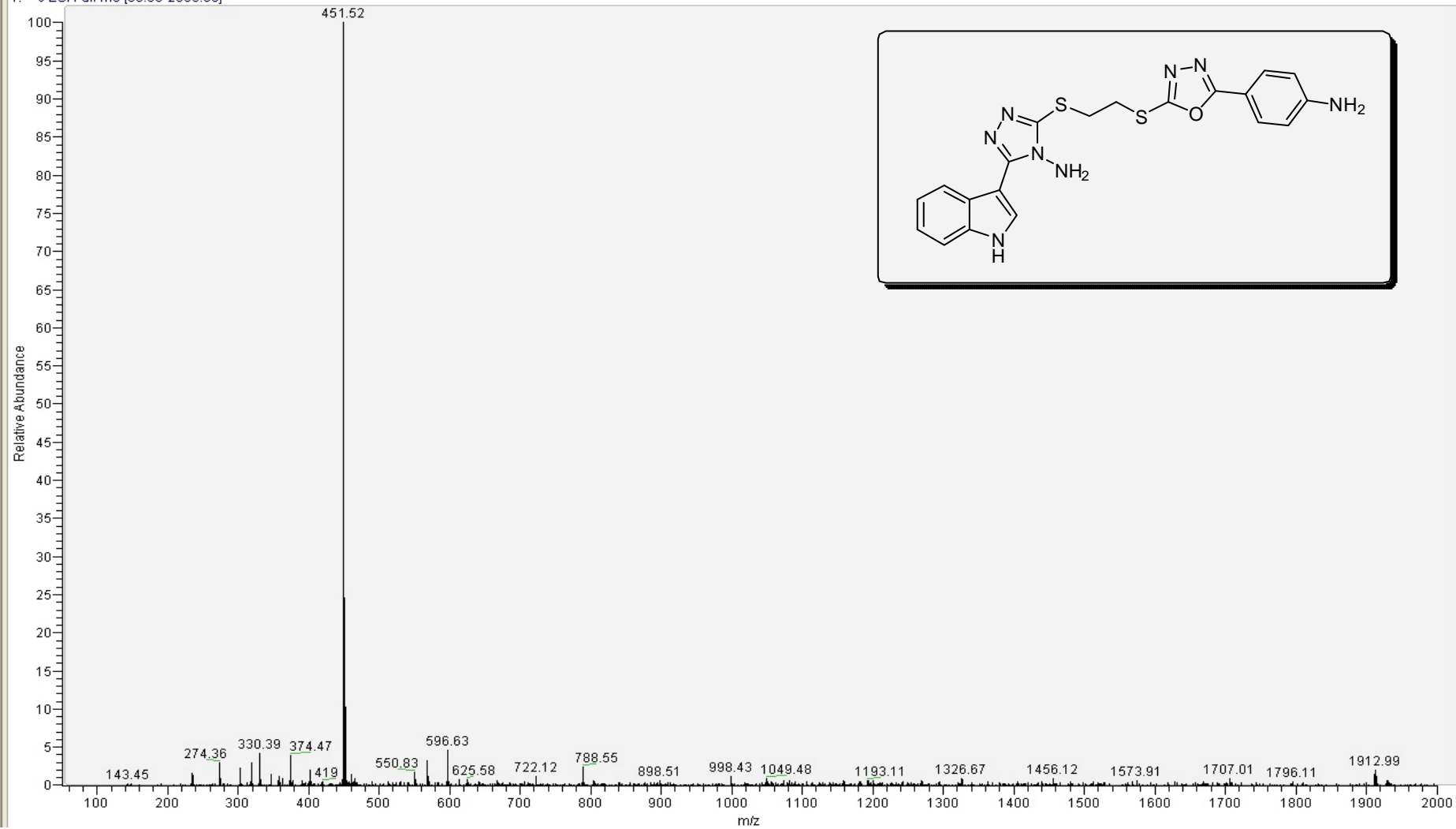
Sample Name:  
S-DXJ  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dmsO  
Data collected on: Jul 24 2014

166.557  
161.337  
152.794  
152.369  
150.874  
136.086  
128.461  
126.162  
125.805  
122.603  
121.784  
120.823  
118.884  
112.095  
109.818  
102.102

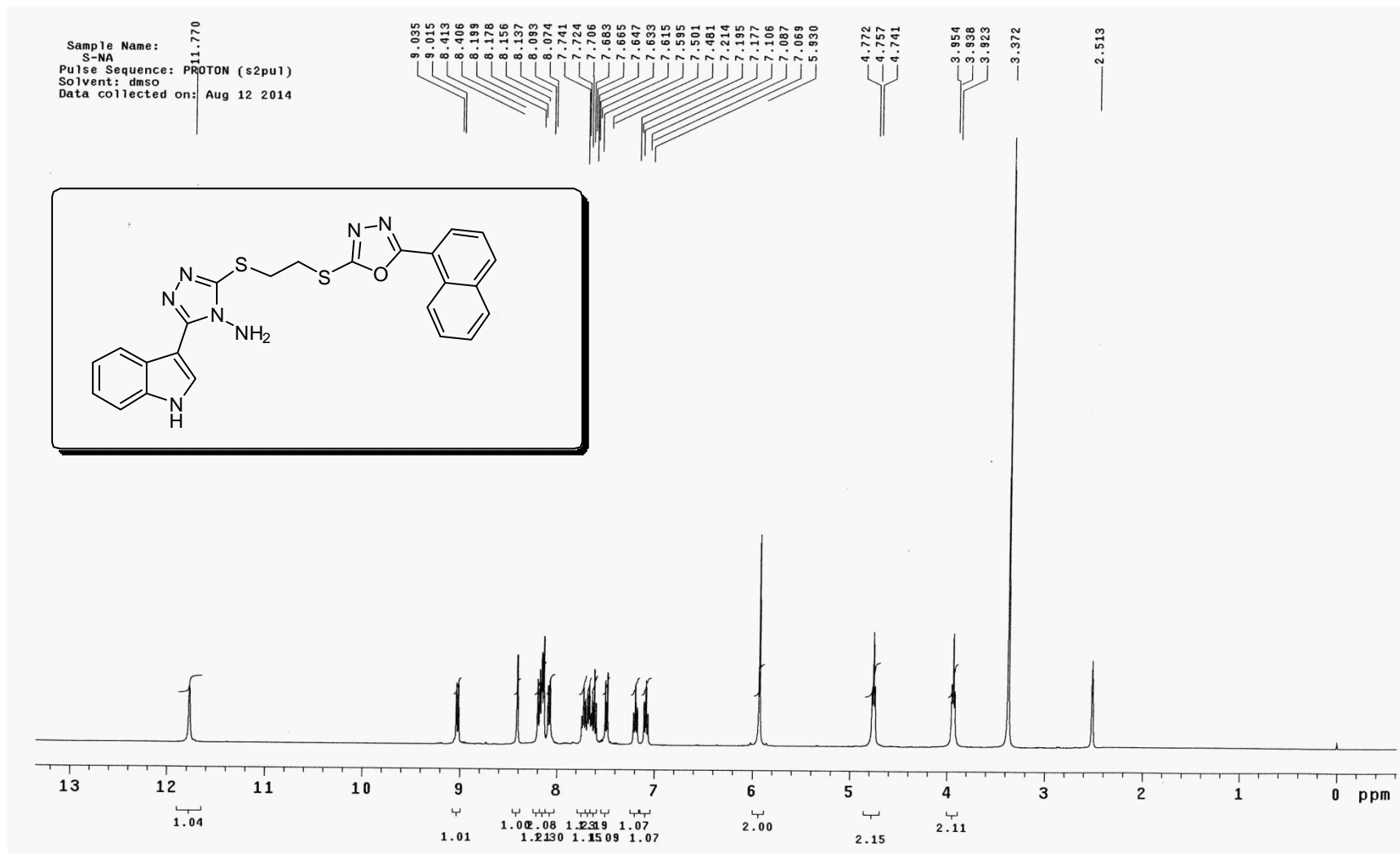
40.575  
40.563  
40.138  
39.890  
39.741  
39.528  
39.323  
32.583  
31.417



T: + c ESI Full ms [50.00-2000.00]



3-(1H-indol-3-yl)-5-[[2-[[5-(naphthalen-1-yl)-1,3,4-oxadiazol-2-yl]thio]ethyl]thio]-4H-1,2,4-triazol-4-amine (10m)





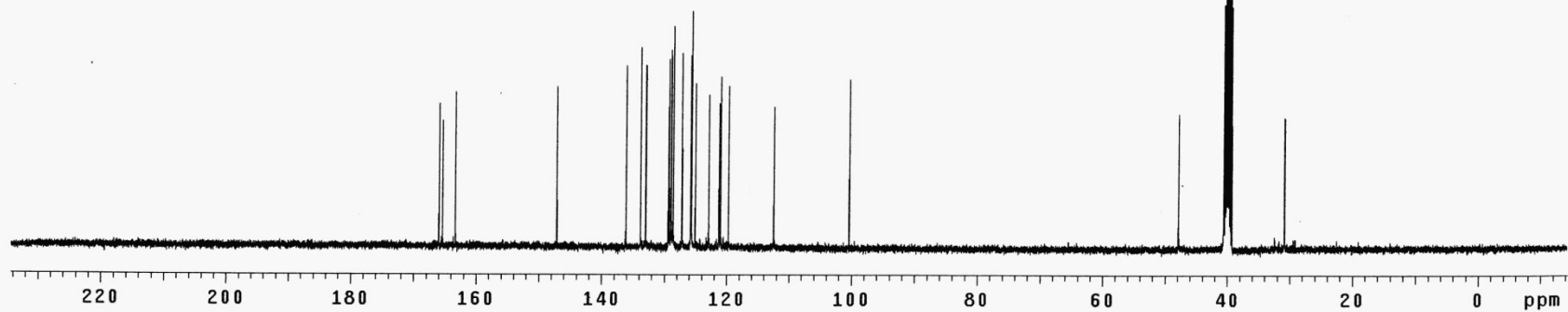
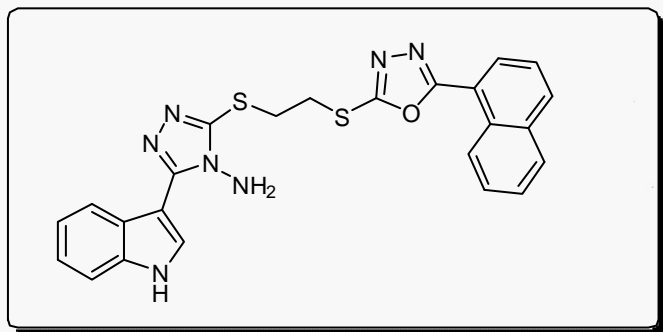
Sample Name:  
S-NA  
Pulse Sequence: CARBON (s2pu1)  
Solvent: dms0  
Data collected on: Aug 12 2014

165.896  
165.412  
163.333

147.134

136.132  
133.803  
132.991  
129.425  
128.268  
128.969  
128.931  
128.613  
127.232  
125.828  
125.692  
125.085  
122.922  
121.283  
121.018  
119.751  
112.436  
100.365

47.897  
40.583  
40.378  
40.166  
38.961  
39.749  
39.544  
39.331  
30.871



T: + c ESI Full ms [50.00-2000.00]

