

Support information

Synthesis, ADMT prediction, *in vitro*, and *in silico* α -glucosidase inhibition evaluations of new quinoline-quinazolinone-thioacetamides

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^cPharmaceutical and Heterocyclic Chemistry Research Laboratory, Department of Chemistry, Iran University of Science and Technology, Tehran, 16846-13114, Iran

^dShahid Beheshti University of Medical Sciences, Tehran, Iran

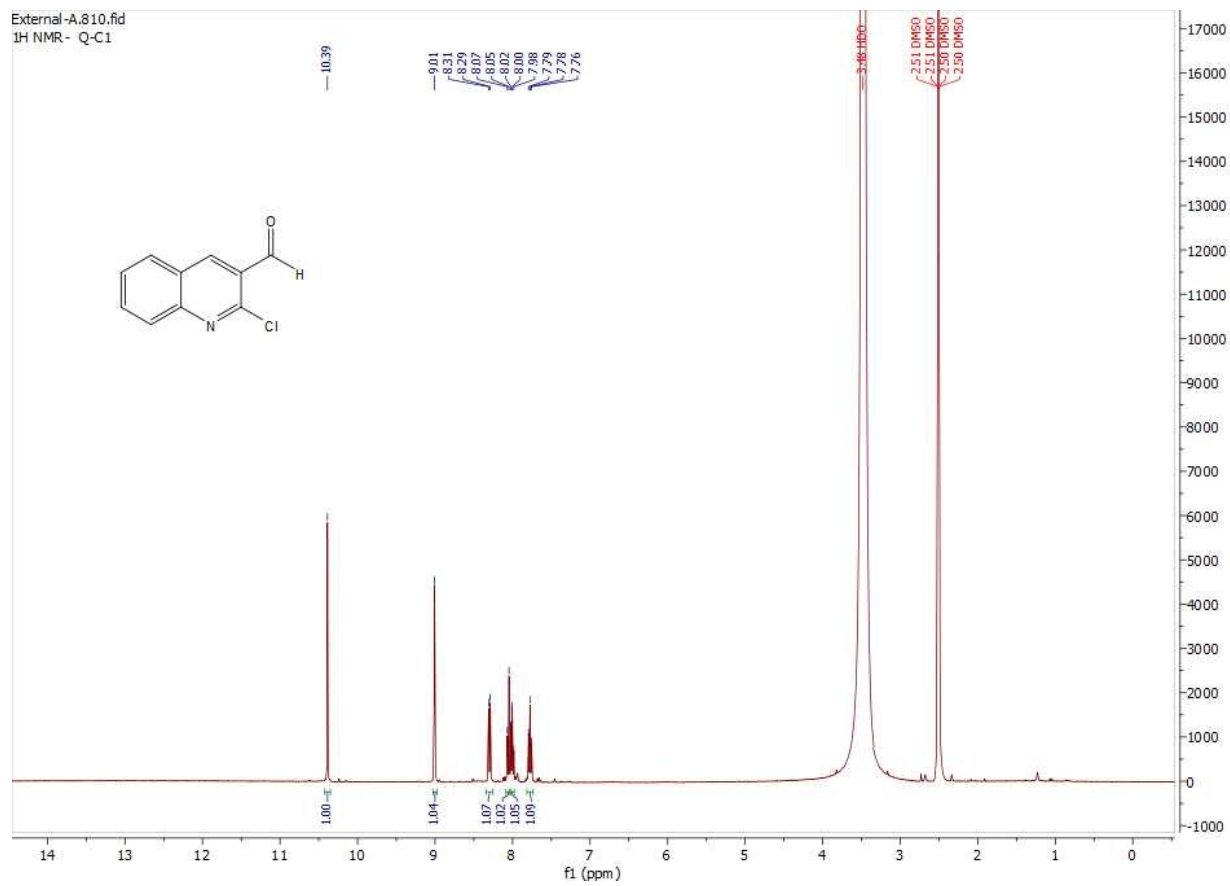
^eDepartment of Pharmaceutical Biotechnology, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran

^fDiabetes Research Center, Endocrinology and Metabolism Clinical Sciences Institute, Tehran University of Medical Sciences, Tehran, Iran

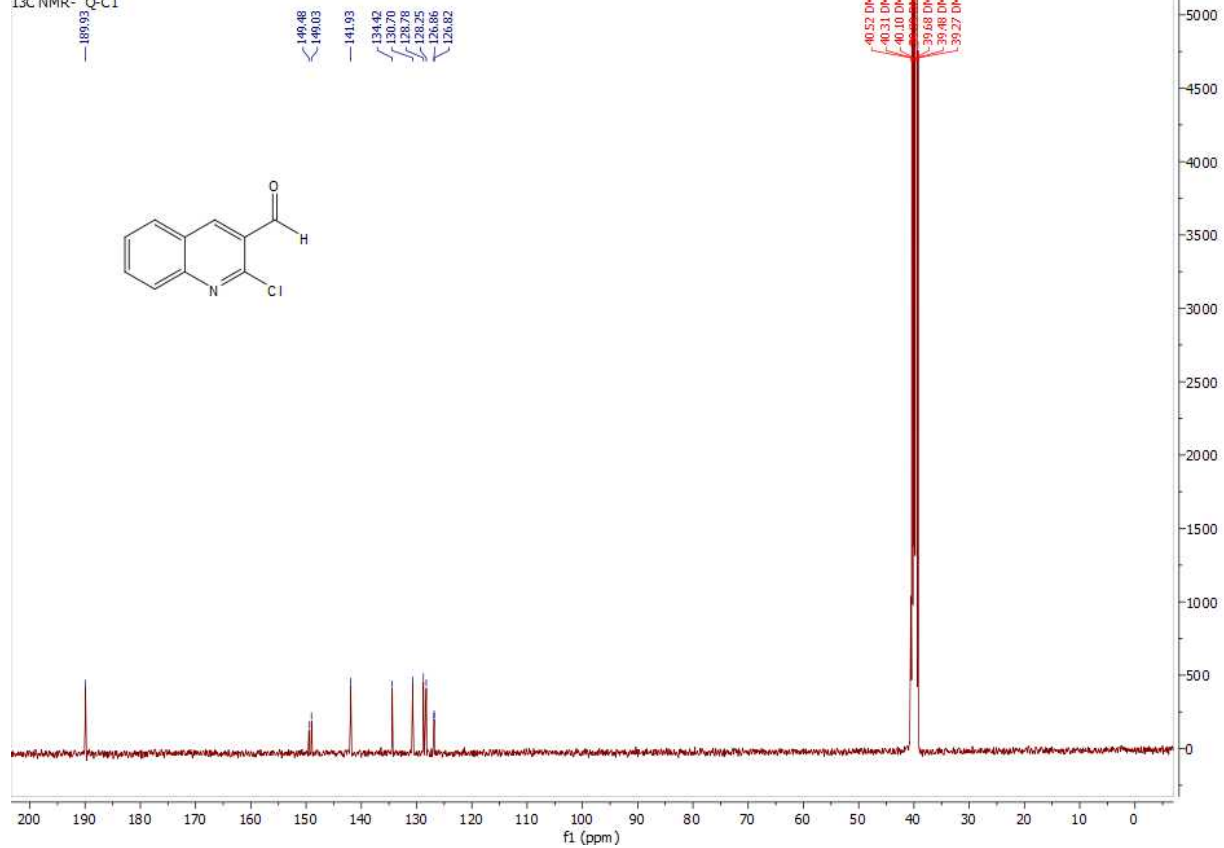
^gFaculty of Pharmacy, Pharmaceutical Sciences Branch, Islamic Azad University, Tehran, Iran

^hCellular and Molecular Biology Research Center, Health Research Institute, Babol University of Medical Sciences, Babol, Iran. E-mail: maryammoha@gmail.com

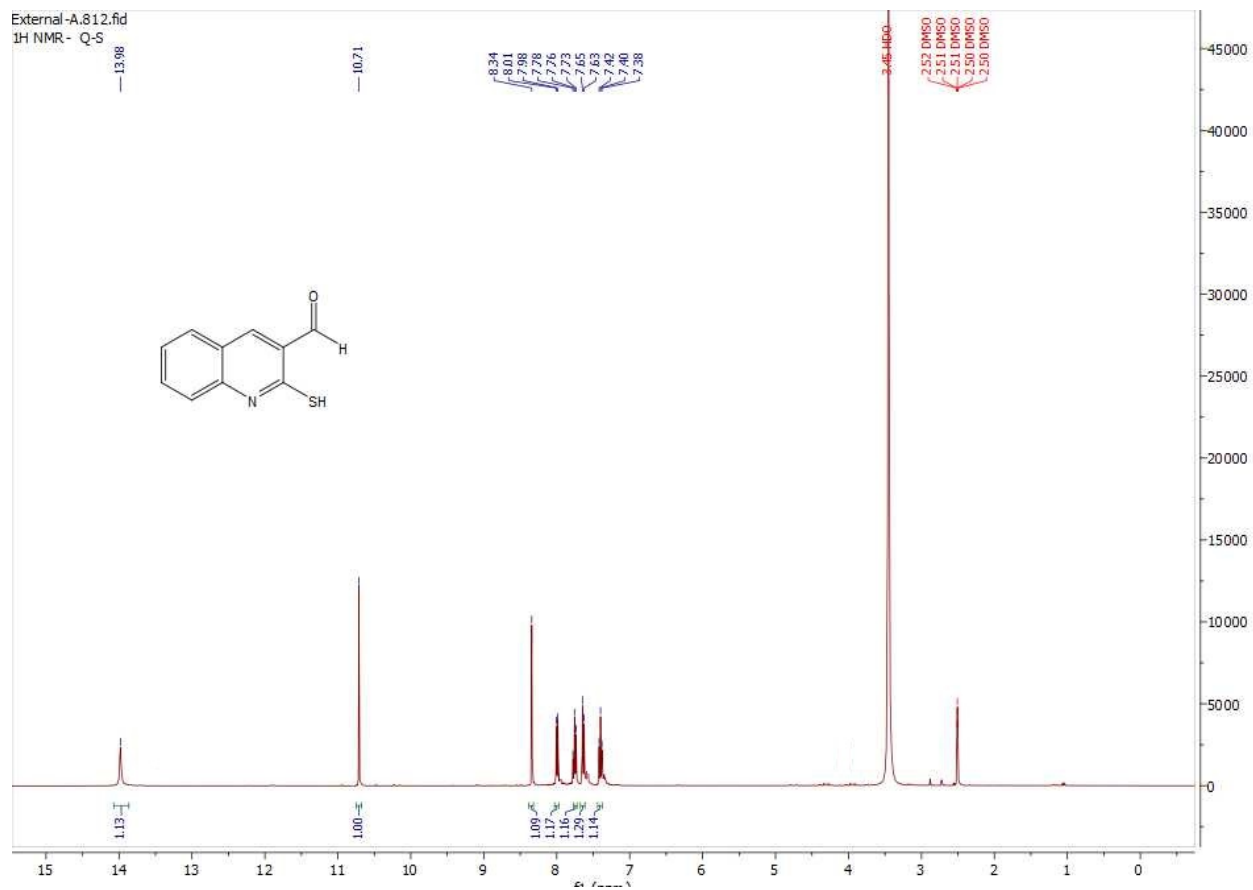
2-chloroquinoline-3-carbaldehyde (2):



External-A.811.fid
13C NMR- Q-C1

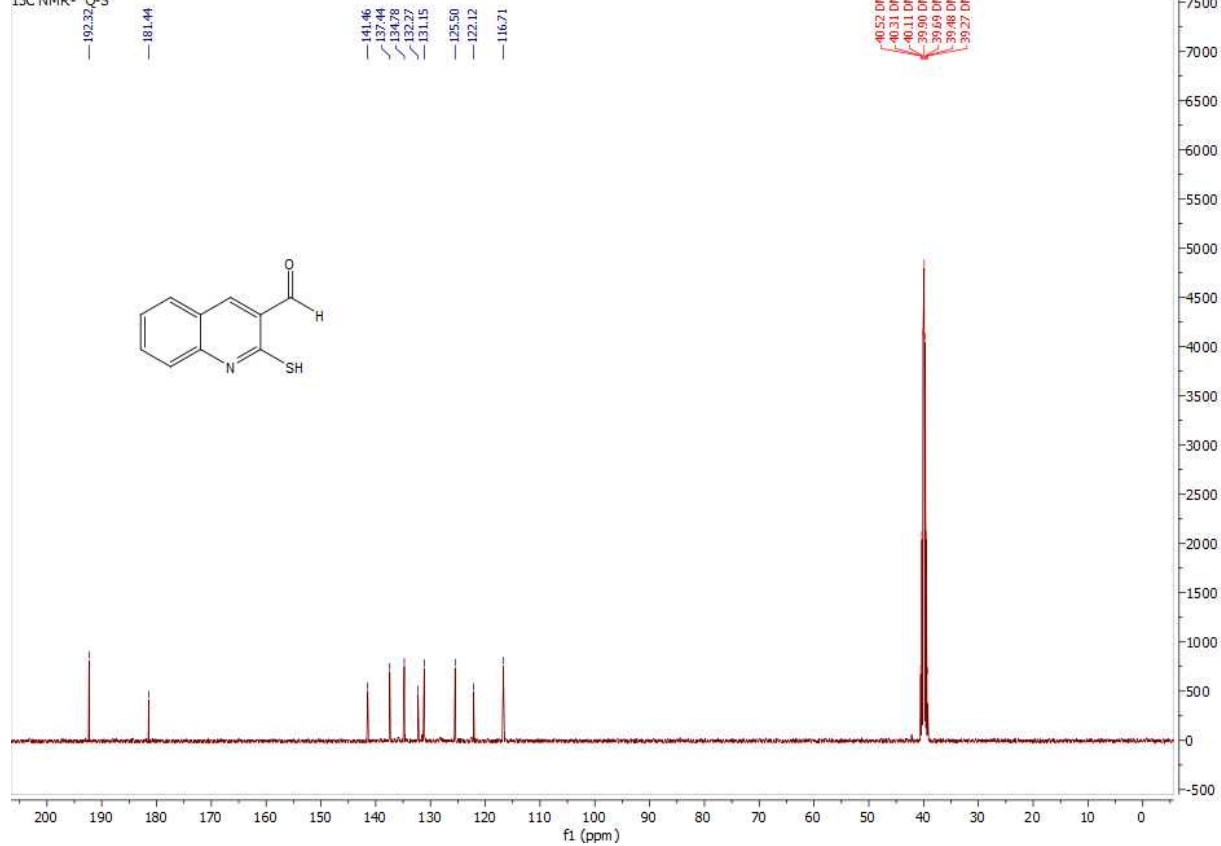


2-mercaptoquinoline-3-carbaldehyde (3):



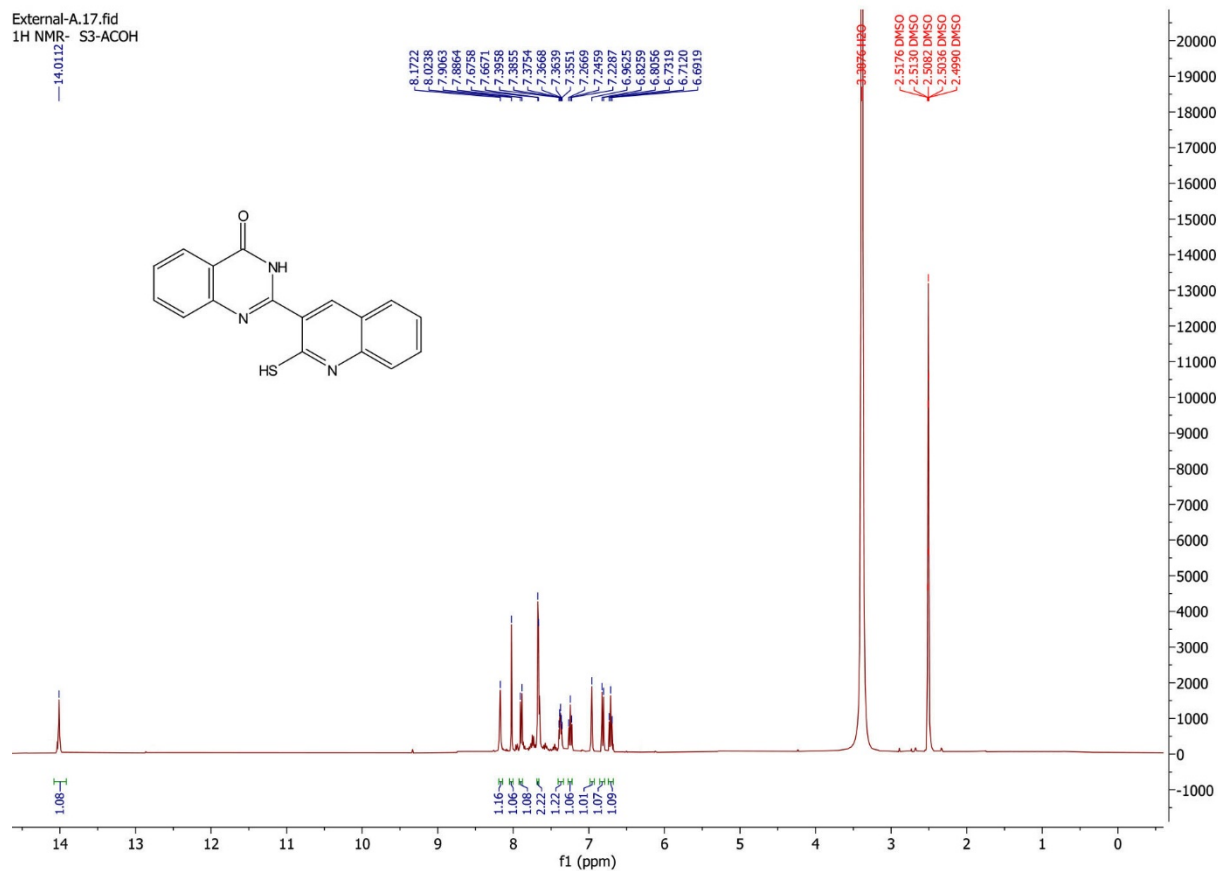
External-A.813.fid

13C NMR- Q-S



2-(2-mercaptoquinolin-3-yl)quinazolin-4(3H)-one

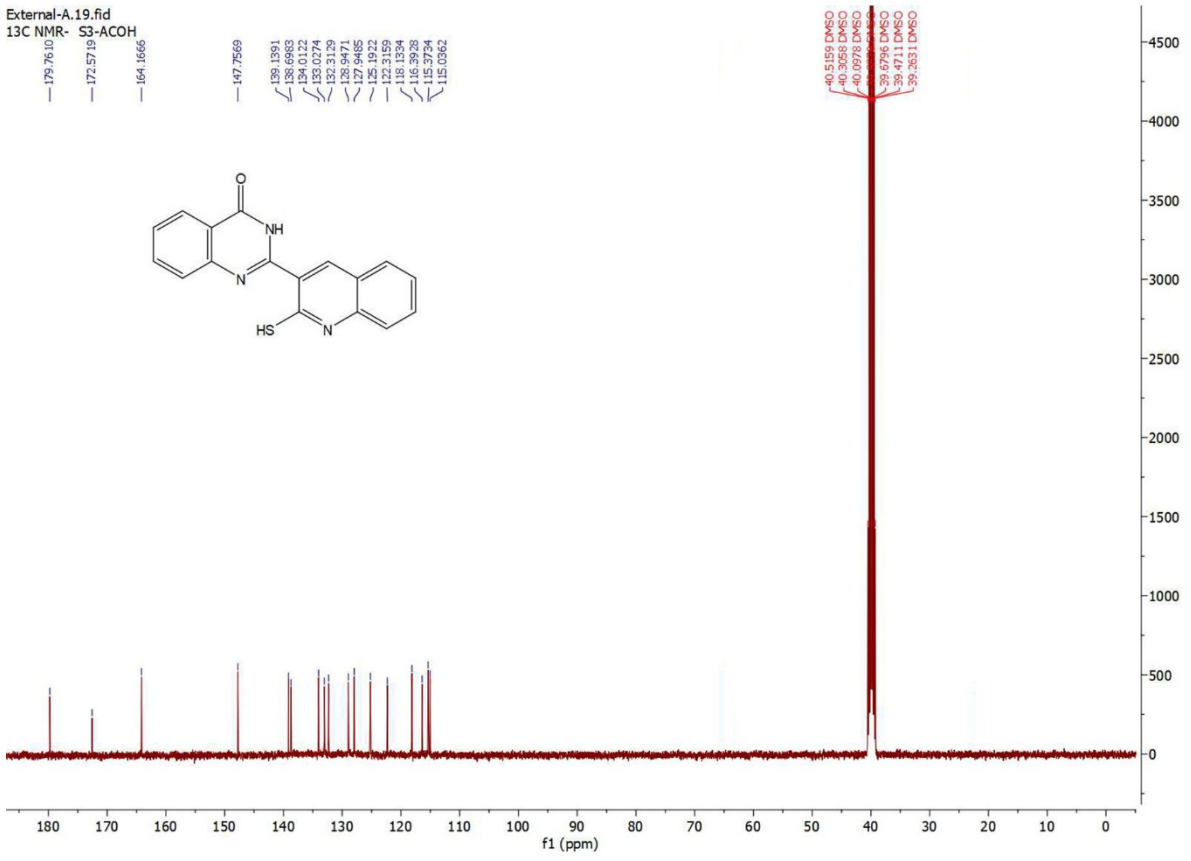
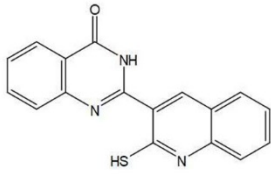
External-A,17.fid
1H NMR - S3-A COH



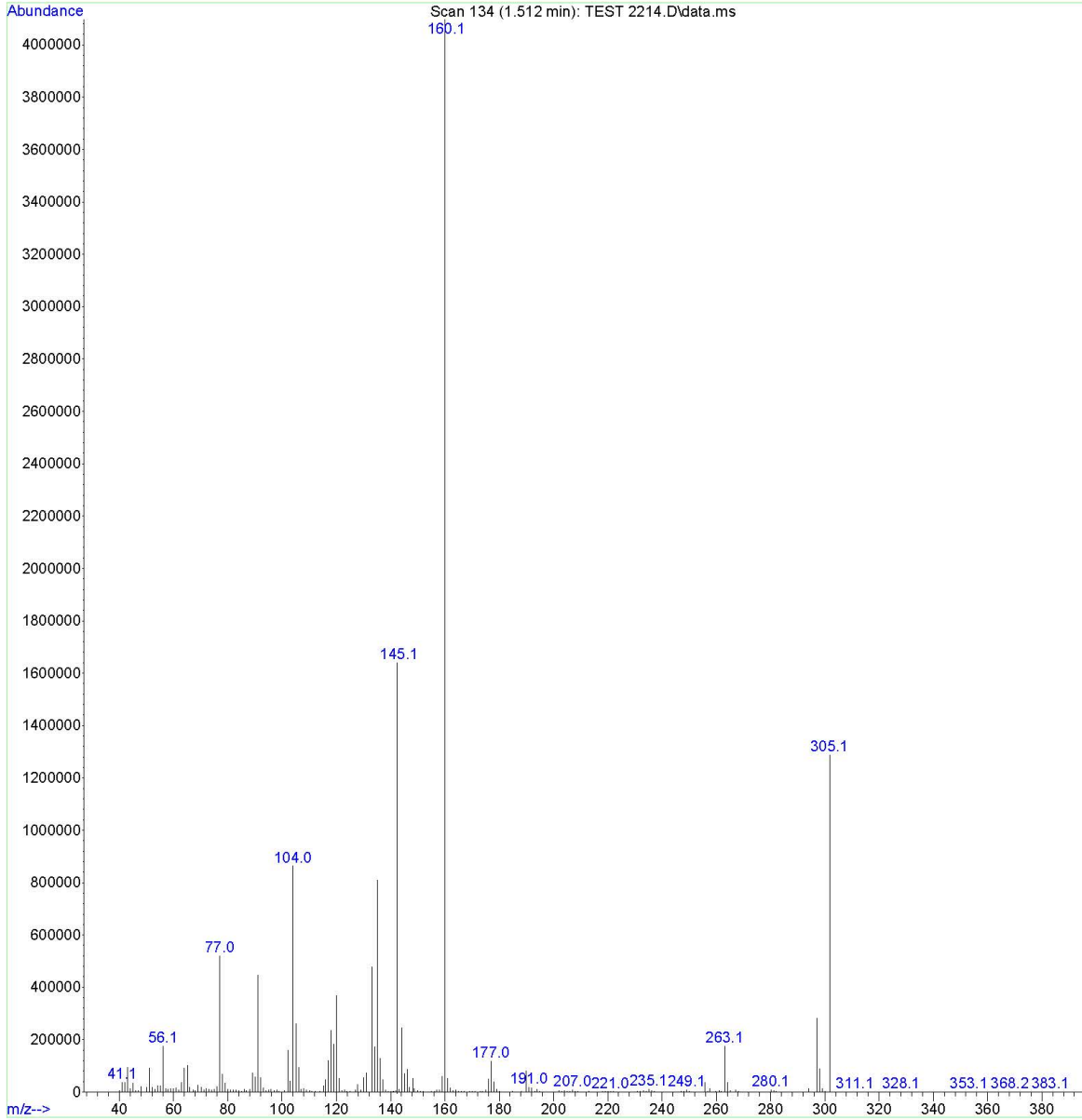
External-A.19.fid
13C NMR- S3-ACOH

179.7610
172.5719
164.1666

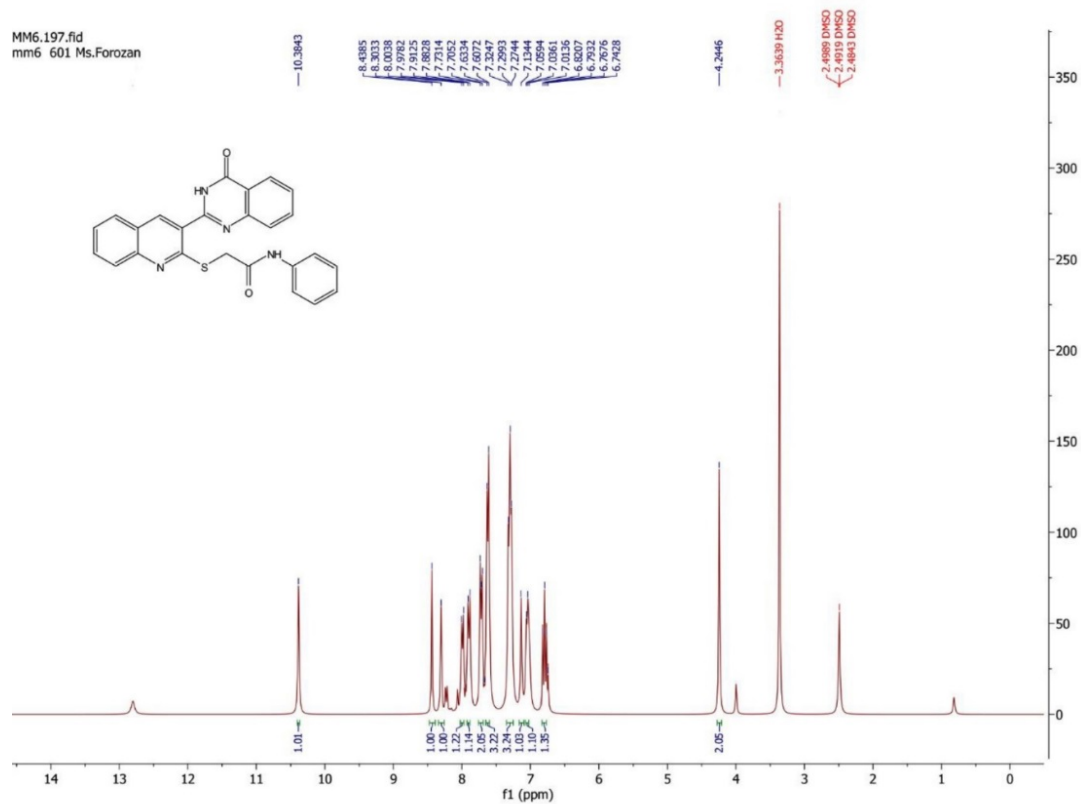
147.7569
138.1391
138.6983
134.0122
133.0274
132.3129
128.9471
127.9485
125.1122
123.1659
118.1334
116.5928
115.3724
115.0362



File :C:\MSDCHEM\3\DATA\Snapshot\TEST 2214.D
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Acquired : 28 Jul 2007 3:35 using AcqMethod test000414.M
Instrument : MSD
Sample Name: intermediate mm6
Misc Info :
Vial Number: 1

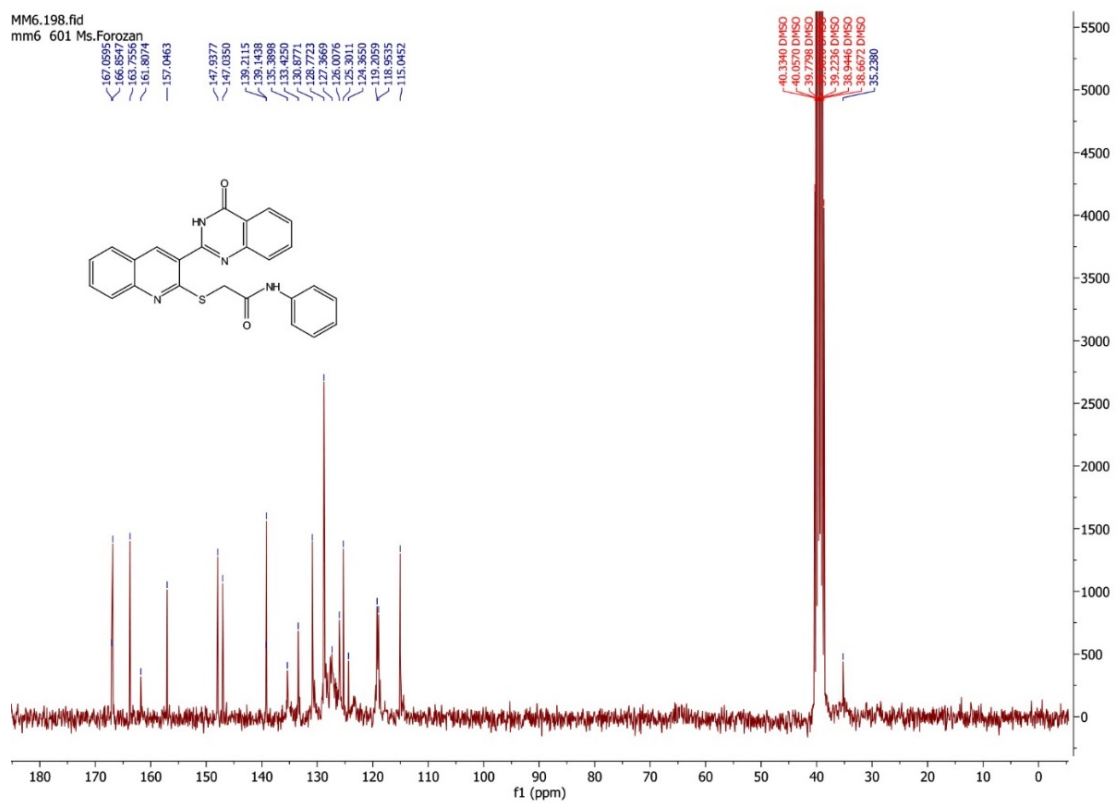
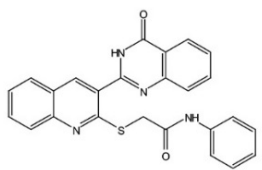


2- $\{[3-(4\text{-Oxo-}3,4\text{-dihydroquinazolin-}2\text{-yl})\text{ quinolin-}2\text{-yl] thio}\}$ -*N*-phenylacetamide (**9a**)

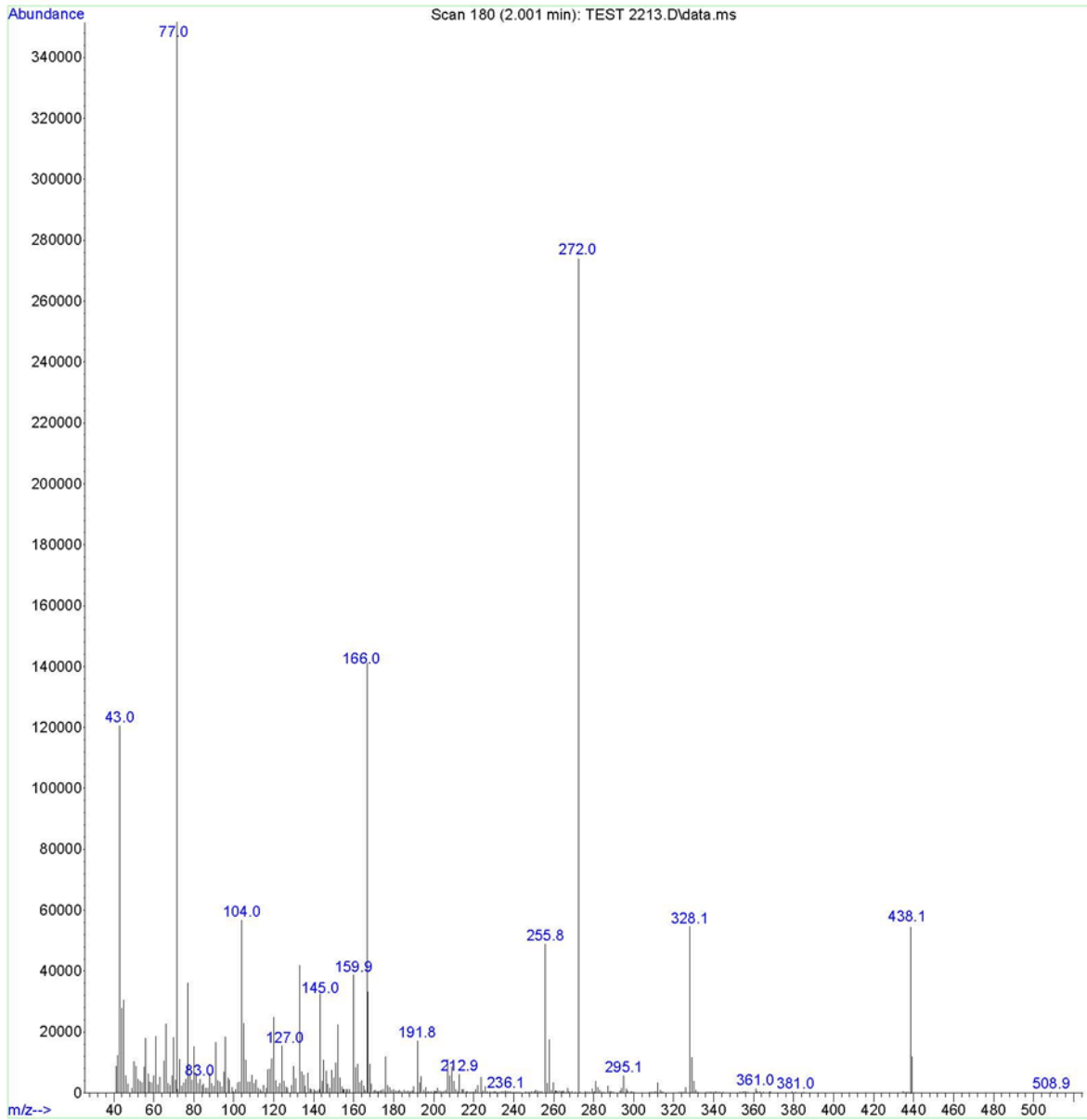


MM6.198.fid
mm6 601 Ms.Forozan

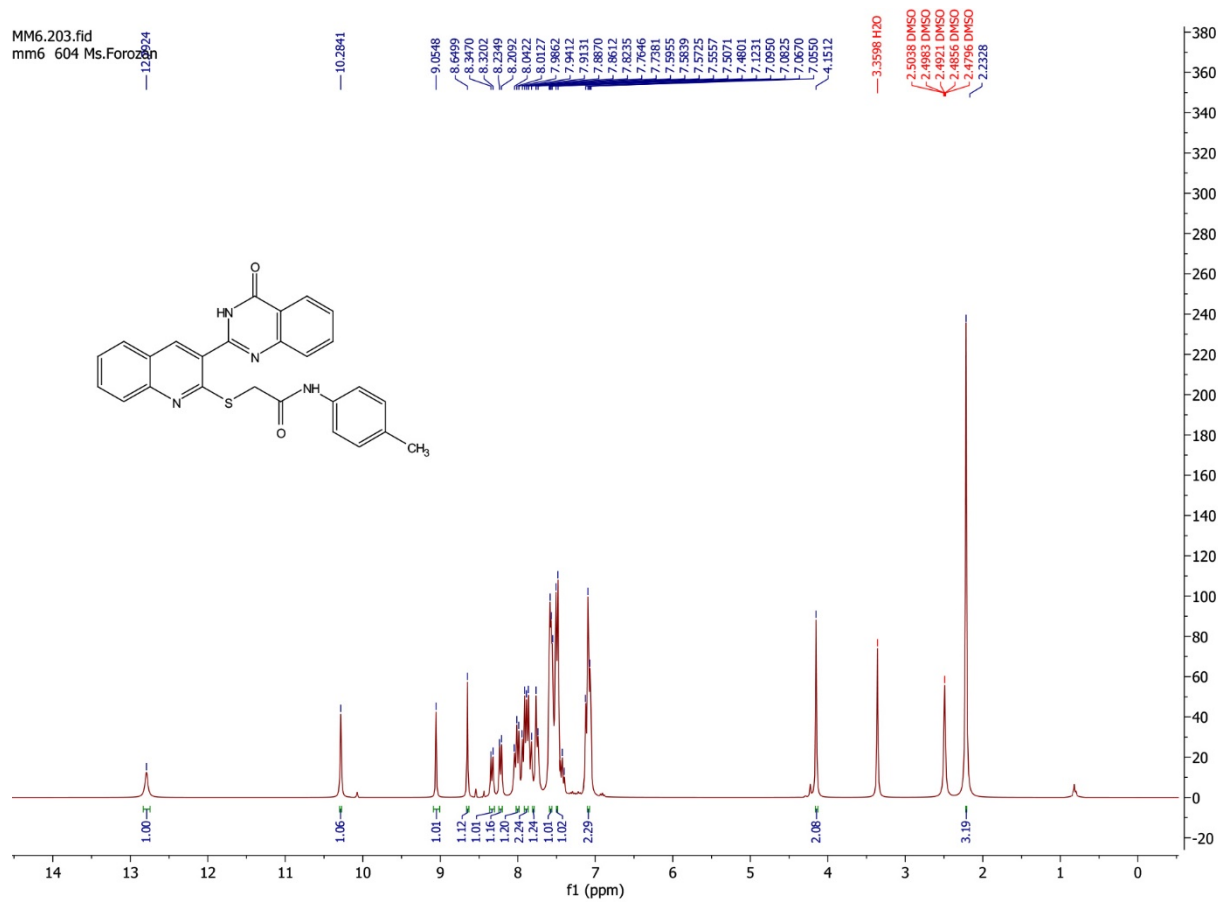
- 167.0595
- 166.8547
- 166.8074
- 157.0463
- 147.0377
- 147.0350
- 139.2115
- 138.1438
- 135.3898
- 133.4250
- 132.8771
- 127.7773
- 127.3669
- 126.0076
- 125.3011
- 124.3650
- 119.2859
- 118.1422
- 115.0452



File :C:\MSDCHEM\3\DATA\Snapshot\TEST 2213.D
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Instrument : MSD
Sample Name: MM6 601
Misc Info :
Vial Number: 1

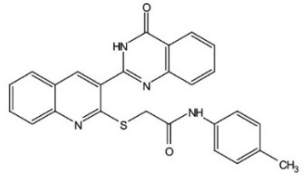


2- $\{[3-(4\text{-Oxo-3,4-dihydroquinazolin-2-yl})\text{quinolin-2-yl}]\text{thio}\}$ - N -(p -tolyl)acetamide (**9b**)



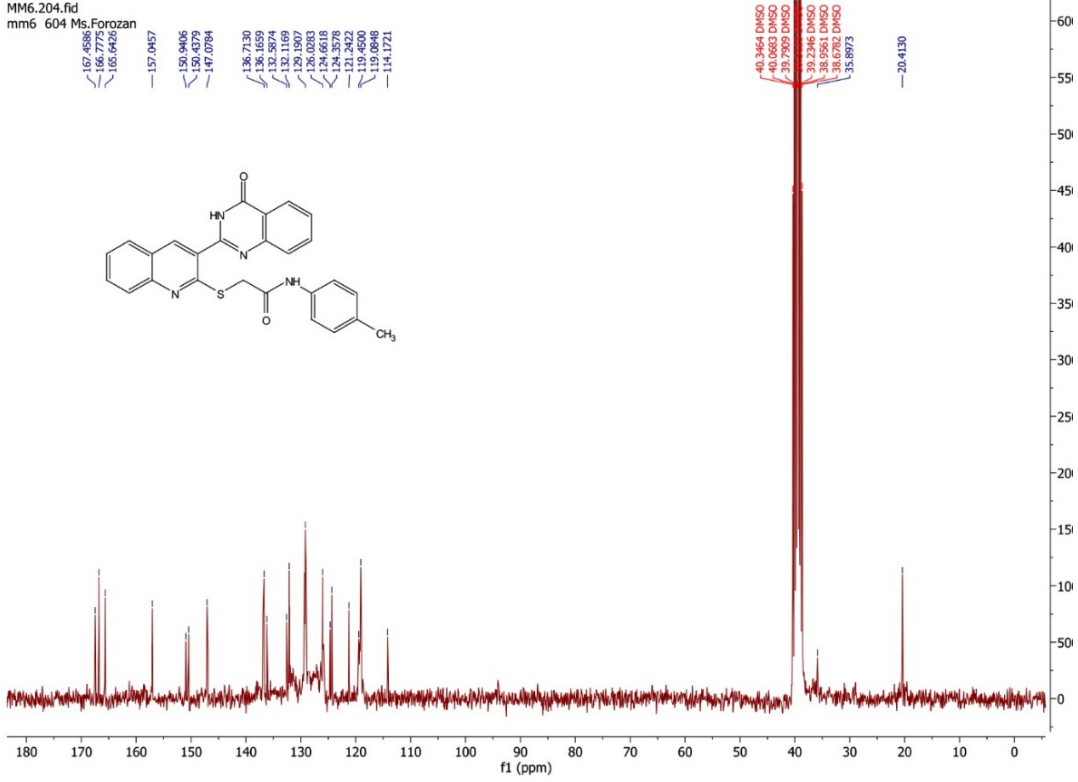
MM6_204.fid
mm6 604 Ms.Forozan

- 167.4586
- 165.6426
- 157.0457
- 150.9406
- 147.0784
- 136.7130
- 135.9574
- 132.8274
- 132.1169
- 129.1907
- 126.0083
- 124.3578
- 121.2422
- 119.6500
- 119.0898
- 114.1721

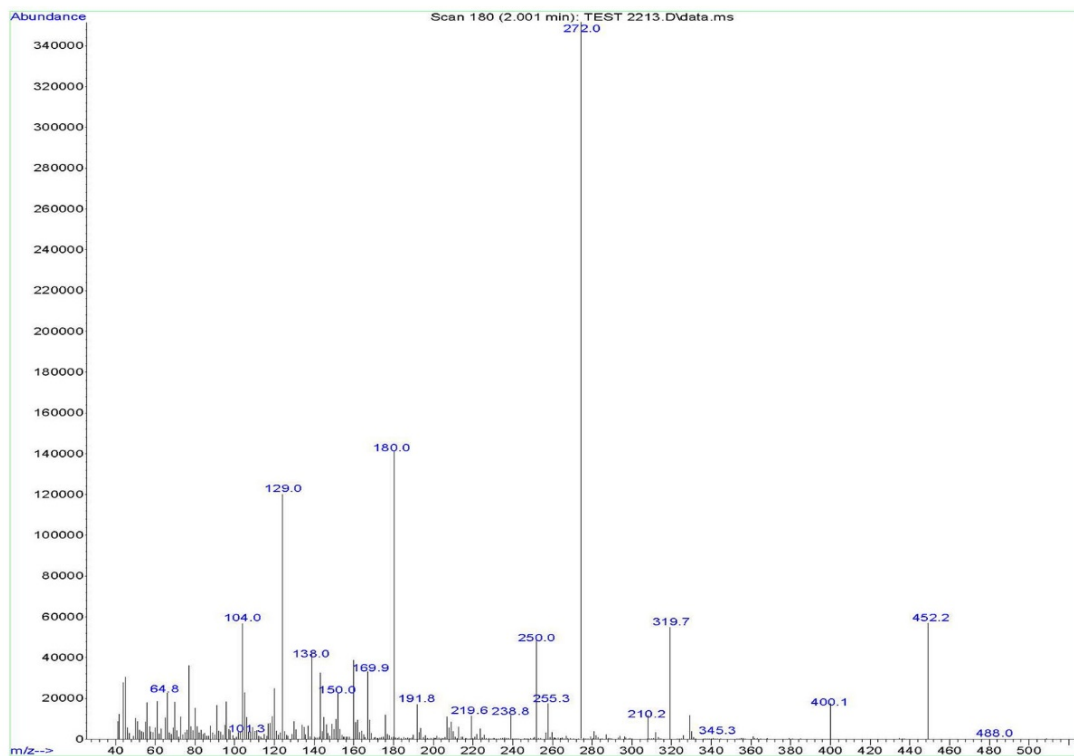


- 40.2464 DMSO
- 39.9990 DMSO
- 39.9990 DMSO
- 39.2346 DMSO
- 38.9951 DMSO
- 38.9951 DMSO
- 35.8973

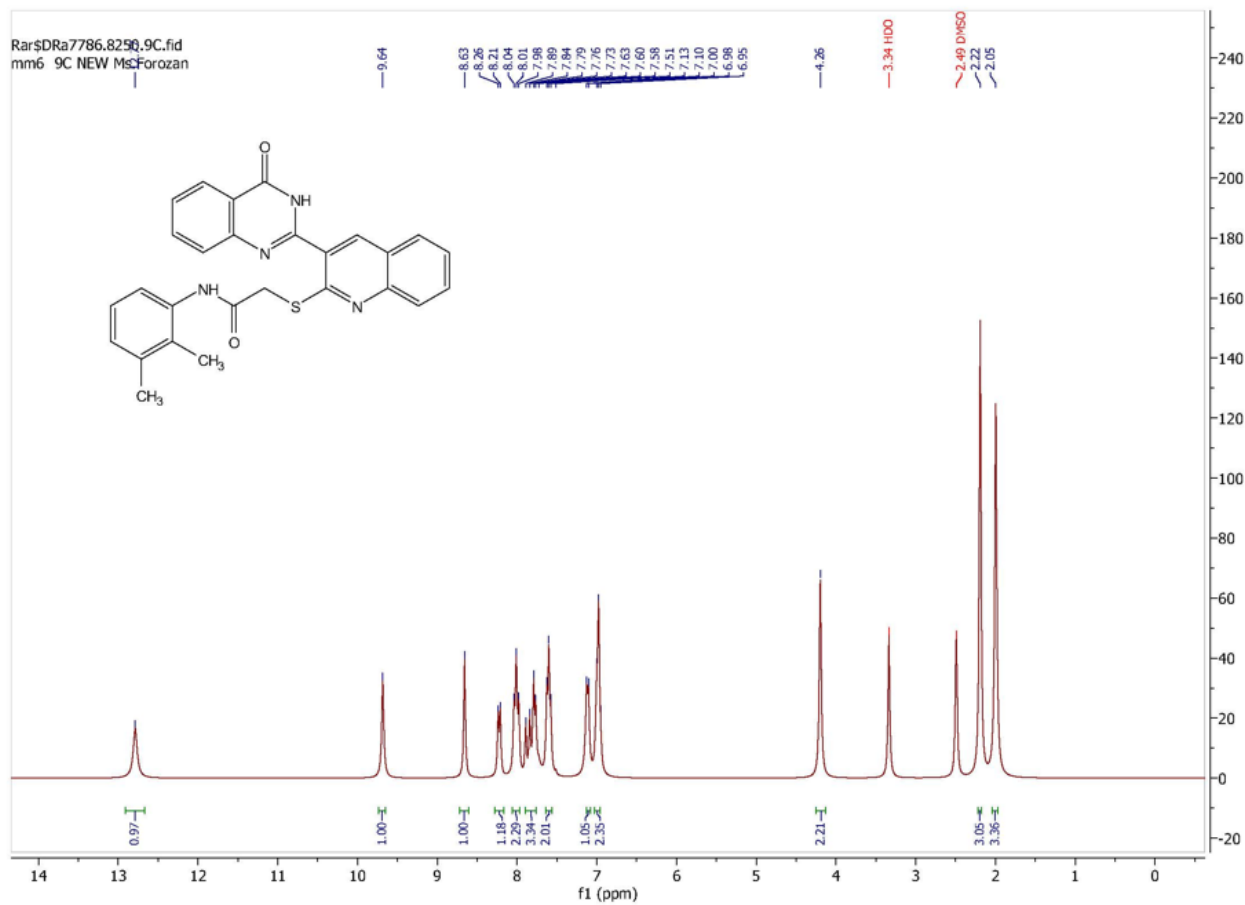
20.4130



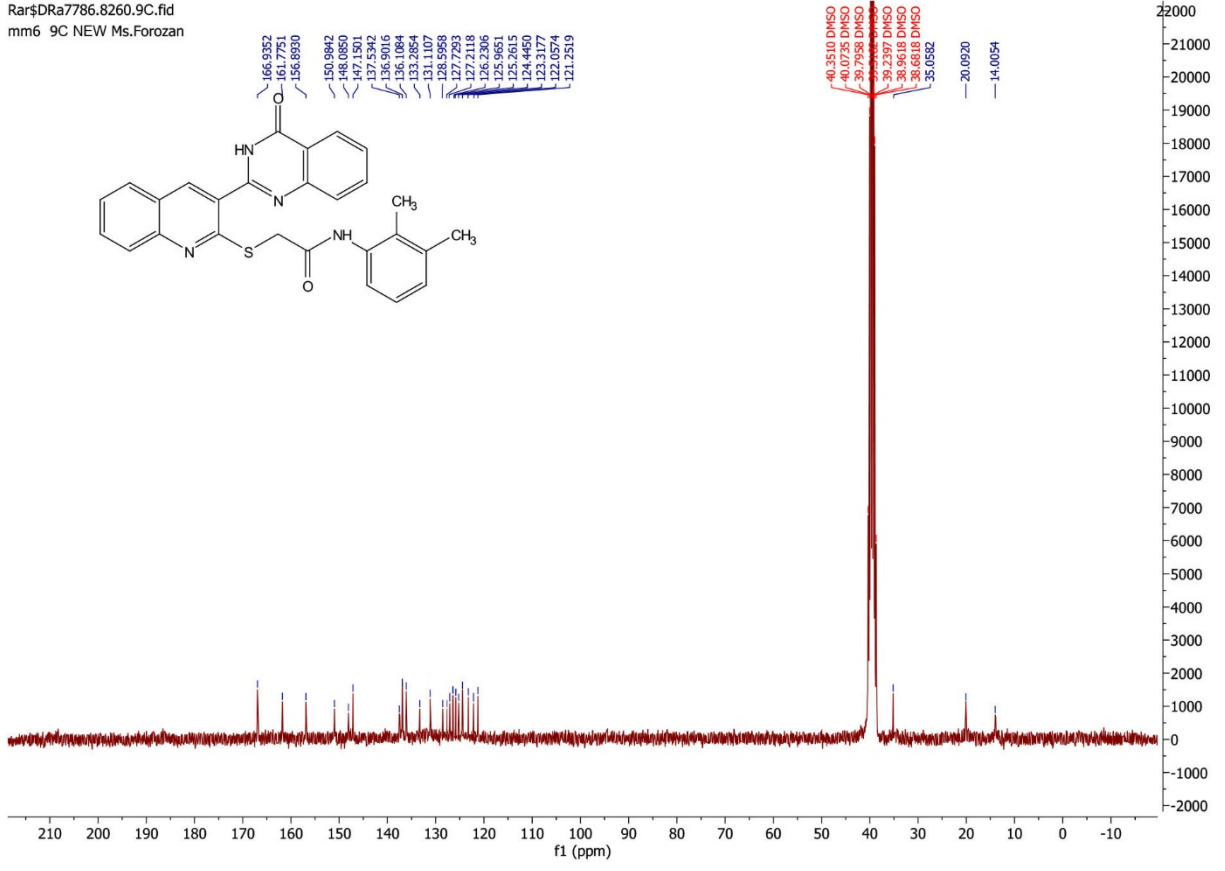
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Instrument : MSD
Sample Name: MM6 604
Misc Info :
Vial Number: 1



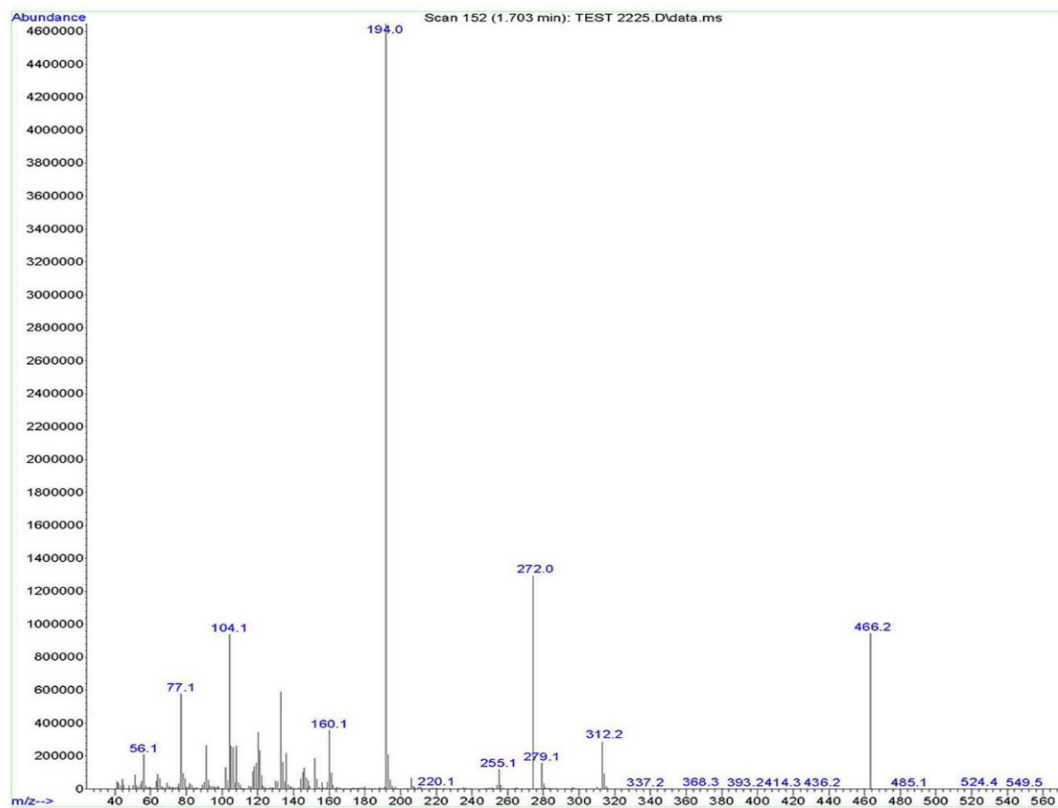
N-(2,3-Dimethylphenyl)-2- $\{[3-(4\text{-oxo-}3,4\text{-dihydroquinazolin-}2\text{-yl})\text{quinolin-}2\text{-yl}]\text{thio}\}$ acetamide
(9c)



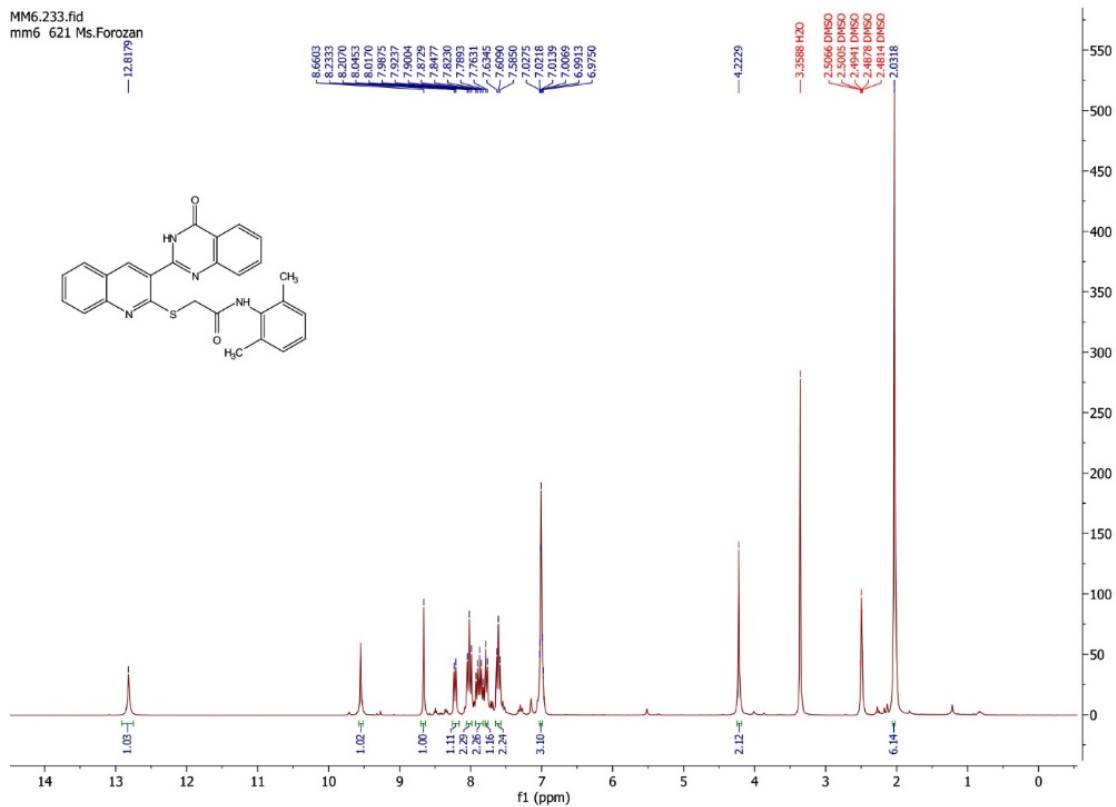
Rar\$DRa7786.8260.9C.fid
mm6 9C NEW Ms.Forozan



File :C:\MSDCHEM\3\DATA\Snapshot\TEST 2225.D
Operator :
Acquired : 28 Jul 2007 4:43 using AcqMethod test000414.M
Instrument : MSD
Sample Name: 607
Misc Info :
Vial Number: 1

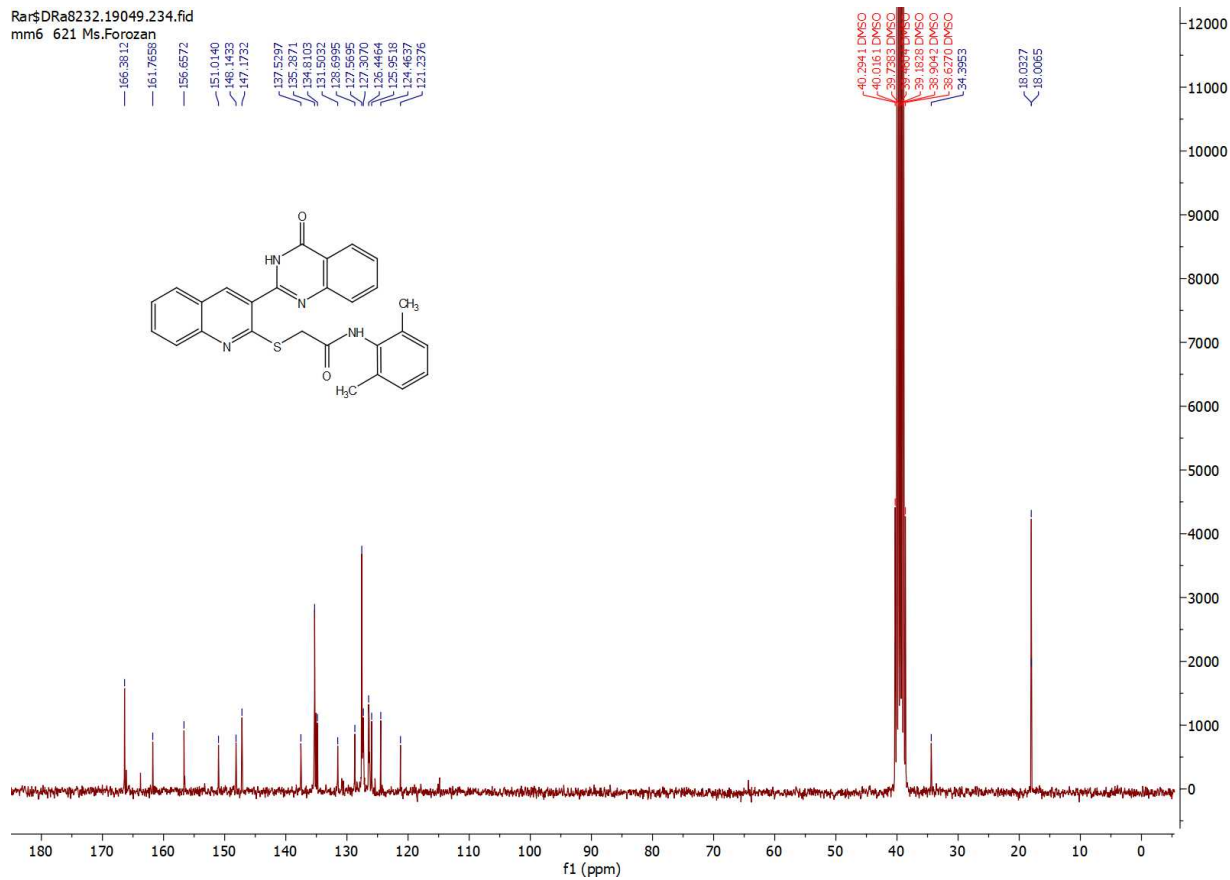
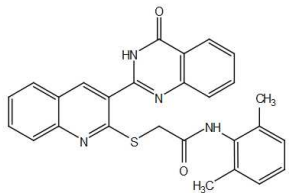


N-(2,6-Dimethylphenyl)-2- $\{[3-(4\text{-oxo-3,4-dihydroquinazolin-2-yl})\text{quinolin-2-yl}]\text{thio}\}$ acetamide
(9d)

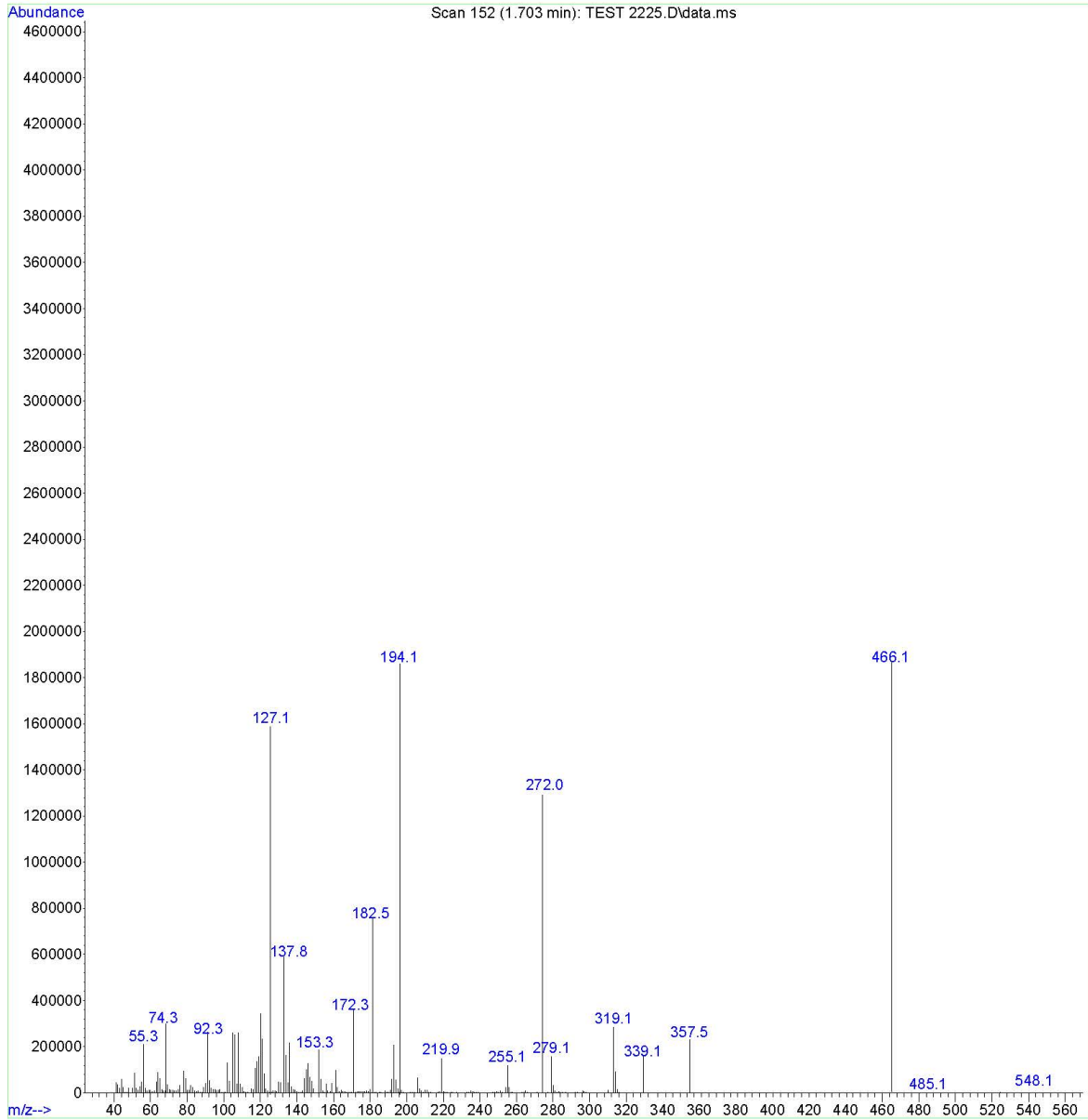


Rar\$DRa8232.19049.234.fid
mm6 621 Ms.Forozan

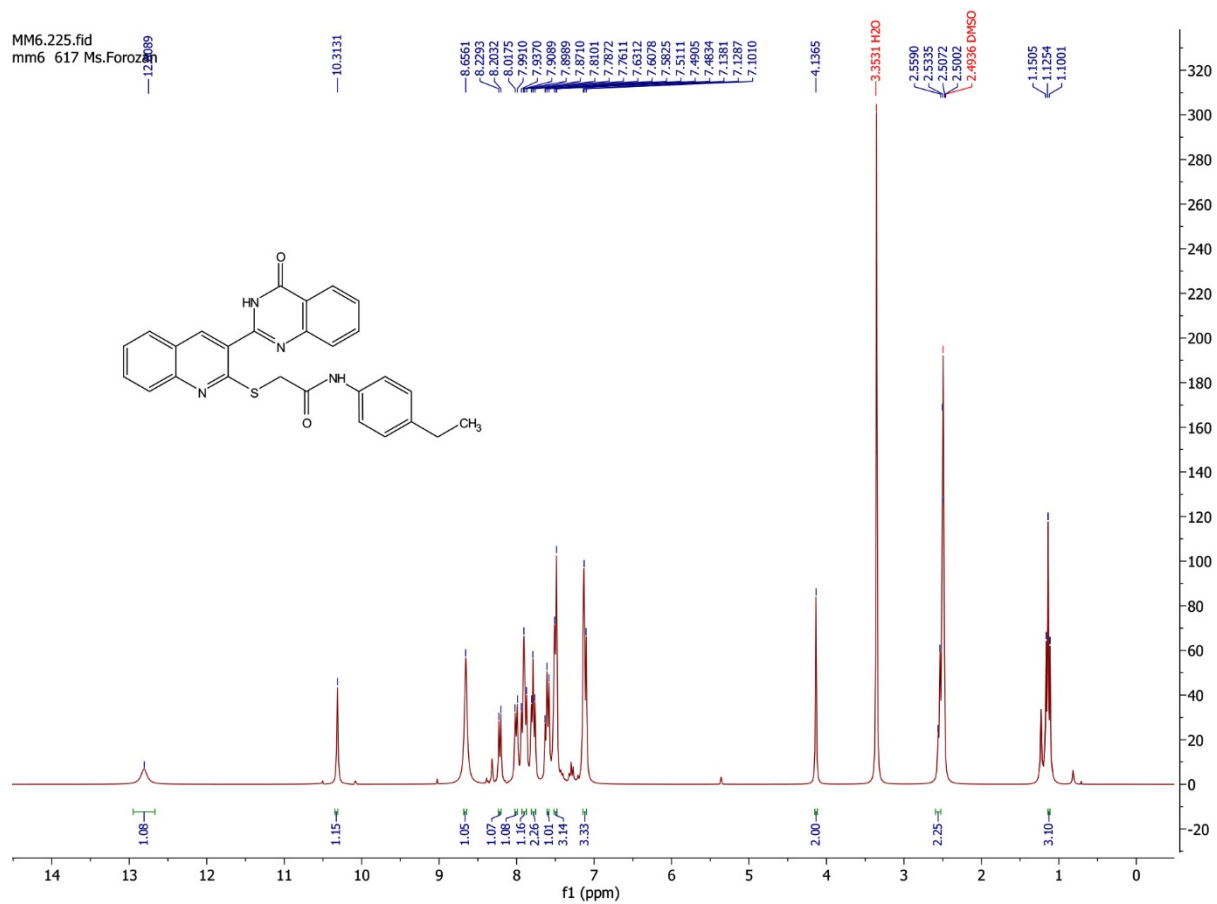
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161.7658
156.6572
151.0140
148.1433
147.1732
137.5297
135.2871
134.8103
131.5032
128.6995
127.9595
127.4424
125.9518
124.4637
121.2376



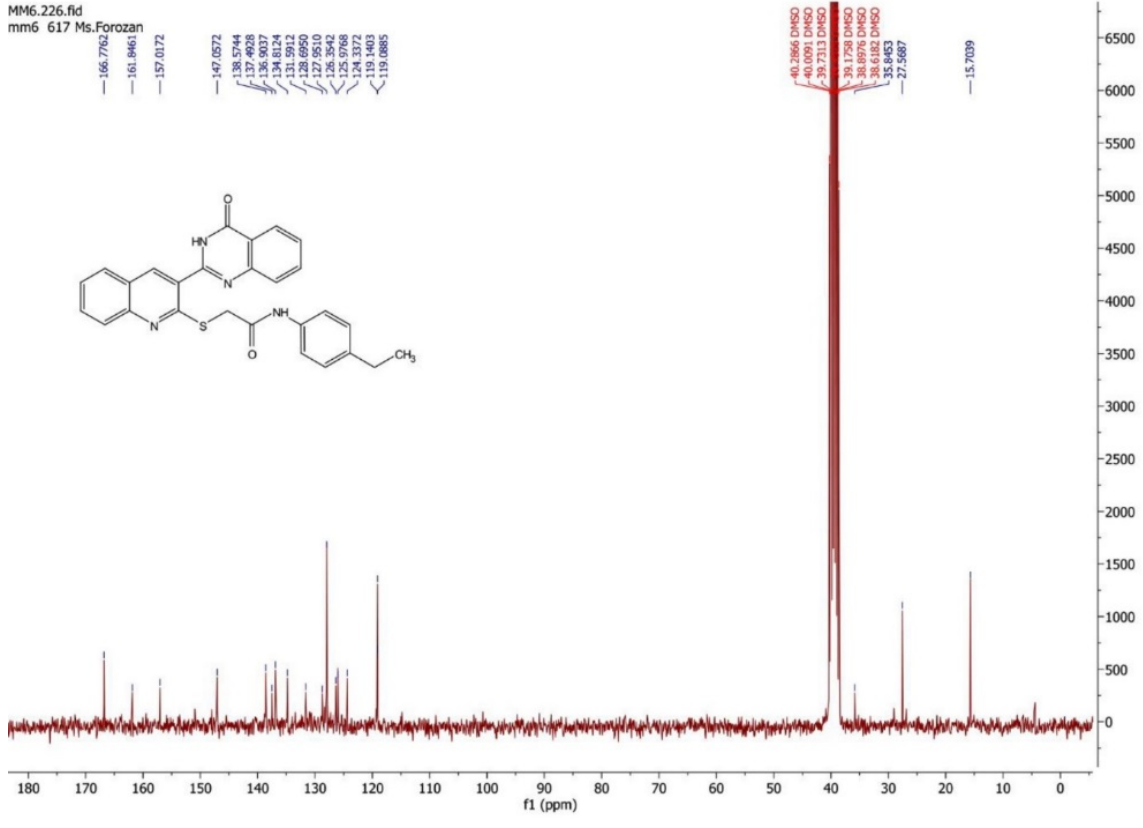
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Operator :
Acquired : 28 Jul 2007 4:43 using AcqMethod test000414.M
Instrument : MSD
Sample Name: MM621
Misc Info :
Vial Number: 1



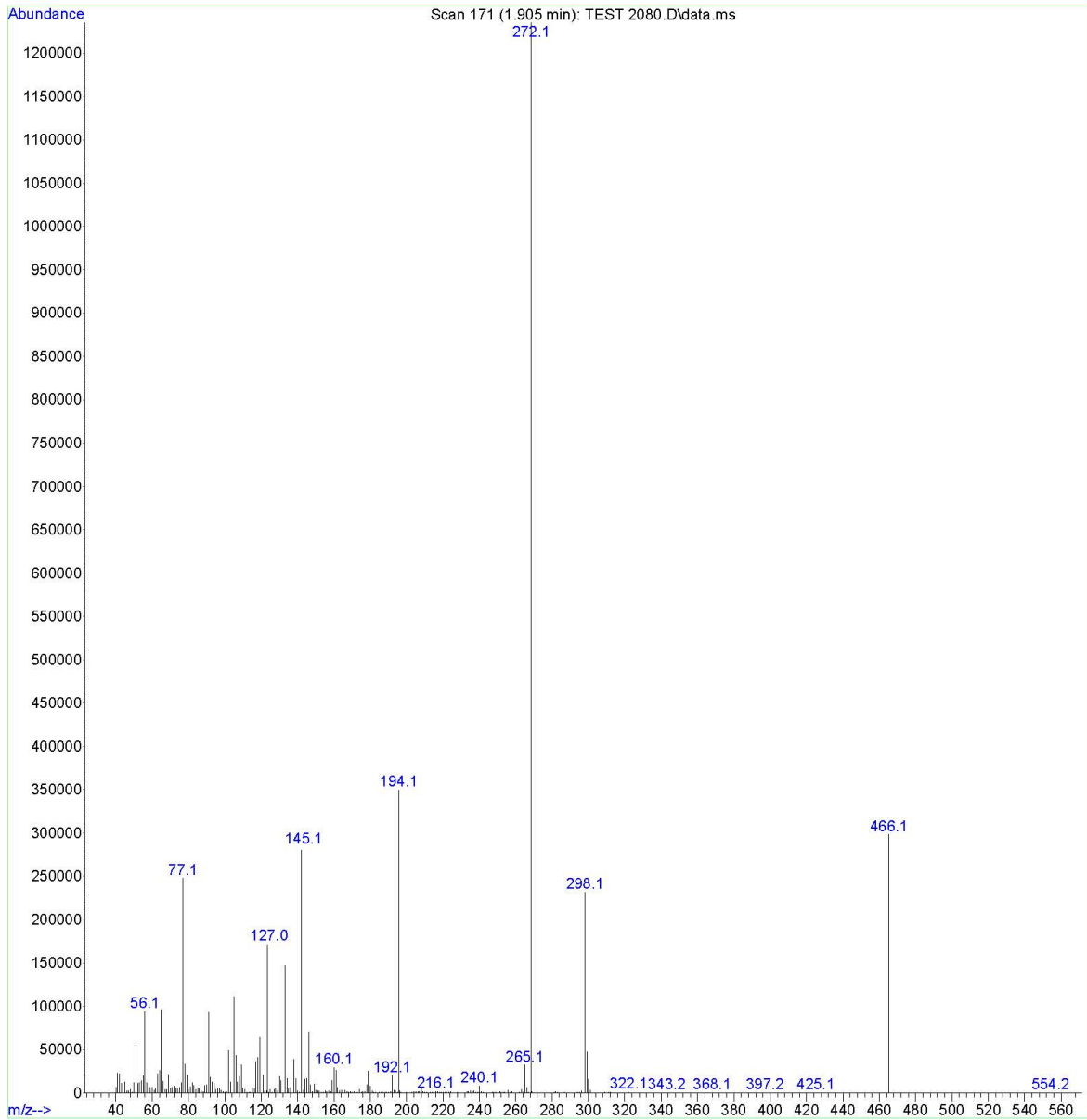
N-(4-Ethylphenyl)-2- $\{$ 3-(4-oxo-3,4-dihydroquinazolin-2-yl)quinolin-2-yl $\}$ thioacetamide (**9e**)



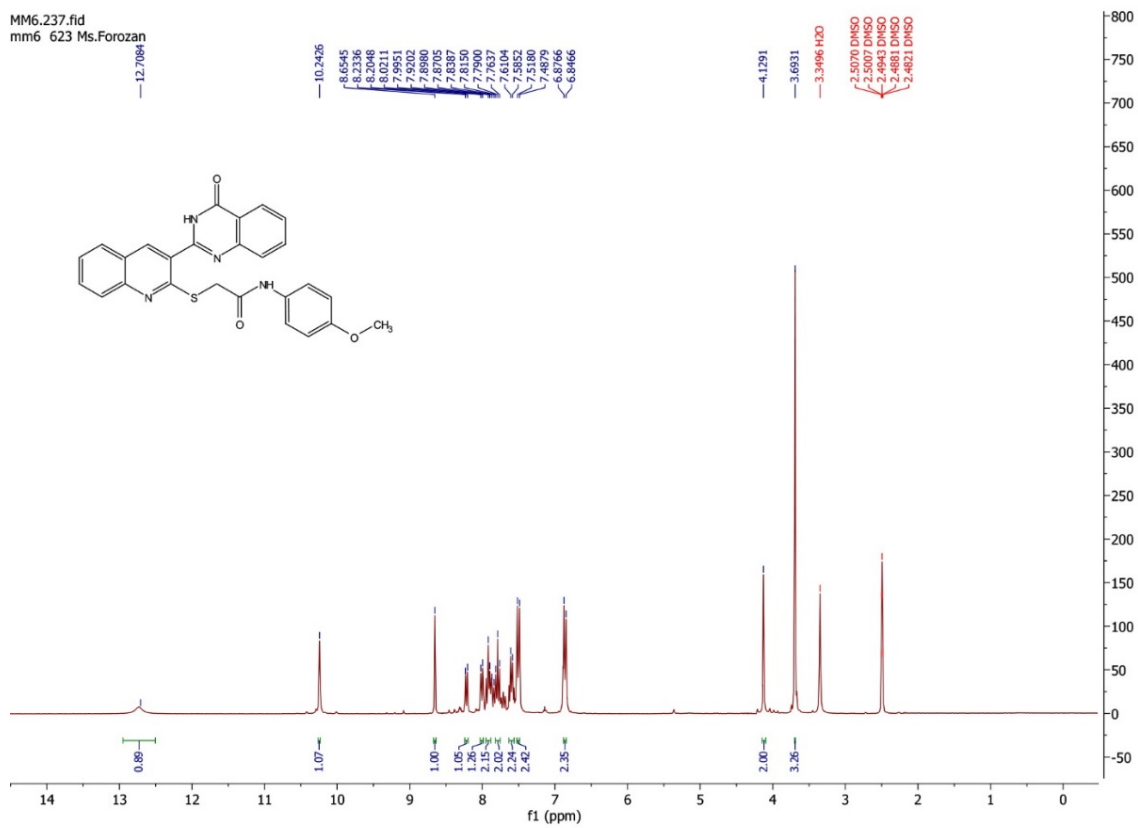
MM6.226.fid
mm6 617 Ms.Forozan



File :C:\MSDCHEM\3\DATA\Snapshot\TEST 2080.D
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Instrument : MSD
Sample Name: MM6 617
Misc Info :
Vial Number: 1

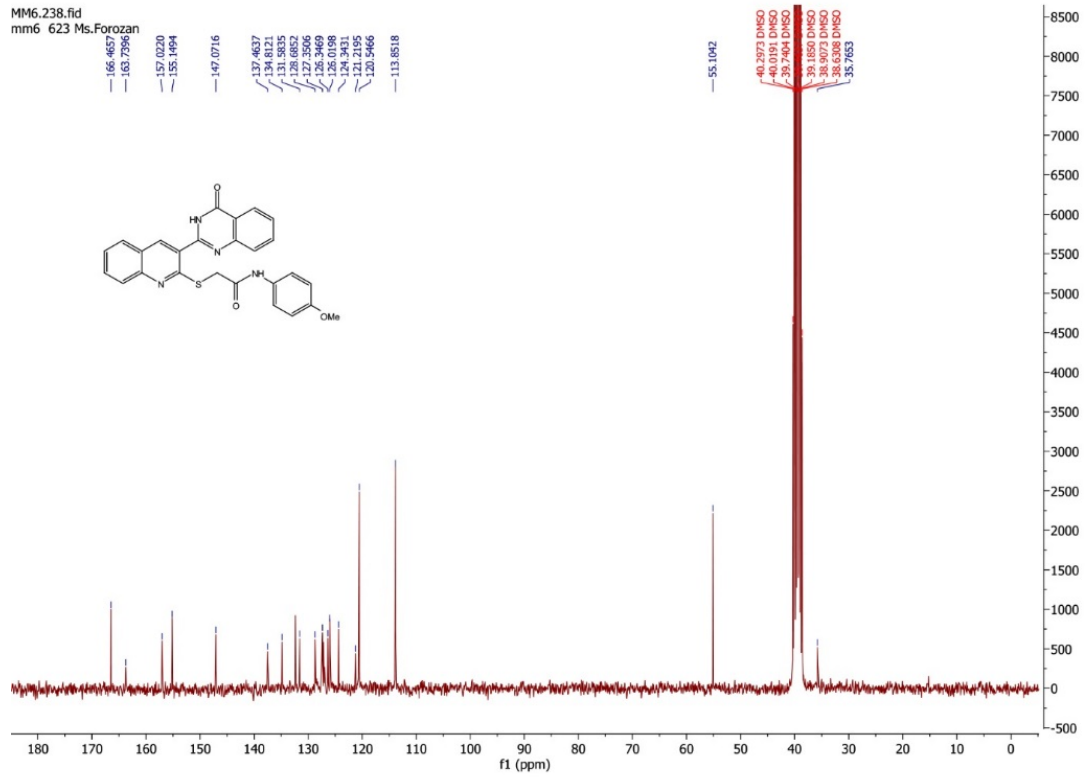
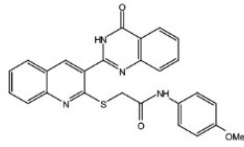


N-(4-Methoxyphenyl)-2- $\{[3-(4\text{-oxo-3,4-dihydroquinazolin-2-yl})\text{quinolin-2-yl}]\text{thio}\}$ acetamide (**9f**)

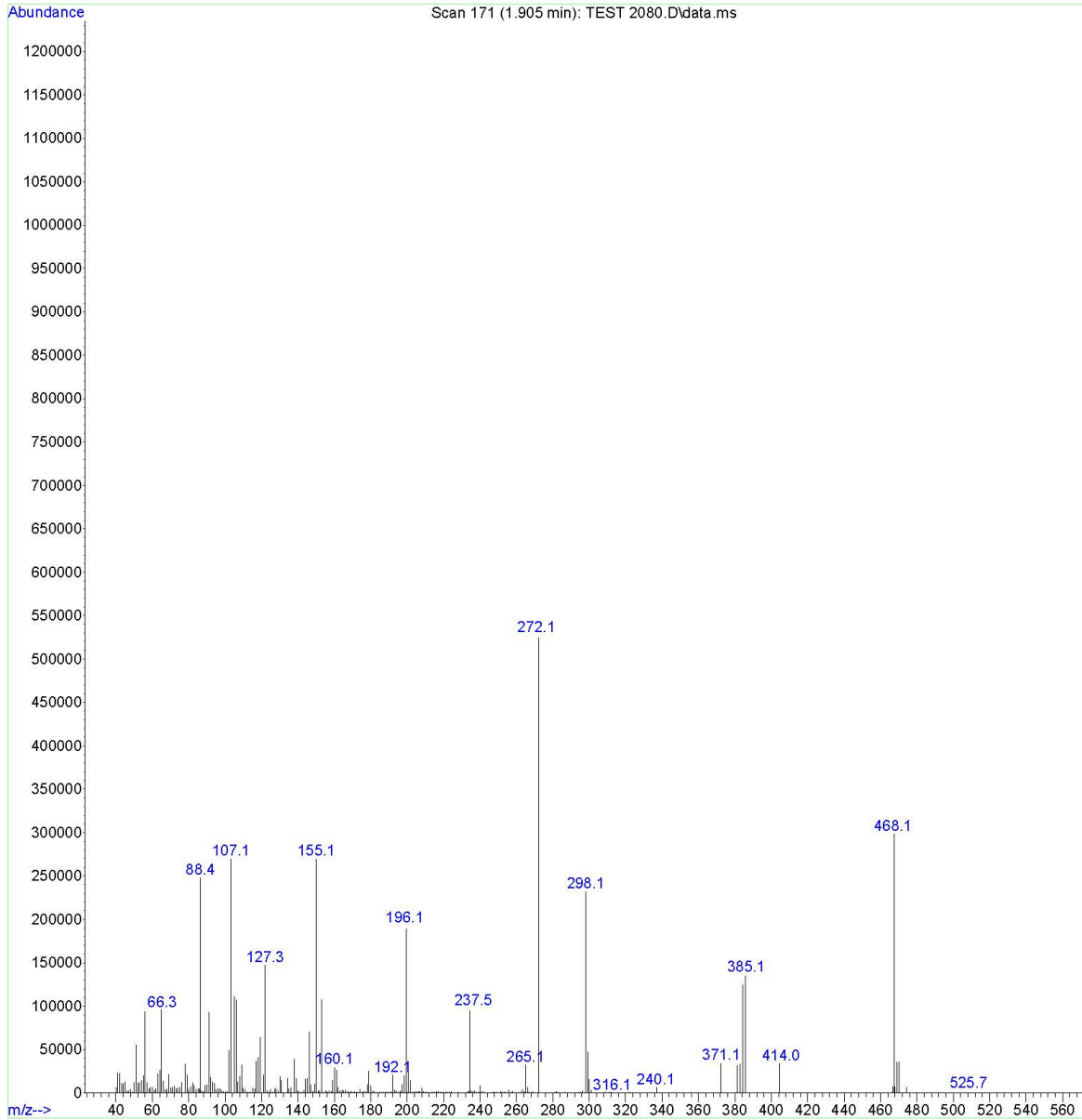


MM6.238.fid
mm6 623 Ms.Forozan

- 166.4657
- 163.7396
- 157.0220
- 155.1494
- 149.0716
- 137.4637
- 134.8121
- 131.5835
- 129.6522
- 127.3266
- 126.3469
- 126.0198
- 124.3431
- 123.4425
- 120.5466
- 113.8518

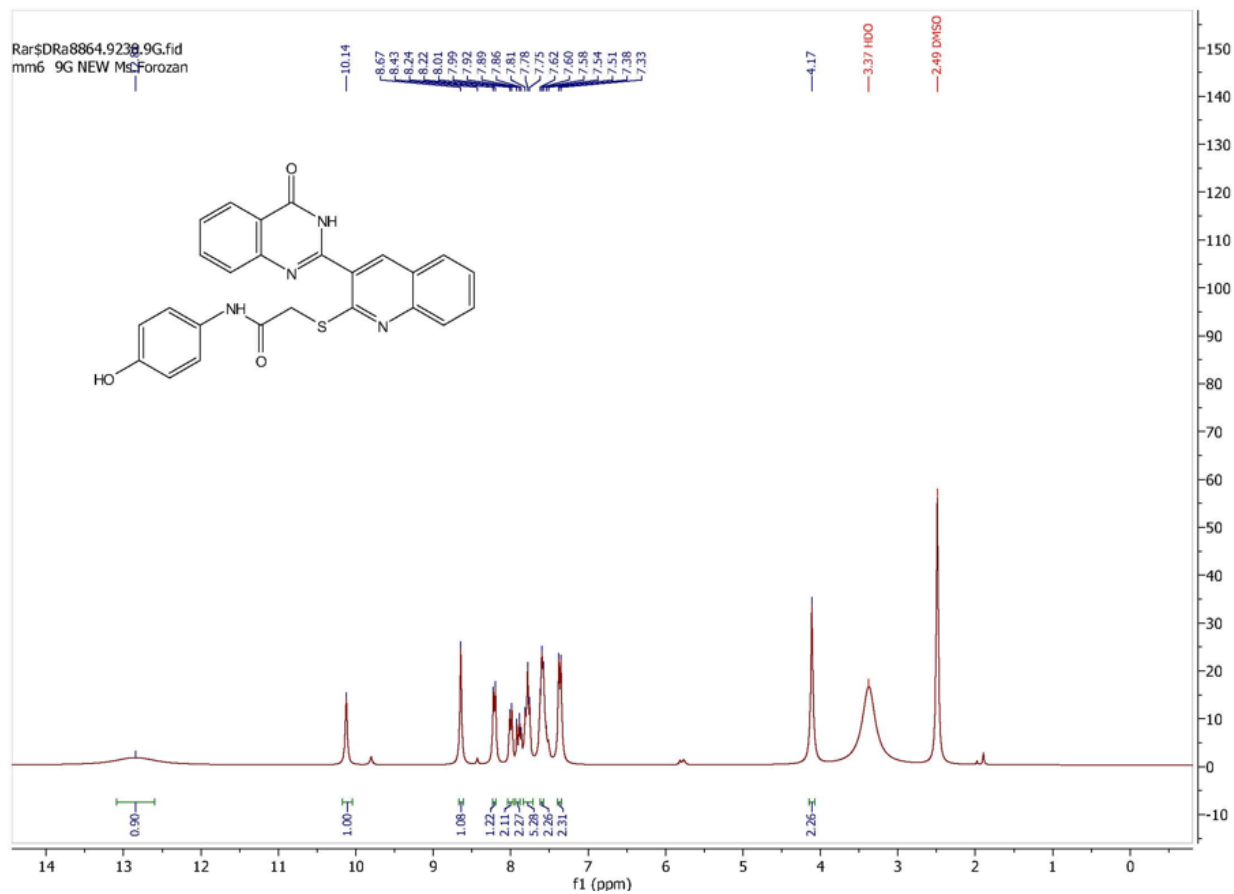


File :C:\MSDCHEM\3\DATA\Snapshot\TEST 2080.D
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Acquired : 22 Jul 2007 1:46 using AcqMethod test000414.M
Instrument : MSD
Sample Name: MM6 623
Misc Info :
Vial Number: 1

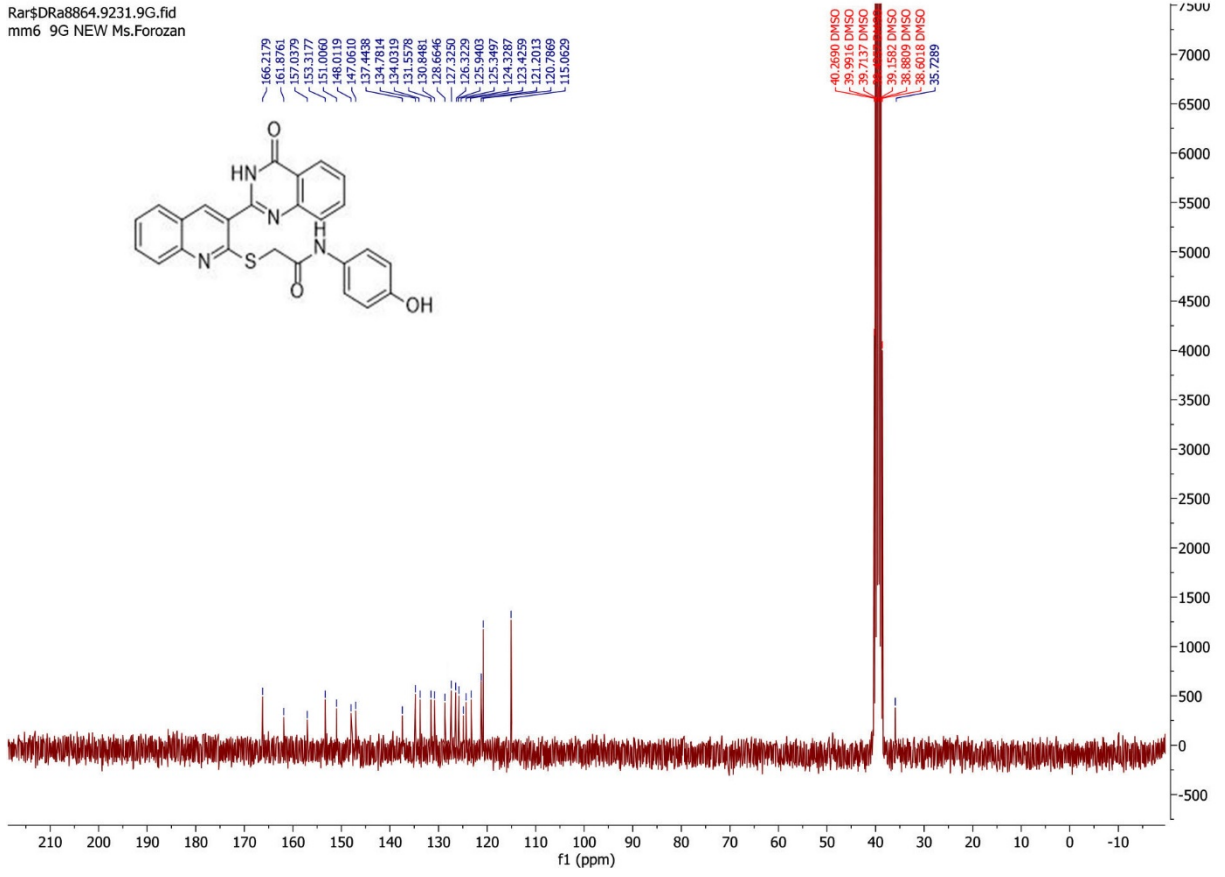


N-(4-Hydroxyphenyl)-2-{[3-(4-oxo-3,4-dihydroquinazolin-2-yl)quinolin-2-yl]thio}acetamide

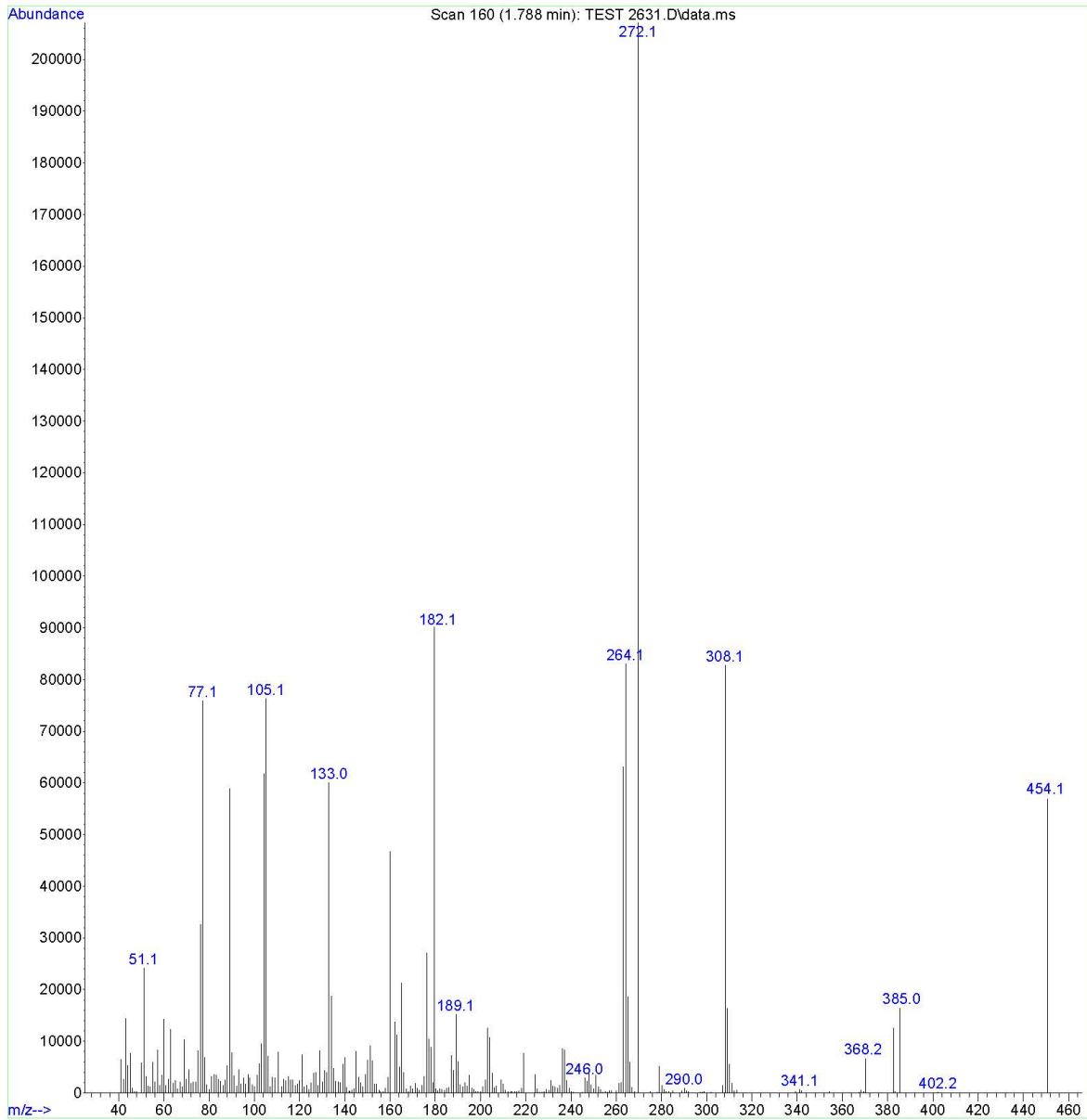
(9g)



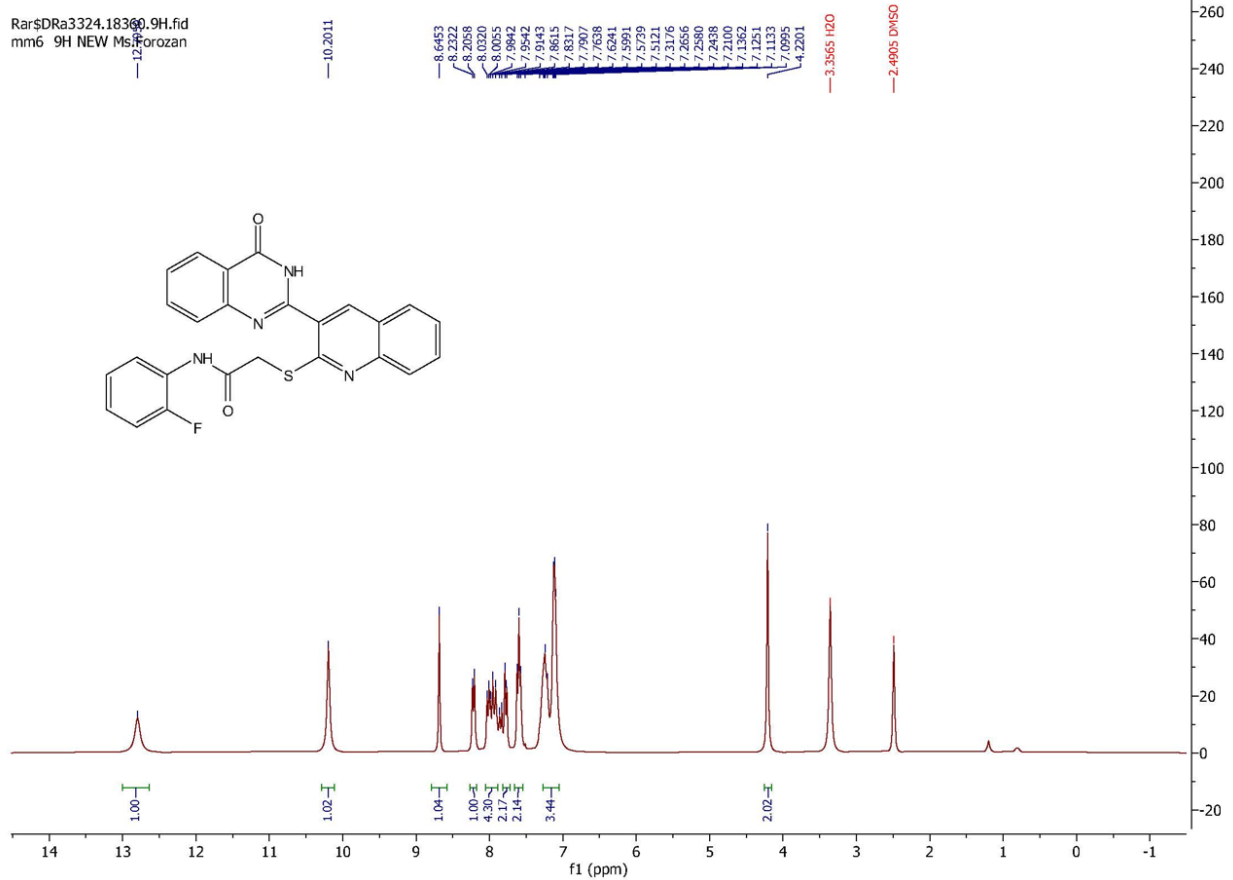
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mm6 9G NEW Ms.Forozan



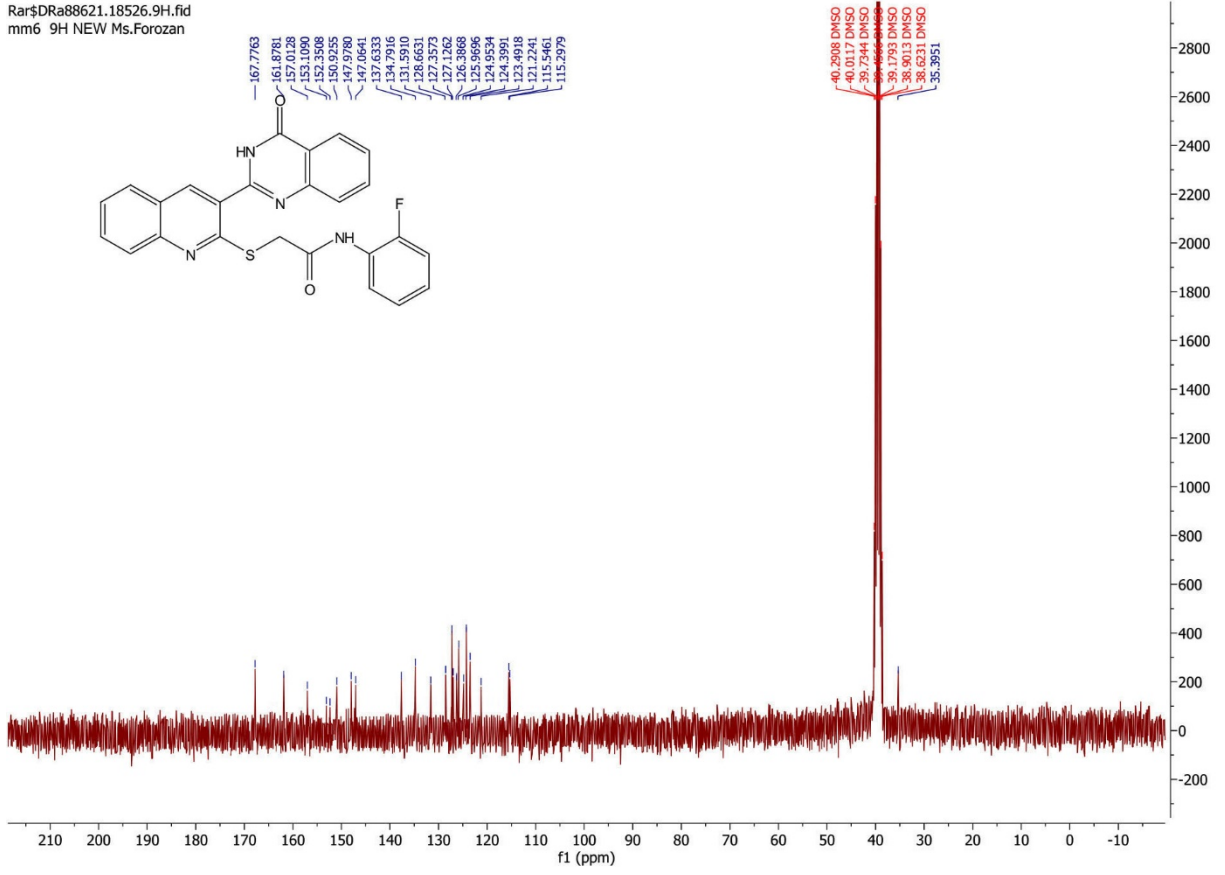
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Operator :
Acquired : 22 Jul 2007 2:46 using AcqMethod test000414.M
Instrument : MSD
Sample Name: MM6 613
Misc Info :
Vial Number: 1



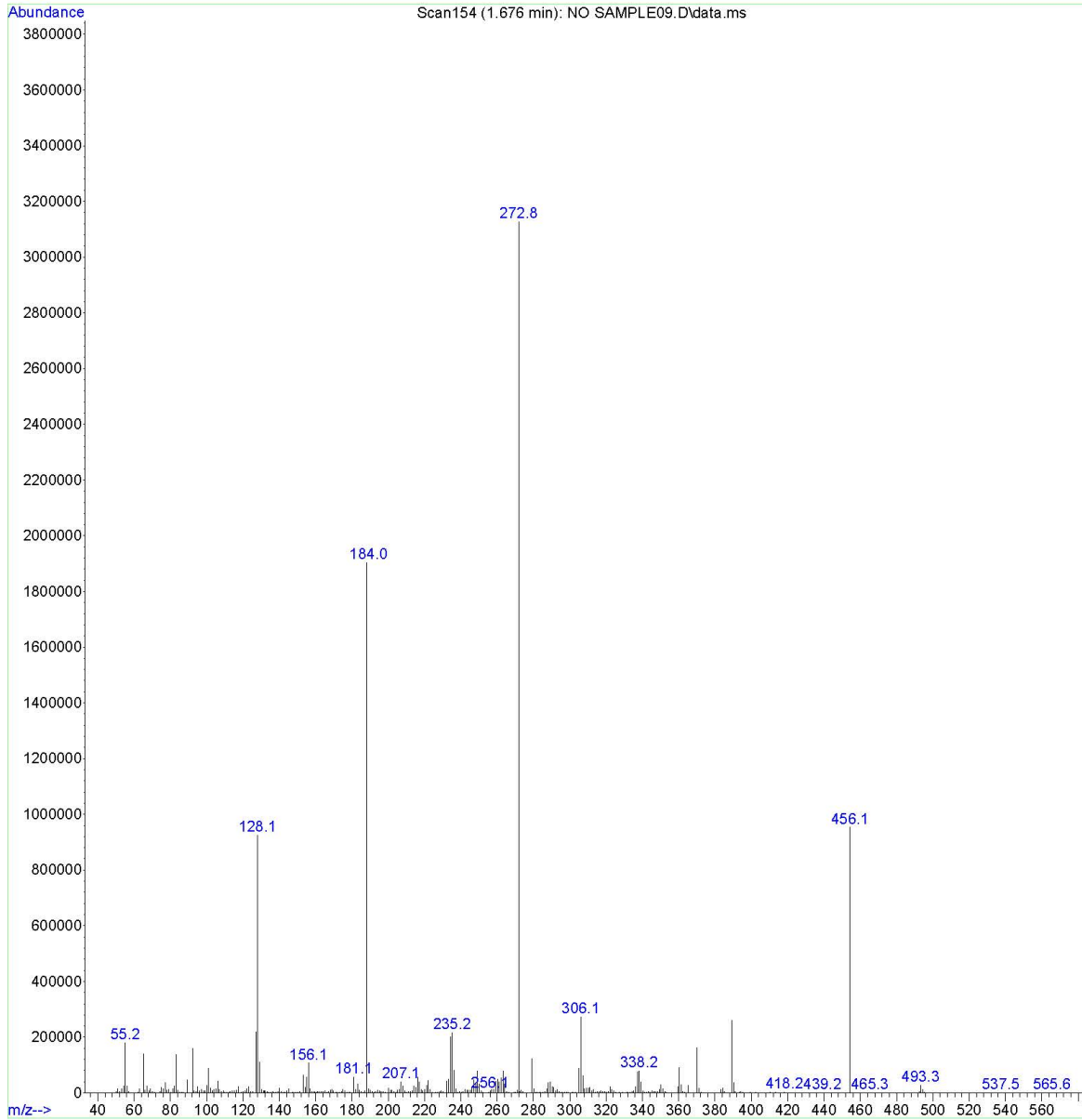
N-(2-Fluorophenyl)-2- $\{[3-(4\text{-oxo-3,4-dihydroquinazolin-2-yl})\text{quinolin-2-yl}]\text{thio}\}$ acetamide (**9h**)



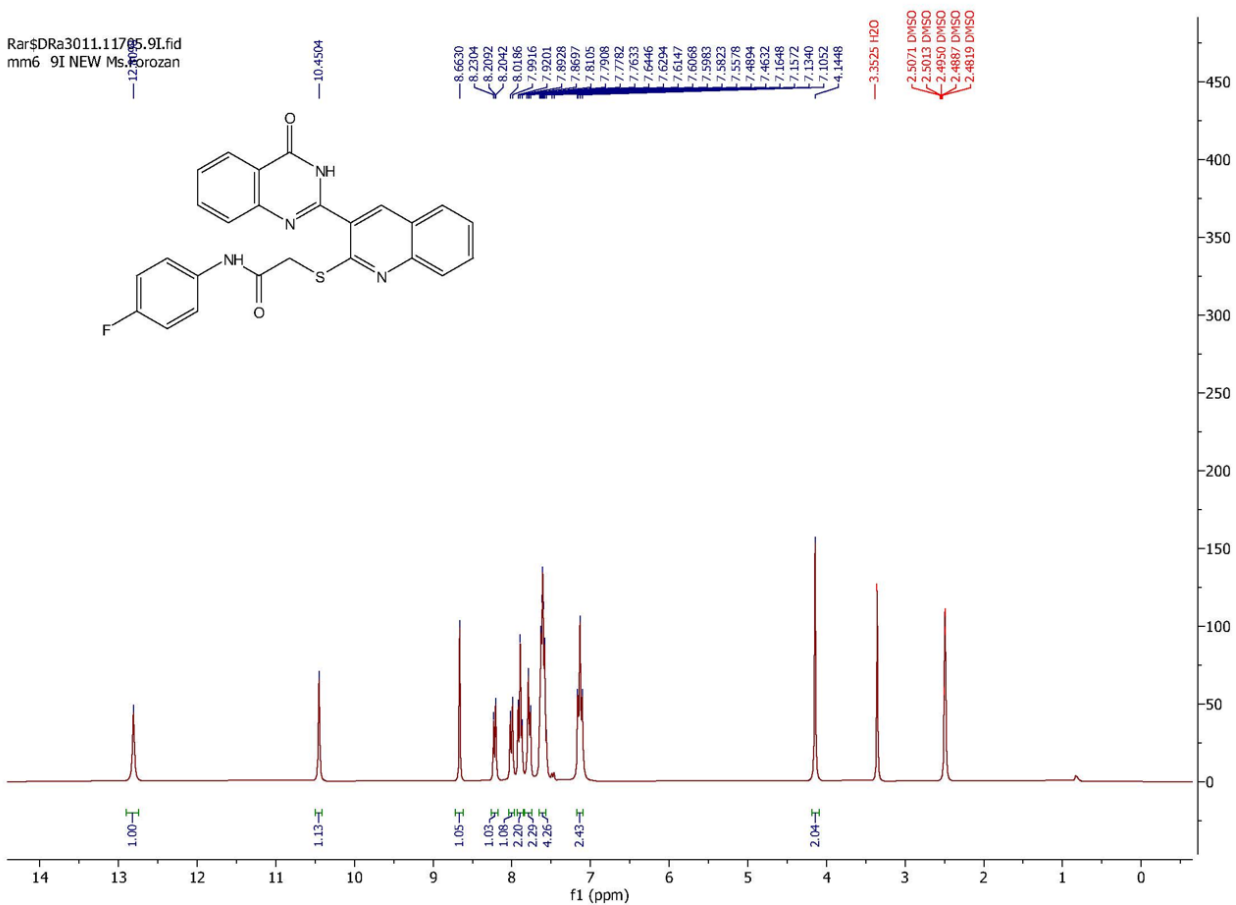
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mm6 9H NEW Ms.Forozan



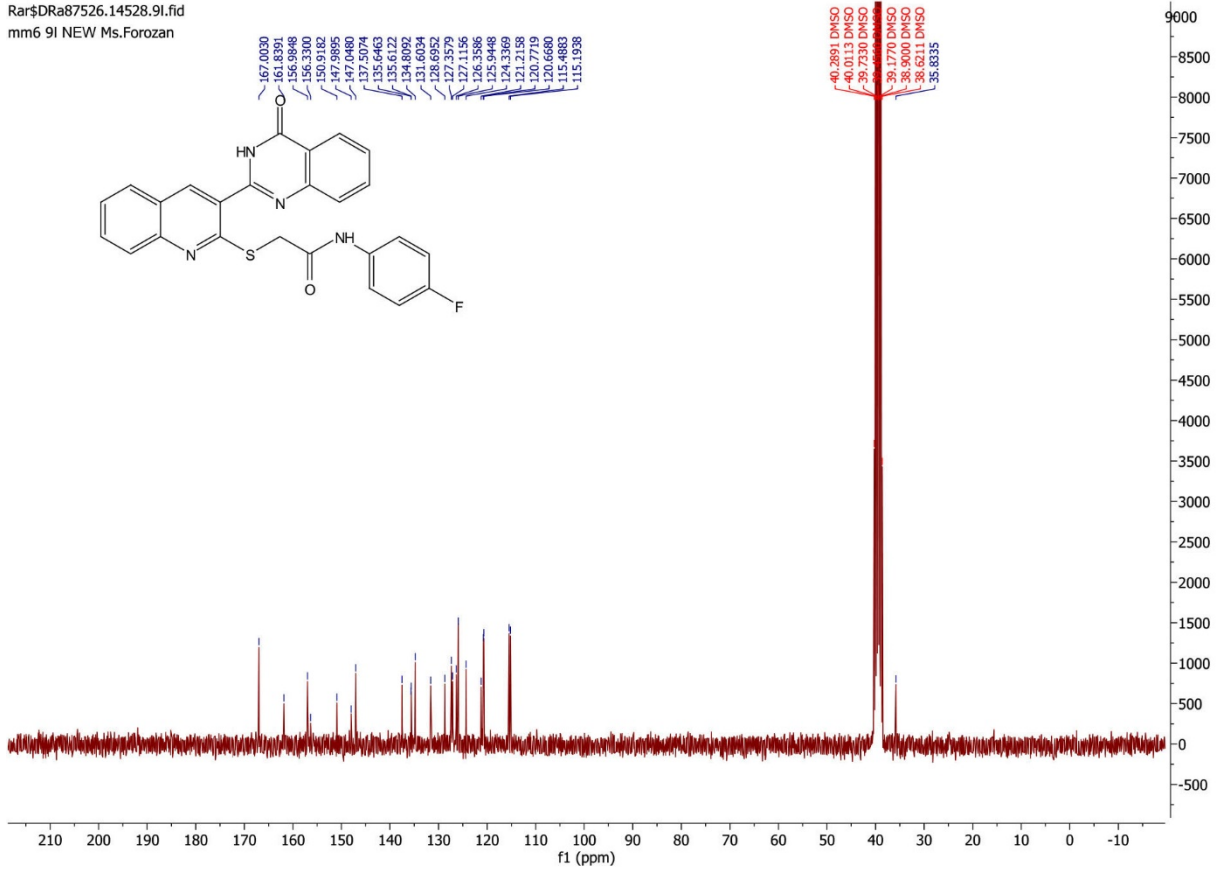
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Instrument : MSD
Sample Name: MM6 612
Misc Info :
Vial Number: 1



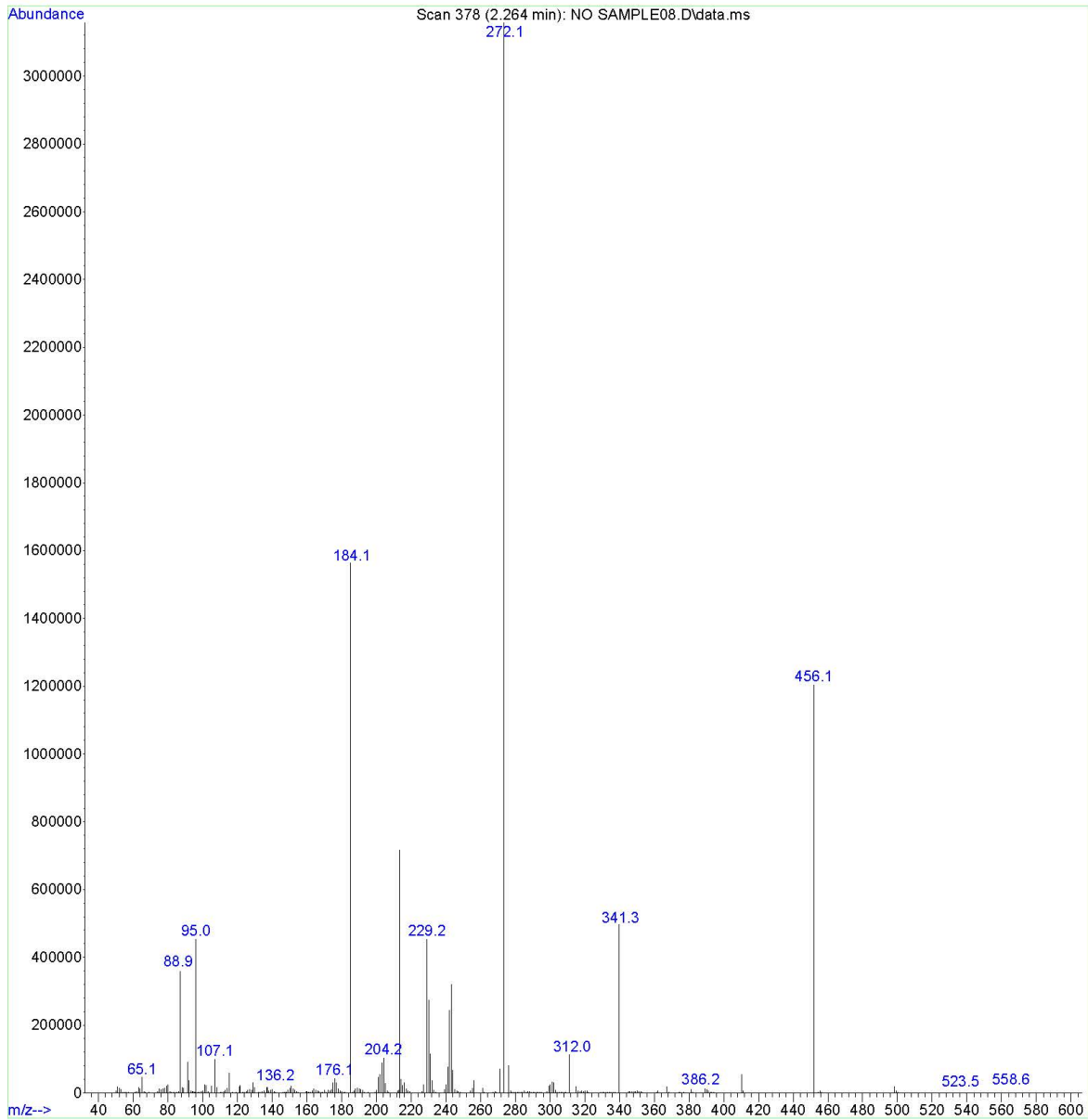
N-(4-Fluorophenyl)-2- $\{[3$ -(4-oxo-3,4-dihydroquinazolin-2-yl)quinolin-2-yl]thio $\}$ acetamide (**9i**)



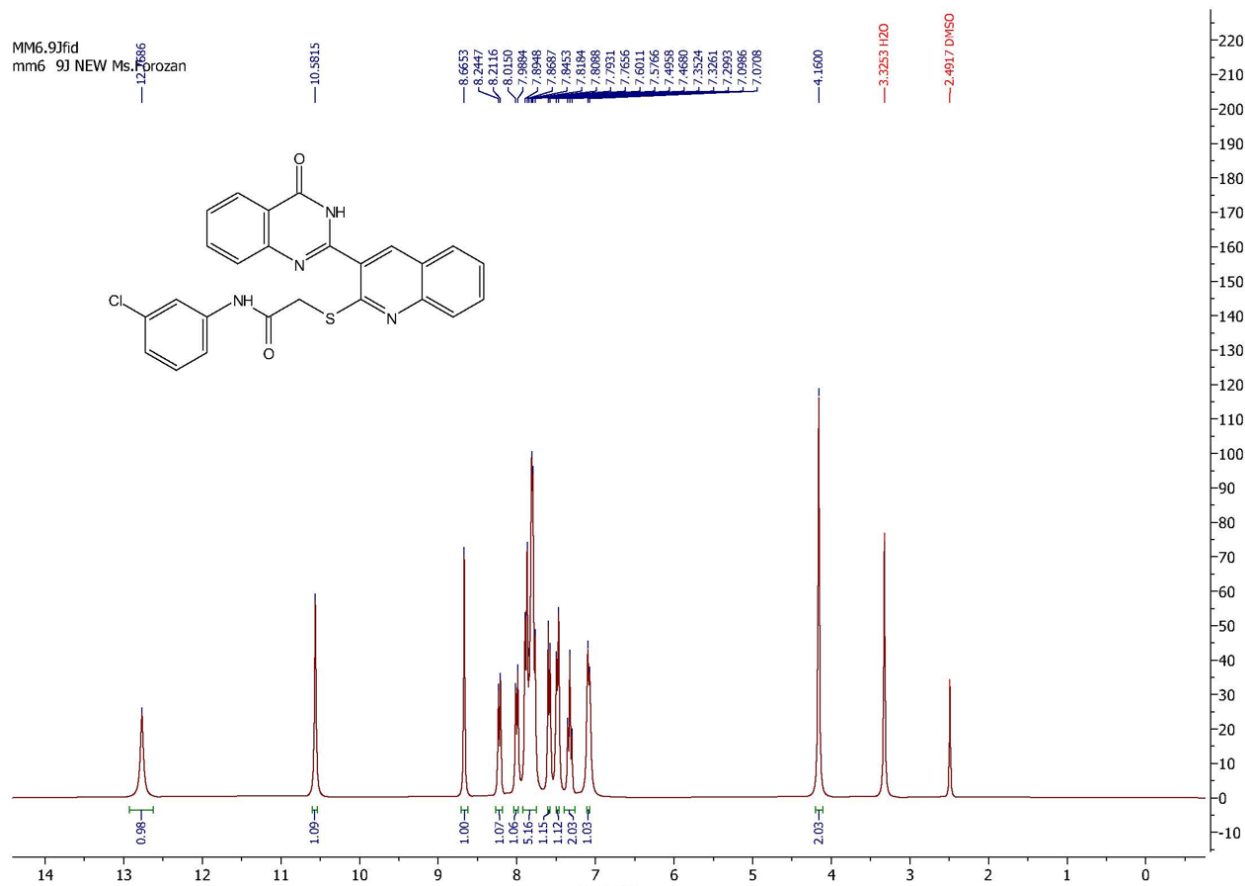
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mm6 9l NEW Ms.Forozan



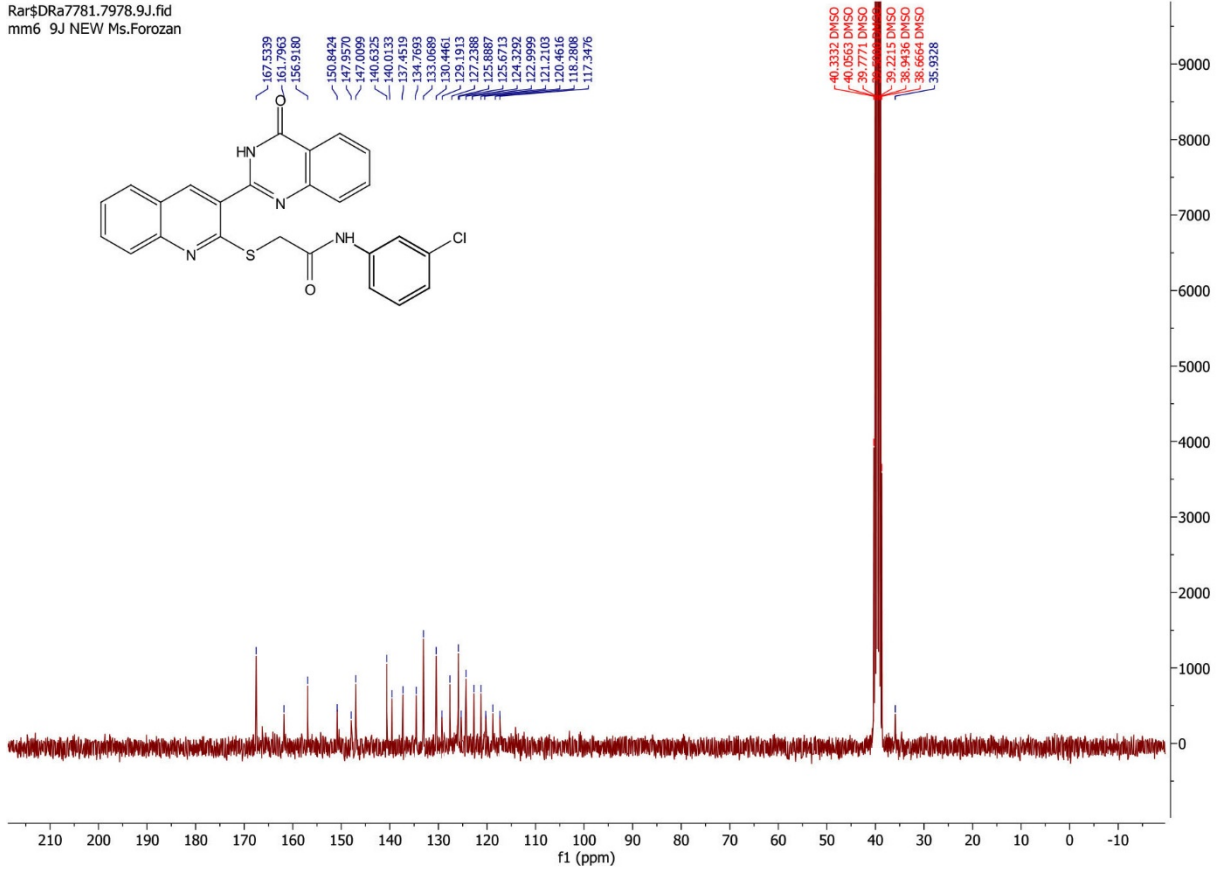
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Operator :
Acquired : 3 Jan 2007 20:41 using AcqMethod f1.M
Instrument : MSD
Sample Name: MM6 618
Misc Info :
Vial Number: 1



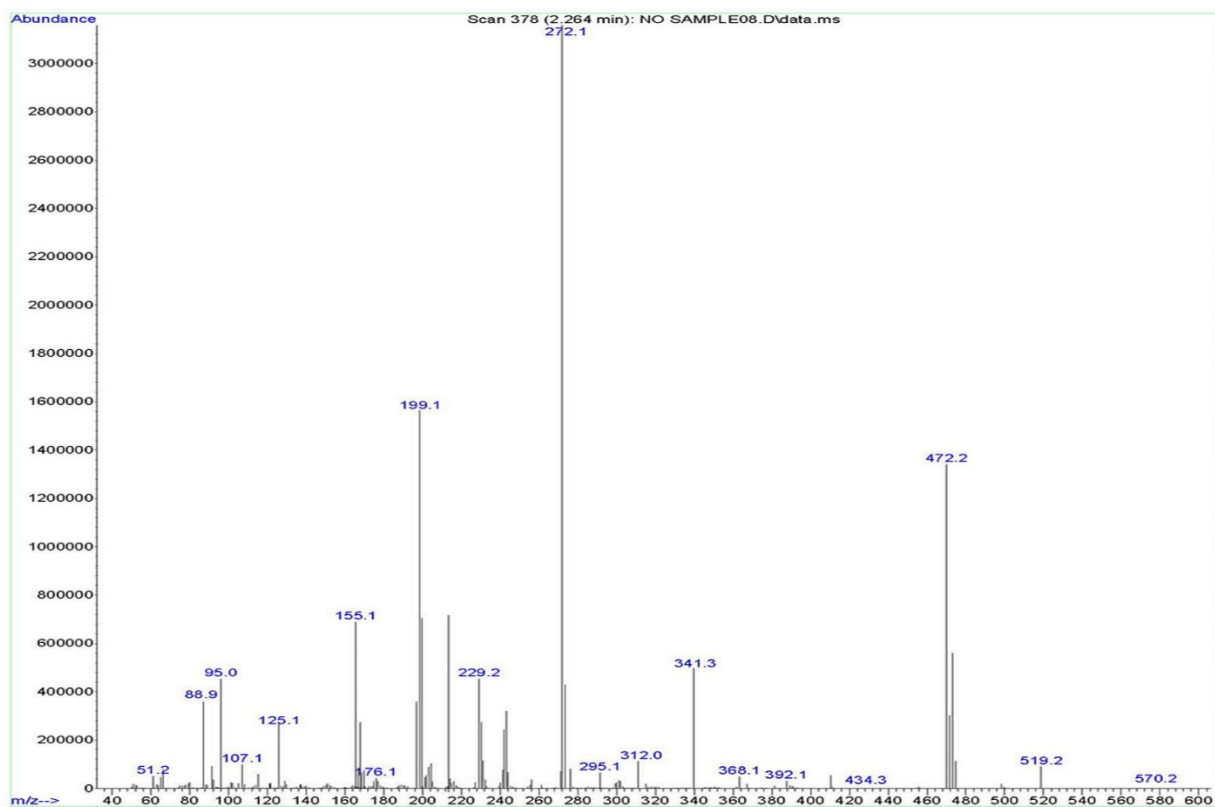
N-(3-Chlorophenyl)-2- $\{[3-(4\text{-oxo-3,4-dihydroquinazolin-2-yl})\text{quinolin-2-yl}]\text{thio}\}$ acetamide (**9j**)



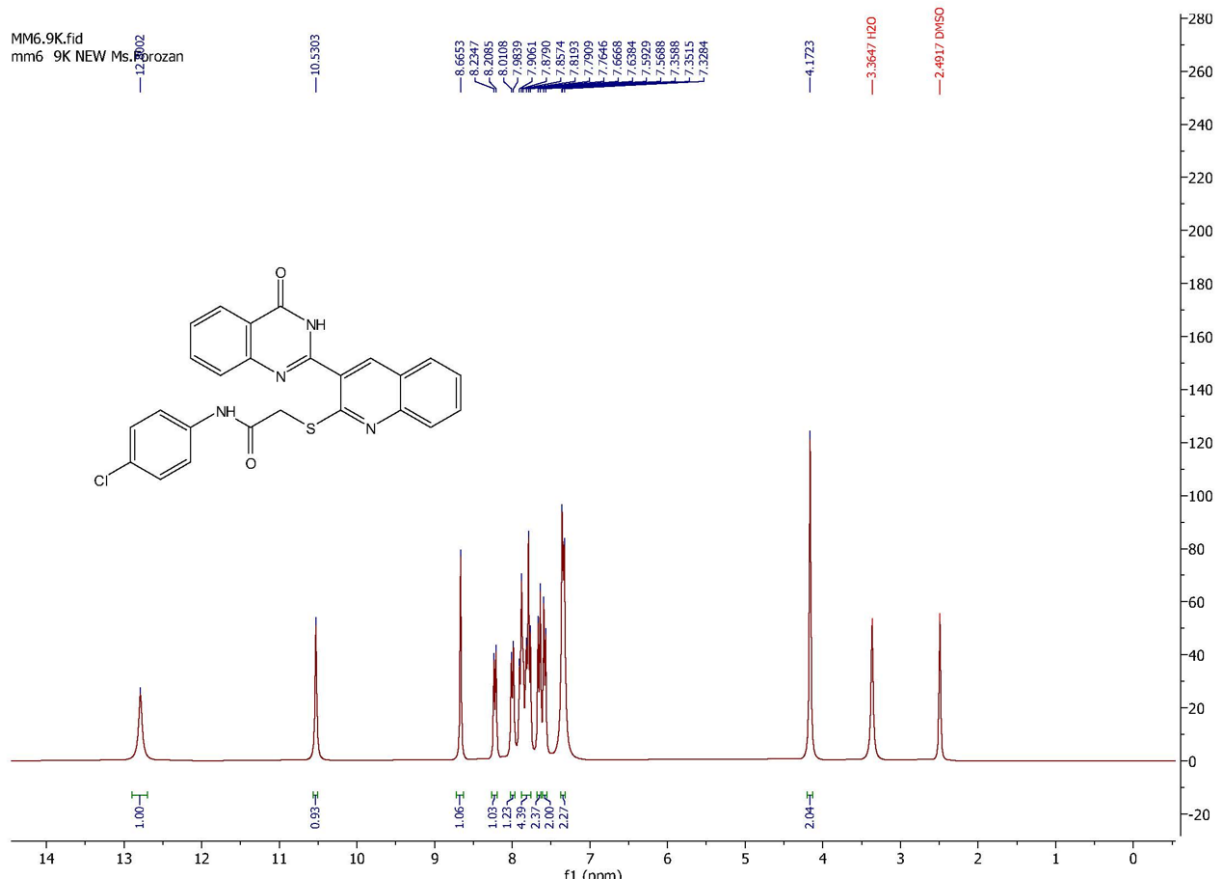
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mm6 9J NEW Ms.Forozan



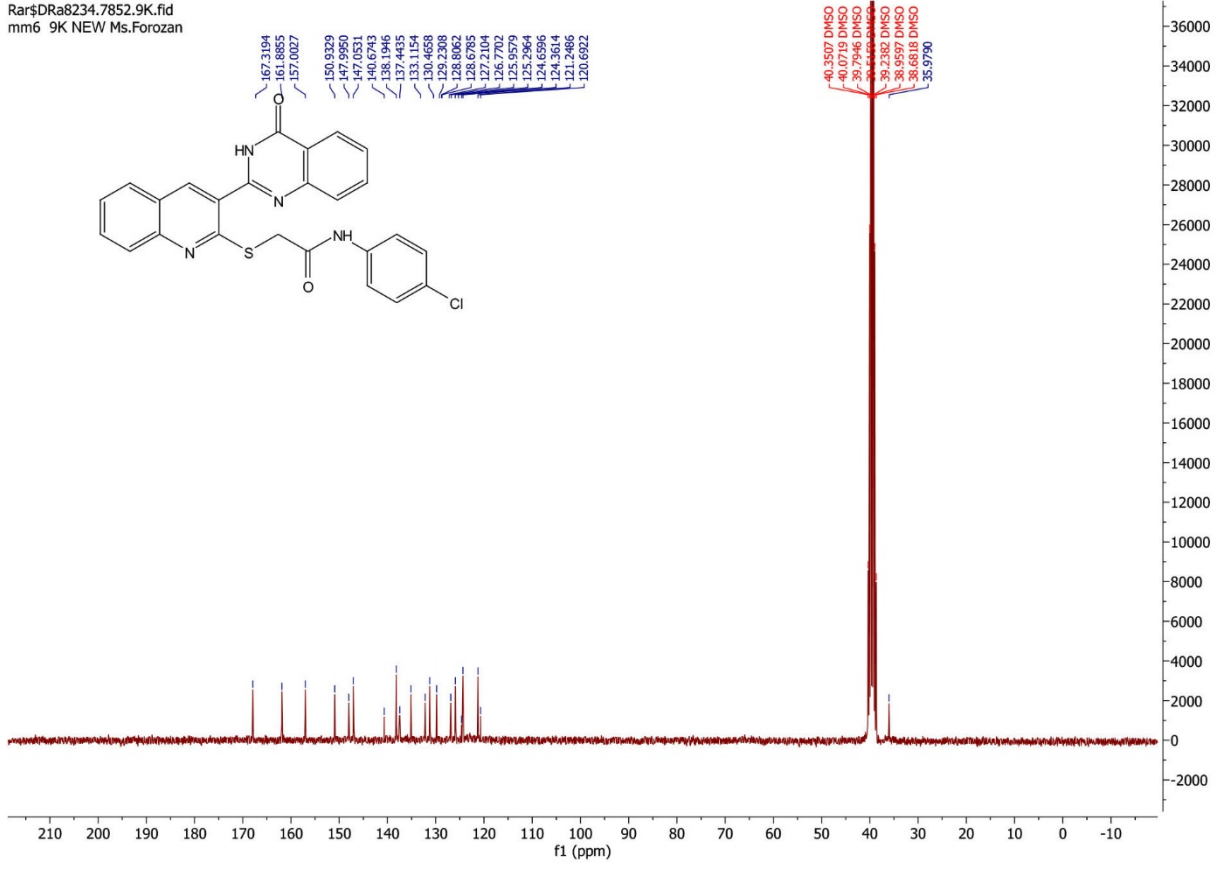
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Operator :
Acquired : 3 Jan 2007 20:41 using AcqMethod f1.M
Instrument : MSD
Sample Name: MM6 606
Misc Info :
Vial Number: 1



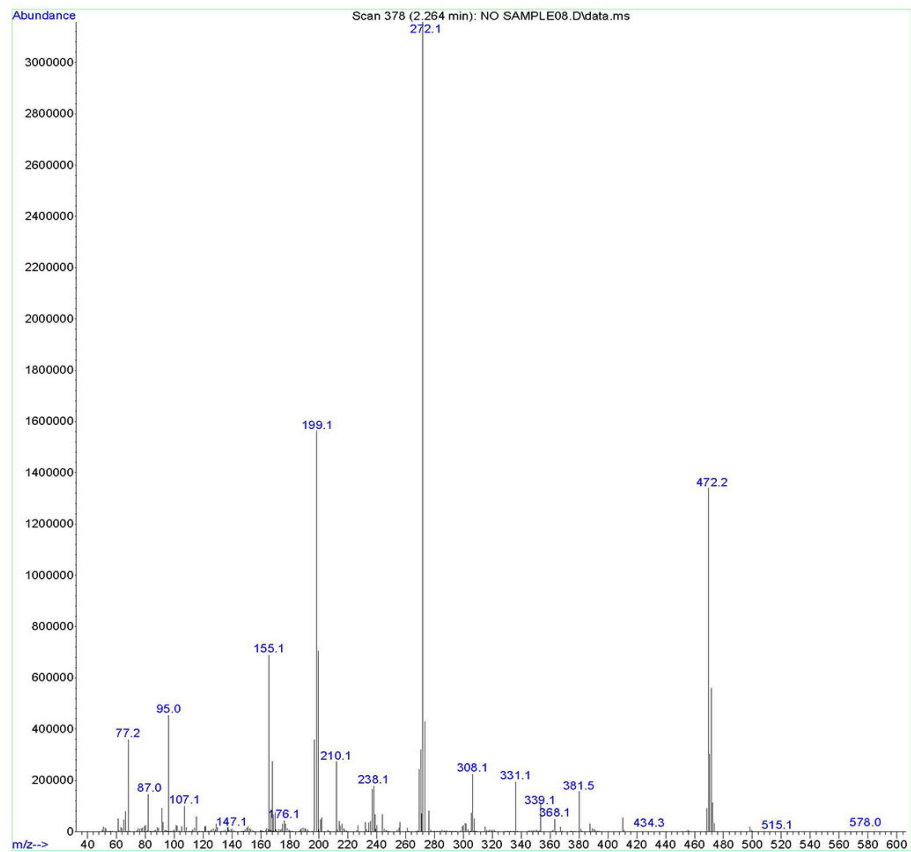
N-(4-Chlorophenyl)-2- $\{[3-(4\text{-oxo-3,4-dihydroquinazolin-2-yl})\text{quinolin-2-yl}] \text{thio}\}$ acetamide
(9k)



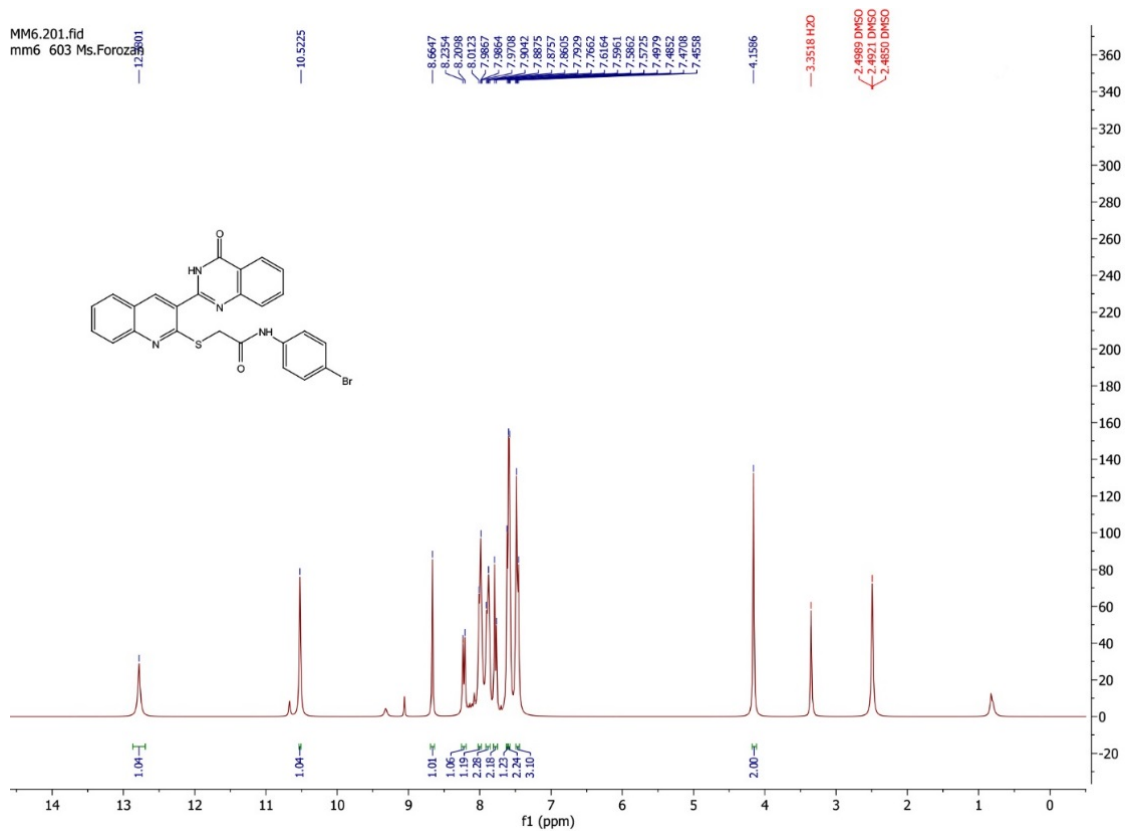
RarşDRa8234.7852.9K.fid
mm6 9K NEW Ms.Forozan



File :C:\MSDCHEM\3\DATA\Snapsho\NO SAMPLE08.D
Operator :
Acquired : 3 Jan 2007 20:41 using AcqMethod f1.M
Instrument : MSD
Sample Name: MM6 602
Misc Info :
Vial Number: 1

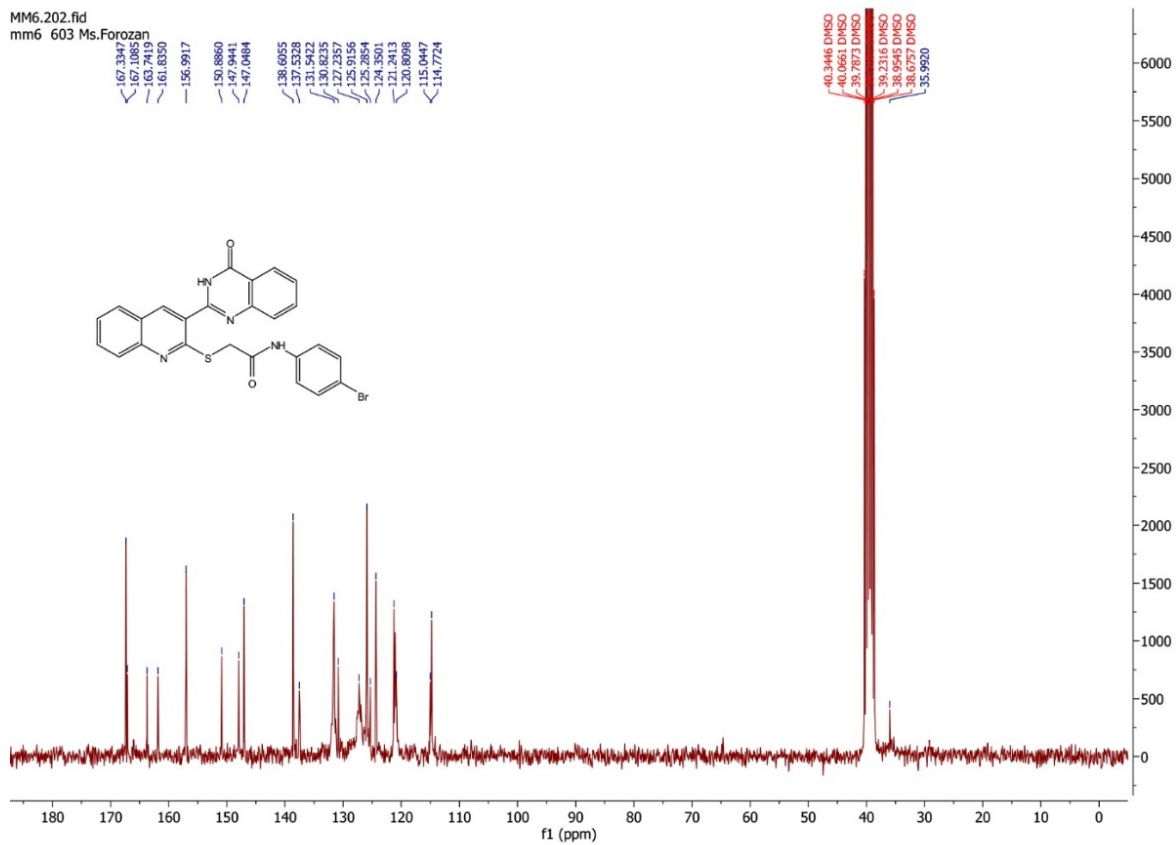
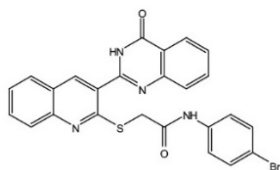


N-(4-Bromophenyl)-2- $\{[3-(4\text{-oxo-3,4-dihydroquinazolin-2-yl})\text{quinolin-2-yl}]\text{thio}\}$ acetamide (**91**)

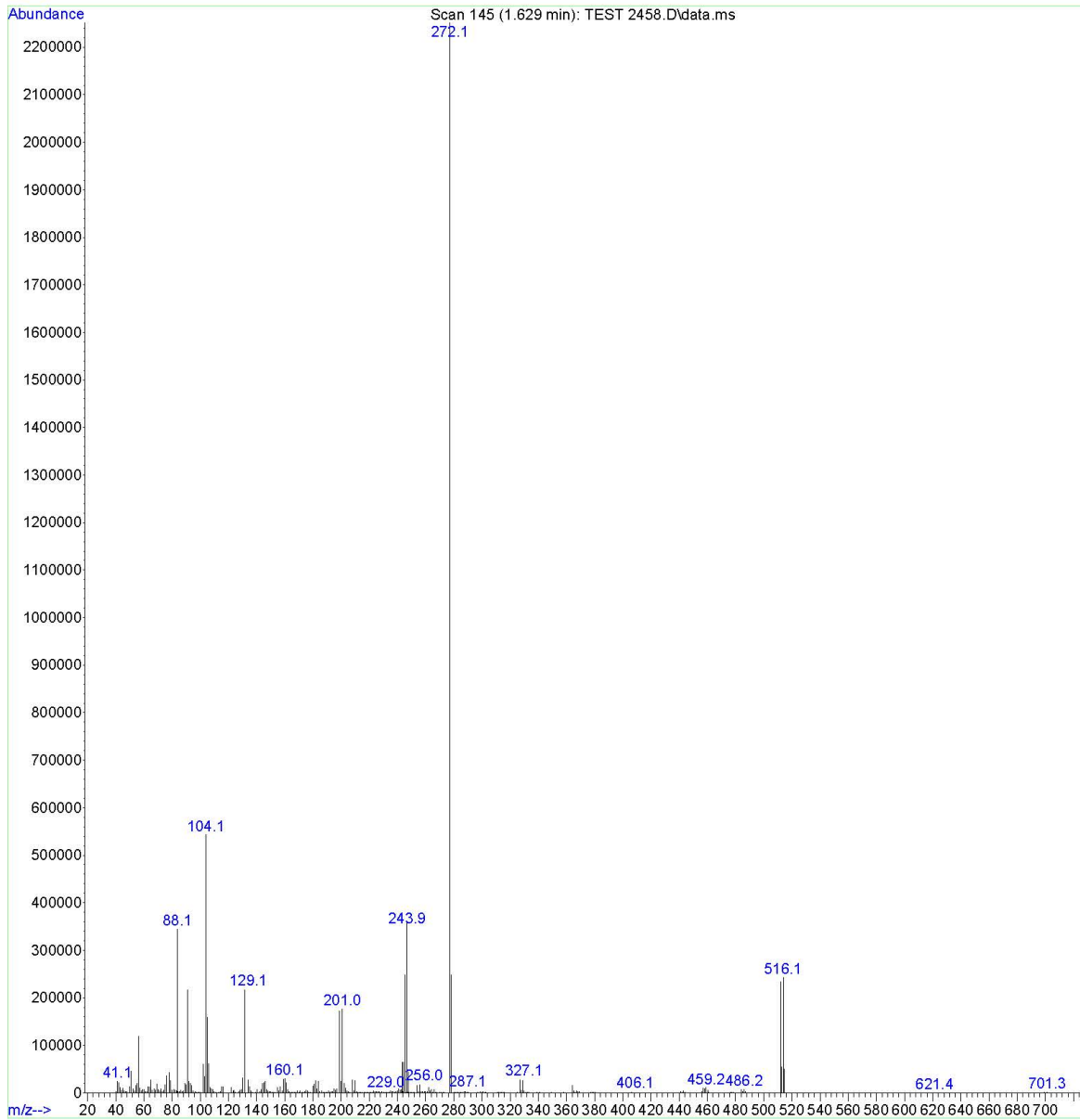


MM6.202.fid
mm6 603 Ms.Forozan

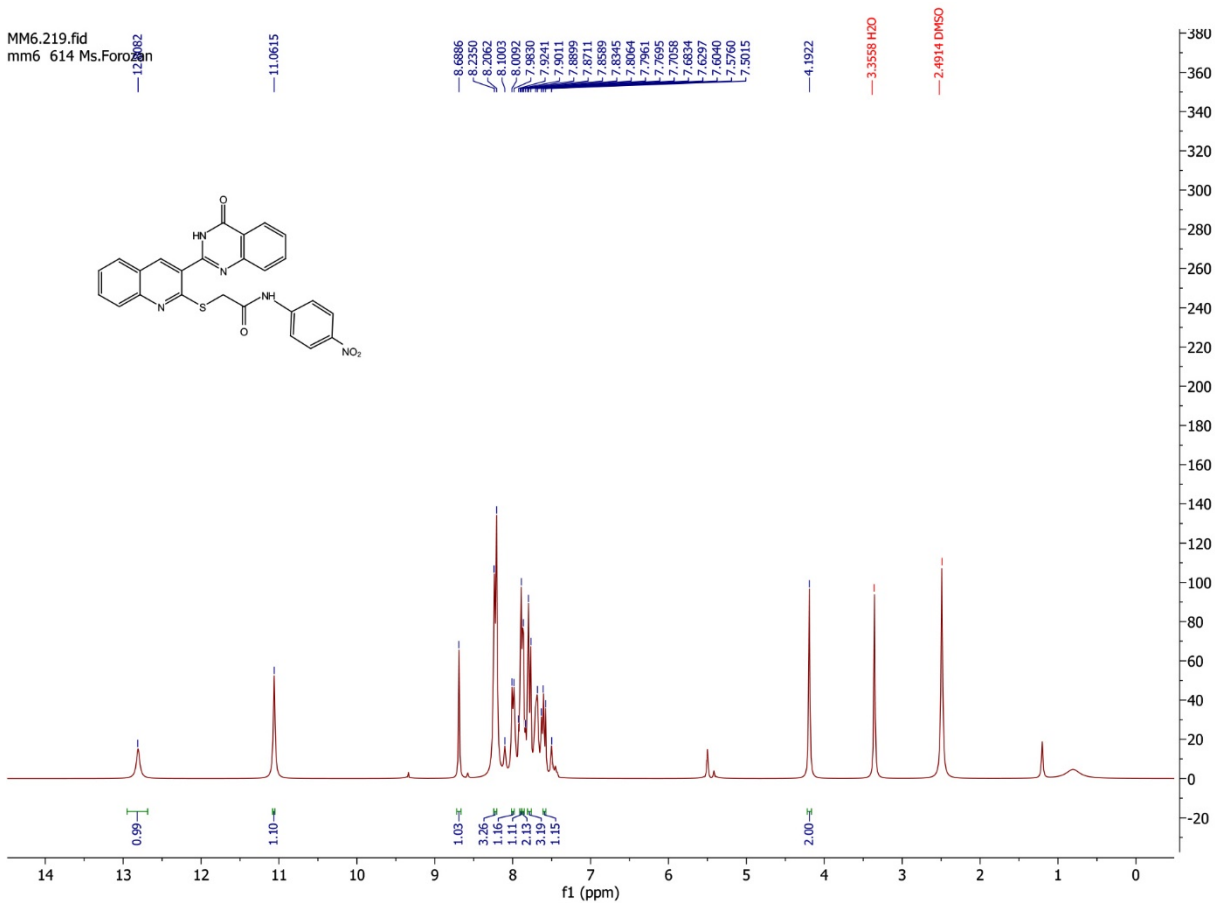
167.3347
167.1085
167.1119
161.8330
156.9917
150.8860
147.9441
147.0484
138.6055
137.5328
131.9422
129.8152
127.2857
125.9156
125.2854
124.3501
121.2413
120.8098
115.0447
114.7724



File :C:\MSDCHEM\3\DATA\Snapshot\TEST 2458.D
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Instrument : MSD
Sample Name: MM6 603
Misc Info :
Vial Number: 1

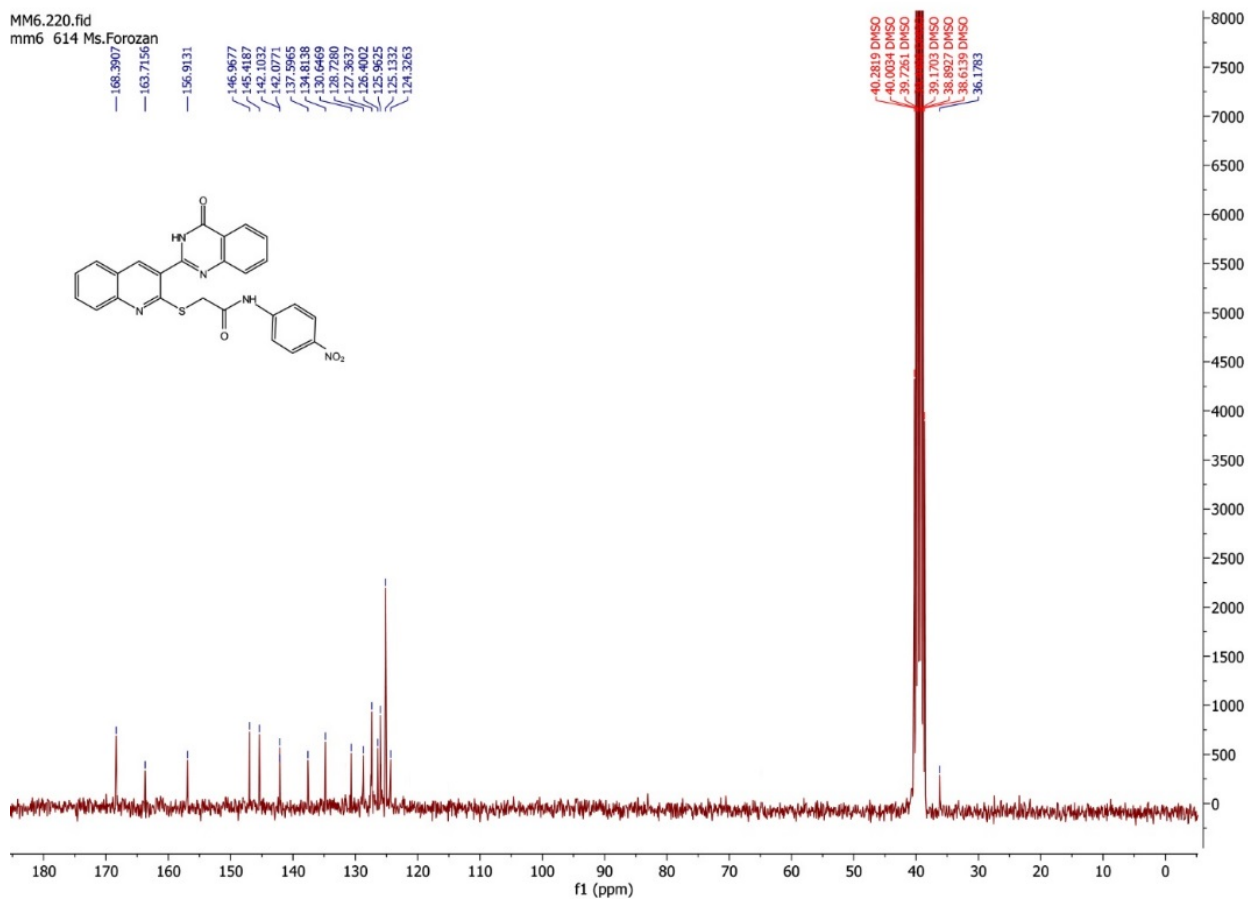
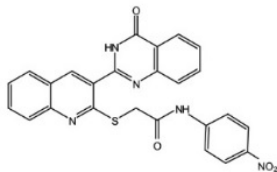


N-(4-Nitrophenyl)-2- $\{$ 3-(4-oxo-3,4-dihydroquinazolin-2-yl)quinolin-2-yl $\}$ thioacetamide (**9m**)

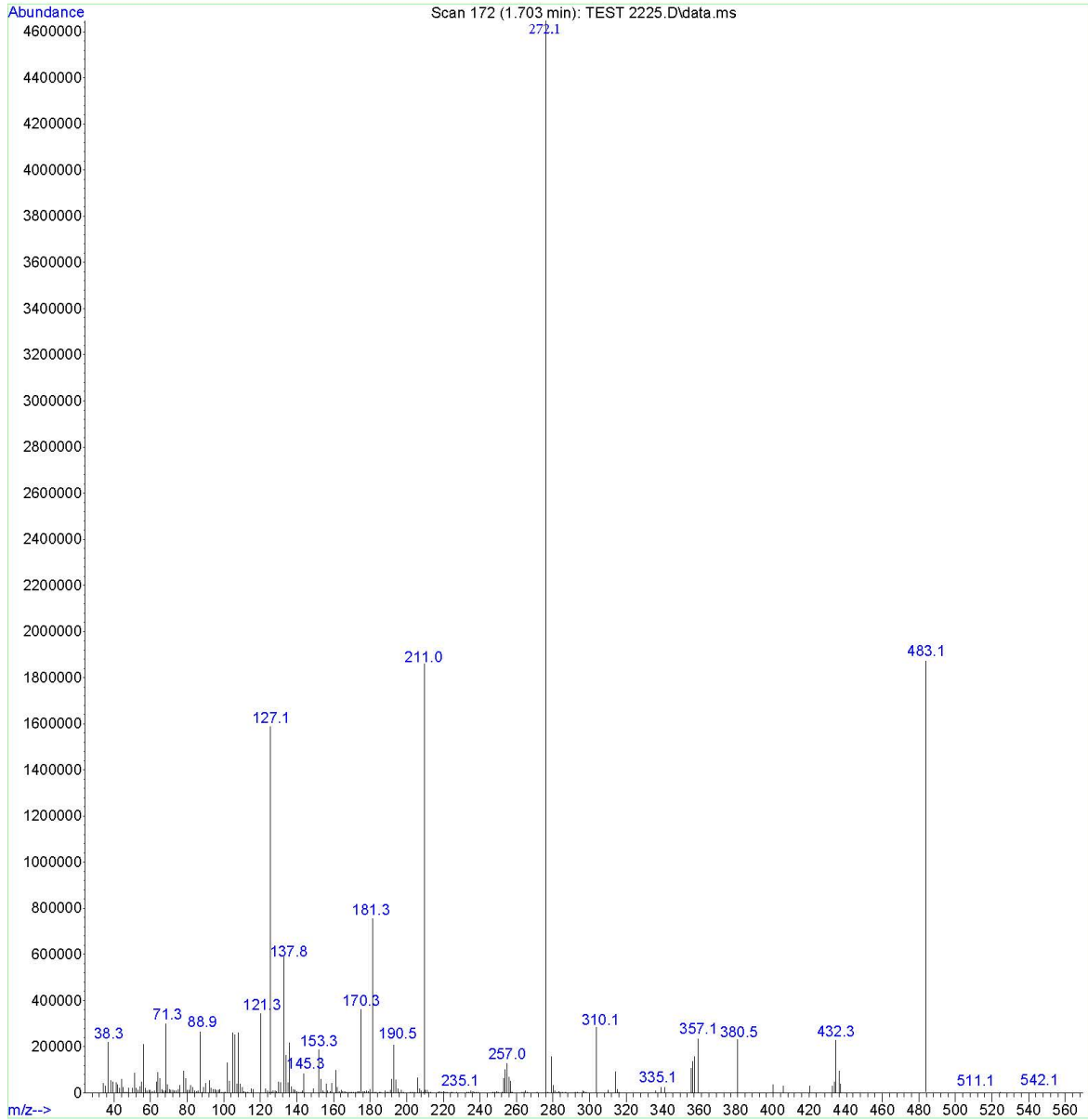


MM6.220.fid
mm6 614 Ms.Forozan

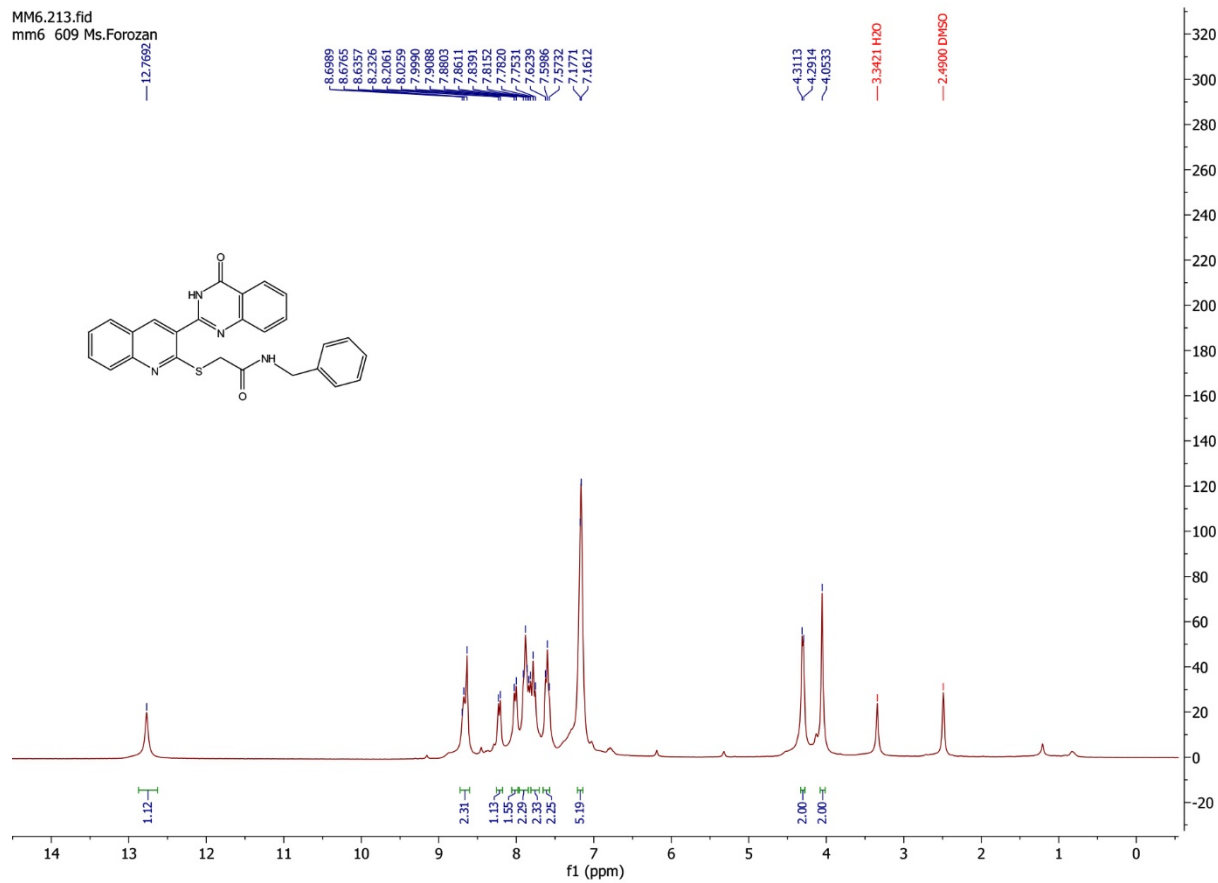
- 168.3907
- 163.7156
- 156.9131
- 146.9577
- 145.4937
- 142.1032
- 142.0771
- 137.5965
- 134.8138
- 130.6469
- 128.7280
- 127.3637
- 126.4002
- 125.9625
- 125.1332
- 124.2663



File :C:\MSDCHEM\3\DATA\Snapshot\TEST 2225.D
Operator :
Acquired : 28 Jul 2007 7:43 using AcqMethod test000414.M
Instrument : MSD
Sample Name: MM6 614
Misc Info :
Vial Number: 1

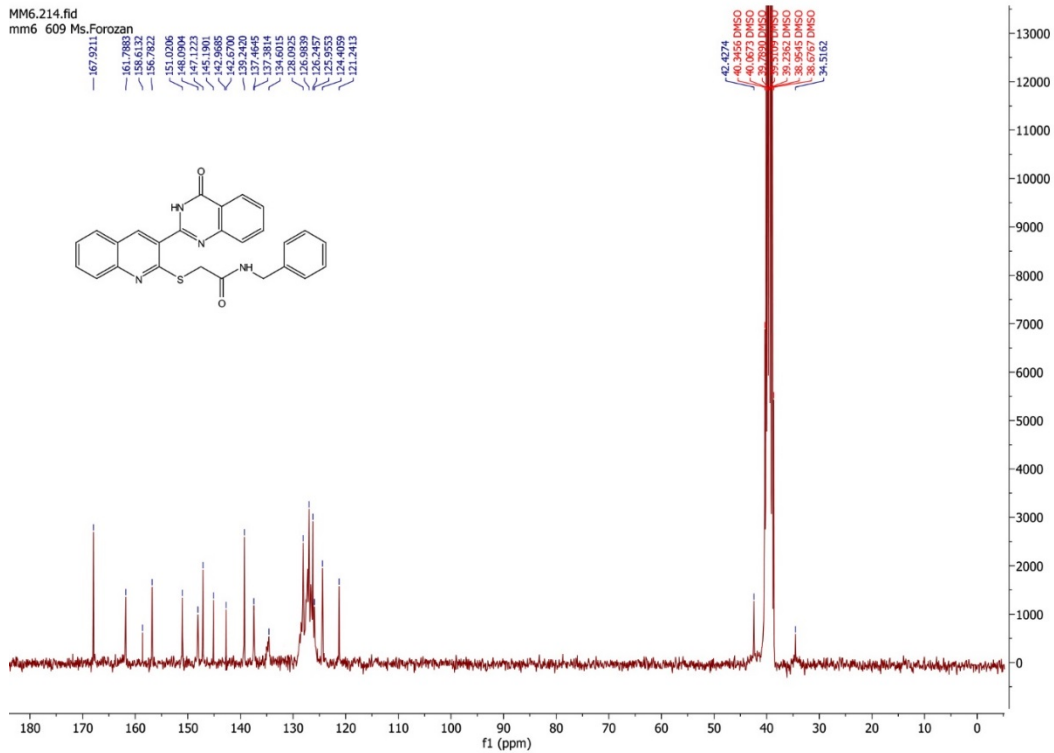
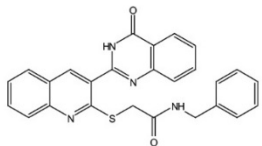


N-Benzyl-2- $\{[3-(4\text{-oxo-}3,4\text{-dihydroquinazolin-}2\text{-yl)quinolin-}2\text{-yl]thio}\}$ acetamide (**9n**)

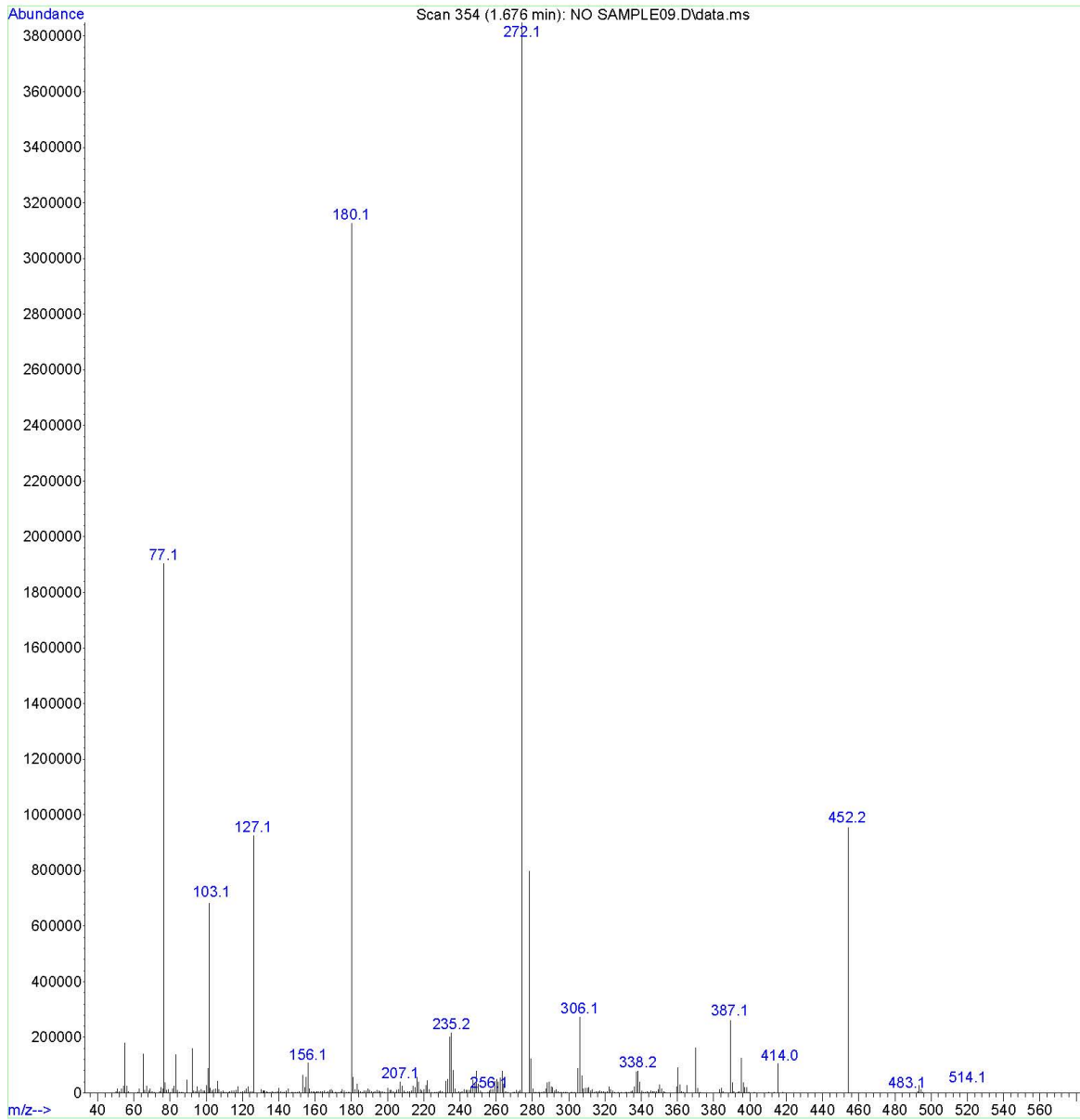


MM6.214.fid
mm6 609 Ms.Forozan

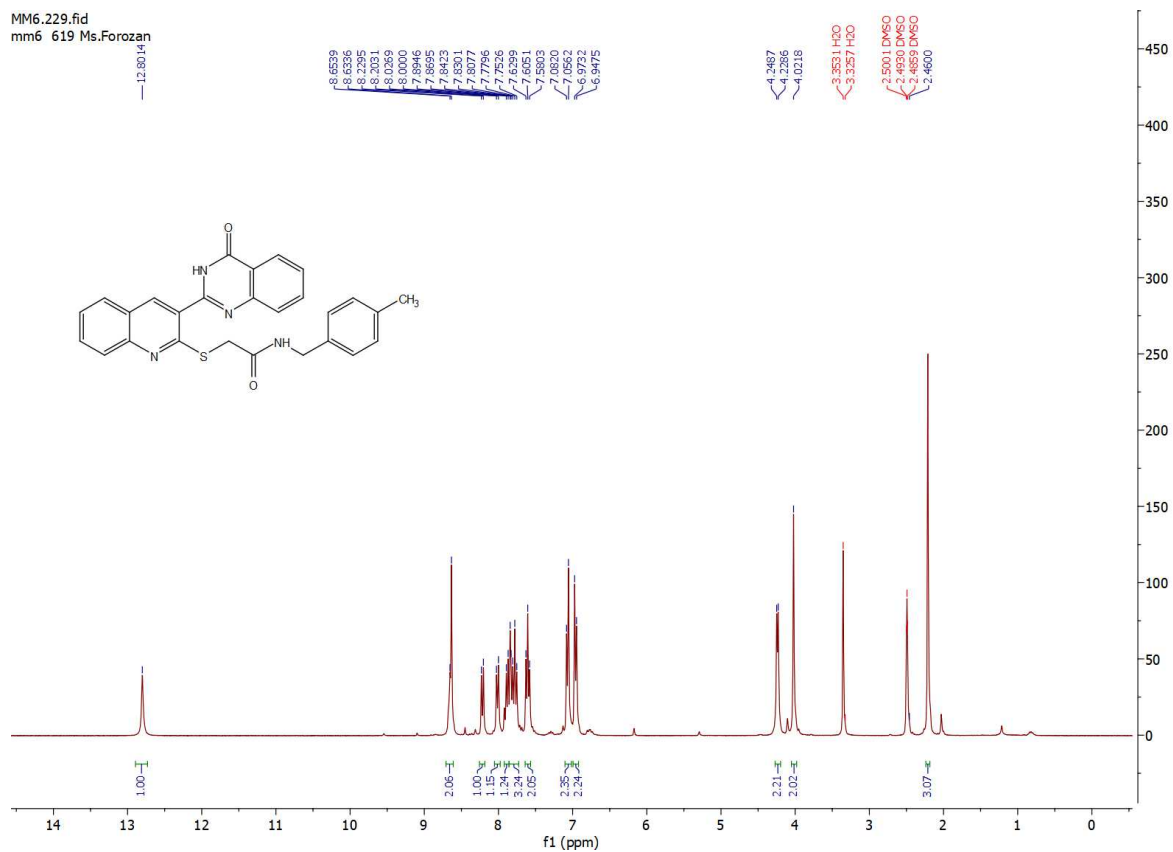
- 167.9211
- 161.7883
- 158.6132
- 156.7822
- 151.0206
- 149.7123
- 145.1901
- 142.9688
- 139.2100
- 137.4645
- 137.3814
- 136.8105
- 126.9839
- 125.9533
- 121.7413



File : C:\MSDCHEM\3\DATA\Snapshot\NO SAMPLE09.D
Operator :
Acquired : 3 Jan 2007 21:03 using AcqMethod f1.M
Instrument : MSD
Sample Name: MM6 609
Misc Info :
Vial Number: 1

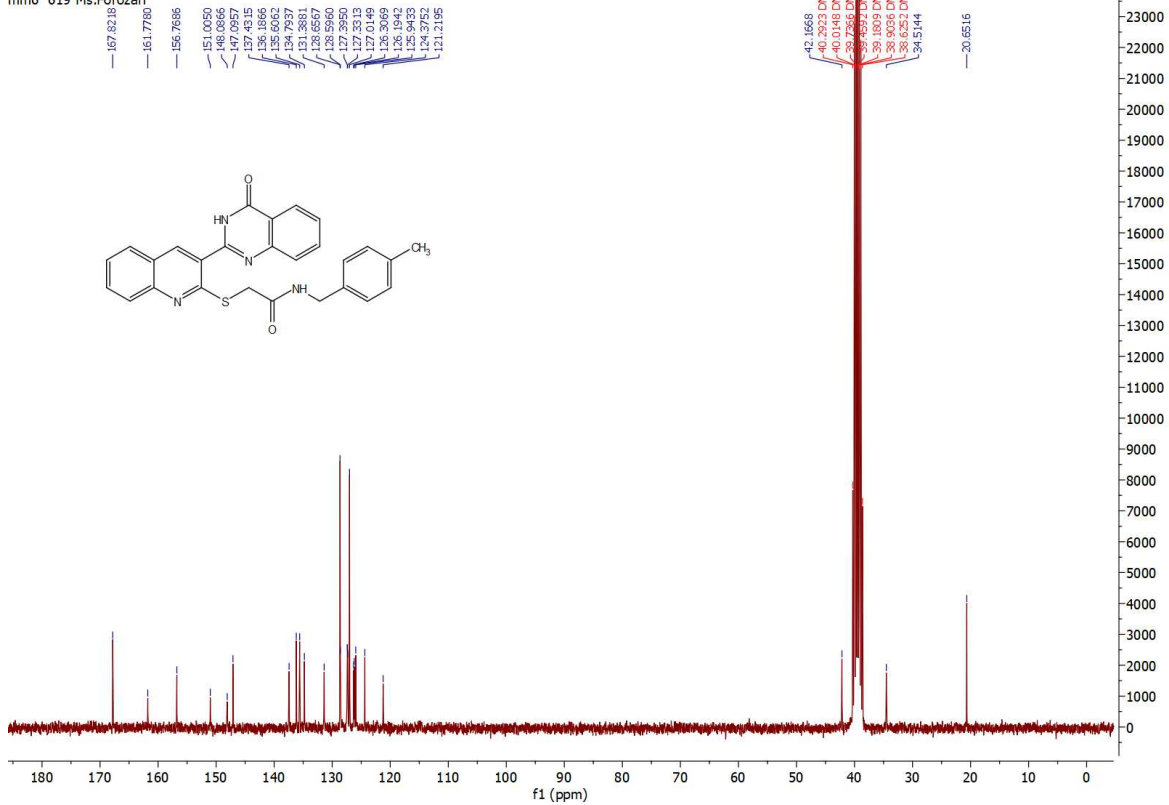


N-(4-Methylbenzyl)-2- $\{[3-(4\text{-oxo-3,4-dihydroquinazolin-2-yl})\text{quinolin-2-yl}]\text{thio}\}$ acetamide (**9o**)

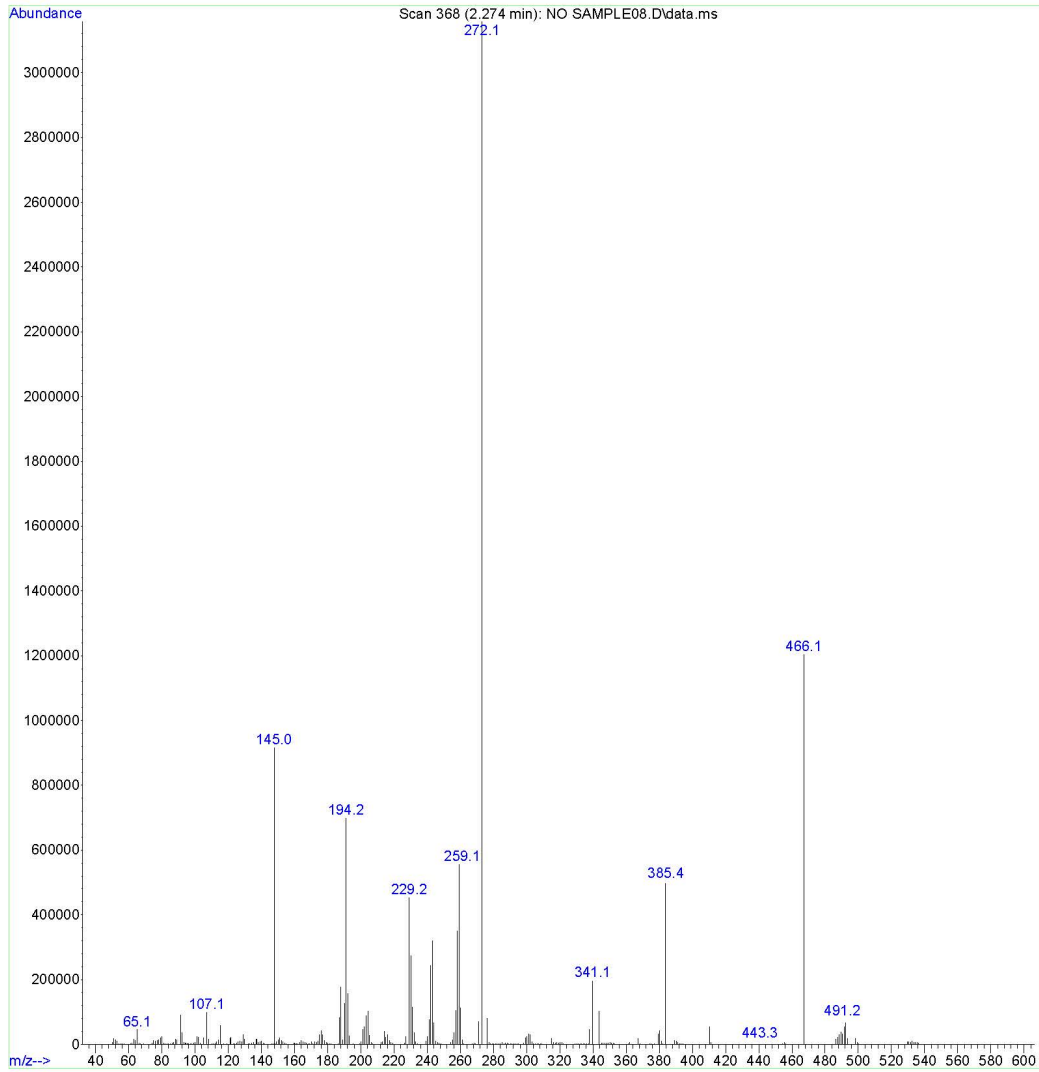


MM6.230.fid

mm6 619 Ms.Forozan

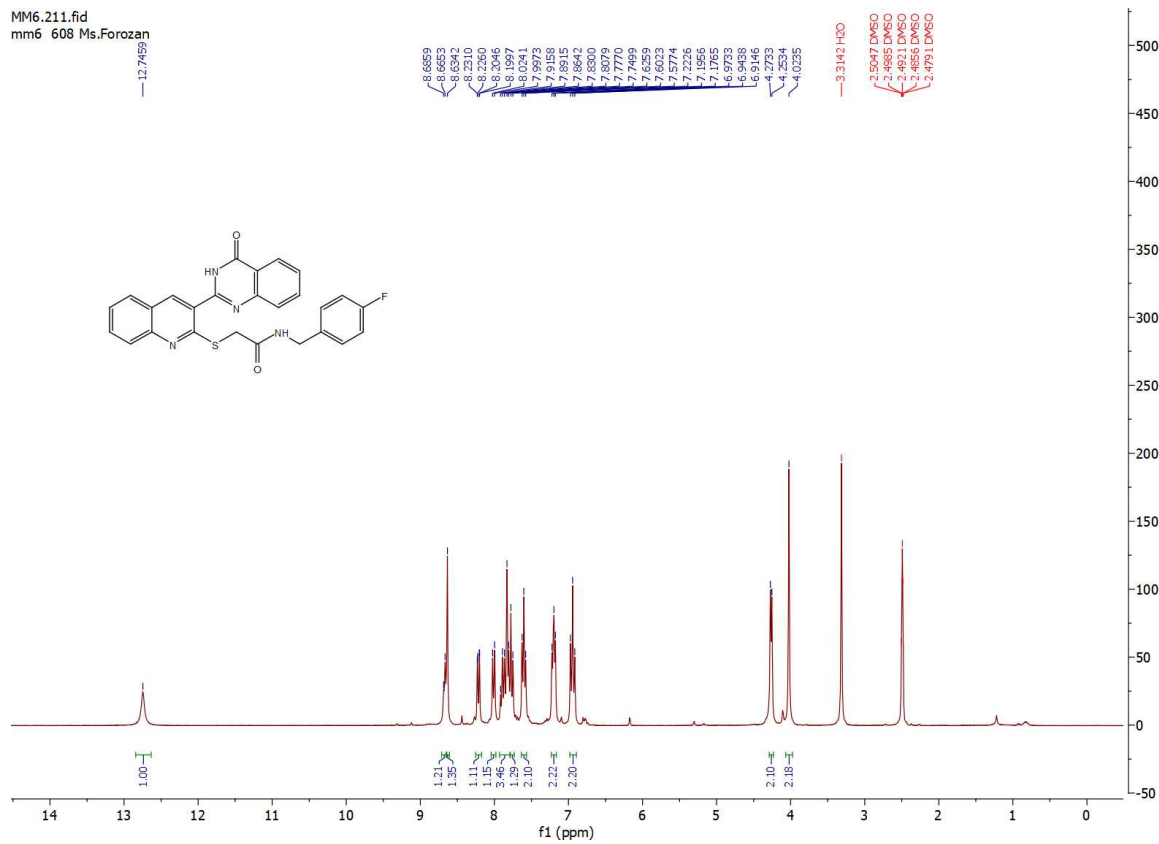


File :C:\MSDCHEM\3\DATA\Snapshot\NO SAMPLE08.D
Operator :
Acquired : 3 Jan 2007 22:41 using AcqMethod f1.M
Instrument : MSD
Sample Name: MM6 619
Misc Info :
Vial Number: 10



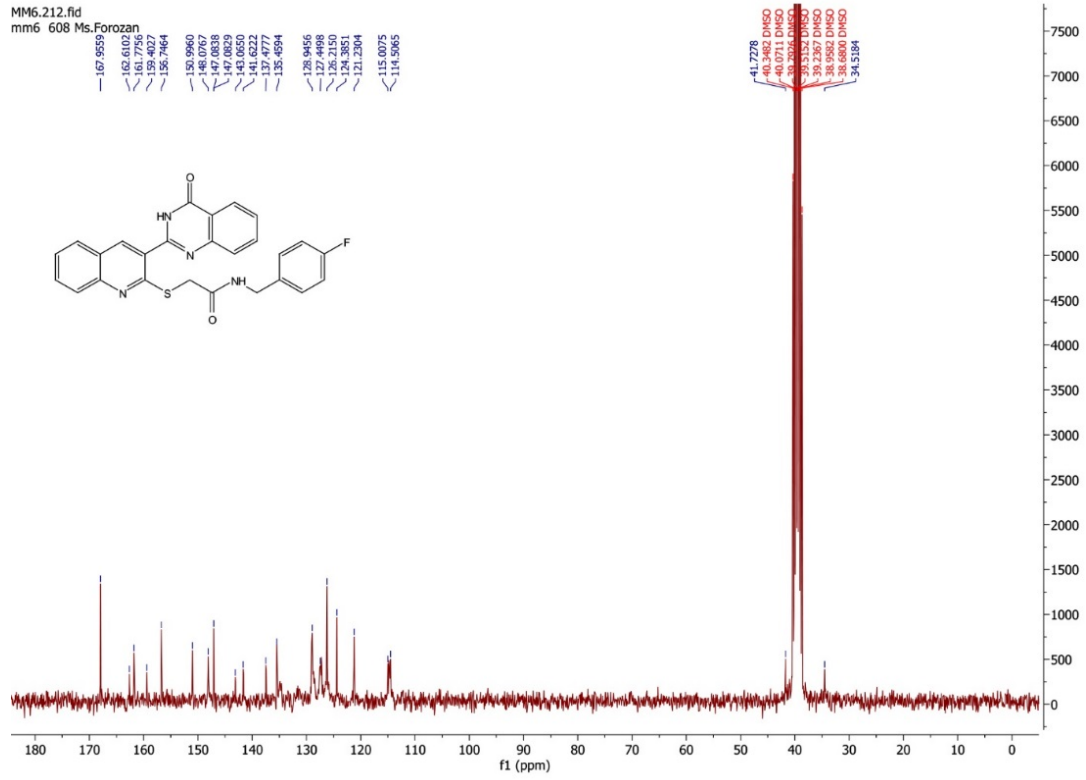
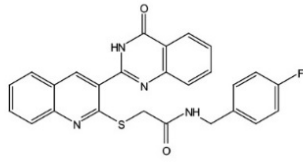
N-(4-Fluorobenzyl)-2-{{3-(4-oxo-3,4-dihydroquinazolin-2-yl)quinolin-2-yl}thio}acetamide (**9p**)

MM6.211.fid
mm6 608 Ms.Forozan



MM6.212.fid
mm6 608 Ms.Forozan

- 167.9559
- 166.6102
- 161.7756
- 159.4027
- 157.7464
- 150.9960
- 148.0767
- 147.0838
- 146.6559
- 143.0650
- 141.6322
- 137.4777
- 135.4594
- 128.9456
- 127.4498
- 126.2150
- 124.3851
- 121.2304
- 115.0075
- 114.5965



File : C:\MSDCHEM\3\DATA\Snapshot\NO SAMPLE09.D
Operator :
Acquired : 3 Jan 2007 21:03 using AcqMethod f1.M
Instrument : MSD
Sample Name: MM6 608
Misc Info :
Vial Number: 1

