

**MOLPRINT 2D-based identification and synthesis of novel chromene based
small molecules that target PLA2: Validation through chemo - and
bioinformatics approach**

Supplementary Information

Table of contents

Retro-synthetic approach for the synthesis of novel DCMB analogues 7(a-n)	Figure 1
Spectral characterization of compound 7a	SI-01
Spectral characterization of compound 7b	SI-02
Spectral characterization of compound 7c	SI-03
Spectral characterization of compound 7d	SI-04
Spectral characterization of compound 7e	SI-05
Spectral characterization of compound 7f	SI-06
Spectral characterization of compound 7g	SI-07
Spectral characterization of compound 7h	SI-08
Spectral characterization of compound 7i	SI-09
Spectral characterization of compound 7j	SI-10
Spectral characterization of compound 7k	SI-11
Spectral characterization of compound 7l	SI-12
Spectral characterization of compound 7m	SI-13
Spectral characterization of compound 7n	SI-14

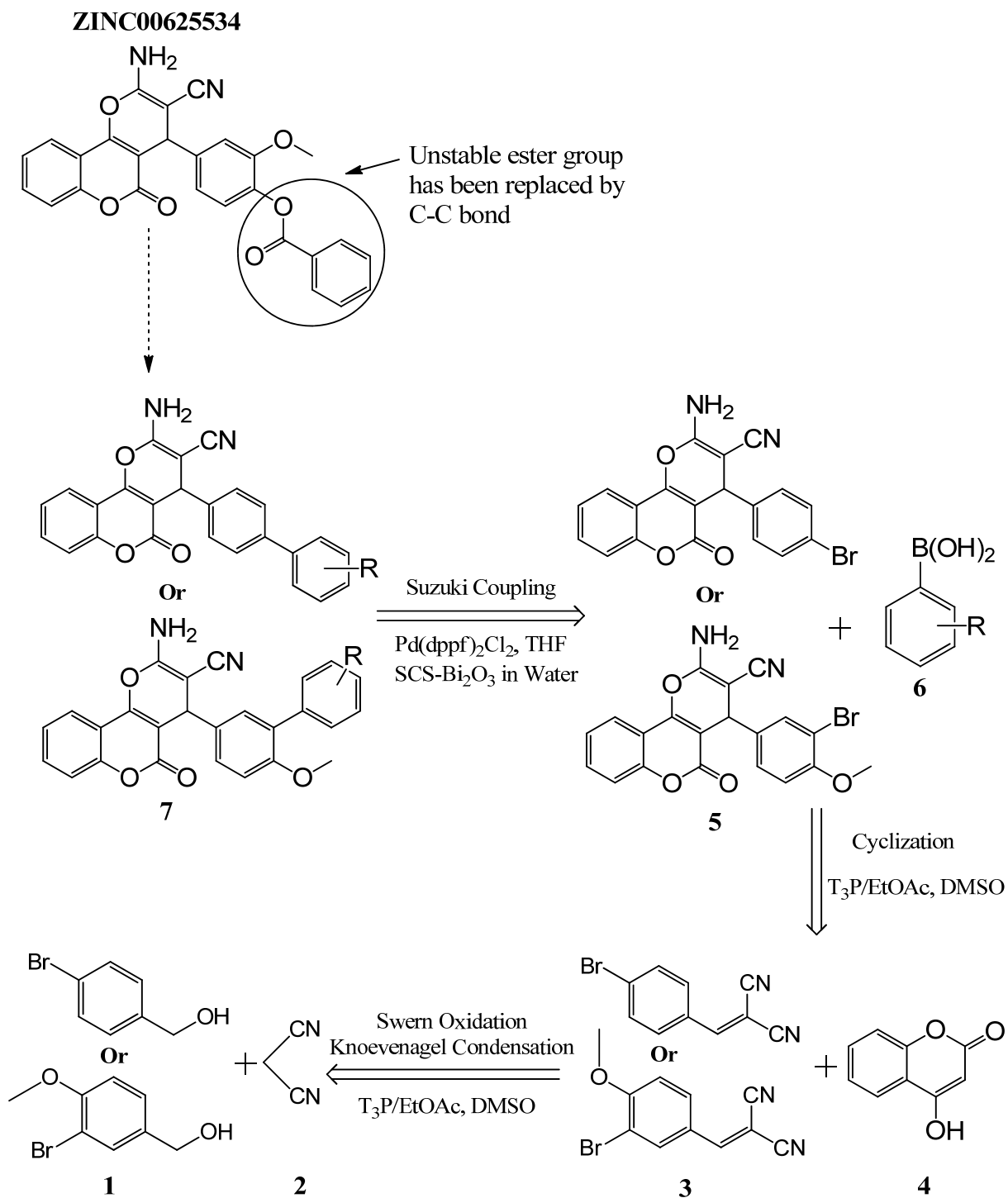
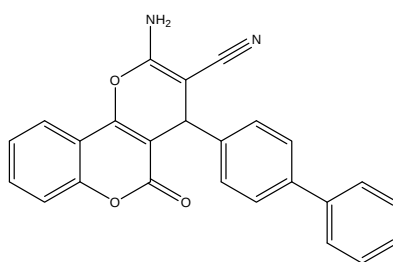
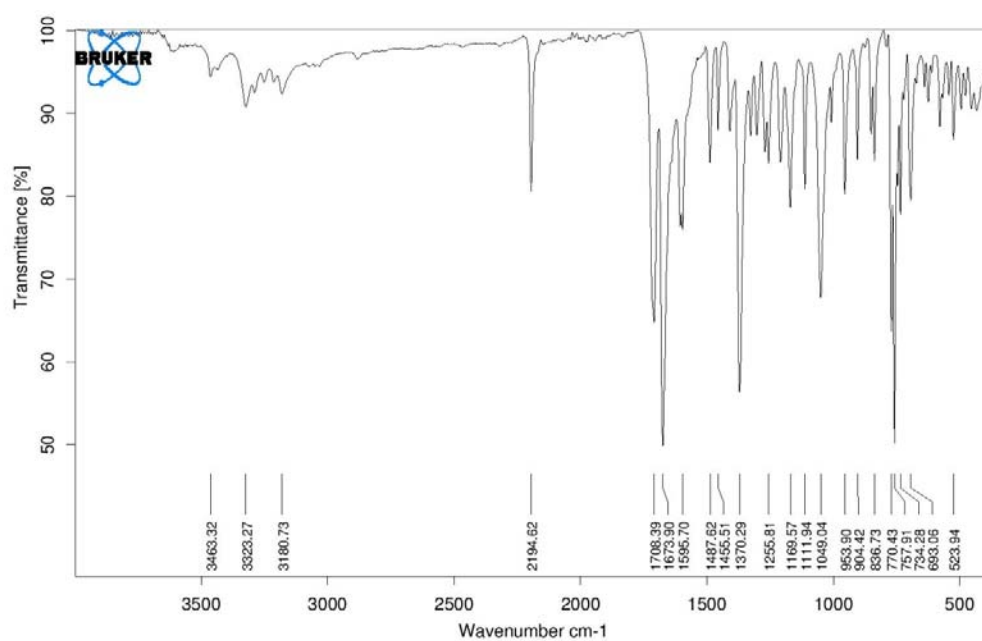
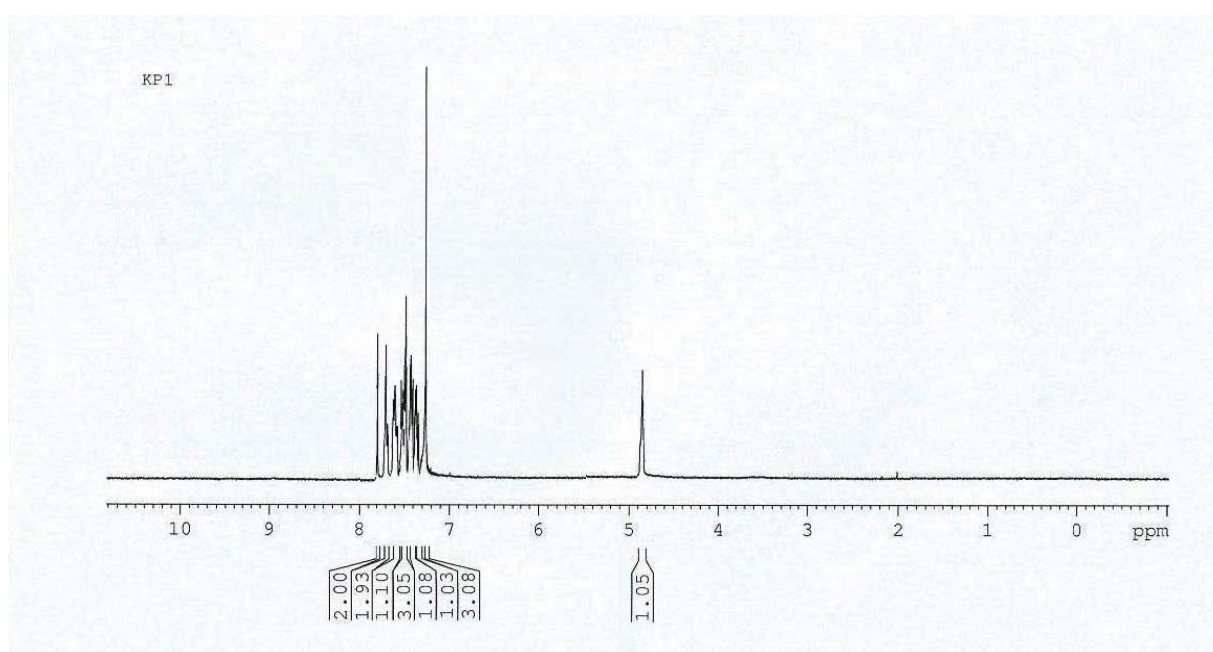
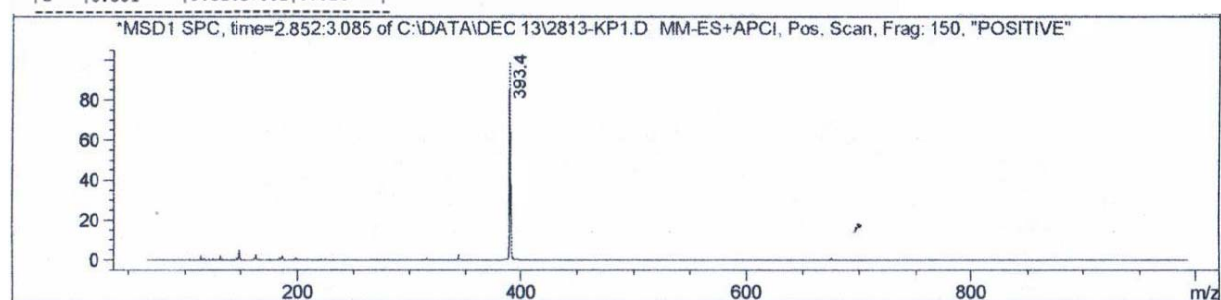
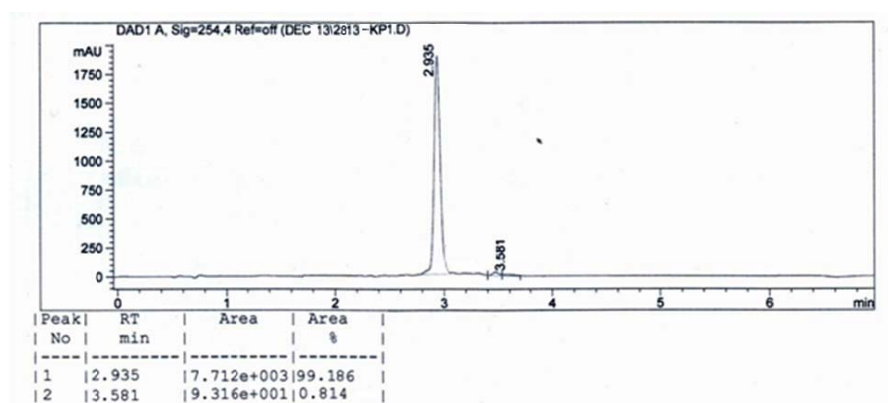


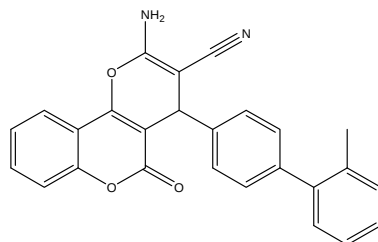
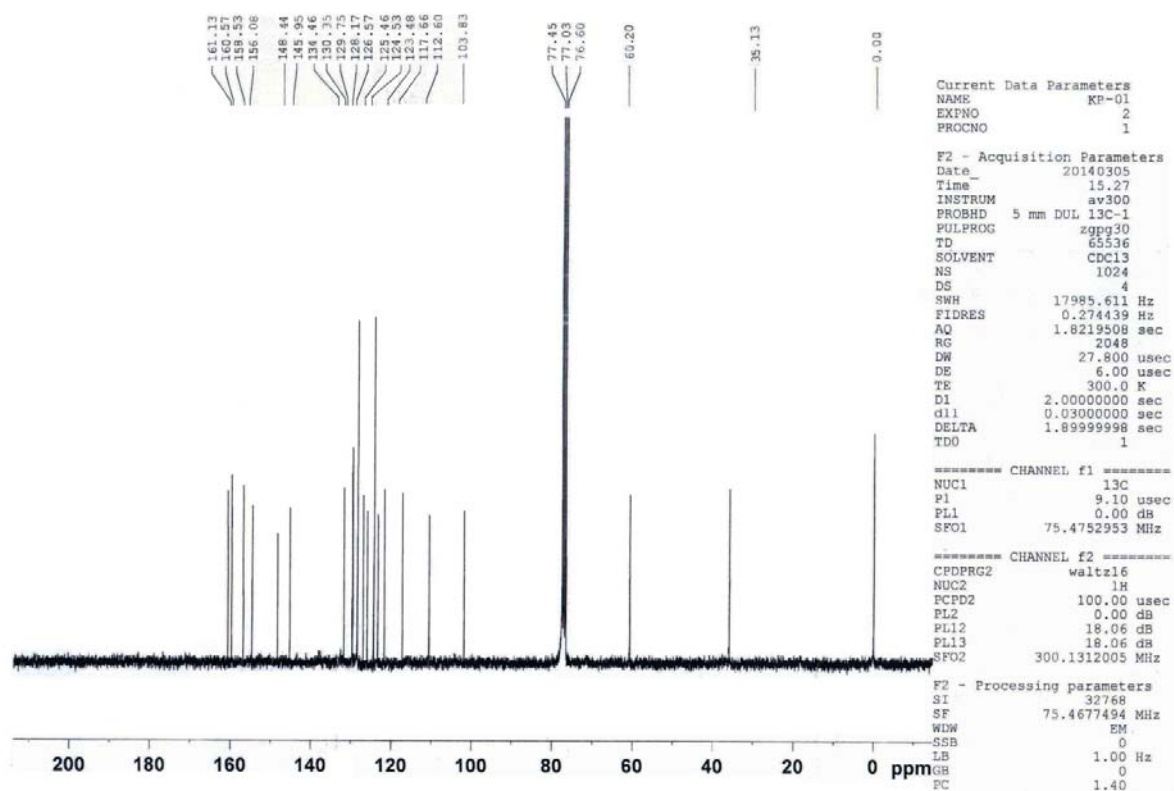
Figure 1



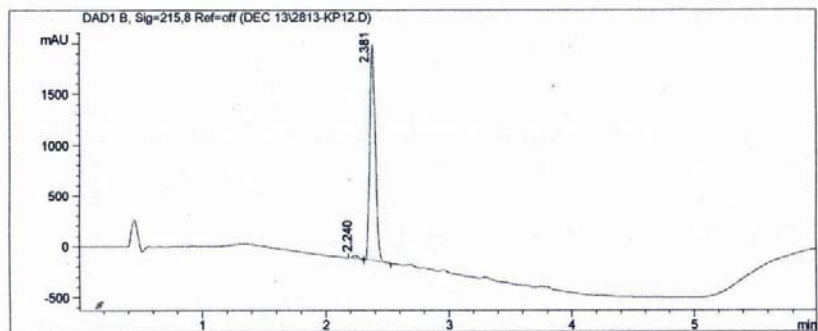
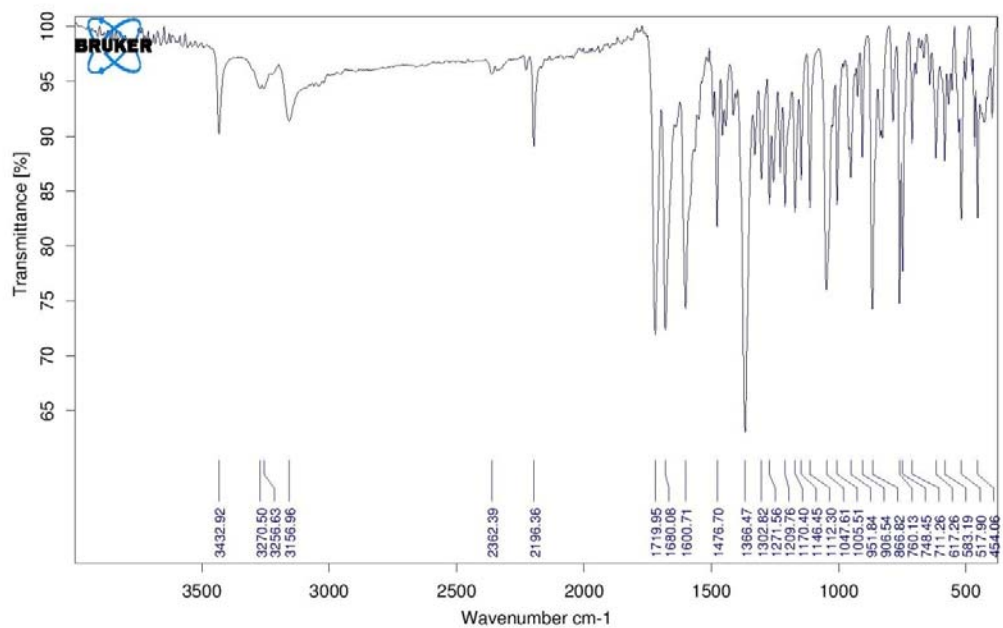
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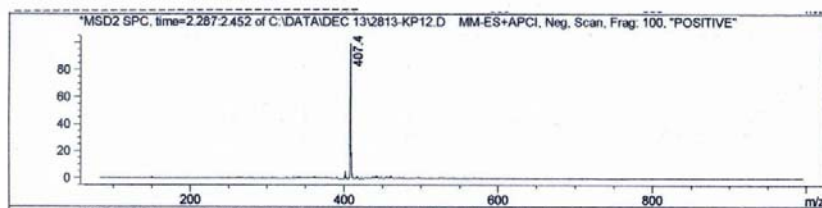


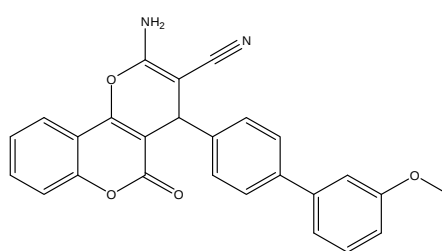
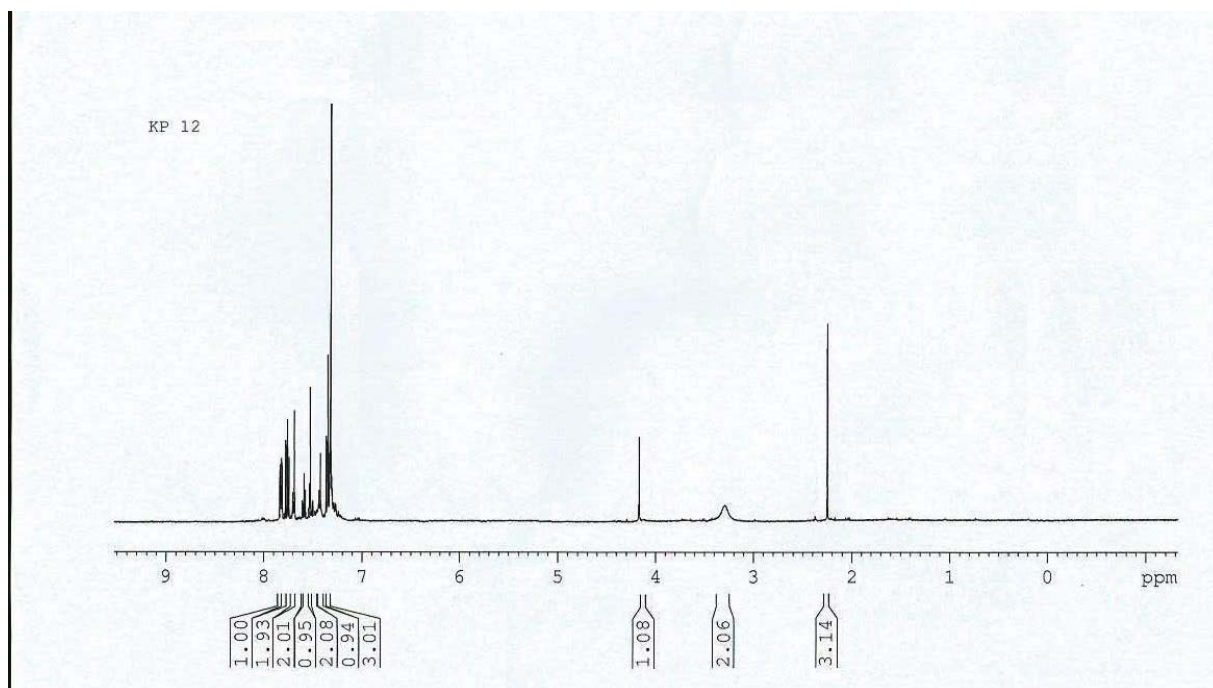


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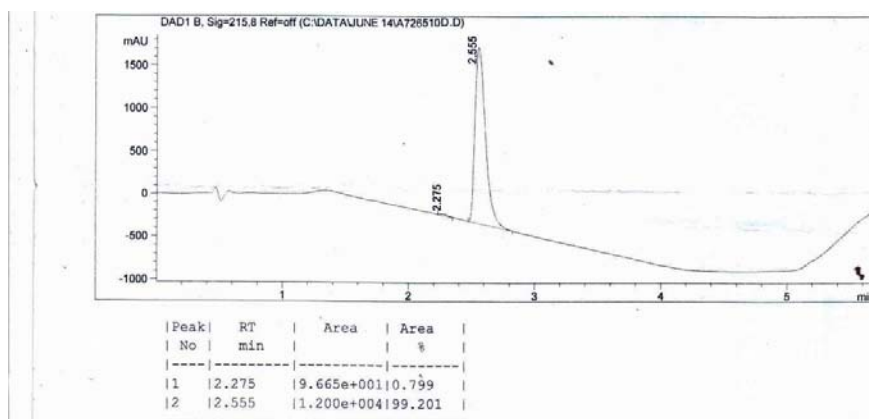
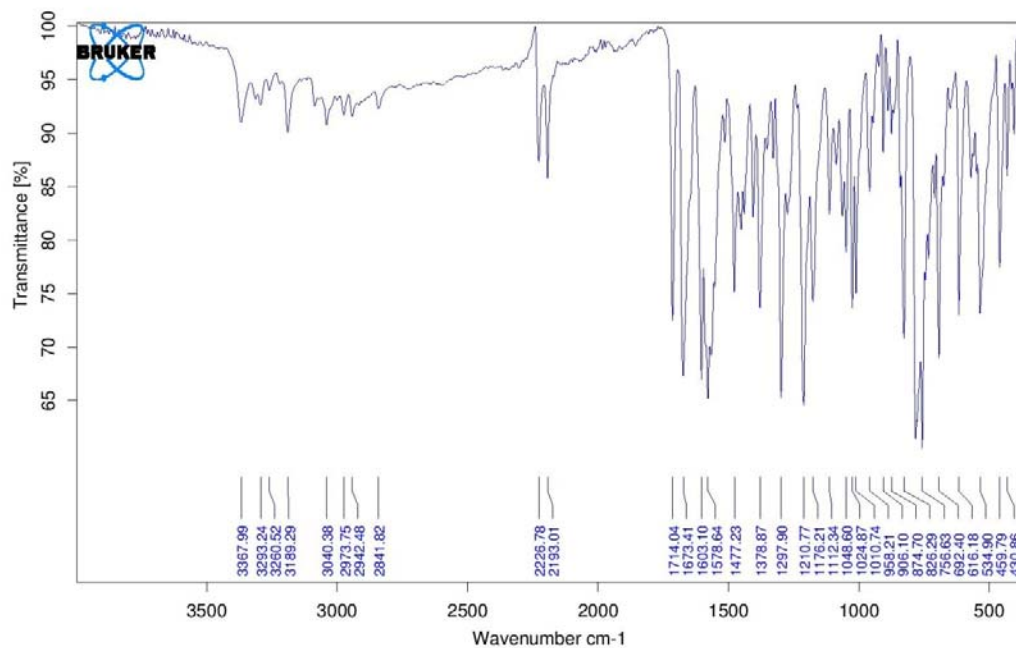


Peak No	RT min	Area	Area %
1	2.240	8.342e+001	1.049
2	2.381	6.613e+003	98.951

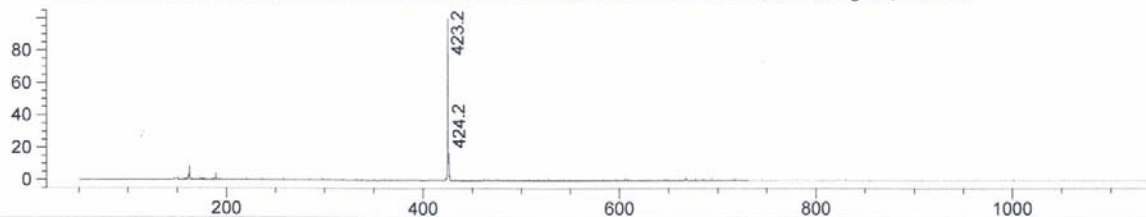




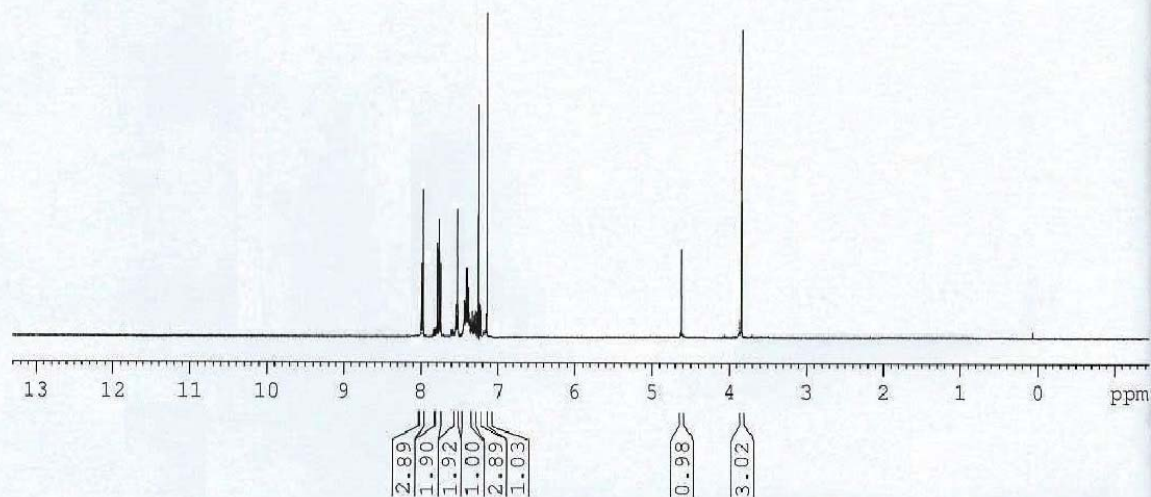
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*MSD1 SPC, time=2.311:2.719 of D:\DATA\MERCK\JUNE14\A726510D.D MM-ES+APCI, Scan, Frag: 50, "Positive"



KP4



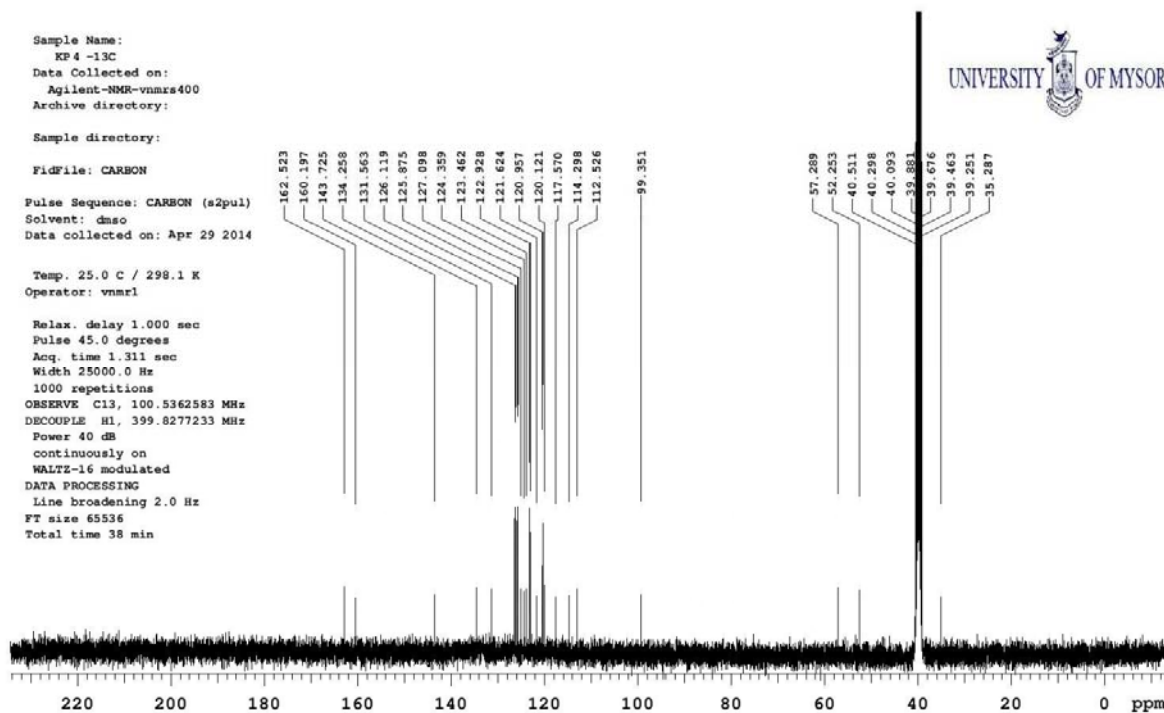
Sample Name:
KP4 -13C
Data Collected on:
Agilent-NMR-vnmrs400
Archive directory:
Sample directory:
FidFile: CARBON

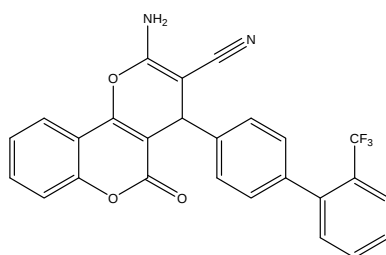
Pulse Sequence: CARBON (a2pul)
Solvent: dmsc
Data collected on: Apr 29 2014

Temp. 25.0 C / 298.1 K
Operator: vnmr1

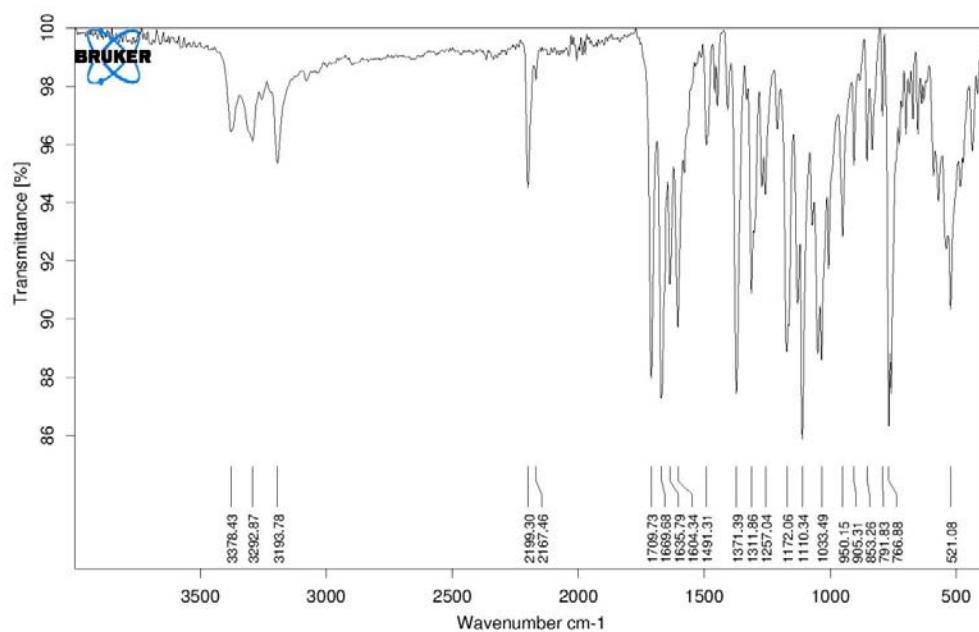
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.311 sec
Width 25000.0 Hz
1000 repetitions
OBSERVE C13, 100.5362583 MHz
DECOUPLE H1, 399.8277233 MHz
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
FT size 65536
Total time 38 min

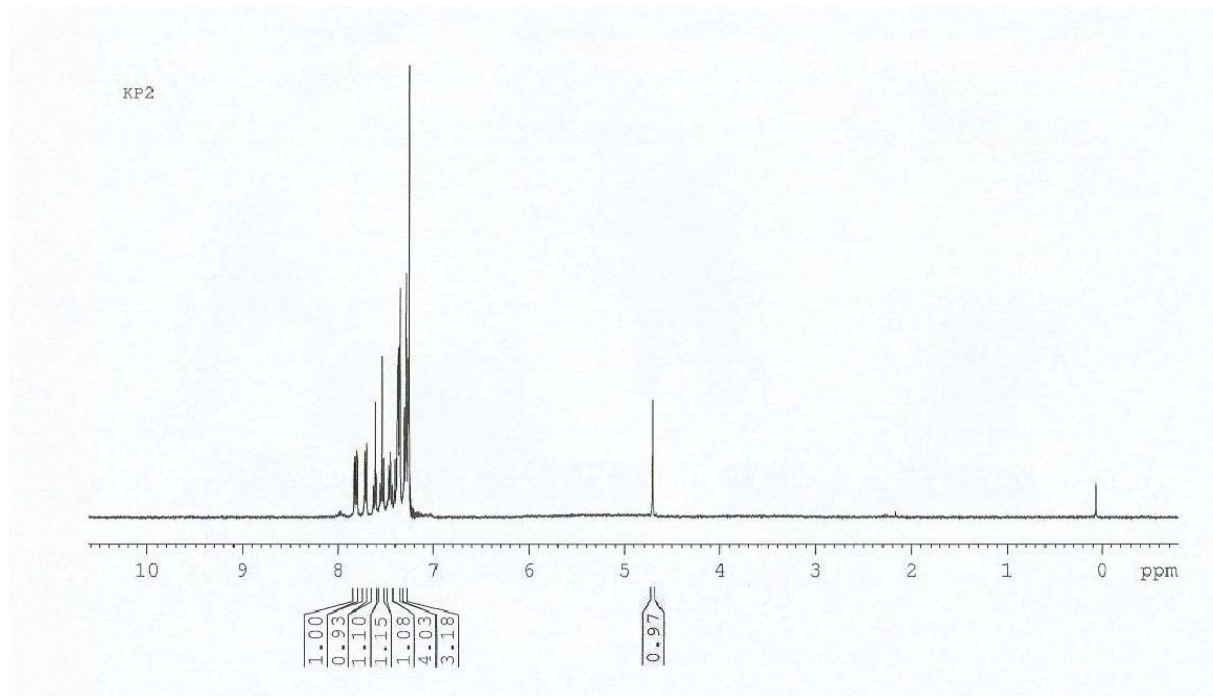
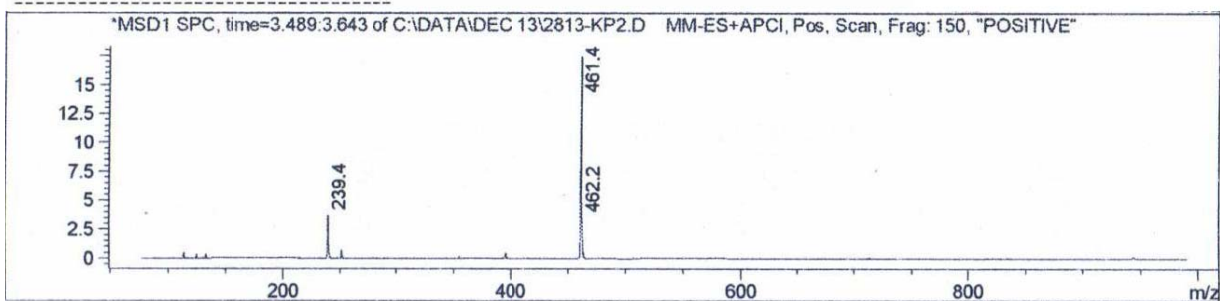
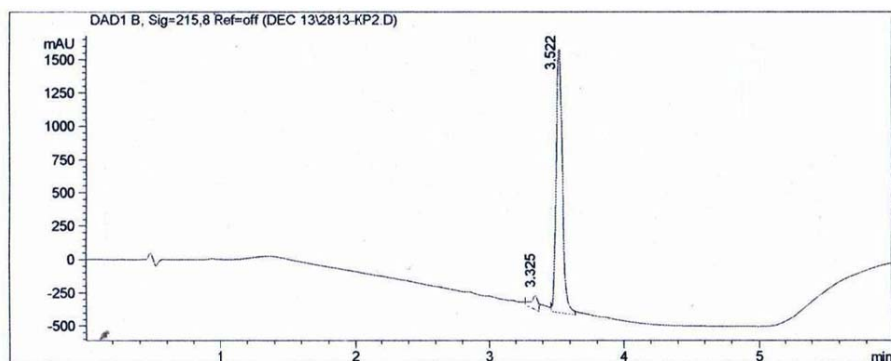
UNIVERSITY OF MYSORE

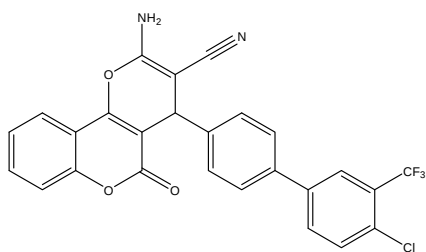
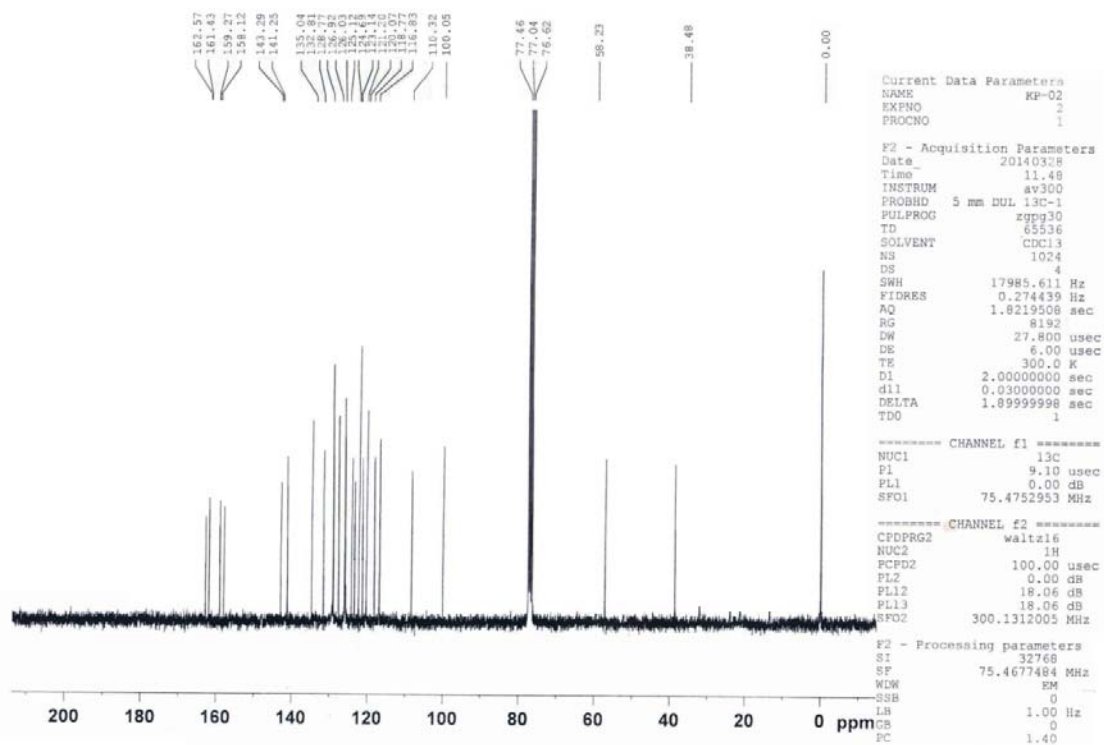




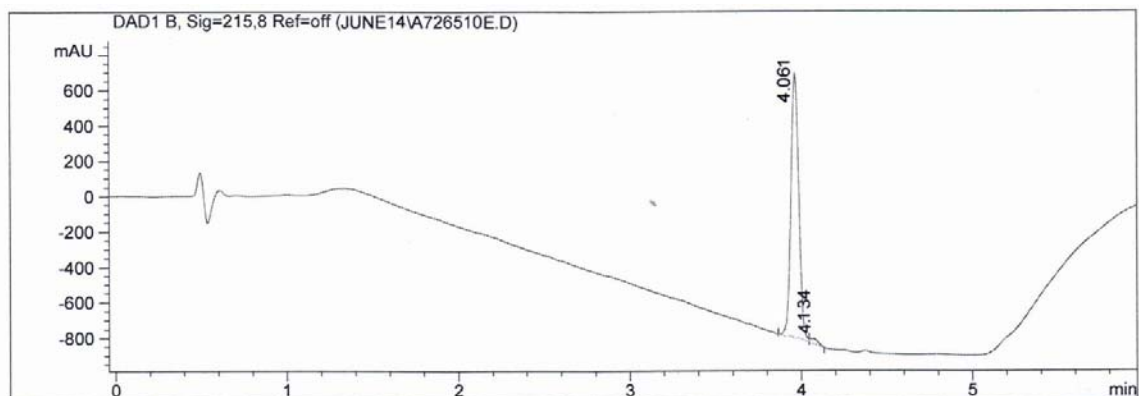
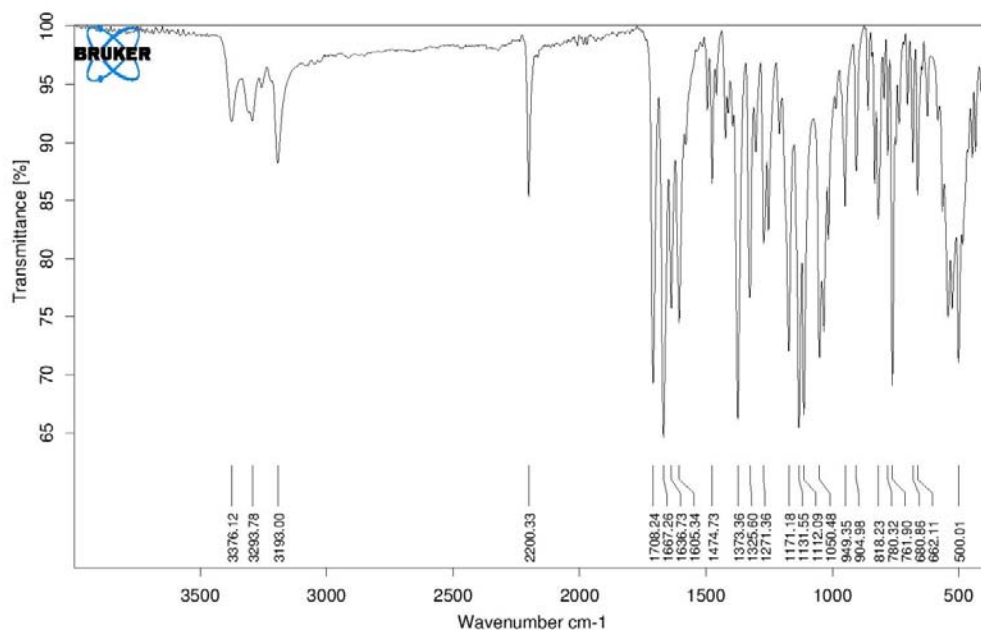
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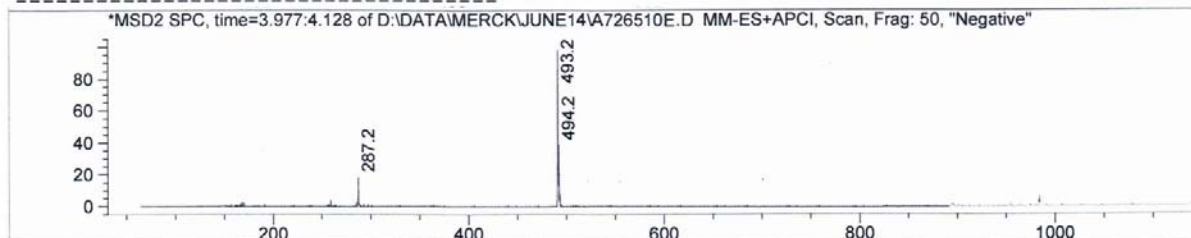


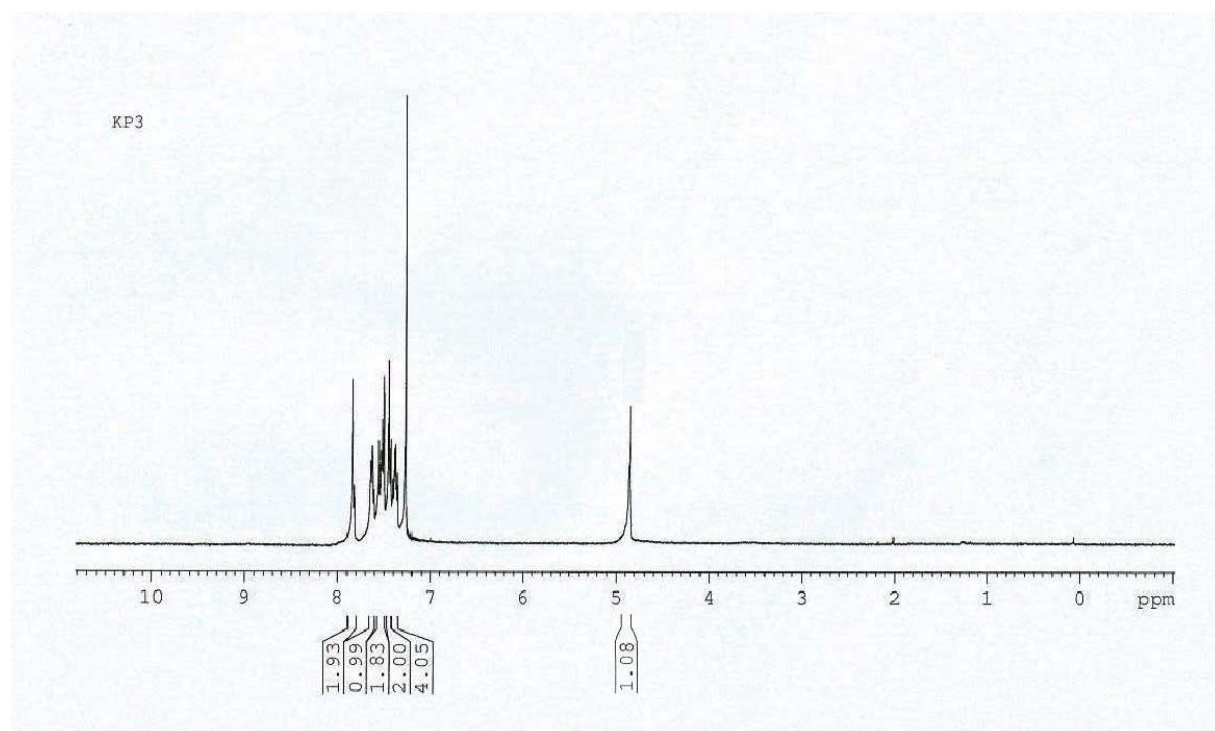


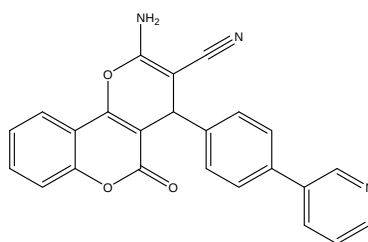
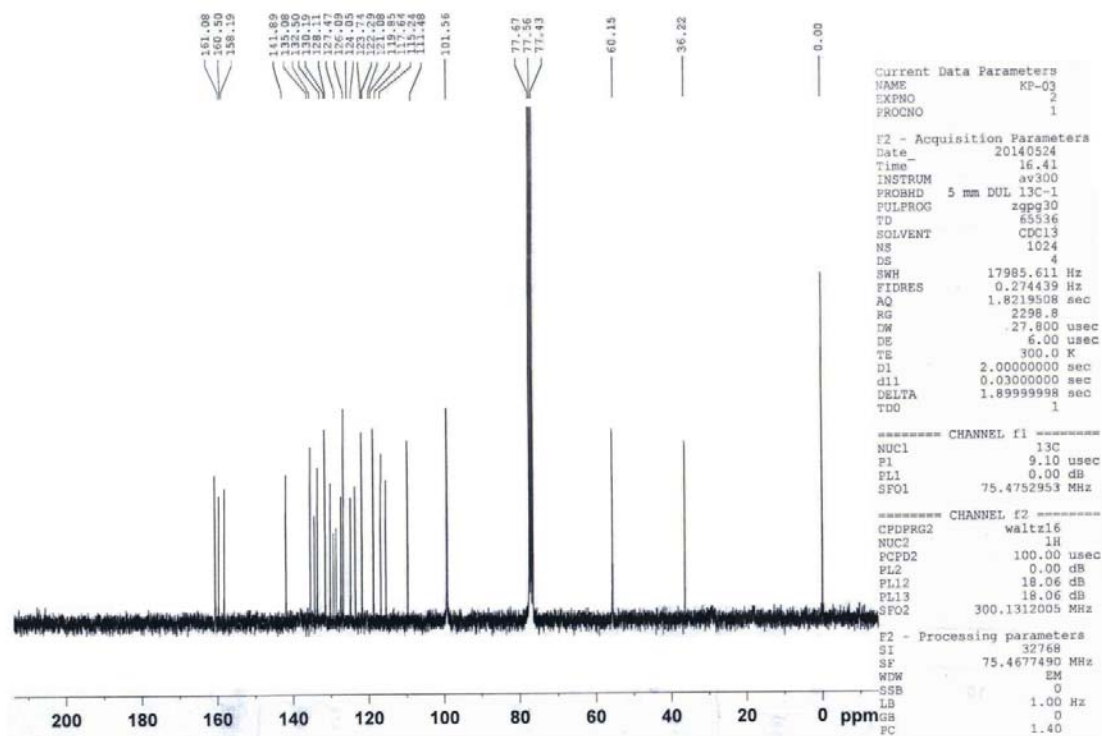
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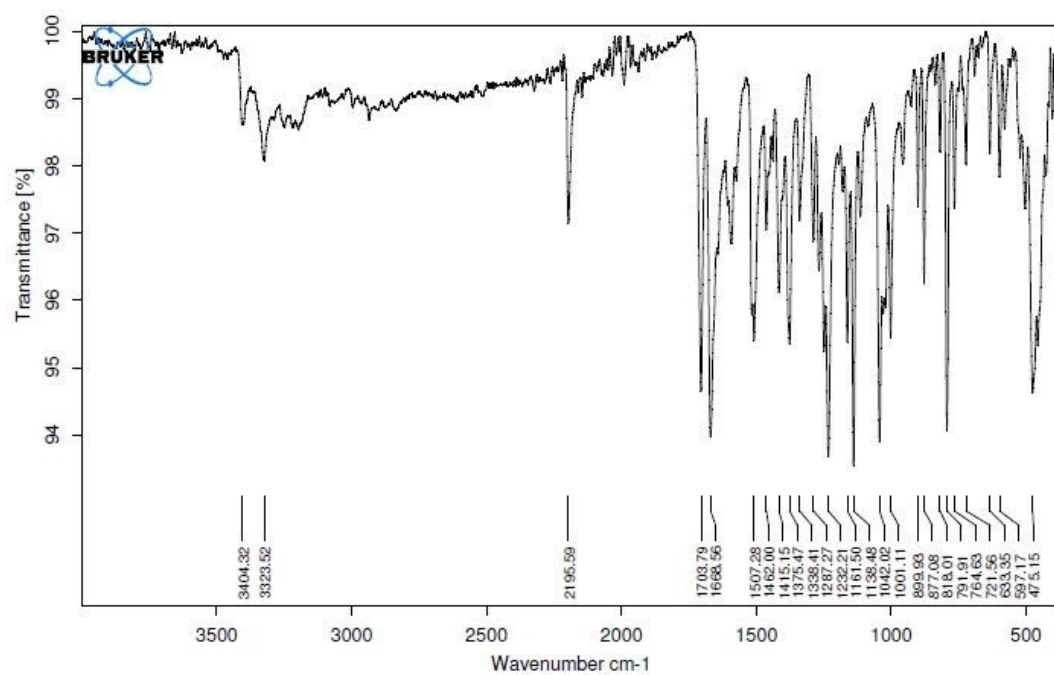
Peak No	RT min	Area	Area %
1	4.061	4.711e+003	98.304
2	4.134	9.092e+001	1.696

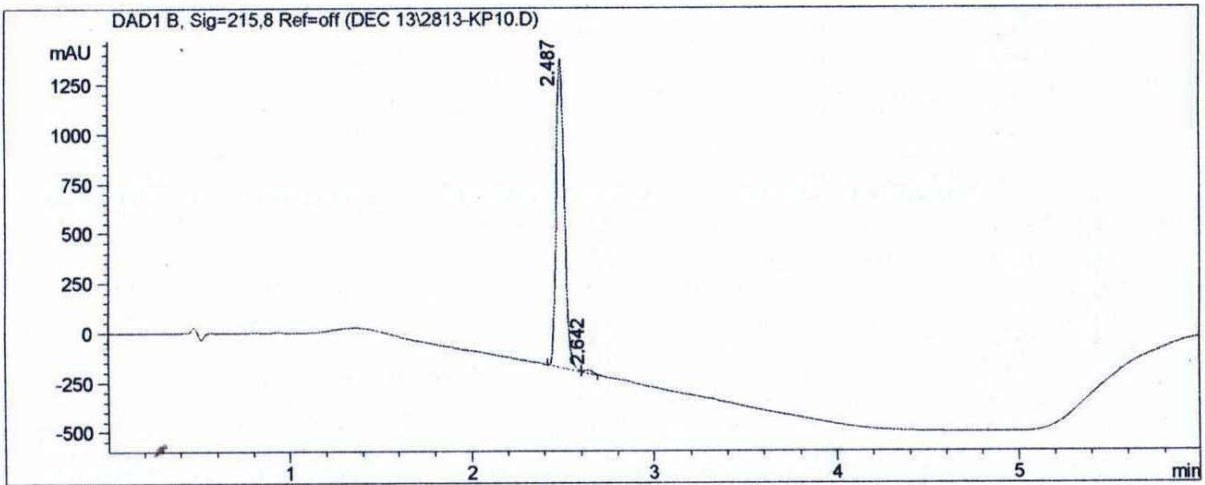




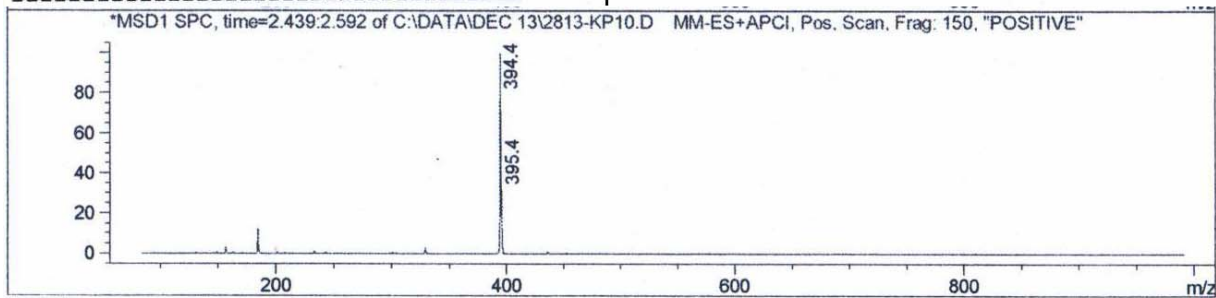


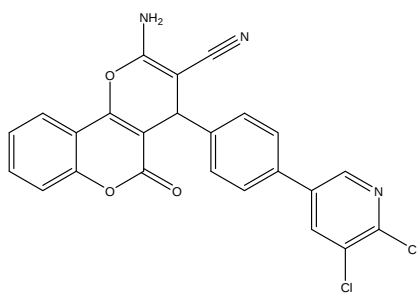
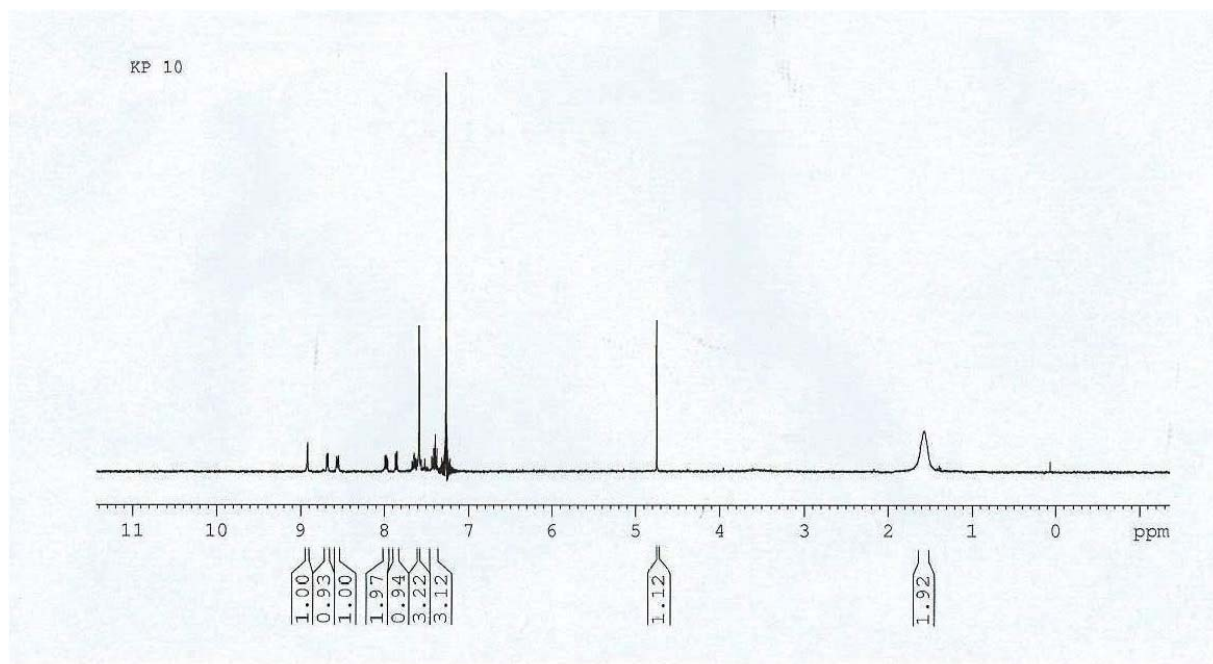
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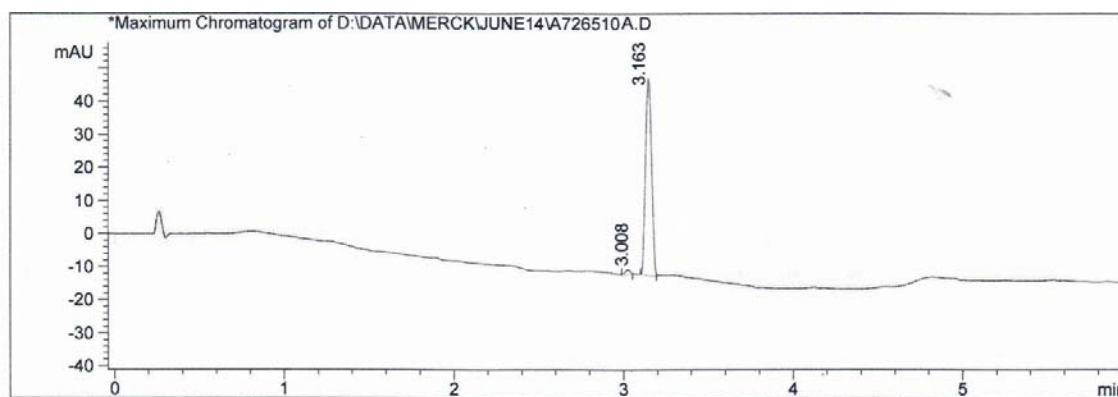
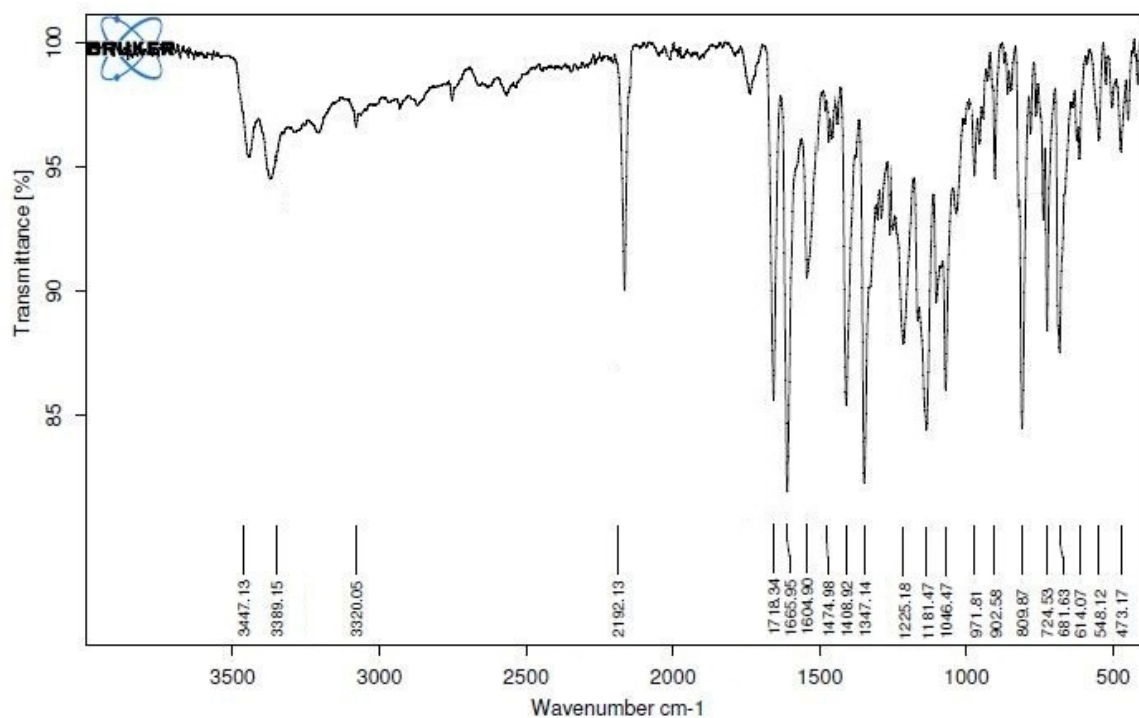


Peak No	RT min	Area	Area %
1	2.487	4.810e+003	98.931
2	2.642	5.744e+001	1.069

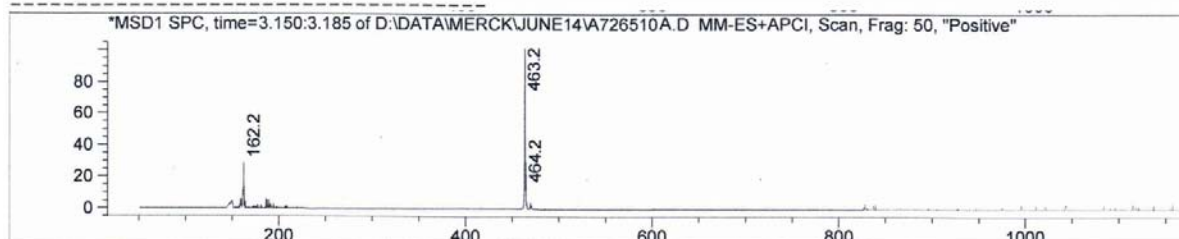


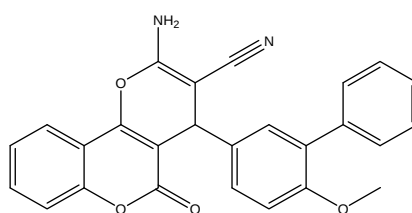
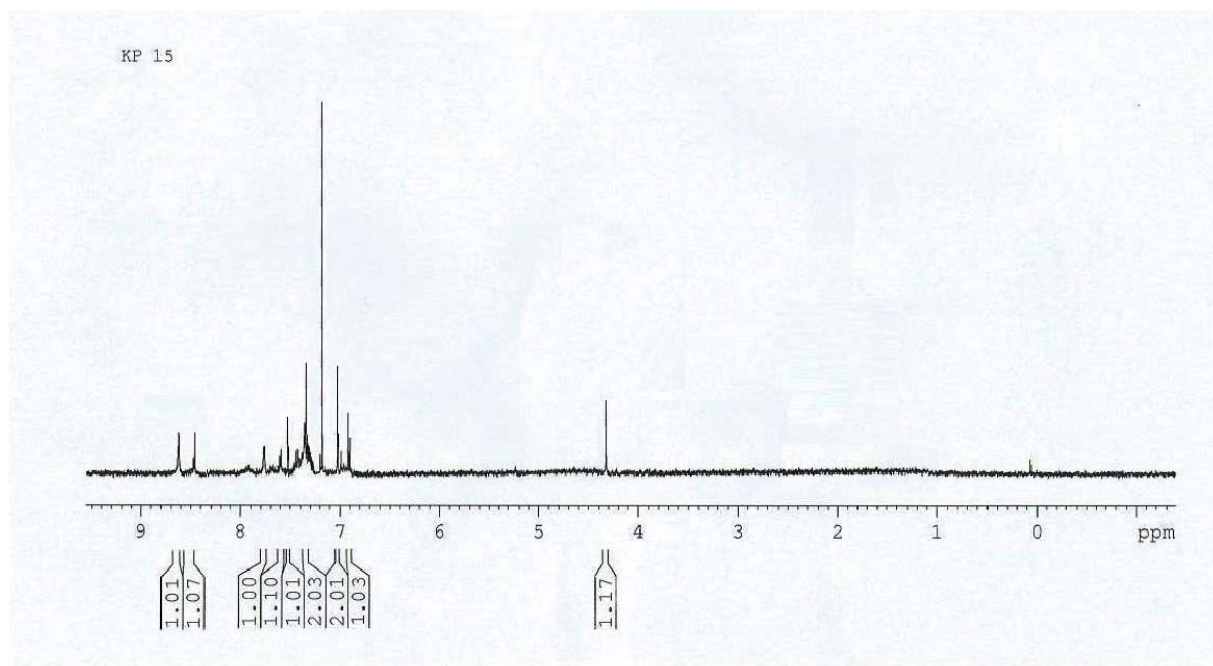


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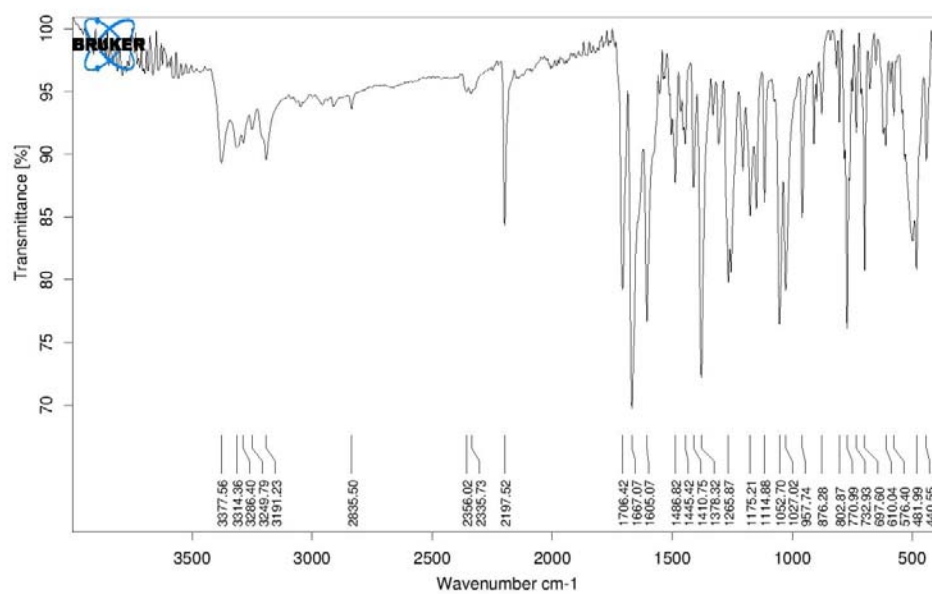


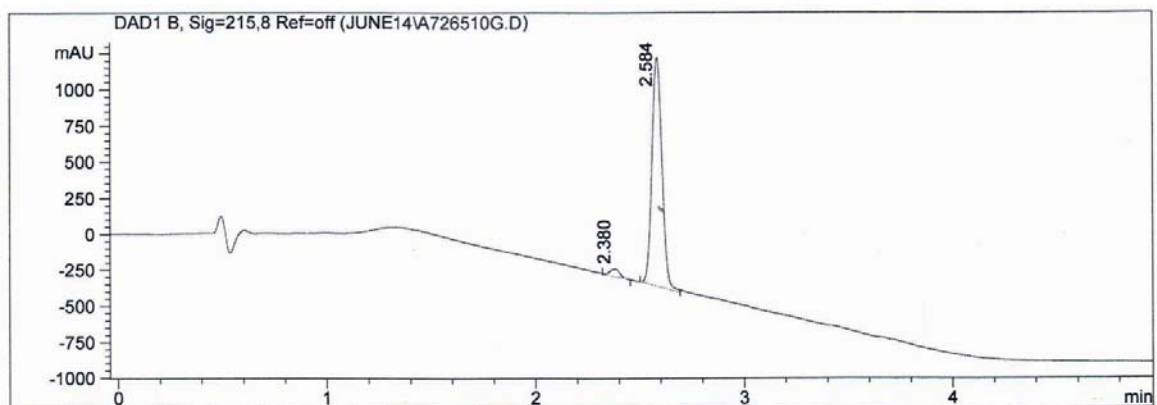
Peak No	RT min	Area	Area %
1	3.008	2.965e+001	1.536
2	3.163	1.496e+002	98.464





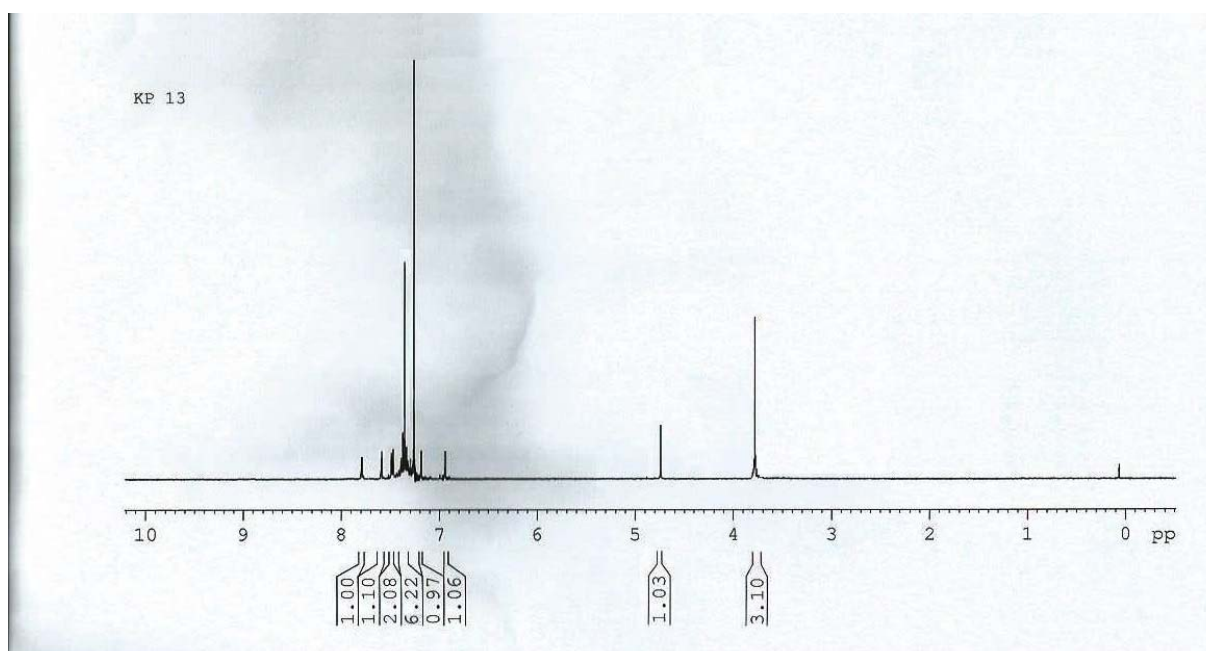
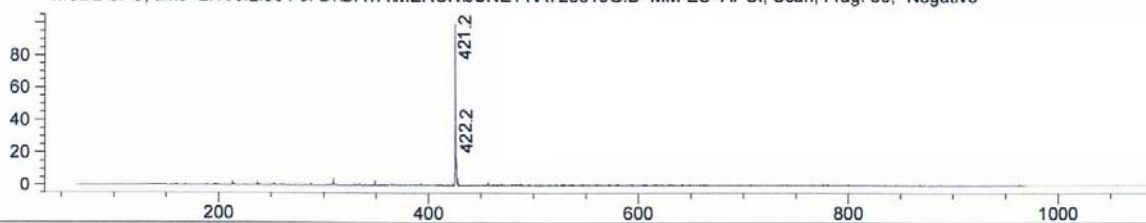
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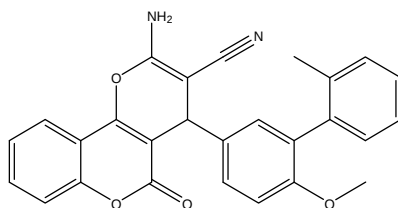




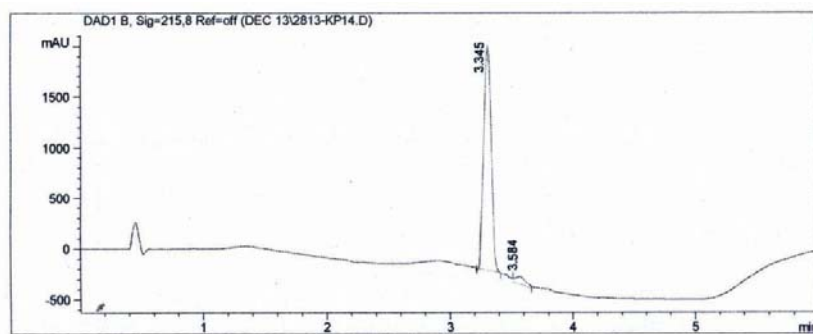
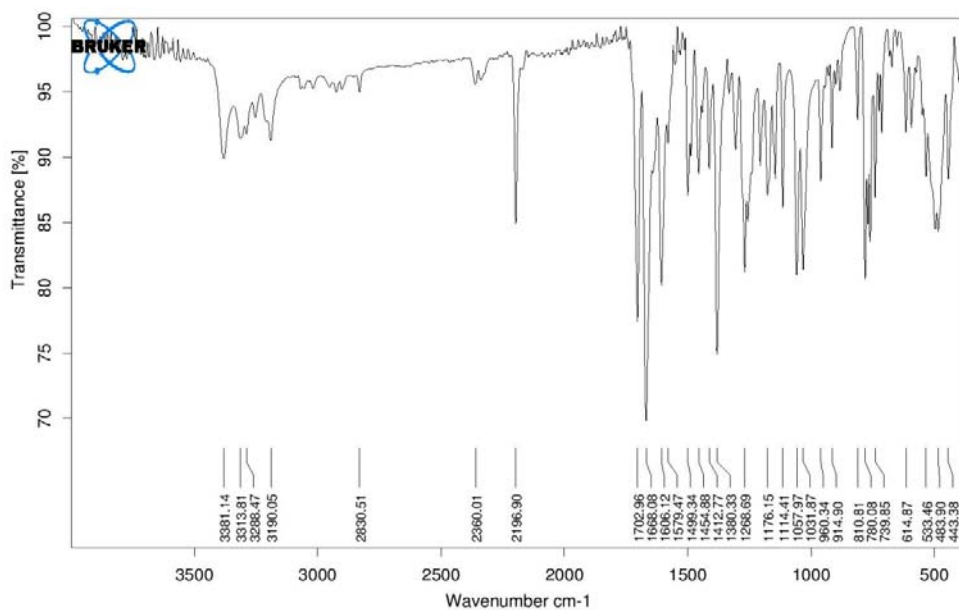
Peak No	RT min	Area	Area %
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2	2.584	5.279e+003	98.121

*MSD2 SPC, time=2.406:2.864 of D:\DATA\MERCK\JUNE14\A726510G.D MM-ES+APCI, Scan, Frag: 50, "Negative"

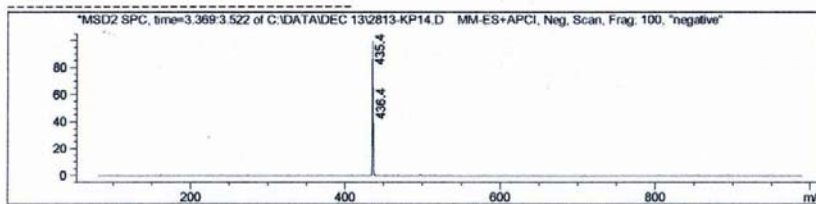


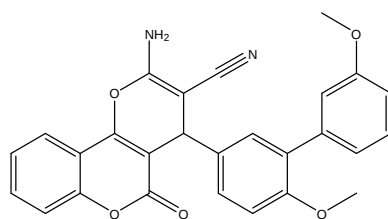
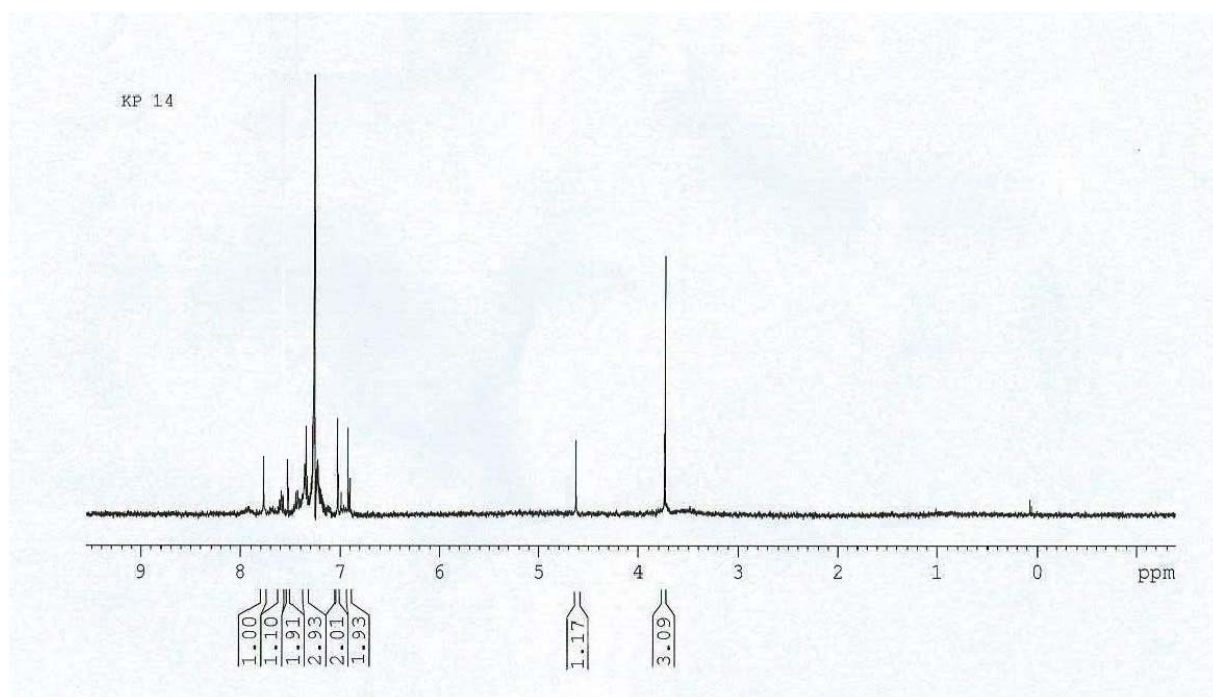


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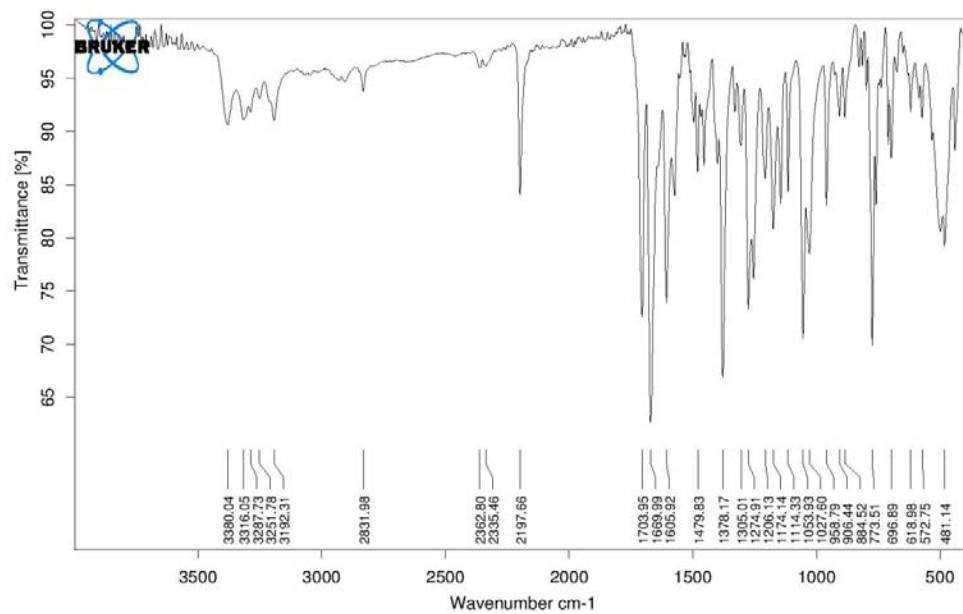


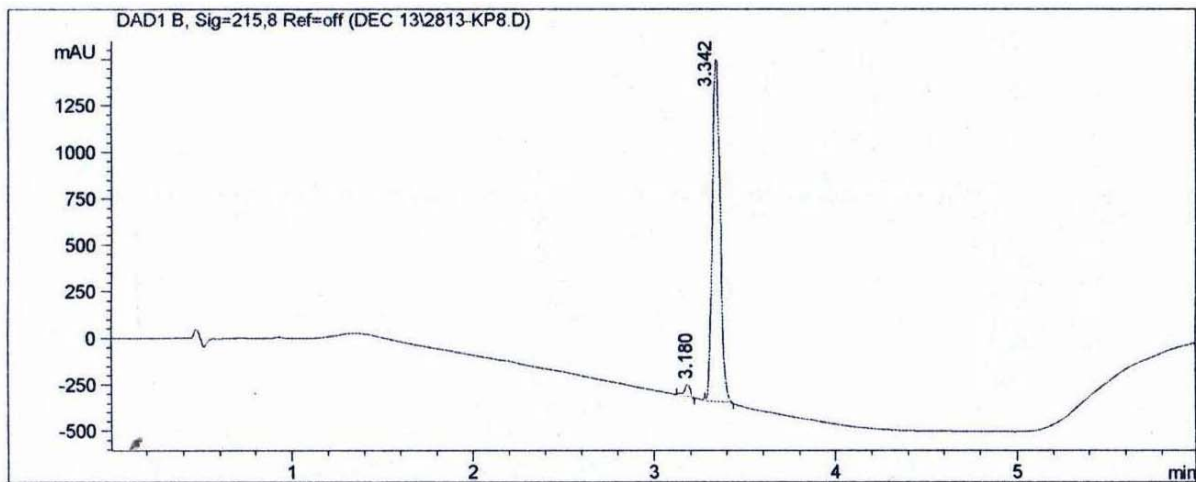
Peak No	RT min	Area	Area %
1	3.345	8.342e+001	98.951
2	3.584	6.613e+003	1.049



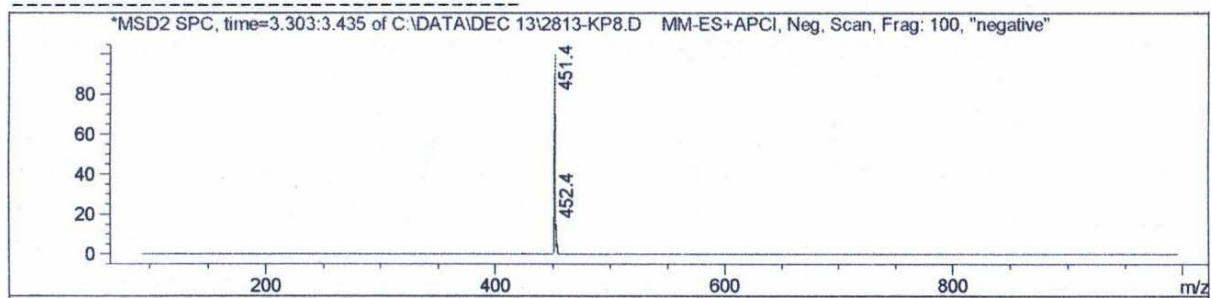


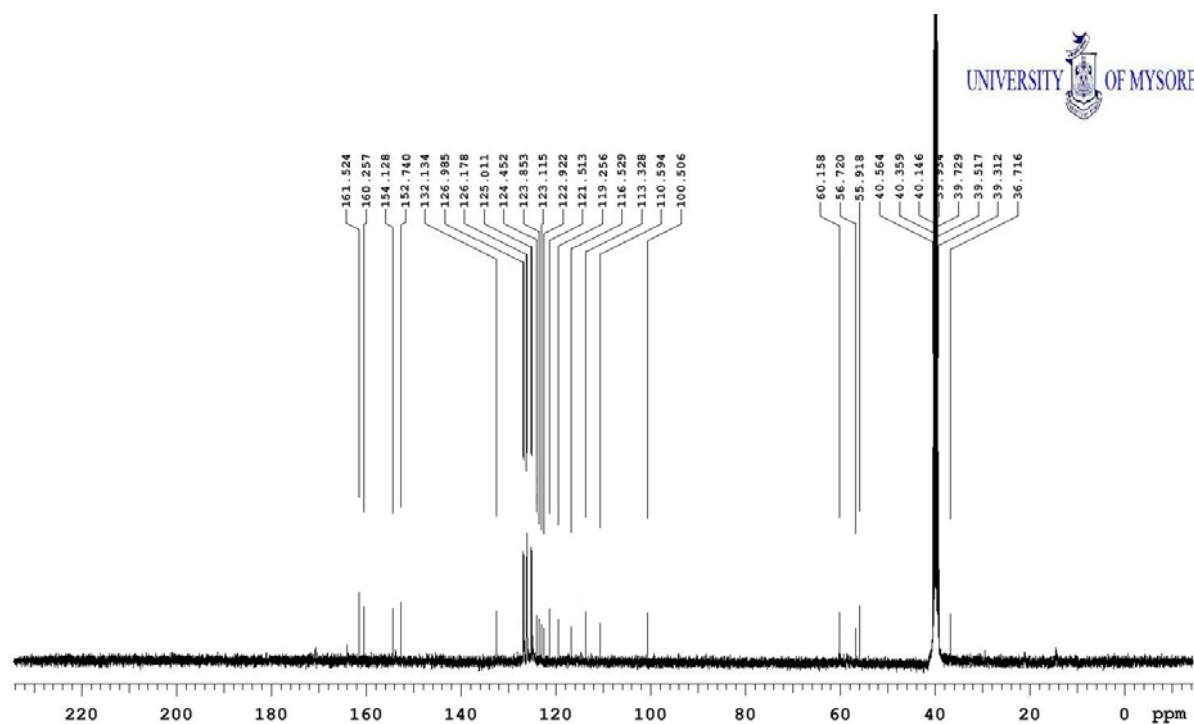
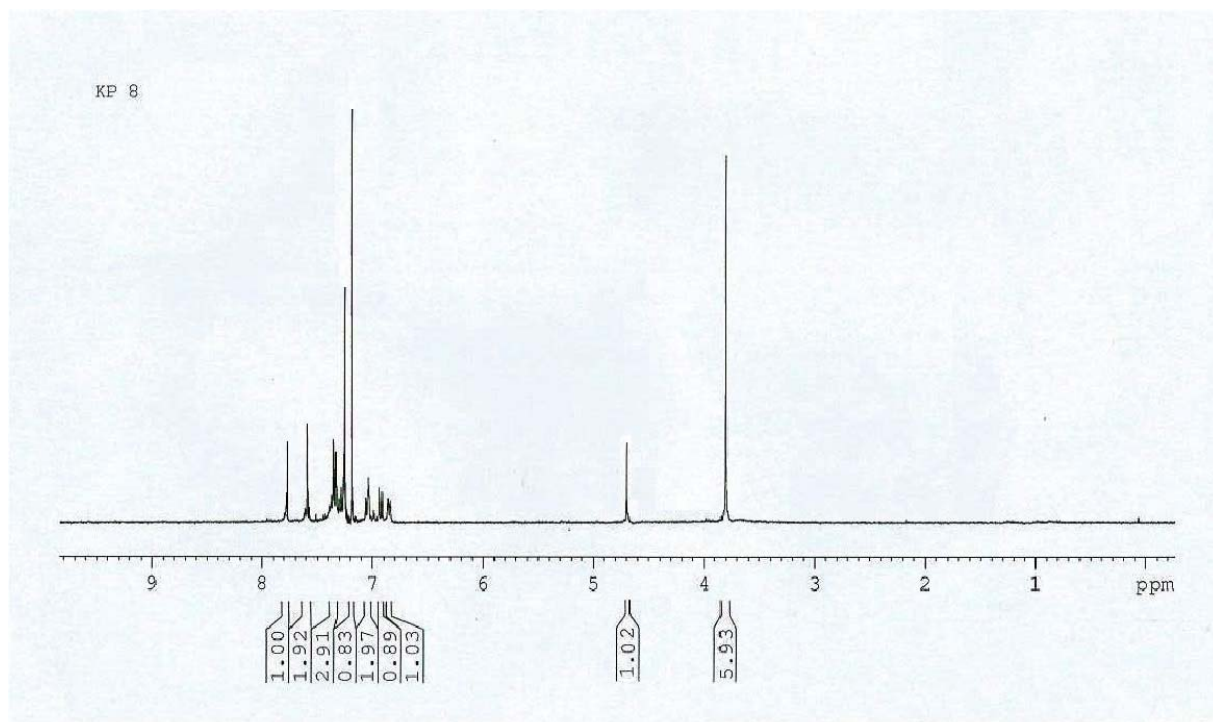
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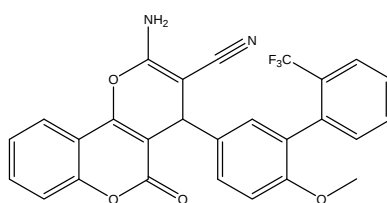


Peak No	RT min	Area	Area %
1	3.180	5.638e+002	1.124
2	3.342	5.615e+003	98.876

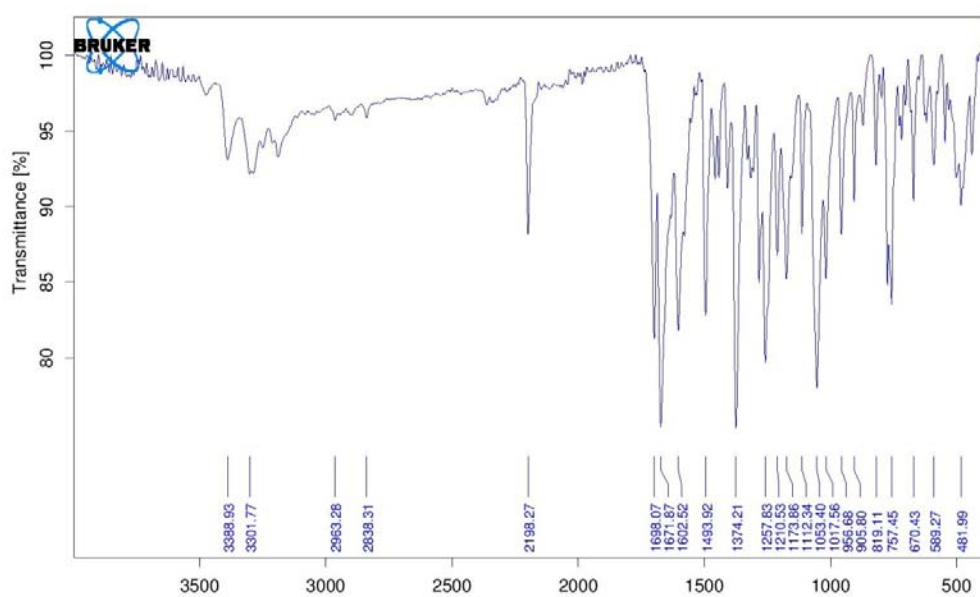


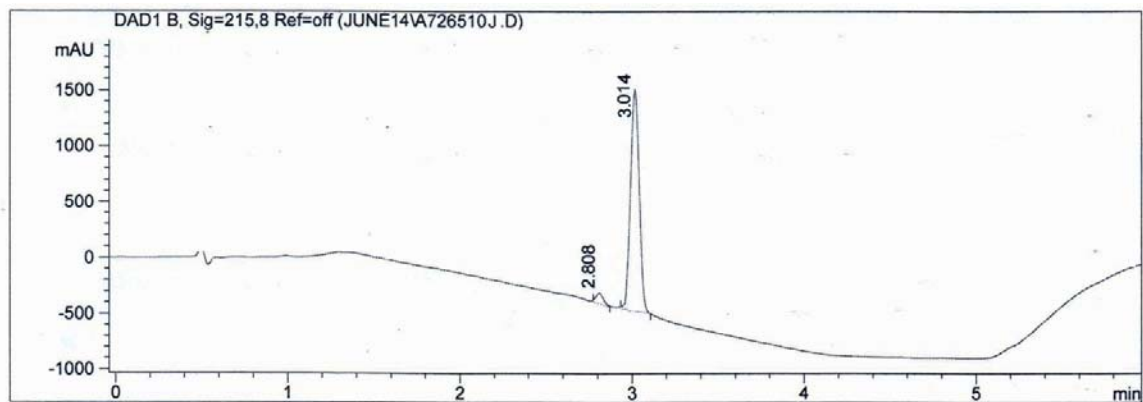


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.311 sec Width 25000.0 Hz 3000 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 40 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 115 minutes	1402373-KP8-13C Solvent: dmsc Ambient temperature Operator: vnmr1 File: 1402373-KP8-13C VNMR5-400 "Agilent-NMR"
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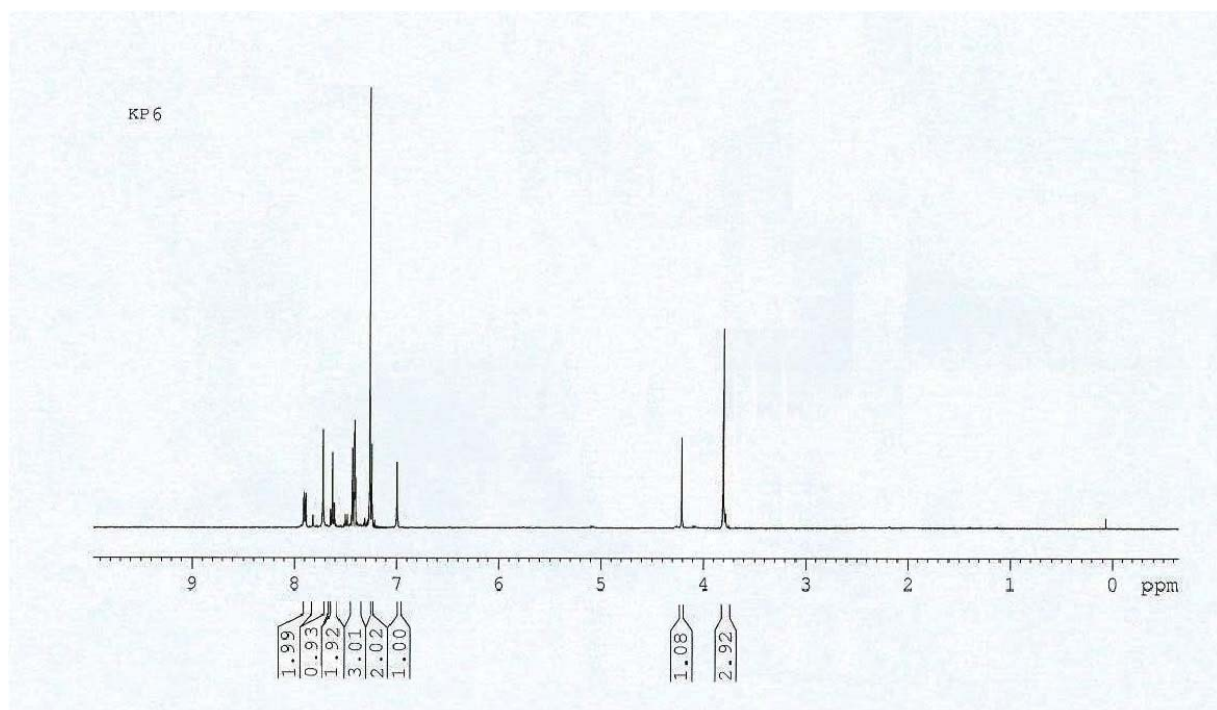
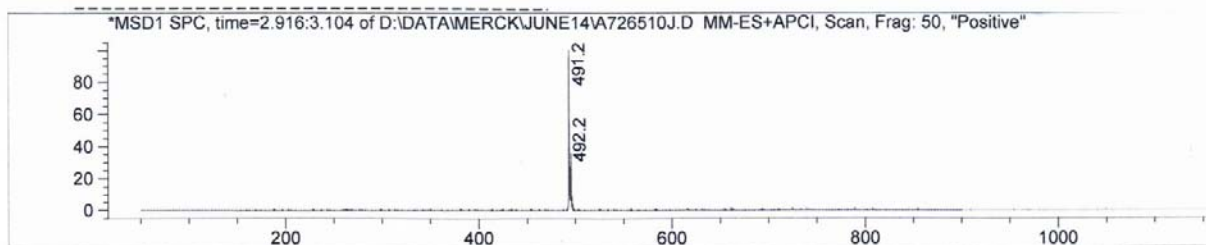


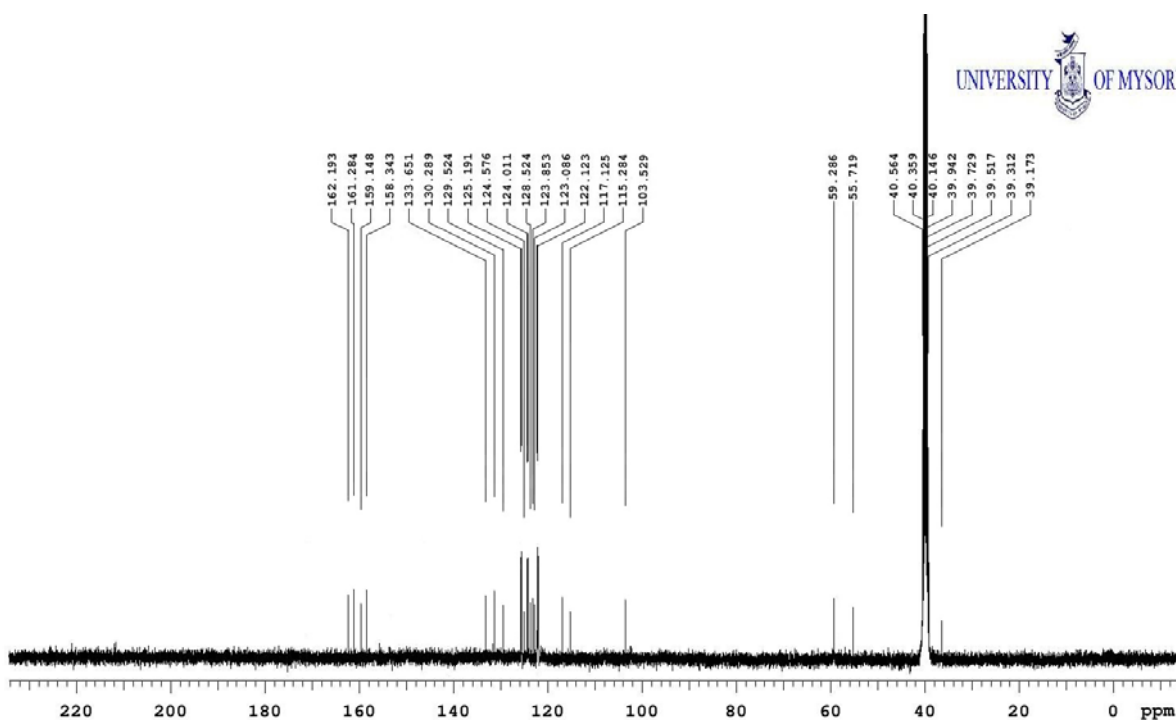
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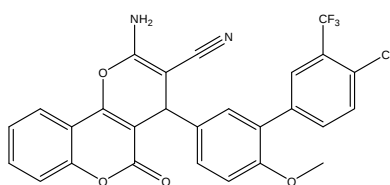


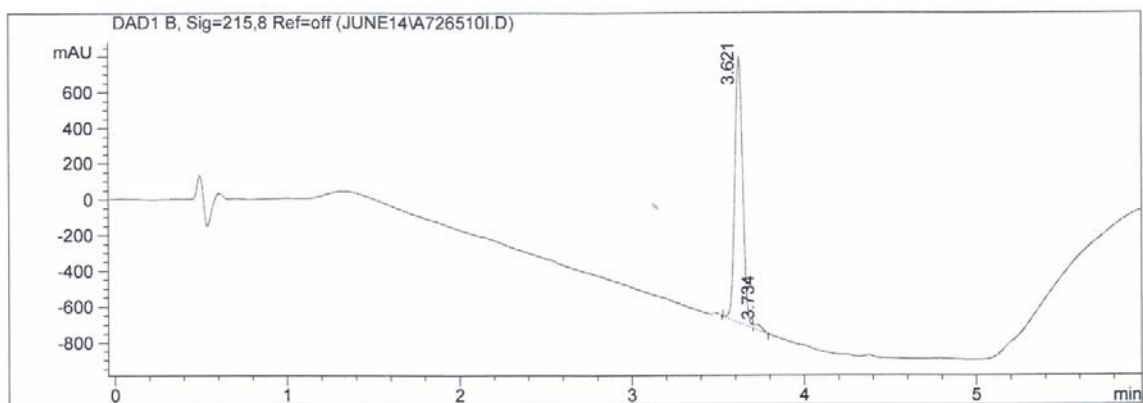
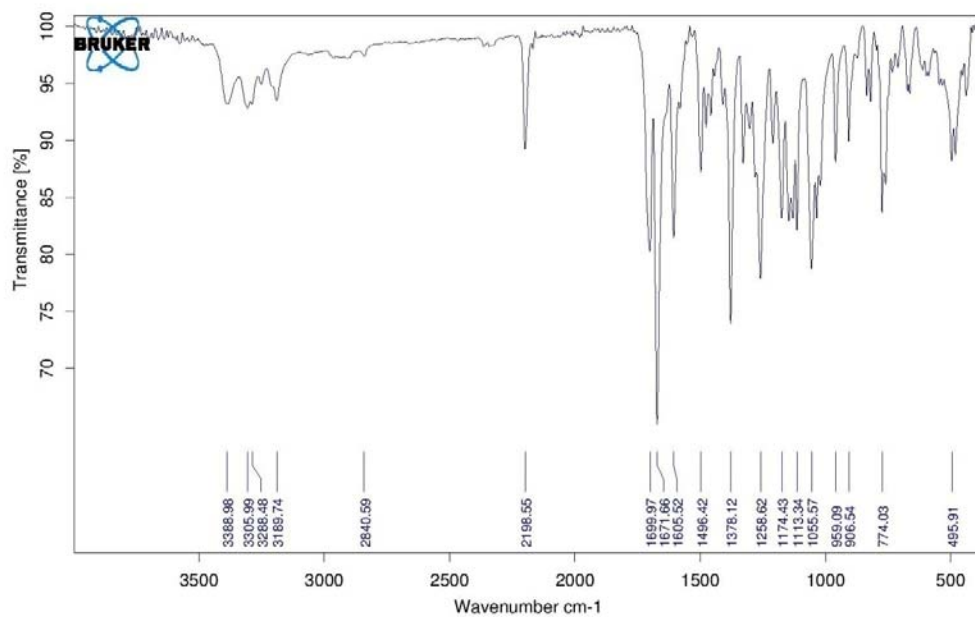
Peak No	RT min	Area	Area %
1	2.808	3.574e+002	1.068
2	3.014	5.282e+001	98.932



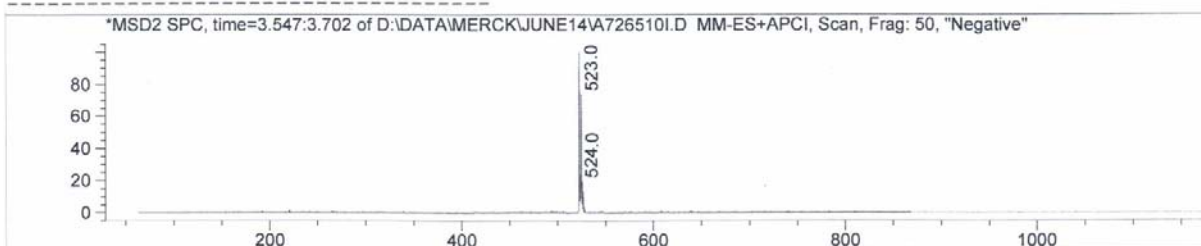


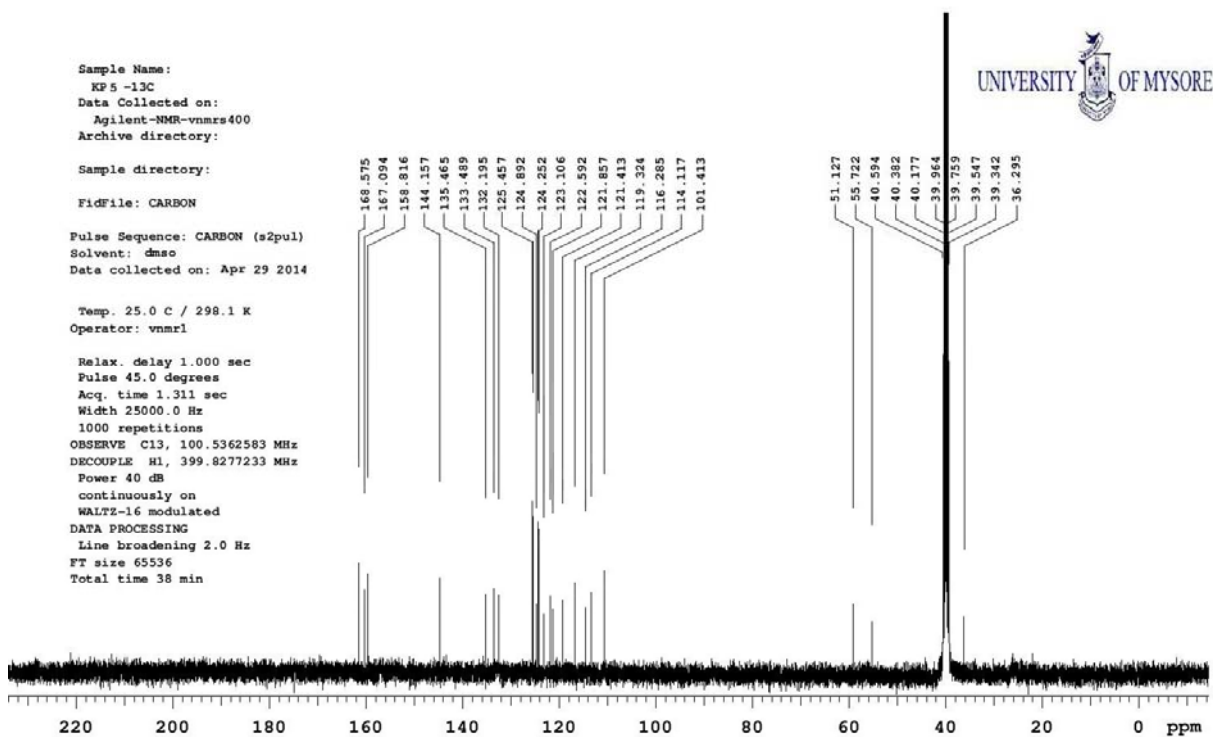
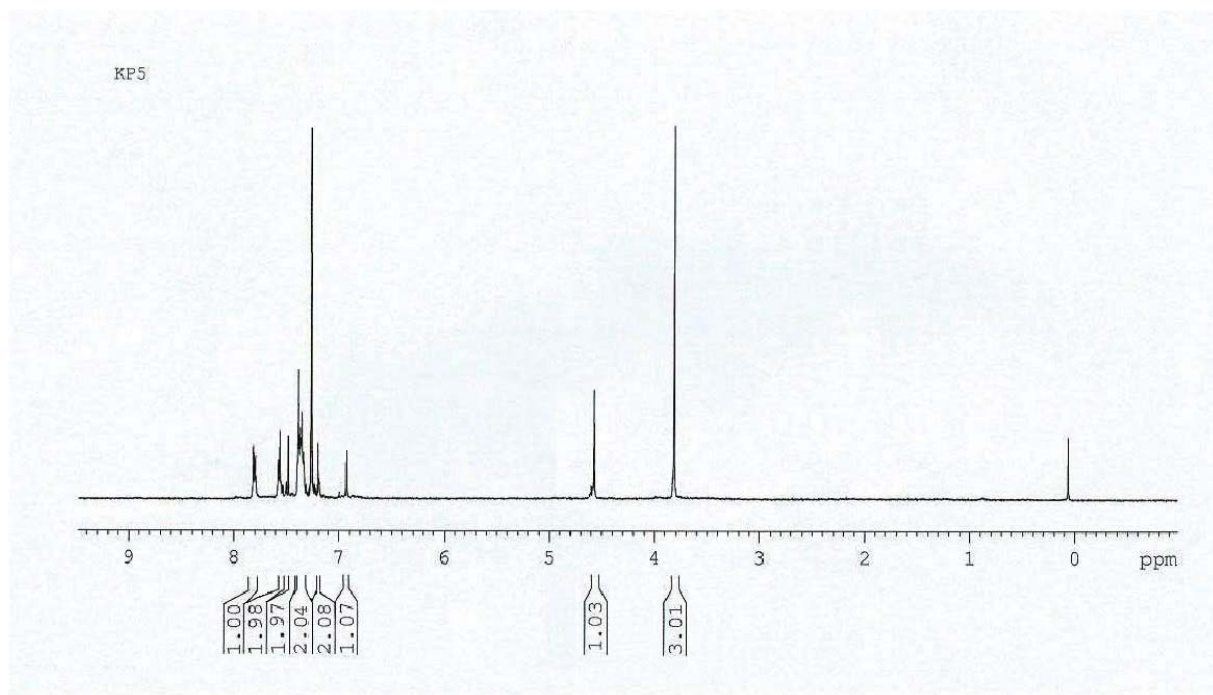
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.311 sec Width 25000.0 Hz 1650 repetitions	OBSERVE C13, 100.5367359 DECOUPLE H1, 399.8296225 Power 40 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536 Total time 63 minutes	1402372-KP-6-13C Solvent: dmsd Ambient temperature Operator: vnmr1 File: 1402372-KP-6-13C VNMR5-400 "Agilent-NMR"
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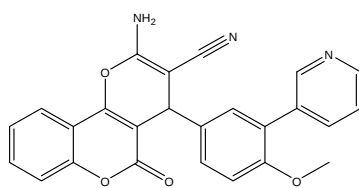




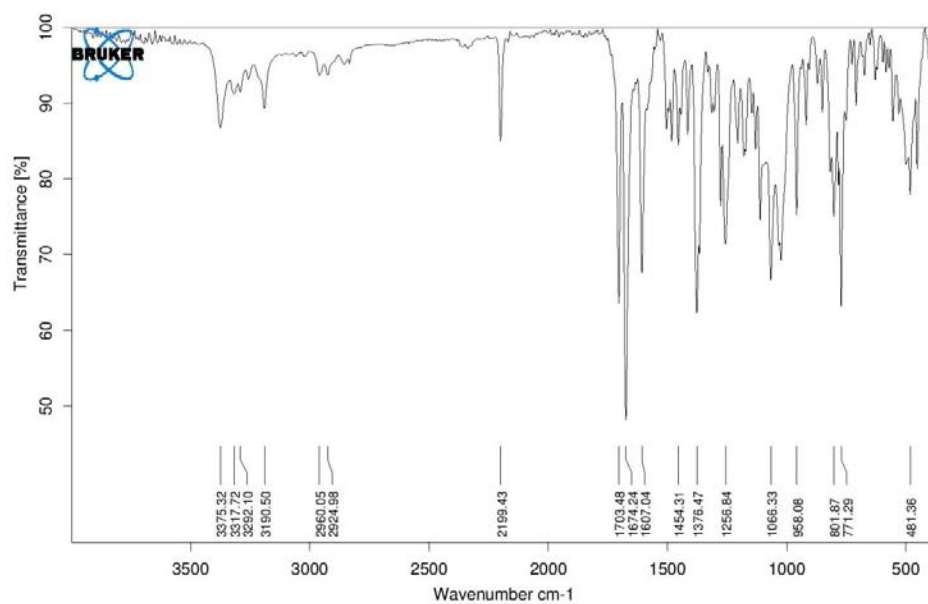
Peak No	RT min	Area	Area %
1	3.621	4.711e+003	98.304
2	3.734	9.092e+001	1.696

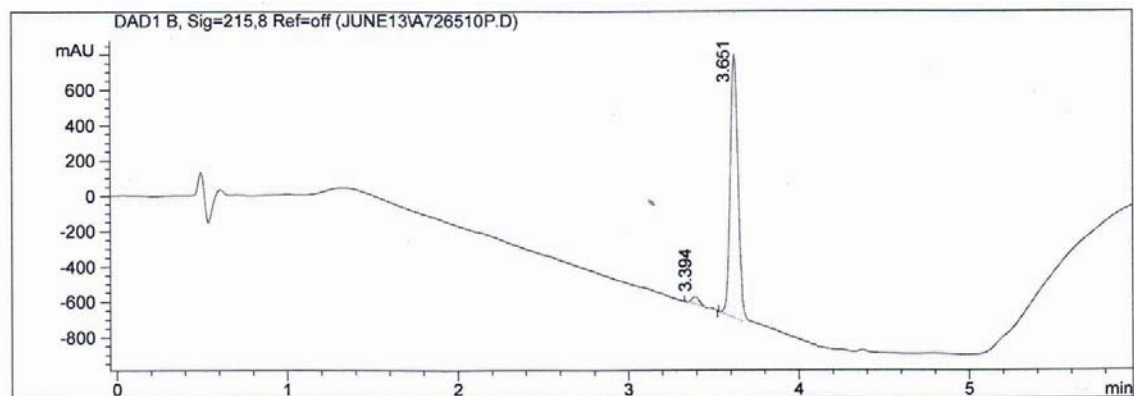




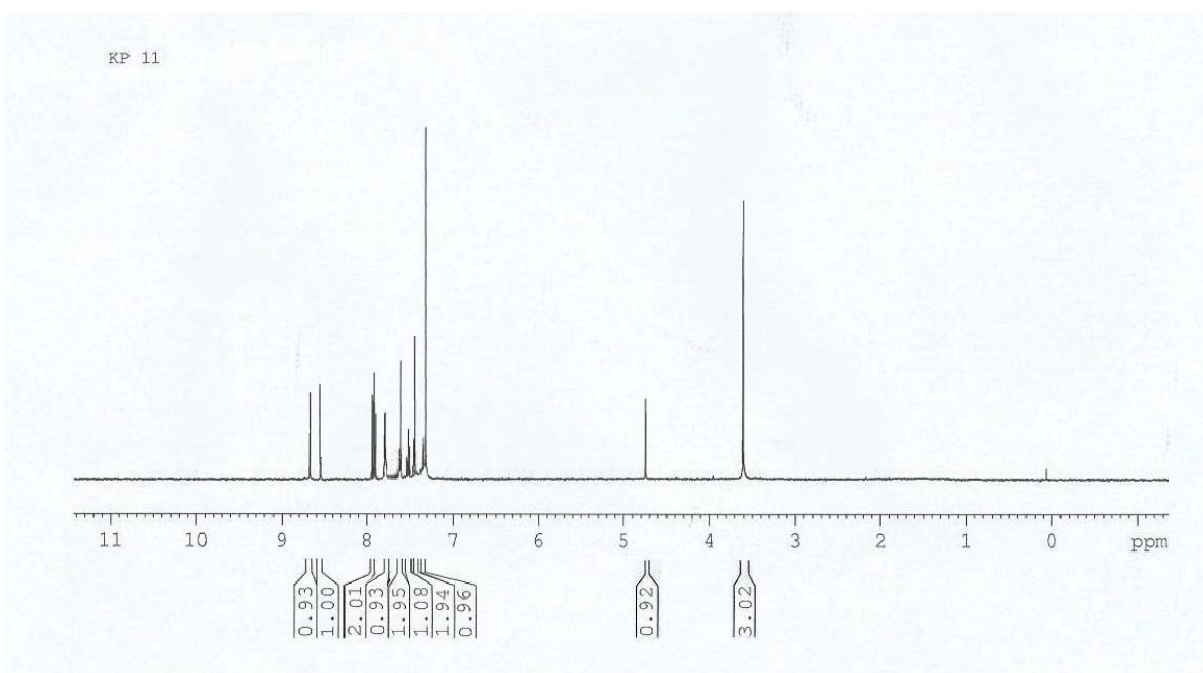
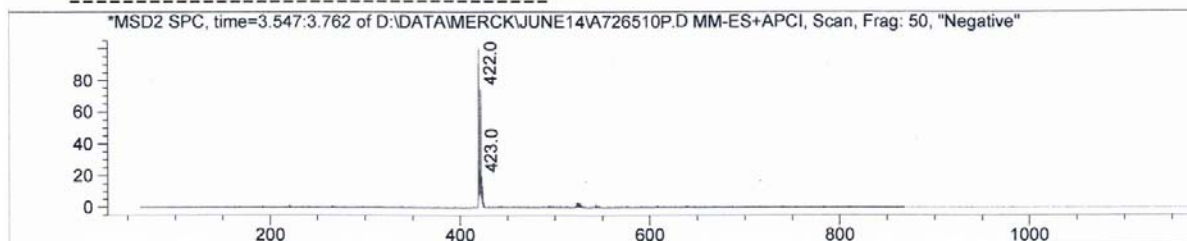


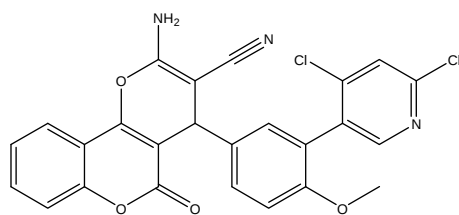
7m



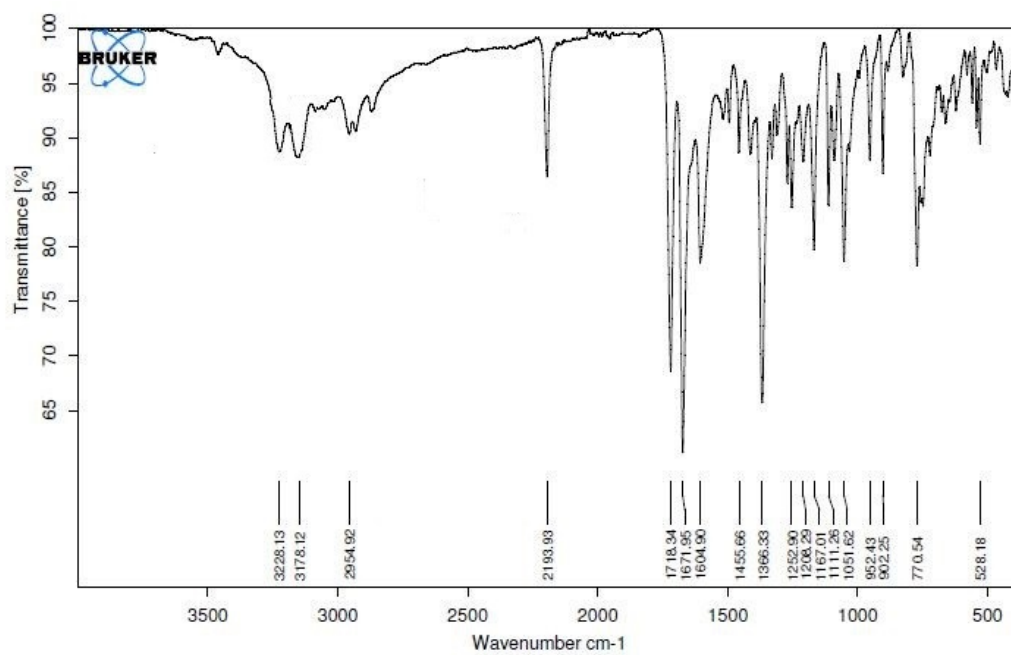


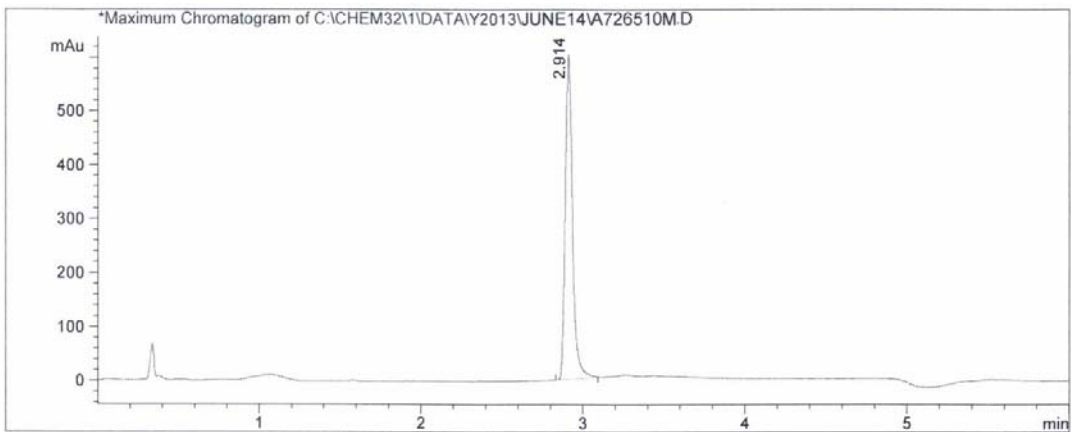
Peak No	RT min	Area	Area %
1	3.394	1.260e+002	1.351
2	3.651	4.711e+003	98.649





7n





Peak No	RT min	Area	Area %
1	2.914	1850.273	100.000

