Supplemental Material

Synthesis of some novel coumarin-pyrimidine hybrid compounds from 8- and 6-acetyl-7-hydroxy-4-methylcoumarin

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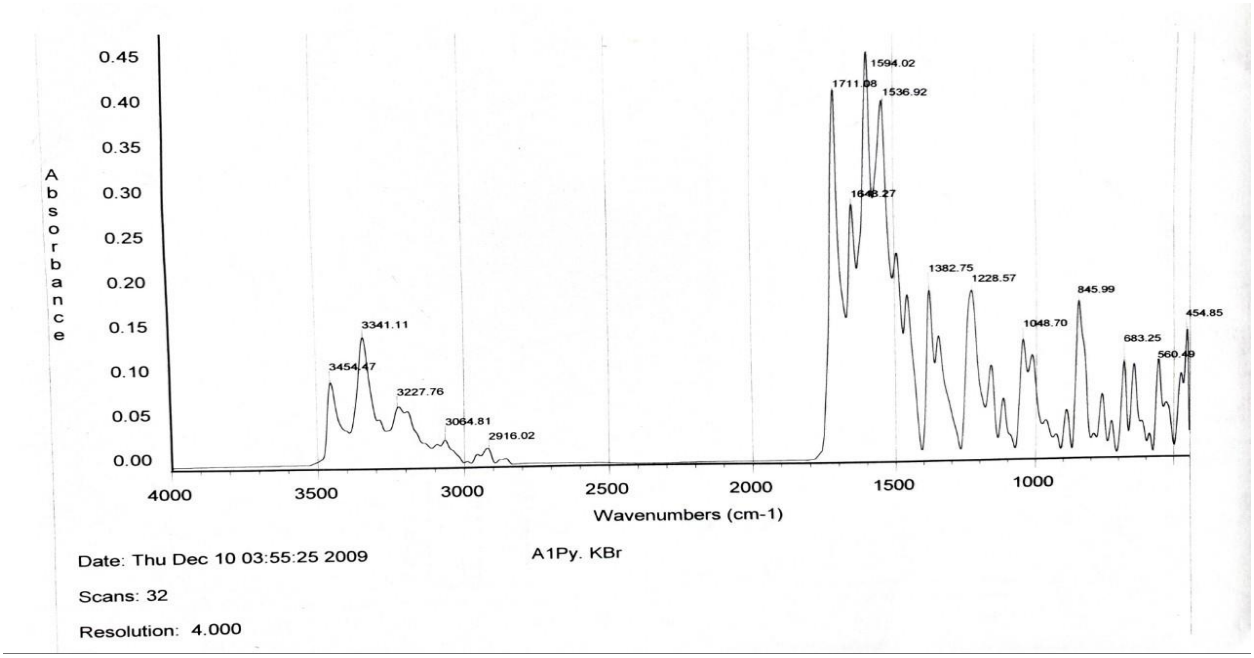
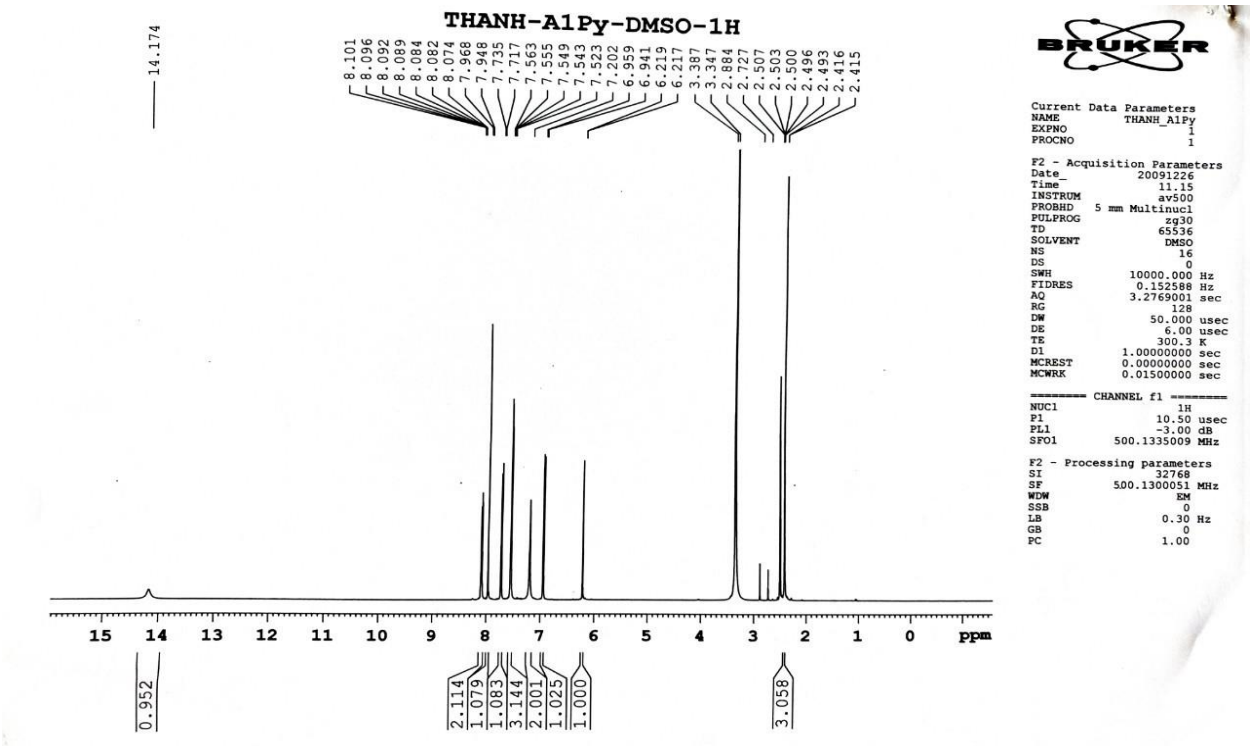
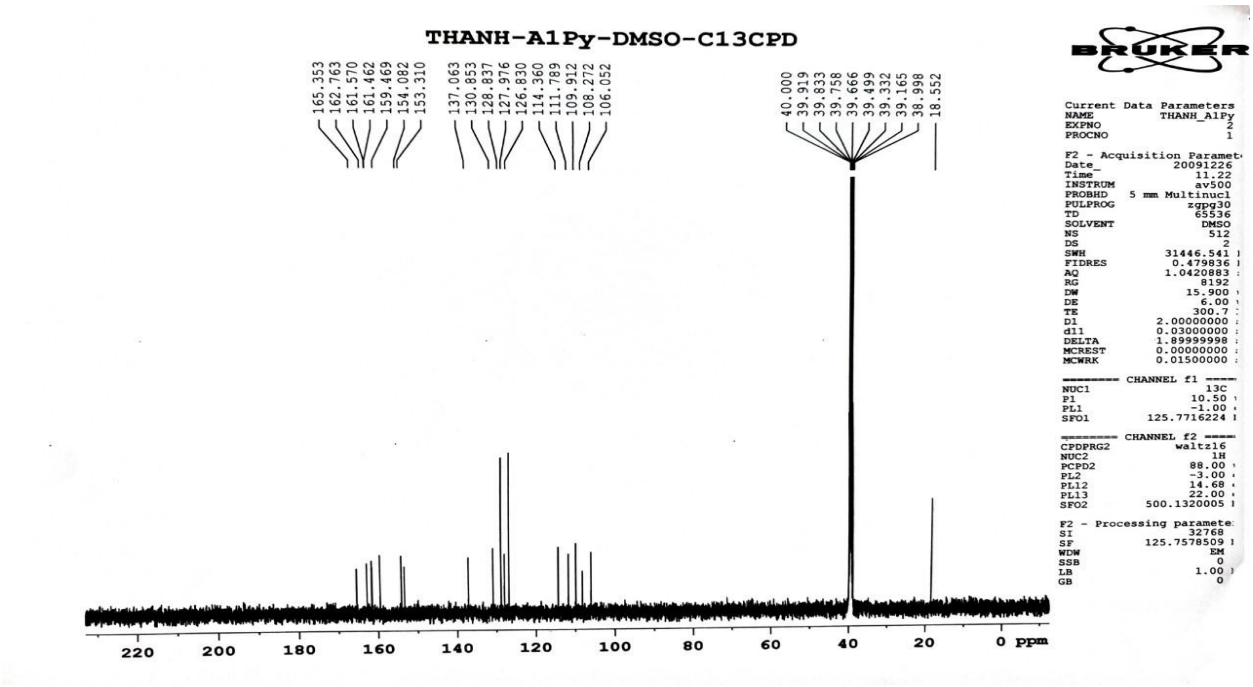
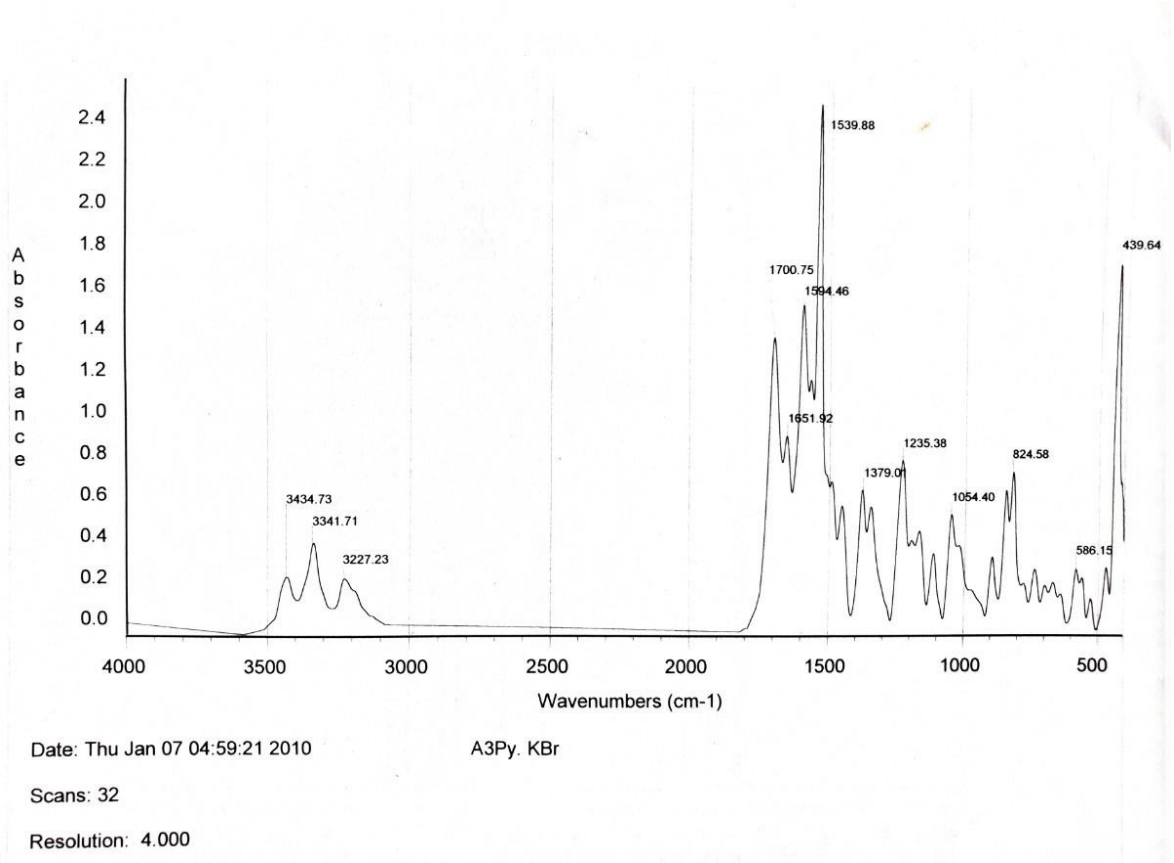
1. IR, NMR spectrum of 8-(2-Amino-6-phenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8a**)

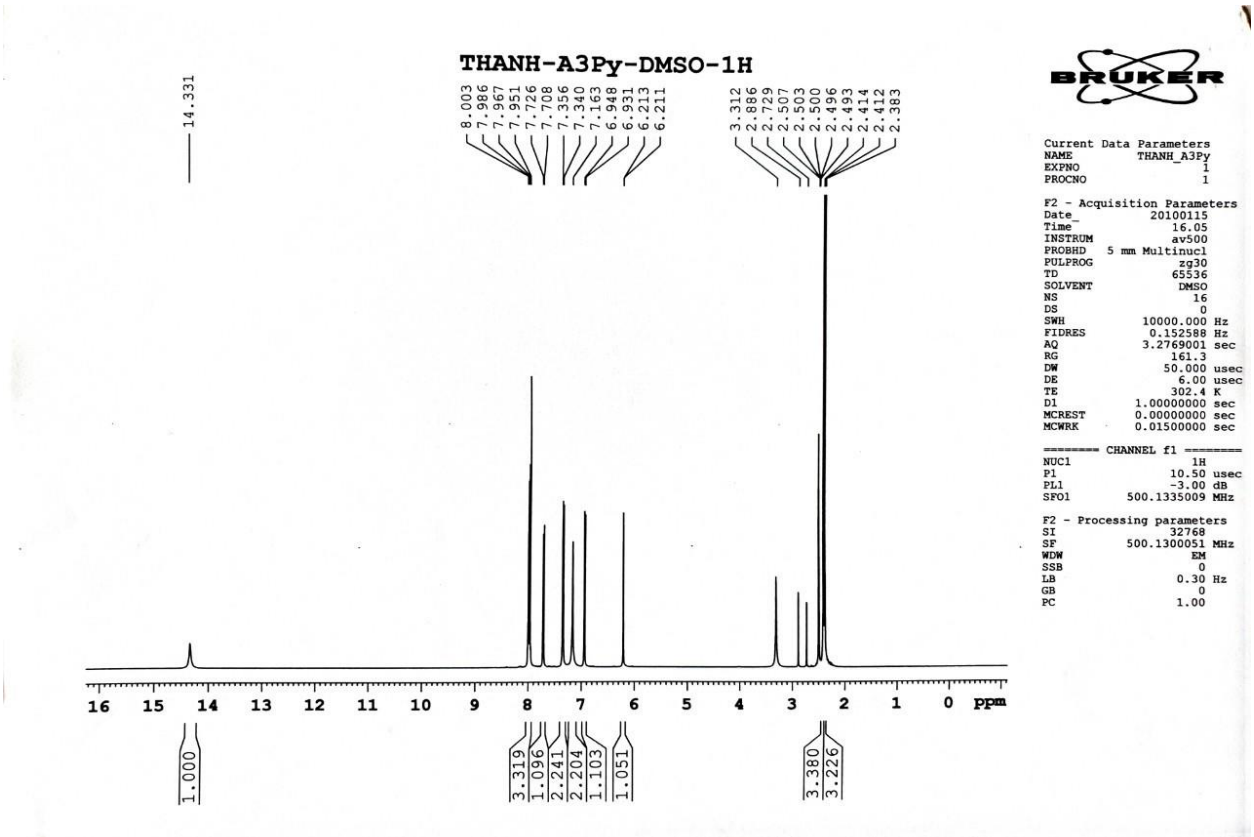






2. IR, NMR and ESI-MS spectrum of 8-(2-Amino-6-p-methoxyphenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8b)**

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7.986
7.967
7.951
7.726
7.708
7.356
7.340
7.163
6.948
6.931
6.213
6.211
3.312
2.886
2.729
2.507
2.503
2.500
2.496
2.493
2.414
2.412
2.383
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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3.319
1.096
2.241
2.204
1.103
1.051
3.380
3.226
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PROCNO 1
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FIDRES 0.152588 Hz
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RG 161.3
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DE 6.00 usec
TE 302.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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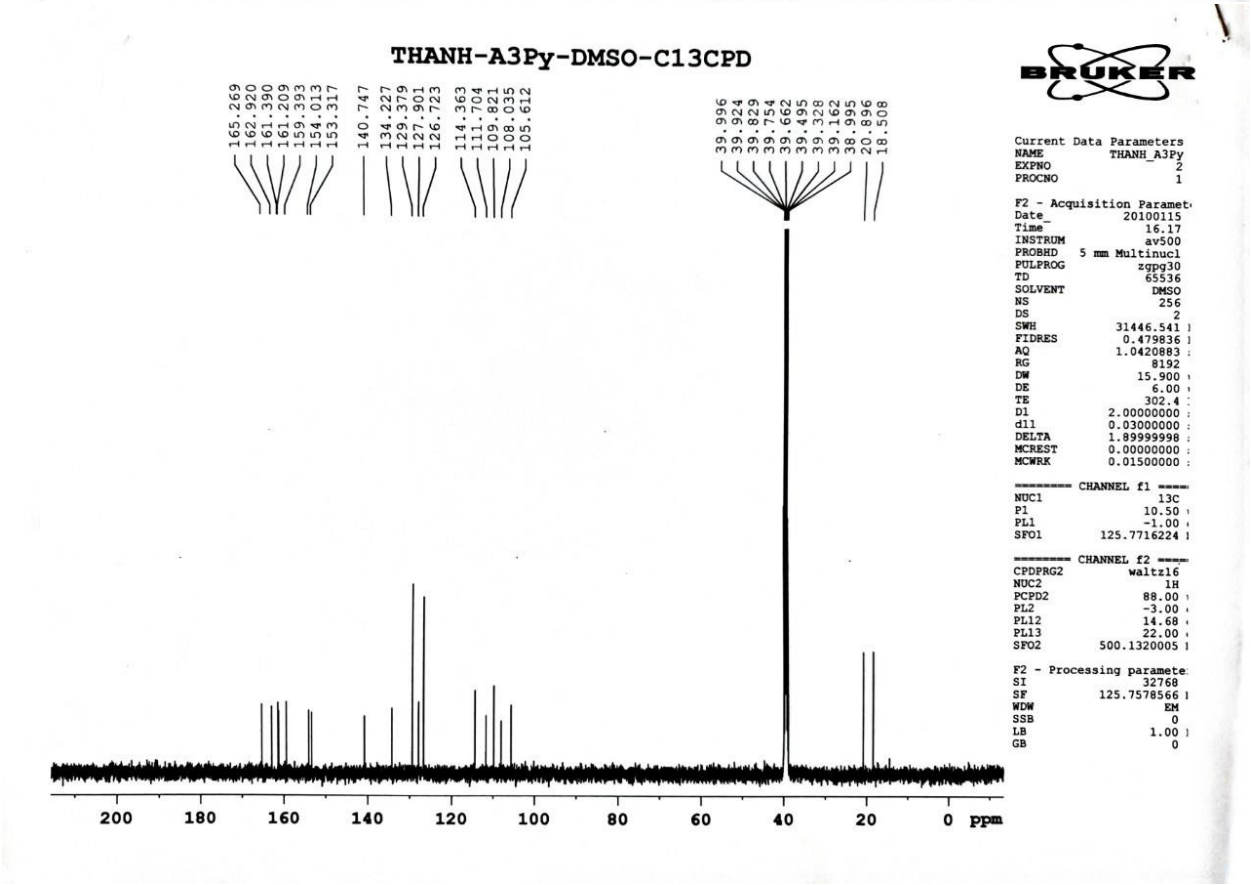
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127.901
126.723
114.363
111.704
109.821
108.035
105.612
39.996
39.924
39.829
39.754
39.662
39.495
39.328
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18.508
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TE 302.4
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PL1 -1.00
SFO1 125.7716224
======== CHANNEL f2 ========
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NUC2 1H
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PL2 -3.00
PL12 14.68
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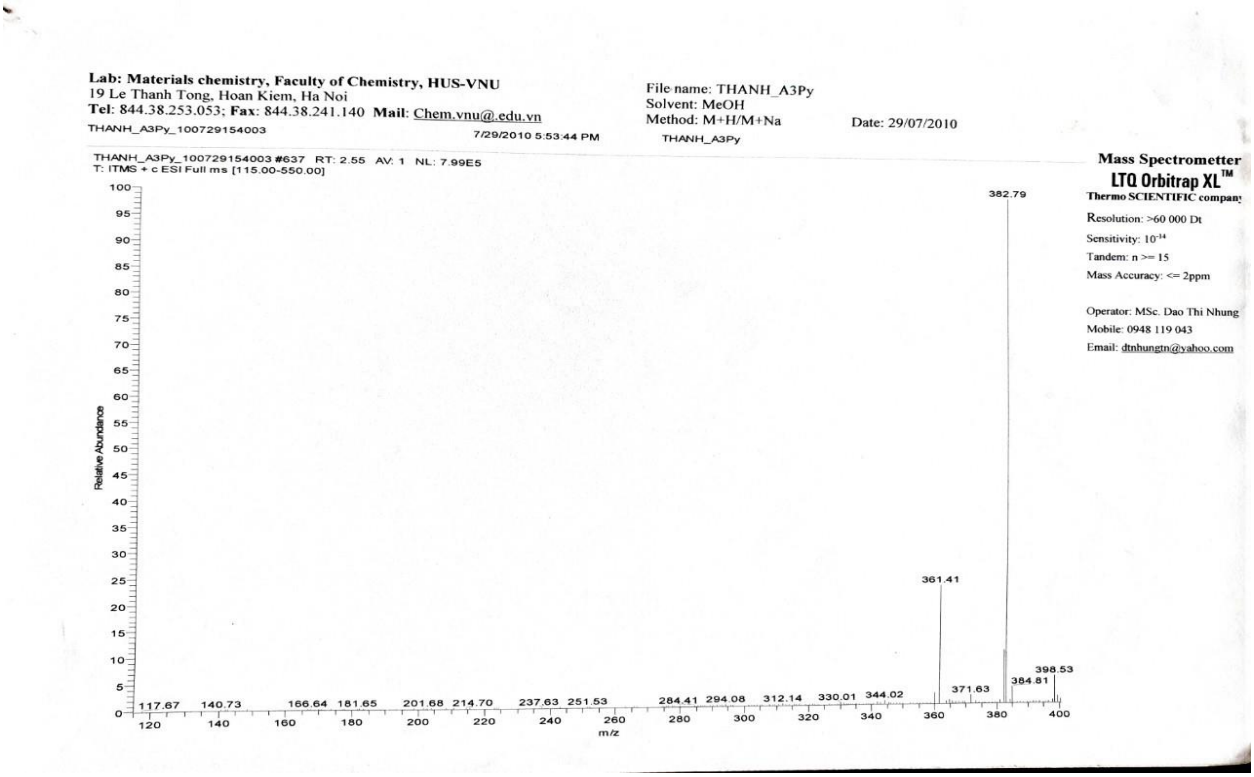
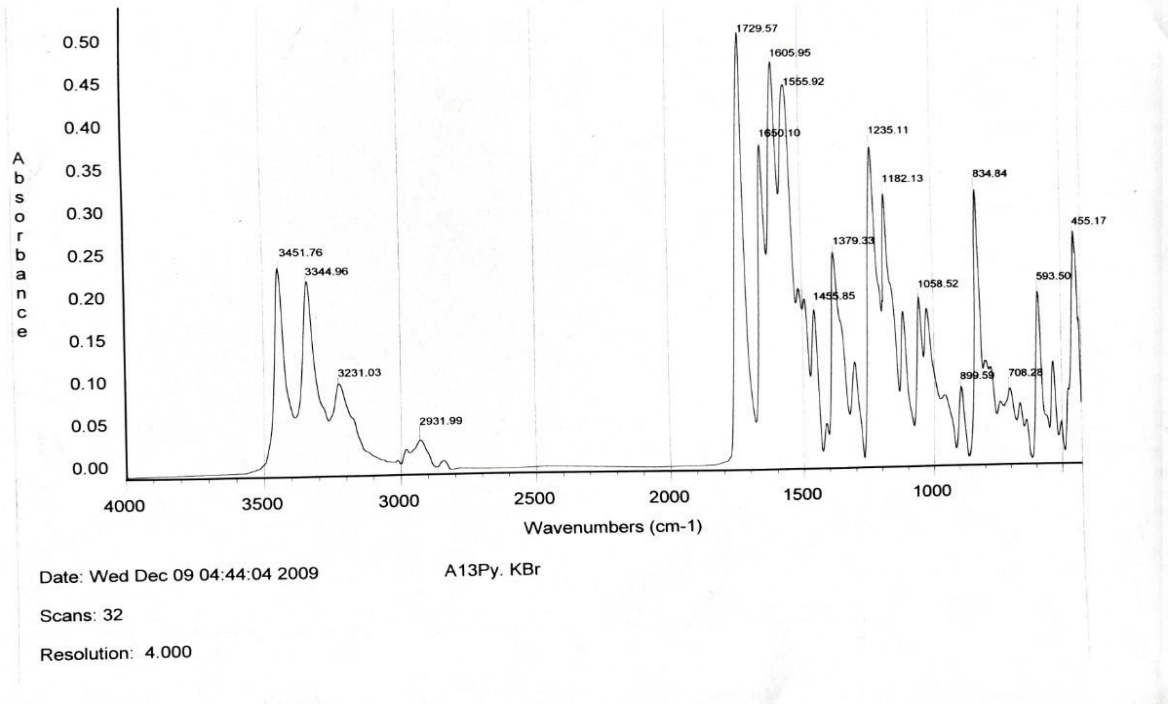
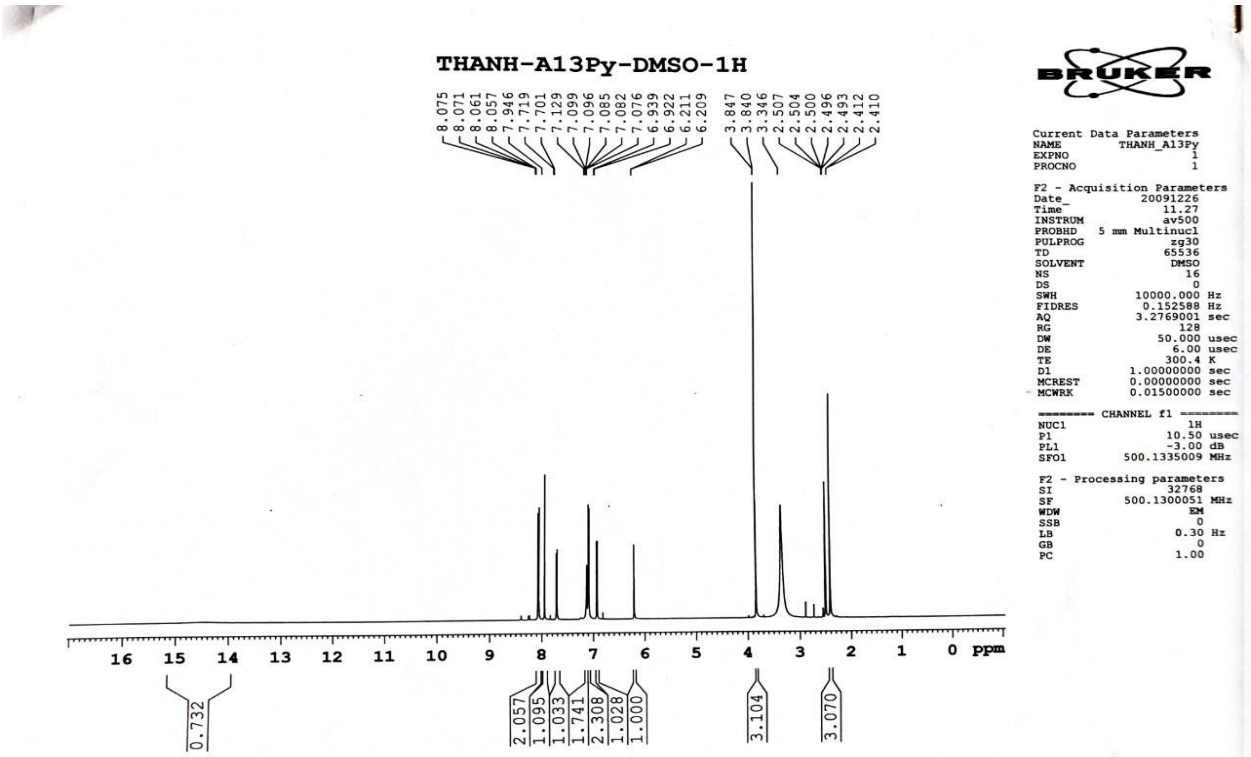


3. IR, NMR and ESI-MS spectrum of 8-(2-Amino-6-p-methoxyphenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8c)**

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8.061
8.057
7.946
7.719
7.701
7.129
7.099
7.096
7.085
7.082
7.076
6.939
6.922
6.211
6.209
3.847
3.840
3.346
2.507
2.504
2.500
2.496
2.493
2.412
2.410
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.732
2.057
1.095
1.033
1.741
2.308
1.028
1.000
3.104
3.070
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FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 300.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
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P1 10.50 usec
PL1 -3.00 dB
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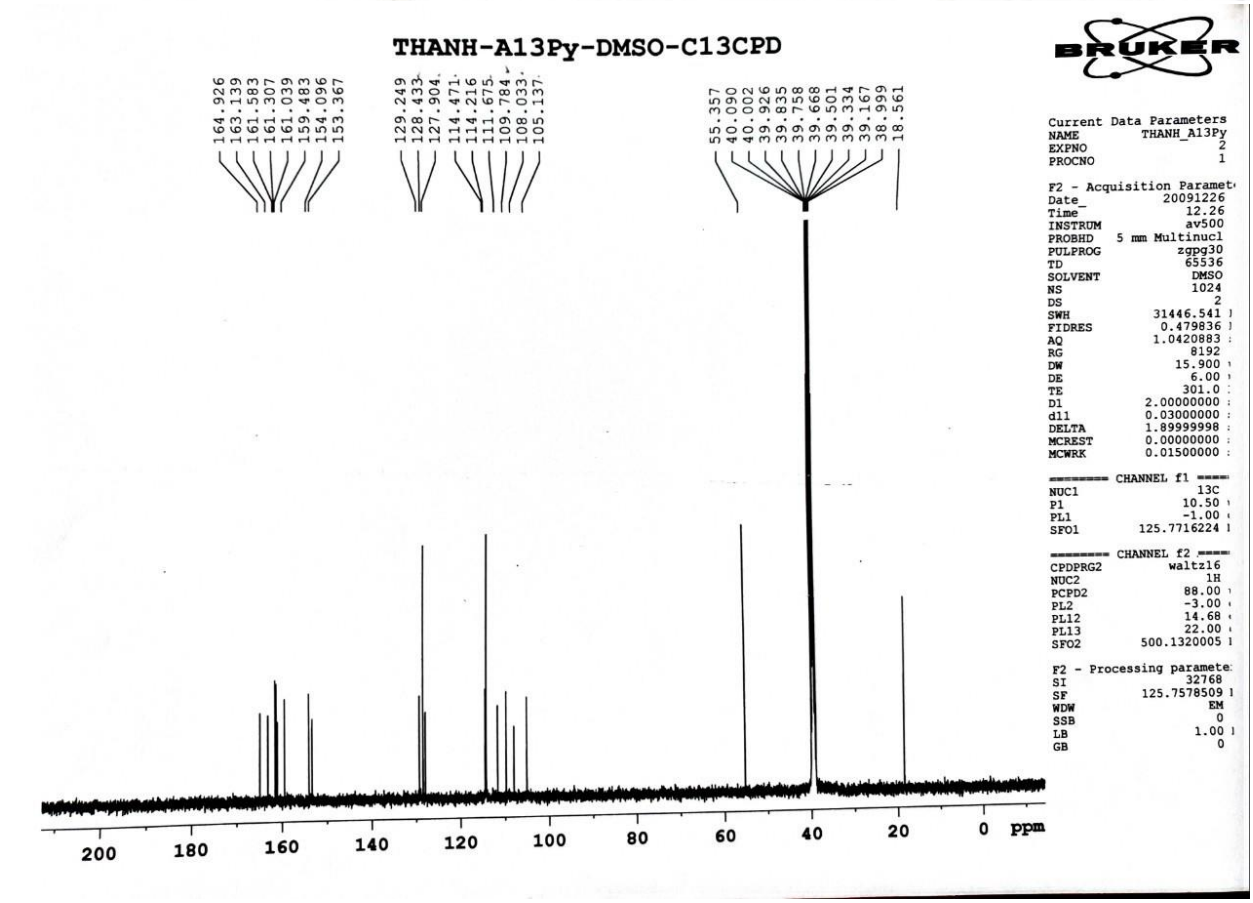
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129.249
128.433
127.904
114.471
114.216
111.675
109.784
108.033
105.137
55.357
40.090
40.002
39.926
39.835
39.758
39.668
39.501
39.334
39.167
38.999
18.561
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
Current Data Parameters
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PROCNO 1
F2 - Acquisition Paramet
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Time 12.26
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
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FIDRES 0.479836
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RG 8192
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DE 6.00
TE 301.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
CHANNEL f1
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
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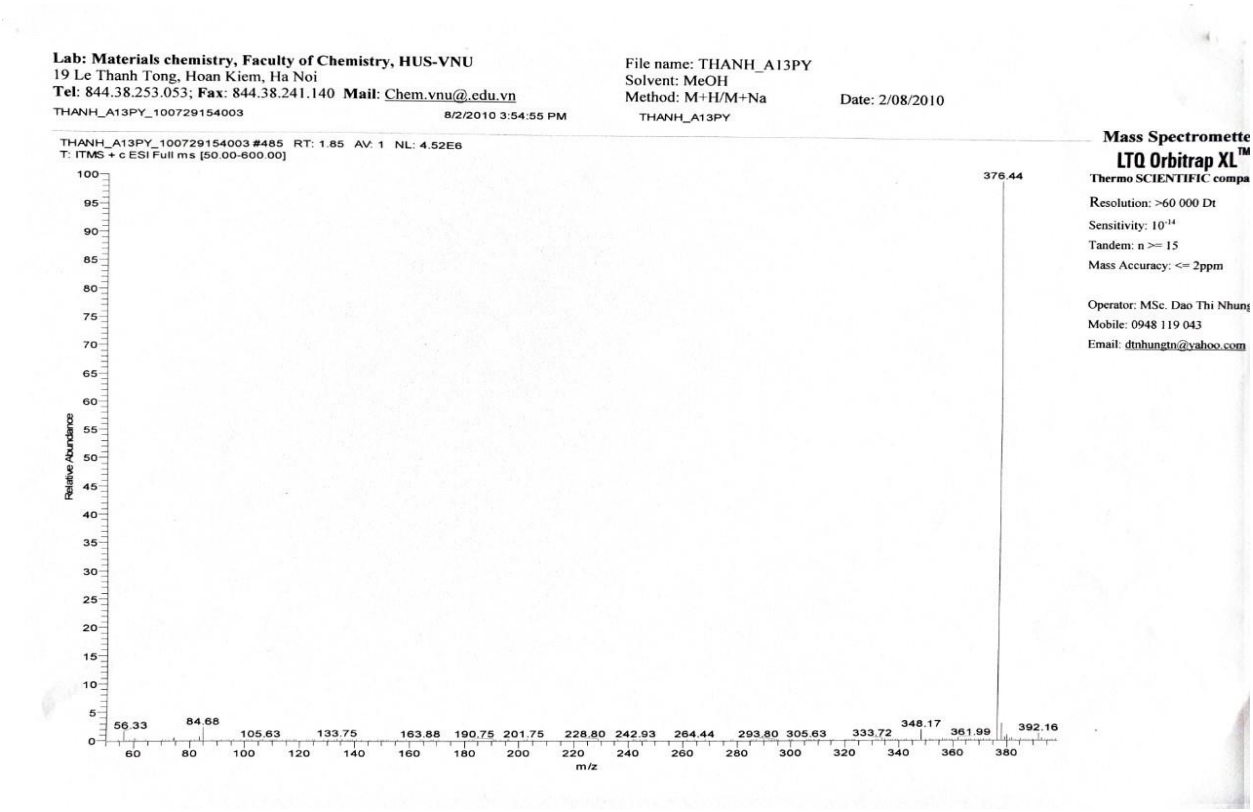
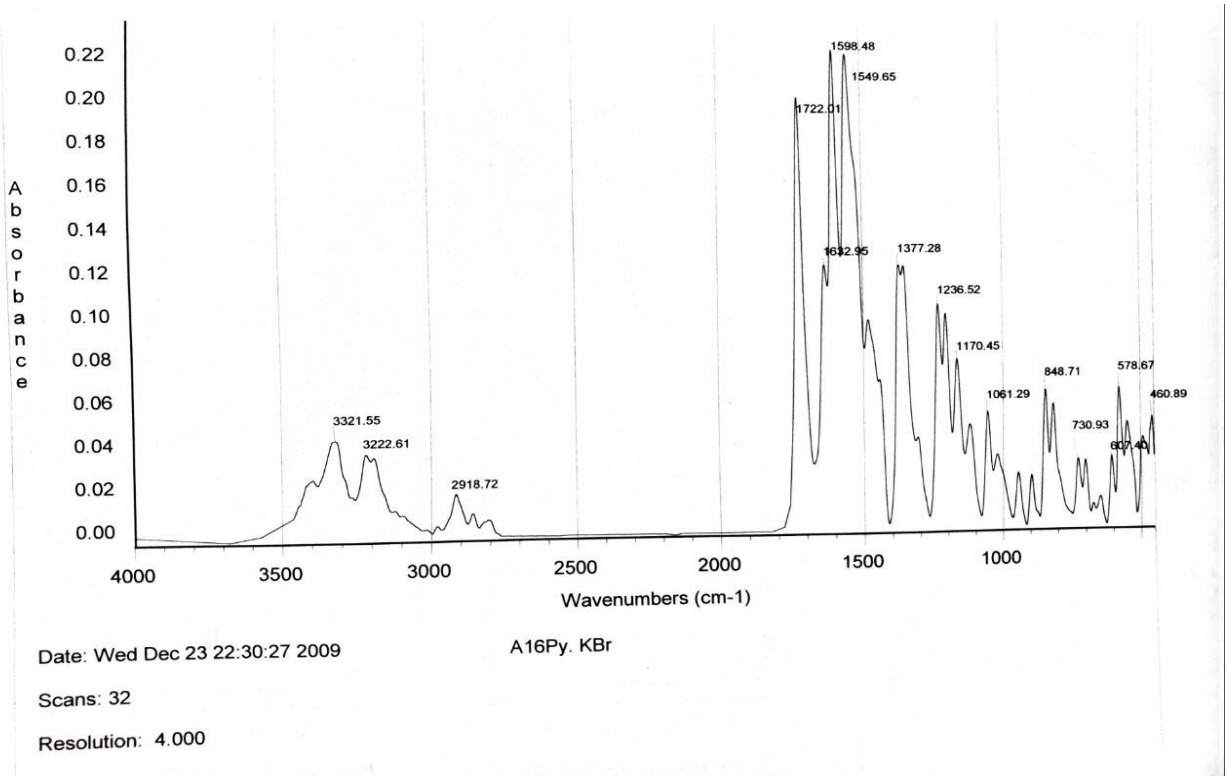
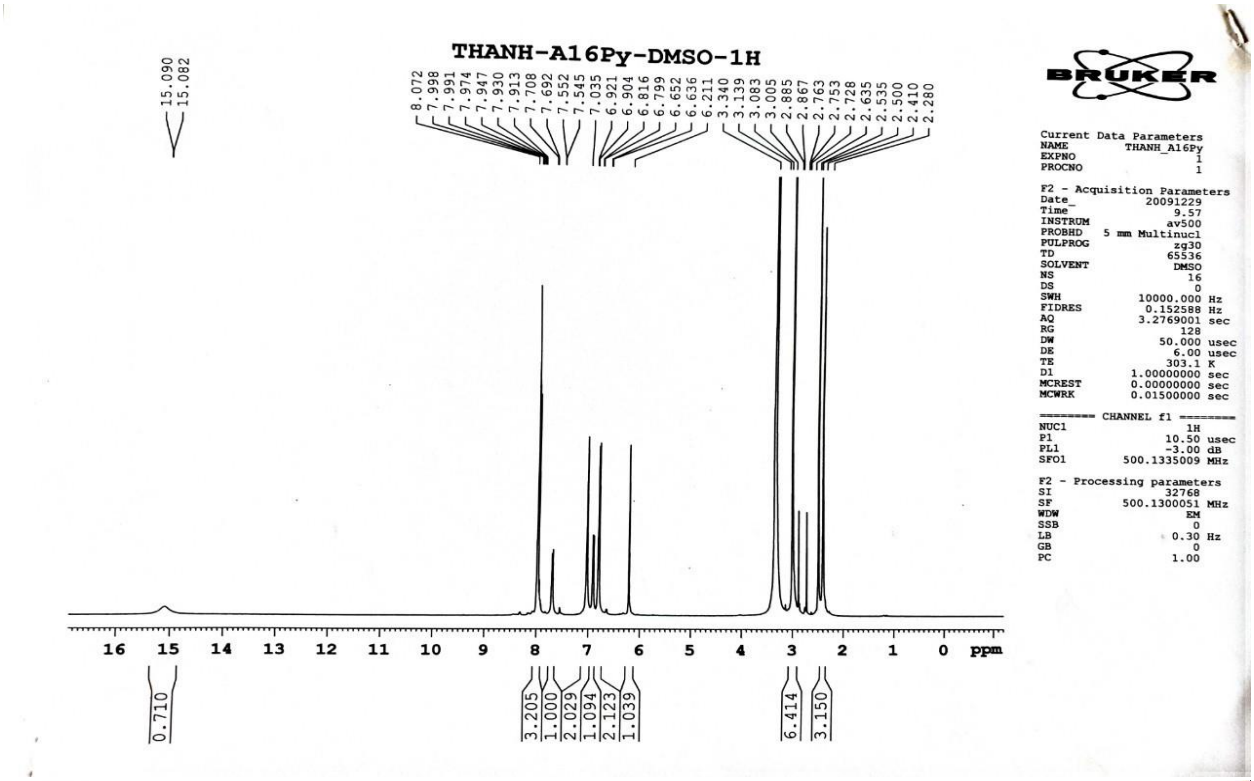


4. IR, NMR spectrum of 8-(2-Amino-6-p-N,N-dimethylaminophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8d)**

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15.082
8.072
7.998
7.991
7.974
7.947
7.930
7.913
7.708
7.692
7.552
7.545
7.035
6.921
6.904
6.816
6.799
6.652
6.636
6.211
3.340
3.139
3.083
3.005
2.885
2.867
2.763
2.753
2.728
2.635
2.535
2.500
2.410
2.280
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.710
3.205
1.000
2.029
1.094
2.123
1.039
6.414
3.150
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RG 128
DW 50.000 usec
DE 6.00 usec
TE 303.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz
F2 - Processing parameters
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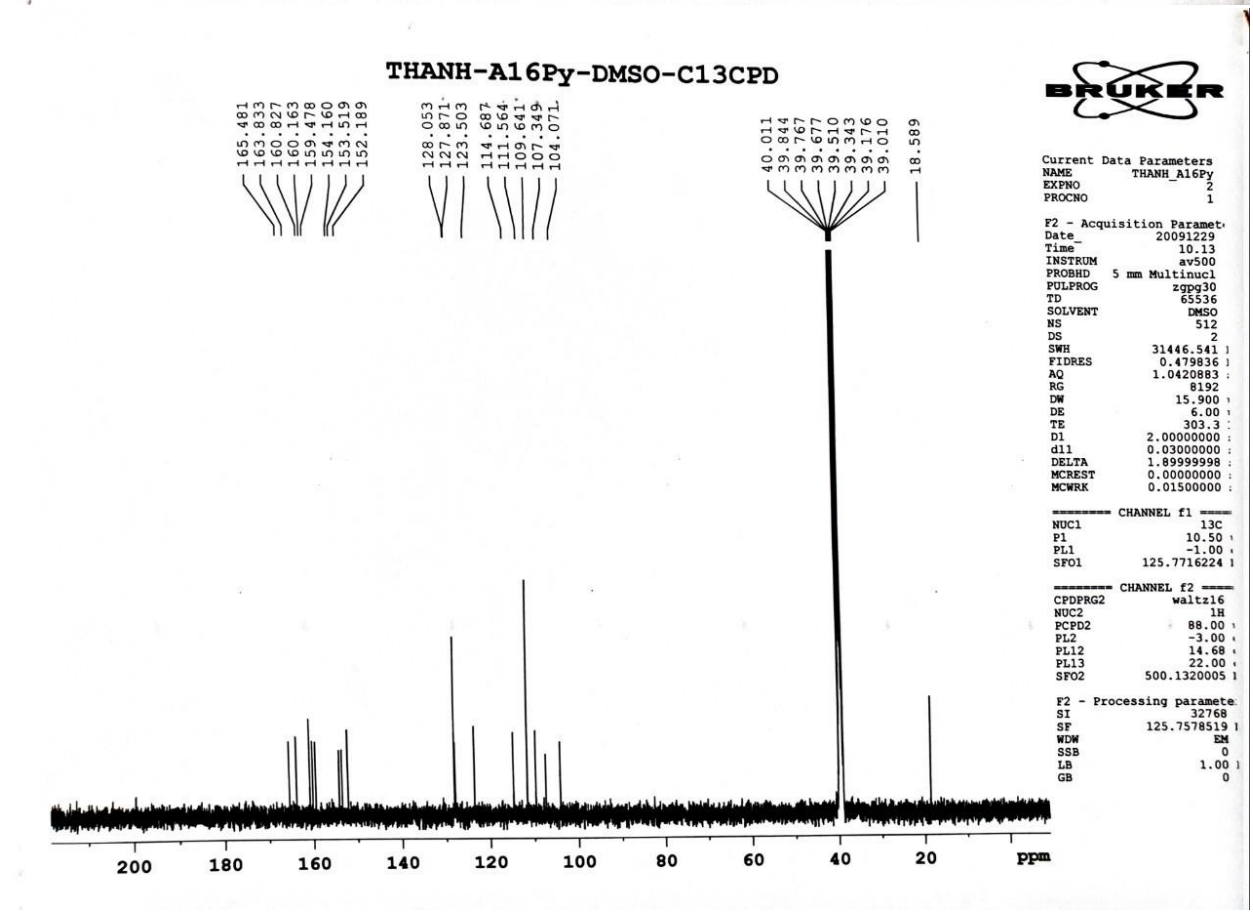
SF 500.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


THANH-A16Py-DMSO-C13CPD
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163.833
160.827
160.163
159.478
154.160
153.519
152.189
128.053
127.871
123.503
114.687
111.564
109.641
107.349
104.071
40.011
39.844
39.767
39.677
39.510
39.343
39.176
39.010
18.589
200 180 160 140 120 100 80 60 40 20 ppm
BRUKER
Current Data Parameters
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PROCNO 1
F2 - Acquisition Paramet
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SOLVENT DMSO
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RG 8192
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DE 6.00
TE 303.3
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
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P1 10.50
PL1 -1.00
SFO1 125.7716224
======== CHANNEL f2 ========
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NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005
F2 - Processing paramete
SI 32768
SF 125.7578519
WDW EM
SSB 0
LB 1.00
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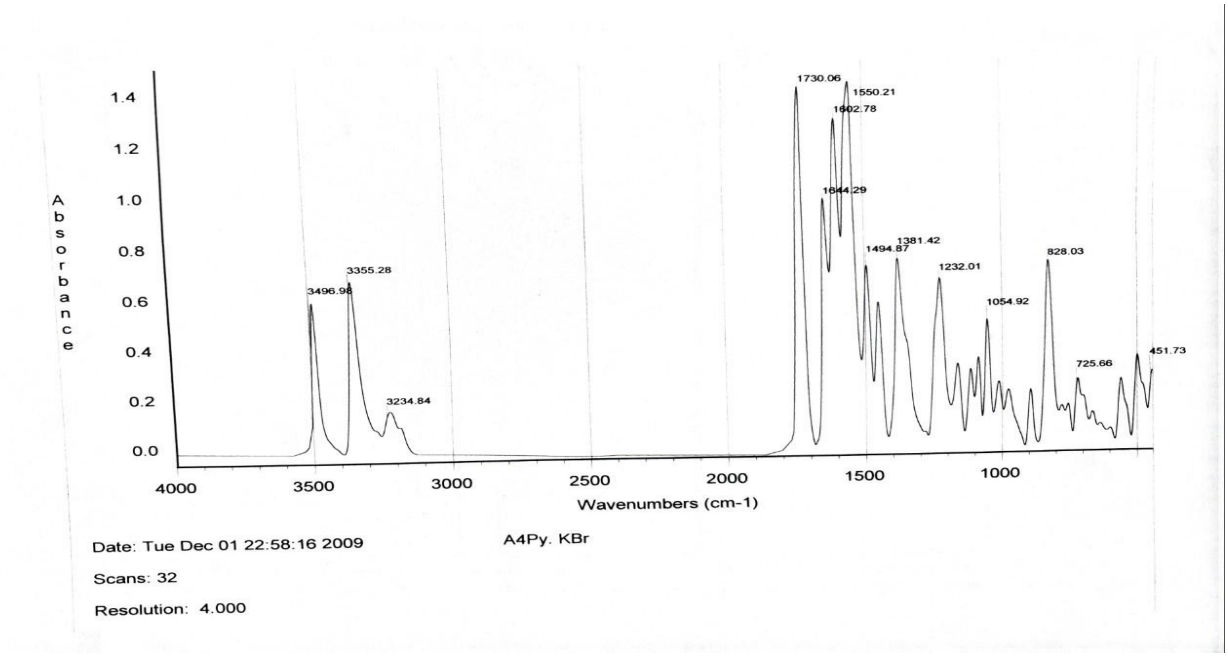
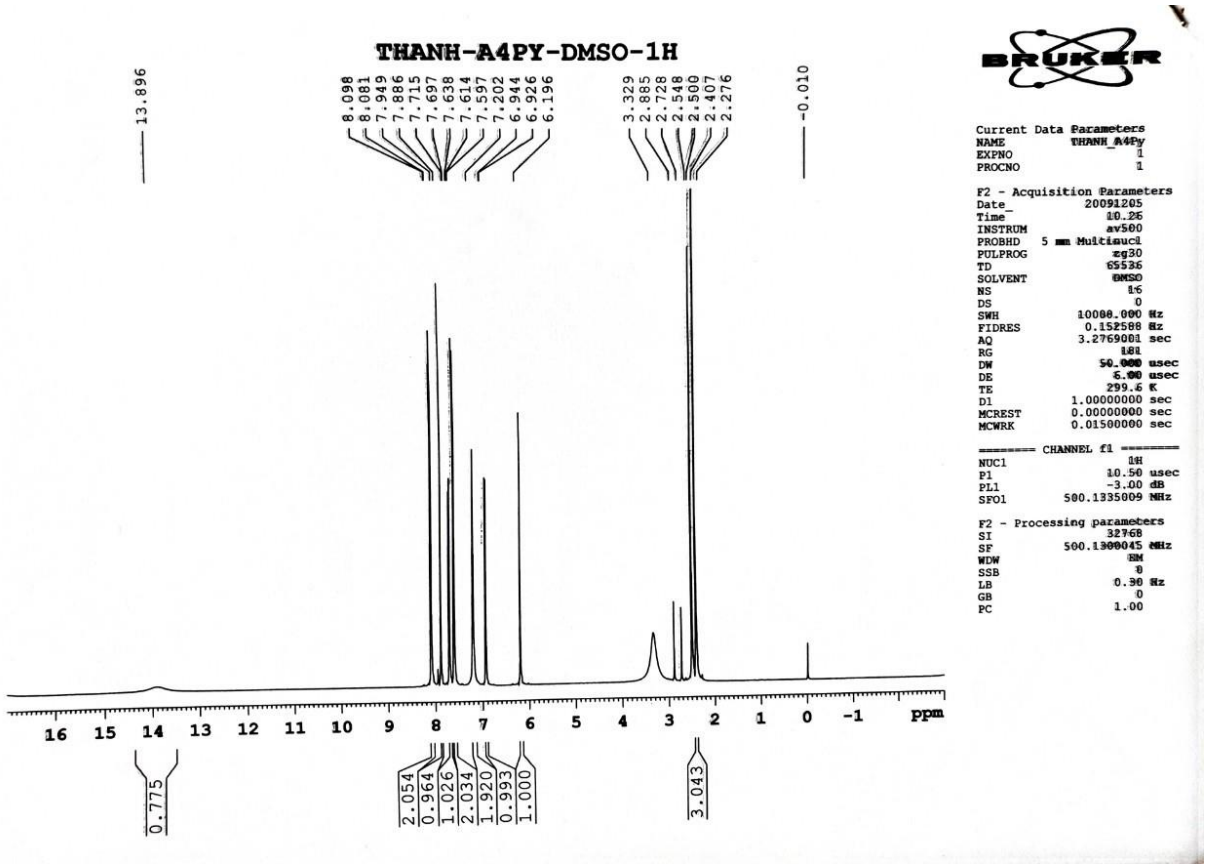
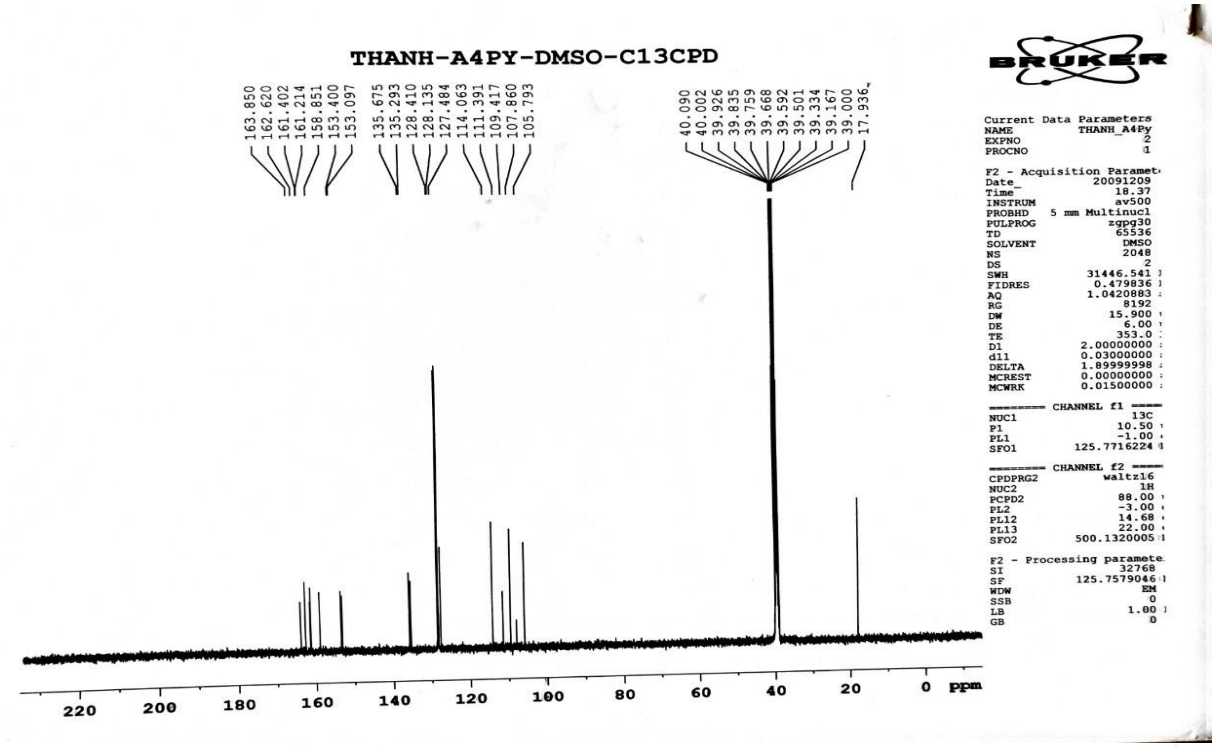
5. IR, NMR and ESI-MS spectrum of 8-(2-Amino-6-p-chlorophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8e)**



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161.402
161.214
158.851
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153.097
135.675
135.293
128.410
128.135
127.484
114.063
111.391
109.417
107.860
105.793
40.090
40.002
39.926
39.835
39.759
39.668
39.592
39.501
39.334
39.167
39.000
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200
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RG 8192
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DE 6.00
TE 353.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
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NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
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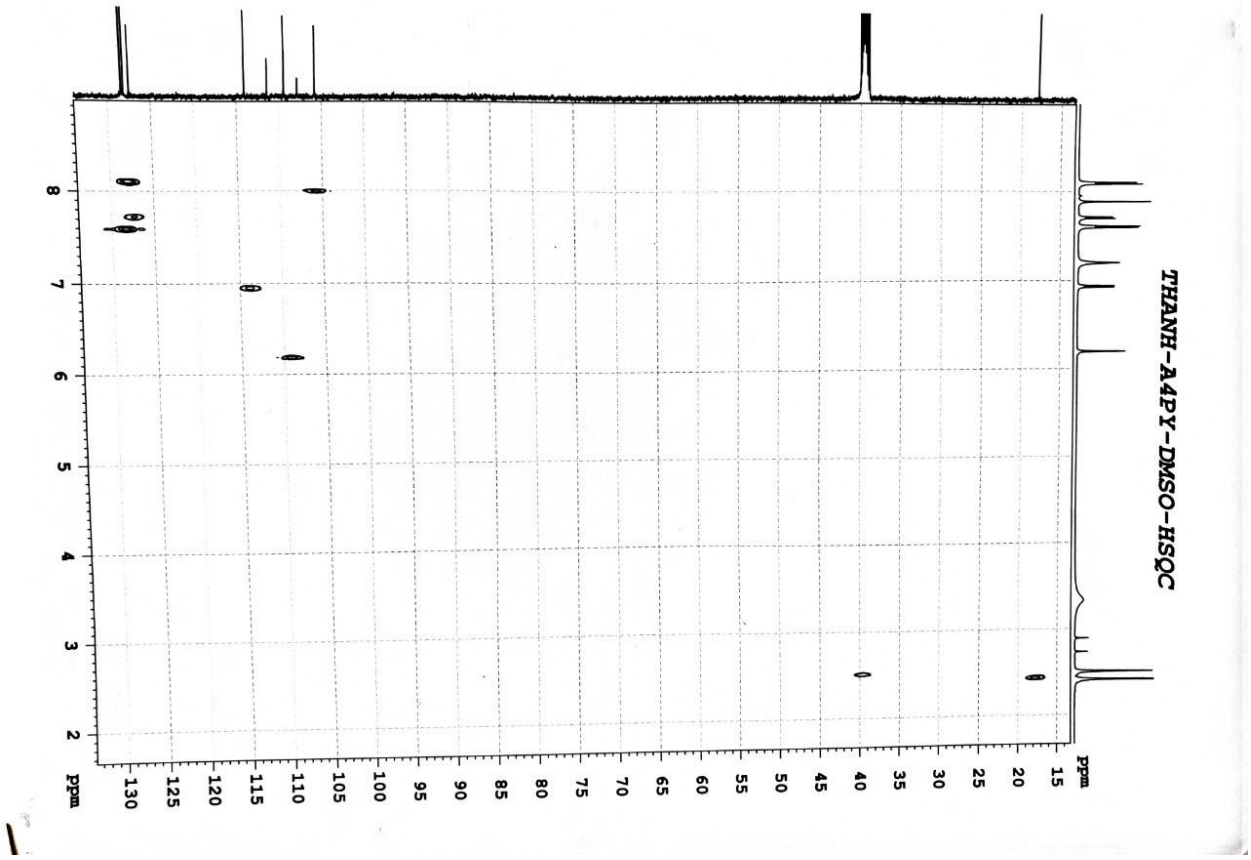
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100
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85
80
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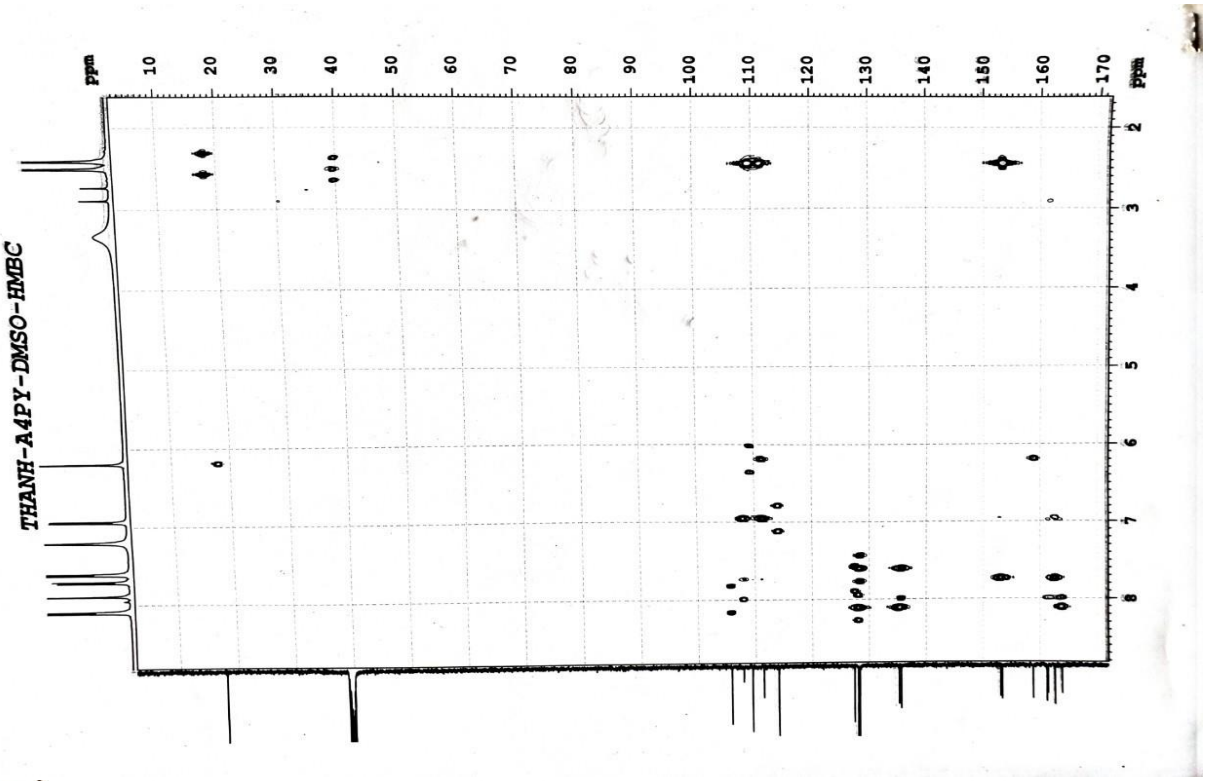
35
30
25
20
15
ppm
8
7
6
5
4
3
2



Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi
Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

File name: THANH_A4PY
Solvent: MeOH
Method: M+H/M+Na Date: 2/08/2010

THANH_A4PY_100729154003 8/2/2010 3:45:53 PM THANH_A4PY

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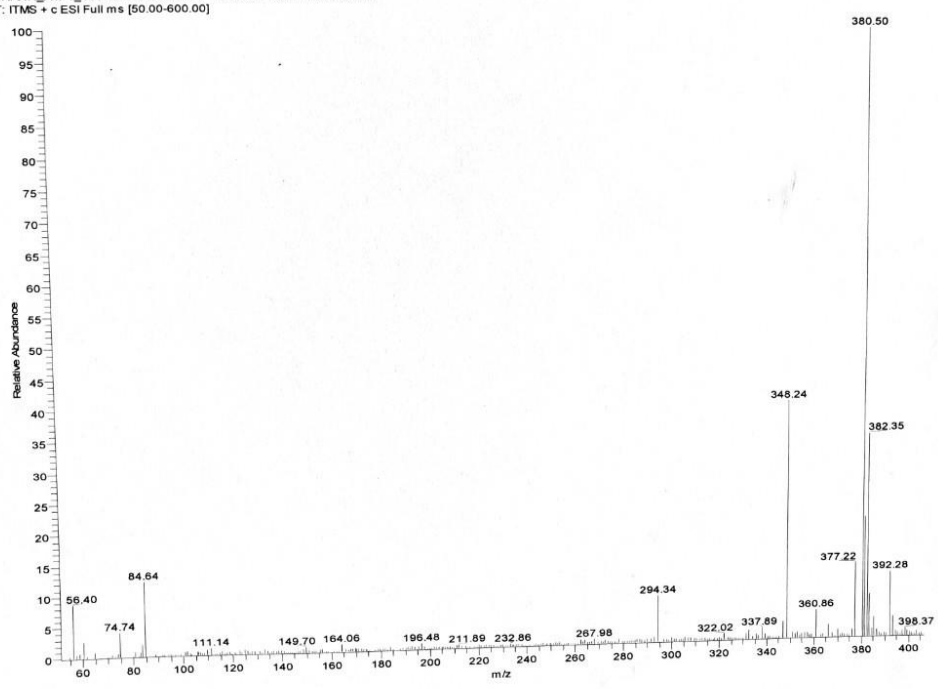
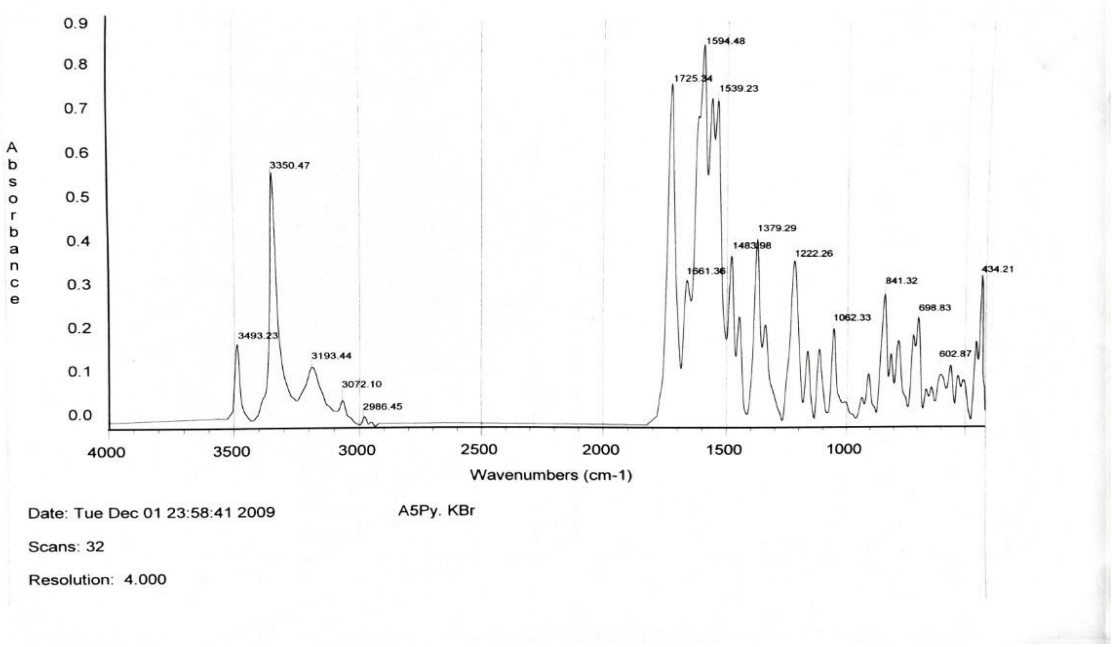
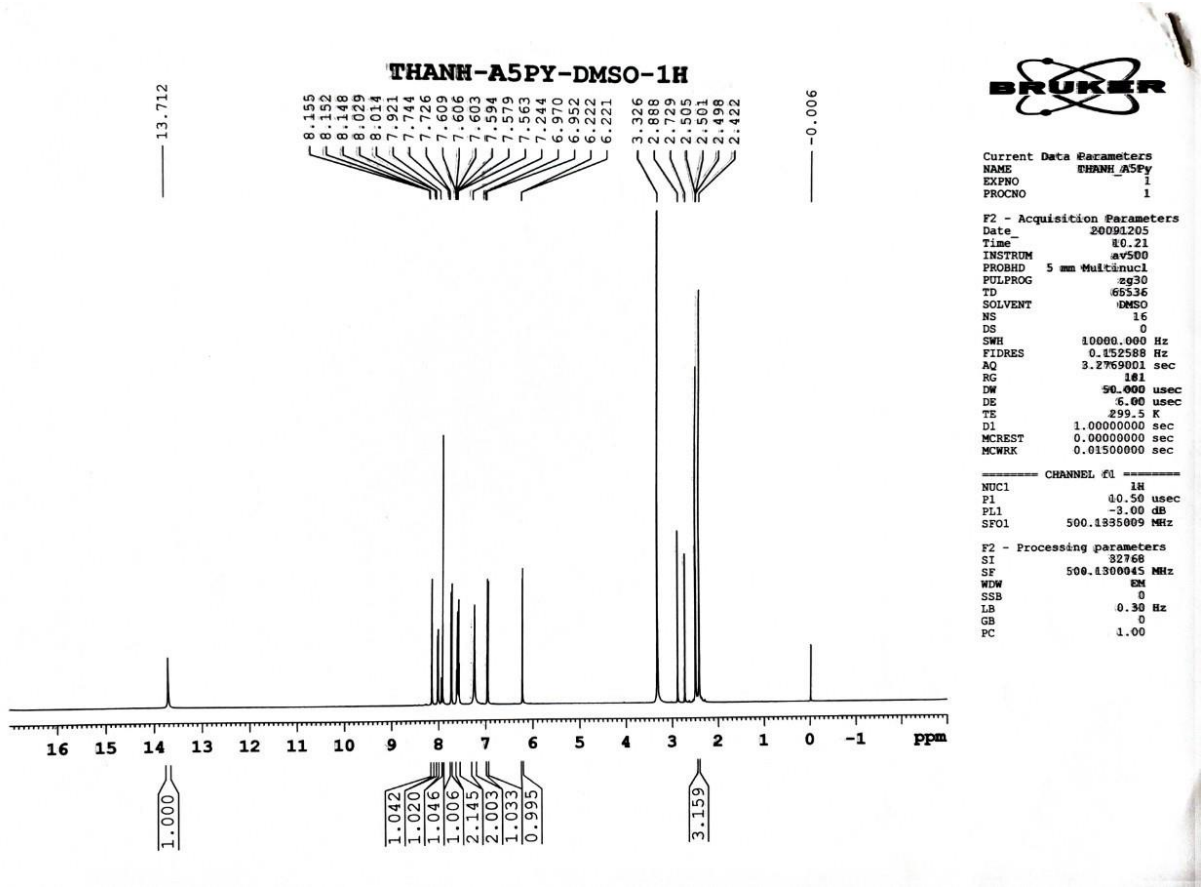


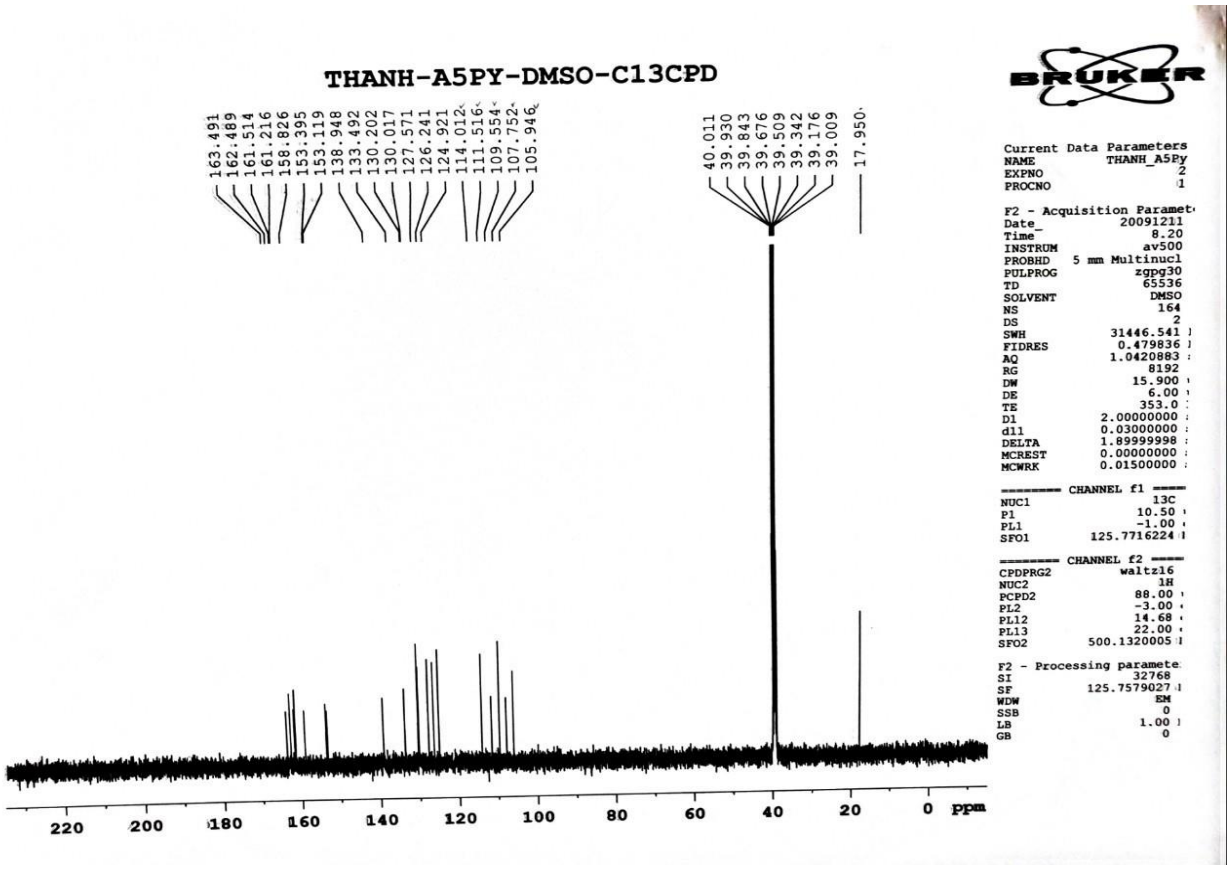
Mass Spectrometer
LTQ Orbitrap XL™
Thermo SCIENTIFIC compar
Resolution: >60 000 Dt
Sensitivity: 10^{-14}
Tandem: n >= 15
Mass Accuracy: <= 2ppm

Operator: MSc. Dao Thi Nhung
Mobile: 0948 119 043
Email: dtnhungtn@yahoo.com

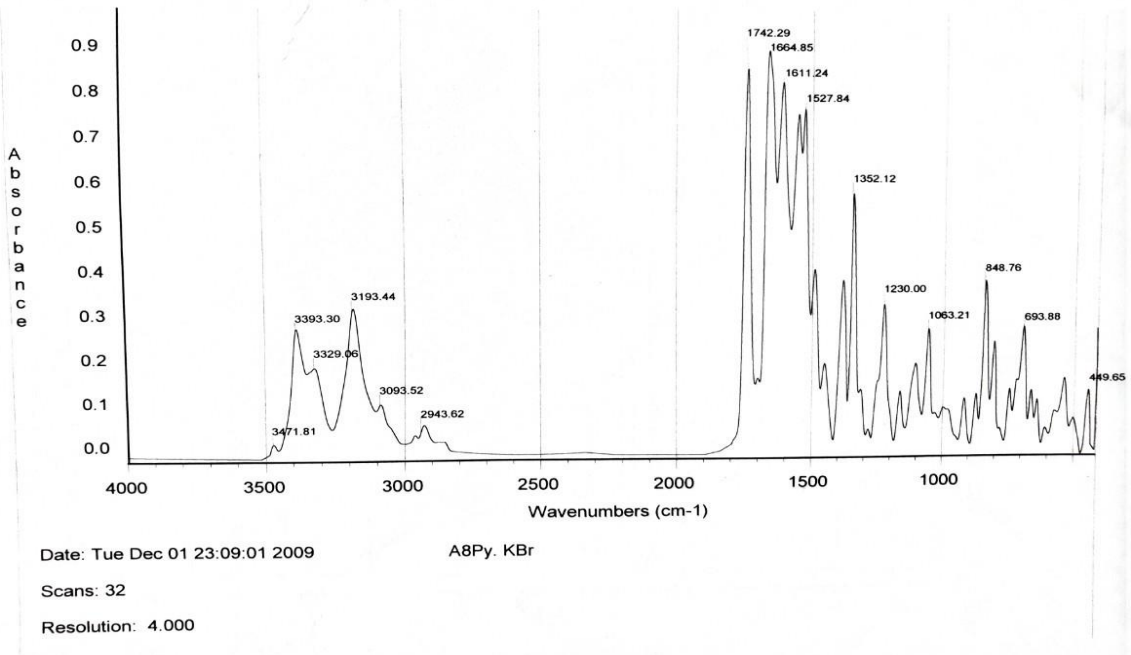
6. IR, NMR spectrum of 8-(2-Amino-6-m-chlorophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8f)**

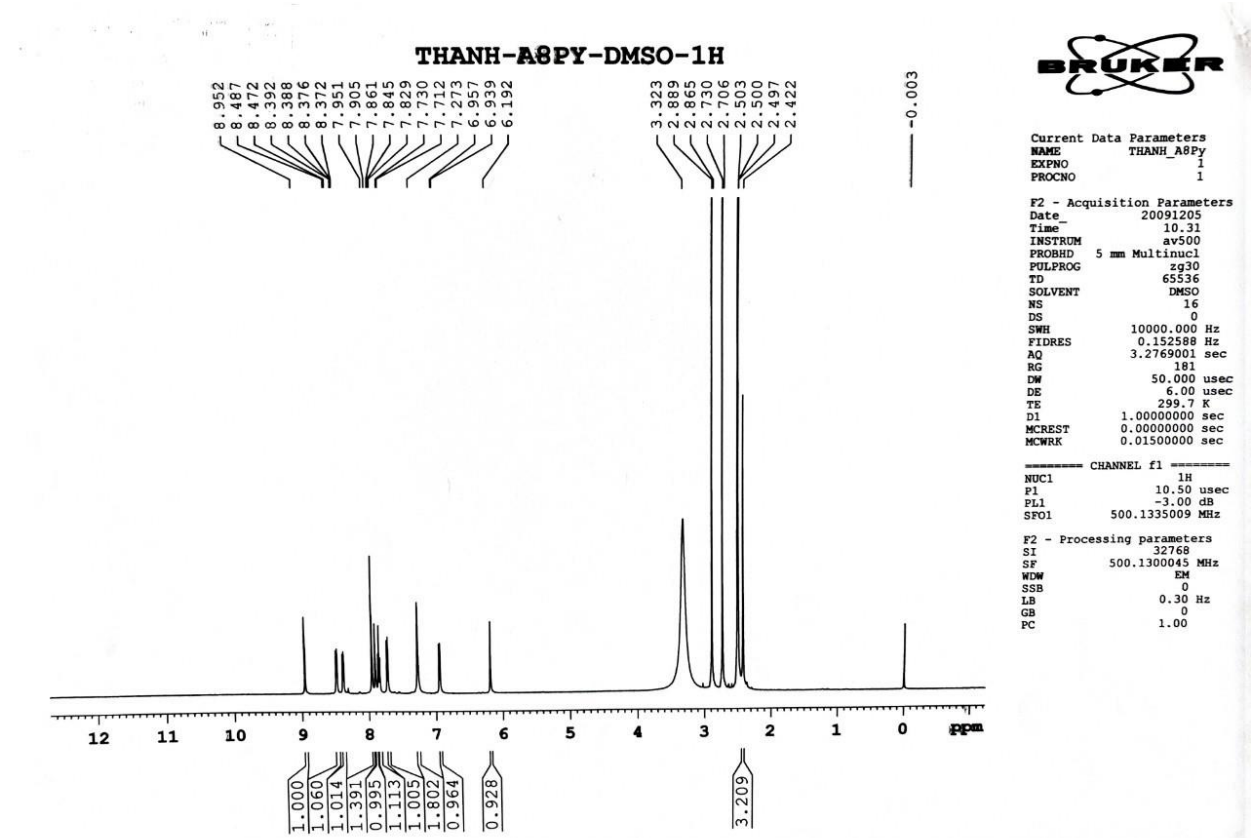






7. IR, NMR spectrum of 8-(2-Amino-6-m-nitrophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8g**)




THANH-A8PY-DMSO-1H
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8.472
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8.388
8.376
8.372
7.951
7.905
7.861
7.845
7.829
7.730
7.712
7.273
6.957
6.939
6.192
3.323
2.889
2.865
2.730
2.706
2.503
2.500
2.497
2.422
-0.003
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1.113
1.005
1.802
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3.209
BRUKER
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PROCNO 1
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PULPROG zg30
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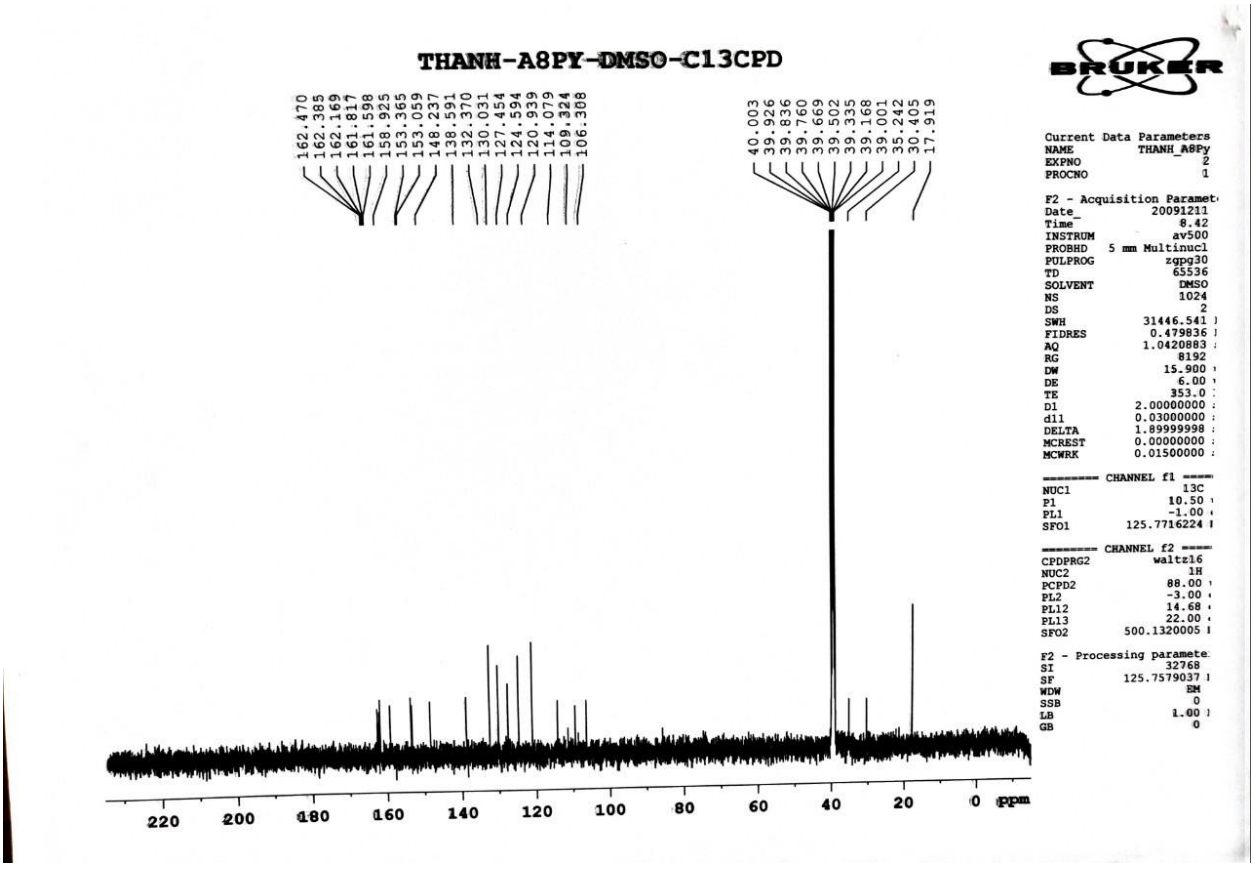
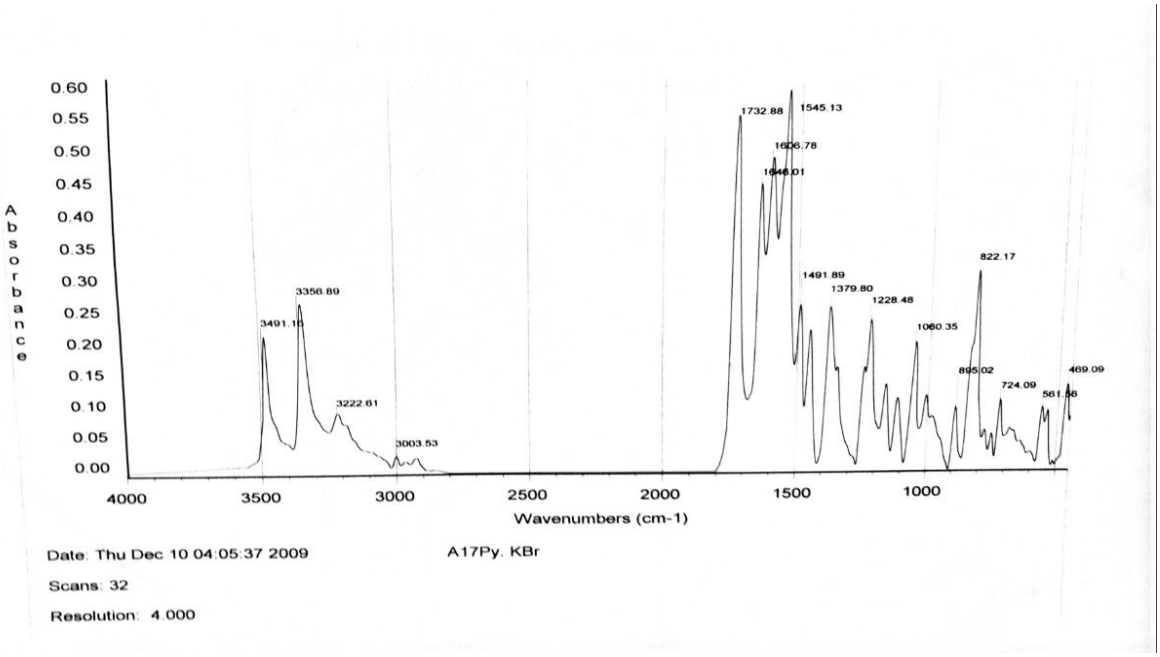
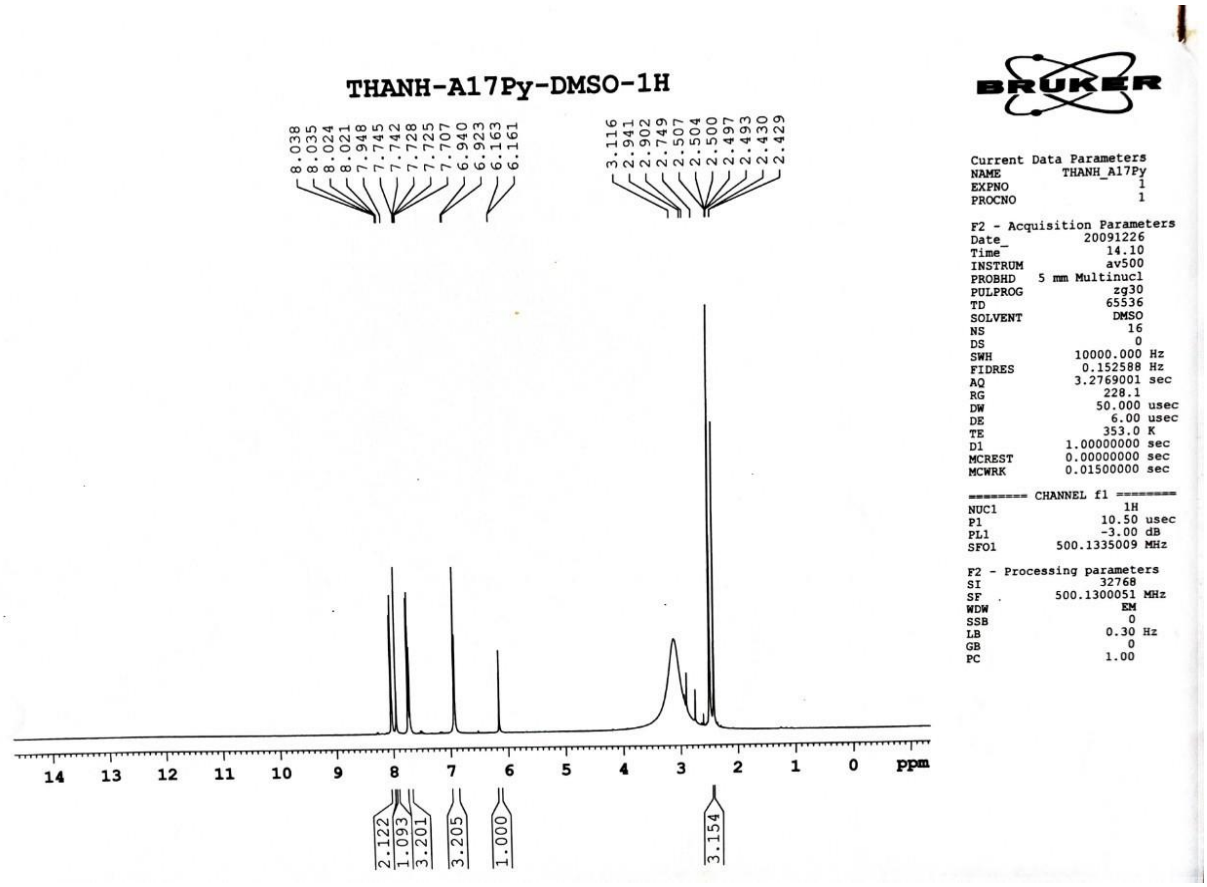
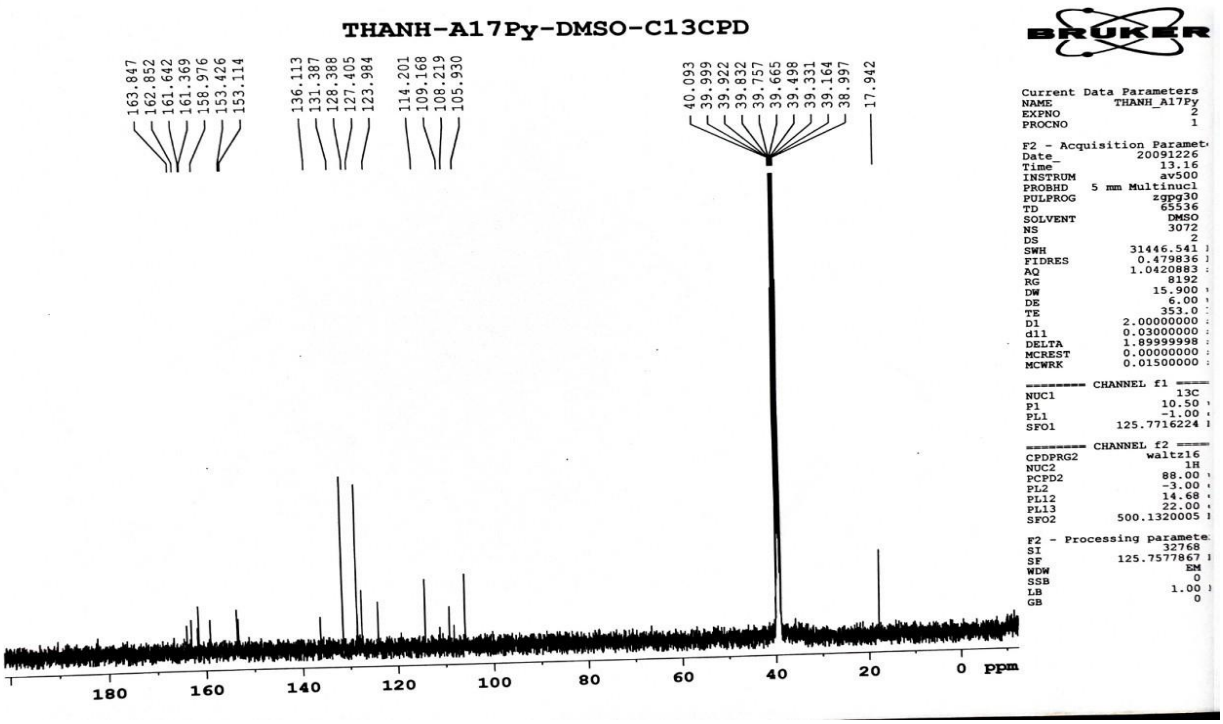
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 181
DW 50.000 usec
DE 6.00 usec
TE 299.7 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz
F2 - Processing parameters
SI 32768
SF 500.1300045 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


THANH-A8PY-DMSO-C13CPD
162.470
162.385
162.169
161.817
161.598
158.925
153.365
153.059
148.237
138.591
132.370
130.031
127.454
124.594
120.939
114.079
109.324
106.308
40.003
39.926
39.836
39.760
39.669
39.502
39.335
39.168
39.001
35.242
30.405
17.919
220 200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
Current Data Parameters
NAME THANH_A8Py
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20091211
Time 8.42
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 353.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
CHANNEL f1
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005
F2 - Processing paramete
SI 32768
SF 125.7579037
WDW EM
SSB 0
LB 1.00
GB 0

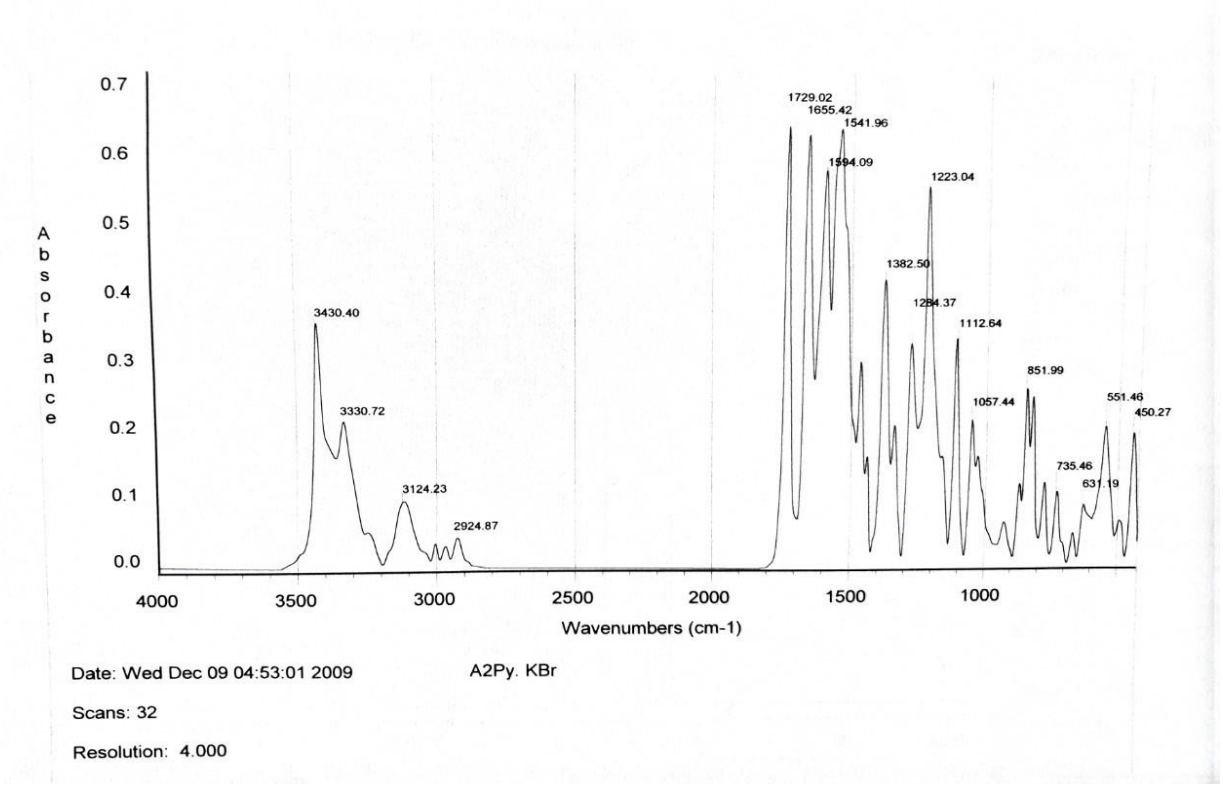
8. IR, NMR spectrum of 8-(2-Amino-6-p-bromophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8h**)

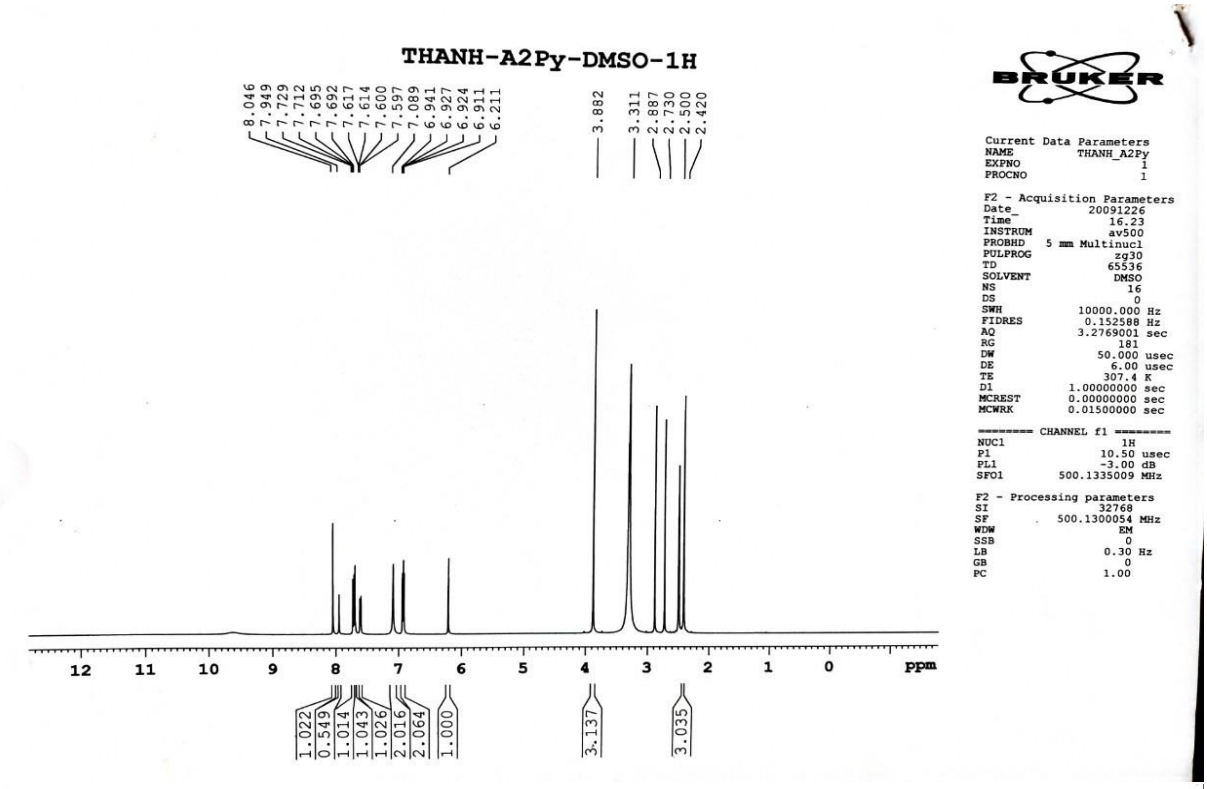






9. IR, NMR and ESI-MS spectrum of 8-(2-Amino-6-(4-hydroxy-3-methoxyphenyl)pyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8i**)





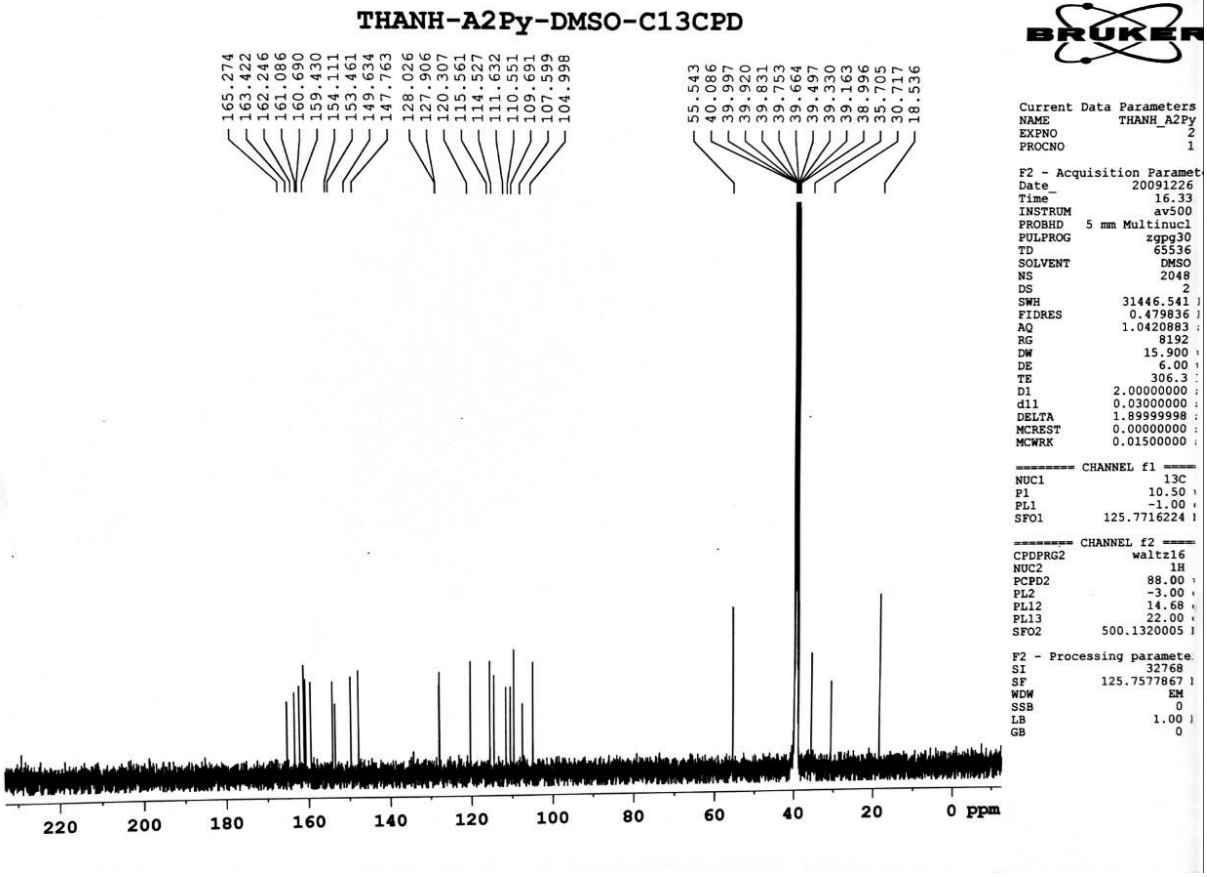
BRUKER

Current Data Parameters
NAME THANH_A2Py
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091226
Time 16.23
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 181
DW 50.000 usec
DE 6.00 usec
TE 307.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz

F2 - Processing parameters
SI 32768
SF 500.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

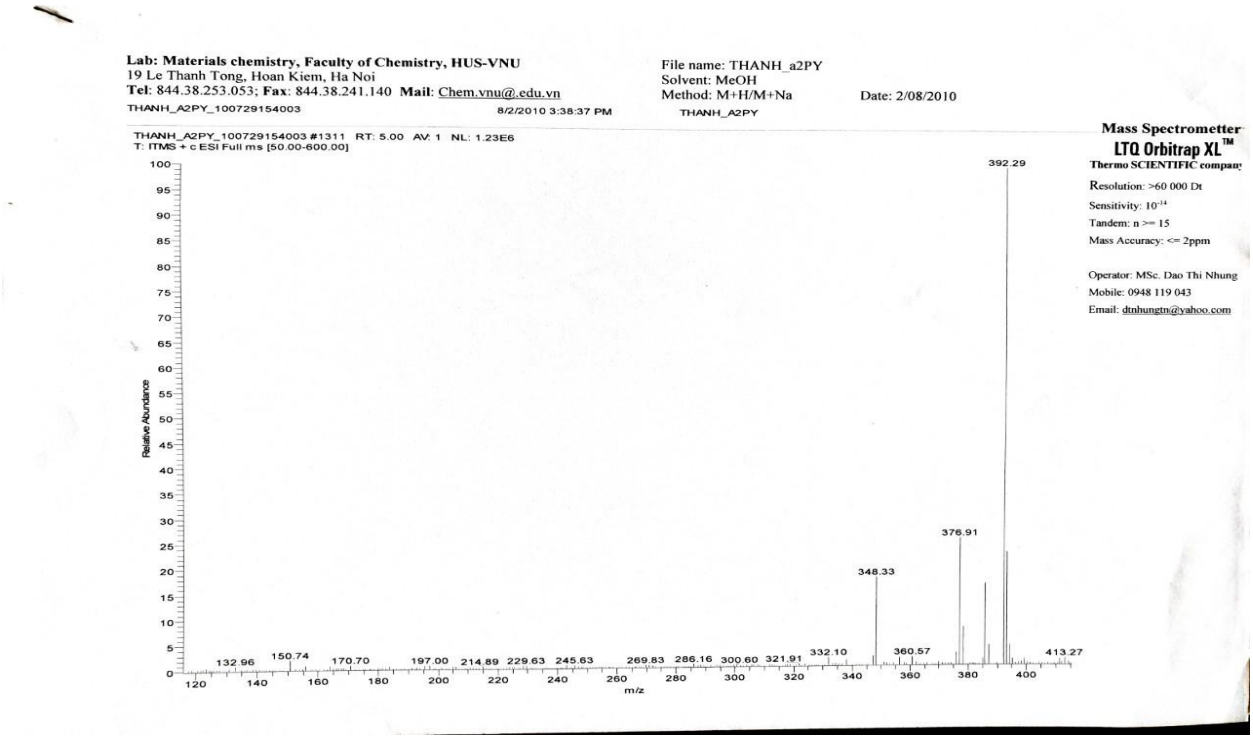
Current Data Parameters
NAME THANH_A2Py
EXPNO 2
PROCNO 1

F2 - Acquisition Paramet
Date_ 20091226
Time 16.33
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 306.3
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000

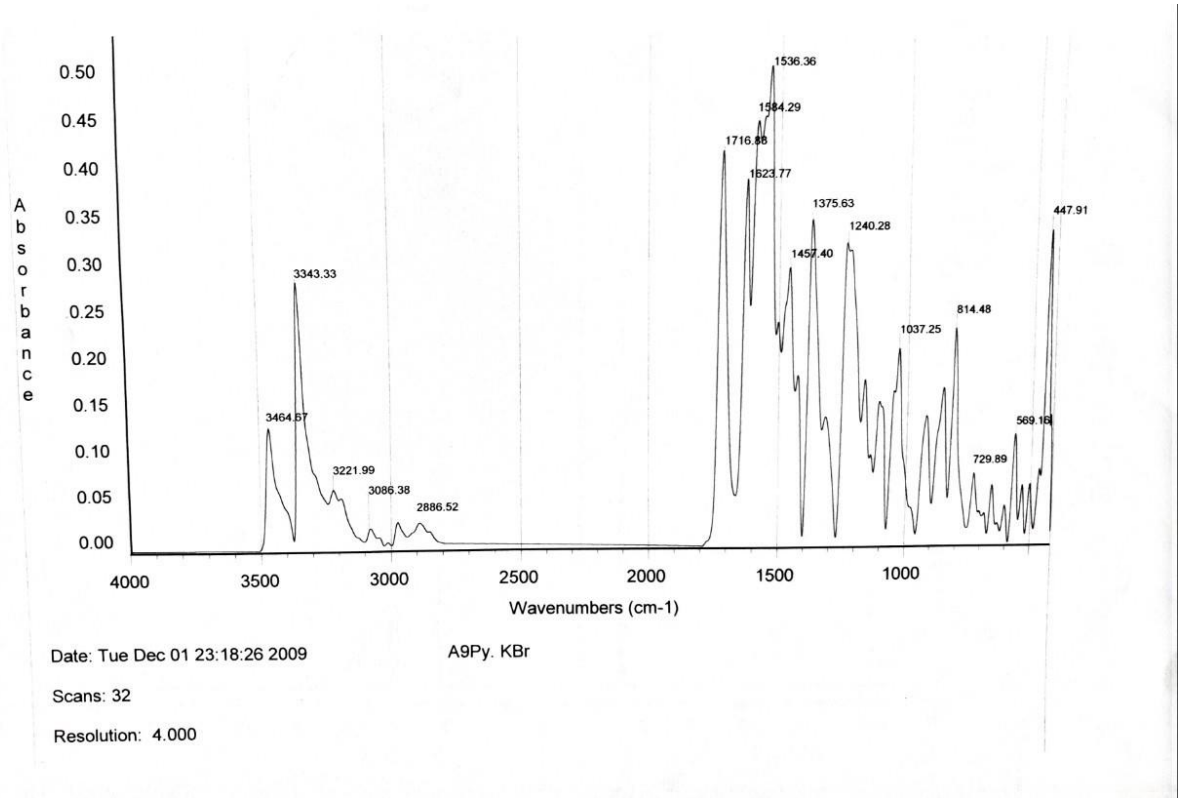
======== CHANNEL f1 ========
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224

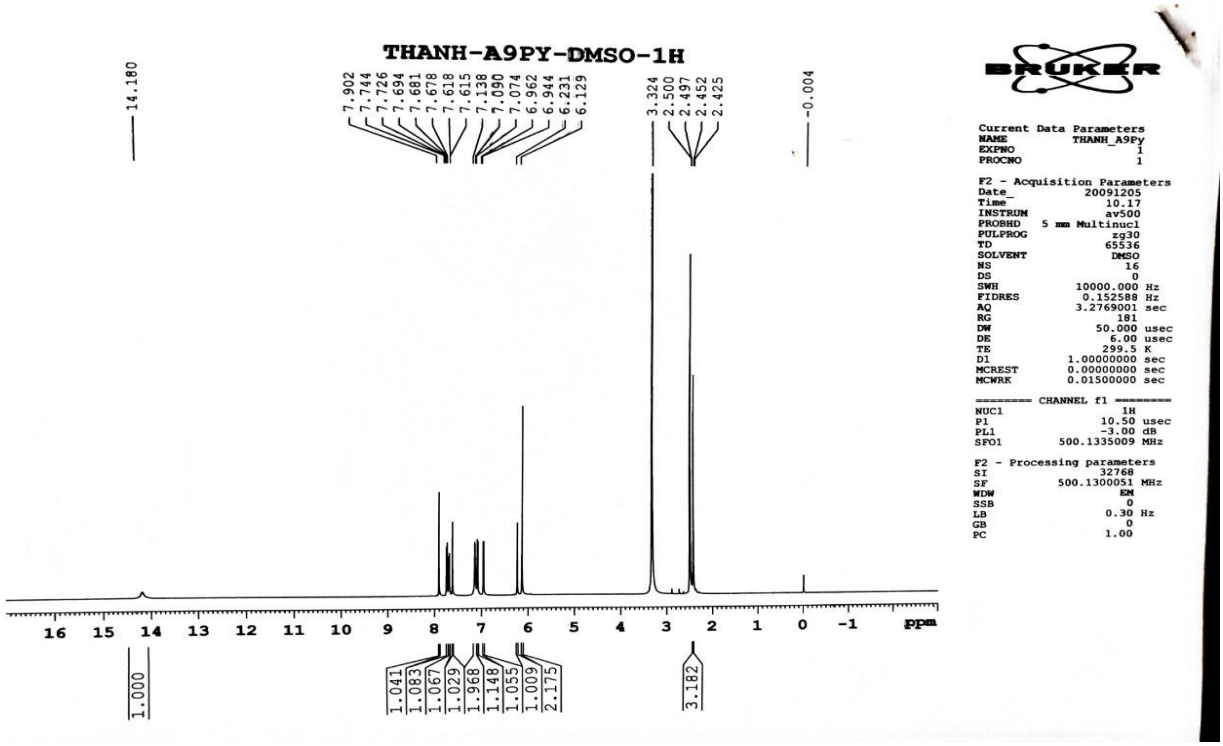
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005

F2 - Processing paramete
SI 32768
SF 125.7577867
WDW EM
SSB 0
LB 1.00
GB 0



10. IR, NMR spectrum of 8-(2-Amino-6-(3,4-methylenedioxyphenyl)pyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**8j**)





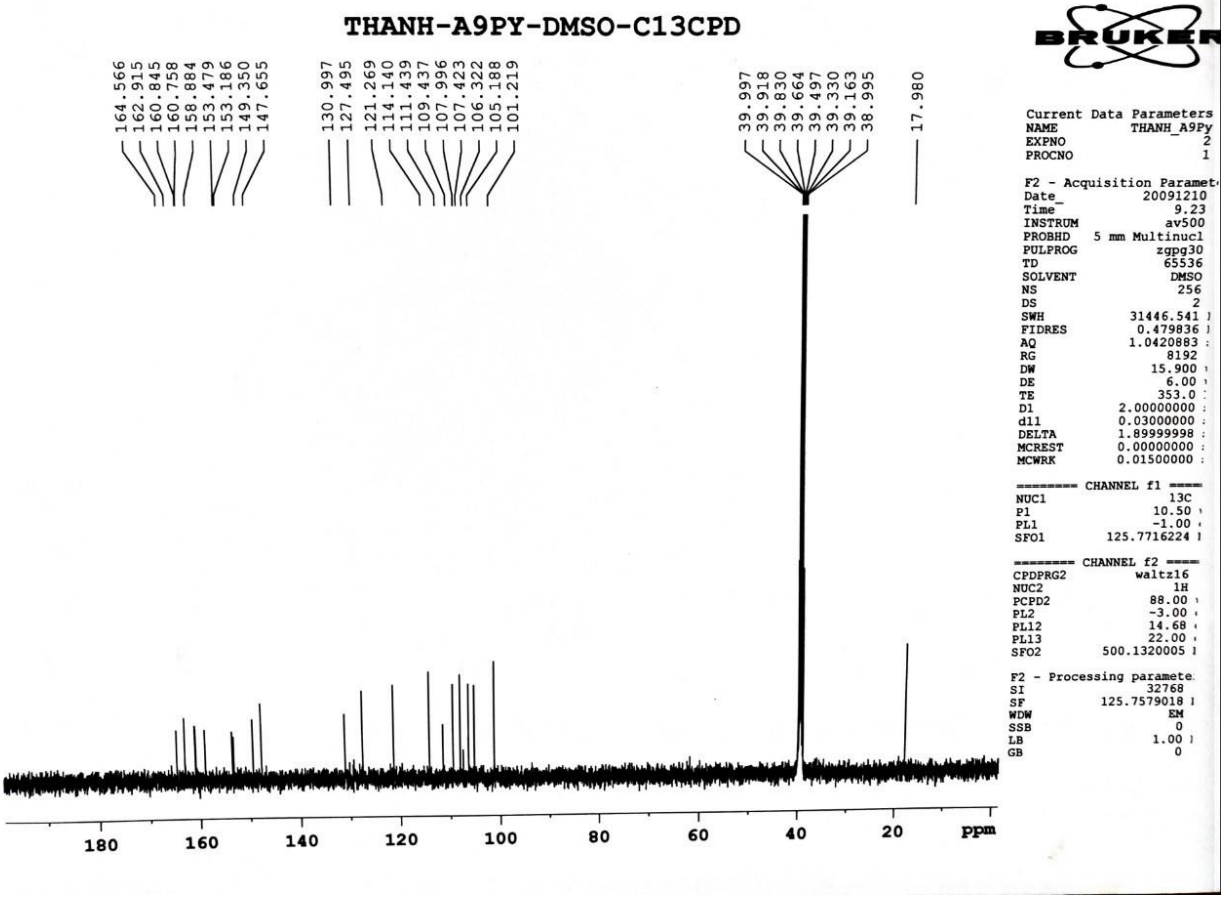
BRUKER

Current Data Parameters
NAME THANH_A9Py
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20091205
Time 10.17
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 181
DW 50.000 usec
DE 6.00 usec
TE 299.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz

F2 - Processing parameters
SI 32768
SF 500.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

Current Data Parameters
NAME THANH_A9Py
EXPNO 2
PROCNO 1

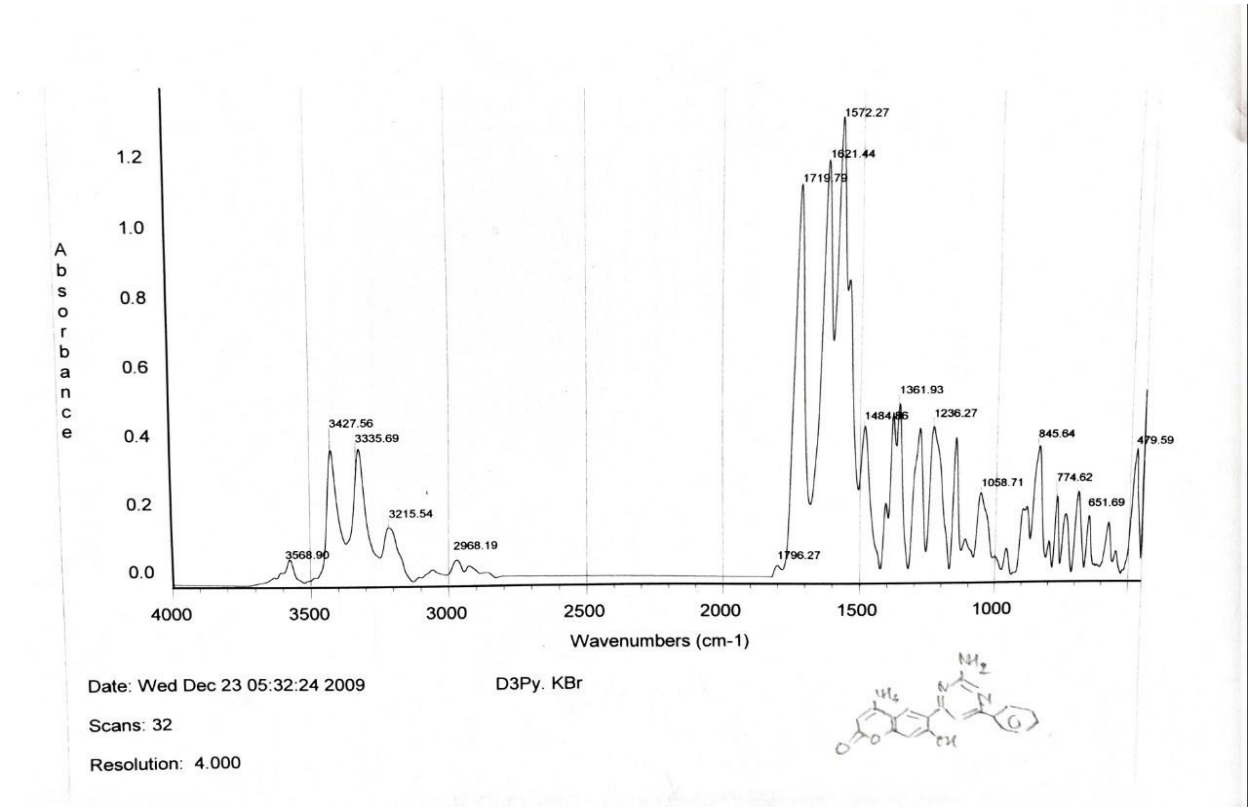
F2 - Acquisition Paramet
Date_ 20091210
Time 9.23
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 353.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000

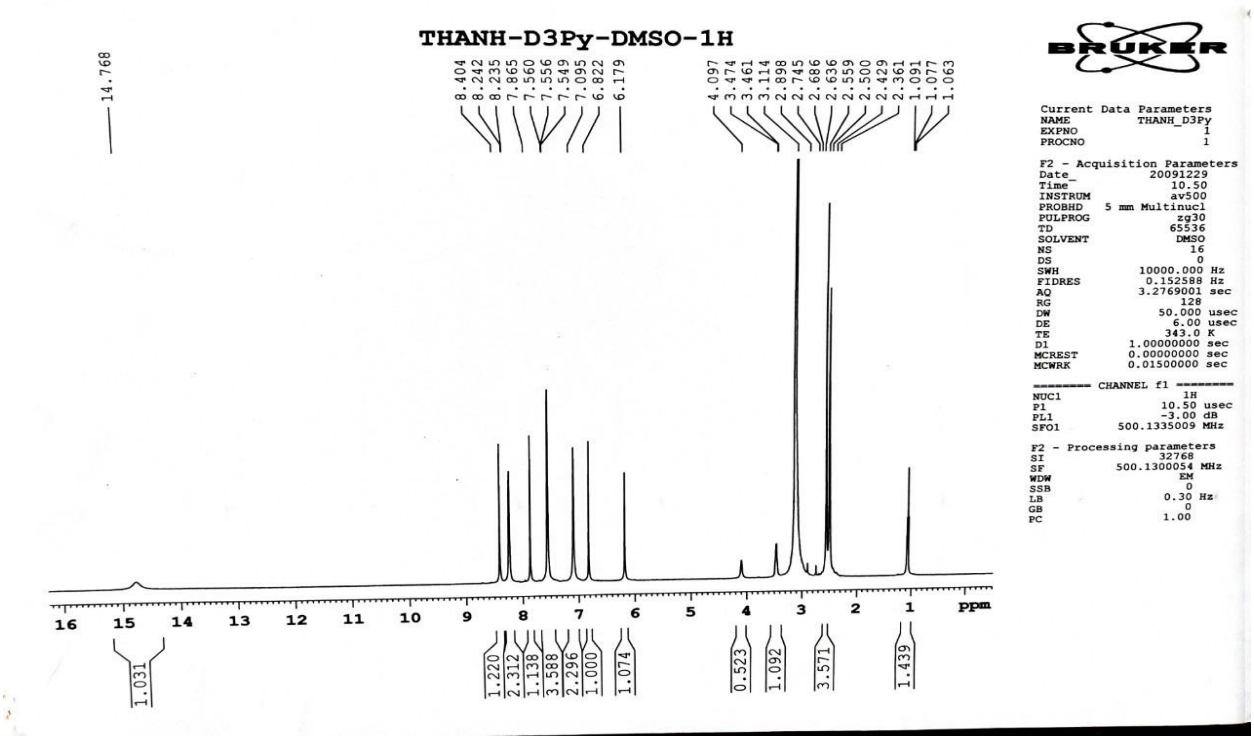
======== CHANNEL f1 ========
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224

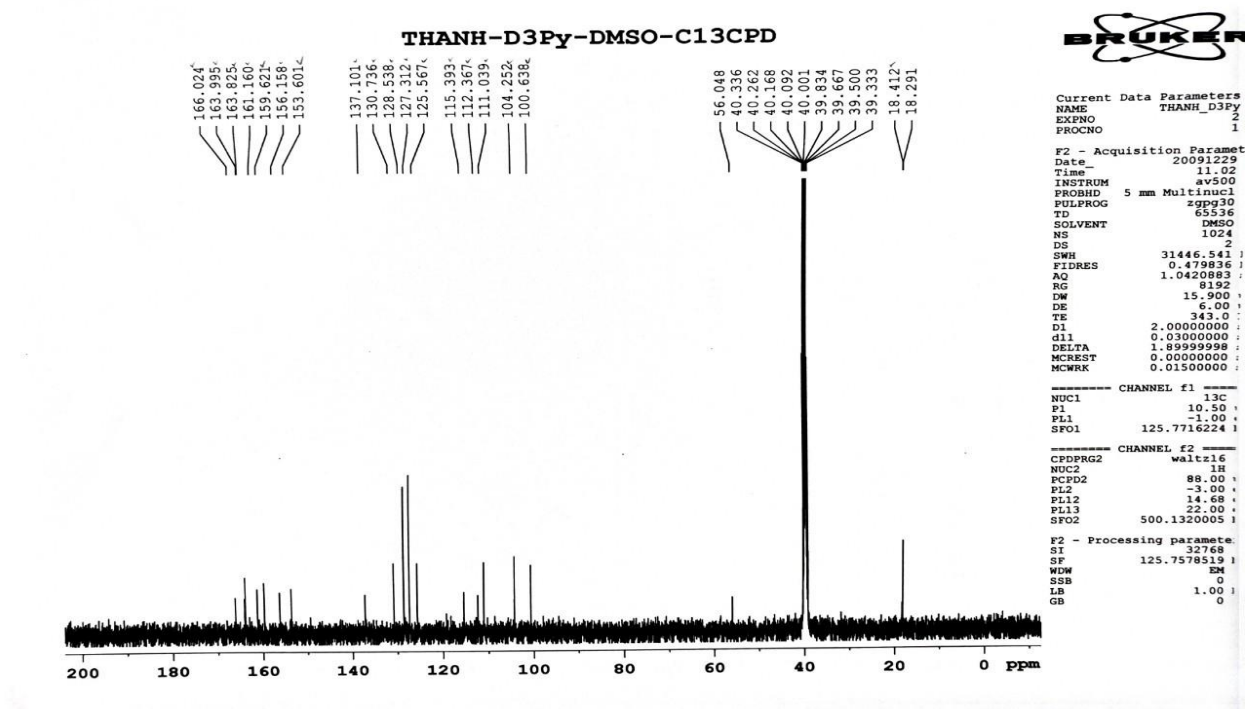
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005

F2 - Processing paramete
SI 32768
SF 125.7579018
WDW EM
SSB 0
LB 1.00
GB 0

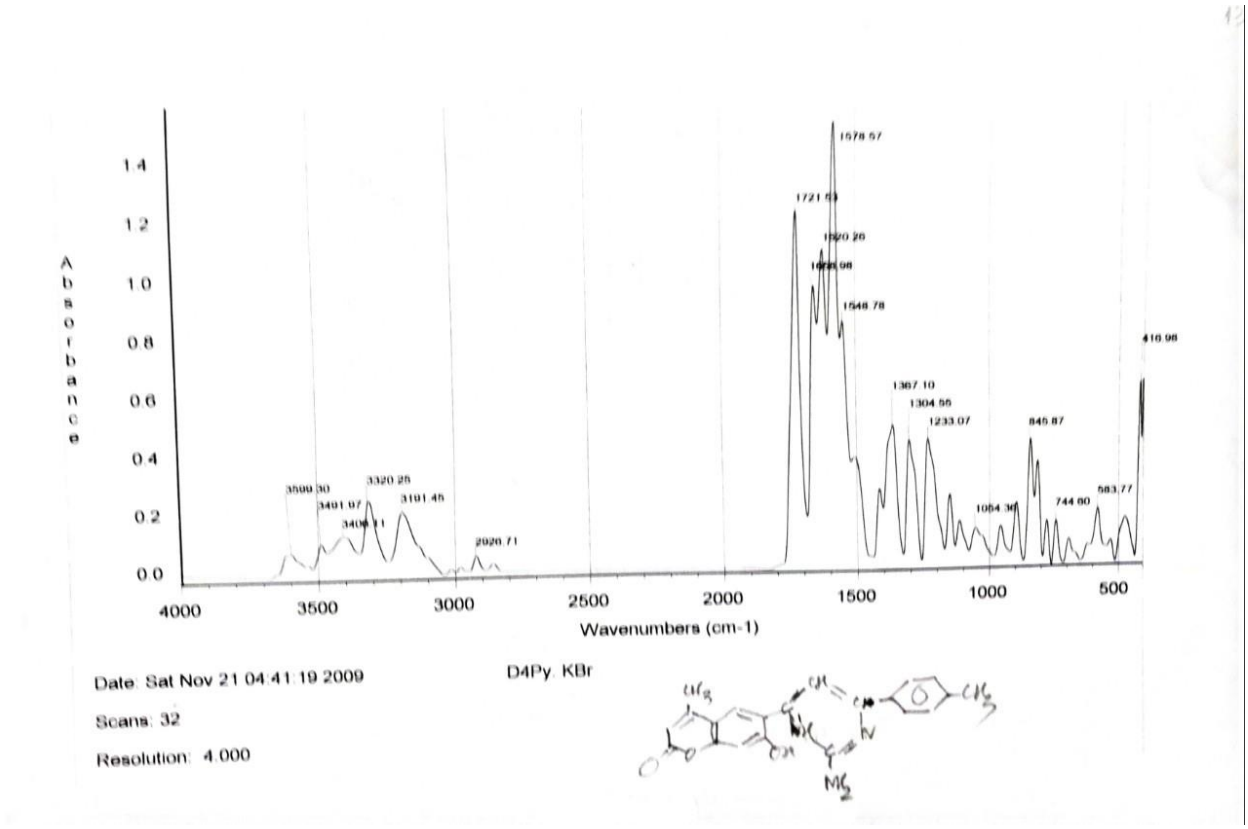
11. IR, NMR spectrum of 6-(2-Amino-6-phenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13a**)

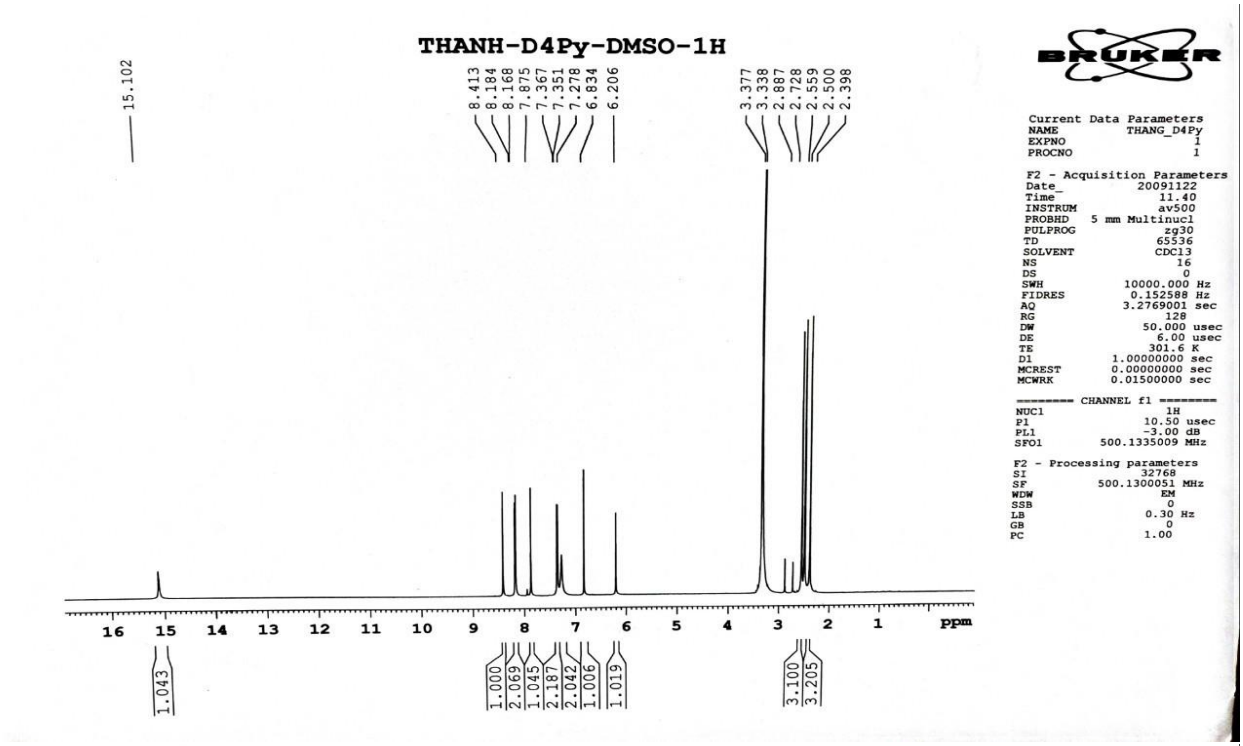


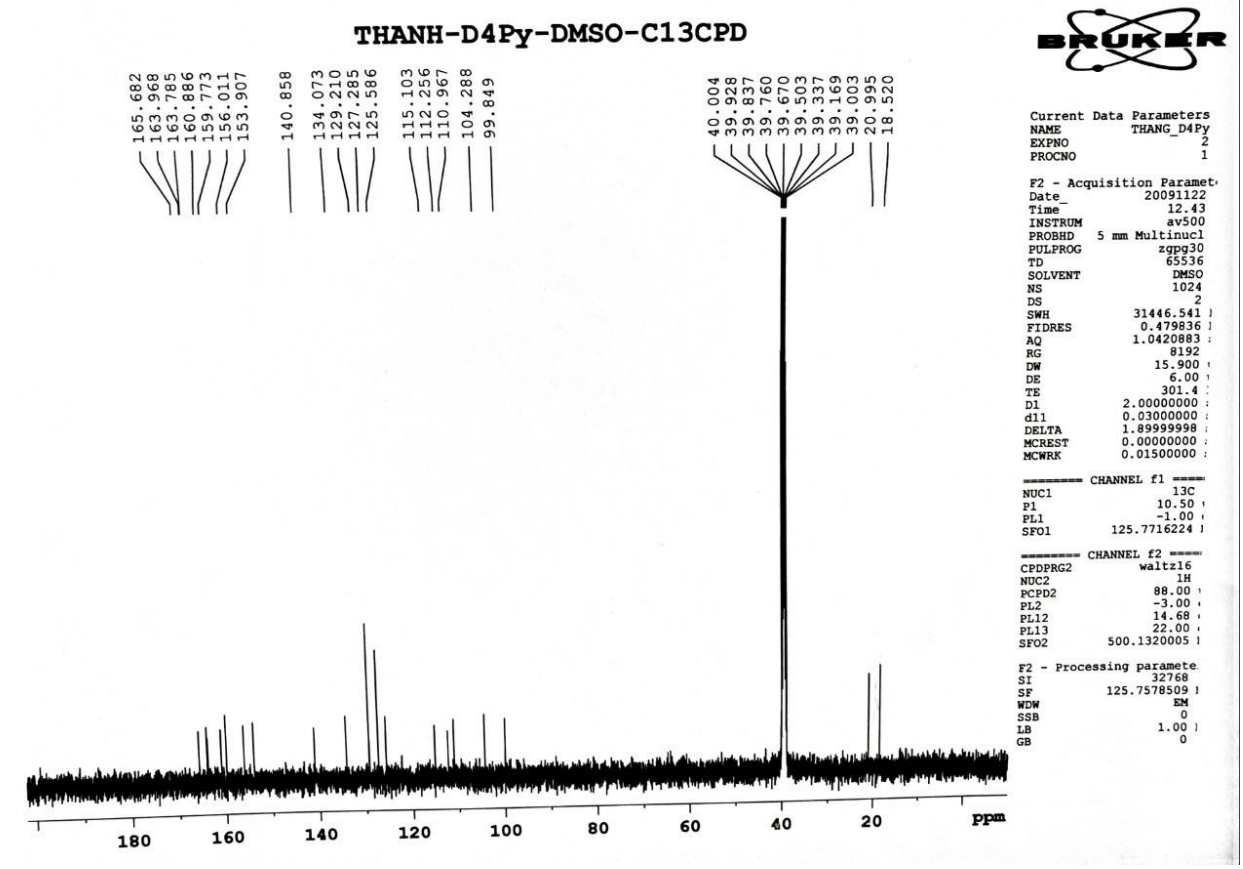


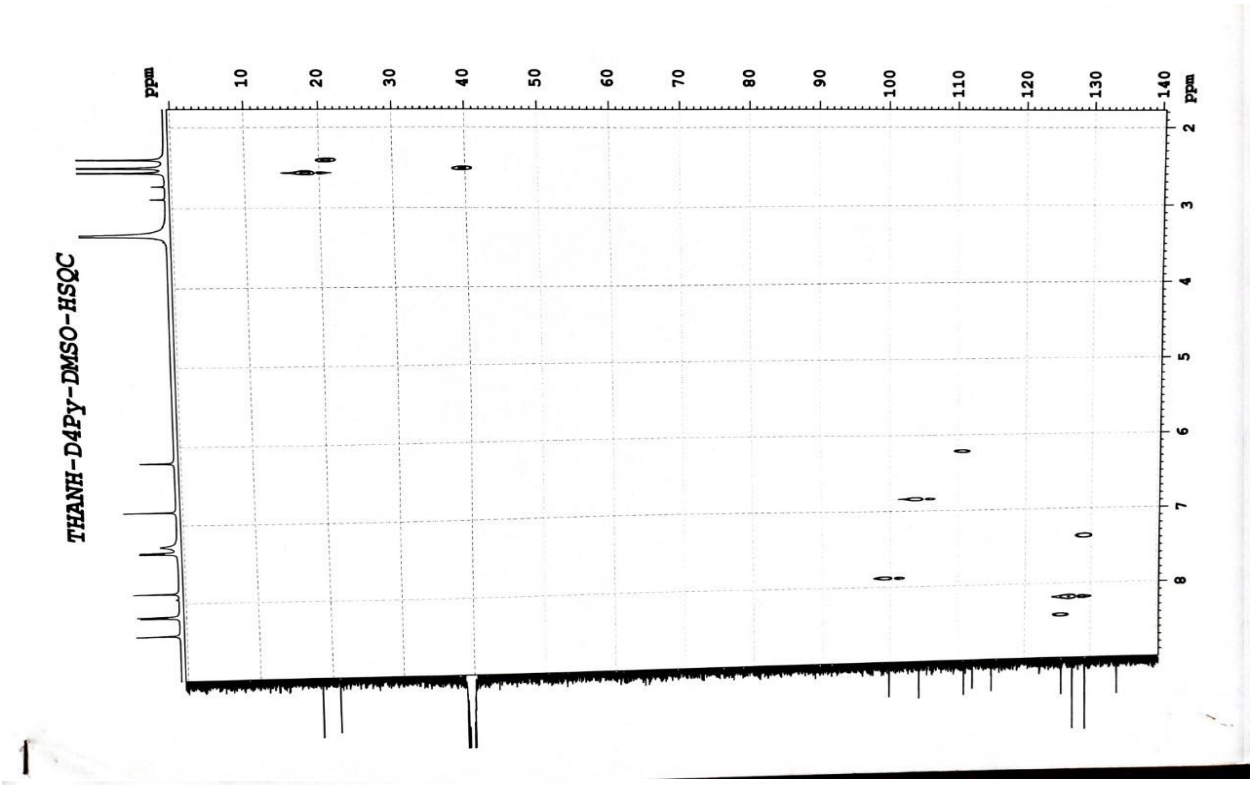


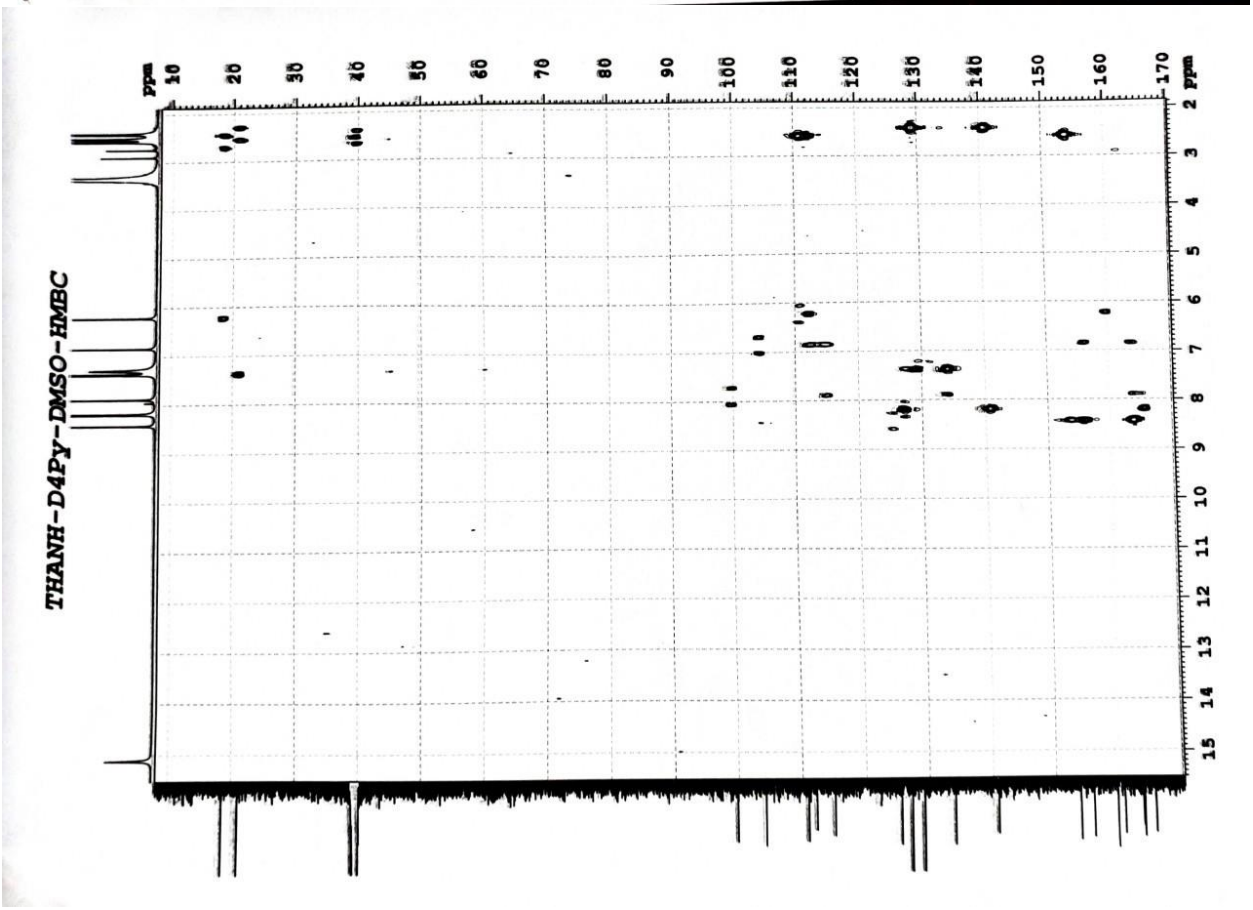
12. IR, NMR spectrum of 6-(2-Amino-6-p-methylphenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13b**)



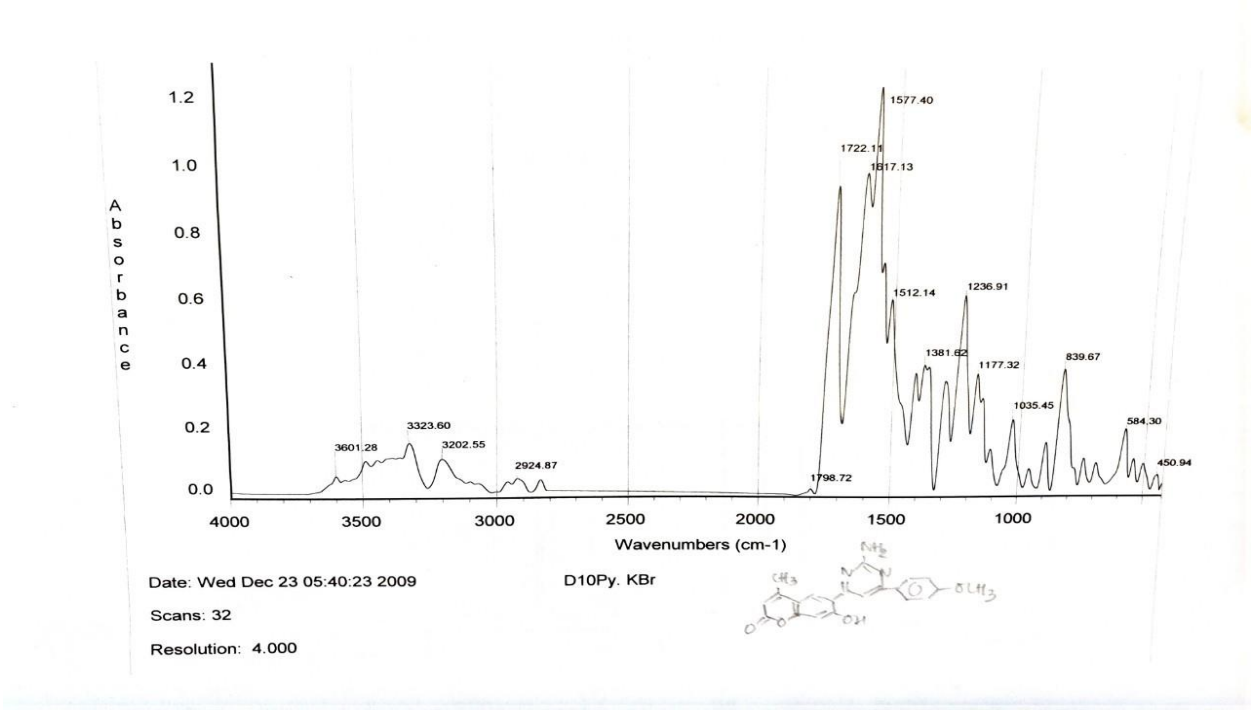

THANH-D4Py-DMSO-1H
15.102
8.413
8.184
8.168
7.875
7.367
7.351
7.278
6.834
6.206
3.377
3.338
2.887
2.728
2.559
2.500
2.398
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.043
1.000
2.069
1.045
2.187
2.042
1.006
1.019
3.100
3.205
BRUKER
Current Data Parameters
NAME THANG_D4Py
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091122
Time 11.40
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 301.6 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz
F2 - Processing parameters
SI 32768
SF 500.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

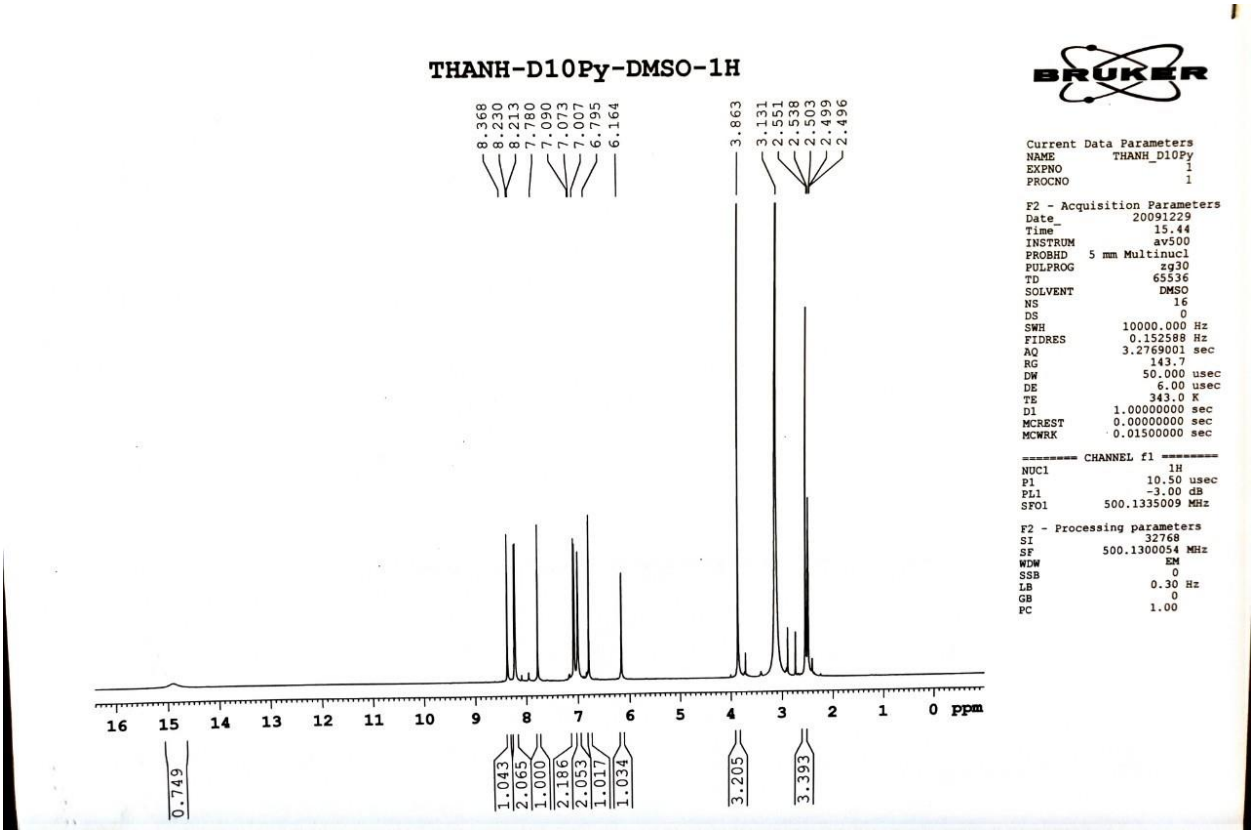

THANH-D4Py-DMSO-C13CPD
165.682
163.968
163.785
160.886
159.773
156.011
153.907
140.858
134.073
129.210
127.285
125.586
115.103
112.256
110.967
104.288
99.849
40.004
39.928
39.837
39.760
39.670
39.503
39.337
39.169
39.003
20.995
18.520
180 160 140 120 100 80 60 40 20 ppm
BRUKER
Current Data Parameters
NAME THANG_D4Py
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20091122
Time 12.43
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 301.4
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
CHANNEL f1
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005
F2 - Processing paramete
SI 32768
SF 125.7578509
WDW EM
SSB 0
LB 1.00
GB 0

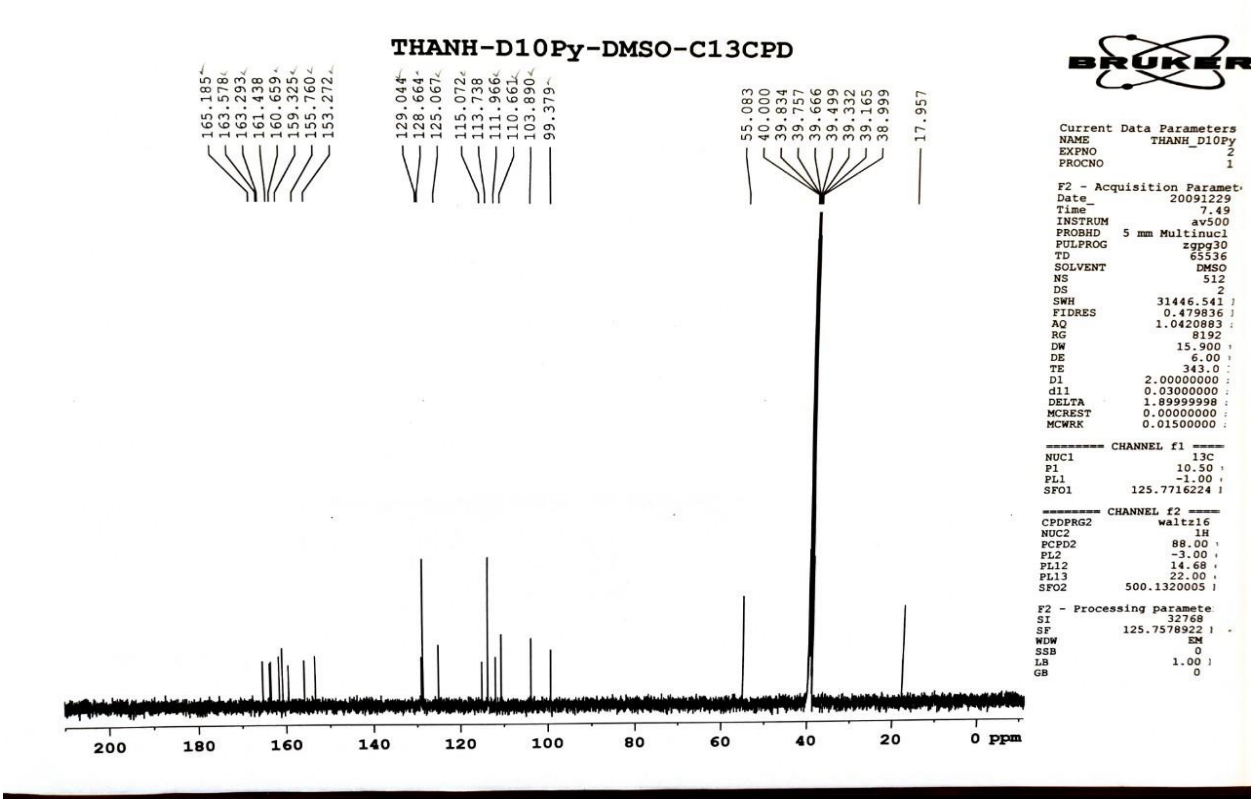

THANH-D4Py-DMSO-HSQC
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
ppm
2
3
4
5
6
7
8


THANH-D4Py-DMSO-HMBC
ppm
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
ppm
2
3
4
5
6
7
8
9
10
11
12
13
14
15

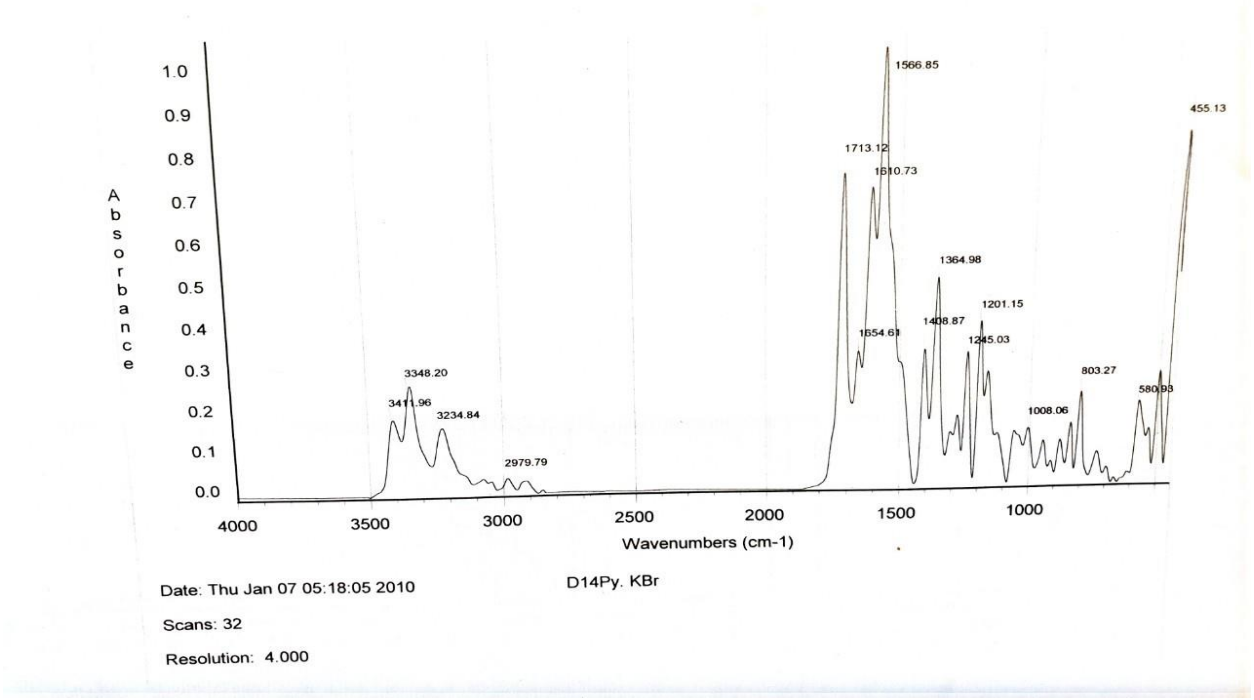
13. IR, NMR spectrum of 6-(2-Amino-6-p-methoxyphenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13c**)

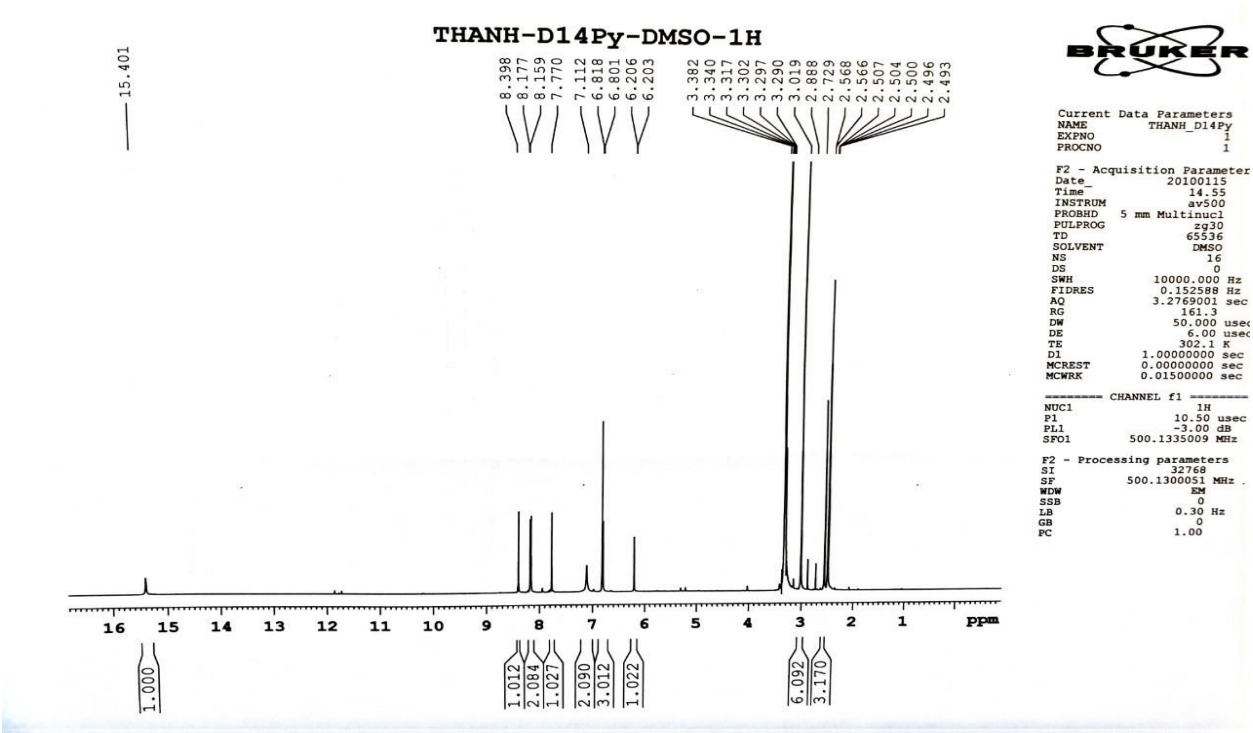


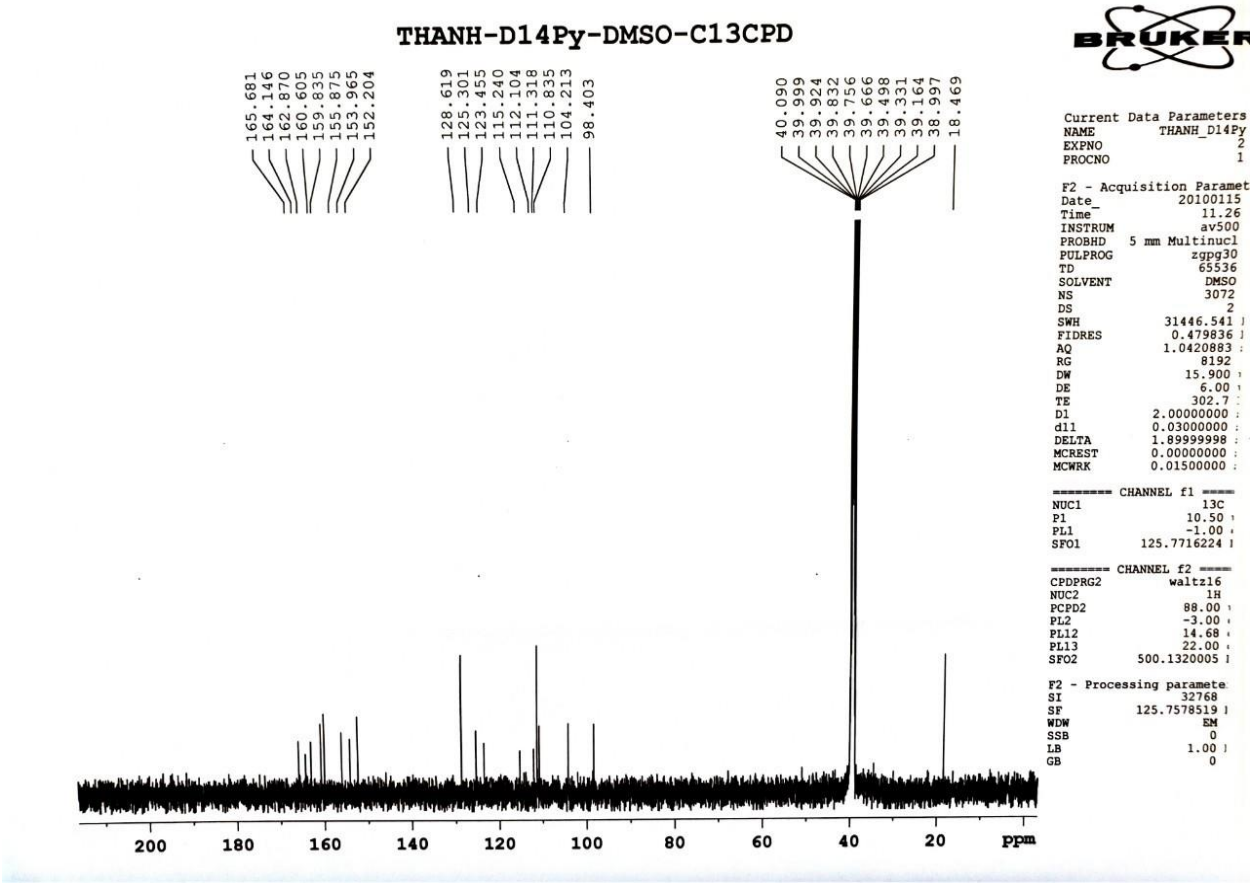




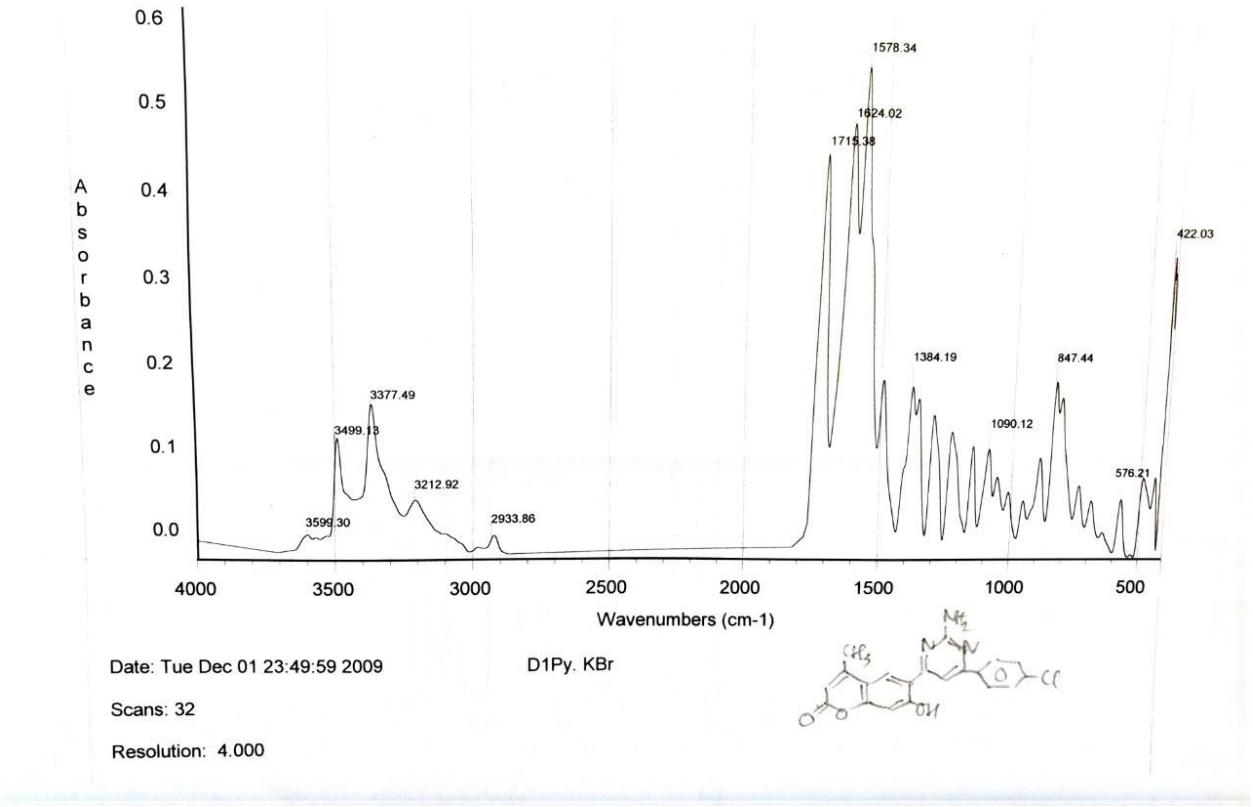
14. IR, NMR spectrum of 6-(2-Amino-6-p-N,N-dimethylaminophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13d**)

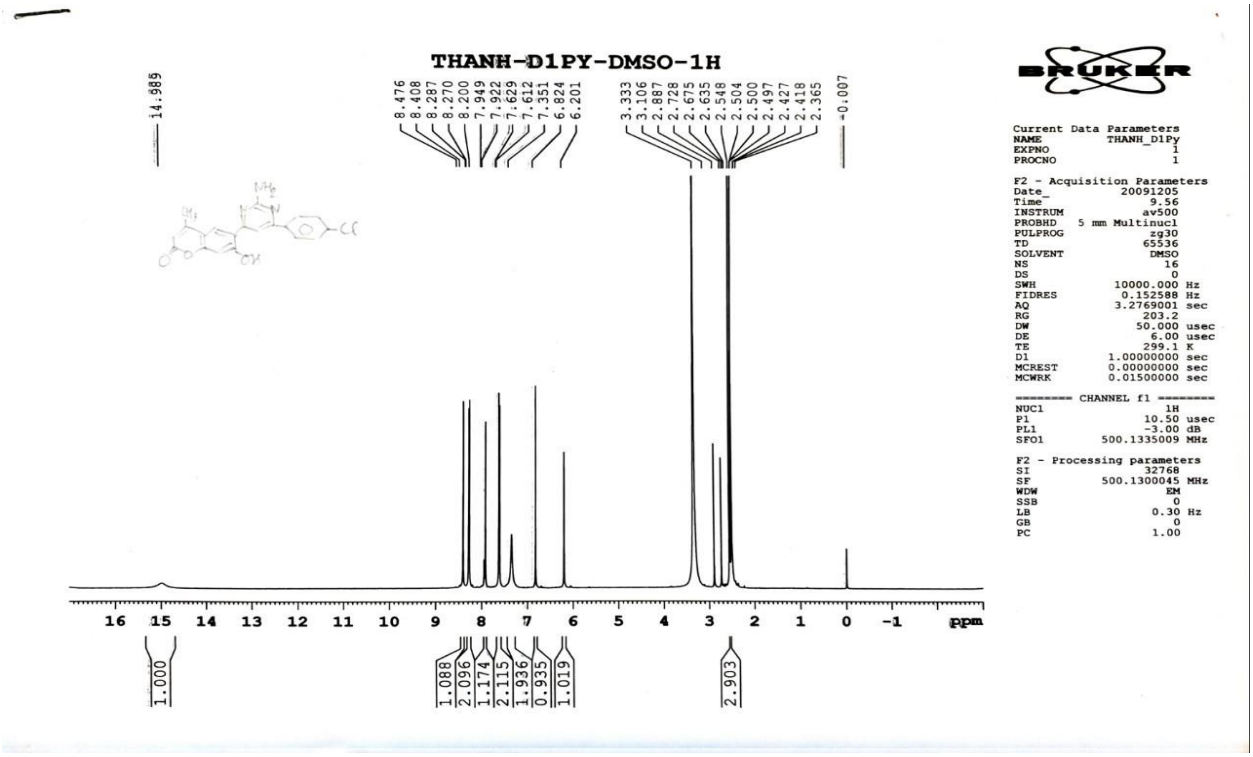


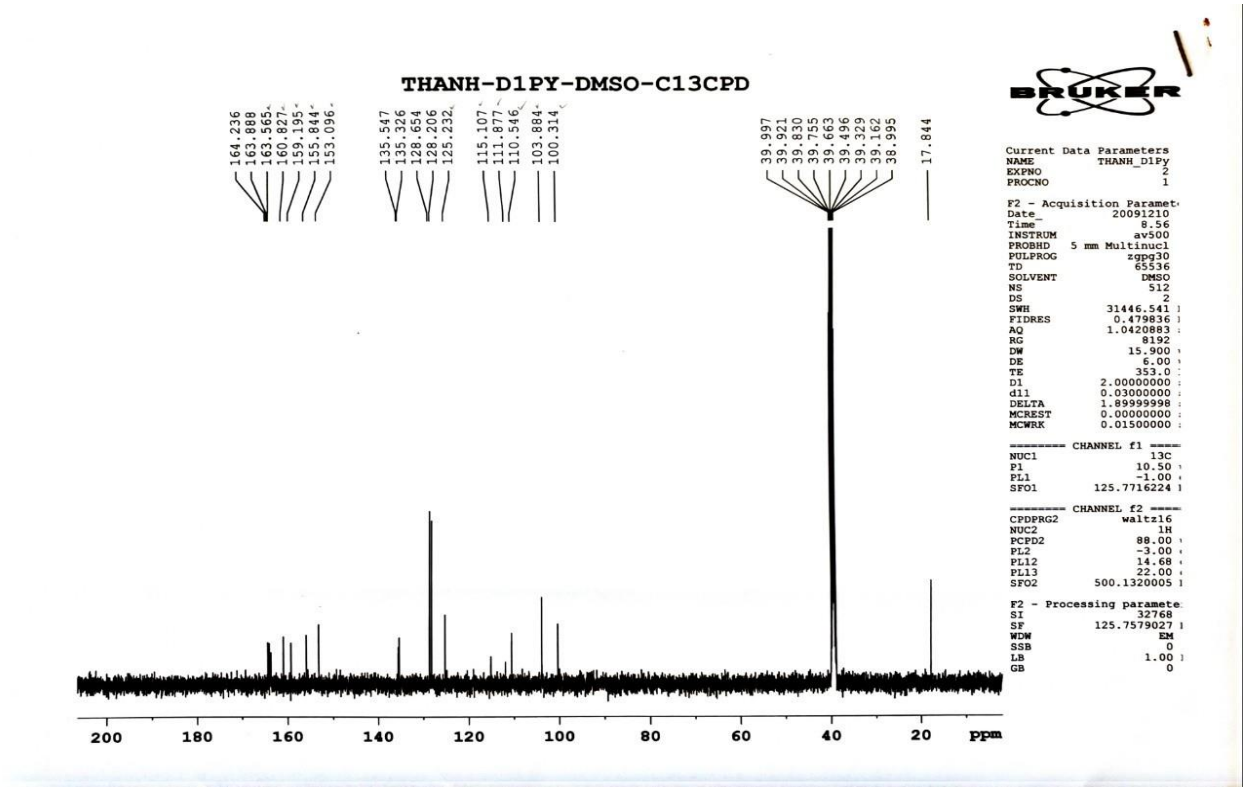

THANH-D14Py-DMSO-1H
15.401
8.398
8.177
8.159
7.770
7.112
6.818
6.801
6.206
6.203
3.382
3.340
3.317
3.302
3.297
3.290
3.019
2.888
2.729
2.568
2.566
2.507
2.504
2.500
2.496
2.493
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm
1.000
1.012
2.084
1.027
2.090
3.012
1.022
6.092
3.170
Current Data Parameters
NAME THANH_D14Py
EXPNO 1
PROCNO 1
F2 - Acquisition Parameter
Date_ 20100115
Time 14.55
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 161.3
DW 50.000 usec
DE 6.00 usec
TE 302.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz
F2 - Processing parameters
SI 32768
SF 500.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


THANH-D14Py-DMSO-C13CPD
165.681
164.146
162.870
160.605
159.835
155.875
153.965
152.204
128.619
125.301
123.455
115.240
112.104
111.318
110.835
104.213
98.403
40.090
39.999
39.924
39.832
39.756
39.666
39.498
39.331
39.164
38.997
18.469
200 180 160 140 120 100 80 60 40 20 ppm
Current Data Parameters
NAME THANH_D14Py
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20100115
Time 11.26
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 3072
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 302.7
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
CHANNEL f1
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005
F2 - Processing paramete
SI 32768
SF 125.7578519
WDW EM
SSB 0
LB 1.00
GB 0

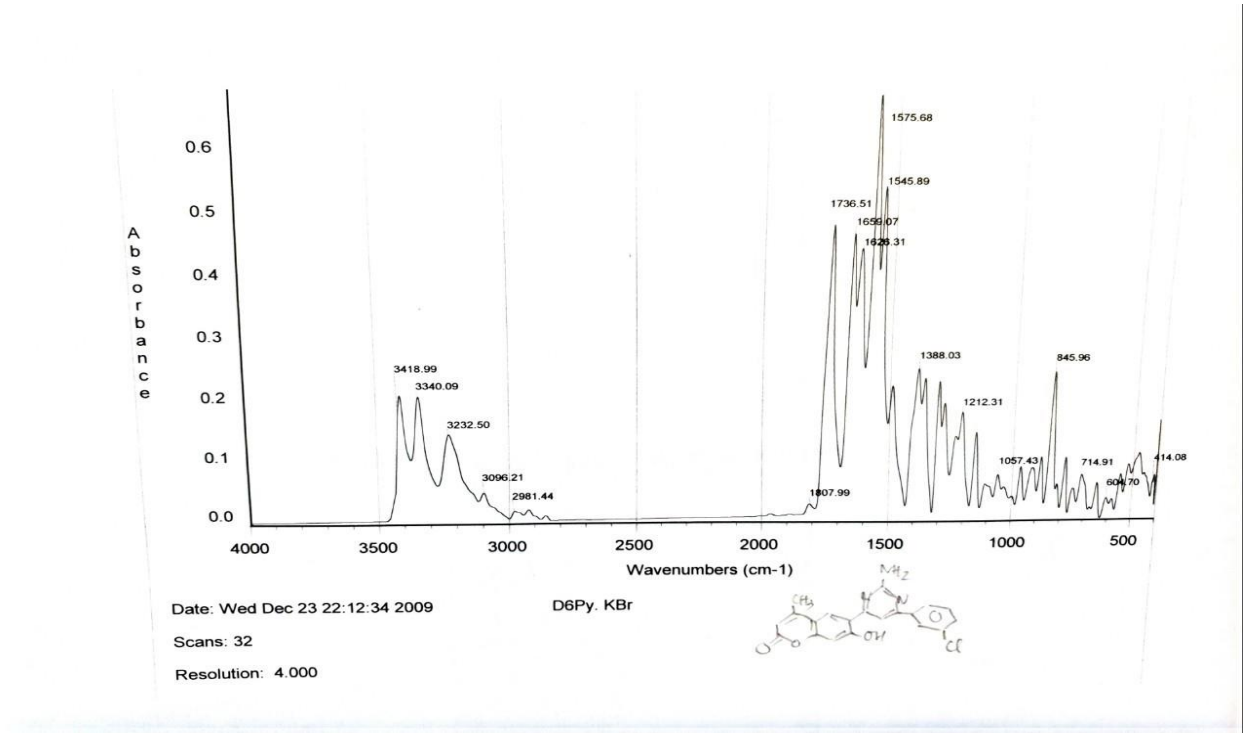
15. IR, NMR spectrum of 6-(2-Amino-6-p-chlorophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13e**)

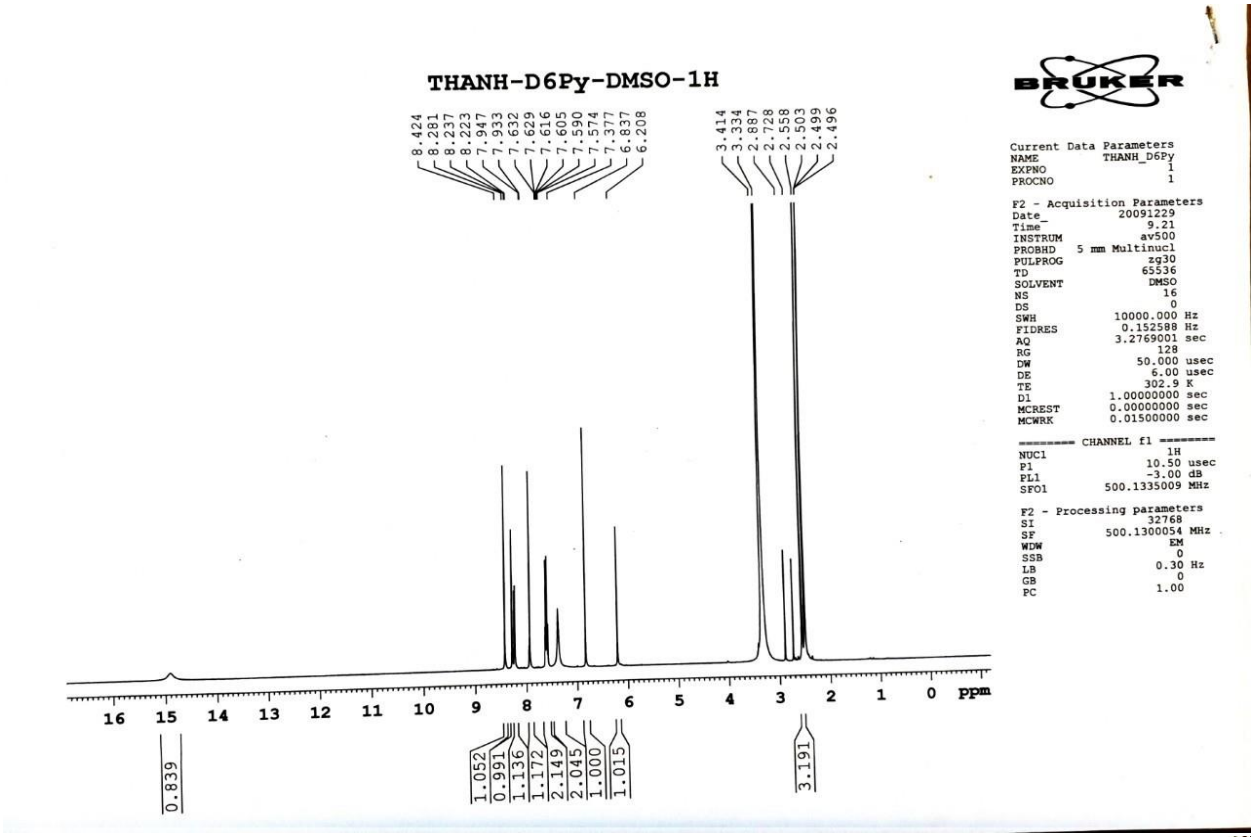


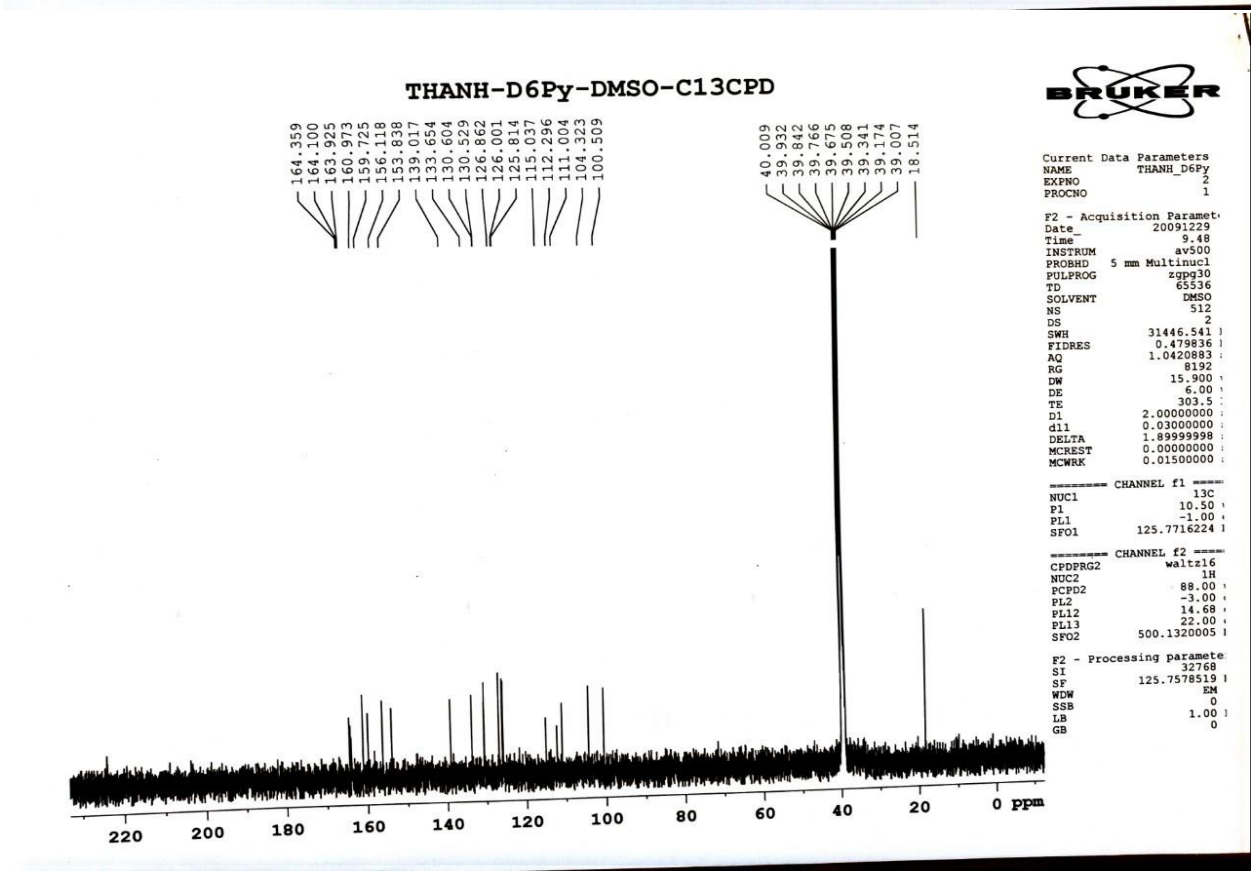




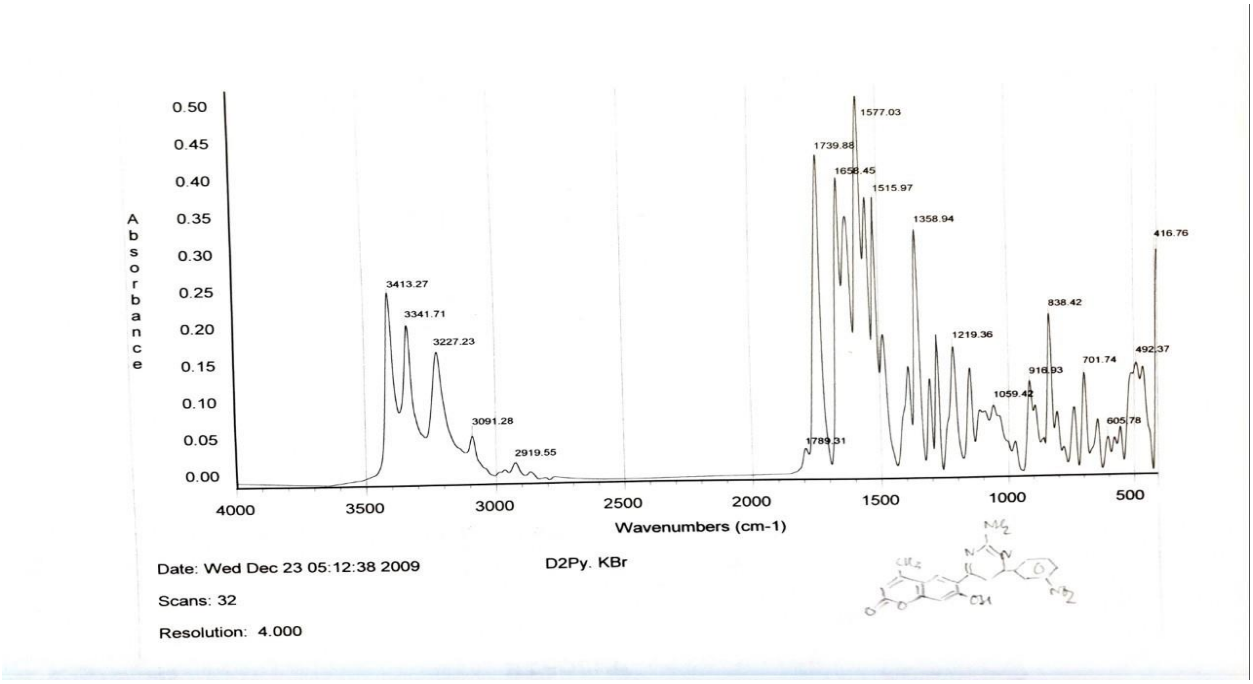
16. IR, NMR spectrum of 6-(2-Amino-6-m-chlorophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13f**)

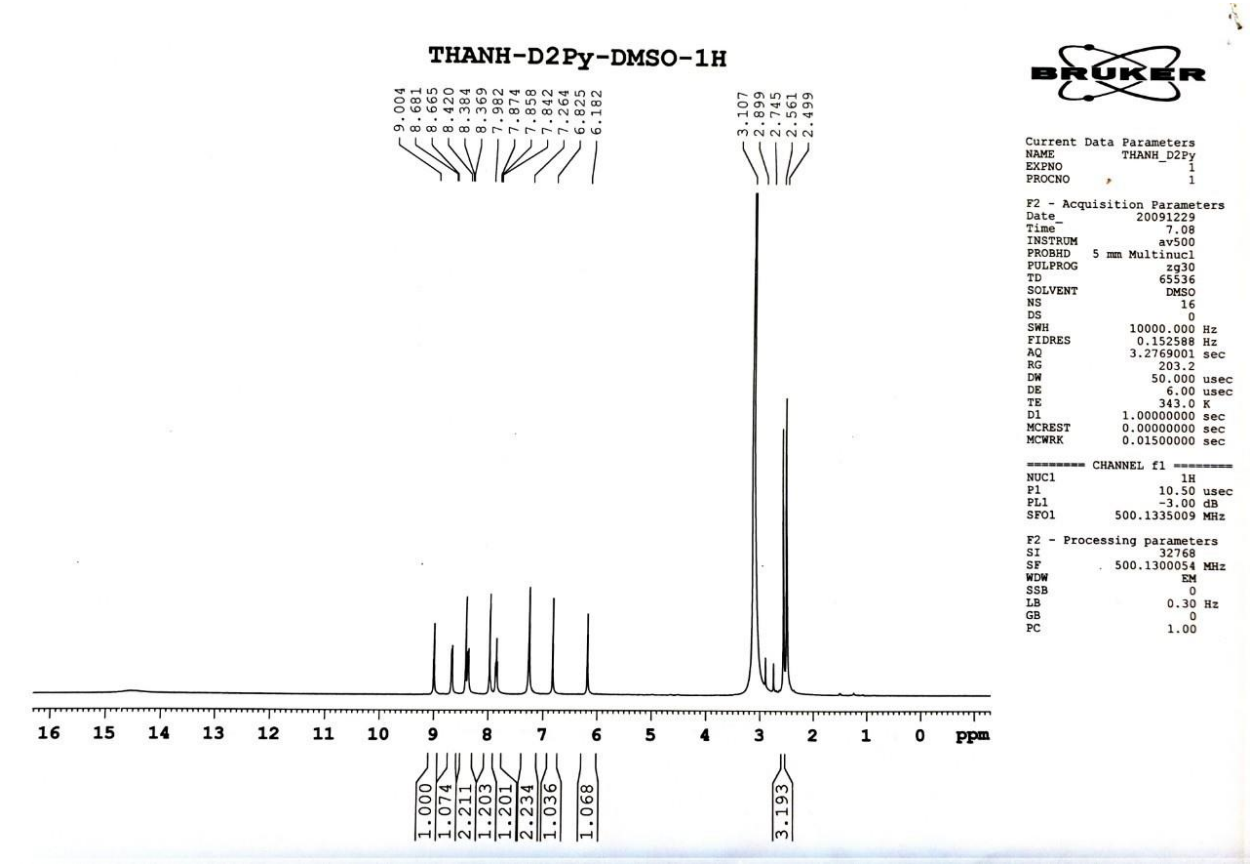



THANH-D6Py-DMSO-1H
8.424
8.281
8.237
8.223
7.947
7.933
7.632
7.629
7.616
7.605
7.590
7.574
7.377
6.837
6.208
3.414
3.334
2.887
2.728
2.558
2.503
2.499
2.496
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.839
1.052
0.991
1.136
1.172
2.149
2.045
1.000
1.015
3.191
BRUKER
Current Data Parameters
NAME THANH_D6Py
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091229
Time 9.21
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 302.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz
F2 - Processing parameters
SI 32768
SF 500.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

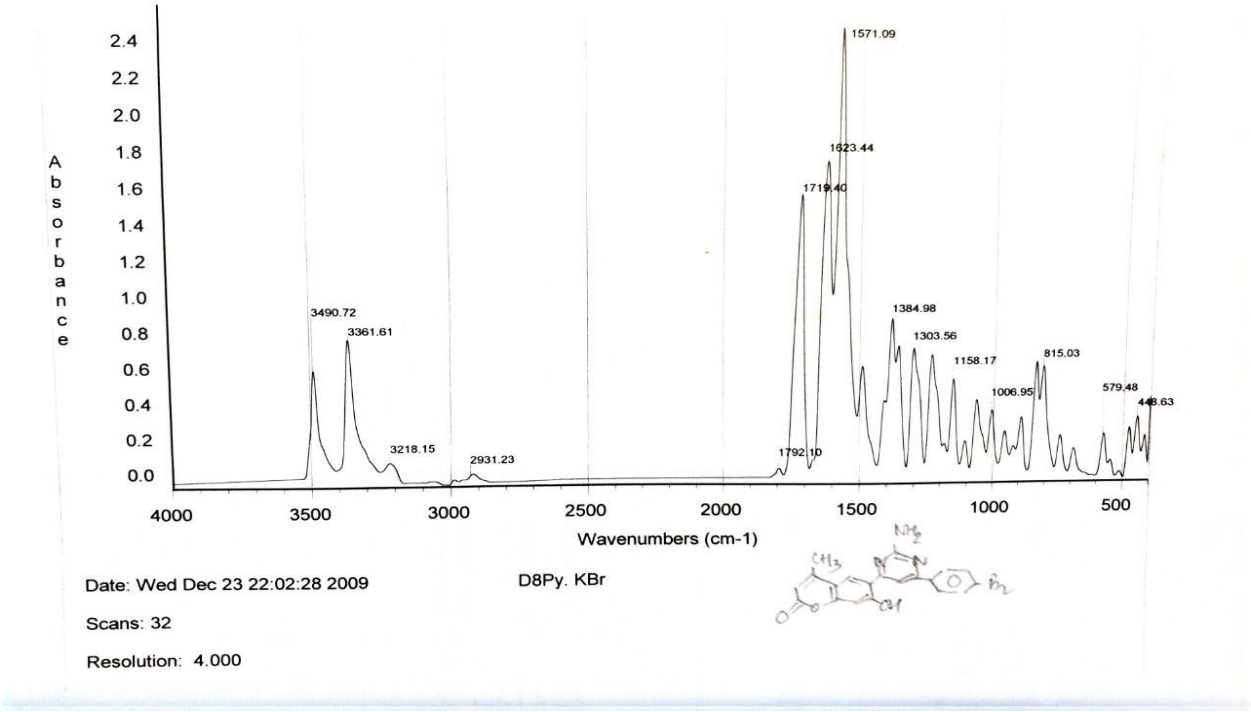

THANH-D6Py-DMSO-C13CPD
164.359
164.100
163.925
160.973
159.725
156.118
153.838
139.017
133.654
130.604
130.529
126.862
126.001
125.814
115.037
112.296
111.004
104.323
100.509
40.009
39.932
39.842
39.766
39.675
39.508
39.341
39.174
39.007
18.514
220 200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
Current Data Parameters
NAME THANH_D6Py
EXPNO 2
PROCNO 1
F2 - Acquisition Parameter
Date_ 20091229
Time 9.48
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 303.5
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
======== CHANNEL f1 ========
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005
F2 - Processing parameter
SI 32768
SF 125.7578519
WDW EM
SSB 0
LB 1.00
GB 0

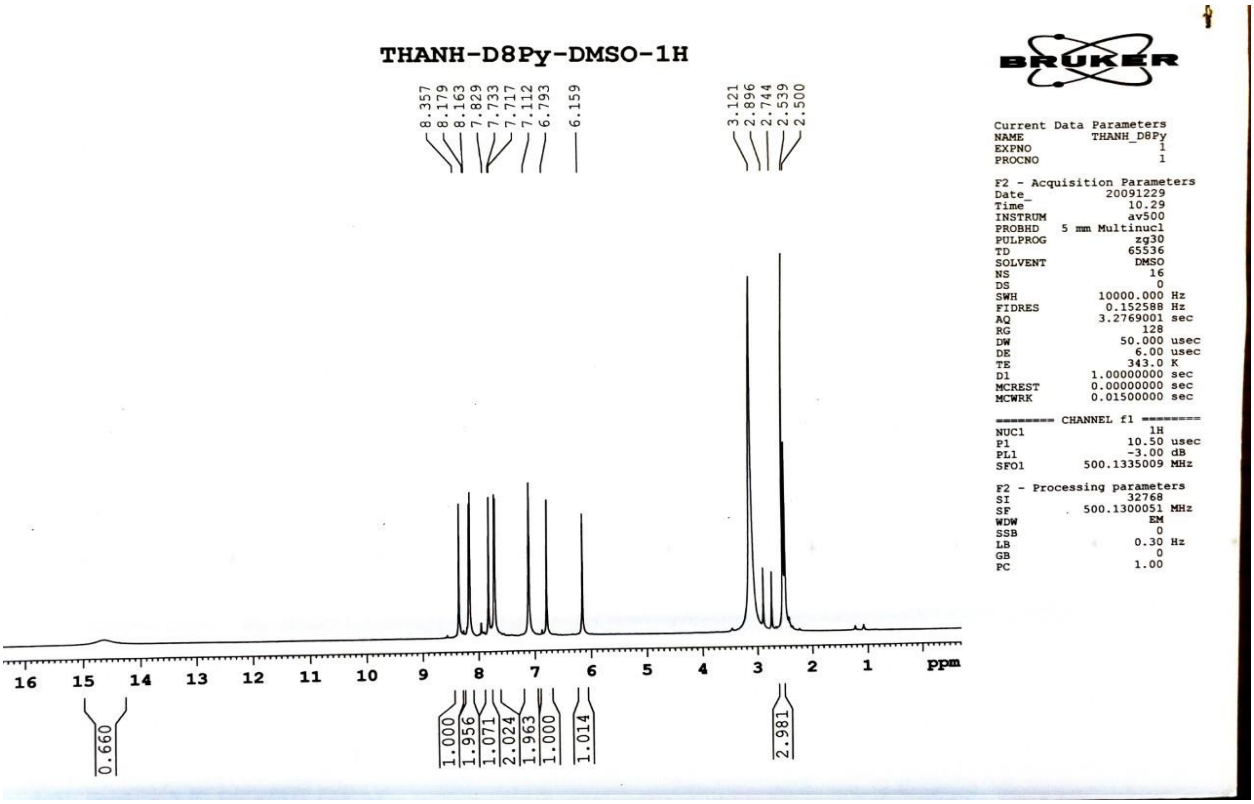
17. IR, NMR spectrum of 6-(2-Amino-6-m-nitrophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13g**)

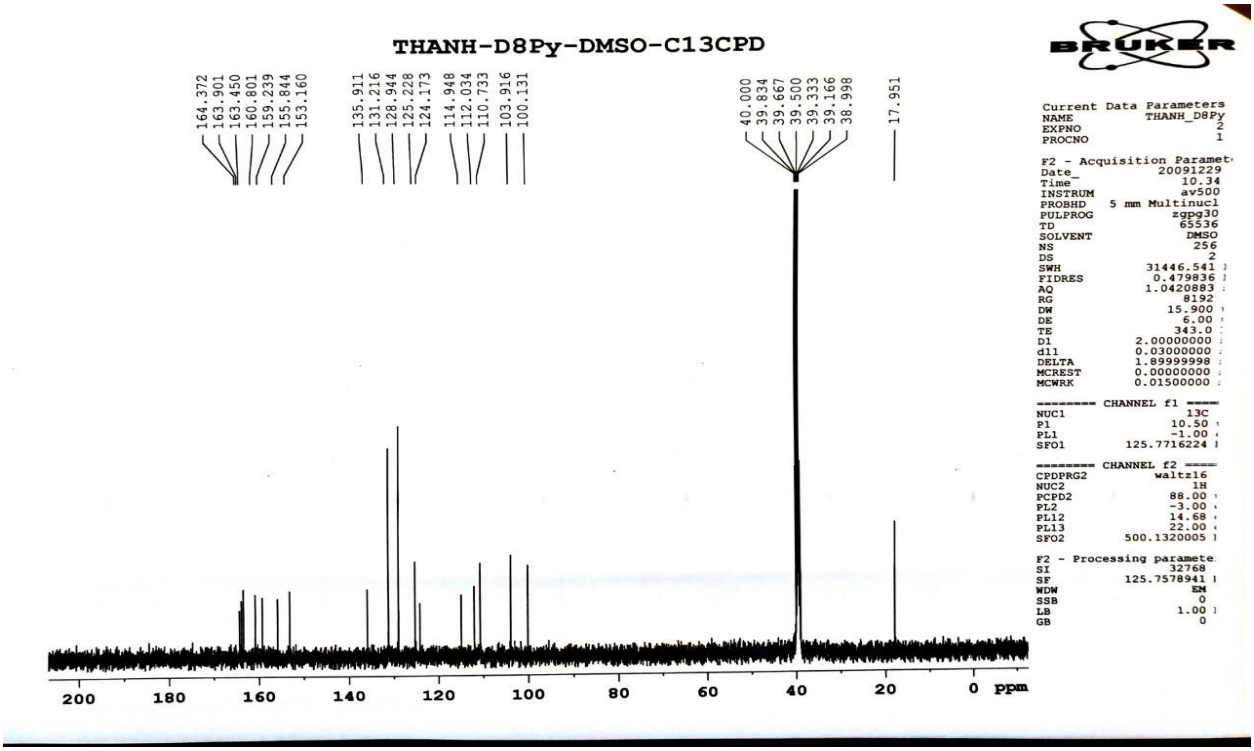




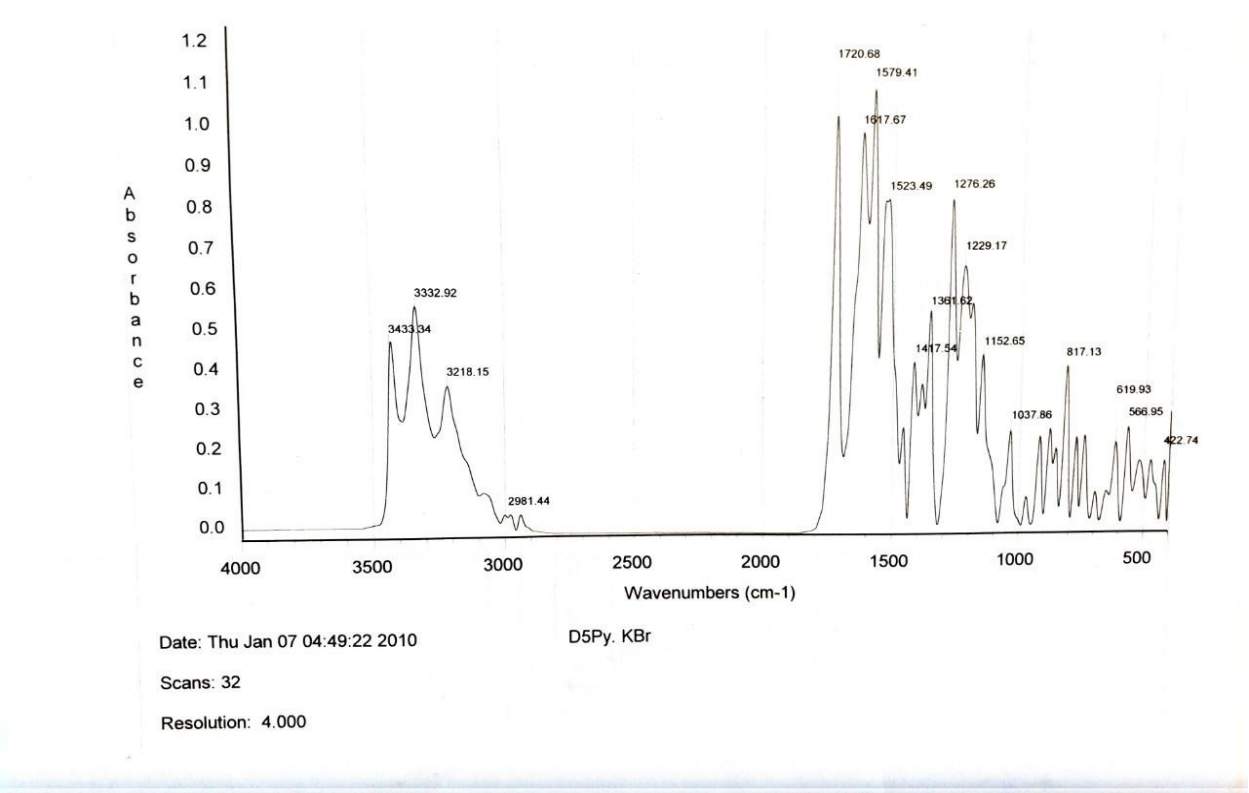
18. IR, NMR spectrum of 6-(2-Amino-6-p-bromophenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13h**)

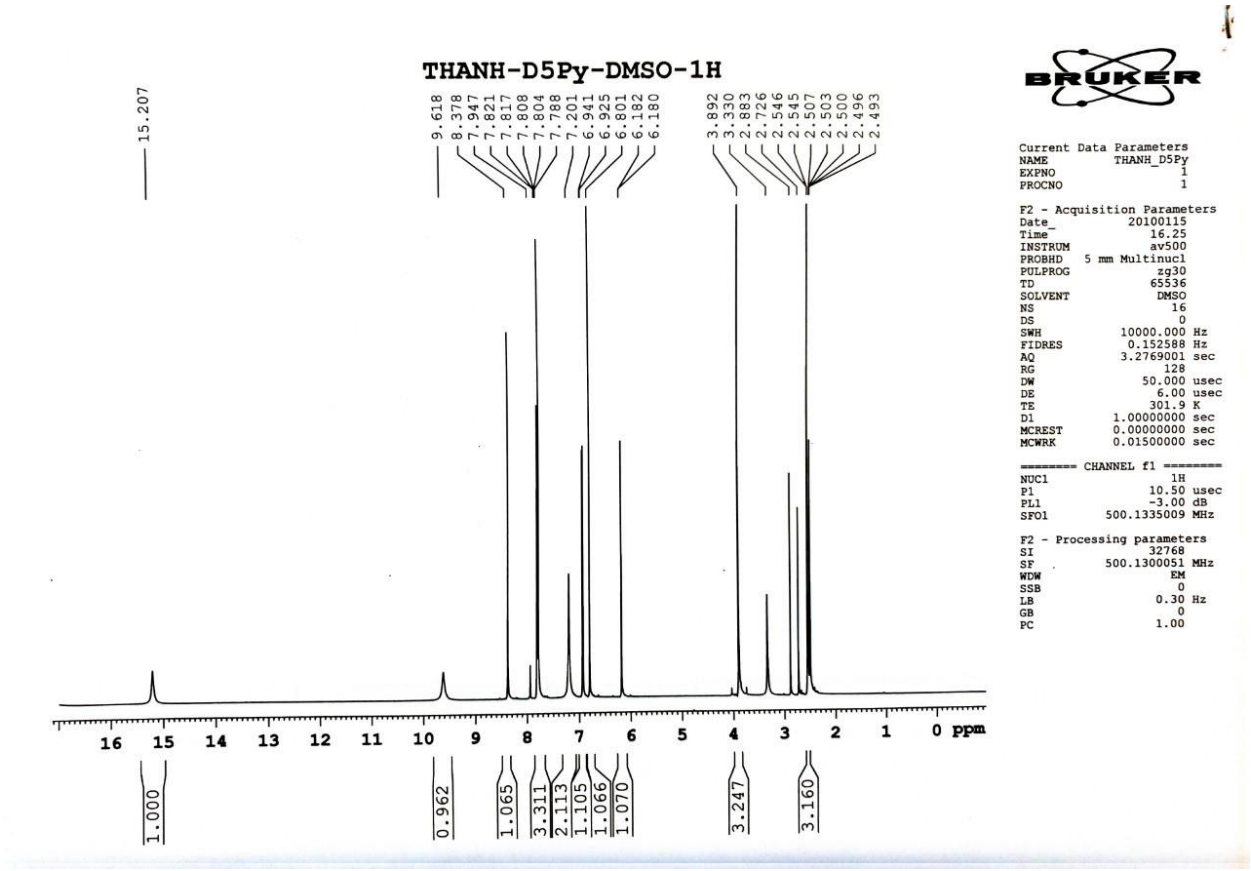


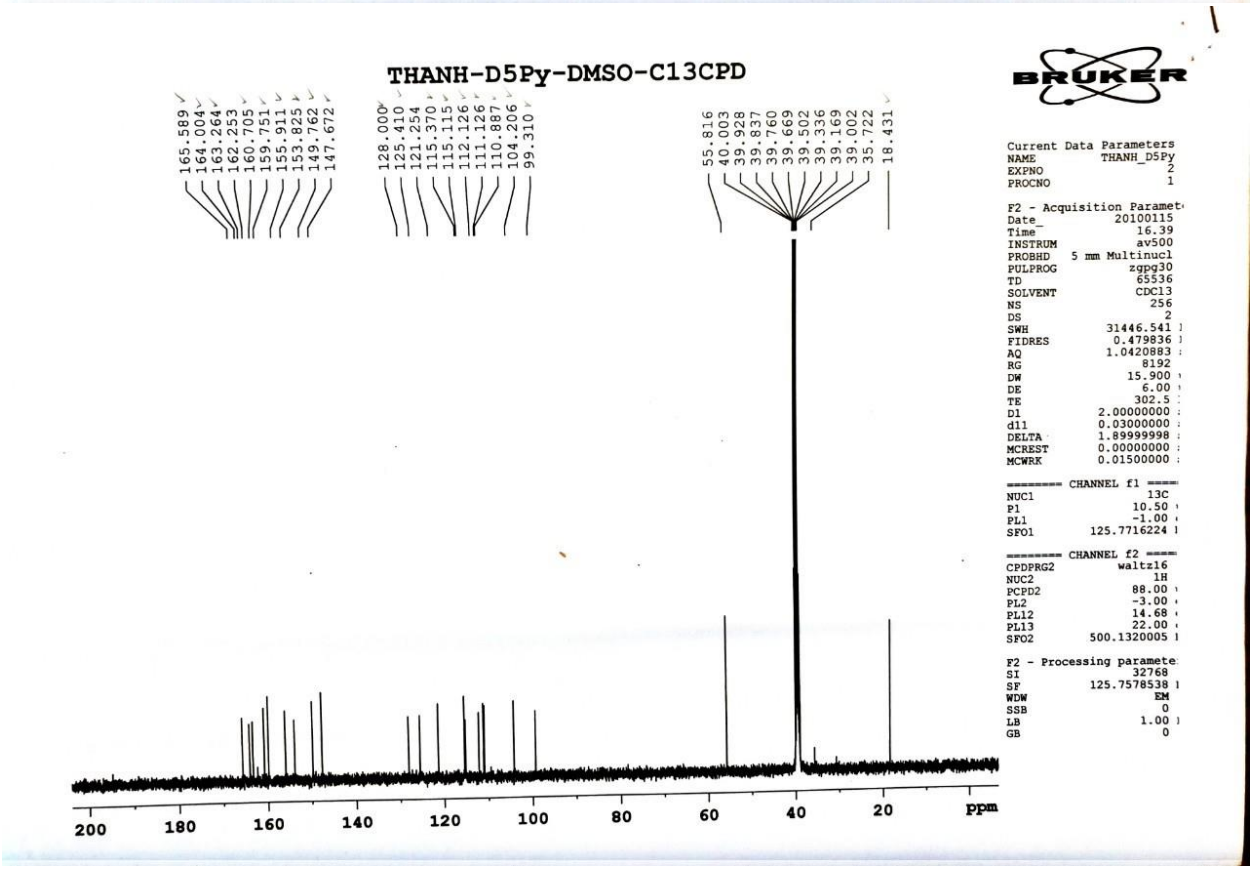


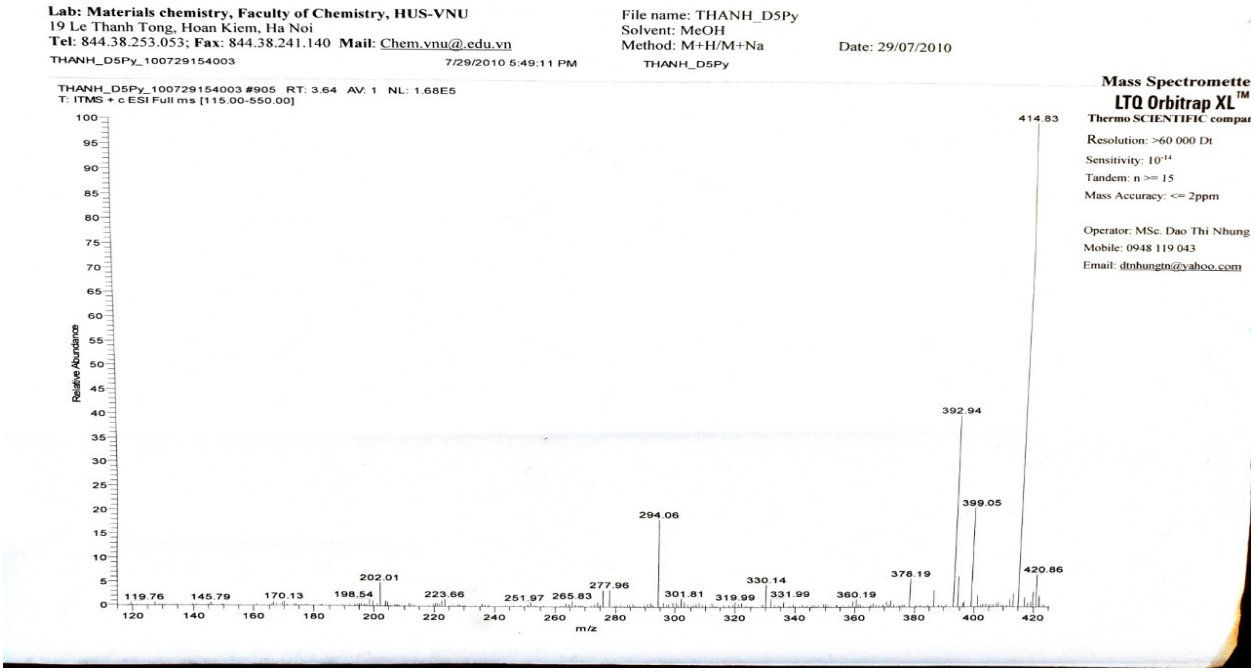


19. IR, NMR and ESI-MS spectrum of 6-(2-Amino-6-(4-hydroxy-3-methoxyphenylpyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13i**)

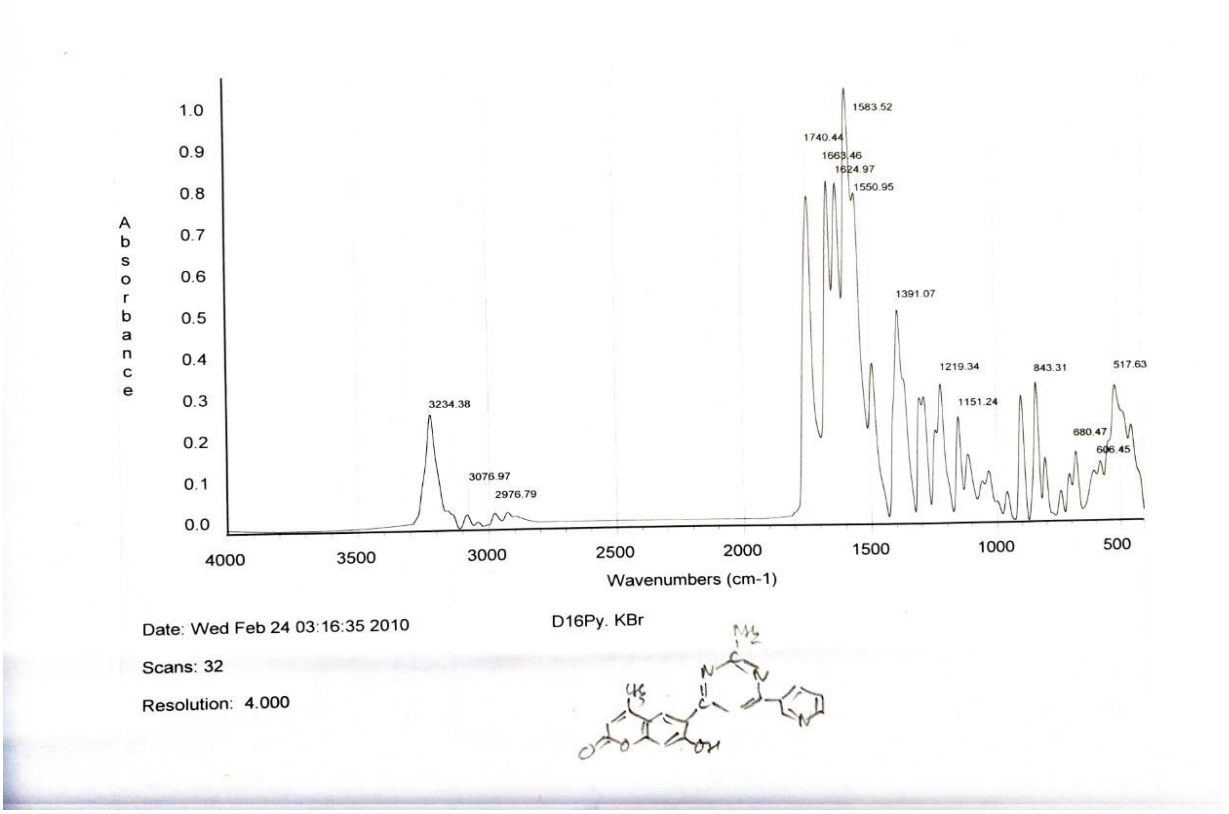


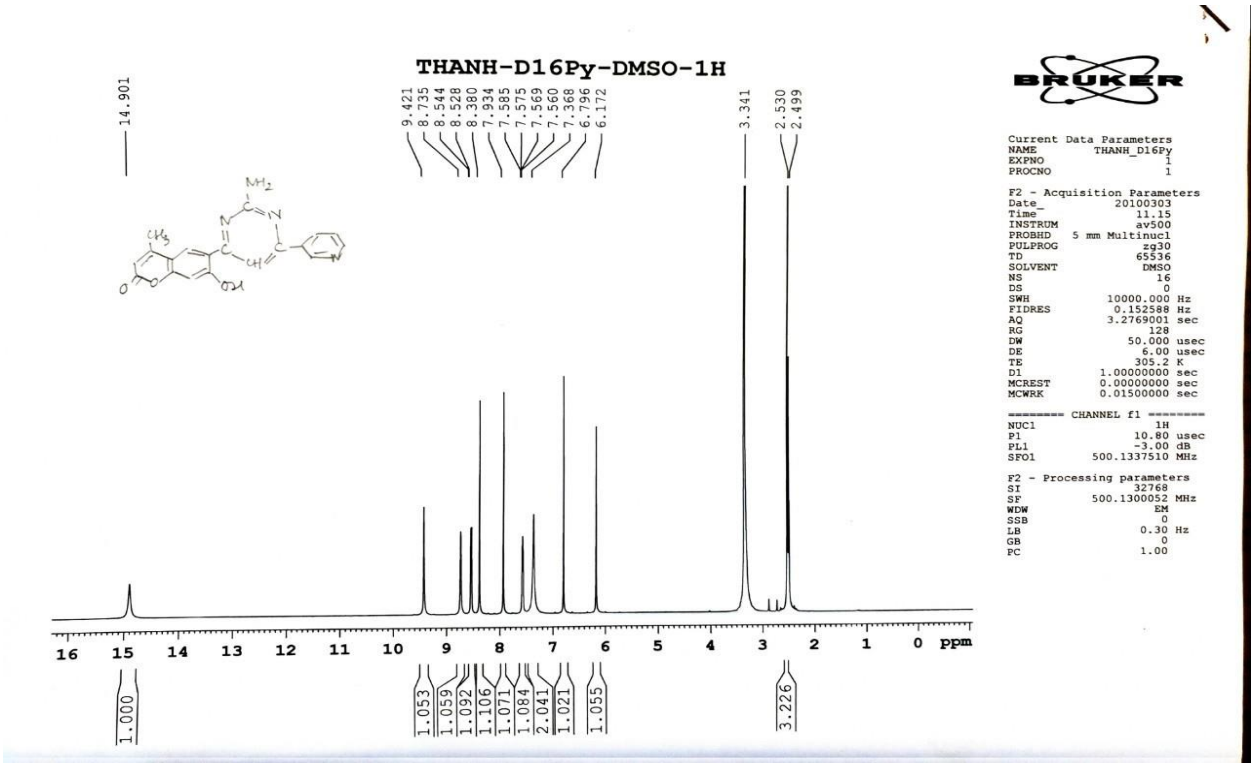

THANH-D5Py-DMSO-1H
15.207
9.618
8.378
7.947
7.821
7.817
7.808
7.804
7.788
7.201
6.941
6.925
6.801
6.182
6.180
3.892
3.330
2.883
2.726
2.546
2.545
2.507
2.503
2.500
2.496
2.493
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
0.962
1.065
3.311
2.113
1.105
1.066
1.070
3.247
3.160
BRUKER
Current Data Parameters
NAME THANH_D5Py
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100115
Time 16.25
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 301.9 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz
F2 - Processing parameters
SI 32768
SF 500.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

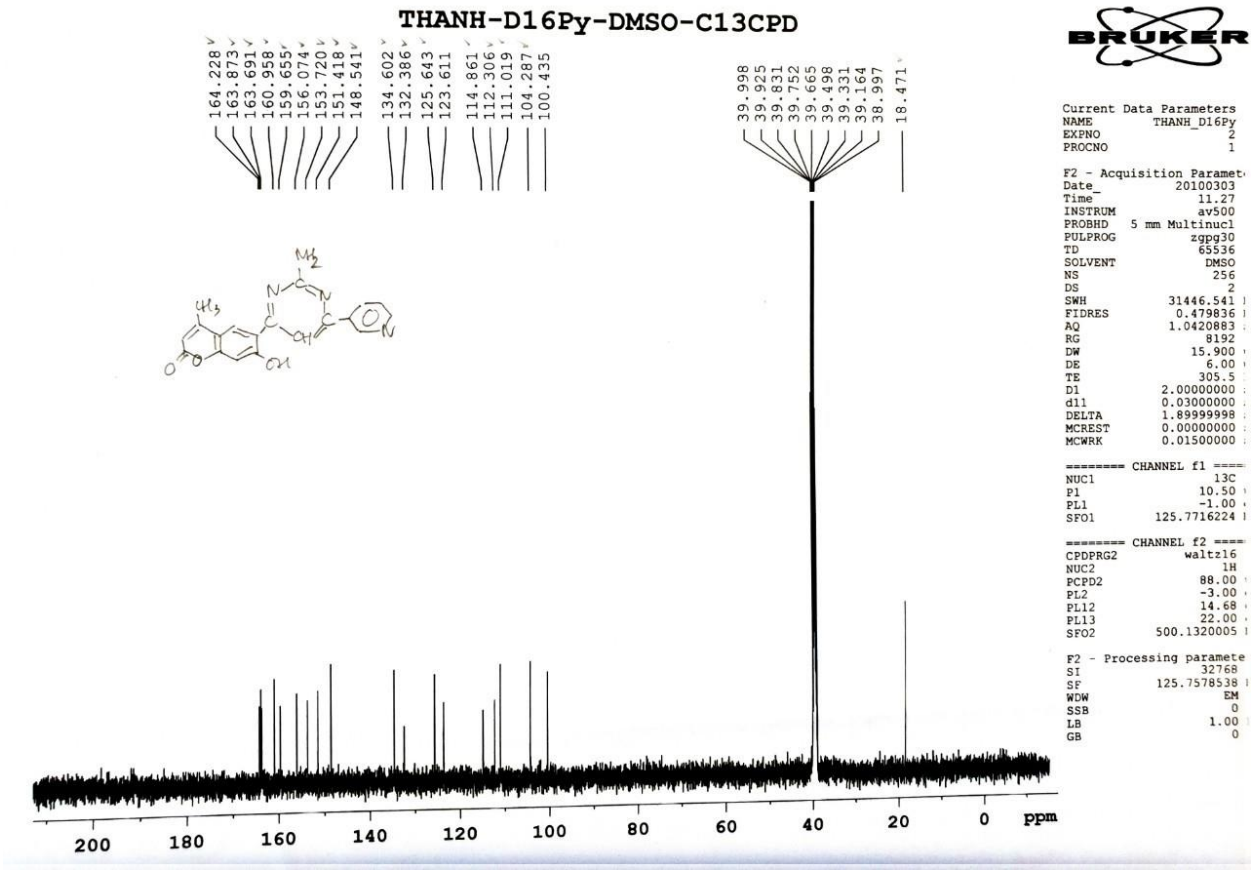

THANH-D5Py-DMSO-C13CPD
165.589
164.004
163.264
162.253
160.705
159.751
155.911
153.825
149.762
147.672
128.000
125.410
121.254
115.370
115.115
112.126
111.126
110.887
104.206
99.310
55.816
40.003
39.928
39.837
39.760
39.669
39.502
39.336
39.169
39.002
35.722
18.431
200 180 160 140 120 100 80 60 40 20 ppm
BRUKER
Current Data Parameters
NAME THANH_D5Py
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20100115
Time 16.39
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 302.5
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
======== CHANNEL f1 ========
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005
F2 - Processing paramete
SI 32768
SF 125.7578538
WDW EM
SSB 0
LB 1.00
GB 0

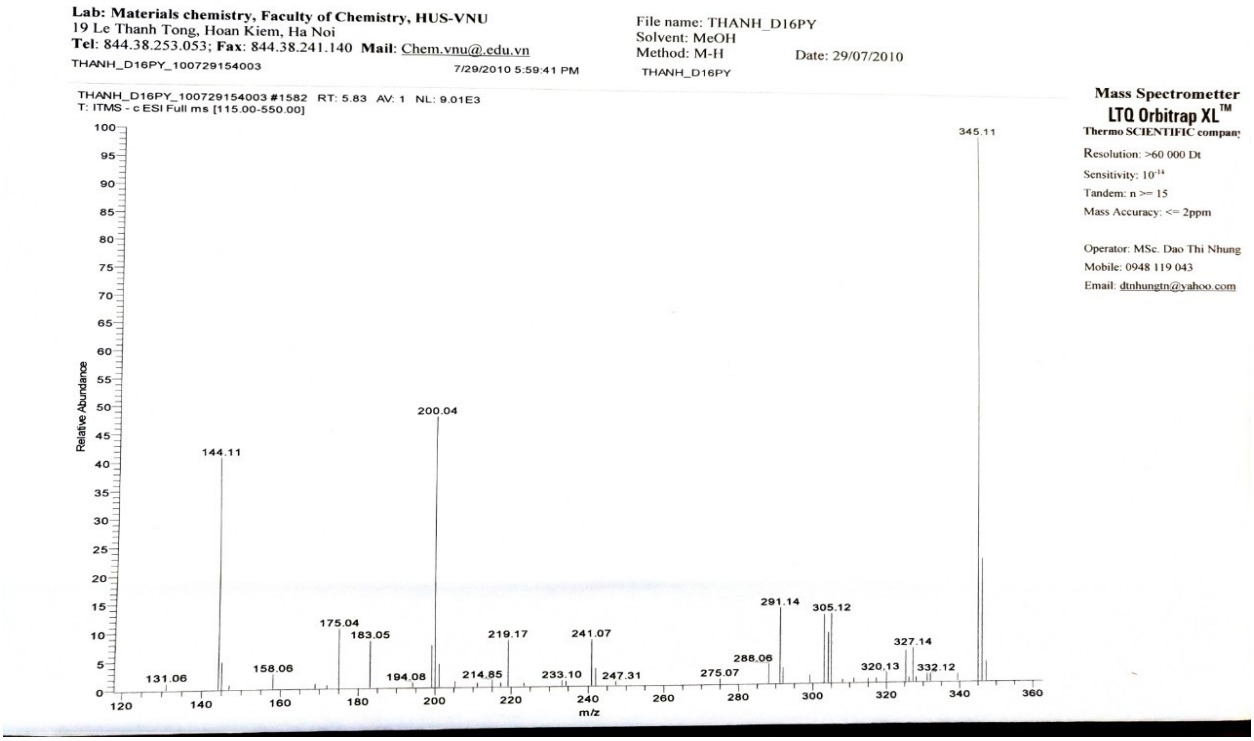


20. IR, NMR and ESI-MS spectrum of 6-(2-Amino-6-(pyridin-3-yl)pyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13j**)

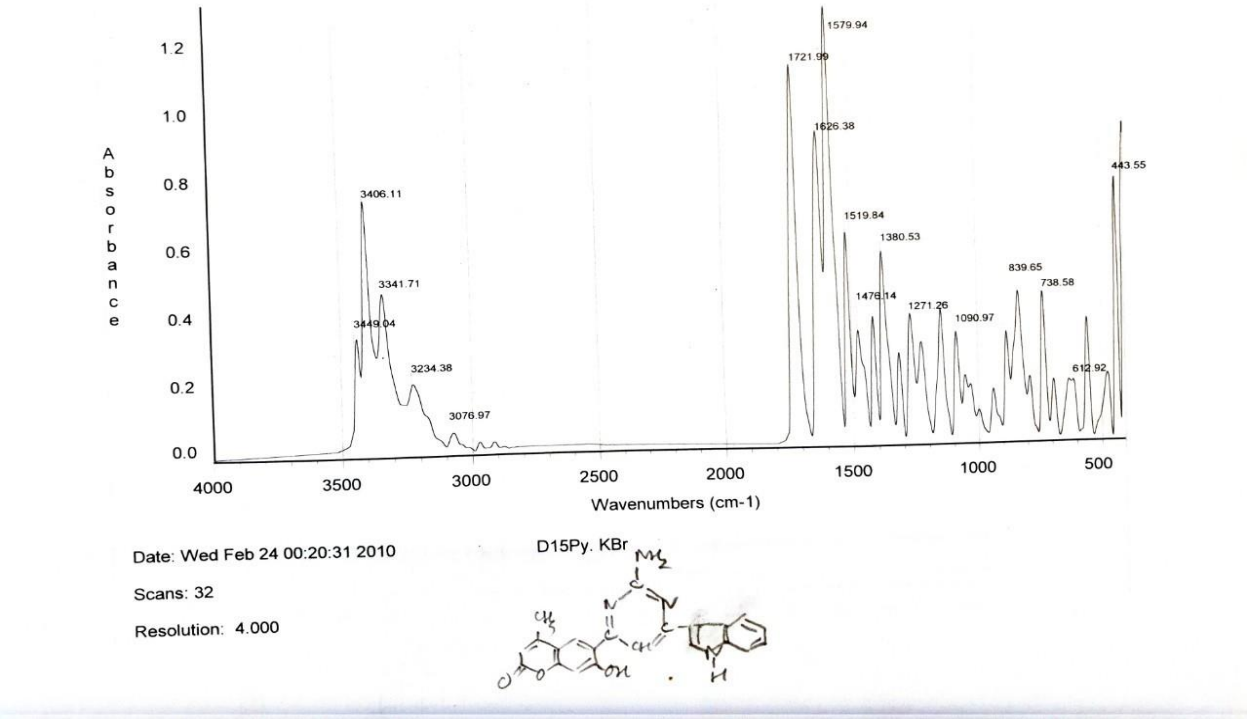


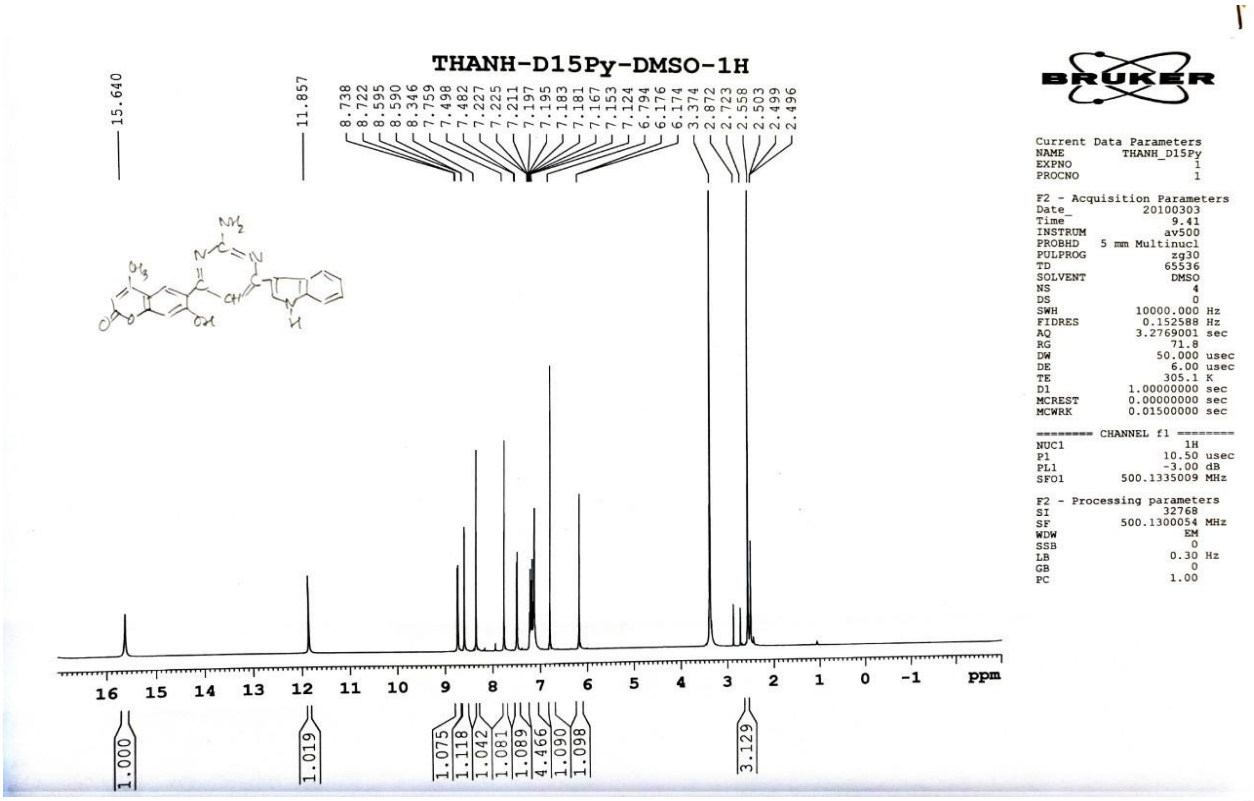

THANH-D16Py-DMSO-1H
14.901
9.421
8.735
8.544
8.528
8.380
7.934
7.585
7.575
7.569
7.560
7.368
6.796
6.172
3.341
2.530
2.499
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.000
1.053
1.059
1.092
1.106
1.071
1.084
2.041
1.021
1.055
3.226
BRUKER
Current Data Parameters
NAME THANH_D16Py
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100303
Time 11.15
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 128
DW 50.000 usec
DE 6.00 usec
TE 305.2 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.80 usec
PL1 -3.00 dB
SFO1 500.1337510 MHz
F2 - Processing parameters
SI 32768
SF 500.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

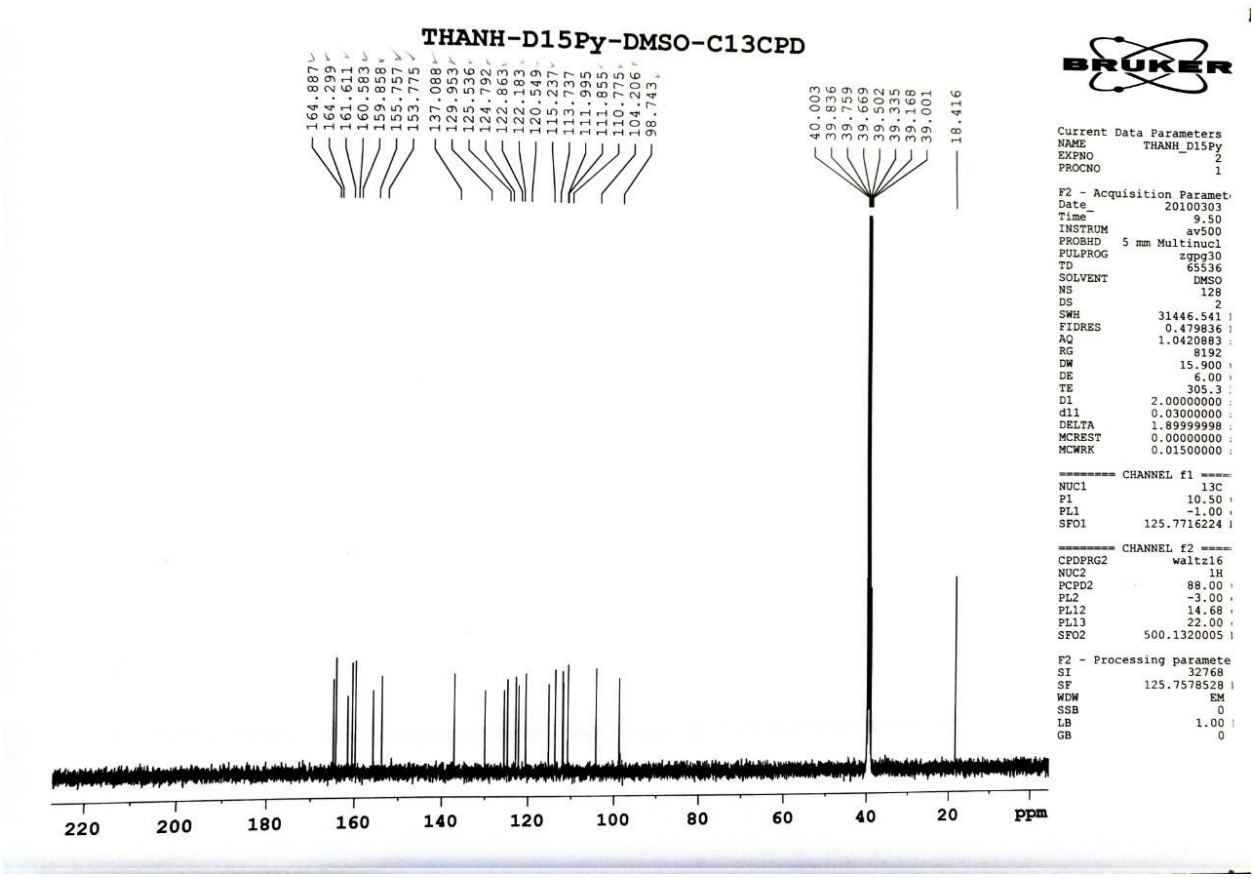

THANH-D16Py-DMSO-C13CPD
164.228
163.873
163.691
160.958
159.655
156.074
153.720
151.418
148.541
134.602
132.386
125.643
123.611
114.861
112.306
111.019
104.287
100.435
39.998
39.925
39.831
39.752
39.665
39.498
39.331
39.164
38.997
18.471
200 180 160 140 120 100 80 60 40 20 0 ppm
BRUKER
Current Data Parameters
NAME THANH_D16Py
EXPNO 2
PROCNO 1
F2 - Acquisition Parameter
Date_ 20100303
Time 11.27
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 256
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 305.5
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
======== CHANNEL f1 ====
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
======== CHANNEL f2 ====
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005
F2 - Processing paramete
SI 32768
SF 125.7578538
WDW EM
SSB 0
LB 1.00
GB 0

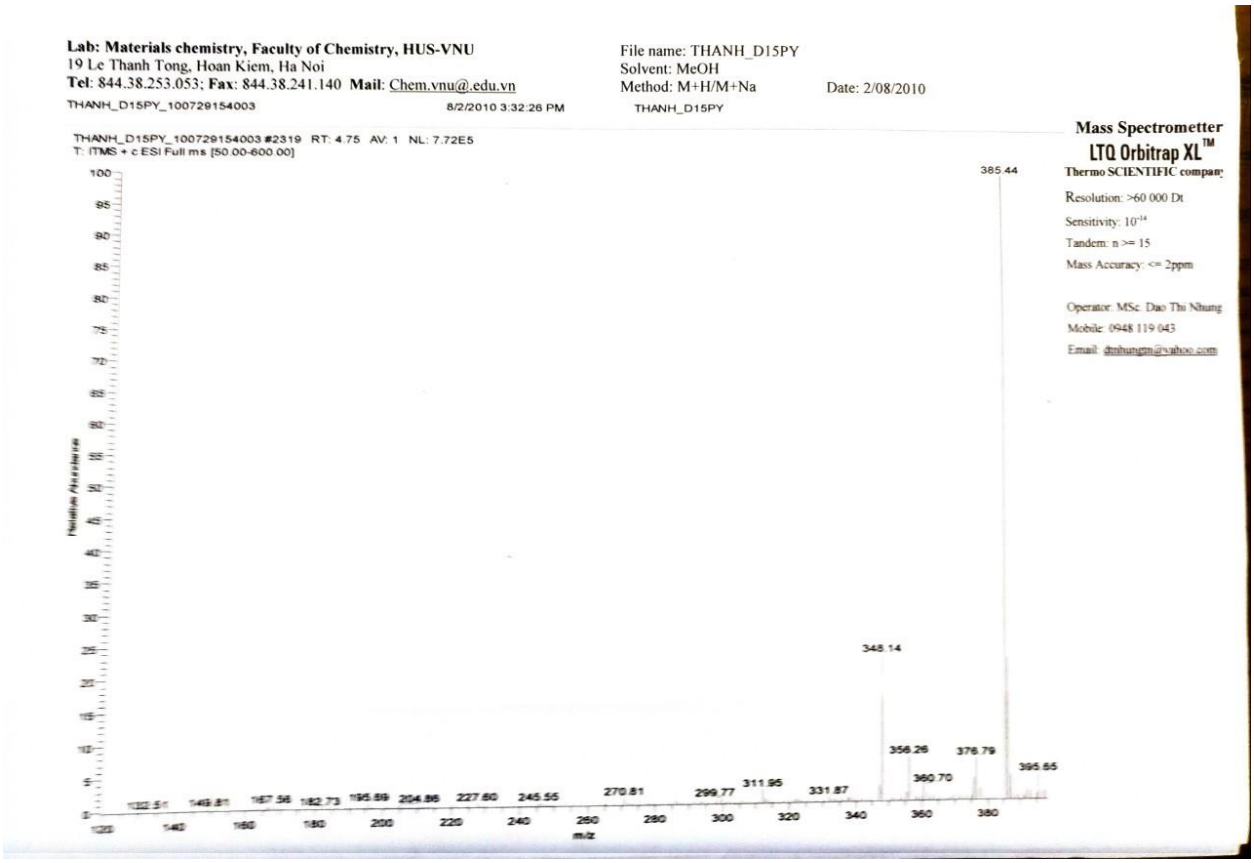


21. IR, NMR and ESI-MS spectrum of 6-(2-Amino-6-(indol-3-yl)pyrimidin-4-yl)-7-hydroxy-4-methylcoumarin (**13k**)




THANH-D15Py-DMSO-1H
15.640
11.857
8.738
8.722
8.595
8.590
8.346
7.759
7.498
7.482
7.227
7.225
7.211
7.197
7.195
7.183
7.181
7.167
7.153
7.124
6.794
6.176
6.174
3.374
2.872
2.723
2.558
2.503
2.499
2.496
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 ppm
1.000
1.019
1.075
1.118
1.042
1.081
1.089
4.466
1.090
1.098
3.129
Current Data Parameters
NAME THANH_D15Py
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100303
Time 9.41
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 4
DS 0
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2769001 sec
RG 71.8
DW 50.000 usec
DE 6.00 usec
TE 305.1 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.50 usec
PL1 -3.00 dB
SFO1 500.1335009 MHz
F2 - Processing parameters
SI 32768
SF 500.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


THANH-D15Py-DMSO-C13CPD
164.887
164.299
161.611
160.583
159.858
155.757
153.775
137.088
129.953
125.536
124.792
122.863
122.183
120.549
115.237
113.737
111.995
111.855
110.775
104.206
98.743
40.003
39.836
39.759
39.669
39.502
39.335
39.168
39.001
18.416
220 200 180 160 140 120 100 80 60 40 20 ppm
Current Data Parameters
NAME THANH_D15Py
EXPNO 2
PROCNO 1
F2 - Acquisition Paramet
Date_ 20100303
Time 9.50
INSTRUM av500
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
DS 2
SWH 31446.541
FIDRES 0.479836
AQ 1.0420883
RG 8192
DW 15.900
DE 6.00
TE 305.3
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
MCREST 0.00000000
MCWRK 0.01500000
CHANNEL f1
NUC1 13C
P1 10.50
PL1 -1.00
SFO1 125.7716224
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 88.00
PL2 -3.00
PL12 14.68
PL13 22.00
SFO2 500.1320005
F2 - Processing paramete
SI 32768
SF 125.7578528
WDW EM
SSB 0
LB 1.00
GB 0


Lab: Materials chemistry, Faculty of Chemistry, HUS-VNU
19 Le Thanh Tong, Hoan Kiem, Ha Noi
Tel: 844.38.253.053; Fax: 844.38.241.140 Mail: Chem.vnu@.edu.vn
THANH_D15PY_100729154003
8/2/2010 3:32:26 PM
File name: THANH_D15PY
Solvent: MeOH
Method: M+H/M+Na
Date: 2/08/2010
THANH_D15PY
THANH_D15PY_100729154003 #2319 RT: 4.75 AV: 1 NL: 7.72E5
T: ITMS + c ESI Full ms [50.00-600.00]
Mass Spectrometter
LTQ Orbitrap XL™
Thermo SCIENTIFIC company
Resolution: >60 000 Dt
Sensitivity: 10-14
Tandem: n >= 15
Mass Accuracy: <= 2ppm
Operator: MSc Dao Thi Nhung
Mobile: 0948 119 043
Email: dtnhungtn@yahoo.com
385.44
348.14
356.26
376.79
360.70
395.65
311.95
299.77
331.87
270.81
245.55
227.60
204.86
195.89
182.73
167.56
149.81
132.51
m/z

