Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Electronic Supplementary Information

Click-on Fluorescent Triazolyl Coumarin Peptidomimetics as Inhibitors of Human Breast Cancer Cell line MCF-7

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Journal: New Journal of Chemistry

[1] Experimental Section

Procedure for the synthesis of 4-Bromomethyl umbeliferone BMU: Placed a solution of 4-methylumbeliferone (176 mg, 10 mmol) in 20 ml glacial acetic acid in a 500 ml flask. 1.598 g (0.4982 ml, 10 mmol) of bromine in 10 ml glacial acetic acid was added to the flask very slowly (about 30 minutes) from a dropping funnel. The mixture was stirred vigorously during the addition of bromine and kept the temperature at 0-5^{0}C. When the addition was completed, it was allowed to stand at room temperature for 30 minutes. Then the mixture was poured into 400 ml water and stirred well. The precipitate was filtered with suction, washed with cold water. Recrystallised from dilute ethanol to afford reasonably pure **BMU** (white powder). 4-(bromomethyl)-7-hydroxy-2H-chromen-2-one. FT-IR (KBr) ν_{max} ;1698,1620,1600,1548,1511,1441,1375,1352,1263,1232,1204,1141,1075,1000,945,848,836,814,750,739,725, 692, 633,618,556,516,499,492,471,458,453,444,434,429,421,413,406,401 cm^{-1} ; ^{1}H-NMR: 2.490 (s, 2H), 6.972-6.994 (d, 2H), 7.682-7.703 (d, 2H), 8.232 (s, 1H) ppm; HRMS (EI) calcd for **$C_{10}H_7BrO_3$** $[M+H]^+$: 254.9579 , found: $[M+H]^+$: 255.0365.

Procedure for the synthesis of 4-Azidomethyl umbeliferone AMU: 4-Bromomethyl umbeliferone (254 mg, 1 mmol), K_2CO_3 (414 mg, 3 mmol) and sodium azide (65 mg, 1 mmol) were stirred at room temperature in DMF. After completion of the reaction, the reaction mixture was poured into ice cold water. The solid product was filtered and dried under vacuum to afford the **4-AMU** in pure form (Brown powder).

4-(azidomethyl)-7-hydroxy-2H-chromen-2-one. FT-IR (KBr) ν_{max} ; 3392,2920,2851,2122,1701,1608, 1550,1507,1445,1377,1340,1315,1261,1201,1161,1146,1105,810,754,725,631,580,552,529,456 cm^{-1} ; ^{1}H-NMR: 2.142 (2, 2H), 6.669 (s, 1H), 6. 732-6. 762 (d, 1H), 6.820-6.841 (d, 1H), 7.361-7.383 (d, 1H), 7.668-7.690 (d, 1H), 8.229 (s, 1H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6): δ 167.01,163.01,156.67,154.65,129.31,127.95,125.01,113.65,112.75,102.13,56.30,40.12,39.91,39.70,39.08, 38.07ppm;HRMS (EI) calcd for **$C_{10}H_7N_3O_3$**$[M]^+$:217.0487 , found: $[M]^+$: 217.0118.

General procedure for the synthesis of type 1 alkynes 1-3: Hydroxycoumarin (1mmol), K_2CO_3 (414 mg, 3 mmol) in DMF were heated to 50 ^{0}c for half an hour. After cooling, propargyl bromide (0.119 ml, I mmol) was added and stirred for 4 hours. The resulting solution is poured into ice water. The precipitate formed was filtered and washed with water to afford pure propargylated coumarin.

Procedure for the synthesis of type 1 alkyne 4: A solution of Coumarin-3-carboxylic acid (1.9 g, 0.01 mol), Propargyl alcohol (0.56 ml, 0.01 mol), N,N-dicyclohexyl cabodiimide (2.3 g, 011 mol), and 4-dimethylaminopyridine (0.122 g, 0.001 mol) in dichloromethane was stirred at room temperature for 6 h. After 6 h, the precipitated N,N-dicyclohexylurea was filtered off and the filtrate was washed with water, 5% acetic acid, and again with water. It was then dried over magnesium sulphate and the solvent was evaporated. The residue obtained was washed with petroleum ether to afford the ester prop-2-yn-1-yl 2-oxo-2Hchromene-3-carboxylate (2.4 g, 96%).

General procedure for the synthesis of type 2 alkynes 5-10: A round bottom flask is charged with propargyl derivative of hydroxy benzaldehyde (2 mmol), ketone (2 mmol), acetyl chloride (2 mL), acetonitrile(1 mL) and catalytic amount of $BF_3.Et_2O$ and kept under stirring for 3h at room temperature. The progress of the reaction was monitored by TLC analysis at regular intervals. After 3h, the mixture was quenched with cold water. The solid residue separated was collected and purified by passing it through a silica gel column. Elution of the column with petroleum ether (60-80 ºC) / ethyl acetate (9: 1 v/v) afforded **5-10**.

General procedure for the Cu (I) 1, 3-dipolar cycloaddition reactions to synthesis TC1-4 & ATC1-6: An equimolar amount of 4-Azidomethyl umbeliferone **4-AMU**(1 mmol) and the alkynes **1-10** (1 mmol) are dissolved in minimum amount of DMSO. To this, 2 ml of *t*-BuOH, 1 ml of water, $CuSO_4$-$5H_2O$ (200 mg) and sodium ascorbate (150 mg) are added and stirred at room temperature for 12 h, and then poured in to cold water. The precipitated click product was filtered, washed with water and dried under vacuum to afford **TC1-4 & ATC1-6** in pure form.

1. 7-hydroxy-4-((4-(((2-oxo-2H-chromen-7-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-2H-chromen-2-one (**TC1**- white powder). FT-IR, KBr, ν_{max} : 3439,2922,2852,1715,1619,1572,1509,1467,1389,1349,1326,1295,1225,1206,1151,1063,1019,984,941, 844, 822,765,686cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d6): δ 2.297-2.321 (d, 3H), 4.022-4.070 (q, 2H), 5.023 (s, 1H), 5.464-5.468 (d, 2H), 5.998 (s, 2H), 6.165 (s, 1H), 7.314-7.438 (m, 3H), 7.554 (s, 1H), 7.570-80121 (m, 4H) ppm;HRMS (EI) calcd for **$C_{23}H_{17}N_3O_6$** $[M+H]^+$: 432.1117 , found: $[M+H]^+$: 432.1188.

2.7-hydroxy-4-((4-(((4-methyl-2-oxo-2H-chromen-7-yl) oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-2H-chromen-2-one (**TC2**- white powder). FT-IR, KBr, ν_{max}: 3422,3165,2923,2853,1726,1685,1615,1573,1557,1508,1466,1402,1354,1322,1283,1228,1159, 1135, 1089,1045,1016,949,906,836,802,765,703,656,620,566,534,507,458cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d6): δ 4.693-4.622 (q, 1H), 5.238 (s, 2H),5.559 (s,1H), 6.502-6.691 (q, 1H), 6.864-6.876 (d, 1H), 7.090-7.354 (m, 8H), 7.963 (s, 1H) ppm;HRMS (EI) calcd for$C_{23}H_{17}N_3O_6$ $[M+H]^+$: 418.0961 , found: $[M+H]^+$: 418.1016.

3. 7-hydroxy-4-((4-(((2-oxo-2H-chromen-4-yl)oxy)methyl)-1H-1,2,3-triazol-1-yl)methyl)-2H-chromen-2-one (**TC3**- white powder). FT-IR, KBr, ν_{max}: 3421,2919,2850,1728,1710,1610,1563,1509,1493,1449,1425,1387,1354,1332,1273,1244, 1197,1156, 1128,1107, 1085,1047,947,882,764,747,655 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d6): δ4.2660-4.3096 (q, 2H), 5.3050 (s,1H), 5.7121-5.7860 (d, 3H), 6.3132 (s, 2H), 6.7602-6.7765 (d, 2H), 7.3075-7.4262 (m, 5H) ppm; ^{13}C NMR (100 MHz, DMSO-d_6): δ 168.20,160.80,160.27,156.05,141.43,135.53,135.07,131.75,130.04,127.80,127.47,127.27,114.52,114.33,87.47,66.48,60.66,48.33,45.33,40.12,39.31,33.24,33.07,30.87,30.66ppm;HRMS (EI) calcd for$C_{22}H_{15}N_3O_6$$[M+H]^+$: 418.0961 , found: $[M+H]^+$: 418.1029.

4. (1-((7-hydroxy-2-oxo-2H-chromen-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methyl 2-oxo-2H-chromene-3-carboxylate (**TC4**- white powder). FT-IR, KBr, ν_{max} : 3431,2925,2852,1717,1693,1648,1617,1576,1555,1456,1401,1369,1289,1258,1233,1181,1033,923,882, 779,759,644,595,464,418cm^{-1}; HRMS (EI) calcd for $C_{23}H_{15}N_3O_7[M+H]^+$: 446.0910 , found: $[M+H]^+$: 446.1774.

5. N-(1-(4-((1-((7-hydroxy-2-oxo-2H-chromen-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-3-oxo-3-phenylpropyl)acetamide (**ATC1**- white powder). FT-IR, KBr, ν_{max} : 3414,2923,2851,1725,1648,1589,1489,1455,1400,1376,1292,1240,1121,1091,1024,818, 754,620,529,470,418cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d6): δ1.517 (s, 3H), 3.271-3.278 (d, 1H), 3.296-3.313 (d, 1H), 4.617-4.653 (q, 2H), 5.229 (s, 1H), 5.485-5.564 (d, 3H), 6.576-6.617 (q, 1H), 6.870 (s, 1H), 7.087-7.368 (m, 11H), 7.998 (s, 1H),8.248 (s, 1H) ppm;HRMS (EI) calcd for$C_{30}H_{26}N_4O_6[M+H]^+$: 539.1852 , found: $[M+H]^+$: 539.2055.

6. N-(3-(4-bromophenyl)-1-(4-((1-((7-hydroxy-2-oxo-2H-chromen-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-3-oxopropyl)acetamide (**ATC2**- white powder). FT-IR, KBr, ν_{max} : 3420,2922,1731,1648,1600,1556,1490,1450,1375,1358,1320, 1240,1160,1122,1088,1016,949,817,754,691,504cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d6): δ 1.502 (s, 3H), 2.297-2.321 (d, 2H), 4.014-4.074 (m, 2H), 5.023 (s,2H), 5.468-5.613 (t, 1H), 6.147 (s, 1H), 7.299-8.121 (m, 13 H),10.074 (s, 1H) ppm;HRMS (EI) calcd for$C_{30}H_{25}BrN_4O_6[M+H]^+$: 617.0957 , found: $[M+H]^+$: 617.1911.

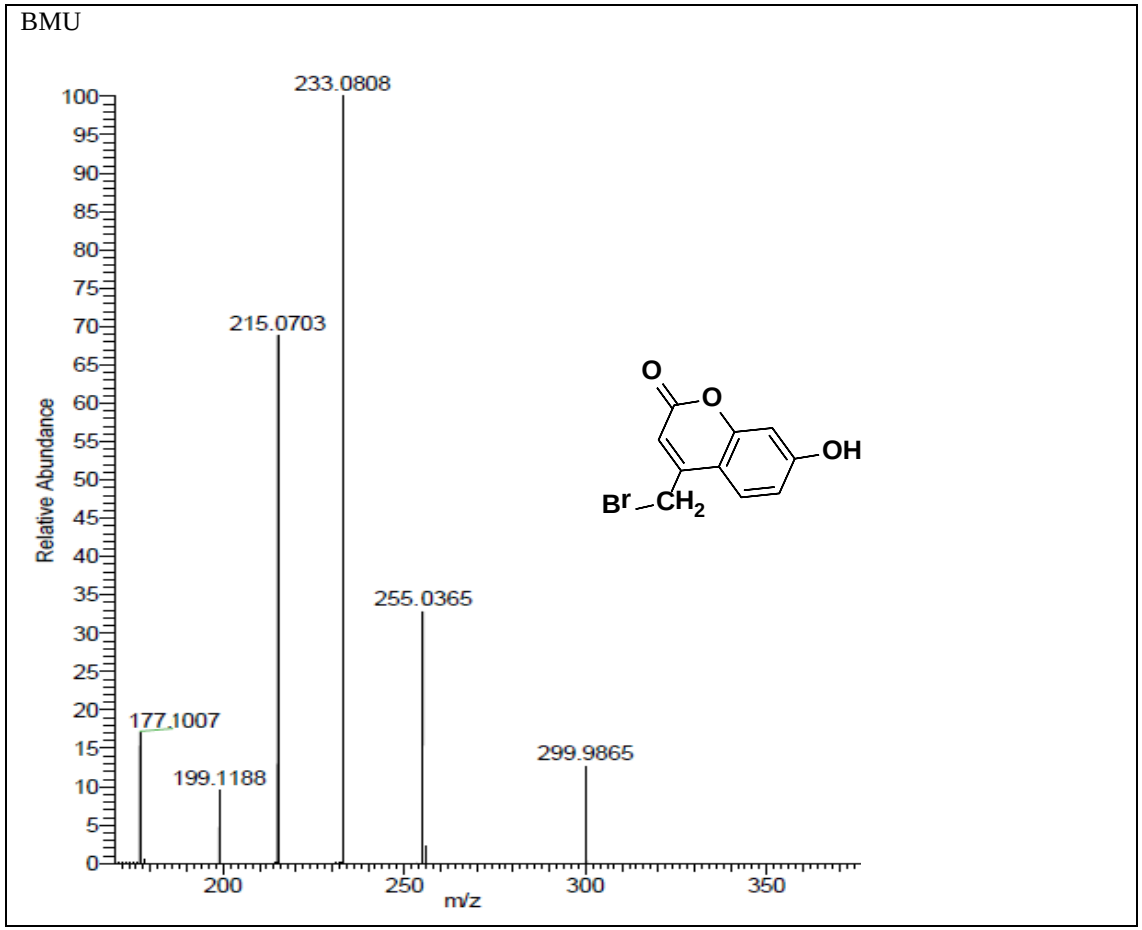
7. N-(1-(2-((1-((7-hydroxy-2-oxo-2H-chromen-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methoxy) phenyl)-3-oxo-3-phenylpropyl)acetamide (**ATC3**- white powder). FT-IR, KBr, ν_{max} : 3423,2922,2852,1728,1655,1599,1508,1466,1419,1383,1323,1248,1171,1125, 1088, 1019,832,763,725,550,502,466cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d6): δ 1.772 (s, 3H), 2.791-2.864 (d, 2H), 4.759-4.794 (d, 2H), 4.836-4.864 (d,1H), 5.875 (s, 1H), 5.891 (s, 1H), 7.225-7.313 (m, 6H), 7.706-7.930 (m, 9H), 10.059 (s, 1H) ppm;HRMS (EI) calcd for$C_{30}H_{26}N_4O_6[M+H]^+$: 539.1852 , found: $[M+H]^+$: 539.1747.

8. N-(3-(4-chlorophenyl)-1-(2-((1-((7-hydroxy-2-oxo-2H-chromen-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-3-oxopropyl)acetamide (**ATC4**- white powder). FT-IR, KBr, ν_{max} : 3385,2983,1700,1647,1579,1591,1445,1351,1301, 1223,1097, 1040,923,808,759,735,689,458,421,cm^{-1};^{1}H NMR (400 MHz, DMSO-d6): δ 1.6795-1.7685 (m, 3H), 2.4337-2.5221 (t, 2H), 4.4094-4.4133 (d, 2H), 5.2202 (s, 1H), 5.3973 (s, 1H), 5.4245 (s, 1H), 6.6648-6.9757 (m, 10 H), 7.3284-7.5221 (m, 2H), 7.9360 (s, 1H), 8.3214 (s, 1H) ppm;^{13}C NMR (100 MHz, DMSO-d_6): δ194.01,194.00,168.43,168.73,161.04,142.20,132.62,130.31,129.92, 129.83,127.62,127.74,122.22,114.74,76.68,55.68,48.73,48.01,39.70,39.50,39.07,34.06,22.52ppm;HRMS (EI) calcd for$C_{30}H_{25}ClN_4O_6$ $[M]^+$: 572.1463 , found: $[M]^+$: 572.1482.

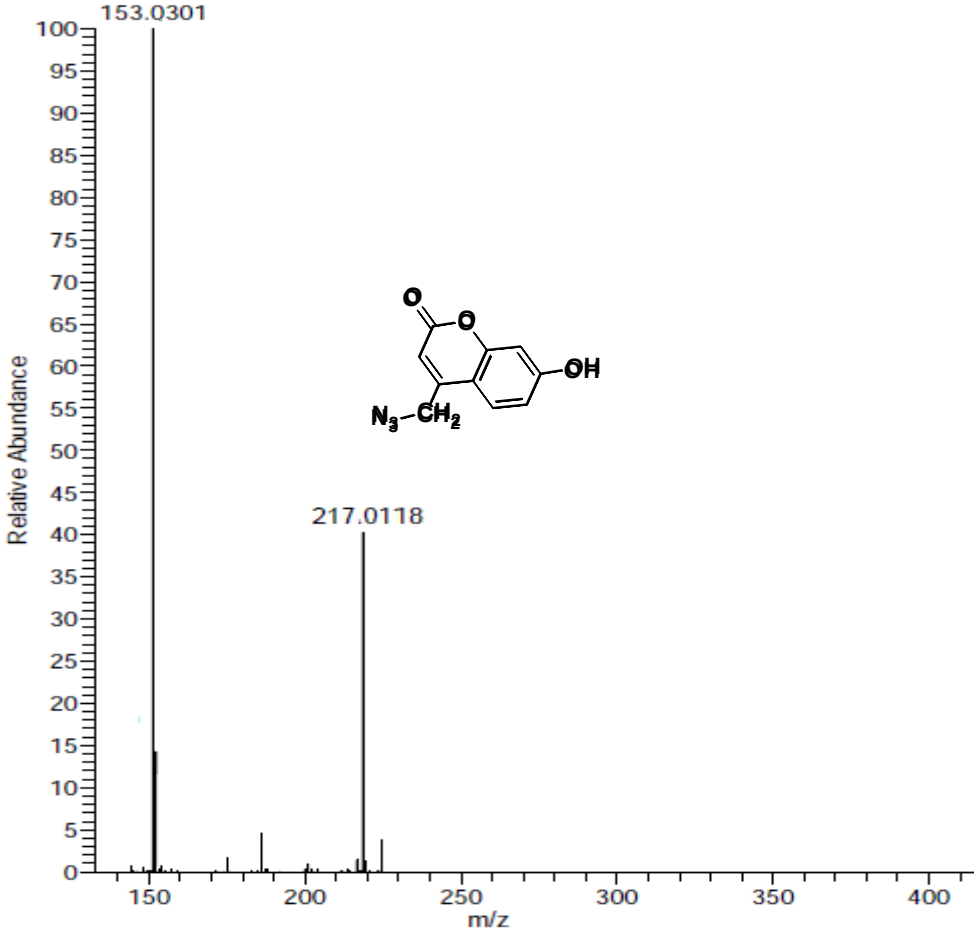
9. N-(3-(4-chlorophenyl)-1-(4-((1-((7-hydroxy-2-oxo-2H-chromen-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-3-oxopropyl)acetamide (**ATC5**- white powder). FT-IR, KBr, ν_{max} : 3433,2923,1787,1765,1650,1596,1557, 1529,1500,1449,1421, 1349,1325,1272,1230,1158,1000,886,860,809,776,700,623,542cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d6): δ 1.6057 (s, 3H), 3.3075-3.2340 (d, 2H), 4.2811- 4.2951 (d, 2H), 5.1848 (s, 1H), 5.3050-5.3096 (d, 2H), 5.5231 (s, 1H), 6.7602-6.7765 (d, 1H), 7.2837-7.3146 (m, 6H), 7.4336-7.6278 (m, 10 H), 8.5555 (s, 1H) ppm;HRMS (EI) calcd for$C_{30}H_{25}ClN_4O_6$$[M+H]^+$: 573.1463 , found: $[M+H]^+$: 573.1219.

10. N-(1-(2-bromophenyl)-3-(4-((1-((7-hydroxy-2-oxo-2H-chromen-4-yl)methyl)-1H-1,2,3-triazol-4-yl)methoxy)phenyl)-3-oxopropyl)acetamide (**ATC6**- white powder). FT-IR, KBr, ν_{max} : 3410,2923,1757,1687,1490,1446,1408,1359,1325,1272,1230, 1180,1157,1091,1014,952,833,754,727,616,585,508,486cm^{-1};HRMS (EI) calcd for$C_{30}H_{25}BrN_4O_6$$[M+H]^+$: 617.0957 , found: $[M+H]^+$: 617.0110.

[2] Mass Spectra of compounds



4-BMU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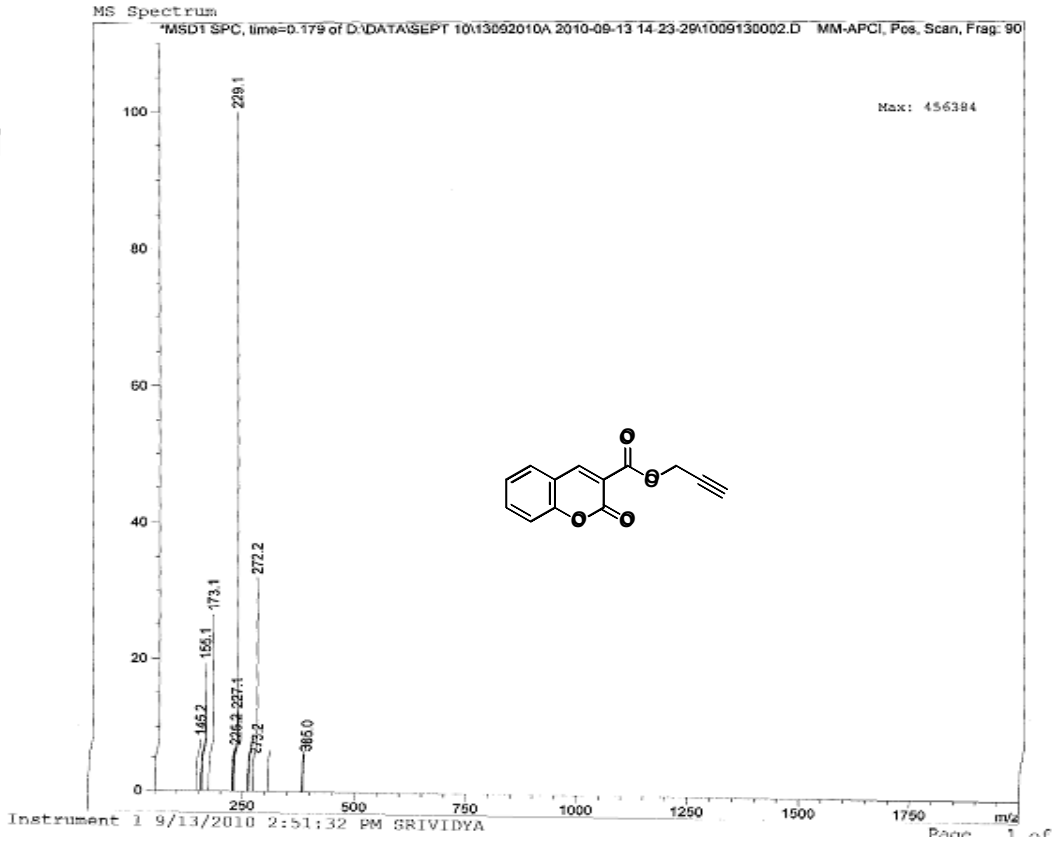
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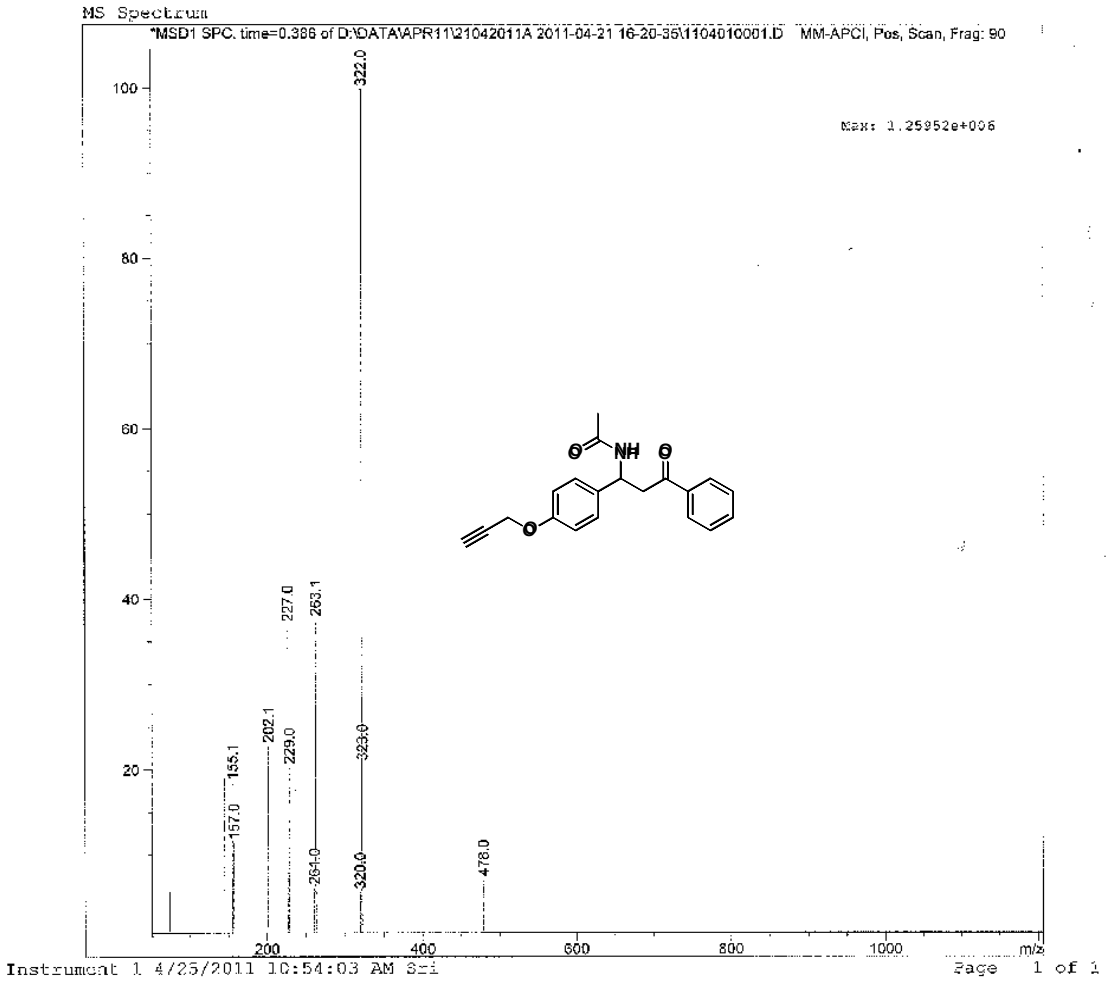
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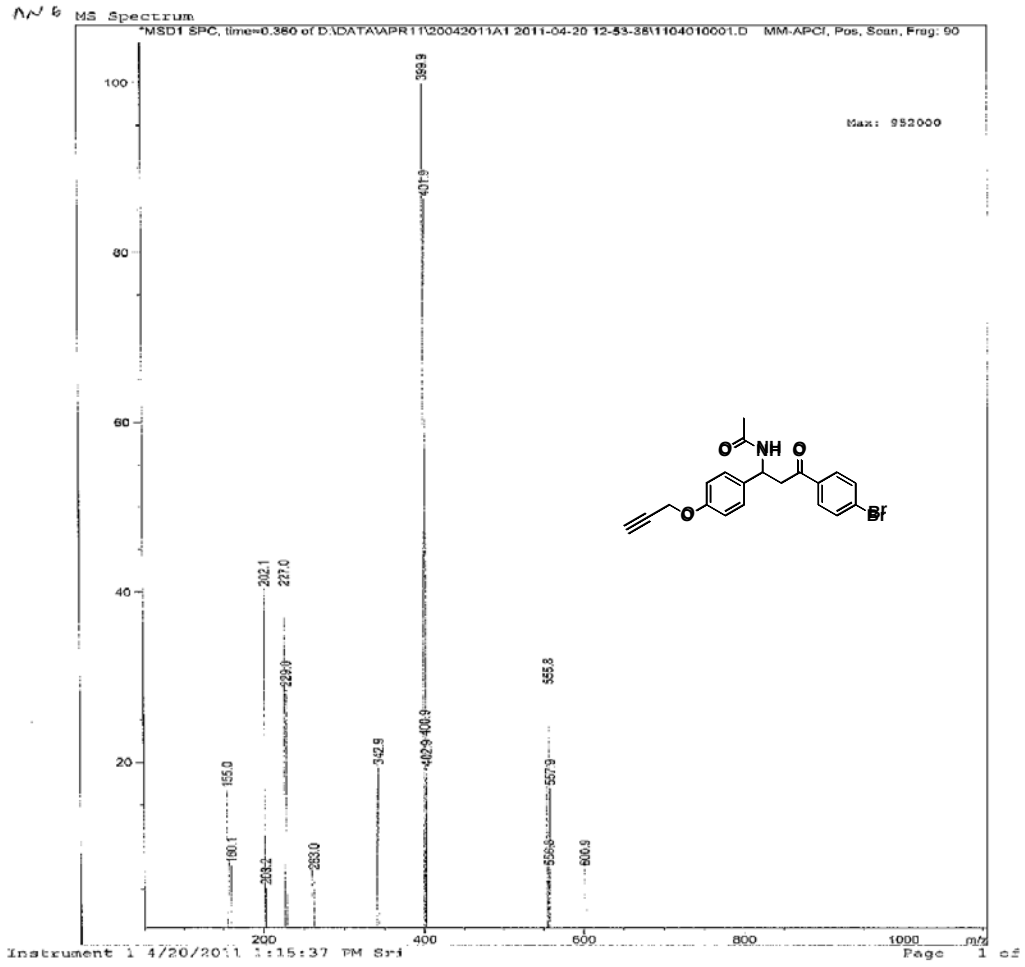
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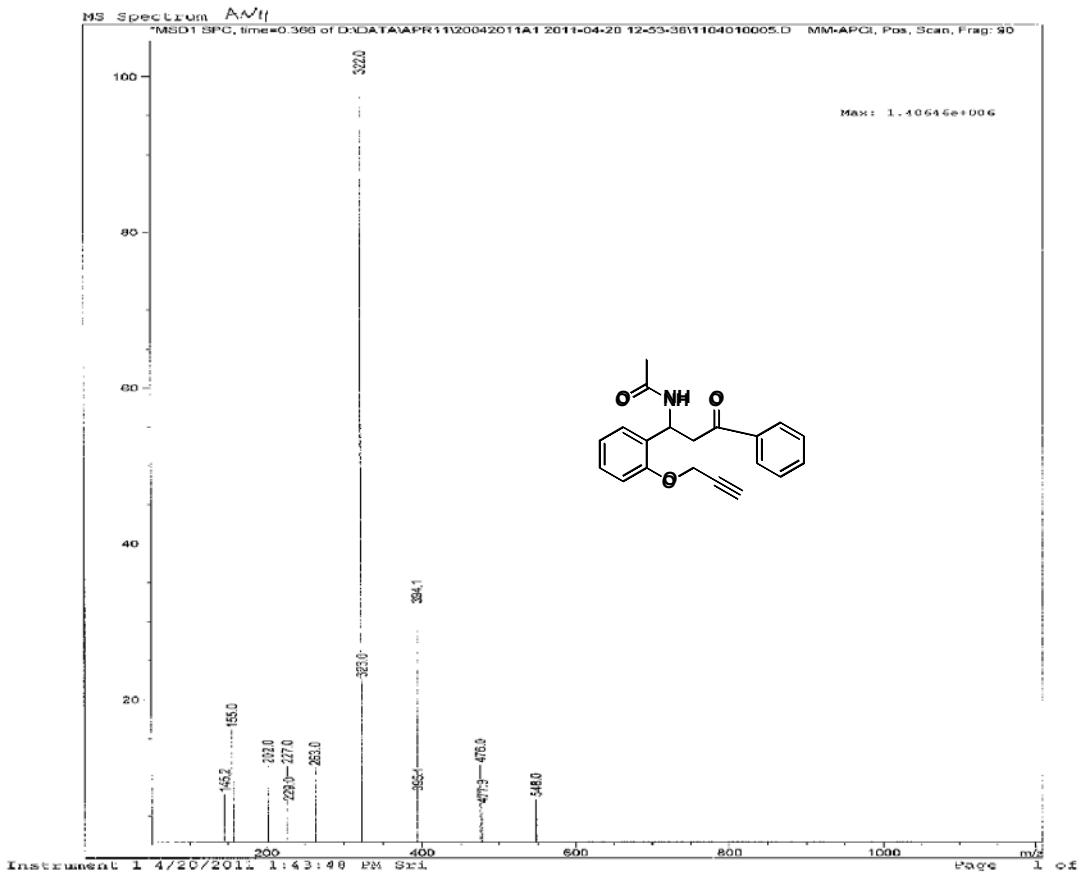
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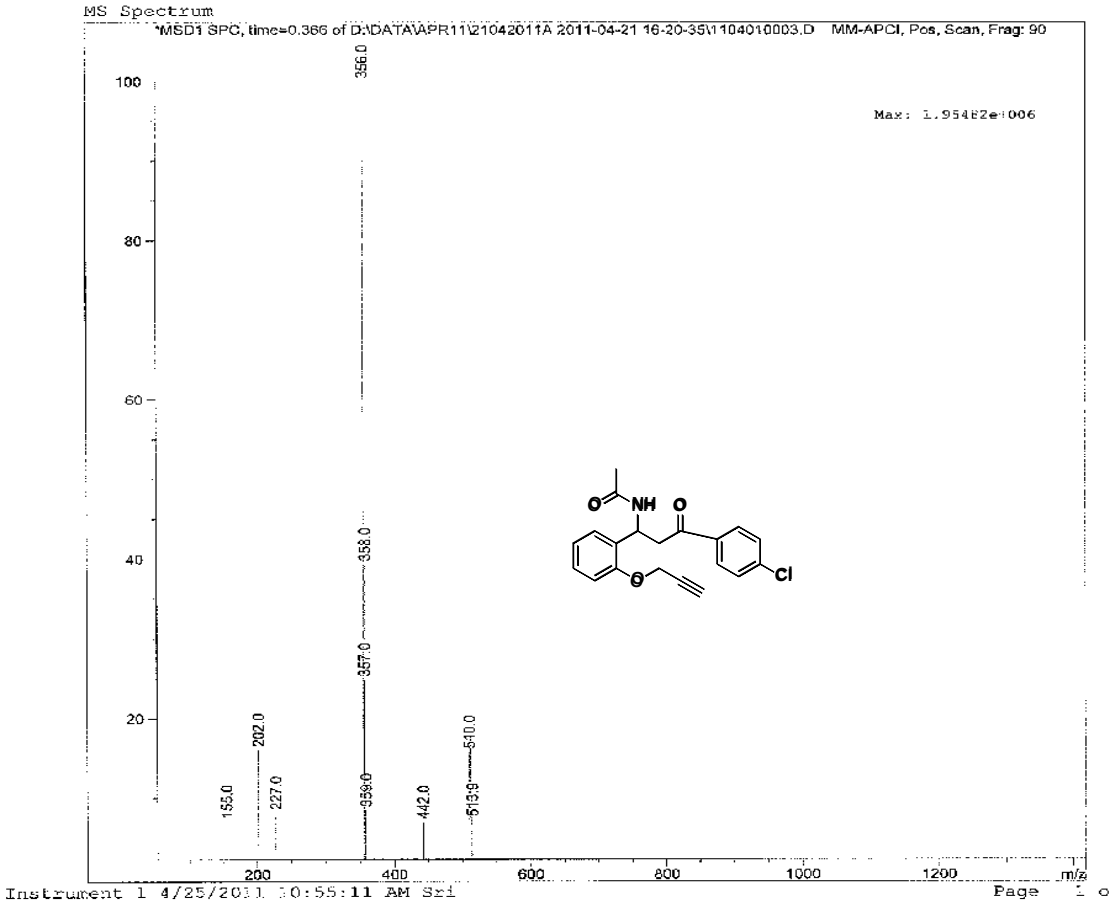
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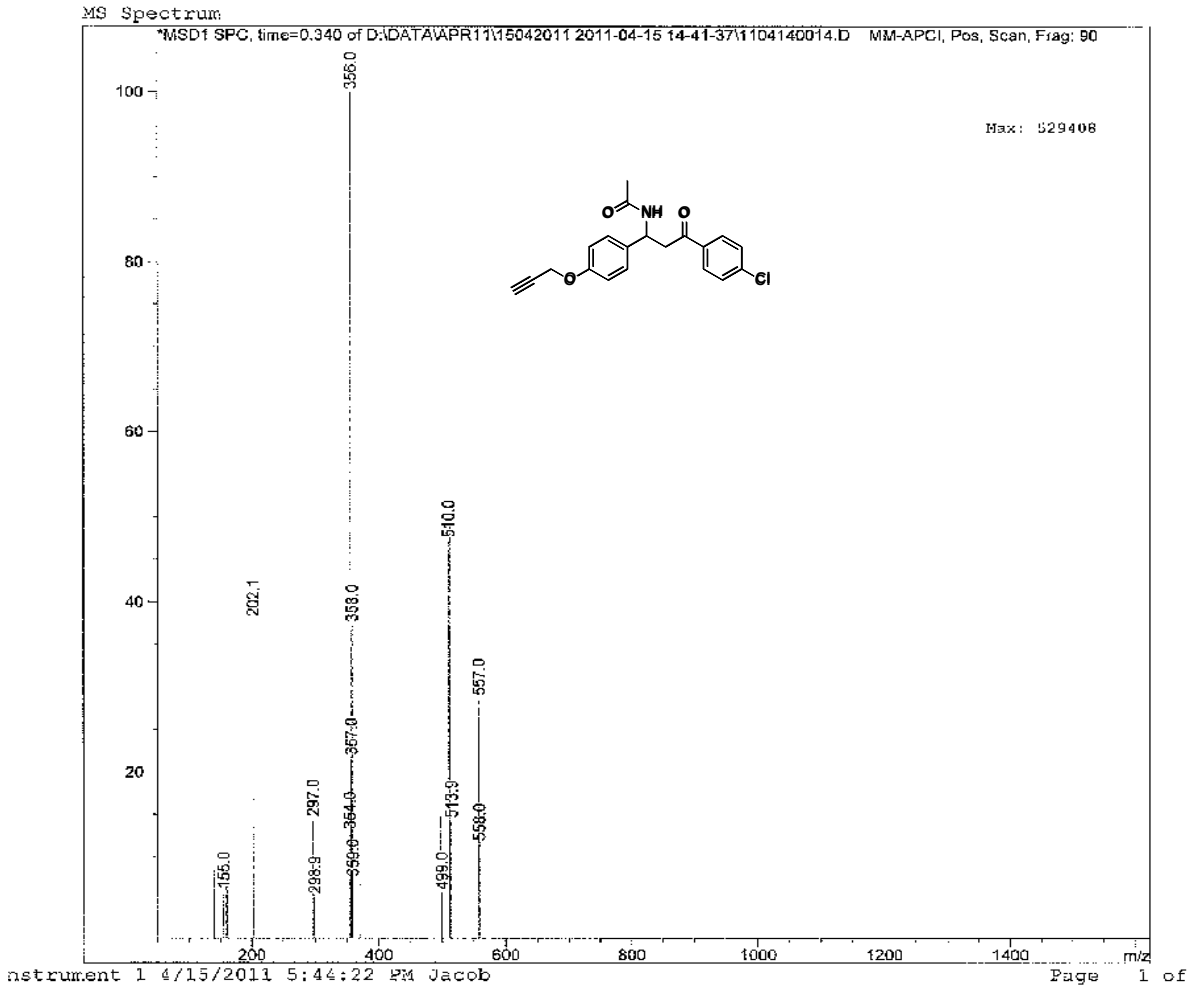
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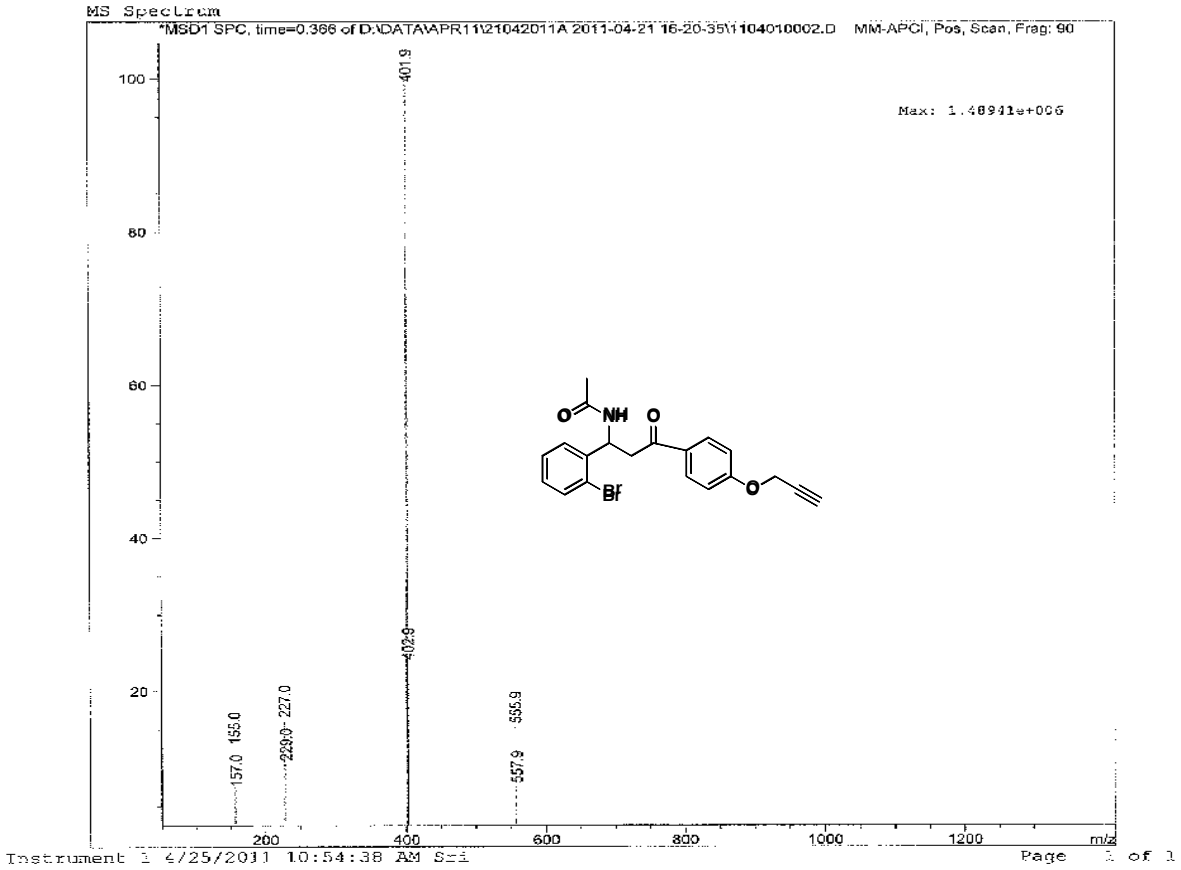
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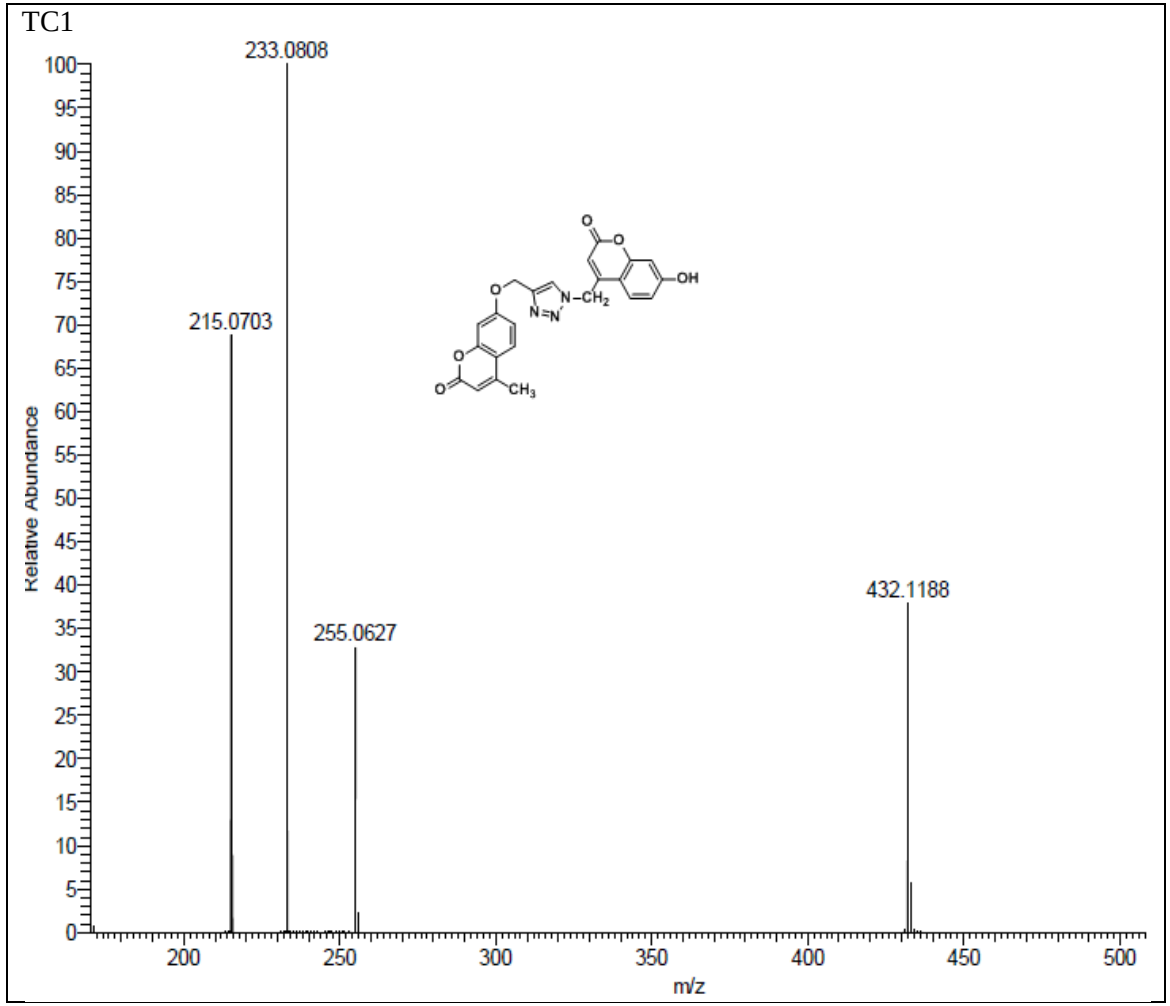
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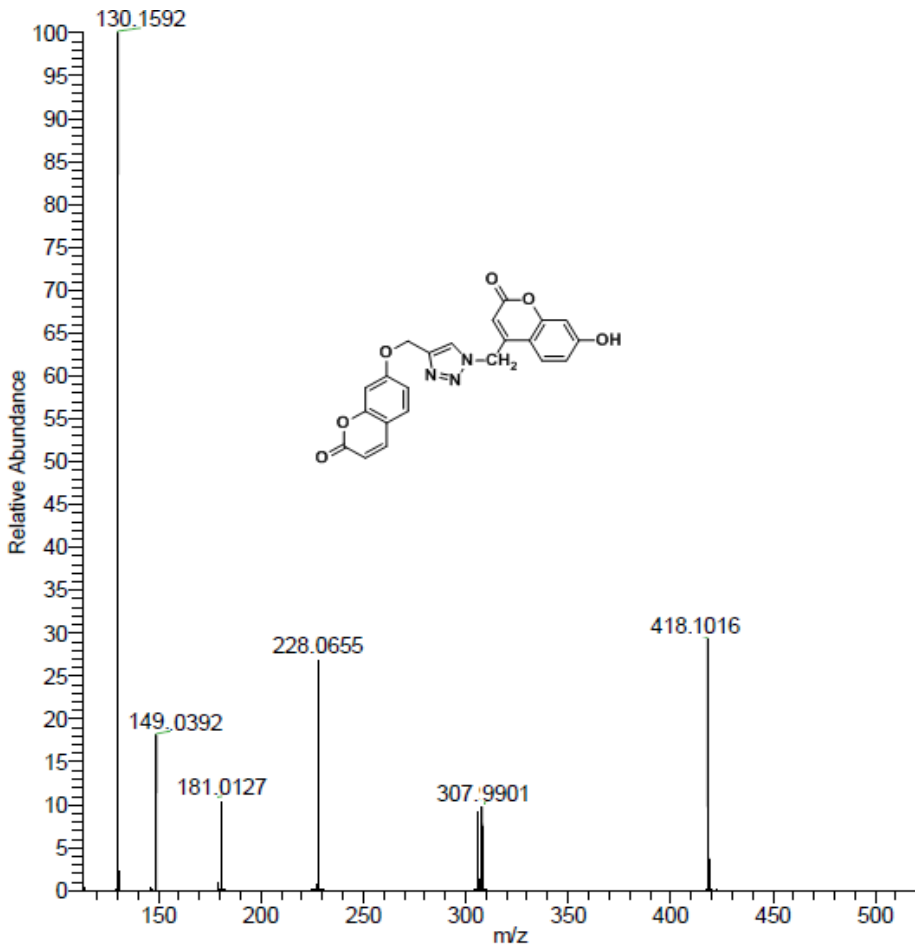
TC2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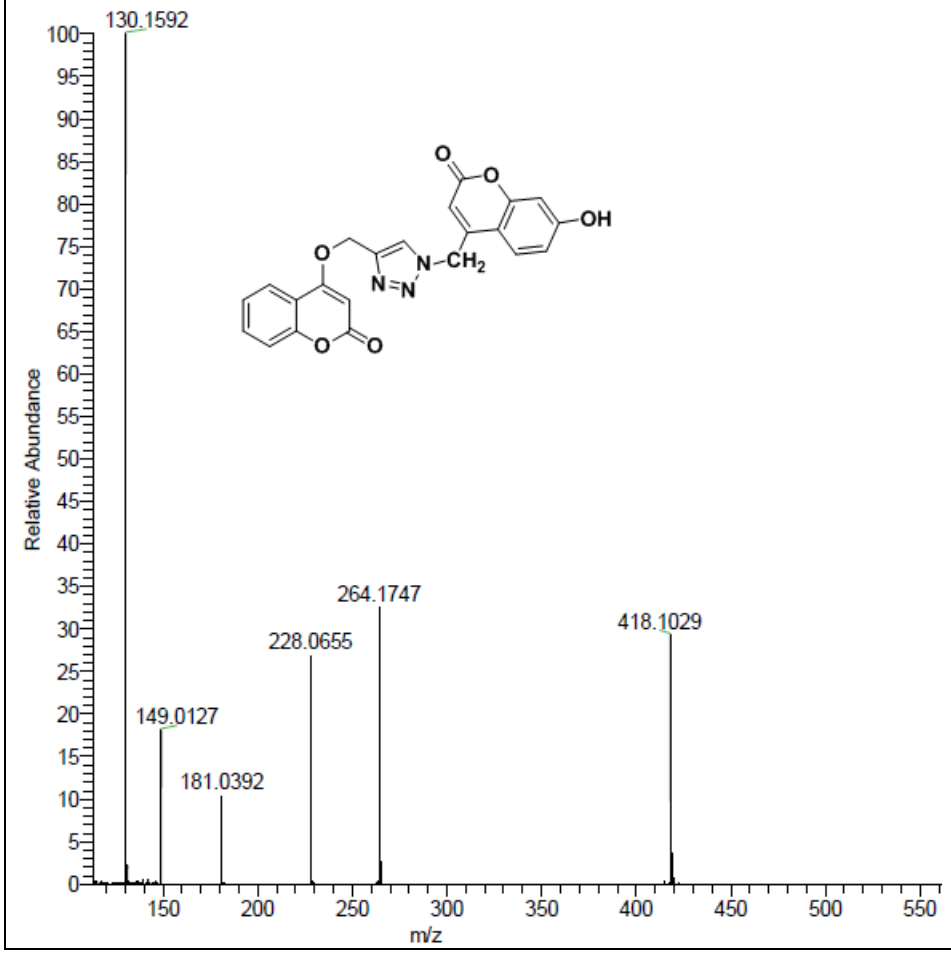
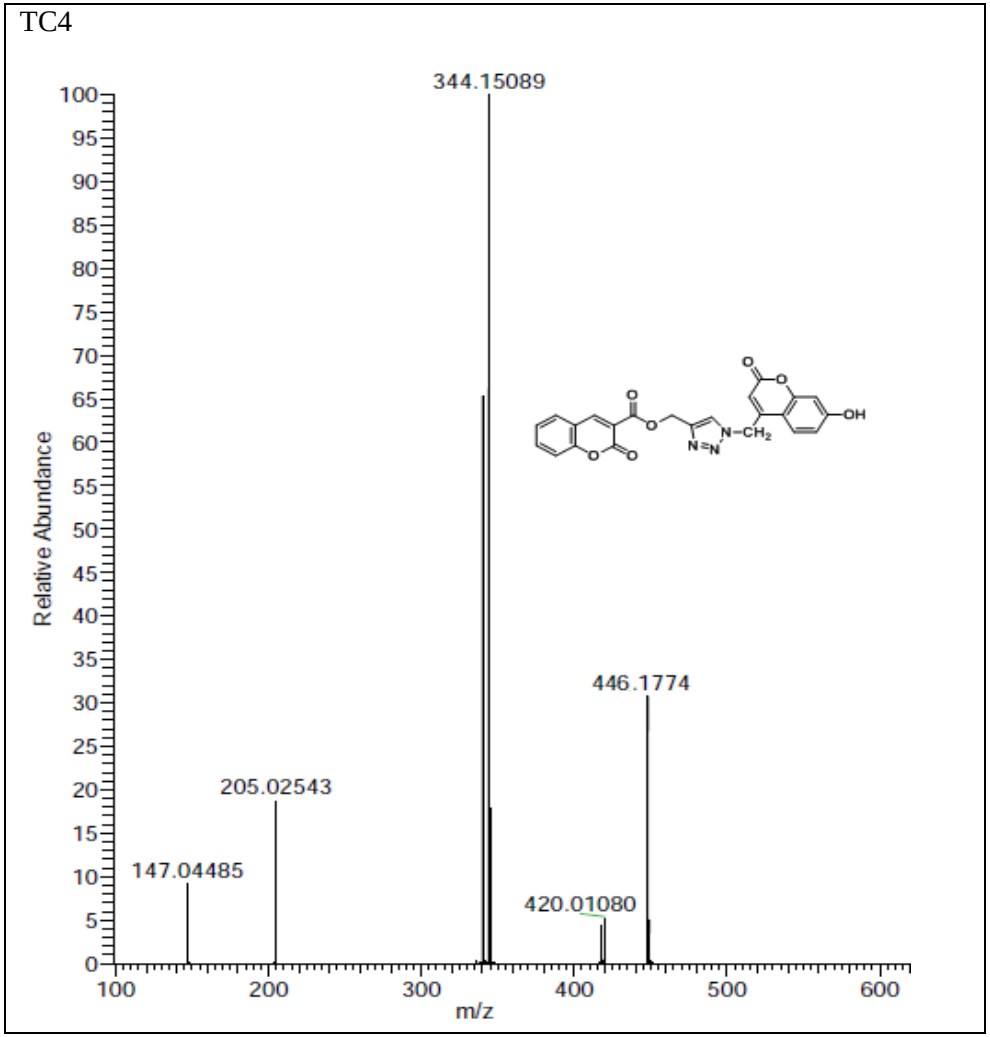
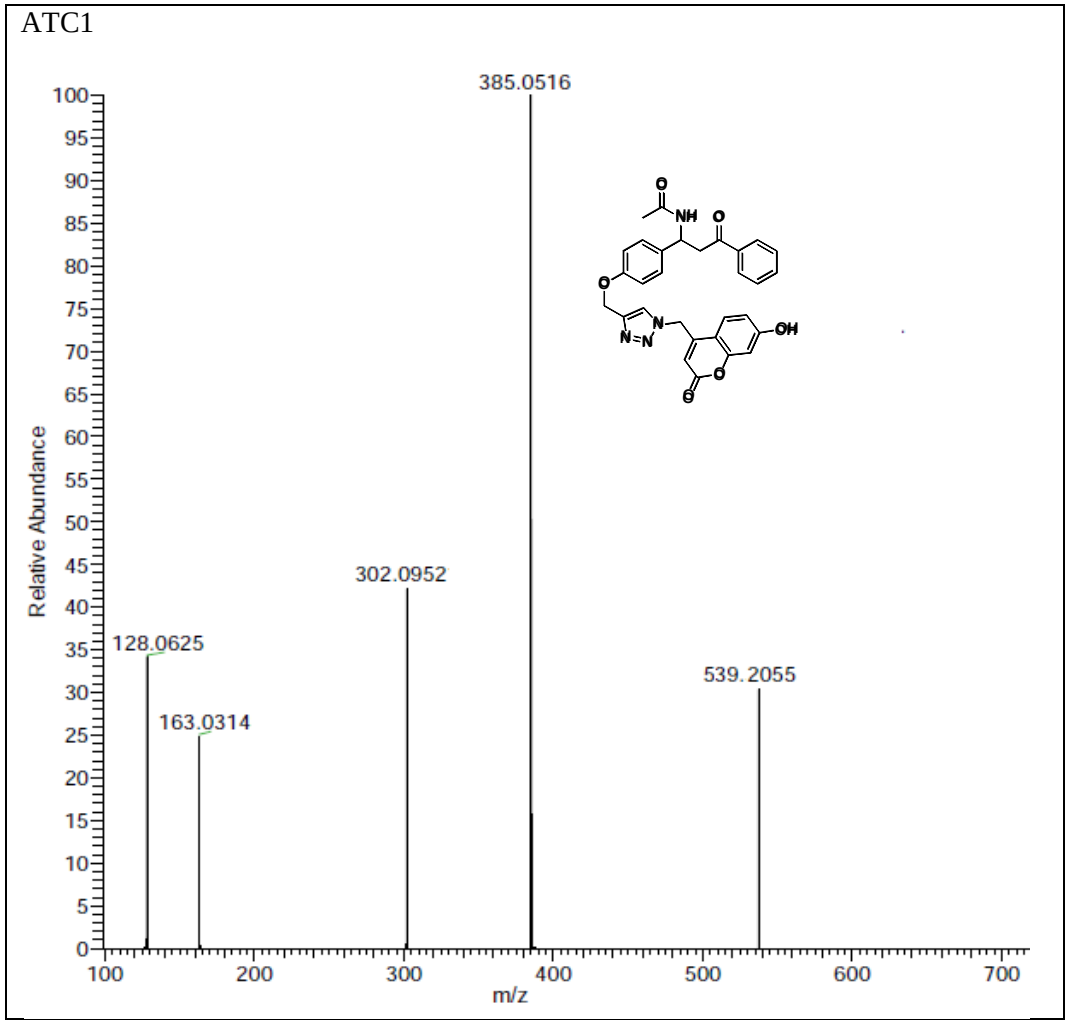
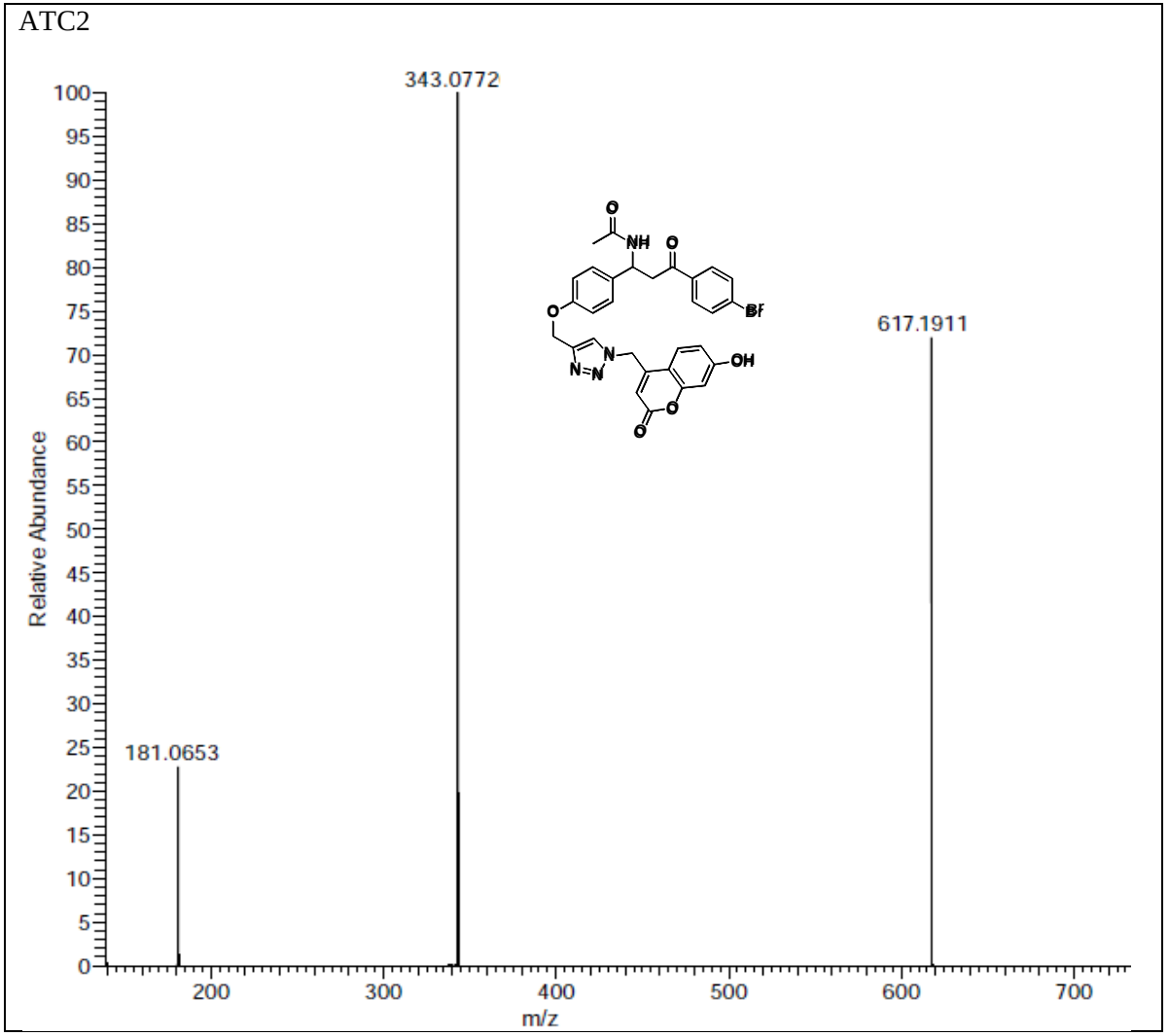
Relative Abundance
m/z
OH

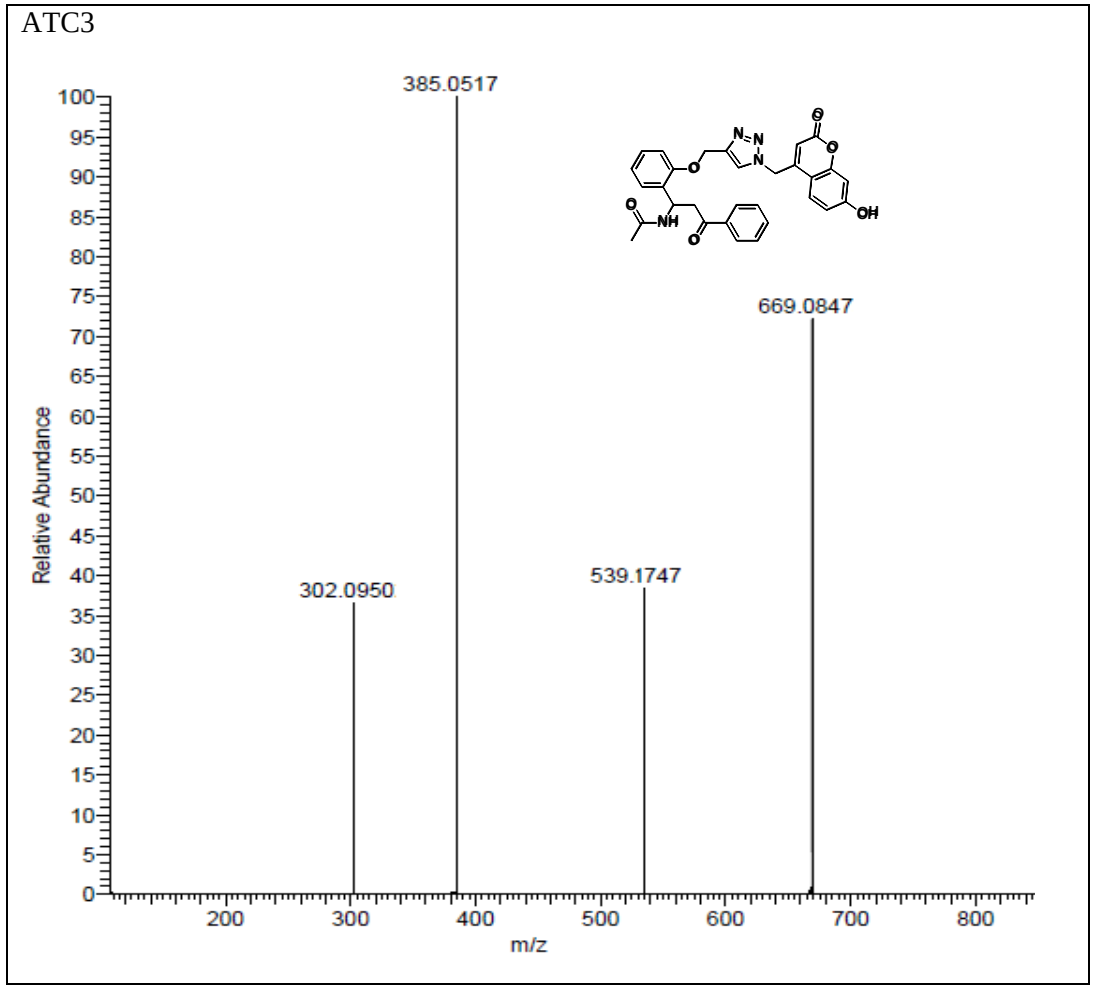
TC3

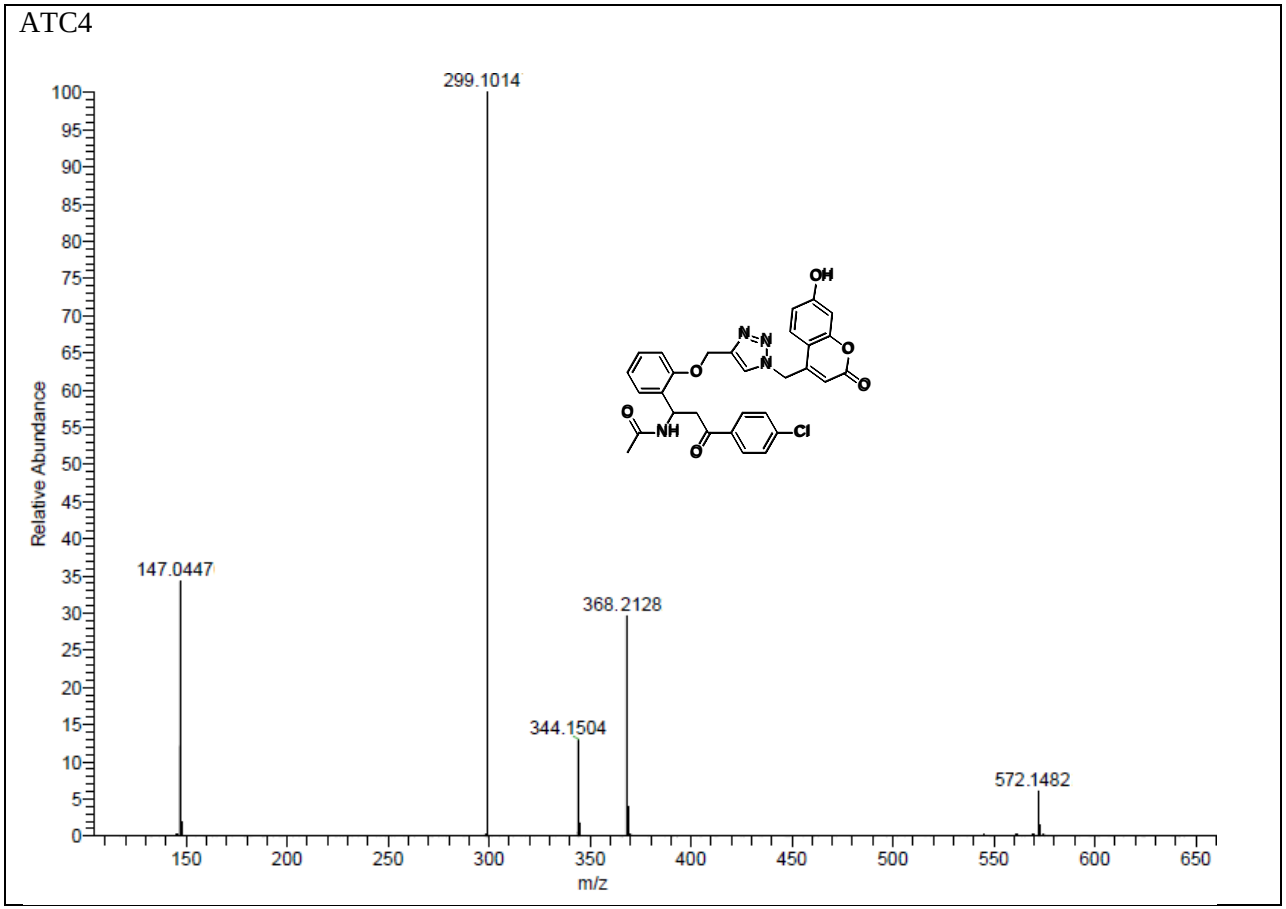

130.1592
264.1747
228.0655
418.1029
149.0127
181.0392
Relative Abundance
m/z
OH
N
N
N
O
O
O
O
O
CH2

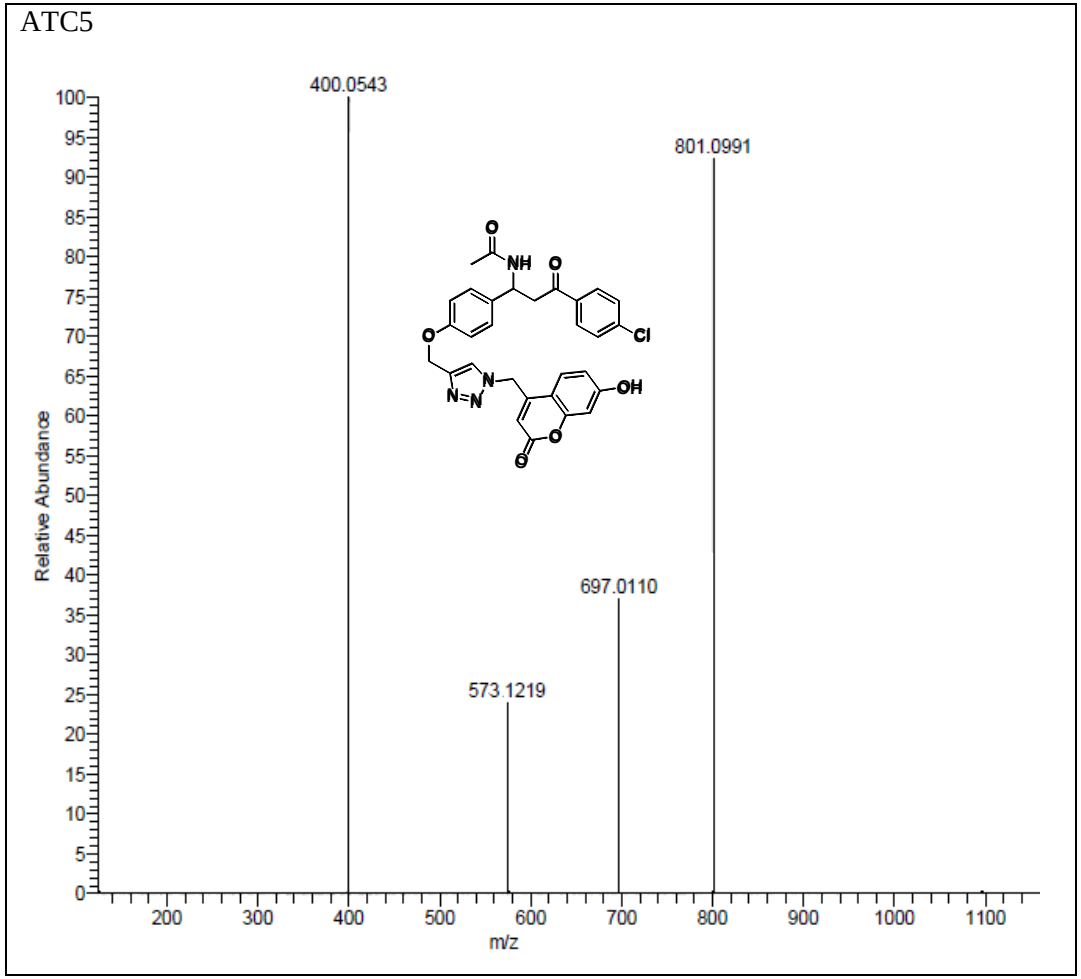

TC4
344.15089
446.1774
205.02543
147.04485
420.01080
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
100
200
300
400
500
600
OH
N=N
N-CH2

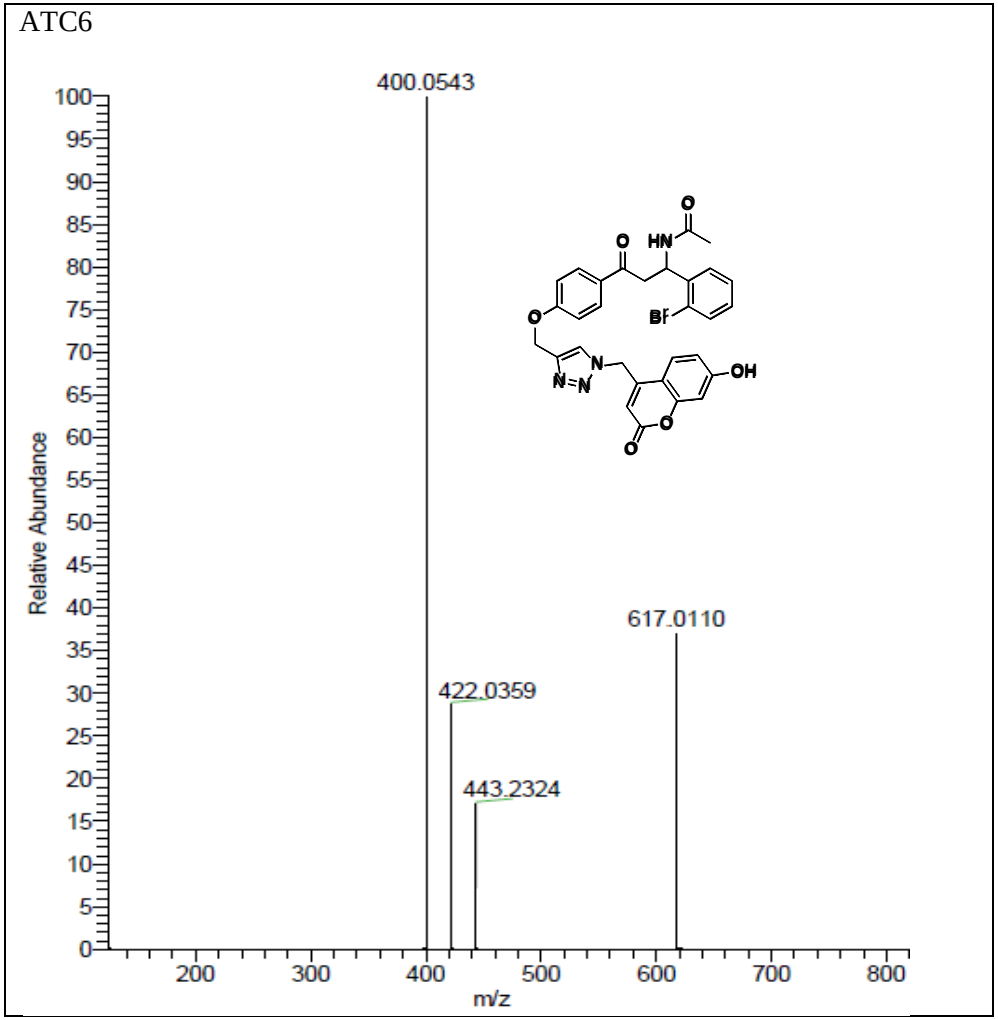

ATC1
385.0516
302.0952
128.0625
163.0314
539.2055
Relative Abundance
m/z
100
200
300
400
500
600
700
NH
OH
N
O


ATC2
343.0772
617.1911
181.0653
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
200
300
400
500
600
700
O
NH
O
O
Br
N
N=N
OH
O
O

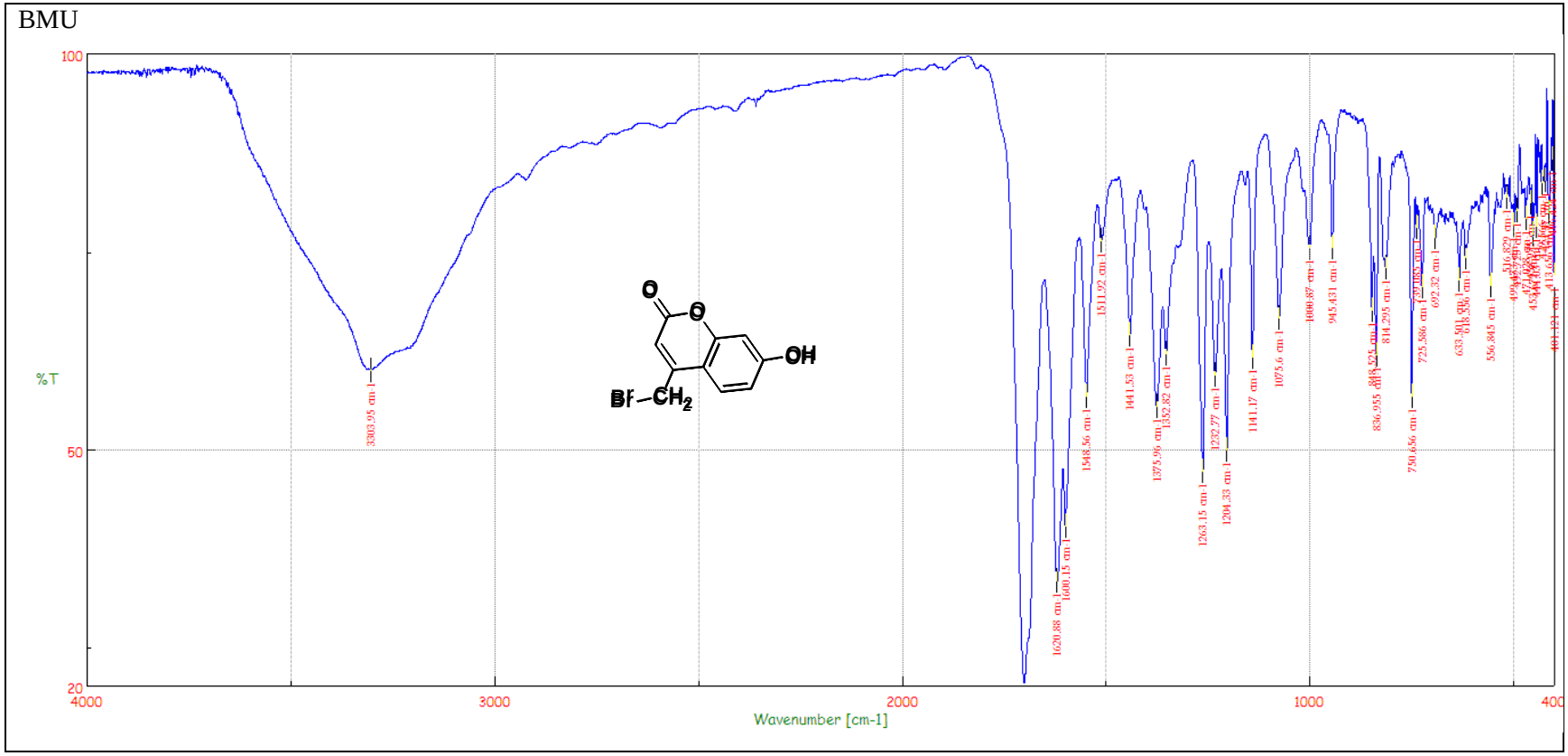

ATC3
385.0517
669.0847
539.1747
302.0950
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
200
300
400
500
600
700
800
N
N
N
O
O
O
O
NH
OH


ATC4
299.1014
147.0447
368.2128
344.1504
572.1482
Relative Abundance
m/z
OH
O
O
N
N
N
O
NH
O
Cl

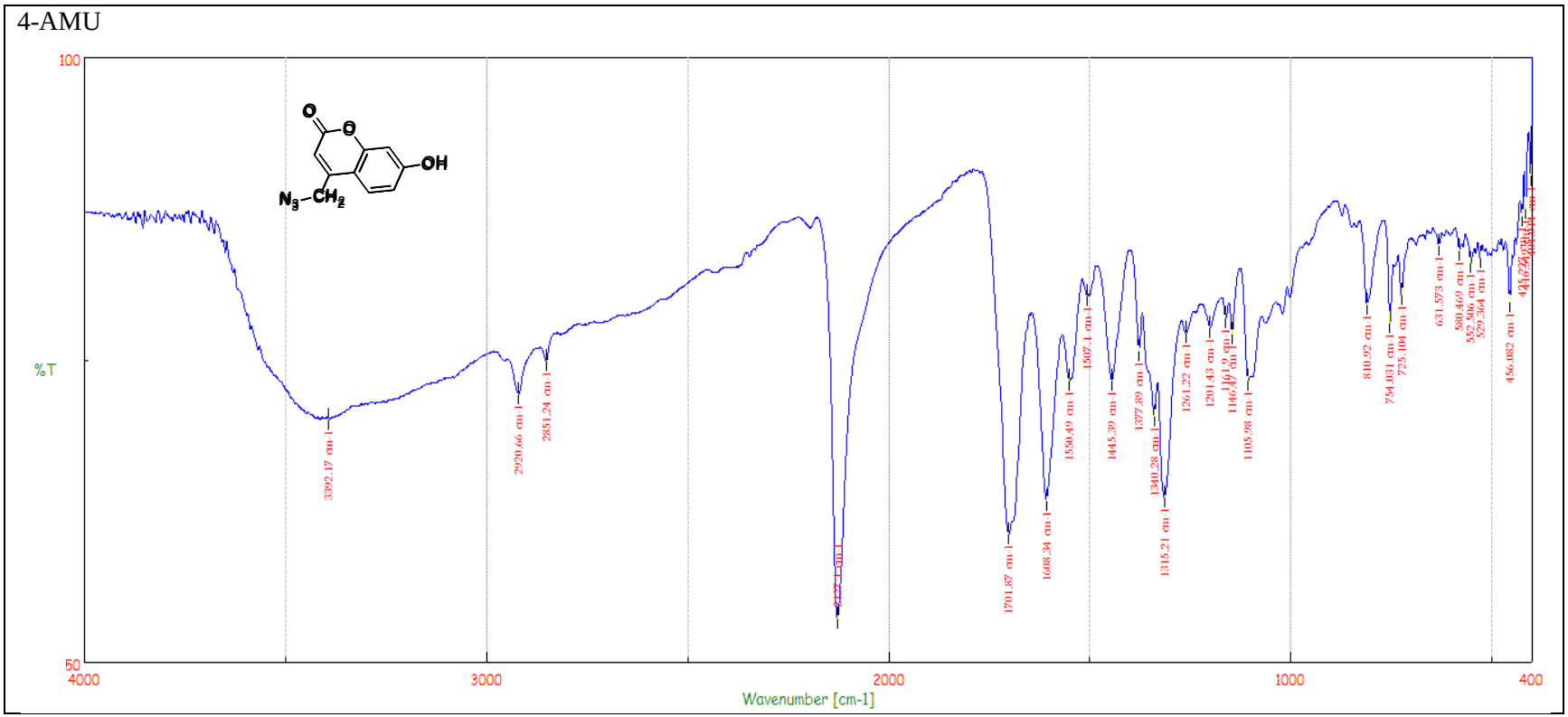

ATC5
400.0543
801.0991
697.0110
573.1219
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
200
300
400
500
600
700
800
900
1000
1100
O
NH
O
Cl
O
N
N=N
OH
O
O


ATC6
400.0543
617.0110
422.0359
443.2324
Relative Abundance
m/z
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
0
200
300
400
500
600
700
800
O
HN
O
Br
O
N
N=N
OH
O
O

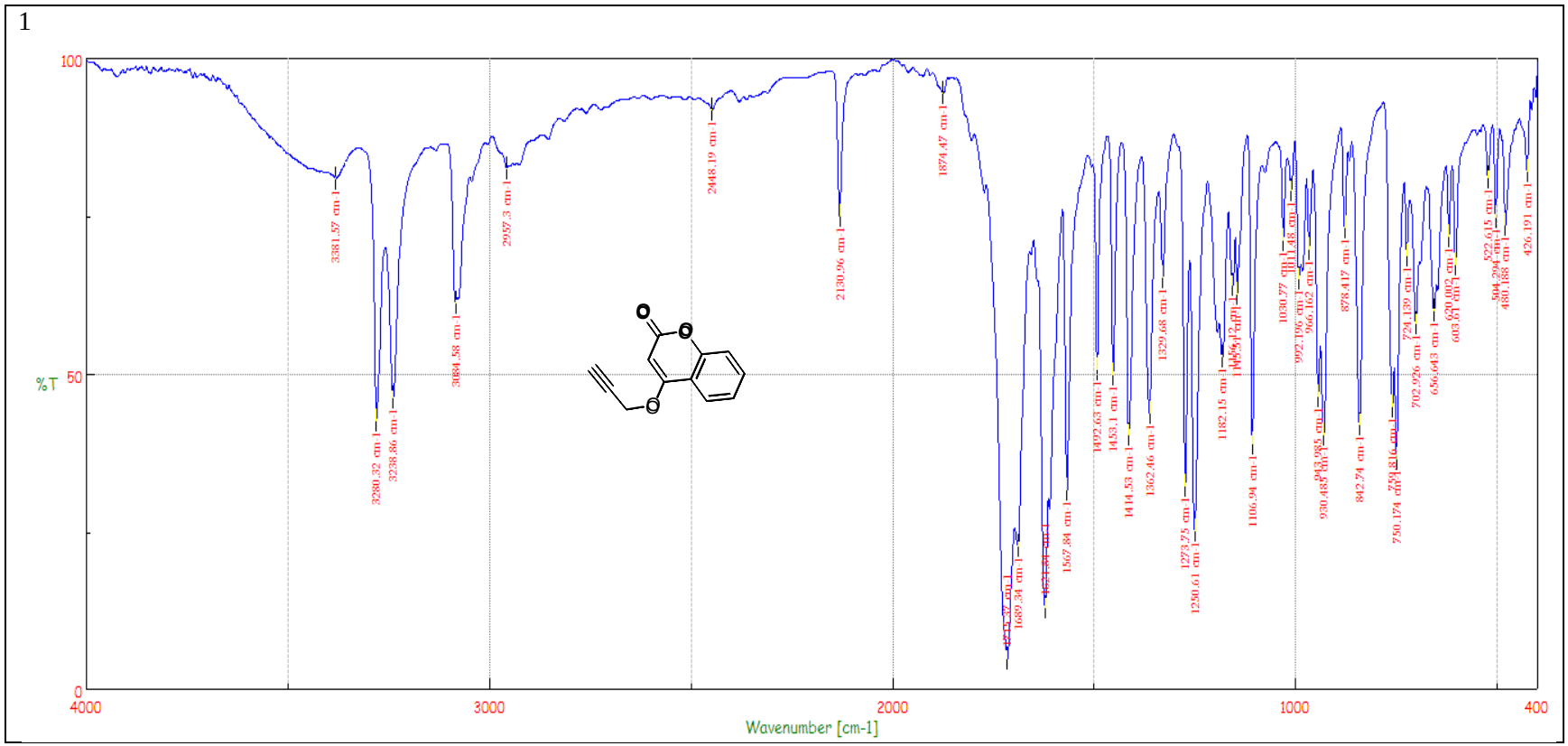
[3] Inrfared Spectra of compounds

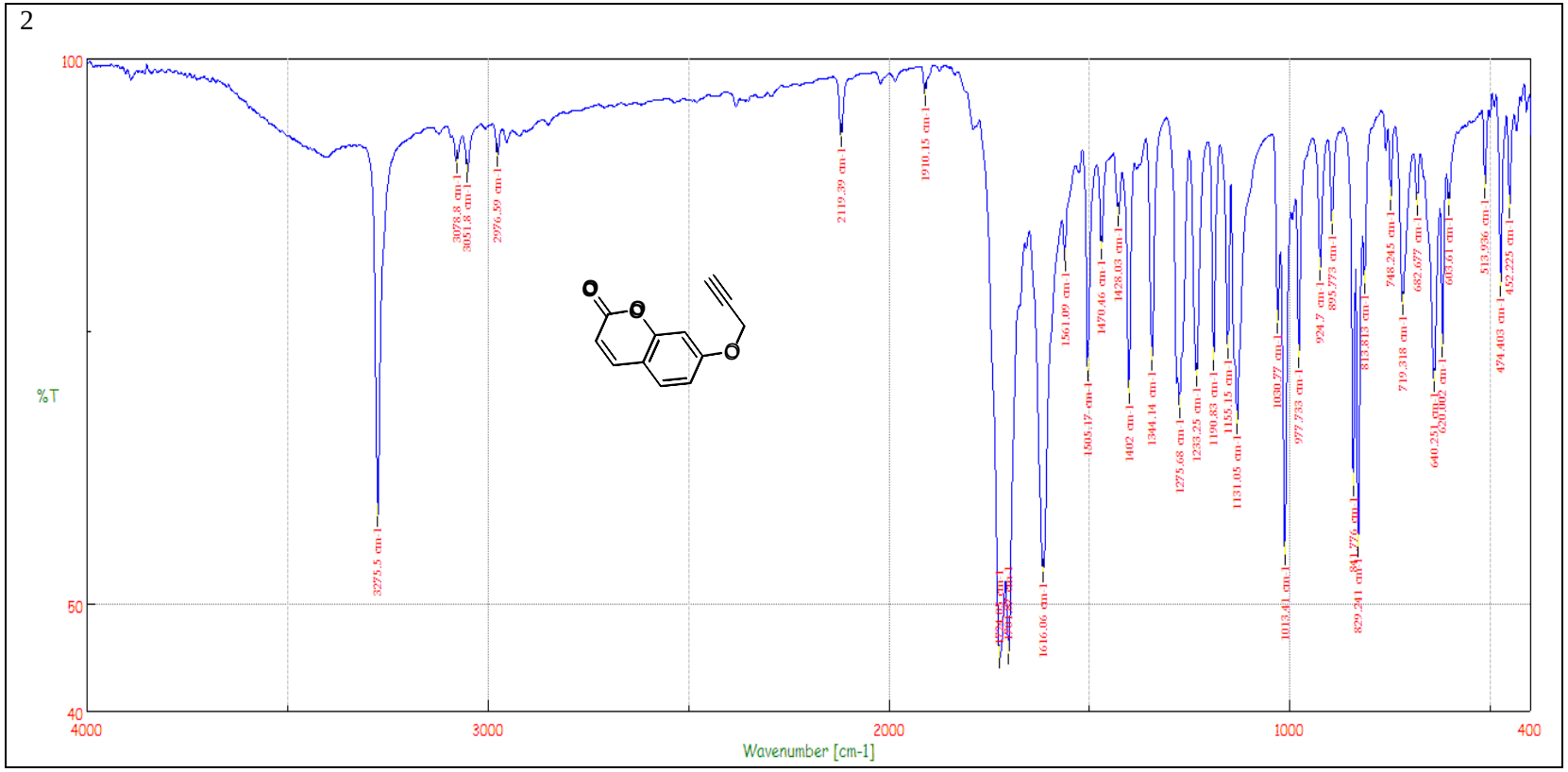


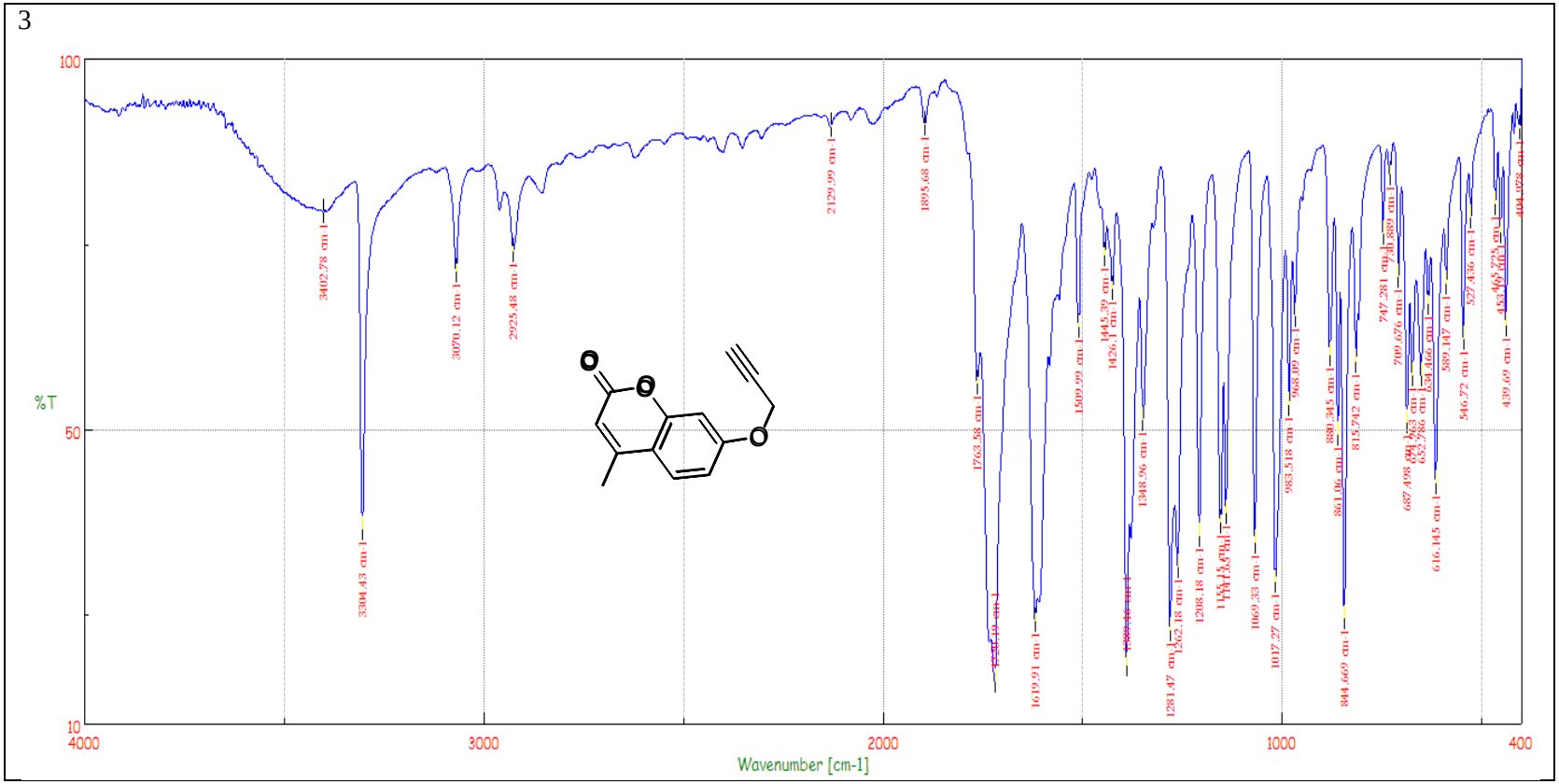
4-AMU


100
50
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
OH
N3–CH2
3392.17 cm-1
2920.66 cm-1
2851.24 cm-1
1701.87 cm-1
1608.34 cm-1
1580.49 cm-1
1507.1 cm-1
1445.39 cm-1
1377.89 cm-1
1340.28 cm-1
1315.21 cm-1
1261.22 cm-1
1201.43 cm-1
1105.98 cm-1
810.92 cm-1
754.031 cm-1
725.104 cm-1
631.573 cm-1
580.469 cm-1
552.506 cm-1
529.364 cm-1
456.082 cm-1

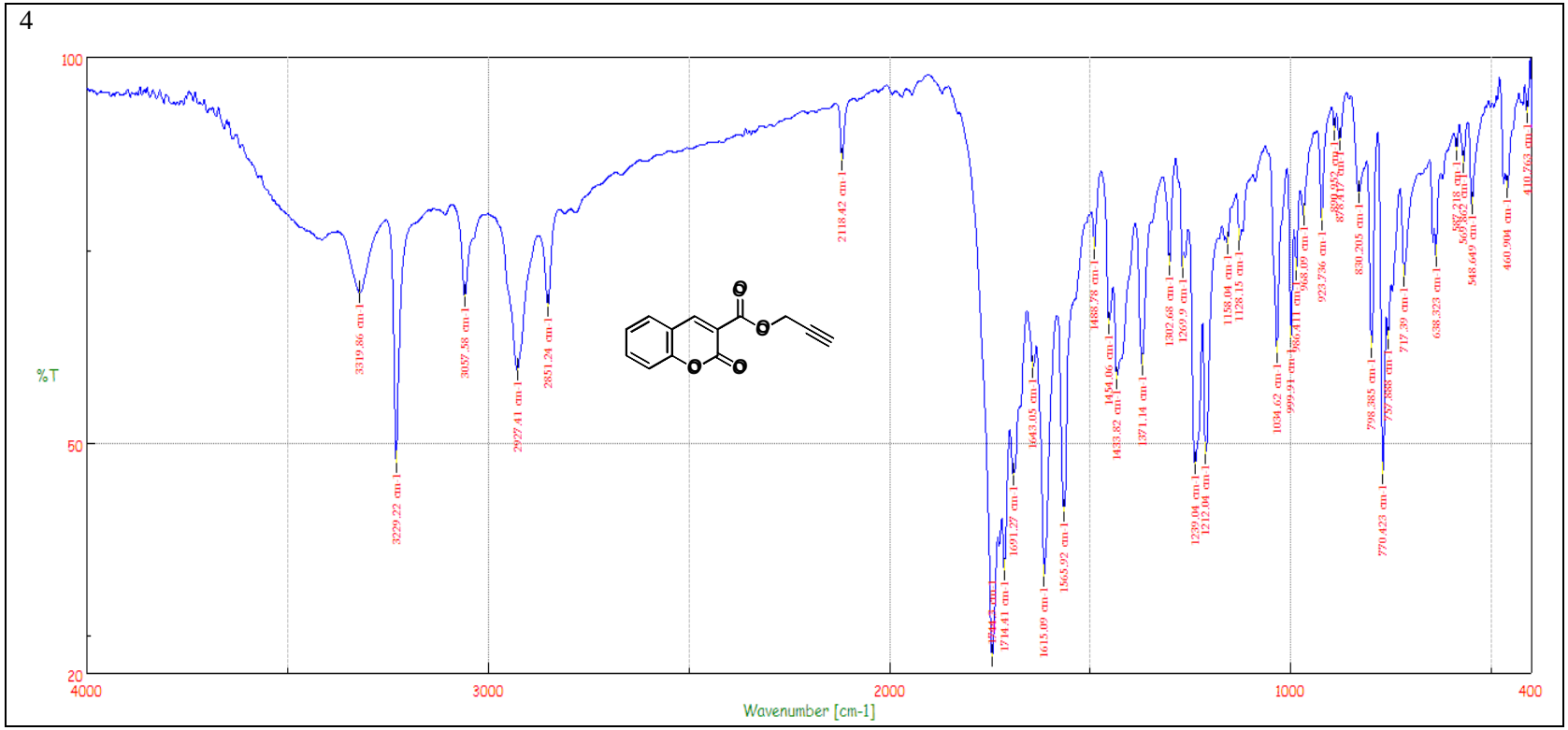
1

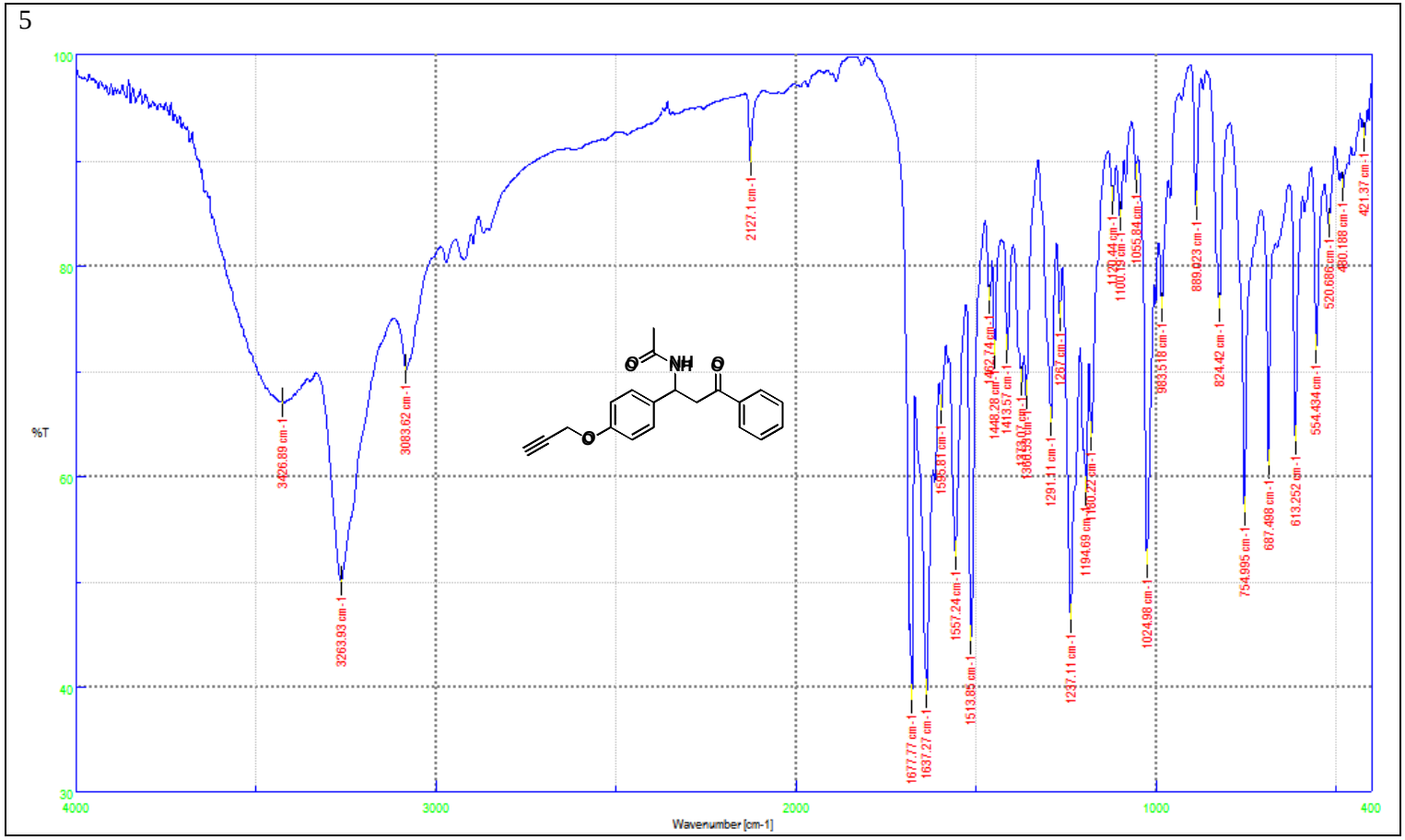

100
50
0
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3381.57 cm-1
3280.32 cm-1
3238.86 cm-1
3084.58 cm-1
2957.3 cm-1
2448.19 cm-1
2130.96 cm-1
1874.47 cm-1
1689.94 cm-1
1567.84 cm-1
1492.63 cm-1
1453.1 cm-1
1414.53 cm-1
1362.46 cm-1
1329.68 cm-1
1273.75 cm-1
1250.61 cm-1
1182.15 cm-1
1106.94 cm-1
1030.77 cm-1
1011.48 cm-1
992.196 cm-1
966.162 cm-1
943.985 cm-1
930.483 cm-1
878.417 cm-1
842.74 cm-1
816 cm-1
759 cm-1
750.174 cm-1
724.139 cm-1
702.926 cm-1
656.643 cm-1
620.002 cm-1
603.651 cm-1
522.615 cm-1
504.294 cm-1
480.188 cm-1
426.191 cm-1


2
100
50
40
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3275.5 cm-1
3078.8 cm-1
3051.8 cm-1
2976.59 cm-1
2119.39 cm-1
1910.15 cm-1
1616.06 cm-1
1561.09 cm-1
1505.17 cm-1
1470.46 cm-1
1428.03 cm-1
1402 cm-1
1344.14 cm-1
1275.68 cm-1
1233.25 cm-1
1199.83 cm-1
1155.15 cm-1
1131.05 cm-1
1030.77 cm-1
1013.41 cm-1
977.733 cm-1
924.7 cm-1
895.773 cm-1
829.241 cm-1
813.813 cm-1
748.245 cm-1
719.318 cm-1
682.677 cm-1
640.25 cm-1
620.962 cm-1
603.61 cm-1
513.936 cm-1
474.403 cm-1
452.225 cm-1

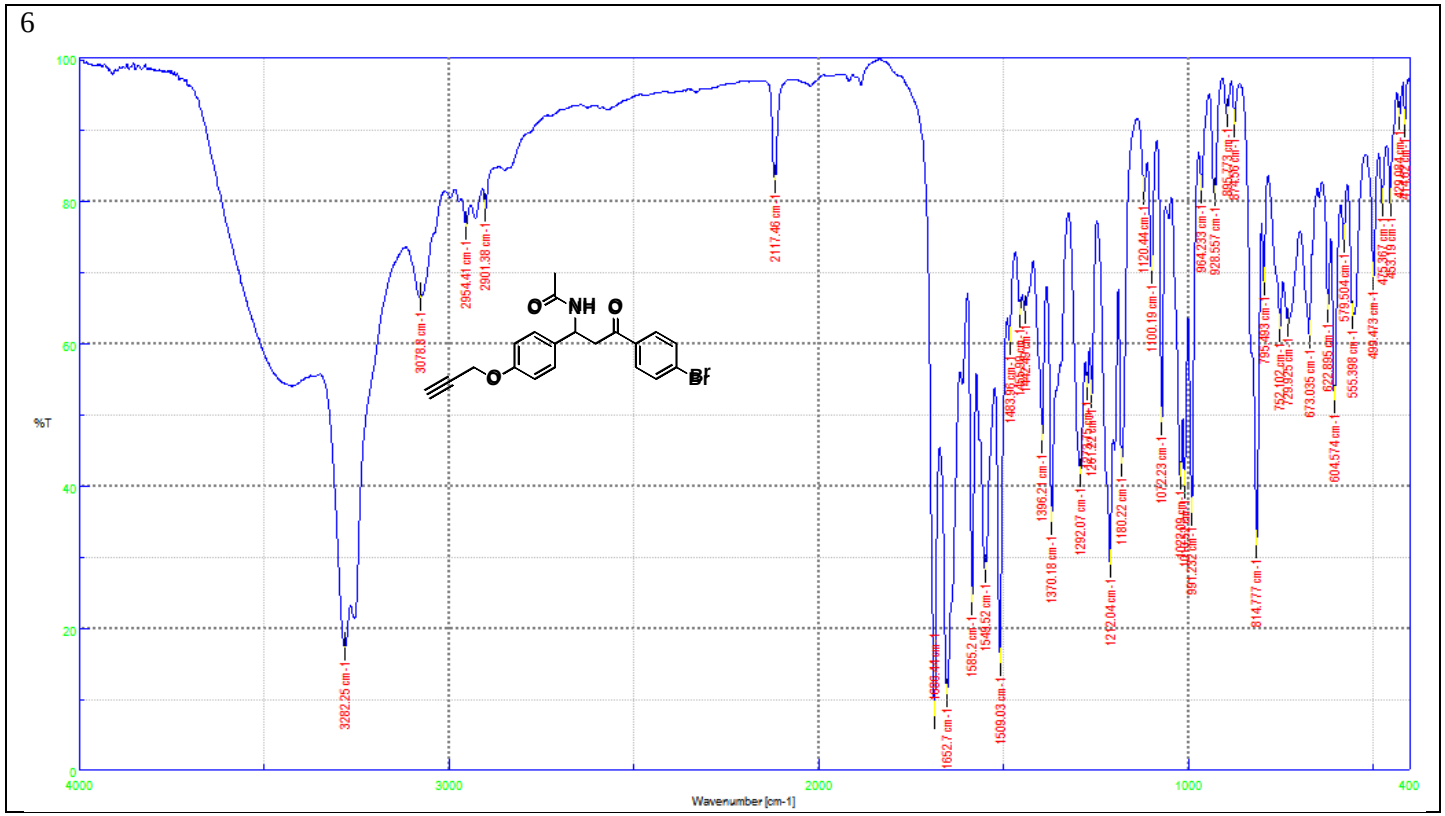

3
100
50
10
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3402.78 cm-1
3304.43 cm-1
3070.12 cm-1
2925.48 cm-1
2129.99 cm-1
1895.68 cm-1
1763.58 cm-1
1619.91 cm-1
1509.99 cm-1
1445.39 cm-1
1426.1 cm-1
1348.96 cm-1
1281.47 cm-1
1262.18 cm-1
1208.18 cm-1
1069.33 cm-1
1017.27 cm-1
983.518 cm-1
968.09 cm-1
880.345 cm-1
861.06 cm-1
844.669 cm-1
815.742 cm-1
747.281 cm-1
730.889 cm-1
709.676 cm-1
687.498 cm-1
652.986 cm-1
634.466 cm-1
616.145 cm-1
589.147 cm-1
546.72 cm-1
527.436 cm-1
439.69 cm-1
O
O
O

4

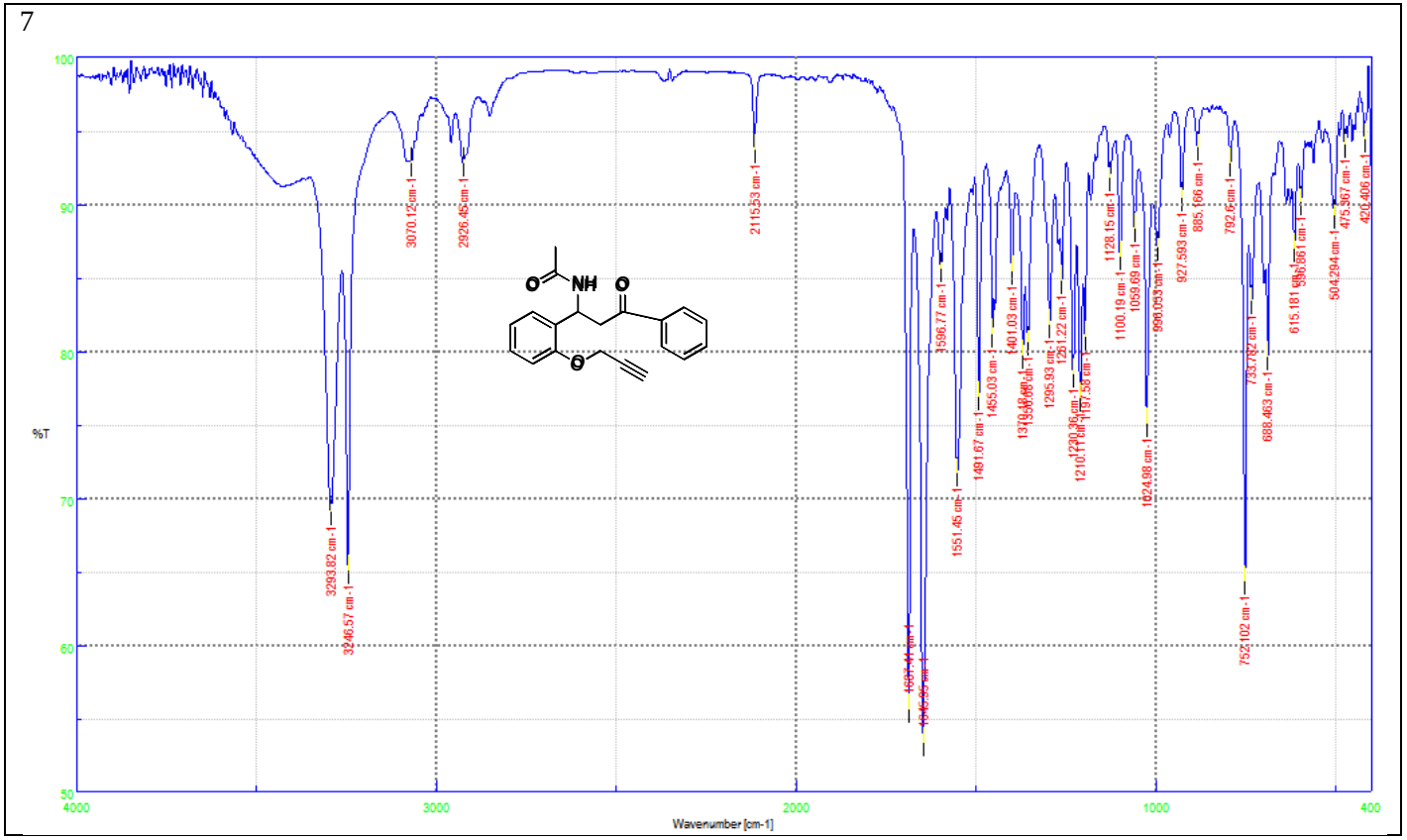

100
50
20
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3319.86 cm-1
3229.22 cm-1
3057.58 cm-1
2927.41 cm-1
2851.24 cm-1
2118.42 cm-1
1714.41 cm-1
1691.27 cm-1
1643.05 cm-1
1615.09 cm-1
1565.92 cm-1
1488.78 cm-1
1454.06 cm-1
1433.82 cm-1
1371.14 cm-1
1302.68 cm-1
1269.9 cm-1
1239.04 cm-1
1212.04 cm-1
1158.04 cm-1
1128.15 cm-1
1034.62 cm-1
999.94 cm-1
966.411 cm-1
968.09 cm-1
923.736 cm-1
878.117 cm-1
830.205 cm-1
798.385 cm-1
770.423 cm-1
757.888 cm-1
717.39 cm-1
638.323 cm-1
587.218 cm-1
569.862 cm-1
548.649 cm-1
460.904 cm-1
410.763 cm-1


5
%T
Wavenumber [cm-1]
4000
3000
2000
1000
400
100
80
60
40
30
3426.89 cm-1
3263.93 cm-1
3083.62 cm-1
2127.1 cm-1
1677.77 cm-1
1637.27 cm-1
1595.81 cm-1
1557.24 cm-1
1513.85 cm-1
1462.74 cm-1
1448.28 cm-1
1413.57 cm-1
1378.87 cm-1
1368.53 cm-1
1291.11 cm-1
1267 cm-1
1237.11 cm-1
1194.69 cm-1
1180.22 cm-1
1178.44 cm-1
1100.78 cm-1
1055.84 cm-1
1024.98 cm-1
983.516 cm-1
889.023 cm-1
824.42 cm-1
754.995 cm-1
687.498 cm-1
613.252 cm-1
554.434 cm-1
520.686 cm-1
480.188 cm-1
421.37 cm-1
NH
O
O
O

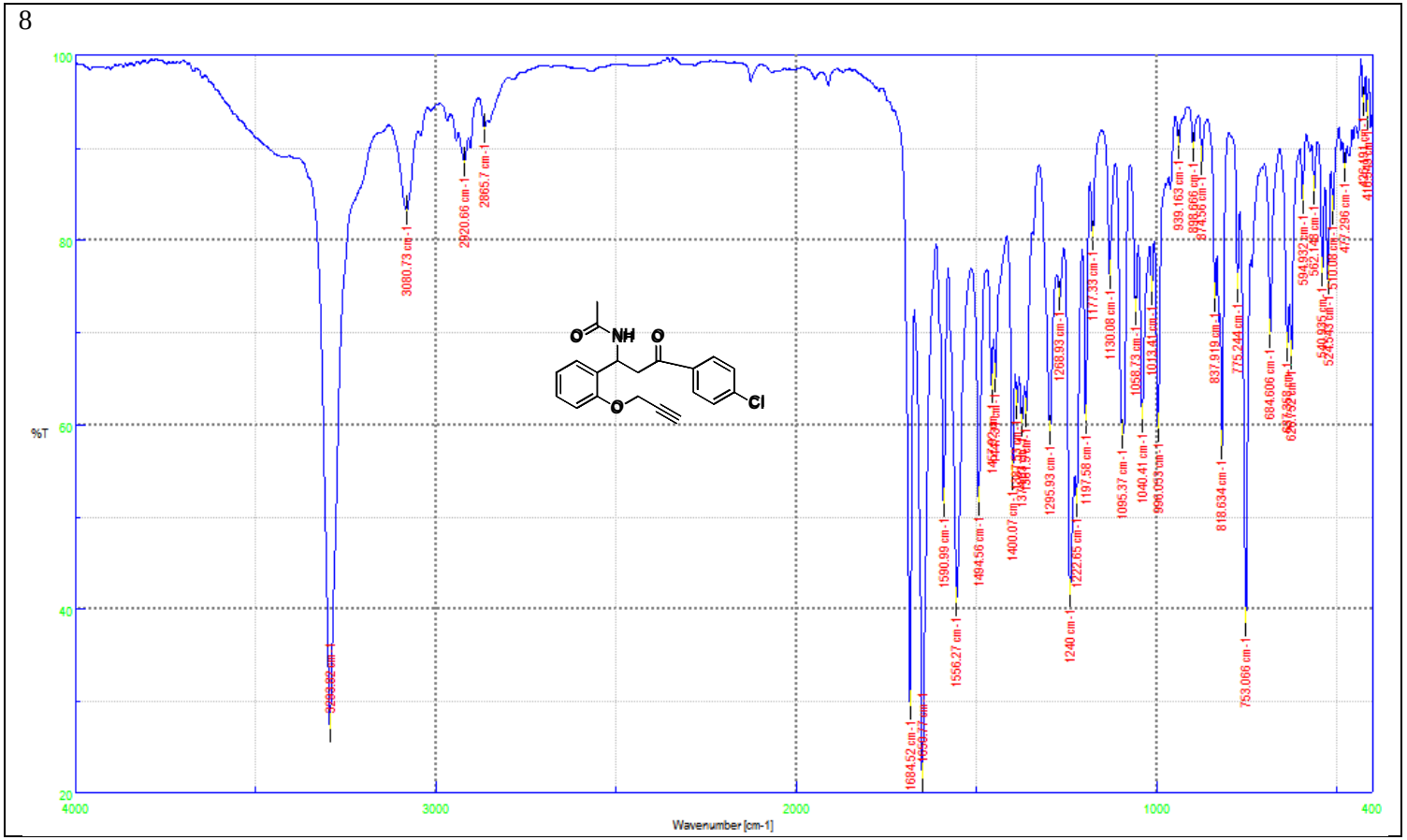
6


%T
Wavenumber [cm-1]
3282.25 cm-1
3078.8 cm-1
2954.41 cm-1
2901.38 cm-1
2117.46 cm-1
1652.7 cm-1
1585.2 cm-1
1548.52 cm-1
1509.03 cm-1
1370.18 cm-1
1292.07 cm-1
1180.22 cm-1
1120.44 cm-1
1100.19 cm-1
964.233 cm-1
928.557 cm-1
795.483 cm-1
673.035 cm-1
622.895 cm-1
604.574 cm-1
579.504 cm-1
555.398 cm-1
499.473 cm-1
463.319 cm-1
NH
O
Br

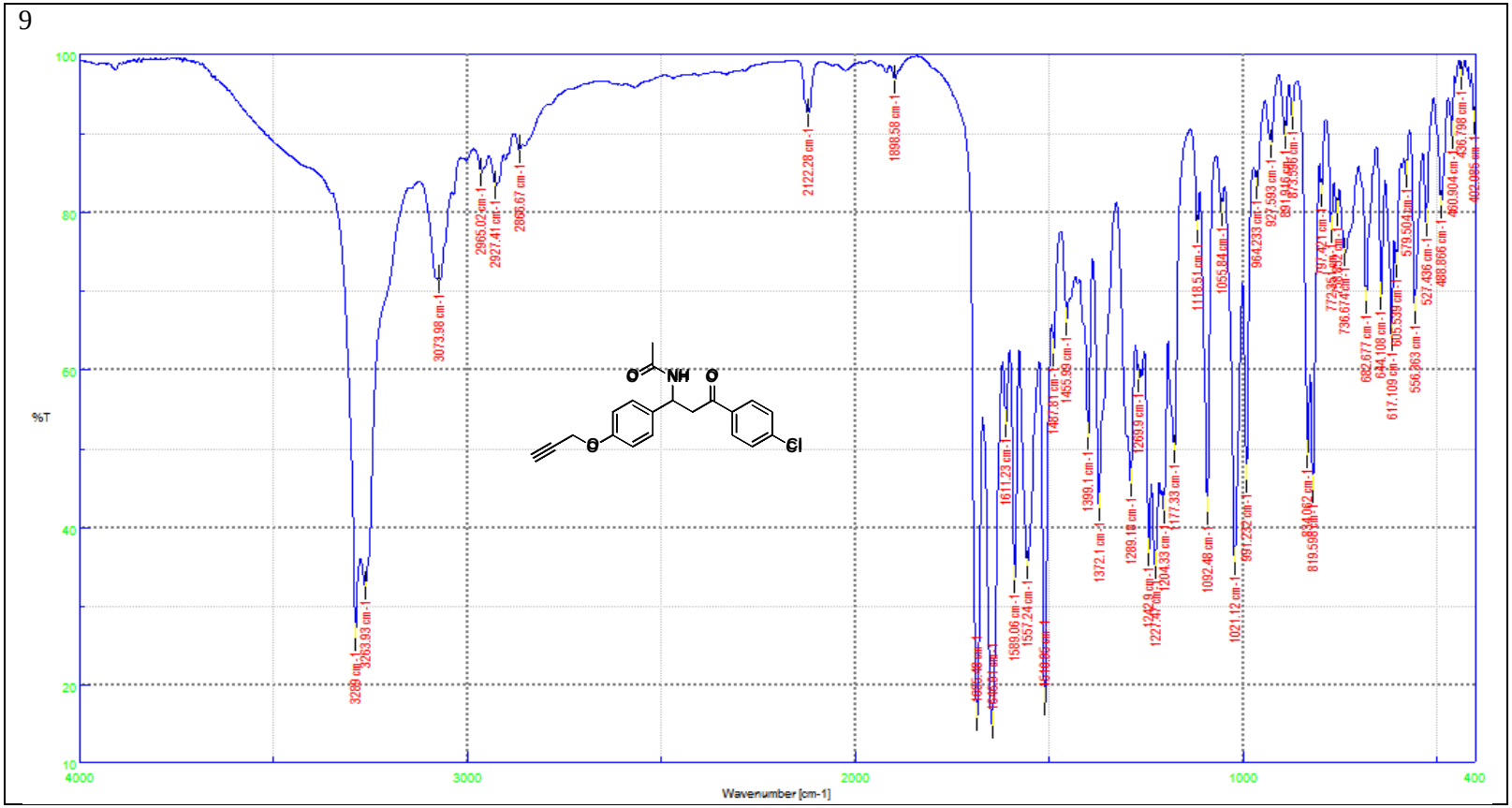
7


%T
Wavenumber [cm-1]
4000
3000
2000
1000
400
100
90
80
70
60
50
3293.82 cm-1
3246.57 cm-1
3070.12 cm-1
2926.45 cm-1
2115.53 cm-1
1596.77 cm-1
1551.45 cm-1
1491.67 cm-1
1455.03 cm-1
1401.03 cm-1
1295.93 cm-1
1128.15 cm-1
1100.19 cm-1
1059.69 cm-1
927.593 cm-1
885.166 cm-1
792.5 cm-1
752.102 cm-1
688.463 cm-1
615.181 cm-1
504.294 cm-1
475.367 cm-1
420.406 cm-1
O
NH
O
O

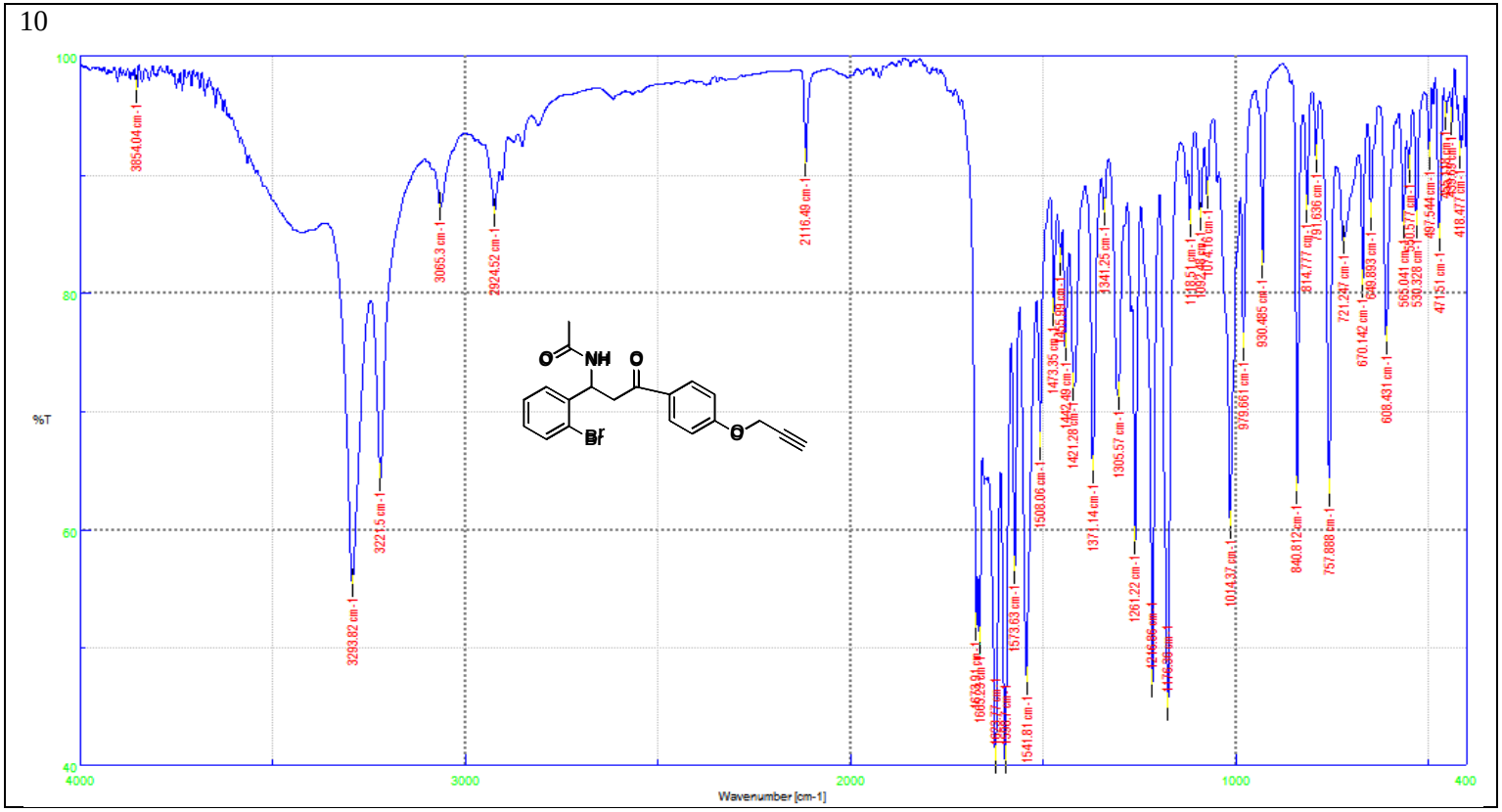
8

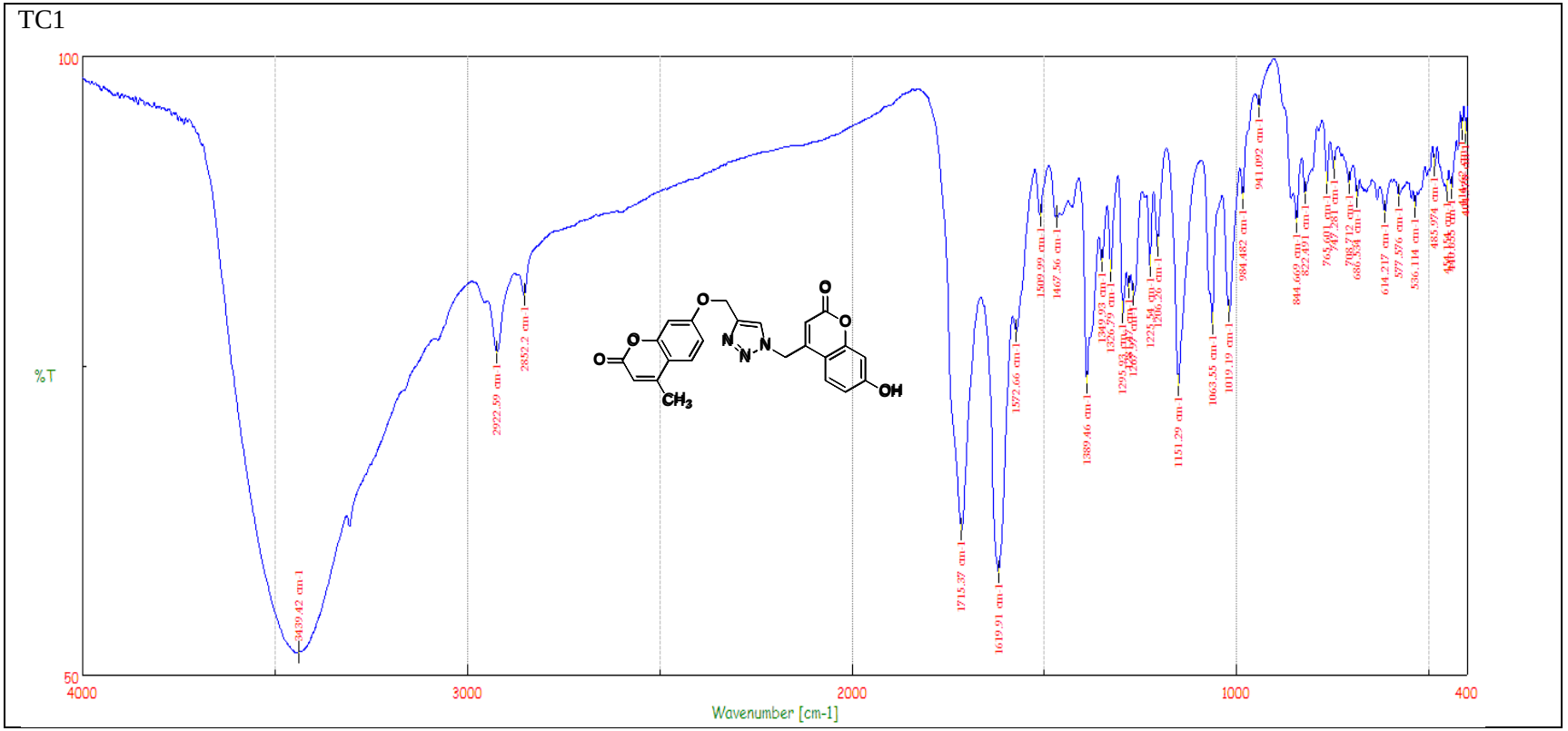

100
80
60
40
20
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3060.73 cm-1
2920.66 cm-1
2865.7 cm-1
1684.52 cm-1
1590.99 cm-1
1556.27 cm-1
1484.56 cm-1
1400.07 cm-1
1295.93 cm-1
1268.93 cm-1
1240 cm-1
1222.65 cm-1
1197.58 cm-1
1177.33 cm-1
1130.08 cm-1
1095.37 cm-1
1058.73 cm-1
1040.41 cm-1
1013.41 cm-1
999.053 cm-1
939.163 cm-1
898.666 cm-1
874.56 cm-1
837.919 cm-1
818.634 cm-1
775.244 cm-1
753.066 cm-1
684.606 cm-1
594.932 cm-1
562.146 cm-1
540.935 cm-1
524.543 cm-1
510.08 cm-1
472.296 cm-1
NH
O
O
Cl

9

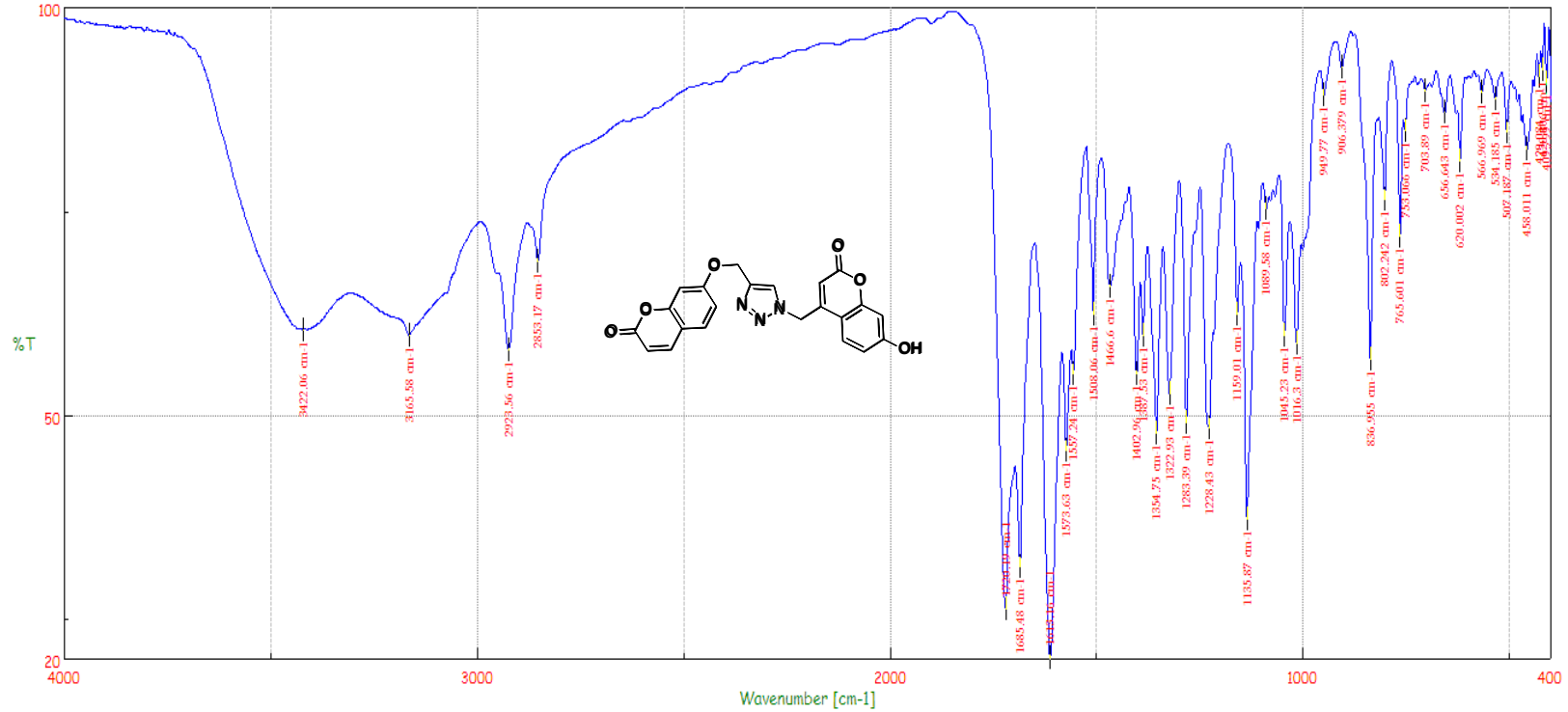

%T
Wavenumber [cm-1]
4000
3000
2000
1000
400
100
80
60
40
20
10
NH
O
O
O
Cl
3263.93 cm-1
3073.98 cm-1
2965.02 cm-1
2927.41 cm-1
2866.67 cm-1
2122.28 cm-1
1898.58 cm-1
1611.23 cm-1
1589.06 cm-1
1537.24 cm-1
1487.81 cm-1
1455.89 cm-1
1399.1 cm-1
1372.1 cm-1
1269.3 cm-1
1204.33 cm-1
1177.33 cm-1
1118.51 cm-1
1092.48 cm-1
1055.84 cm-1
1021.12 cm-1
964.233 cm-1
927.593 cm-1
891.946 cm-1
819.583 cm-1
772.958 cm-1
736.674 cm-1
682.677 cm-1
644.108 cm-1
617.109 cm-1
605.539 cm-1
579.504 cm-1
556.863 cm-1
527.436 cm-1
488.866 cm-1
460.904 cm-1
436.796 cm-1

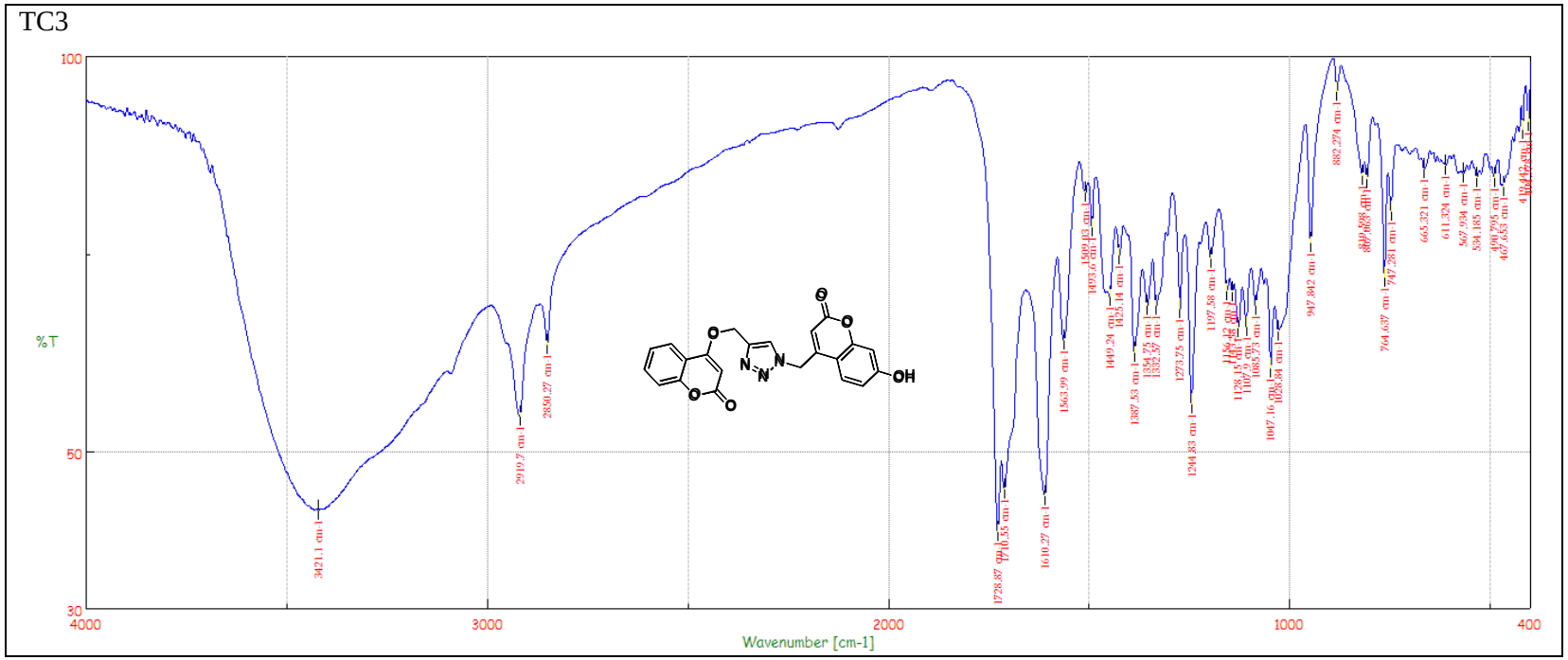
10

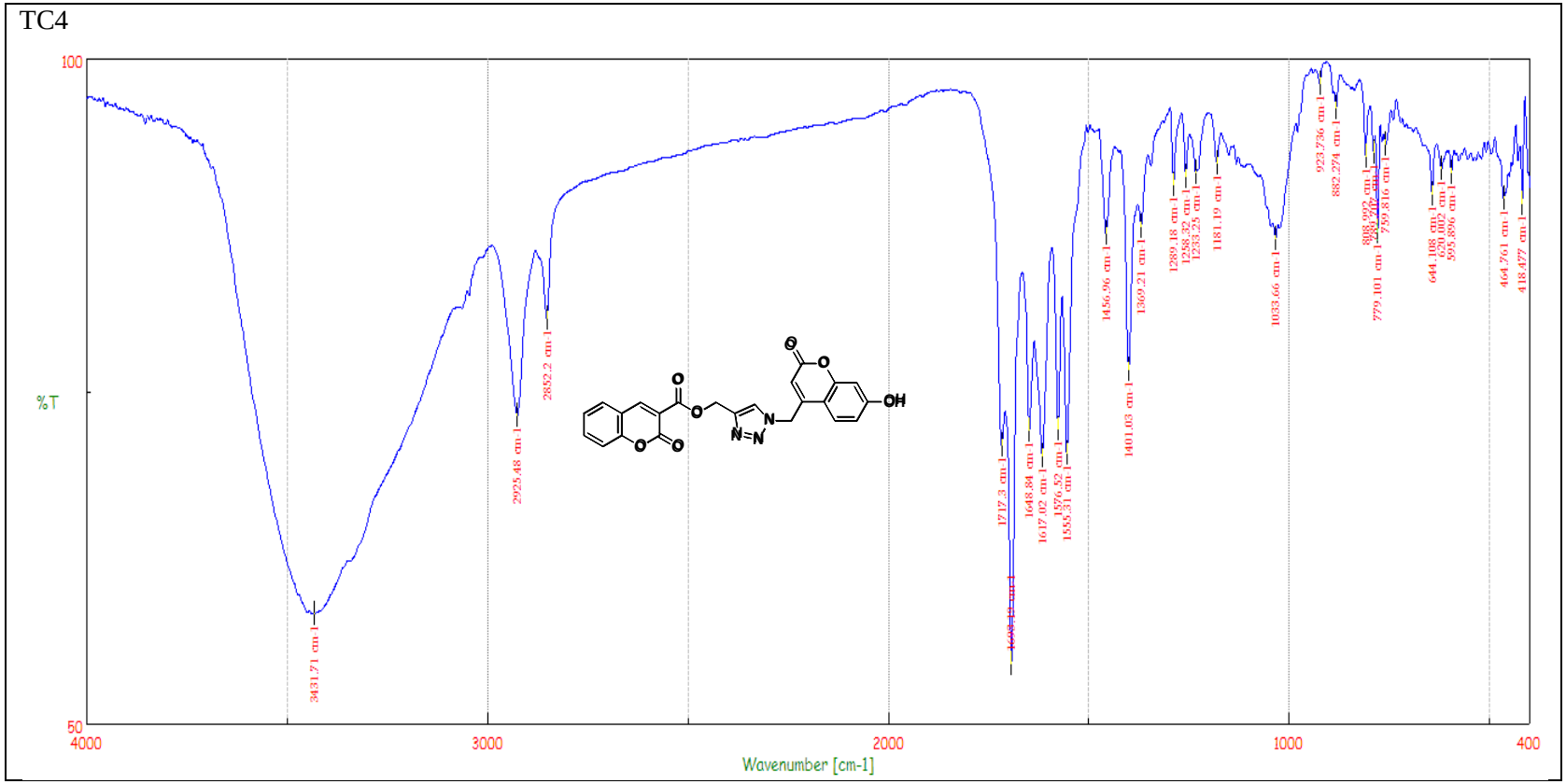

100
80
60
40
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3854.04 cm-1
3293.82 cm-1
3221.5 cm-1
3065.3 cm-1
2924.52 cm-1
2116.49 cm-1
1541.81 cm-1
1573.63 cm-1
1508.06 cm-1
1473.35 cm-1
1421.28 cm-1
1371.14 cm-1
1305.57 cm-1
1261.22 cm-1
1014.37 cm-1
979.661 cm-1
930.485 cm-1
840.812 cm-1
757.888 cm-1
721.297 cm-1
670.142 cm-1
608.431 cm-1
814.777 cm-1
O
NH
O
Br
O

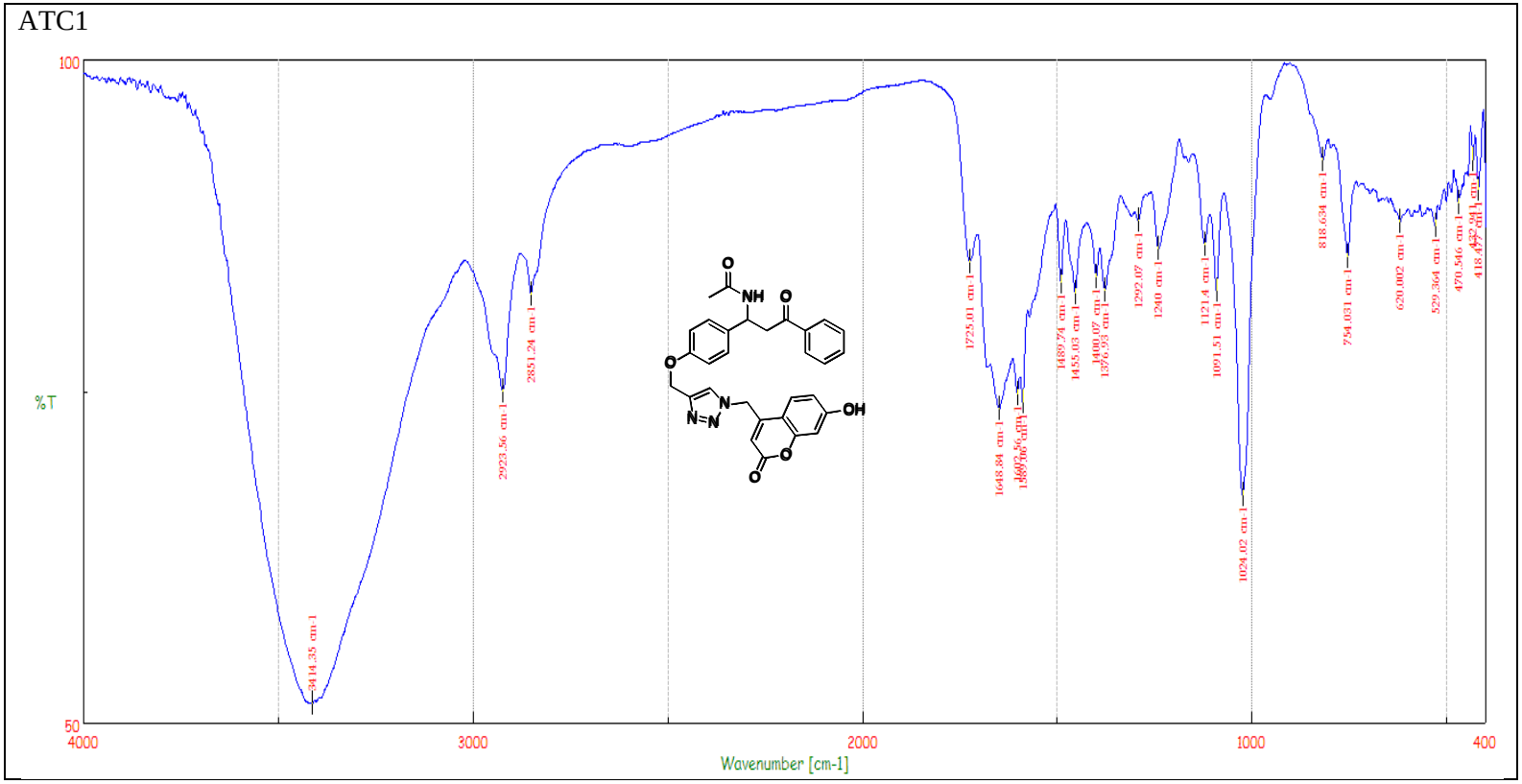

TC1
100
%T
50
4000
3000
2000
1000
400
Wavenumber [cm-1]
3439.42 cm-1
2922.59 cm-1
2852.2 cm-1
1715.37 cm-1
1619.91 cm-1
1572.66 cm-1
1509.99 cm-1
1467.56 cm-1
1389.46 cm-1
1349.93 cm-1
1326.79 cm-1
1295.93 cm-1
1268.97 cm-1
1225.58 cm-1
1206.26 cm-1
1151.29 cm-1
1063.55 cm-1
1019.19 cm-1
984.482 cm-1
941.092 cm-1
844.669 cm-1
822.491 cm-1
765.69 cm-1
708.712 cm-1
686.854 cm-1
614.217 cm-1
577.576 cm-1
536.114 cm-1
485.994 cm-1
O
O
O
N
N
N
CH3
O
O
OH

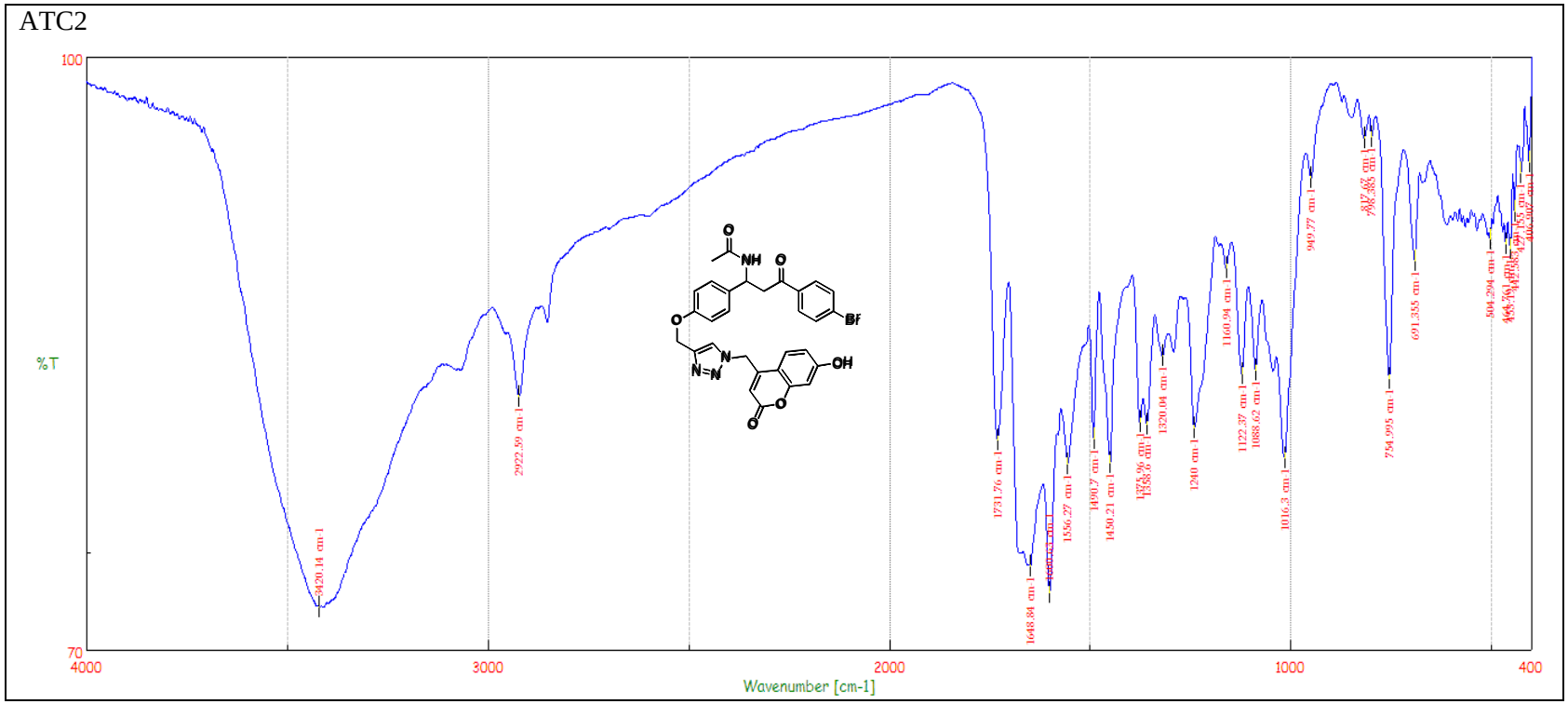
TC2

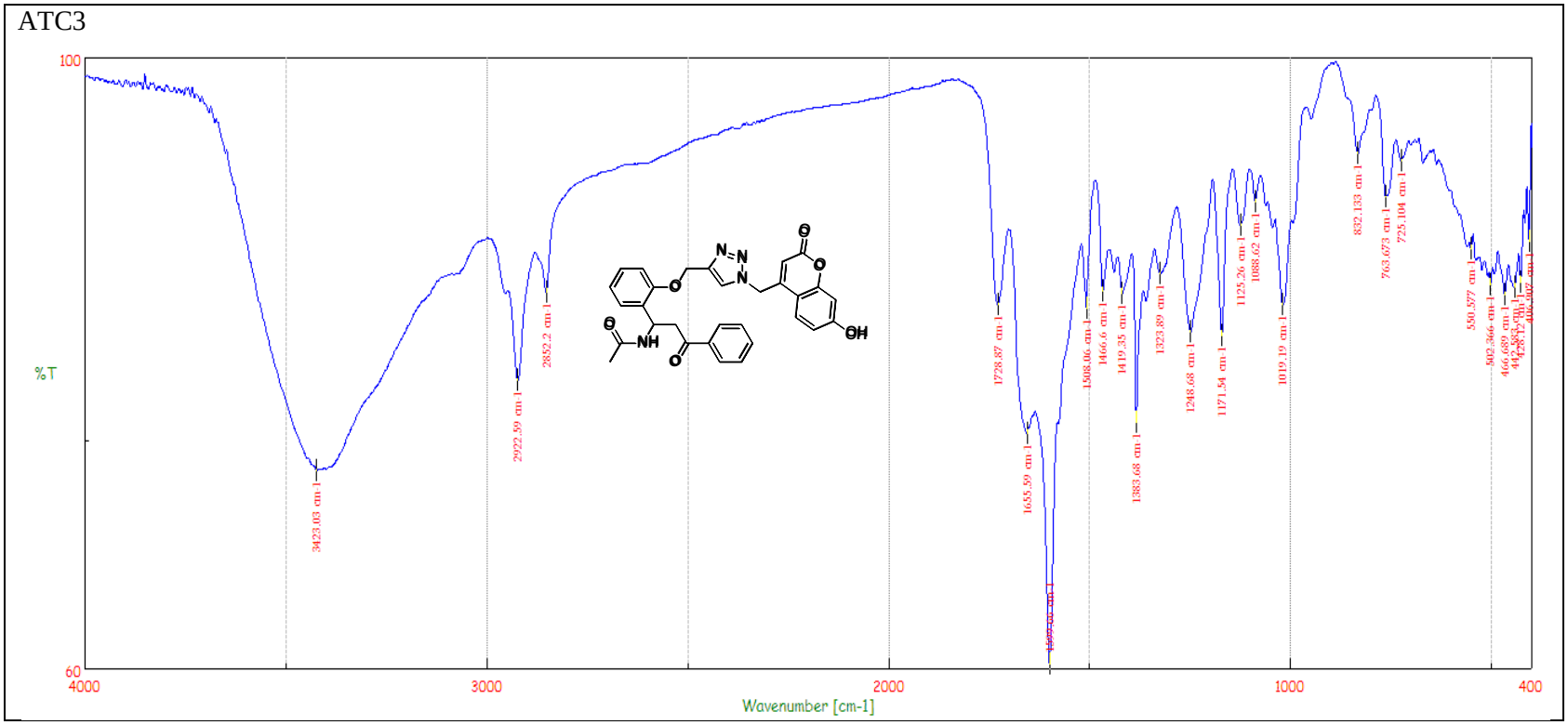

100
50
20
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3422.06 cm-1
3165.58 cm-1
2923.56 cm-1
2853.17 cm-1
1685.48 cm-1
1573.63 cm-1
1557.24 cm-1
1508.06 cm-1
1466.6 cm-1
1402.96 cm-1
1389.53 cm-1
1354.75 cm-1
1322.93 cm-1
1283.39 cm-1
1228.43 cm-1
1159.01 cm-1
1135.87 cm-1
1089.58 cm-1
1045.23 cm-1
1016.3 cm-1
949.77 cm-1
906.379 cm-1
836.955 cm-1
802.242 cm-1
765.601 cm-1
755.066 cm-1
703.89 cm-1
656.643 cm-1
620.002 cm-1
566.969 cm-1
534.185 cm-1
502.187 cm-1
458.011 cm-1
O
O
O
N
N
N
O
O
OH

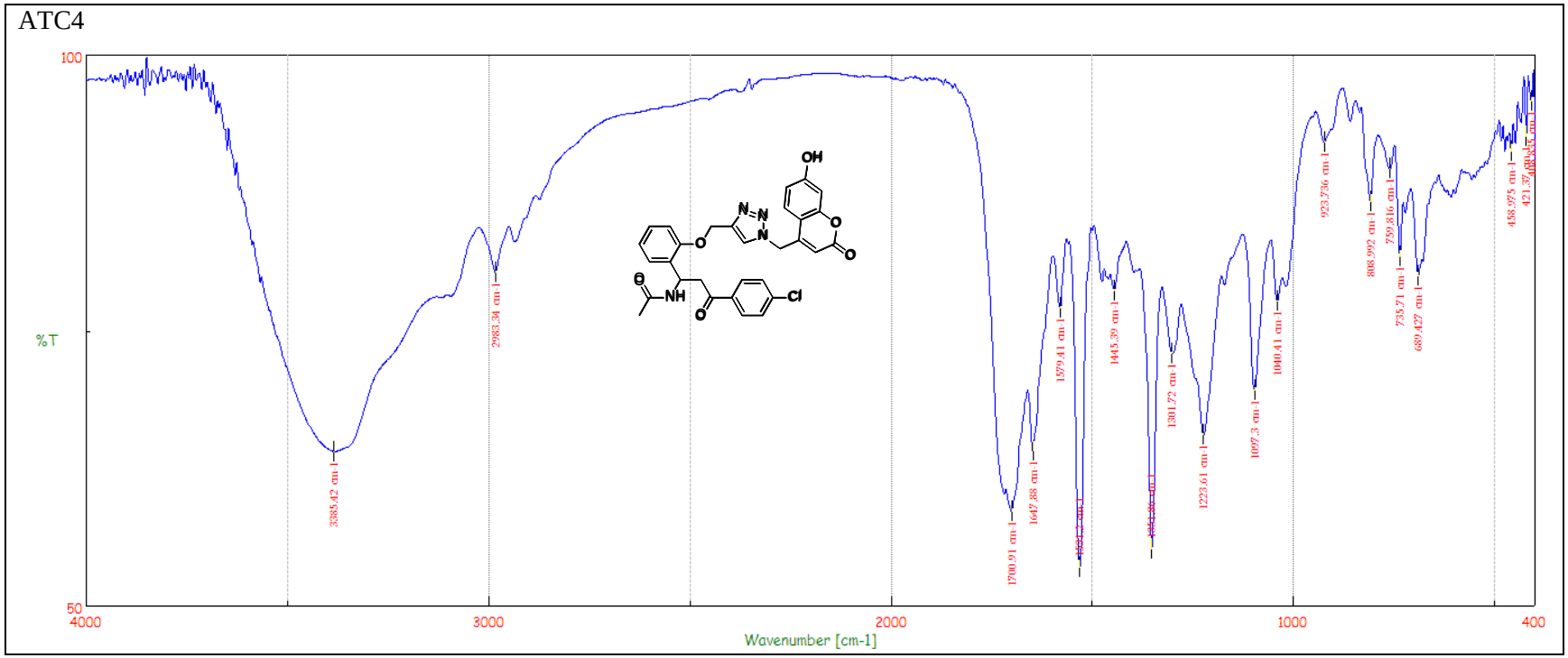

TC3
100
50
30
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3421.1 cm-1
2919.57 cm-1
2850.27 cm-1
1728.87 cm-1
1710.35 cm-1
1610.27 cm-1
1563.99 cm-1
1493.03 cm-1
1449.24 cm-1
1425.14 cm-1
1387.53 cm-1
1354.75 cm-1
1332.59 cm-1
1293.75 cm-1
1244.83 cm-1
1197.58 cm-1
1128.15 cm-1
1107.9 cm-1
1085.73 cm-1
1047.16 cm-1
947.842 cm-1
882.274 cm-1
764.637 cm-1
747.281 cm-1
665.321 cm-1
611.324 cm-1
567.934 cm-1
534.185 cm-1
490.795 cm-1
467.553 cm-1
OH

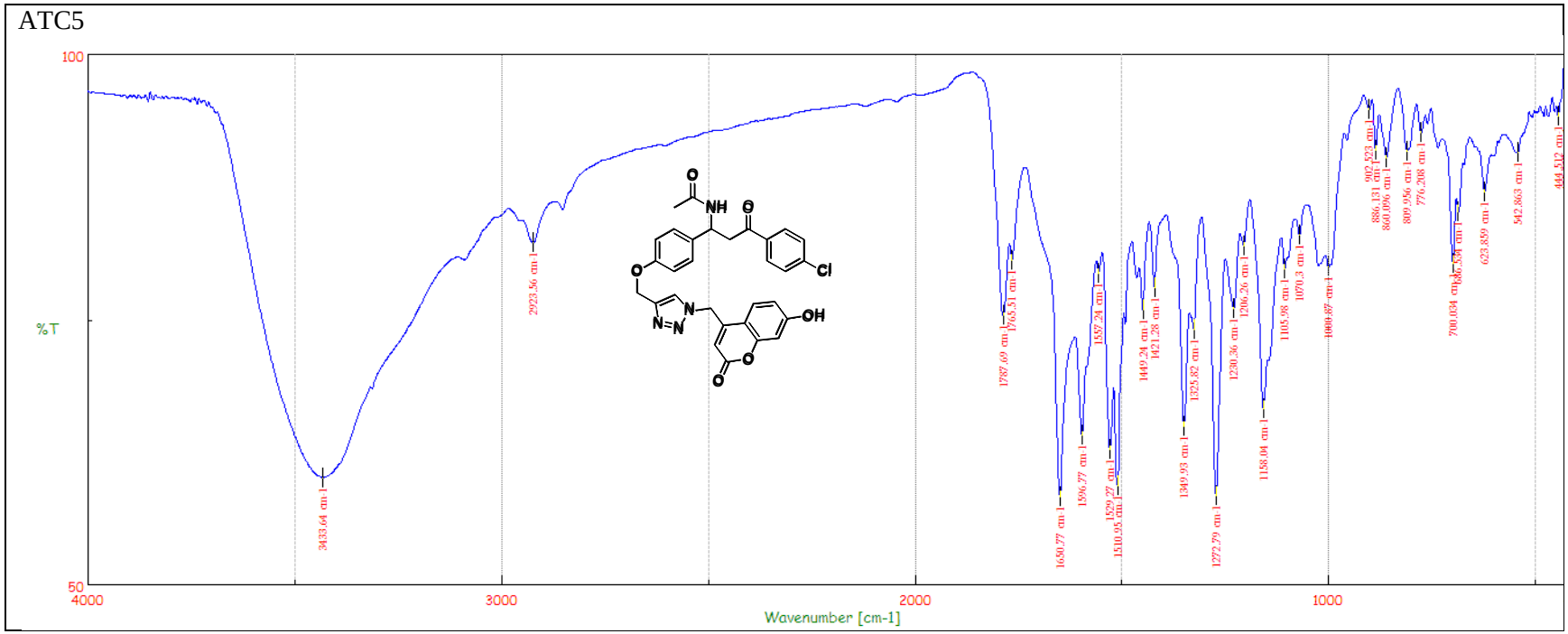

TC4
100
%T
50
4000
3000
2000
1000
400
Wavenumber [cm-1]
3431.71 cm-1
2925.48 cm-1
2852.2 cm-1
1717.3 cm-1
1648.84 cm-1
1617.02 cm-1
1576.52 cm-1
1555.31 cm-1
1456.96 cm-1
1401.03 cm-1
1369.21 cm-1
1289.18 cm-1
1258.32 cm-1
1235.25 cm-1
1181.19 cm-1
1033.66 cm-1
923.736 cm-1
882.274 cm-1
808.992 cm-1
779.101 cm-1
759.816 cm-1
644.108 cm-1
691.002 cm-1
595.896 cm-1
464.761 cm-1
418.477 cm-1
OH

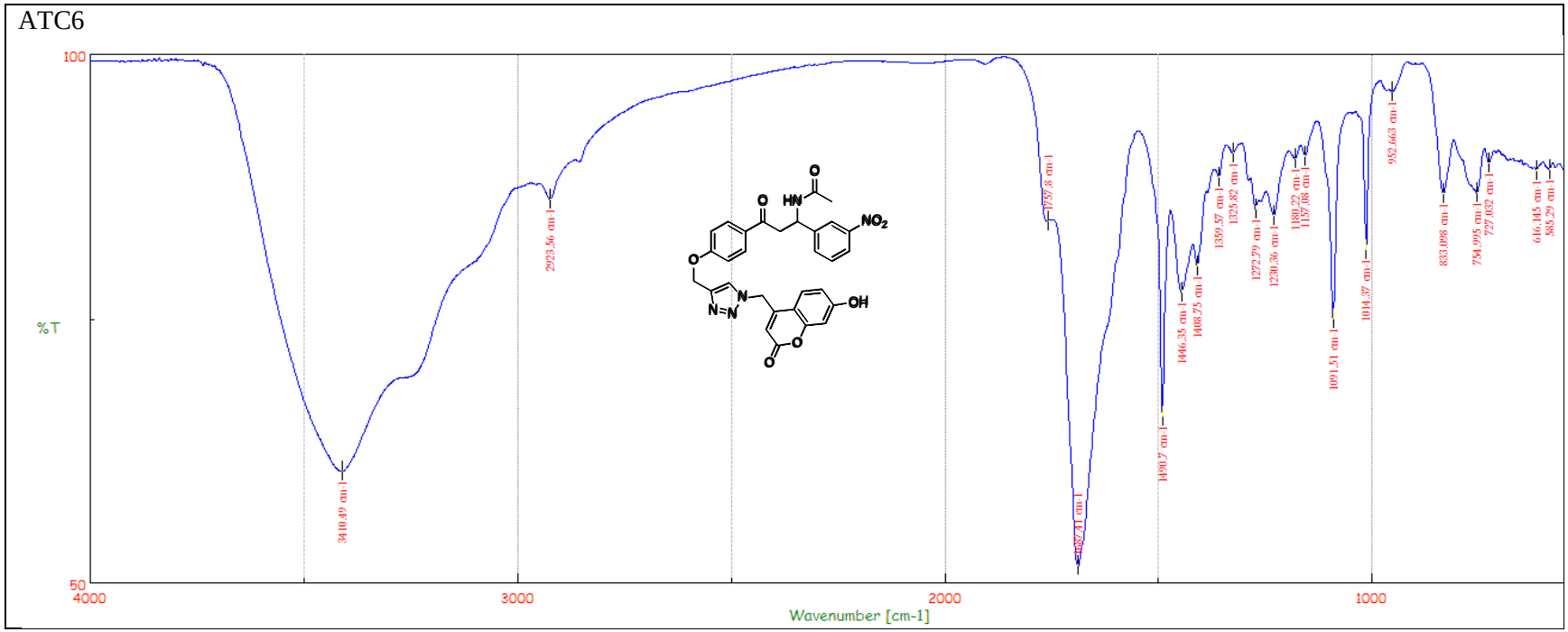

ATC1
100
%T
50
4000
3000
2000
1000
400
Wavenumber [cm-1]
3414.35 cm-1
2923.56 cm-1
2851.24 cm-1
1725.01 cm-1
1648.84 cm-1
1489.74 cm-1
1455.03 cm-1
1400.07 cm-1
1376.93 cm-1
1292.07 cm-1
1240 cm-1
1121.4 cm-1
1091.51 cm-1
1024.02 cm-1
818.634 cm-1
754.031 cm-1
620.002 cm-1
529.364 cm-1
470.546 cm-1
NH
O
N
OH


ATC2
100
70
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3420.14 cm-1
2922.59 cm-1
1731.76 cm-1
1648.84 cm-1
1556.27 cm-1
1490.7 cm-1
1450.21 cm-1
1375.96 cm-1
1358.6 cm-1
1320.04 cm-1
1240 cm-1
1160.94 cm-1
1122.37 cm-1
1088.62 cm-1
1016.3 cm-1
949.77 cm-1
817.67 cm-1
754.995 cm-1
691.355 cm-1
504.294 cm-1
NH
O
Br
OH
N
O

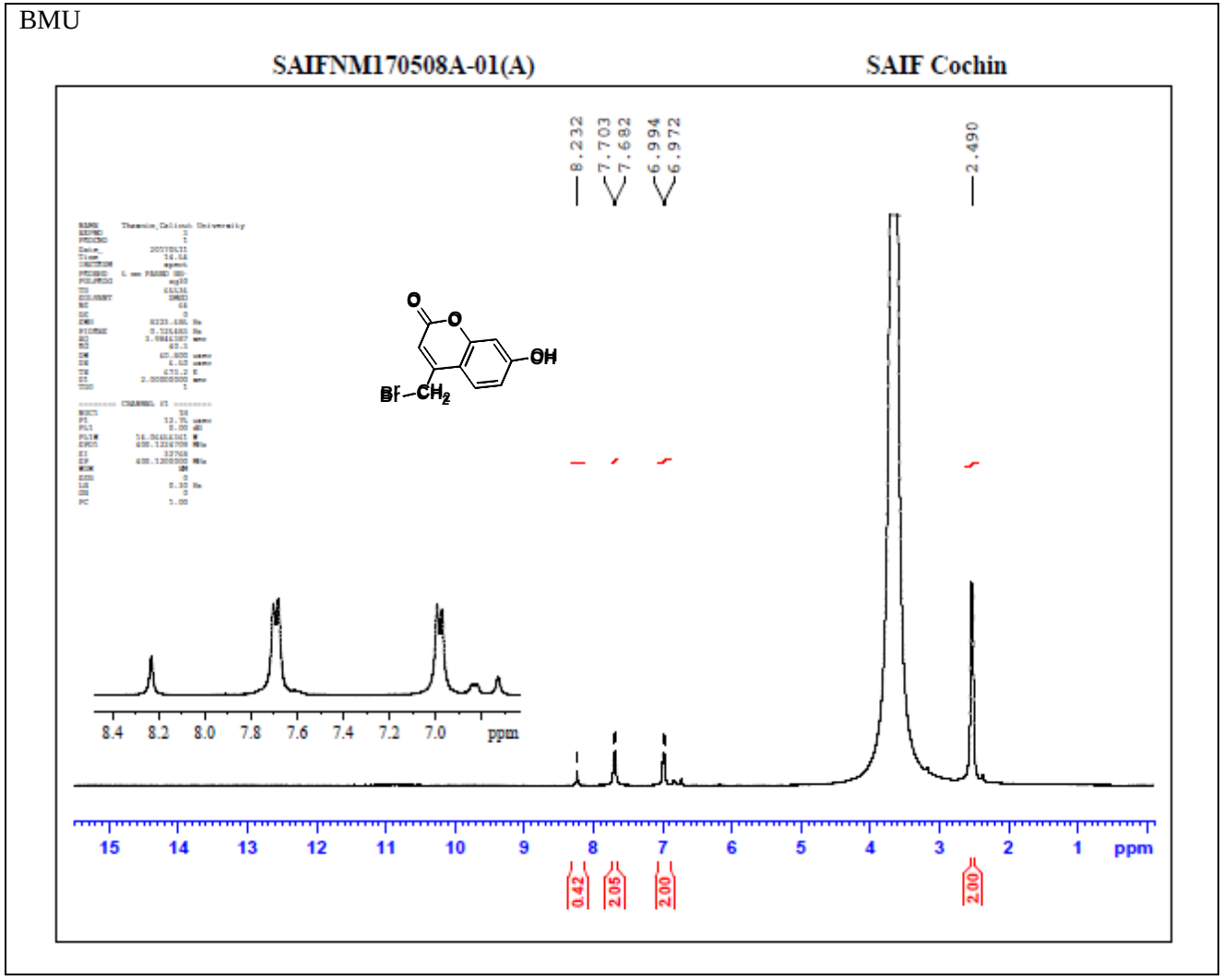

ATC3
100
60
%T
4000
3000
2000
1000
400
Wavenumber [cm-1]
3423.03 cm-1
2922.59 cm-1
2852.2 cm-1
1655.59 cm-1
1508.06 cm-1
1466.6 cm-1
1419.35 cm-1
1383.68 cm-1
1323.89 cm-1
1248.68 cm-1
1171.54 cm-1
1125.26 cm-1
1088.62 cm-1
1019.19 cm-1
832.133 cm-1
763.673 cm-1
725.104 cm-1
550.577 cm-1
502.366 cm-1
466.689 cm-1
NH
OH


ATC4
100
%T
50
4000
3000
2000
1000
400
Wavenumber [cm-1]
3385.42 cm-1
2983.34 cm-1
1700.91 cm-1
1647.88 cm-1
1579.41 cm-1
1445.39 cm-1
1301.72 cm-1
1223.61 cm-1
1097.3 cm-1
1040.41 cm-1
923.736 cm-1
808.992 cm-1
759.816 cm-1
735.71 cm-1
689.427 cm-1
458.975 cm-1
OH
O
N
N
N
O
O
NH
O
Cl

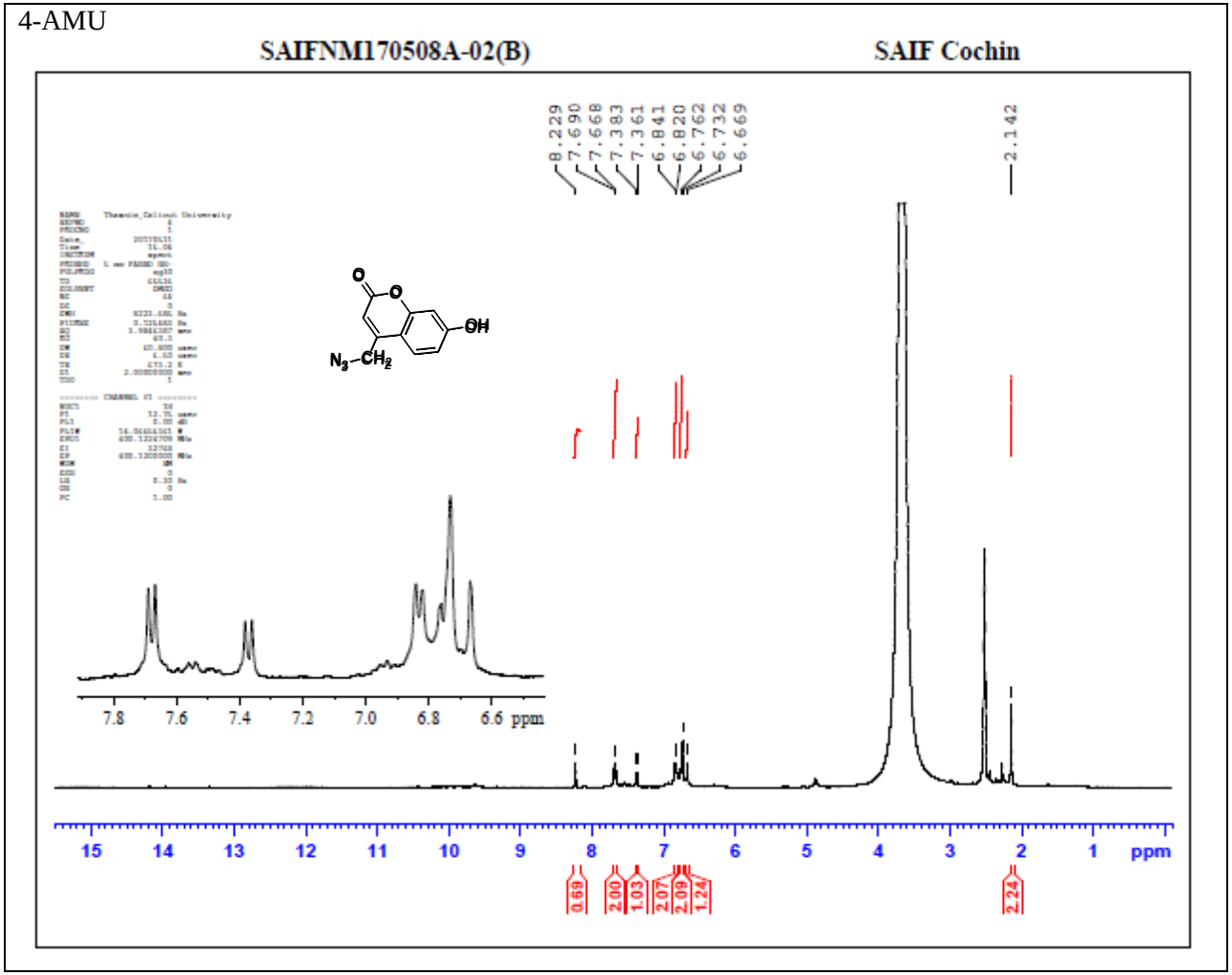

ATC5
100
%T
50
4000
3000
2000
1000
Wavenumber [cm-1]
3433.64 cm-1
2923.56 cm-1
1787.69 cm-1
1765.51 cm-1
1680.77 cm-1
1596.77 cm-1
1559.24 cm-1
1529.27 cm-1
1510.93 cm-1
1449.24 cm-1
1421.28 cm-1
1349.93 cm-1
1325.82 cm-1
1272.79 cm-1
1230.36 cm-1
1206.26 cm-1
1158.04 cm-1
1105.96 cm-1
1070.3 cm-1
1000.87 cm-1
902.323 cm-1
886.131 cm-1
860.1096 cm-1
809.956 cm-1
776.208 cm-1
700.034 cm-1
623.859 cm-1
542.863 cm-1
444.512 cm-1
NH
O
Cl
OH
N
O


ATC6
100
50
%T
4000
3000
2000
1000
Wavenumber [cm-1]
3410.49 cm-1
2923.56 cm-1
1737.8 cm-1
1587.41 cm-1
1490.7 cm-1
1446.35 cm-1
1408.75 cm-1
1359.57 cm-1
1325.82 cm-1
1272.79 cm-1
1230.36 cm-1
1180.22 cm-1
1157.08 cm-1
1091.51 cm-1
1014.37 cm-1
952.663 cm-1
833.098 cm-1
754.995 cm-1
727.052 cm-1
616.945 cm-1
585.29 cm-1
O
HN
O
NO2
O
N
N=N
OH
O
O

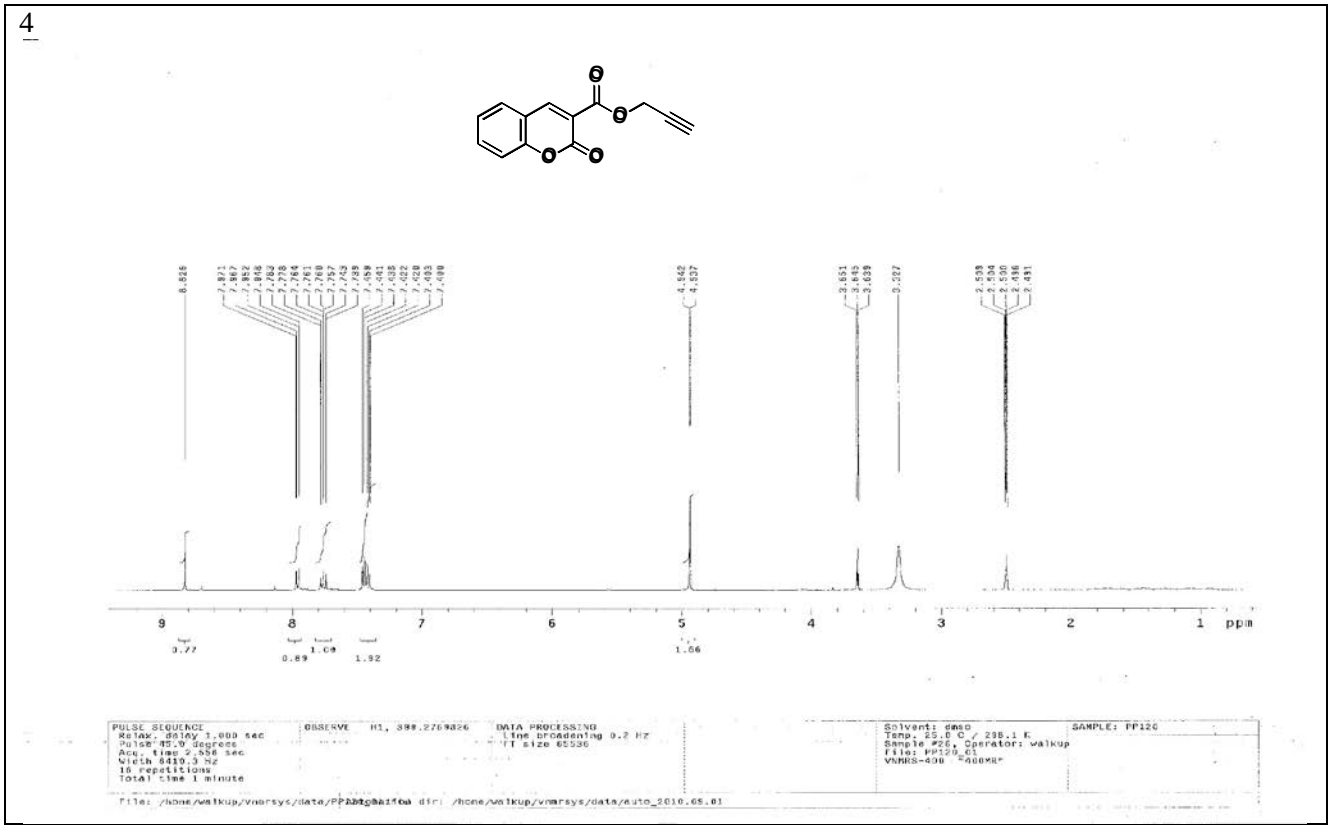
[4] ^{1}H NMR spectra of compounds

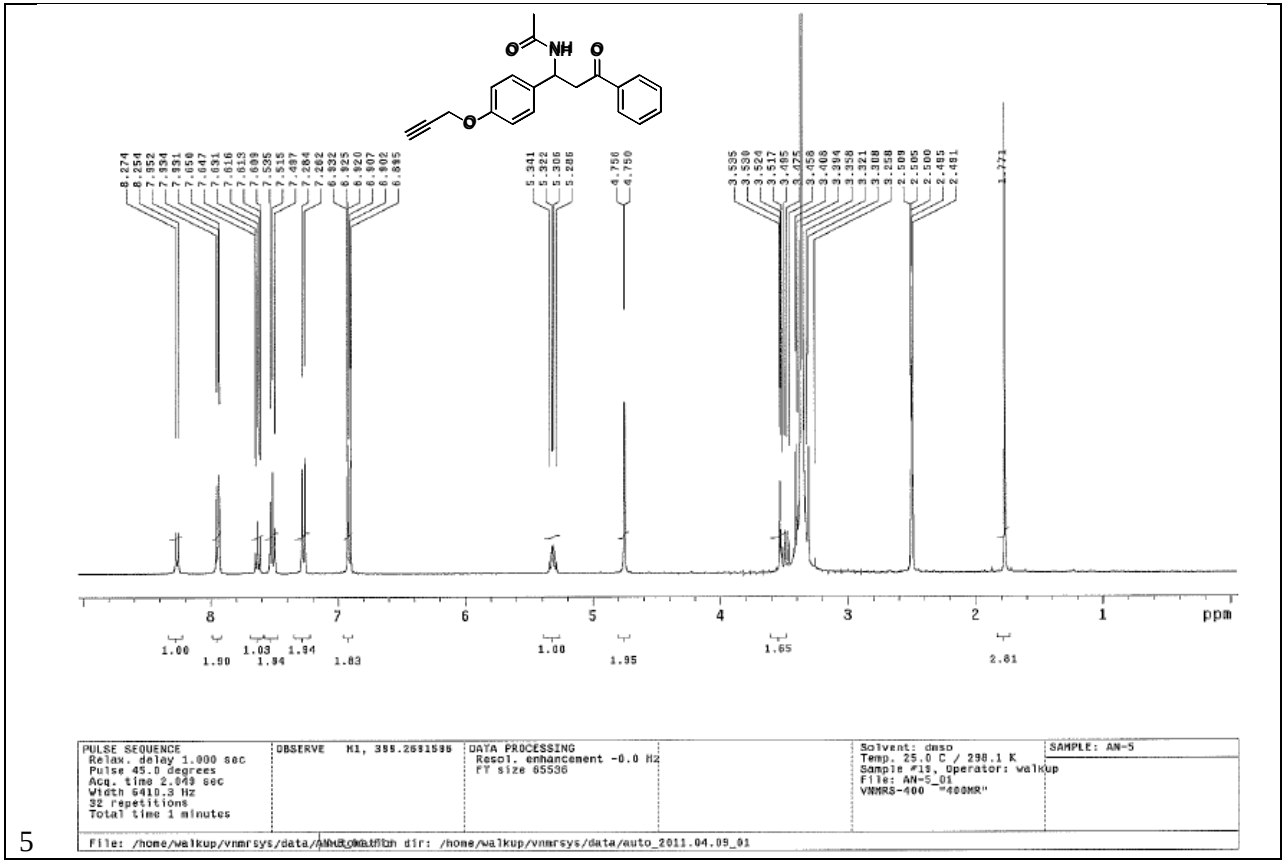


4-AMU


SAIFNM170508A-02(B)
SAIF Cochin
8.229
7.690
7.668
7.383
7.361
6.841
6.820
6.762
6.732
6.669
2.142
OH
N3–CH2
7.8
7.6
7.4
7.2
7.0
6.8
6.6 ppm
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.69
2.00
1.03
2.07
2.09
1.24
2.24

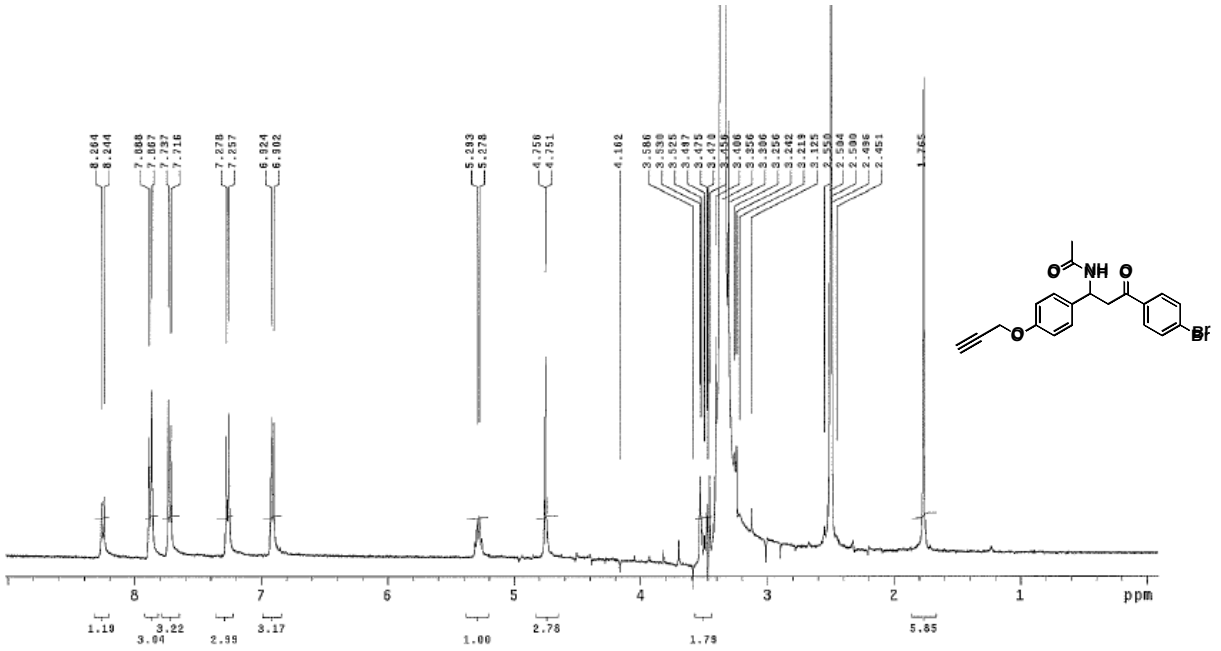
4


8.026
7.871
7.867
7.852
7.848
7.763
7.759
7.746
7.761
7.760
7.757
7.743
7.739
7.659
7.461
7.438
7.422
7.428
7.403
7.400
4.542
4.537
3.651
3.645
3.639
3.227
2.538
2.534
2.530
2.496
2.491
9
8
7
6
5
4
3
2
1
ppm
3.27
0.89
1.00
1.92
1.66
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.556 sec
Width 6410.3 Hz
16 repetitions
Total time 1 minute
OBSERVE H1, 399.7769826
DATA PROCESSING
Line broadening 0.2 Hz
FT size 65536
Solvent: dmso
Temp. 25.0 C / 298.1 K
Sample #26, Operator: walkup
File: PP120_01
VNMRS-400 "400MR"
SAMPLE: PP120
File: /home/walkup/vnmrsys/data/PP120_01.fid dir: /home/walkup/vnmrsys/data/auto_2010.05.01


NH
O
O
O
8.274
8.254
7.952
7.934
7.931
7.630
7.627
7.611
7.616
7.613
7.609
7.535
7.515
7.497
7.284
7.282
6.932
6.925
6.920
6.907
6.902
6.885
5.341
5.322
5.306
5.286
4.756
4.750
3.535
3.530
3.524
3.517
3.495
3.475
3.458
3.408
3.394
3.358
3.321
3.308
3.258
3.168
2.505
2.500
2.485
2.481
1.771
8
7
6
5
4
3
2
1
ppm
1.00
1.50
1.03
1.94
1.94
1.83
1.00
1.95
1.65
2.61
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 5410.3 Hz
32 repetitions
Total time 1 minutes
OBSERVE H1, 399.2691595
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Solvent: dmso
Temp. 25.0 C / 298.1 K
Sample #13, Operator: walkup
File: AN-5_01
VNMRS-400 "400MR"
SAMPLE: AN-5
File: /home/walkup/vnmrsys/data/AN-5_01.fid dir: /home/walkup/vnmrsys/data/auto_2011.04.09_01

5

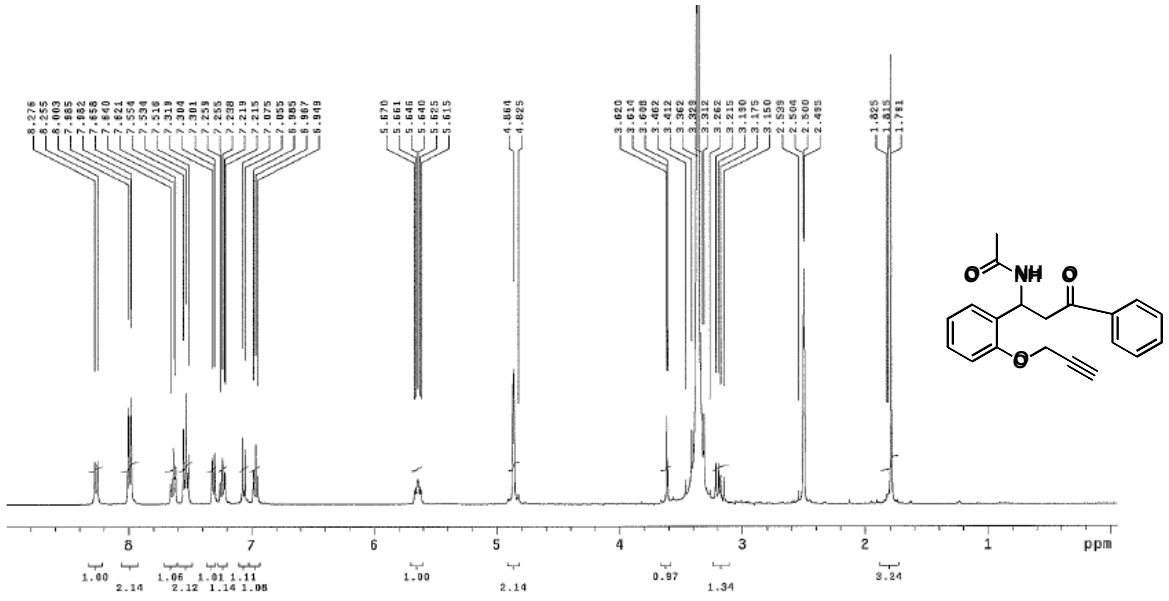
6



PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.049 sec Width 6410.3 Hz 32 repetitions Total time 1 minutes	OBSERVE H1, 399.2691595	DATA PROCESSING Resol. enhancement -0.0 Hz FT size 65536		Solvent: dmso Temp. 25.0 C / 298.1 K Sample #20, Operator: walkup File: AN-6_01 VNMRS-400 "400MR"	SAMPLE: AN-6

File: /home/walkup/vnmrsys/data/AN-6_01.fid dir: /home/walkup/vnmrsys/data/auto_2011.04.08_01

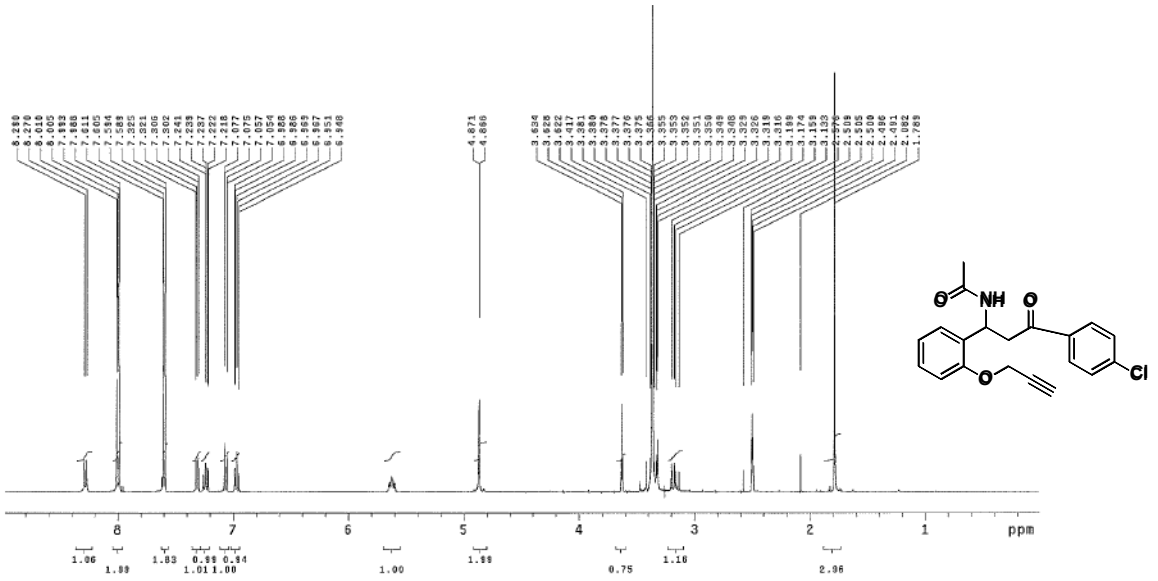
7



PULSE SEQUENCE	OBSERVE H1, 388.2691587	DATA PROCESSING		Solvent: dmso	SAMPLE: An-11
Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.049 sec Width 6410.3 Hz 32 repetitions Total time 1 minutes		Resol. enhancement -0.0 Hz FT size 65536		Temp. 25.0 C / 298.1 K Sample #36, Operator: walkup File: An-11_01 VNMRS-400 "400MR"	

File: /home/walkup/vnmrsys/data/AnAutoUnits dir: /home/walkup/vnmrsys/data/auto_2011.04.08_01

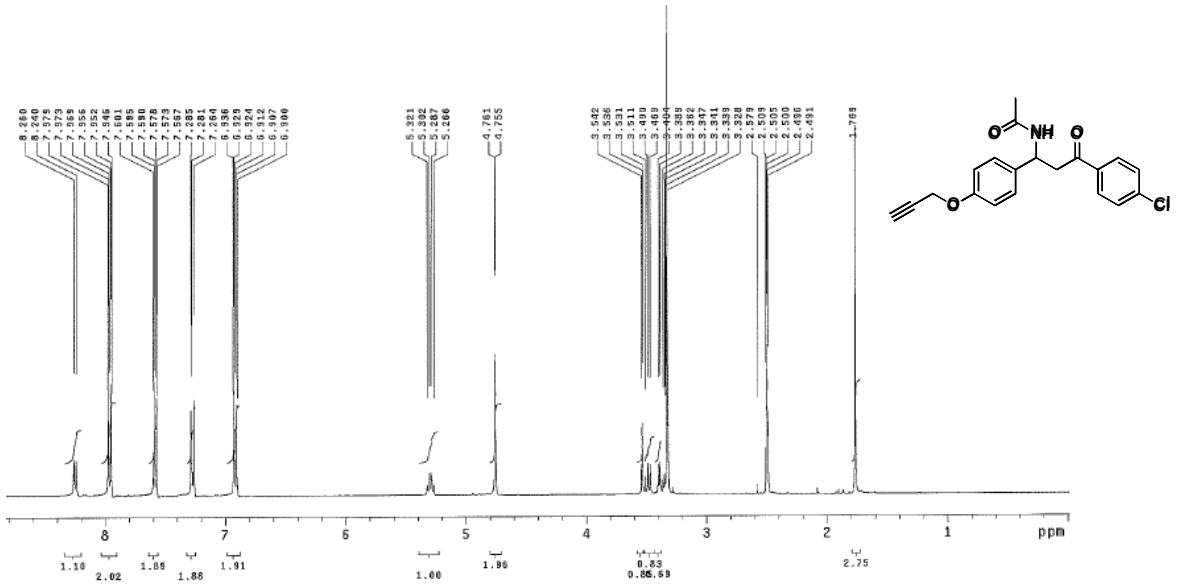
8



PULSE SEQUENCE	OBSERVE H1, 399.2681597	DATA PROCESSING		Solvent: dmso	SAMPLE: An-12
Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.048 sec Width 8410.3 Hz 32 repetitions Total time 1 minutes		Resol. enhancement -0.0 Hz FT size 65536		Temp. 25.0 C / 298.1 K Sample #37, Operator: walkup File: An-12_01 VNMRS-400 "400MR"	

File: /home/walkup/vnmrsys/data/An-12_01.fid Acquisition dir: /home/walkup/vnmrsys/data/auto_2011.04.09_01

9


8.260
8.240
7.975
7.973
7.969
7.956
7.952
7.946
7.601
7.595
7.590
7.578
7.573
7.567
7.285
7.281
7.264
6.936
6.929
6.924
6.912
6.907
6.900
5.321
5.302
5.287
5.266
4.761
4.755
3.542
3.536
3.531
3.511
3.489
3.483
3.468
3.462
3.389
3.382
3.347
3.341
3.339
3.328
2.579
2.509
2.505
2.500
2.496
2.491
1.769
NH
O
O
O
Cl
8
7
6
5
4
3
2
1
ppm
1.10
2.02
1.89
1.88
1.91
1.00
1.96
0.83
0.86
0.69
2.75
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
32 repetitions
Total time 1 minutes
OBSERVE H1, 399.2691598
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Solvent: dmso
Temp. 25.0 C / 298.1 K
Sample #26, Operator: walkup
File: An68_01
VNMRS-400 "400MR"
SAMPLE: An68
File: /home/walkup/vnmrsys/data/An68_01.fid Data dir: /home/walkup/vnmrsys/data/auto_2011.04.08_01

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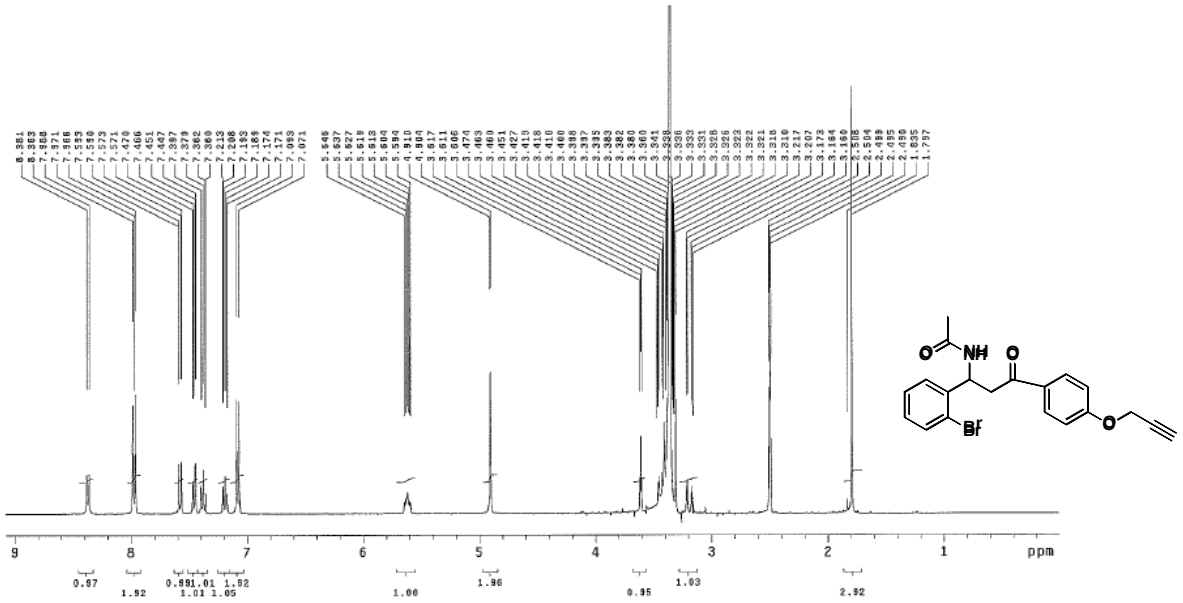
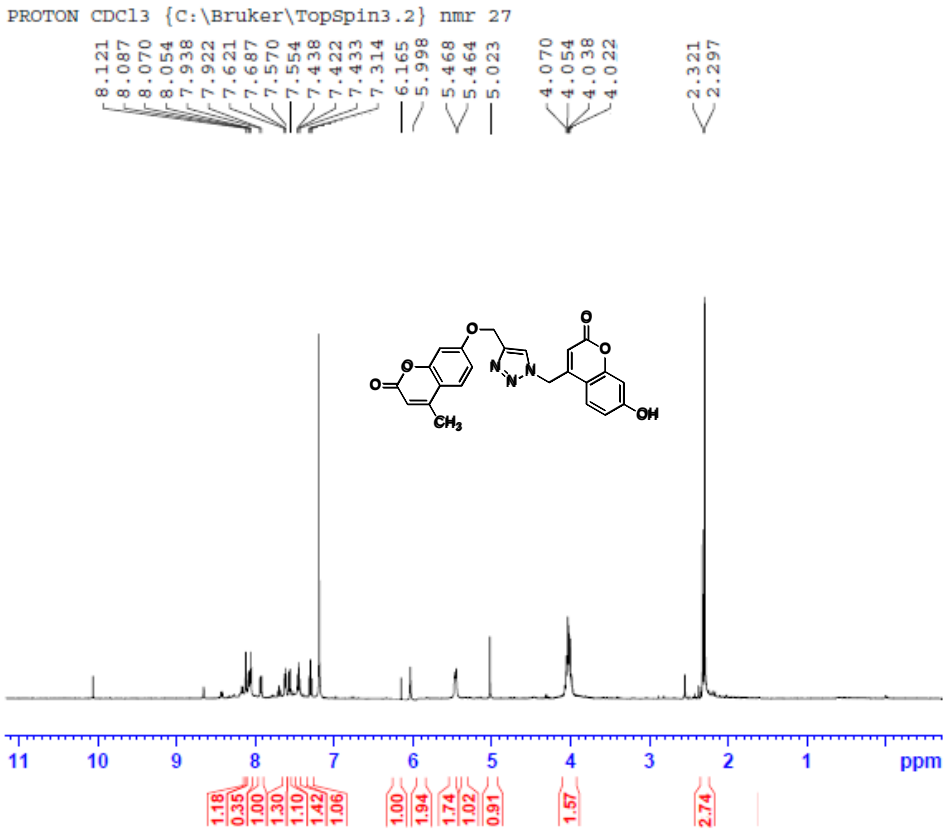


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 2.049 sec Width 6410.3 Hz 32 repetitions Total time 1 minutes	OBSERVE H1, 399.2591600	DATA PROCESSING Resol. enhancement -0.0 Hz FT size 65536		Solvent: dmso Temp. 25.0 C / 298.1 K Sample #28, Operator: walkup File: An-10_01 VNMRS-400 "400MR"	SAMPLE: An-10

File: /home/walkup/vnmrsys/data/An-10_01.fid Auto-built dir: /home/walkup/vnmrsys/data/auto_2011.04.09_01

TC1



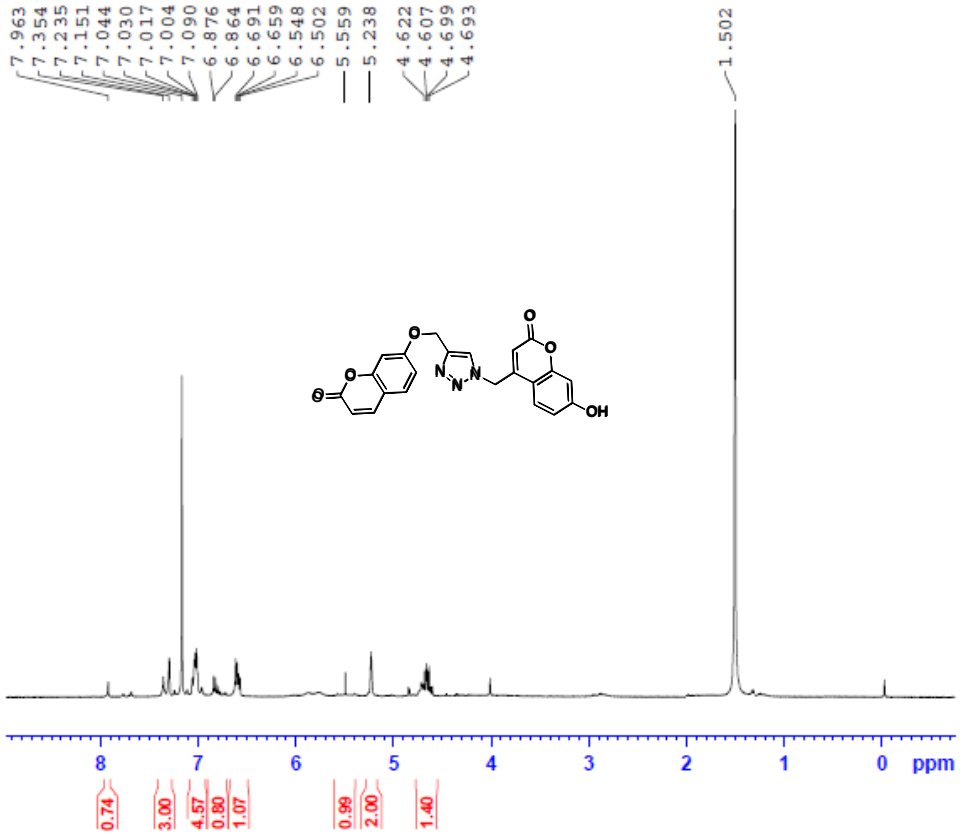

```
Current Data Parameters
NAME                  Soumya
EXPNO                      6
PROCNO                     1

P2 - Acquisition Parameters
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES            0.152588 Hz
AQ                3.2767999 sec
RG                      181
DW                   50.000 usec
DE                    6.50 usec
TE                   301.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             500.2330891 MHz
NUC1                      1H
P1                     9.04 usec
PLW1            27.16399956 W

P2 - Processing parameters
SI                    65536
SF               500.2300475 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

TC2



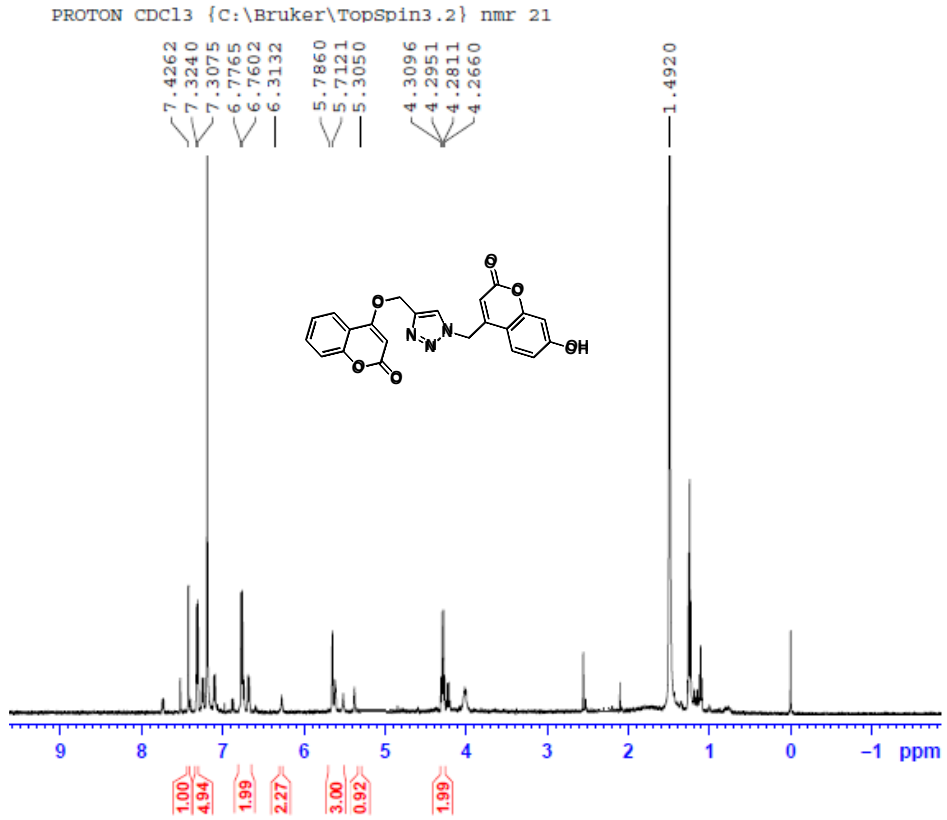

```
Current Data Parameters
NAME                  Soumya
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES                 0.152588 Hz
AQ                 3.2767999 sec
RG                       203
DW                    50.000 usec
DE                     6.50 usec
TE                     298.9 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             500.2330891 MHz
NUC1                    1H
P1                      9.04 usec
PLW1            27.16399956 W

F2 - Processing parameters
SI                     65536
SF               500.2300597 MHz
WDW                      EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```

TC3



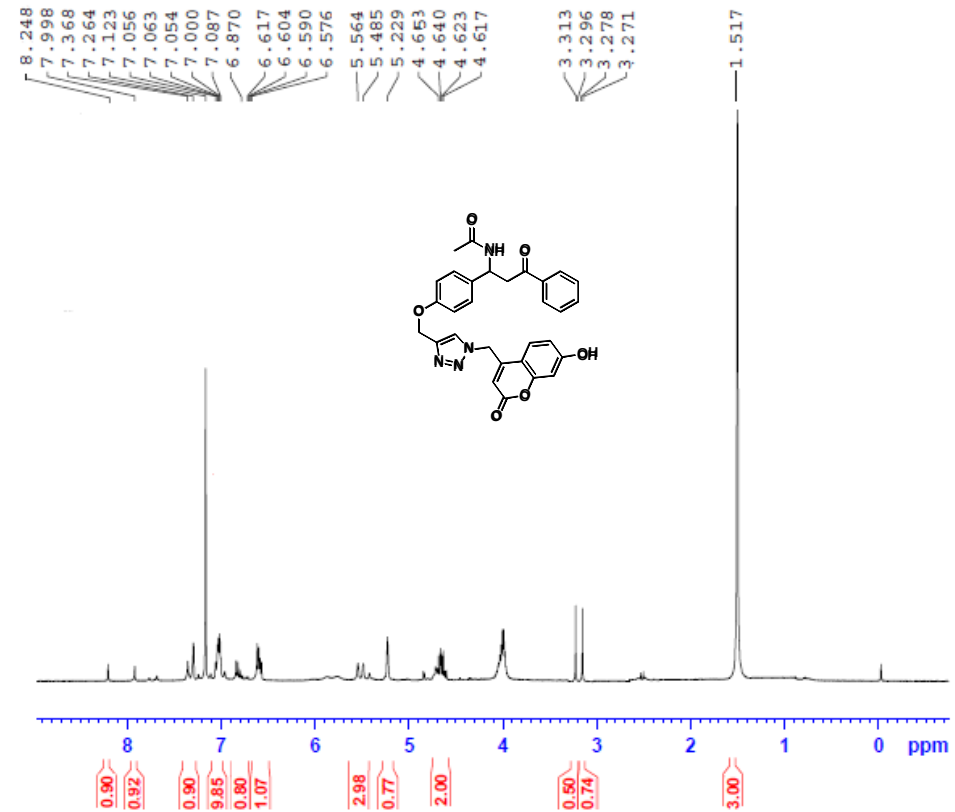

```
Current Data Parameters
NAME                  Soumya
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                3.2767999 sec
RG                      144
DW                   50.000 usec
DE                    6.50 usec
TE                   298.0 K
D1             1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           500.2330891 MHz
NUC1                   1H
P1                   9.04 usec
PLW1          27.16399956 W

F2 - Processing parameters
SI                    65536
SF             500.2300453 MHz
WDW                    EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

ATC1



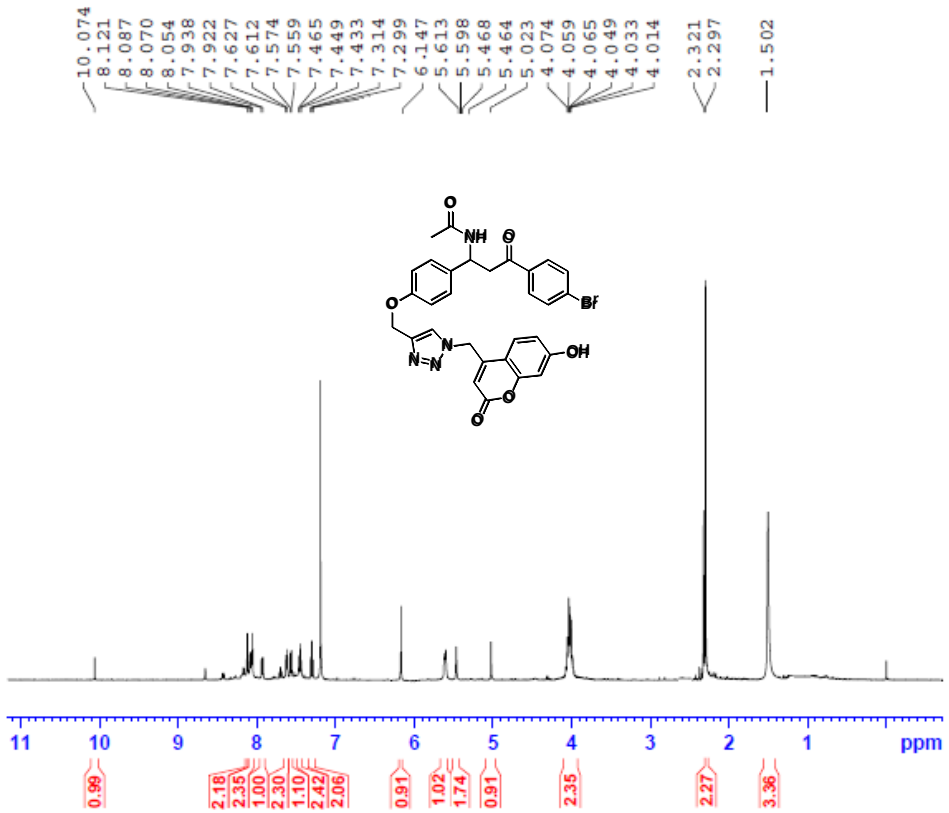

```
Current Data Parameters
NAME                  Soumya
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                3.2767999 sec
RG                       203
DW                   50.000 usec
DE                    6.50 usec
TE                    298.9 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            500.2330891 MHz
NUC1                      1H
P1                     9.04 usec
PLW1           27.16399956 W

F2 - Processing parameters
SI                     65536
SF              500.2300597 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

ATC2




```
Current Data Parameters
NAME                  Soumya
EXPNO                      6
PROCNO                     1

F2 - Acquisition Parameters
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                3.2767999 sec
RG                       181
DW                  50.000 usec
DE                   6.50 usec
TE                   301.0 K
D1                1.00000000 sec
TD0                        1

-------- CHANNEL f1 --------
SFO1           500.2330891 MHz
NUC1                     1H
P1                    9.04 usec
PLW1          27.16399956 W

F2 - Processing parameters
SI                    65536
SF             500.2300475 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
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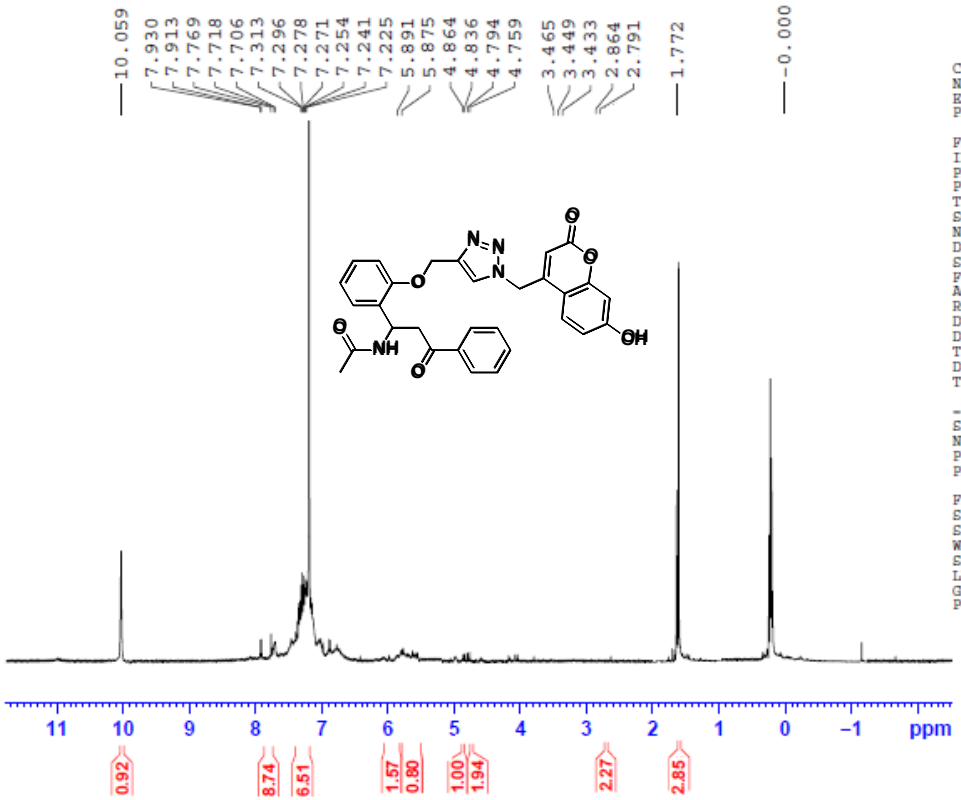
ATC3



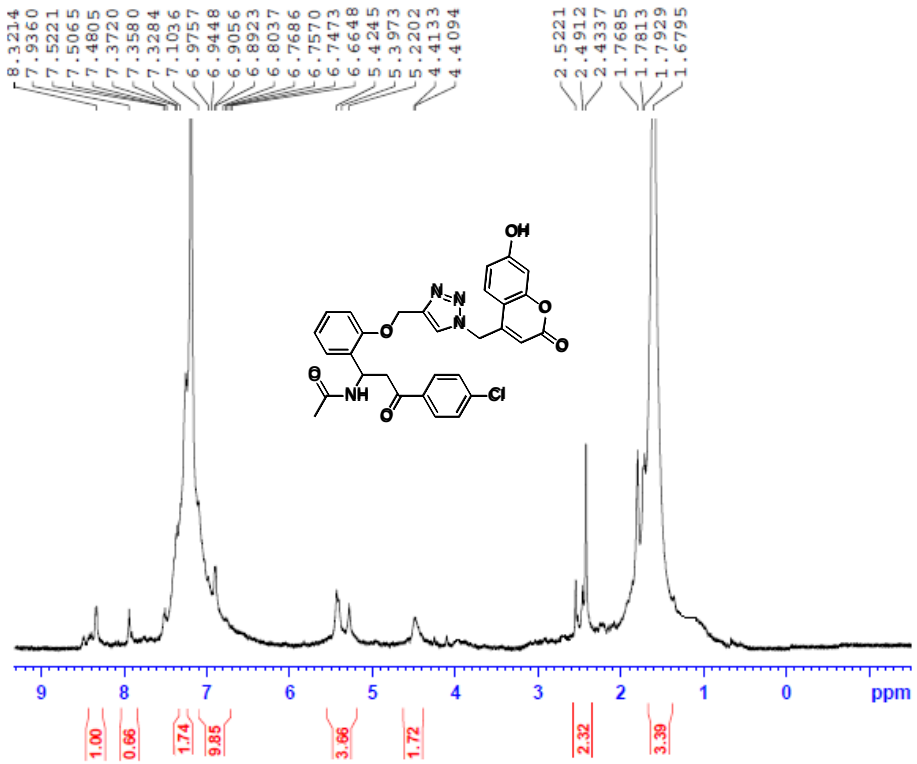

```
Current Data Parameters
NAME                  Soumya
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                3.2767999 sec
RG                       203
DW                    50.000 usec
DE                     6.50 usec
TE                     301.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           500.2330891 MHz
NUC1                    1H
P1                   9.04 usec
PLW1          27.16399956 W

F2 - Processing parameters
SI                     65536
SF             500.2300476 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                     1.00
```

ATC4



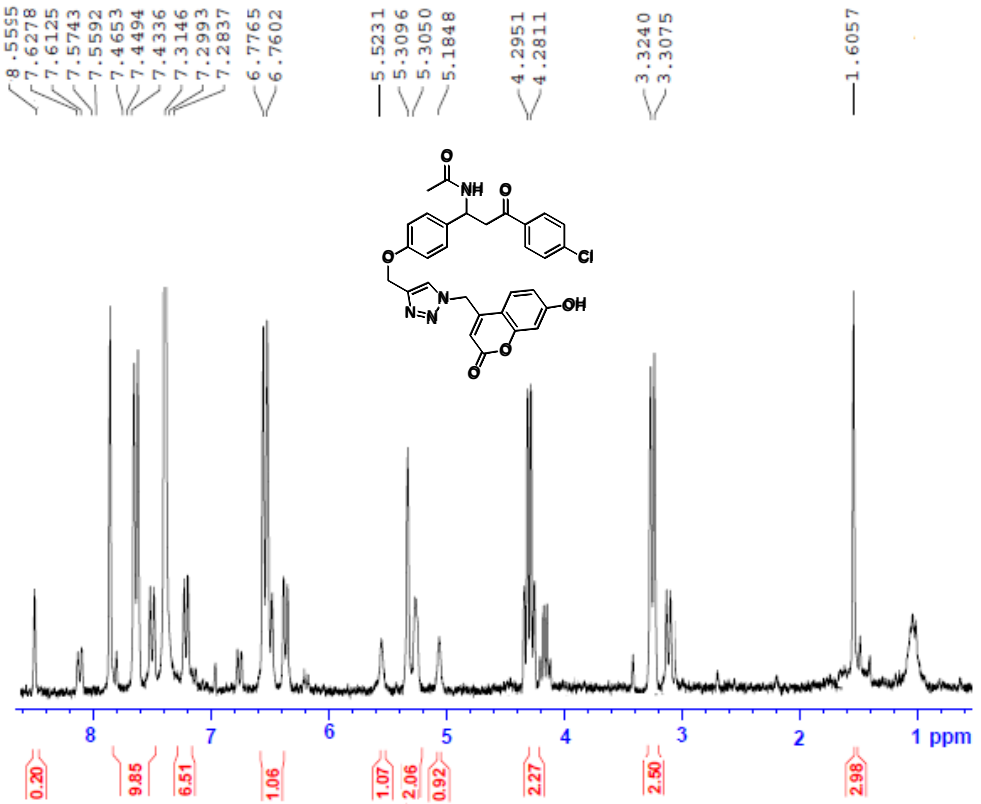

```
Current Data Parameters
NAME                  Soumya
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2767999 sec
RG                       144
DW                    50.000 use
DE                     6.50 use
TE                    298.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1           500.2330891 MHz
NUC1                    1H
P1                    9.04 use
PLW1          27.16399956 W

F2 - Processing parameters
SI                     65536
SF             500.2300453 MHz
WDW                       EM
SSB                    0
LB                     0.30 Hz
GB                     0
PC                     1.00
```

ATC5



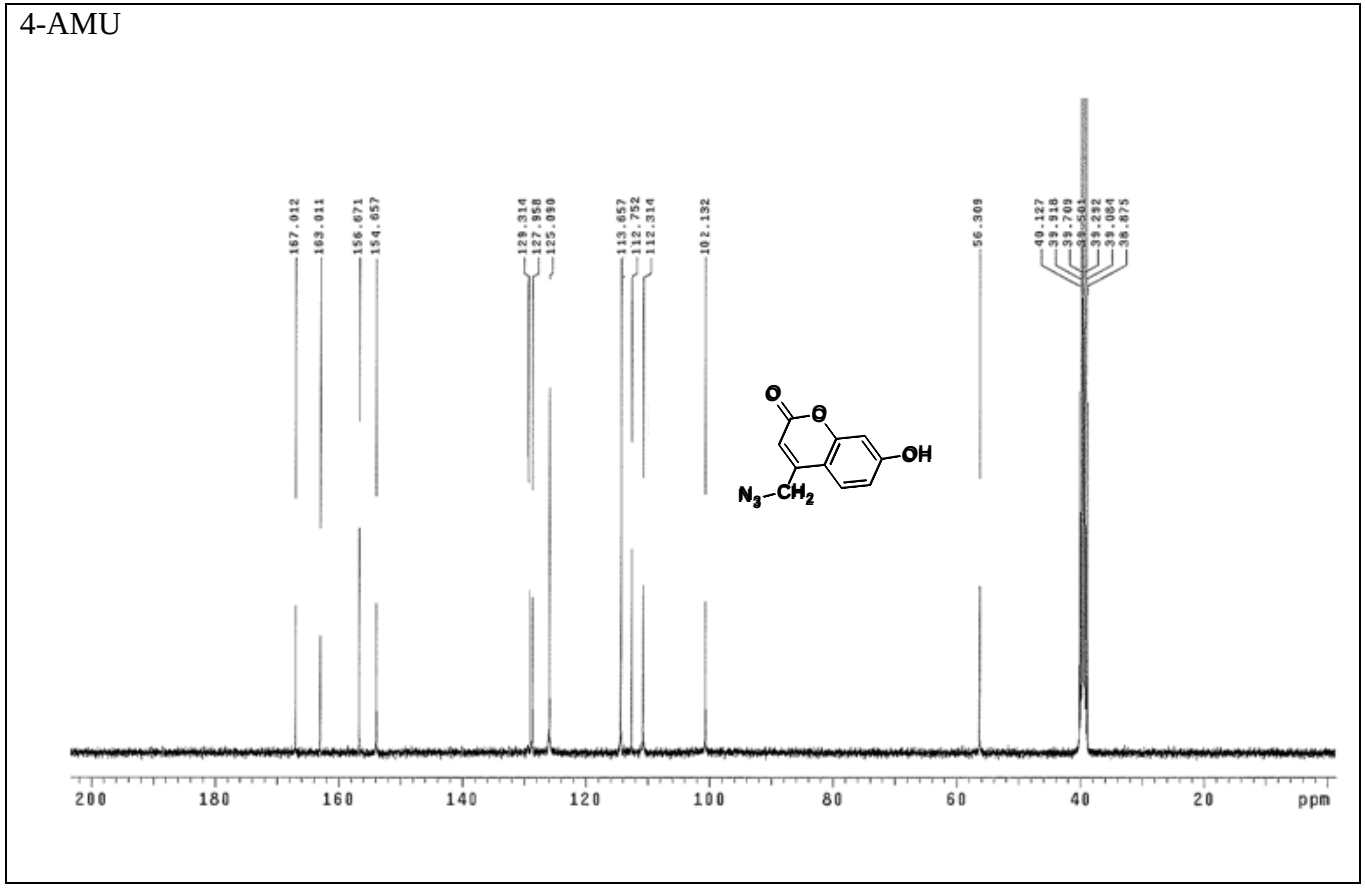

```
Current Data Parameters
NAME                  Soumya
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2767999 sec
RG                       203
DW                    50.000 usec
DE                     6.50 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                        1

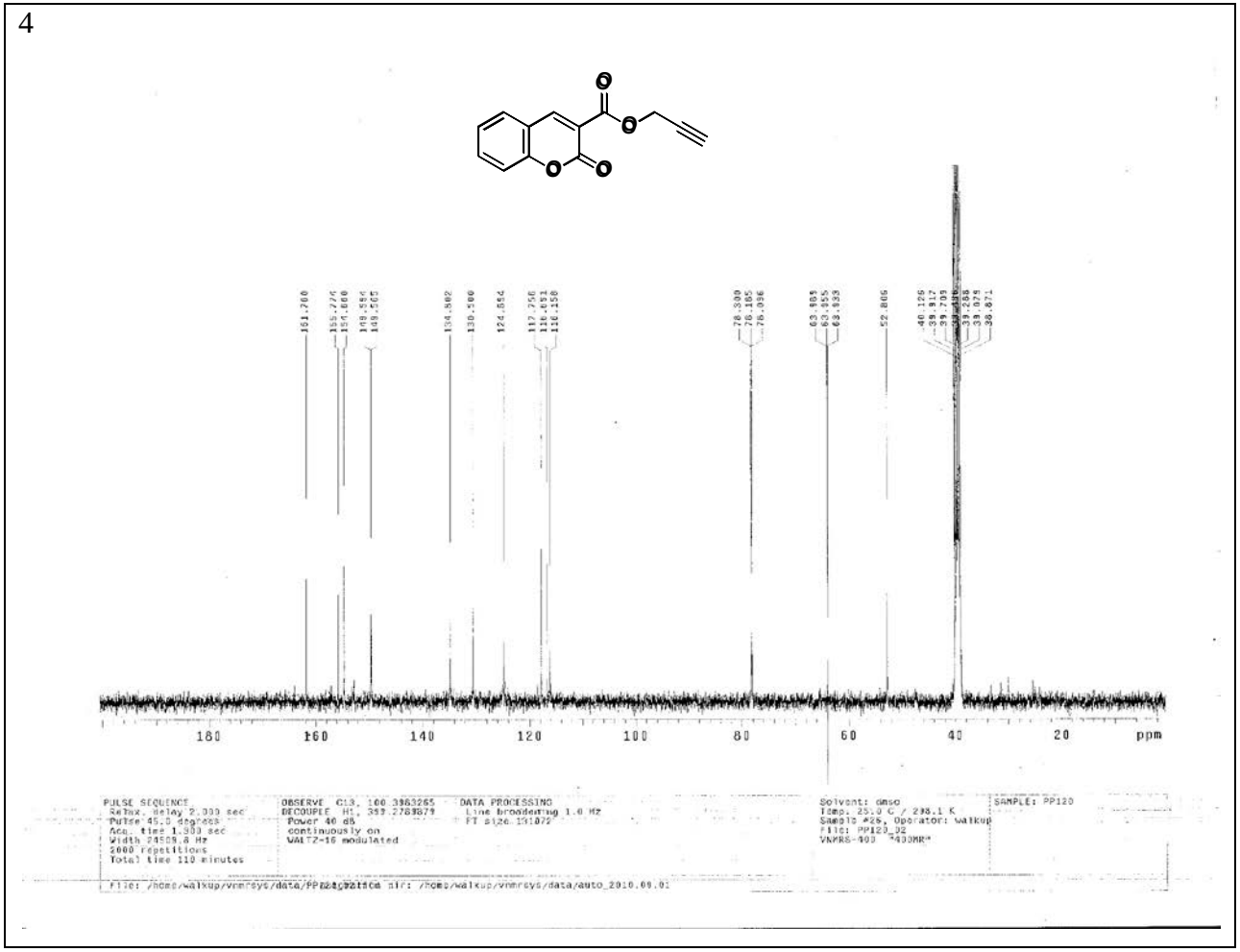
======== CHANNEL f1 ========
SFO1           500.2330891 MHz
NUC1                    1H
P1                     9.04 usec
PLW1          27.16399956 W

F2 - Processing parameters
SI                     65536
SF             500.2300458 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

[5] ^{13}C NMR Spectra of compounds



4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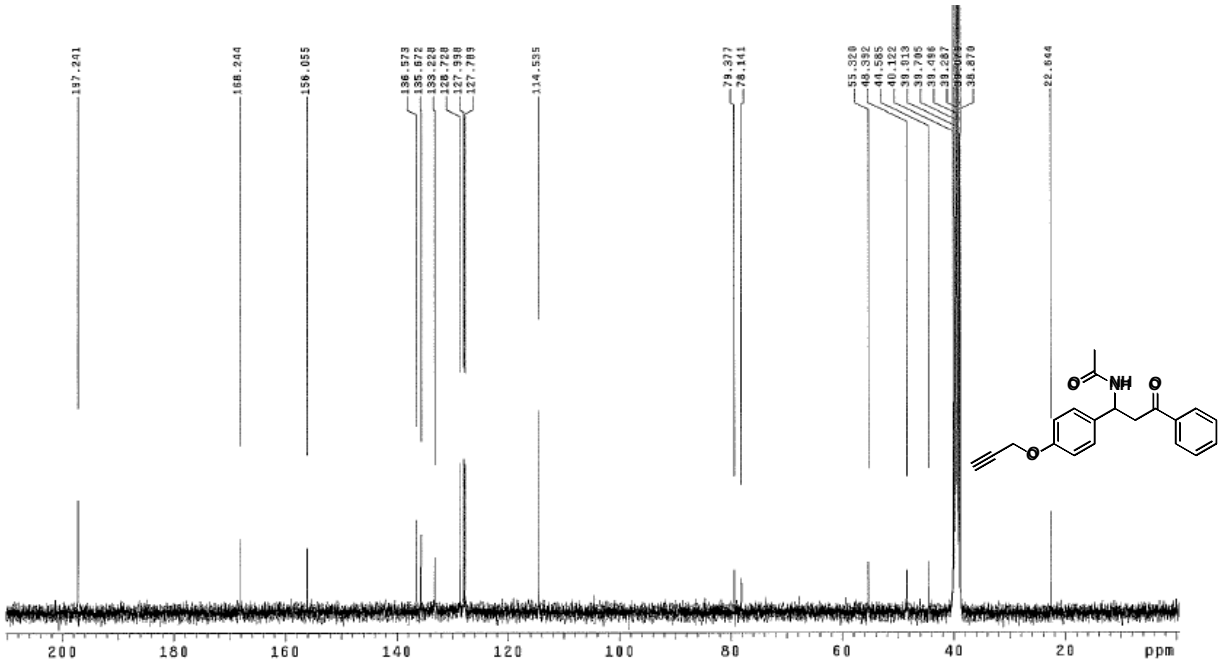
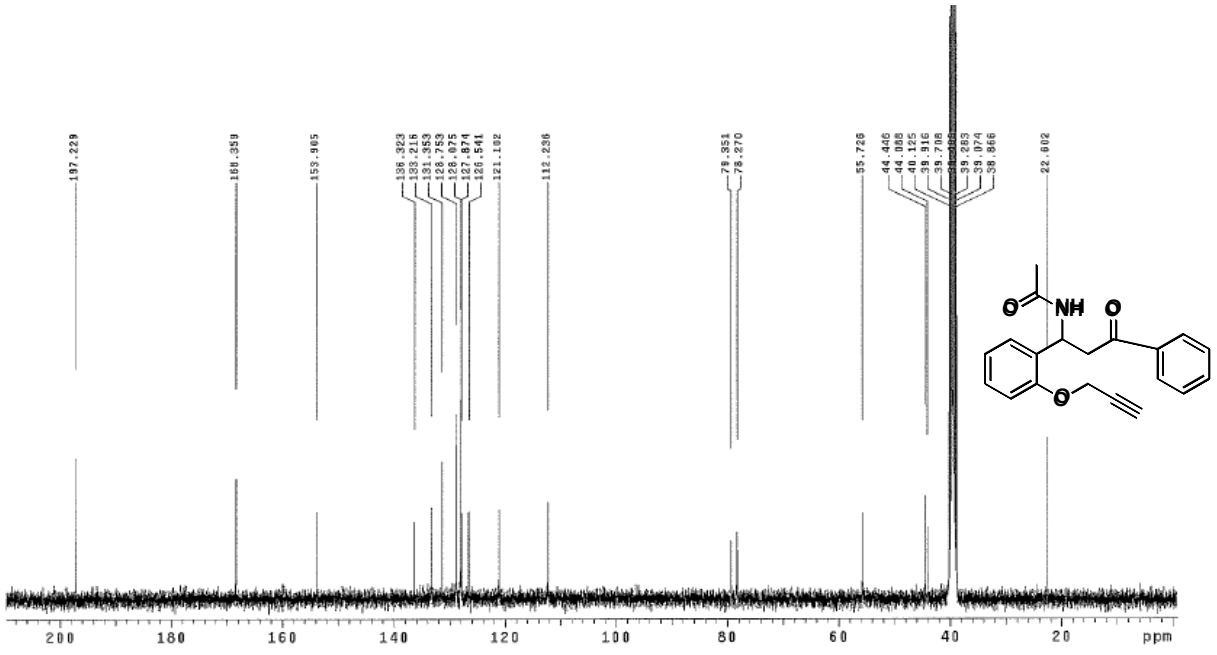
155.276
154.660
149.584
149.565
134.582
130.590
124.654
117.756
116.651
116.158
78.380
78.105
76.056
63.865
63.955
63.633
52.805
40.126
39.917
39.709
39.501
39.293
39.084
38.876
38.671
180
160
140
120
100
80
60
40
20
ppm
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
2000 repetitions
Total time 110 minutes
OBSERVE C13, 100.3863265
DECOUPLE H1, 399.7783879
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Solvent: dmso
Temp. 25.0 C / 298.1 K
Sample #26, Operator: walkup
File: PP120_02
VNMRS-400 "400MR"
SAMPLE: PP120
File: /home/walkup/vnmrsys/data/PP120_02.fid
/home/walkup/vnmrsys/data/auto_2010.09.01

5



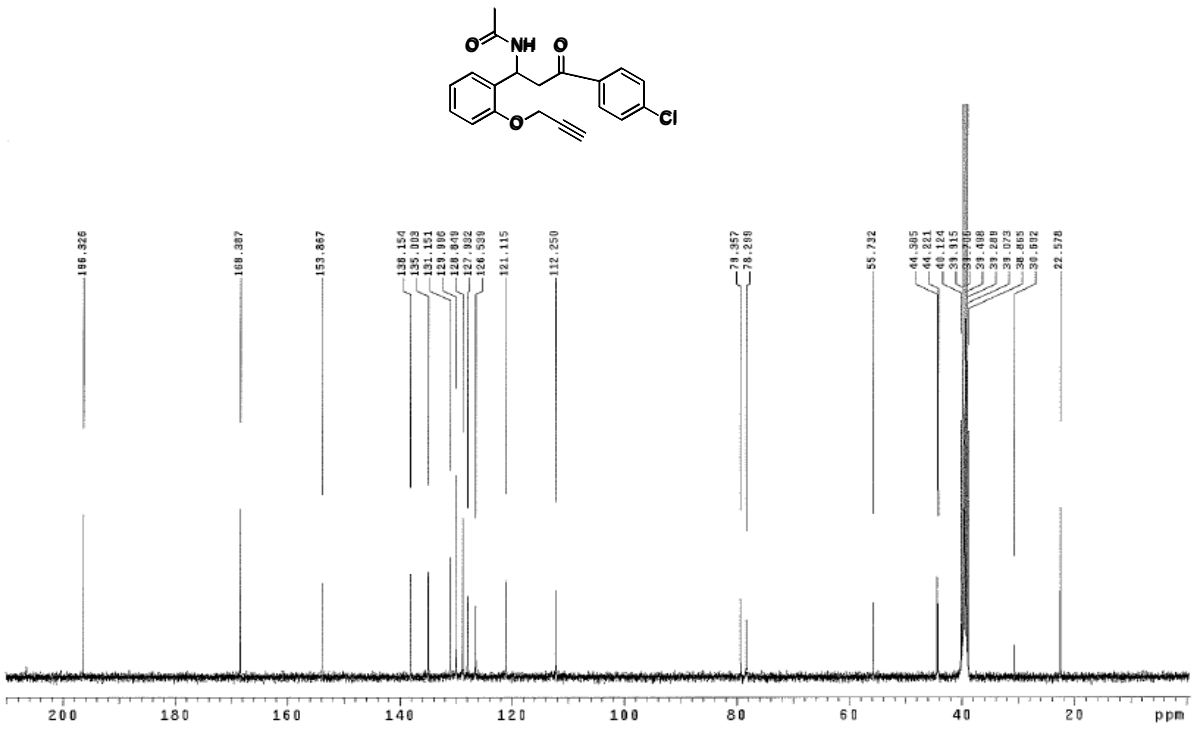
PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 24509.8 Hz 5000 repetitions Total time 3.2 hours	OBSERVE C13, 100.3963563 DECOUPLE H1, 399.2711702 Power 40 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536		Solvent: dmso Temp. 25.0 C / 298.1 K Sample #19, Operator: walkup File: AN-5_03 VNMRS-400 "400MR"	SAMPLE: AN-5
File: /home/walkup/vnmrsys/data/AN-5_03.fid dir: /home/walkup/vnmrsys/data/auto_2011.04.09_01					

6

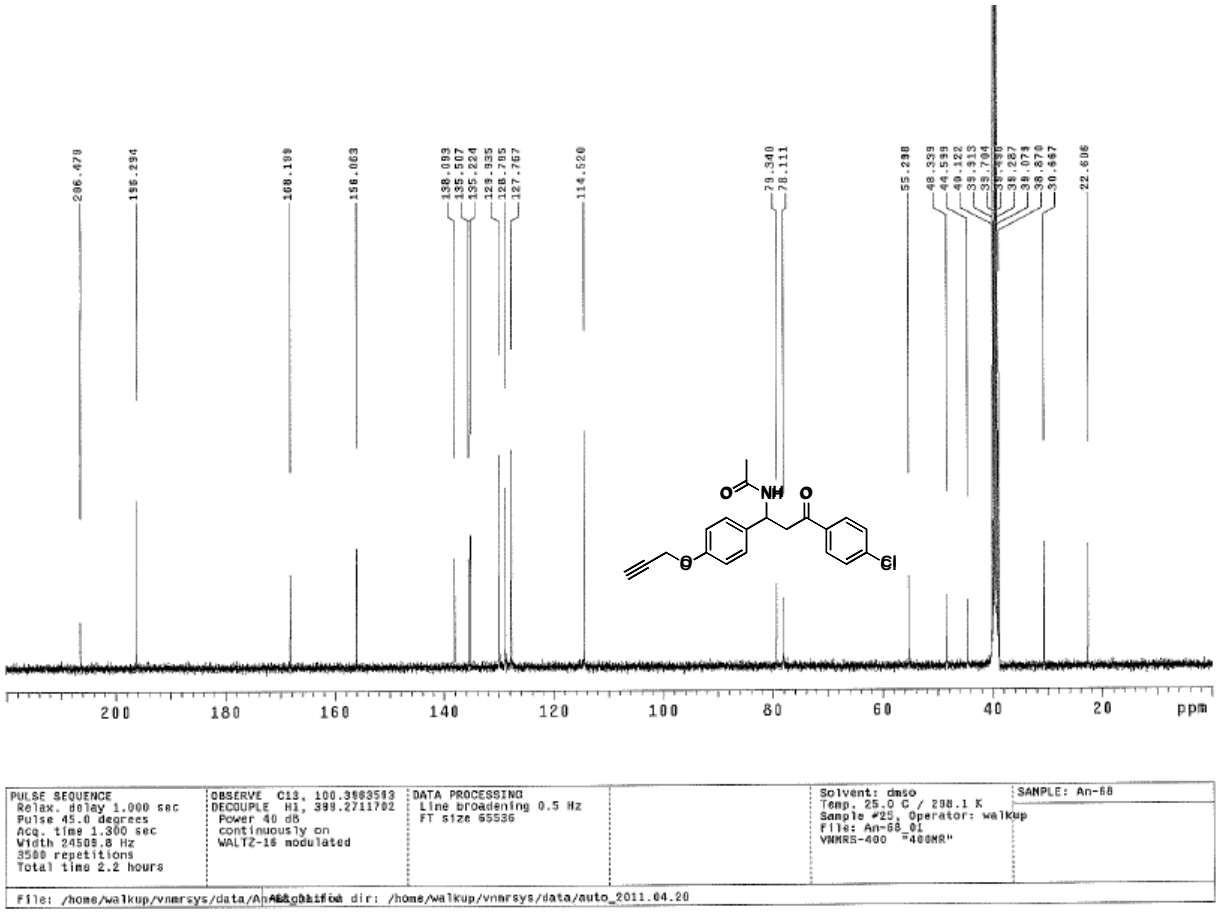


PULSE SEQUENCE Relax. delay 1.000 sec Pulse 45.0 degrees Acq. time 1.300 sec Width 24509.8 Hz 3000 repetitions Total time 115 minutes	OBSERVE C13, 100.3963560 DECOUPLE H1, 399.2711702 Power 40 dB continuously on WALTZ-16 modulated	DATA PROCESSING Line broadening 0.5 Hz FT size 65536		Solvent: dmso Temp. 25.0 C / 298.1 K Sample #36, Operator: walkup File: An-11_02 VNMRS-400 "400MR"	SAMPLE: An-11
File: /home/walkup/vnmrsys/data/AnAu1_02/fid dir: /home/walkup/vnmrsys/data/auto_2011.04.09_01					

7


NH
O
O
O
Cl
196.326
168.387
153.867
138.154
135.008
131.151
129.986
128.849
127.932
126.539
121.115
112.250
79.357
78.268
55.732
44.385
44.221
40.124
39.915
39.706
39.498
39.289
39.073
38.865
30.692
22.578
200
180
160
140
120
100
80
60
40
20
ppm
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
3000 repetitions
Total time 115 minutes
OBSERVE C13, 100.3963562
DECOUPLE H1, 399.2711702
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Solvent: dmso
Temp. 25.0 C / 298.1 K
Sample #37, Operator: walkup
File: An-12_02
VNMRS-400 "400MR"
SAMPLE: An-12
File: /home/walkup/vnmrsys/data/An-12_02.fid dir: /home/walkup/vnmrsys/data/auto_2011.04.08_01

8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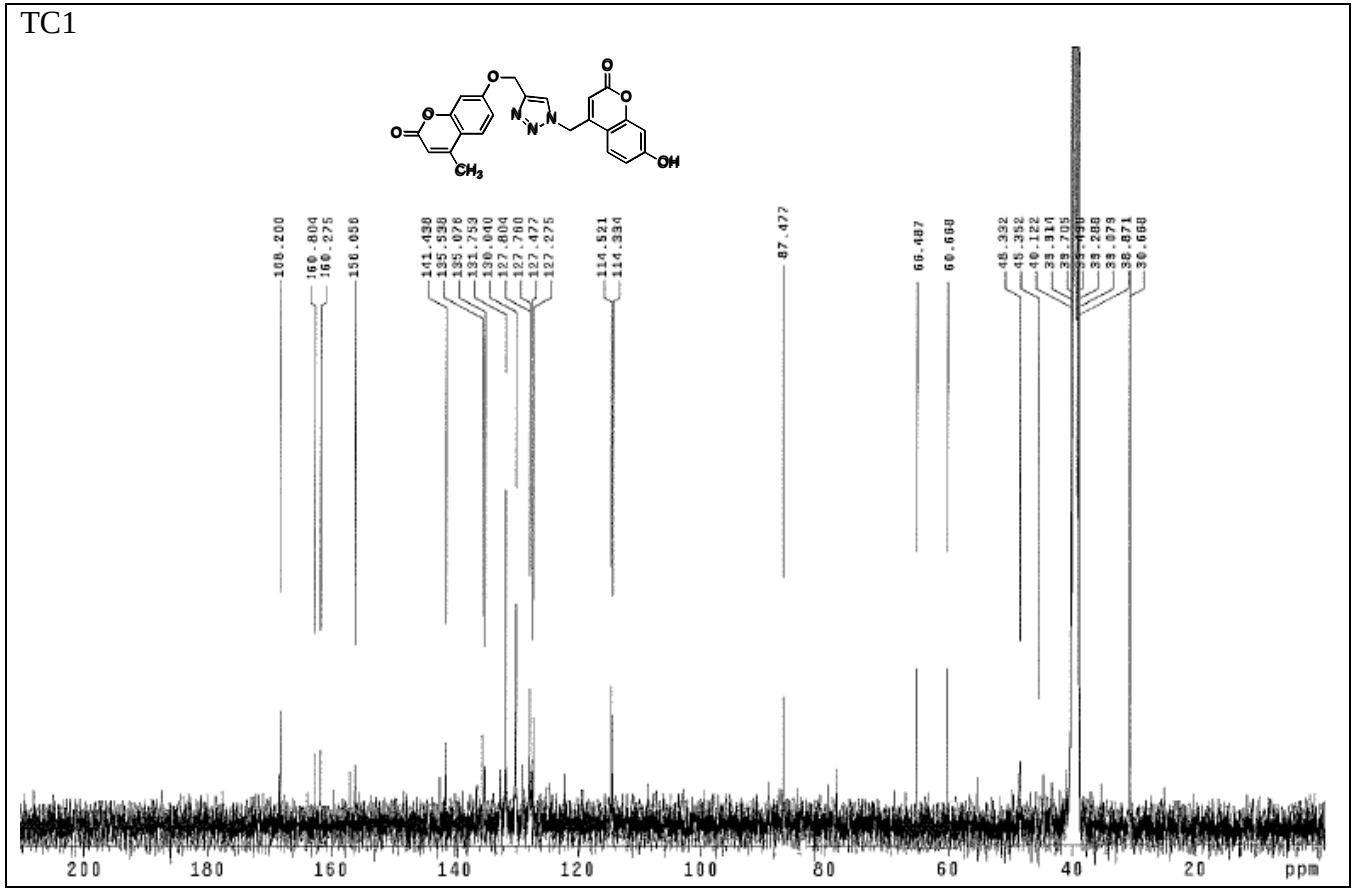
150.063
138.093
135.507
135.224
129.935
128.785
127.767
114.520
79.340
78.111
55.298
48.339
44.549
40.122
39.913
39.704
39.496
39.287
39.079
38.870
30.667
22.606
NH
O
O
O
Cl
200
180
160
140
120
100
80
60
40
20
ppm
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24508.8 Hz
3500 repetitions
Total time 2.2 hours
OBSERVE C13, 100.3603593
DECOUPLE H1, 399.2711702
Power 40 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Solvent: dmso
Temp. 25.0 C / 298.1 K
Sample #25, Operator: walkup
File: An-68_01
VNMRS-400 "400NR"
SAMPLE: An-68
File: /home/walkup/vnmrsys/data/An-68_01.fid
dir: /home/walkup/vnmrsys/data/auto_2011.04.20


TC1
O
O
O
O
N
N
N
O
CH3
OH
168.200
160.804
160.275
156.050
141.430
135.538
135.076
131.753
130.040
127.804
127.760
127.477
127.275
114.521
114.334
87.477
66.487
60.668
48.332
45.352
40.122
39.916
39.705
39.490
39.288
39.079
38.871
30.668
200
180
160
140
120
100
80
60
40
20
ppm

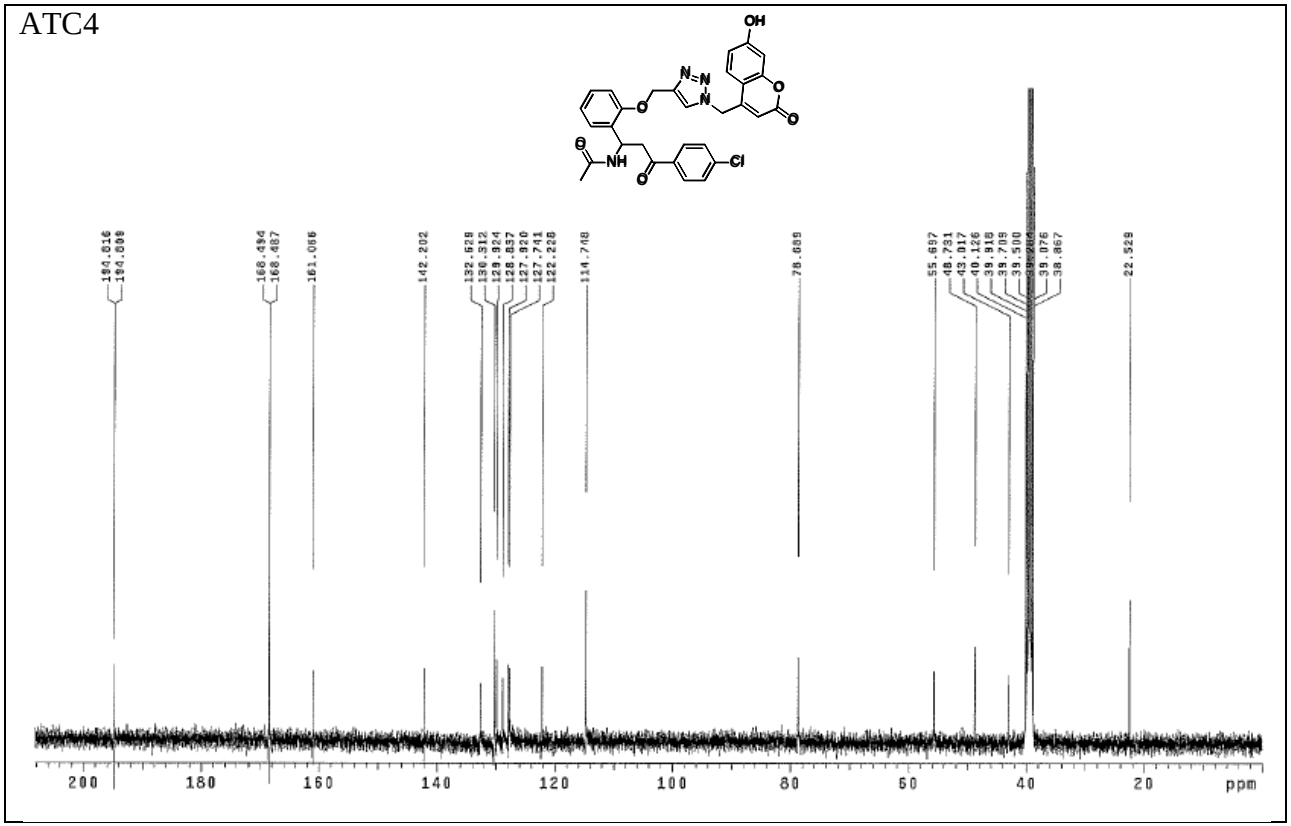

ATC4
OH
O
N
N
N
O
O
O
NH
O
Cl
194.016
194.098
168.494
168.487
161.056
142.292
132.528
130.312
129.924
128.837
127.920
127.741
122.228
114.748
78.685
55.697
48.731
43.017
40.126
39.718
39.705
39.500
39.076
38.867
22.529
200
180
160
140
120
100
80
60
40
20
ppm

Table S1 : Drug like properties of click products TC1-4 & ATC1-6

Compound	MW	natoms	TPSA	volume	miLogP	nON	nOHNH	nviolations	nrotb
TC1	431.40	32	120.60	360.17	3.27	9	1	0	5
TC2	417.38	31	120.60	343.61	2.84	9	1	0	5
TC3	417.38	31	120.60	343.61	2.89	9	1	0	5
TC4	445.39	33	137.67	362.59	2.62	10	1	0	6
ATC1	538.56	40	136.56	471.03	2.46	10	2	1	10
ATC2	617.46	41	136.56	488.92	3.27	10	2	1	10
ATC3	538.56	40	136.56	471.03	2.41	10	2	1	10
ATC4	573.00	41	136.56	484.57	3.09	10	2	1	10
ATC5	573.00	41	136.56	484.57	3.14	10	2	1	10
ATC6	597.58	44	182.38	511.17	1.99	13	2	2	12

Cytotoxicity evaluation results of TC1 against Human Breast Cancer Cell line MCF-7

The MCF-7 cells were maintained in RPMI medium 1640 supplemented with 10% fetal bovine serum as well as 100 µg/mL streptomycin, 100 U/mL penicillin, 2 mM L-glutamine and Earle's BSS adjusted to contain 1.5 g/L Na bicarbonate, 0.1 mM nonessential amino acids, and 1.0 mM of Na pyruvate in a humidified atmosphere containing 5% CO_2 at 37 °C. The MCF-7cells in the log phase were seeded in 96-well plates at a concentration of 1.0 x 104cells/well and incubated overnight at 37 °C in 5%CO_2 humidified environment. The cells were then treated with different concentrations of the **TC1** such as 10, 20, 30, 40, 50,60, 70, 80, 90, and 100 µM/mL (dissolved with RPMI medium1640), respectively. Controls were also cultivated under same conditions without the addition of **TC1**. The treated cells were incubated for 48 h and then subjected for MTT assay.

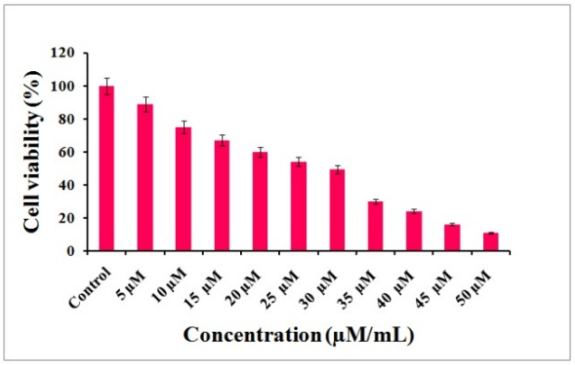
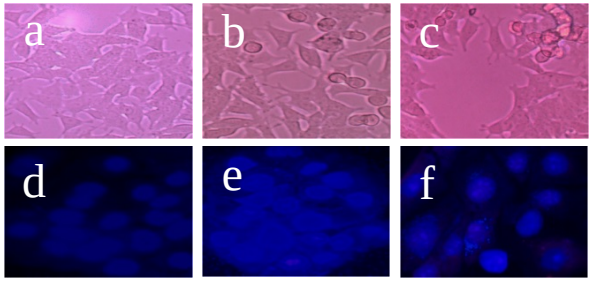


Figure S1.MTT assay results confirming the in vitro cytotoxicity effect of **TC1** against the MCF-7 cells. The detected IC50 concentration was 30 µM/mL.

The stock concentration (5 mg/mL) of MTT-(3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) was prepared and 100 µL of MTT was added in each **TC1** treated wells and incubated for 4h. Purple colourformazan crystals were observed and these crystals were dissolved in 100 µL of dimethyl sulphoxide (DMSO), and read at 620 nm in a multiwell ELISA plate reader (Thermo, Multiskan). The dose dependent cytotoxicity was observed in **TC1** treated MCF-7cells. [30] Fifty percentage of cell death, which determines the inhibitory concentration (IC50) value of **TC1** against MCF-7 cells holds at 30 µM in 48 h (figure S1).

In order to study the morphological changes, MCF-7 cells were grown (1 x 105 cells/cover slip) and incubated with **TC1** at its IC50concentration (30 µM/mL) and then they were fixed in a mixture of methanol and acetic acid (3:1, v/v). The cover slips were gently mounted on glass slides for the morphometric analysis. Morphological changes of MCF-7 cells were analyzed under a Nikon (Japan) bright field inverted light microscope at 40x magnification. The most recognizable morphological changes of **TC1** treated cells observed in this study were the cytoplasmic condensation, cell shrinkage, production of numerous cell surface protuberances at the plasma membrane blebbing and hyper condensed chromatin as shown in treated MCF-7 cells.



FigureS2.Bright field inverted light microscopy images (a) (Control), (b) (IC25) and (c) (IC50) and fluorescence microscopy images (d) (Control), (e) (IC25) and (f) (IC50) of **TC1** treated MCF-7 cells.

Followed by this, DAPI (4,6-diamidino-2-phenylindole, dihydrochloride) staining was carried out. For this, the MCF-7 cells incubated with **TC1** at its IC50 concentration (30 µM/mL) for 48 h and then they were fixed in a mixture of methanol and acetic acid (3:1, v/v) prior to washing with PBS. The washed cells were then stained with 1 mg/mL DAPI (4,6-diamidino-2-phenylindole, dihydrochloride) for 20 min. in a dark atmosphere. The stained images were recorded using a fluorescent microscope with appropriate excitation filter. The bright field and fluorescence microscopic images are shown in Figure S2. As shown in figure S2 , the strong bluish fluorescence and cellular uptake observed in the imaging studies with **TC1** reveals that these molecules have high potency against breast cancer cell lines (MCF-7).