Supplementary Materials for

Novel thiazoline-coumarin hybrid compounds containing sugar moieties: Synthesis, biological evaluation and molecular docking study as antiproliferative agents

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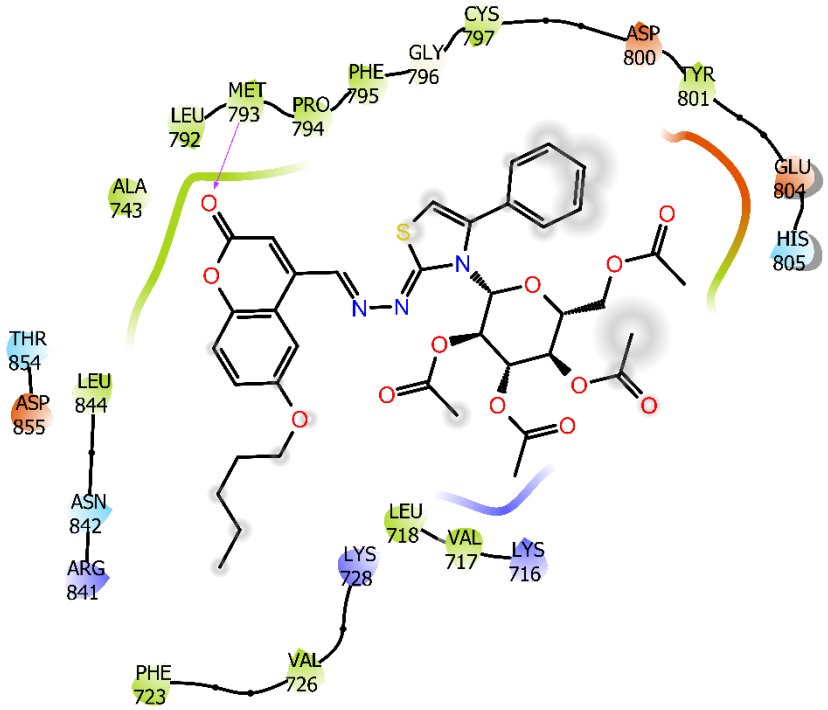
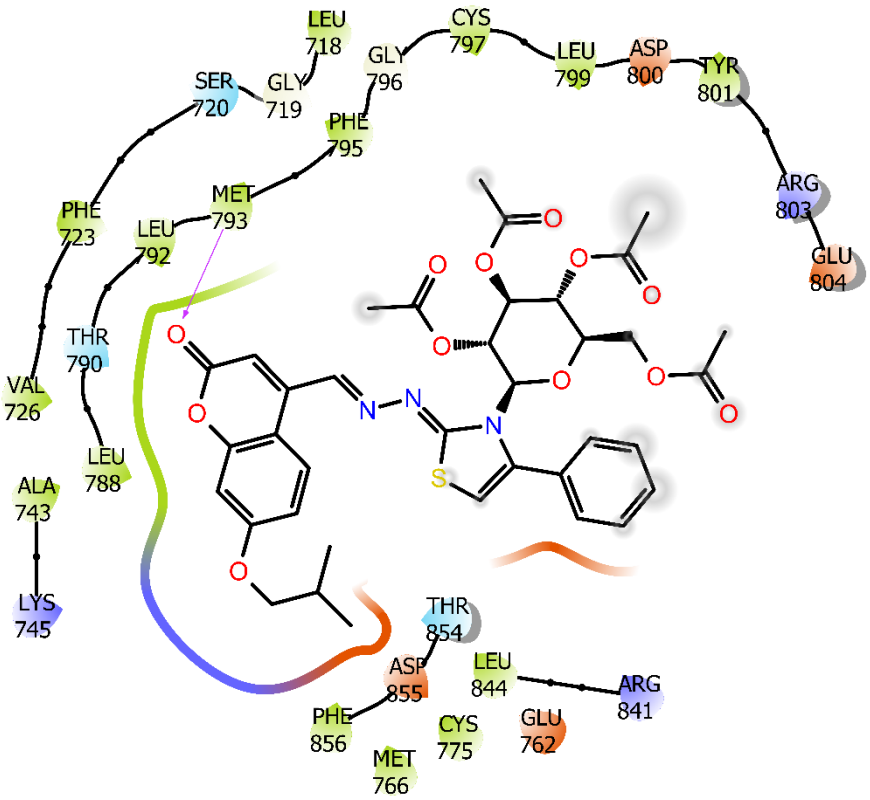
1.1. 2D interactions with EGFR (enzyme 5UGB) of selected compounds 4d,4e, and 4f (A−C) and of Sorafenib (D)

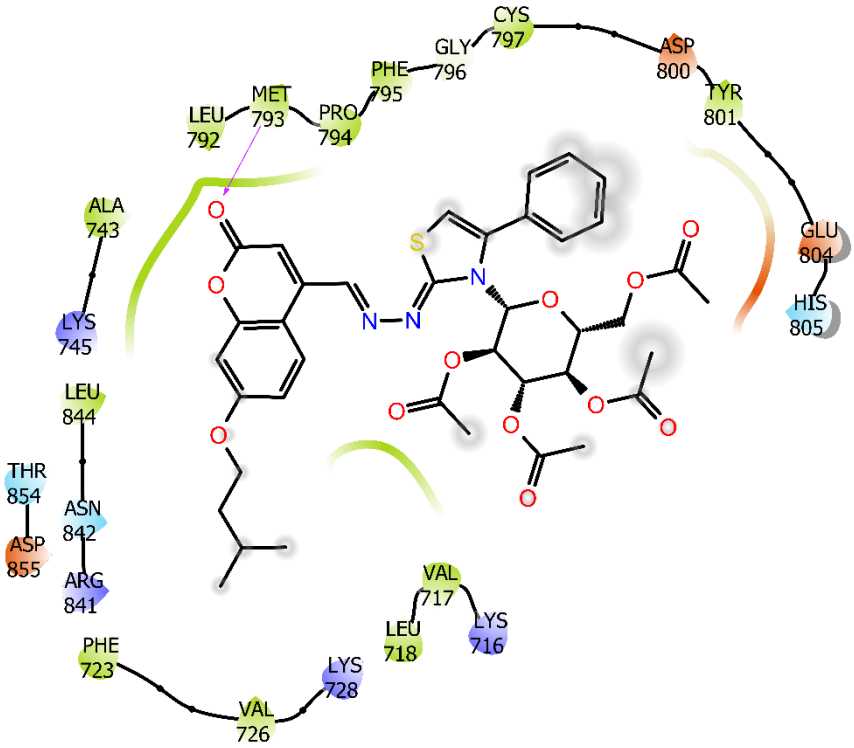
(A) Compound **4d** (R = 6-OC_5H_{11})



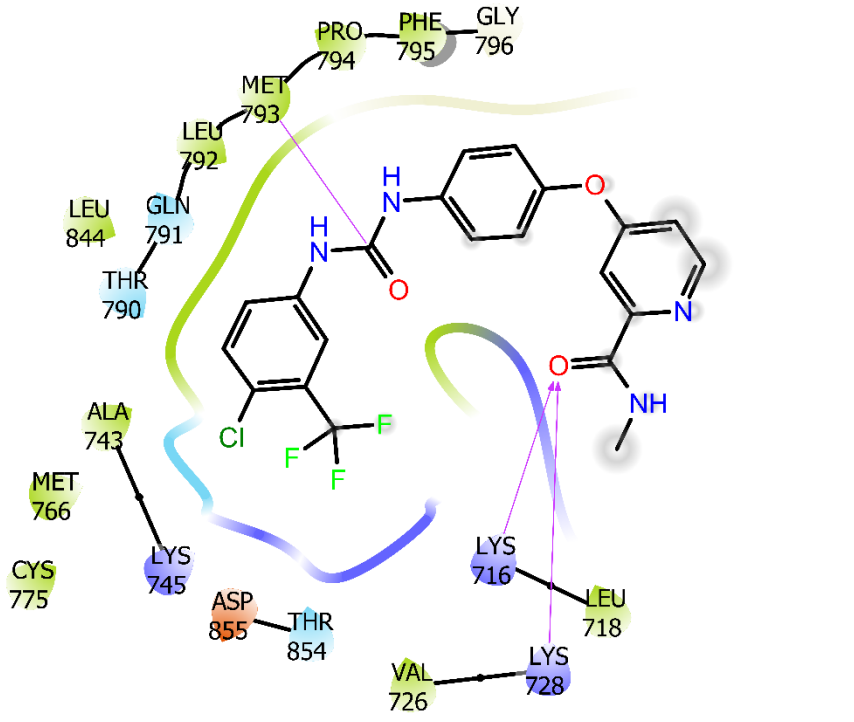
(B) Compound **4e** (R = 7-O^iC_4H_9)



(C) Compound **4f** (R = 7-O^{i}C$_5$H$_{11}$)

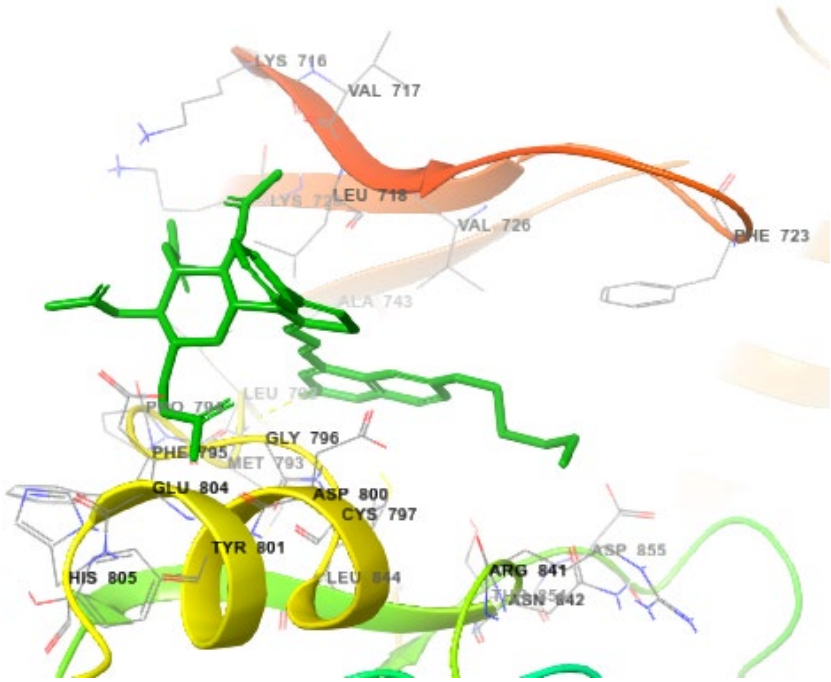


(D) Sorafenib

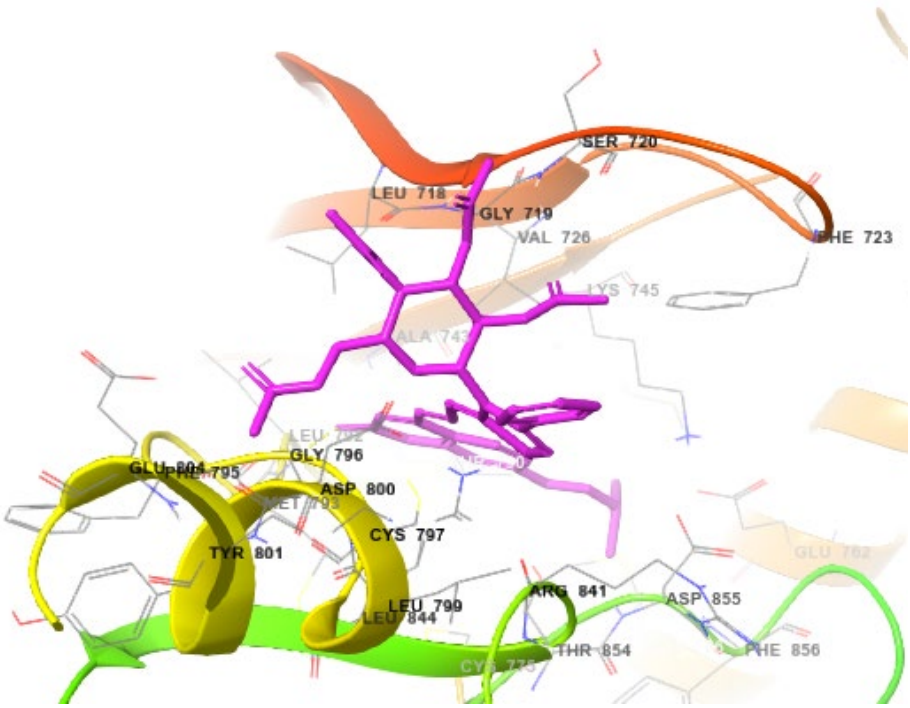


1.2. 3D interactions with EGFR of selected compounds 4d,4e, and 4f (A−C) and of Sorafenib (D)

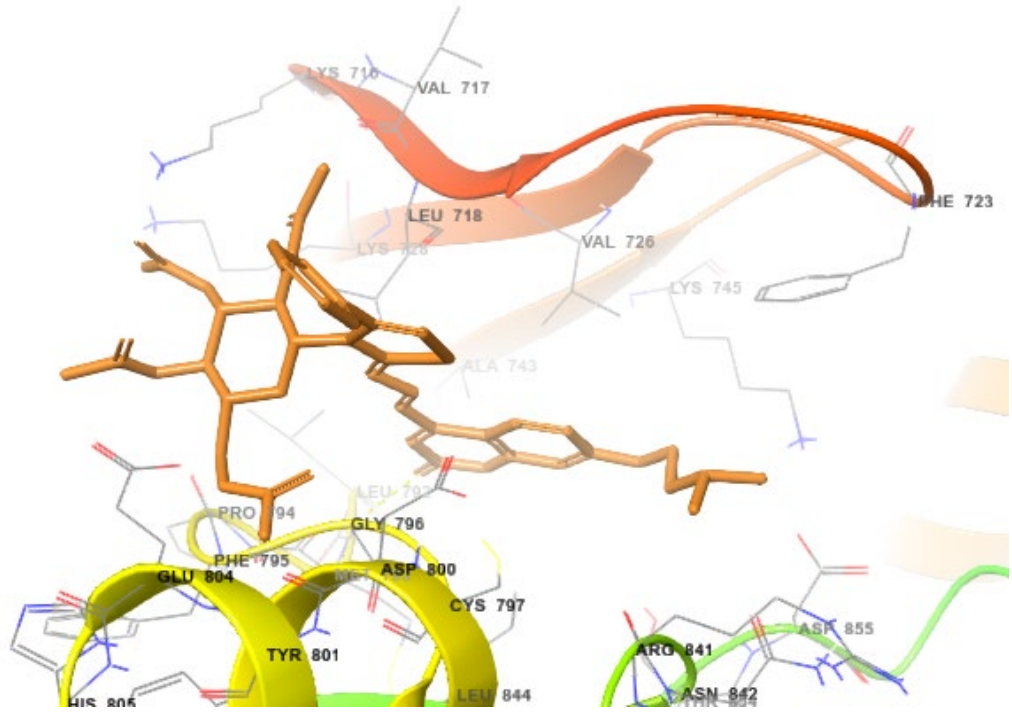
(A) Compound **4d** (R = 6-OC_5H_{11})



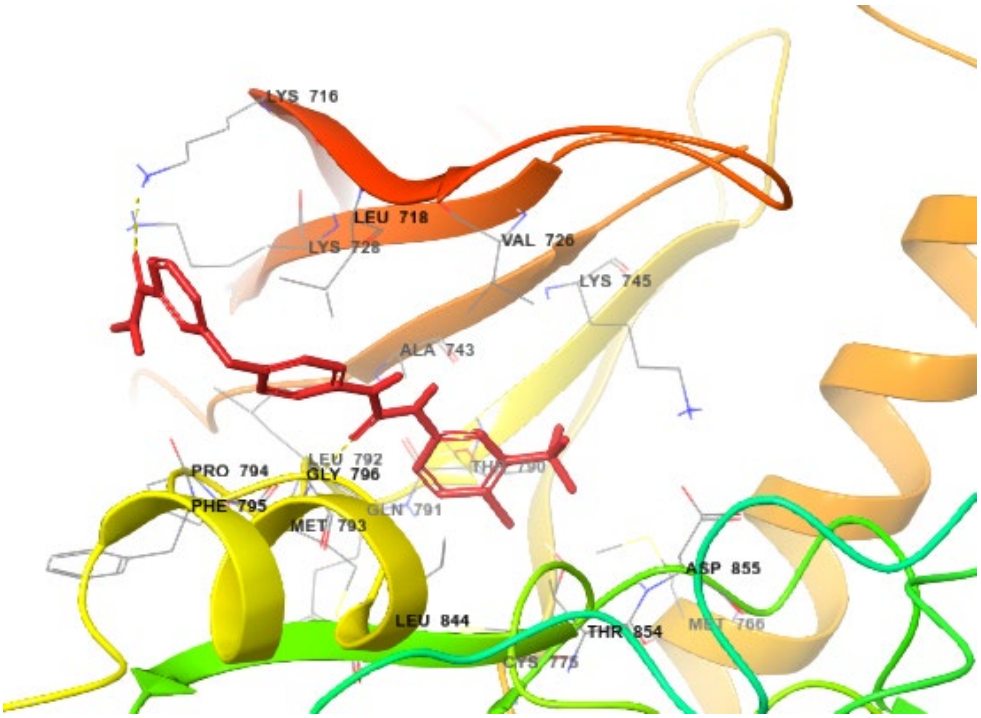
(B) Compound **4e** (R = 7-$O^iC_4H_9$)



(C) Compound **4f** (R = 7-O^{i}C$_5$H$_{11}$)

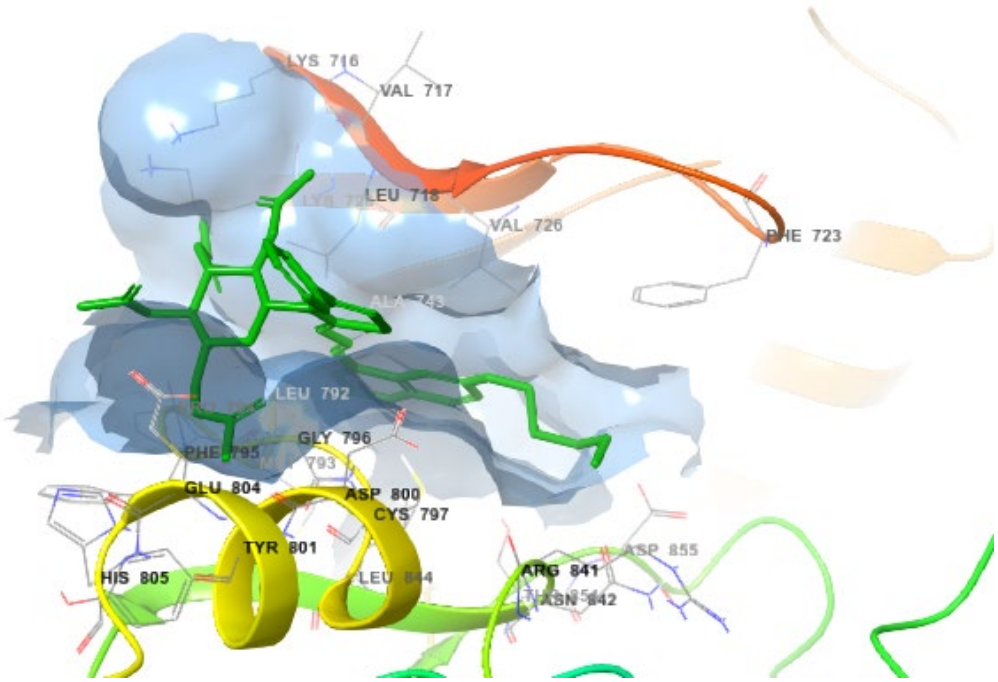


(D) Sorafenib

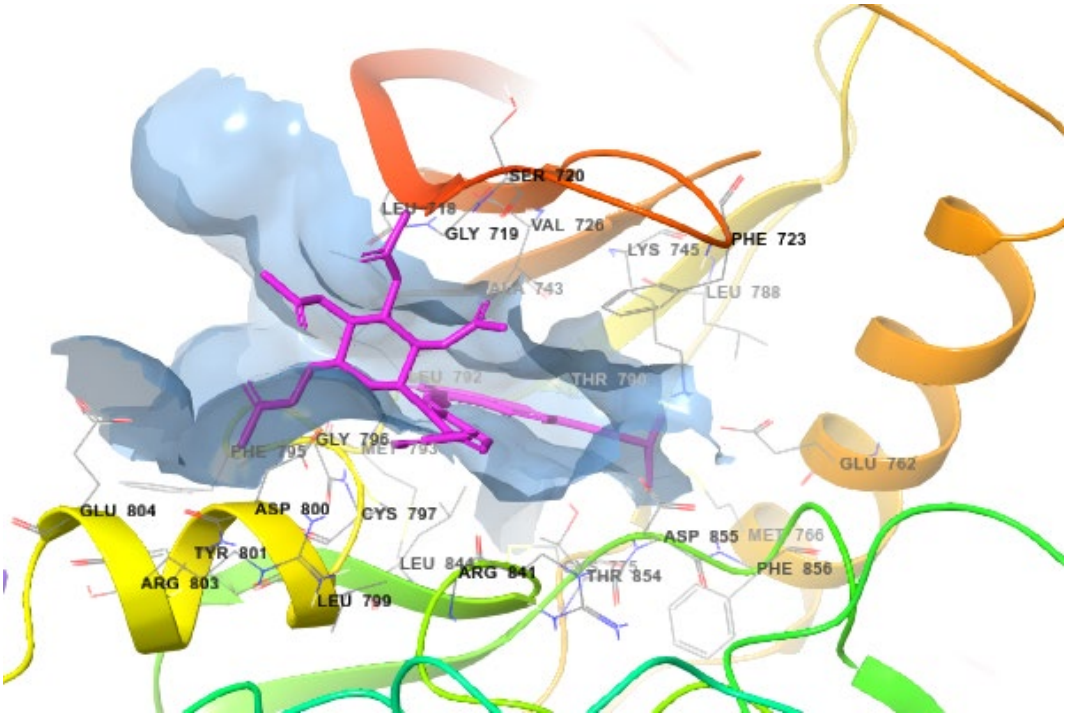


1.3. Alignments in binding pocket of EGFR (enzyme 5UGB) of selected compounds 4d,4e, and 4f (A−C) and of Sorafenib (D)

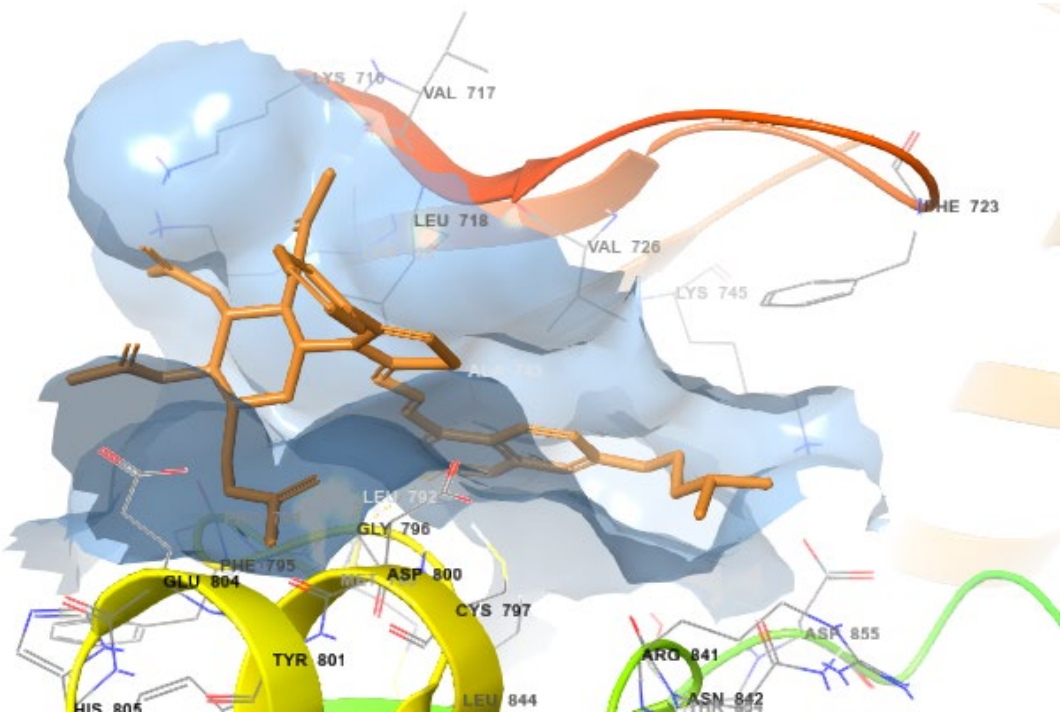
(A) Compound **4d** (R = 6-OC_5H_{11})



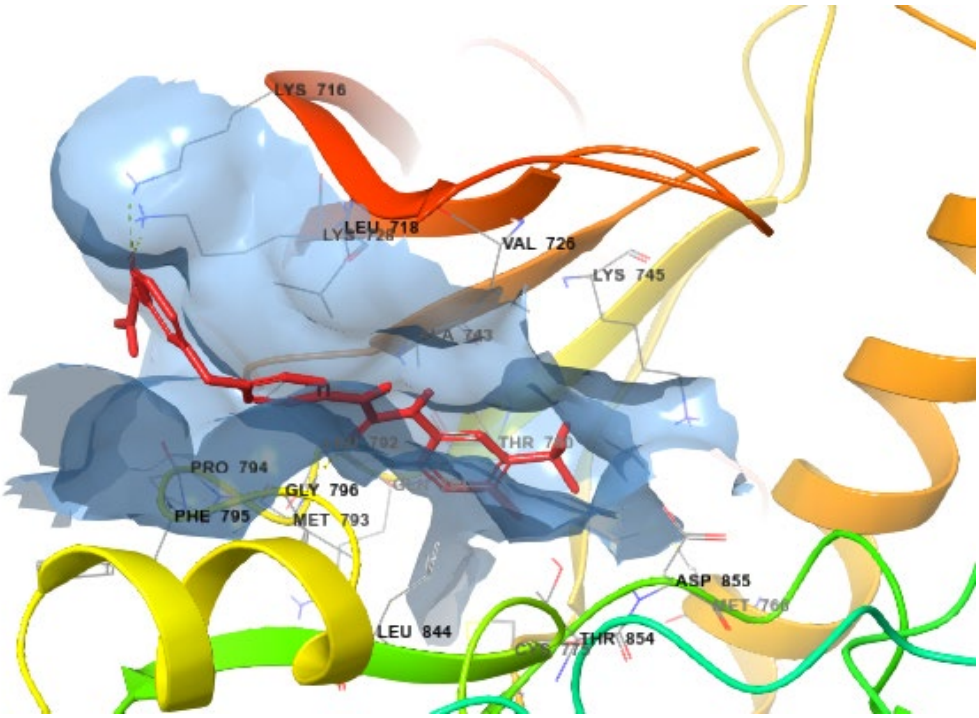
(B) Compound **4e** (R = 7-$O^iC_4H_9$)



(C) Compound **4f** (R = 7-O^{i}C$_5$H$_{11}$)

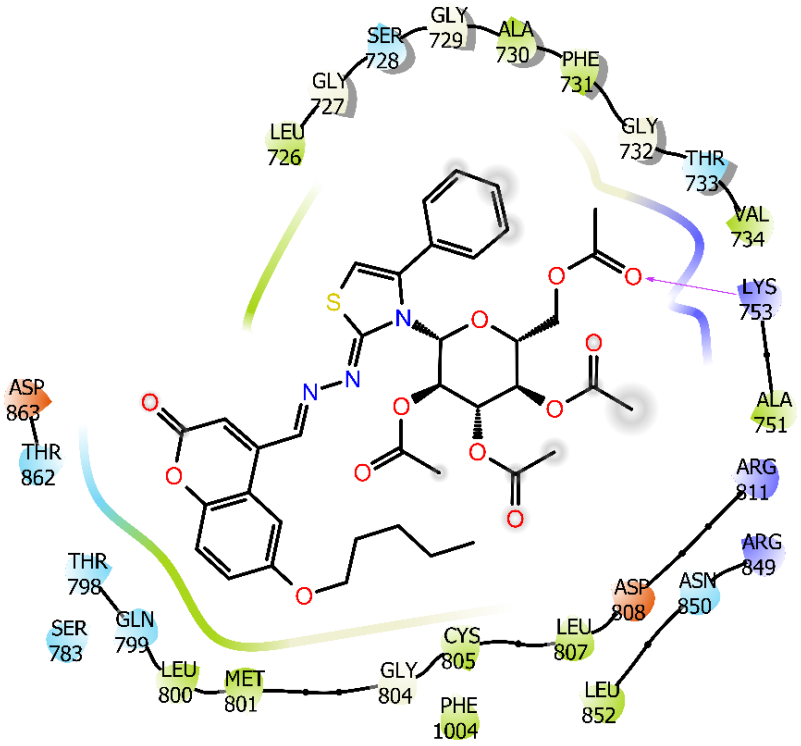


(D) Sorafenib

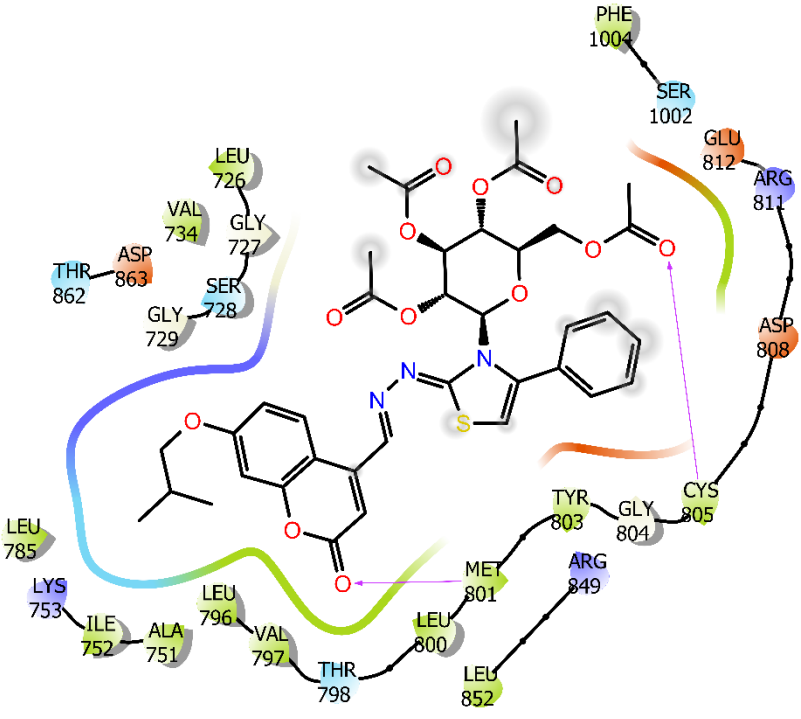


1.4. 2D interactions with HER2 (enzyme 3CRD) of selected compounds 4d,4e, and 4f (A−C) and of Sorafenib (D)

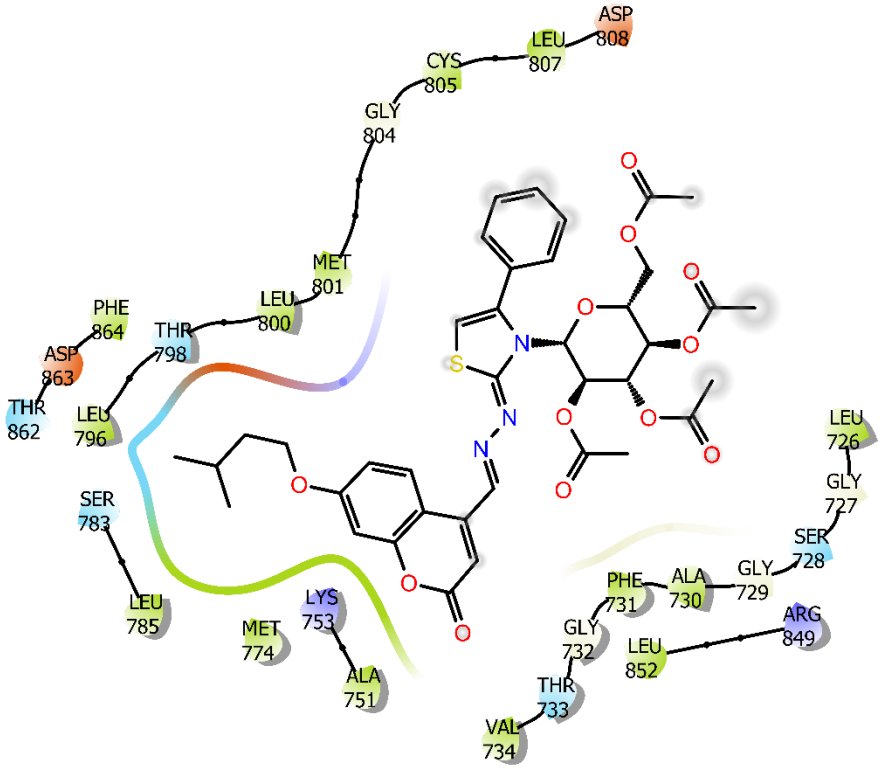
(A) Compound **4d** (R = 6-OC_5H_{11})



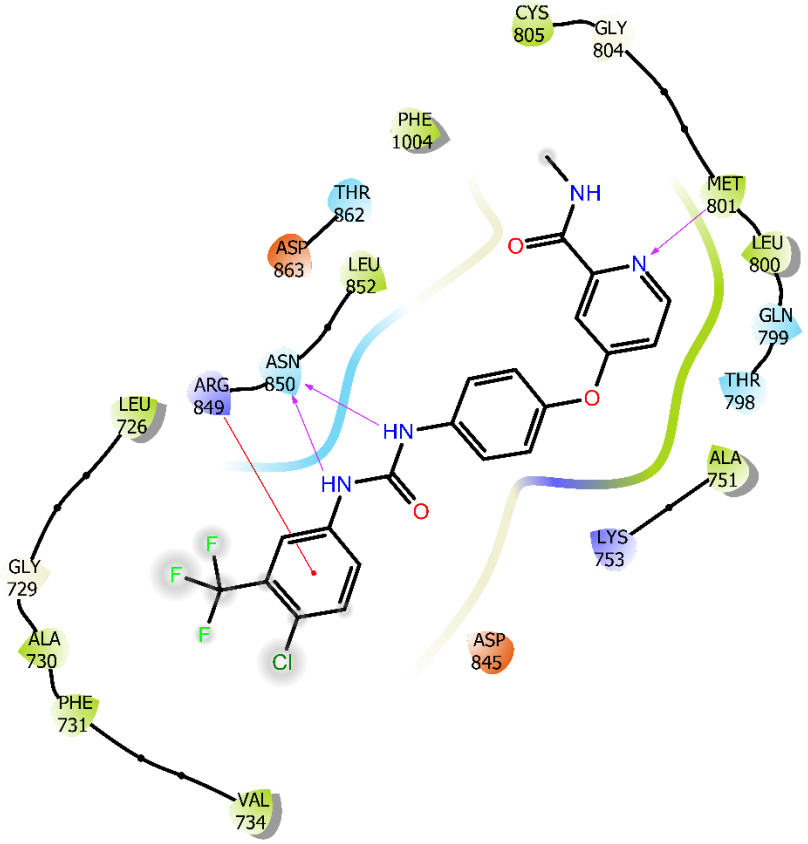
(B) Compound **4e** (R = 7-O^iC_4H_9)



(C) Compound **4f** (R = 7-O^{i}C$_5$H$_{11}$)



(D) Sorafenib



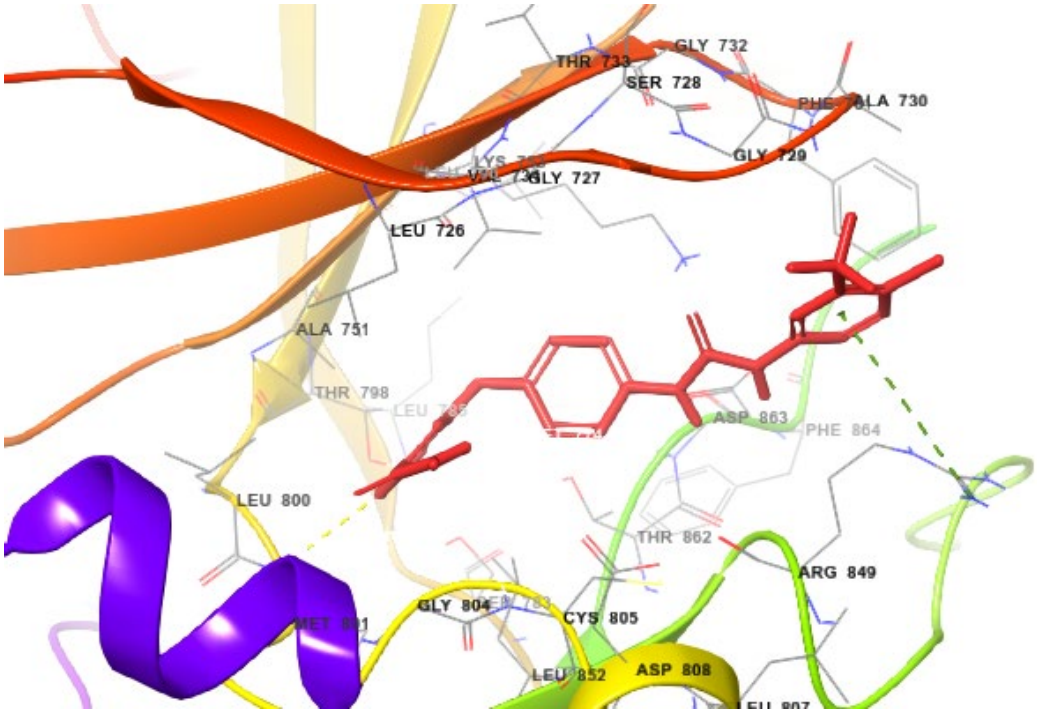
1.5. 3D interactions with HER2 of selected compounds 4d,4e, and 4f (A−C) and of Sorafenib (D)

(A) Compound **4d** (R = 6-OC_5H_{11})

(B) Compound **4e** (R = 7-$O^iC_4H_9$)

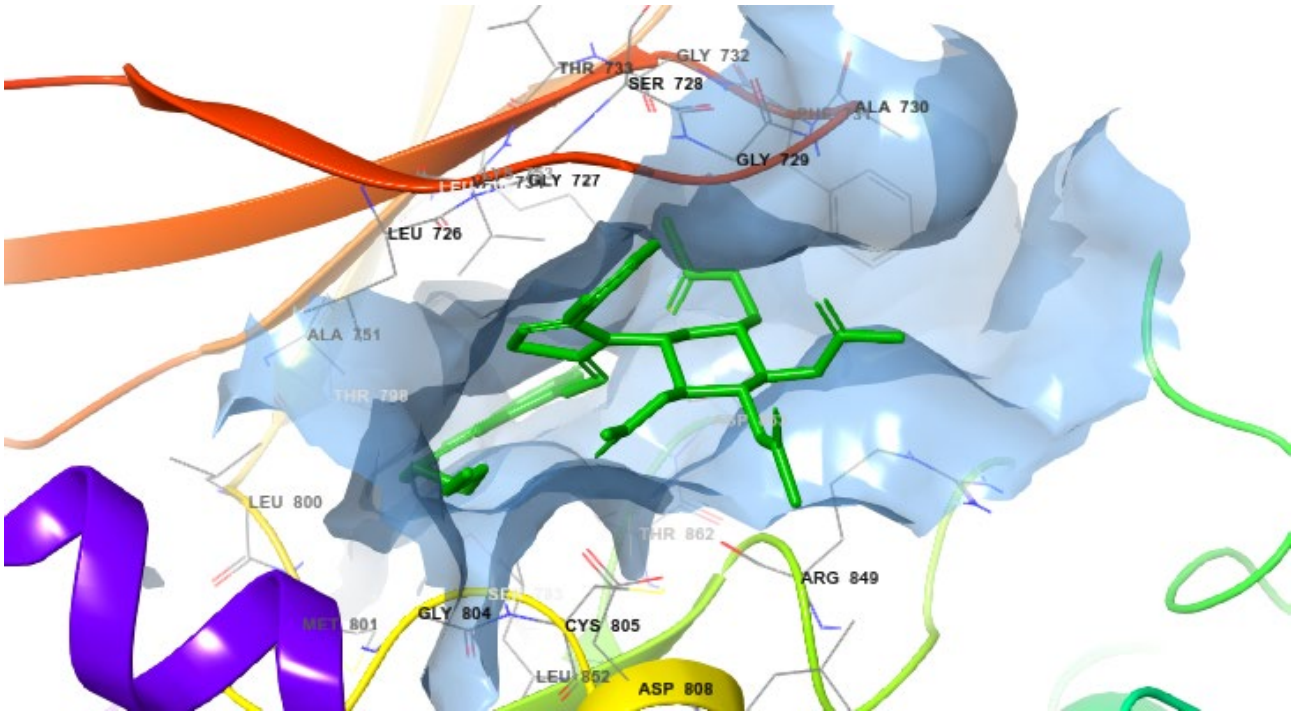
(C) Compound **4f** (R = 7-O^{i}C$_5$H$_{11}$)

(D) Sorafenib

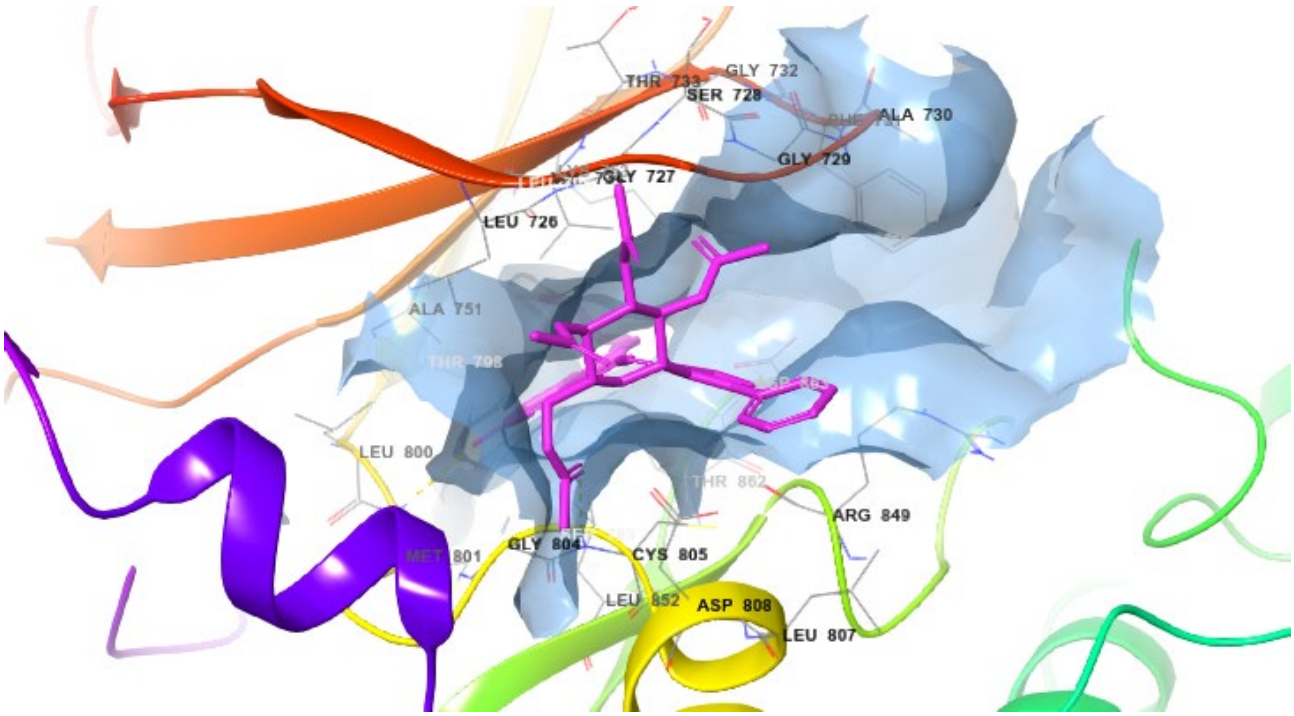


1.6. Alignments in binding pocket HER2 (enzyme 3CRD) of selected compounds 4d,4e, and 4f (A−C) and of Sorafenib (D)

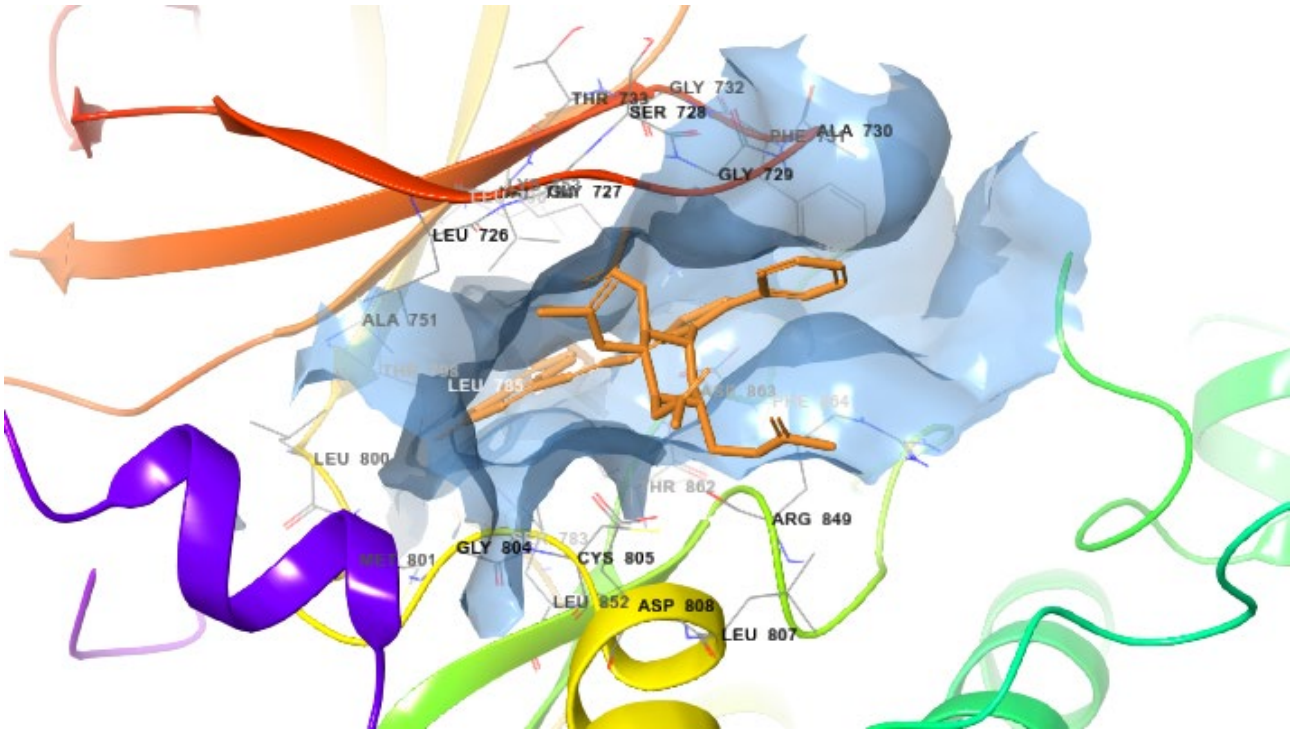
(A) Compound **4d** (R = 6-OC_5H_{11})



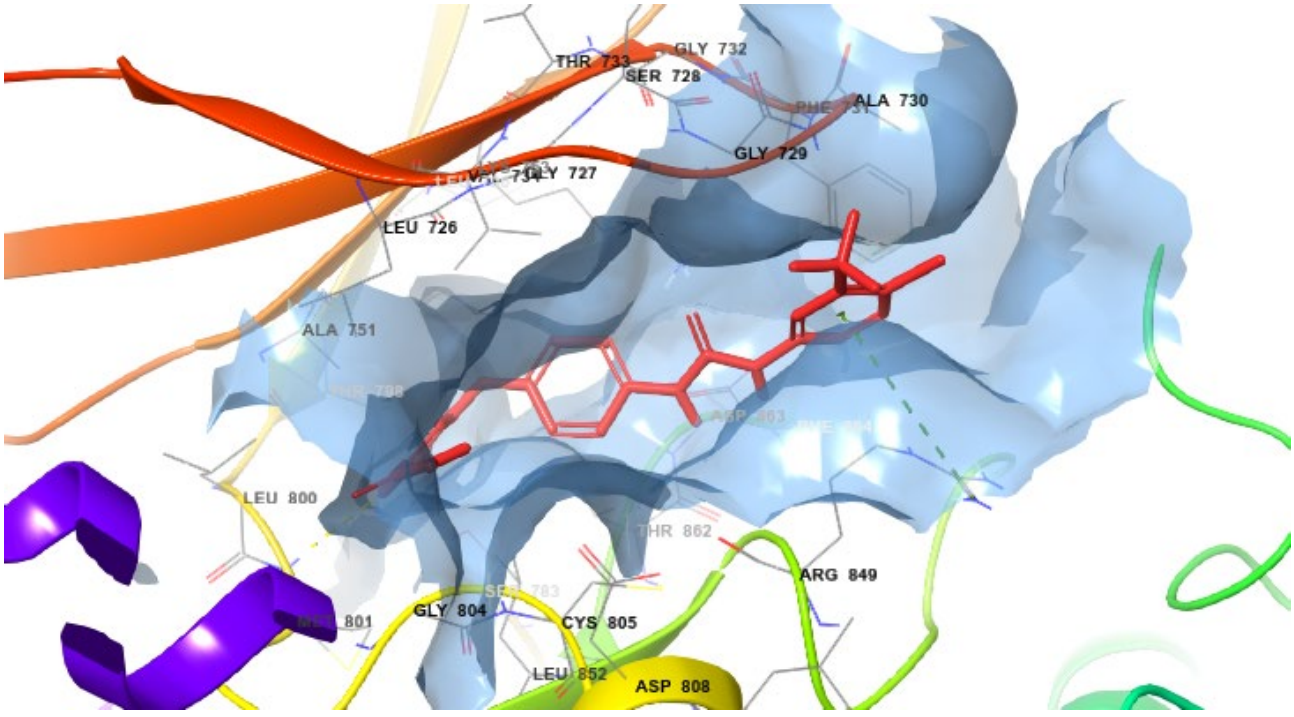
(B) Compound **4e** (R = 7-$O^iC_4H_9$)



(C) Compound **4f** (R = 7-O^{i}C$_5$H$_{11}$)

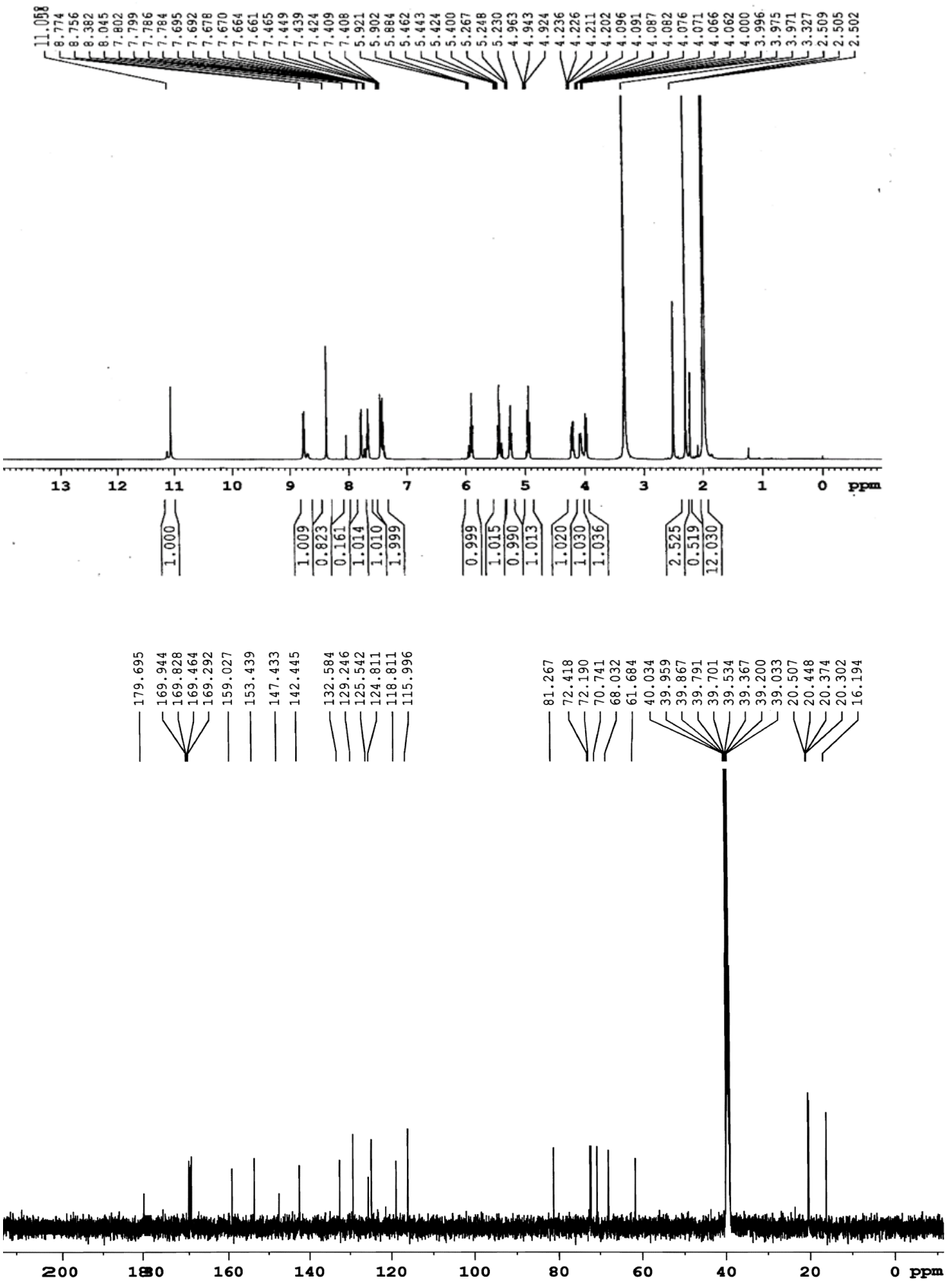


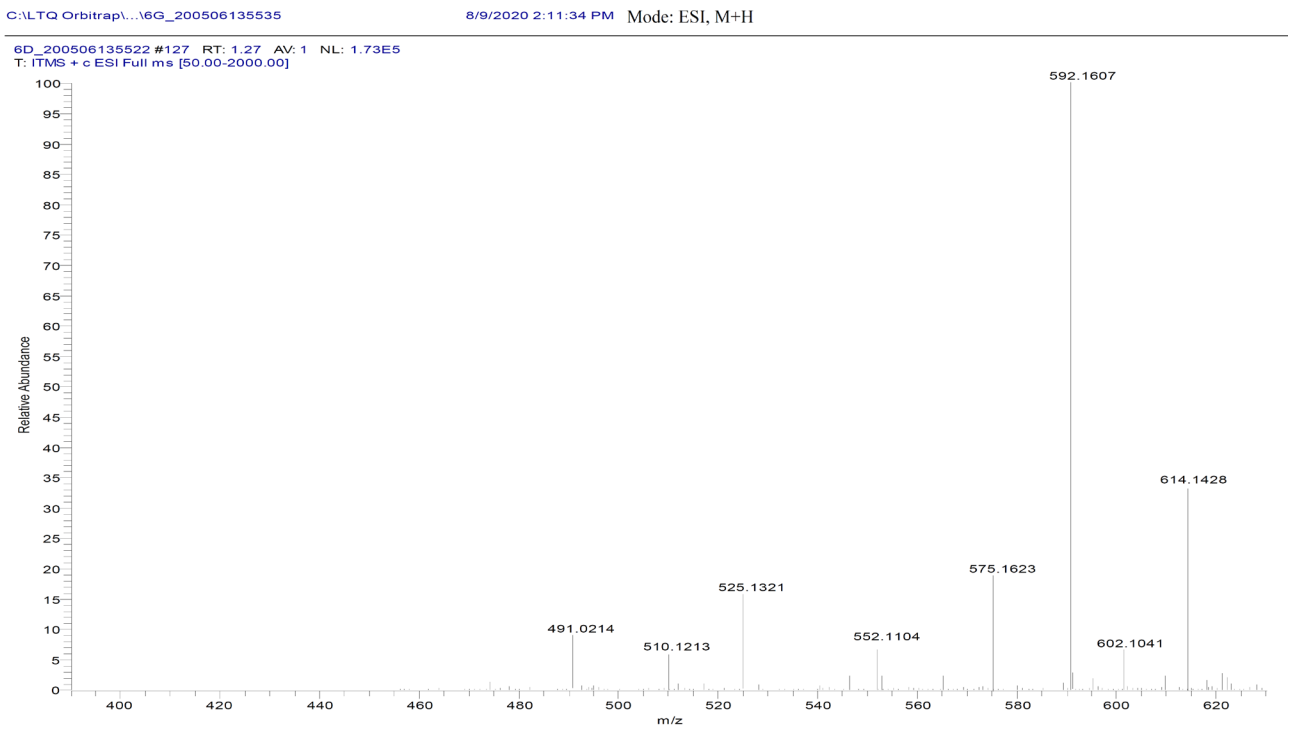
(D) Sorafenib



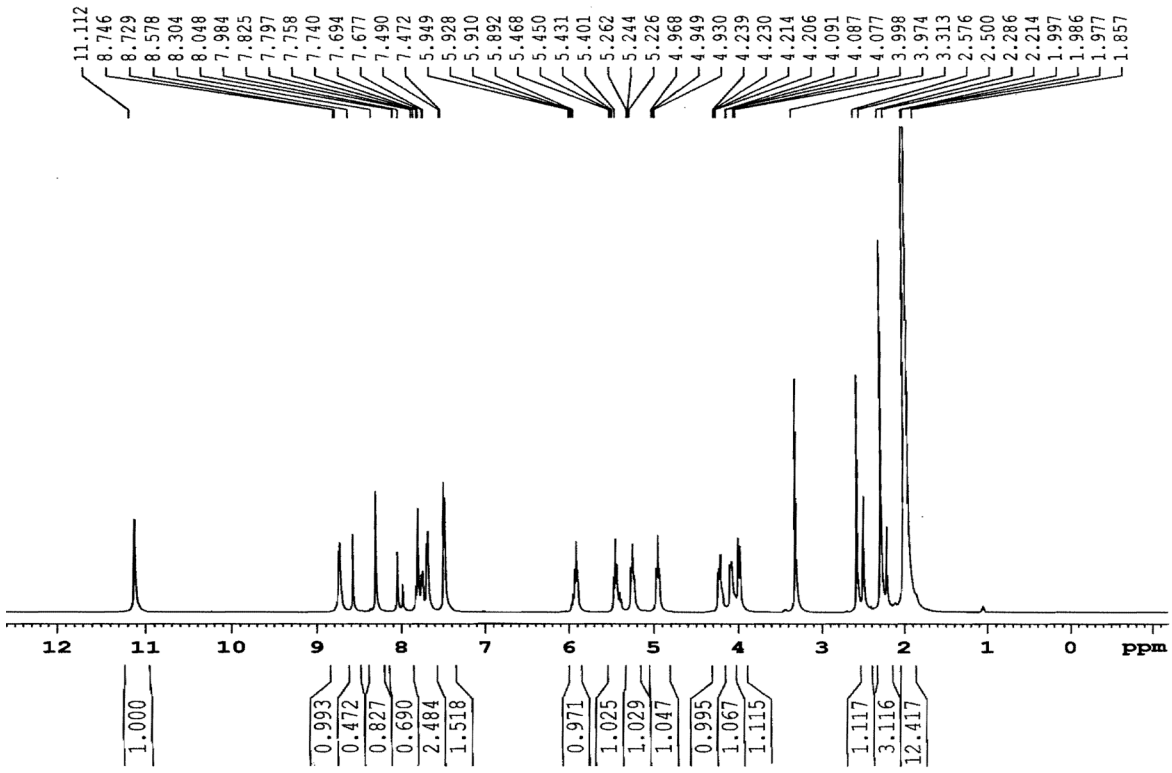
2. Selected spectra of substituted 3′-acetylcoumarin *N*-(2,3,4,6-tetra-*O*-acetyl-β-D-glycopyranosyl)thiosemicarbazones (3a-g)

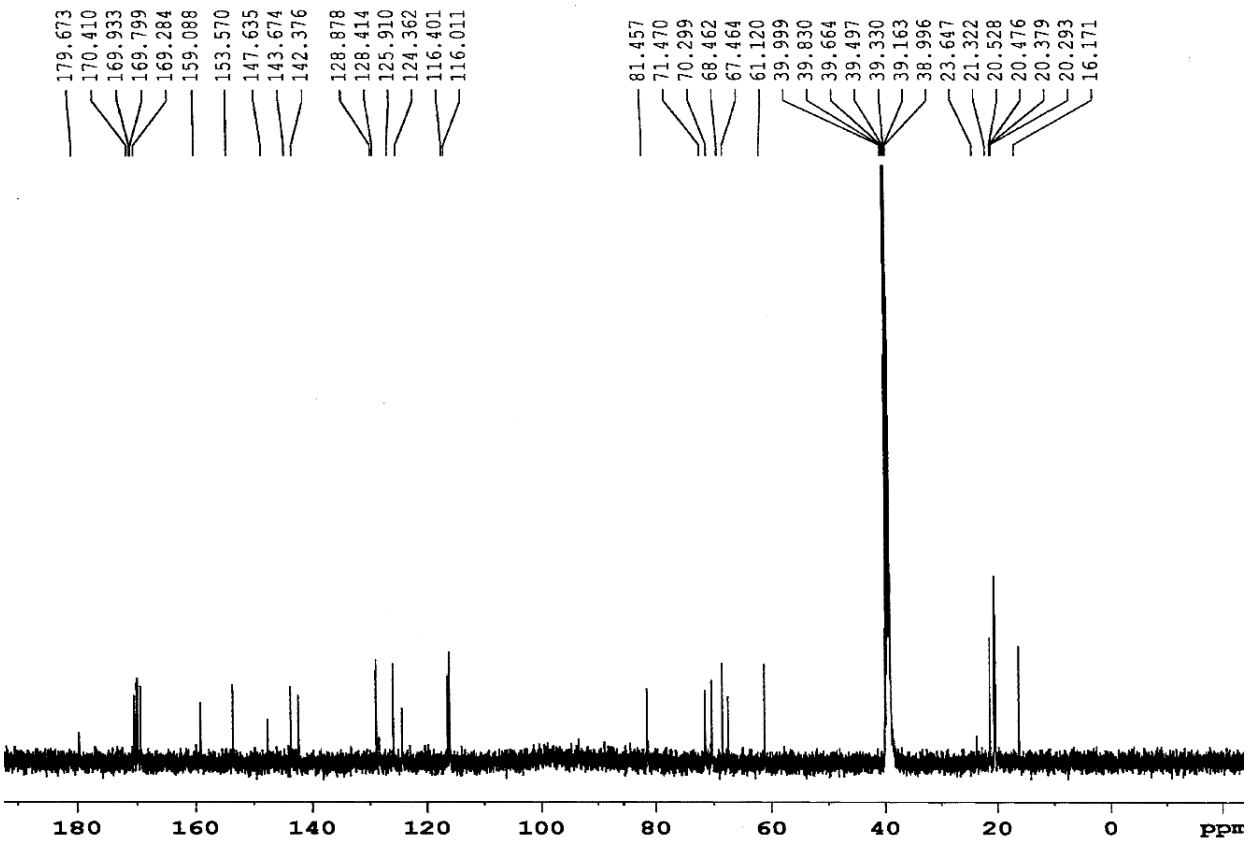
*3'-Acetylcoumarin N-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)thiosemicarbazone (**3a**)*





*3'-Acetyl-6'-chlorocoumarin N-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)thiosemicarbazone (**3b**)*

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170.410
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169.799
169.284
159.088
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142.376
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125.910
124.362
116.401
116.011
81.457
71.470
70.299
68.462
67.464
61.120
39.999
39.830
39.664
39.497
39.330
39.163
38.996
23.647
21.322
20.528
20.476
20.379
20.293
16.171
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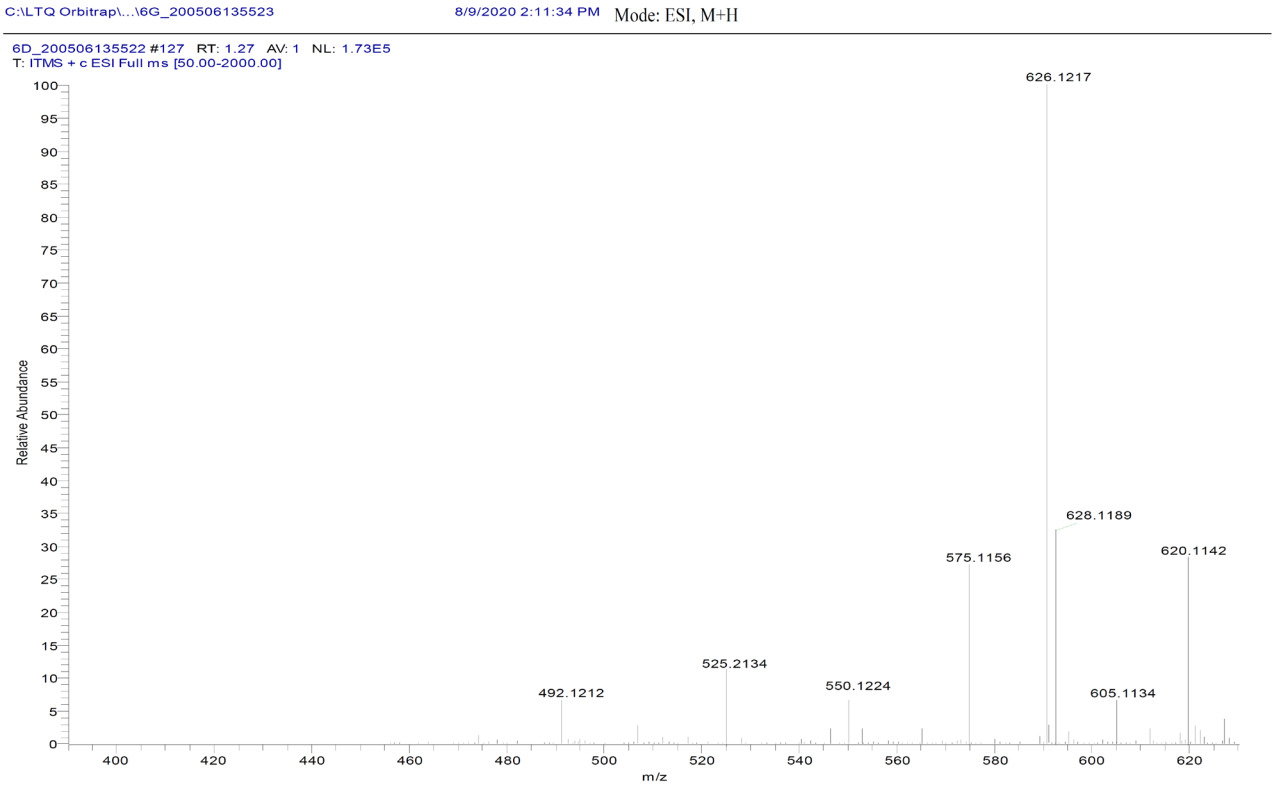
160
140
120
100
80
60
40
20
0
ppm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Relative Abundance
m/z
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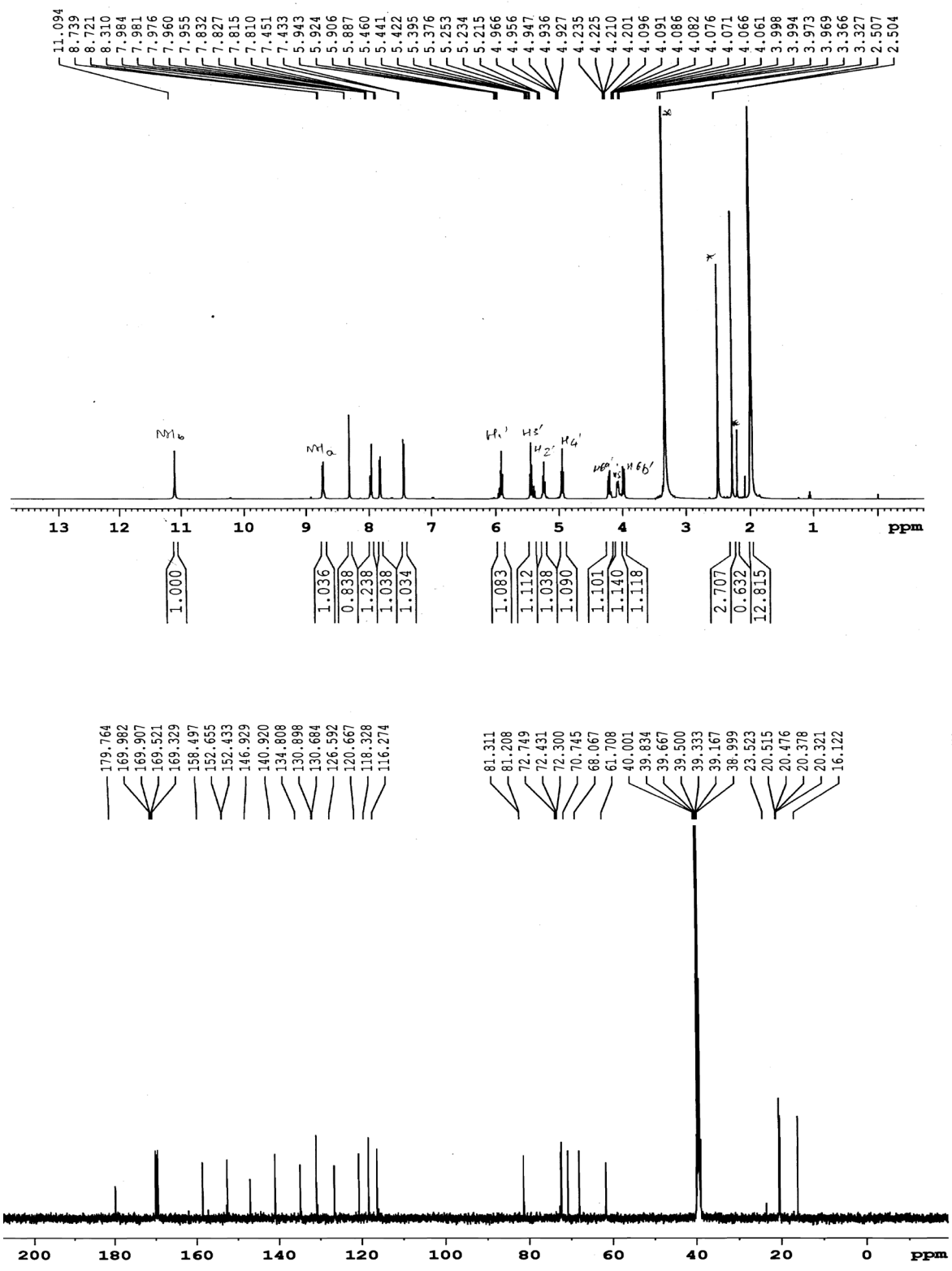
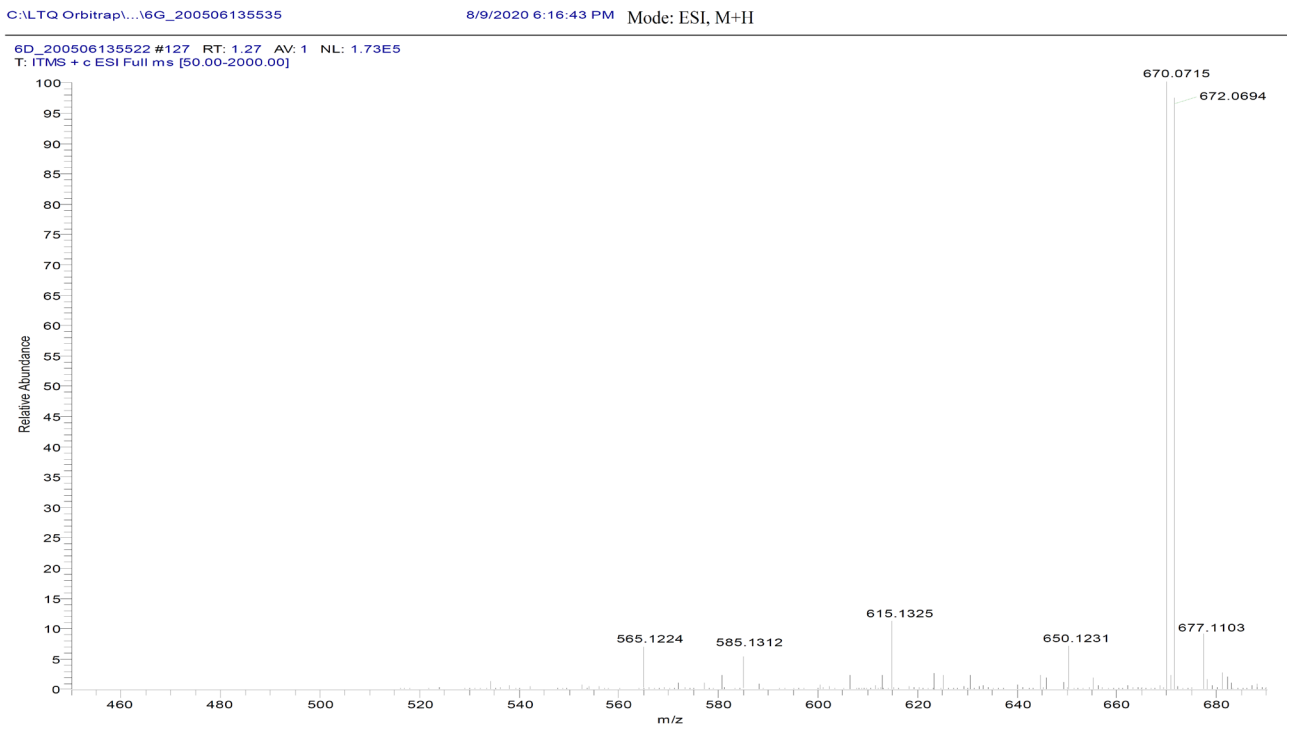
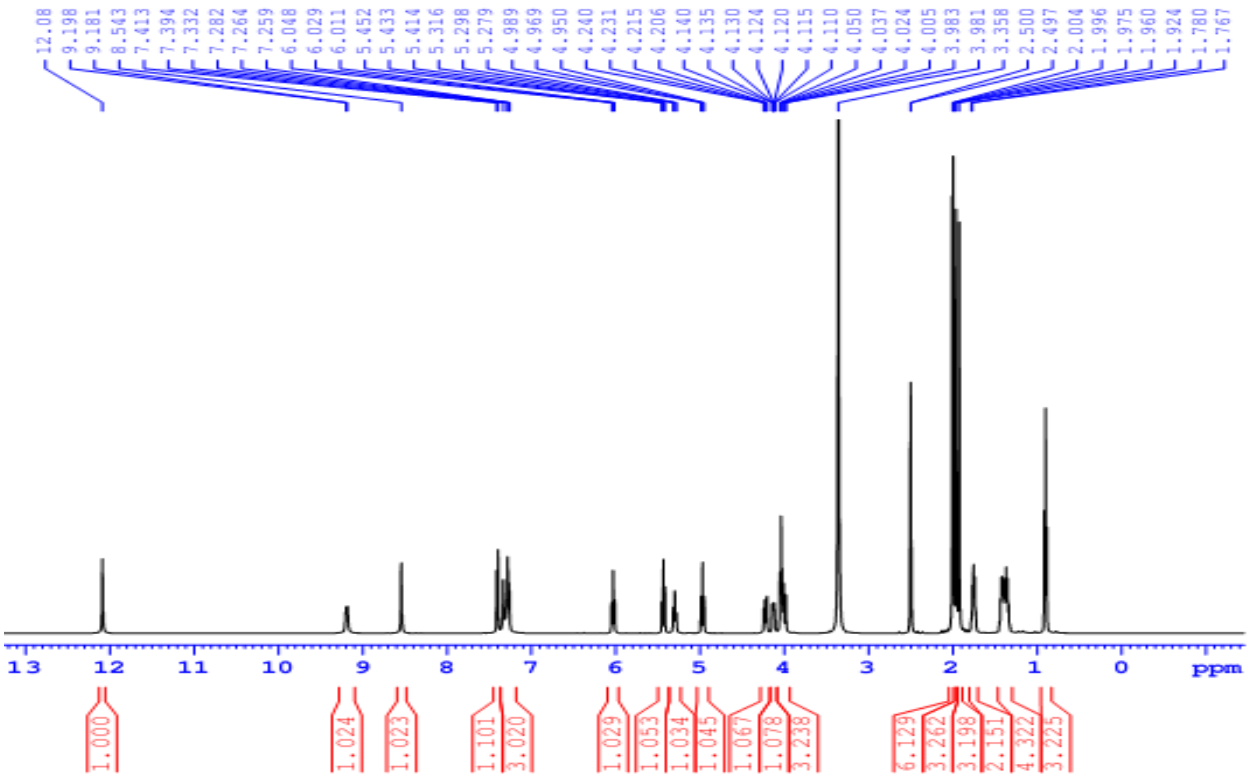
628.1189
620.1142
575.1156
525.2134
550.1224
492.1212
605.1134

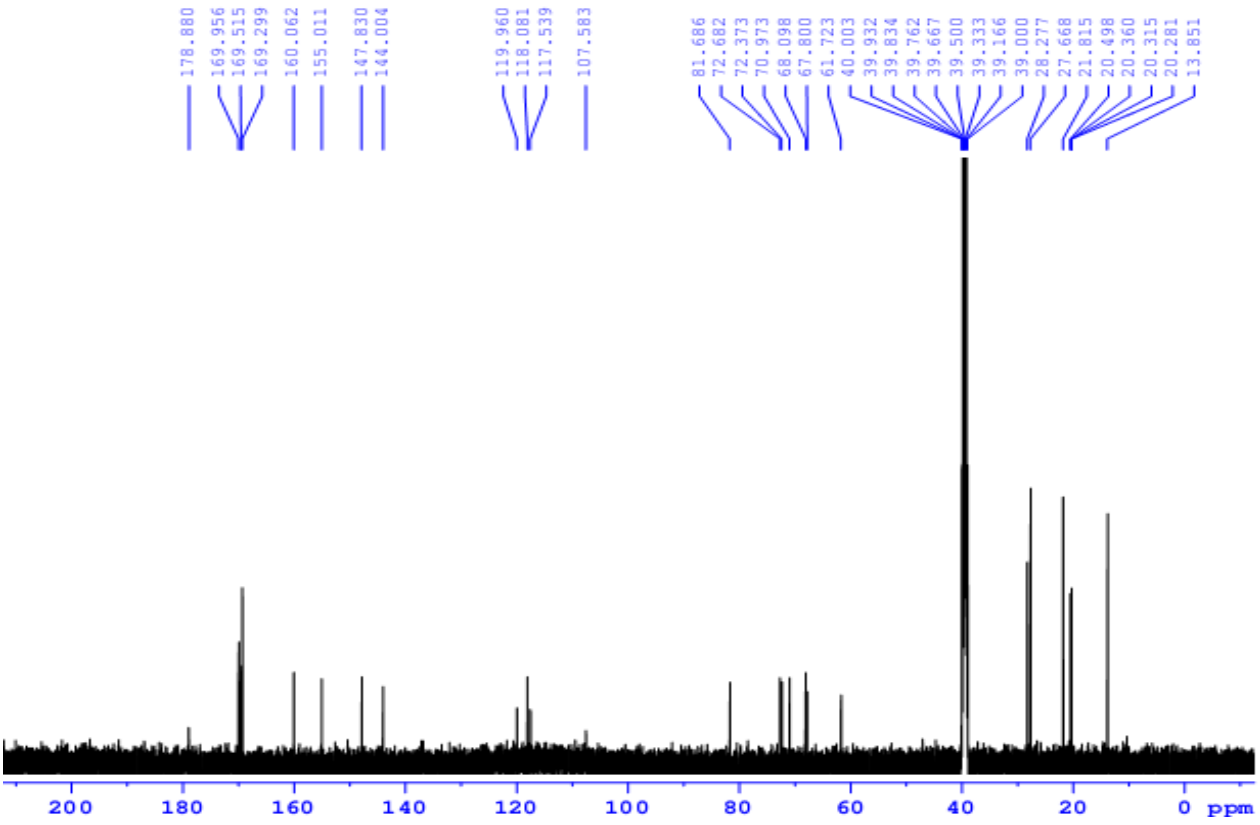
*3'-Acetyl-6'-bromocoumarin N-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)thiosemicarbazone (**3c**)*





6-Pentoxy-4-formylcoumarin N-(2',3',4',6'-tetra-O-acetyl-β-D-glucopyranosyl)thiosemicarbazone ***(3d)***





Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Sample name : 6OPen4MeCouGlc
Mode: ESI, M+H

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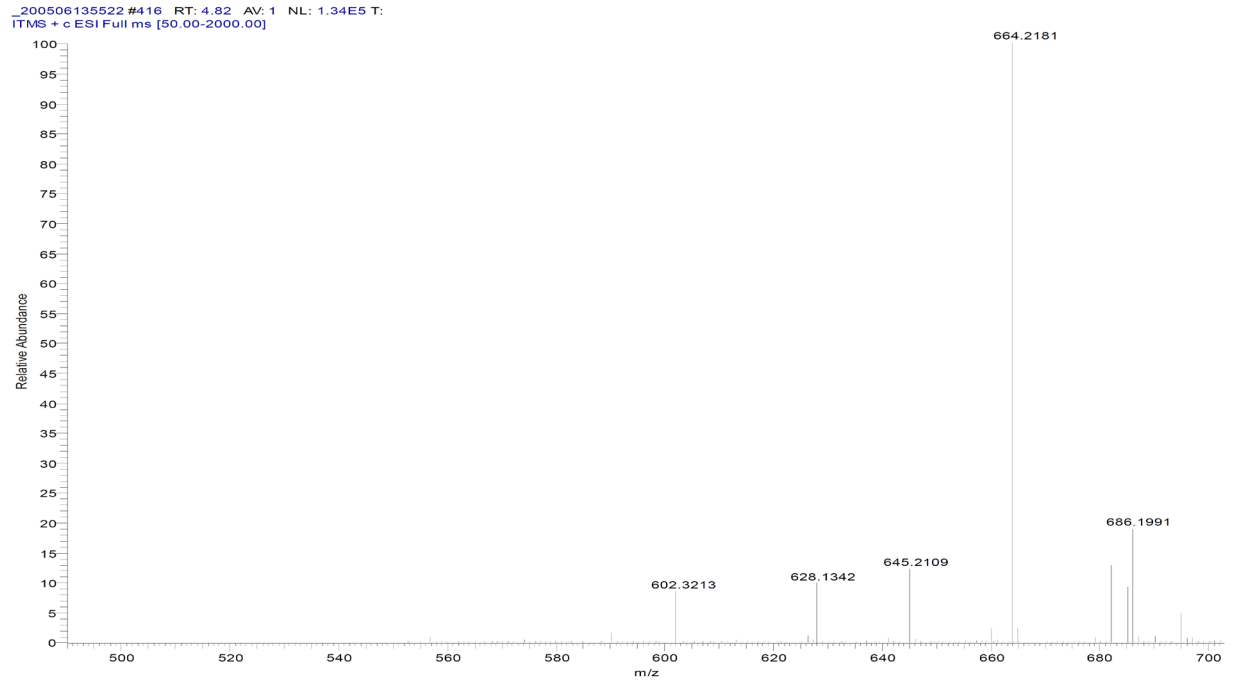
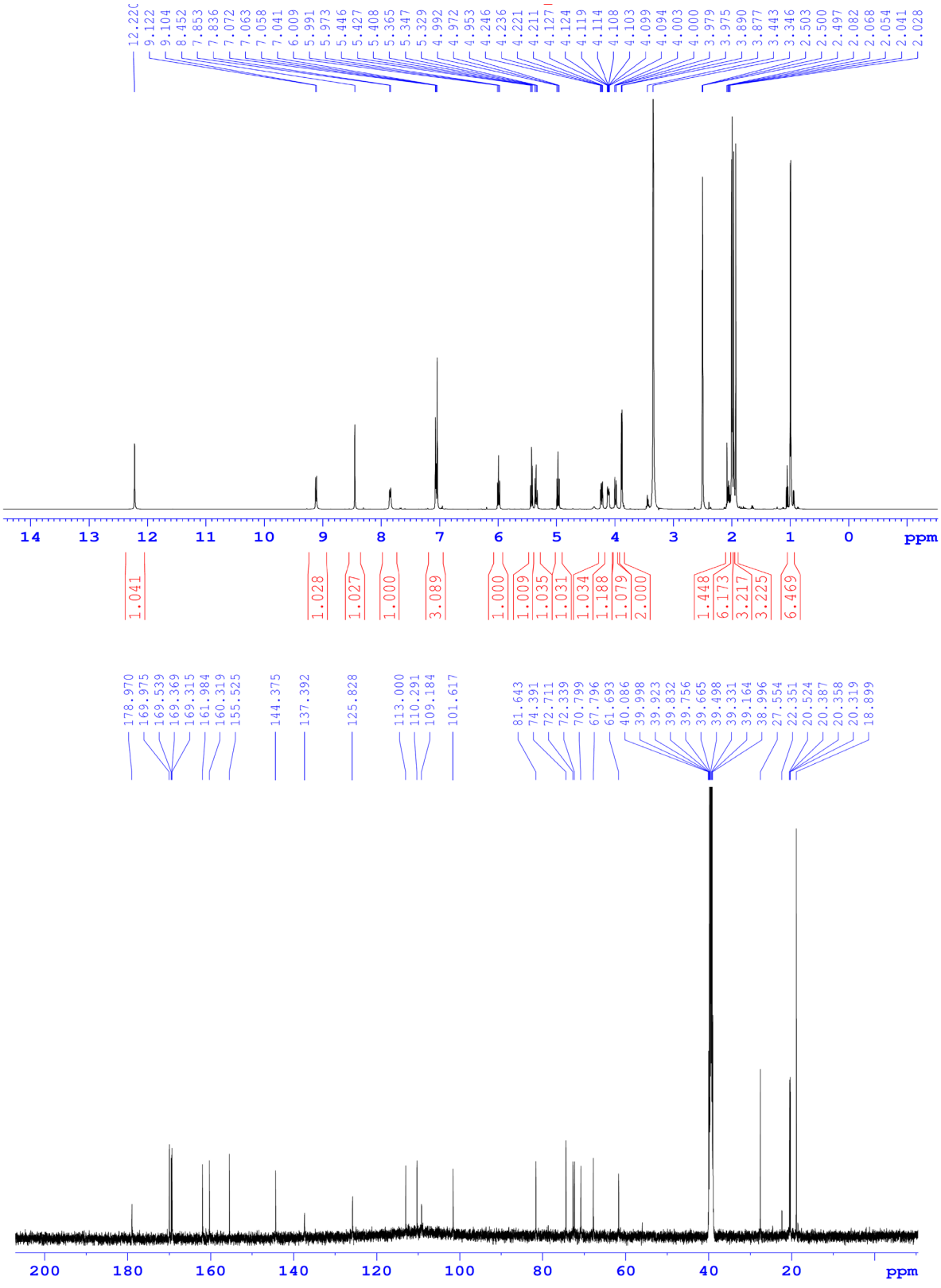


7-Isobutoxy-4-formylcoumarin 4-(2',3',4',6'-tetra-O-acetyl-β-D-glucopyranosyl)thiosemicarbazone ***(3e)***



Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Sample name : /tOBu4ForCouGlc
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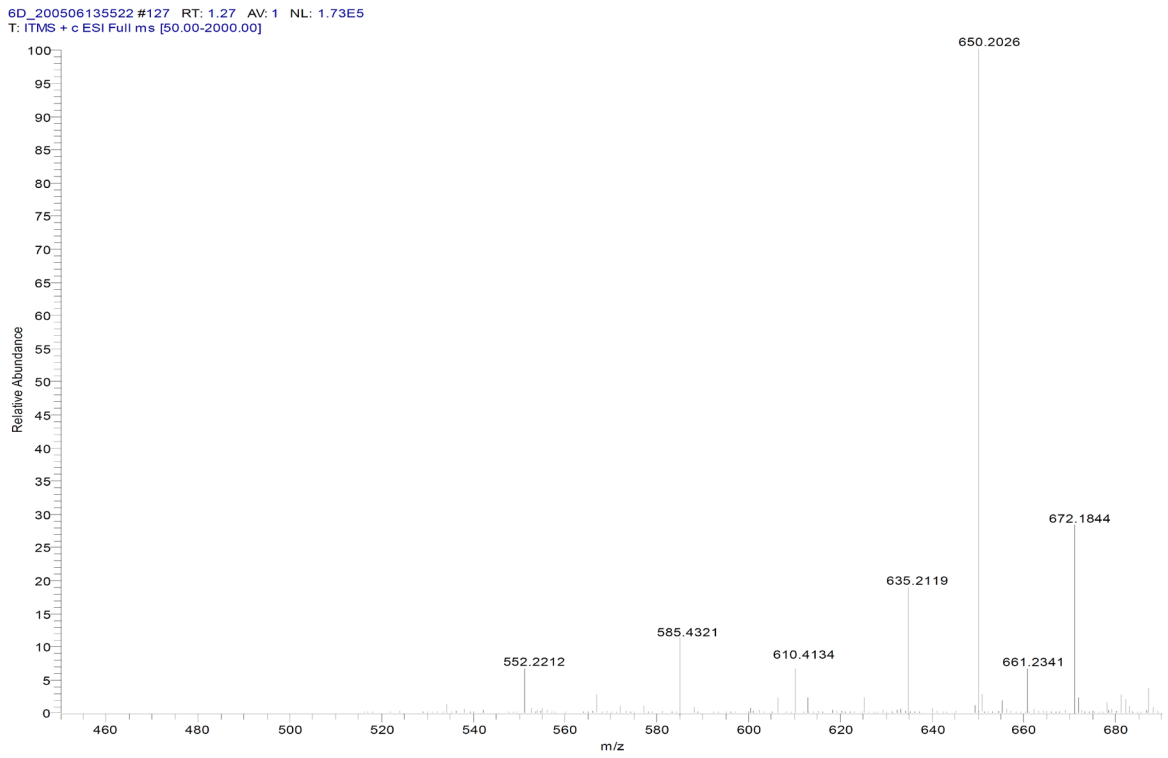
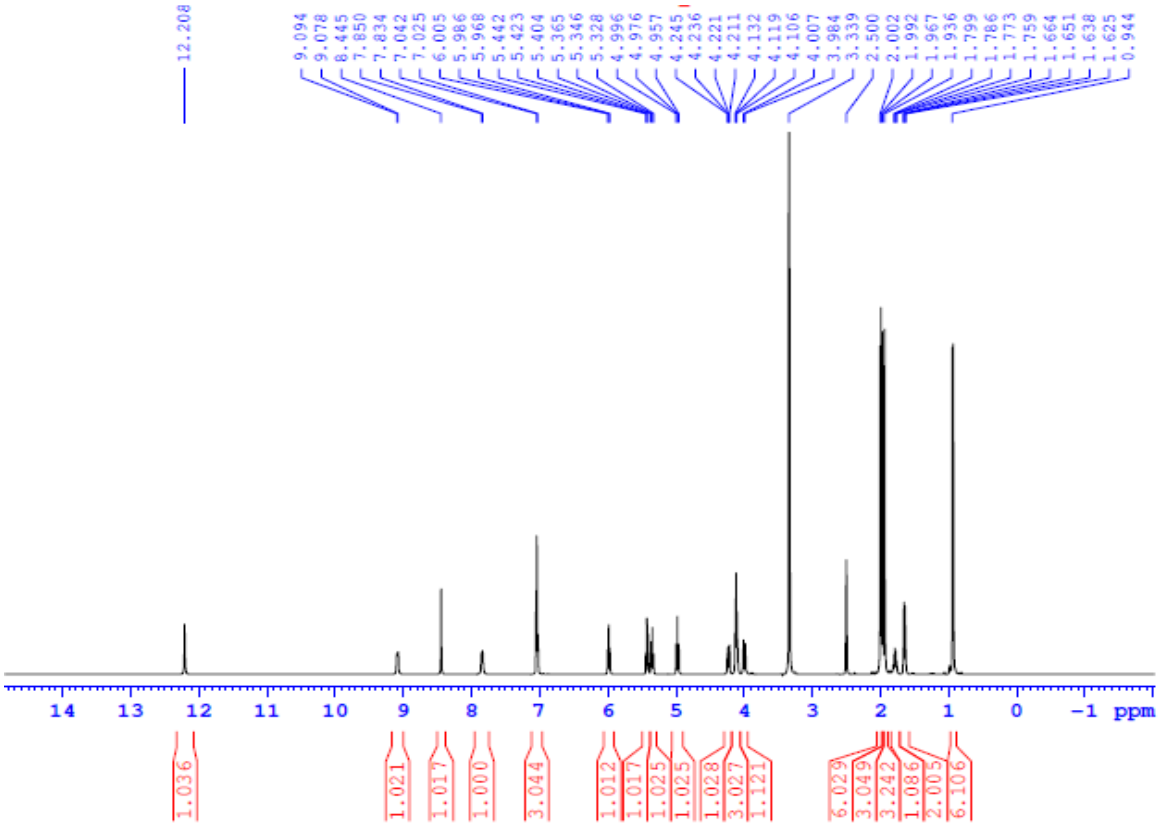
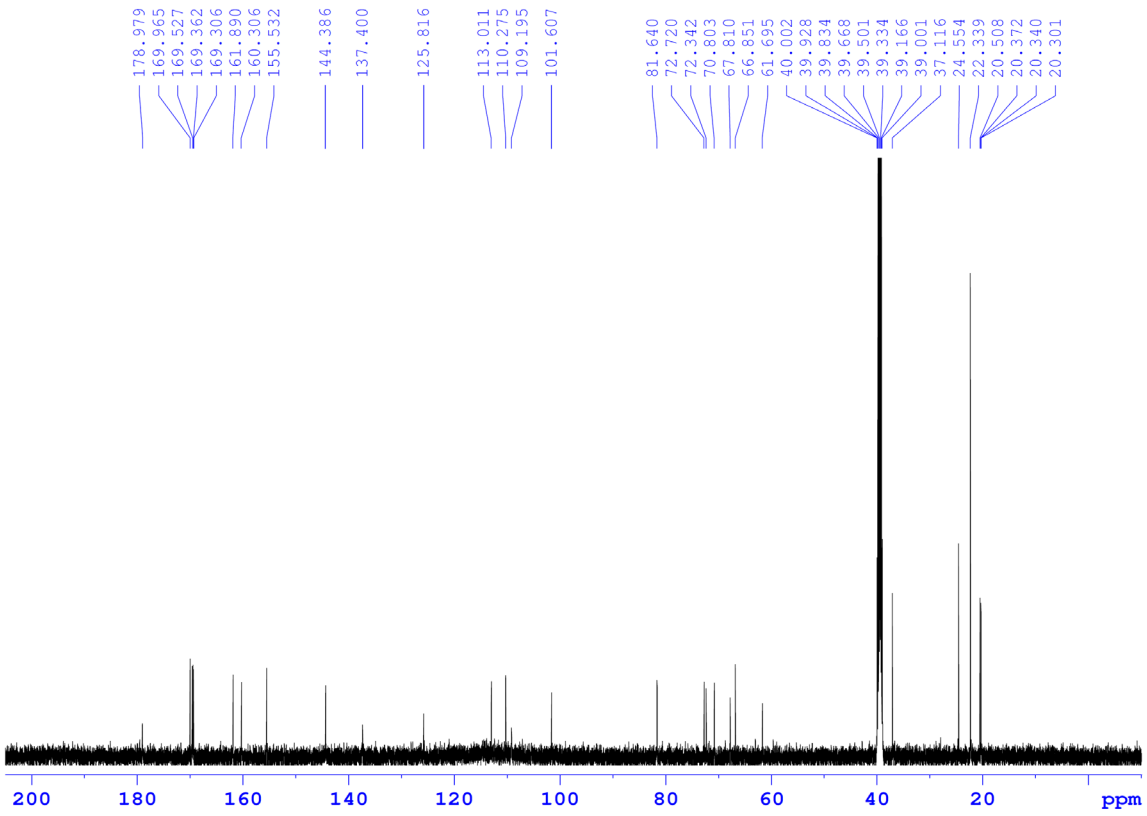


7-Isopentoxy-4-formylcoumarin N-(2',3',4',6'-tetra-O-acetyl-β-D-glucopyranosyl)thiosemicarbazone ***(3f)***





Tel: 844.38.253.053; **Fax**: 844.38.241.140 **Mail**: Chem.vnu@.edu.vn

Mode: ESI, M+H

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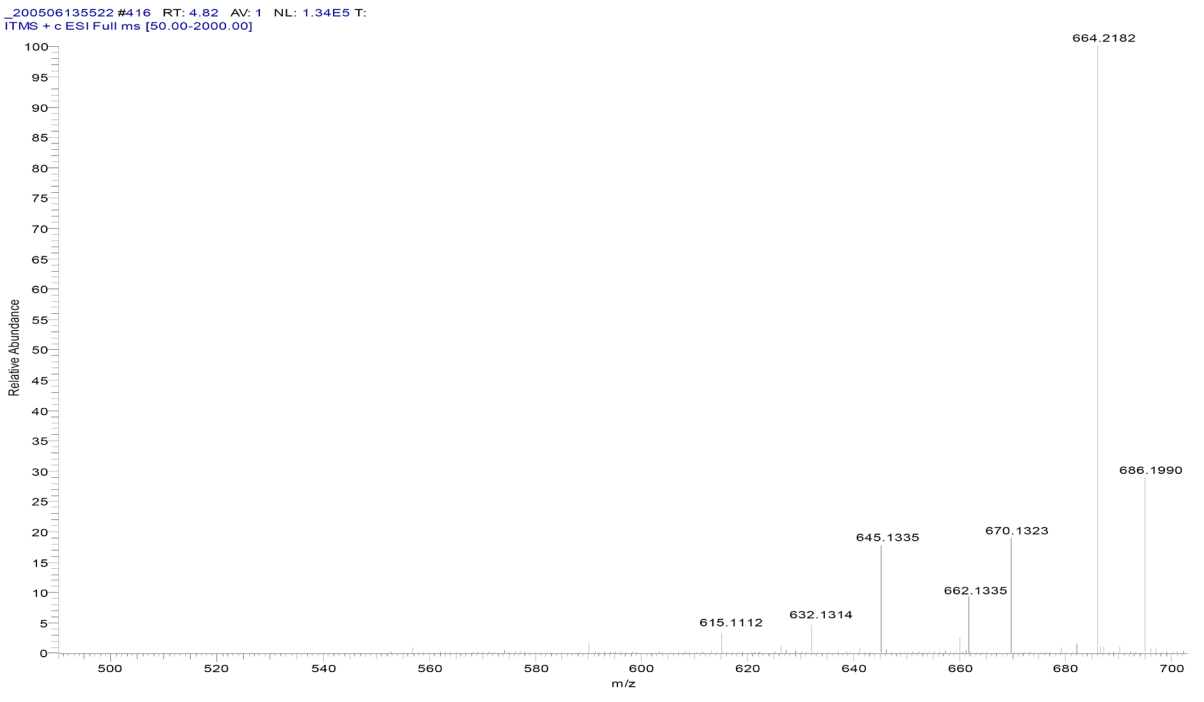
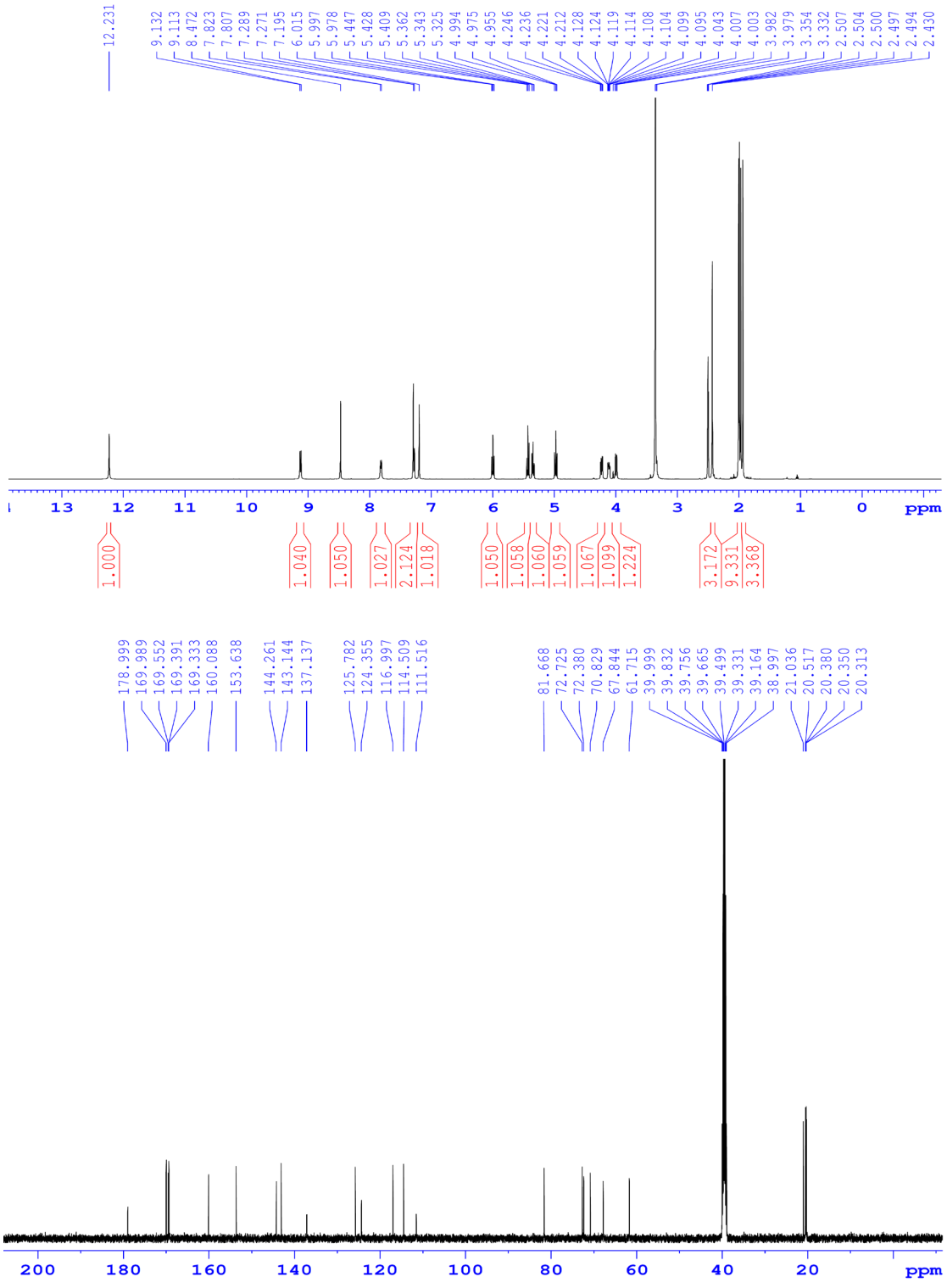
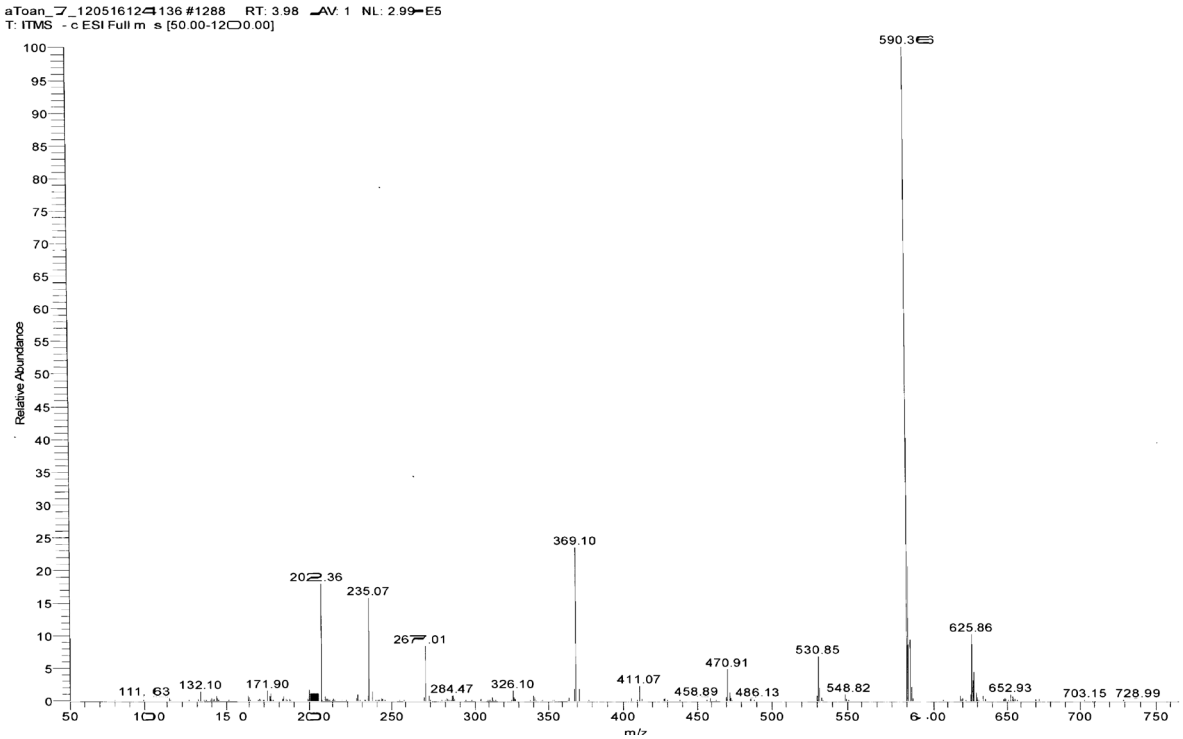


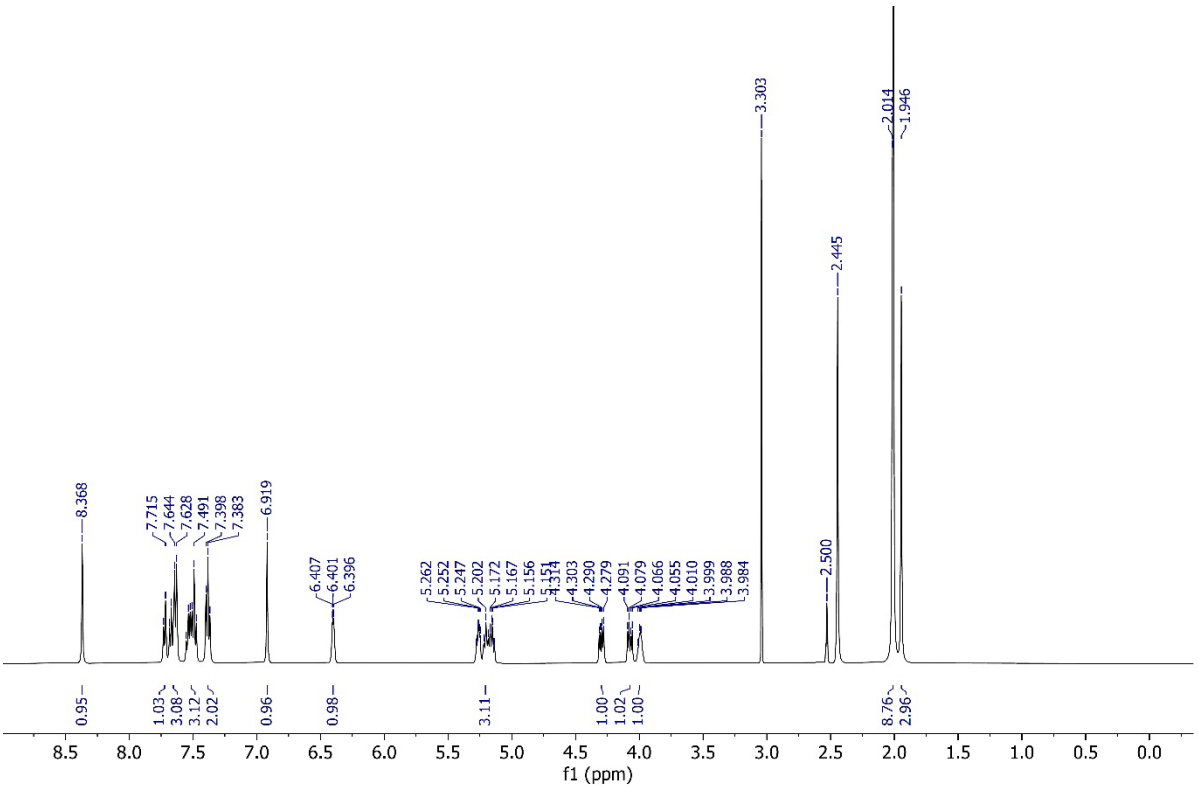
7-Methyl-4-formylcoumarin N-(2',3',4',6'-tetra-O-acetyl-β-D-glucopyranosyl)thiosemicarbazone ***(3g)***

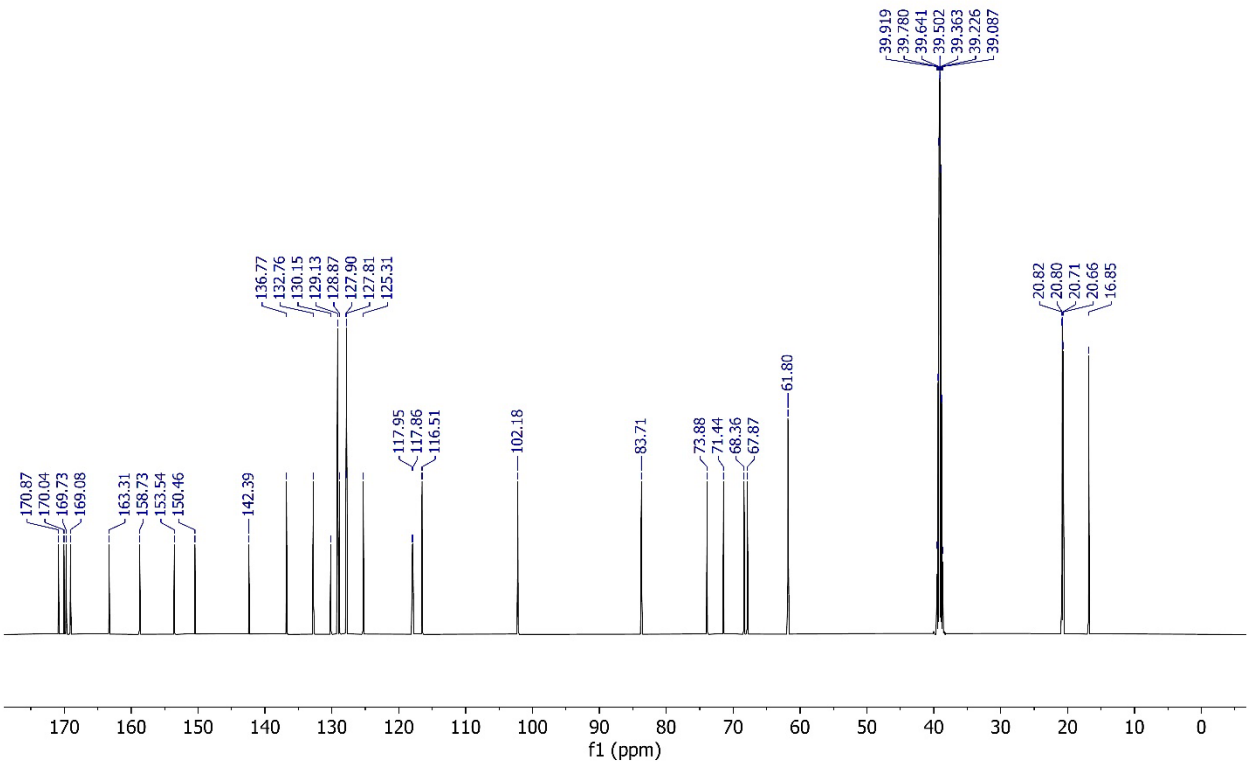




3. Spectra of substituted 2,3-dihydro-2(3*H*)-thiazoles (4a-g)

*3-(4'-Phenyl-3'-(2'',3'',4'',6''-tetra-O-acetyl-β-D-glucopyranosyl)thiazol-2'(3'H)-ylidene)hydrazono)ethyl)coumarin (**4a**)*

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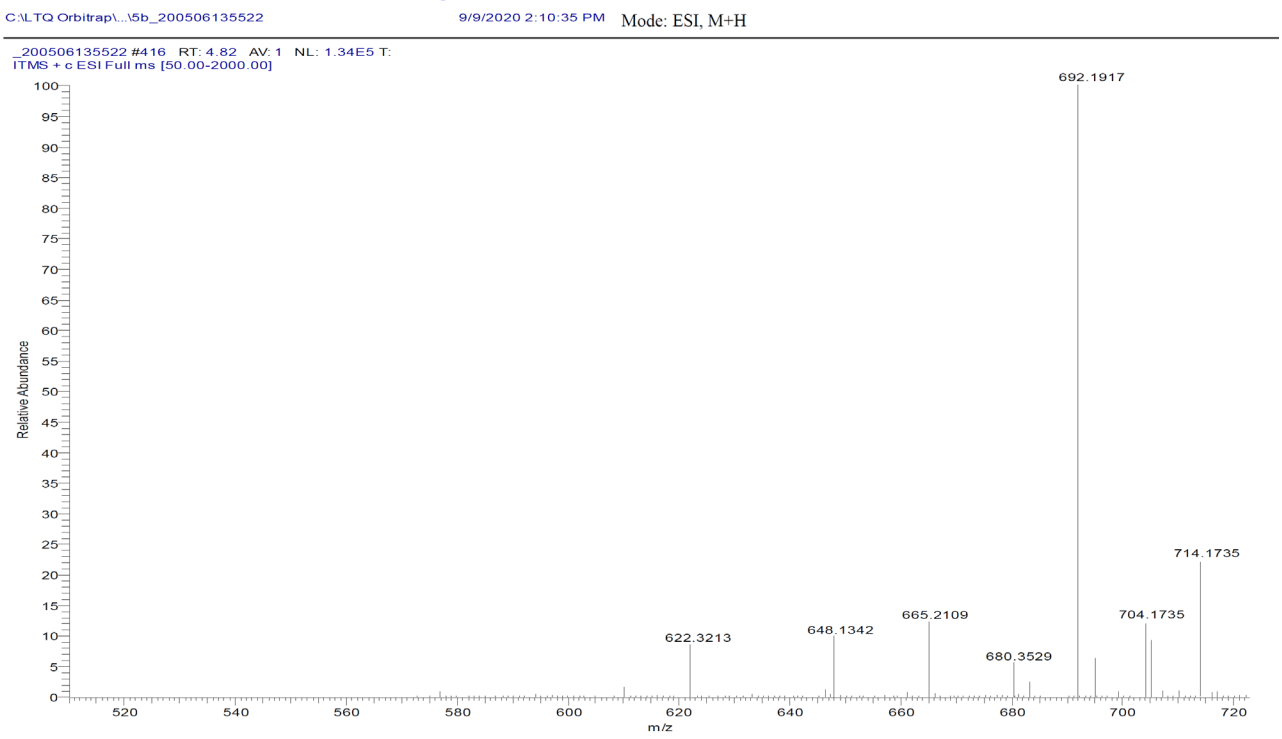
39.780
39.641
39.502
39.363
39.226
39.087
136.77
132.76
130.15
129.13
128.87
127.90
127.81
125.31
20.82
20.80
20.71
20.66
16.85
61.80
117.95
117.86
116.51
102.18
83.71
73.88
71.44
68.36
67.87
170.87
170.04
169.73
169.08
163.31
158.73
153.54
150.46
142.39
f1 (ppm)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9/9/2020 2:10:35 PM
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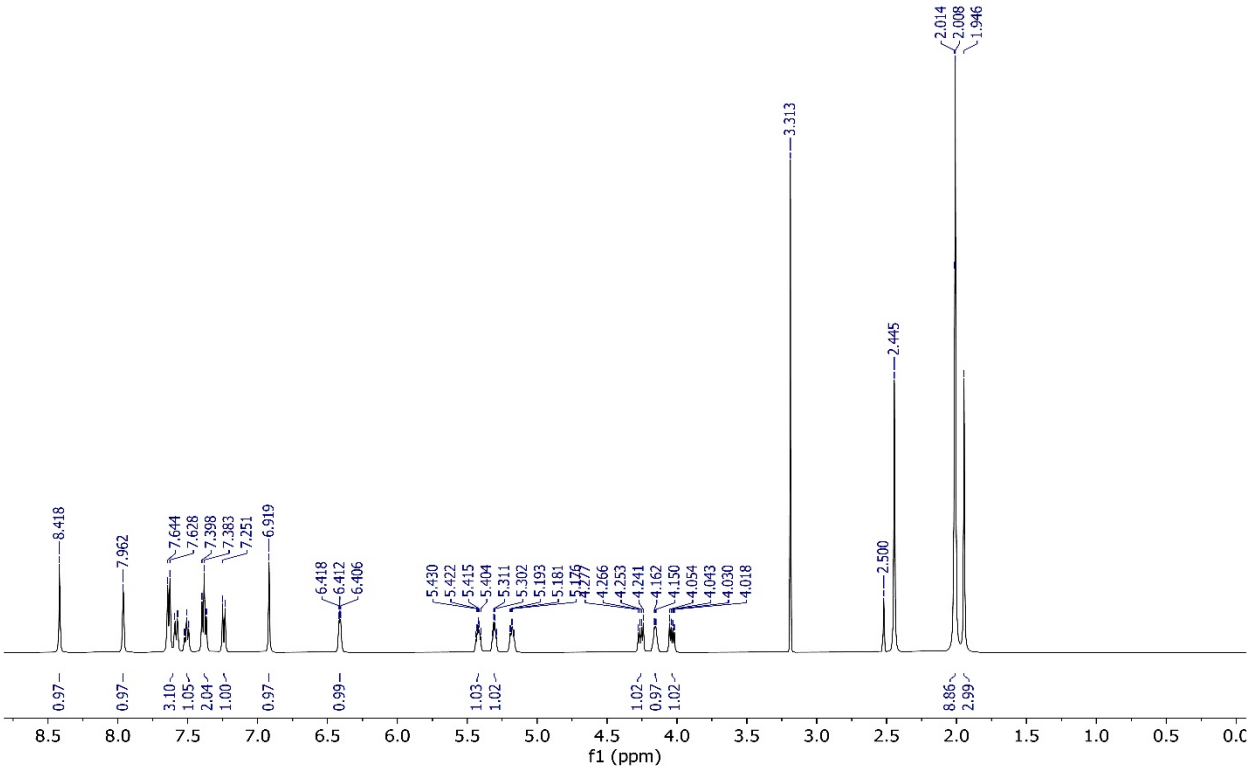
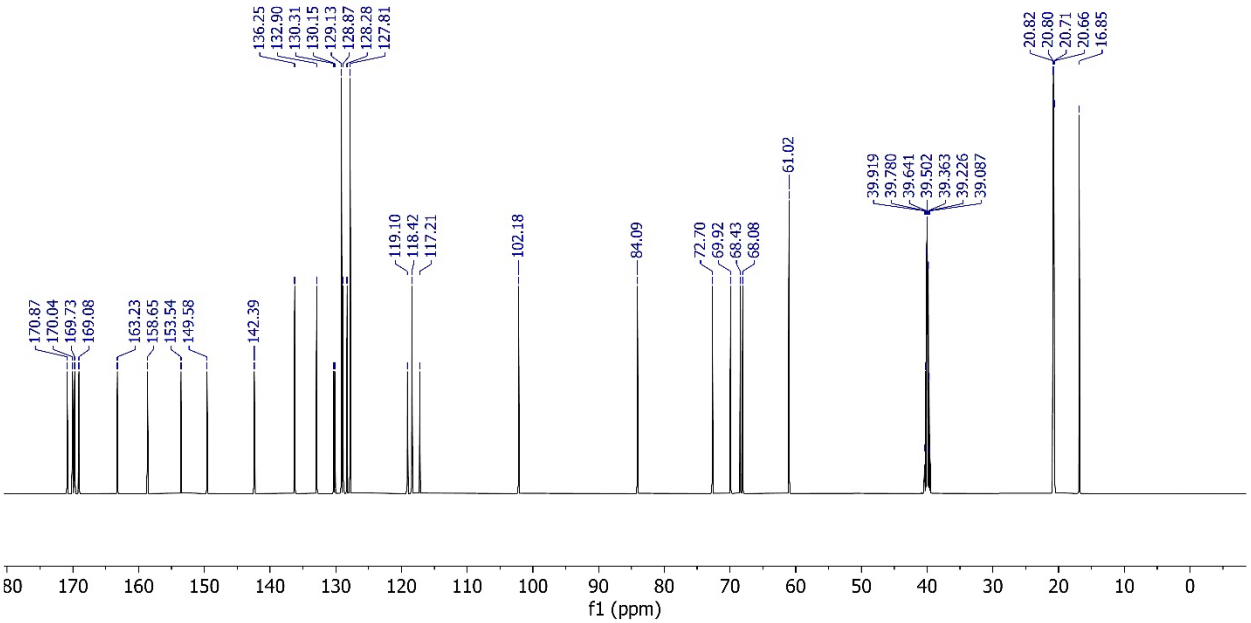
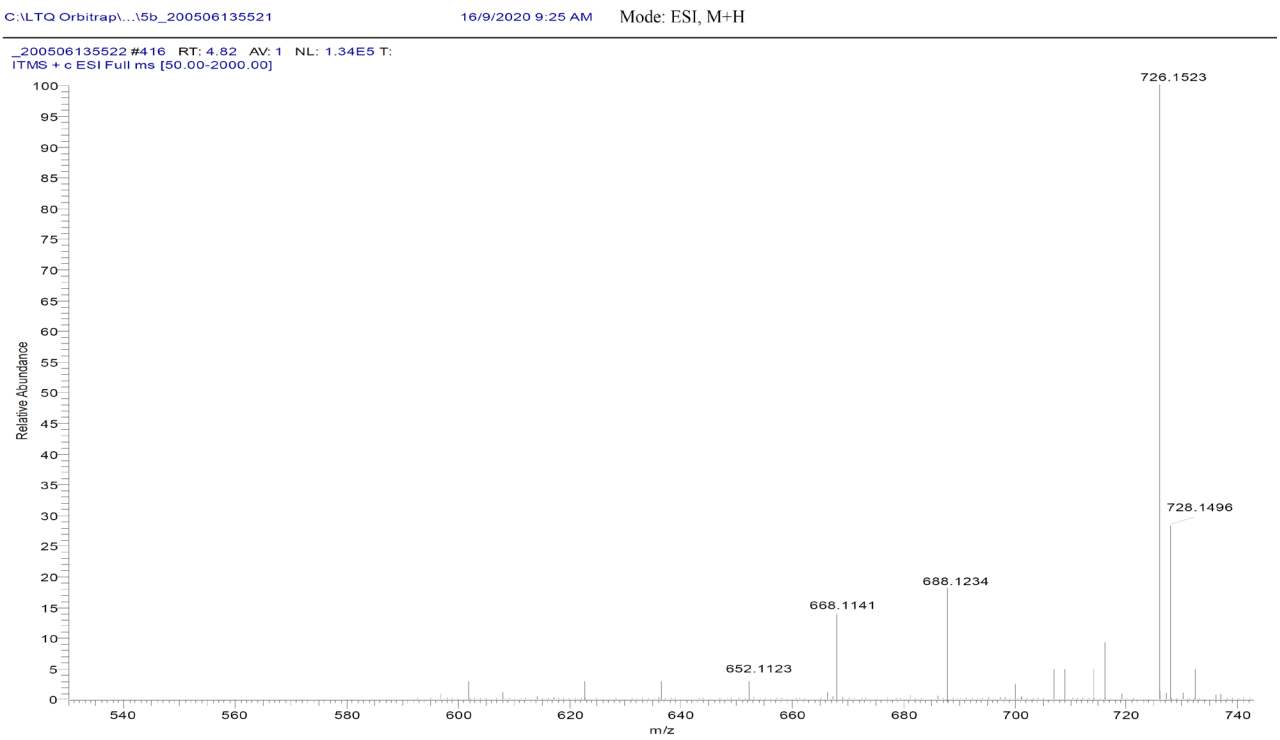
692.1917
714.1735
704.1735
665.2109
648.1342
622.3213
680.3529
Relative Abundance
m/z

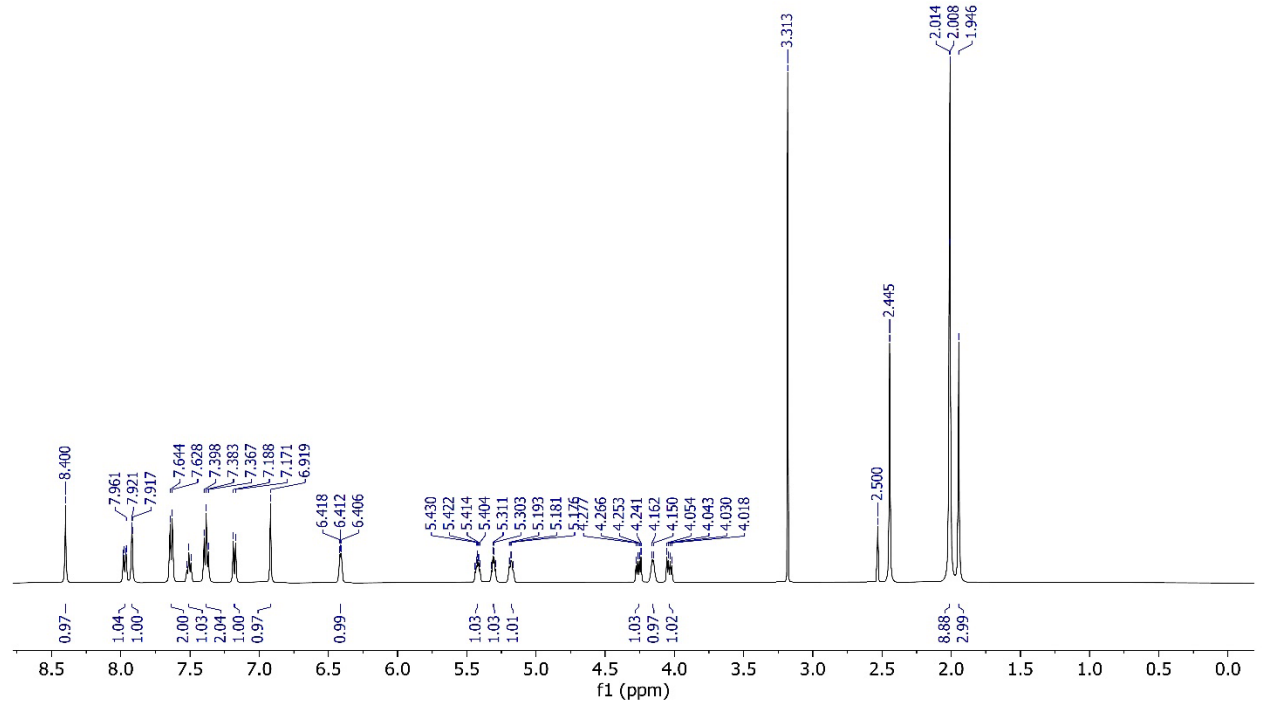
*3-(4'-Phenyl-3'-(2'',3'',4'',6''-tetra-O-acetyl-β-D-galactopyranosyl)thiazol-2'(3'H)-ylidene)hydrazono)ethyl)-6-chlorocoumarin (**4b**)*

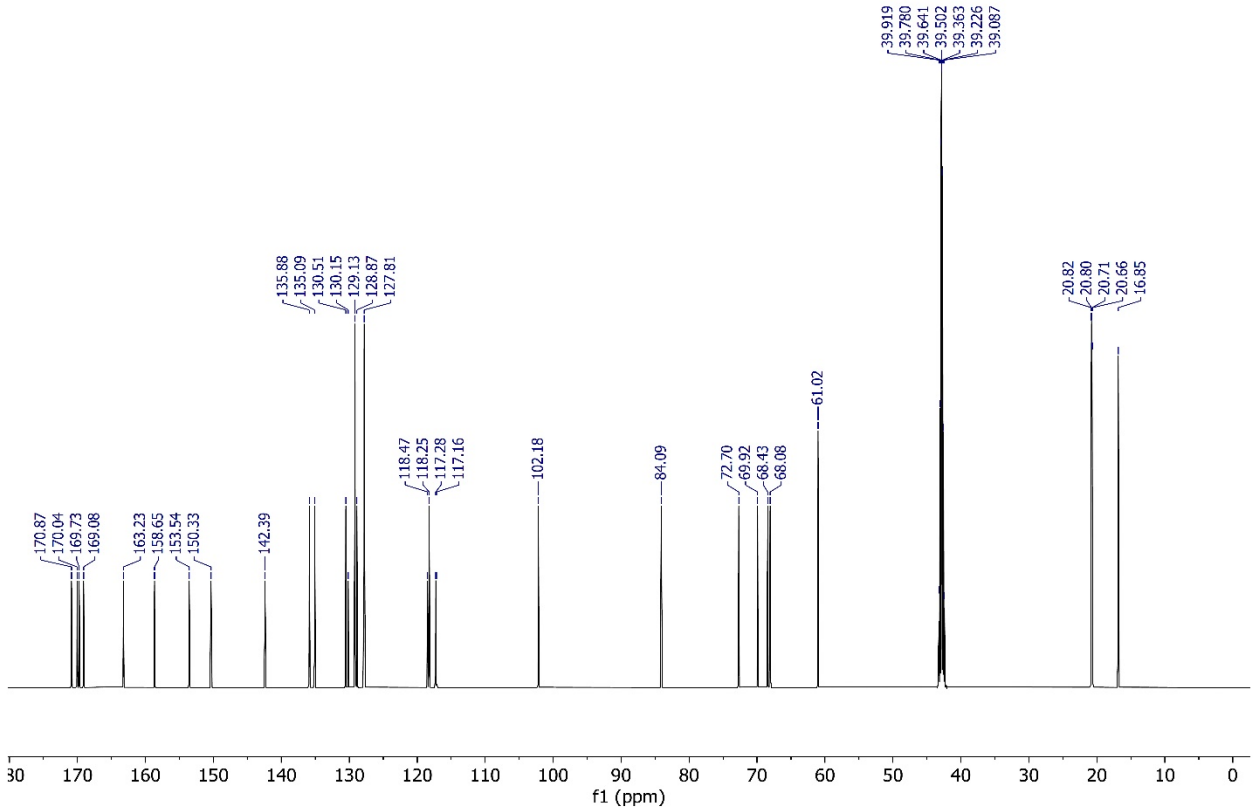


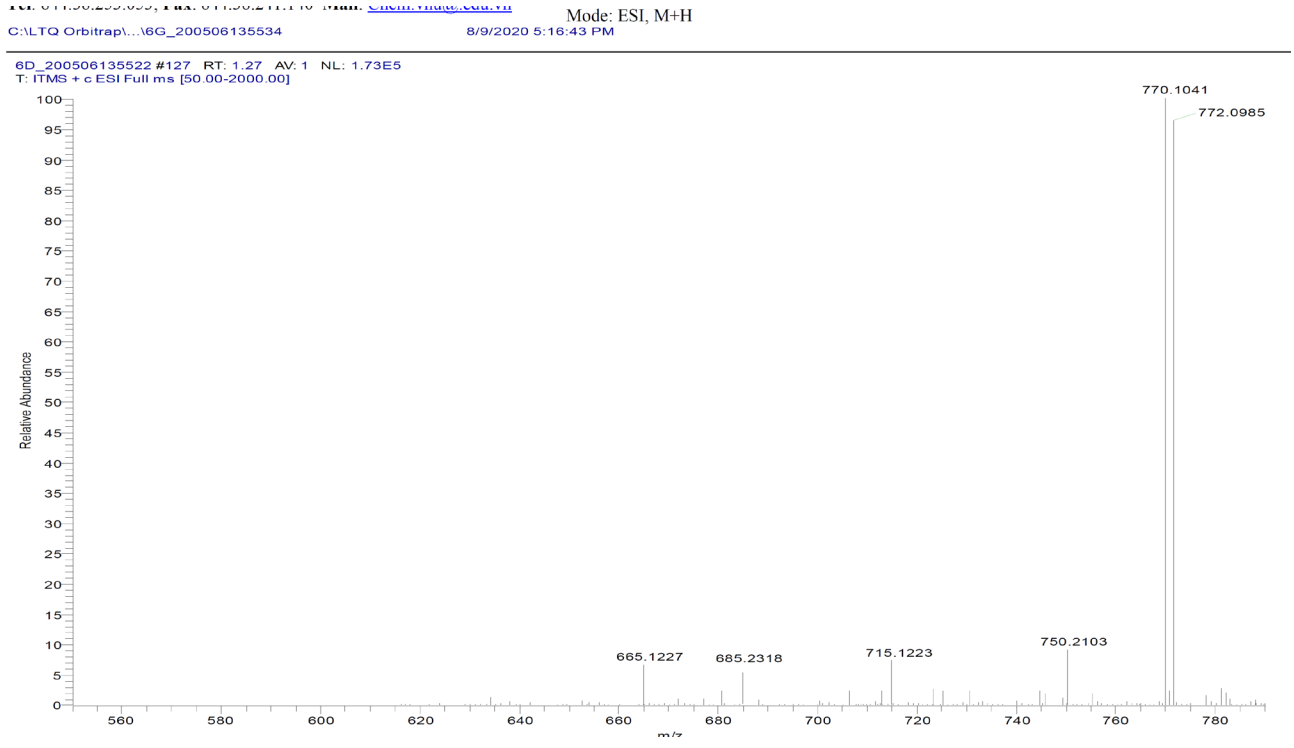




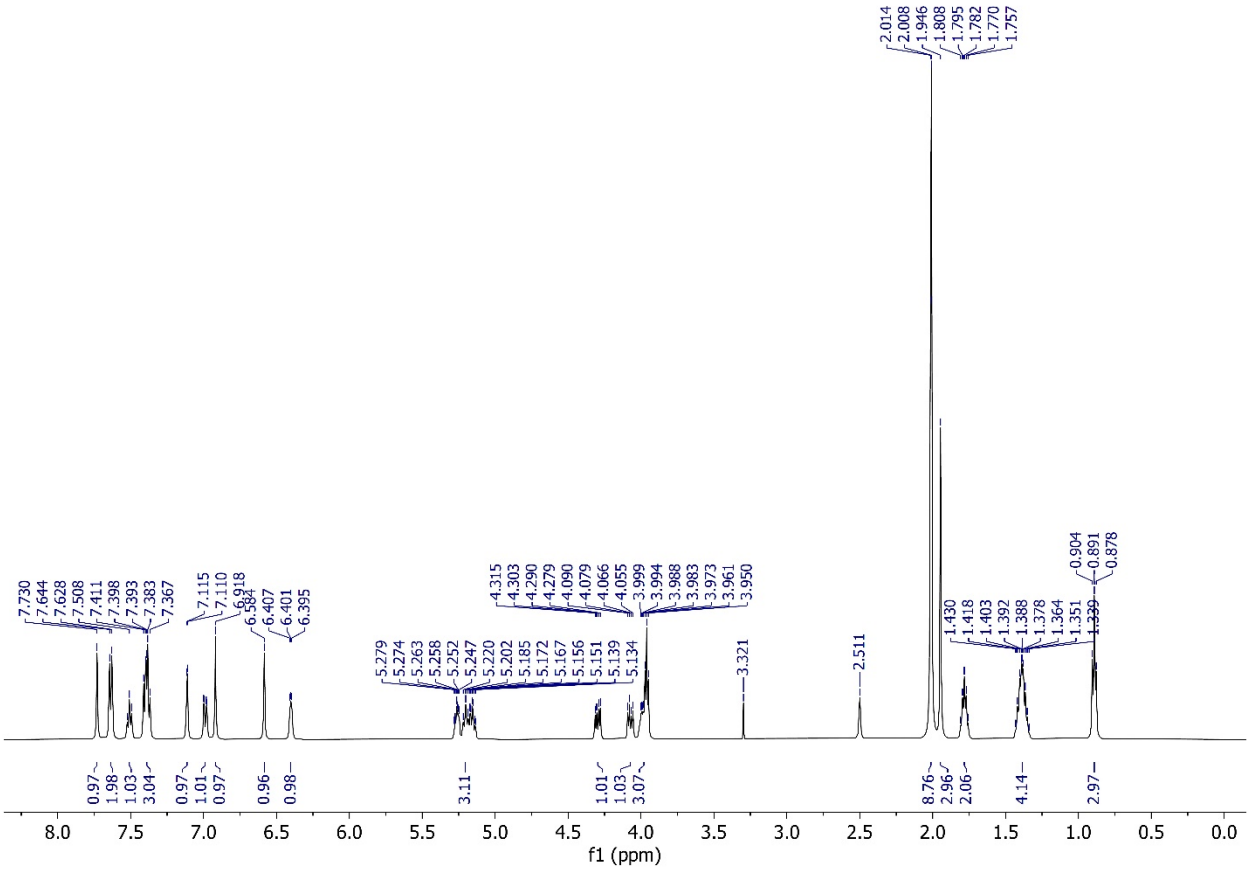
*3-(4'-Phenyl-3'-(2'',3'',4'',6''-tetra-O-acetyl-β-D-galactopyranosyl)thiazol-2'(3'H)-ylidene)hydrazono)ethyl)-6-bromocoumarin (**4c**)*

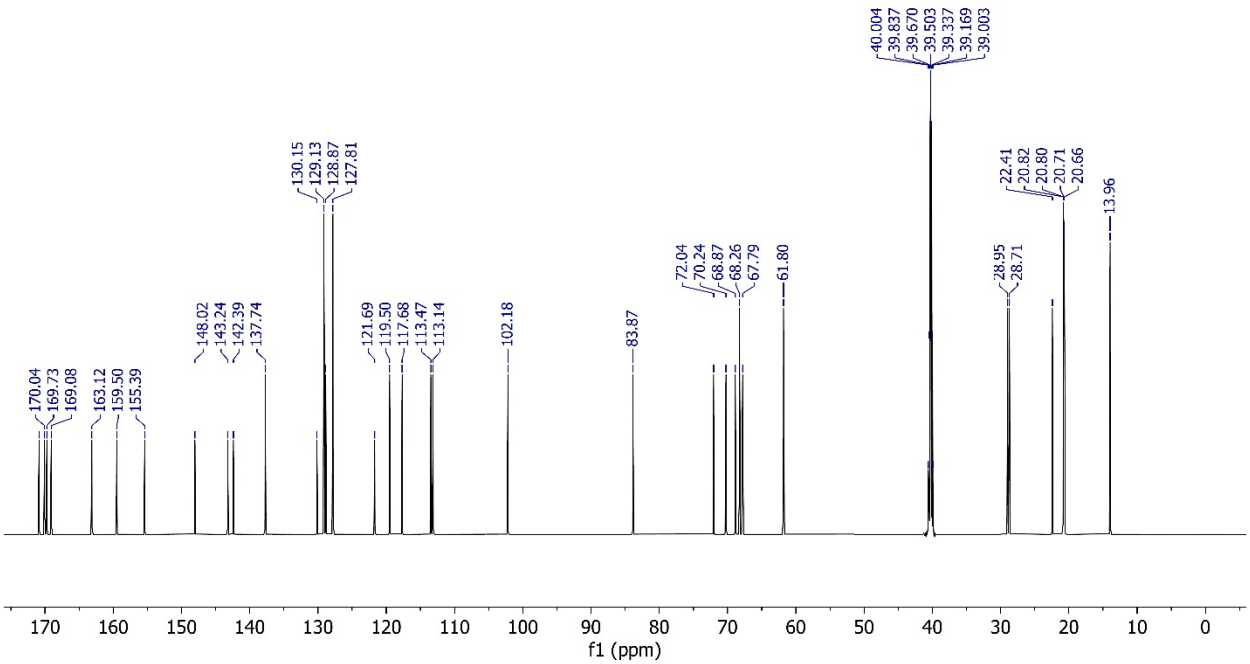


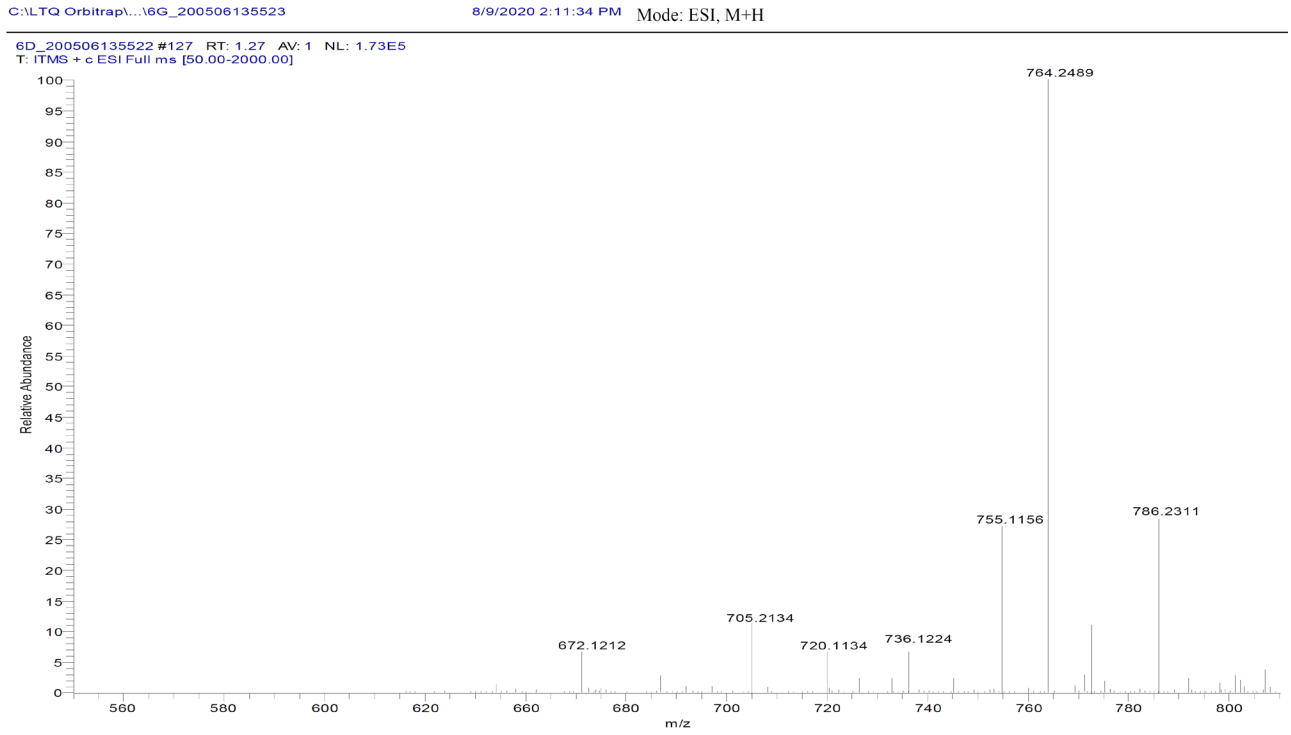

39.919
39.780
39.641
39.502
39.363
39.226
39.087
135.88
135.09
130.51
130.15
129.13
128.87
127.81
20.82
20.80
20.71
20.66
16.85
61.02
118.47
118.25
117.28
117.16
102.18
84.09
72.70
69.92
68.43
68.08
170.87
170.04
169.73
169.08
163.23
158.65
153.54
150.33
142.39
f1 (ppm)


Mode: ESI, M+H
C:\LTQ Orbitrap\...\6G_200506135534
8/9/2020 5:16:43 PM
6D_200506135522 #127 RT: 1.27 AV: 1 NL: 1.73E5
T: ITMS + c ESI Full ms [50.00-2000.00]
770.1041
772.0985
665.1227
685.2318
715.1223
750.2103
Relative Abundance
m/z

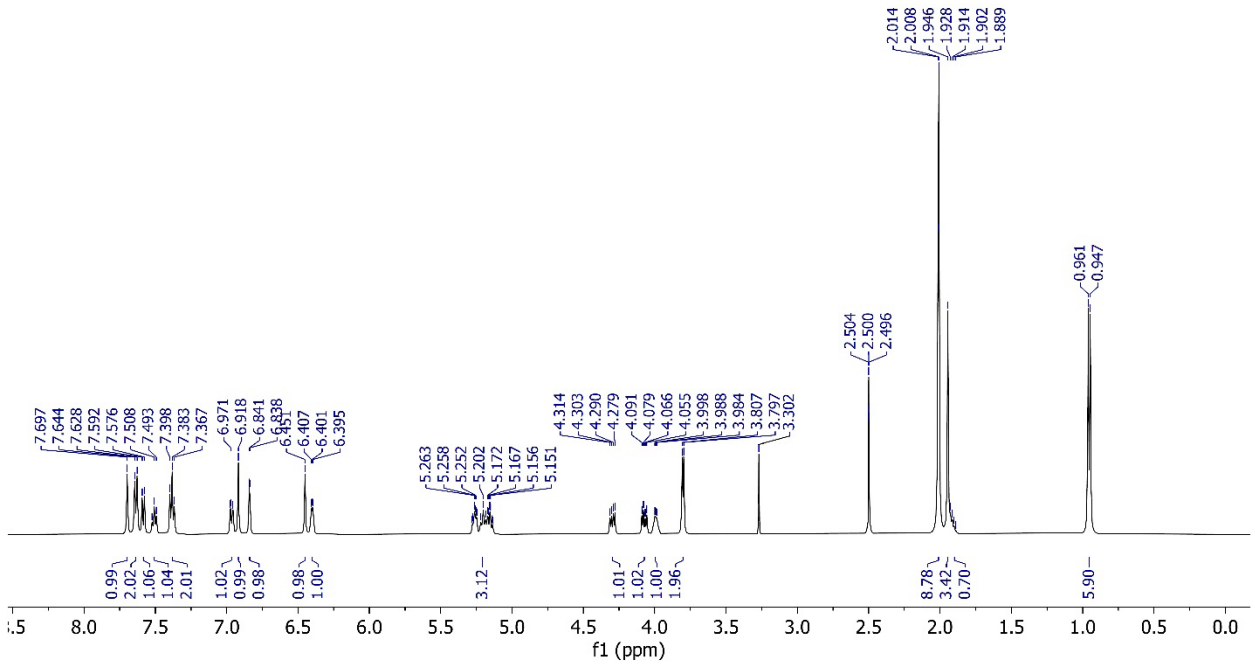
*4-(4'-Phenyl-3'-(2'',3'',4'',6''-tetra-O-acetyl-β-D-glucopyranosyl)thiazol-2'(3'H)-ylidene)hydrazono)methyl)-6-pentoxycoumarin (**4d**)*

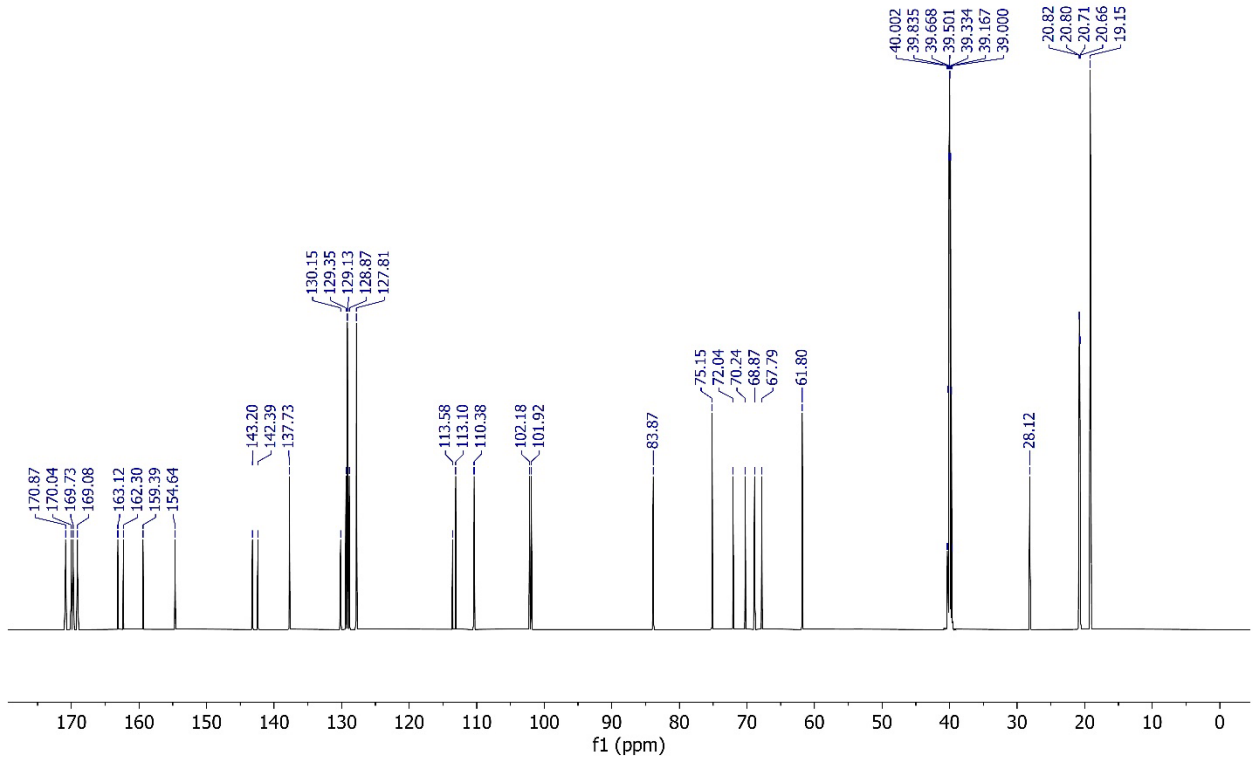


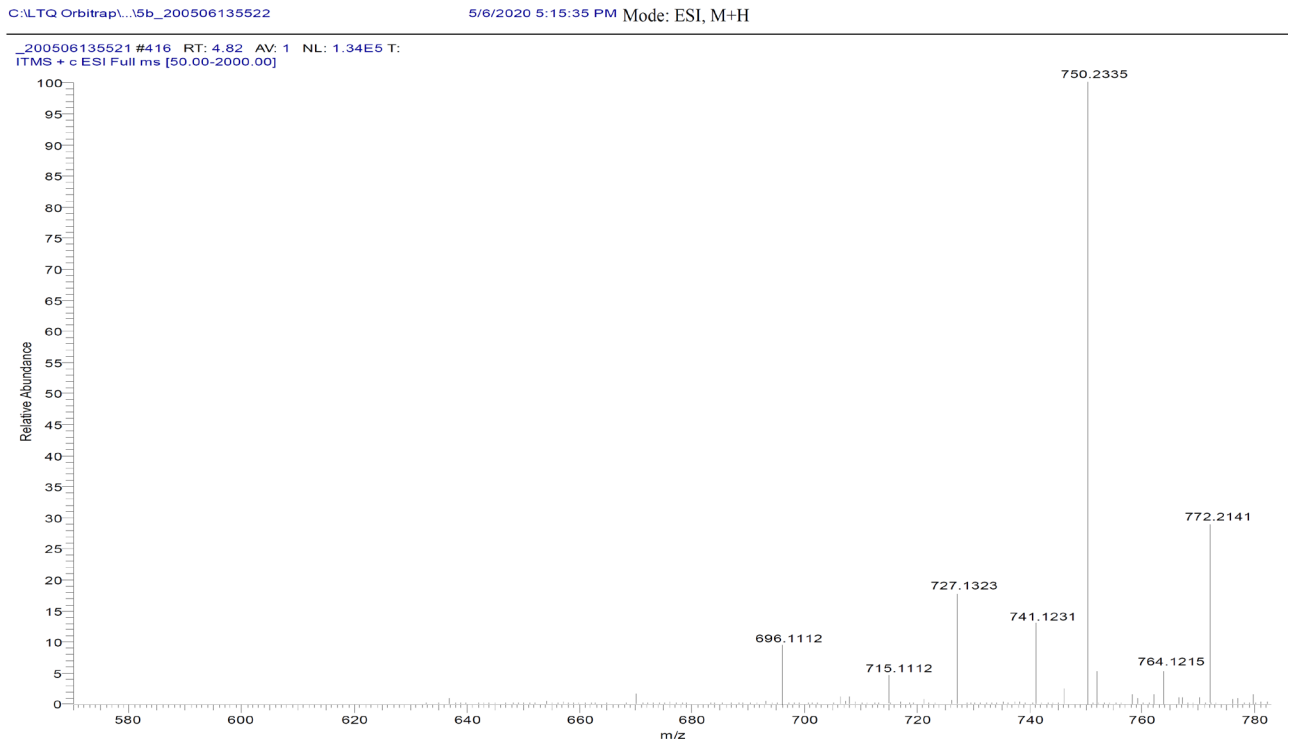




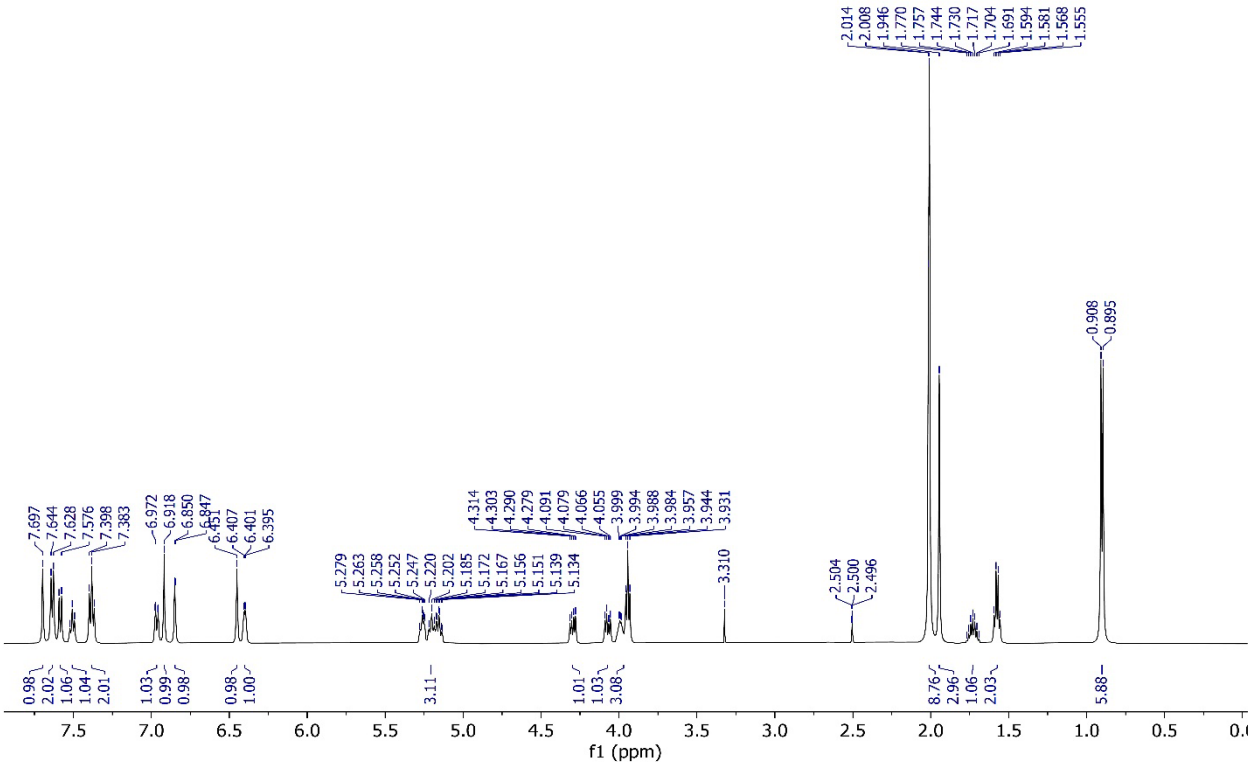
*4-(4'-Phenyl-3'-(2'',3'',4'',6''-tetra-O-acetyl-β-D-glucopyranosyl)thiazol-2'(3'H)-ylidene)hydrazono)methyl)-7-isobutoxycoumarin (**4e**)*

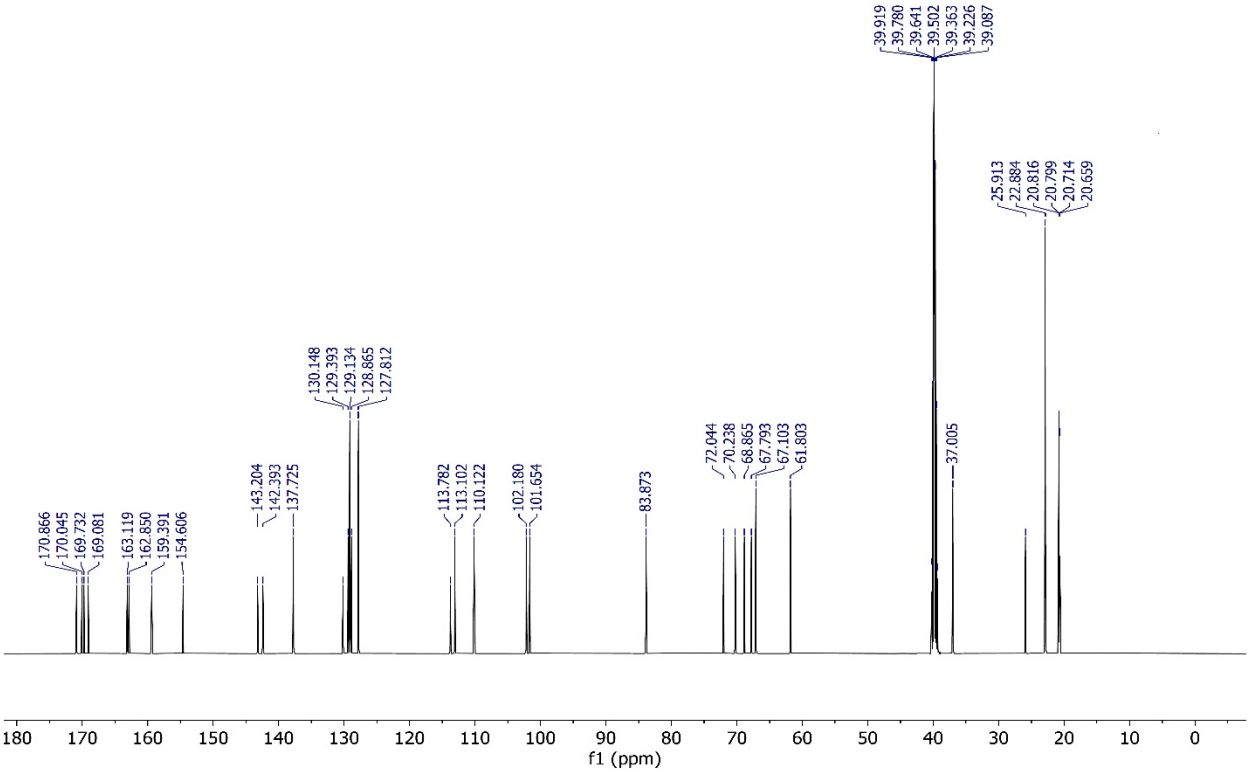


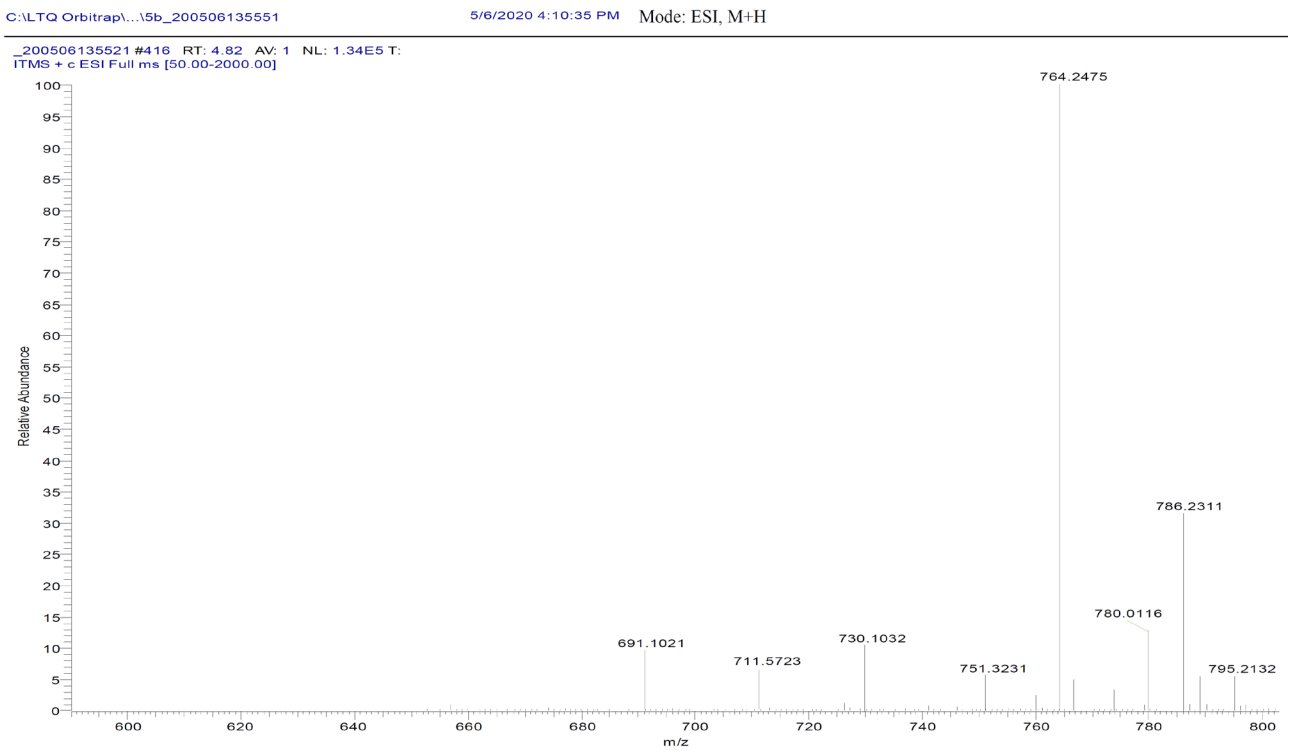

40.002
39.835
39.668
39.501
39.334
39.167
39.000
20.82
20.80
20.71
20.66
19.15
130.15
129.35
129.13
128.87
127.81
75.15
72.04
70.24
68.87
67.79
61.80
143.20
142.39
137.73
113.58
113.10
110.38
102.18
101.92
83.87
28.12
170.87
170.04
169.73
169.08
163.12
162.30
159.39
154.64
f1 (ppm)


C:\LTQ Orbitrap\...\5b_200506135522
5/6/2020 5:15:35 PM Mode: ESI, M+H
_200506135521 #416 RT: 4.82 AV: 1 NL: 1.34E5 T:
ITMS + c ESI Full ms [50.00-2000.00]
750.2335
772.2141
727.1323
741.1231
696.1112
715.1112
764.1215
Relative Abundance
m/z

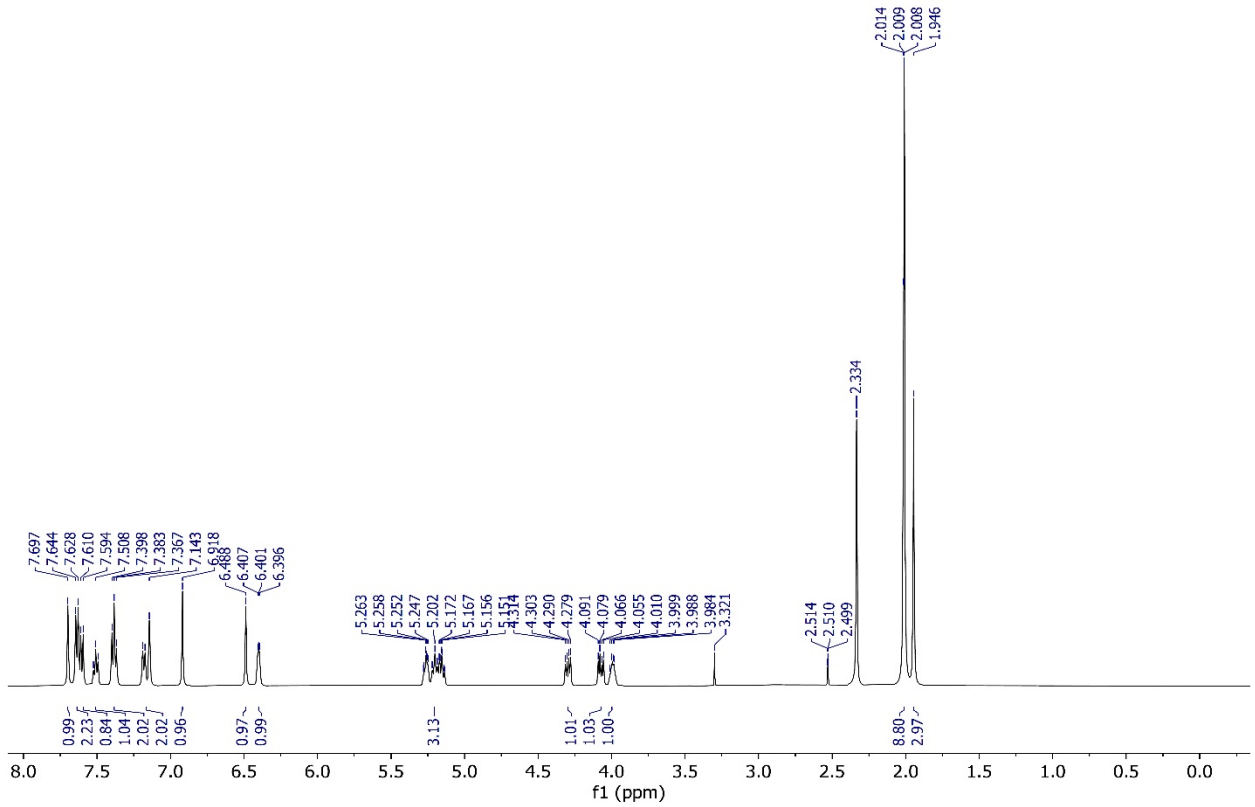
*4-(4'-Phenyl-3-(2,3,4,6-tetra-O-acetyl-β-D-glucopyranosyl)thiazol-2'(3'H)-ylidene)hydrazono)methyl)-7-isopentoxycoumarin (**4f**)*

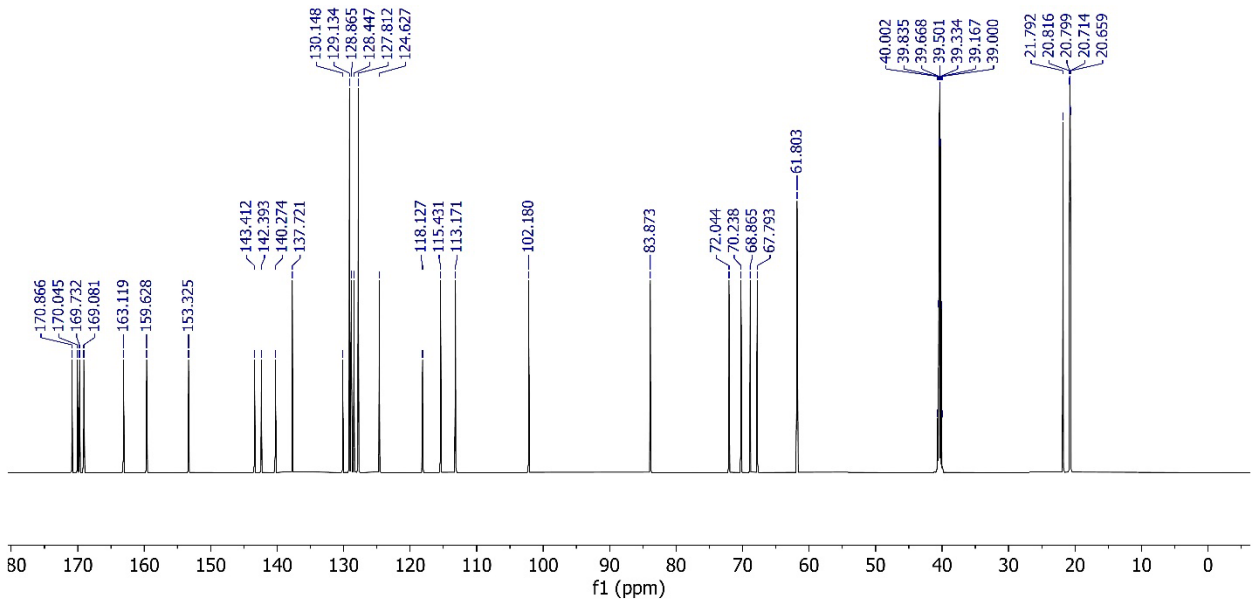


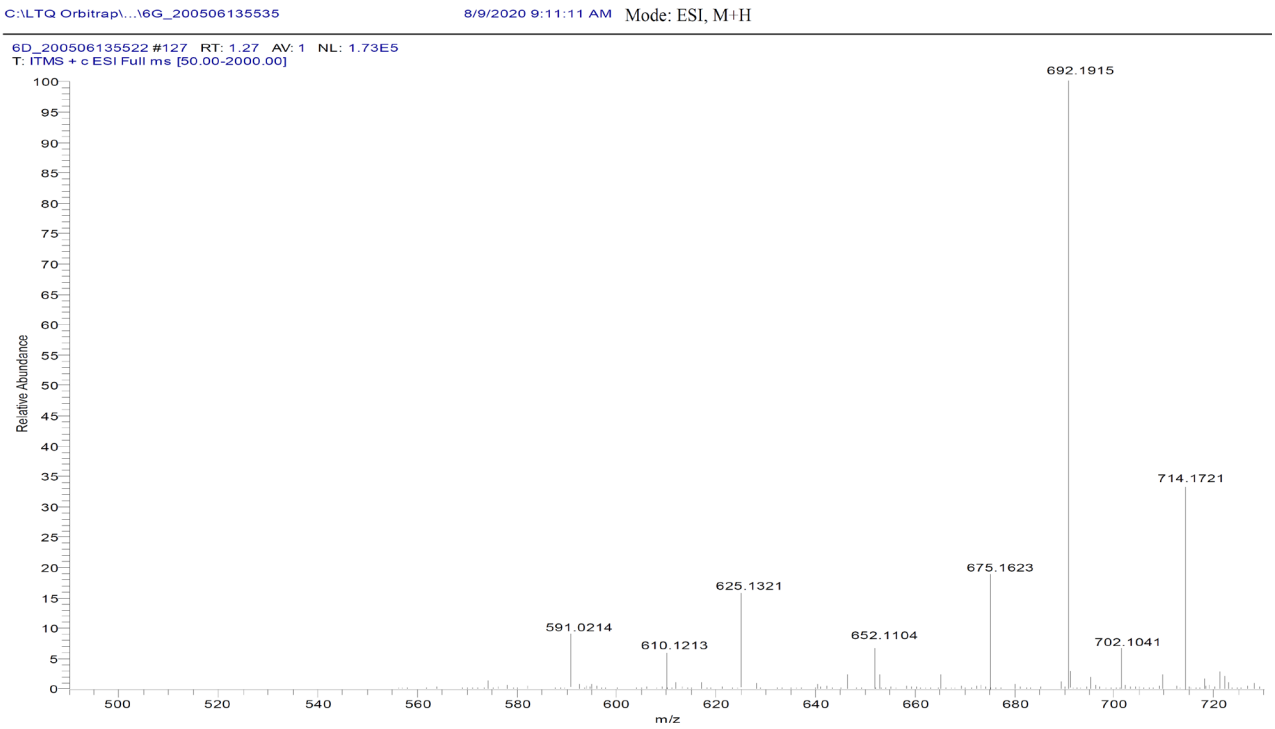




*4-(4'-Phenyl-3'-(2'',3'',4'',6''-tetra-O-acetyl-β-D-glucopyranosyl)thiazol-2'(3'H)-ylidene)hydrazono)methyl)-7-methylcoumarin (**4g**)*




130.148
129.134
128.865
128.447
127.812
124.627
40.002
39.835
39.668
39.501
39.334
39.167
39.000
21.792
20.816
20.799
20.714
20.659
61.803
143.412
142.393
140.274
137.721
118.127
115.431
113.171
102.180
83.873
72.044
70.238
68.865
67.793
170.866
170.045
169.732
169.081
163.119
159.628
153.325
f1 (ppm)


C:\LTQ Orbitrap\...\6G_200506135535
8/9/2020 9:11:11 AM
Mode: ESI, M+H
6D_200506135522 #127 RT: 1.27 AV: 1 NL: 1.73E5
T: ITMS + c ESI Full ms [50.00-2000.00]
692.1915
714.1721
675.1623
625.1321
591.0214
610.1213
652.1104
702.1041
Relative Abundance
m/z