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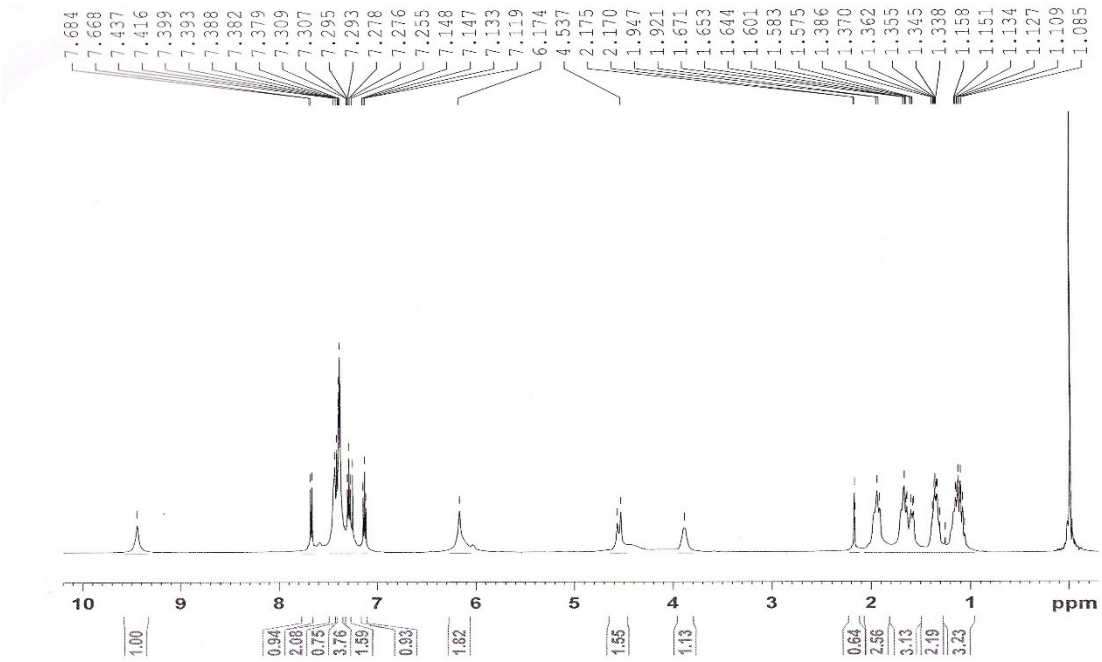
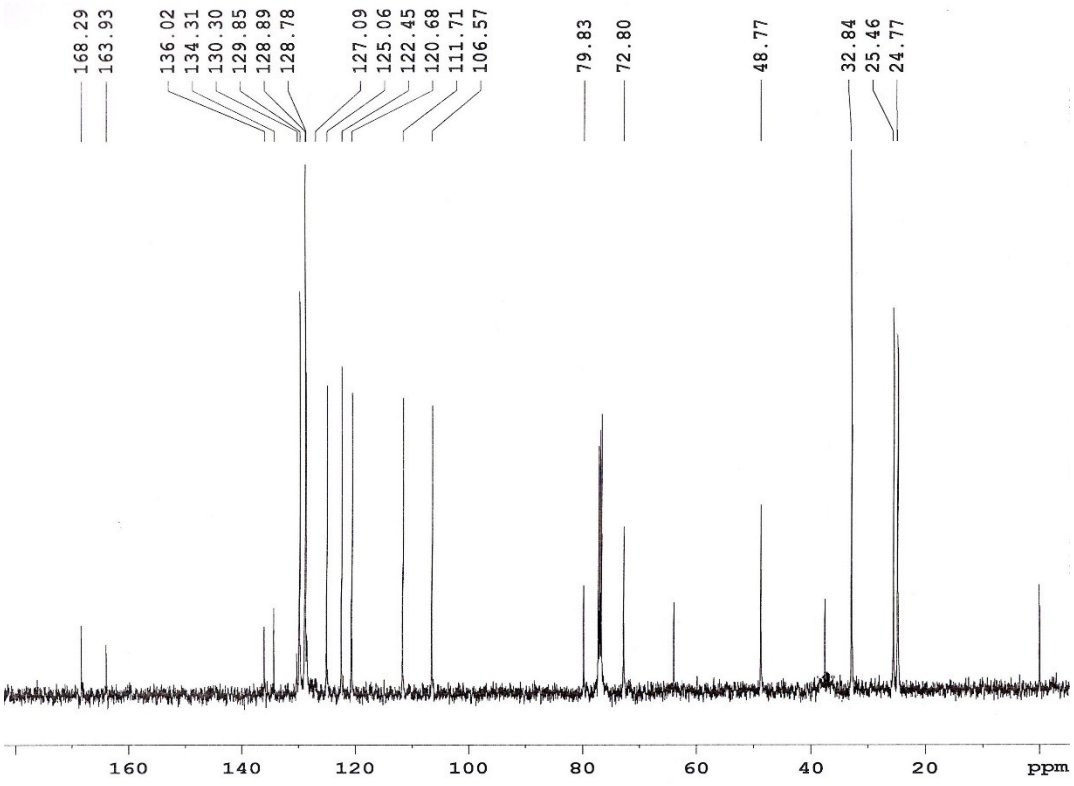
Supporting Information

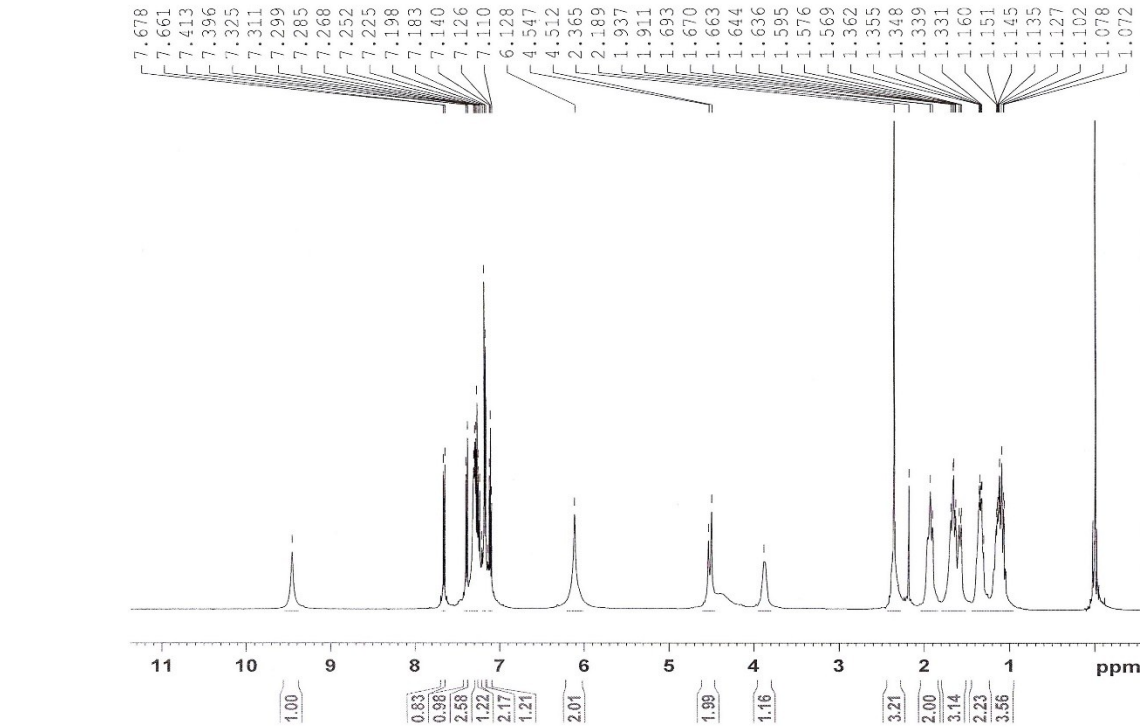
Experimental and Computational Evidences for KO*t*Bu-Promoted Synthesis of Oxopyrazino[1,2-*a*]indoles

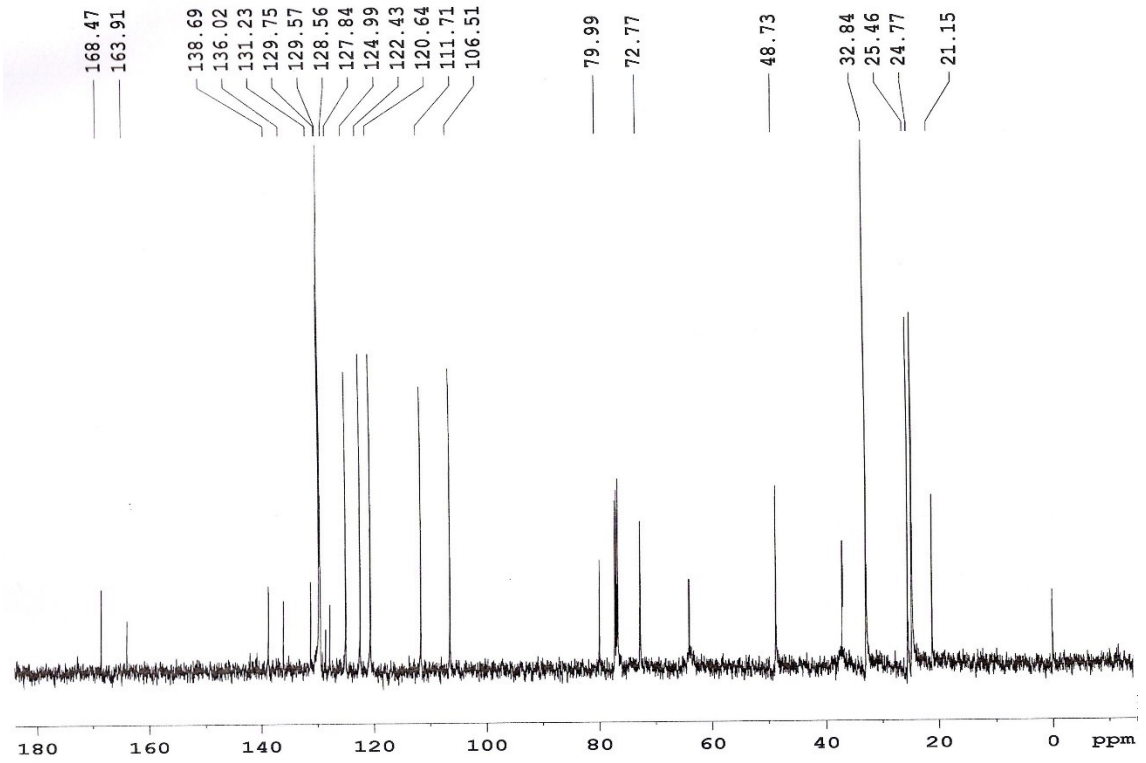
N-(2-(Cyclohexylamino)-2-oxo-1-phenylethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1a***



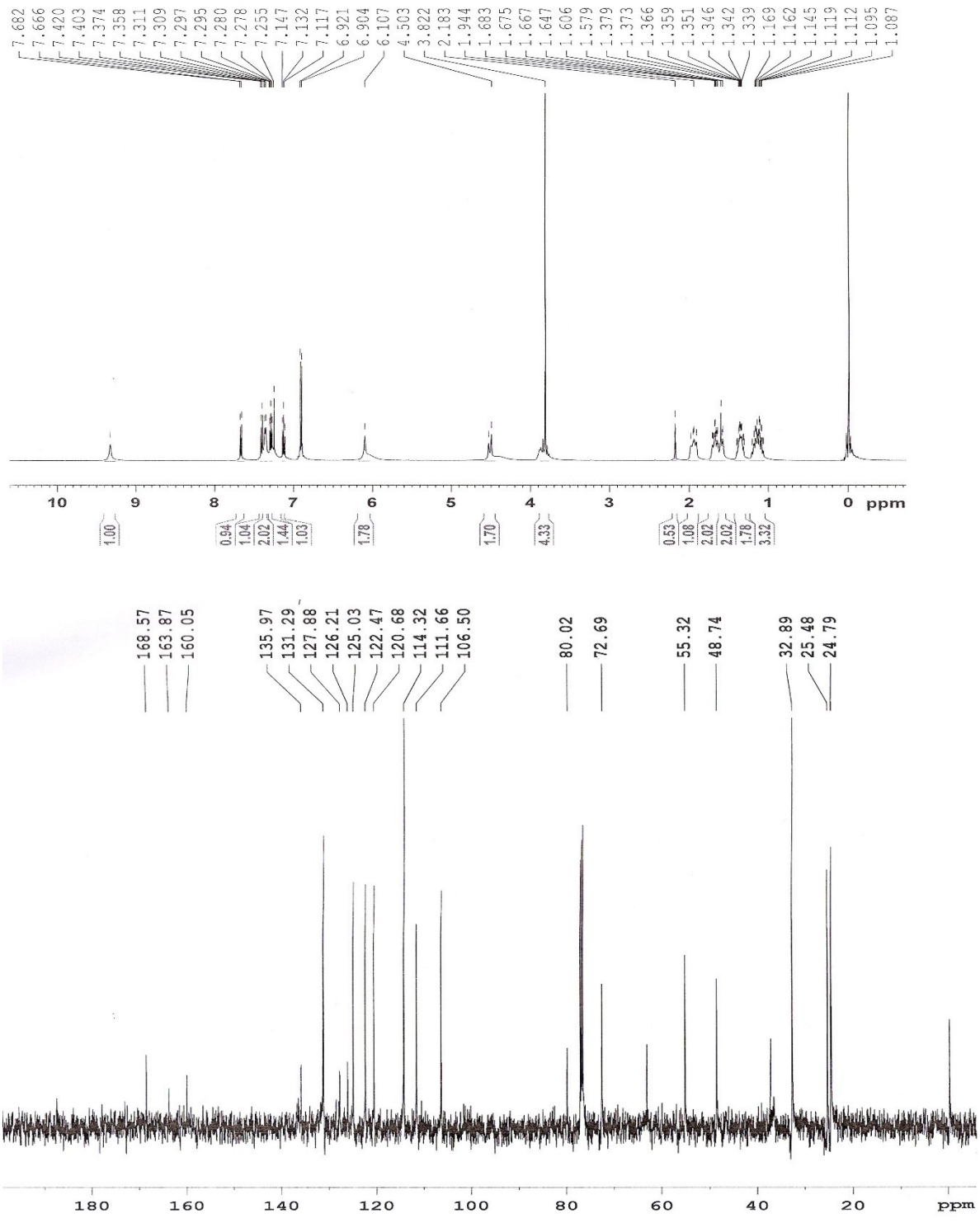


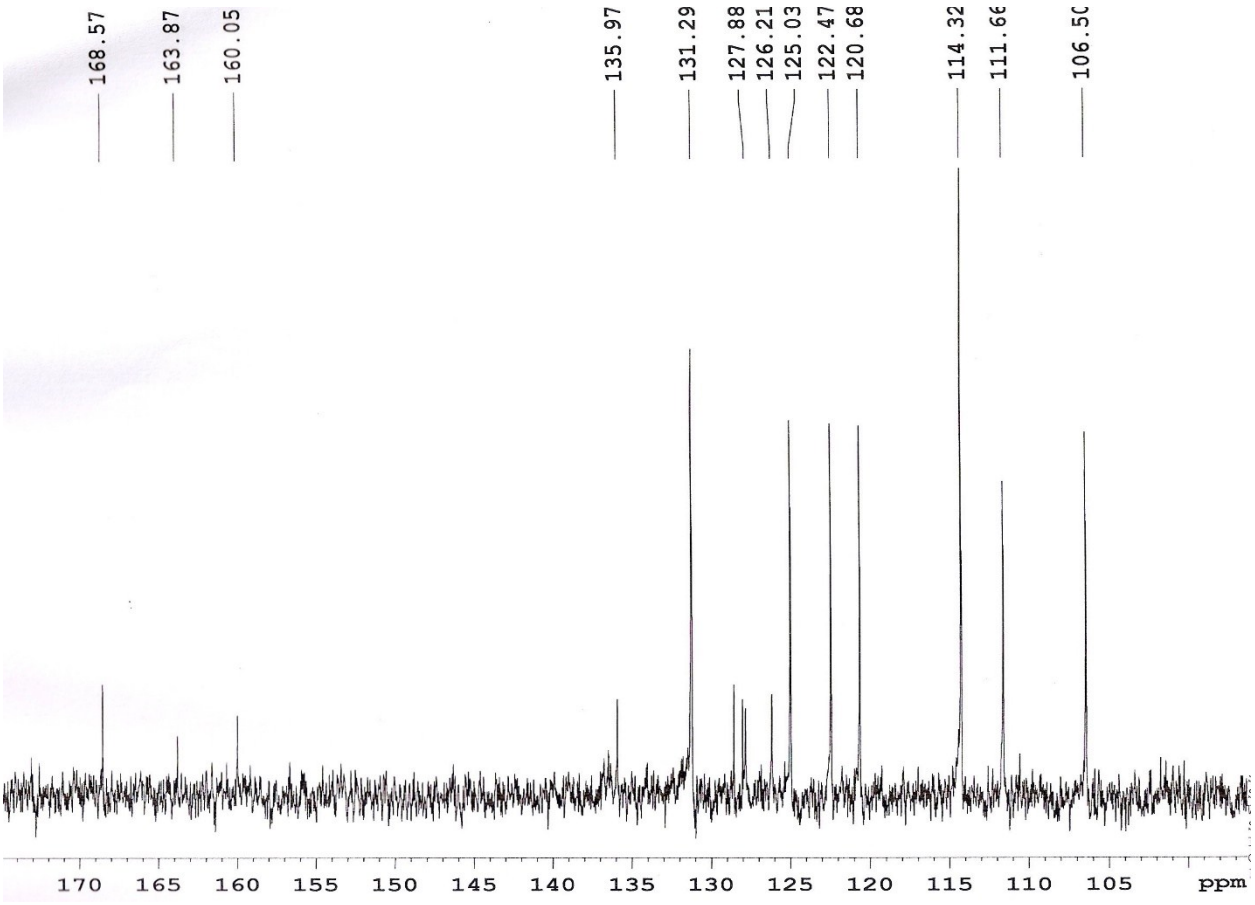
N-(2-(Cyclohexylamino)-2-oxo-1-(p-tolyl)ethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1b***





N-(2-(Cyclohexylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1c***

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163.87
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127.88
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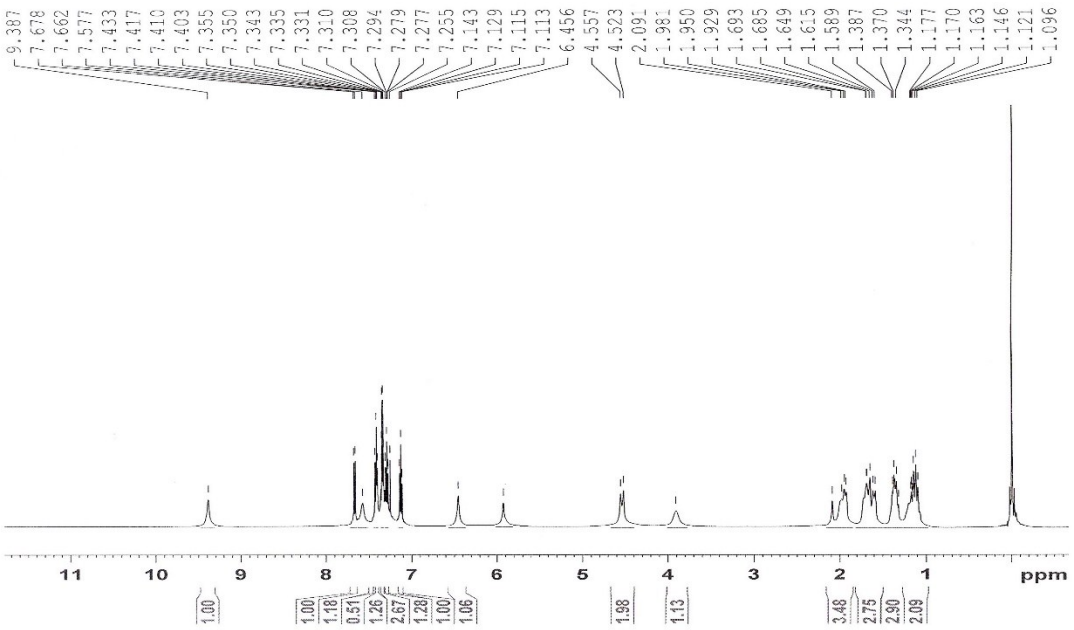
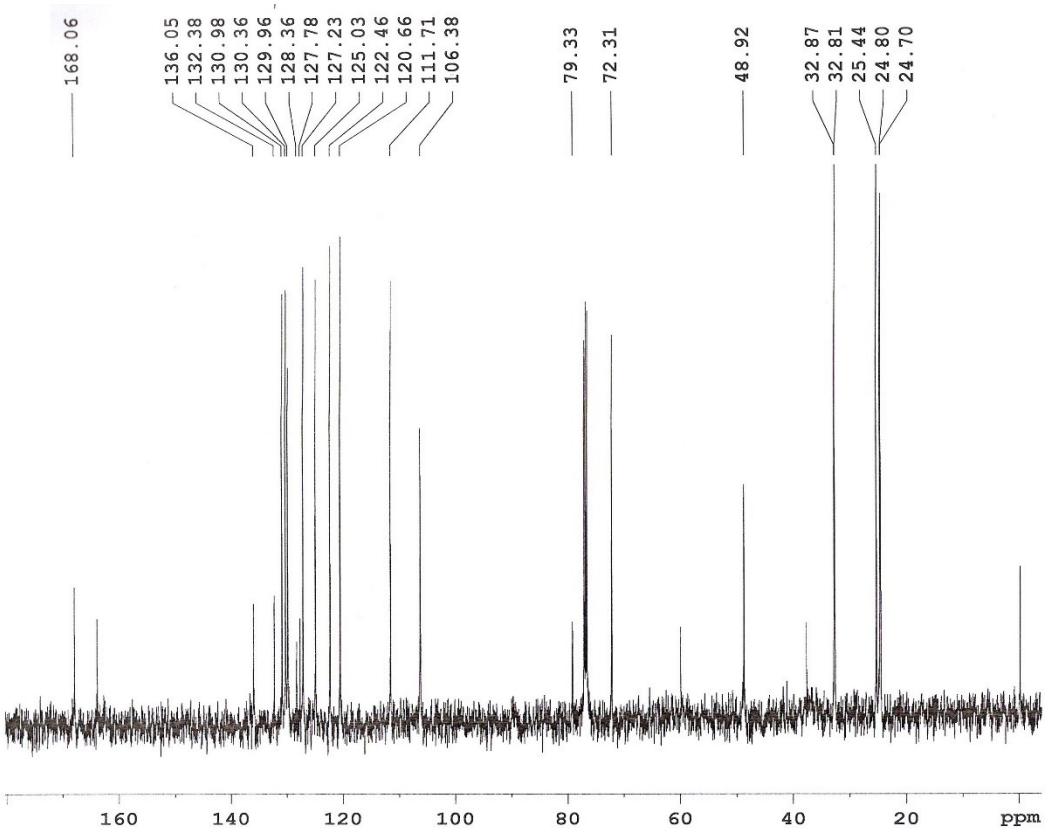
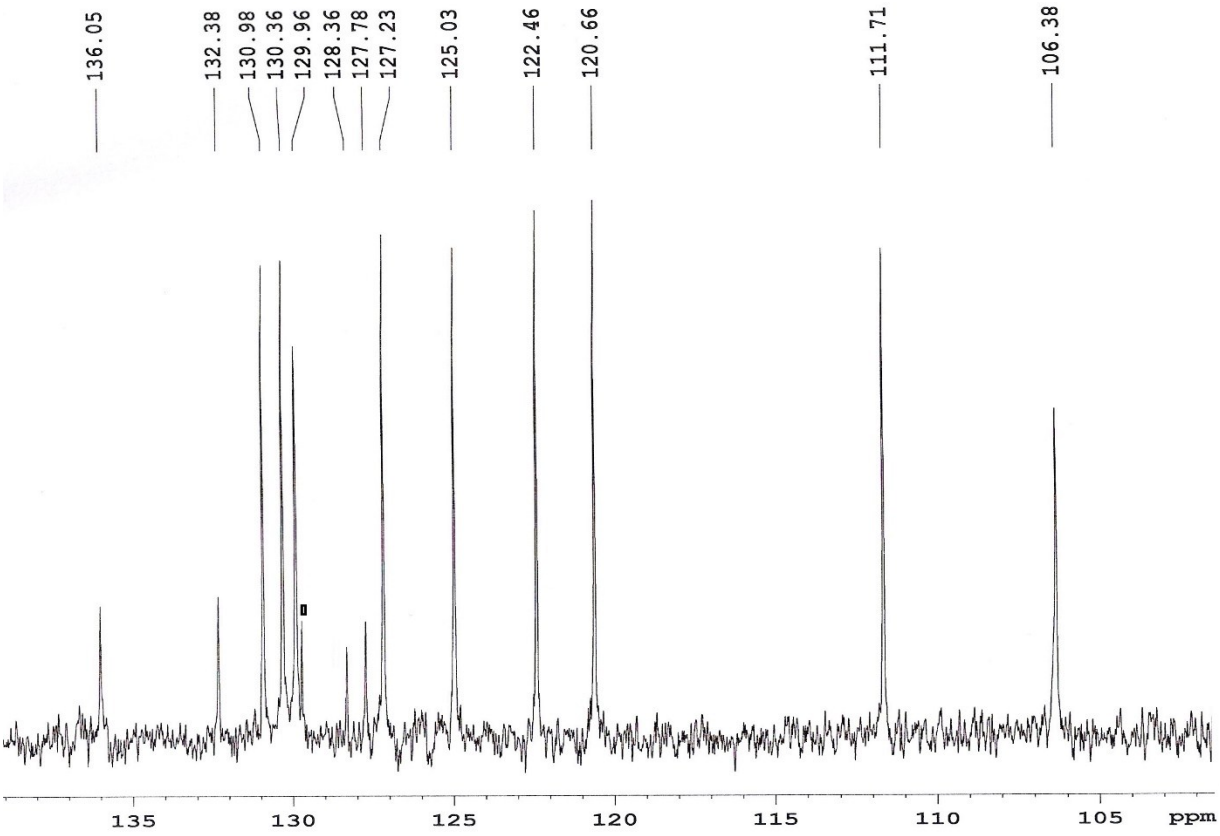
125.03
122.47
120.68
114.32
111.66
106.50
170
165
160
155
150
145
140
135
130
125
120
115
110
105
ppm

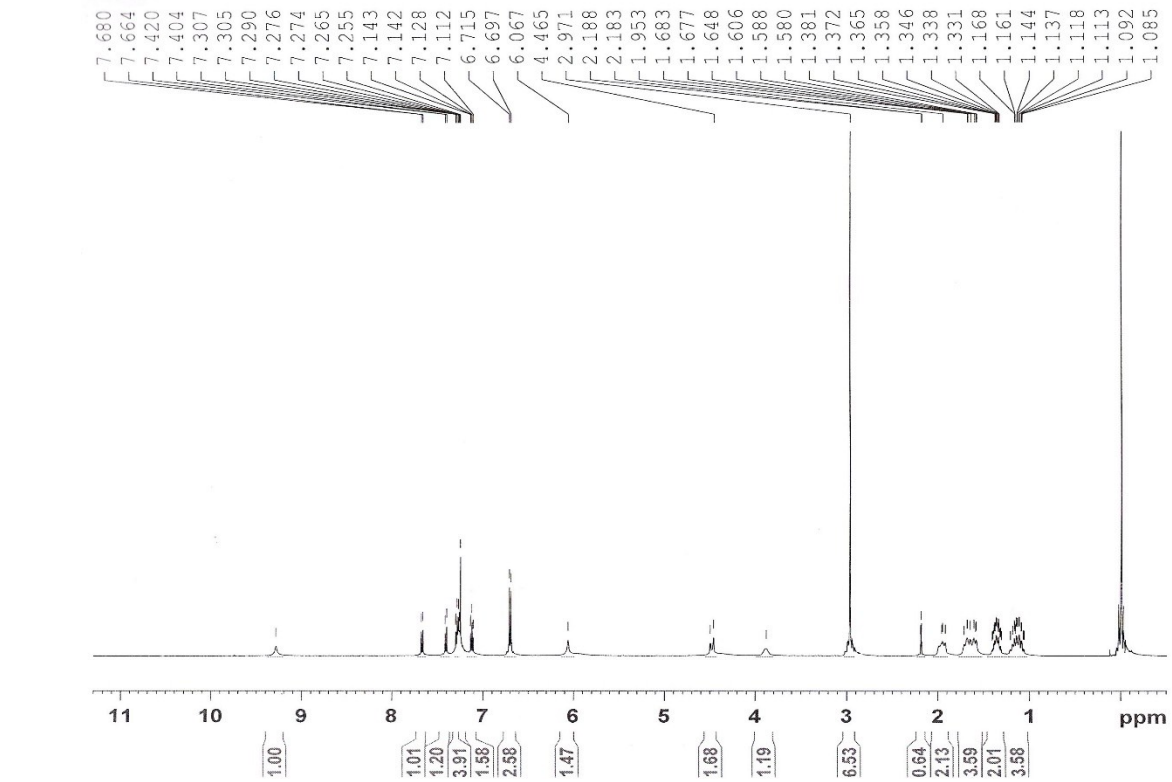
N-(1-(2-Chlorophenyl)-2-(cyclohexylamino)-2-oxoethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1d***

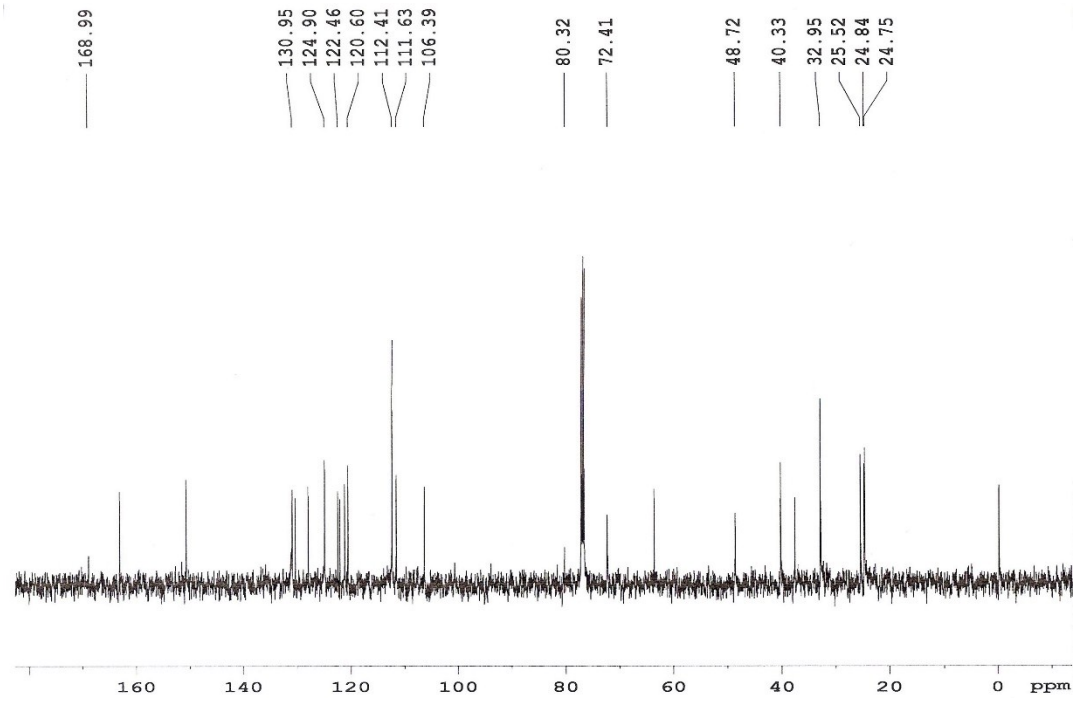


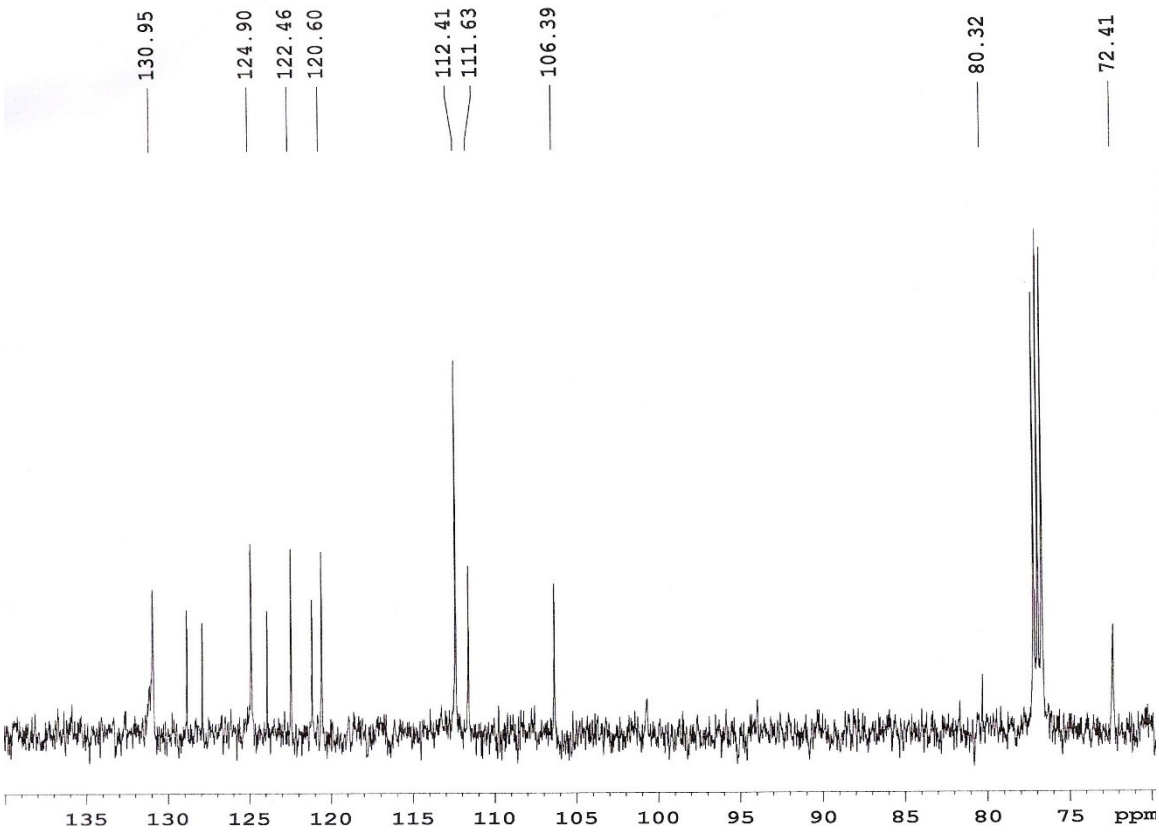



136.05
132.38
130.98
130.36
129.96
128.36
127.78
127.23
125.03
122.46
120.66
111.71
106.38
135
130
125
120
115
110
105
ppm

N-(2-(Cyclohexylamino)-1-(4-(dimethylamino)phenyl)-2-oxoethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1e***



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124.90
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135
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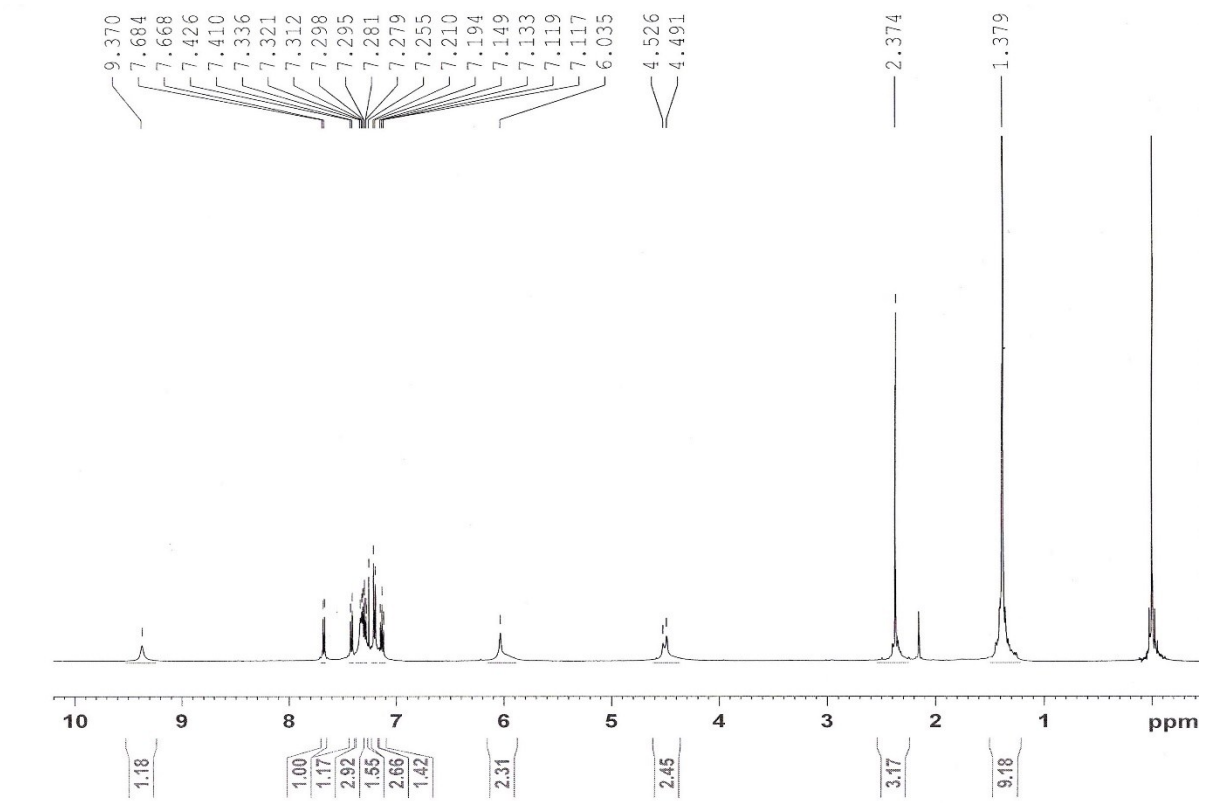
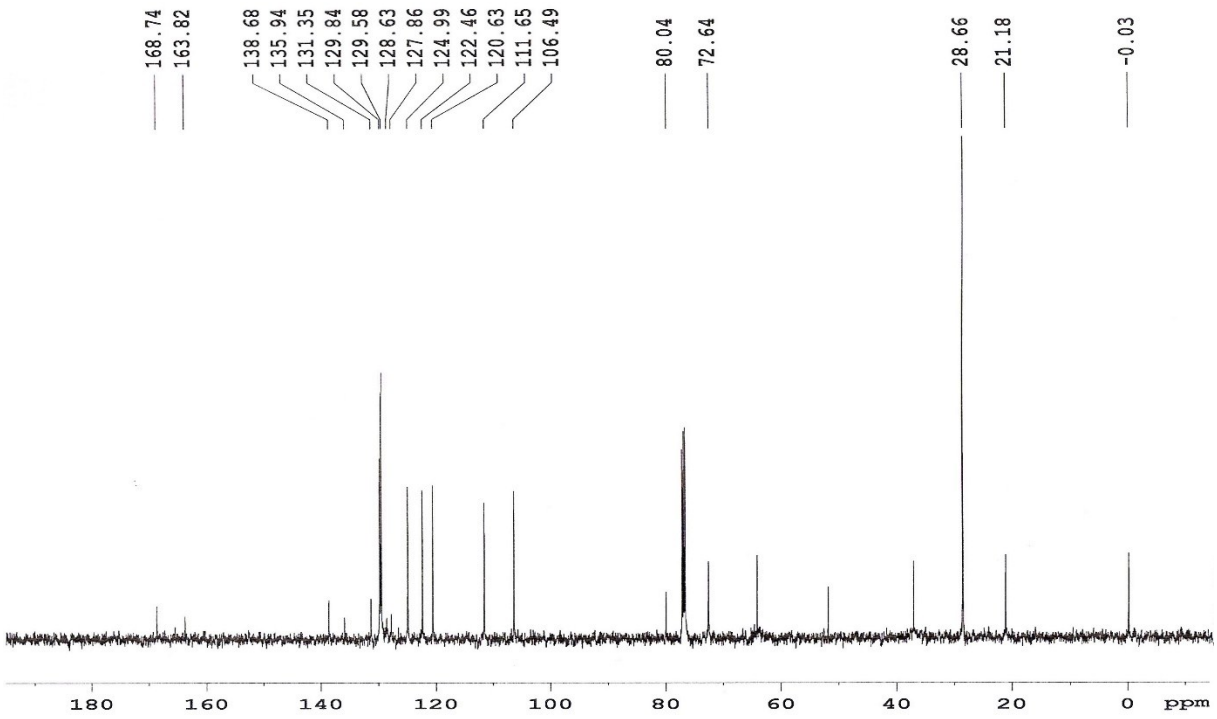
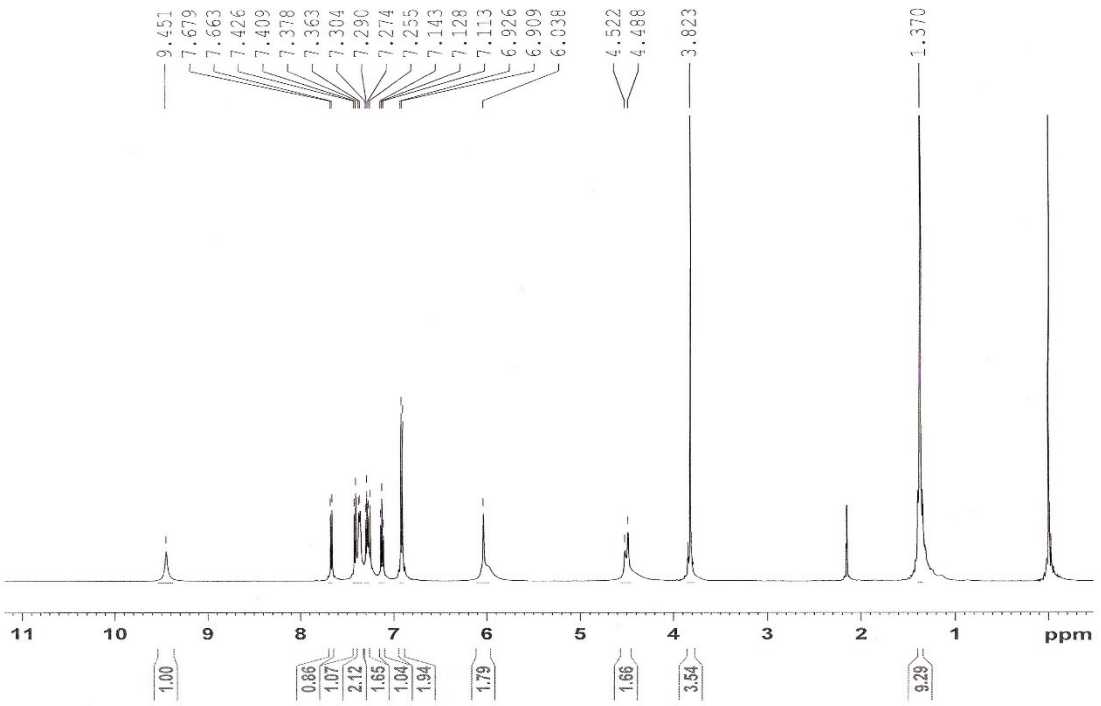
125
120
115
110
105
100
95
90
85
80
75
ppm

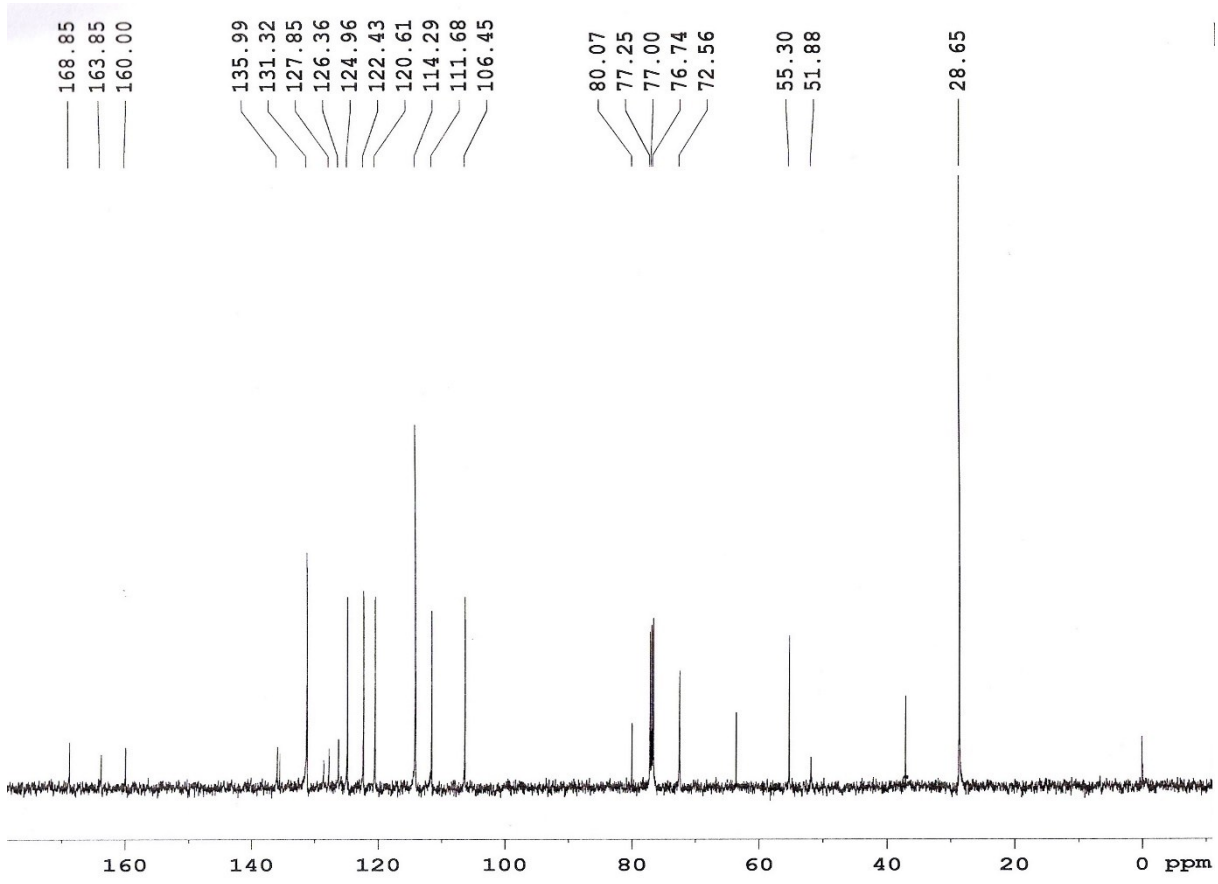
N-(2-(tert-Butylamino)-2-oxo-1-(p-tolyl)ethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1f***

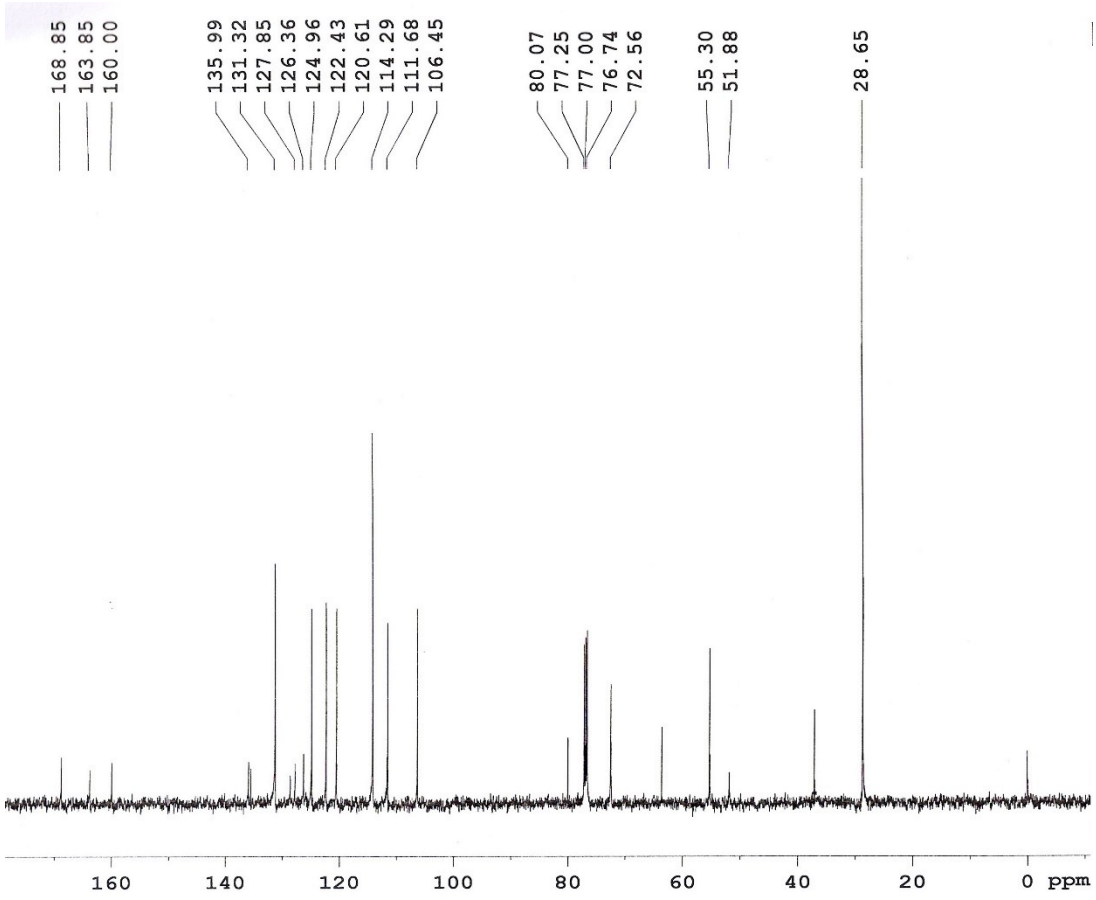




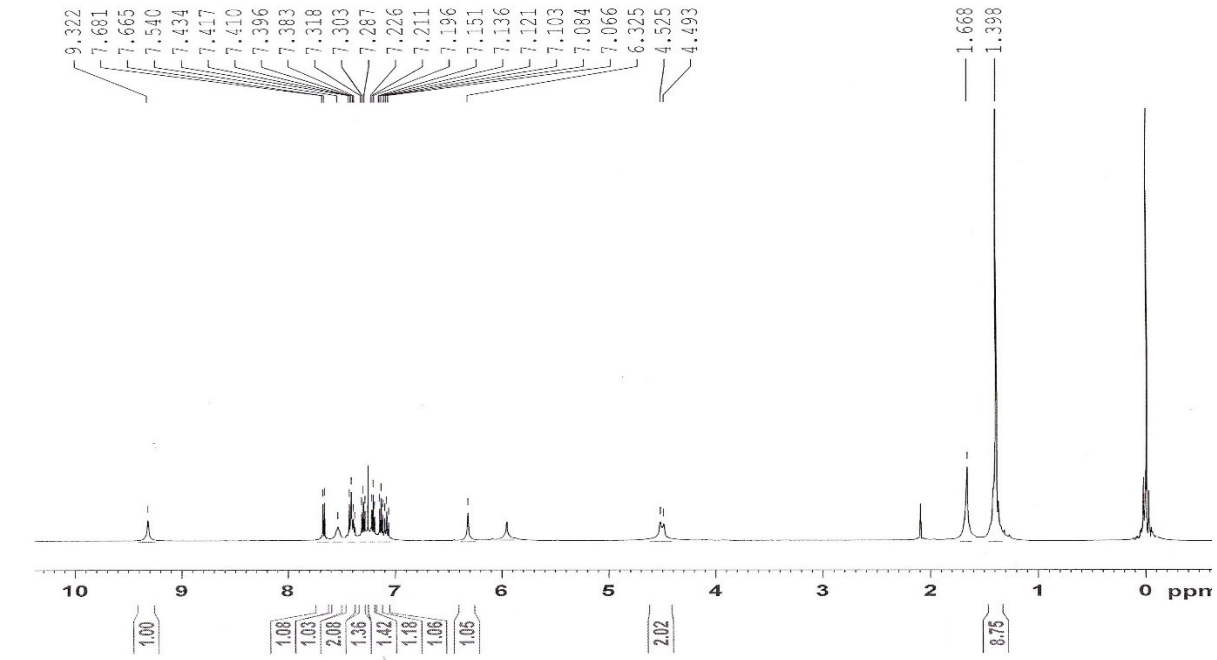
N-(2-(tert-Butylamino)-1-(4-methoxyphenyl)-2-oxoethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1g***

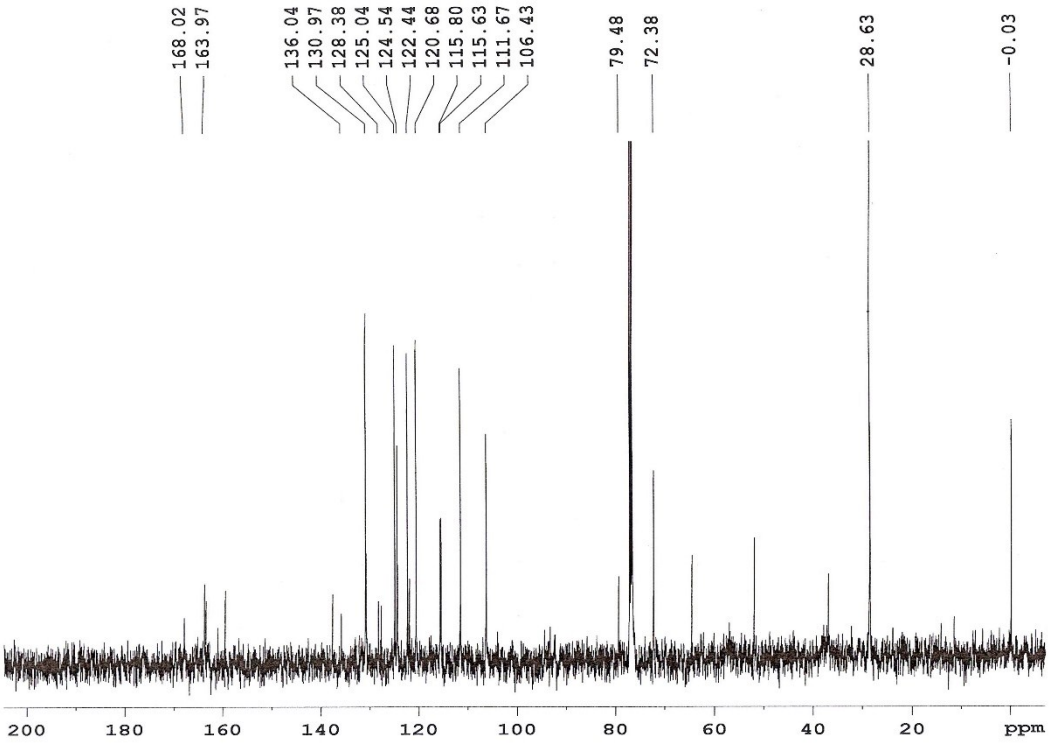


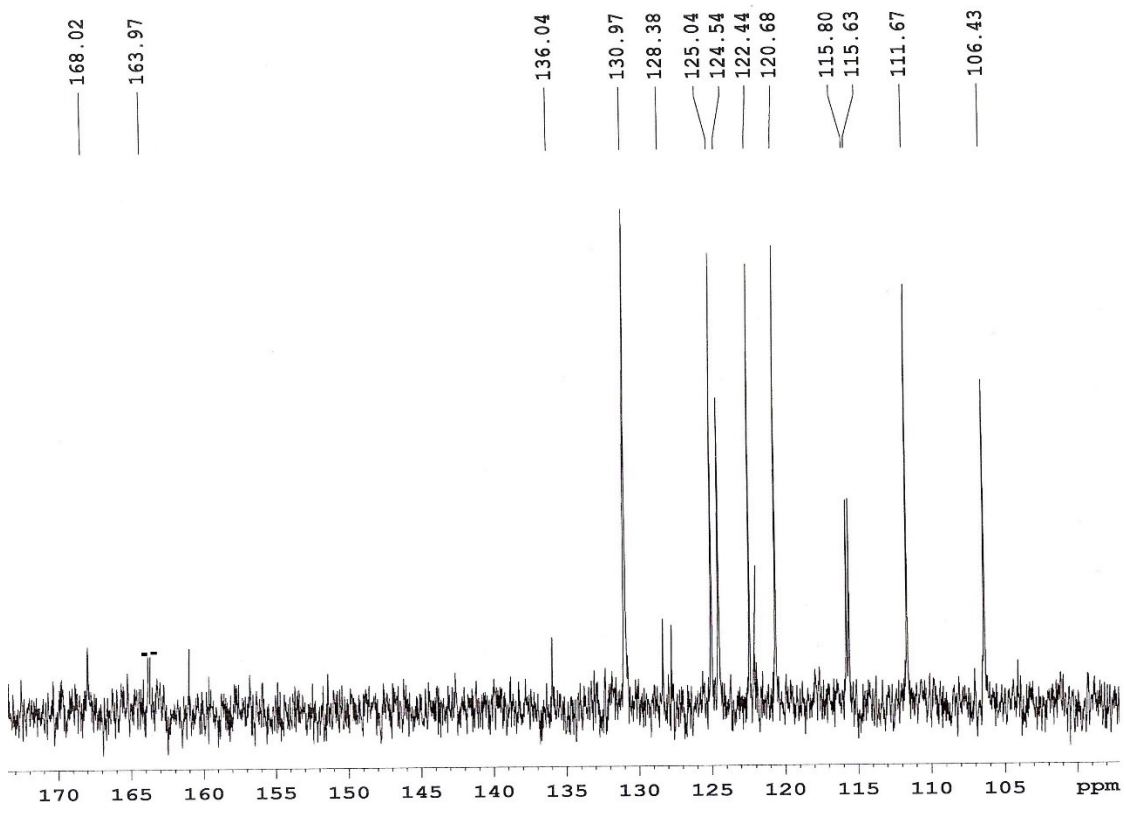



168.85
163.85
160.00
135.99
131.32
127.85
126.36
124.96
122.43
120.61
114.29
111.68
106.45
80.07
77.25
77.00
76.74
72.56
55.30
51.88
28.65
160
140
120
100
80
60
40
20
0 ppm

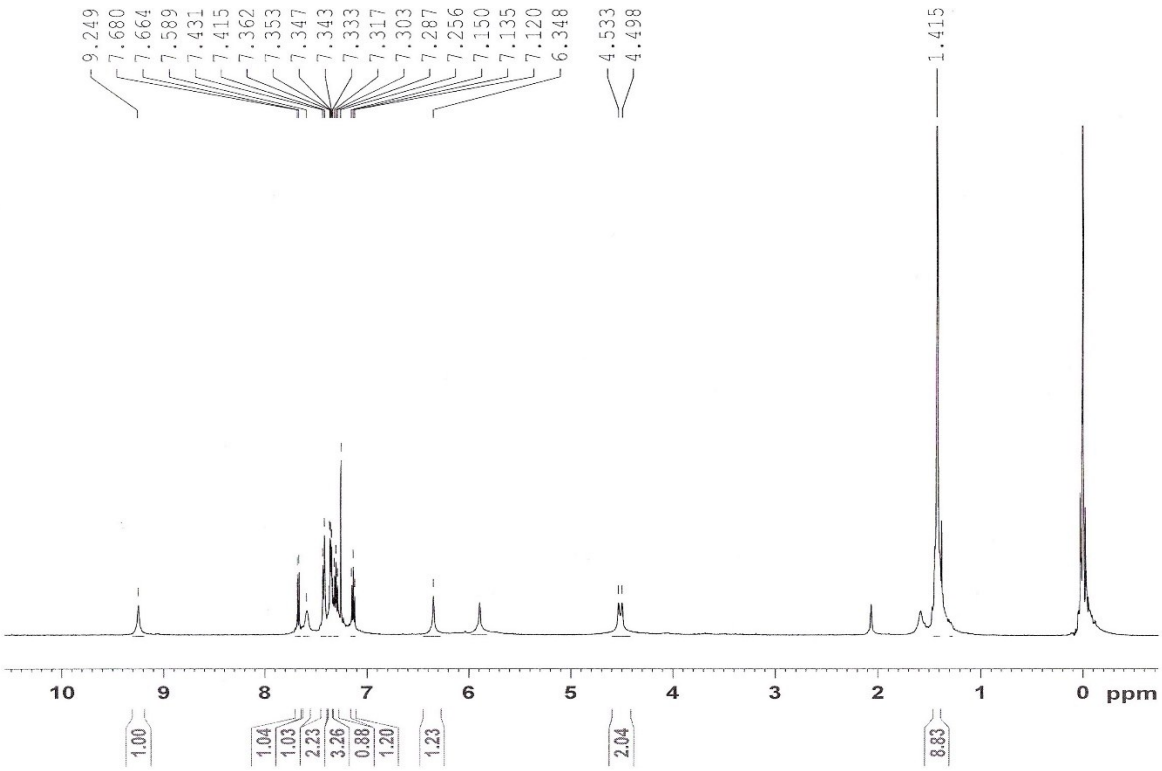
N-(2-(tert-Butylamino)-1-(2-fluorophenyl)-2-oxoethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1h***

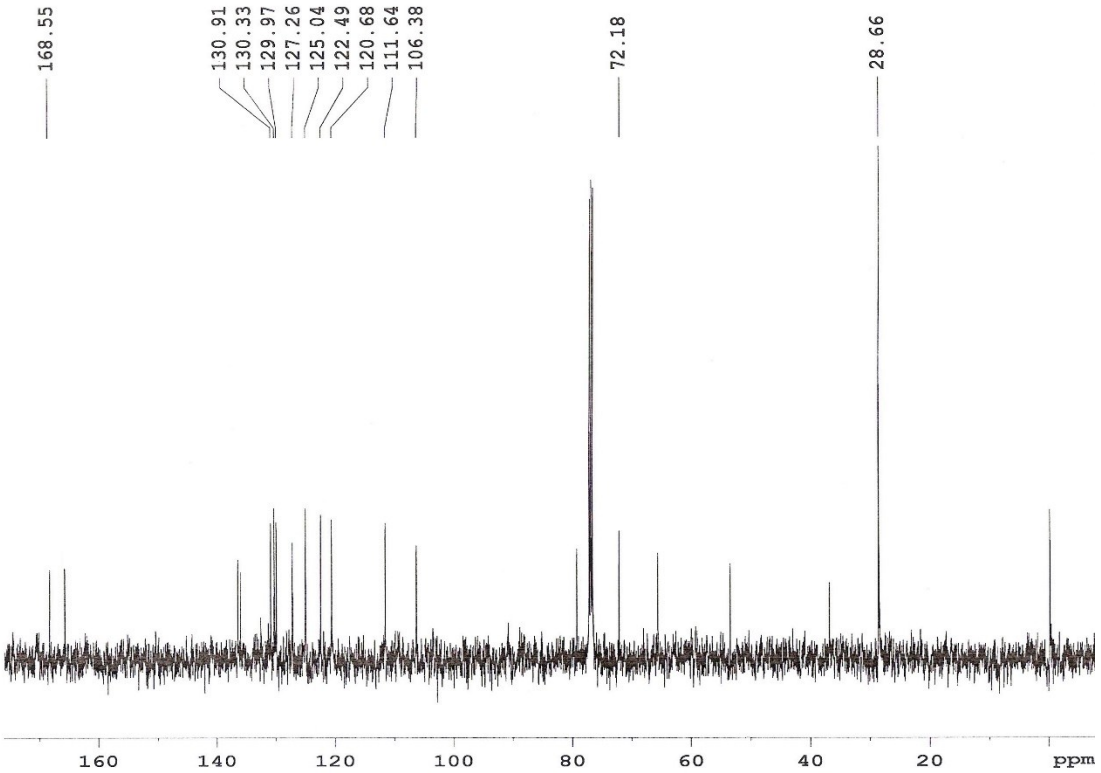


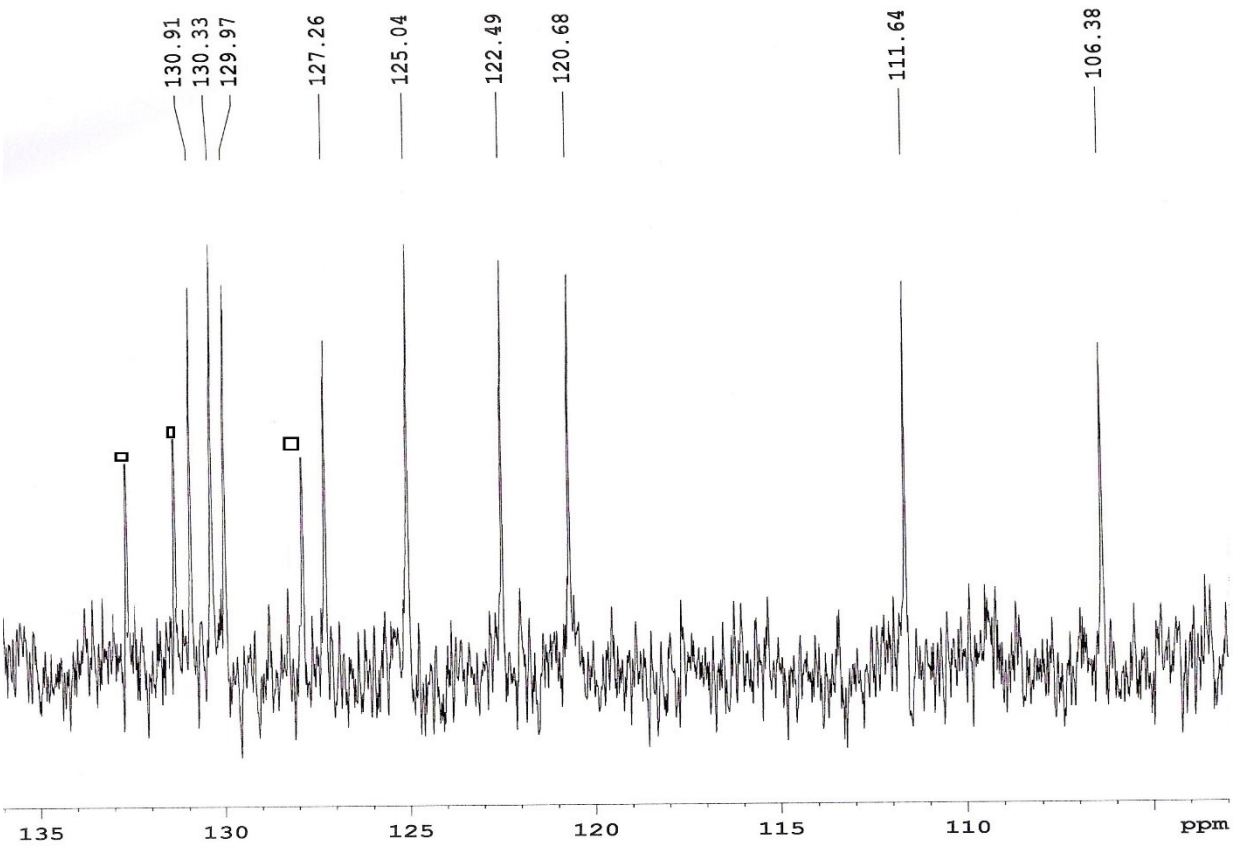



168.02
163.97
136.04
130.97
128.38
125.04
124.54
122.44
120.68
115.80
115.63
111.67
106.43
170
165
160
155
150
145
140
135
130
125
120
115
110
105
ppm

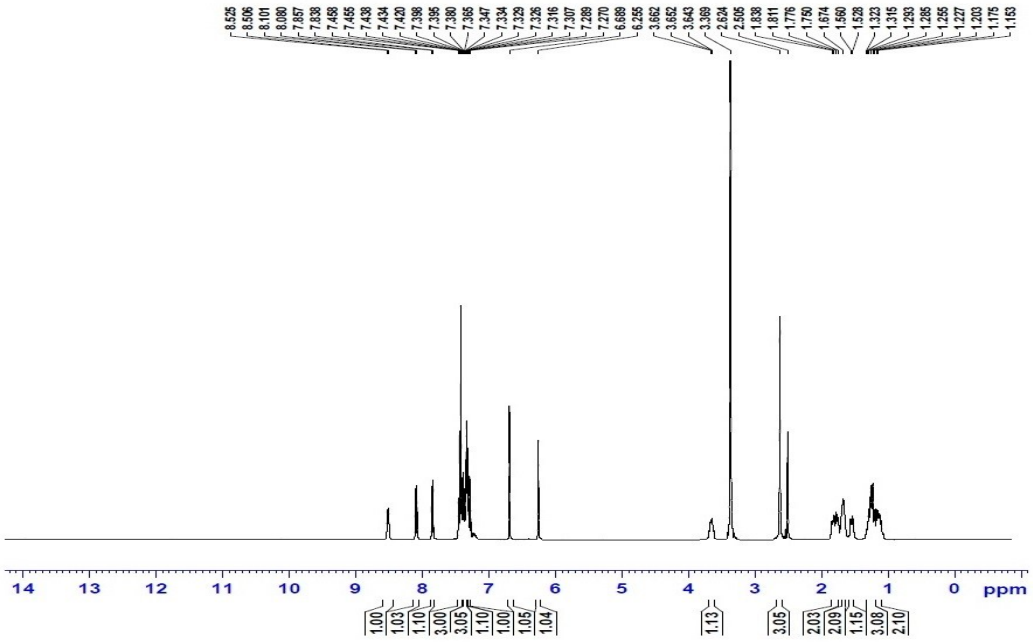
N-(2-(tert-Butylamino)-1-(2-chlorophenyl)-2-oxoethyl)-N-(prop-2-yn-1-yl)-1H-indole-2-carboxamide ***1i***

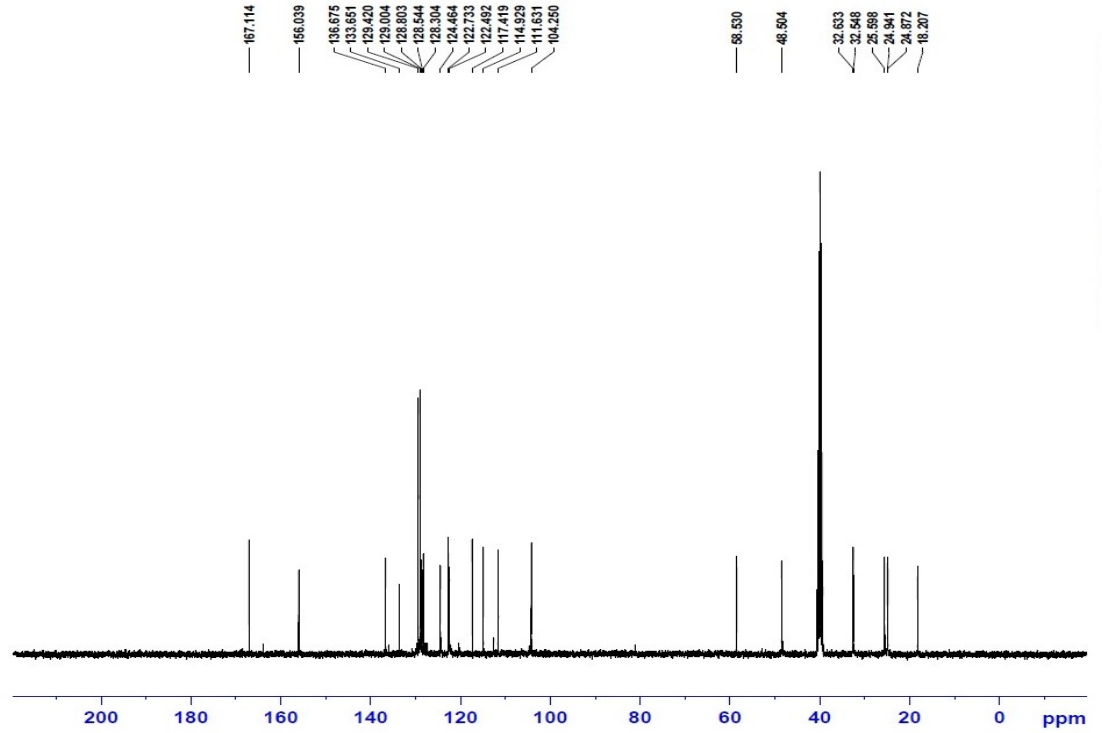





130.91
130.33
129.97
127.26
125.04
122.49
120.68
111.64
106.38
135
130
125
120
115
110
ppm

N-Cyclohexyl-2-(4-methyl-1-oxopyrazino[1,2-a]indol-2(1H)-yl)-2-phenylacetamide ***2a***





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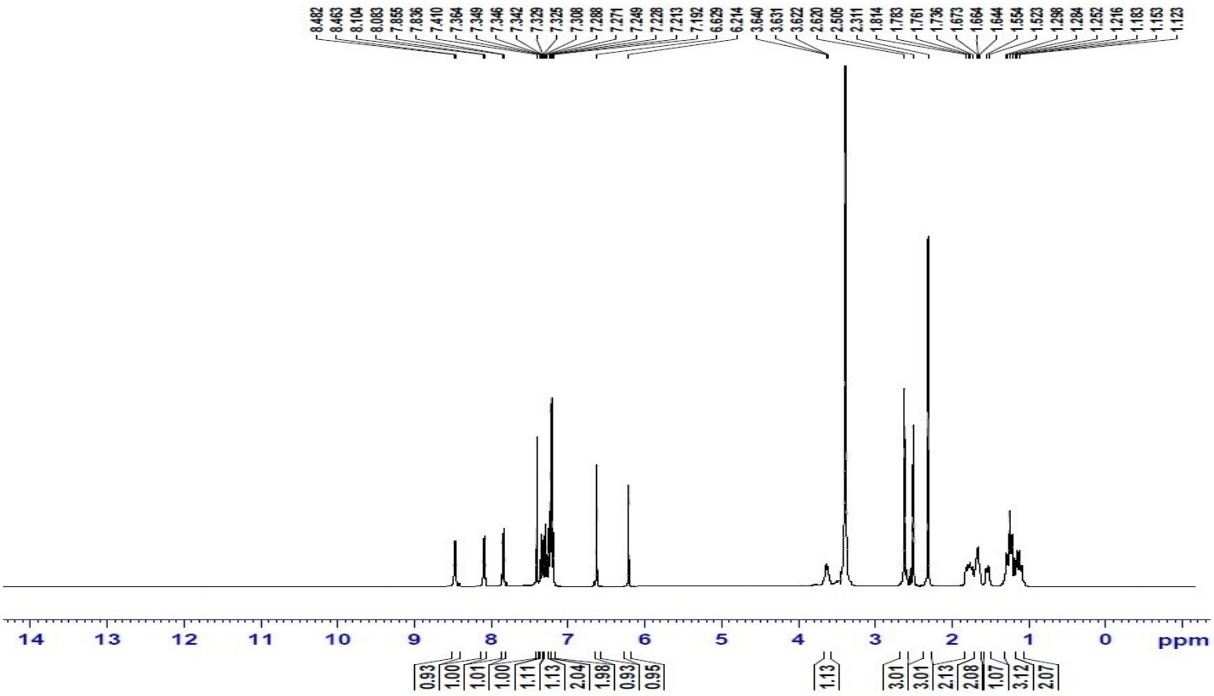
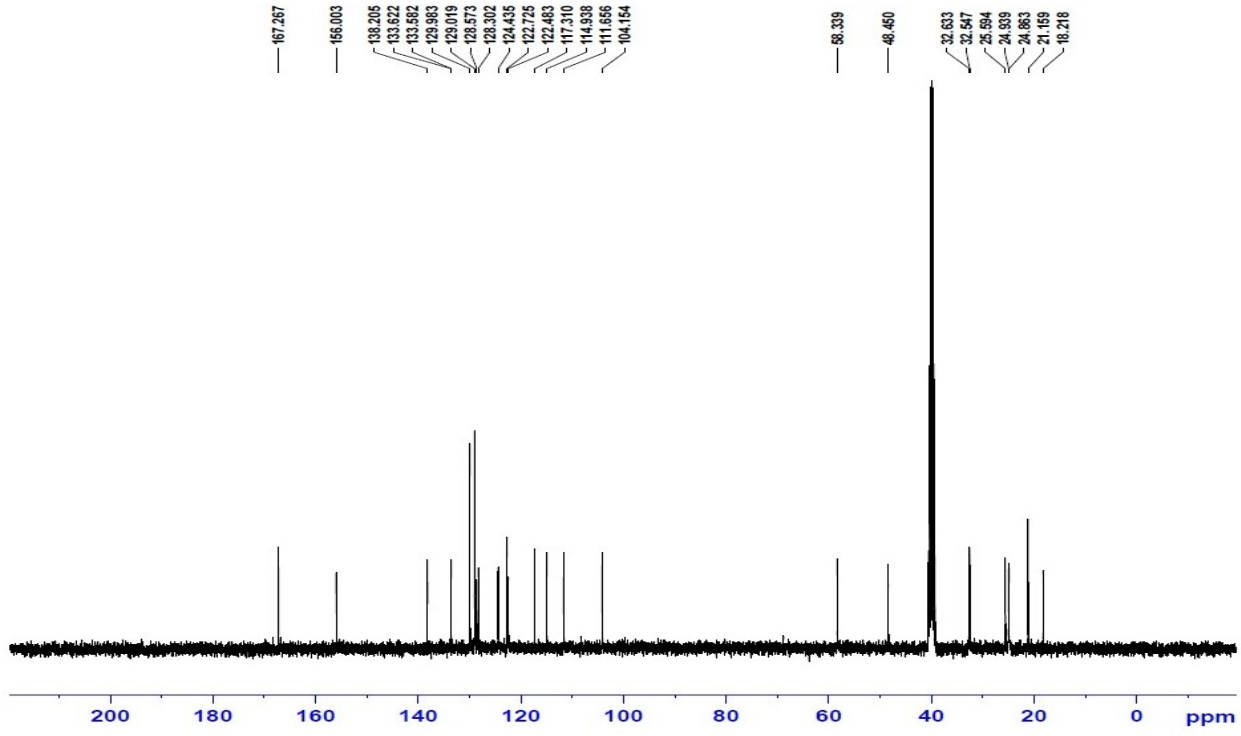
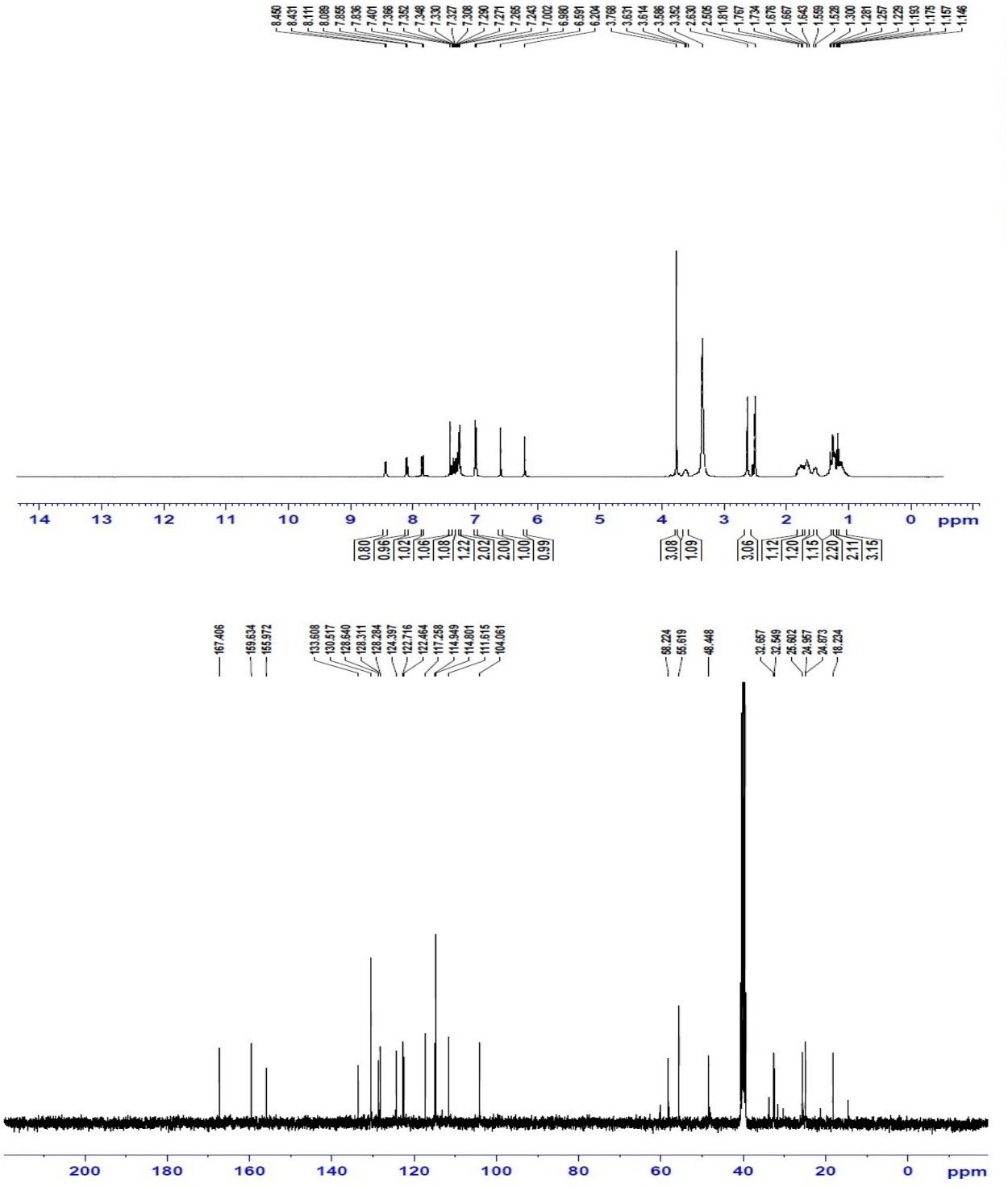




N-Cyclohexyl-2-(4-methoxyphenyl)-2-(4-methyl-1-oxopyrazino[1,2-a]indol-2(1H)-yl)acetamide ***2c***



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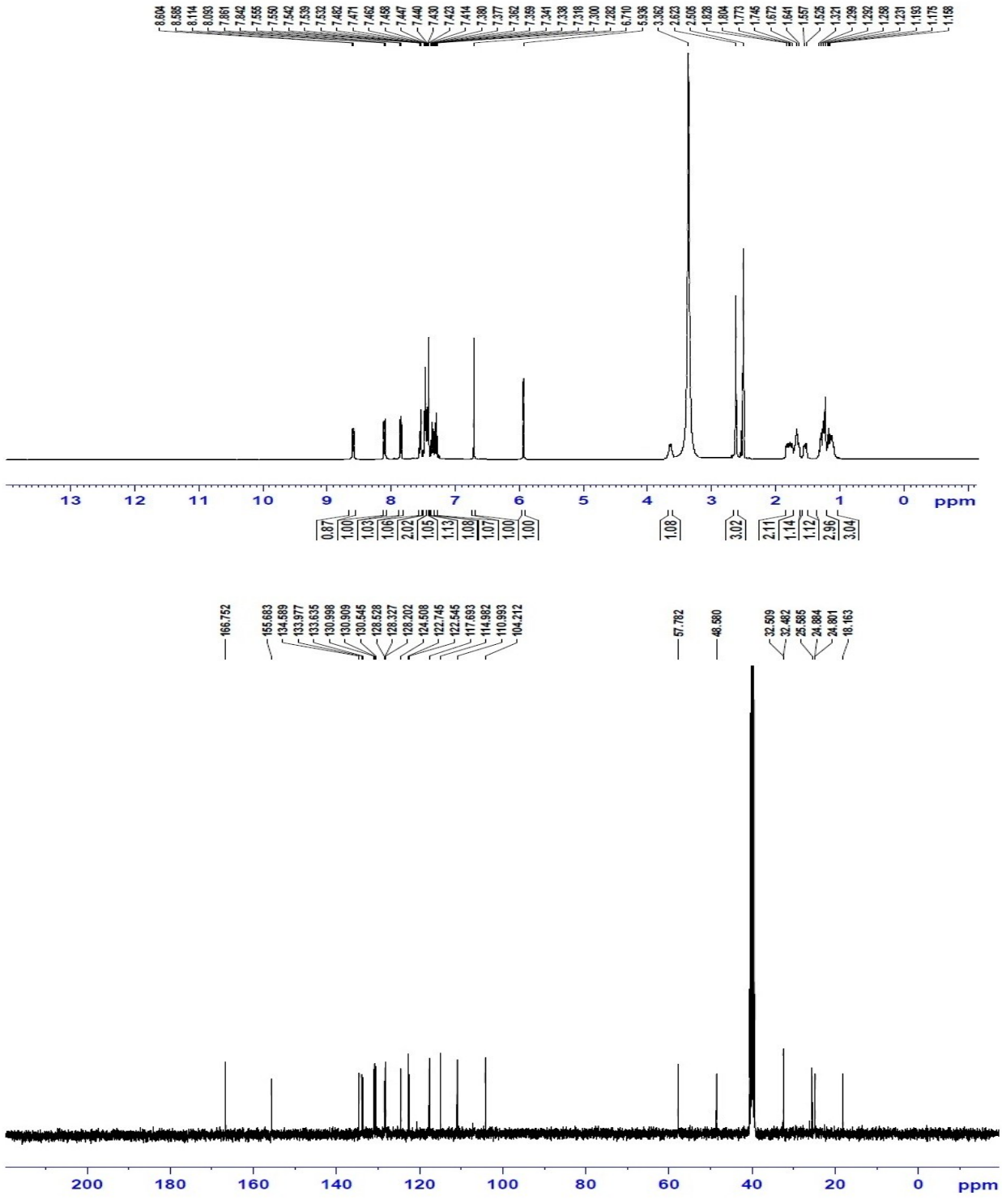
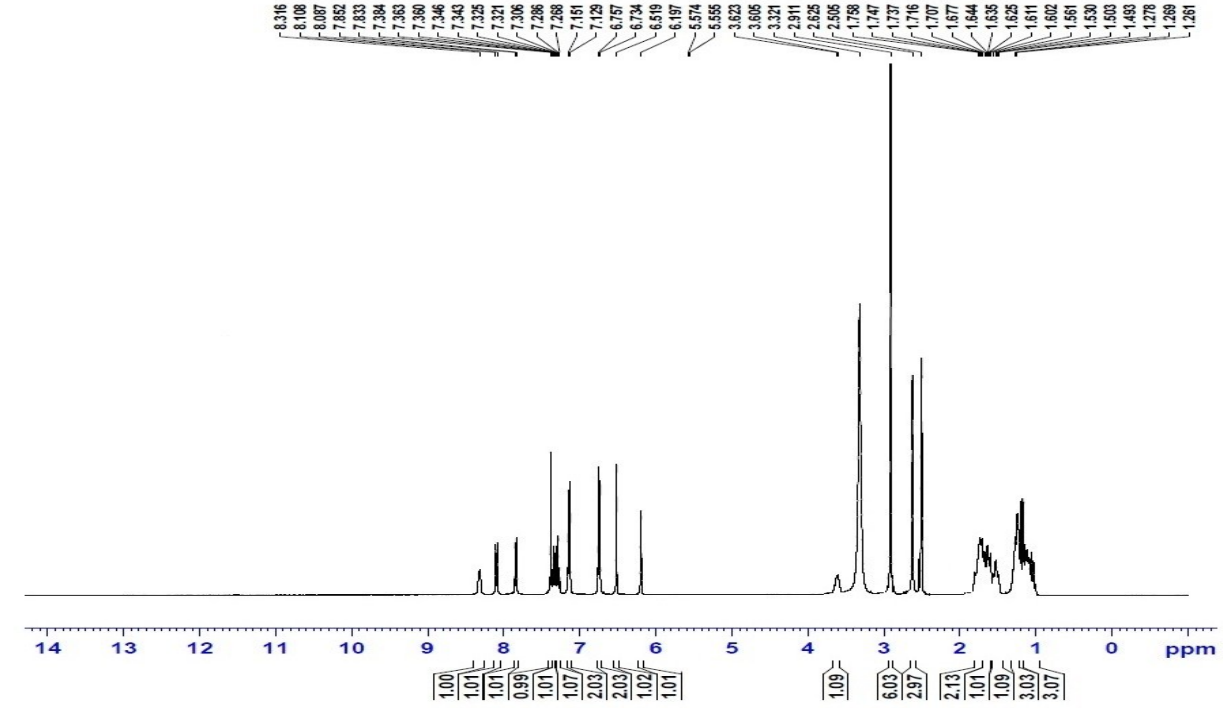
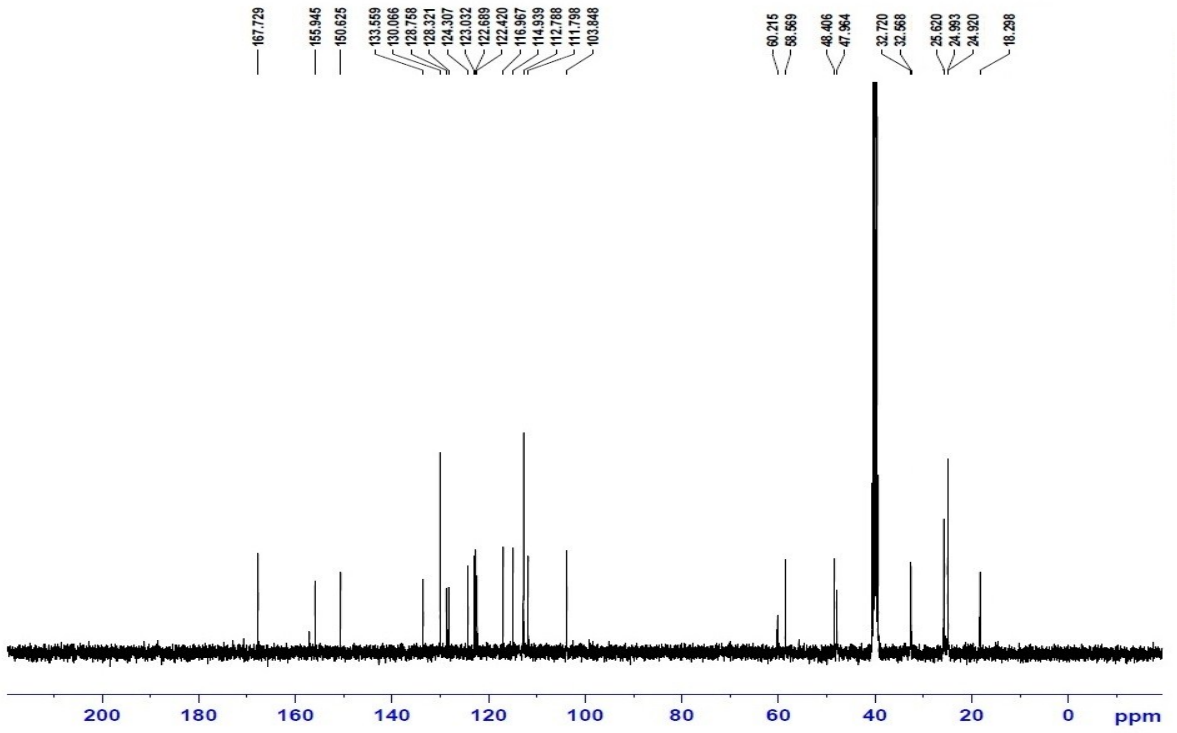
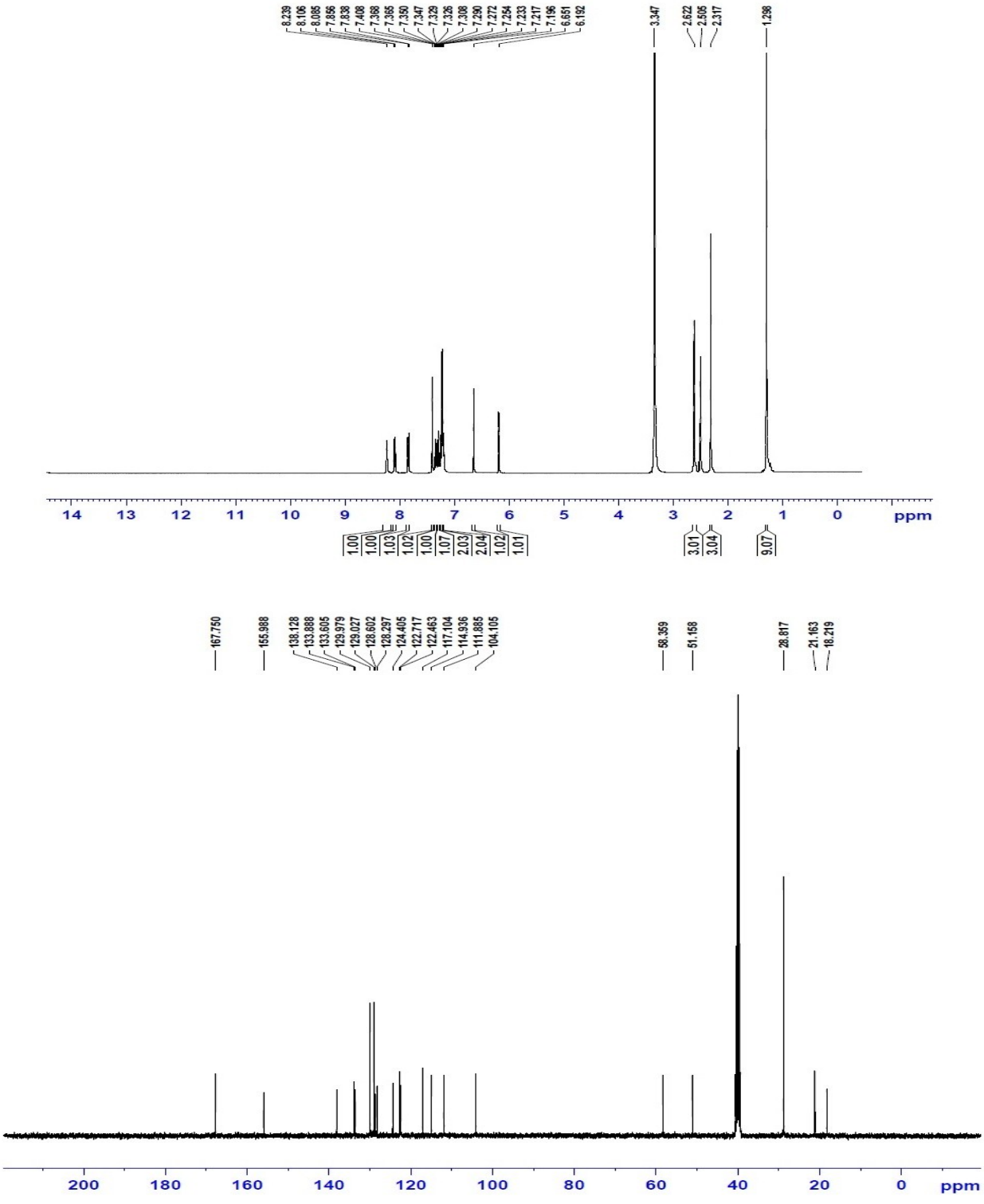


N-Cyclohexyl-2-(4-(dimethylamino)phenyl)-2-(4-methyl-1-oxopyrazino[1,2-a]indol-2(1H)-yl)acetamide ***2e***

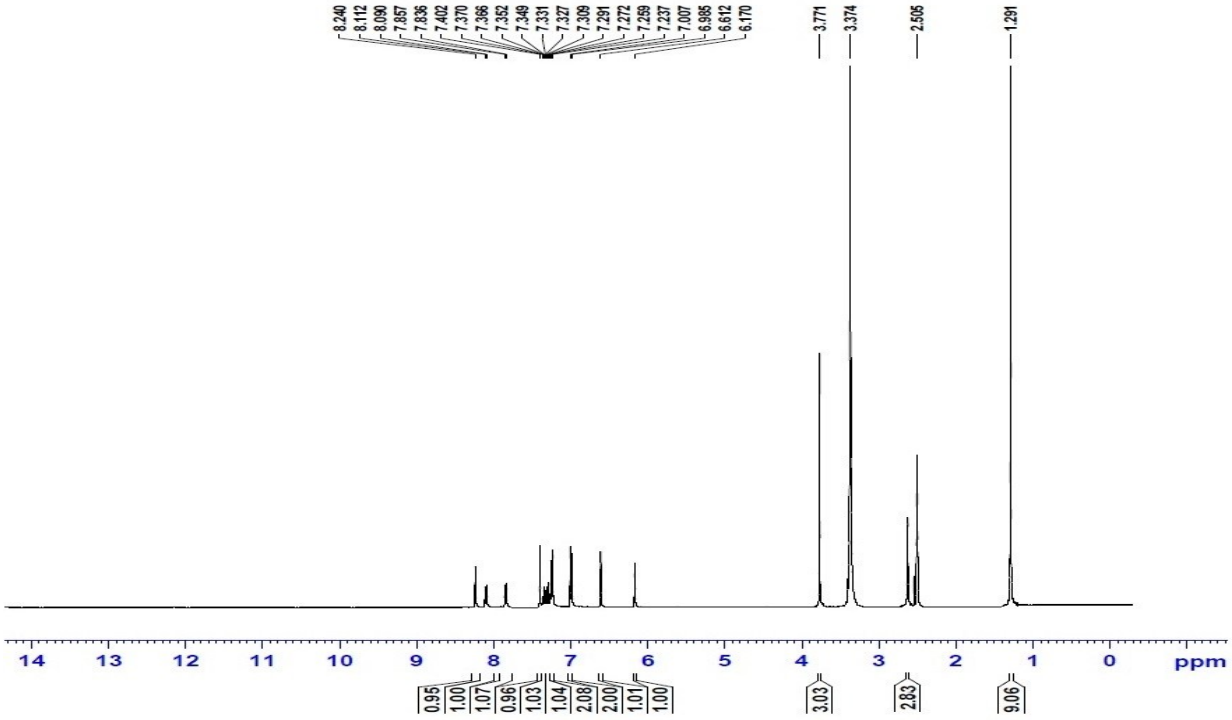


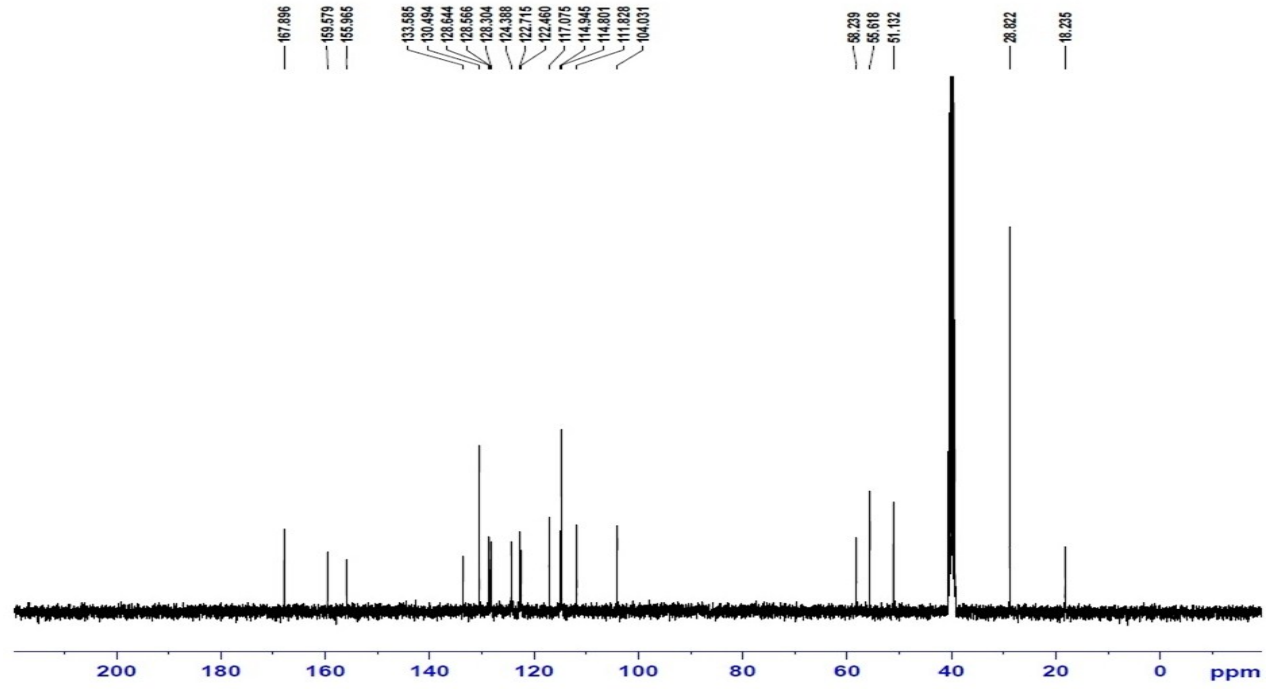


N-(tert-Butyl)-2-(4-methyl-1-oxopyrazino[1,2-a]indol-2(1H)-yl)-2-(p-tolyl)acetamide ***2f***

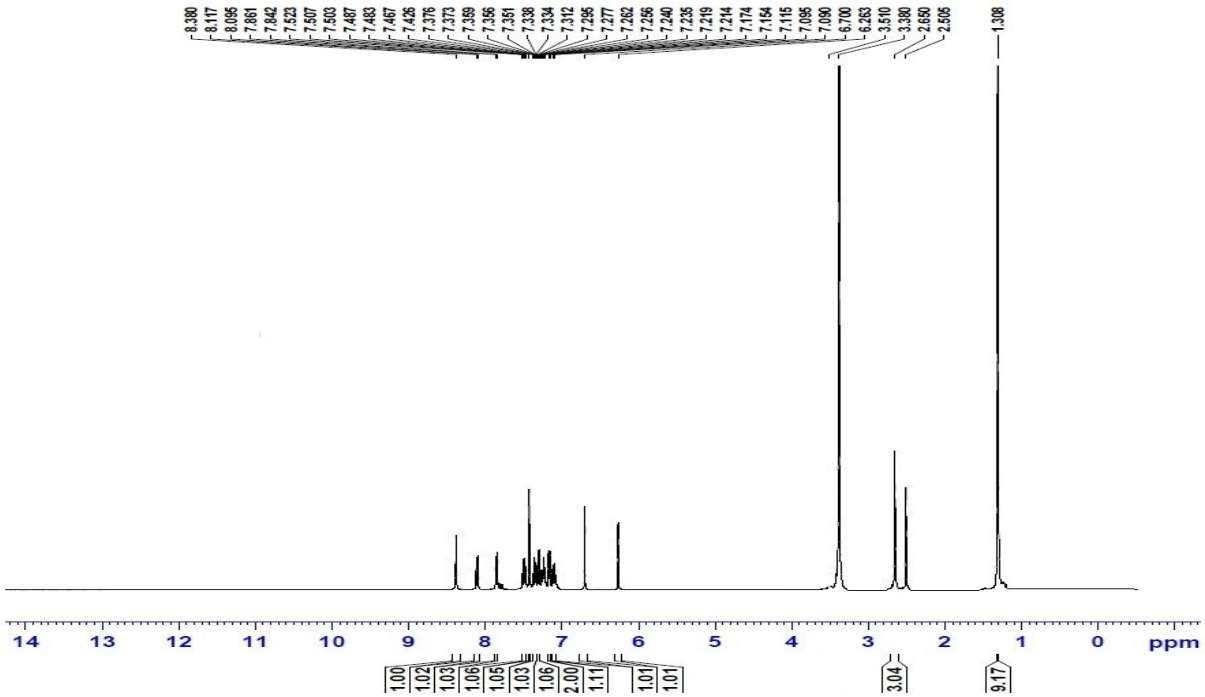


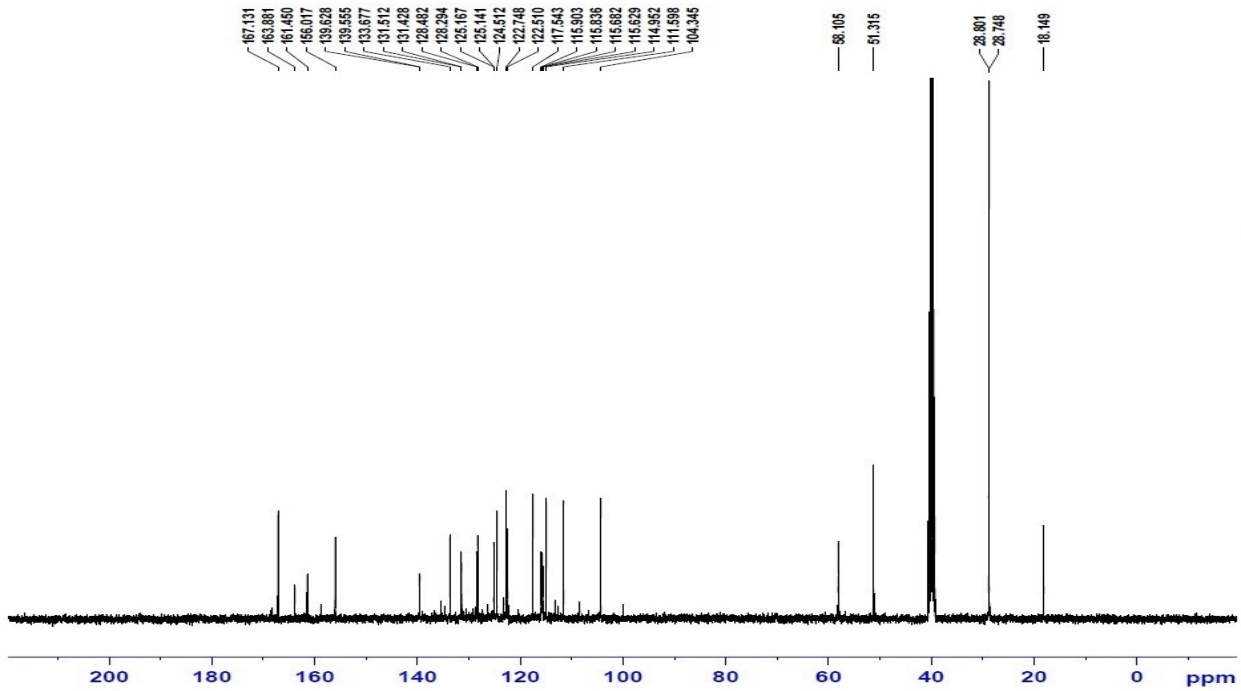
N-(tert-Butyl)-2-(4-methoxyphenyl)-2-(4-methyl-1-oxopyrazino[1,2-a]indol-2(1H)-yl)acetamide ***2g***



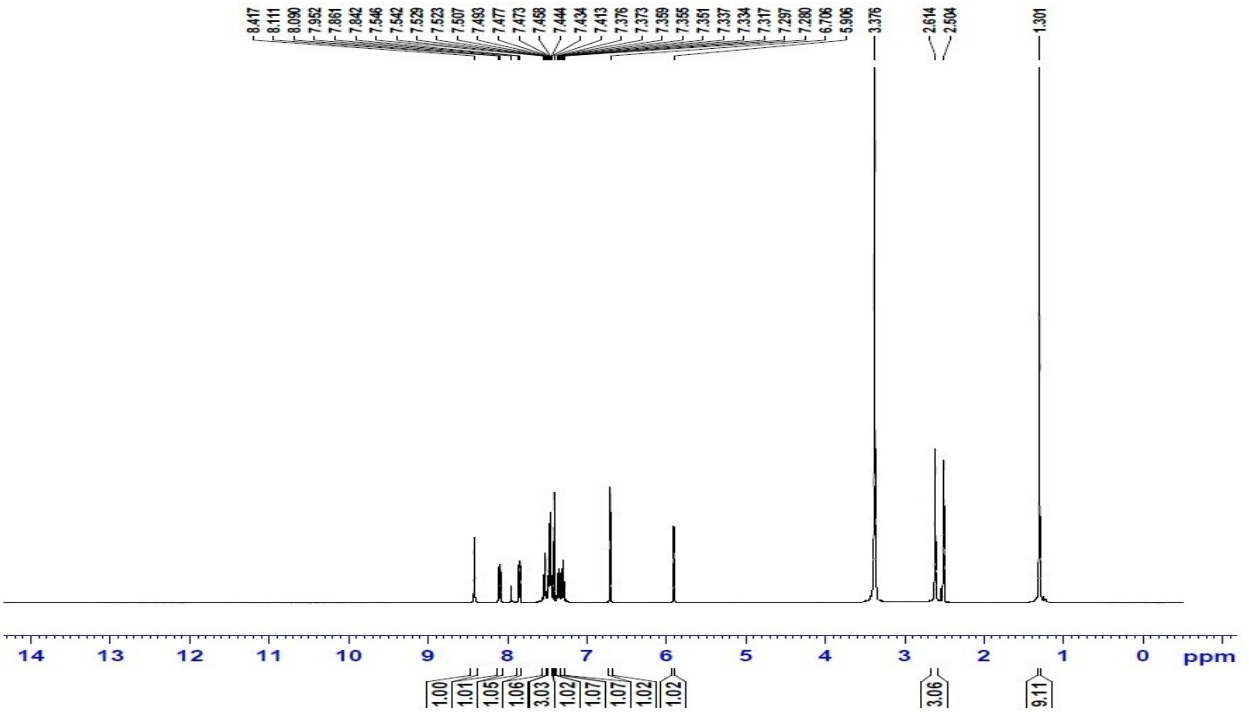


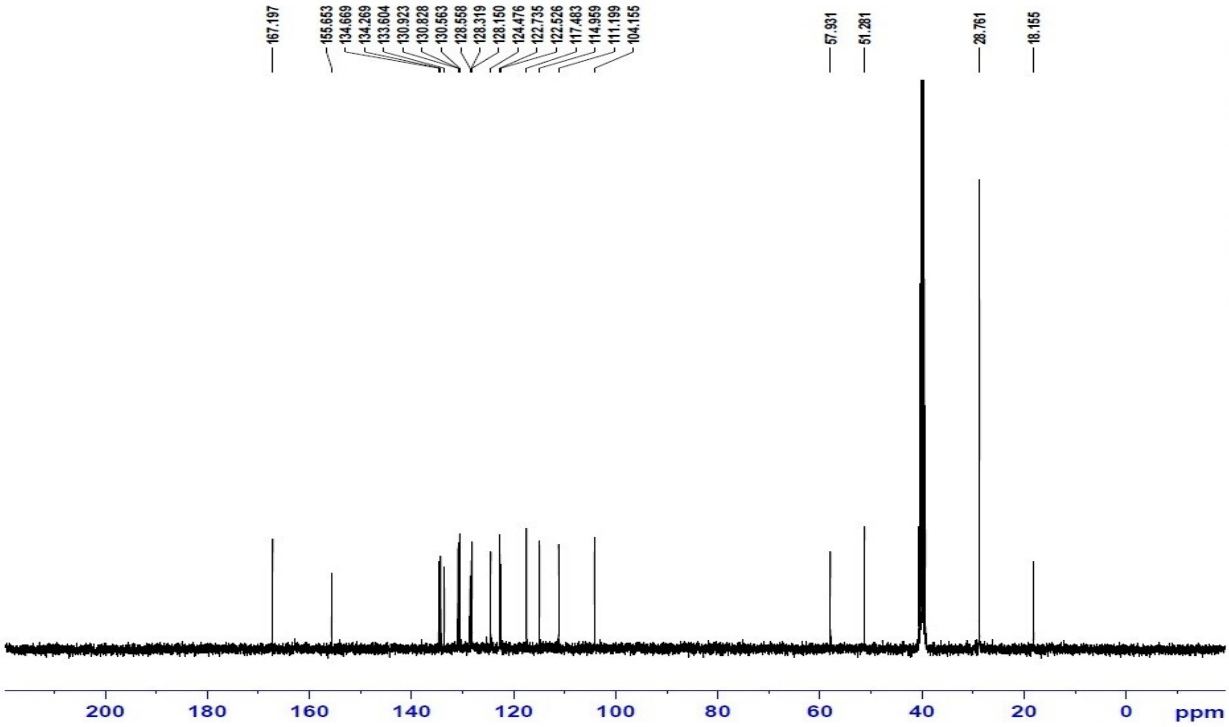
N-(tert-Butyl)-2-(4-fluorophenyl)-2-(4-methyl-1-oxopyrazino[1,2-a]indol-2(1H)-yl)acetamide ***2h***





N-(tert-Butyl)-2-(2-chlorophenyl)-2-(4-methyl-1-oxopyrazino[1,2-a]indol-2(1H)-yl)acetamide ***2i***





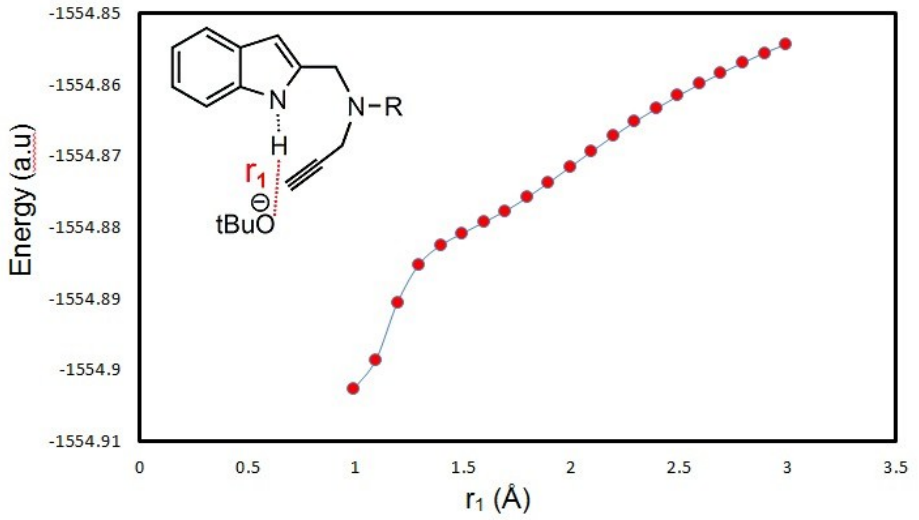


Figure S1 Relaxed PES scan calculated at the B3LYP/BS1 level of theory in DMF using the CPCM solvation model. This plot suggests that corresponding deprotonation does not have any enthalpic activation barrier.

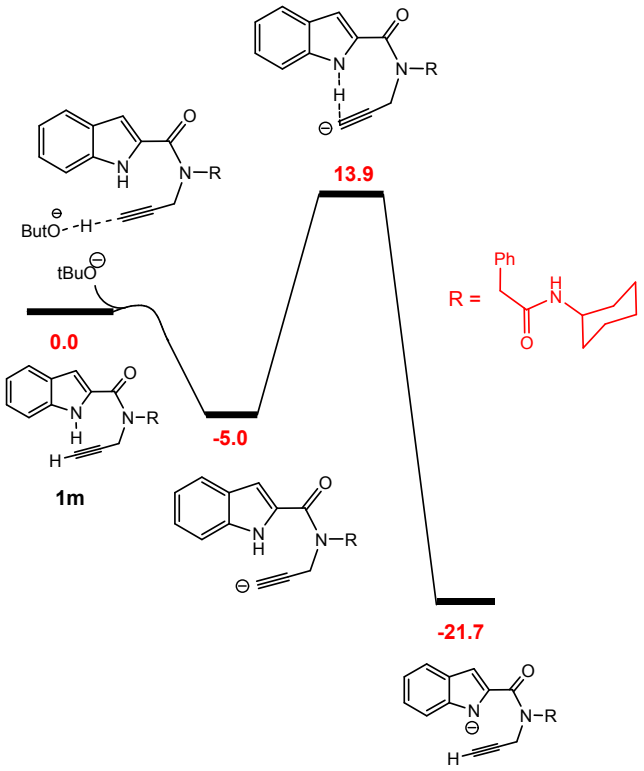


Figure S2 Another alternative pathway for deprotonation of indole N-H bond (pathway C). The relative free energies obtained from the M06/6-311+G(2d,p)//B3LYP/6-31G(d) calculations in DMF are given in kcal/mol.

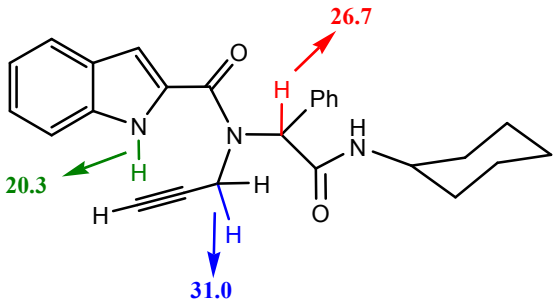


Figure S3 The pKa values for some selective protons calculated based on the methodology given in the following reference: H. Batebi, F. Zarkoob, K. Daraei, B. Y. Yates, A. Ariafard, *J. Organomet*. **2013, 748**, 89.