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SUPPORTING INFORMATION

Convenient synthesis of 2,3-disubstituted quinazolin-4(3H)-ones and 2-styryl-3-substituted quinazolin-4(3H)-ones: Applications towards the synthesis of drugs

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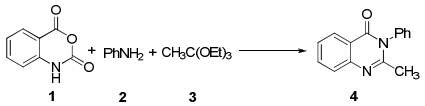
1. Tables

Table 1. The 3-MCR of **1**, **2**, and **3** under various solvent conditions to form **4**



Entry	Temperature (°C)	Time (h)	Solvent (3 mL)	Yield (%)[b]
1	reflux	4	MeOH	65
2	reflux	4	EtOH	68
3	reflux	4	^{i}PrOH	44
4	reflux	4	^{t}BuOH	41
5	reflux	4	EG[c]	45
6	reflux	4	PhMe	72
7	reflux	4	1,4-dioxane	68
8	reflux	4	MeCN	52
9	reflux	4	DCE	46
10	reflux	4	DMF	32
11	reflux	4	THF	39
12	120	4	PEG-200	42

[a]The mixture of **1** (1 mmol), **2** (1 mmol, 1 equiv), and **3** (1 mmol, 1 equiv) was treated under different condition. [b]Isolated yield of **4**. [c]Ethylene Glycol

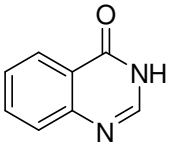
Table 2. Optimization of the synthesis of **4** under microwave irradiation.[a]

Entry	Temp. (°C)	Time (min)	Yield (%)[b]
1	100	10	15
2	100	20	35
3	100	30	52
4	120	10	21
5	120	20	44
6	120	30	65
4	130	10	29
5	130	20	50
6	130	30	72
7	140	10	32
8	140	20	90
9	140	30	91
10	150	10	32
11	150	20	90
12	150	30	90
13	140	30	79
14	140	20	91

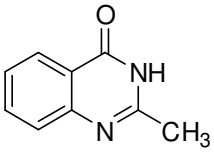
15	140	10	78
16	140	20	90
17	100	30	90

[a]**1** (1 mmol) was treated with **2** (1 mmol, 1 equiv) and **3** (1 mmol, 1 equiv) under neat condition at different temperatures, microwave input power at 150 W.[b]Isolated Yield.

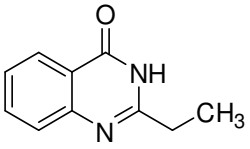
2. Spectral Data



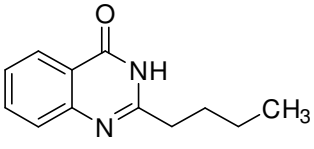
Quinazolin-4(1*H*)-one[1-3] (Entry 1, Table 2):White solid;mp = 225-227 °C; IR (KBr) ν_{max} = 3461, 2923, 1664, 1613cm^{-1};^{1}H NMR (400 MHz, DMSO):δ = 12.22 (s, 1H), 8.07-8.12 (m, 2H), 7.80 (t, *J* = 7.0 Hz, 1H), 7.66 (d, *J* = 7.9 Hz, 1H), 7.51 (t, *J* = 7.1 Hz, 1H);MS(APCI) m/z: 147.26 (M+H)$^+$.



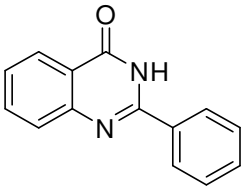
2-Methylquinazolin-4(1*H*)-one[1-3] (Entry 2, Table 2): White solid; mp = 238-240 °C; IR (KBr) ν_{max} = 1675, 1462, 1258, 750 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$):δ = 12.07 (s, 1H), 8.29 (d, *J* = 7.9 Hz, 1H), 7.77 (t, *J* =8.0 Hz, 1H), 7.68 (d, *J* =8.1 Hz, 1H), 7.47 (t, *J* = 7.1 Hz, 1H), 2.60 (s, 3 H);MS(APCI) m/z: 161.28 (M+H)$^+$.



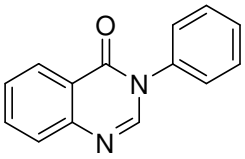
2-Ethylquinazolin-4(1*H*)-one[1, 4, 5] (Entry 3, Table 2): White solid; mp = 236-237 °C;IR (KBr) ν_{max} =2914, 1683, 1621, 1469, 1202 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$):δ = 12.16 (s, 1H), 8.30 (d, *J*=8.0 Hz, 1H), 7.77 (t, *J*=7.6 Hz,1H), 7.71 (d, *J*= 8.0 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 2.86 (q,*J* = 7.6 Hz, 2H), 1.46 (t, *J*= 7.6 Hz, 3H); MS(APCI) m/z:175.32 (M+H)$^+$.



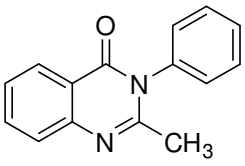
2-Butylquinazolin-4(1*H*)-one[6, 7](Entry 4, Table 2): White solid; mp = 198-200 °C; IR (KBr) ν_{max} =2927, 1677, 1618, 1471 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$)δ: 12.09 (s, 1H), 8.31 (d, *J*=7.9 Hz, 1H), 7.81-7.71 (m, 2H), 7.49 (t, *J*=7.4 Hz, 1H), 2.83 (t, *J* = 7.8 Hz, 2H), 1.94-1.86 (m, 2H), 1.57-1.48 (m, 2H), 1.57-1.48 (m, 2H), 1.07-1.00 (m, 3H);MS(APCI) *m/z 203*.36 (M+H)$^+$.



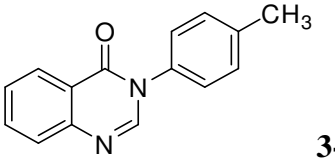
2-Phenylquinazolin-4(1*H*)-one[2, 8, 9](Entry 5, Table 2):White solid; mp = 236-237 °C; IR (KBr) ν_{max} =2956, 1668, 1602, 1471, 1296 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$)δ: 11.72 (s, 1H), 8.33 (d, *J*=7.1 Hz, 1), 8.28-8.25 (m, 2H), 7.85-7.79 (m, 2H), 7.61-7.57 (m, 3H), 7.53-7.49 (m, 1H);MS(APCI) *m/z 223.25* $(M+H)^+$



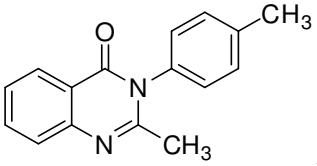
3-Phenylquinazolin-4(3*H*)-one[2, 10](Entry 6, Table 2):White solid; mp = 135-136 °C IR (KBr) ν_{max} = 3056,1672,1611,1474, 764 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.36 (d, *J* = 7.7Hz, 1H), 8.12 (s, 1H), 7.82-7.75 (m, 2H), 7.57-7.47 (m, 4H), 7.43 (d, *J*= 8.2Hz, 2H); MS(APCI) *m/z* 223.24 $(M+H)^+$.



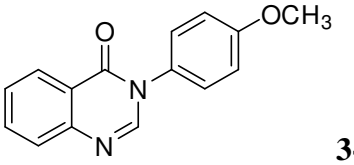
2-Methyl-3-phenylquinazolin-4(3*H*)-one[11](Entry 7, Table 2):White solid; mp = 147-148 °C; IR (KBr) ν_{max} = 2930, 1678, 1586, 1471, 1267 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.27 (d, *J* = 7.5 Hz, 1H), 7.76 (d, *J* = 7.2 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.51 (m, 4H), 7.27 (d, *J* = 6.0 Hz, 2H), 2.24 (s, 3H); MS(APCI) *m/z* 237.30 $(M+H)^+$.



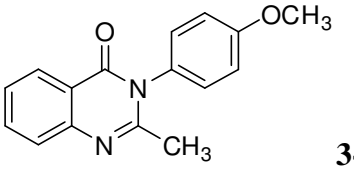
3-*p*-Tolylquinazolin-4(3*H*)-one[10] (Entry 8, Table 2):White solid; mp = 143-144 °C; IR (KBr) ν_{max} = 2960, 1676, 1602, 1467 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.37 (d, *J* = 8 Hz, 1H), 8.11 (s, 1H), 7.75-7.82 (m, 2H), 7.52-7.56 (m, 1H), 7.26-7.36 (m, 4H), 2.44 (s, 3H);MS(APCI) *m/z* 237.03 $(M+H)^+$.



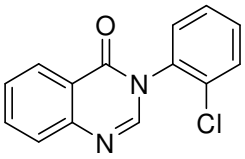
2-Methyl-3-p-tolylquinazolin-4(3*H*)-one[12](Entry 9, Table 2):White solid; mp =150-152 °C; IR (KBr) ν_{max} = 2923, 1677, 1602, 1468, 1262 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.27 (d, *J* = 7.78 Hz, 1H), 7.78-7.74 (m, 1H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.48-7.44 (m, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.15-7.12 (m, 2H) 3.13 (s, 3H), 2.34 (s, 3); MS(APCI) *m/z* 251.26 $(M+H)^+$.



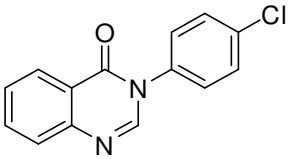
3-(4-Methoxyphenyl)quinazolin-4(3*H*)-one[10, 13](Entry 10, Table 2): White solid; mp =132-134 °C; IR (KBr) ν_{max} = 2989, 1680, 1266 cm $^{-1}$; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.36 (d,*J* = 7.8Hz, 1H), 8.12 (s, 1H), 7.82-7.75 (m, 2H), 7.55 (t, *J* = 7.2Hz, 1H), 7.34 (d, *J* = 8.6 Hz, 2H), 7.05 (d, *J* = 8.6Hz, 2H), 3.87 (s, 3H);MS(APCI) *m/z* 253.25 $(M+H)^+$.



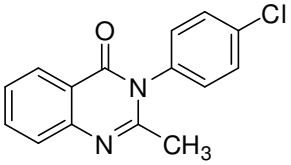
3-(4-Methoxyphenyl)-2-methylquinazolin-4(3*H*)-one[13, 14](Entry 11, Table 2):White solid; mp = 167-170 °C; IR (KBr) ν_{max} = 2975, 1676, 1474, 1260 cm $^{-1}$; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.26 (d, *J*=8.3Hz, 1H), 7.76-7.74 (m, 1H), 7.66 (d, *J* = 8.1Hz, 1H), 7.45 (t, *J* = 7.2 Hz, 1H), 7.17 (d, *J*=6.8Hz, 2H), 7.05 (d, *J*=7.1Hz, 2H), 3.87 (s, 3H) 2.26 (s, 3H);MS(APCI) *m/z* 253.25 $(M+H)^+$.



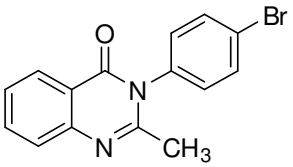
3-(2-Chlorophenyl)quinazolin-4(3*H*)-one[15](Entry 12, Table 2):White solid; mp = 118-120 °C; IR (KBr) ν_{max} = 3012, 1685, 1470, 1265 cm $^{-1}$; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.38 (d, *J* = 7.4 Hz, 1H), 7.97 (s, 1H), 7.85-7.78 (m, 2H), 7.63-7.54 (m, 2H), 7.51-7.43 (m, 3H); MS(APCI) *m/z* 257.35 $(M+H)^+$.



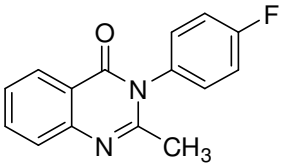
3-(4-Chlorophenyl)quinazolin-4(3*H*)-one[10] (Entry 13, Table 2):White solid; mp = 124-125 °C; IR (KBr) ν_{max} = 3006, 1675, 1472, 1258 cm $^{-1}$; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.35 (d, *J* = 7.8 Hz, 1H), 8.09 (s, 1H), 7.75-7.83 (m, 2H), 7.51-7.57 (m, 3H), 7.38 (d, *J* = 8.5 Hz, 2H); MS(APCI) *m/z* 257.25 $(M+H)^+$.



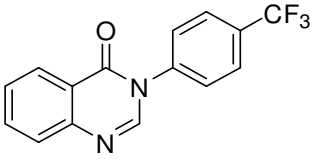
3-(4-Chlorophenyl)-2-methylquinazolin-4(3*H*)-one[16](Entry 14, Table 5): Yellow solid; mp = 159-160 °C; IR (KBr) ν_{max} = 2923, 1677, 1602, 1468, 1262 cm $^{-1}$; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.25 (d, *J*=7.9 Hz, 1H), 7.76 (t, *J*=7.5 Hz, 1H), 7.67 (d, *J* = 7.9 Hz, 1H), 7.54-7.47 (m, 3H), 7.22 (d, *J*=6.6 Hz, 2H), 2.25 (s, 3H);MS(APCI) *m/z* 271.24 $(M+H)^+$.



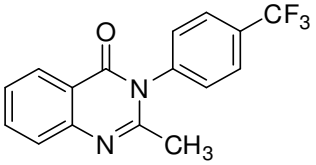
3-(4-Bromophenyl)-2-methylquinazolin-4(3*H*)-one[17](Entry 15, Table 2): Black solid; mp = 168-169 °C; IR (KBr) ν_{max} = 2923, 1684, 1605, 1472, 1227 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.25 (d, *J*=8.0 Hz, 1H), 7.79-7.75 (m, 1H), 7.71-7.66 (m, 3H), 7.47 (t, *J*= 7.5 Hz, 1H), 7.17-7.13 (m, 2H), 2.25 (s, 3H); MS(APCI) *m/z* 315.29$(M+H)^+$.



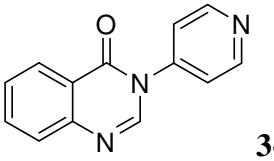
3-(4-Fluorophenyl)-2-methylquinazolin-4(3*H*)-one[18](Entry 16, Table 2): White solid; mp = 132-134 °C; IR (KBr) ν_{max} = 2919, 1684, 1607, 1378, 1261 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.25 (d, *J*=8.0 Hz, 1H), 7.76 (t, *J*=7.2 Hz, 1H), 7.67 (d, *J*=8.0 Hz, 1H), 7.47 (t, *J*= 7.5 Hz, 1H), 7.27-7.25 (m, 3H), 2.25 (s, 3H);MS(APCI) *m/z* 255.29 $(M+H)^+$.



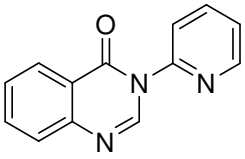
3-(4-(Trifluoromethyl)phenyl)quinazolin-4(3*H*)-one[19, 20] (Entry 17, Table 2):White solid; mp = 183-184 °C; IR (KBr) ν_{max} = 2917, 1682, 1602, 1120 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.38 (d, *J* = 8.0 Hz, 1H), 8.12 (s, 1H), 7.84 (d, *J* = 8.2 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H),7.61-7.57 (m, 3H);MS(APCI) *m/z* 291.21 $(M+H)^+$.



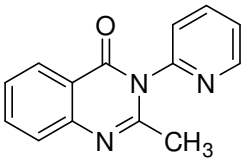
2-Methyl-3-(4-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one[20](Entry 18, Table 2): white solid; mp = 146-148°C; IR (KBr) ν_{max} = 2917, 1682, 1602, 1120 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.26 (d, *J* = 7.8 Hz, 1H), 7.86-7.78 (m, 3H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.51-7.44 (m, 3H), 2.26 (s, 3H); MS(APCI) *m/z* 305.33 $(M+H)^+$.



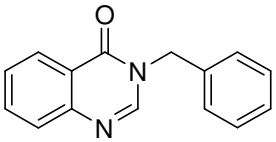
3-(Pyridin-4-yl)quinazolin-4(3*H*)-one (Entry 19, Table 2): White solid; mp = 148-150°C; IR (KBr) ν_{max} = 3000, 1645, 1623, 1258 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.84 (s, 2H), 8.37 (d, *J* = 7.7 Hz, 1H), 8.12 (s, 1H), 7.84 (t, *J* = 7.3 Hz, 1H), 7.78 (d, *J* = 7.5 Hz, 1H), 7.59 (t, *J* = 7.0 Hz, 1H), 7.47 (d, *J* = 1.4 Hz, 2H);^{13}C NMR (100 MHz, $CDCl_3$) δ : 160.0, 151.4, 147.5, 144.8, 144.5, 135.1, 128.1, 127.8, 127.3, 122.0, 121.3;MS(APCI) *m/z* 224.19 $(M+H)^+$; HRMS (ESI) m/z calcd for $C_{13}H_9N_3ONa^+$ [M + Na^+], 246.0638; Found 246.0641.



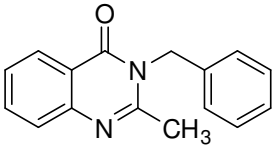
3-(Pyridin-2-yl)quinazolin-4(3*H*)-one[26](Entry 20, Table 2): White solid; mp = 135-137 °C; IR (KBr) ν_{max} = 3000, 1645, 1623, 1258 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.64 (d, *J* = 4.0 Hz, 2H), 8.39 (d, *J* = 8.0 Hz, 1H), 7.92 (d,*J* = 10.6 Hz, 1H), 7.83-7.77 (m, 2H), 7.78 (d, *J* = 7.5 Hz, 1H), 7.56 (t, *J* = 7.7 Hz, 1H), 7.42-7.38 (m, 1H);MS(APCI) *m/z* 224.20 $(M+H)^+$.



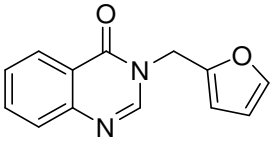
2-Methyl-3-(pyridin-2-yl)quinazolin-4(3*H*)-one[27](Entry 21, Table 2): White solid; mp = 176 °C; IR (KBr) ν_{max} = 3007, 1684, 1607, 1276 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.70 (d, *J* = 3.4 Hz, 1H), 8.27 (d, *J* = 7.9 Hz, 1H), 7.96-7.92 (m, 1H), 7.78-7.75 (m, 1H), 7.68 (d, J = 8.1 Hz, 1H), 7.48-7.39 (m, 3H), 2.22 (s, 3H);MS(APCI) m/z 238.27 $(M+H)^+$.



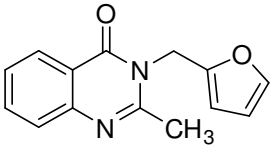
3-Benzylquinazolin-4(3*H*)-one[19] (Entry 22, Table 2):White solid; mp = 116-117 °C; IR (KBr) ν_{max} = 2923,1676,1610,1474 cm^{-1}: ^{1}H NMR (400 MHz, $CDCl_3$)δ:8.13 (d, *J* = 8.0Hz , 1H), 7.96 (s, 1H),7.51 (d, *J* = 3.5Hz, 2H), 7.29-7.25 (m, 1H), 7.17-7.07 (m, 5H), 4.98 (s, 2H);MS(APCI) *m/z* 237.05 $(M+H)^+$.



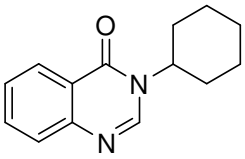
3-Benzyl-2-methylquinazolin-4(3*H*)-one[13](Entry 23, Table 2):Yellow solid; mp = 231-232 °C; IR (KBr) ν_{max} = 2989,1684,1506, 1276 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.33 (d, *J*= 8.0 Hz, 1H), 7.73 (d, *J* = 7.1 Hz, 1H), 7.63 (d, *J*= 8.0 Hz, 1H), 7.47 (t, *J* = 7.9 Hz, 1H), 7.32-7.26 (m, 3H), 7.19 (d, *J* =7.2 Hz, 2H), 5.40 (s, 2H), 2.55 (s, 3H); MS(APCI) *m/z* 251.27$(M+H)^+$.



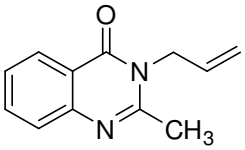
3-(Furan-2-ylmethyl)quinazolin-4(3*H*)-one[28](Entry 24, Table 2): Brown solid; mp = 127-128 °C; IR (KBr) ν_{max} = 2917, 1684, 1559, 1506, 1260 cm^{-1};^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.31 (d, *J*= 7.6 Hz, 1H), 8.17 (s, 1H), 7.77-7.69 (m, 2H), 7.50 (d, *J*= 6.9 Hz, 1H), 7.38 (s, 1H), 6.47 (s, 1H), 6.35 (s, 1H), 5.19 (s, 2H).



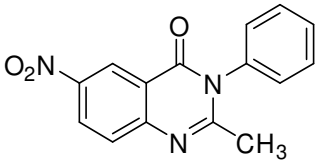
3-(Furan-2-ylmethyl)-2-methylquinazolin-4(3*H*)-one (Entry 25, Table 2): brown solid; mp = 162-165; IR (KBr) ν_{max} = 3007, 1677, 1598, 1260 cm $^{-1}$;^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.26-8.23 (m, 1H), 7.72-7.68 (m, 1H), 7.60 (d, *J*=15.7 Hz, 1H), 7.42 (t, *J*= 7.6 Hz, 1H), 7.34 (s, 1H), 6.41-6.40 (m, 1H), 6.33-6.31 (m, 1H), 5.30 (s, 2H), 2.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ :161.8, 154.2, 149.2, 147.2, 142.4, 134.4, 126.9, 126.7, 126.5, 120.4, 110.7, 109.5, 40.6, 23.4; MS(APCI) *m/z* 241.06 $(M+H)^+$; HRMS (ESI) m/z calcd for $C_{14}H_{12}N_2O_2Na^+$ [M + Na^+], 263.0791; Found 263.0795.



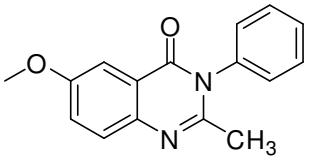
3-Cyclohexylquinazolin-4(3*H*)-one[29](Entry 26, Table 2): White solid; mp = 112-114 °C; IR (KBr) ν_{max} = 3005, 1674, 1457, 1275 cm $^{-1}$;^{1}H NMR (400 MHz, $CDCl_3$)δ: 9.61 (s, 1H), 8.11 (d, *J* = 8 Hz, 1H), 7.61-7.57 (m, 1H), 7.26-7.19 (m, 1H), 7.04 (d, *J* = 8.1 Hz, 1H), 4.94-4.88 (m, 1H), 2.56-2.46 (m, 2H), 1.90-1.83 (m, 2H), 1.72-1.60 (m, 3H), 1.47-1.30 (m, 3H);MS(APCI) *m/z* 229.36 $(M+H)^+$.



3-Allyl-2-methylquinazolin-4(3*H*)-one[30](Entry 27, Table 2):Syrupy liquid; mp = 80-81 °C; IR (KBr) ν_{max} = 2923, 1668, 1594, 1473, 1276 cm $^{-1}$;^{1}H NMR (400 MHz, $CDCl_3$)δ: 8.26 (d, *J*=8.0 Hz, 1H), 7.72 (t, *J*=7.3 Hz, 1H), 7.61 (d, *J*=8.2 Hz, 1H), 7.44 (t, *J*= 7.8 Hz, 1H), 6.01-5.91 (m, 1H), 5.25 (d, *J*=10.4 Hz, 1H), 5.12 (d, *J*=13.1 Hz, 1H), 4.77 (d, *J*= 3.4 Hz, 2H), 2.62 (s, 3H); MS(APCI) *m/z* 201.15$(M+H)^+$.

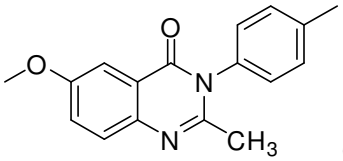


2-Methyl-6-nitro-3-phenylquinazolin-4(3*H*)-one[21] (Entry 28, Table 2): Yellow solid; mp = 223-224 °C; IR (KBr) ν_{max} = 2917, 1682, 1602, 1120 cm $^{-1}$;^{1}H NMR (400 MHz, $CDCl_3$)δ: 9.12 (d, *J*=2.6 Hz, 1H), 8.55 (d, *J* = 9.0 Hz, 1H), 7.79 (d, *J* = 8.9 Hz, 1H), 7.62-7.54 (m, 3H), 7.29-7.26 (m, 2H), 2.30 (s, 3H); MS(APCI) *m/z* 282.21$(M+H)^+$.

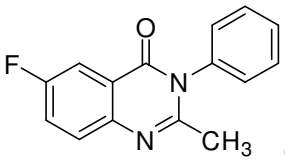


6-Methoxy-2-methyl-3-phenylquinazolin-4(3*H*)-one[22](Entry 29, Table 2): White solid; mp = 230-232 °C; IR (KBr) ν_{max} = 2919, 1655, 1595, 1114 cm $^{-1}$;^{1}H

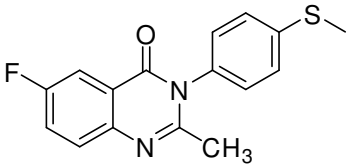
NMR (400 MHz, $CDCl_3$)δ: 7.51-7.66 (m, 5H), 7.39 (dd, *J* = 8.96, 3.0 Hz, 1H), 7.27-7.30 (m, 2H), 3.93 (s, 3H), 2.24 (s, 3H); MS(APCI) *m/z* 267.21$(M+H)^+$.



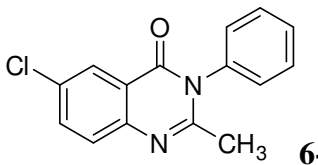
6-Methoxy-2-methyl-3-p-tolylquinazolin-4(3H)-one (Entry 30, Table 2): White solid; mp = 234-236°C; IR (KBr) ν_{max} = 2980, 1643, 1625, 1254 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 7.62-7.65 (m, 2H), 7.36-7.39 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 2H), 3.92 (s, 3H), 2.47 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 162.3, 158.2, 152.2, 142.1, 139.3, 135.3, 130.6, 128.3, 127.7, 124.7, 121.5, 106.5, 55.8, 24.2, 21.3; HRMS (ESI) m/z calcd for $C_{13}H_9N_3ONa^+$ [M + Na^+], 303.1109; Found 303.1104.



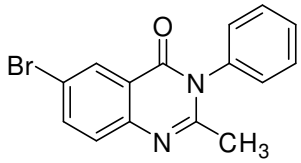
6-Fluoro-2-methyl-3-phenylquinazolin-4(3H)-one[23](Entry 31, Table 2): White solid; mp = 154-155 °C; IR (KBr) ν_{max} = 2917, 1697, 1475, 1260 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 7.91 (dd, *J* = 8.36, 3.0 Hz, 1H), 7.71 (dd, *J* = 8.96, 4.8 Hz, 1H), 7.50-7.61 (m, 2H), 7.27-7.29 (m, 2H), 2.25 (s, 3H); MS(APCI) *m/z* 255.36 $(M+H)^+$.



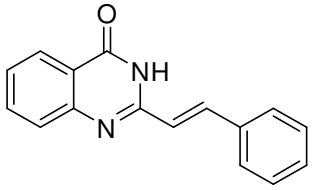
6-Fluoro-2-methyl-3-(4-(methylthio)phenyl)quinazolin-4(3H)-one (Entry 32, Table 2): White solid; mp = 218-220 °C; IR (KBr) ν_{max} = 2985, 1635, 1258 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 7.89 (dd, *J* = 8.40, 3.0 Hz, 1H), 7.68(dd, *J* = 8.92, 4.76 Hz, 1H), 7.46-7.51 (m, 1H), 7.39-7.41 (m, 2H), 7.15-7.17 (m, 2H), 2.54 (s, 3H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ : 161.9, 161.8, 161.7, 159.5, 153.6, 153.5, 144.2, 144.1, 140.8, 134.1, 129.2, 128.2, 127.3, 123.3, 123.0, 122.0, 121.0, 112.0, 111.8, 24.3, 15.5; HRMS (ESI) m/z calcd for $C_{13}H_9N_3ONa^+$ [M + Na^+], 323.0630; Found 323.0634.



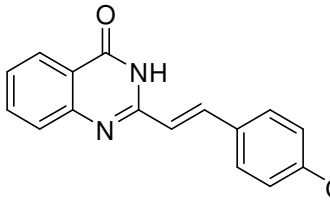
6-Chloro-2-methyl-3-phenylquinazolin-4(3*H*)-one[24, 25](Entry 33, Table 2): White solid; mp = 154-155 °C; IR (KBr) ν_{max} = 2919, 1695, 1473, 1275 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.24 (d, *J*=2.4 Hz, 1H), 7.73-7.70 (m, 1H), 7.64 (d, *J*=8.7 Hz, 1H), 7.61-7.52 (m, 3H), 7.29-7.26 (m, 2H), 2.25 (s, 3H); MS(APCI) *m/z* 271.28 $(M+H)^+$.



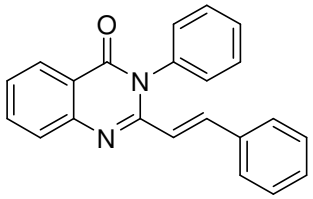
6-Bromo-2-methyl-3-phenylquinazolin-4(3*H*)-one[16, 21](Entry 34, Table 2): White solid; mp = 123 °C; IR (KBr) ν_{max} = 2918, 1691, 1588, 1470, 1275 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.38 (d, *J*=2.3 Hz, 1H), 7.84 (d, *J*=8.6 Hz, 1H), 7.59-7.52 (m, 4H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ :161.1, 154.8, 146.4, 137.8, 137.5, 130.1, 129.6, 129.5, 128.7, 127.9, 122.2, 120.1, 24.5; MS(APCI) *m/z* 315.27$(M+H)^+$.



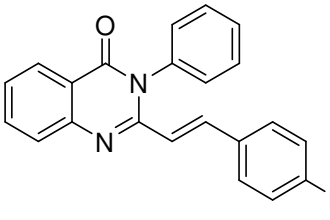
(*E*)-2-Styrylquinazolin-4(3*H*)-one[21, 30] (Entry 1,Table 3): white solid; mp = 252-253°C; IR (KBr) ν_{max} = 3415, 1660, 1632, 1252, 1172 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 11.90 (s, 1 H, NH), 8.34 (d, *J* = 8.04 Hz, 1 H), 8.01 (d, *J* = 16.5 Hz, 1 H), 7.76–7.82 (m, 2 H), 7.68 (d, *J* = 7.1 Hz, 2 H), 7.39-7.52 (m, 4 H), 7.00 (d, *J* = 16.5 Hz, 1 H); MS (APCI) m/z: 249.29 $(M + H)^+$.



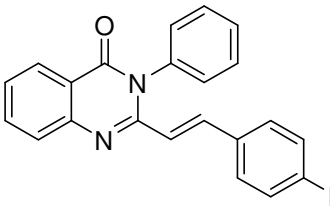
(*E*)-2-(4-Methoxystyryl)quinazolin-4(3*H*)-one[31] (Entry 2,Table 3): white solid; mp = 278-279 °C; IR (KBr) ν_{max} = 3448, 1674, 1598, 1472, 1250 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 10.31 (s, 1 H, NH), 8.30 (dd, *J* = 1.1 Hz &*J* = 8.0 Hz, 1 H), 7.71-7.80 (m, 3 H), 7.58 (d, *J* = 8.7 Hz, 2 H) 7.45–7.49 (m, 1 H), 6.97 (d, *J* = 8.7 Hz, 2 H), 6.78 (d, *J* = 16.3 Hz, 1 H), 3.87 (s, 3H); MS (APCI) m/z: 279.32 $(M + H)^+$.



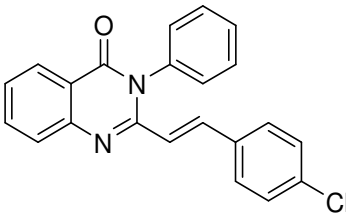
(*E*)-3-Phenyl-2-styrylquinazolin-4(3H)-one[31] (Entry 3,Table 3): white solid; mp = 196-197 °C; IR (KBr) ν_{max} = 3442, 1676, 1545, 1472, 1258, 1132 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.30 (d, *J* = 7.9 Hz, 1 H), 7.97 (d,*J* = 15.5 Hz, 1 H), 7.79 (d, *J* = 3.4 Hz, 2 H) 7.53- 7.61 (m, 3 H), 7.47-7.50 (m, 1 H), 7.28-7.34 (m, 7 H), 6.39 (d, *J* = 15.5 Hz, 1 H); MS (APCI) m/z: 325.21 $(M + H)^+$.



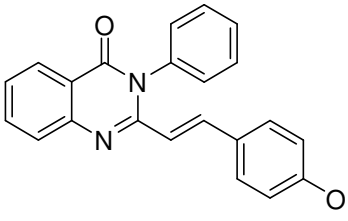
(*E*)-2-(4-Methylstyryl)-3-phenylquinazolin-4(3*H*)-one[32] (Entry 4,Table 3): white solid; mp = 168-170°C; IR (KBr) ν_{max} = 3445, 1672, 1536, 1472, 1252, 1042, 956 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.31 (d, *J* = 7.8 Hz, 1 H), 7.96 (d, *J* = 15.5 Hz, 1 H), 7.79 (d, *J* = 3.6 Hz, 2 H) 7.62 –7.54 (m, 3 H), 7.51-7.45 (m, 1 H), 7.34 (d, *J* = 1.5 Hz, 2 H), 7.22 (d, *J* = 1.5 Hz, 2 H), 7.12 (d, *J* = 7.9 Hz, 2 H), 6.35 (d, *J* = 15.5 Hz, 1 H), 2.35 (s, 3 H); MS (APCI) m/z: 339.42 $(M + H)^+$.



(*E*)-2-(4-Bromostyryl)-3-phenylquinazolin-4(3*H*)-one[31](Entry 5,Table 3): white solid; mp = 262-263 °C; IR (KBr) ν_{max} = 3452, 1652, 1542, 1145, 1345, 1052 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.30 (d, *J* = 8.2 Hz, 1 H), 7.89 (d, *J* = 15.5 Hz, 1 H), 7.79-7.82 (m, 2 H) 7.51 –7.61 (m, 3 H), 7.36-7.50 (m, 3 H), 7.27-7.32 (m, 2H), 7.16 (d, *J* = 8.3 Hz, 2 H), 6.35 (d, *J* = 15.5 Hz, 1 H); MS (APCI) m/z: 404.28 $(M + H)^+$.

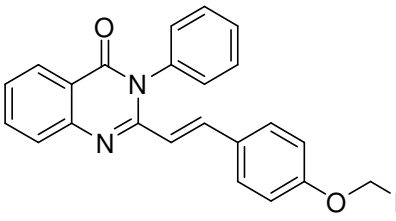


(*E*)-3-Phenyl-2-(4-(trifluoromethyl)styryl)quinazolin-4(3H)-one(Entry 6,Table 3): white solid; mp = 175-177°C; IR (KBr) ν_{max} = 3372, 1684, 1552, 1323, 1122, 1067, 824 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.32 (d, *J* = 7.9 Hz, 1 H), 7.98 (d, *J* = 15.5 Hz, 1 H), 7.80-7.85 (m, 2 H) 7.55–7.67 (m, 5H),7.40-8.53 (m,1H),7.31-7.38 (m, 4H),6.48(d, *J* = 15.6 Hz, 1 H); (^{13}C NMR ($CDCl_3$, 100 MHz): 161.1, 151.0, 147.6, 138.67, 137.9, 136.8, 134.7, 131.2, 130.9, 130.0, 129.5, 128.6, 127.8, 127.4, 127.2, 126.9, 125.7, 125.7, 125.6, 125.1, 122.4, 122.4, 121.0; MS (APCI) m/z: 393.39 $(M + H)^+$;HRMS (ESI) m/z calcd for $C_{23}H_{15}F_3N_2ONa^+$ [M + Na^+], 415.1029; Found 413.1031.

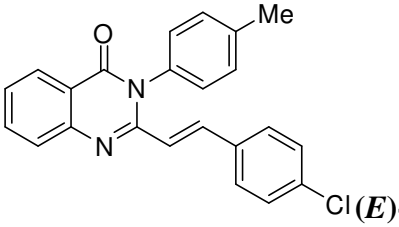


(*E*)-2-(4-Methoxystyryl)-3-phenylquinazolin-4(3*H*)-one[31](Entry 7,Table 3): white solid; mp = 165-167 °C; IR (KBr) ν_{max} = 3324, 2963, 1656, 1524, 1245, 1132 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.29 (dd, *J* = 7.9 Hz, 1 H), 7.93 (d, *J* = 15.4 Hz, 1 H), 7.76-7.85 (m, 2 H) 7.54-7.60 (m, 3 H), 7.42-7.46 (m, 1 H), 7.24-7.35 (m, 4H),

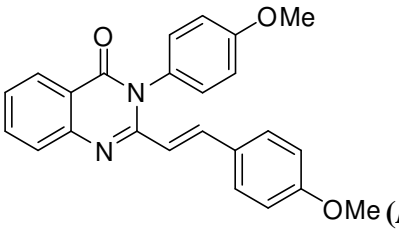
6.62 (d, *J* = 8.7 Hz, 2 H), 6.23 (d, *J* = 15.4 Hz, 1 H), 3.71 (s, 3H); (^{13}C NMR ($CDCl_3$, 100 MHz):162.4, 160.92, 152.1, 147.9, 139.6, 139.7, 137.1, 134.5, 129.8, 129.3, 129.2, 128.7, 128.1, 127.2, 127.1, 126.3, 120.8, 117.5, 114.2, 55.3;MS (APCI) m/z: 355.42 $(M + H)^+$.



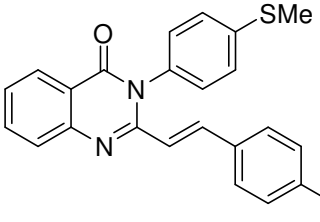
(*E*)-2-(4-(Benzyloxy)styryl)-3-phenylquinazolin-4(3*H*)-one (Entry 8,Table 3): white solid; mp = 168-170°C; IR (KBr) ν_{max} = 3296, 1668, 1548, 1210, 1050 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.28-8.30 (m, 1 H), 7.93 (d, *J* = 15.4 Hz, 1 H), 7.76-7.80 (m, 2 H), 7.53-7.61 (m, 3 H), 7.43-7.47 (m, 1 H), 7.36-7.41 (m, 9H), 6.87-6.91 (m, 2 H), 6.23 (d, *J* = 15.4 Hz, 1 H), 5.06 (s, 2 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.4, 160.0, 152.0, 147.9, 139.5, 137.1, 136.4, 134.5, 129.9, 129.4, 129.3, 128.7, 128.6, 128.3, 128.1, 127.4, 127.2, 127.1, 126.3, 120.8, 117.6, 115.1, 70.0; MS (APCI) m/z: 431.49 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{29}H_{22}N_2O_2Na^+$ $[M + Na^+]$, 453.1573; Found 453.1581.



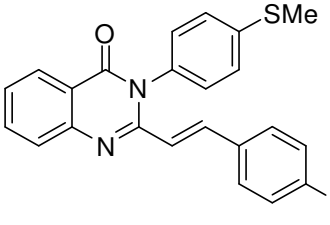
(*E*)-3-(4-Chlorostyryl)-2-(p-tolyl)isoquinolin-1(2*H*)-one[31] (Entry 9,Table 3): white solid; mp = 208-210°C; IR (KBr) ν_{max} = 3412, 1680, 1641, 1522, 1242cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.29 (d, *J* = 7.8 Hz, 1 H), 7.90 (d, *J* = 15.5 Hz, 1 H), 7.75-7.77 (m, 2 H), 7.44-7.48 (m, 1 H), 7.37 (d, *J* = 8.0 Hz, 2 H), 7.23-7.28 (m, 4H),7.18 (d, *J* = 8.1 Hz, 2 H), 6.40 (d, *J* = 15.5 Hz, 1 H), 2.48 (s, 3 H);MS (APCI) m/z: 372.79 $(M + H)^+$.



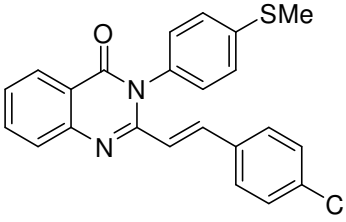
(*E*)-3-(4-Methoxyphenyl)-2-(4-methoxystyryl)quinazolin-4(3*H*)-one (Entry 10,Table 3): white solid; mp = 167-169°C; IR (KBr) ν_{max} = 2965, 1671, 1495, 1352, 1260 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz): δ = 8.28 (d, *J* = 7.8 Hz, 1 H), 7.93 (d, *J* = 15.4 Hz, 1 H), 7.76 (m, 2 H), 7.21-7.44 (m, 5 H), 7.08 (d, *J* = 8.6 Hz, 2 H), 6.84 (d, *J* = 8.4 Hz, 2 H), 6.31 (d, *J* = 15.4 Hz, 1 H), 3.90 (s, 3 H), 3.80 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.6, 160.8, 159.8, 152.5, 147.9, 139.5, 134.5, 129.6, 129.5, 129.4, 128.1, 127.1, 126.2, 120.7, 117.6, 115.1, 114.2, 55.6, 55.3; MS (APCI) m/z: 385.44 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{24}H_{20}N_2O_3Na^+$ $[M + Na^+]$, 407.1366; Found 407.1366.



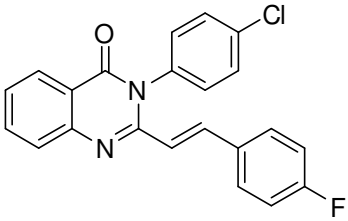
(*E*)-2-(4-Methoxystyryl)-3-(4-(methylthio)phenyl)quinazolin-4(3H)-one (Entry 11,Table 3): white solid; mp = 192-195°C; IR (KBr) ν_{max} = 2933, 1679, 1545, 1255 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ =8.28 (d, *J* = 7.9 Hz, 1 H), 7.94 (d, *J* = 15.4 Hz, 1 H), 7.77-7.80 (m, 2 H), 7.40-7.45 (m, 3 H), 7.30 (d, *J* = 8.6 Hz, 2 H), 7.23 (t, *J* = 9.4 Hz, 2 H), 6.85 (d, *J* = 8.6 Hz, 2 H), 6.29 (d, *J* = 15.4 Hz, 1 H), 3.81 (s, 3 H), 2.57 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.5, 160.9, 152.1, 147.9, 140.4, 139.8, 134.6, 133.7, 129.5, 128.9, 128.0, 127.2, 127.1, 126.3, 126.3, 120.7, 117.4, 114.3, 55.3, 15.5; MS (APCI) m/z: 401.52 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{24}H_{20}N_2O_2SNa^+$ [$M + Na^+$], 423.1138; Found 423.1139.



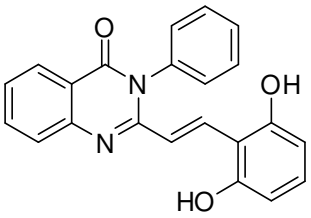
(*E*)-2-(4-(Dimethylamino)styryl)-3-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one(Entry 12, Table 3): white solid; mp = 195-197°C; IR (KBr) ν_{max} = 3321, 2961, 1686, 1555, 1242, 1031 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.28 (d, *J* = 7.7 Hz, 1 H), 7.93 (d, *J* = 15.3 Hz, 1 H), 7.72-7.76 (m, 2 H), 7.38-7.42 (m, 5 H), 7.21-7.25 (m, 2 H), 6.84 (d, *J* = 8.8 Hz, 2 H), 6.18 (d, *J* = 15.3 Hz, 1 H), 2.99 (s, 6 H), 2.56 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.6, 152.7, 151.3, 148.1, 140.6, 140.1, 140.6, 140.1, 134.5, 134.0, 129.5, 129.0, 127.1, 127.1, 127.0, 125.8, 123.2, 120.5, 114.4, 111.8, 40.1, 15.5; MS (APCI) m/z: 414.55 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{25}H_{23}N_3OSNa^+$ [$M + Na^+$], 436.1454; Found 436.1458.



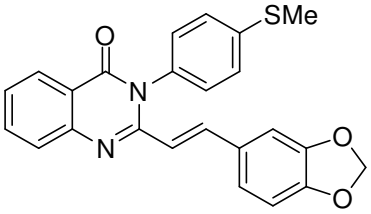
(*E*)-2-(4-Chlorostyryl)-3-(4-(methylthio)phenyl)quinazolin-4(3H)-one(Entry 13, Table 3):white solid; mp = 182-184°C; IR (KBr) ν_{max} = 3345, 1662, 1523, 1210, 1049 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.29 (d, *J* = 7.9 Hz, 1 H), 7.92 (d, *J* = 15.5 Hz, 1 H), 7.76-7.81 (m, 2 H), 7.41-7.49 (m, 3 H), 7.21-7.31 (m, 6 H), 6.18 (d, *J* = 15.5 Hz, 1 H), 2.56 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.3, 151.4, 147.6, 140.6, 138.6, 135.5, 134.7, 133.7, 133.4, 129.0, 129.0, 128.9, 127.3, 127.2, 127.1, 126.7, 120.8, 120.3, 15.4; MS (APCI) m/z: 405.92 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{23}H_{17}ClN_2OSNa^+$ [$M + Na^+$], 427.0642; Found 427.0642.



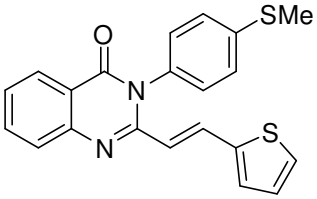
(*E*)-3-(4-Chlorophenyl)-2-(4-fluorostyryl)quinazolin-4(3*H*)-one(Entry 14, Table 3):white solid; mp = 187-188°C; IR (KBr) ν_{max} = 3332, 1668, 1498,, 1225, 1066 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.29 (d, *J* = 7.4 Hz, 1 H), 7.95 (d, *J* = 15.4 Hz, 1 H), 7.76-7.83 (m, 2 H), 7.57 (d, *J* = 8.6 Hz, 2 H), 7.41-7.52 (m, 1H), 7.21-7.35 (m, 4 H), 7.02 (t, *J* = 8.6 Hz, 2 H), 6.29 (d, *J* = 15.4 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 164.8, 162.3, 162.2, 151.2, 147.6, 139.1, 135.4, 135.4, 134.8, 131.3, 131.3, 130.2, 130.1, 129.7, 129.6, 127.4, 127.1, 126.84, 120.7, 119.1, 119.1, 116.1, 115.9; MS (APCI) m/z: 377.83 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{22}H_{14}ClFN_2ONa^+$ [M + Na^+], 399.0671; Found 399.0676



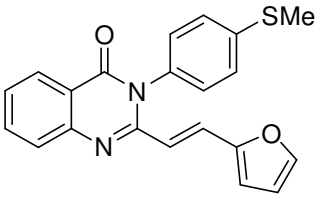
(*E*)-2-(2,6-Dihydroxystyryl)-3-phenylquinazolin-4(3*H*)-one(Entry 15, Table 3):white solid; mp = 160-162 °C; IR (KBr) ν_{max} = 3326, 3245, 1676, 1245, 1156, 1023 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.28 (d, *J* = 7.4 Hz, 1 H), 7.67-7.95 (m, 3 H), 7.54-7.60 (m, 3 H), 7.45 (t, *J* = 6.9 Hz, 1 H), 7.30 (t, *J* = 7.8 Hz, 3 H), 6.54 (d, *J* = 2.8 Hz, 1 H), 6.40 (d, *J* = 2.8 Hz, 1 H), 6.25 (d, *J* = 15.2 Hz, 1 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.3, 151.7, 151.6, 147.8, 144.2, 136.9, 134.5, 129.9, 129.3, 128.6, 127.2, 127.1, 126.5, 126.4, 120.8, 117.4, 114.0, 112.2; MS (APCI) m/z: 357.41 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{22}H_{16}N_2O_3Na^+$ [M + Na^+], 379.1053; Found 379.1056.



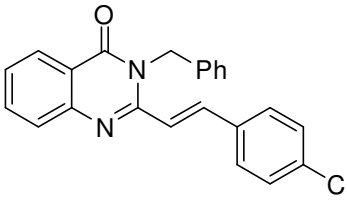
(*E*)-2-(2-(Benzo[d][1,3]dioxol-5-yl)vinyl)-3-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one(Entry 16, Table 3):white solid; mp = 170-171°C; IR (KBr) ν_{max} = 3345, 2962, 1648, 1542, 1245, 1042 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.27 (d, *J* = 7.6 Hz, 1 H), 7.9 (d, *J* = 15.4 Hz, 1 H), 7.59-7.78 (m, 2 H), 7.40-7.45 (m, 3 H), 7.20-7.23 (m, 2 H), 6.90-6.92 (m, 1 H), 6.77 (d, *J* = 8.0 Hz, 2 H), 6.25 (d, *J* = 15.3 Hz, 1 H), 5.97 (s, 2 H), 2.57 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.4, 151.9, 149.1, 148.1, 147.8, 140.5, 139.8, 134.6, 133.5, 129.7, 128.9, 127.2, 127.1, 126.4, 124.1, 120.7, 117.8, 108.5, 106.3, 101.4, 15.4; MS (APCI) m/z: 415.49 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{24}H_{18}N_2O_3SNa^+$ [M + Na^+], 437.0930; Found 437.0934.



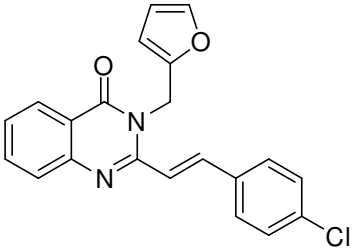
(*E*)-3-(4-(Methylthio)phenyl)-2-(2-(thiophen-2-yl)vinyl)quinazolin-4(3*H*)-one(Entry 17, Table 3):white solid; mp = 181-183°C; IR (KBr) ν_{max} = 3362, 1665, 1525, 1162, 1046 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.28 (d, *J* = 7.6 Hz, 1 H), 8.09 (d, *J* = 15.2 Hz, 1 H), 7.74-7.80 (m, 2 H), 7.41-7.47 (m, 3 H), 7.27 (t, *J* = 5.0 Hz, 1 H), 7.18-7.22 (m, 3 H), 6.99-7.02 (m, 1H), 6.22 (d, *J* = 15.2 Hz, 1 H), 2.57 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.3, 151.5, 147.7, 140.6, 140.6, 134.7, 133.4, 132.7, 129.9, 128.9, 128.1, 127.7, 127.2, 127.2, 126.5, 125.2, 120.7, 118.6, 15.6; MS (APCI) m/z: 377.49 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{21}H_{16}N_2OS_2Na^+$ $[M + Na^+]$, 399.0596; Found 399.0594.



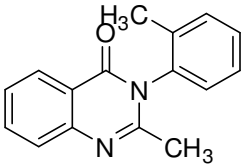
(*E*)-2-(2-(furan-2-yl)vinyl)-3-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one(Entry 18, Table 3):white solid; mp = 195-196°C; IR (KBr) ν_{max} = 3323, 1645, 1552, 1145, 1023 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.28 (dd, *J* = 8.0 Hz &*J* = 1.0 Hz, 1 H), 7.72-7.80 (m, 3 H), 7.38-7.47 (m, 4 H), 7.20-7.22 (m, 2 H), 6.55 (d, *J* = 3.2 Hz, 1 H), 6.42 (m, 1 H), 6.32 (d, *J* = 15.1 Hz, 1 H), 2.57 (s, 3 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.4, 151.8, 151.7, 147.8, 144.3, 140.4, 134.6, 133.6, 128.9, 127.2, 127.1, 126.7. 126.5, 120.8, 117.3, 114.2, 112.2, 15.5; MS (APCI) m/z: 361.45 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{21}H_{16}N_2O_2SNa^+$[M + Na^+], 383.0825; Found 383.0828.



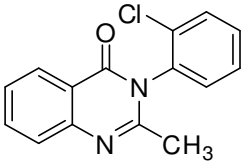
(*E*)-3-Benzyl-2-(4-chlorostyryl)quinazolin-4(3*H*)-one(Entry 19, Table 3):white solid; mp = 158-160°C; IR (KBr) ν_{max} = 3330, 1668, 1546, 1157, 1042 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.38 (dd, *J* = 8.2 Hz & 1.0 Hz, 1 H), 7.86 (d, *J* = 15.4 Hz, 1 H), 7.72-7.79 (m, 2 H), 7.46-7.50 (m, 1 H), 7.26-7.35 (m, 9H), 6.22 (d, *J* = 15.4 Hz, 1 H), 5.51 (s, 2 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 162.4, 152.2, 147.5, 139.6, 136.3, 135.5, 134.5, 133.8, 129.1, 129.1, 128.8, 127.8, 127.3, 127.2, 126.7, 126.5, 120.5, 119.9, 46.9; MS (APCI) m/z: 373.86 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{23}H_{17}ClN_2ONa^+$[M + Na^+], 395.0922; Found 395.0922.



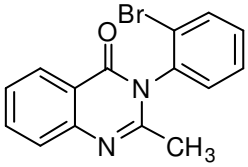
(*E*)-2-(4-Chlorostyryl)-3-(furan-2-ylmethyl)quinazolin-4(3*H*)-one(Entry 20, Table 3):White solid; mp = 195-197°C; IR (KBr) ν_{max} = 3325, 1668, 1492, 1142, 1023 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.38 (dd, *J* = 8.1 Hz & 1.0 Hz, 1 H), 7.86 (d, *J* = 15.4 Hz, 1 H), 7.70-7.78 (m, 2 H), 7.53-7.56 (m, 2 H), 7.43-7.47 (m, 2 H), 7.38-7.40-7.45 (m, 3 H), 6.45-6.46 (m, 1 H), 6.35-6.37 (m, 1 H), 5.43 (s, 2 H); ^{13}C NMR ($CDCl_3$, 100 MHz): 161.9, 151.9, 149.4, 147.4, 142.5, 139.7, 135.6, 134.4, 133.9, 129.2, 129.0, 127.3, 127.0, 126.6, 120.5, 119.9, 110.8, 109.5, 40.2; MS (APCI) m/z: 363.82 $(M + H)^+$; HRMS (ESI) m/z calcd for $C_{21}H_{15}ClN_2O_2Na^+$ $[M + Na^+]$, 385.0714; Found 385.0721



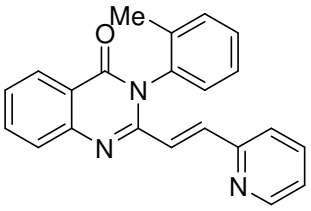
2-Methyl-3-*o*-tolylquinazolin-4(3*H*)-one (**Methaqualone**)[33]: White solid; mp = 118-119 °C; IR (KBr) ν_{max} = 3008, 1683, 1600, 1471, 1274 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.29 (d, *J* = 7.9 Hz, 1H), 7.78 (t, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.41-7.36 (m, 3H), 7.16 (d, *J* = 7.3 Hz, 1H), 2.19 (s, 3H), 2.13 (s, 3H);MS(APCI) *m/z* 251.41 $(M+H)^+$.



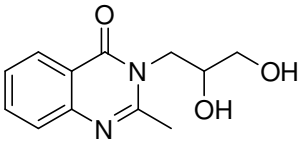
3-(2-Chlorophenyl)-2-methylquinazolin-4(3*H*)-one (Mecloqualone)[33]:Brown solid; mp = 126-128 °C; IR (KBr) ν_{max} = 2925, 1688, 1608, 1471, 1281 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.28 (d, *J* = 6.8 Hz, 1H), 7.78 (t, *J* = 8.2 Hz, 1H), 7.70 (d, *J* = 7.6 Hz, 1H), 7.62-7.60 (m, 1H), 7.50-7.46 (m, 3H), 7.36-7.33 (m, 1H), 2.23 (s, 3H);MS(APCI) *m/z* 271.24 $(M+H)^+$



3-(2-Bromophenyl)-2-methylquinazolin-4(3*H*)-one (Mebroqualone)[33]: White solid; mp = 143-145 °C; IR (KBr) ν_{max} = 2923, 1687, 1607, 1471, 1281 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$)δ: 8.28 (d, *J* = 7.9 Hz, 1H), 8.27-7.76 (m, 2H), 7.70 (d, *J* = 7.5 Hz, 1H), 7.51-7.47 (m, 2H), 7.40-7.36 (m, 2H), 2.22 (s, 3H); MS(APCI) *m/z* 315.12 $(M+H)^+$



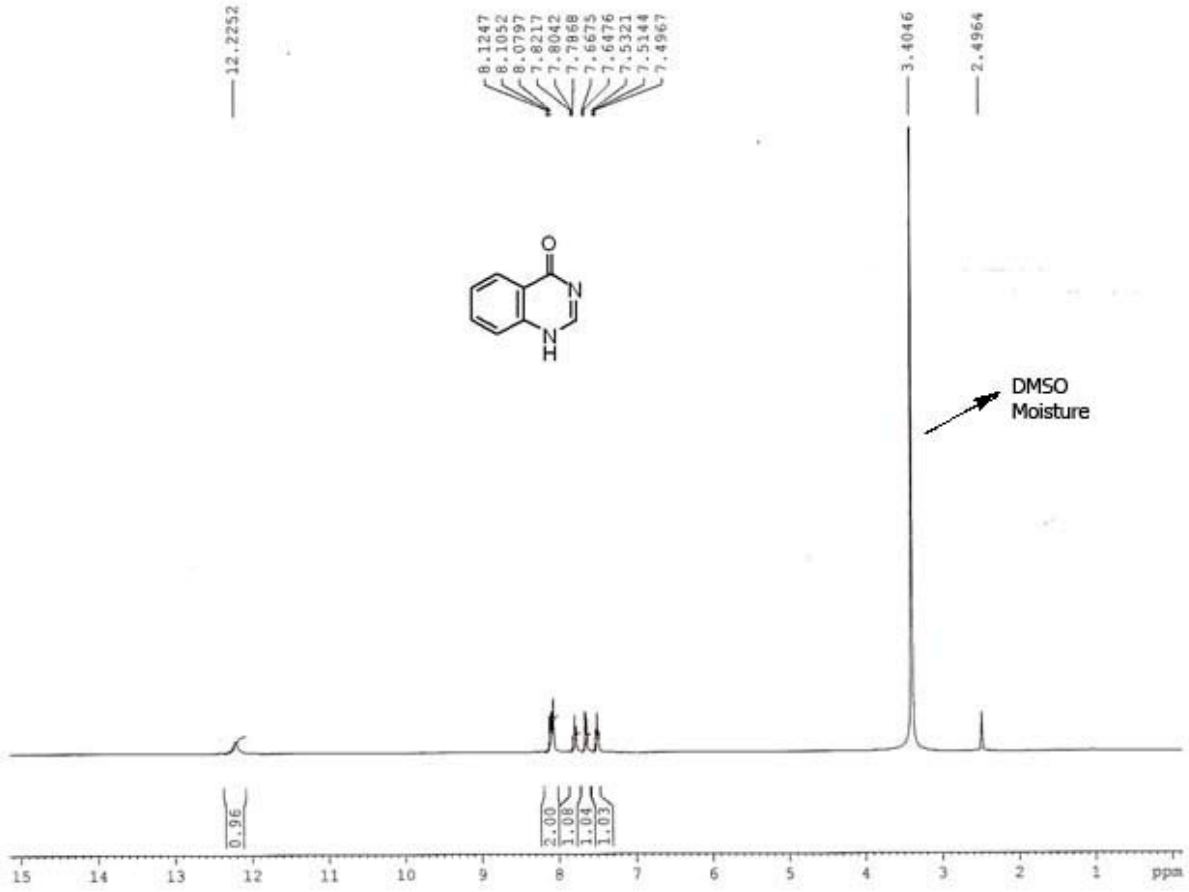
(*E*)-2-(2-(pyridin-2-yl)vinyl)-3-(*o*-tolyl)quinazolin-4(3*H*)-one (Piriquialone)[33]: white solid; mp = 195-196 °C; IR (KBr) ν_{max} = 3326, 1645, 1525, 1126, 1023 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz): δ = 8.50 (d, *J* = 3.9 Hz, 1 H), 8.31-8.34 (m, 1 H), 8.00 (d, *J* = 15.0 Hz, 1 H), 7.80-7.82 (m, 2 H), 7.61-7.63 (m, 1 H), 7.48-7.52 (m, 1 H), 7.40-7.46 (m, 3 H), 7.30 (d, *J* = 7.8 Hz, 1 H), 7.22 (d, *J* = 7.6 Hz, 1 H), 7.14-7.18 (m, 1 H), 6.92 (d, *J* = 15.0 Hz, 1 H), 2.13 (s, 3H); MS (APCI) m/z: 340.42 $(M + H)^+$.



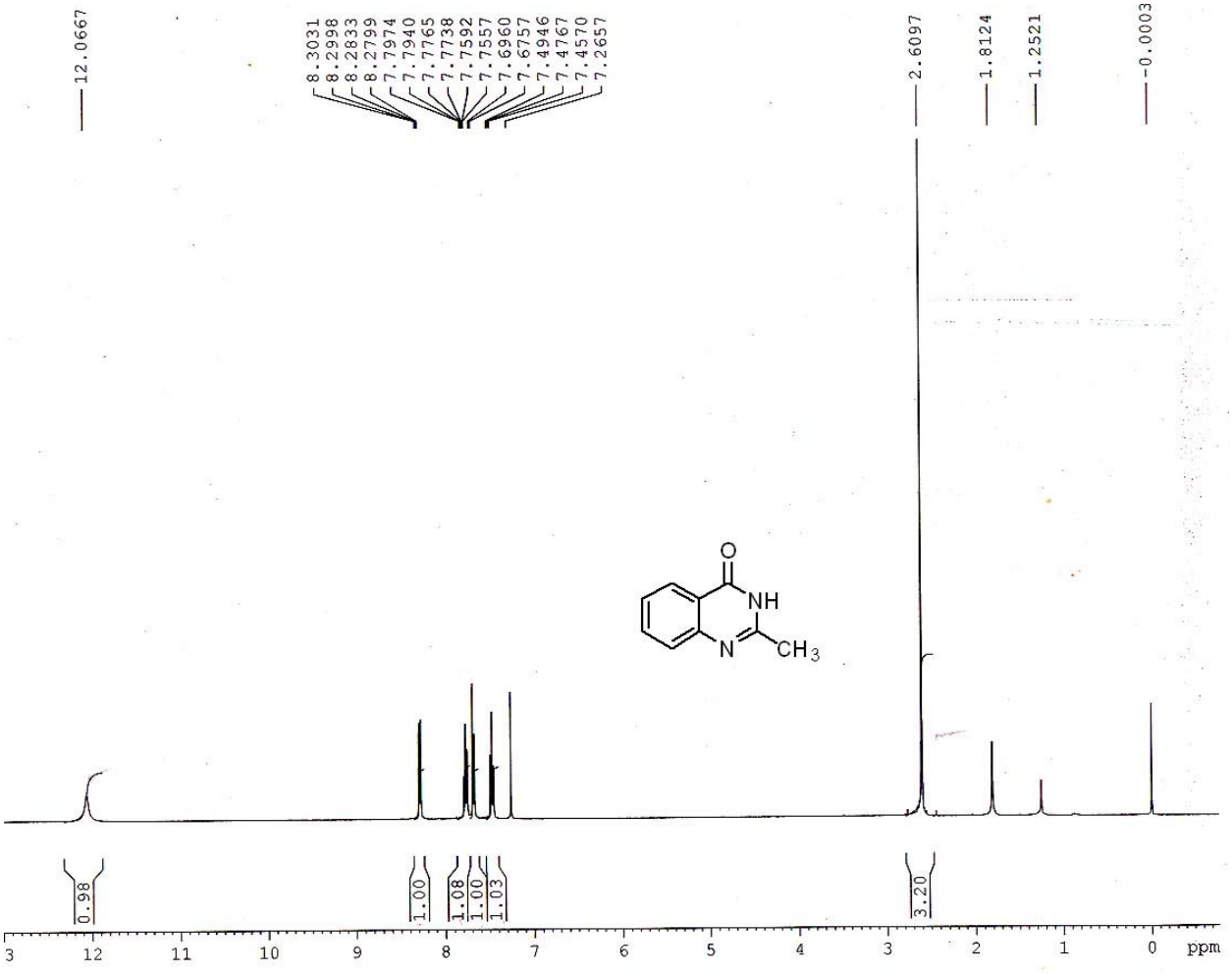
3-(2,3-dihydroxypropyl)-2-methylquinazolin-4(3H)-one (Diproqualone)[34]: white solid; mp = 210-212 °C; IR (KBr) ν_{max} = 3318, 1641, 1531 cm^{-1}; ^1H NMR (DMSO, 400 MHz): δ = 8.10 (d, *J* = 7.92 Hz, 1 H), 7.76-7.80 (m, 1 H), 7.58 (d, *J* = 8.16 Hz, 1 H), 7.47 (t, *J* = 7.16 Hz, 1H), 5.08 (d, *J* = 4.52 Hz, 1 H), 4.79 (t, *J* = 5.64 Hz, 1 H), 4.26-4.32 (m, 1H), 3.82-3.91 (m, 2H), 2.71(s, 3H); MS (APCI) m/z: 235.12 $(M + H)^+$.

3. Scanned NMR Spectra

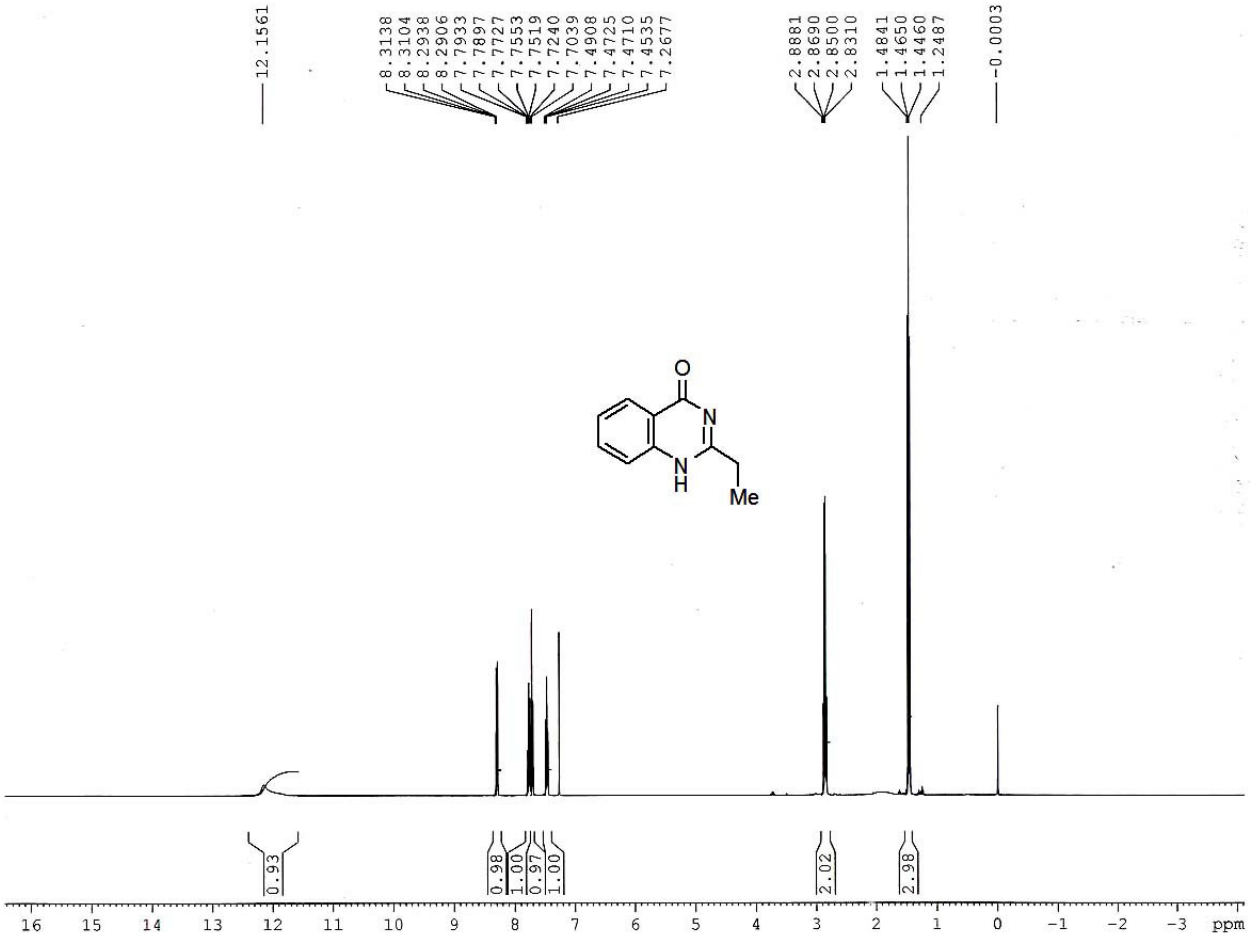
Quinazolin-4(1*H*)-one(Entry 1, Table 2)



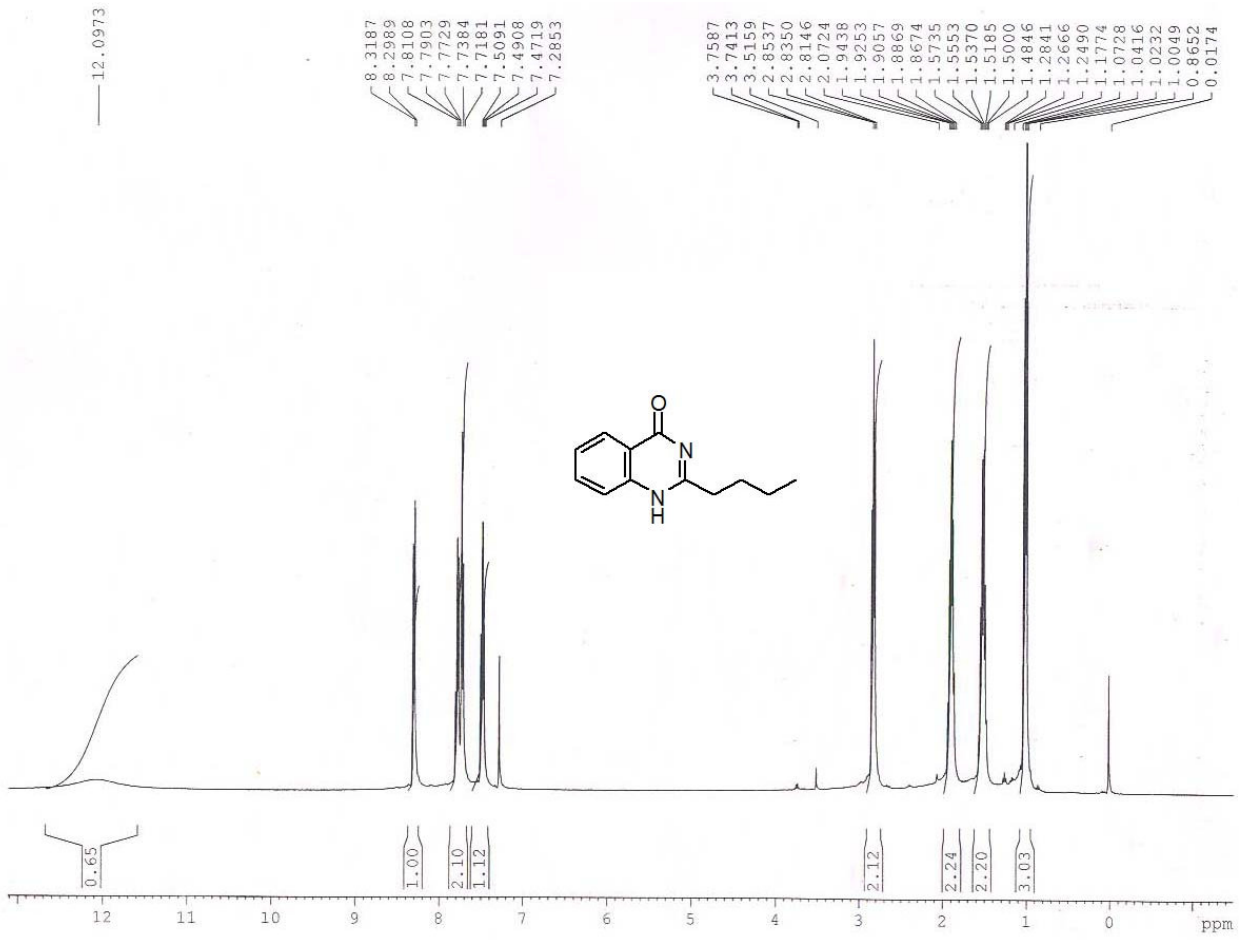
2-Methylquinazolin-4(1*H*)-one(Entry 2, Table 2)



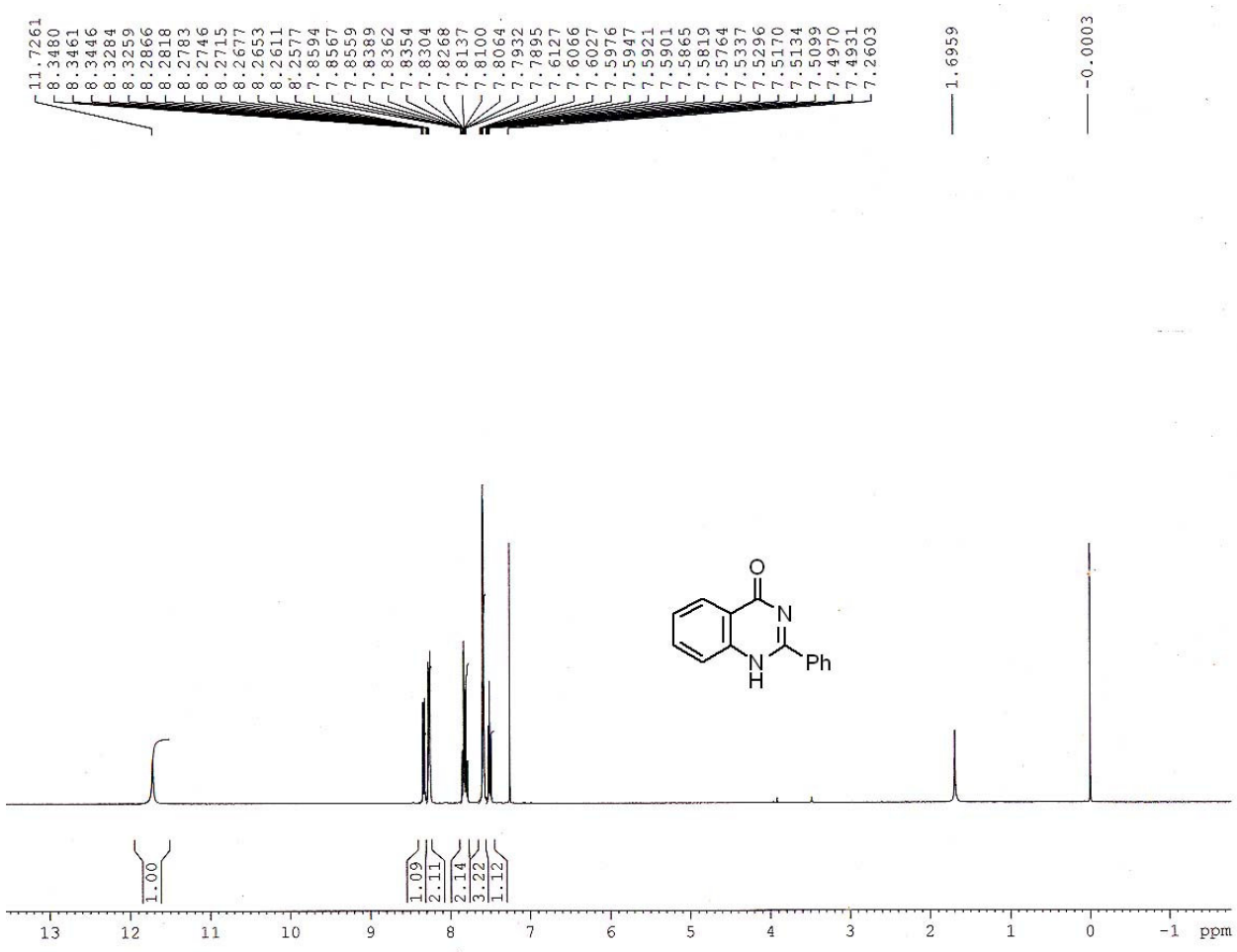
2-Ethylquinazolin-4(1*H*)-one(Entry 3, Table 2)



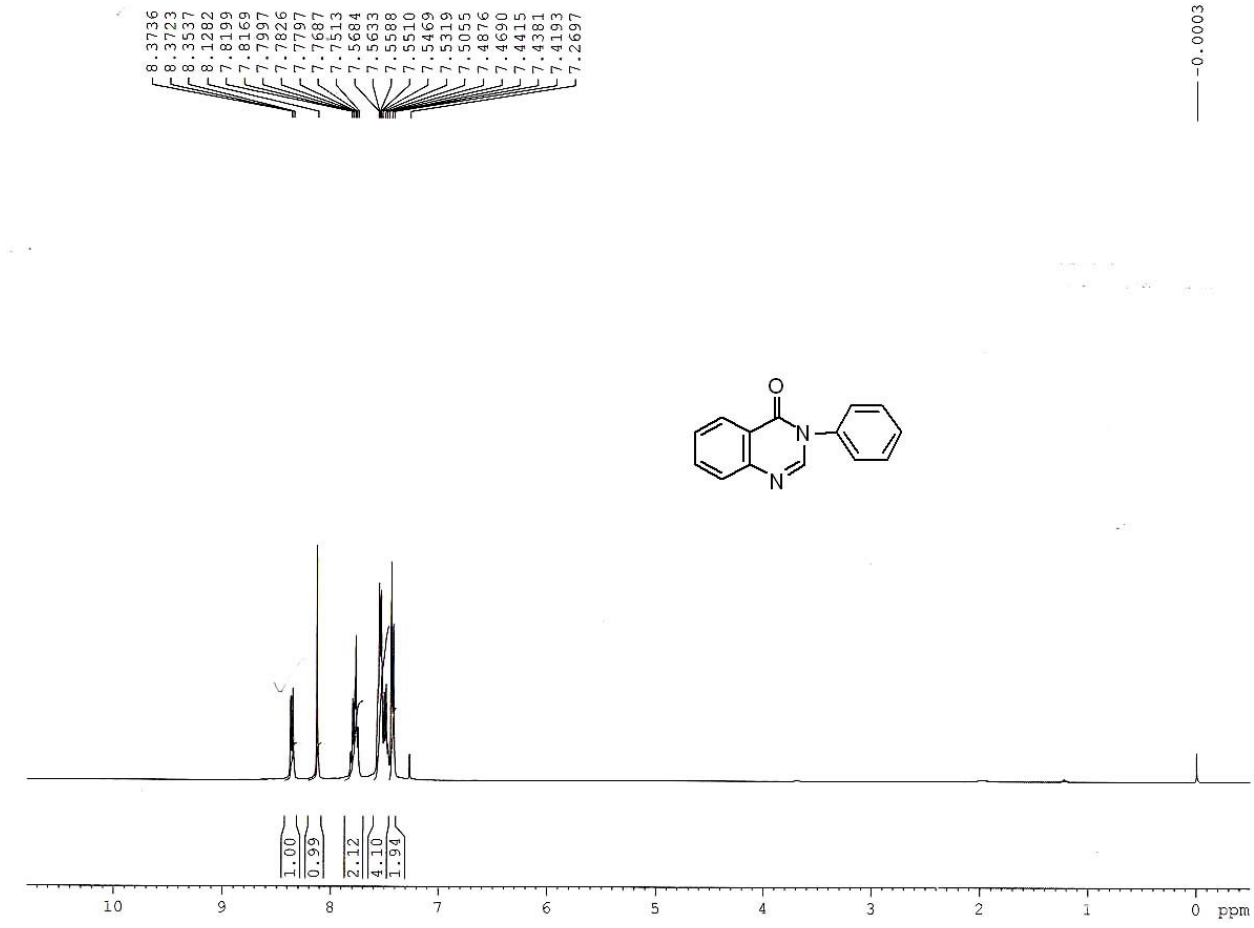
2-Butylquinazolin-4(1*H*)-one(Entry 4, Table 2)



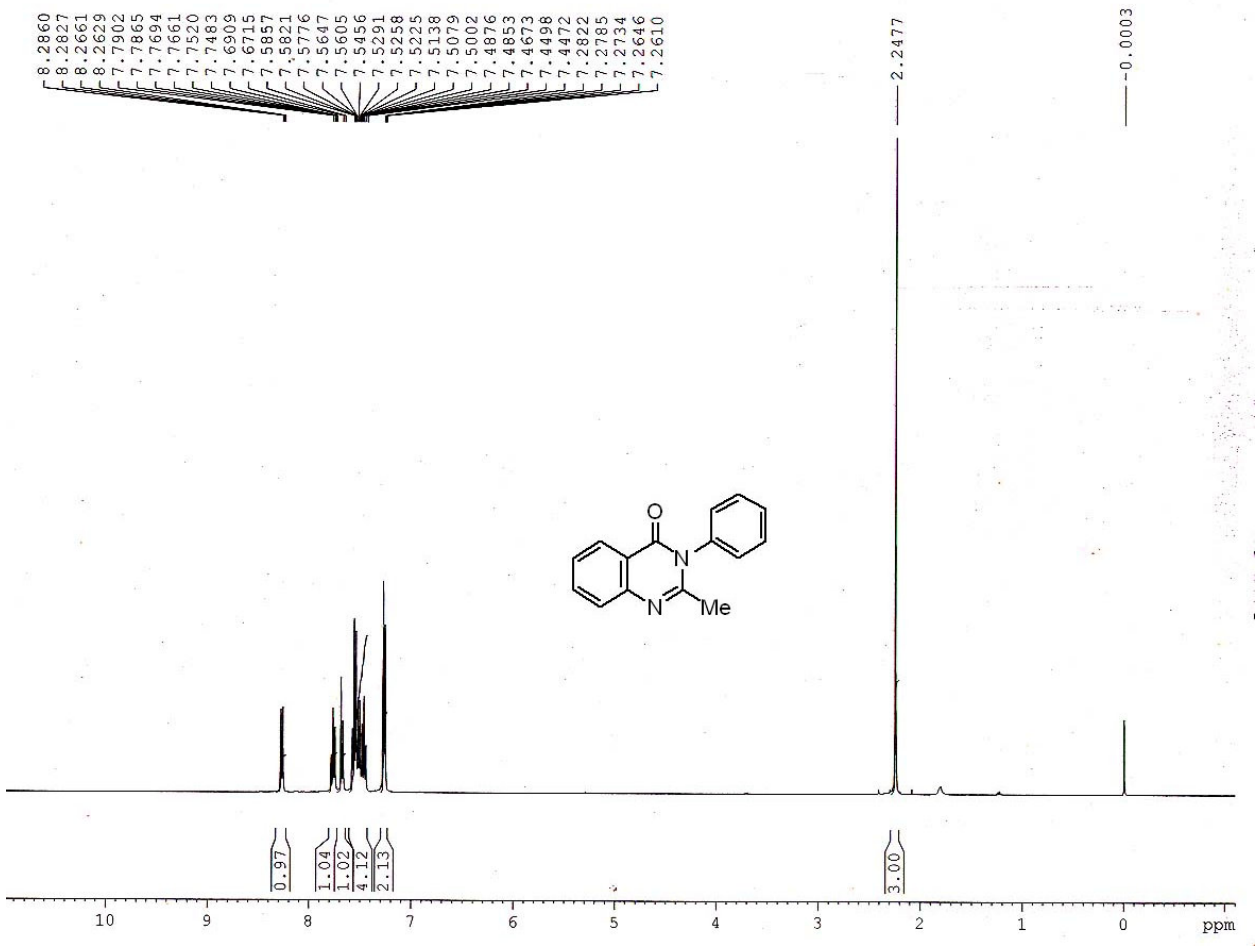
2-Phenylquinazolin-4(1*H*)-one(Entry 5, Table 2)



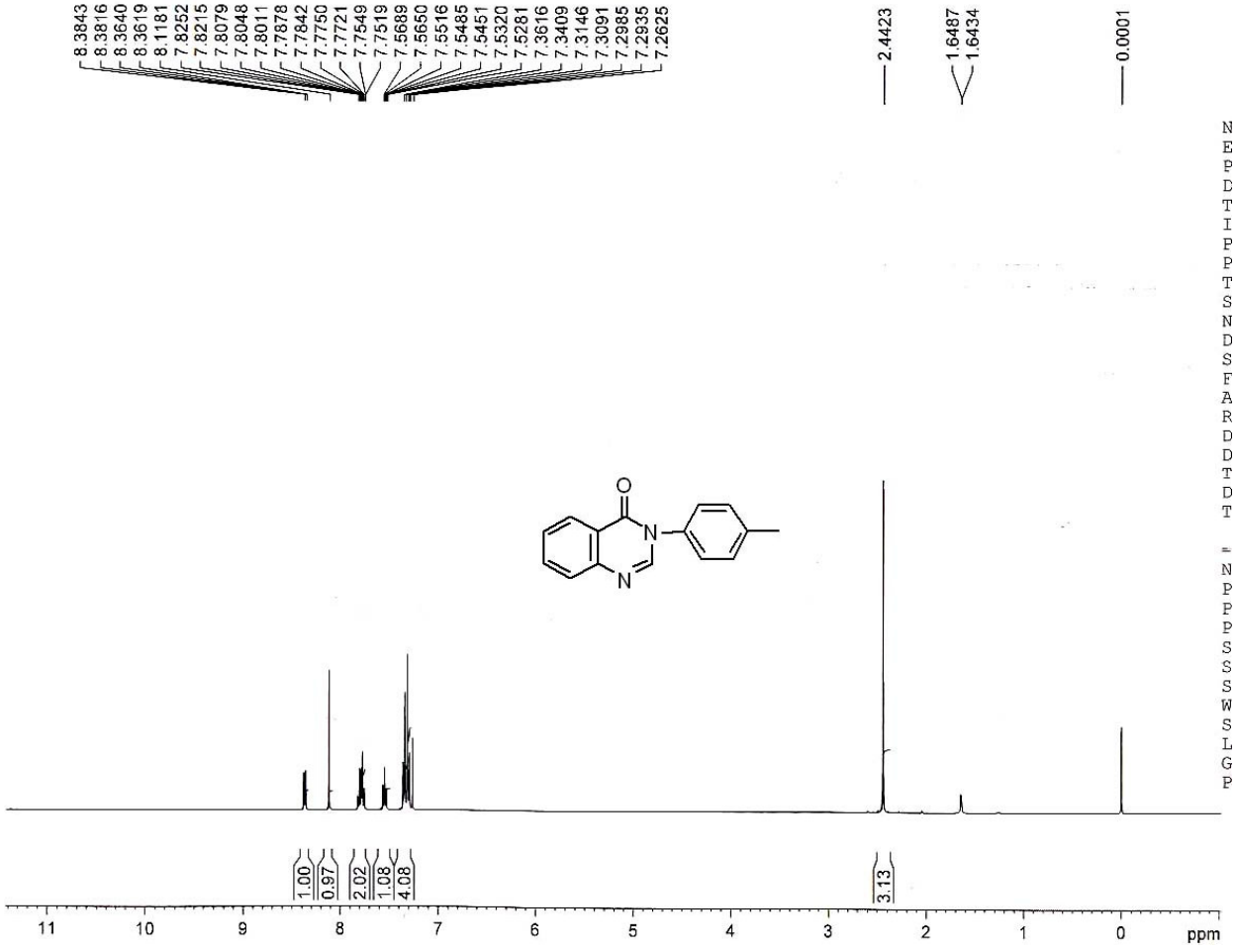
3-Phenylquinazolin-4(3*H*)-one(Entry 6, Table 2)



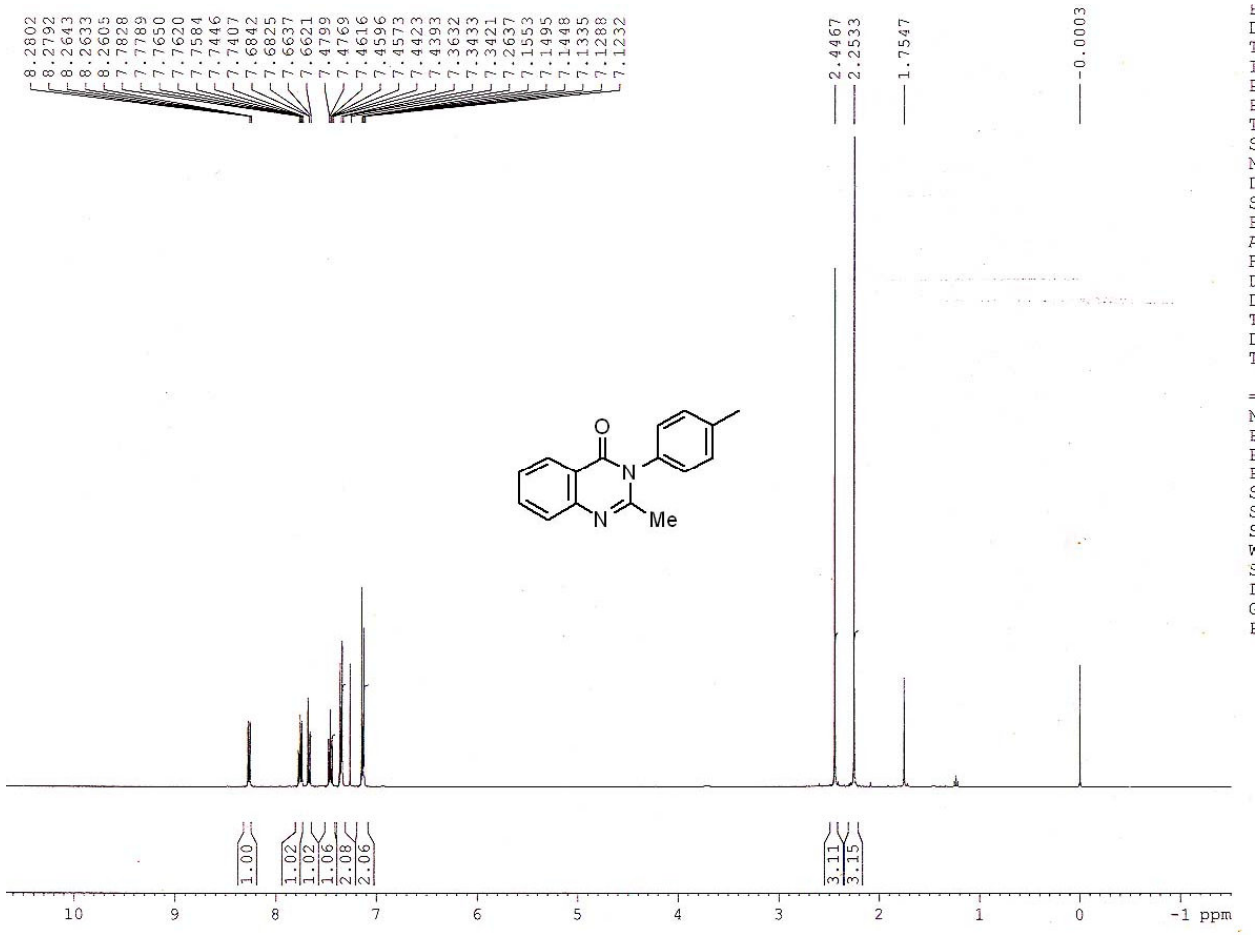
2-Methyl-3-phenylquinazolin-4(3*H*)-one(Entry 7, Table 2)



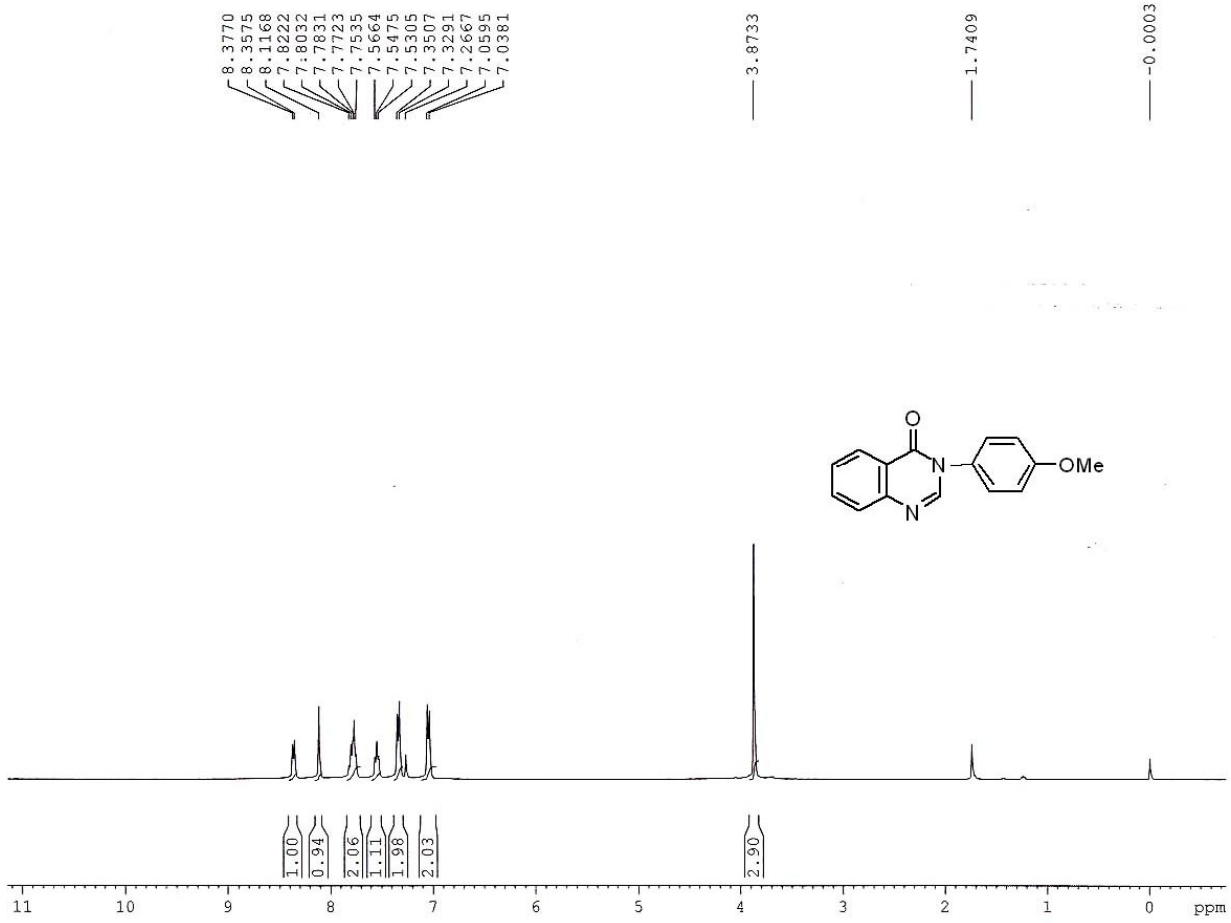
3-p-Tolylquinazolin-4(3*H*)-one(Entry 8, Table 2)



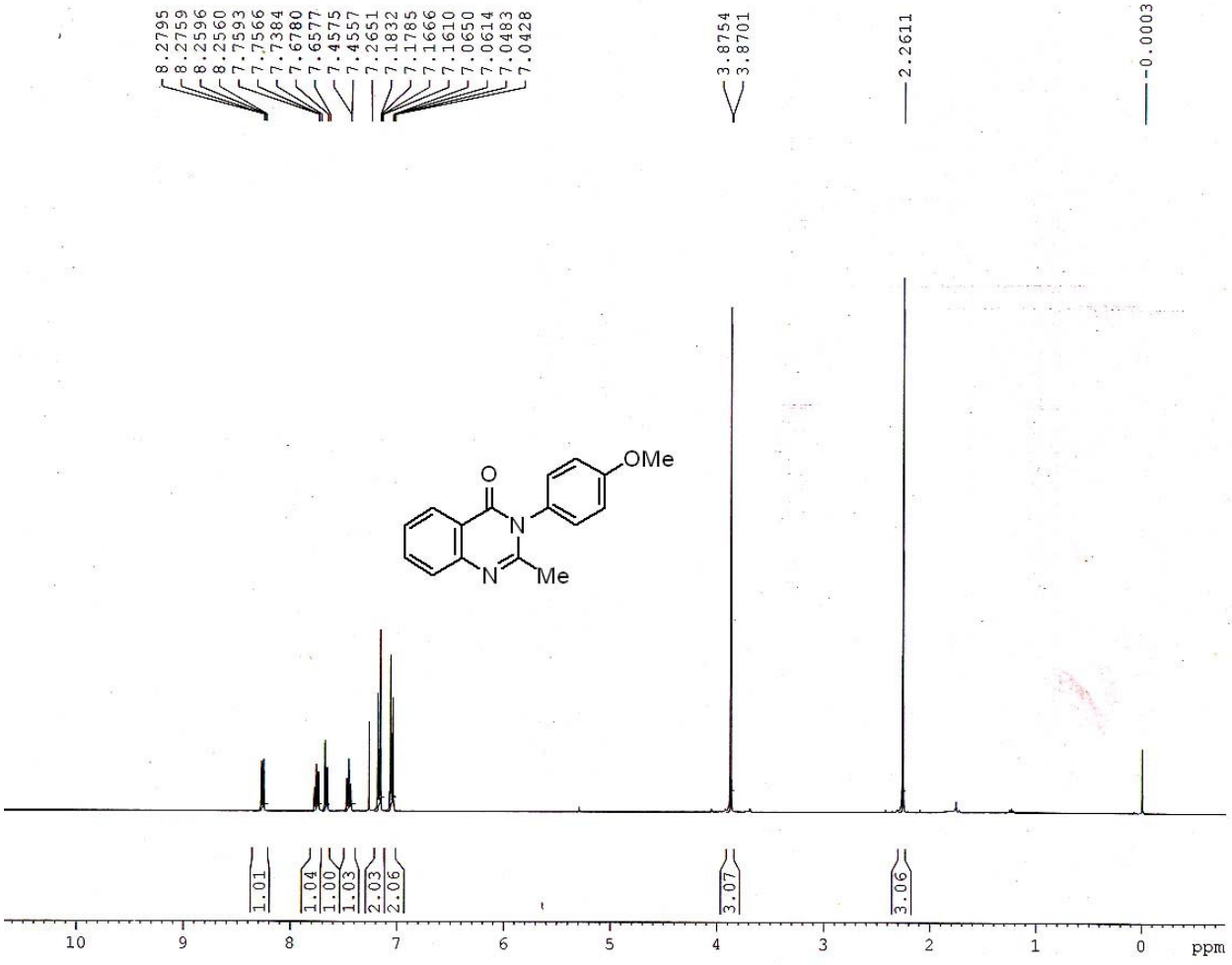
2-Methyl-3-p-tolylquinazolin-4(3*H*)-one(Entry 9, Table 2)



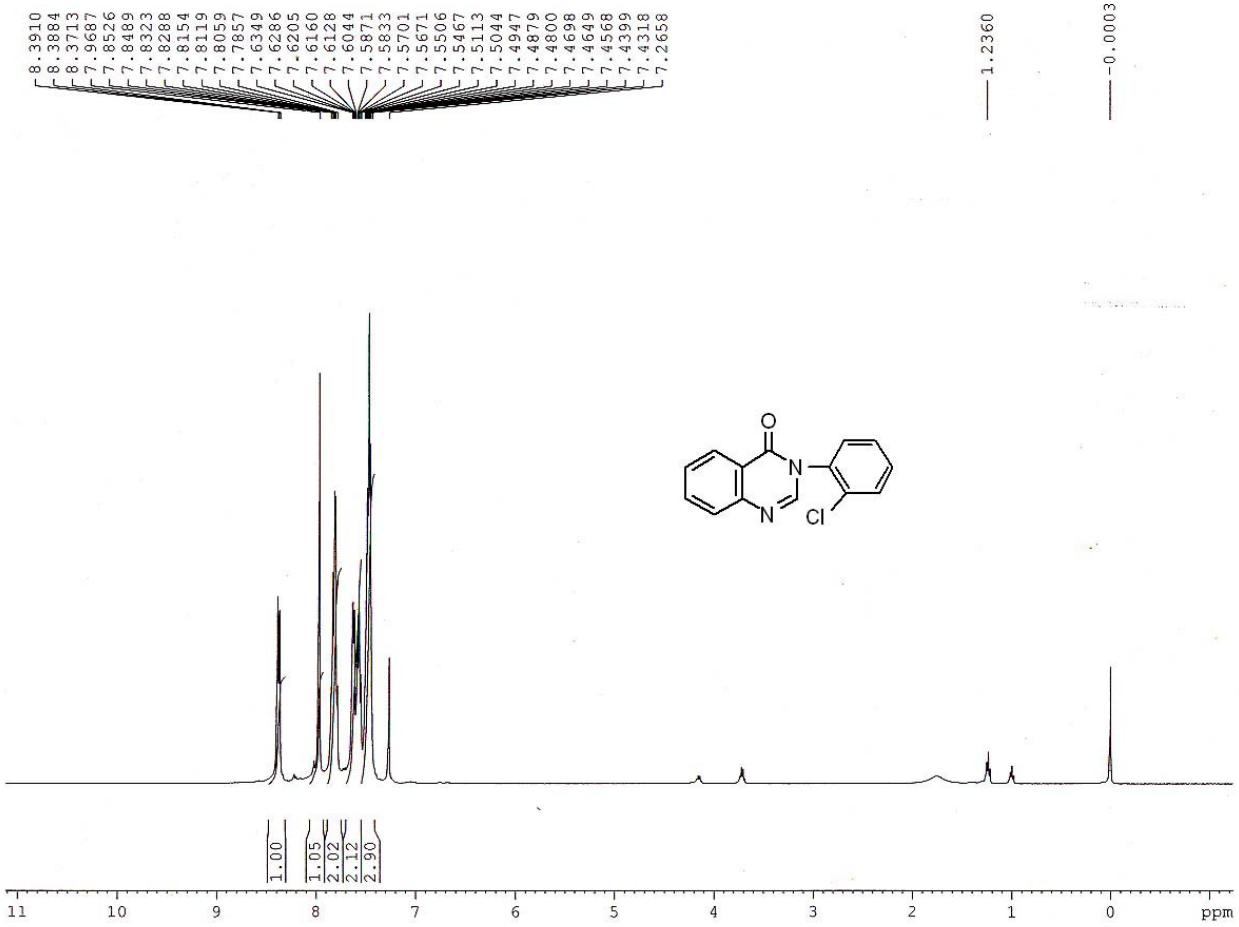
3-(4-Methoxyphenyl)quinazolin-4(3*H*)-one(Entry 10, Table 2)



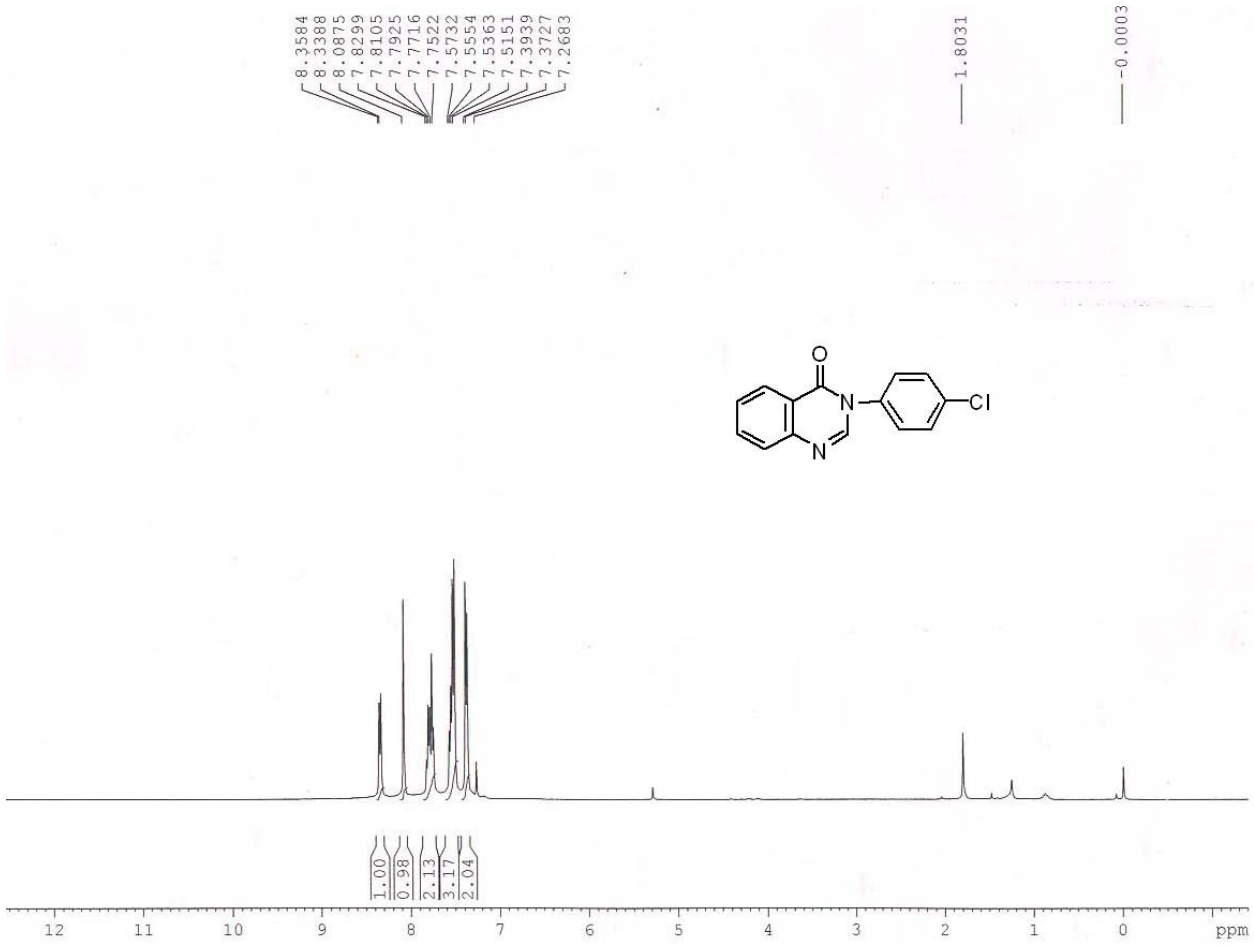
3-(4-Methoxyphenyl)-2-methylquinazolin-4(3*H*)-one(Entry 11, Table 2)



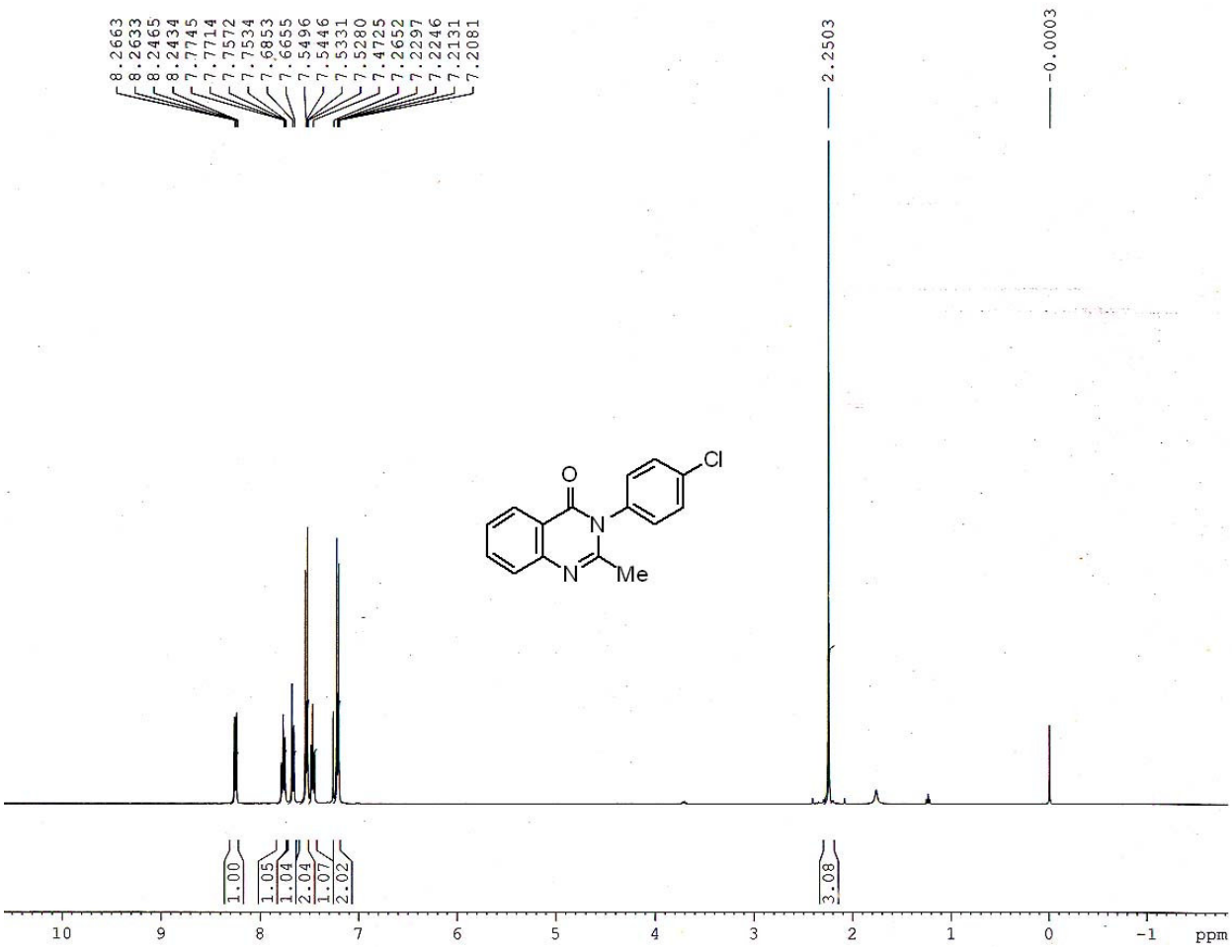
3-(2-Chlorophenyl)quinazolin-4(3*H*)-one (Entry 12, Table 2)



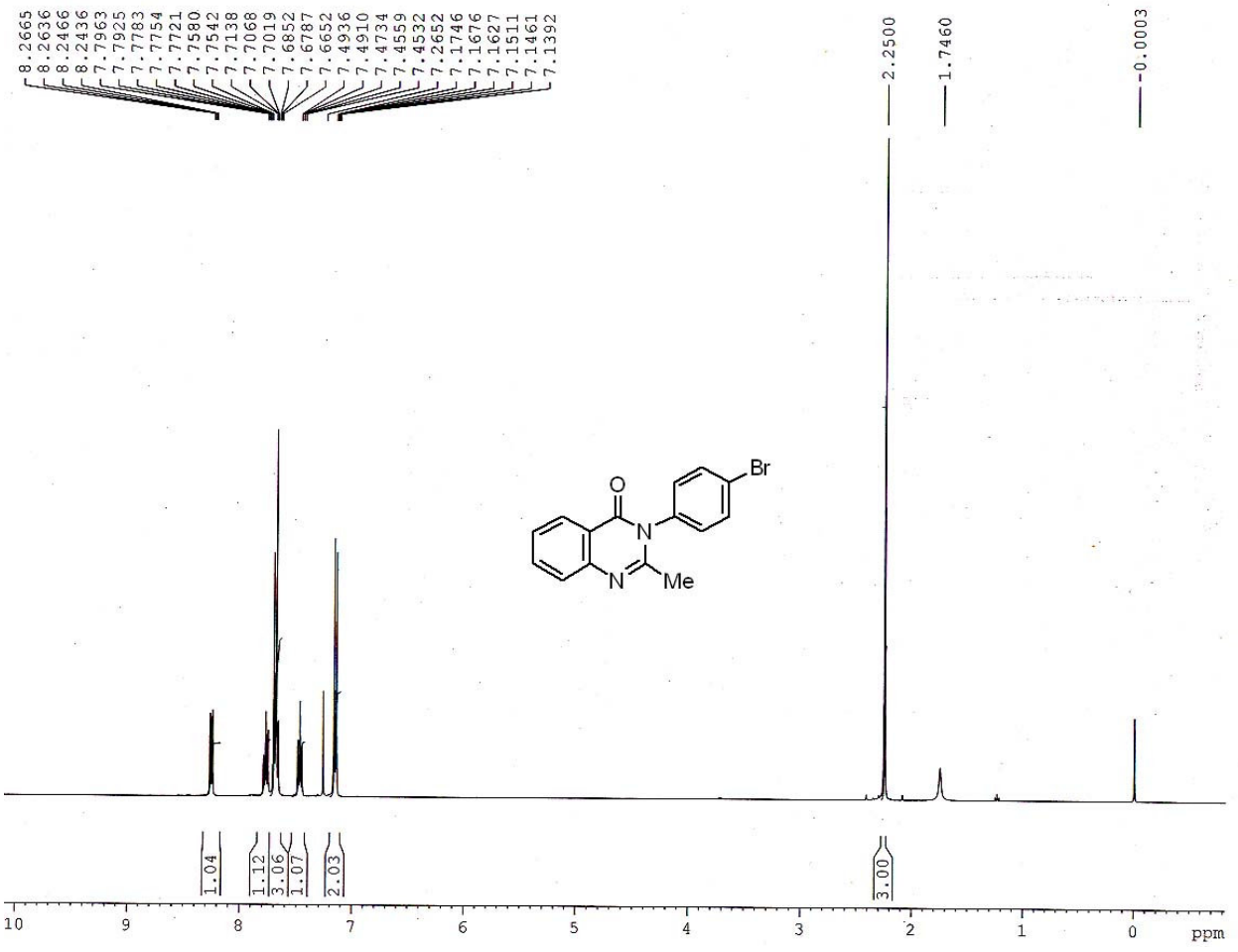
3-(4-Chlorophenyl)quinazolin-4(3*H*)-one (Entry 13, Table 2)



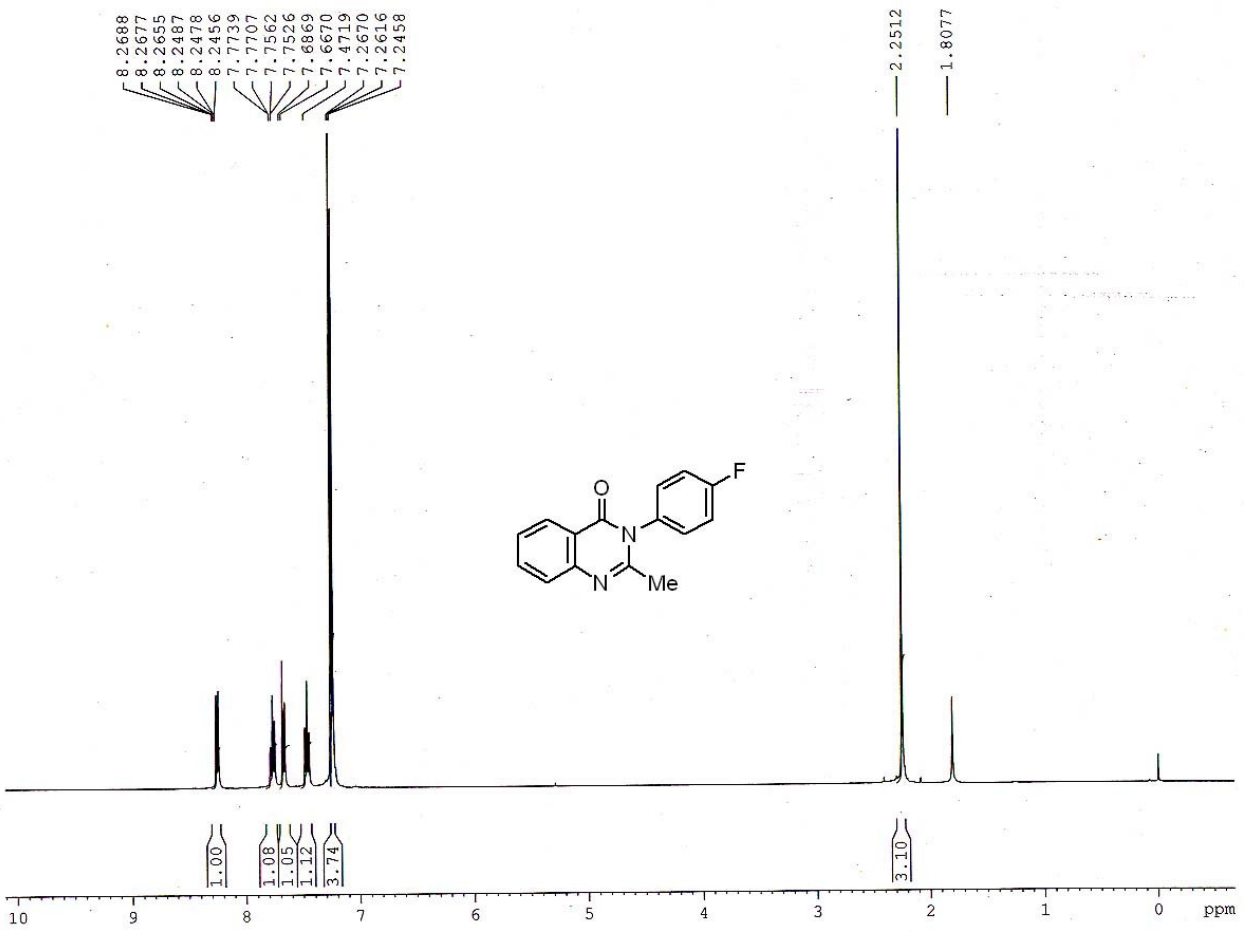
3-(4-Chlorophenyl)-2-methylquinazolin-4(3*H*)-one(Entry 14, Table 2)



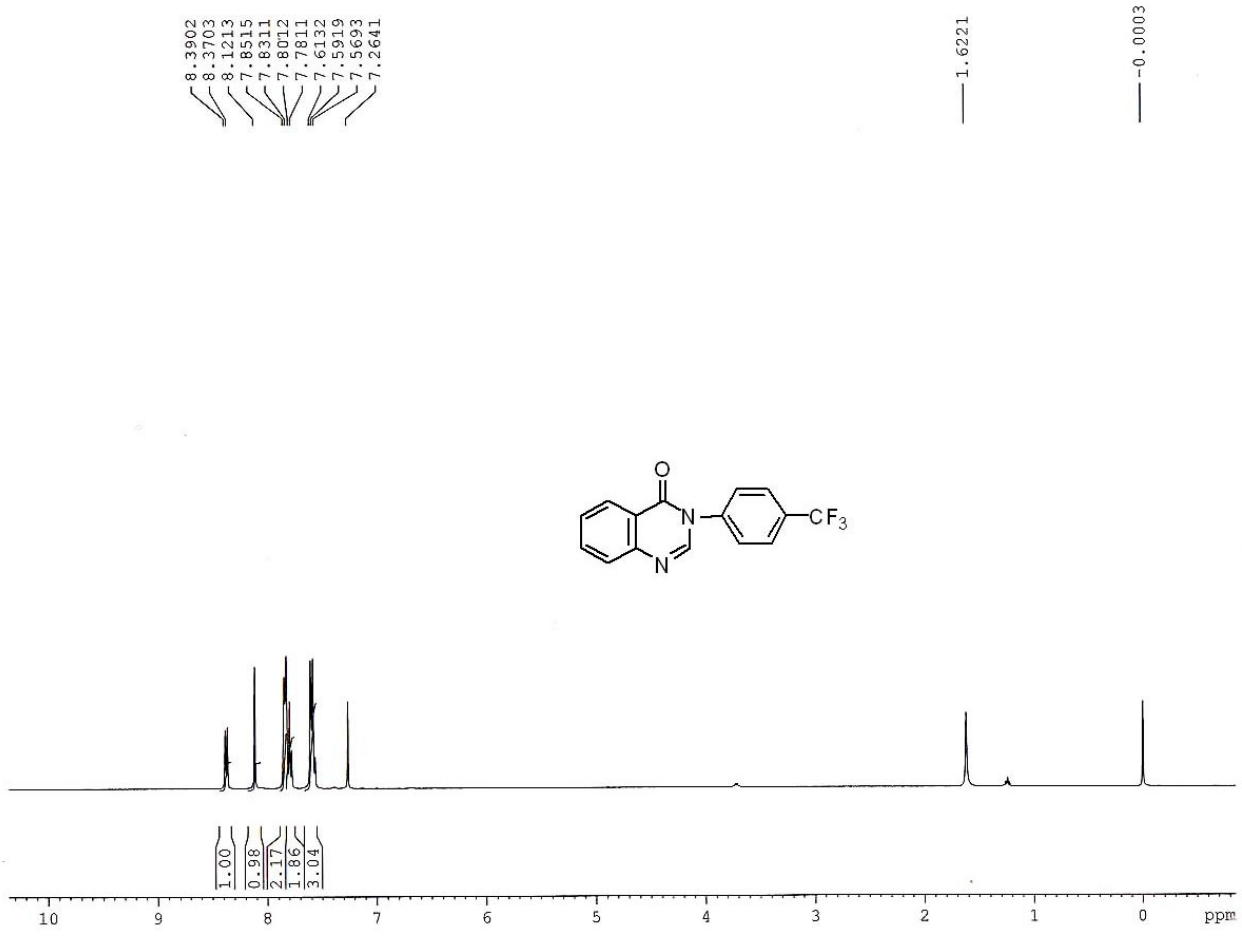
3-(4-Bromophenyl)-2-methylquinazolin-4(3*H*)-one(Entry 15, Table 2)



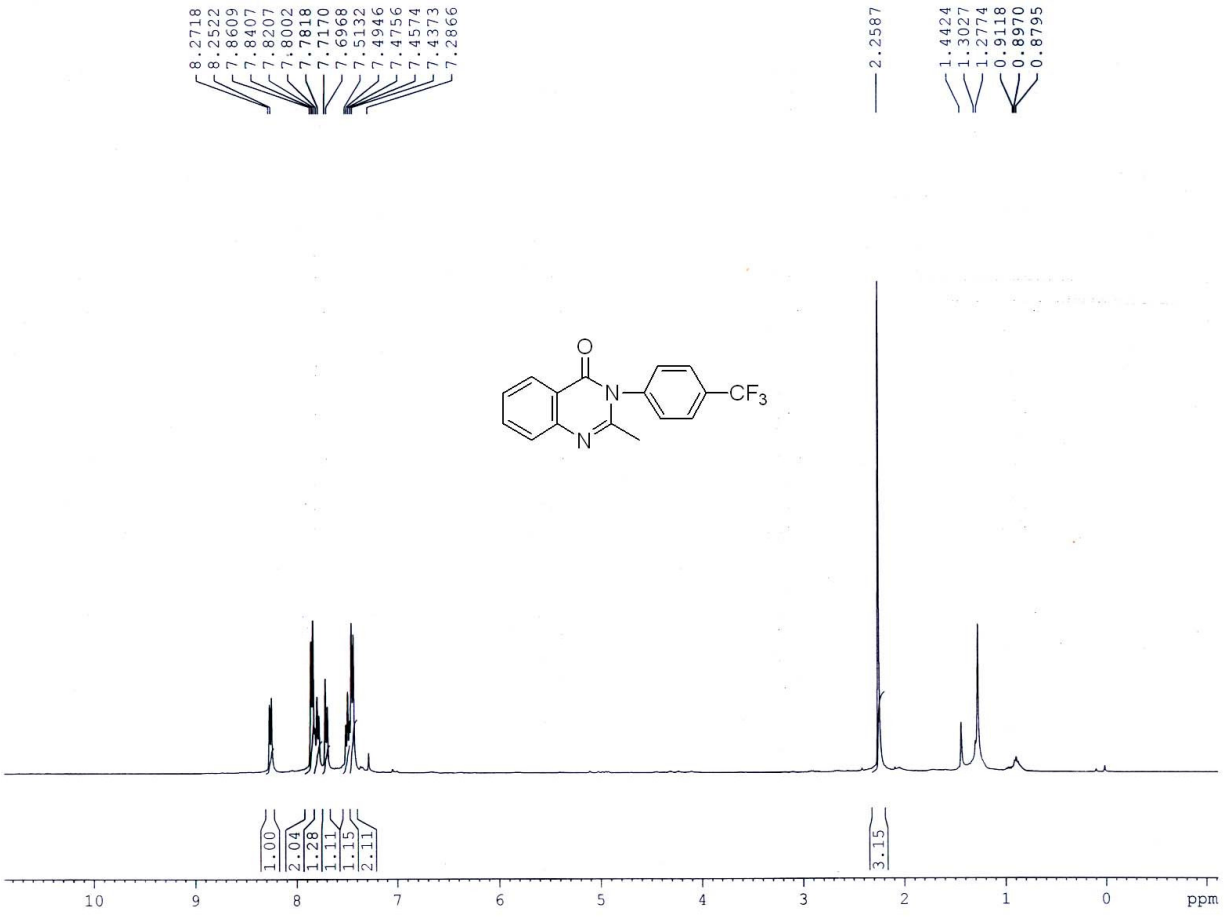
3-(4-Fluorophenyl)-2-methylquinazolin-4(3*H*)-one(Entry 16, Table 2)



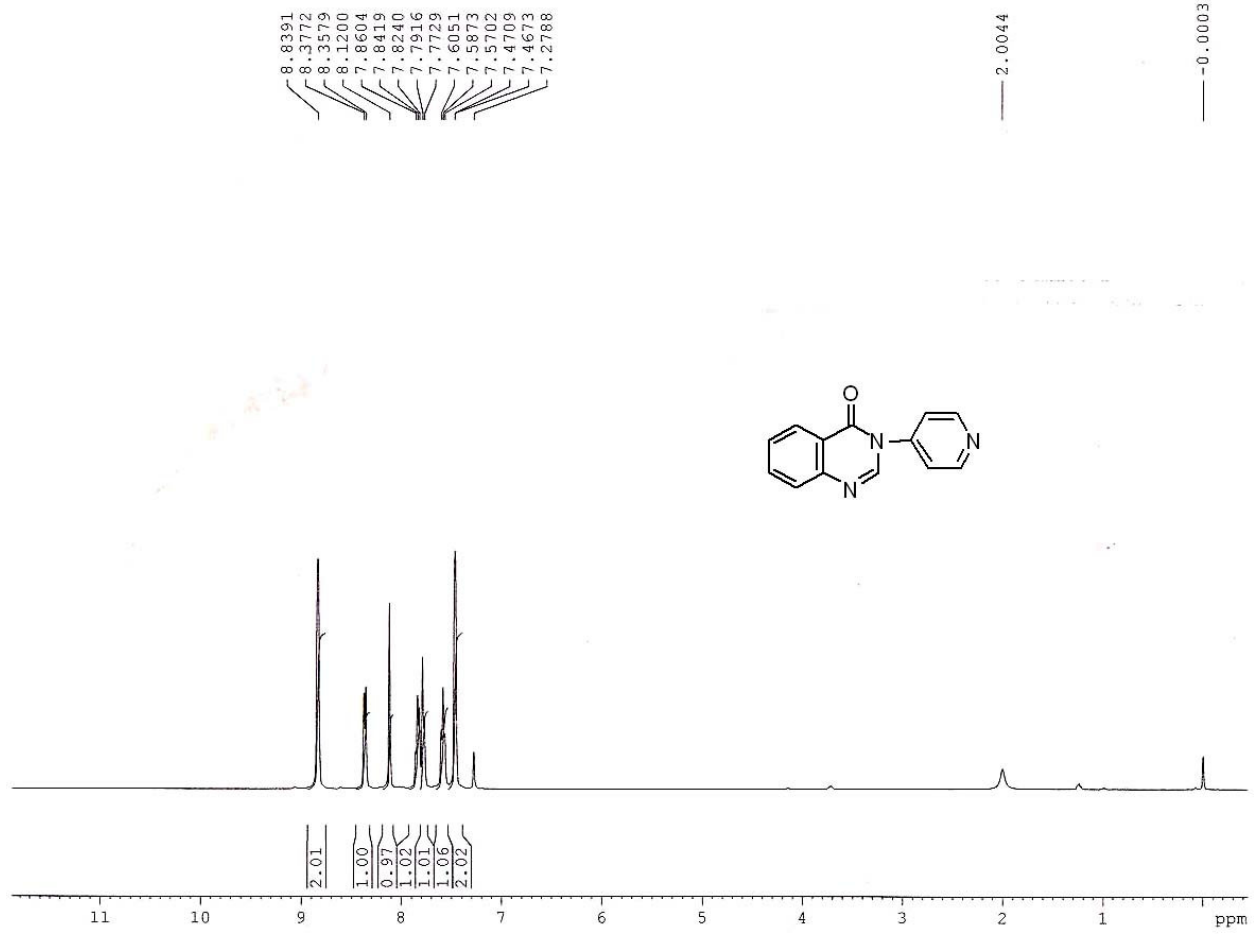
3-(4-(Trifluoromethyl)phenyl)quinazolin-4(3*H*)(Entry 17, Table 2)

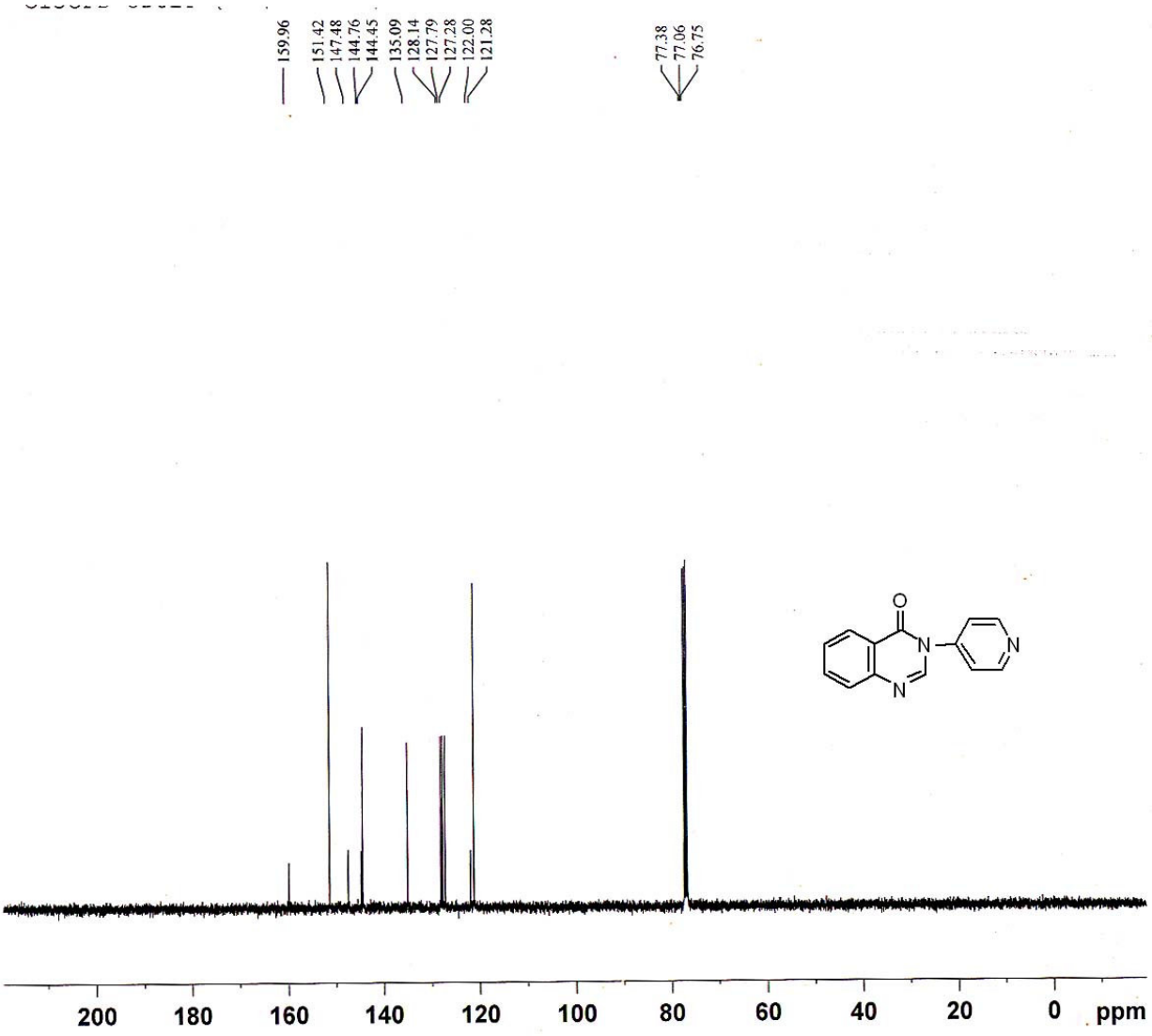


2-Methyl-3-(4-(trifluoromethyl)phenyl)quinazolin-4(3*H*)-one(Entry 18, Table 2)

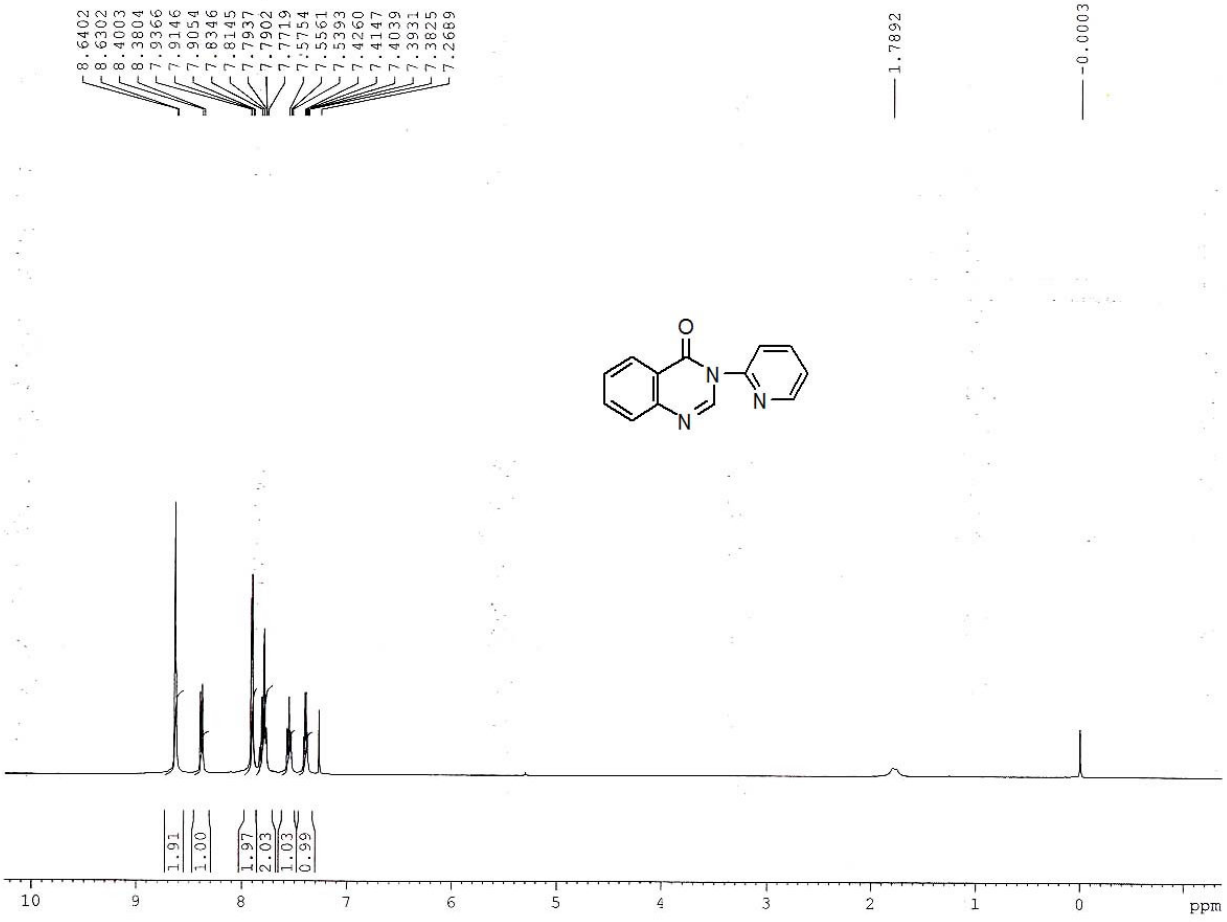


3-(Pyridin-4-yl)quinazolin-4(3*H*)-one(Entry 19, Table 2)

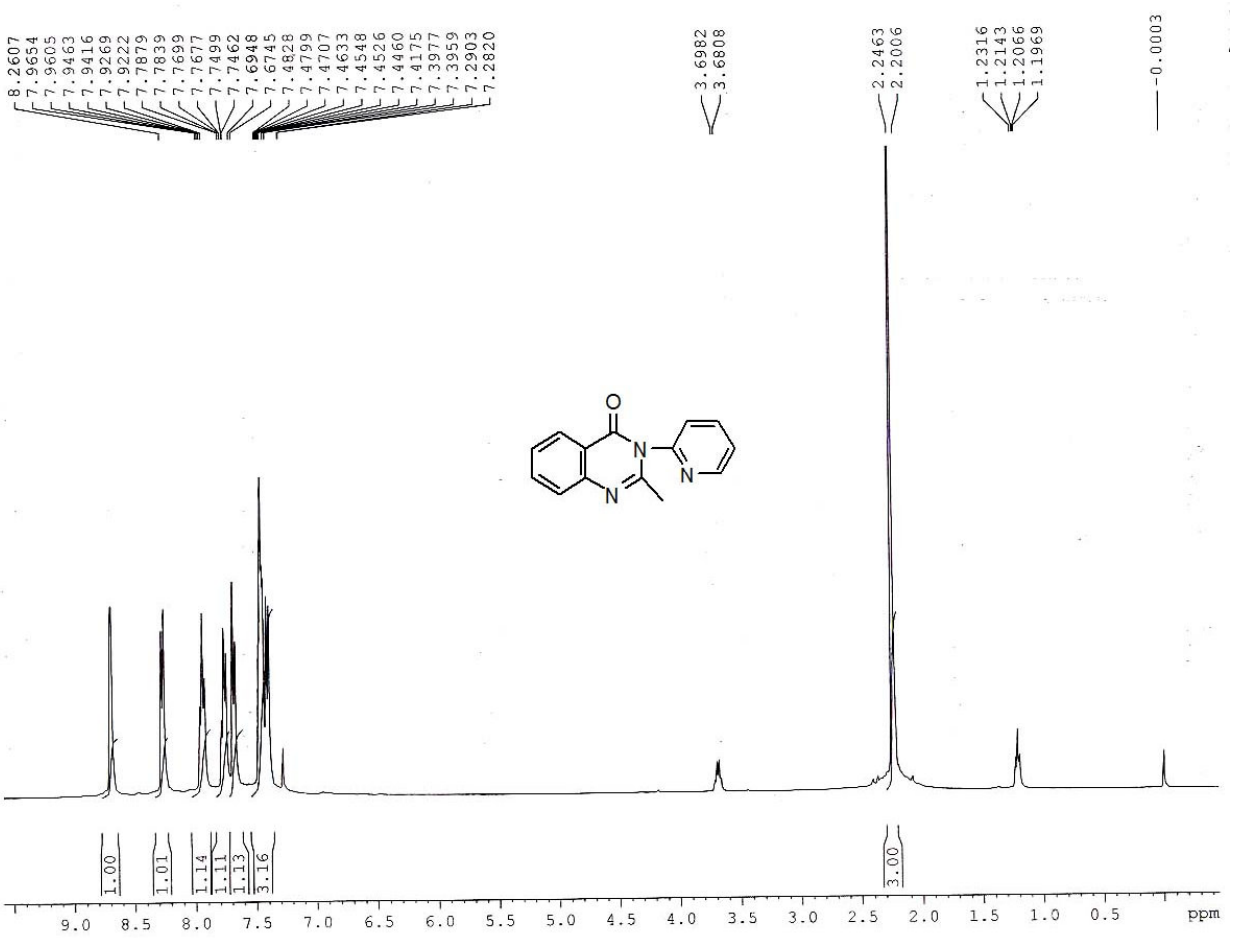



159.96
151.42
147.48
144.76
144.45
135.09
128.14
127.79
127.28
122.00
121.28
77.38
77.06
76.75
O
N
N
N
200
180
160
140
120
100
80
60
40
20
0
ppm

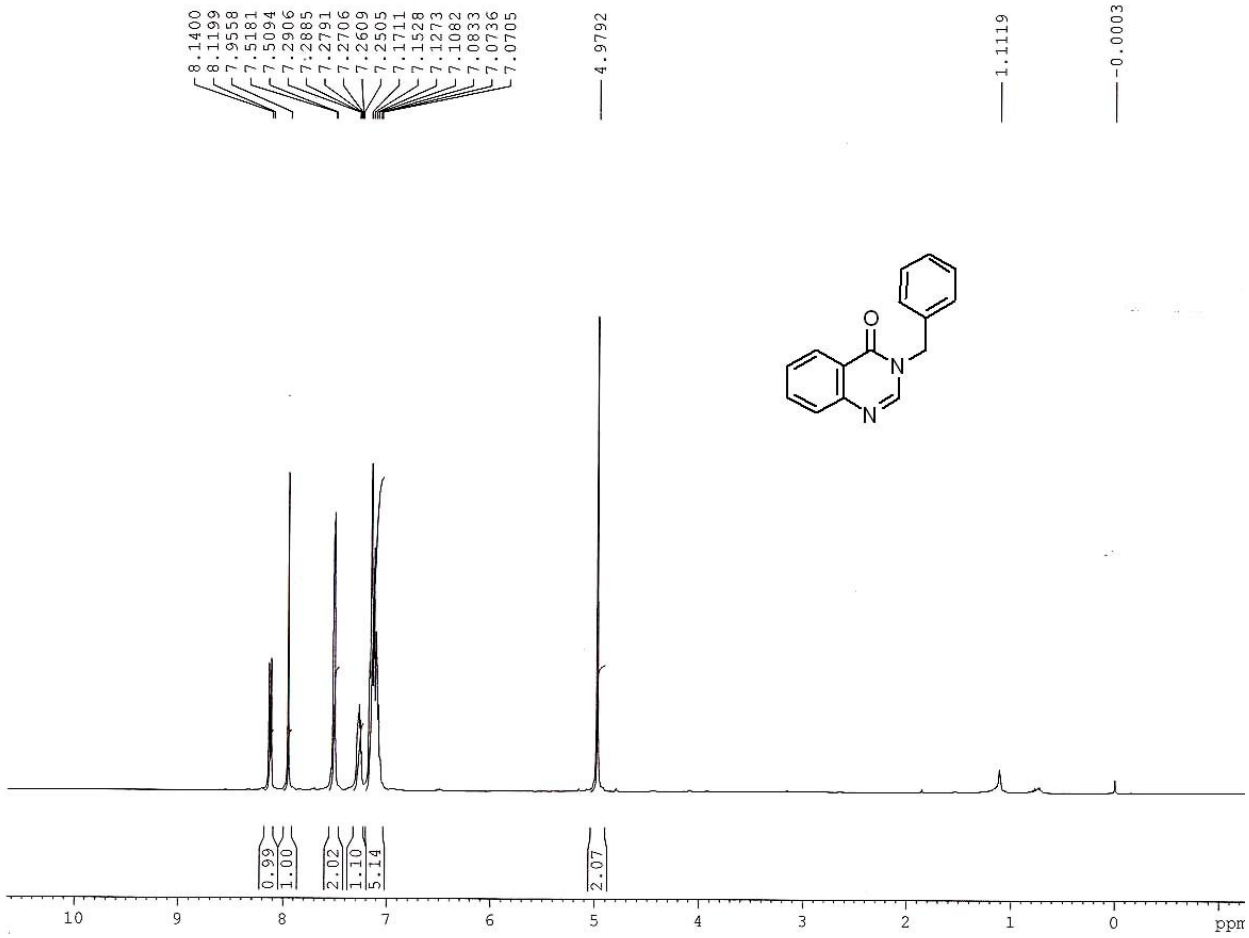
3-(Pyridin-2-yl)quinazolin-4(3*H*)-one(Entry 20, Table 2)



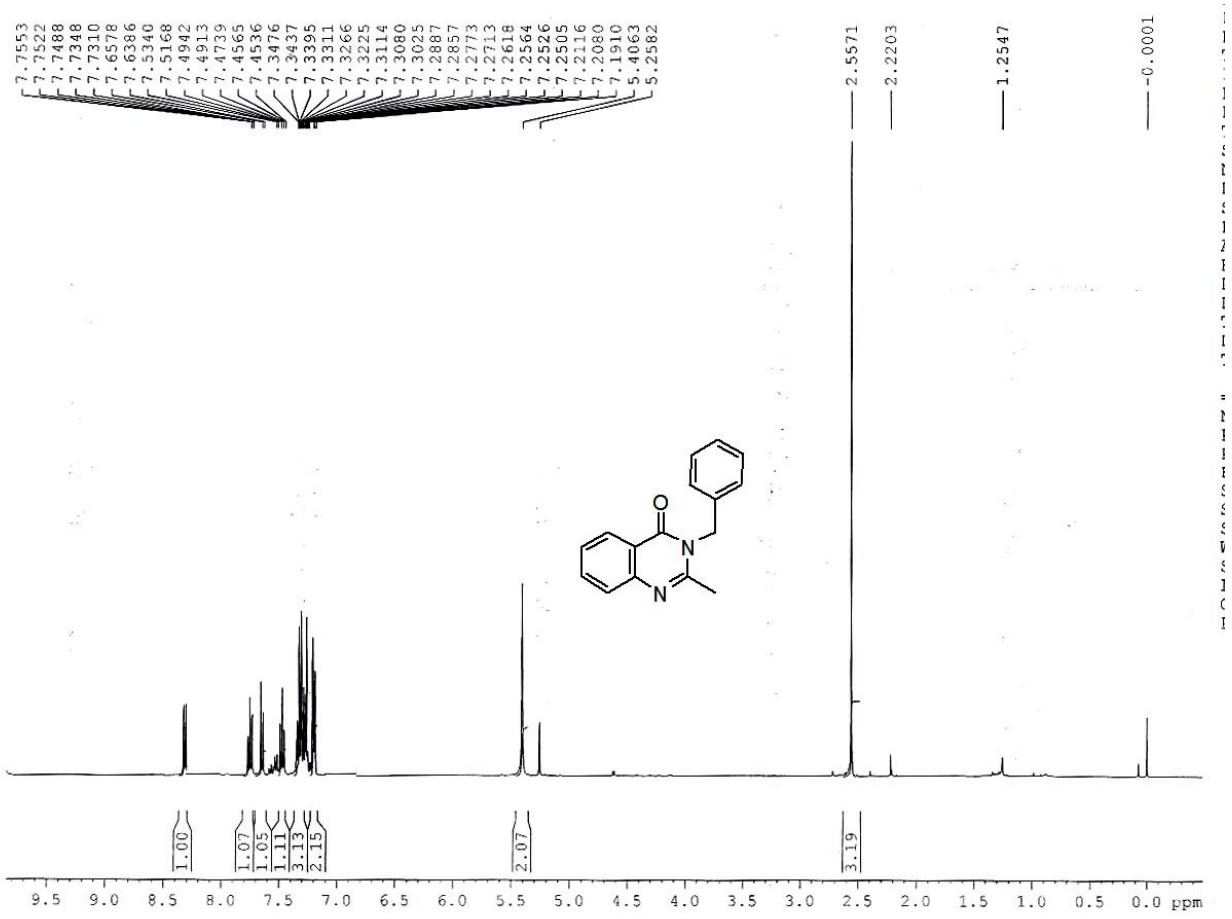
2-Methyl-3-(pyridin-2-yl)quinazolin-4(3*H*)-one(Entry 21, Table 2)



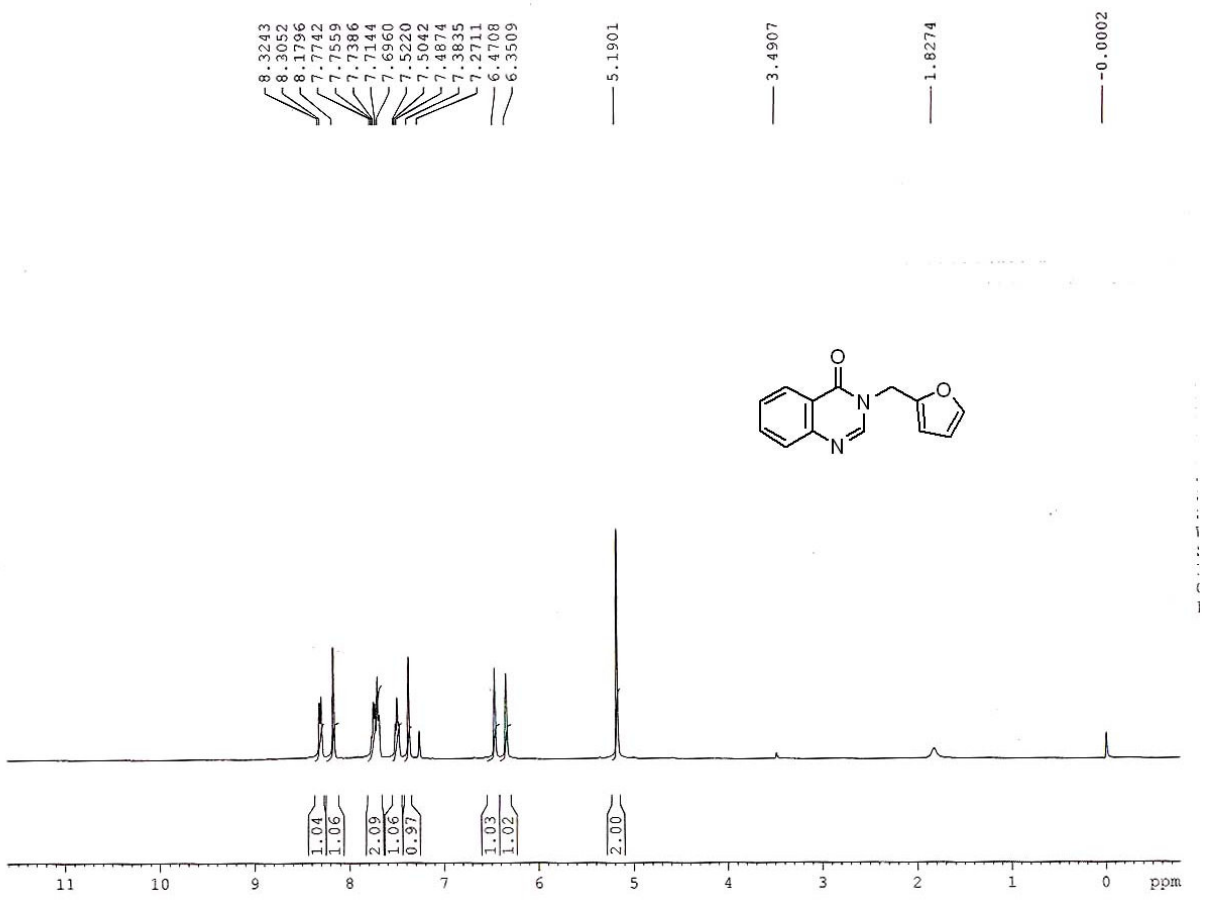
3-Benzylquinazolin-4(3*H*)-one(Entry 22, Table 2)



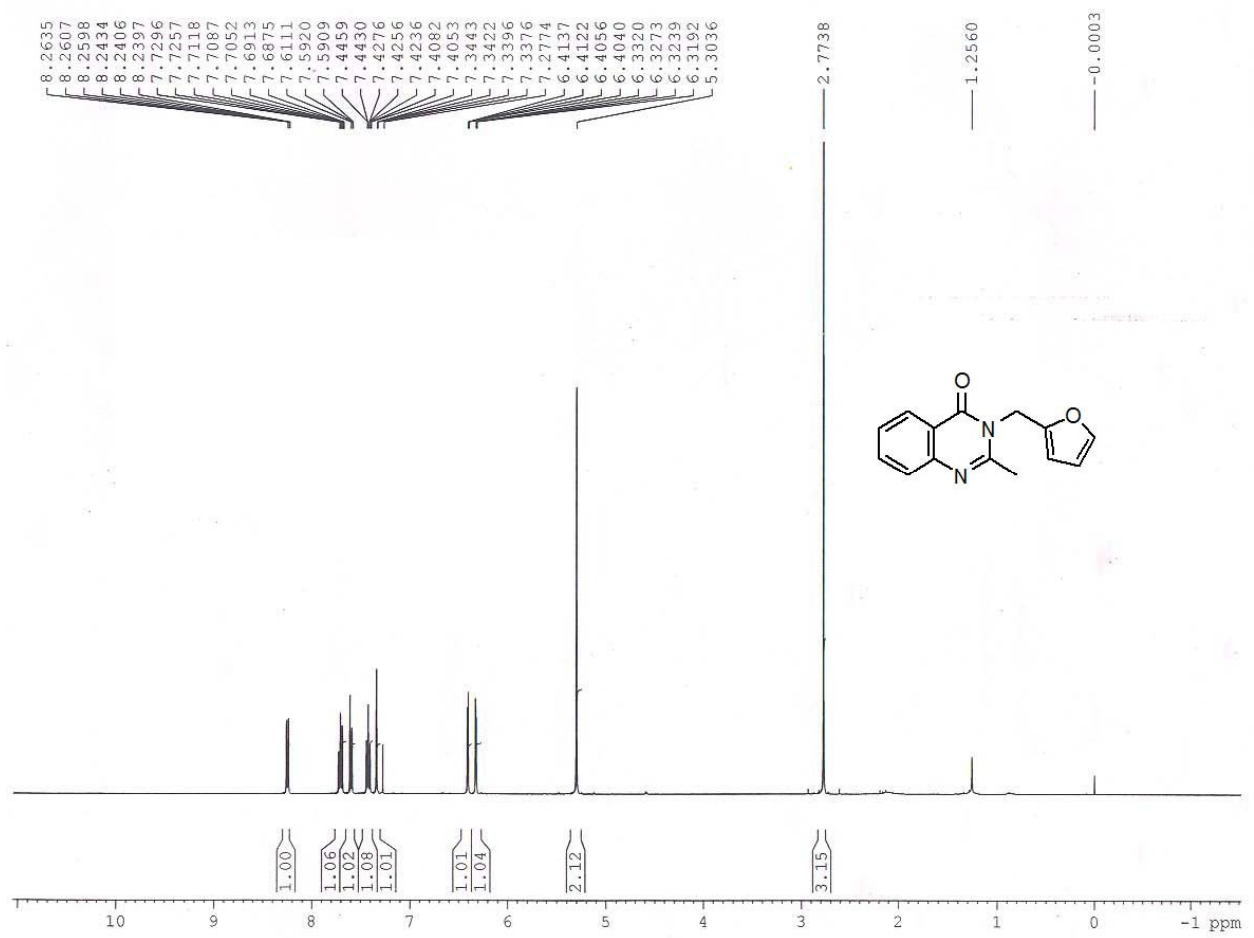
3-Benzyl-2-methylquinazolin-4(3*H*)-one(Entry 23, Table 2)



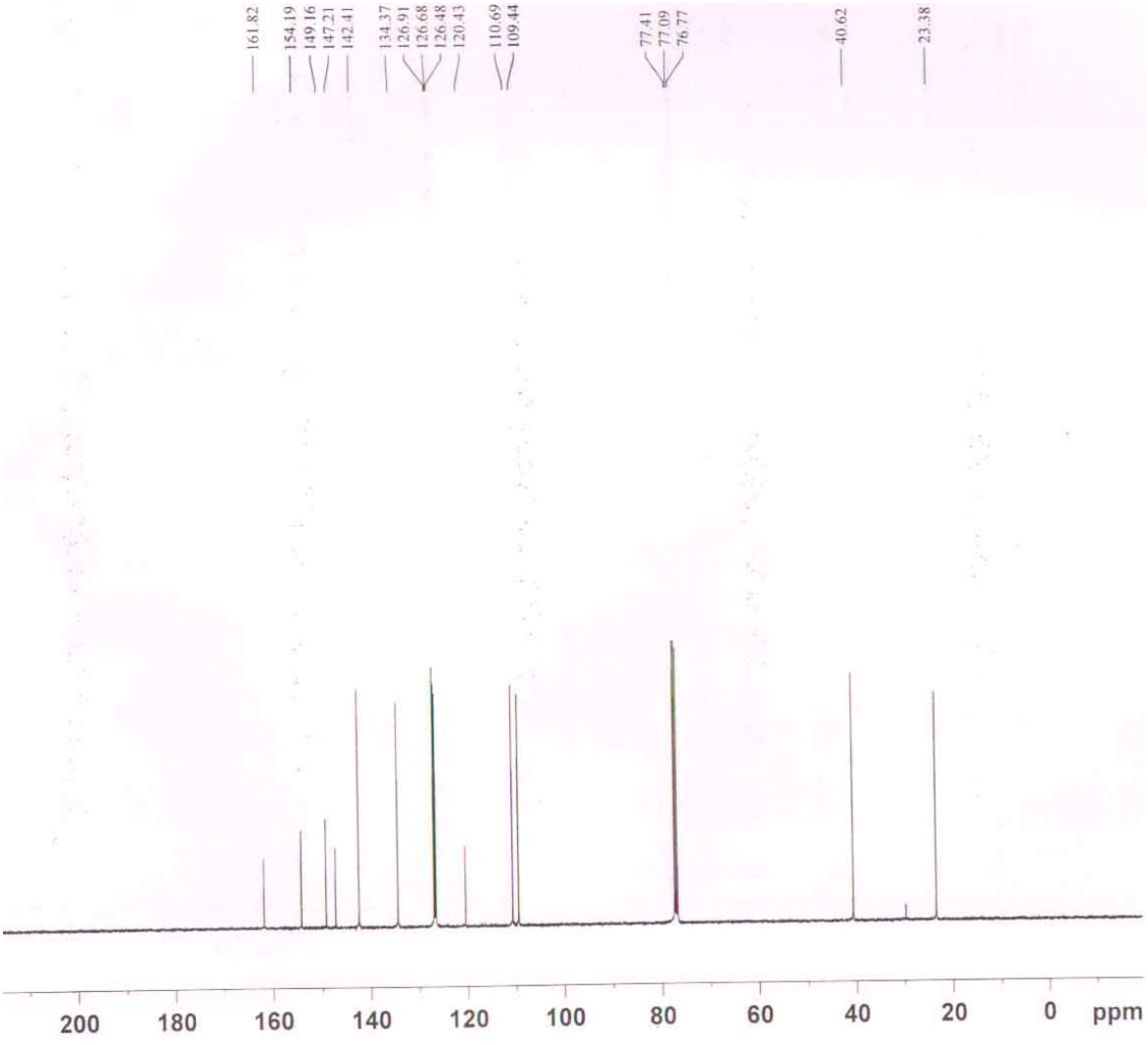
3-(Furan-2-ylmethyl)quinazolin-4(3H)-one(Entry 24, Table 2)



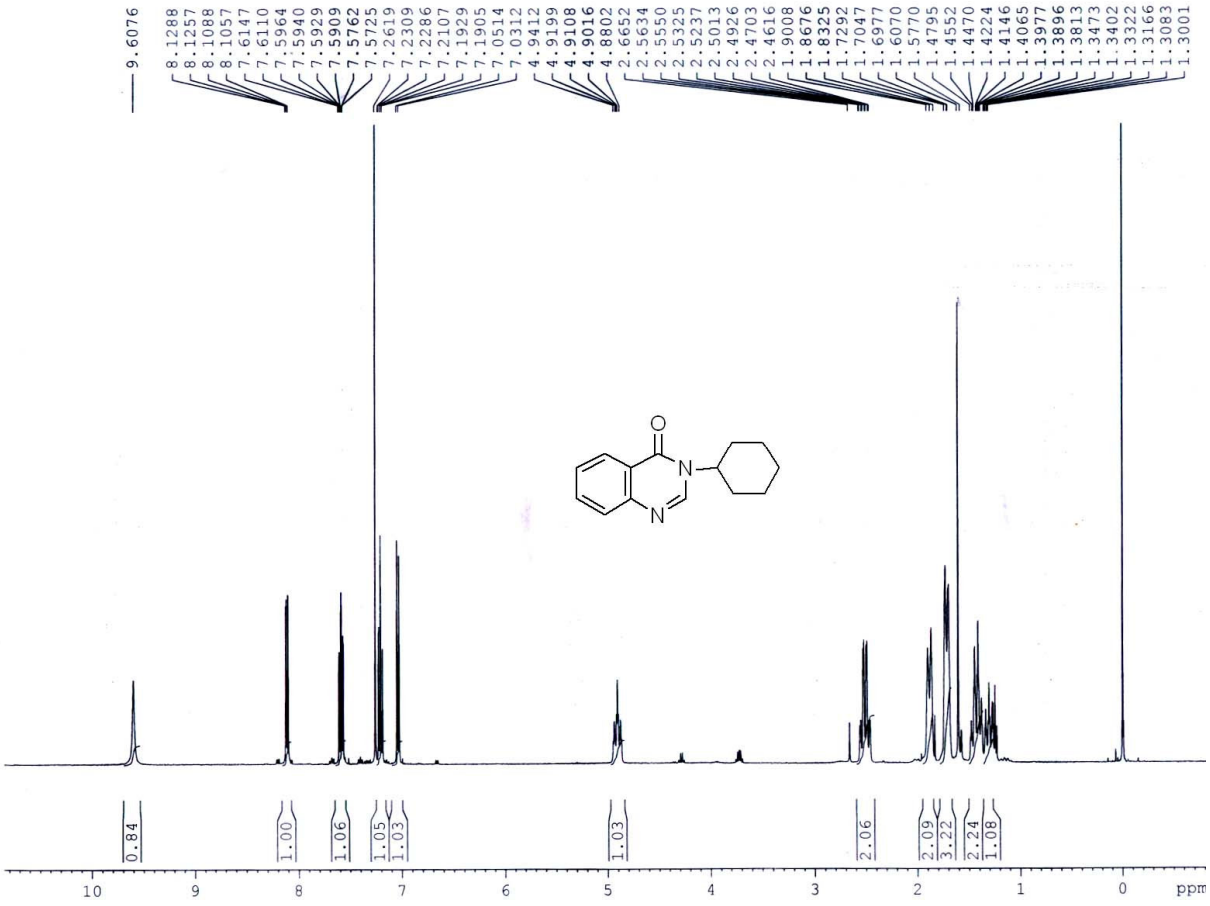
3-(Furan-2-ylmethyl)-2-methylquinazolin-4(3*H*)-one(Entry 25, Table 2)



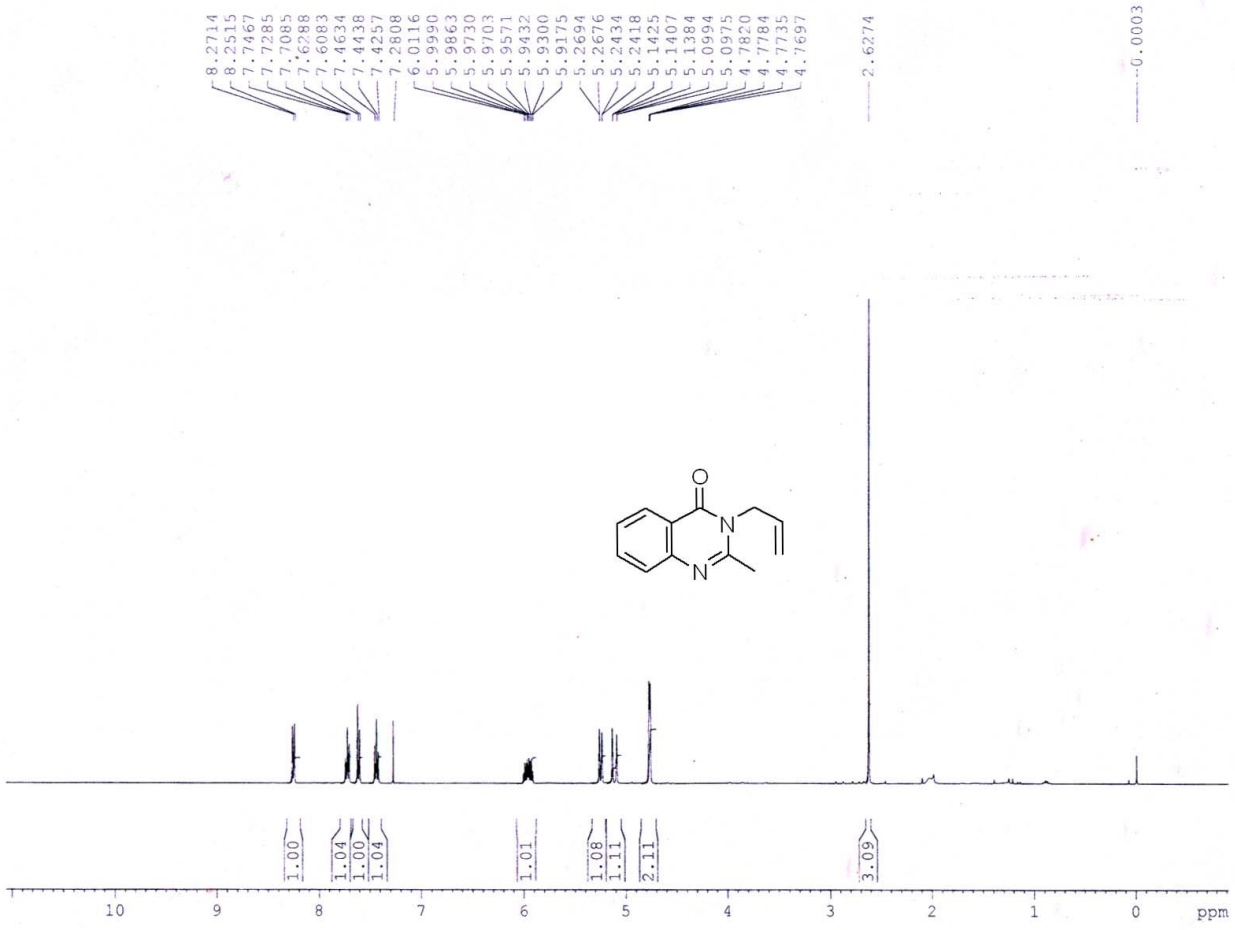
3-(Furan-2-ylmethyl)-2-methylquinazolin-4(3*H*)-one(Entry 25, Table 2)



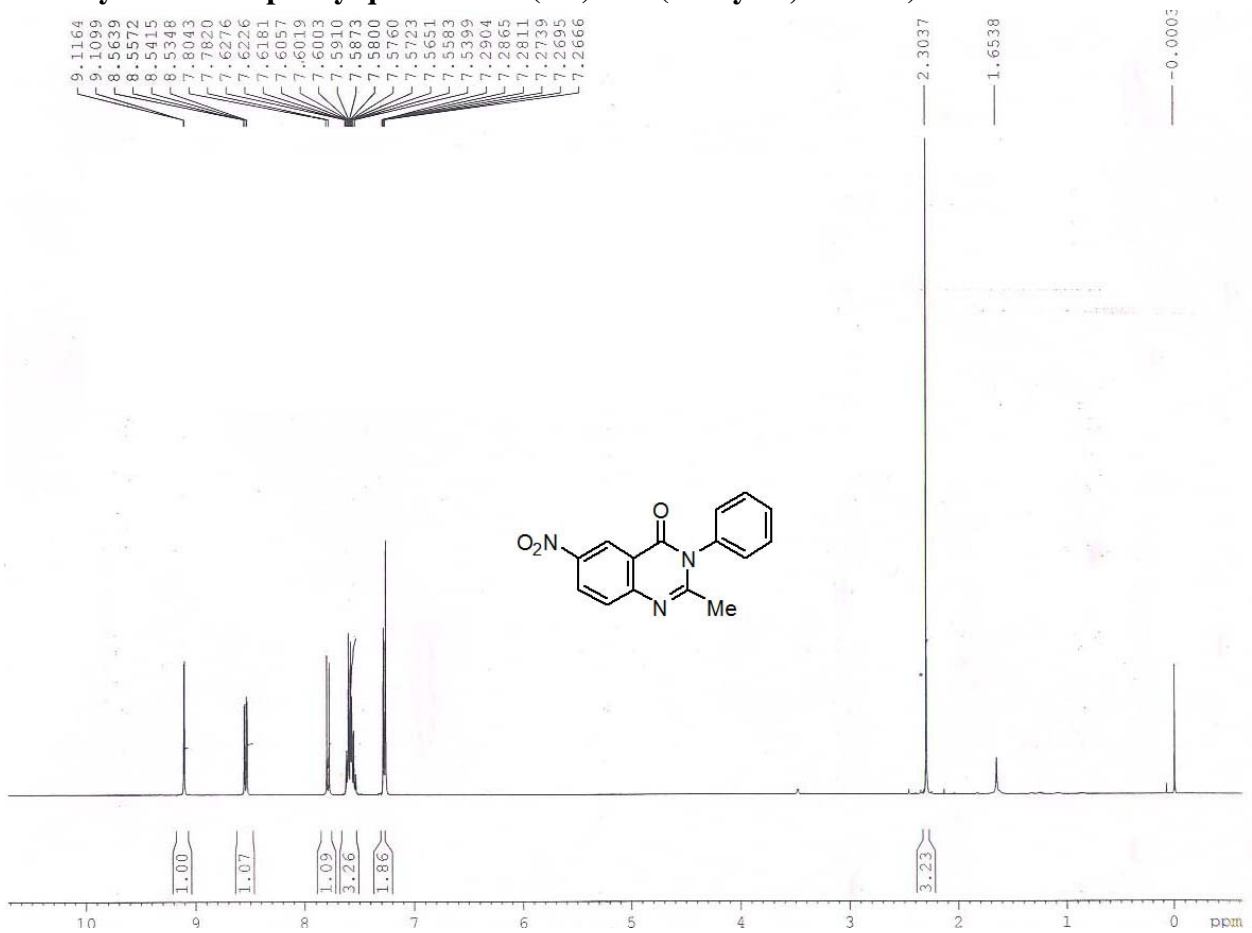
3-Cyclohexylquinazolin-4(3*H*)-one(Entry 26, Table 2)



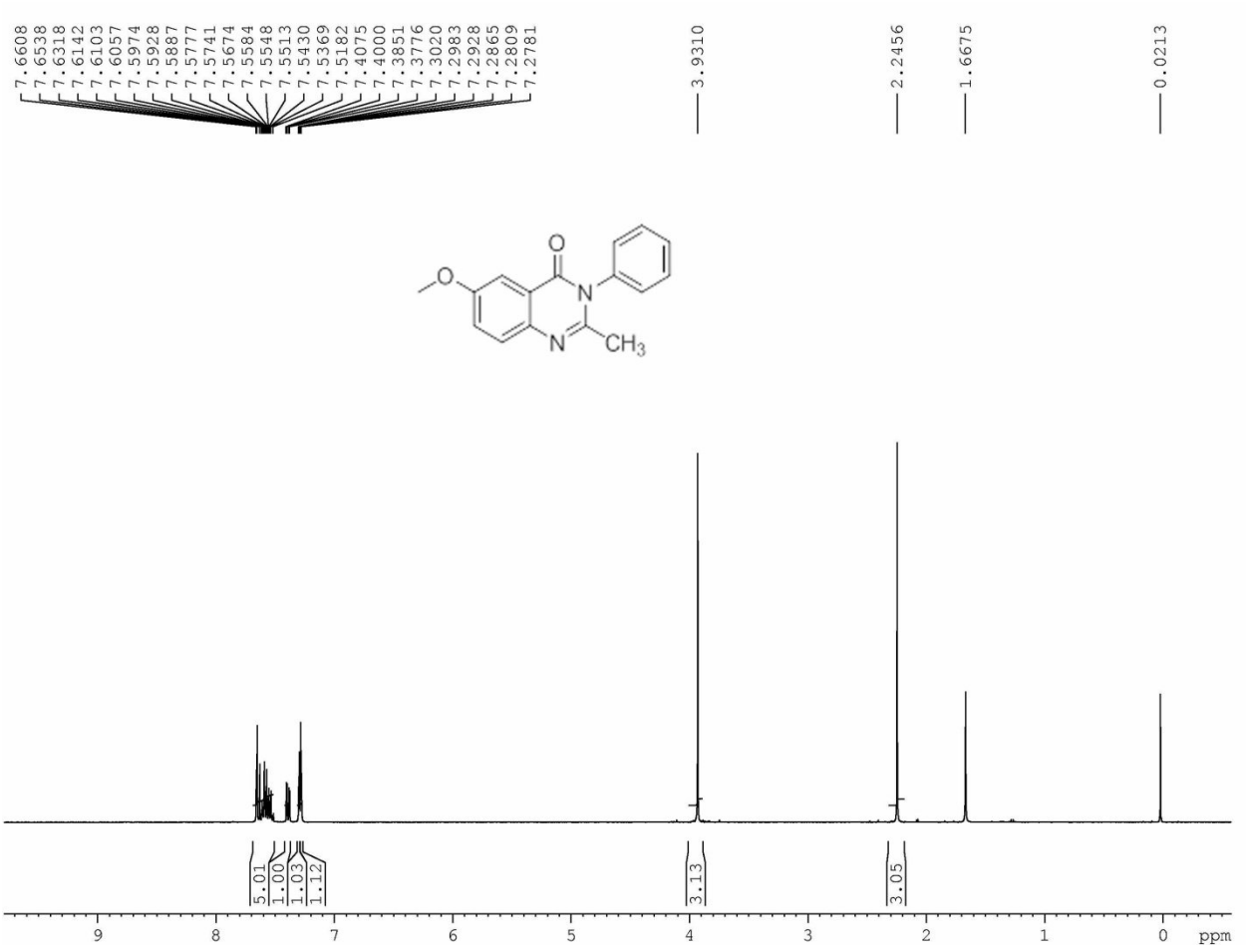
3-Allyl-2-methylquinazolin-4(3H)-one(Entry 27, Table 2)



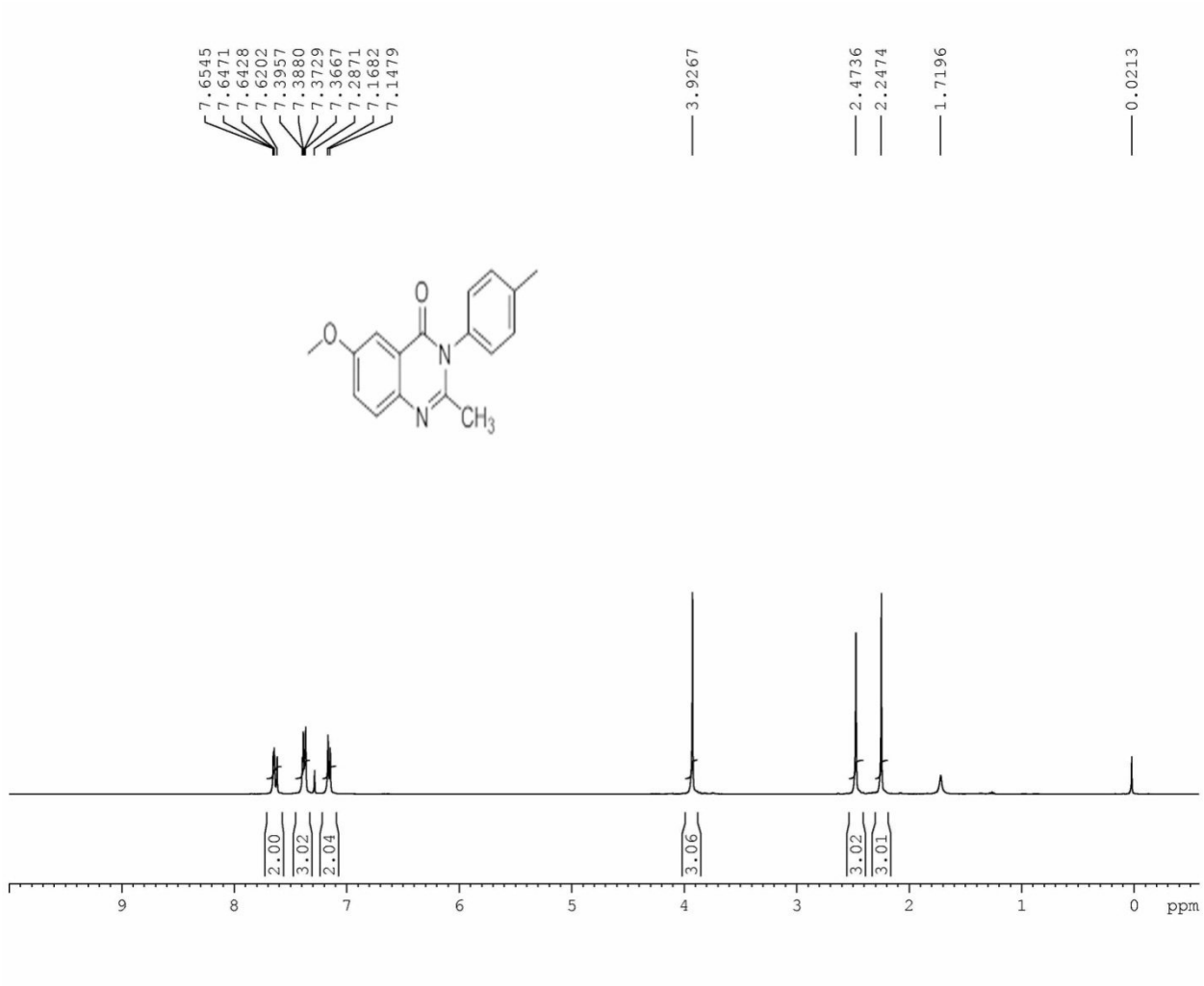
2-Methyl-6-nitro-3-phenylquinazolin-4(3*H*)-one (Entry 28, Table 2)



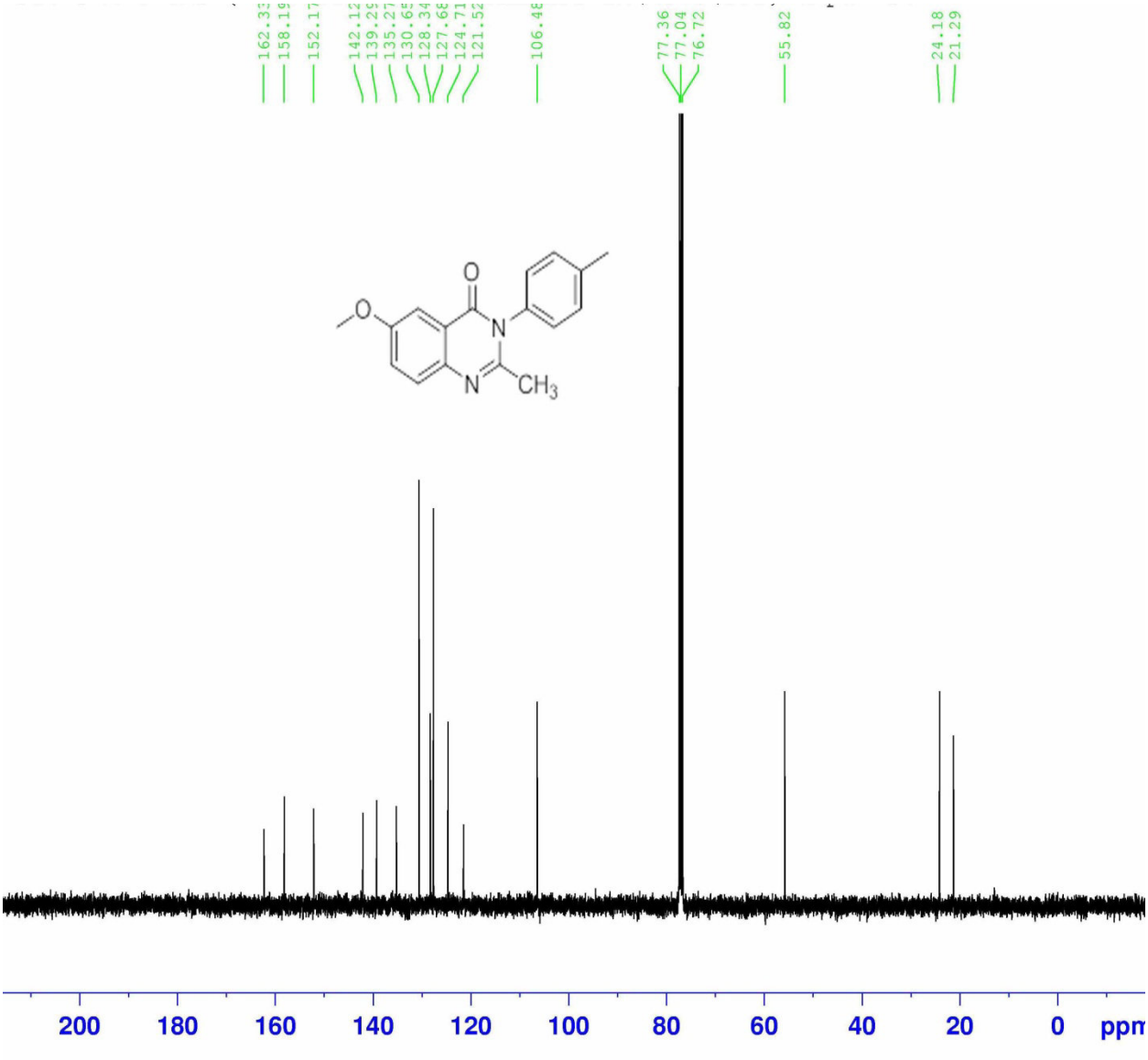
6-Methoxy-2-methyl-3-phenylquinazolin-4(3*H*)-one(Entry 29, Table 2):



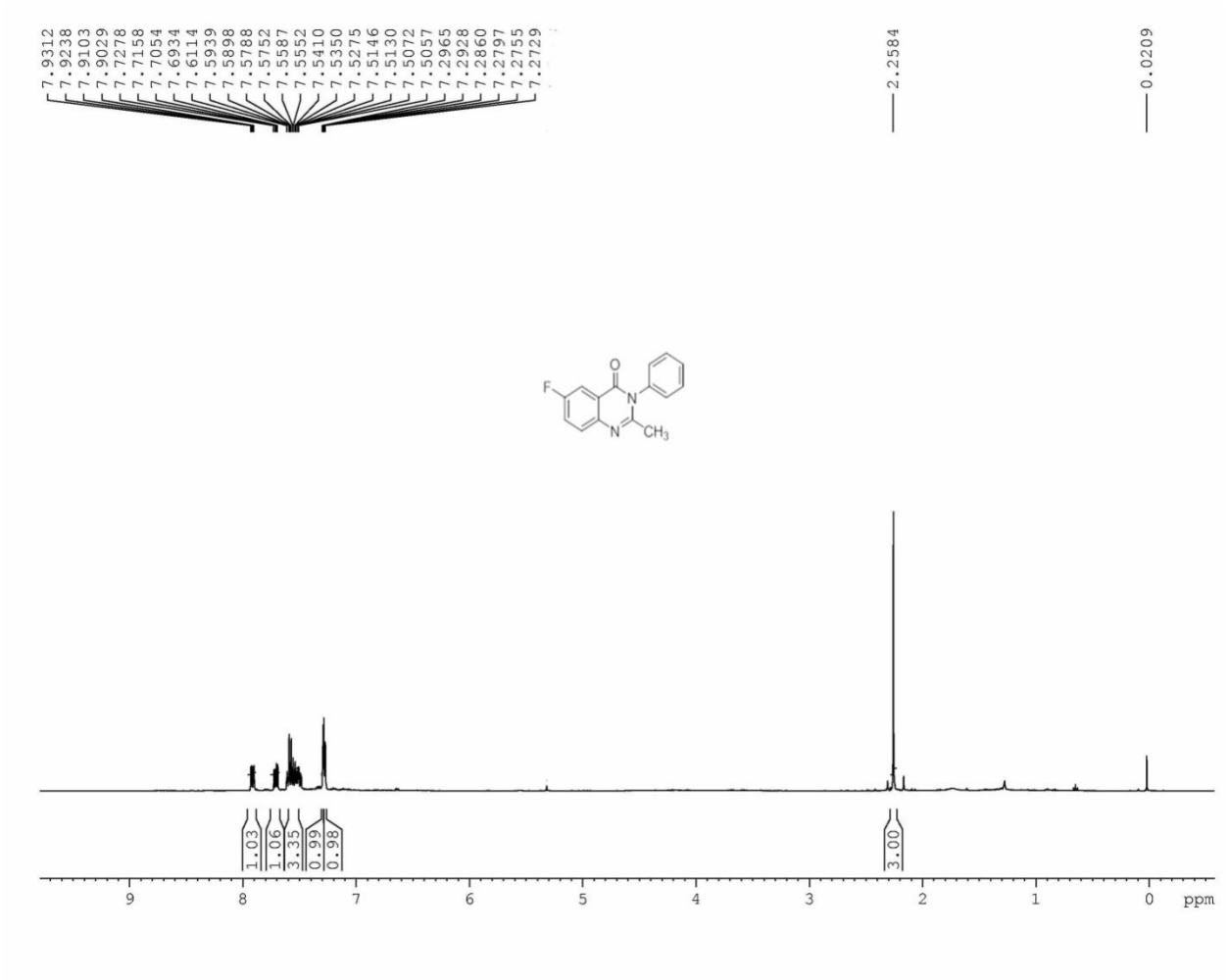
6-Methoxy-2-methyl-3-p-tolylquinazolin-4(3H)-one (Entry 30, Table 2):



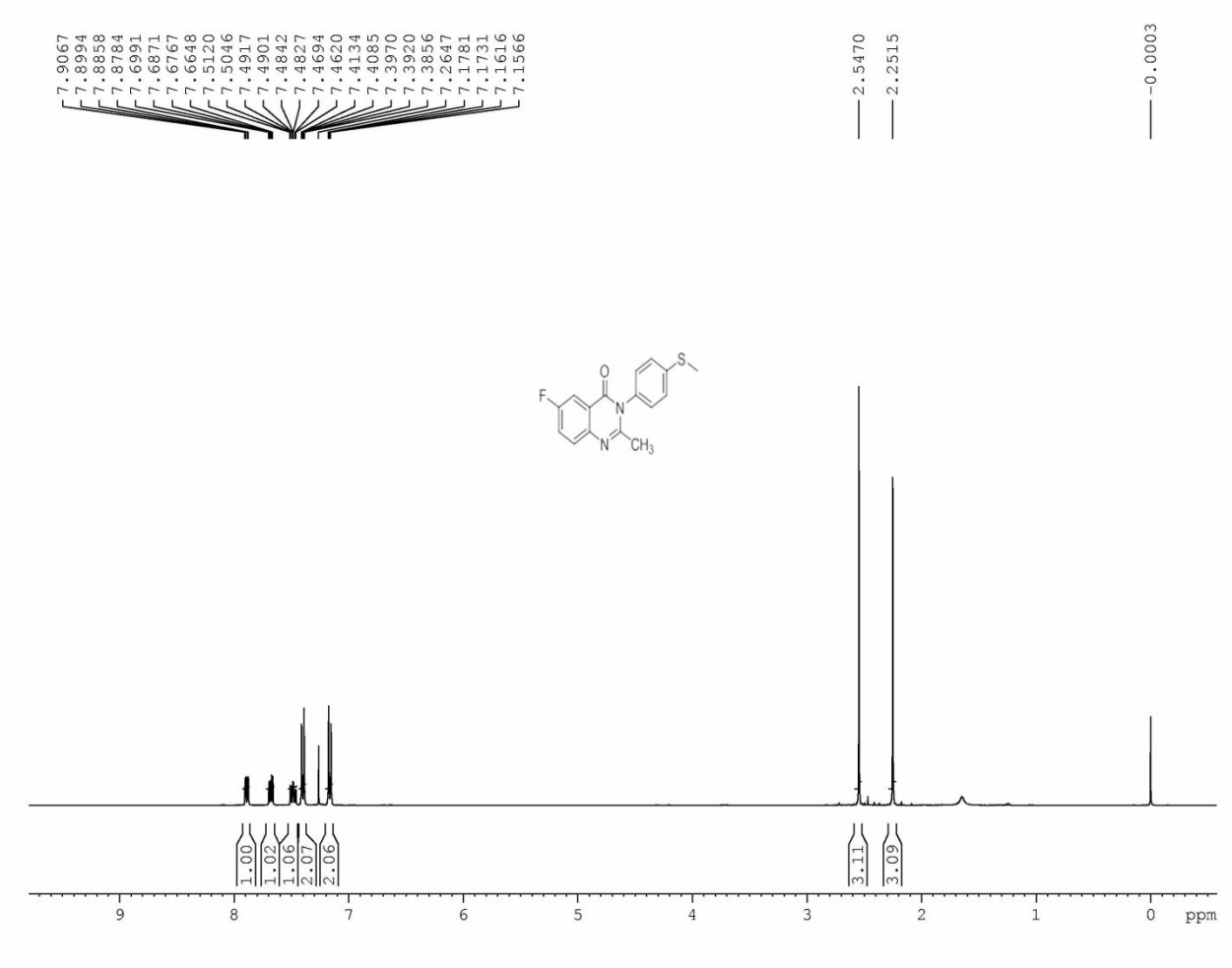
6-Methoxy-2-methyl-3-p-tolylquinazolin-4(3H)-one (Entry 30, Table 2):



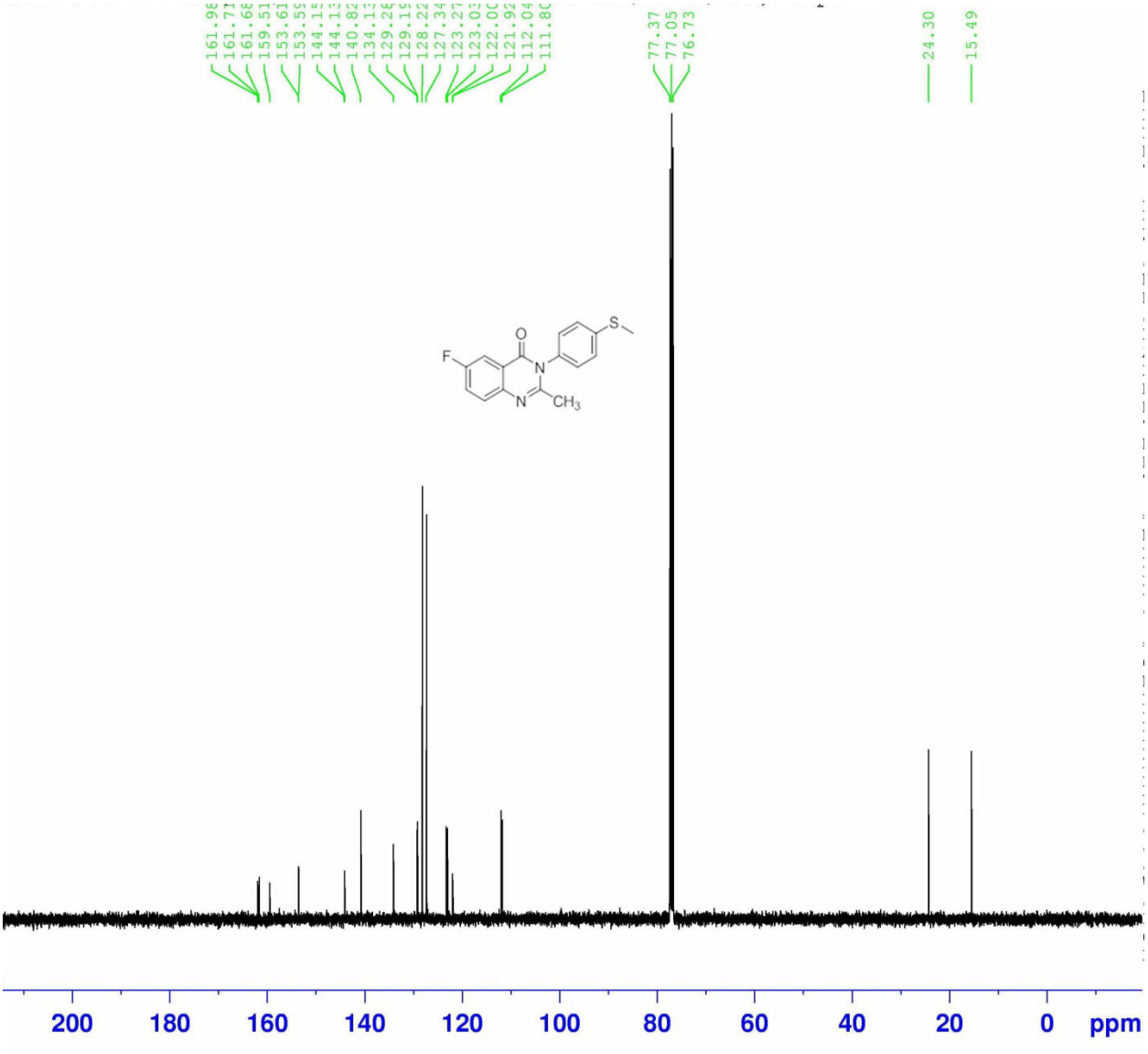
6-Fluoro-2-methyl-3-phenylquinazolin-4(3H)-one (Entry 31, Table 2):



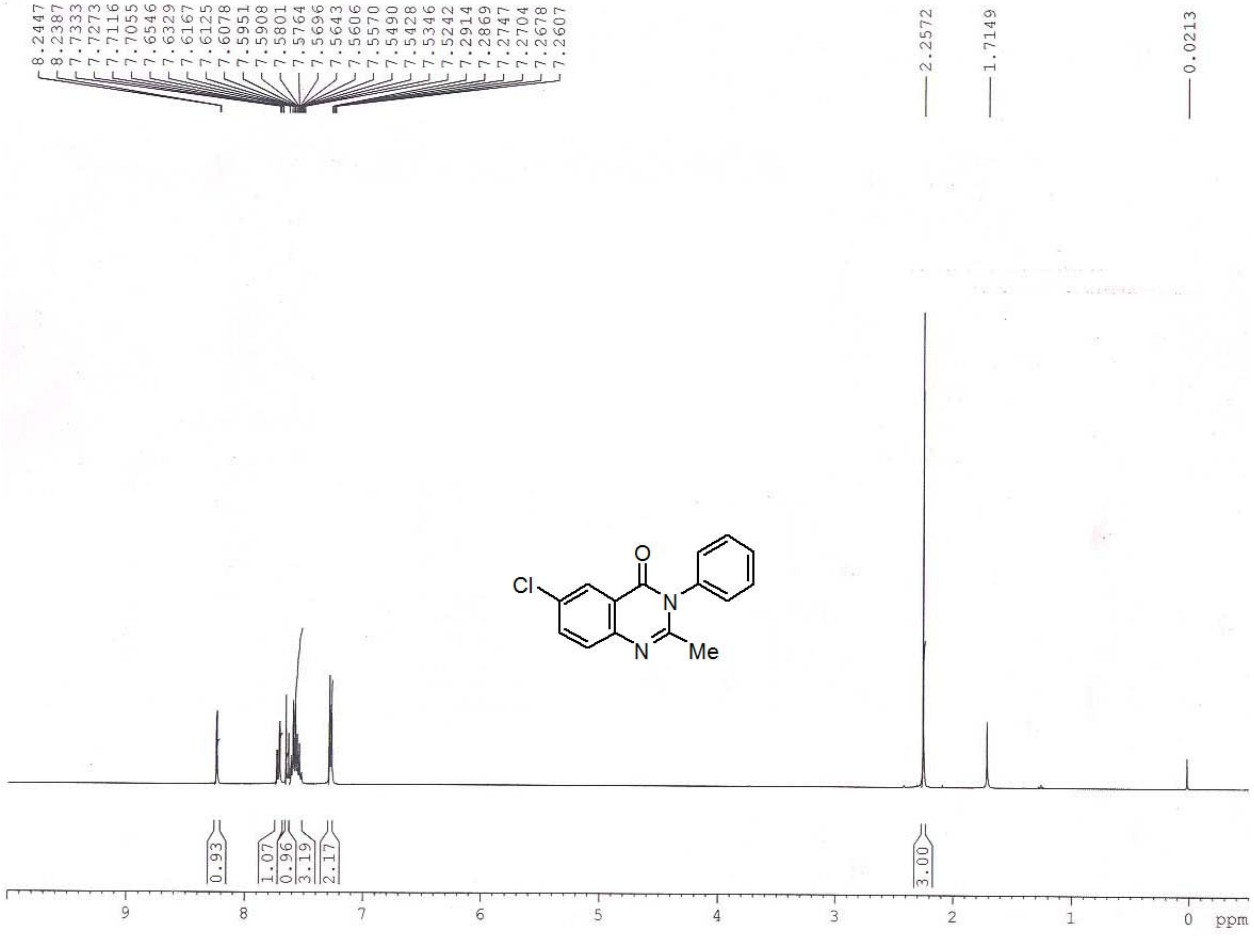
6-Fluoro-2-methyl-3-(4-(methylthio)phenyl)quinazolin-4(3H)-one (Entry 32, Table 2):

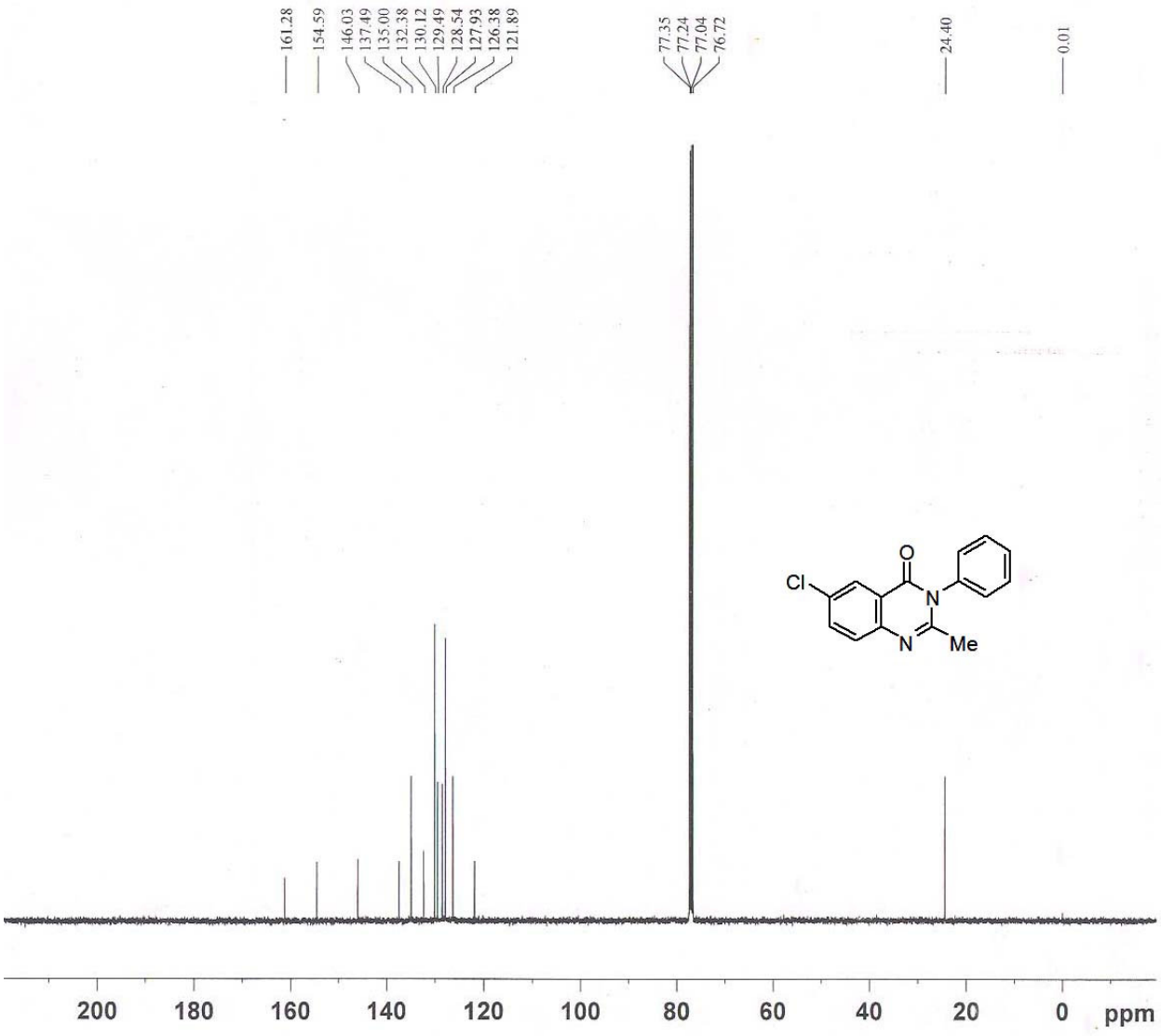


6-Fluoro-2-methyl-3-(4-(methylthio)phenyl)quinazolin-4(3H)-one (Entry 32, Table 2):

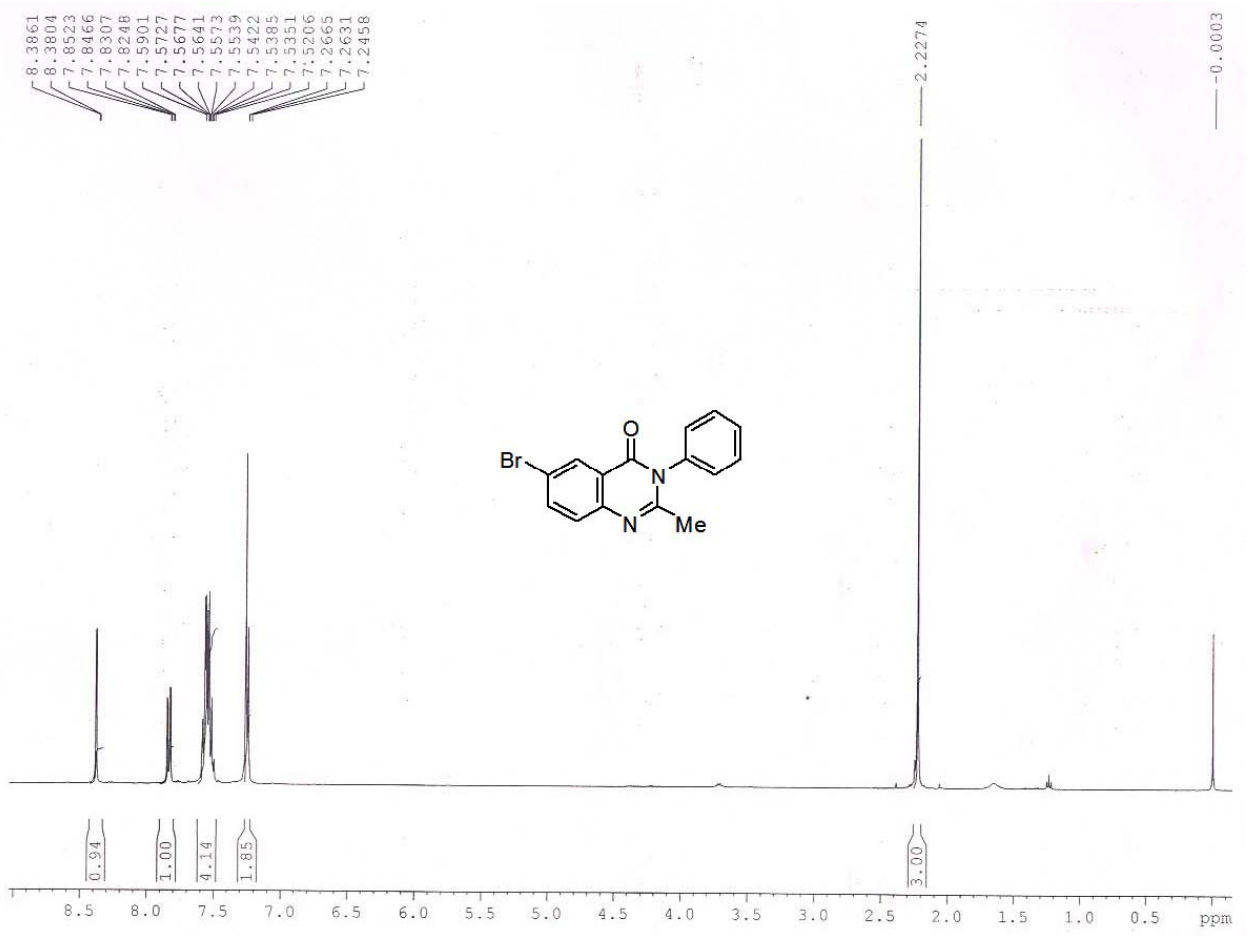


6-Chloro-2-methyl-3-phenylquinazolin-4(3*H*)-one(Entry 33, Table 2)

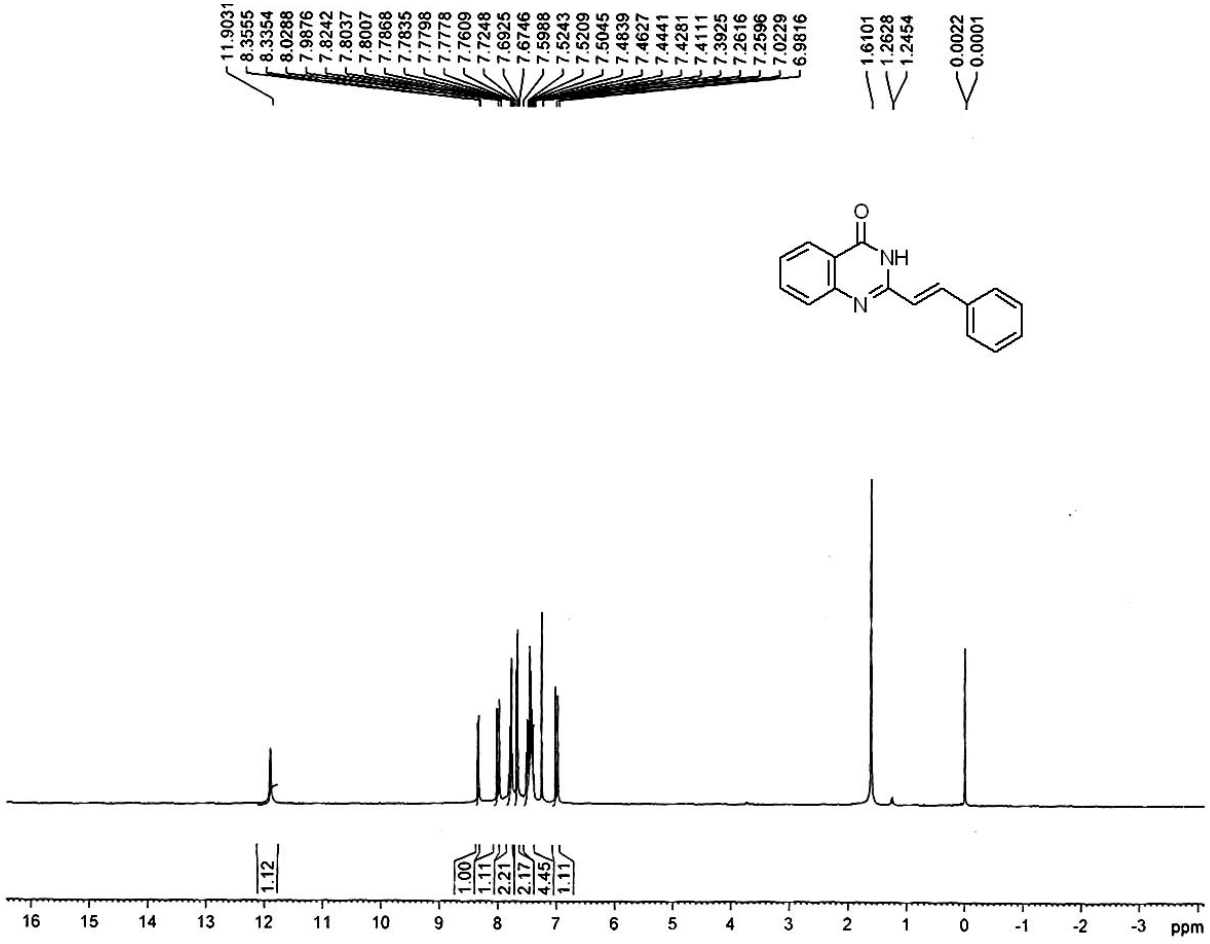



161.28
154.59
146.03
137.49
135.00
132.38
130.12
129.49
128.54
127.93
126.38
121.89
77.35
77.24
77.04
76.72
24.40
0.01
Cl
O
N
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

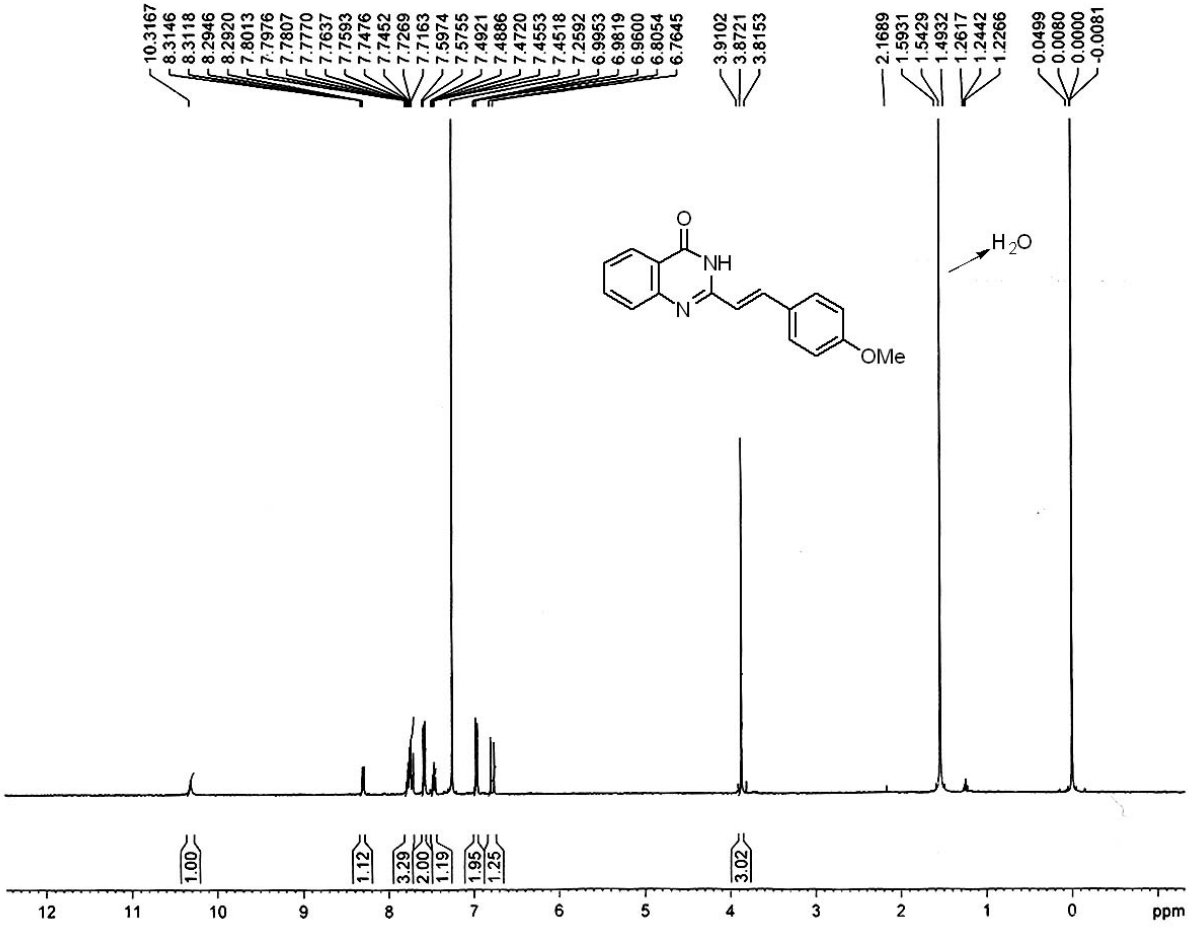
6-Bromo-2-methyl-3-phenylquinazolin-4(3*H*)-one(Entry 34, Table 2)



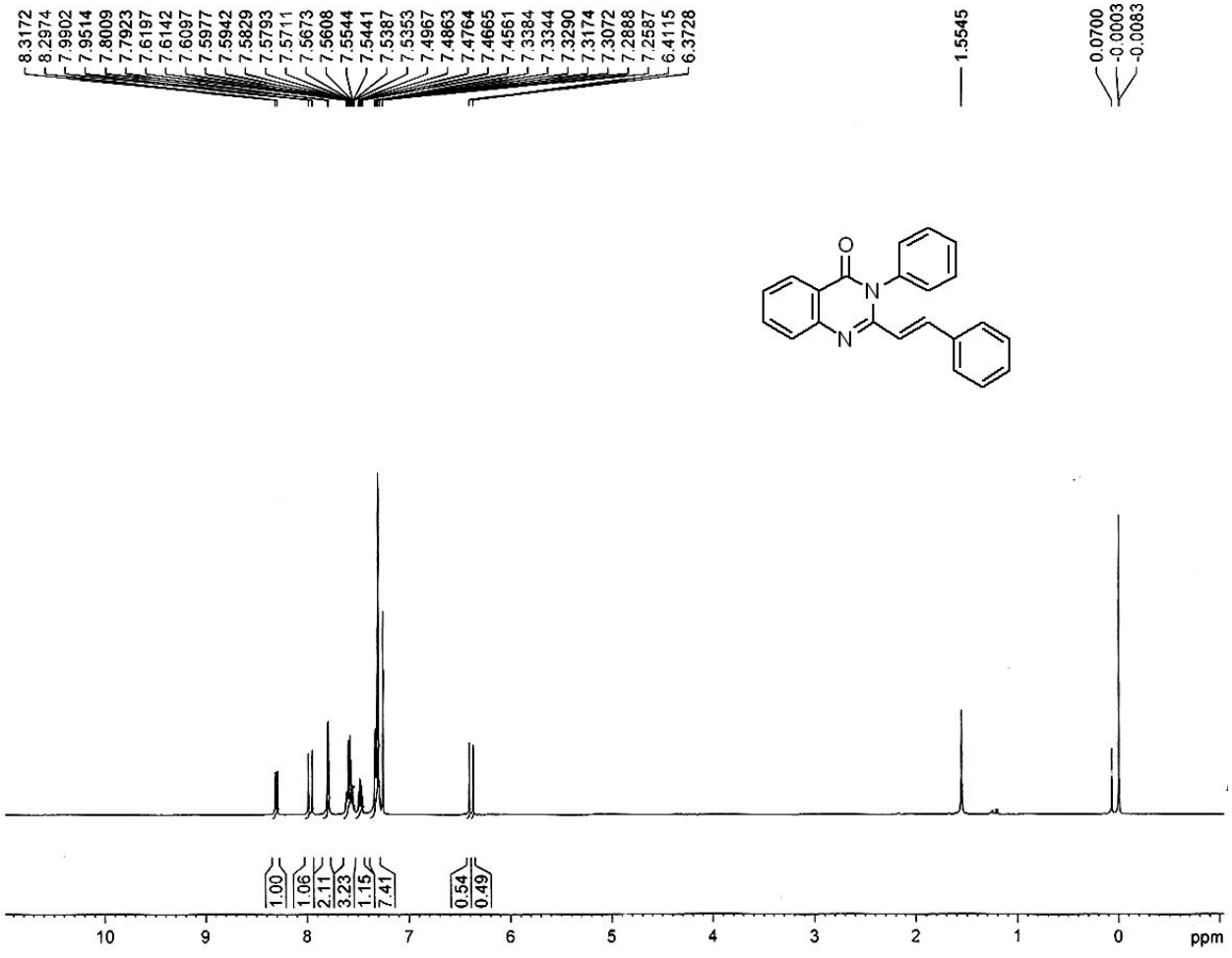
(*E*)-2-Styrylquinazolin-4(3*H*)-one (Entry 1, Table 3)



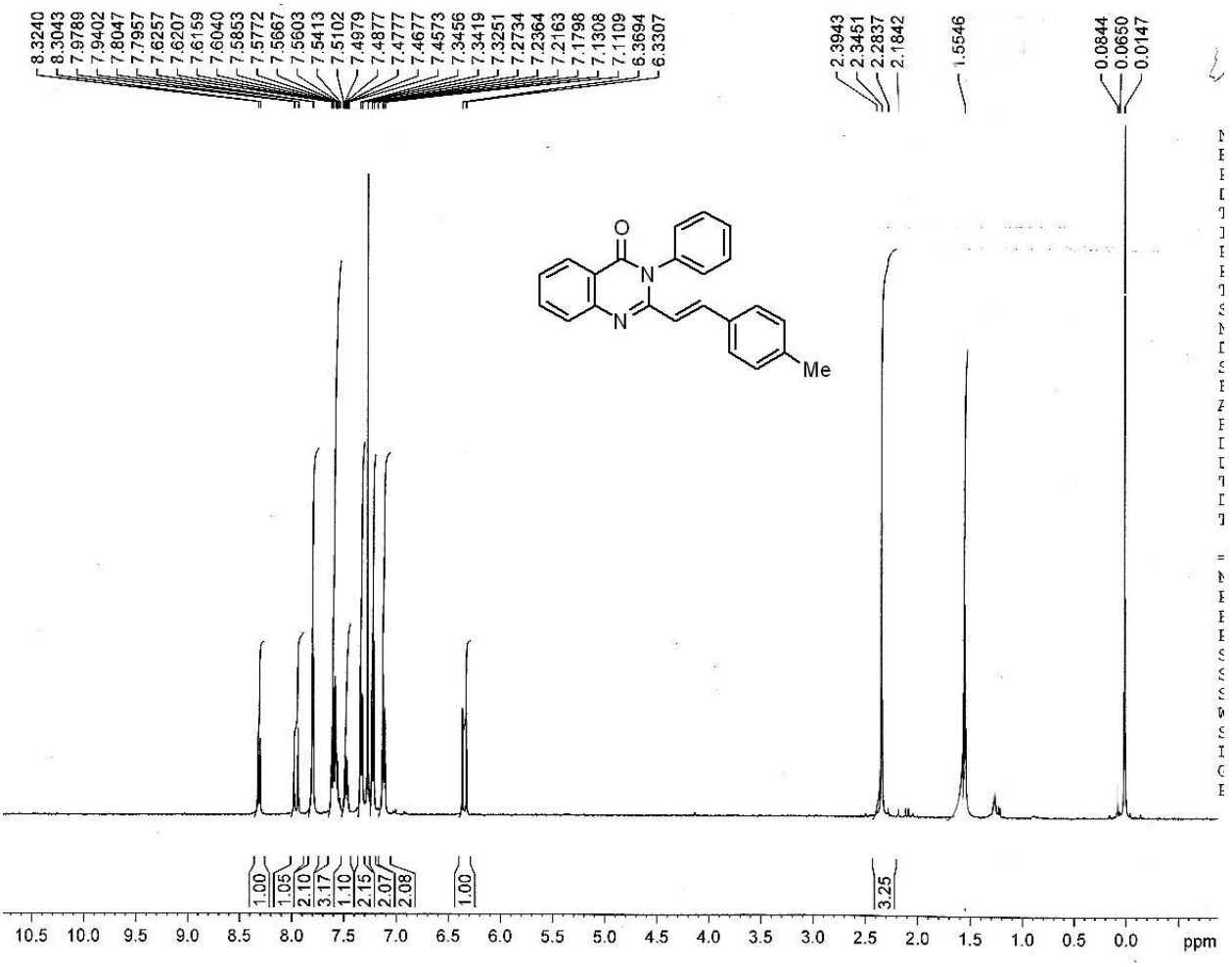
(*E*)-2-(4-Methoxystyryl)quinazolin-4(3*H*)-one (Entry 2,Table 3)



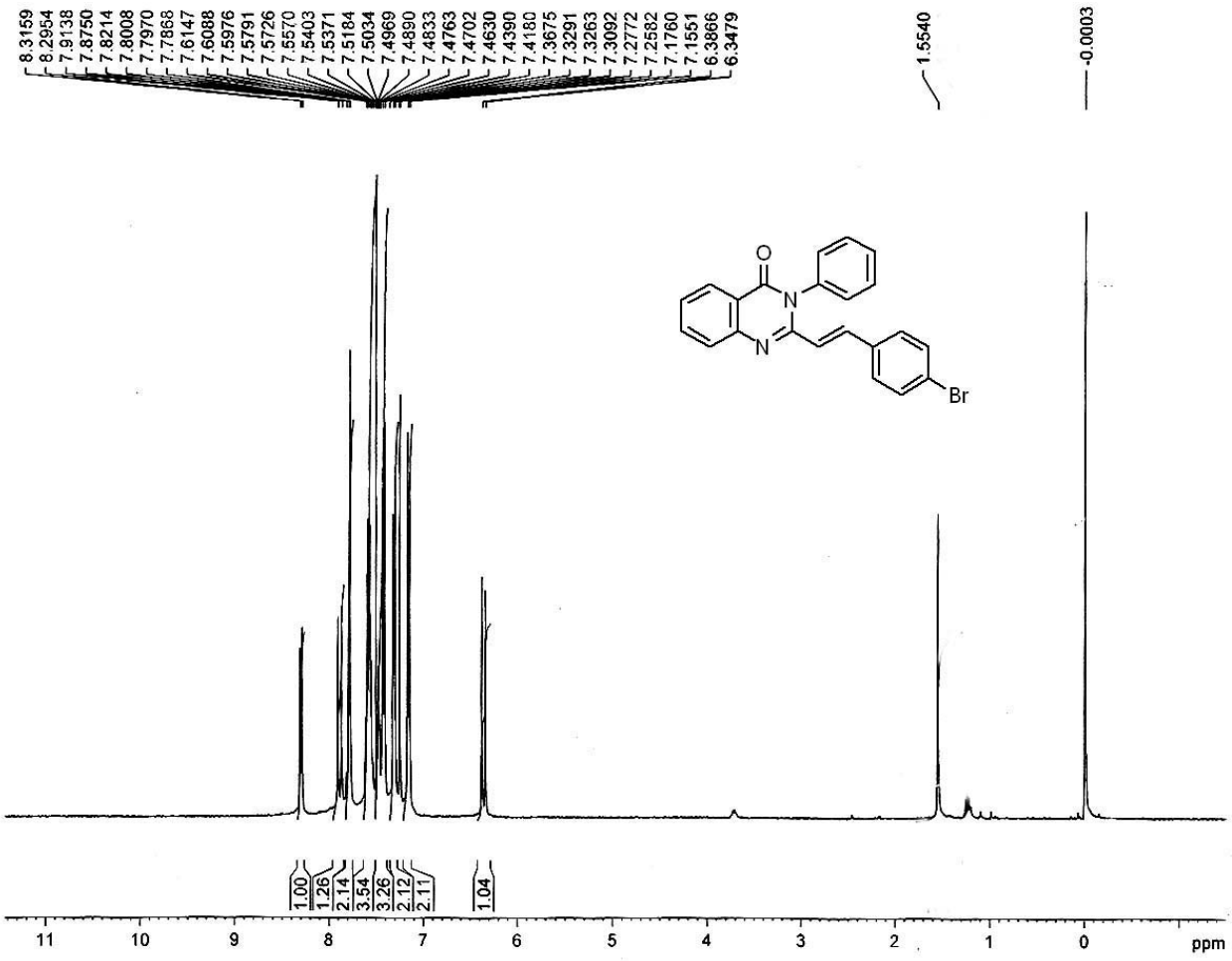
(*E*)-3-Phenyl-2-styrylquinazolin-4(3H)-one (Entry 3,Table 3)



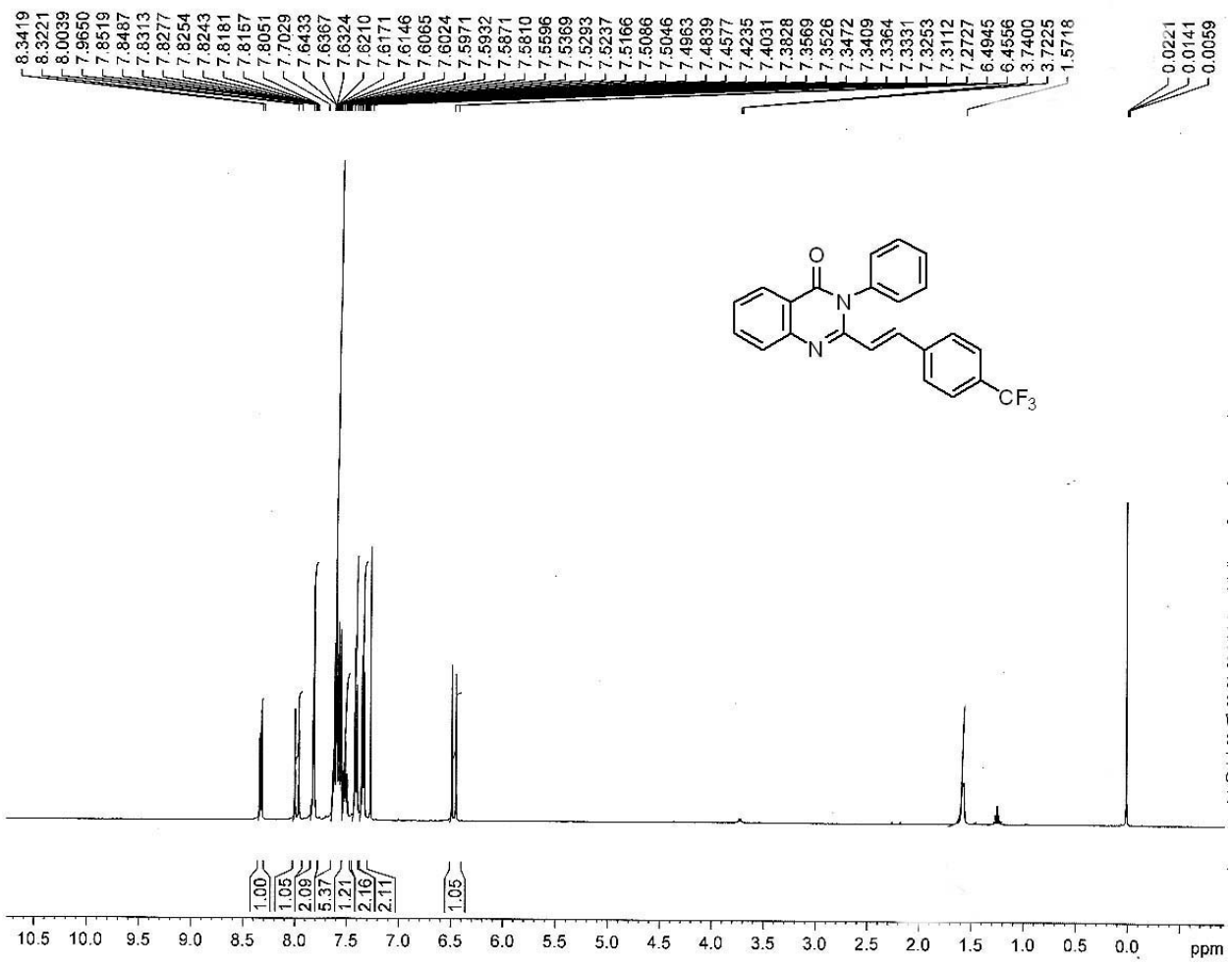
(*E*)-2-(4-Methylstyryl)-3-phenylquinazolin-4(3*H*)-one (Entry 4, Table 3)

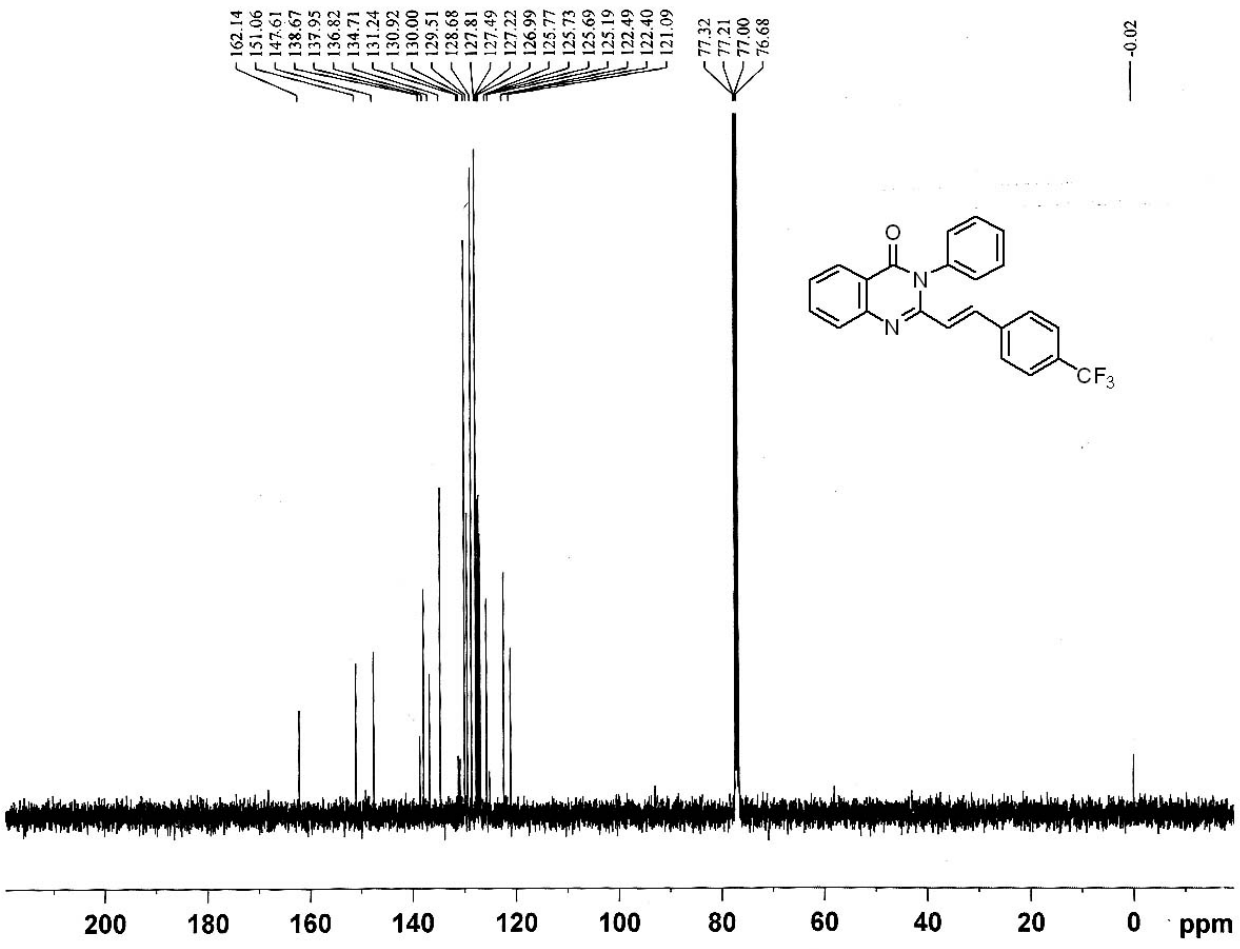


(*E*)-2-(4-Bromostyryl)-3-phenylquinazolin-4(3*H*)-one (Entry 5,Table 3)

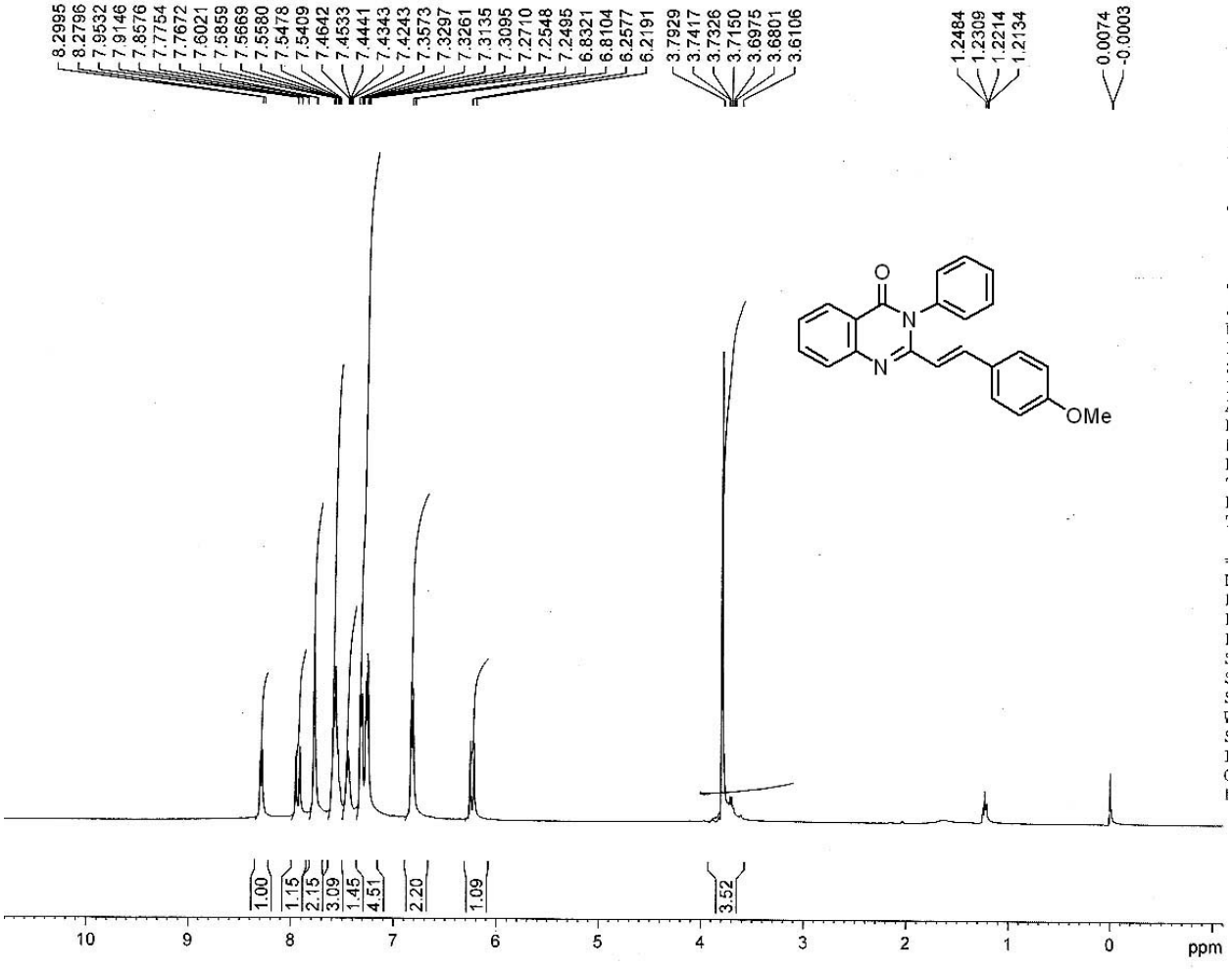


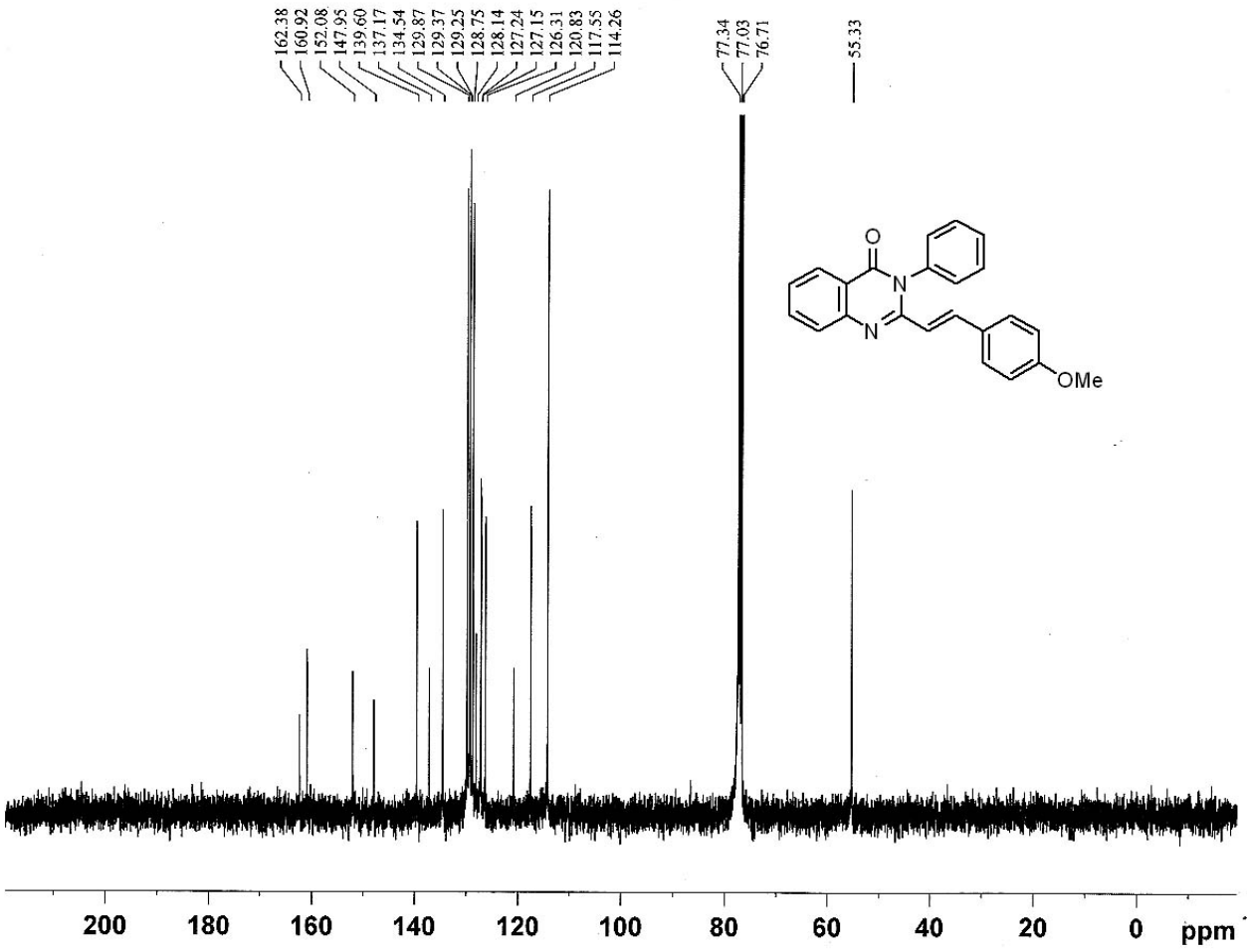
(*E*)-3-Phenyl-2-(4-(trifluoromethyl)styryl)quinazolin-4(3*H*)-one (Entry 6,Table 3)



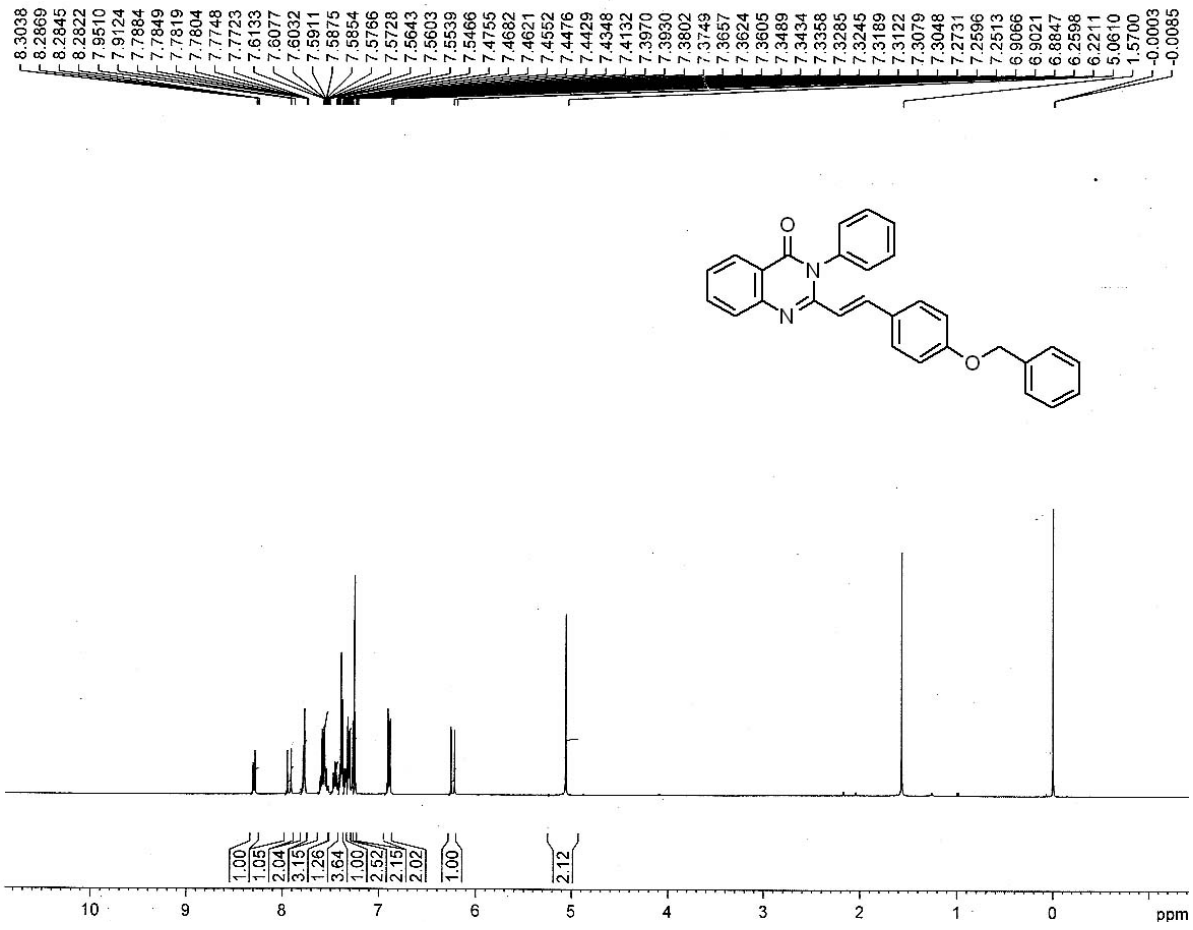

162.14
151.06
147.61
138.67
137.95
136.82
134.71
131.24
130.92
130.00
129.51
128.68
127.81
127.49
127.22
126.99
125.77
125.73
125.69
125.19
122.49
122.40
121.09
77.32
77.21
77.00
76.68
-0.02
O
N
N
CF3
200
180
160
140
120
100
80
60
40
20
0
ppm

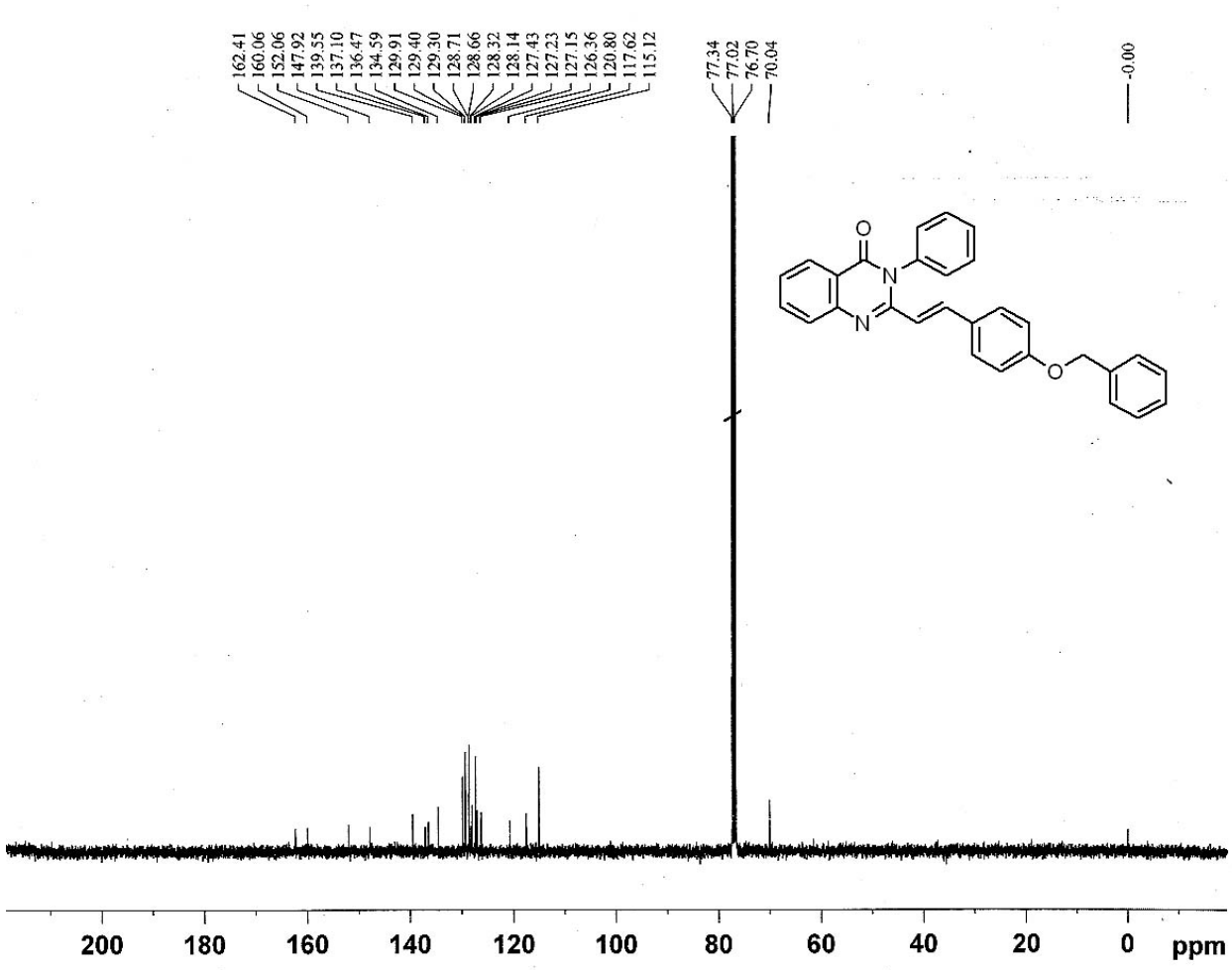
(*E*)-2-(4-Methoxystyryl)-3-phenylquinazolin-4(3*H*)-one(Entry 7,Table 3)



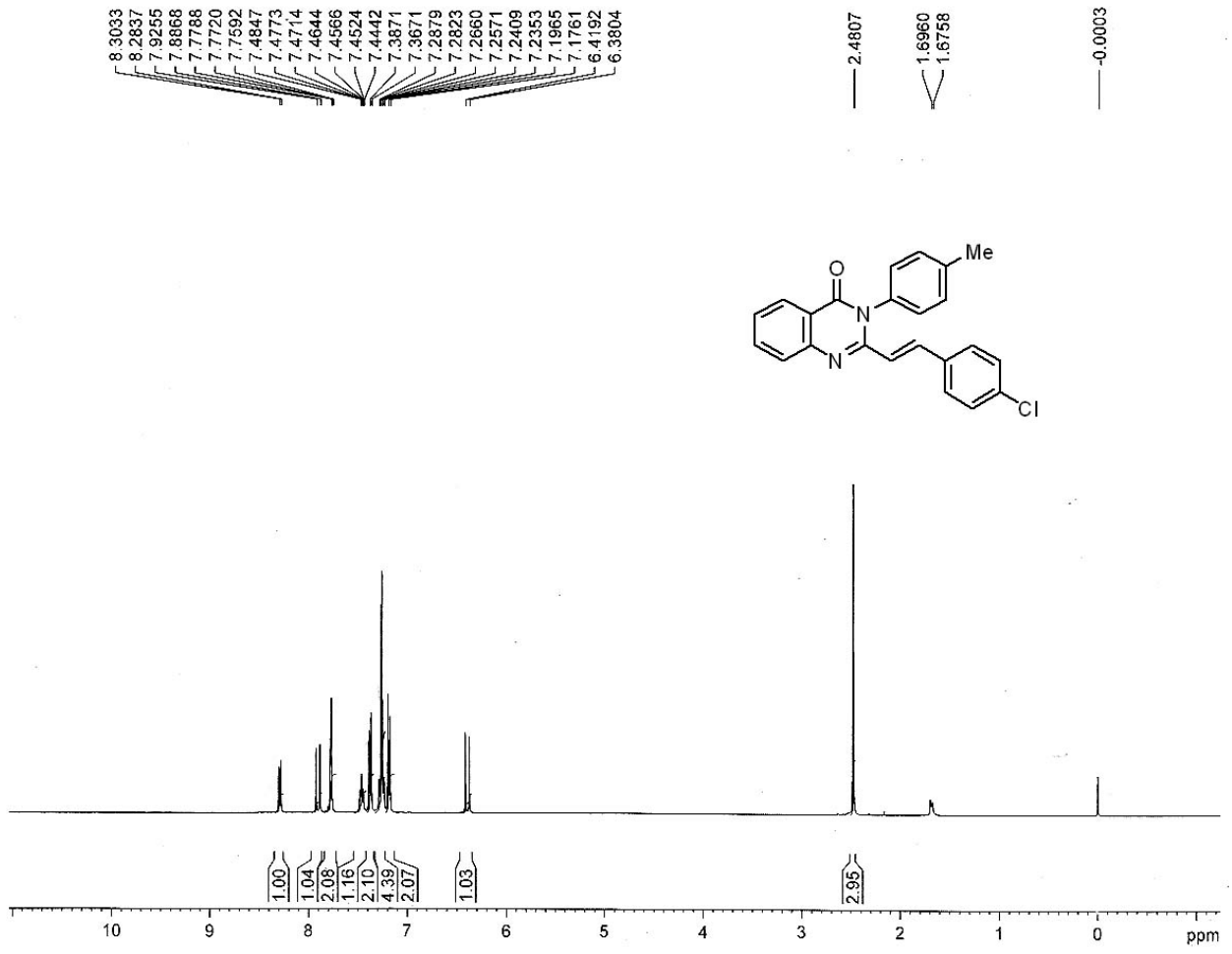

162.38
160.92
152.08
147.95
139.60
137.17
134.54
129.87
129.37
129.25
128.75
128.14
127.24
127.15
126.31
120.83
117.55
114.26
77.34
77.03
76.71
55.33
O
N
N
OMe
200
180
160
140
120
100
80
60
40
20
0
ppm

(*E*)-2-(4-(Benzyloxy)styryl)-3-phenylquinazolin-4(3*H*)-one (Entry 8,Table 3)

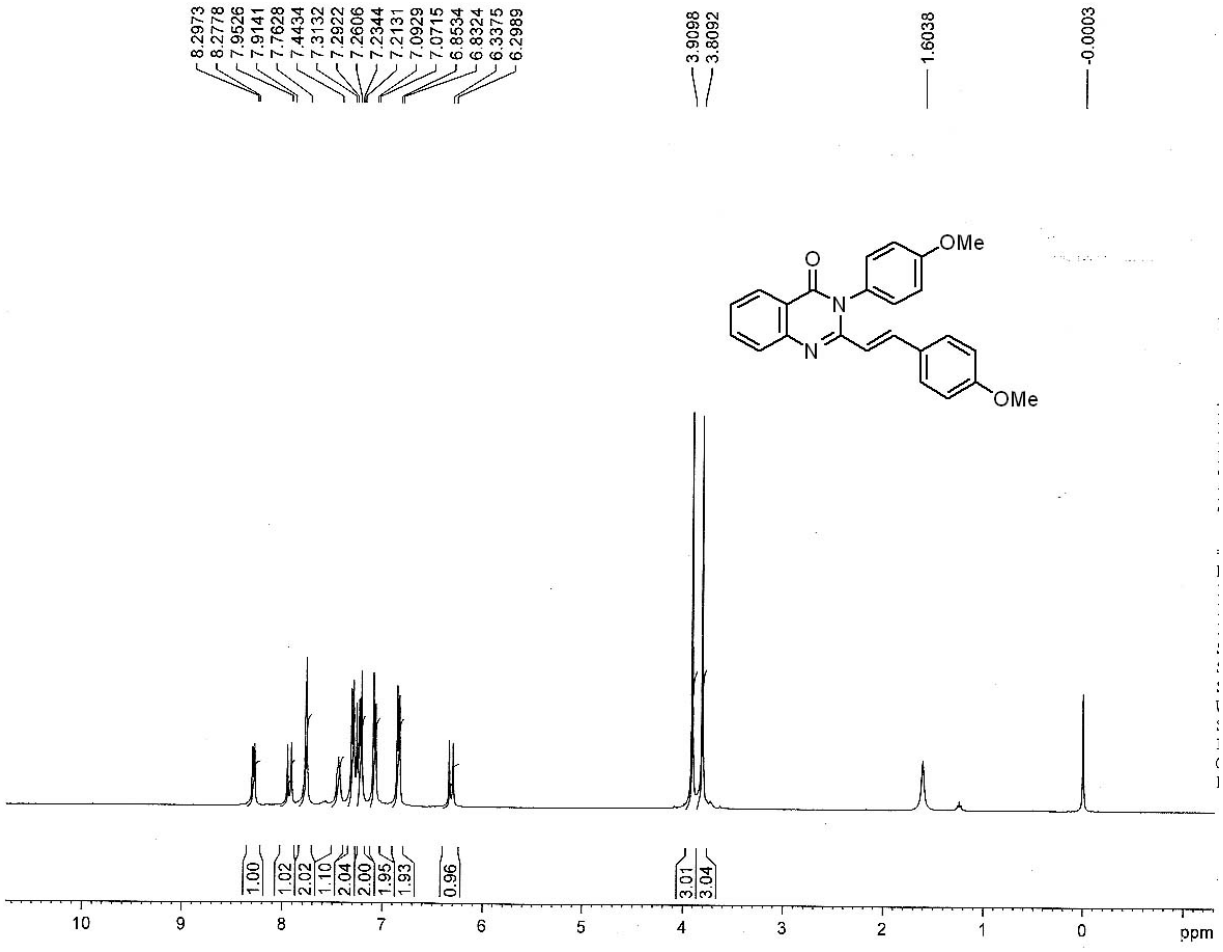


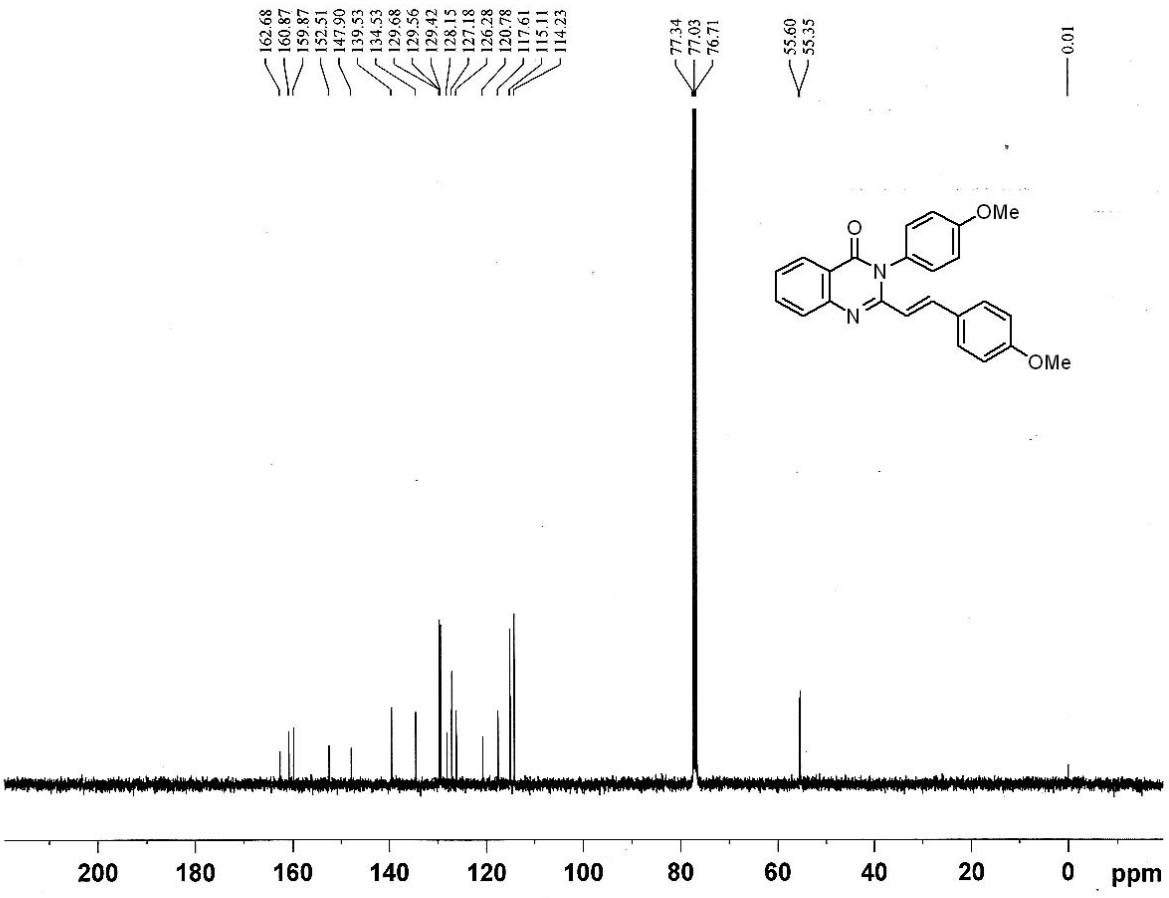

162.41
160.06
152.06
147.92
139.55
137.10
136.47
134.59
129.91
129.40
129.30
128.71
128.66
128.32
128.14
127.43
127.23
127.15
126.36
120.80
117.62
115.12
77.34
77.02
76.70
70.04
-0.00
O
N
N
O
200
180
160
140
120
100
80
60
40
20
0
ppm

(*E*)-3-(4-Chlorostyryl)-2-(p-tolyl) quinazolin-4(3*H*)-one (Entry 9,Table 3)

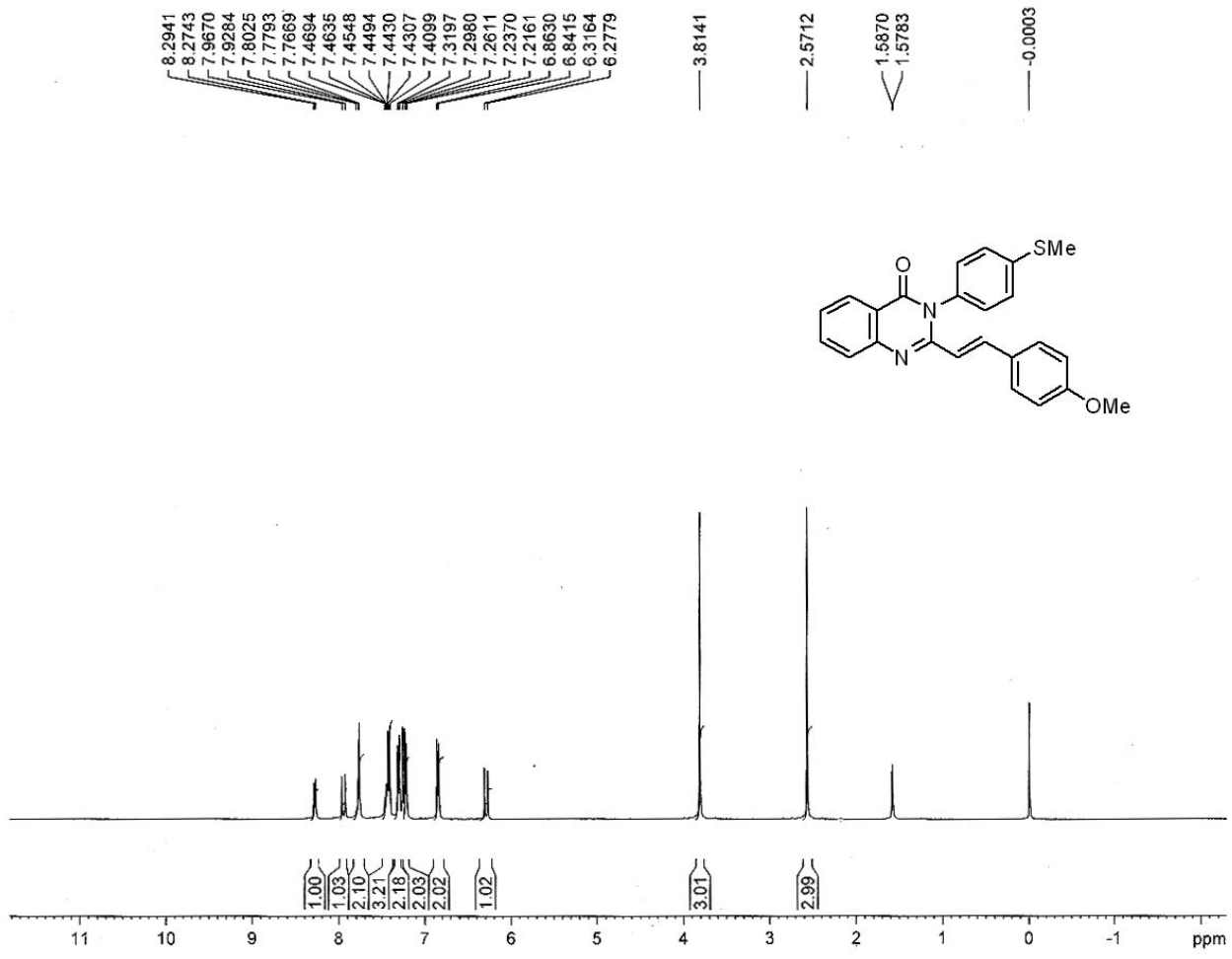


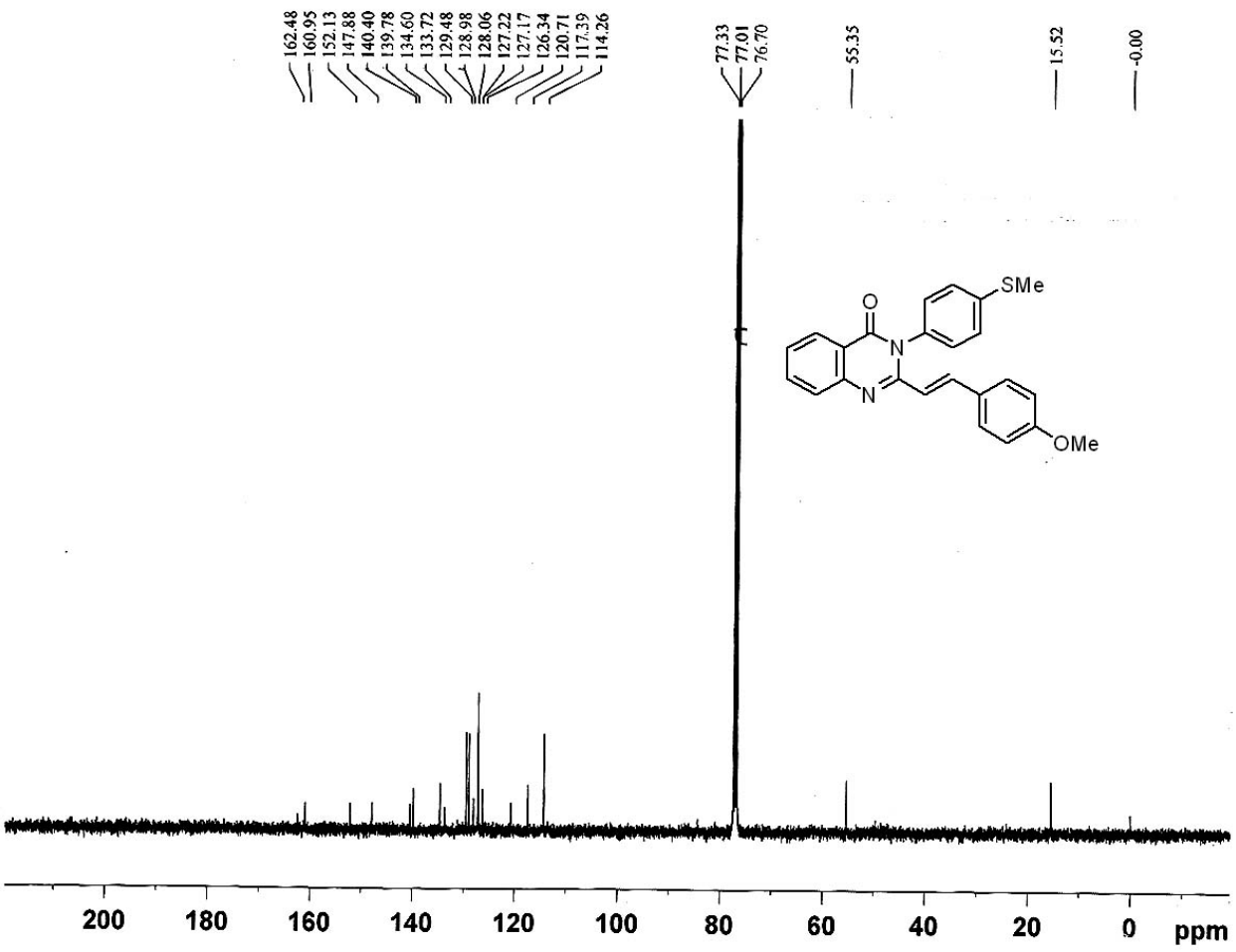
(*E*)-3-(4-Methoxyphenyl)-2-(4-methoxystyryl)quinazolin-4(3*H*)-one (Entry 10,Table 3)



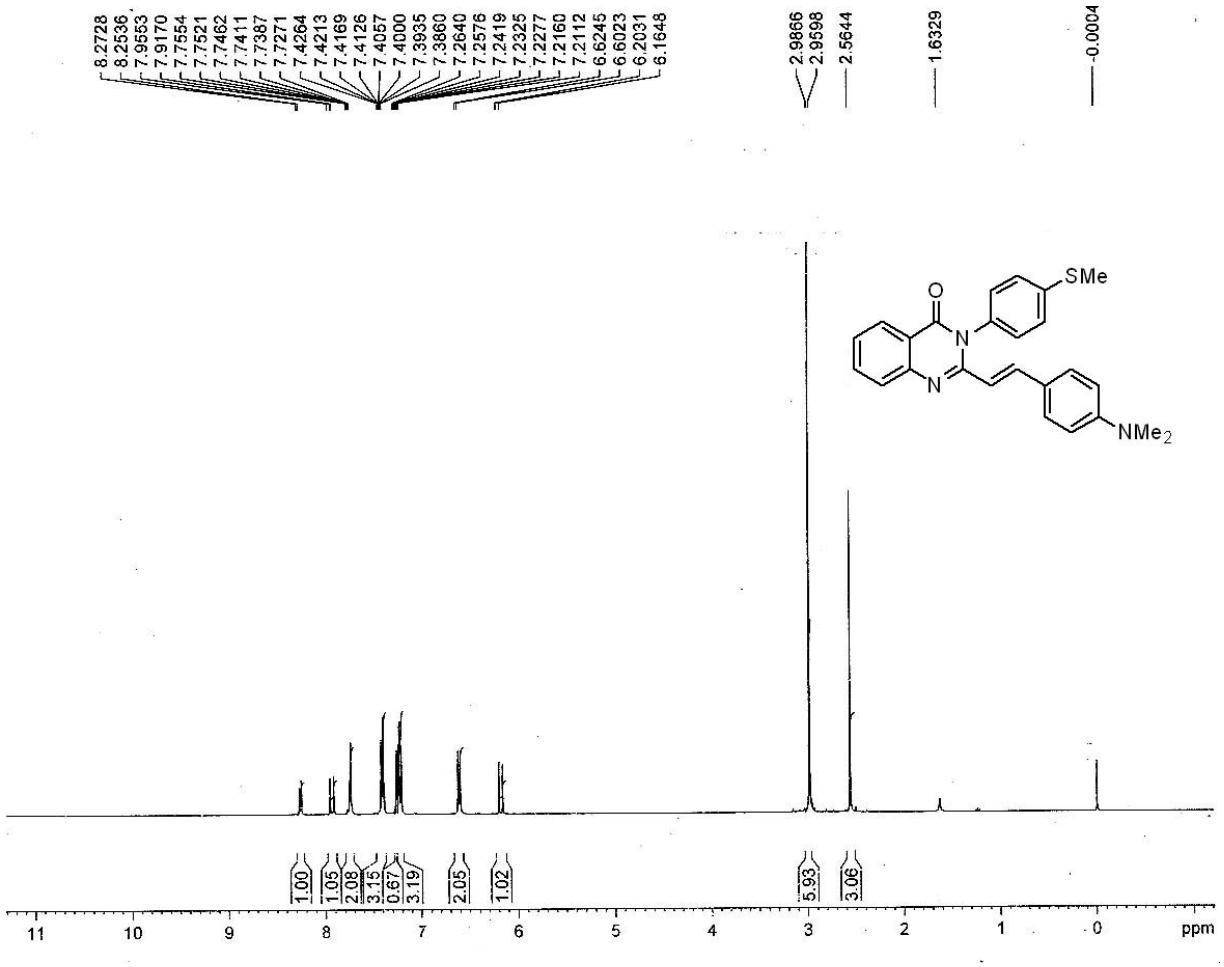

162.68
160.87
159.87
152.51
147.90
139.53
134.53
129.68
129.56
129.42
128.15
127.18
126.28
120.78
117.61
115.11
114.23
77.34
77.03
76.71
55.60
55.35
0.01
OMe
OMe
O
N
N
200
180
160
140
120
100
80
60
40
20
0
ppm

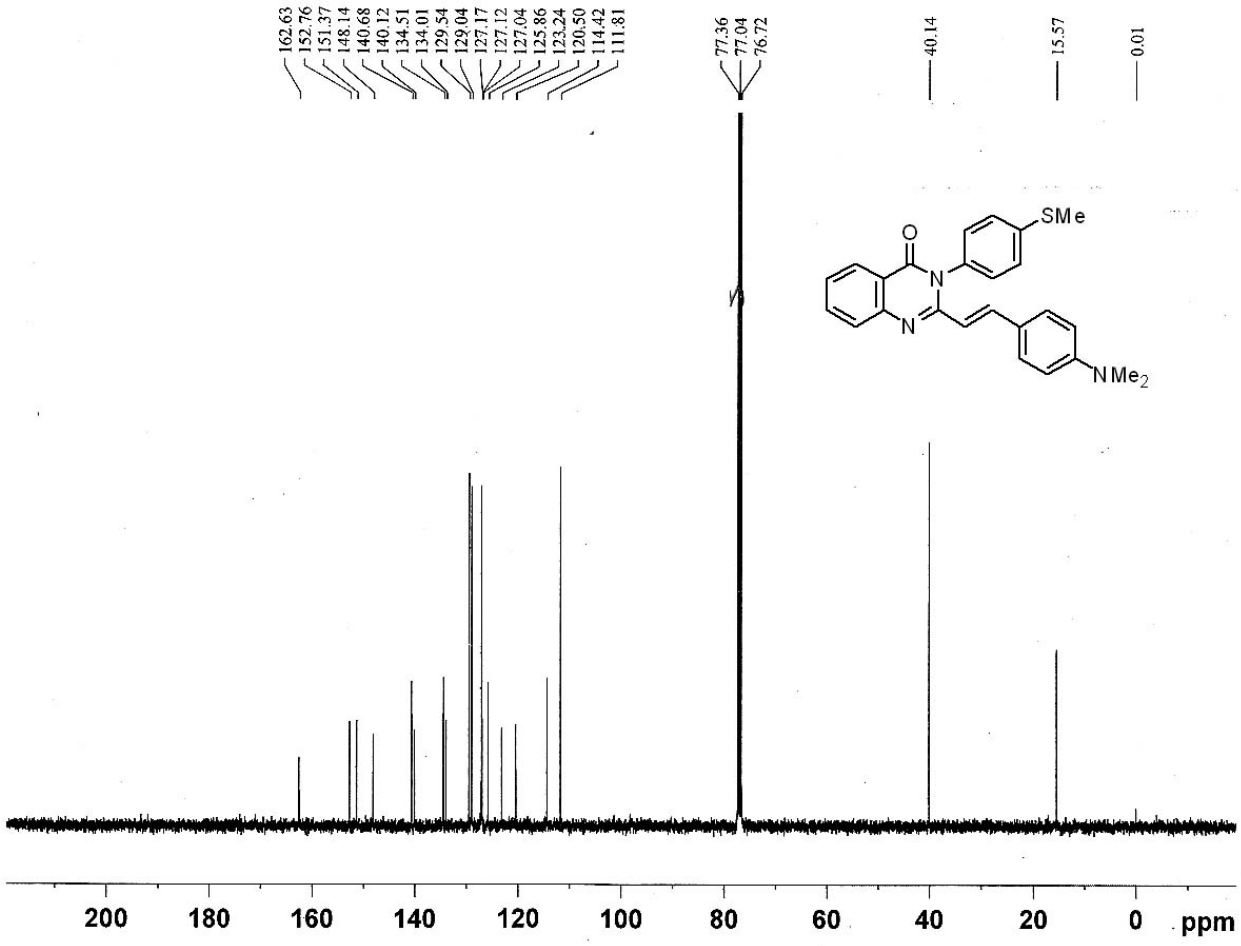
(*E*)-2-(4-Methoxystyryl)-3-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one (Entry 11,Table 3)



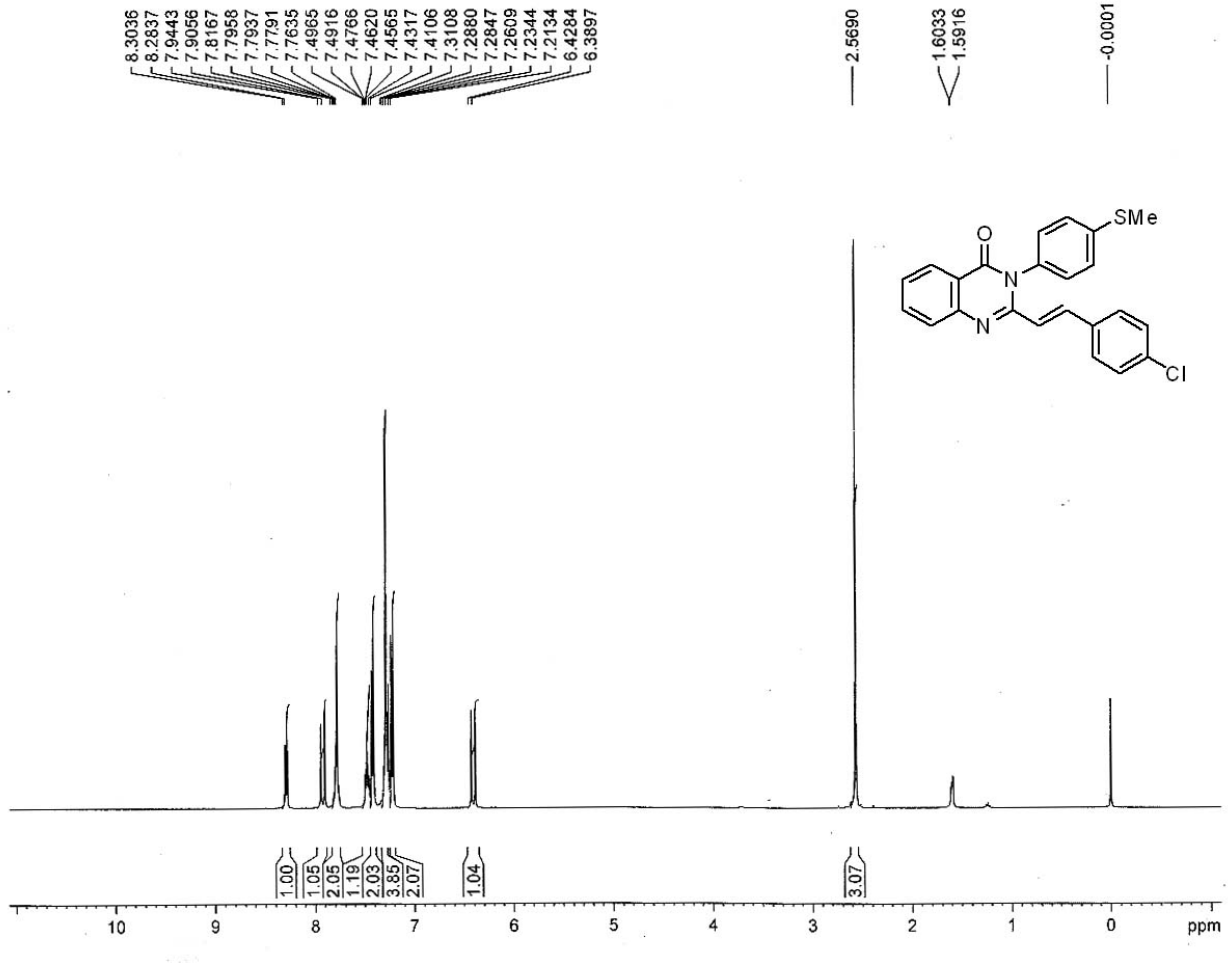

162.48
160.95
152.13
147.88
140.40
139.78
134.60
133.72
129.48
128.98
128.06
127.22
127.17
126.34
120.71
117.39
114.26
77.33
77.01
76.70
55.35
15.52
-0.00
SMe
O
N
N
OMe
200
180
160
140
120
100
80
60
40
20
0
ppm

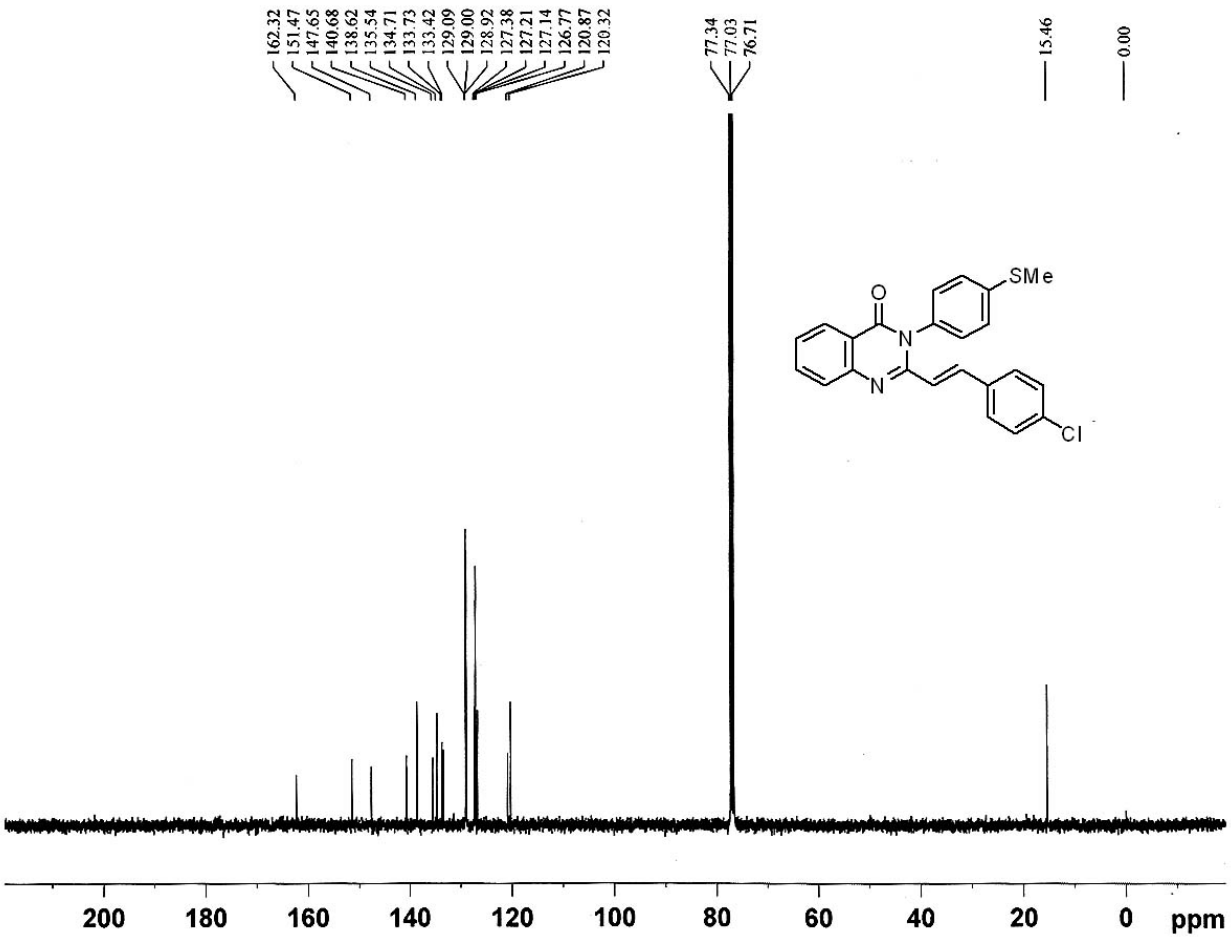
***(E)*-2-(4-(Dimethylamino)styryl)-3-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one(Entry 12, Table 3)**



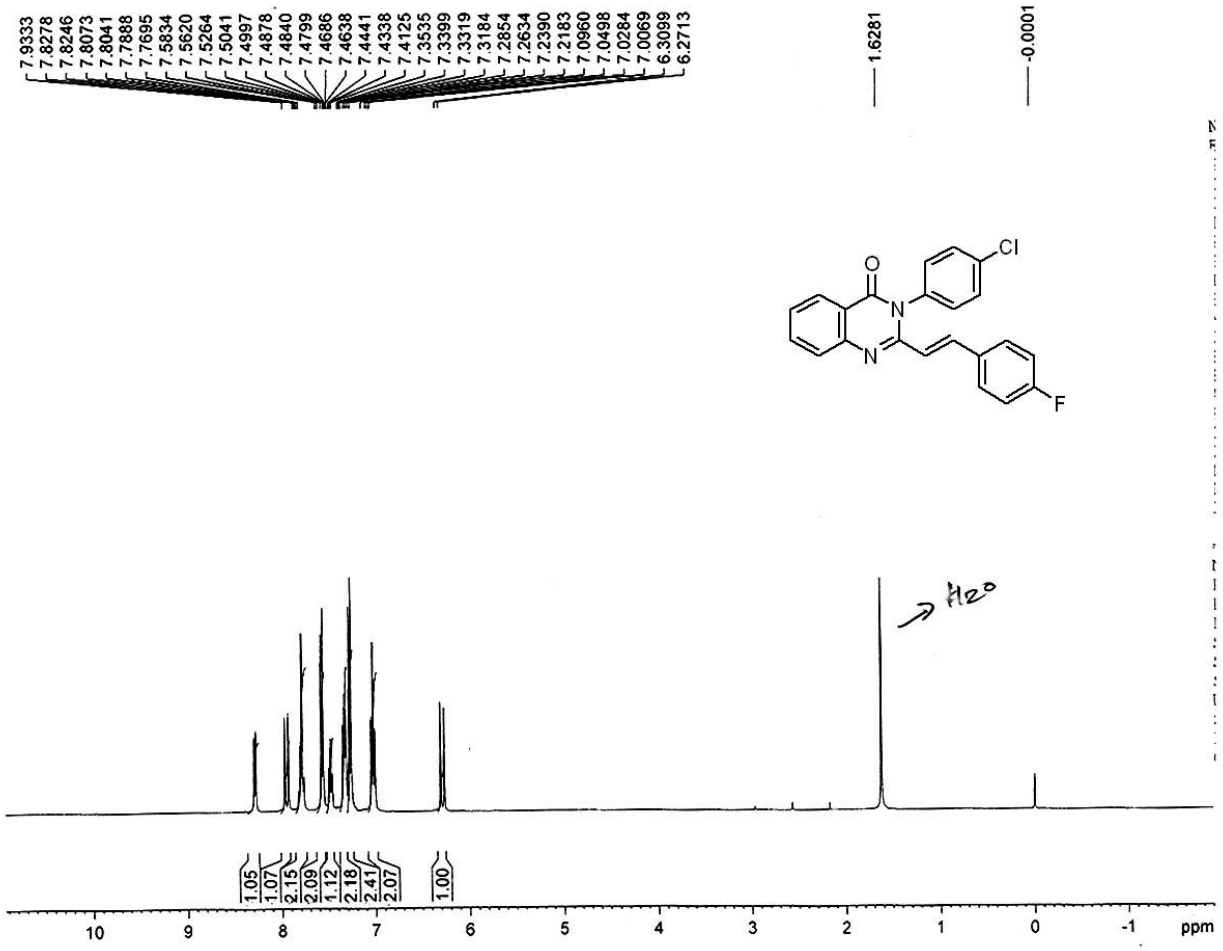

162.63
152.76
151.37
148.14
140.68
140.12
134.51
134.01
129.54
129.04
127.17
127.12
127.04
125.86
123.24
120.50
114.42
111.81
77.36
77.04
76.72
40.14
15.57
0.01
SMe
O
N
N
NMe2
200
180
160
140
120
100
80
60
40
20
0
ppm

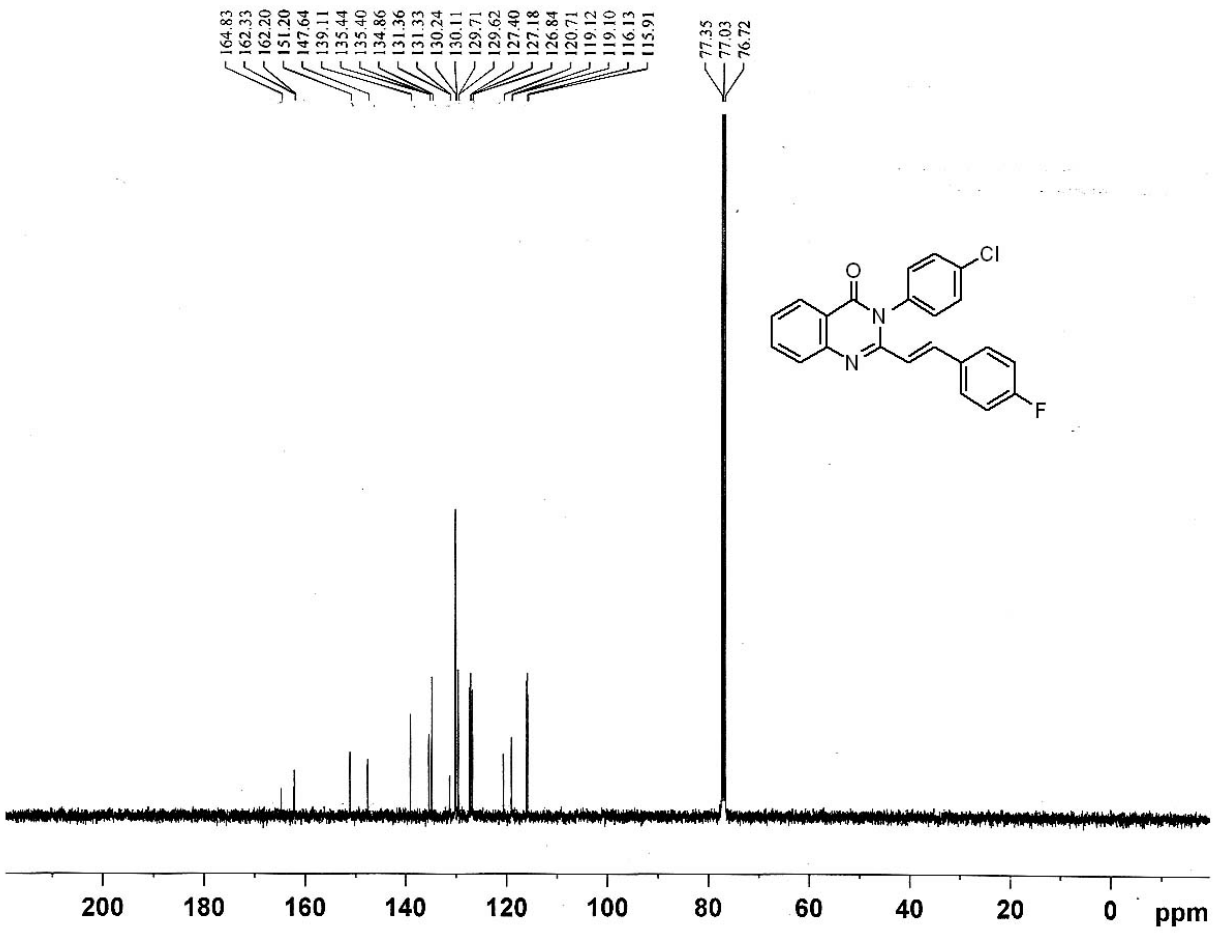
***(E)*-2-(4-Chlorostyryl)-3-(4-(methylthio)phenyl)quinazolin-4(3H)-one (Entry 13, Table 3)**



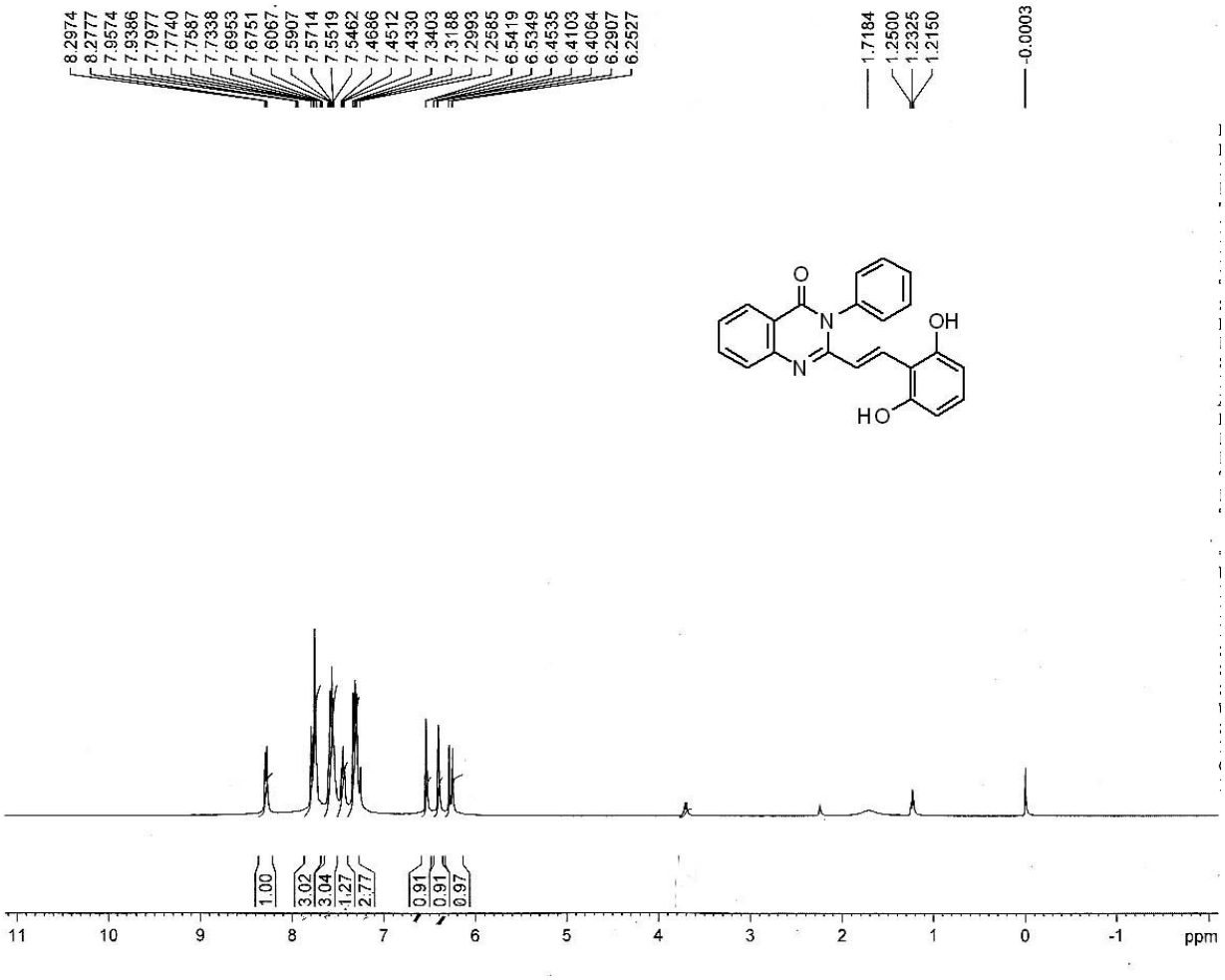

162.32
151.47
147.65
140.68
138.62
135.54
134.71
133.73
133.42
129.09
129.00
128.92
127.38
127.21
127.14
126.77
120.87
120.32
77.34
77.03
76.71
15.46
0.00
SMe
O
N
N
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

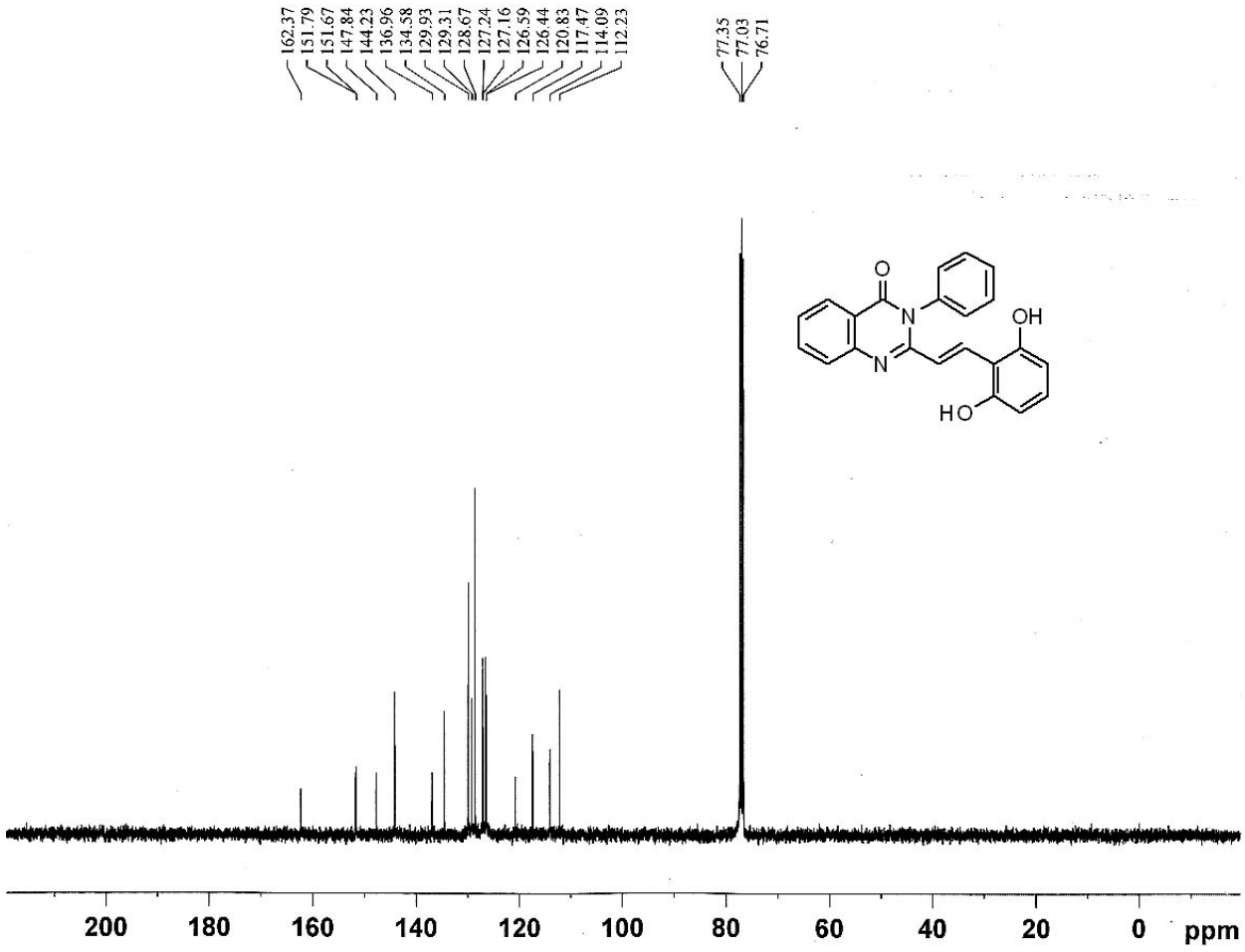
(*E*)-3-(4-Chlorophenyl)-2-(4-fluorostyryl)quinazolin-4(3*H*)-one(Entry 14, Table 3)



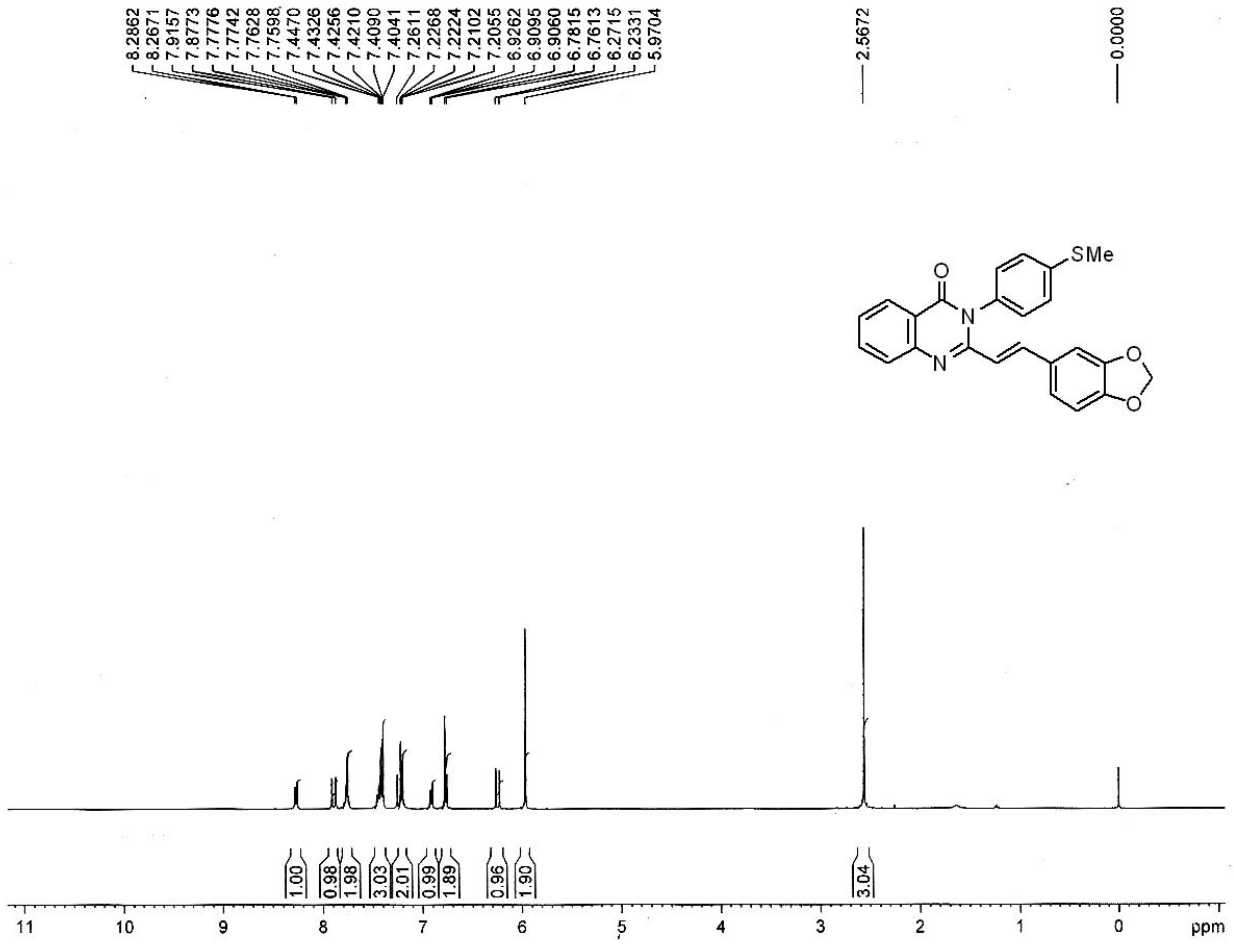

164.83
162.33
162.20
151.20
147.64
139.11
135.44
135.40
134.86
131.36
131.33
130.24
130.11
129.71
129.62
127.40
127.18
126.84
120.71
119.12
119.10
116.13
115.91
77.35
77.03
76.72
O
N
N
Cl
F
200
180
160
140
120
100
80
60
40
20
0
ppm

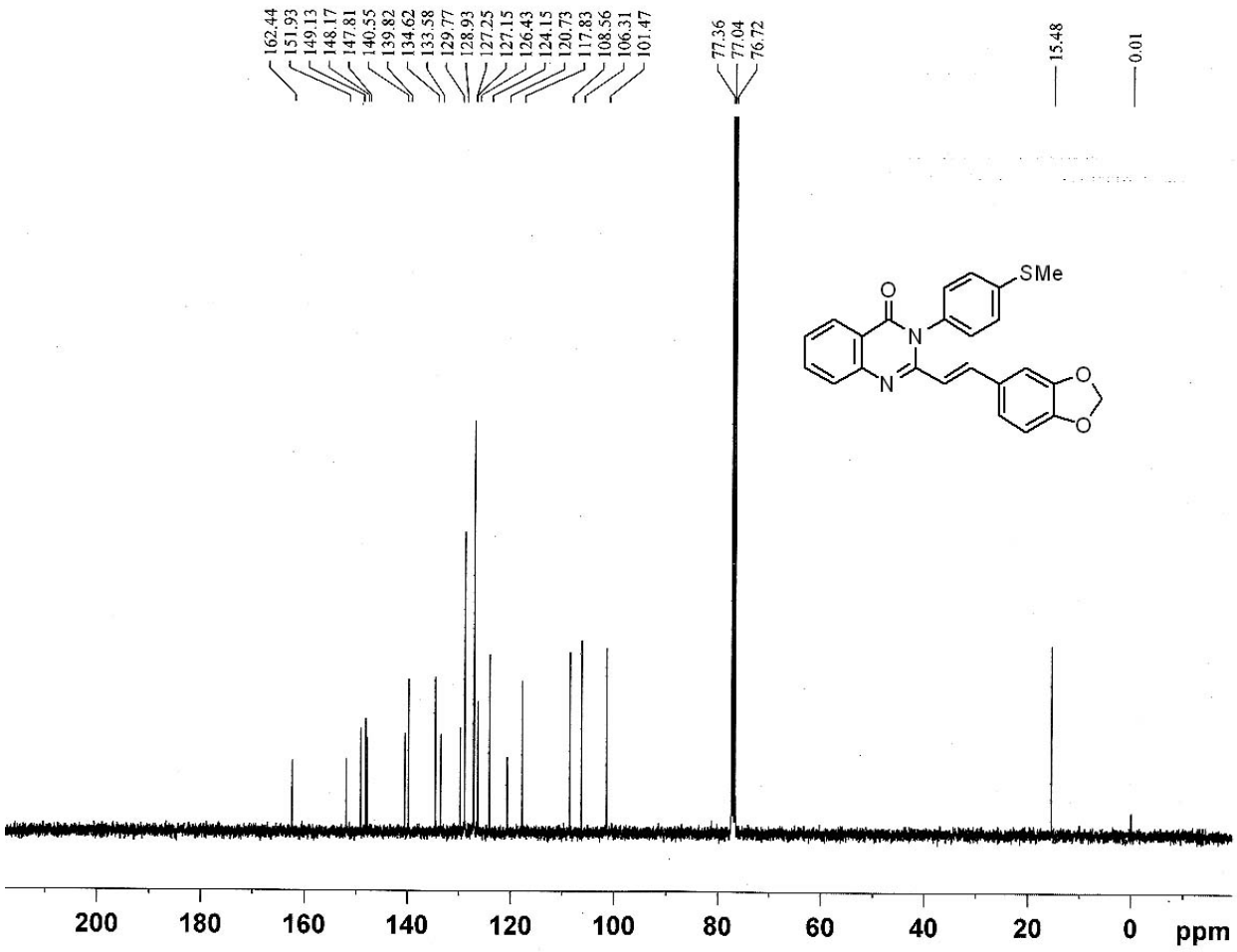
(*E*)-2-(2,6-Dihydroxystyryl)-3-phenylquinazolin-4(3*H*)-one(Entry 15, Table 3)



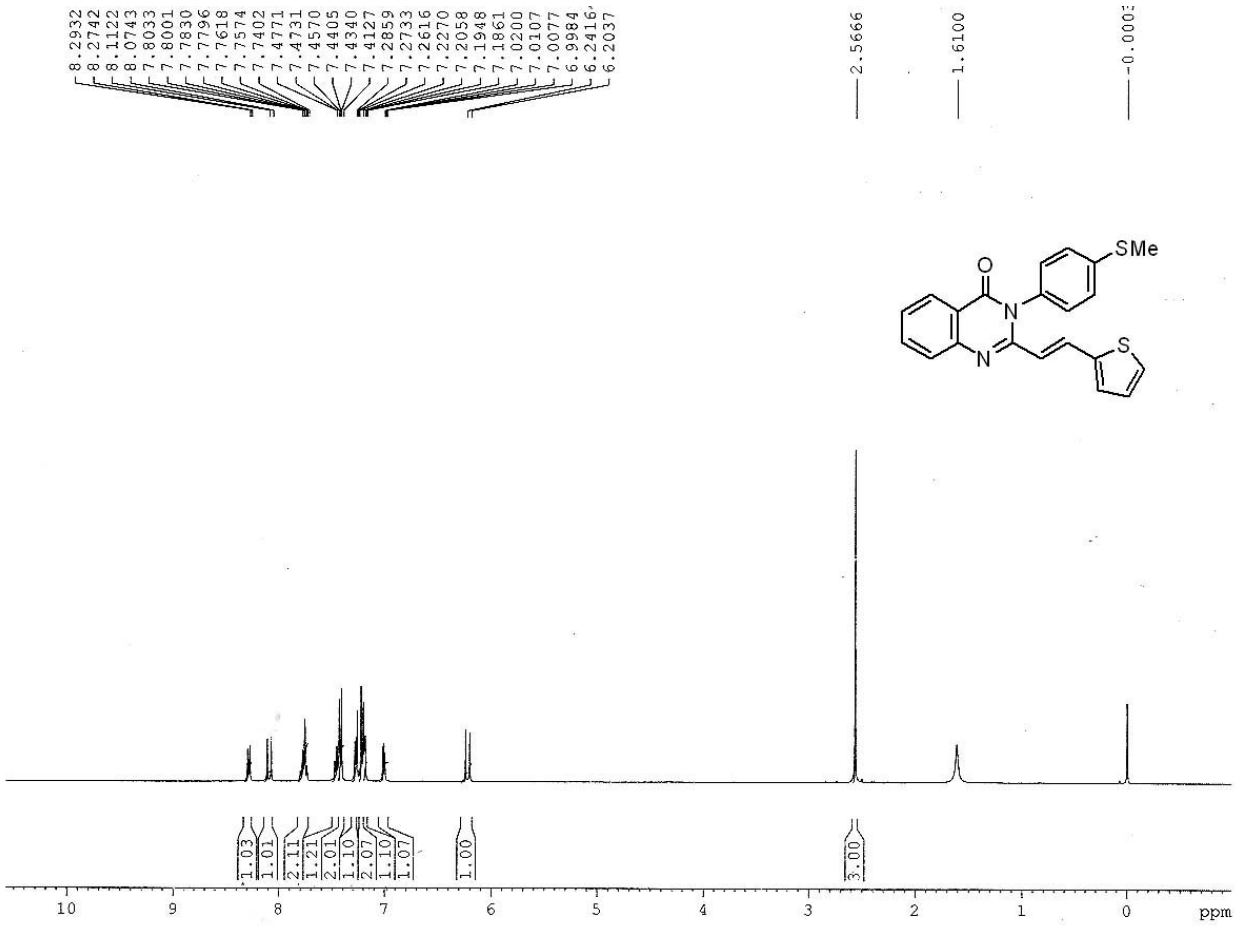

162.37
151.79
151.67
147.84
144.23
136.96
134.58
129.93
129.31
128.67
127.24
127.16
126.59
126.44
120.83
117.47
114.09
112.23
77.35
77.03
76.71
O
N
N
OH
HO
200
180
160
140
120
100
80
60
40
20
0
ppm

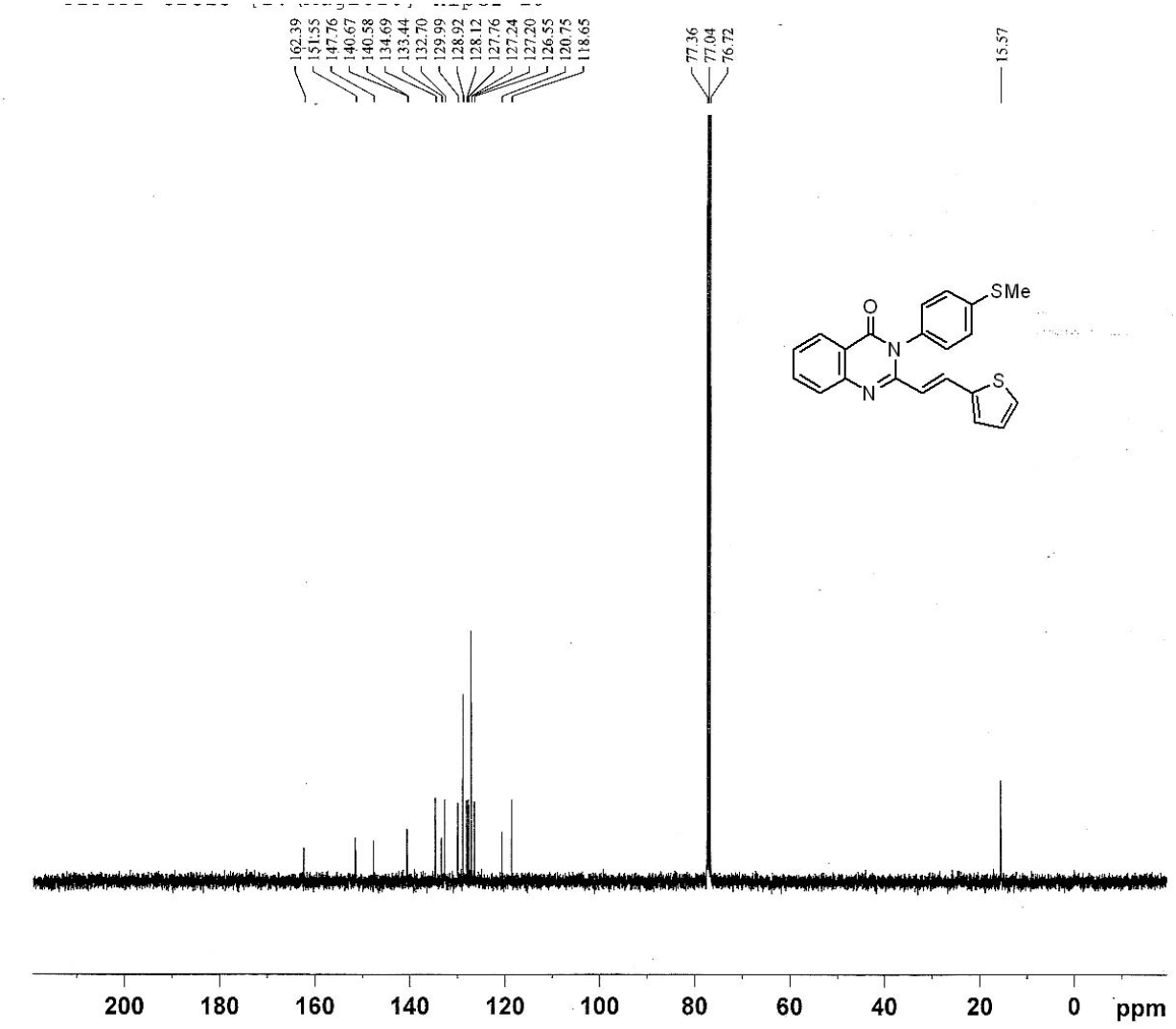
(*E*)-2-(2-(Benzo[d][1,3]dioxol-5-yl)vinyl)-3-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one (Entry 16, Table 3)



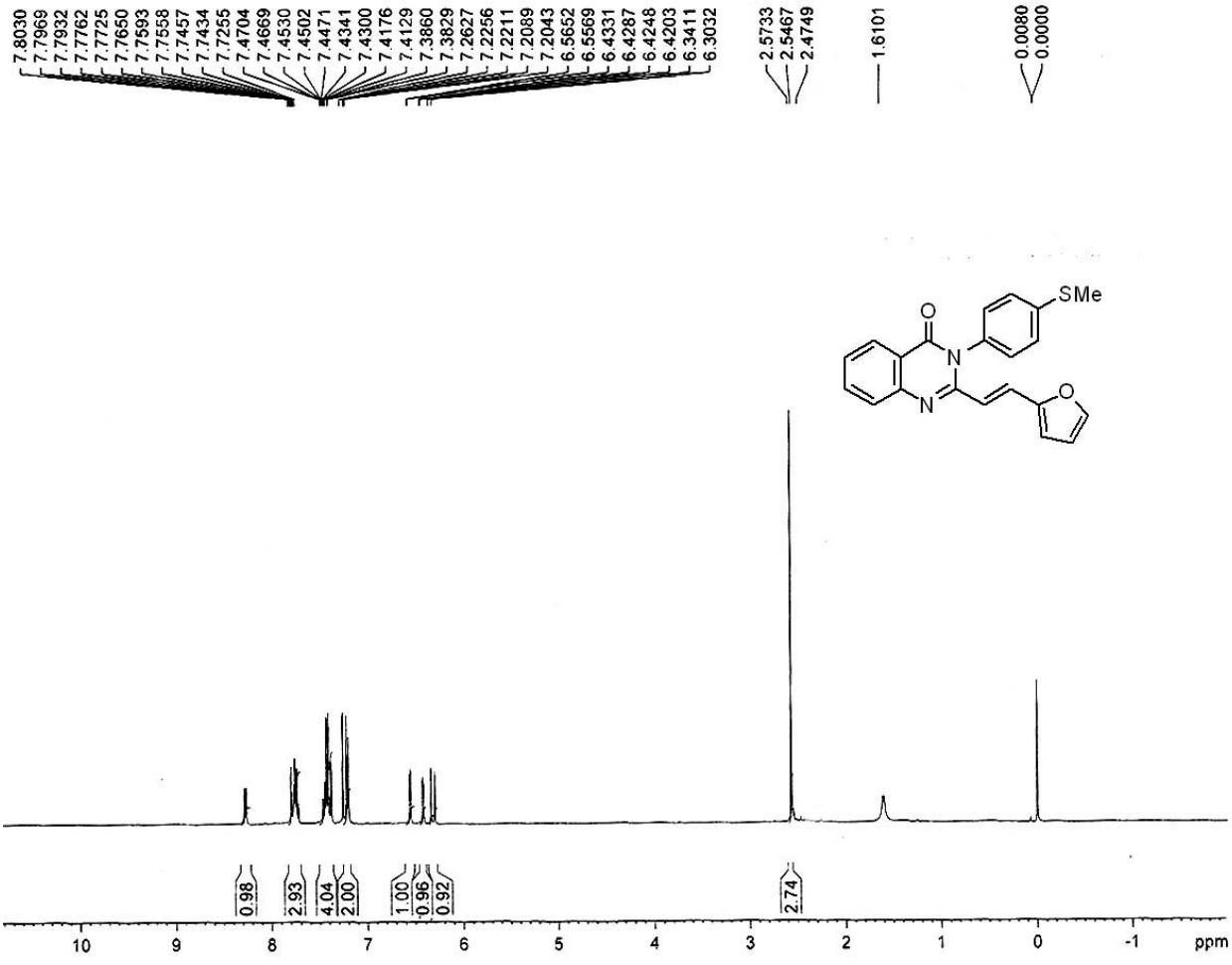

162.44
151.93
149.13
148.17
147.81
140.55
139.82
134.62
133.58
129.77
128.93
127.25
127.15
126.43
124.15
120.73
117.83
108.56
106.31
101.47
77.36
77.04
76.72
15.48
0.01
SMe
O
N
N
O
O
200
180
160
140
120
100
80
60
40
20
0
ppm

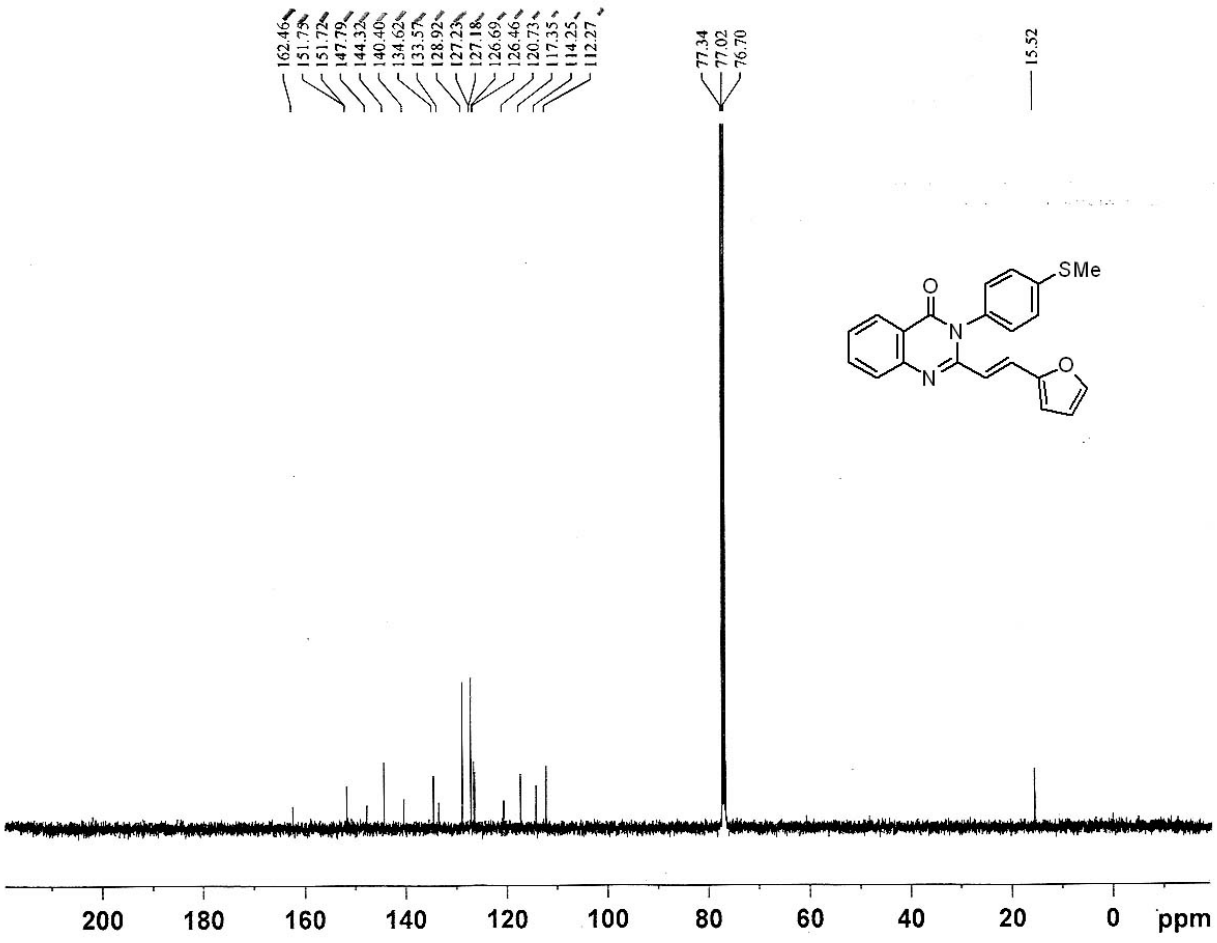
(*E*)-3-(4-(Methylthio)phenyl)-2-(2-(thiophen-2-yl)vinyl)quinazolin-4(3*H*)-one (Entry 17, Table 3)



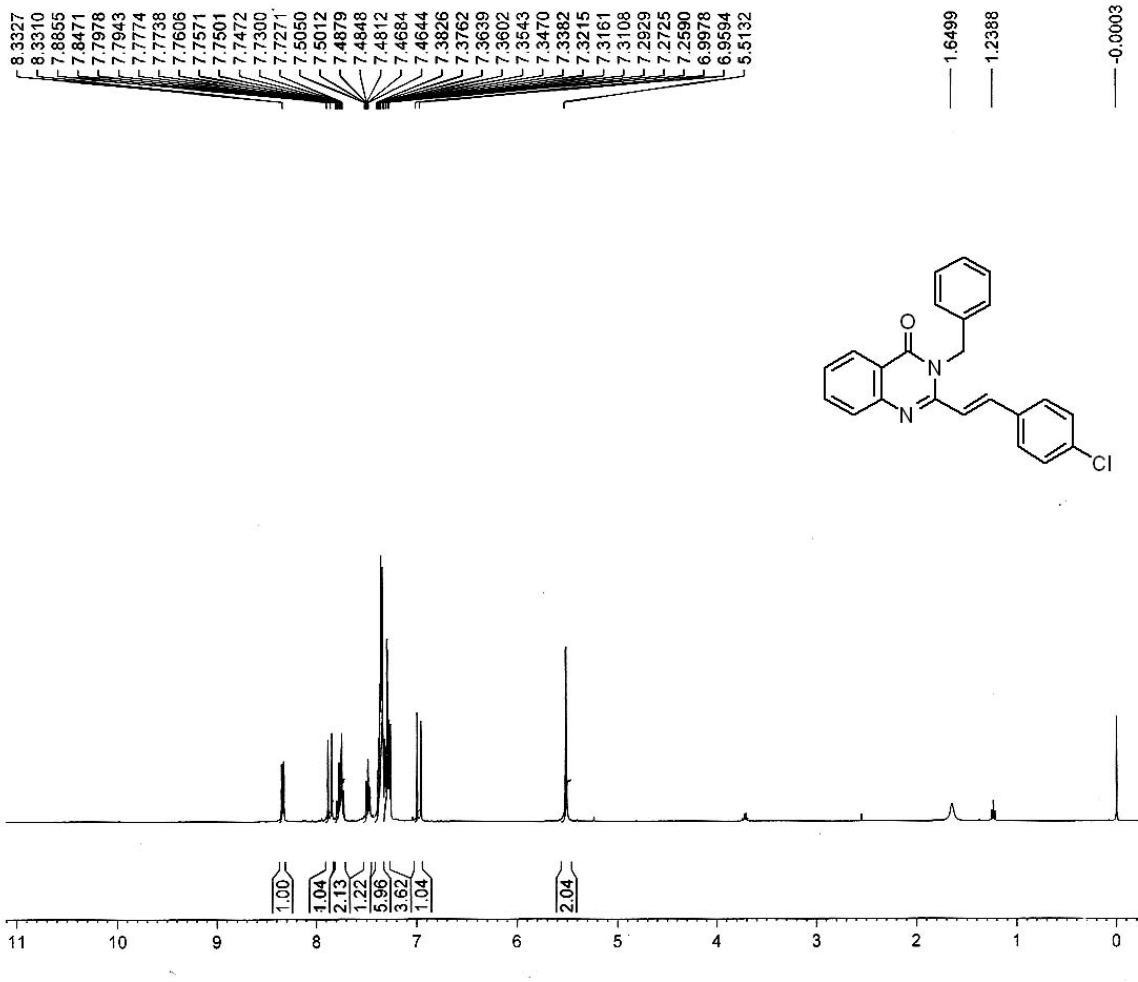

162.39
151.55
147.76
140.67
140.58
134.69
133.44
132.70
129.99
128.92
128.12
127.76
127.24
127.20
126.55
120.75
118.65
77.36
77.04
76.72
15.57
SMe
O
N
N
S
200
180
160
140
120
100
80
60
40
20
0
ppm

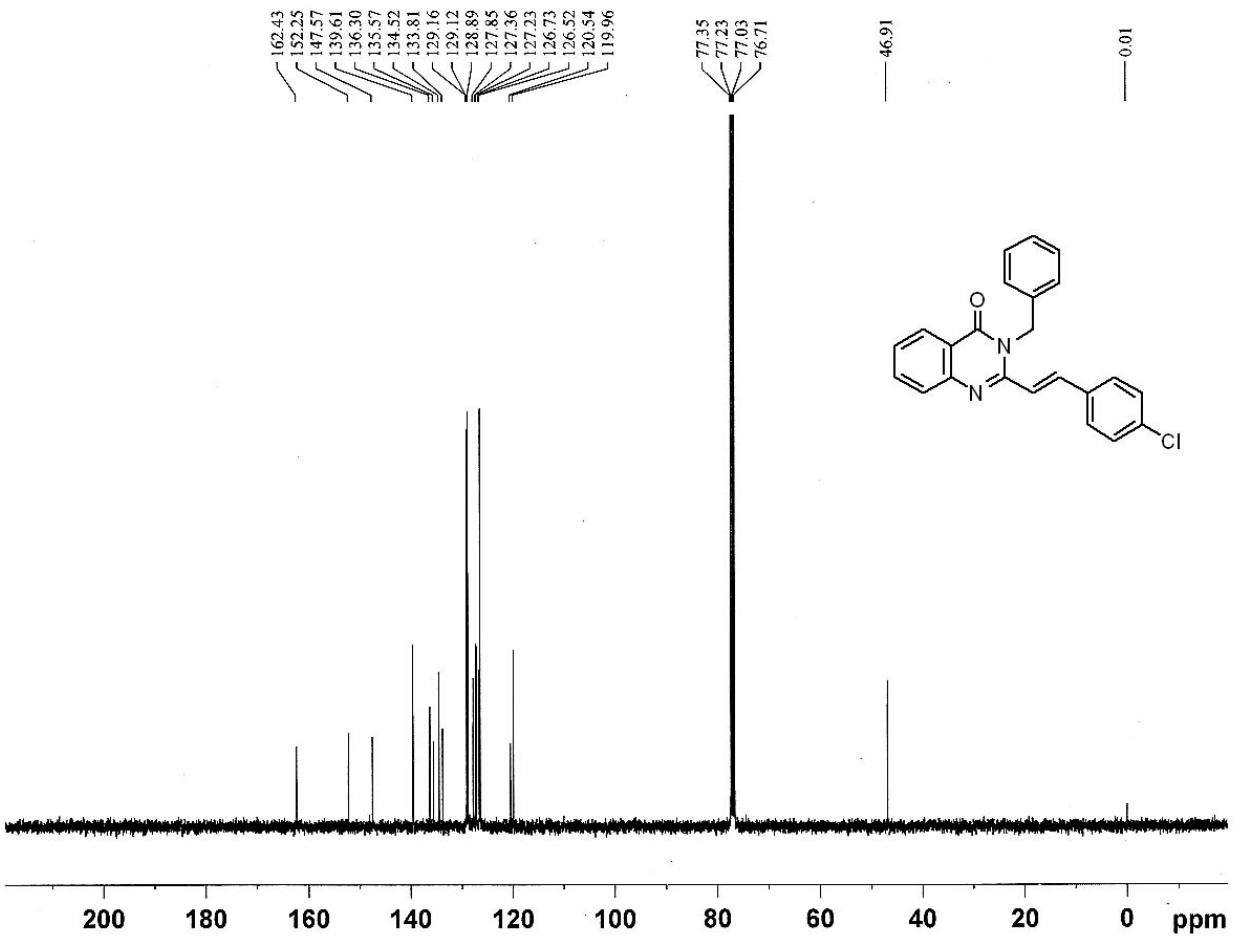
(*E*)-2-(2-(furan-2-yl)vinyl)-3-(4-(methylthio)phenyl)quinazolin-4(3*H*)-one(Entry 18, Table 3)



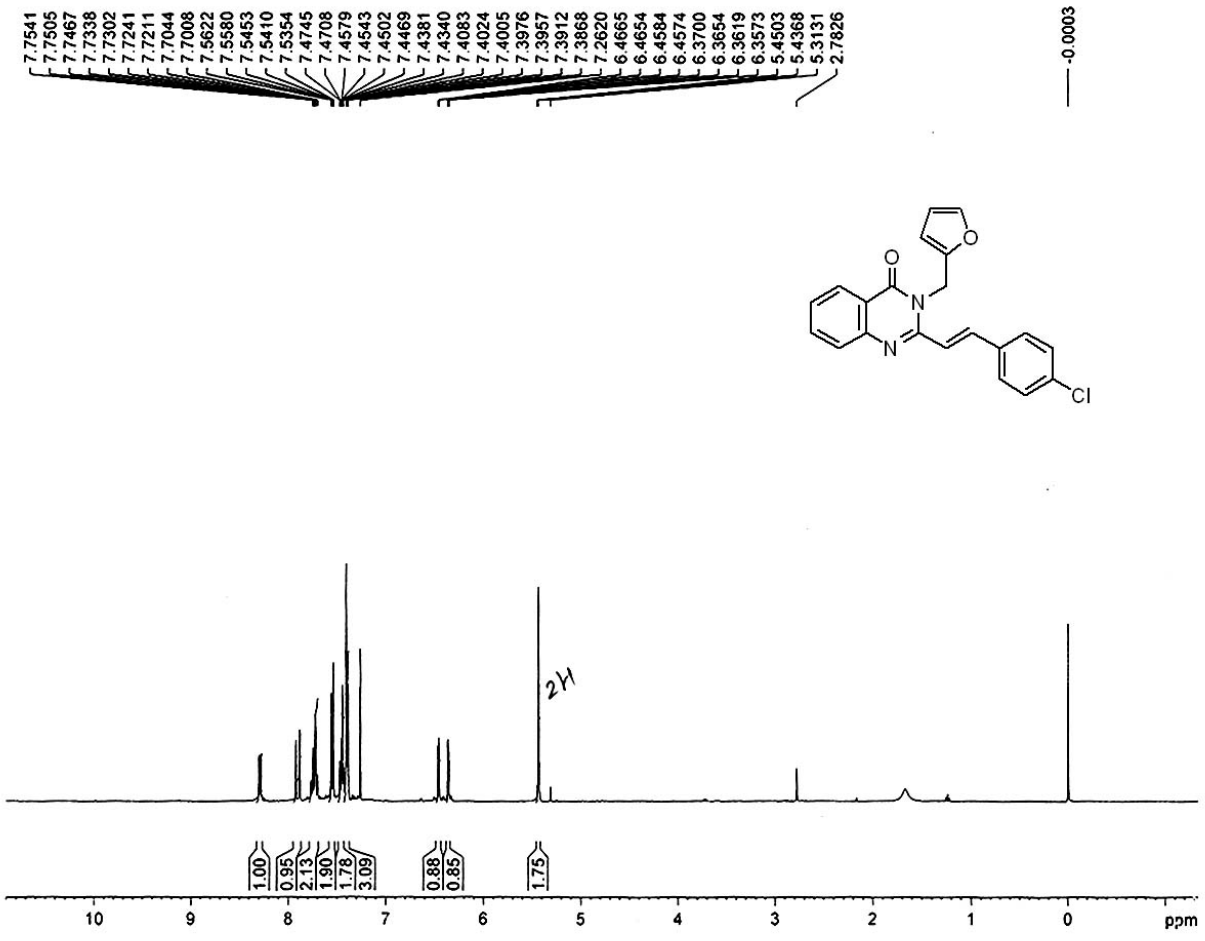

162.46
151.79
151.72
147.79
144.32
140.40
134.62
133.57
128.92
127.23
127.18
126.69
126.46
120.73
117.35
114.25
112.27
77.34
77.02
76.70
15.52
SMe
O
N
N
O
200
180
160
140
120
100
80
60
40
20
0
ppm

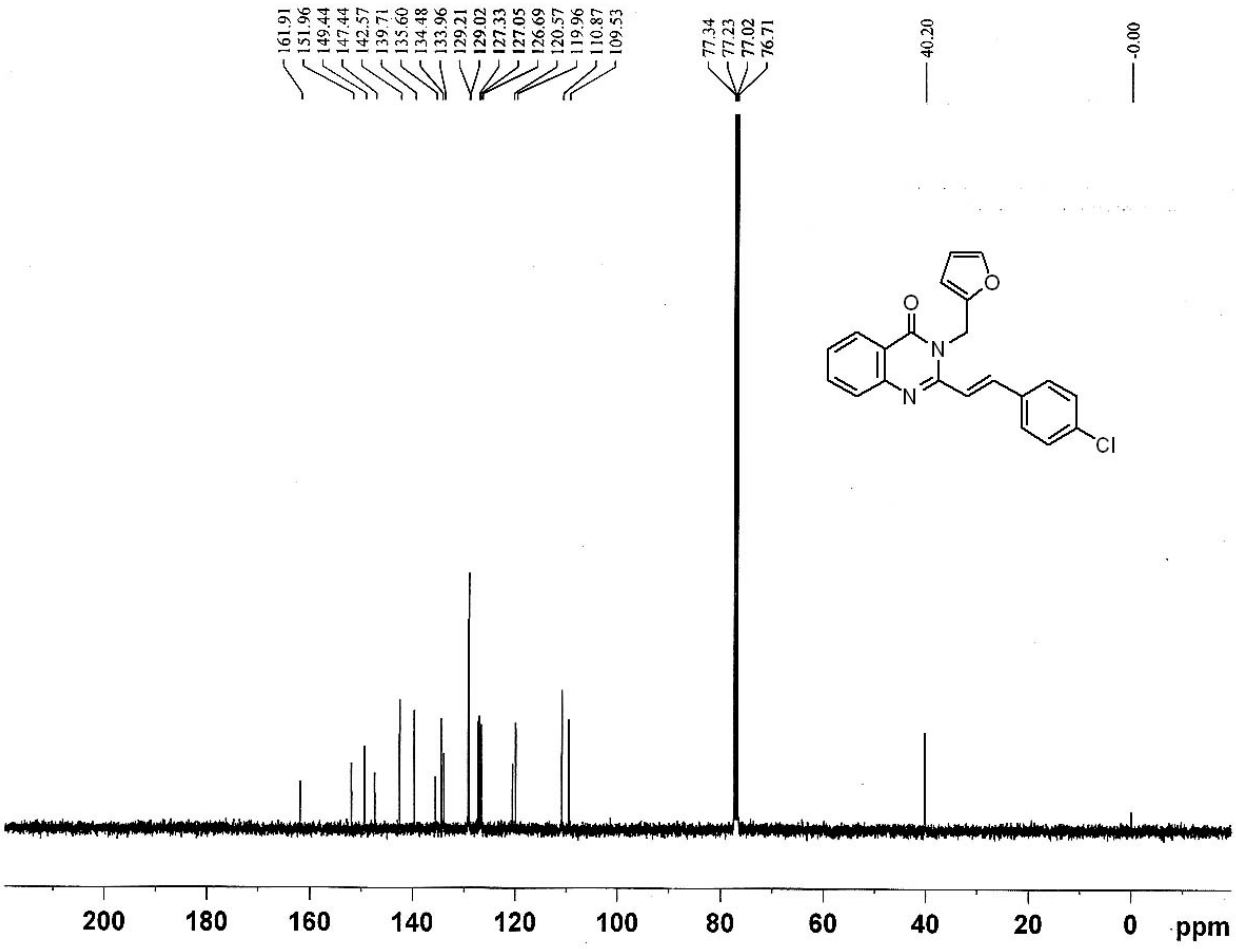
(*E*)-3-Benzyl-2-(4-chlorostyryl)quinazolin-4(3*H*)-one(Entry 19, Table 3)



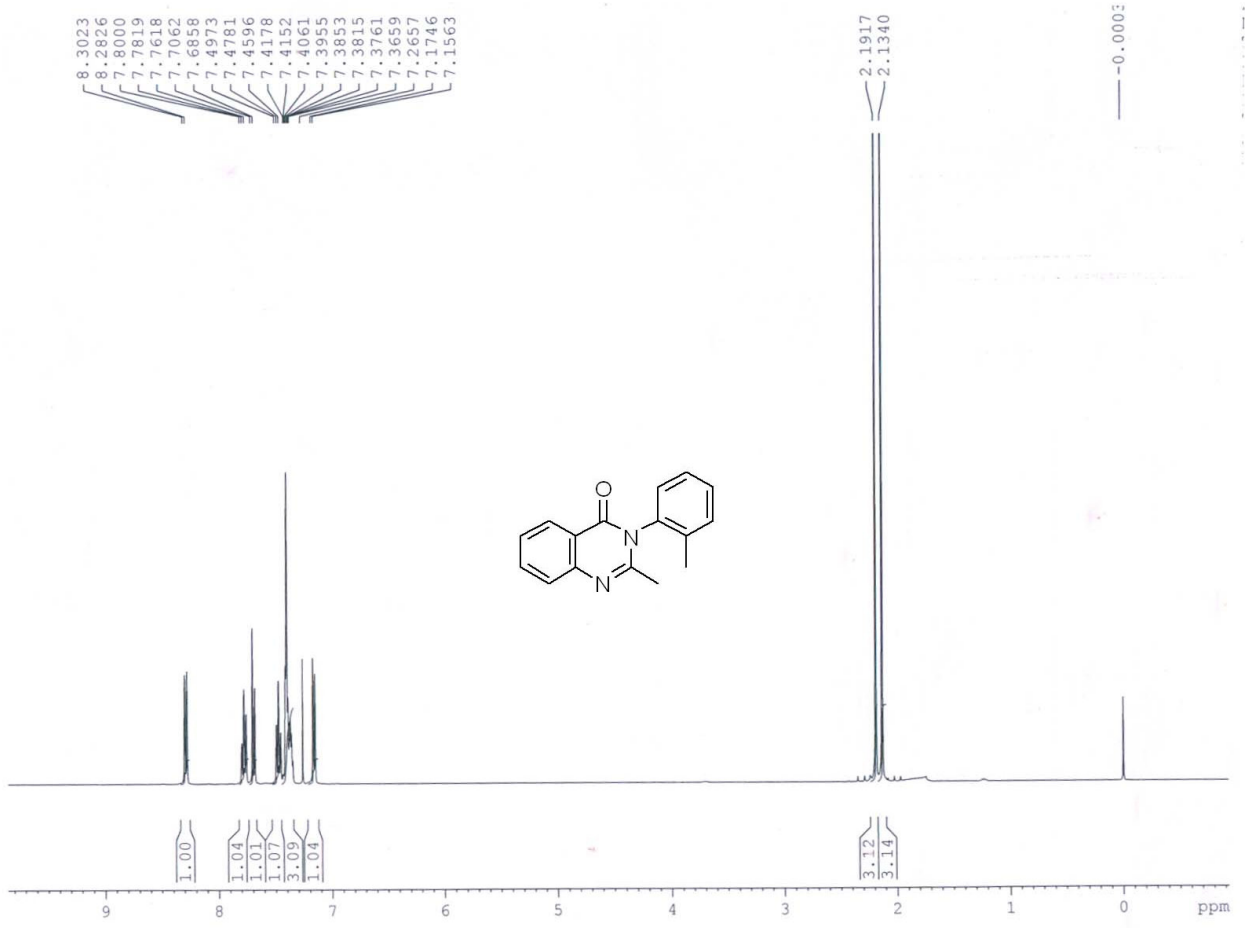

162.43
152.25
147.57
139.61
136.30
135.57
134.52
133.81
129.16
129.12
128.89
127.85
127.36
127.23
126.73
126.52
120.54
119.96
77.35
77.23
77.03
76.71
46.91
0.01
O
N
N
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

(*E*)-2-(4-Chlorostyryl)-3-(furan-2-ylmethyl)quinazolin-4(3*H*)-one (Entry 20, Table 3)

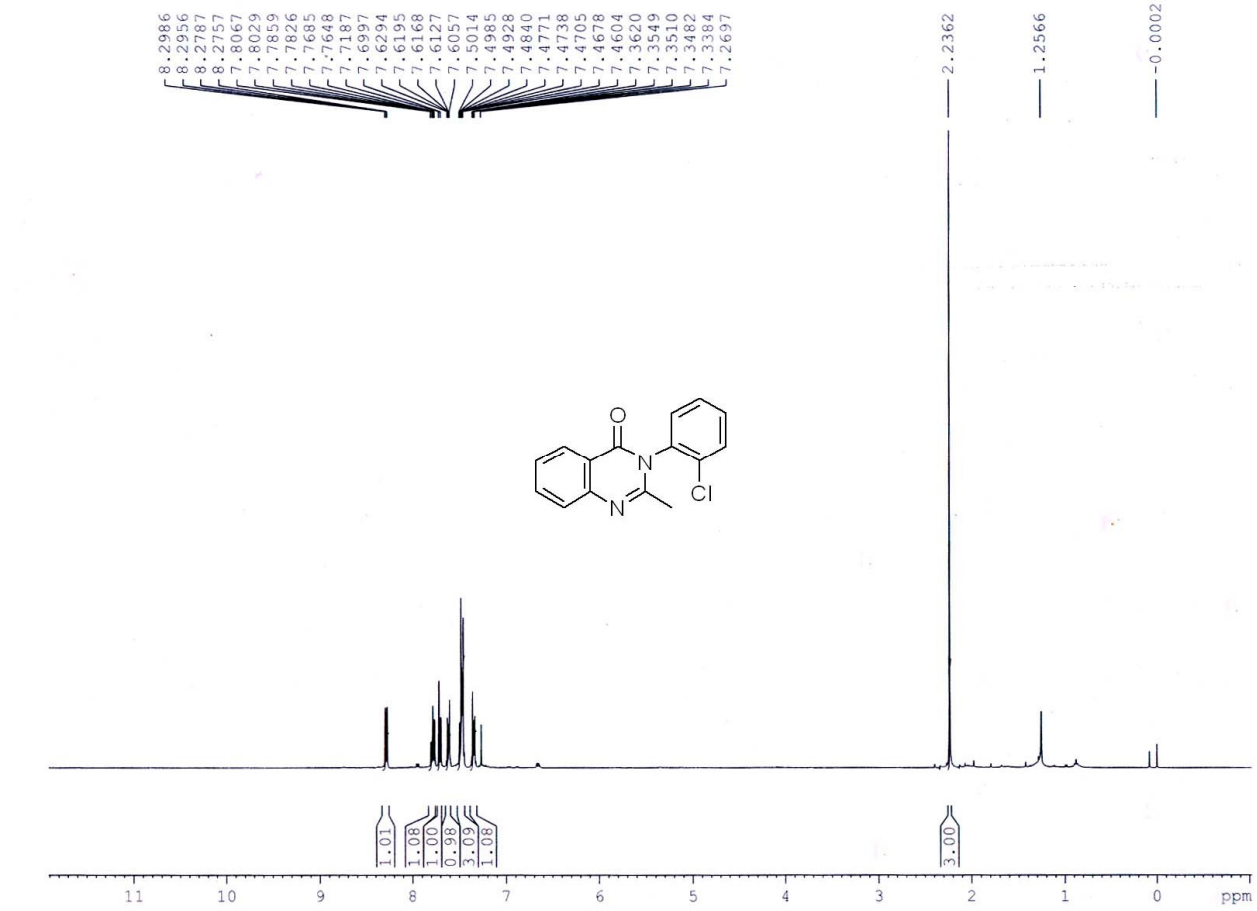



161.91
151.96
149.44
147.44
142.57
139.71
135.60
134.48
133.96
129.21
129.02
127.33
127.05
126.69
120.57
119.96
110.87
109.53
77.34
77.23
77.02
76.71
40.20
-0.00
O
N
N
O
Cl
200
180
160
140
120
100
80
60
40
20
0
ppm

Methaqualone

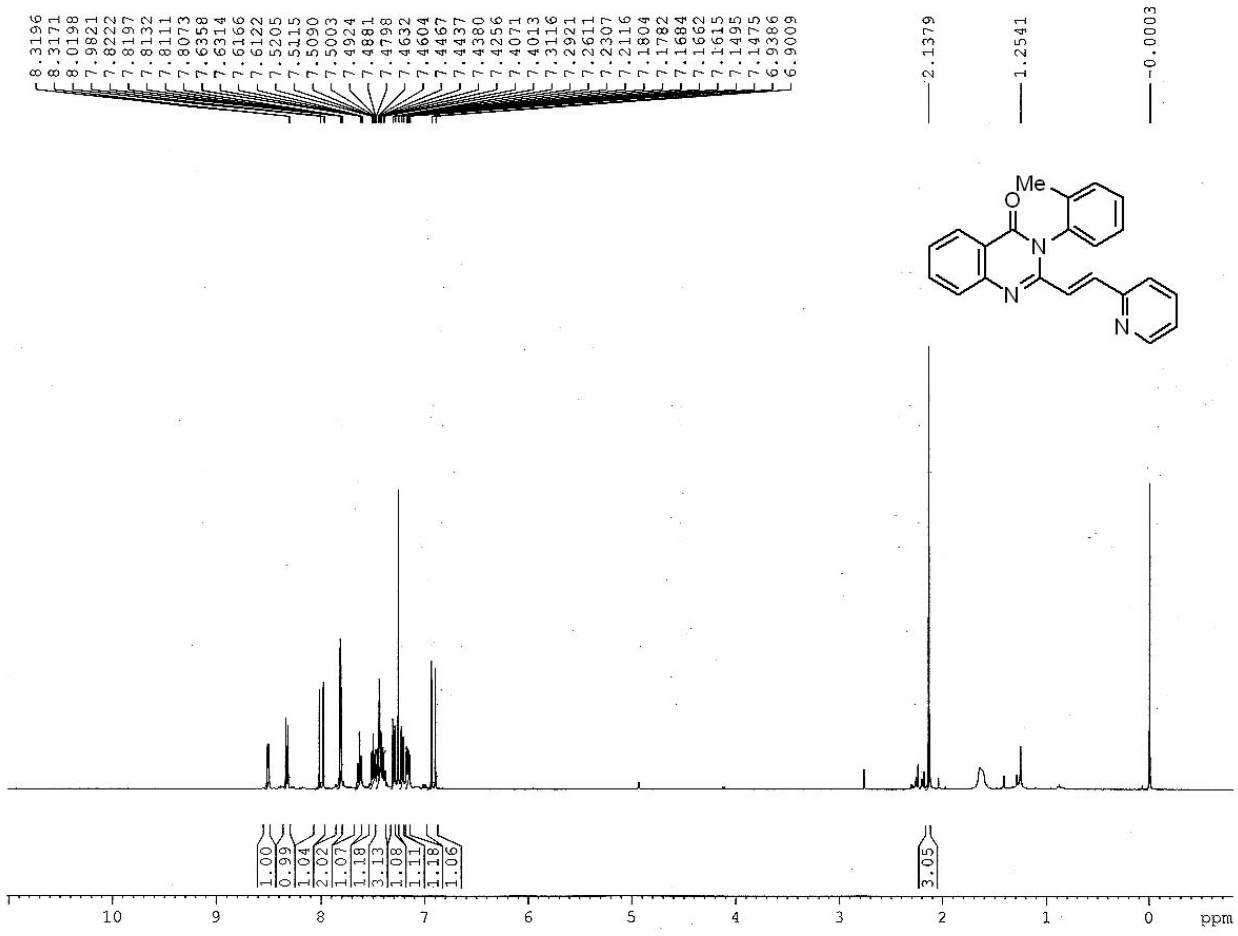


Mecloqualone

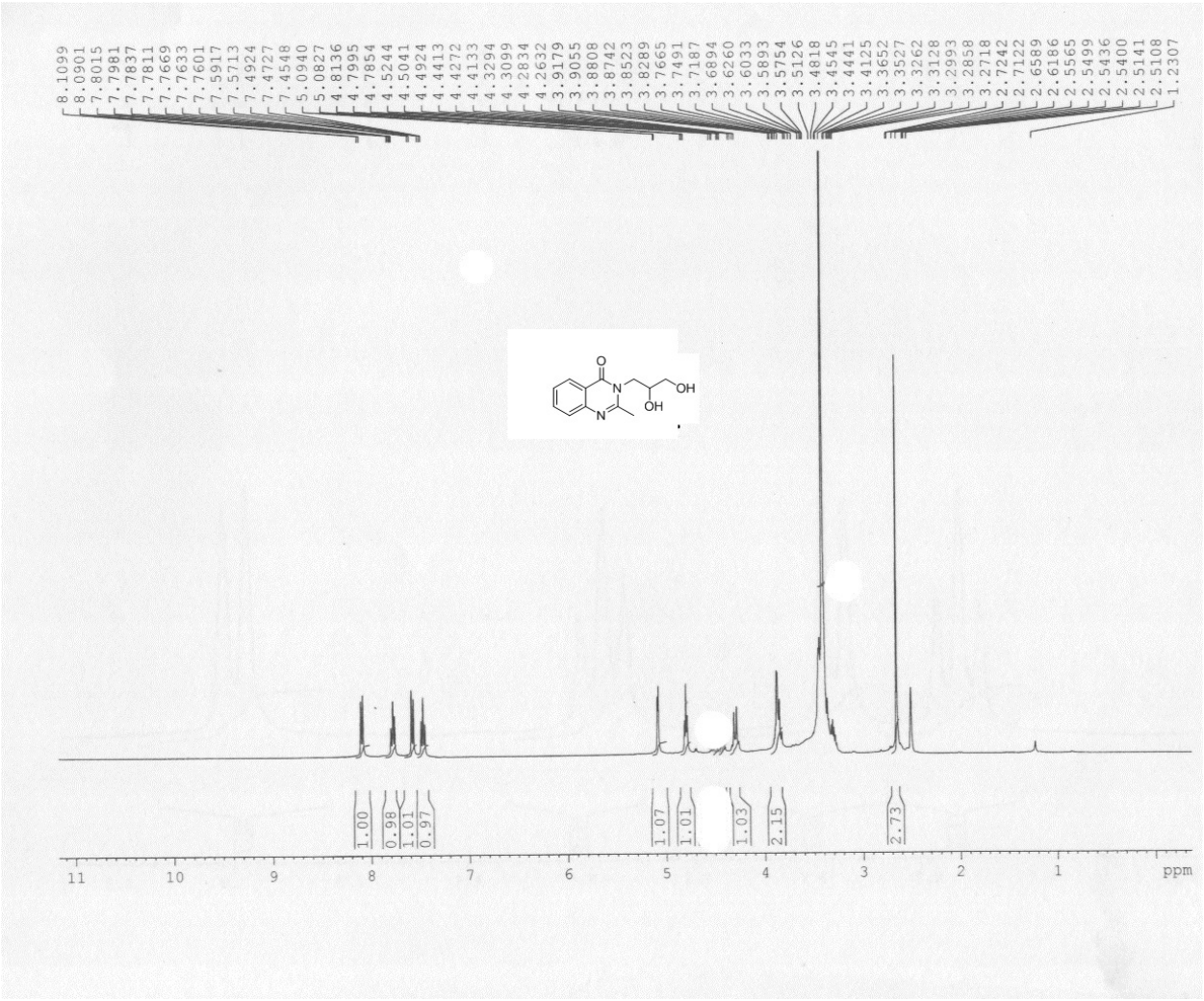


Mebroqualone

Piriquialone



Diproqualone



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