Supporting Information

New Chemistry of 1,3-Diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one:

Chemistry at C-6, C-7 and C-8 positions

Panayiotis A. Koutentis*, Harry Krassos and Daniele Lo Re

Department of Chemistry, University of Cyprus, P.O. Box 20537, 1678 Nicosia,

Cyprus, koutenti@ucy.ac.cy

Table of Contents

1. Section A

1.1. Experimental

1.1.1. General Procedures

Acetonitrile was distilled over CaH_2 and THF was distilled over Na before use. Reactions were protected by $CaCl_2$ drying tubes. Anhydrous Na_2SO_4 was used for drying organic extracts and all volatiles were removed under reduced pressure. All reaction mixtures and column eluents were monitored by TLC using commercial glass backed thin layer chromatography (TLC) plates (Kieselgel 60 F_{254}). The plates were observed under UV light at 254 and 365 nm. The technique of dry flash chromatography was used throughout for all non-TLC scale chromatographic separations using silica gel 60 (less than 0.063 mm). Melting points were determined using a hotstage microscope apparatus. Solvents used for recrystallization are indicated after the melting point. Inflections in the UV spectra are identified by the abbreviation "inf". FTIR spectra were recorded using a Ge ATR accessory and strong, medium and weak peaks are represented by s, m and w respectively. ^{1}H NMR spectra were recorded at either 300 or 500 MHz and ^{13}C NMR spectra were recorded at either 75 and 125 MHz, respectively. DEPT 135 NMR studies identified quaternary and tertiary carbons, which are indicated by (s) and (d) notations, respectively. Deuterated solvents were used for homonuclear lock and the signals are referenced to the deuterated solvent peaks. Low resolution (EI) mass spectra were recorded on a GCMS with direct inlet probe.

1.1.2. Preparation of (benzotriazinylidene)malononitrile

*1.1.2.1. 2-(1,3-Diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-ylidene)propanedinitrile (**11**).* To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1

mmol) in PhCl (1 ml), TCNE (23 mg, 0.18 mmol) was added and the mixture heated to *ca.* 140 ^{o}C for 18 h. TLC (*t*-BuOMe/hexane, 2:1) showed the absence of the starting material and the presence of a new less polar green product. The mixture was diluted with THF (2 ml) and cooled until *ca.* 0 ^{o}C. The precipitate was filtered and dissolved in DCM (5 ml). To this solution was added silica gel (100 mg) and the mixture stirred for 10 min and then filtered. The solvent was evaporated *in vacuo* and the residue crystallized to afford the *title compound* **11** (6 mg, 17%) as green plates, mp 306-311 ^{o}C (from $CHCl_3$), R_f 0.61 (*t*-BuOMe/hexane, 3:1); (found: C, 75.9; H, 3.7; N, 20.1. $C_{22}H_{13}N_5$ requires C, 76.1; H, 3.8; N, 20.2%); λ_{max}(DCM)/nm 277 (log ε 3.06), 345 inf (3.24), 360 (3.37), 377 (3.42), 421 (2.98), 610 inf (2.90), 647 (3.04), 702 (3.08), 774 inf (2.84); ν_{max}/cm^{-1} 3063w (Ar CH), 2203m (C≡N), 1612w, 1551w, 1508s, 1489w, 1472w, 1454w, 1449w, 1427w, 1402w, 1377m, 1364w, 1341w, 1306m, 1267m, 1227w, 1207w, 1188w, 1153w, 1136w, 1069w, 1028w, 1003w, 983w, 989w, 924w, 887w, 860w, 841m, 833w 816w, 800w, 781w; δ_H(300 MHz, $CDCl_3$) 8.28-8.25 (2H, m, Ar *H*), 7.94 (1H, d, *J* 9.5, 1.9, *H*-6), 7.72-7.59 (6H, m, Ar *H*), 7.52-7.46 (3H, m, Ar *H*), 6.59 (1H, d, *J* 2.0, *H*-8); δ_H(125 MHz; $CDCl_3$) 156.5 (s), 154.1 (s), 153.1 (s), 140.7 (s), 137.8 (d), 134.7 (s), 133.3 (s), 131.5 (d), 131.2 (d), 130.6 (d), 130.6, (d), 129.1 (d), 127.2 (d), 125.4 (d), 116.1 (s), 116.0 (s), 95.1 (d); *m*/*z* (EI) 348 (M^++1, 26%), 347 (M^+, 100), 319 (3), 244 (4), 215 (6), 188 (3), 139 (16), 112 (11), 103 (6), 91 (6), 77 ($C_5H_5^+$, 41), 51 (21).

1.1.3. C-6 Substituted Benzotriazinones

*1.1.3.1. 6-Hydroxy-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**15**).* To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (29.9 mg, 0.1 mmol) in THF/H_2O (4:1) (1 ml), KOH (16.8 mg, 0.3 mmol) was added and the reaction mixture was heated at 90^{o}C for 18 h. TLC (*t*-BuOMe) show the absence of

the starting material and the presence of a very polar red compound. Conc. HCl was added (51 μl, 0.61 mmol), followed by an excess of hexane (10 ml) and the precipitate that formed was filtered, washed (water) and recrystallized to afford the *title compound* **15** (28.9 mg, 92%) as light red plates, mp 250-255 ^{o}C (from PhH), R_f 0.74 (DCM/MeOH, 5:1); (found: C, 72.3; H, 4.1; N, 13.4. $C_{19}H_{13}N_3O_2$ requires C, 72.4; H, 4.2; N, 13.3%); λ_{max}(DCM)/nm 251 (log ε 3.41), 309 (3.72), 366 inf (2.91), 386 inf (2.83), 508 (2.82); ν_{max}/cm^{-1} 3161w (OH), 1580s, 1555s, 1495m, 1470m, 1404m, 1385s, 1364m, 1314s, 1290m, 1261w, 1229m, 1190m, 1163m, 1070w, 1026w, 1003w, 984w, 928w, 854m, 818w, 781m, 750w, 717m; δ_H(300 MHz; TFA-d_1) OH peak missing 8.32 (2H, d, *J* 7.7, Ar *H*), 7.83-7.61 (7H, m, Ar *H*), 7.53 (2H, dd, *J* 7.5, 7.5, Ar *H*), 7.19 (1H, m, Ar *H*); δ_C(75 MHz; TFA-d_1) 167.1 (Ar *C*=O), 161.5 (s), 158.7 (s), 148.5 (s), 142.2 (s), 140.1 (s), 135.4 (d), 134.3 (d), 131.7 (d), 130.9 (s), 130.7 (d), 129.3 (d), 126.3 (d), 108.1 (d), 100.2 (d); *m*/*z* (EI) 316 (M^++1, 24%), 315 (M^+, 100), 298 (4), 287 (26), 277 (6), 258 (2), 184 (13), 155 (9), 144 (17), 128 (10), 117 (8), 104 (12), 89 (5), 77 (62), 51 (33).

*1.1.3.2. 6-Ethoxy-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**14**) (Method 1).* To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in EtOH (1 ml), Hünig's base (342 μl, 2 mmol) was added, and the reaction mixture was heated at reflux for 48 h. TLC (*t*-BuOMe) showed the absence of the starting material and the presence of a new red compound. The mixture was diluted with DCM (8 ml) and adsorbed onto silica gel. Dry flash chromatography (*t*-BuOMe) gave the *title compound* **14** (15 mg, 44%) as red needles, mp 212-214 ^{o}C (from PhH), R_f 0.29 (*t*-BuOMe); (found: C, 73.6; H, 4.9; N, 12.2. $C_{21}H_{17}N_3O_2$ requires C, 73.5; H, 5.0; N, 12.2%); λ_{max}(DCM)/nm 246 (log ε 3.39), 311 (3.72), 363 inf (3.03), 381 inf (2.77), 520 (2.83); ν_{max}/cm^{-1} 3107w, 3061w and 3036w (Ar CH), 2990w, 1607s,

1591m, 1560s, 1516m, 1493m, 1458w, 1447w, 1408w, 1393w, 1379w, 1352w, 1314w, 1281m, 1256m, 1242m, 1227w, 1206w, 1196w, 1155w, 1136w, 1107w, 1084w, 1067w, 1024m, 986w, 970w, 926w, 901w, 866w, 849m, 824m; δ_H(300 MHz; $CDCl_3$) 8.32-8.29 (2H, m, Ar *H*), 7.62-7.57 (4H, m, Ar *H*), 7.51-7.48 (4H, m, Ar *H*), 7.01 (1H, s, *H*-5), 6.31 (1H, s, *H*-8), 4.34 (2H, q, *J* 6.8, O*CH*$_2$), 1.62 (3H, t, *J* 7.0, C*H*$_3$); δ_C(75 MHz; $CDCl_3$) 175.3 (*C*=O), 163.4 (s), 155.3 (s), 151.4 (s), 141.5 (s), 135.2 (s), 134.6 (s), 130.6 (d), 130.2 (d), 130.1 (d), 128.9 (d), 126.9 (d), 125.9 (d), 104.6 (d), 97.3 (d), 65.9 (O*C*H$_2$), 14.3 (*C*H$_3$); *m/z* (EI) 344 (M^++1, 10%), 343 (M^+, 31), 328 (100), 314 (9), 300 (48), 271 (7), 195 (3), 184 (2), 168 (11), 155 (8), 144 (12), 128 (5), 116 (10), 103 (9), 89 (7), 77 (72), 57 (12), 51 (22).

*1.1.3.3. 6-Ethoxy-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**14**) (Method 2).* To a stirred solution of 6-hydroxy-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**15**) (31.5 mg, 0.1 mmol) in MeCN (1 ml), EtI (32.5 μl, 0.4 mmol) and Hünig's base (137 μl, 0.8 mmol) were added. The mixture was stirred at reflux for 19 h. TLC (*t*-BuOMe) showed the absence of the starting material and the presence of a less polar compound. Dry flash chromatography (*t*-BuOMe) of the residue gave the title compound **14** (24.3 mg, 71%) as red needles, mp 212-214 °C (from PhH), R_f 0.29 (*t*-BuOMe), identical to that described above.

*1.1.3.4. 6-(Isobutylthio)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**16**) (typical procedure).* To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in THF (1 ml), 2-methylpropane-1-thiol (32 μl, 0.3 mmol) and Hünig's base (19 μl, 0.11 mmol) were added. The mixture was stirred at *ca.* 20 °C for 30 min. TLC (*t*-BuOMe) showed the absence of the starting material and the presence of a less polar brown compound. The mixture was diluted with DCM (5 ml)

and adsorbed onto silica gel. Dry flash chromatography (*t*-BuOMe/hexane, 1:2) of the residue gave the *title compound* **16** (35.3 mg, 91%) as brown needles, mp 205-209 ^{o}C (from DCM/MeOH, 1:2); R_f 0.76 (*t*-BuOMe/hexane, 3:1); (found: C, 71.2; H, 5.3; N, 10.7. $C_{23}H_{21}N_3OS$ requires C, 71.3; H, 5.5; N, 10.8%); λ_{max}(DCM)/nm 267 (log ε 3.23), 324 (3.37), 341 inf (3.26), 425 (3.15), 519 inf (2.50), 550 (2.55), 603 inf (2.27); ν_{max}/cm^{-1} 2955w, 2922w, 2855w, 1580s, 1522s, 1508s, 1493m, 1452w, 1429w, 1371w, 1339w, 1314m, 1287w, 1215w, 1198w, 1171w, 1144w, 1069w, 1024w, 1009m, 928w, 847m, 812w; δ_H(300 MHz, $CDCl_3$) 8.29-8.26 (2H, m, Ar *H*), 7.63-7.55 (5H, m, Ar *H*), 7.47-7.45 (3H, m, Ar *H*), 7.36 (1H, s, *H*-5), 6.15 (1H, s, *H*-8), 2.88 (2H, d, *J* 6.5, SCH_2), 2.13 (1H, hept, *J* 6.8, C*H*Me$_2$), 1.16 [6H, d, *J* 6.8, CH(CH_3)$_2$]; δ_C(75 MHz, $CDCl_3$) 177.4 (*C*=O), 160.5 (s), 151.8 (s), 151.5 (s), 141.5 (s), 136.1 (s), 134.5 (s), 130.6 (d), 130.3 (d), 130.1 (d), 128.9 (d), 126.9 (d), 125.9 (d), 119.9 (d), 95.7 (d), 39.9 (S*C*H$_2$), 27.6 (*C*H), 22.6 (2 × *C*H$_3$); *m*/*z* (EI) 387 (M$^+$, 13%), 372 (10), 354 (100), 344 (92), 331 (52), 313 (10), 303 (16), 299 (5), 200 (6), 180 (9), 168 (8), 160 (6), 116 (16), 103 (6), 94 (11), 77 (71), 69 (6), 51 (15).

*1.1.3.5. 6-(Benzylthio)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* ***(17)***. Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) with benzyl-mercaptan (35 μl, 0.3 mmol) and Hünig's base (19 μl, 0.11 mmol) at *ca.* 20 ^{o}C for 20 min gave the *title compound* **17** (34.9 mg, 83%) as brown needles, mp 232-234 ^{o}C (from DCM/MeOH, 1:3); R_f 0.69 (*t*-BuOMe/hexane, 3:1); (found: C, 74.0; H, 4.6; N, 10.1. $C_{26}H_{19}N_3OS$ requires C, 74.1; H, 4.5; N, 10.0%); λ_{max}(DCM)/nm 265 (log ε 3.40), 324 (3.45), 339 (3.36), 420 (3.20), 518 inf (2.60), 555 (2.64), 604 inf (2.38); ν_{max}/cm^{-1} 3028w (Ar CH), 2922w, 2855w, 1580m, 1524s, 1510m, 1493w, 1452w, 1391w, 1371w, 1337w, 1315m, 1285w, 1240w, 1217w, 1204w, 1171w, 1142w, 1069w, 1026w, 1011m, 928w, 851m, 818w, 783w, 774w;

δ_H(300 MHz, $CDCl_3$) 8.29-8.25 (2H, m, Ar *H*), 7.63-7.55 (5H, m, Ar *H*), 7.49-7.46 (6H, m, Ar *H*), 7.39-7.28 (3H, m, Ar *H*), 6.16 (1H, s, *H*-8), 4.26 (2H, s, CH_2Ph); δ_C(75 MHz, $CDCl_3$) 177.3 (*C*=O), 159.4 (s), 151.9 (s), 151.5 (s), 141.4 (s), 136.1 (s), 134.7 (s), 134.4 (s), 130.6 (d), 130.3 (d), 130.1 (d), 129.1 (d), 128.9 (d), 128.8 (d), 127.9 (d), 126.9 (d), 125.8 (d), 120.4 (d), 95.6 (d), 35.9 (S*C*H_2); *m*/*z* (EI) 422 (M^++1, 27%), 421 (M^+, 100), 388 (52), 360 (5), 344 (8), 300 (28), 271 (9), 210 (4), 180 (5), 168 (10), 140 (6), 116 (13), 93 (7), 91 (40), 77 (41), 65 (13), 51 (8).

*1.1.3.6. 1,3-Diphenyl-6-(phenylsulfanyl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**18**)*. To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in EtOH (2 ml), Hünig's base (19 μl, 0.11 mmol) and thiophenol (20 μl, 0.2 mmol) were added and the reaction heated at reflux for 30 min. TLC (*t*-BuOMe/hexane, 3:1) showed the absence of the starting material and the presence of a new brown compound. The mixture was diluted with DCM (15 ml) and then washed with 1 M HCl (10 ml) and 5% aq. $NaHCO_3$ (15 ml). The organics layers were combined, dried (Na_2SO_4), filtered and concentrated *in vacuo*. Dry flash chromatography (*t*-BuOMe) gave the *title compound* **18** (40.7 mg, 100%) as brown plates, mp 299-301 ^oC (from PhH), R_f 0.76 (*t*-BuOMe); (found: C, 73.6; H, 4.2; N, 10.3. $C_{25}H_{17}N_3OS$ requires C, 73.7; H, 4.2; N, 10.3%); λ_{max}(DCM)/nm 262 (log ε 3.13), 326 (3.21), 419 (2.94), 517 inf (2.36), 556 (2.41), 601 inf (2.18); ν_{max}/cm^{-1} 3075w and 3032w (Ar CH), 1584s, 1526s, 1510m, 1491m, 1454w, 1437w, 1395w, 1373m, 1337w, 1314m, 1283w, 1219w, 1196w, 1175w, 1157w, 1142w, 1067w, 1026w, 1001m, 926w, 916w, 862m, 845m, 820m, 775m, 750s, 727w; δ_H(300 MHz; $CDCl_3$) 8.22-8.18 (2H, m, Ar *H*), 7.67-7.56 (10H, m, Ar *H*), 7.45-7.41 (3H, m, Ar *H*), 6.92 (1H, s, *H*-5), 6.20 (1H, s, *H*-8); δ_C(75 MHz; $CDCl_3$) 177.2 (*C*=O), 161.6 (s), 152.1 (s), 151.8 (s), 141.5 (s), 136.3 (s), 135.9 (d), 134.4 (s), 130.6 (d), 130.5 (d),

130.4 (d), 130.4 (d), 130.2 (d), 129.3 (s), 128.9 (d), 127.0 (d), 125.9 (d), 121.3 (d), 95.7 (d); *m*/*z* (EI) 408 (M^++1, 32%), 407 (M^+, 100), 390 (42), 378 (6), 302 (29), 298 (6), 204 (12), 171 (11), 140 (9), 127 (5), 116 (11), 104 (6), 93 (7), 77 (89), 65 (5), 51 (24).

*1.1.3.7. 6-Amino-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**19**)*. To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in DMF (2 ml) at *ca*. 120 ^{o}C, a steady stream of NH_3 (g) was passed through for 6 h. After an additional 6 h at *ca*. 120 ^{o}C TLC (*t*-BuOMe) showed the disappearance of the starting material. The mixture was allowed to cool to *ca*. 20 $^{\circ}$C, diluted with DCM (20 ml) and washed with H_2O (15 ml). The organic layer was separated, dried (Na_2SO_4) and adsorbed onto silica. Dry flash chromatography (*t*-BuOMe) gave the *title compound* **19** (20 mg, 64%) as a light orange needles, mp 279-282 ^{o}C (from PhH); R_f 0.21 (*t*-BuOMe/hexane, 3:1); (found: C, 72.7; H, 4.4; N, 17.9. $C_{19}H_{14}N_4O$ requires C, 72.6; H, 4.5; N, 17.8%); λ_{max}(DCM)/nm 274 (log ε 3.49), 302 inf (3.46), 312 (3.48), 332 inf (3.29), 401 inf (3.25), 417 (3.30), 504 (2.60); ν_{max}/cm^{-1} 3416w (Ar NH), 3283w, 3221br w, 3154br w (Ar CH), 1639w, 1581m, 1566m, 1555s, 1541s, 1491m, 1449w, 1422w, 1391w, 1360w, 1312w, 1292w, 1275w, 1231w, 1190w, 1173w, 1098w, 1067w, 1026w, 1003w, 980w, 916w, 854w, 835w,m, 824m, 812w; δ_H(300 MHz; TFA-d_1) NH peak missing 8.09 (2H, d, *J* 7.6, Ar *H*), 7.78-7.64 (7H, m, Ar *H*), 7.58-7.48 (3H, m, Ar *H*); δ_C(75 MHz; TFA-d_1) 161.8 (*C*=O), 158.9 (s), 154.1 (s), 143.7 (s), 142.0 (s), 141.2 (s), 136.8 (d), 134.9 (d), 131.9 (d), 131.4 (d), 129.5 (d), 127.8 (s), 126.5 (d), 101.8 (d), 99.0 (d); *m*/*z* (EI) 315 (M^++1, 23%), 314 (M^+, 100), 297 (3), 286 (12), 183 (9), 155 (9), 143 (7), 116 (8), 104 (13), 89 (7), 77 (100), 67 (9), 63 (5), 51 (61).

*1.1.3.8. 6-(Ethylamino)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**20**).* To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in $EtNH_2$ 2 M in THF (1 ml, 20 mmol) was added and the mixture was stirred at *ca.* 20 °C for 2 h. The solution was cooled to *ca.* 0 °C and filtered to afford the *title compound* **20** (24.8 mg, 72%) as an orange plates, mp 297-301 °C (from PhH), R_f 0.69 (*t*-BuOMe); (found: C, 73.6; H, 5.4; N, 16.2. $C_{21}H_{18}N_4O$ requires C, 73.7; H, 5.3; N, 16.4%); λ_{max}(DCM)/nm 280 inf (log ε 3.44), 287 (3.46), 301 (3.45), 311 inf (3.41), 336 inf (3.06), 352 inf (2.94), 412 inf (3.29), 430 (3.39); ν_{max}/cm^{-1} 3240br w (NH), 2980w, 2864w, 1562w, 1547s, 1518w, 1489m, 1477m, 1449w, 1383w, 1354w, 1312m, 1298w, 1271w, 1200w, 1171w, 1134w, 1070w, 1051w, 1024w, 989w, 924w, 866w, 843w, 816w, 806w, 779w; δ_H(300 MHz; TFA-d_1) NH peak missing 7.99 (2H, d, *J* 8.0, Ar *H*), 7.70-7.56 (6H, m, Ar *H*), 7.52-7.47 (2H, m, Ar *H*), 7.24 (1H, s, *H*-5 or 8), 6.96 (1H, s, *H*-5 or 8), 3.75 (2H, q, *J* 7.1, NC*H*$_2$), 1.40 (3H, t, *J* 7.1, C*H*$_3$); δ_C(75 MHz; TFA-d_1) 155.8 (*C*=O), 153.4 (s), 144.1 (s), 144.1 (s), 142.0 (s), 141.0 (s), 136.7 (d), 134.7 (d), 132.0 (d), 131.4 (d), 129.4 (d), 127.9 (s), 126.5 (d), 100.9 (d), 95.2 (d), 42.4 (N*C*H$_2$), 13.1 (*C*H$_3$); *m*/*z* (EI) 343 (M$^+$+1, 24%), 342 (M$^+$, 100), 327 (26), 300 (17), 284 (4), 271 (5), 197 (4), 180 (8), 134 (11), 118 (7), 104 (10), 89 (5), 77 (60), 64 (7), 51 (17).

*1.1.3.9. 1,3-Diphenyl-6-(phenylamino)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**21**).* To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in EtOH (1 ml), Hünig's base (19 μl, 0.15 mmol) and aniline (14 μl, 0.15 mmol) were added and the reaction mixture was heated at reflux for 12 h. The reaction mixture was then allowed to cool to *ca.* 20 °C and the precipitate that formed was filtered and washed with cold ethanol to afford the *title compound* **21** (26.2 mg; 67%) as orange plates, mp > 300 °C (from PhH), R_f 0.58 (*t*-BuOMe/hexane, 3:1);

(found: C, 76.7; H, 4.5; N, 14.2. $C_{25}H_{18}N_4O$ requires C, 76.9; H, 4.7; N, 14.4%); λ_{max}(DCM)/nm 253 inf (log ε 2.99), 295 (3.32), 329 inf (3.02), 445 (3.16); ν_{max}/cm^{-1} 3200m (Ar NH), 3051w (Ar CH), 1616w, 1568m, 1549s, 1526m, 1491s, 1456w, 1447m, 1391w, 1379m, 1312m, 1296m, 1279w, 1256w, 1233w, 1200w, 1186w, 1169w, 1138w, 1069w, 1024w, 1005w, 991m, 920w, 876m, 839m, 822m, 791m, 768m, 746m, 710m; δ_H(300 MHz; TFA-d_1) NH peak missing 7.57 (2H, d, *J* 7.8, Ar *H*), 7.31-7.17 (6H, m, Ar *H*), 7.13-7.04 (5H, m, Ar *H*), 7.00-6.96 (3H, m, Ar *H*), 6.61 (1H, s, *H*-5 or 8); δ_C(75 MHz; TFA-d_1) 165.0 (*C*=O), 153.1 (s), 152.8 (s), 144.2 (s), 141.6 (s), 141.0 (s), 135.7 (s), 134.7 (d), 133.4 (d), 131.2 (d), 130.9 (d), 130.5 (d), 129.7 (s), 129.3 (d), 128.9 (d), 126.3 (d), 125.1 (d), 99.5 (d), 97.2 (d); *m*/*z* (EI) 391 (M^++1, 30%), 390 (M^+, 100), 373 (14), 361 (2), 313 (4), 298 (2), 286 (23), 258 (4), 195 (8), 180 (6), 155 (7), 143 (4), 128 (4), 116 (6), 104 (6), 89 (4), 77 (51), 51 (16).

*1.1.3.10. 6-(4-Phenylpiperazin-1-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**22**)*. To a stirred mixture of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in THF (0.5 ml), at *ca.* 20 °C and protected with $CaCl_2$ drying tube, 4-phenylpiperazine (30.5 μl, 0.2 mmol) was added and the reaction mixture was stirred at *ca.* 20 °C for 9 h until no starting material remained (TLC). The reaction mixture was then diluted (DCM, 15 ml) and washed (5% HCl, 10 ml) to remove unreacted amine. The organic layer separated, dried (Na_2SO_4) and adsorbed onto silica. Dry flash chromatography (*t*-BuOMe/hexane/DCM, 1:2:7) gave the *title compound **22*** (41.8 mg, 91%) as red needles, mp 280-282 °C (from PhH); R_f 0.50 (*t*-BuOMe/hexane, 1:1); (found: C, 75.6; H, 5.4; N, 15.3. $C_{29}H_{25}N_5O$ requires C 75.8, H 5.5, N 15.2%); λ_{max}(DCM)/nm 255 (log ε 3.47), 277 (3.51), 299 (3.57), 318 inf (3.49), 339 inf (3.17), 358 inf (3.02), 453 (3.45); ν_{max}/cm^{-1} 3067w, 3022w (Ar CH), 2972w, 2837w, 1593m, 1535s, 1506m, 1495m, 1452m, 1441m, 1429w, 1395w, 1377m,

1346w, 1315m, 1296m, 1287m, 1229s, 1211m, 1180w, 1152m, 1090w, 1069w, 1051w, 1028m, 1003w, 991w, 932m, 891m, 847m, 835m, 818m, 783w, 773m, 750m, 737w; δ_H(300 MHz; $CDCl_3$) 8.30-8.27 (2H, m, Ar *H*), 7.63-7.55 (5H, m, Ar *H*), 7.50-7.45 (3H, m, Ar *H*), 7.36-7.28 (2H, m, Ar *H*), 6.97-6.88 (4H, m, Ar *H*), 6.11 (1H, s, Ar *H*), 4.09 (4H, br t, *J* 5.1, NCH_2), 3.41 (4H, br t, *J* 5.2, NCH_2); δ_C(75 MHz; $CDCl_3$) 177.3 (*C*=O), 155.8 (s), 153.3 (s), 152.0 (s), 150.8 (s), 141.8 (s), 135.4 (s), 135.0 (s), 130.2 (d), 130.0 (d), 129.9 (d), 129.5 (d), 128.8 (d), 127.0 (d), 126.0 (d), 120.3 (d), 116.2 (d), 105.6 (d), 97.8 (d), 49.1 (*C*H_2), 48.7 (*C*H_2); *m/z* (EI) 459 (M^+, 9%), 340 (22), 327 (16), 314 (21), 299 (3), 229 (5), 180 (3), 168 (2), 144 (4), 132 (100), 117 (4), 104 (32), 91 (7), 77 (31), 51 (5).

*1.1.3.11. 6-(*N-*Methyl*-N-*phenylamino)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**23**)*. Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) and *N*-methylaniline (0.4 ml, 3.69 mmol) heated to *ca.* 80 °C for 3 d gave the *title compound* **23** (37.7 mg, 93%) as red cubes, mp 238-240 °C (from EtOH); R_f 0.32 (*t*-BuOMe/hexane, 1:1); (found: C, 77.1; H, 5.1; N, 13.8. $C_{26}H_{20}N_4O$ requires C, 77.2; H, 5.0; N, 13.9%); λ_{max}(DCM)/nm 299 (log ε 3.52), 339 inf (3.16), 360 inf (2.97), 451 (3.37); ν_{max}/cm^{-1} 3059w (Ar CH), 2928w, 1597w, 1585m, 1524s, 1491m, 1450m, 1389w, 1356m, 1314m, 1294m, 1252w, 1188w, 1169w, 1146w, 1109w, 1070w, 1024w, 1001w, 982m, 924w, 862m, 843w, 831w, 816w, 777m; δ_H(300 MHz; $CDCl_3$) 8.26-8.23 (2H, m, Ar *H*), 7.62-7.53 (5H, m, Ar *H*), 7.45-7.40 (5H, m, Ar *H*), 7.32-7.27 (1H, m, Ar *H*), 7.23-7.20 (2H, m, Ar *H*), 6.75 (1H, s, *H*-5 or 8), 6.05 (1H, s, *H*-5 or 8), 3.73 (3H, s, CH_3); δ_C(75 MHz; $CDCl_3$) one Ar CH missing 176.7 (*C*=O), 154.9 (s), 153.1 (s), 151.8 (s), 148.0 (s), 141.9 (s), 135.5 (s), 135.0 (s), 130.0 (d), 129.9 (d), 129.8 (d), 128.7 (d), 126.9 (d), 126.7 (d), 126.0 (d), 125.4 (d), 106.6 (d), 97.5 (d), 43.7 (*C*H_3); *m/z* (EI) 405 (M^++1, 33%), 404 (M^+, 100), 390 (8),

327 (10), 312 (4), 300 (11), 271 (3), 202 (14), 196 (10), 180 (5), 168 (8), 155 (3), 140 (4), 128 (3), 116 (6), 104 (11), 91 (9), 77 (64), 65 (4), 51 (16).

*1.1.3.12. 6-(*N-*Cyclohexyl*-N-*methylamino)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1H)-one (**24**)*. Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) with *N*-methylcyclohexylamine (0.4 ml, 3.03 mmol) at *ca.* 20 ^{o}C for 20 h gave the *title compound* **24** (35.5 mg, 87%) as orange needles, mp 162-165 ^{o}C (from pentane); R_f 0.47 (*t*-BuOMe/hexane, 1:1); (found: C, 76.0; H, 6.3; N, 13.6. $C_{26}H_{26}N_4O$ requires C, 76.1; H, 6.4; N, 13.7%); λ_{max}(DCM)/nm 278 inf (log ε 3.58), 299 (3.63), 321 inf (3.46), 339 inf (3.08), 366 inf (2.89), 456 (3.52); ν_{max}/cm^{-1} 3055w (Ar CH), 2926w, 2853w, 1591m, 1533s, 1493m, 1449m, 1406w, 1393w, 1366w, 1344w, 1315m, 1296m, 1248w, 1207w, 1179w, 1150w, 1121w, 1088w, 1026w, 1003w, 991w, 928w, 887w, 856w, 841w, 831m, 820m, 772m; δ_H(300 MHz; $CDCl_3$) 8.28-8.25 (2H, m, Ar *H*), 7.59-7.52 (5H, m, Ar *H*), 7.48-7.41 (3H, m, Ar *H*), 6.72 (1H, s, Ar *H*), 6.03 (1H, s, Ar *H*), 4.78 (1H, br s, NC*H*), 3.15 (3H, s, NCH_3), 1.93-1.83 (4H, m, CH_2), 1.73-1.35 (6H, m, CH_2); δ_C(75 MHz; $CDCl_3$) 177.6 (*C*=O), 155.9 (s), 152.8 (s), 152.1 (s), 142.0 (s), 135.8 (s), 134.9 (s), 129.9 (d), 129.8 (d), 129.7 (d), 128.6 (d), 126.9 (d), 126.1 (d), 103.0 (d), 97.6 (d), 59.8 (*C*H) 34.1 (*C*H_3), 30.7 (*C*H_2), 25.8 (*C*H_2), 25.8 (*C*H_2); *m/z* (EI) 411 (M^++1, 32%), 410 (M^+, 94), 395 (100), 327 (62), 315 (5), 300 (5), 205 (9), 180 (10), 132 (5), 112 (5), 104 (6), 91 (6), 77 (49), 55 (19).

*1.1.3.13. 1,3-Diphenyl-6-(piperidin-1-yl)benzo[e][1,2,4]triazin-7(1H)-one (**25**)*. Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) with piperidine (0.4 ml, 4.05 mmol) at *ca.* 20 ^{o}C for 10 min gave the *title compound* **25** (37.7 mg, 99%) as orange needles, mp 183-185 ^{o}C (from cyclohexane), R_f 0.29 (*t*-BuOMe/hexane, 1:1); (found: C, 75.2; H, 5.7; N, 14.6. $C_{24}H_{22}N_4O$ requires

C, 75.4; H, 5.8; N, 14.7%); λ_{max}(DCM)/nm 278 (log ε 3.55), 302 (3.61), 319 inf (3.51), 338 inf (3.17), 364 inf (2.95), 458 (3.53); ν_{max}/cm^{-1} 3053w (Ar CH), 2926w (Ar CH), 2853w (Ar CH), 1584m, 1537s, 1493m, 1449m, 1406w, 1395w, 1371w, 1346w, 1314m, 1292m, 1238m, 1221w, 1190w, 1171w, 1096m, 1069w, 1024w, 1003w, 991w, 901s, 824m, 773m, 745m; δ_H(300 MHz; $CDCl_3$) 8.28-8.25 (2H, m, Ar *H*), 7.62-7.51 (5H, m, Ar *H*), 7.48-7.43 (3H, m, Ar *H*), 6.87 (1H, s, *H*-5), 6.06 (1H, s, *H*-8), 3.90-3.87 (4H, m, C*H*$_2$N), 1.79-1.75 (6H, m, C*H*$_2$); δ_C(75 MHz; $CDCl_3$) 177.4 (*C*=O), 156.2 (s), 153.0 (s), 152.0 (s), 142.0 (s), 135.7 (s), 134.9 (s), 130.0 (d), 129.9 (d), 129.8 (d), 128.7 (d), 126.9 (d), 126.1 (d), 104.8 (d), 97.7 (d), 50.7 (*C*H$_2$N), 26.4 (*C*H$_2$), 24.6 (*C*H$_2$); *m/z* (EI) 383 (M$^+$+1, 27%), 382 (M$^+$, 100), 353 (6), 339 (9), 326 (7), 314 (12), 299 (18), 271 (8), 191 (6), 174 (5), 168 (8), 140 (4), 104 (6), 77 (41), 63 (4), 51 (9).

Alternatively, to a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]-triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in THF (1 ml) at *ca.* 20 ^{o}C, piperidine (20.0 μl, 0.2 mmol) was added. After 3 h no starting material remained (TLC). Dry flash chromatography (*t*-BuOMe/hexane/DCM, 1:2:7) gave the *title compound* **25** (35.3 mg, 93%) as orange needles, mp 183-185 ^{o}C (from cyclohexane), identical to that describe above.

*1.1.3.14. 6-[3,4-Dihydroisoquinolin-2(1H)-yl]-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**26**).* Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) with 1,2,3,4-tetrahydroisoquinoline (0.6 ml, 4.79 mmol) heated to *ca.* 50 ^{o}C for 30 min gave the *title compound* **26** (34.9 mg, 81%) as orange plates, mp 197-199 ^{o}C (from cyclohexane); R_f 0.38 (*t*-BuOMe/hexane, 1:1); (found: C, 78.1; H, 5.0; N, 13.0. $C_{28}H_{22}N_4O$ requires C, 78.1; H, 5.1; N, 13.0%); λ_{max}(DCM)/nm 278 inf (log ε 3.47), 299 (3.54), 344 inf (3.11), 363 inf (2.96), 435 inf (3.38), 455 (3.43); ν_{max}/cm^{-1} 3057w, 3030w (Ar CH), 2903w, 2874w, 2839w, 1595m, 1584m, 1537s,

1493m, 1449m, 1439m, 1395w, 1373m, 1314m, 1294m, 1236m, 1198w, 1186m, 1148w, 1111w, 1070w, 1055w, 1026w, 1003w, 993w, 912m, 849w, 818m, 773m; δ_H(300 MHz; $CDCl_3$) 8.29-8.26 (2H, m, Ar *H*), 7.62-7.51 (5H, m, Ar *H*), 7.49-7.44 (3H, m, Ar *H*), 7.25-7.17 (4H, m, Ar *H*), 6.88 (1H, s, *H*-5 or 8), 6.08 (1H, s, *H*-5 or 8), 5.05 (2H, s, C*H*$_2$N), 4.15 (2H, dd, *J* 5.7, 5.7, C*H*$_2$N), 3.10 (2H, dd, *J* 5.7, 5.7 C*H*$_2$); δ_C(75 MHz, $CDCl_3$) one Ar *C*H missing 177.4 (*C*=O), 155.1 (s), 153.1 (s), 152.1 (s), 141.9 (s), 135.6 (s), 135.1 (s), 135.0 (s), 133.6 (s), 130.1 (d), 129.9 (d), 129.8 (d), 128.7 (d), 128.5 (d), 127.1 (d), 127.0 (d), 126.6 (d), 126.1 (d), 103.7 (d), 97.6 (d), 51.2 (*C*H$_2$N), 47.3 (*C*H$_2$N), 29.1 (*C*H$_2$); *m/z* (EI) 431 (M^++1, 34%), 430 (M^+, 100), 413 (4), 325 (15), 314 (30), 301 (21), 286 (6), 271 (6), 222 (12), 215 (10), 197 (7), 180 (5), 168 (9), 140 (6), 129 (13), 115 (22), 104 (13), 91 (11), 77 (58), 63 (8), 51 (17).

*1.1.3.15. 6-(4-Methylpiperazin-1-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**27**)*. Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) with 1-methylpiperazine (0.5 ml, 4.51 mmol) heated to *ca*. 50 ^oC for 15 min gave the *title compound* **27** (33.4 mg, 84%) as red needles, mp 198-199 ^oC (from EtOH); R_f 0.29 (*t*-BuOMe/MeOH, 5:1); (found: C, 72.6; H, 5.9; N, 17.5. $C_{24}H_{23}N_5O$ requires C, 72.5; H, 5.8; N, 17.6%); λ_{max}(DCM)/nm 277 (log ε 3.36), 294 (3.35), 308 (3.38), 319 (3.39), 335 inf (3.22), 437 (3.25), 543 inf (2.47); ν_{max}/cm^{-1} 3065w (Ar CH), 2953w, 1591m, 1537s, 1497m, 1477w, 1452m, 1433w, 1385w, 1364w, 1315m, 1294m, 1285m, 1250m, 1229w, 1213w, 1188w, 1161w, 1144w, 1090w, 1072w, 1059w, 1026w, 1020w, 1003w, 978m, 922w, 901m, 851m, 826m, 781w, 773m, 750m; δ_H(300 MHz; $CDCl_3$) 8.27 (2H, dd, *J* 6.6, 3.0, Ar *H*), 7.65-7.55 (5H, m, Ar *H*), 7.47-7.45 (3H, m, Ar *H*), 6.94 (1H, s, *H*-5 or 8), 6.22 (1H, s, *H*-5 or 8), 4.56 (2H, d, *J* 13.5, C*H*$_2$), 3.84 (2H, dd, *J* 12.3. 12.6, C*H*$_2$), 3.61 (2H, d, *J* 11.7, C*H*$_2$), 3.21-3.12 (2H, m, C*H*$_2$), 2.87 (3H, d, *J* 3.9, C*H*$_3$); δ_C(75 MHz; $CDCl_3$) 176.6 (*C*=O), 155.4 (s), 153.5

(s), 152.0 (s), 141.5 (s), 135.0 (s), 134.6 (s), 130.5 (d), 130.2 (d), 130.0 (d), 128.8 (d), 126.9 (d), 125.8 (d), 108.4 (d), 97.7 (d), 53.6 (N*C*H_2), 45.4 (N*C*H_2), 43.7 (N*C*H_3); *m/z* (EI), 397 (M^+, 14%), 340 (10), 327 (21), 314 (12), 299 (4), 180 (3), 168 (2), 140 (2), 116 (2), 103 (2), 77 (16), 70 (100), 51 (4).

*1.1.3.16. 1,3,6-Triphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**28**) (typical procedure).* To a stirred solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in dry THF (0.6 ml) at *ca.* 20 ^oC undrer an Ar atmosphere, PhMgBr 1 M in THF (0.4 ml, 0.4 mmol) was added and the mixture was stirred for 12 h. TLC (*t*-BuOMe/hexane, 3:1) showed the absence of the starting material and the presence of a new less polar purple product. The mixture was diluted with MeOH (1 ml) and stirred during 10 min. Dry flash chromatography (*t*-BuOMe) gave the *title compound* **28** (30.8 mg, 82%) as purple needles, mp 262-265 ^oC (from DCM/MeOH, 1:3), R_f 0.60 (*t*-BuOMe/hexane, 3:1); (found: C, 79.9; H, 4.4; N, 11.1. $C_{25}H_{17}N_3O$ requires C, 80.0; H, 4.6; N, 11.2%); λ_{max}(DCM)/nm 253 (log ε 3.39), 272 inf (3.32), 327 (3.56), 405 inf (2.73), 568 (2.72), 617 inf (2.54); ν_{max}/cm^{-1} 3061w (Ar CH), 1611w, 1601w, 1585m, 1541s, 1520s, 1489m, 1456w, 1439w, 1396w, 1373w, 1344w, 1314m, 1281w, 1267w, 1202m, 1179w, 1169w, 1157w, 1136w, 1078w, 1067w, 1028w, 1001w, 989w, 930w, 916w, 905w, 849m, 839m, 829m, 785m, 777m, 762s; δ_H(300 MHz; $CDCl_3$) 8.30-8.27 (2H, m, Ar *H*), 7.84 (1H, s, *H*-5 or 8), 7.78-7.75 (2H, m, Ar *H*), 7.63-7.57 (5H, m, Ar *H*), 7.48-7.47 (6H, m, Ar *H*), 6.23 (1H, s, *H*-5 or 8); δ_C(75 MHz; $CDCl_3$) 180.7 (*C*=O), 155.1 (s), 151.6 (s), 151.1 (s), 141.3 (s), 136.1 (s), 135.7 (s), 134.2 (s), 130.6 (d), 130.2 (d), 130.2 (d), 129.8 (d), 129.7 (d), 128.9 (d), 128.4 (d), 126.8 (d), 125.8 (d), 98.4 (d); *m*/*z* (EI) 376 (M^++1, 19%), 375 (M^+, 72), 374 (M^+-1, 100), 347 (4), 270 (9), 243 (8), 188 (4), 166 (7), 139 (14), 103 (3), 89 (7), 77 (42), 63 (4), 51 (13).

*1.1.3.17. 1,3-Diphenyl-6-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**29**).* Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) with (thien-2-yl)MgBr 1 M in THF (0.4 ml, 0.4 mmol) at *ca.* 20 ^{o}C in Ar atmosphere for 18 h gave the *title compound* **29** (24.1 mg, 63%) as a brown needles, mp 264-268 ^{o}C (from DCM/MeOH, 1:3), R_f 0.86 (*t*-BuOMe/hexane, 3:1); (found: C, 72.4; H, 3.9; N, 10.9. $C_{23}H_{15}N_3OS$ requires C, 72.4; H, 4.0; N, 11.0%); λ_{max}(DCM)/nm 294 (log ε 3.27), 329 (3.20), 455 (3.07), 561 inf (2.43), 596 (2.44), 647 inf (2.19); ν_{max}/cm^{-1} 3067w (Ar CH), 1585m, 1533s, 1516m, 1493s, 1454w, 1406m, 1391w, 1360w, 1333w, 1315m, 1285m, 1263w, 1229w, 1200w, 1175w, 1157w, 1136w, 1090w, 1078w, 1067w, 1045w, 1024w, 1001w, 988m, 972w, 920w, 880m, 858w, 851w, 835m, 814w; δ_H(500 MHz; $CDCl_3$) 8.34-8.31 (2H, m, Ar *H*), 8.18 (1H, s, Ar *H*), 8.08 (1H, d, *J* 3.8, Ar *H*), 7.71 (1H, d, *J* 5.0, Ar *H*), 7.67-7.59 (5H, m, Ar *H*), 7.53-7.49 (3H, m, Ar *H*), 7.22-7.20 (1H, m, Ar *H*), 6.39 (1H, s, Ar *H*); δ_C(75 MHz; $CDCl_3$) 179.3 (*C*=O), 153.9 (s), 151.6 (s), 143.1 (s), 141.4 (s), 136.2 (s), 135.8 (s), 134.6 (d), 134.4 (s), 130.6 (d), 130.3 (d), 130.2 (d), 129.8 (d), 128.9 (d), 127.2 (d), 126.9 (d), 125.8 (d), 123.4 (d), 97.7 (d); *m*/*z* (EI) 382 (M^++1, 28%), 381 (M^+, 100), 364 (3), 353 (52), 320 (5), 250 (15), 235 (3), 221 (6), 205 (3), 191 (6), 186 (7), 173 (5), 145 (12), 116 (4), 108 (3), 101 (5), 89 (6), 77 (61), 69 (7), 51 (19).

1.1.4. Halogenation at C-8 using NXS

*1.1.4.1. 8-Chloro-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**30**) (typical procedure).* To a solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in dry DCM (2 ml), NCS (15 mg, 0.11 mmol) was added. The mixture was stirred at *ca.* 20 ^{o}C for 12 h or until all the starting material was consumed. The reaction mixture was then adsorbed onto silica using DCM. Dry flash chromatography (*t*-BuOMe) of the residue gave the *title compound* **30** (33 mg, 99%) as shiny blue

crystals, mp 187-189 ^{o}C (from cyclohexane); R_f 0.80 (*t*-BuOMe/hexane, 3:1); (found: C, 68.3; H, 3.7; N, 12.5. $C_{19}H_{12}ClN_3O$ requires C, 68.4; H, 3.6; N, 12.6%); λ_{max}(DCM)/nm 241 (log ε 3.07), 301 (3.30), 313 inf (3.26), 358 (2.96), 568 (2.55); ν_{max}/cm^{-1} 3054w (Ar CH), 1615m, 1605m, 1536w, 1517s, 1490w, 1455w, 1430w, 1389w, 1376w, 1312w, 1198w, 1175w, 1137w, 1108m, 1088w, 1073w, 1027w, 1000w, 946w, 921w, 903w, 840m, 811w, 799w; δ_H(300 MHz, $CDCl_3$) 8.29-8.26 (2H, m, Ar *H*), 7.77 (1H, d, *J* 9.7, Ar *H*), 7.54-7.47 (9H, m, Ar *H*); δ_C(75 MHz, $CDCl_3$) 176.2 (*C*=O), 154.8 (s), 150.8 (s), 143.3 (s), 140.5 (d), 133.0 (s), 131.8 (s), 131.8 (d), 130.9 (d), 129.3 (d), 128.8 (d), 126.7 (d), 125.3 (d), 105.4 (*C*-8); *m*/*z* (EI) 335 (M^++2, 24%), 333 (M^+, 54), 298 (100), 270 (6), 167 (12), 139 (16), 114 (4), 104 (6), 97 (24), 77 (70), 62 (10), 51 (27).

*1.1.4.2. 8-Bromo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**31**).* Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) with NBS (89 mg, 0.5 mmol) at *ca.* 20 ^{o}C for 12 h gave the *title compound* **31** (38 mg, 100%) as dark blue shiny needles, mp 180-183 ^{o}C (from cyclohexane), R_f 0.75 (*t*-BuOMe/hexane, 3:1); (found: C, 60.3; H, 3.1; N, 11.1. $C_{19}H_{12}BrN_3O$ requires C, 60.3; H, 3.2; N, 11.1%); λ_{max}(DCM)/nm 244 (log ε 3.19), 301 (3.37), 317 inf (3.32), 358 (3.12), 571 (2.68); ν_{max}/cm^{-1} 3052w (Ar CH), 1602m, 1558w, 1533w, 1509s, 1487m, 1455w, 1426w, 1386w, 1371w, 1322w, 1309w, 1243w, 1226w, 1195m, 1172w, 1156w, 1133m, 1102m, 1086w, 1072w, 1023w, 985m, 940w, 925w, 915w, 877w, 836m, 790m; δ_H(300 MHz, $CDCl_3$) 8.30-8.26 (2H, m, Ar *H*), 7.77 (1H, d, *J* 9.6, Ar *H*), 7.54-7.48 (9H, m, Ar *H*); δ_C(75 MHz, $CDCl_3$) 176.4 (*C*=O), 154.8 (s), 150.7 (s), 143.0 (s), 140.1 (d), 134.1 (s), 133.0 (s), 131.9 (d), 130.9 (d), 129.3 (d), 128.9 (d), 128.8 (d), 126.7 (d), 125.7 (d), 96.7 (*C*-8); *m*/*z* (EI) 379 (M^++2, 19%), 377

(M^+, 18), 298 (100), 270 (6), 242 (2), 193 (3), 167 (11), 139 (23), 114 (5), 103 (7), 89 (7), 77 (65), 62 (13), 51 (29).

*1.1.4.3. 8-Iodo-1,3-diphenylbenzo[e][1,2,4]triazin-7(1H)-one (**32**).* Similar treatment of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) with NIS (112 mg, 0.5 mmol) at *ca.* 20 ^oC for 12 h gave the *title compound* **32** (42.3 mg, 100%) as shiny dark blue needles, mp 200-203 ^oC (from cyclohexane), R_f 0.75 (*t*-BuOMe/hexane, 3:1); (found: C, 53.7; H, 2.7; N, 9.7. $C_{19}H_{12}IN_3O$ requires C, 53.7; H, 2.8; N, 9.9%); λ_{max}(DCM)/nm 239 (log ε 3.03), 252 (3.04), 298 (3.17), 362 (2.94), 575 (2.45); ν_{max}/cm^{-1} 3049w (Ar CH), 1614m, 1591s, 1537w, 1479s, 1460m, 1433m, 1391w, 1375m, 1327m, 1308m, 1277m, 1198w, 1177w, 1165w, 1136m, 1111m, 1086w, 1076w, 1022w, 1001w, 980m, 939w, 860w, 827m, 791m, 775m, 727w; δ_H(300 MHz, $CDCl_3$) 8.30-8.26 (2H, m, Ar *H*), 7.73 (1H, d, *J* 9.6, Ar *H*), 7.60-7.43 (9H, m, Ar *H*); δ_C(75 MHz, $CDCl_3$) 178.2 (*C*=O), 155.0 (s), 150.6 (s), 142.1 (s), 138.5 (d), 138.3 (s), 133.0 (s), 132.2 (d), 130.9 (d), 129.4 (d), 129.2 (d), 128.8 (d), 126.8 (d), 126.6 (d), 75.5 (*C*-8); *m*/*z* (EI) 426 (M^++1, 7%), 425 (M^+, 30), 298 (100), 270 (6), 243 (2), 189 (9), 167 (11), 153 (6), 140 (25), 114 (7), 103 (6), 89 (8), 77 (64), 62 (12), 51 (27).

*1.1.4.4. 8-Iodo-1,3,6-triphenylbenzo[e][1,2,4]triazin-7(1H)-one (**33**).* Similar treatment of 1,3,6-triphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**28**) (37.5 mg, 0.1 mmol) with NIS (44.8 mg, 0.2 mmol) at *ca.* 20 ^oC during 12 h gave the *title compound* **33** (38.1 mg, 76%) as shiny dark blue needles, mp 96-101 ^oC (DCM/MeOH, 1:3), R_f 0.43 (*t*-BuOMe/hexane, 1:4); (found: C, 59.8; H, 3.2; N, 8.3. $C_{25}H_{16}IN_3O$ requires C, 59.9 H, 3.2; N, 8.4%); λ_{max}(DCM)/nm 257 (log ε 3.52), 346 (3.51), 402 inf (2.88), 588 (2.72); ν_{max}/cm^{-1} 3055w (Ar CH), 2924w, 2851w, 1730w, 1601m, 1591m, 1537w, 1504m, 1485s, 1454m, 1422w, 1371w, 1329w, 1312m,

1279w, 1219m, 1167m, 1130w, 1084w, 1070w, 1026w, 1003w, 995w, 949w, 887w, 837w, 789m, 770m, 762m; δ_H(300 MHz, $CDCl_3$) 8.31-8.28 (2H, m, Ar *H*), 7.86-7.85 (1H, m, Ar *H*), 7.81-7.78 (2H, m, Ar *H*), 7.58-7.53 (11H, m, Ar *H*); δ_C(75 MHz, $CDCl_3$) 176.8 (*C*=O), 155.4 (s), 150.9 (s), 148.3 (s), 142.3 (s), 138.1 (s), 135.7 (s), 133.5 (s), 130.9 (d), 130.0 (d), 129.9 (d), 129.6 (d), 129.5 (d), 129.4 (d), 129.0 (d), 128.4 (d), 127.0 (d), 126.9 (d), 76.9 (*C*-8); *m*/*z* (EI) 502 (M^++1, 9%), 501 (M^+, 28), 374 (100), 346 (6), 265 (4), 251 (3), 242 (25), 229 (12), 216 (15), 189 (6), 166 (11), 140 (26), 113 (9), 103 (7), 89 (7), 77 (76), 63 (8), 51 (29).

*1.1.4.5. 8-Iodo-1,3-diphenyl-6-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**34**).* Similar treatment of 1,3-diphenyl-6-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**29**) (37.5 mg, 0.1 mmol) with NIS (44.8 mg, 0.2 mmol) at *ca.* 20 ^oC for 12 h gave the *title compound* **34** (34 mg, 67%) as green needles, mp 230-294 ^oC (DCM/MeOH, 1:4), R_f 0.46 (*t*-BuOMe/hexane, 1:4); (found: C, 54.4; H, 2.6; N, 8.2. $C_{23}H_{14}IN_3OS$ requires C, 54.5 H, 2.8; N, 8.3%); λ_{max}(DCM)/nm 296 (log ε 3.36), 362 (3.33), 458 (3.19), 602 (2.54); ν_{max}/cm^{-1} 3069w, 1585m, 1557w, 1528w, 1504m, 1479s, 1454m, 1427m, 1406w, 1369m, 1312m, 1281w, 1242m, 1202w, 1161w, 1132w, 1090w, 1074w, 1047w, 1026w, 1003w, 991w, 939w, 922w, 874m, 849w, 841w, 831w, 826w, 777w; δ_H(500 MHz, $CDCl_3$) 8.33-8.31 (2H, m, Ar H), 8.16 (1H, s, Ar H), 8.06 (1H, dd, *J* 0.9, 3.9, Ar H), 7.73 (1H, dd, *J* 1.0, 5.1, Ar H), 7.59-7.50 (8H, m, Ar H), 7.23 (1H, s, *J* 5.1, 4.2, Ar H); δ_C(125 MHz, $CDCl_3$) one Ar CH missing 176.1 (s), 154.5 (s), 151.4 (s), 142.4 (s), 140.0 (s), 137.9 (s), 136.7 (s), 134.8 (d), 133.8 (s), 131.0 (d), 130.0 (d), 129.7 (d), 129.4 (d), 129.0 (d), 127.4 (d), 127.1 (d), 123.3 (d), 75.1 (s); *m*/*z* (EI) 508 (M^++1, 14%), 506 (M^+, 39), 380 (100), 335 (10), 313 (5), 285 (5), 248 (15), 235 (10), 222 (15), 207 (5), 169 (18), 147 (15), 134 (6), 119 (9), 114 (7), 100 (7), 77 (43), 69 (17), 51 (14).

*1.1.4.6. 8-Bromo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**31**) via bromination using Br_2.* To a solution of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) (30 mg, 0.1 mmol) in dry DCM (1.5 ml), Br_2 (11 μl, 0.2 mmol) was added. The mixture was stirred at *ca.* 20 °C for 0.5 h. Then the DCM was evaporated and the solid residue was dissolved in MeOH (1 ml) and then precipitated by adding excess of water. The precipitate was filtered and dried giving the *title compound* **31** (37.6 mg, 100%) as dark blue shiny needles, mp 180-183 °C (from cyclohexane), identical to that described above.

1.1.5. Reaction of 8-halobenzotriazinones with nucleophiles

1.1.5.1. *8-Bromo-1,3-diphenyl-6-(pyrrolidin-1-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**35**).* To a stirred solution of 8-bromo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**31**) (37.8 mg, 0.100 mmol) in DCM (2 ml), at *ca.* 20 °C, protected with a $CaCl_2$ drying tube, pyrrolidine (18.2 μl, 0.200 mmol) was added and the reaction mixture was stirred at this temperature for 36 hours until no starting material remained (TLC). The reaction mixture was then diluted (DCM) and washed (5% HCl) to remove unreacted amine. The organic layer was separated, dried (Na_2SO_4) and evaporated to afford the *title compound* **35** (33.1 mg, 74%) as red crystals, mp 254-255 °C (from cyclohexane); (Found C, 61.9; H, 4.2 N, 12.6. $C_{23}H_{19}BrN_4O$ requires C, 61.8; H, 4.3; N, 12.5%); λ_{max}(DCM)/nm 283 inf (log ε 3.53), 307 (3.69), 327 inf (3.53), 354 inf (3.10), 368 inf (3.02), 440 inf (3.49), 459 (3.60); ν_{max}/cm^{-1} 2968w, 2924w (Ar CH), 2878w (Ar CH), 2849w, 1609m, 1584m (Ar C-C), 1564s, 1531s, 1495m, 1468m, 1454m, 1443w, 1404m, 1371m, 1302s, 1290m, 1256w, 1225w, 1200w, 1171w, 1157w, 1119w, 1107w, 1092w, 1069w, 1026w, 993w, 937m, 922w, 905w, 883w, 856w, 843w, 816m, 782w, 768m; δ_H(300 MHz; $CDCl_3$) 8.27-8.24 (2H, m, Ph C*H*), 7.50-7.42 (8H, m, Ph C*H*), 6.57 (1H, s, Ph C*H*), 4.335 (2H, s, CH_2), 3.533 (2H, s,

C*H*$_2$), 2.00 (4H, s, C*H*$_2$); δ_C(75 MHz; $CDCl_3$) 172.0 (*C*=O), 153.1, 152.05, 150.6, 144.2, 135.2, 133.8, 130.5 (d), 129.25 (d), 129.2 (d), 128.9 (d), 127.4 (d), 126.8, 100.15, 27.3 (*C*H_2); m/z (EI) 448 (M^++1, 55), 447 (M^+, 14), 446 (M^++1, 57), 393 (4), 367 (M^++Br, 4), 339 (M^+-C_2H_4Br, 20), 298 (M^+-C_4H_8NBr, 4), 238 (13), 180 (7), 167 (5), 152 (5), 140 (7), 116 (7), 103 (12), 91 (13), 77 (100), 70 (12).

*1.1.5.2. 8-Iodo-1,3,6-triphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**33**) (typical procedure)*. To a stirred solution of 8-iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**) (42.5 mg, 0.1 mmol) in dry THF (0.6 ml) at *ca.* 20 ^oC in Ar atmosphere, PhMgBr 1 M in THF (0.4 ml, 0.4 mmol) was added and the mixture was stirred for 18 h. TLC (*t*-BuOMe/hexane, 1:1) showed the absence of the starting material and the presence of a new less polar blue product. The mixture was diluted with MeOH (1 ml), stirred for 10 min, adsorbed onto silica gel and dry flash chromatography (EtOAc/hexane, 1:2) gave the *title compound* **33** (11 mg, 22%) as a blue needles, mp 96-101 ^oC (DCM/MeOH, 1:3), R_f 0.43 (*t*-BuOMe/hexane, 1:4), identical to that describe above.

*1.1.5.3. 8-Iodo-1,3-diphenyl-6-(thien-2-yl)benzo[e][1,2,4]triazin-7(1*H*)-one (**34**)*. Similar treatment of 8-iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**) (42.5 mg, 0.1 mmol) with (thien-2-yl)MgBr 1 M in THF (0.4 ml, 0.4 mmol) gave the *title compound* (**34**) (25.0 mg, 49%) as a green needles, mp 230-294 ^oC (DCM/MeOH, 1:4), R_f 0.46 (*t*-BuOMe/hexane, 1:4), identical to that describe above.

1.1.6. C-C coupling reactions

1.1.6.1. Suzuki Coupling at C-8

*1.1.6.1.1. 1,3,8-Triphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**36**) (typical procedure).* To a stirred solution of 8-iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**) (42.5 mg, 0.1 mmol) in dioxane/water 3:1 (0.8 ml), Pd(dppf)Cl_2·DCM (8 mg, 0.01 mmol), K_2CO_3 (27.6 mg, 0.2 mmol) and phenylboronic acid (24.4 mg, 0.2 mmol) were added and the mixture was heated at reflux for 2.5 h. TLC (*t*-BuOMe/hexane, 1:1), showed the absence of the starting material and the presence of a new slightly more polar blue product. The mixture was dried (Na_2SO_4) filtered, adsorbed onto silica gel and dry flash chromatography (*t*-BuOMe/hexane, 1:2) gave the *title compound* **36** (29.4 mg, 78%) as shiny blue needles, mp 219-222 ^oC (from DCM/MeOH 1:1); R_f 0.70 (*t*-BuOMe/hexane 3:1); (found: C, 80.1; H, 4.5; N, 11.1. $C_{25}H_{17}N_3O$ requires C, 80.0; H, 4.6; N, 11.2%); λ_{max}(DCM)/nm 230 inf (log ε 3.46), 240 (3.47), 256 (3.44), 288 (3.58), 309 inf (3.47), 360 (3.28), 584 (2.76); ν_{max}/cm^{-1} 3055w (Ar CH), 2920w, 2849w, 1624w, 1599w, 1582m, 1537m, 1524m, 1483m, 1456m, 1435s, 1396w, 1373m, 1321w, 1310m, 1287w, 1234m, 1175m, 1132m, 1107m, 1088m, 1074m, 1026w, 989w, 951m, 910w, 891w, 835m; δ_H(300 MHz, $CDCl_3$) 8.31-8.28 (2H, m, Ar *H*), 7.78 (1H, d, *J* 9.7, Ar *H*), 7.52-7.48 (3H, m, Ar *H*), 7.42 (1H, d, *J* 9.7, Ar *H*), 7.16-7.11 (2H, m, Ar *H*), 7.05-6.95 (6H, m, Ar *H*), 6.92-6.88 (2H, m, Ar *H*); δ_C(75 MHz, $CDCl_3$) 181.2 (*C*=O), 155.9 (s), 150.7 (s), 143.5 (s), 141.6 (d), 133.8 (s), 133.6 (s), 132.6 (s), 132.2 (d), 131.0 (d), 130.7 (d), 128.9 (d), 128.5 (d), 128.1 (d), 127.7 (d), 127.0 (d), 126.7 (d), 124.8 (d), 112.7 (s); *m*/*z* (EI) 376 (M^++1, 29%), 375 (M^+, 100), 346 (38), 330 (5), 298 (23), 284 (6), 271 (42), 243 (15), 215 (14), 187 (6), 180 (9), 166 (9), 139 (26), 114 (9), 104 (11), 89 (22), 77 (54), 63 (10), 51 (21).

*1.1.6.1.2. 8-(4-Chlorophenyl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**37**).* Similar treatment of 8-iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**) (42.5 mg, 0.1 mmol) with Pd(dppf)Cl_2·DCM (8 mg, 0.01 mmol), K_2CO_3 (27.6 mg, 0.2 mmol) and 4-chlorophenylboronic acid (31.2 mg, 0.2 mmol) heated at reflux for 1.5 h gave the *title compound* **37** (37.2 mg, 91%) as blue needles, mp 215-219 ^oC (from DCM/MeOH 1:1), R_f 0.65 (*t*-BuOMe/hexane, 3:1); (found: C, 73.1; H, 3.8; N, 10.2. $C_{25}H_{16}ClN_3O$ requires C, 73.3; H, 3.9; N, 10.3%); λ_{max}(DCM)/nm 238 (log ε 3.39), 254 inf (3.34), 299 (3.49), 314 (3.36), 360 (3.23), 577 (2.68); ν_{max}/cm^{-1} 3055w (Ar CH), 2918m, 2848w, 1622w, 1593m, 1584m, 1539m, 1518m, 1481m, 1454m, 1439s, 1400w, 1369m, 1317s, 1296m, 1283w, 1231w, 1173w, 1155w, 1130m, 1105w, 1090m, 1072w, 1028w, 1015m, 989w, 966w, 953m, 914w, 835s, 891w; δ_H(300 MHz, $CDCl_3$) 8.31-8.27 (2H, m, Ar *H*), 7.78 (1H, d, *J* 9.7, Ar *H*), 7.51-7.49 (3H, m, Ar *H*), 7.41 (1H, d, *J* 9.7, Ar *H*), 7.17-7.10 (5H, m, Ar *H*), 6.96-6.93 (2H, m, Ar *H*), 6.84-6.81 (2H, m, Ar *H*); δ_C(75 MHz, $CDCl_3$) 181.0 (*C*=O), 155.9 (s), 151.0 (s), 143.5 (s), 141.6 (d), 133.7 (s), 132.8 (s), 132.7 (s), 132.4 (d), 132.3 (d), 132.2 (s), 130.8 (d), 129.0 (d), 128.8 (d), 128.5 (d), 127.7 (d), 126.8 (d), 125.0 (d), 111.3 (s); *m*/*z* (EI) 410 (M^++1, 34), 409 (M^+, 100), 380 (40), 374 (12), 364 (5), 346 (16), 332 (8), 304 (20), 278 (8), 242 (13), 215 (11), 187 (7), 180 (9), 173 (18), 166 (9), 140 (21), 123 (13), 104 (9), 87 (5), 77 (65), 63 (6), 51 (25).

*1.1.6.1.3. 8-(3-Methoxyphenyl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**38**).* Similar treat-ment of 8-iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**) (42.5 mg, 0.1 mmol) with Pd(dppf)Cl_2·DCM (8 mg, 0.01 mmol), K_2CO_3 (27.6 mg, 0.2 mmol) and 3-methoxyphenylboronic acid (30.4 mg, 0.2 mmol) heated at reflux for 1 h gave the *title compound* **38** (38.8 mg; 96%) as blue needles, mp 187-190 ^oC (from DCM/MeOH, 1:1), R_f 0.65 (*t*-BuOMe/hexane 3:1); (found: C, 77.1; H, 4.6; N, 10.4.

$C_{26}H_{19}N_3O_2$ requires C, 77.0; H, 4.7; N, 10.4%); λ_{max}(DCM)/nm 235 (log ε 3.51), 252 inf (3.45), 286 (3.58), 361 (3.26), 573 (2.73); ν_{max}/cm^{-1} 3071w, 3002w (Ar CH), 2925w, 2848w, 1596m, 1582m, 1557w, 1540s, 1521s, 1484w, 1476w, 1457m, 1436s, 1393w, 1363m, 1314s, 1280m, 1249m, 1204m, 1183w, 1162m, 1125m, 1102w, 1079w, 1046m, 1019w, 994w, 948m, 919w, 873w; δ_H(300 MHz, $CDCl_3$) 8.31-8.27 (2H, m, Ar *H*), 7.79 (1H, d, *J* 9.7, Ar *H*), 7.52-7.48 (3H, m, Ar C*H*), 7.42 (1H, d, *J* 9.7, Ar *H*), 7.17-7.14 (2H, m, Ar *H*), 7.09-7.06 (3H, m, Ar *H*), 6.92 (1H, dd, *J* 7.9, 7.9, Ar *H*), 6.57 (1H, ddd, *J* 7.6, 1.1, 1.1, Ar *H*), 6.50 (1H, ddd, *J* 8.3, 2.6, 0.8, Ar *H*), 6.35 (1H, dd, *J* 2.4, 1.6, Ar *H*), 3.67 (3H, s, OCH_3); δ_C(75 MHz, $CDCl_3$) 181.2 (*C*=O), 156.6 (s), 155.9 (s), 150.8 (s), 143.6 (s), 141.6 (d), 134.9 (s), 133.8 (s), 132.7 (s), 132.2 (d), 130.7 (d), 129.0 (d), 128.8 (d), 128.5 (d), 128.2 (d), 126.8 (d), 124.8 (d), 123.8 (d), 116.5 (d), 113.1 (d), 112.5 (s); *m*/*z* (EI) 406 (M^++1, 34%), 405 (M^+, 100), 388 (16), 374 (72), 362 (12), 346 (12), 333 (14), 328 (17), 314 (5), 301 (31), 285 (6), 273 (2), 257 (9), 231 (9), 202 (17), 195 (8), 180 (13), 169 (11), 154 (7), 139 (9), 126 (29), 104 (14), 89 (7), 77 (77), 51 (30).

*1.1.6.1.4. 1,3,6,8-Tetraphenylbenzo[e][1,2,4]triazin-7(1*H*)-one (**42**). (Suzuki procedure).* To a stirred solution of 8-iodo-1,3,6-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**28**) (50.1 mg, 0.1 mmol) in dioxane/water 3:1 (0.8 ml), Pd(dppf)Cl_2·DCM (8 mg, 0.01 mmol), K_2CO_3 (27.6 mg, 0.2 mmol) and phenylboronic acid (24.4 mg, 0.2 mmol) were added and the mixture was heated at reflux for 2.5 h. The mixture was dried (Na_2SO_4) filtered, adsorbed onto silica gel and dry flash chromatography (EtOAc/hexane, 1:2) gave the *title compound* **42** (34.8 mg, 77%) as shiny blue needles, mp 205-209 ^oC (from DCM/MeOH, 1:3), R_f 0.37 (*t*-BuOMe/hexane, 1:4); (found: C, 82.3; H, 4.7; N, 9.2. $C_{31}H_{21}N_3O$ requires C, 82.5; H, 4.7; N, 9.3%); λ_{max}(DCM)/nm 230 inf (log ε 3.62), 255 (3.70), 285 inf (3.57), 339 (3.76), 585 (2.93);

ν_{max}/cm^{-1} 3055w (Ar CH), 2963w, 2916w, 1601m, 1587s, 1547s, 1524s, 1487s, 1454w, 1445w, 1431m, 1369w, 1335w, 1310m, 1285s, 1258m, 1209m, 1182w, 1146w, 1124w, 1076w, 1069w, 1028w, 1005w, 953w, 920w, 907w, 883w, 839w, 802m; δ_H(500 MHz; $CDCl_3$) 8.33-8.31 (2H, m, Ar H), 7.95 (1H, s, Ar H), 7.81-7.82 (2H, m, Ar H), 7.53-7.45 (6H, m, Ar H), 7.20-7.18 (2H, m, Ar H), 7.08-7.04 (3H, m, Ar H), 7.00-6.94 (5H, m, Ar H); δ_C(125 MHz; $CDCl_3$) one Ar *C*H missing 179.8 (s), 155.9 (s), 151.0 (s), 150.3 (s), 143.6 (s), 136.0 (s), 134.3 (s), 134.1 (s), 132.2 (s), 131.3 (d), 130.6 (d), 130.0 (d), 129.7 (d), 128.9 (d), 128.5 (d), 128.3 (d), 128.1 (d), 127.6 (d), 126.9 (d), 126.8 (d), 125.0 (d), 112.9 (s); *m*/*z* (EI) 452 (M^++1, 31%), 451 (M^+, 100), 450 (M^+-1, 46), 423 (35), 374 (18), 347 (18), 319 (13), 285 (3), 242 (8), 216 (14), 189 (9), 180 (11), 165 (6), 104 (7), 89 (15), 77 (33), 69 (7), 51 (10).

1.1.6.2. Stille Coupling at C-8

*1.1.6.2.1. 8-(Furan-2-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* ***(39)*** *(typical procedure)*. To a stirred solution of 8-iodo-1,3-diphenylbenzo[*e*][1,2,4]-triazin-7(1*H*)-one (**32**) (42.5 mg, 0.1 mmol) in DMF (2 ml), 2-(tributylstannyl)furan (91 μl, 0.29 mmol) and $Pd(OAc)_2$ (3.4 mg, 0.015 mmol) were added and the solution was heated at *ca.* 100 ^oC under an Ar atmosphere for 21 h. TLC (*t*-BuOMe/hexane, 1:1) showed the absence of the starting material and the presence of a new more polar product. The reaction mixture was cooled, filtered, diluted with EtOAc (10 ml) and washed with water (15 ml). The combined organic layers were dried (Na_2SO_4), filtered and the residue dry flash chromatographed (*t*-BuOMe/hexane, 1:2) to give the *title compound* **39** (25.9 mg, 71%) as shiny blue needles, mp 189-192 ^oC (from cyclohexane); R_f 0.65 (*t*-BuOMe/hexane, 3:1); (found: C, 75.5; H, 4.1; N, 11.4. $C_{23}H_{15}N_3O_2$ requires C, 75.6; H, 4.1; N, 11.5%); λ_{max}(DCM)/nm 218 (log ε 3.83), 252 (3.11), 298 (3.14), 378 (2.72), 602 (2.53); ν_{max}/cm^{-1} 3140w, 3113w, 3065w (Ar CH),

1626m, 1599m, 1585m, 1539w, 1514m, 1485w, 1470m, 1454w, 1437s, 1391w, 1364m, 1329m, 1317m, 1277w, 1232m, 1215w, 1188w, 1169m, 1155m, 1126m, 1101m, 1088w, 1076m, 1024m, 1003w, 986w, 949m, 935w, 883w, 858w, 831s; δ_H(300 MHz, $CDCl_3$) 8.33-8.30 (2H, m, Ar *H*), 7.76 (1H, d, *J* 9.7, Ar *H*), 7.54-7.48 (3H, m, Ar *H*), 7.41-7.37 (3H, m, Ar *H*), 7.24-7.17 (3H, m, Ar *H*), 6.78-6.77 (1H, m, Ar *H*), 6.57 (1H, dd, *J* 3.1, 0.7, Ar *H*), 6.11 (1H, dd, *J* 3.3, 1.9, Ar *H*); δ_C(75 MHz, $CDCl_3$) one Ar CH missing 179.8 (*C*=O), 155.3 (s), 151.5 (s), 145.3 (s), 143.2 (s), 141.8 (d), 141.4 (d), 133.7 (s), 132.2 (d), 131.9 (s), 130.8 (d), 128.9 (d), 128.5 (d), 128.3 (d), 127.0 (d), 123.2 (d), 113.1 (d), 111.3 (d), 102.8 (s); *m*/*z* (EI) 366 (M^++1, 28%), 365 (M^+, 100), 336 (80), 322 (40), 308 (17), 260 (5), 232 (10), 219 (5), 205 (25), 191 (5), 176 (17), 169 (7), 152 (12), 129 (15), 103 (18), 88 (4), 77 (87), 63 (7), 51 (52).

*1.1.6.2.2. 1,3-Diphenyl-8-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**40**).* Similar treatment of 8-iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**) (42.5 mg, 0.1 mmol) with 2-(tributylstannyl)thiophene (95 μl, 0.3 mmol) and $Pd(OAc)_2$ (3.4 mg, 0.015 mmol) heated at *ca.* 100 ^oC under an Ar atmosphere for 25 h gave the *title compound* **40** (30.1 mg, 79%) as shiny blue needles, mp 215-217 ^oC (from DCM/MeOH, 1:3); R_f 0.79 (*t*-BuOMe); (found: C, 72.6; H, 3.9; N, 10.8. $C_{23}H_{15}N_3OS$ requires C, 72.4; H, 4.0; N, 11.0%); λ_{max}(DCM)/nm 255 (log ε 3.45), 288 (3.49), 364 (3.28), 593 (2.66); ν_{max}/cm^{-1} 3071w, 3038w (Ar CH), 1624w, 1595s, 1547w, 1532w, 1504w, 1489s, 1456w, 1437s, 1422m, 1369m, 1356w, 1327w, 1312s, 1283m, 1229m, 1209w, 1167w, 1157w, 1128w, 1209w, 1179w, 1072w, 1038w, 1030w, 1003w, 980w, 974w, 947w, 920w, 883w, 866w, 845w, 833m, 818m, 791w, 761m; δ_H(300 MHz, $CDCl_3$) 8.33-8.30 (2H, m, Ar *H*), 7.79 (1H, d, *J* 9.5, Ar *H*), 7.55-7.49 (3H, m, Ar *H*), 7.42 (1H, d, *J* 9.7, Ar *H*), 7.26-7.22 (2H, m, Ar *H*), 7.15-7.09 (4H, m, Ar *H*),

6.52 (1H, dd, *J* 5.1, 3.7, Ar *H*), 6.29 (1H, dd, *J* 3.6, 0.9, Ar *H*); δ_C(75 MHz, $CDCl_3$) 181.0 (*C*=O), 155.7 (s), 151.3 (s), 143.3 (s), 141.0 (d), 133.7 (s), 132.8 (s), 132.4 (s), 132.4 (d), 130.8 (d), 129.1 (d), 129.0 (d), 128.6 (d), 128.3 (d), 126.9 (d), 126.7 (d), 126.0 (d), 123.3 (d), 106.1 (s); *m*/*z* (EI) 382 (M^++1, 28%), 381 (M^+, 100), 364 (33), 352 (59), 336 (5), 324 (4), 298 (7), 276 (47), 249 (12), 221 (24), 189 (6), 180 (5), 145 (33), 120 (5), 103 (12), 95 (12), 77 (71), 69 (13), 51 (36).

*1.1.6.2.3. 1,3-Diphenyl-8-vinylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**41**).* Similar treatment of 8-iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**) (42.5 mg, 0.1 mmol) with tributyl-(vinyl)stannane (100 μl, 0.33 mmol) and $Pd(OAc)_2$ (3.4 mg, 0.015 mmol) heated at *ca.* 100 ^oC under an Ar atmosphere for 24 h gave the *title compound* **41** (16.4 mg, 51%) as shiny blue needles, mp 154-157 ^oC (from cyclohexane), R_f 0.66 (*t*-BuOMe/hexane, 3:1); (found: C, 77.4; H, 4.7; N, 12.8. $C_{21}H_{15}N_3O$ requires C, 77.5; H, 4.7; N, 12.9%); λ_{max}(DCM)/nm 242 (log ε 3.58), 256 inf (3.55), 289 (3.69), 367 (3.44), 594 (2.92); ν_{max}/cm^{-1} 3063w, 3017w (Ar CH), 2924w, 2853w, 1620m, 1609m, 1585m, 1580m, 1537m, 1504m, 1493m, 1487m, 1454s, 1438s, 1400m, 1371m, 1337m, 1310m, 1279w, 1207m, 1173w, 1159w, 1130m, 1088m, 1070w, 1028w, 1009m, 943w, 908m, 833m, 772m; δ_H(300 MHz, $CDCl_3$) 8.30-8.26 (2H, m, Ar *H*), 7.68 (1H, d, *J* 9.7, Ar *H*), 7.51-7.44 (7H, m, Ar *H*), 7.41-7.35 (1H, m, Ar *H*), 7.30 (1H, d, *J* 9.7, Ar *H*), 5.97 (1H, dd, *J* 17.7, 11.5, C*H*), 5.35 (1H, dd, *J* 17.7, 2.0, C*H*), 4.97 (1H, dd, *J* 11.6, 2.0, C*H*); δ_C(75 MHz, $CDCl_3$) 182.1 (*C*=O), 155.6 (s), 151.1 (s), 145.0 (s), 141.5 (d), 133.7 (s), 132.3 (s), 131.6 (d), 130.7 (d), 129.5 (d), 128.9 (d), 128.7 (d), 128.3 (d), 126.8 (d), 124.4 (d), 119.2 (CH_2), 109.2 (s); *m*/*z* (EI) 326 (M^++1, 24%), 325 (M^+, 100), 296 (30), 268 (5), 248 (17), 221 (37), 194 (24), 180 (9), 165 (49), 139 (7), 117 (7), 104 (10), 89 (17), 77 (57), 63 (25), 51 (27).

*1.1.6.2.4. 1,3-Diphenyl-6,8-di(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**43**).* (Stille procedure). To a stirred solution of 8-iodo-1,3-diphenyl-6-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**29**) (50.7 mg, 0.1 mmol) in DMF (2 ml), 2-(tributylstannyl)thiophene (95 μl, 0.3 mmol) and $Pd(OAc)_2$ (3.4 mg, 0.015 mmol) were added and the solution was heated at *ca.* 100 ^{o}C under an Ar atmosphere for 15 h. TLC (*t*-BuOMe/hexane, 2:1) showed the absence of the starting material and the presence of a new more polar product. The reaction mixture was cooled to *ca.* 20 ^{o}C, filtered, diluted with Et_2O (10 ml) and washed with water (15 ml). The combined organic layers were dried (Na_2SO_4), filtered, evaporated *in vacuo* and dry flash chromatographed (EtOAc/hexane, 1:3) of the residue gave the *title compound* **43** (37.6 mg, 81%) as green-brown needles, mp 223-236 ^{o}C (from DCM/MeOH, 1:4), R_f 0.43 (*t*-BuOMe/hexane, 1:4); (found: C, 69.9; H, 3.7; N, 8.9. $C_{27}H_{17}N_3OS_2$ requires C, 70.0; H, 3.7; N, 9.1%); λ_{max}(DCM)/nm 285 (log ε 4.06), 363 (2.97), 456 (3.82), 619 (3.06); ν_{max}/cm^{-1} 3078w, 2963w, 1582m, 1574w, 1537s, 1501w, 1489s, 1454w, 1429m, 1420m, 1404w, 1383w, 1373w, 1356w, 1312m, 1283m, 1261m, 1229w, 1211w, 1196w, 1173w, 1161w, 1088w, 1069m, 1057w, 1045w, 1028m, 991w, 945w, 908w, 881w, 847w, 833s, 820w, 800w, 798m, 768w; δ_H(500 MHz; $CDCl_3$) 8.37-8.35 (2H, m, Ar H), 8.25 (1H, s, Ar H), 8.09 (1H, s, *J* 1.0, 4.2, Ar H), 7.72 (1H, s, *J* 1.0, 5.1, Ar H), 7.55-7.49 (3H, m, Ar H), 7.27-7.25 (2H, m, Ar H), 7.23 (1H, dd, *J* 4.2, 5.1, Ar H), 7.19-7.13 (3H, m , Ar H), 7.11 (1H, dd, *J* 1.0, 5.1, Ar H), 6.55 (1H, dd, *J* 3.5, 5.3, Ar H), 6.35 (1H, dd, *J* 1.1, 3.4, Ar H); δ_C(125 MHz; $CDCl_3$) 178.9 (s), 154.6 (s), 151.9 (s), 143.5 (s), 141.8 (s), 136.4 (s), 134.5 (d), 134.1 (s), 133.6 (s), 132.2 (s), 130.7 (d), 129.7 (d), 129.5 (d), 129.0 (d), 128.6 (d), 128.5 (d), 127.1 (d), 127.0 (d), 126.7 (d), 126.0 (d), 123.8 (d), 123.5 (d), 105.4 (s); *m*/*z* (EI) 464 (M^++1, 32%), 463 (M^+, 100), 446 (28), 434 (47), 402 (4), 358 (31), 332 (8), 271 (7), 228 (16), 210 (7)

190 (7), 180 (6), 171 (6), 151 (4), 139 (10), 127 (5), 111 (8), 95 (13), 77 (64), 69 (12), 51 (23).

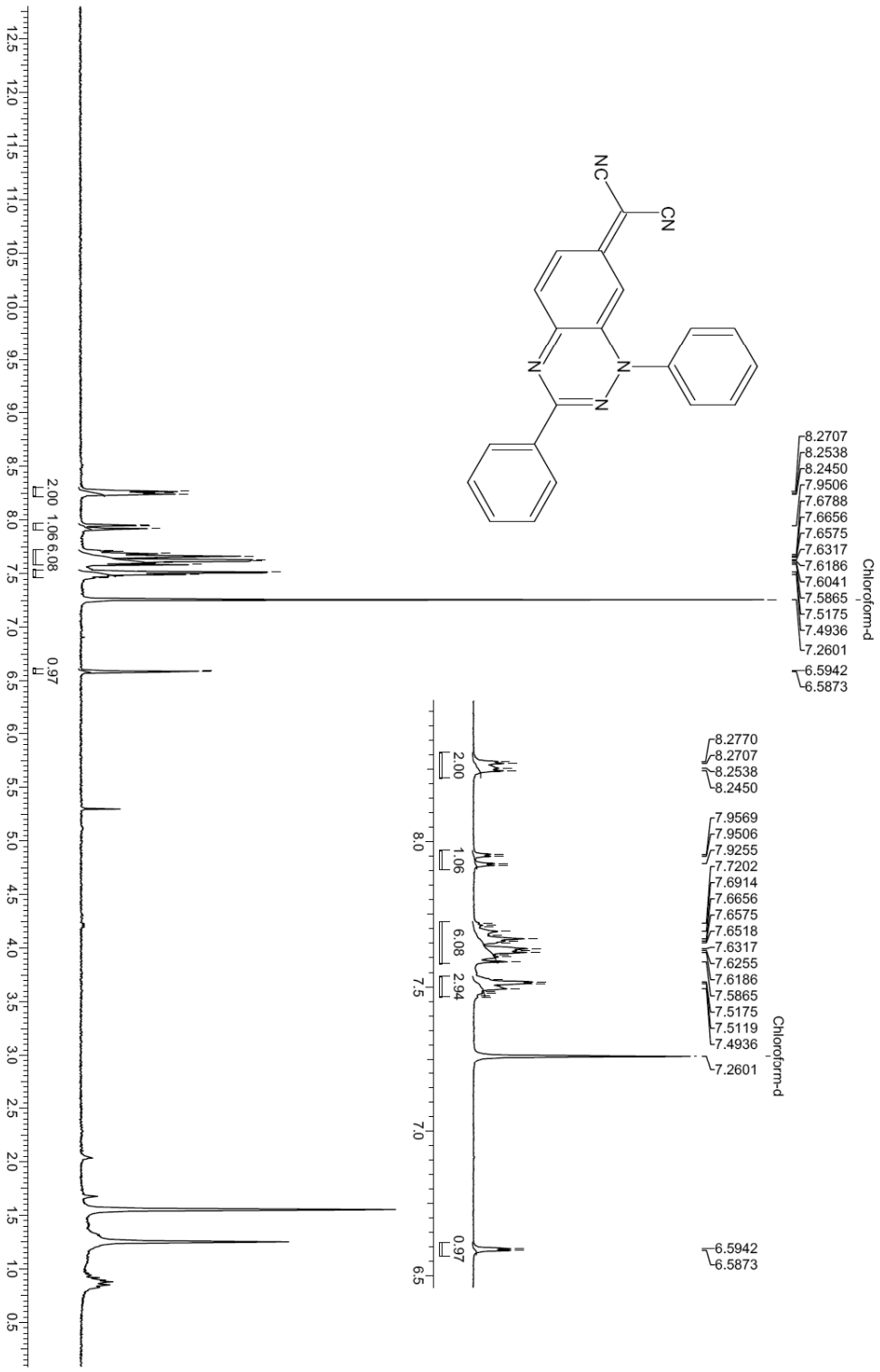
1.1.7. Preparation of 1,3,6,8-tetraarylbenzotriazinones via Grignard reaction at C-6

*1.1.7.1. 1,3,6,8-Tetraphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**42**) (typical procedure)*. To a stirred solution of 1,3,8-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**28**) (37.5 mg, 0.1 mmol) in dry THF (0.6 ml) at *ca.* 20 ^{o}C in Ar atmosphere, PhMgBr 1 M in THF (0.4 ml, 0.4 mmol) was added and the mixture stirred for 18 h. TLC (*t*-BuOMe/hexane, 1:1) showed the absence of the starting material and the presence of a new less polar blue product. The mixture was diluted with MeOH (1 ml) and stirred for 10 min. Dry flash chromatography (EtOAc/hexane, 1:2) gave the *title compound* **42** (35.5 mg, 79%) as blue needles, mp 205-209 ^{o}C (from DCM/MeOH, 1:3), R_f 0.37 (*t*-BuOMe/hexane, 1:4), identical to that describe above.

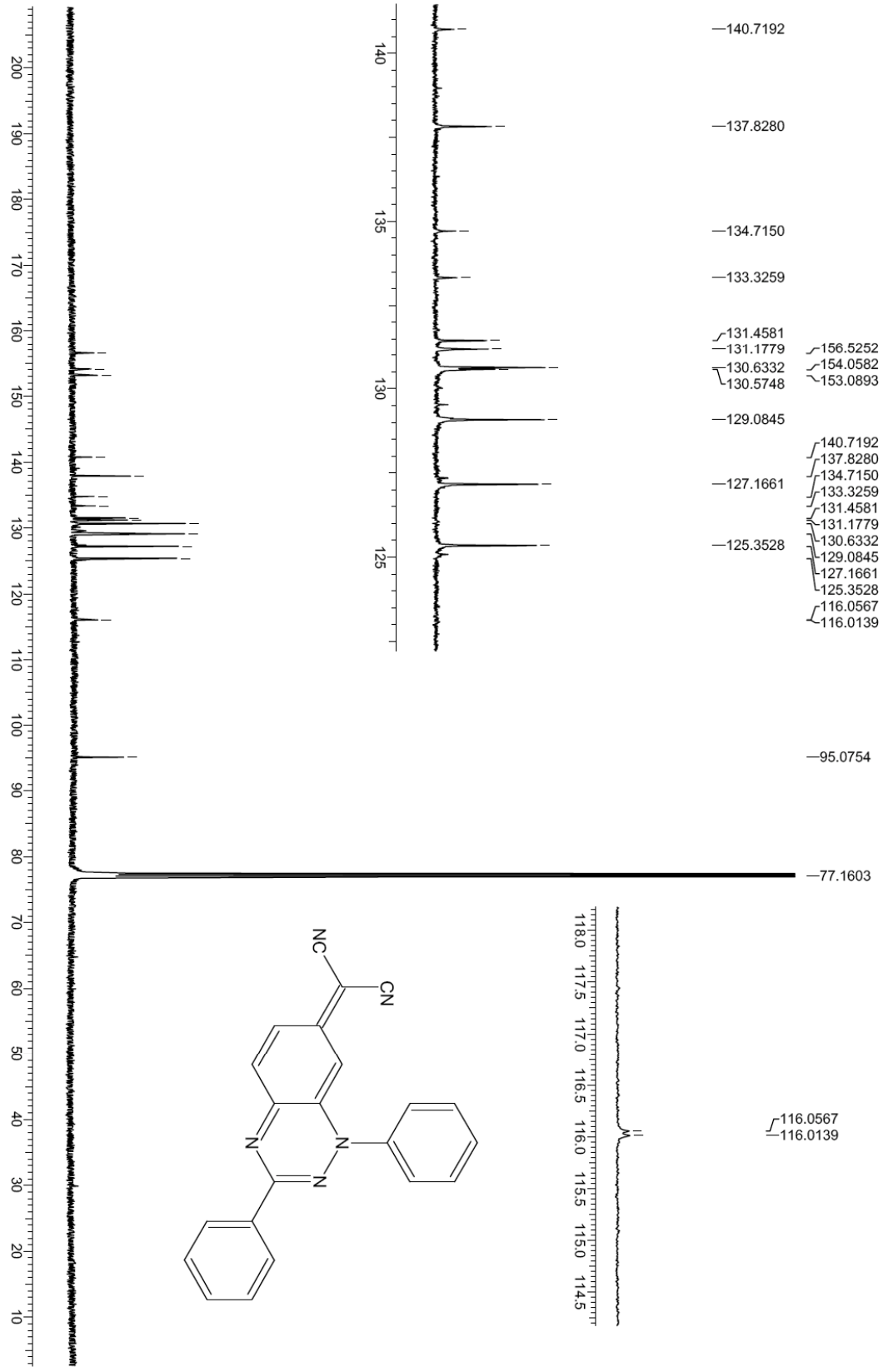
*1.1.7.2. 1,3-Diphenyl-6,8-di(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**43**).* To a stirred solution of 1,3-diphenyl-8-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**29**) (38.1 mg, 0.1 mmol) in dry THF (0.6 ml), (thien-2-yl)MgBr 1 M in THF (0.4 ml, 0.4 mmol) and the mixture stirred at *ca.* 20 ^{o}C in Ar atmosphere for 16 h. TLC (*t*-BuOMe/hexane, 3:1) showed the absence of the starting material and the presence of a new less polar green-brown product. The mixture was diluted with MeOH (1 ml) and stirred for 10 min. Dry flash chromatography (EtOAc/hexane, 1:3) gave the *title compound* **43** (26.3 mg, 57%) as a green-brown needles, mp 223-236 ^{o}C (from DCM/MeOH, 1:4), R_f 0.43 (*t*-BuOMe/hexane, 1:4), identical to that describe above.

2. Section B: ^{1}H and ^{13}C NMR Spectra

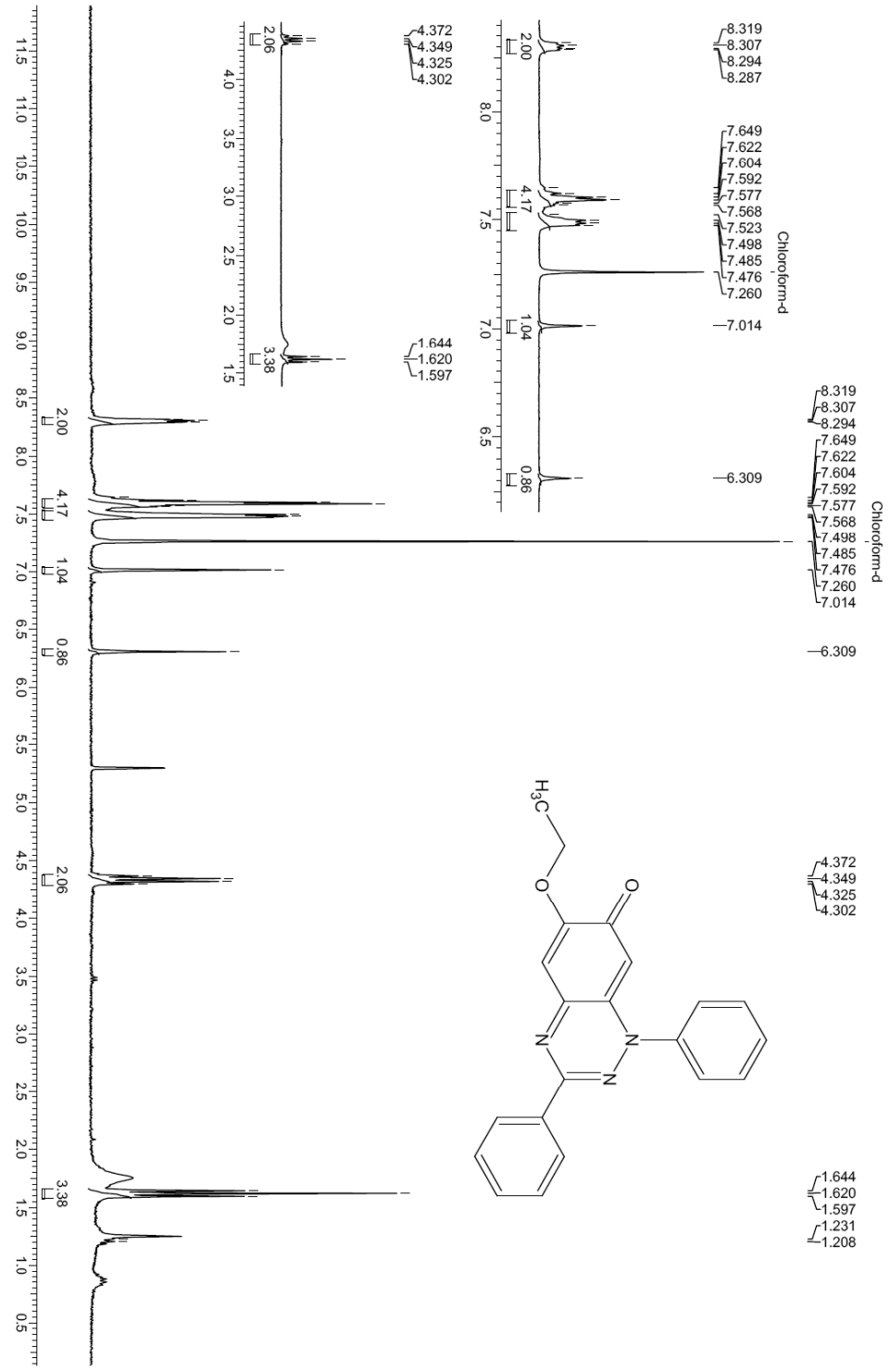
^{1}H NMR of *2-(1,3-Diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-ylidene)propanedinitrile* ***(11)***



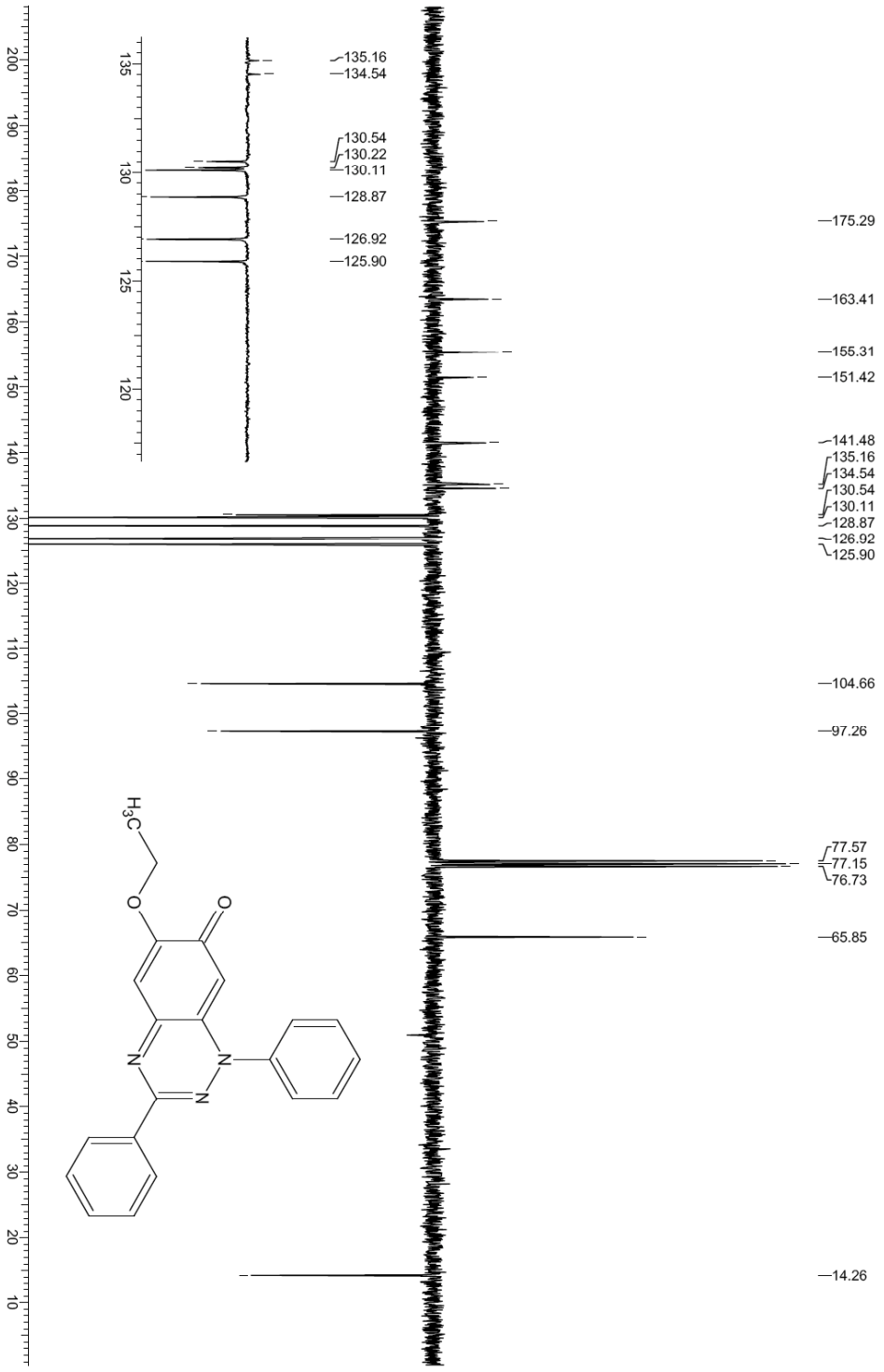
^{13}C NMR of *2-(1,3-Diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-ylidene)propanedinitrile* ***(11)***



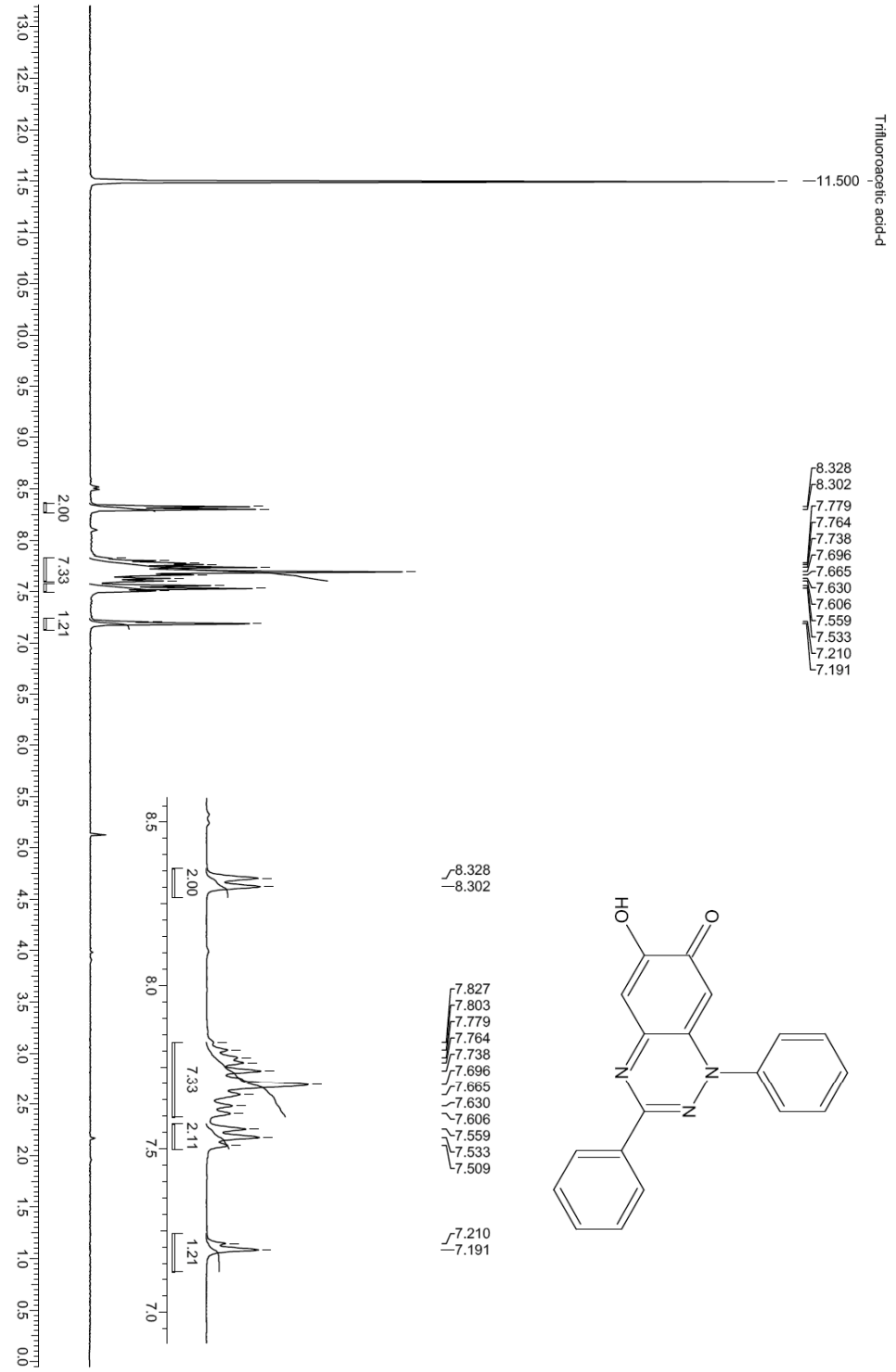
^{1}H NMR of *6-Ethoxy-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**14**)*



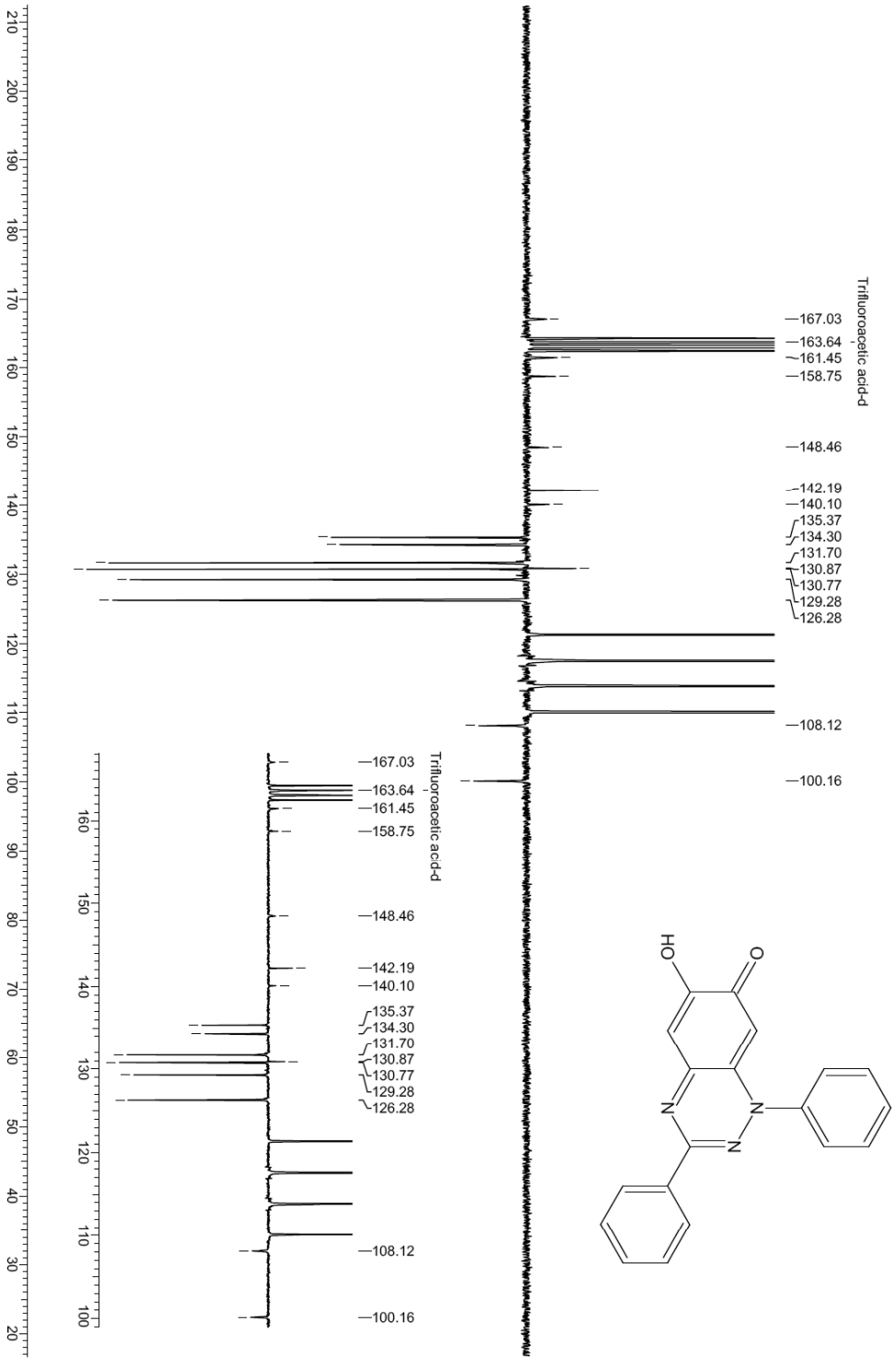
^{13}C NMR of *6-Ethoxy-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* (***14***)



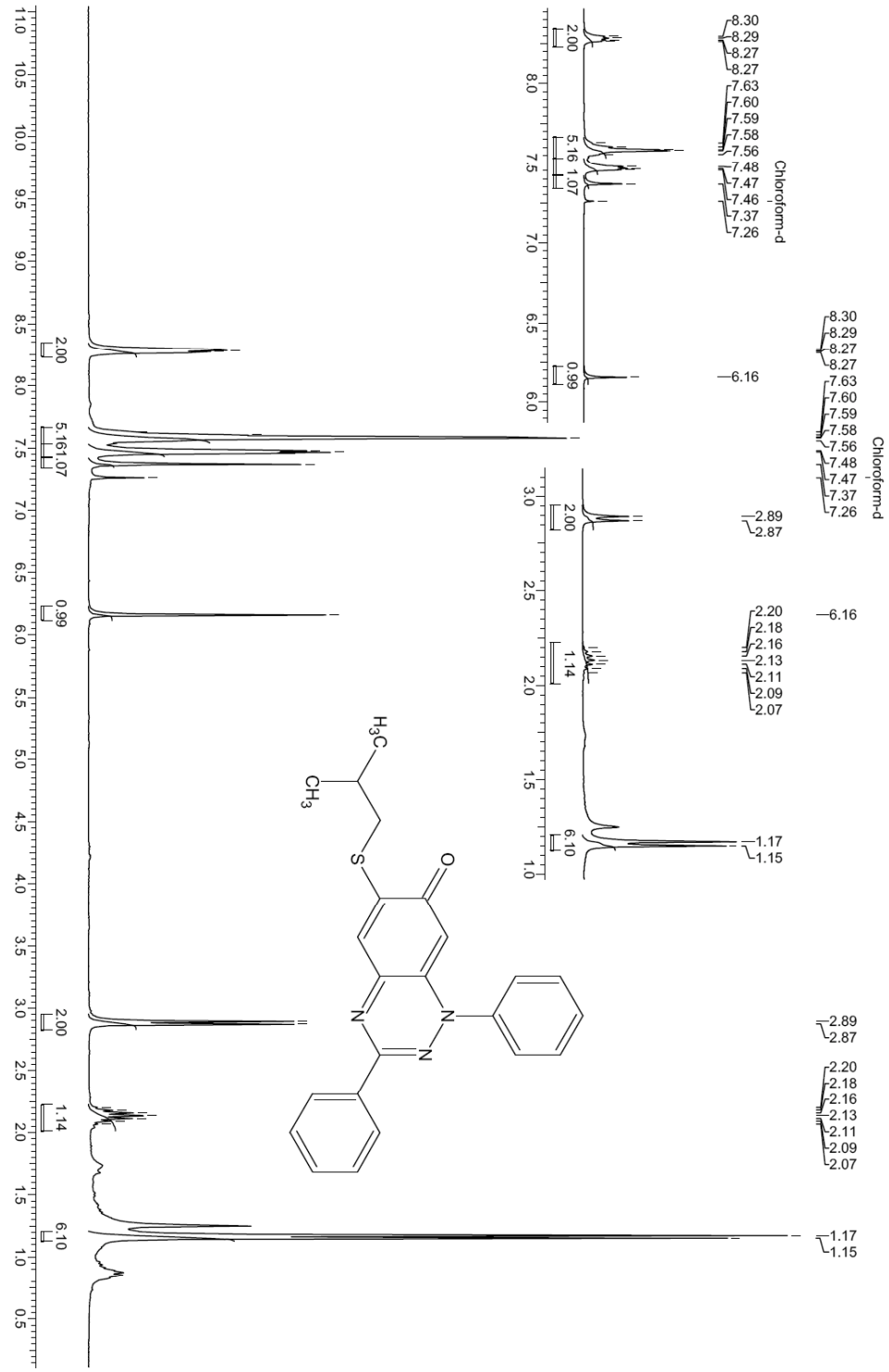
[1]H NMR of *6-Hydroxy-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**15**)*



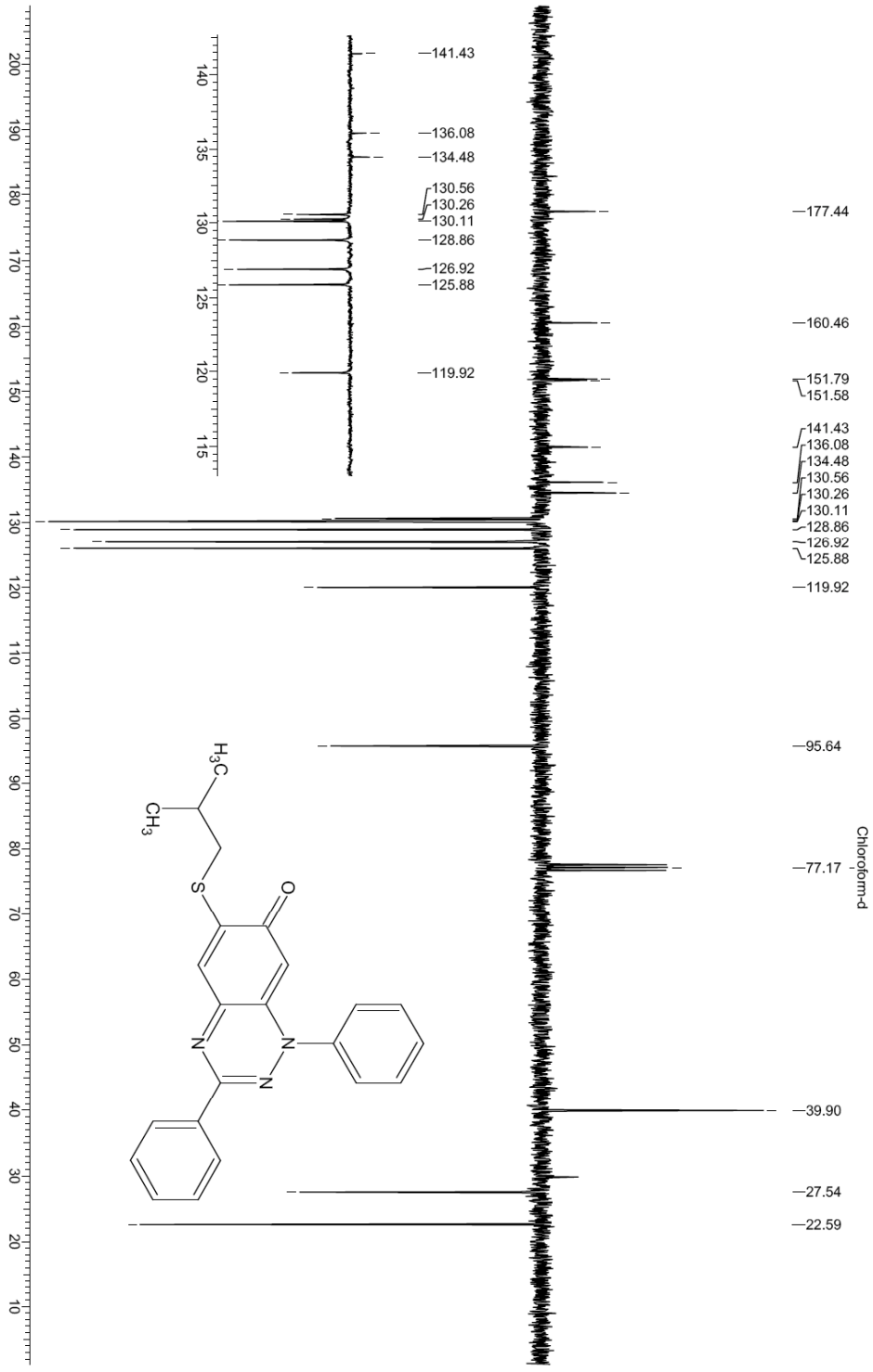
^{13}C NMR of *6-Hydroxy-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**15**)*



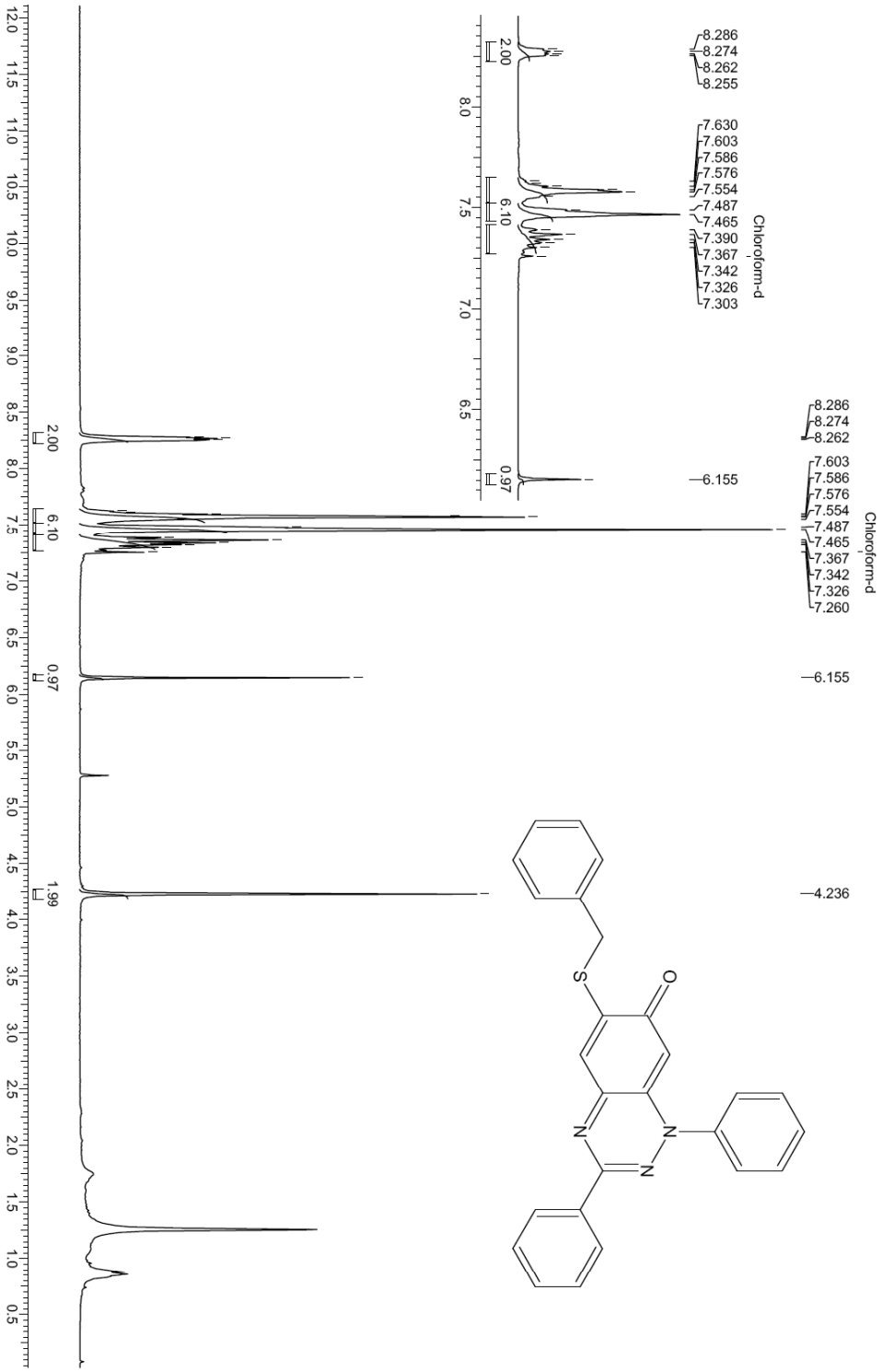
^{1}H NMR of *6-(Isobutylthio)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**16**)*



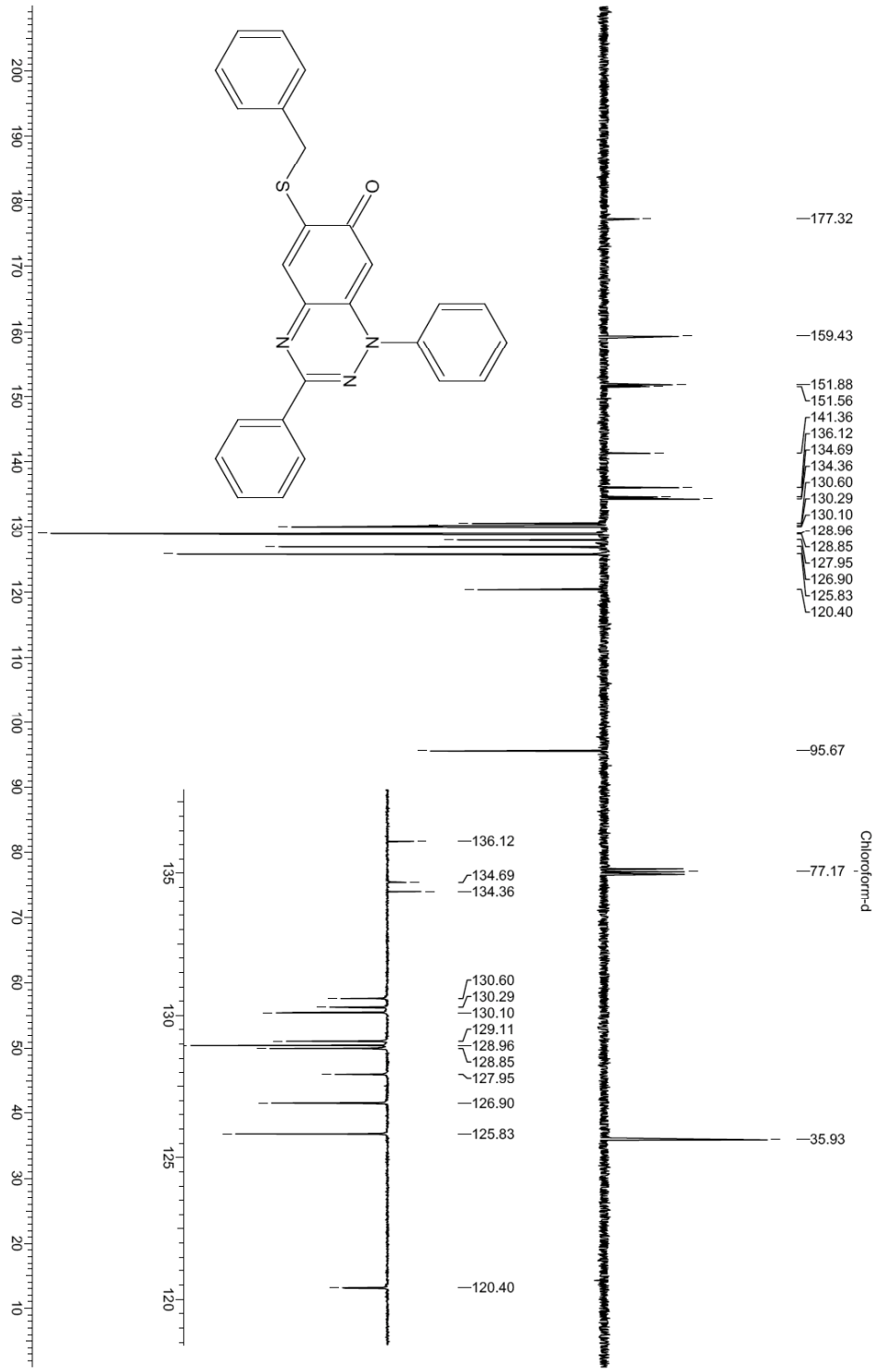
^{13}C NMR of *6-(Isobutylthio)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**16**)*



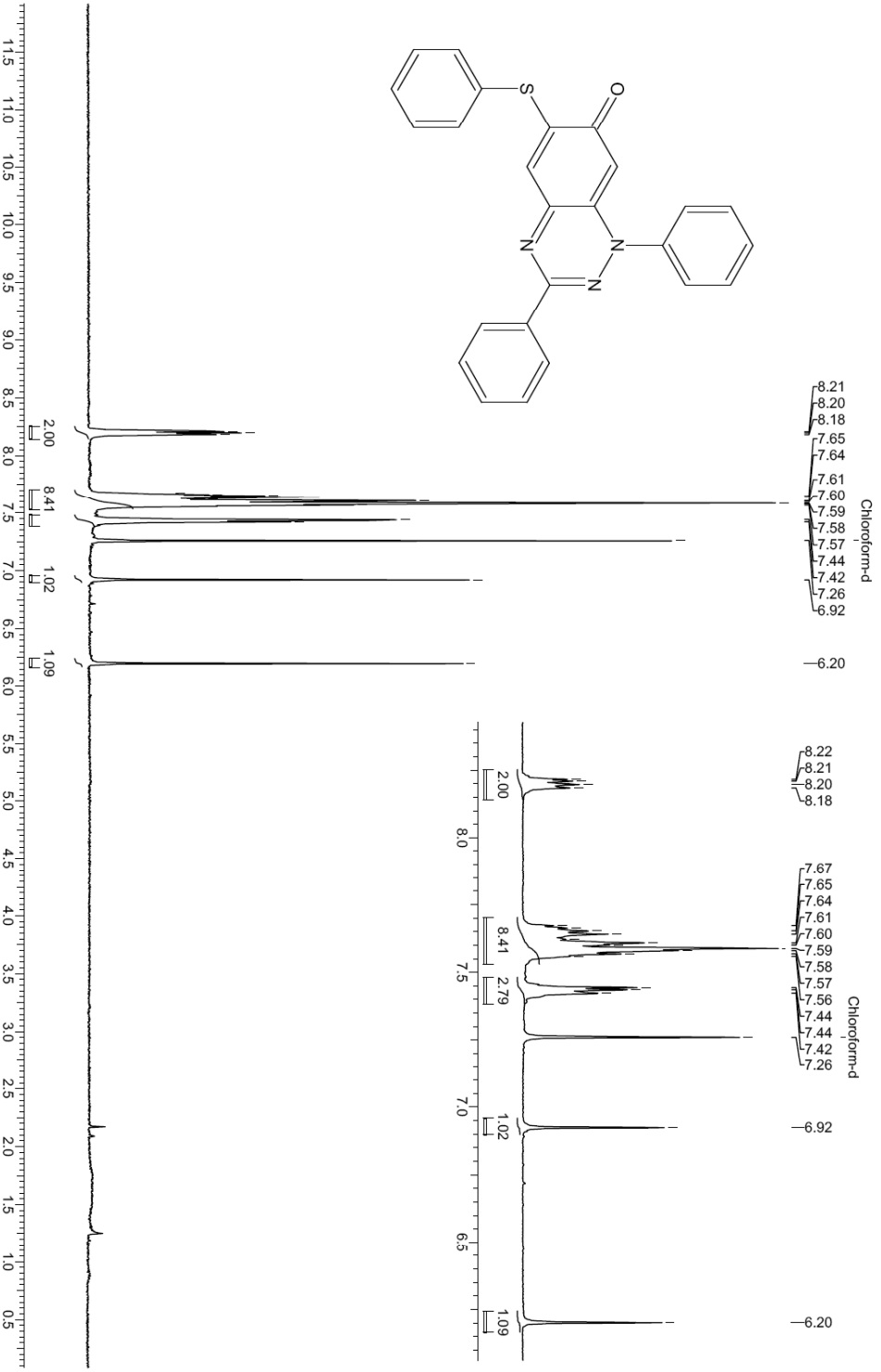
^{1}H NMR of *6-(Benzylthio)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**17**)*



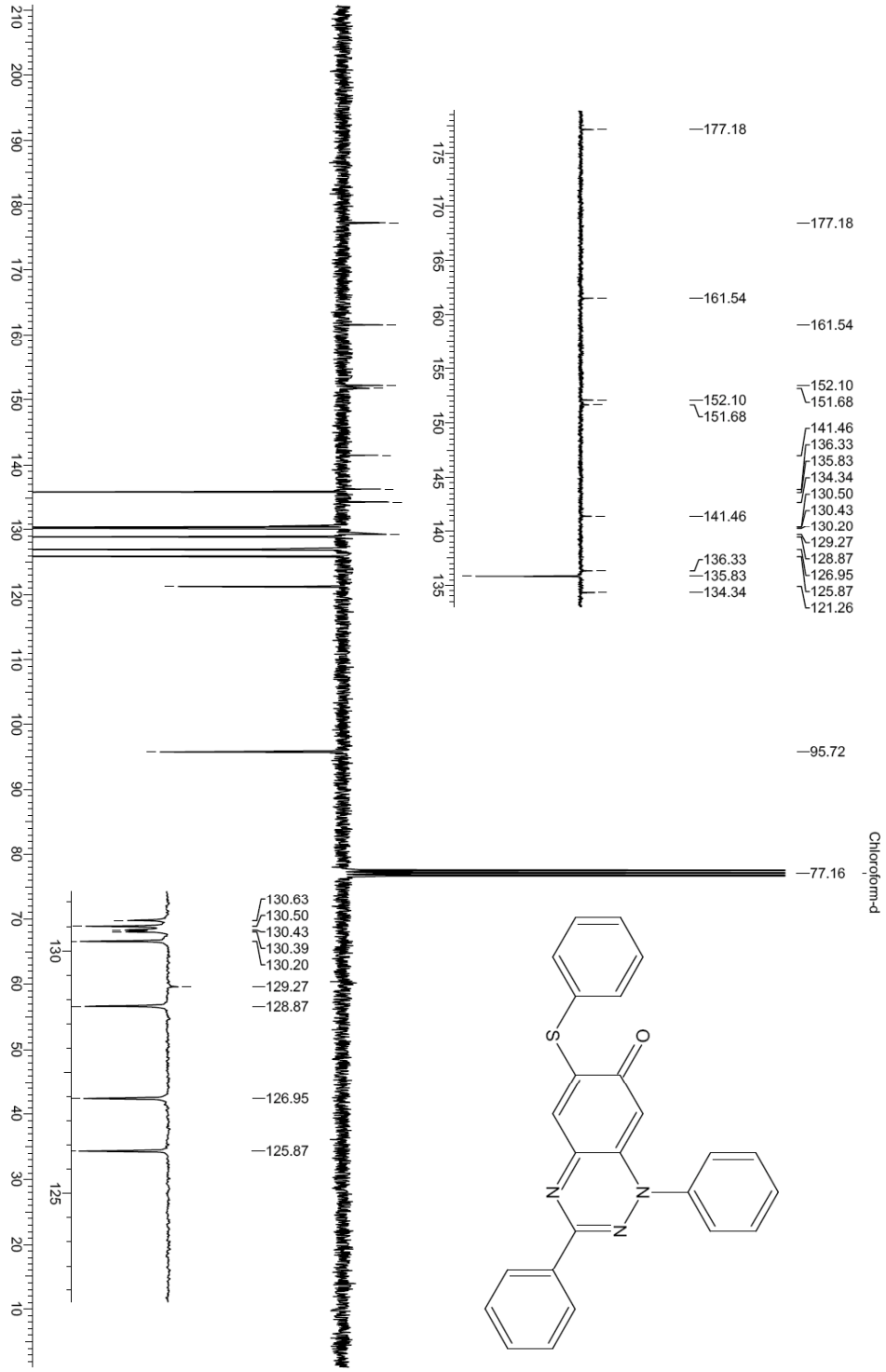
^{13}C NMR of *6-(Benzylthio)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**17**)*



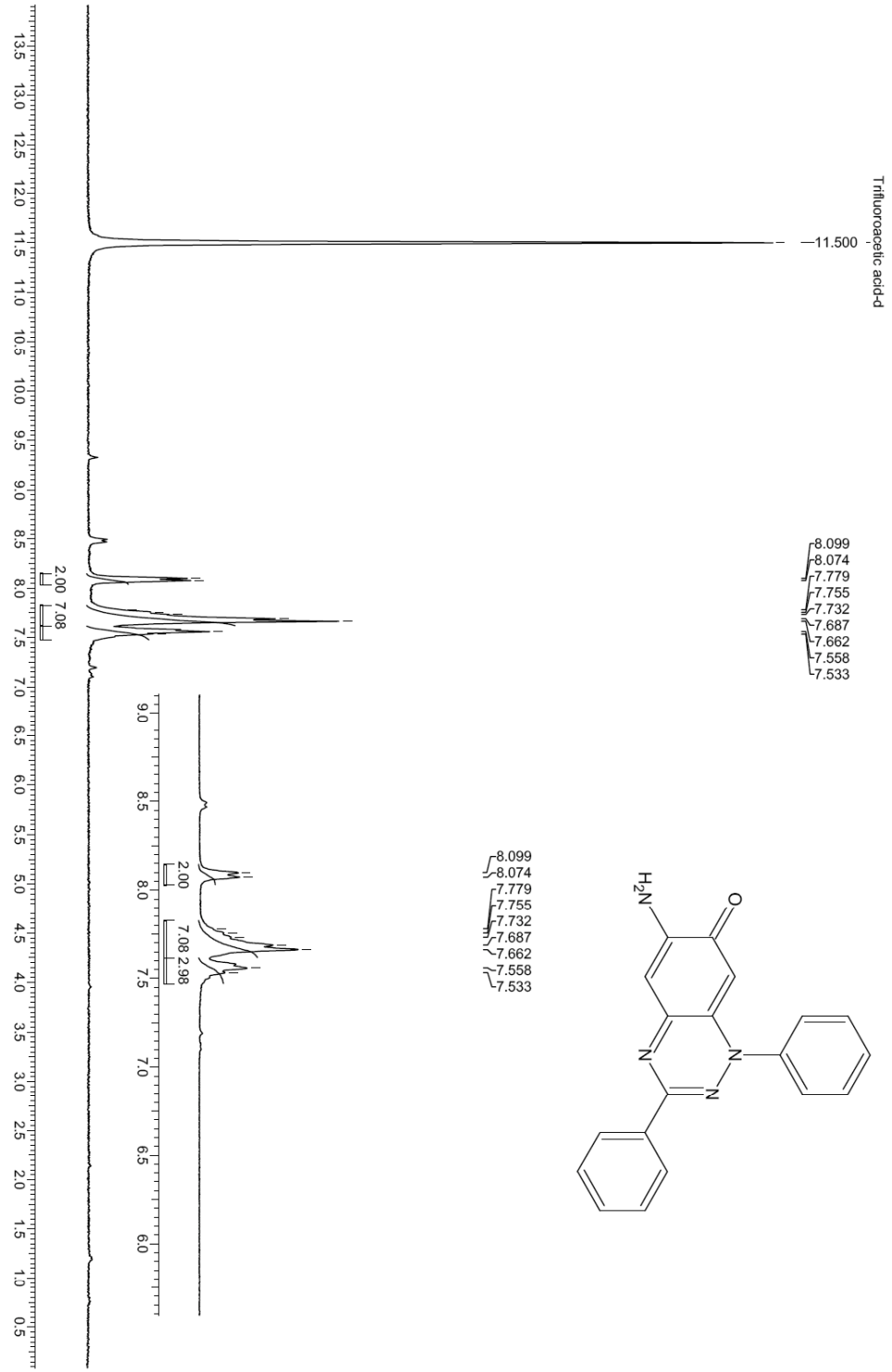
^{1}H NMR of *1,3-Diphenyl-6-(phenylthio)benzo[*e*][1,2,4]triazin-7(1*H*)-one* (***18***)



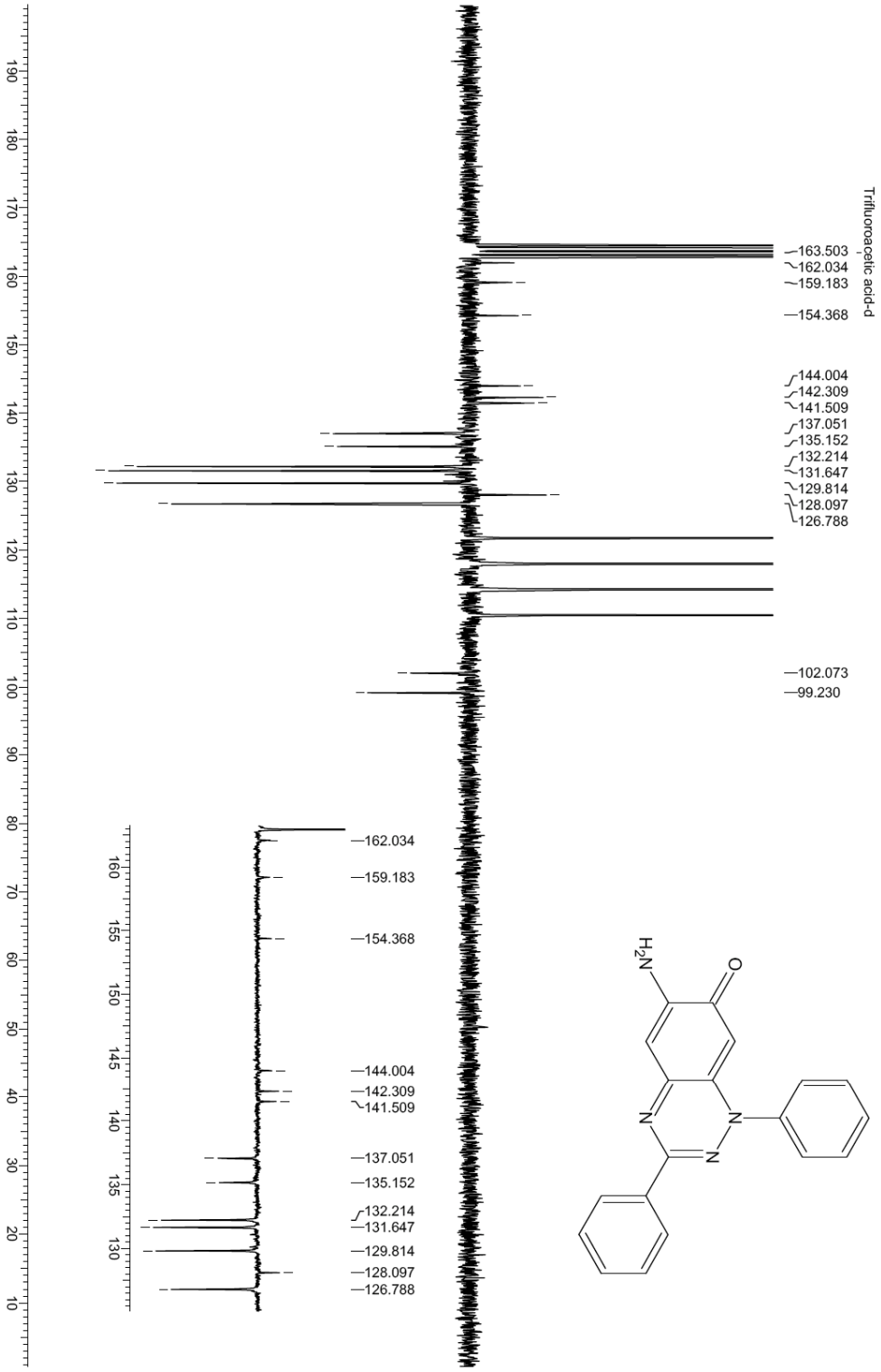
^{13}C NMR of *1,3-Diphenyl-6-(phenylthio)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**18**)*



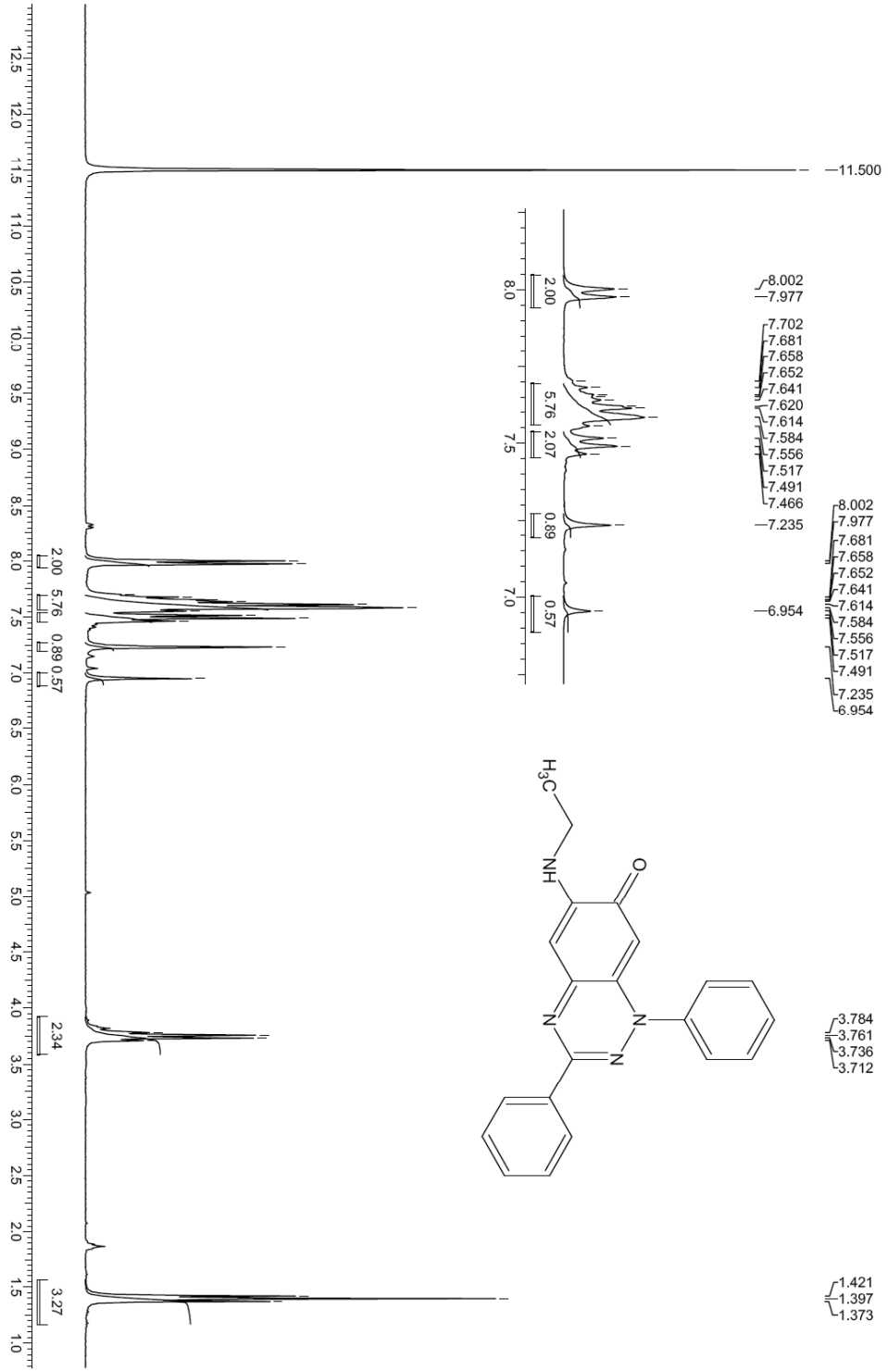
^{1}H NMR of *6-Amino-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**19**)*



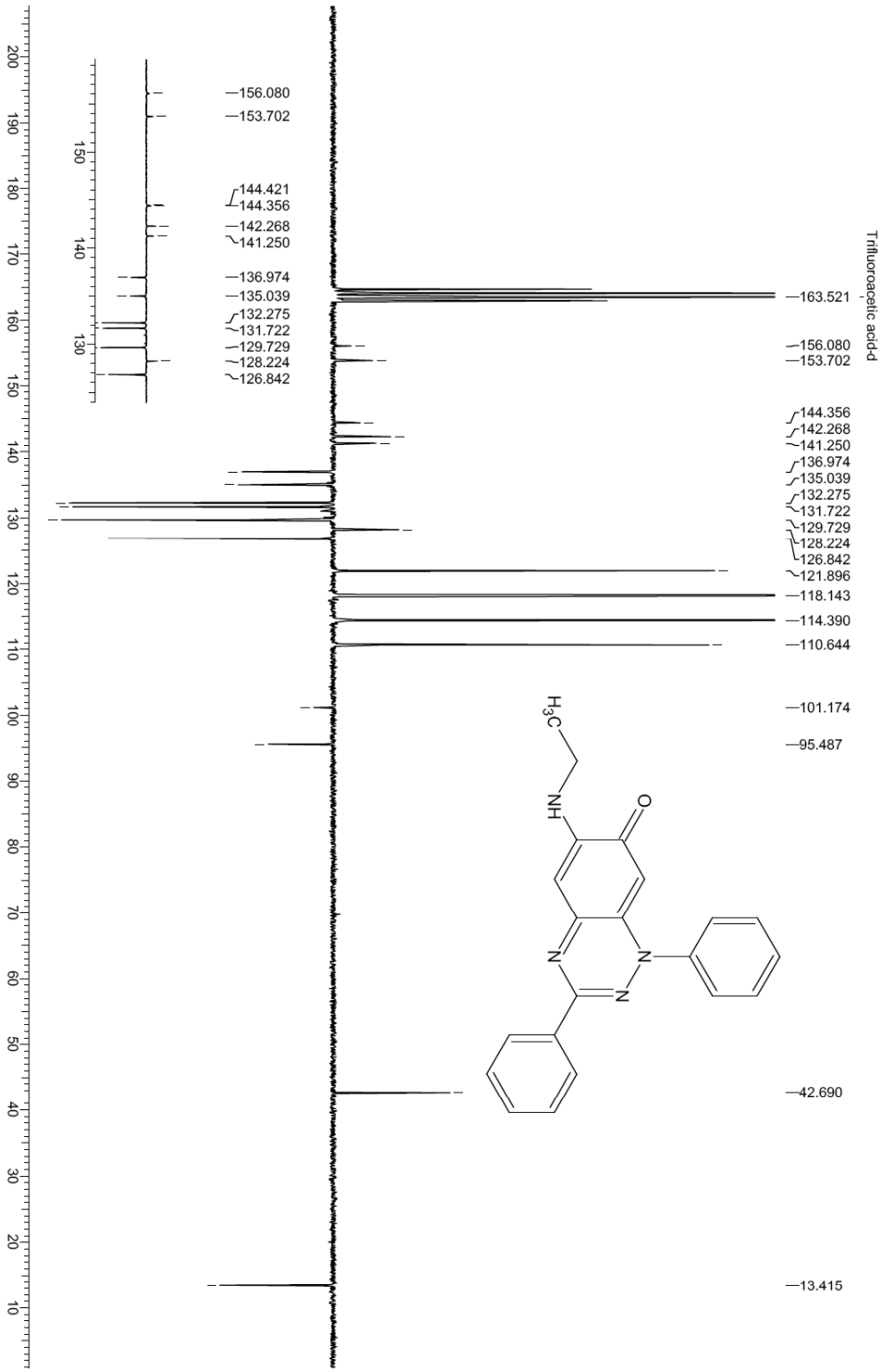
^{13}C NMR of *6-Amino-1,3-diphenylbenzo*[e]*[1,2,4]triazin-7(1*H*)-one* (***19***)



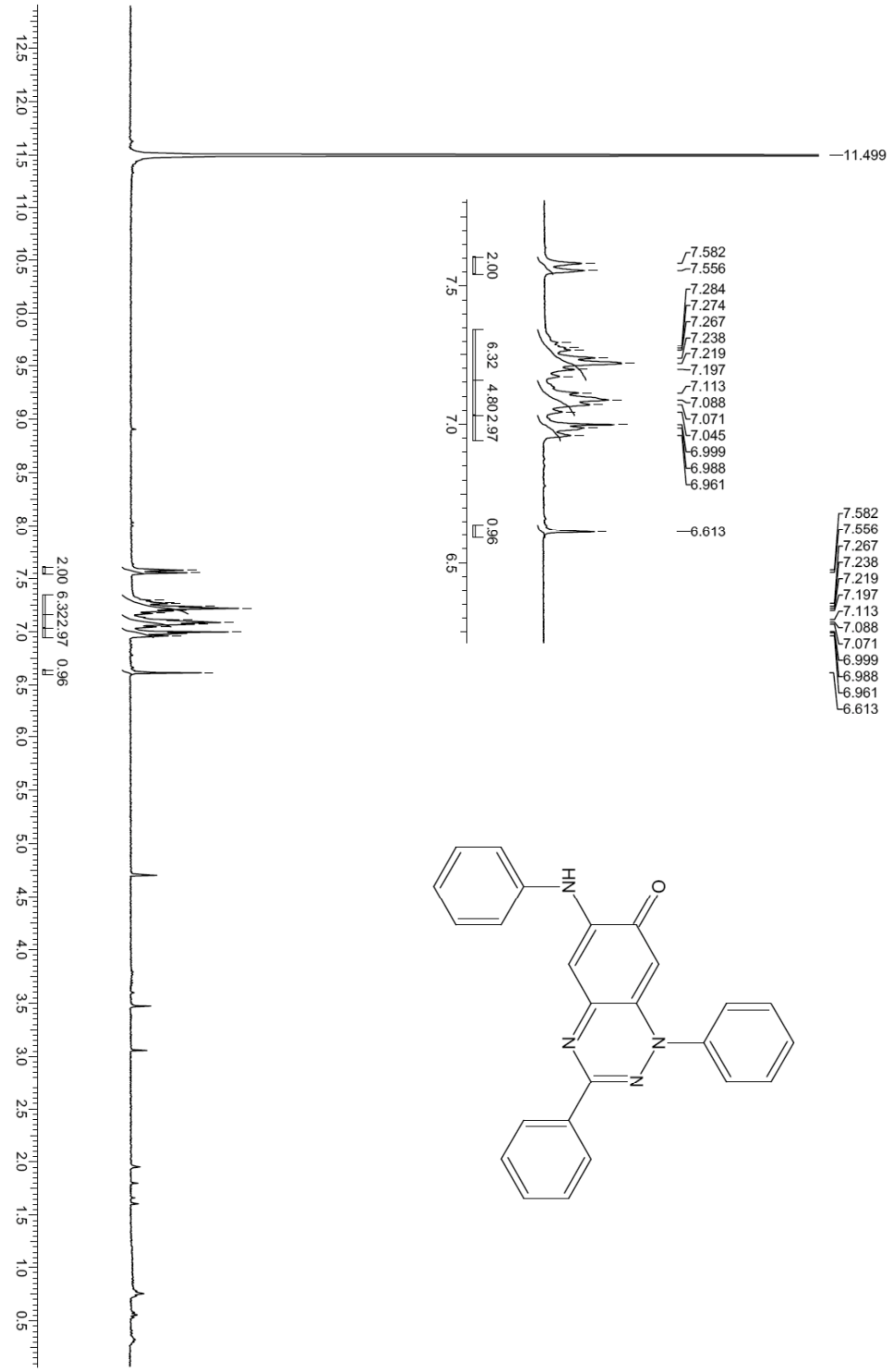
^{1}H NMR of *6-(Ethylamino)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**20**)*



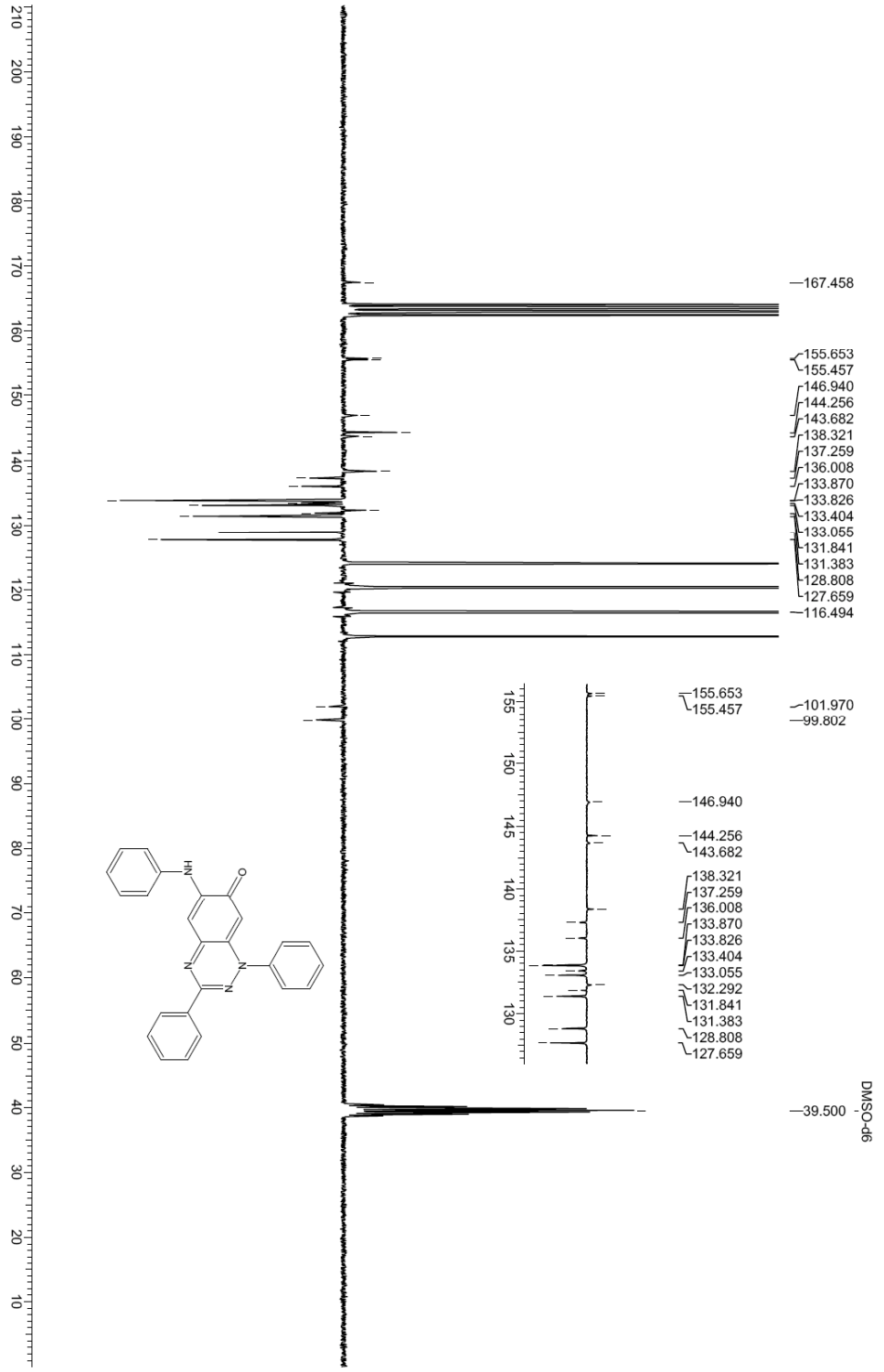
^{13}C NMR of *6-(Ethylamino)-1,3-diphenylbenzo*[e]*[1,2,4]triazin-7(1*H*)-one* (***20***)



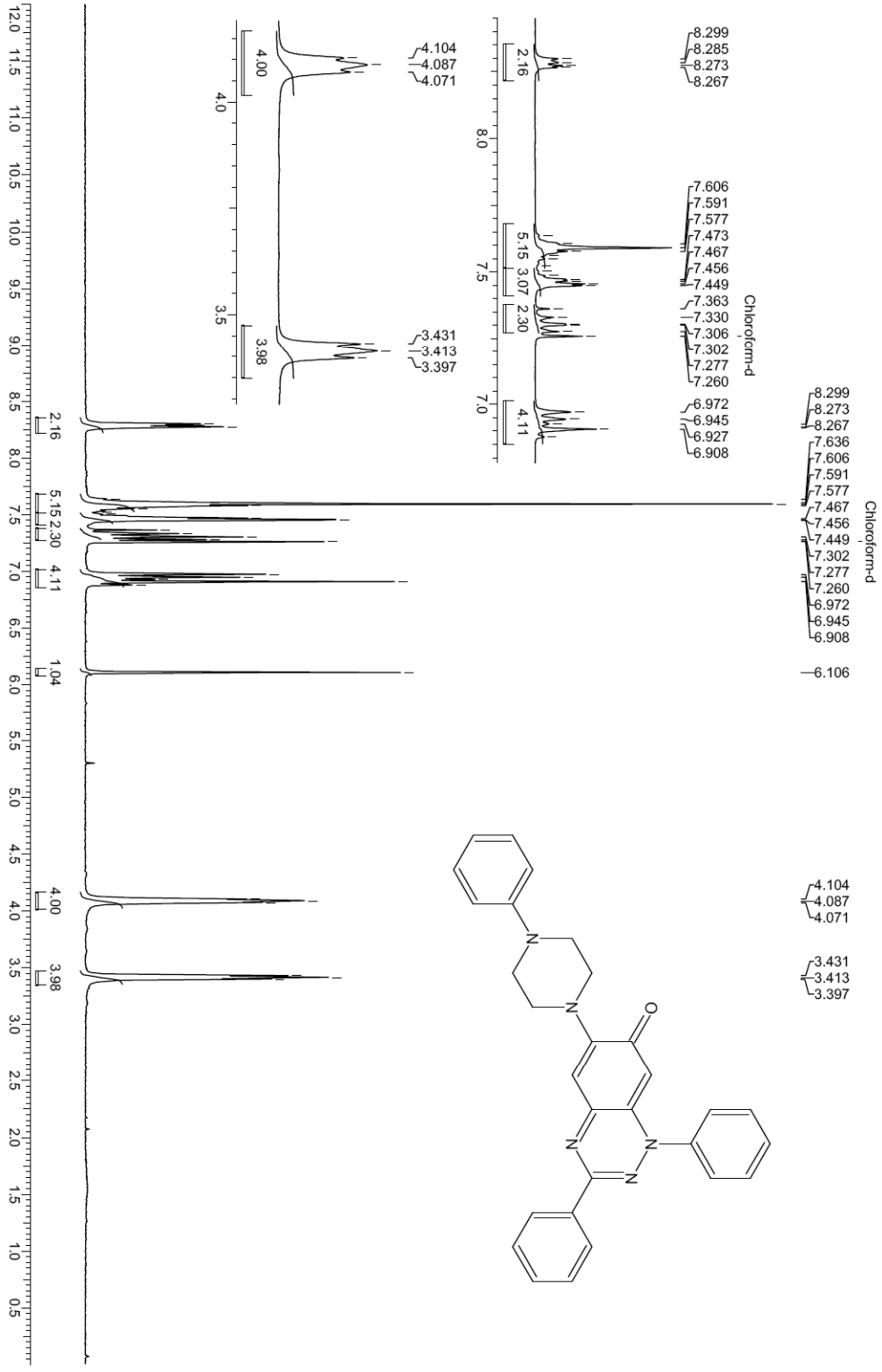
^{1}H NMR of *1,3-Diphenyl-6-(phenylamino)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**21**)*



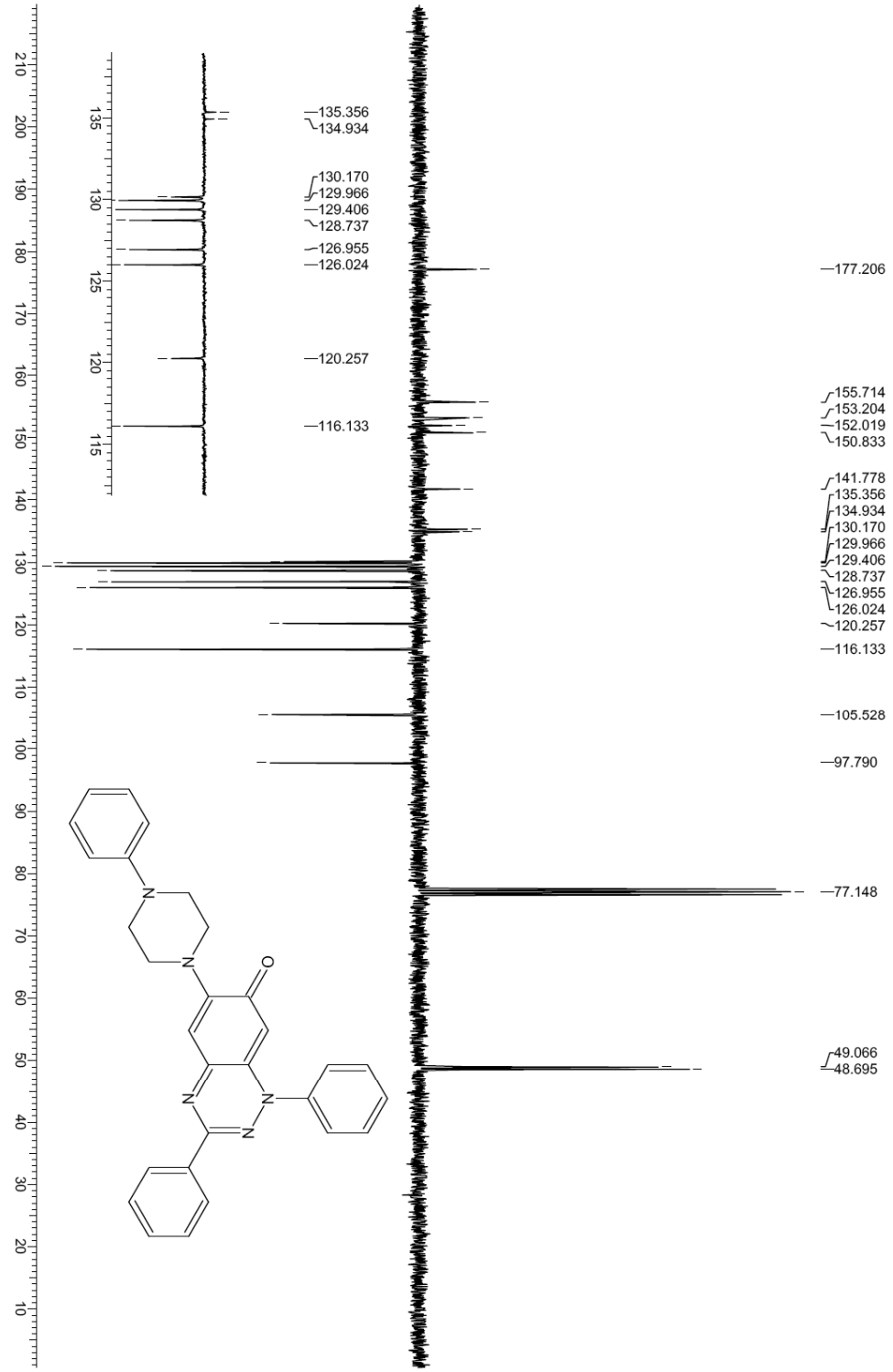
^{13}C NMR of *1,3-Diphenyl-6-(phenylamino)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**21**)*



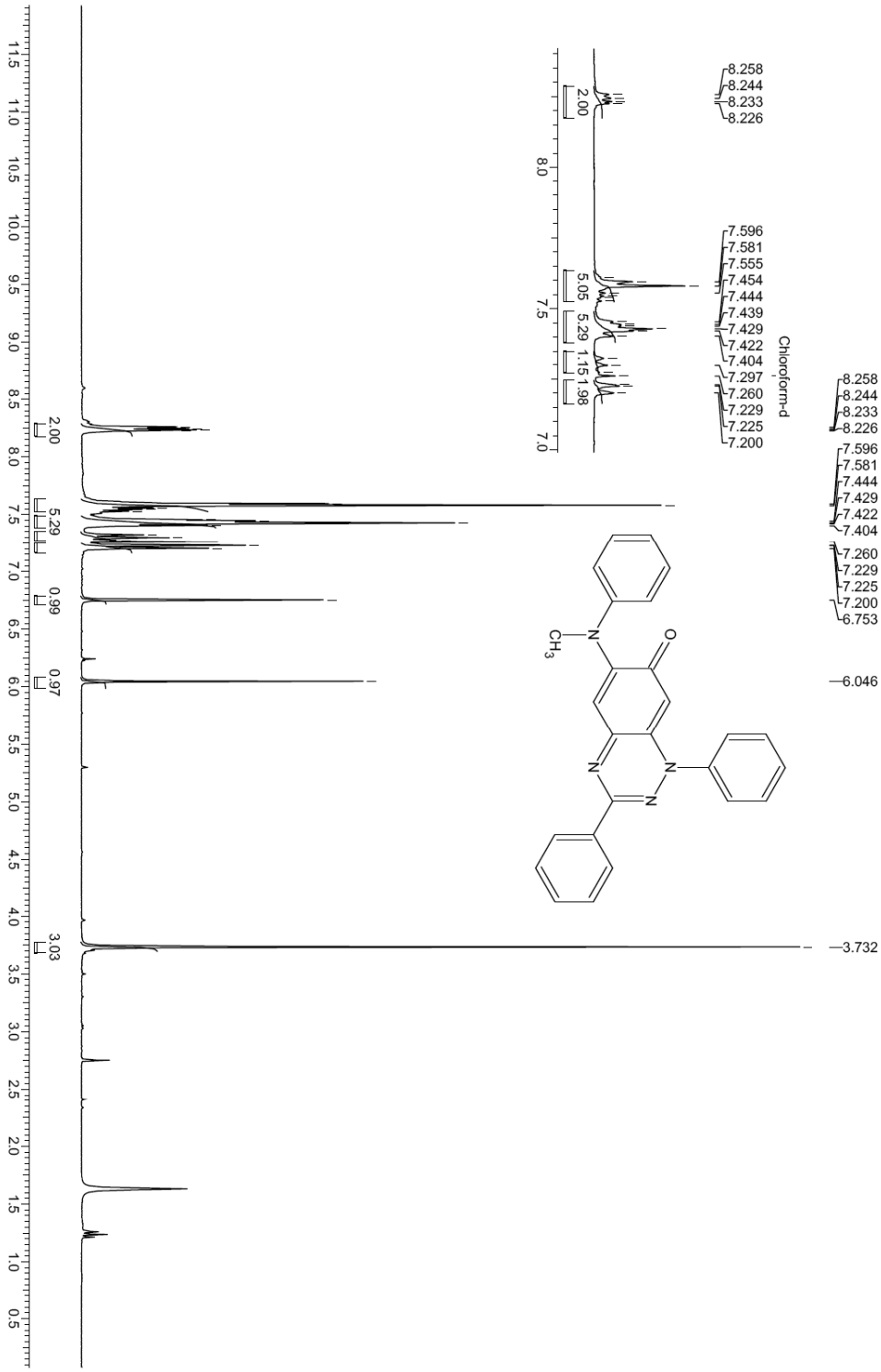
^{1}H NMR of *6-(4-Phenylpiperazin-1-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**22**)*



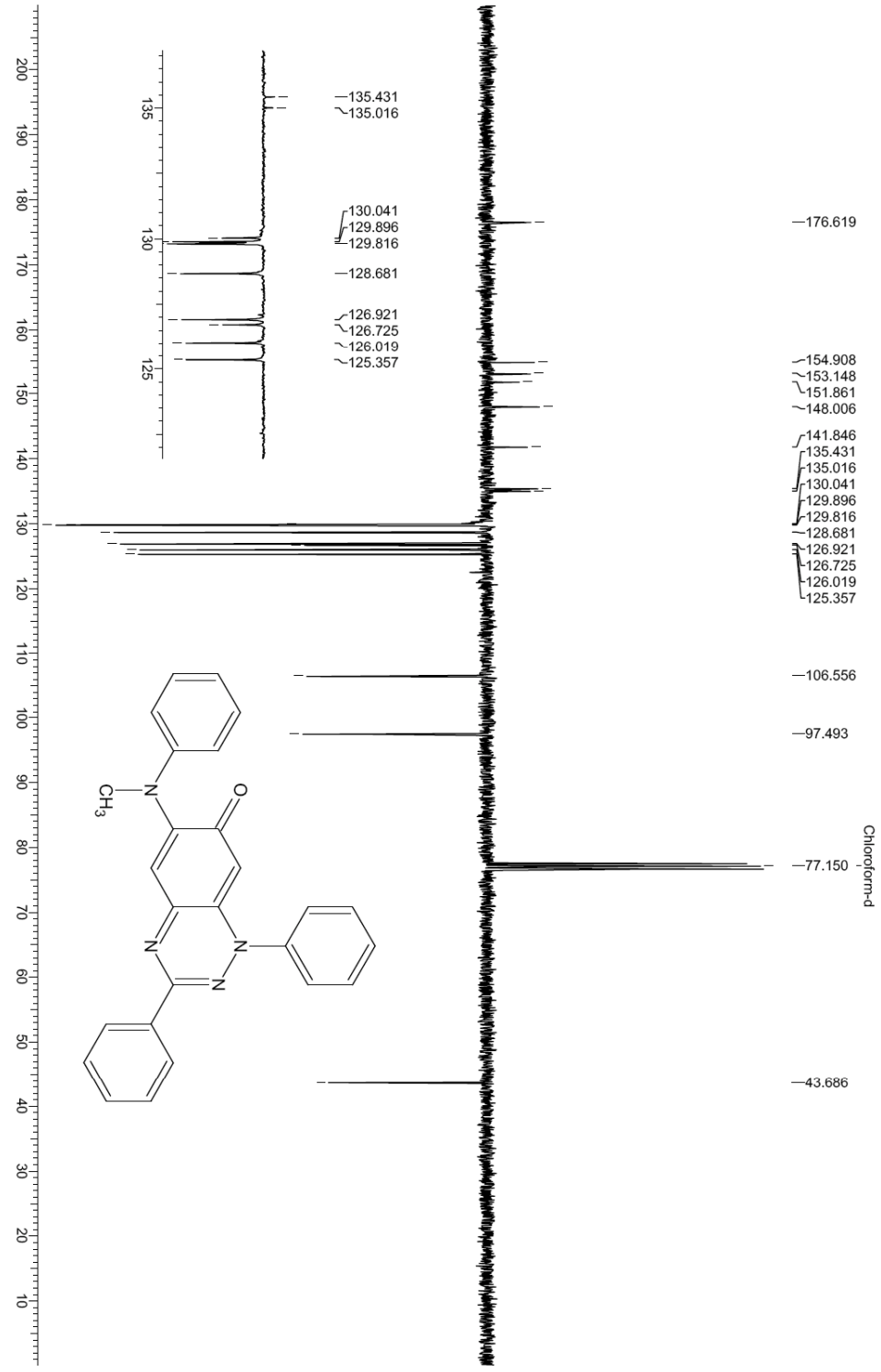
^{13}C NMR of *6-(4-Phenylpiperazin-1-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**22**)*



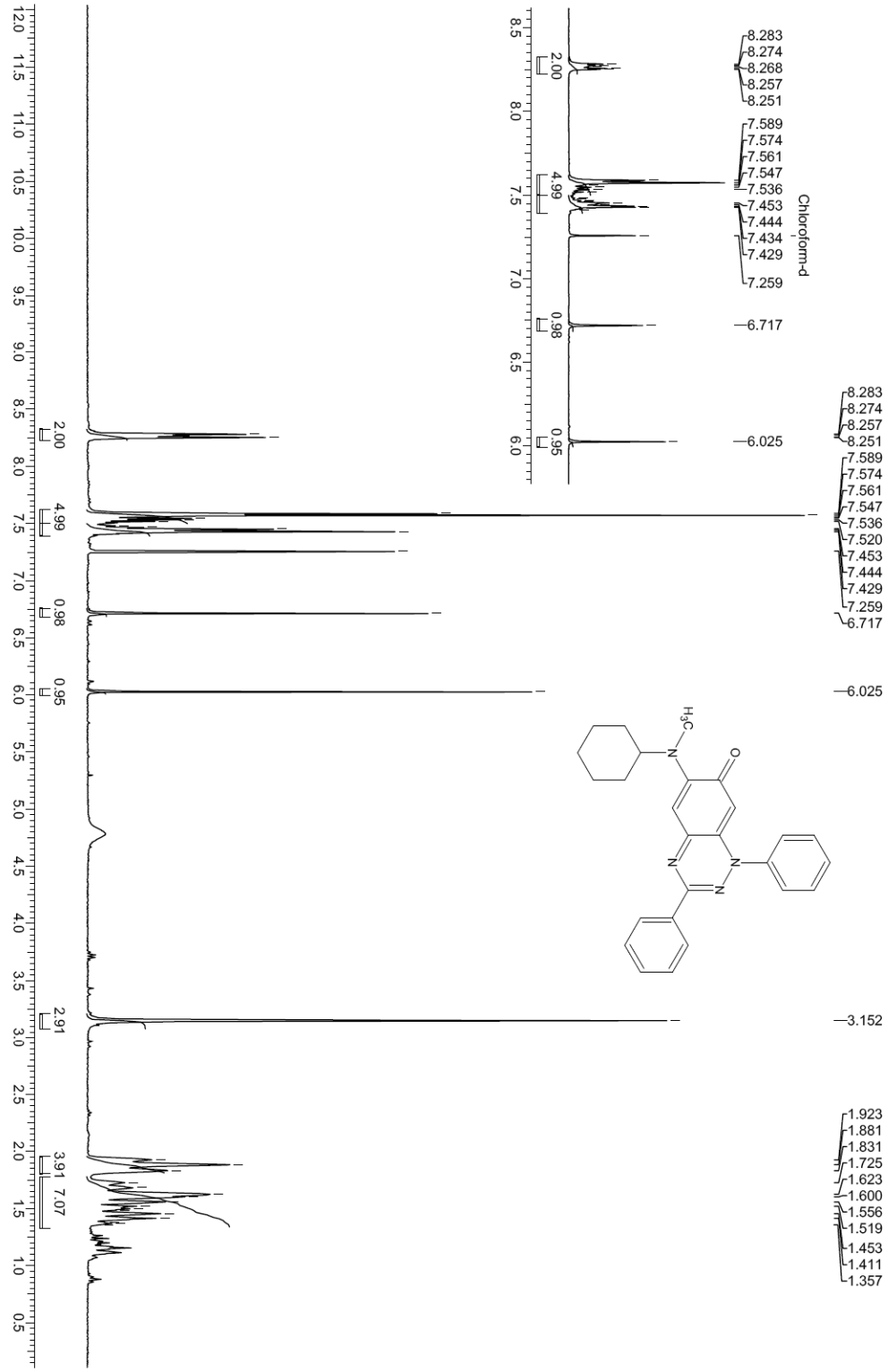
^{1}H NMR of *6-(*N-*Methyl*-N-*phenylamino)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**23**)*



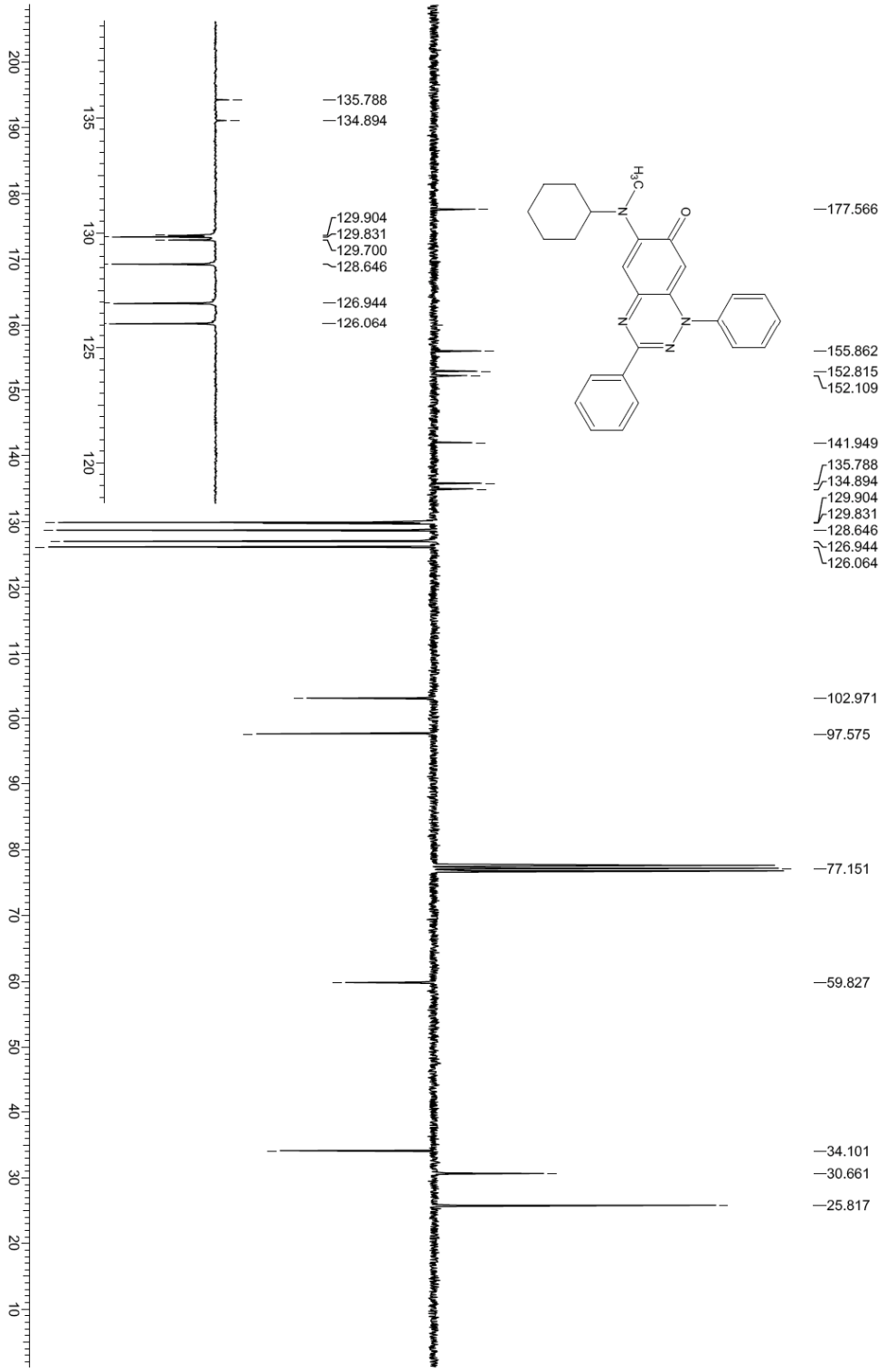
^{13}C NMR of *6-(*N-*Methyl*-N-*phenylamino)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**23**)*



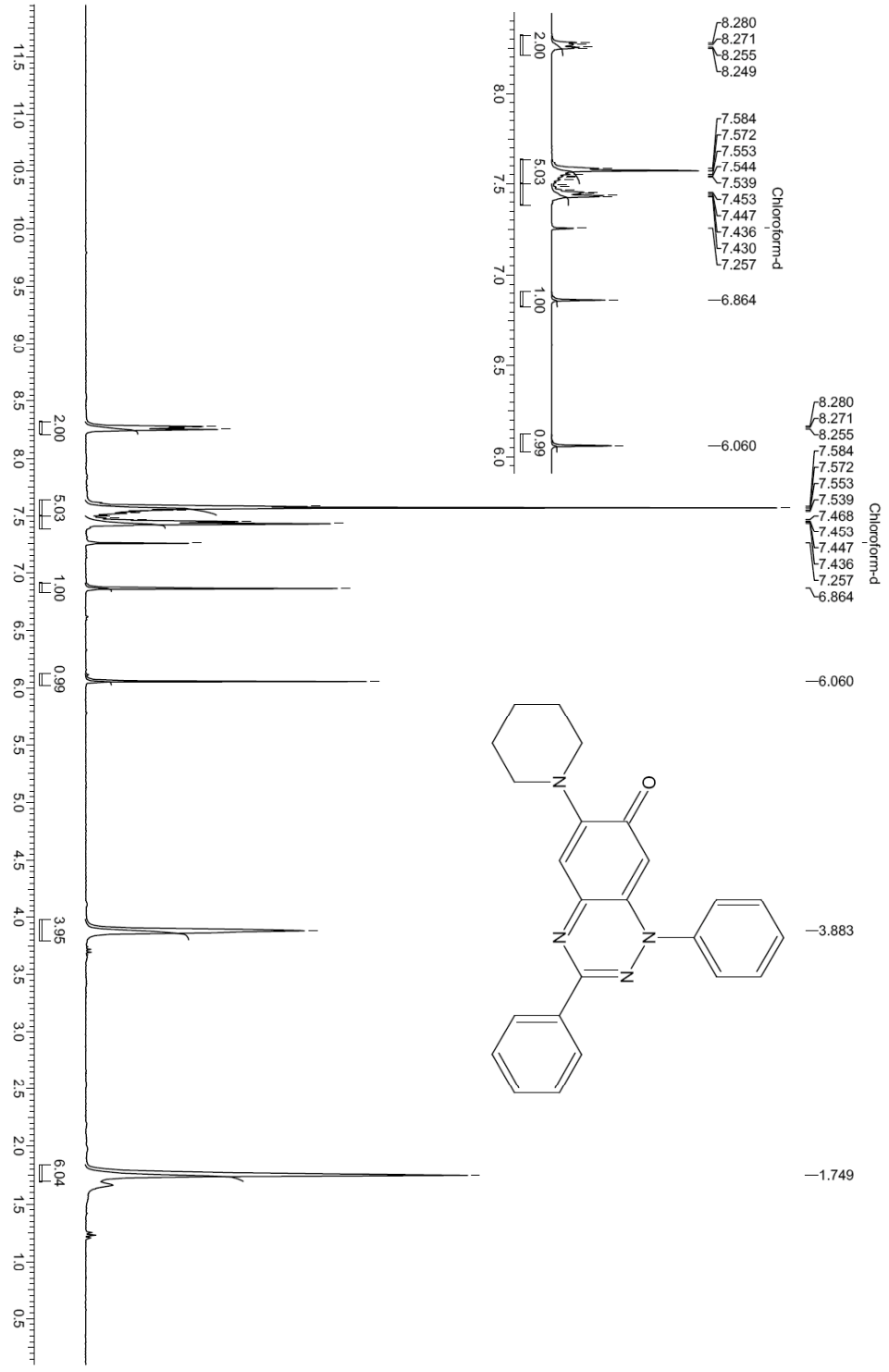
^{1}H NMR of *6-(*N-*Cyclohexyl*-N-*methylamino)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**24**)*



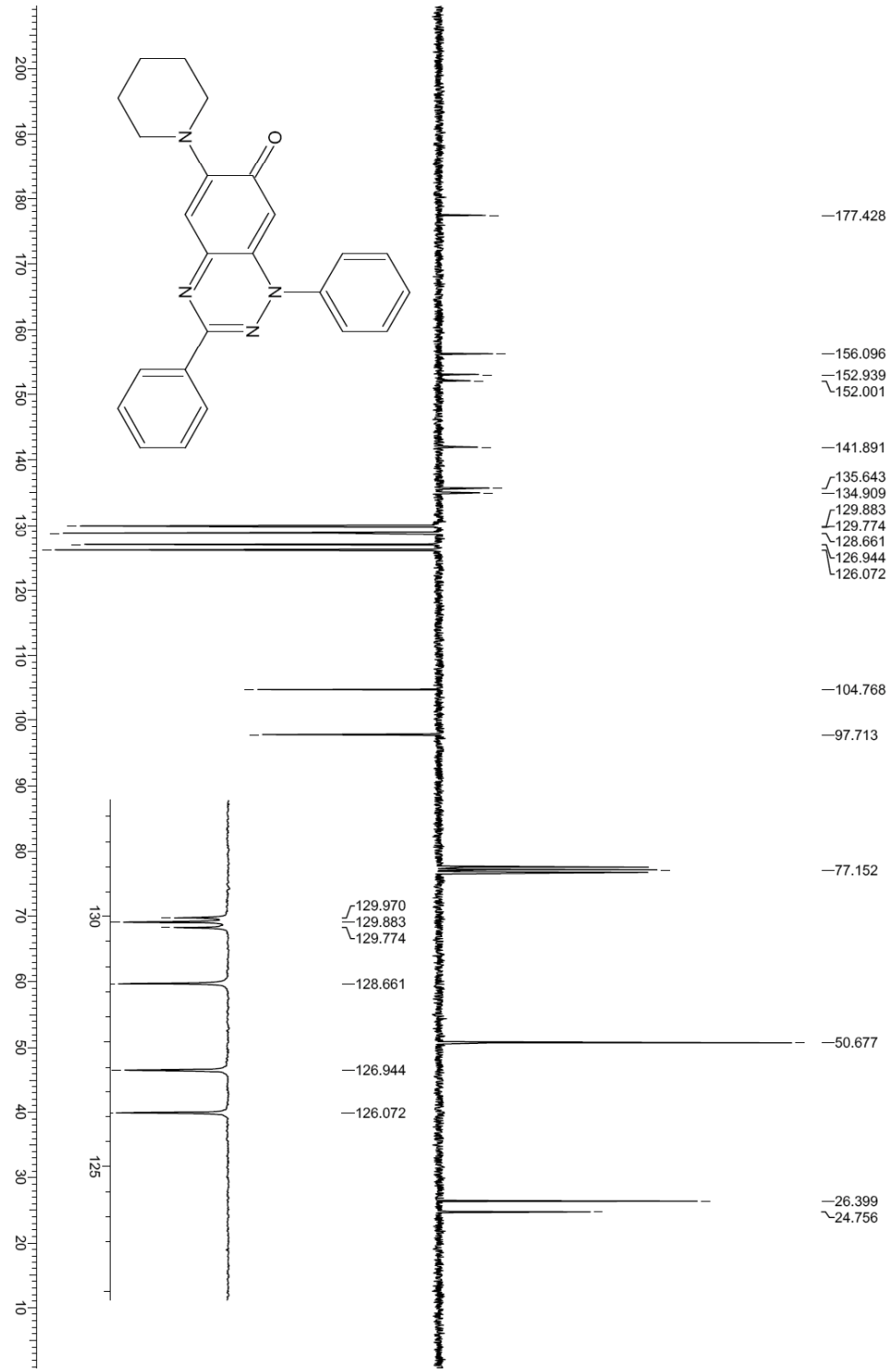
^{13}C NMR of *6-(*N-*Cyclohexyl*-N-*methylamino)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**24**)*



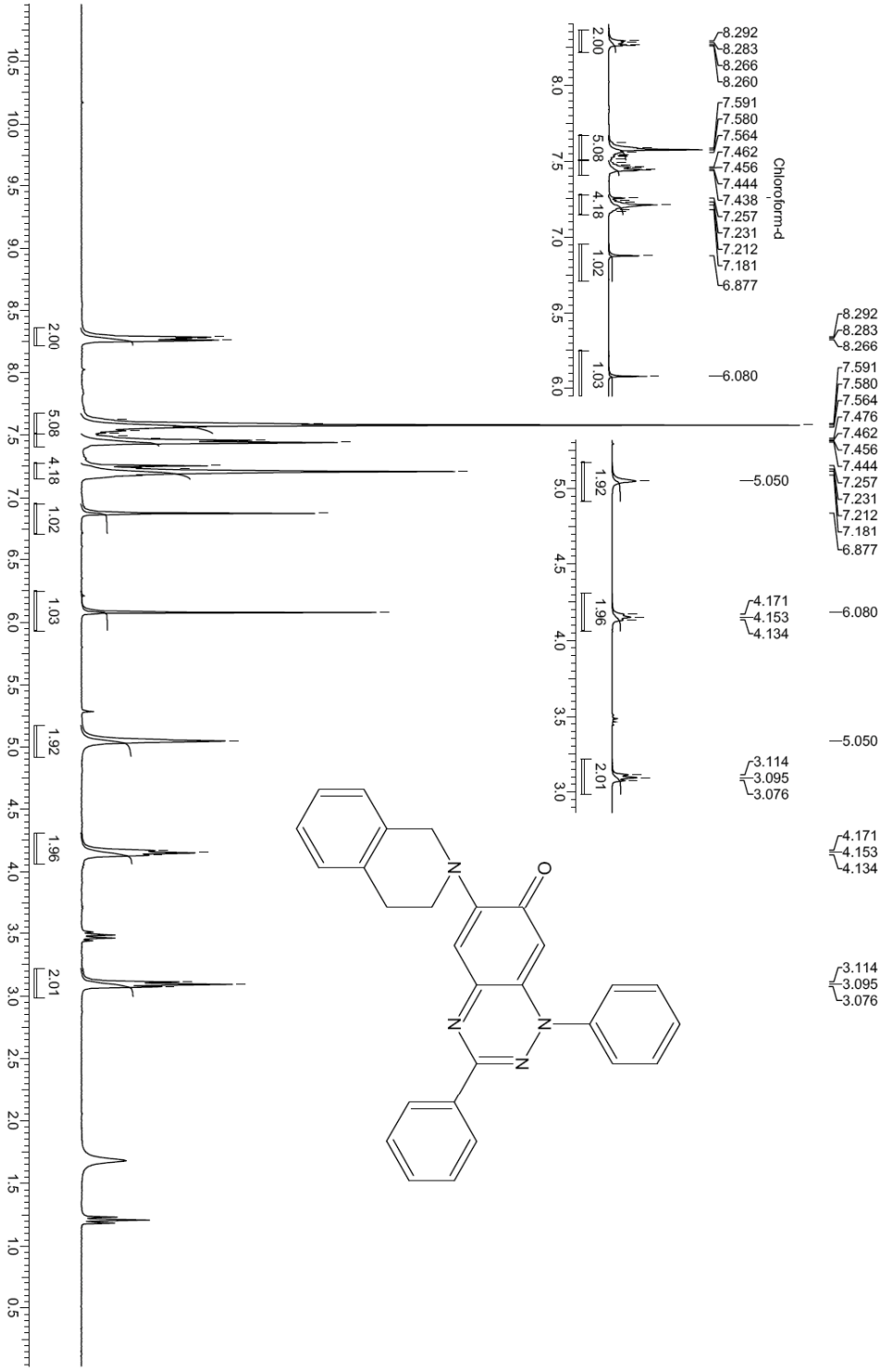
^{1}H NMR of ,*3-Diphenyl-6-(piperidin-1-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**25**)*



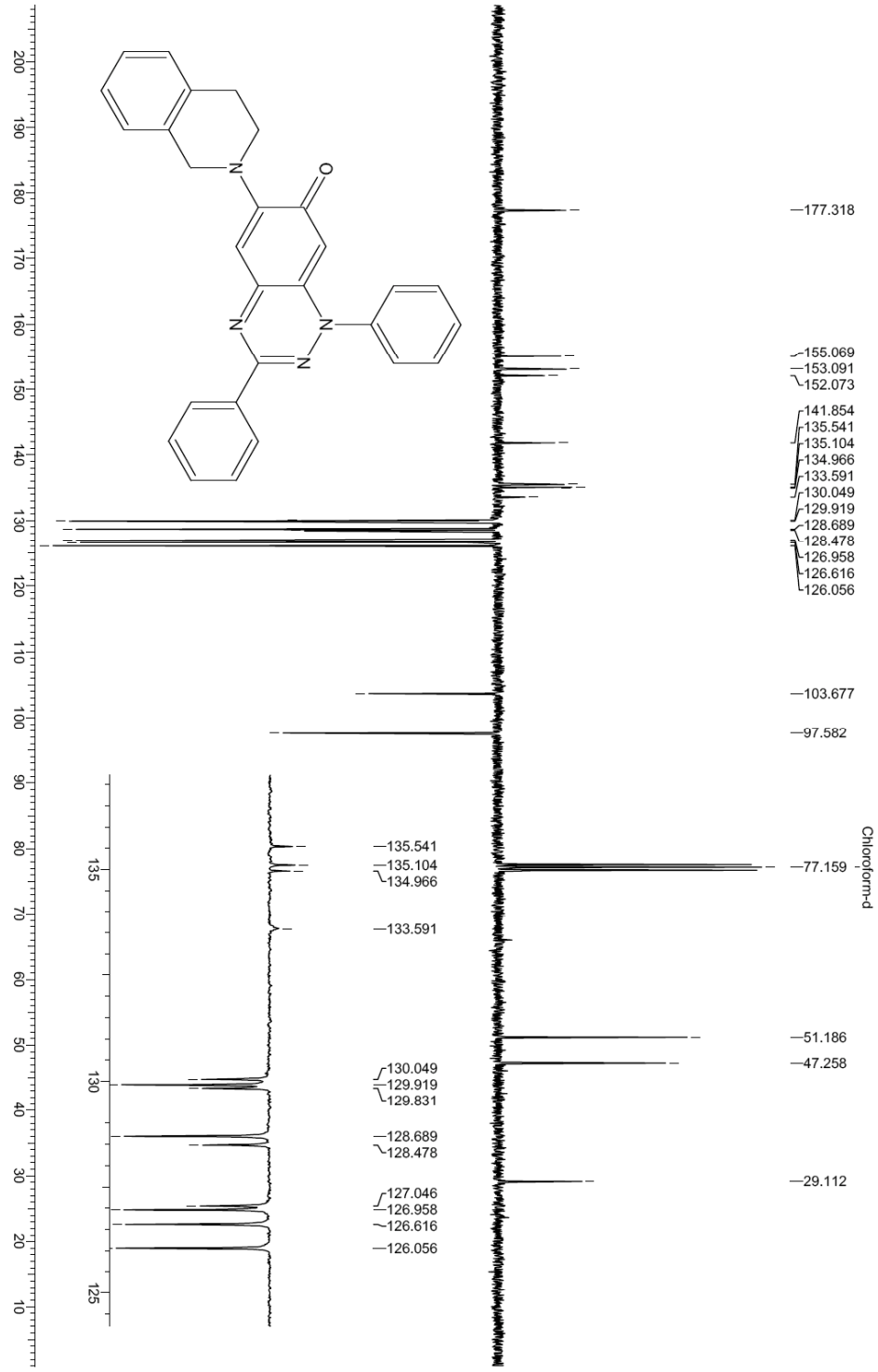
^{13}C NMR of *,3-Diphenyl-6-(piperidin-1-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**25**)*



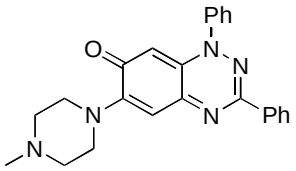
^{1}H NMR of *6-[3,4-Dihydroisoquinolin-2(1H)-yl]-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**26**)*

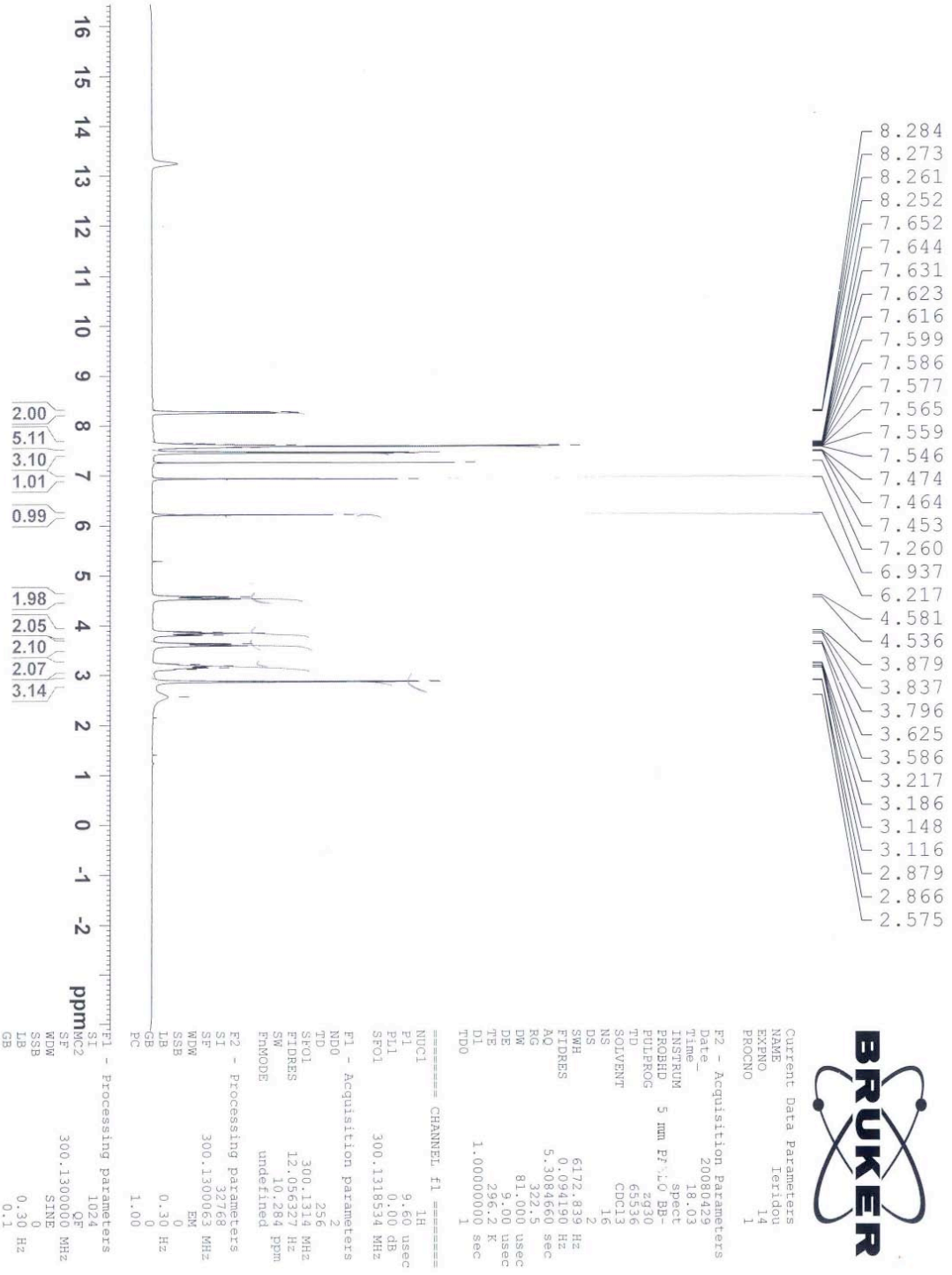


^{13}C NMR of *6-[3,4-Dihydroisoquinolin-2(1H)-yl]-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**26**)*

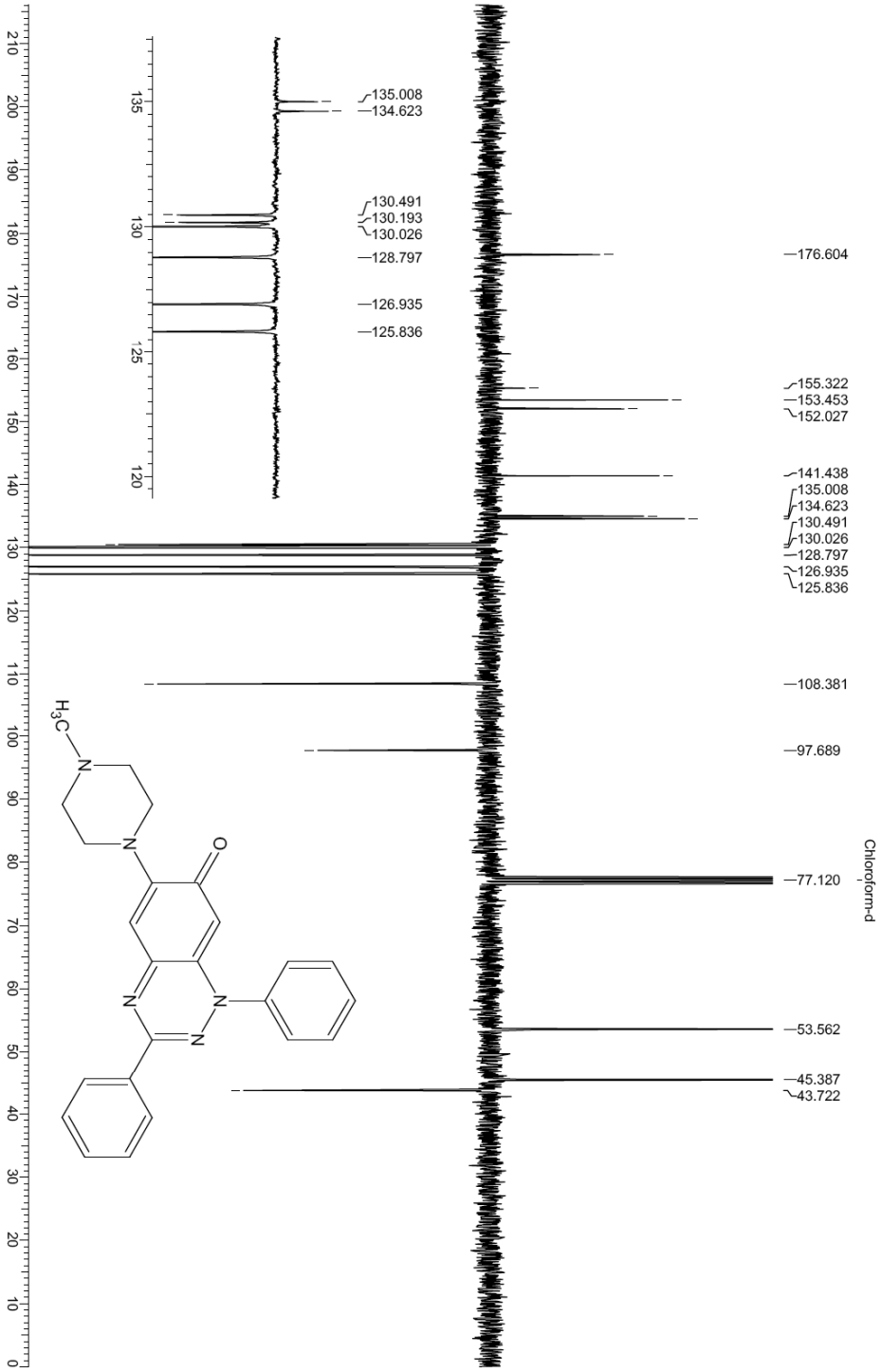


^{1}H NMR of *(4-Methylpiperazin-1-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**27**)*

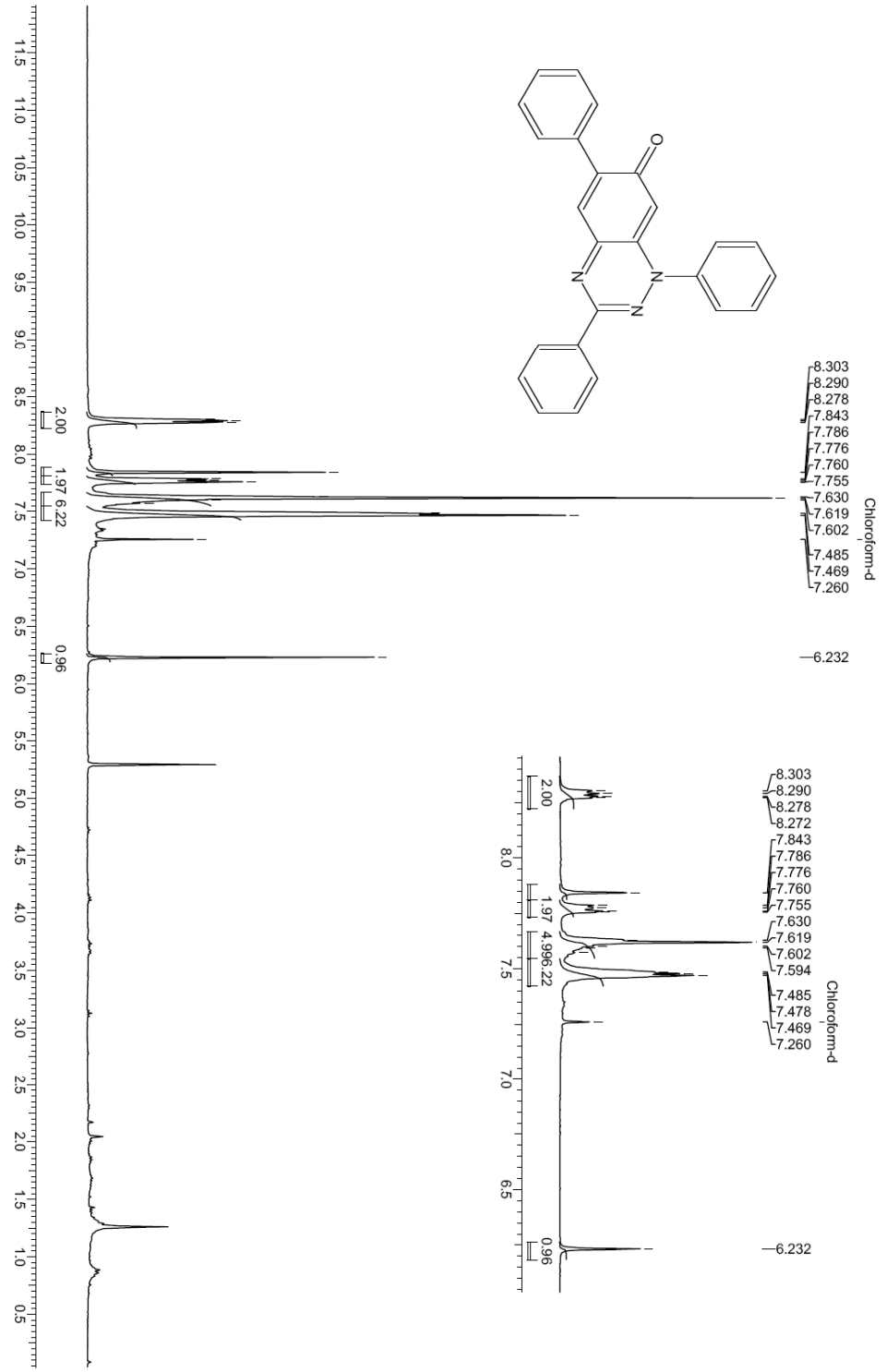




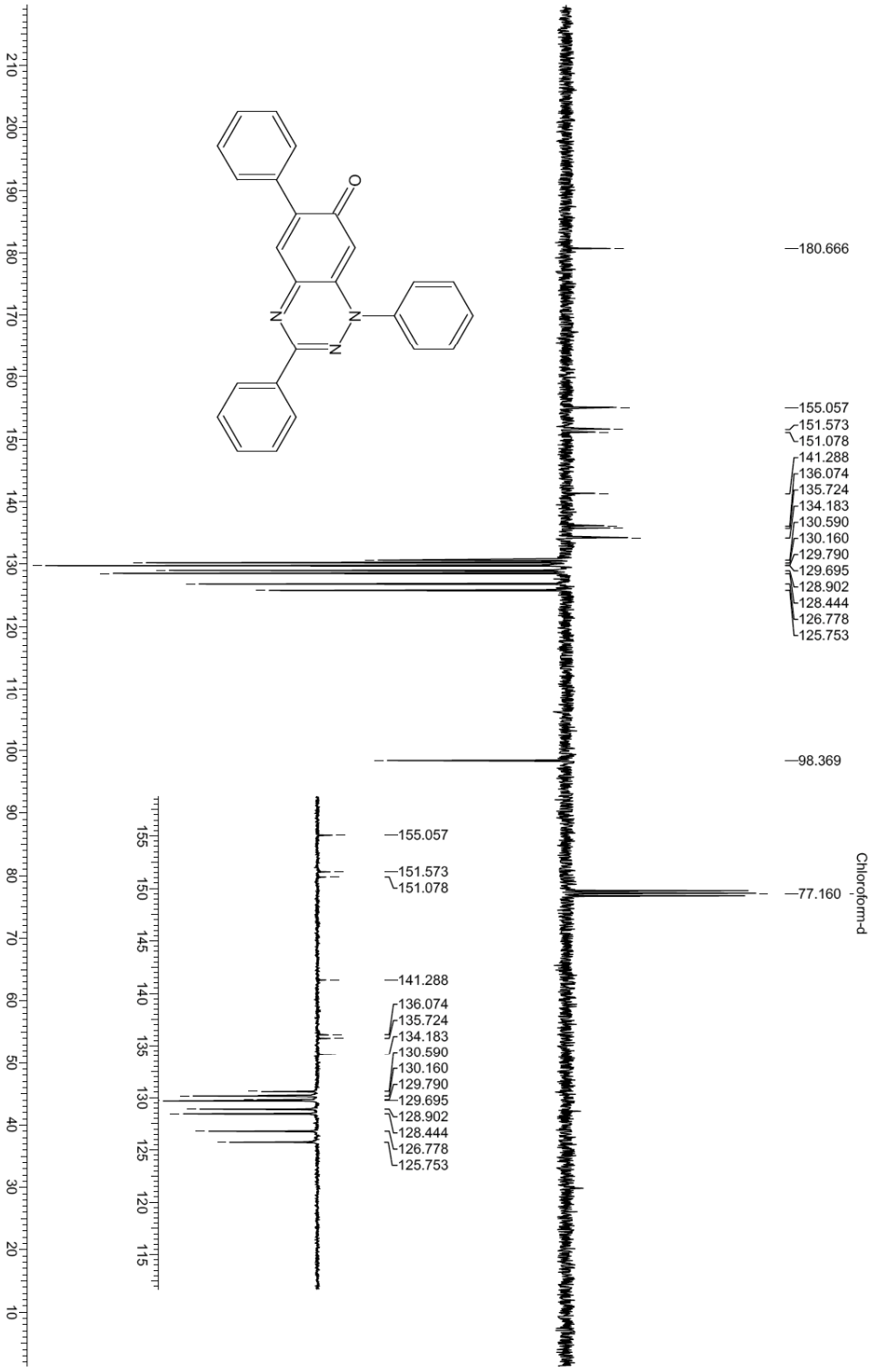
^{13}C NMR of *(4-Methylpiperazin-1-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**27**)*



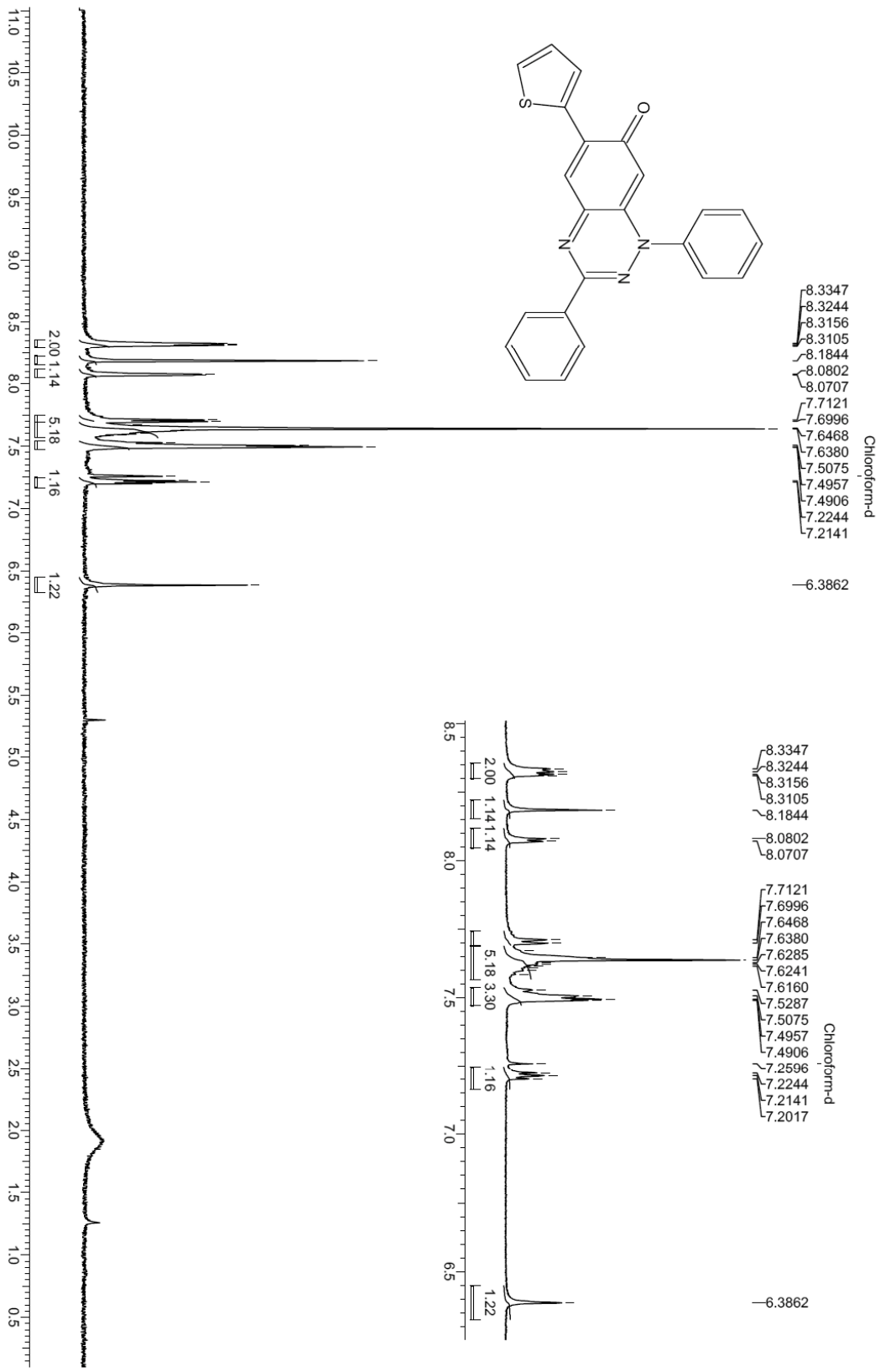
^{1}H NMR of *1,3,6-Triphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* ***(28)***



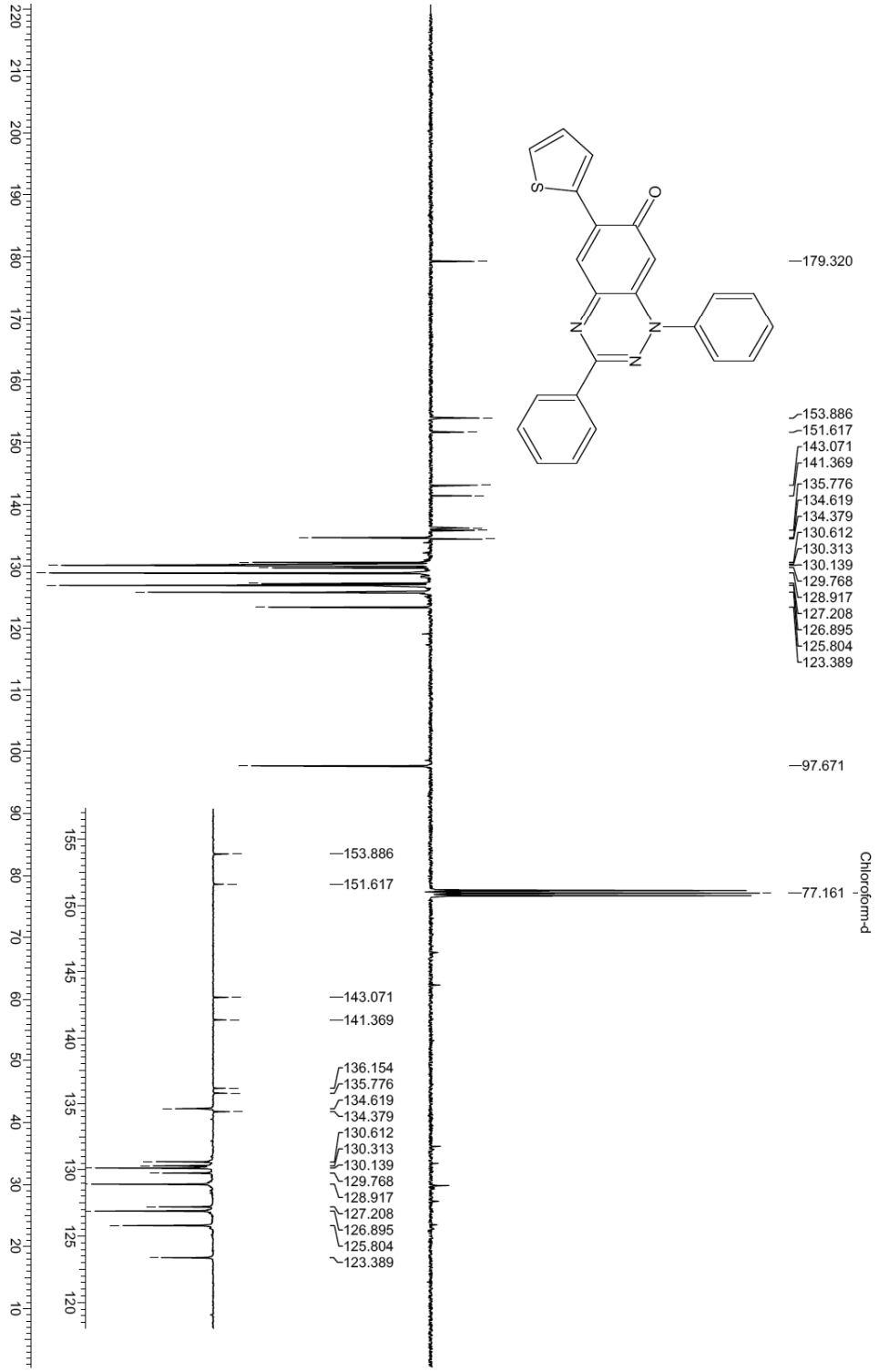
^{13}C NMR of *1,3,6-Triphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**28**)*



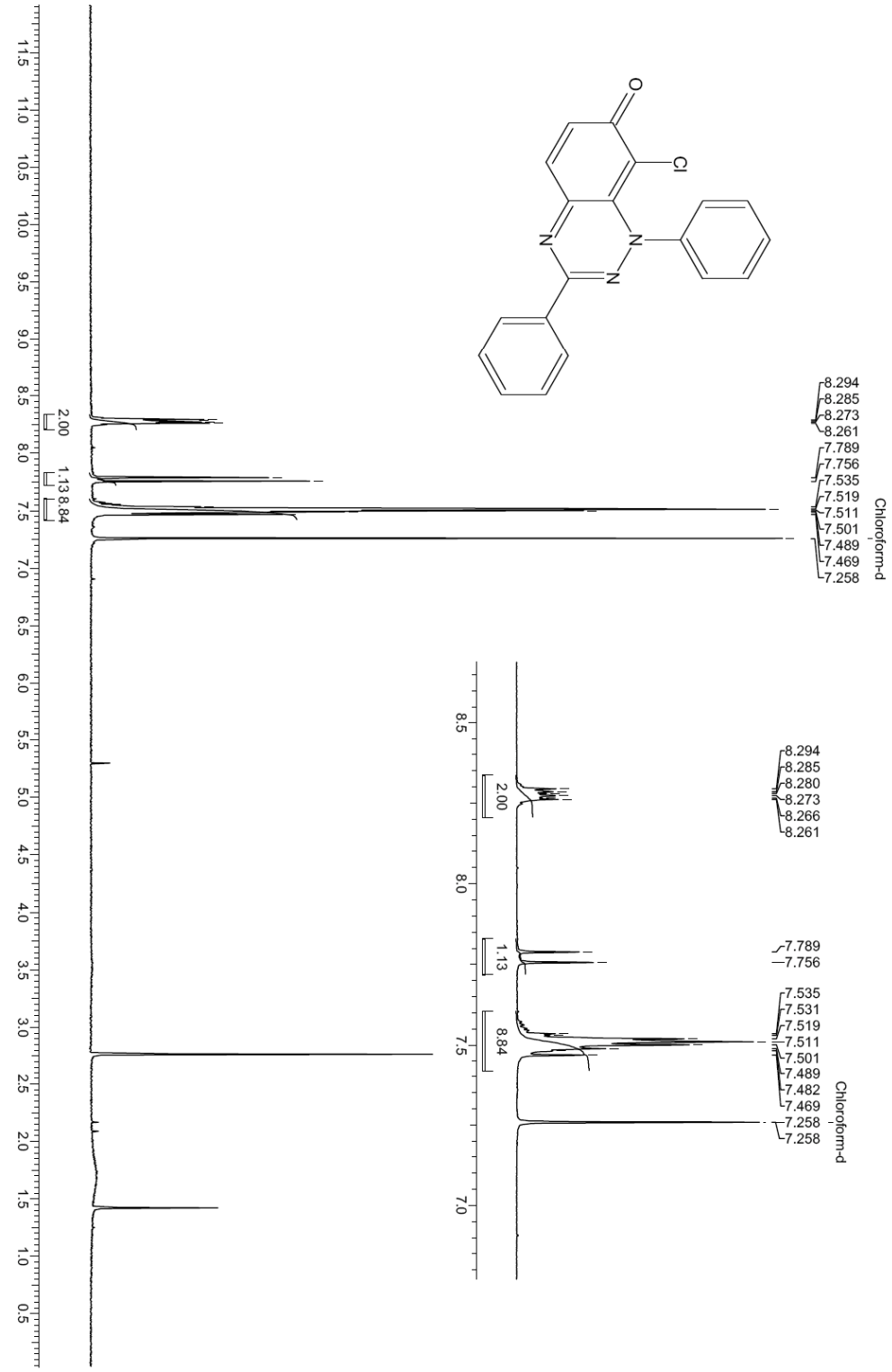
^{1}H NMR of *1,3-Diphenyl-6-(thiophen-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**29**)*



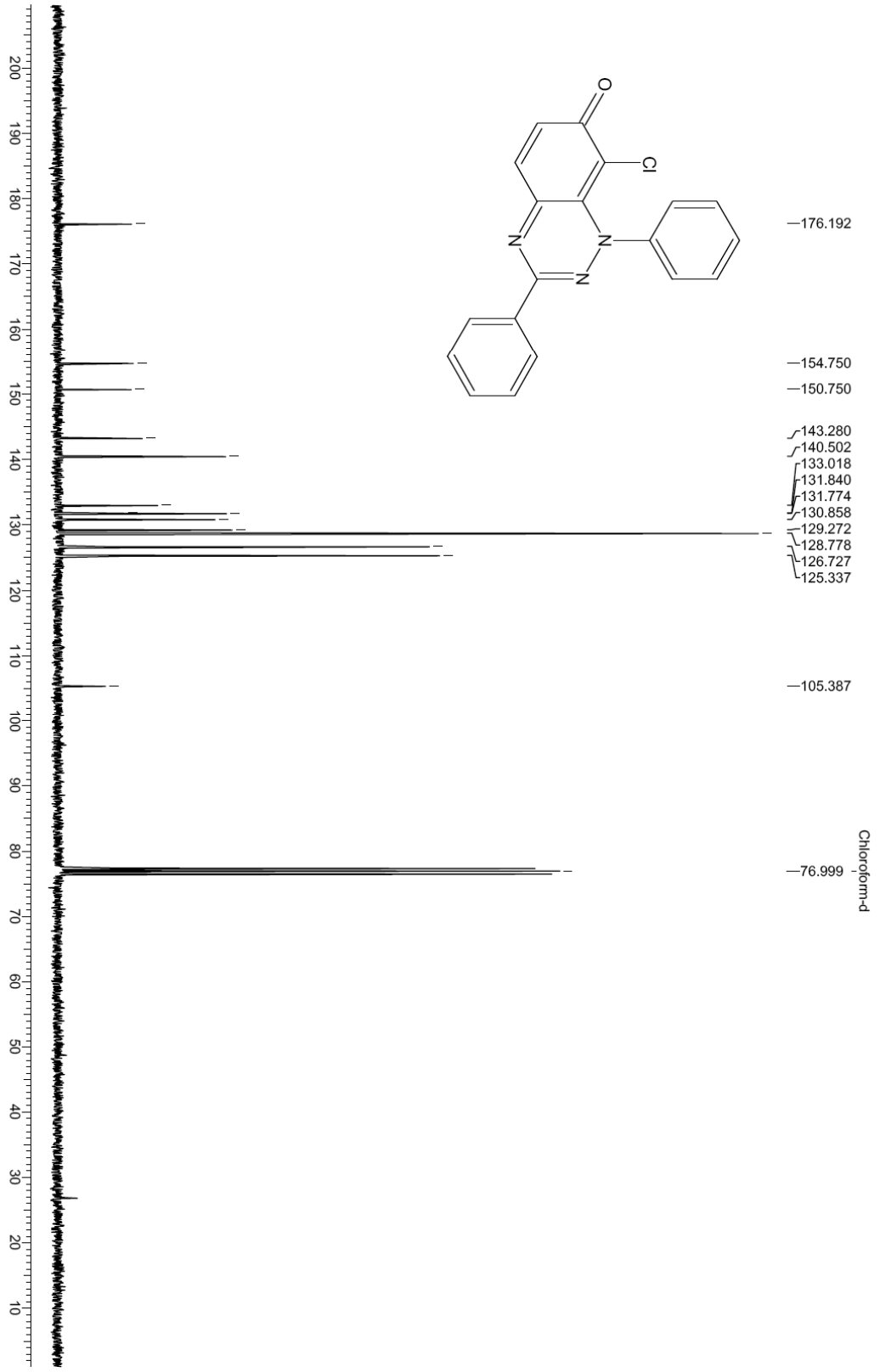
^{13}C NMR of *1,3-Diphenyl-6-(thiophen-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one* (***29***)



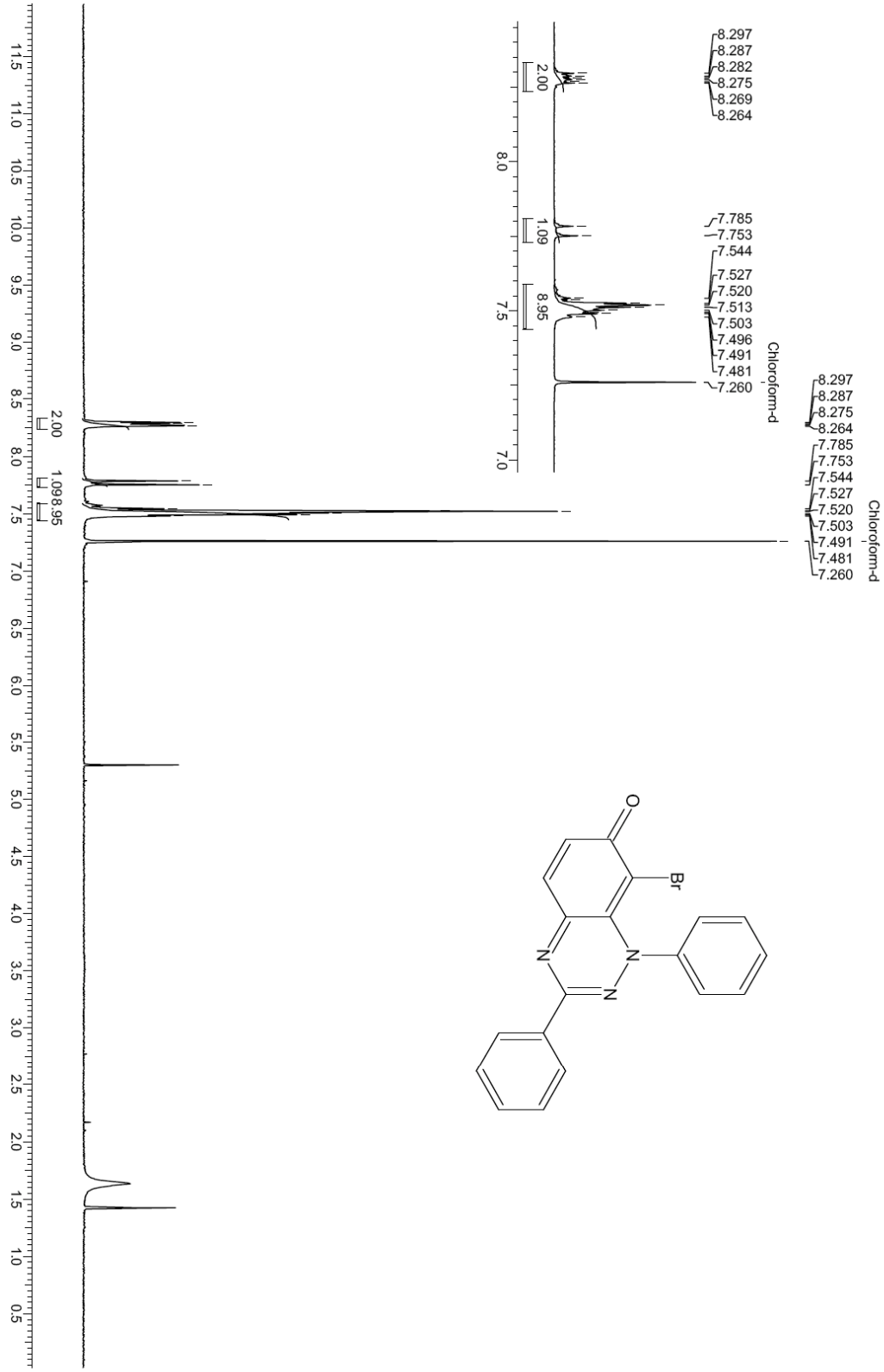
^{1}H NMR of *8-Chloro-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* ***(30)***



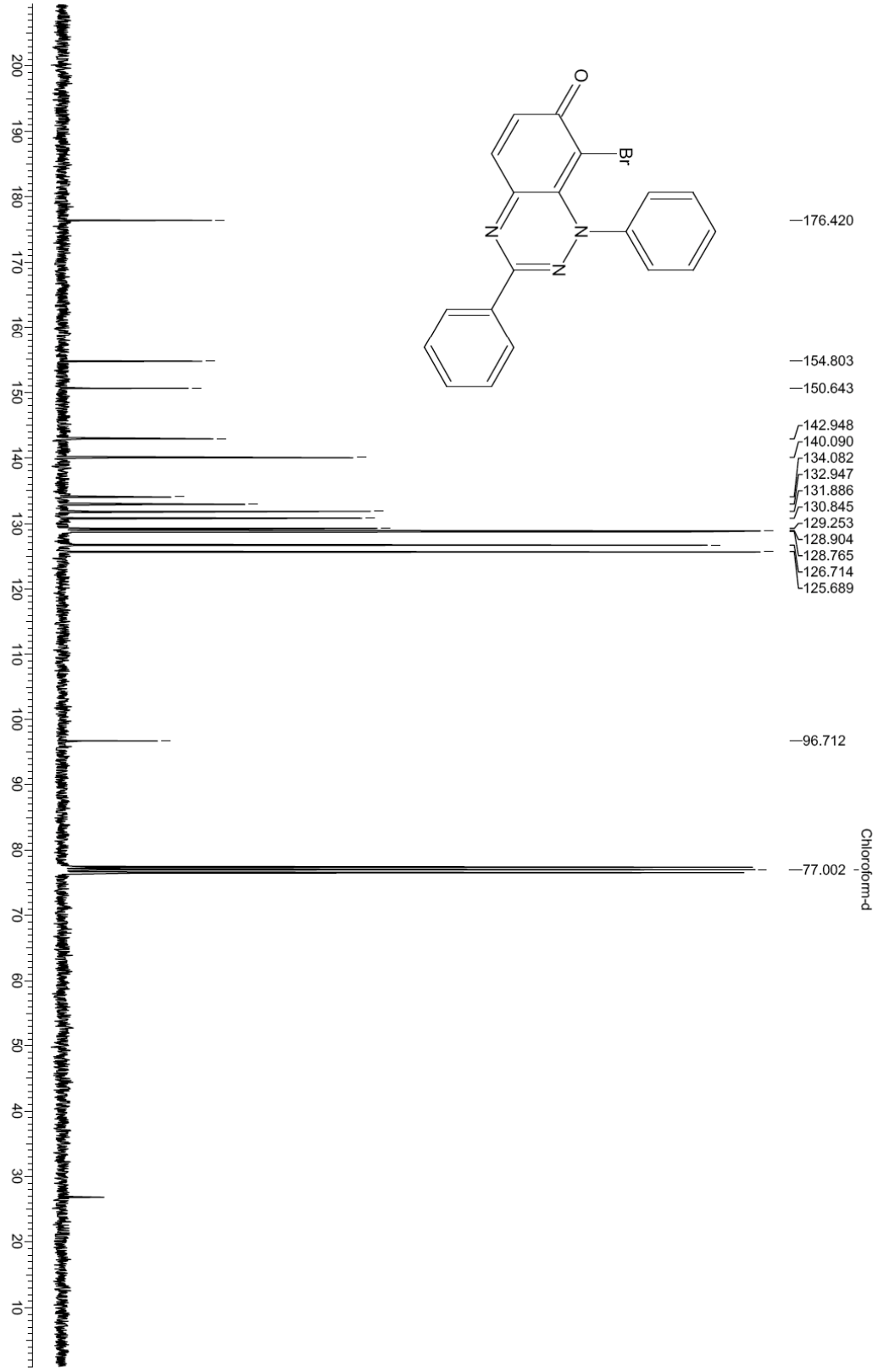
^{13}C NMR of *8-Chloro-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* ***(30)***



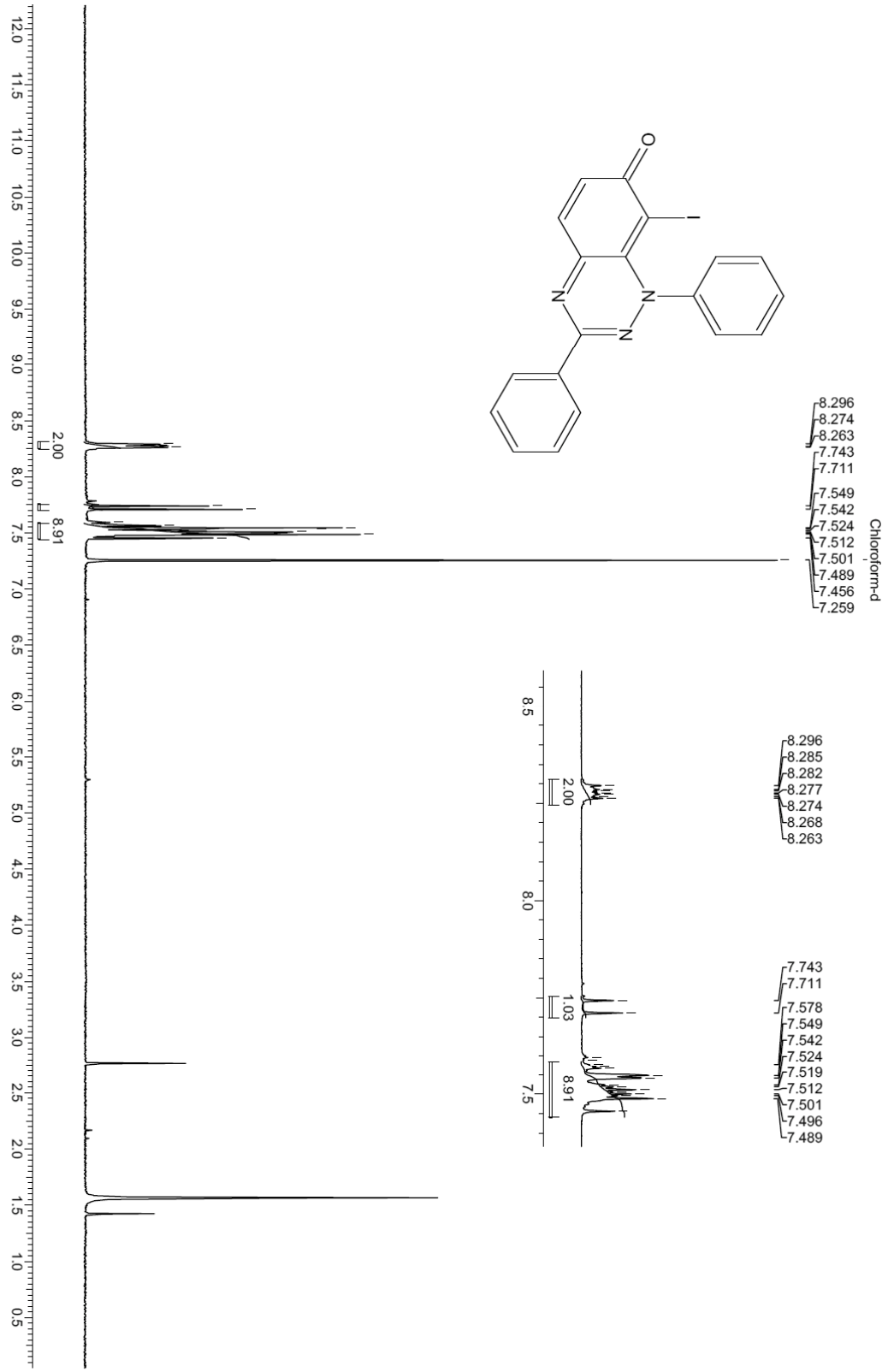
^{1}H NMR of *8-Bromo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* ***(*****31*****)***



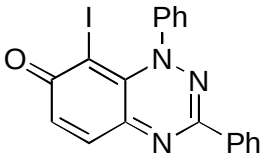
^{13}C NMR of *8-Bromo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* ***(31)***

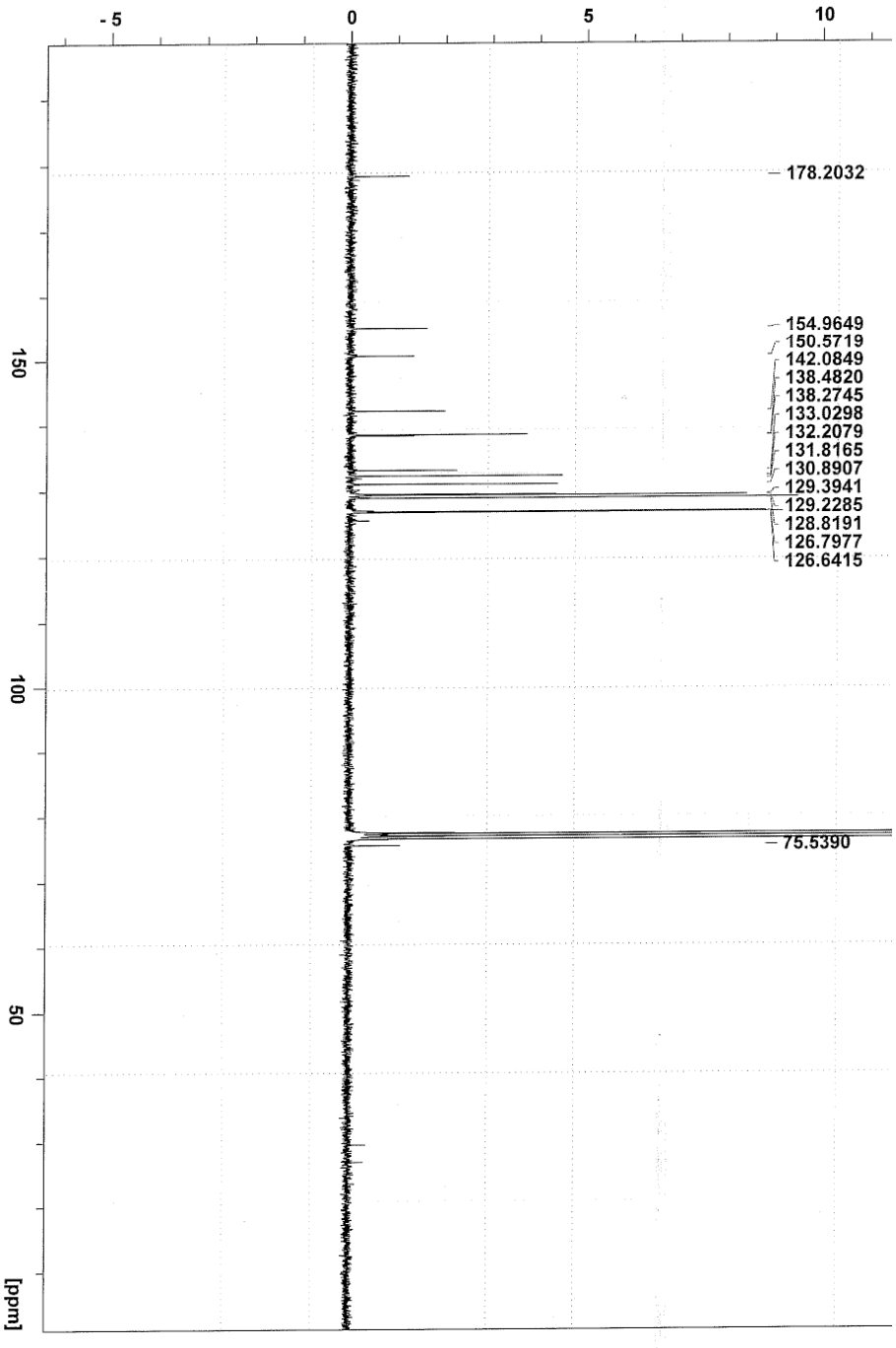


^{1}H NMR of *8-Iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**)*

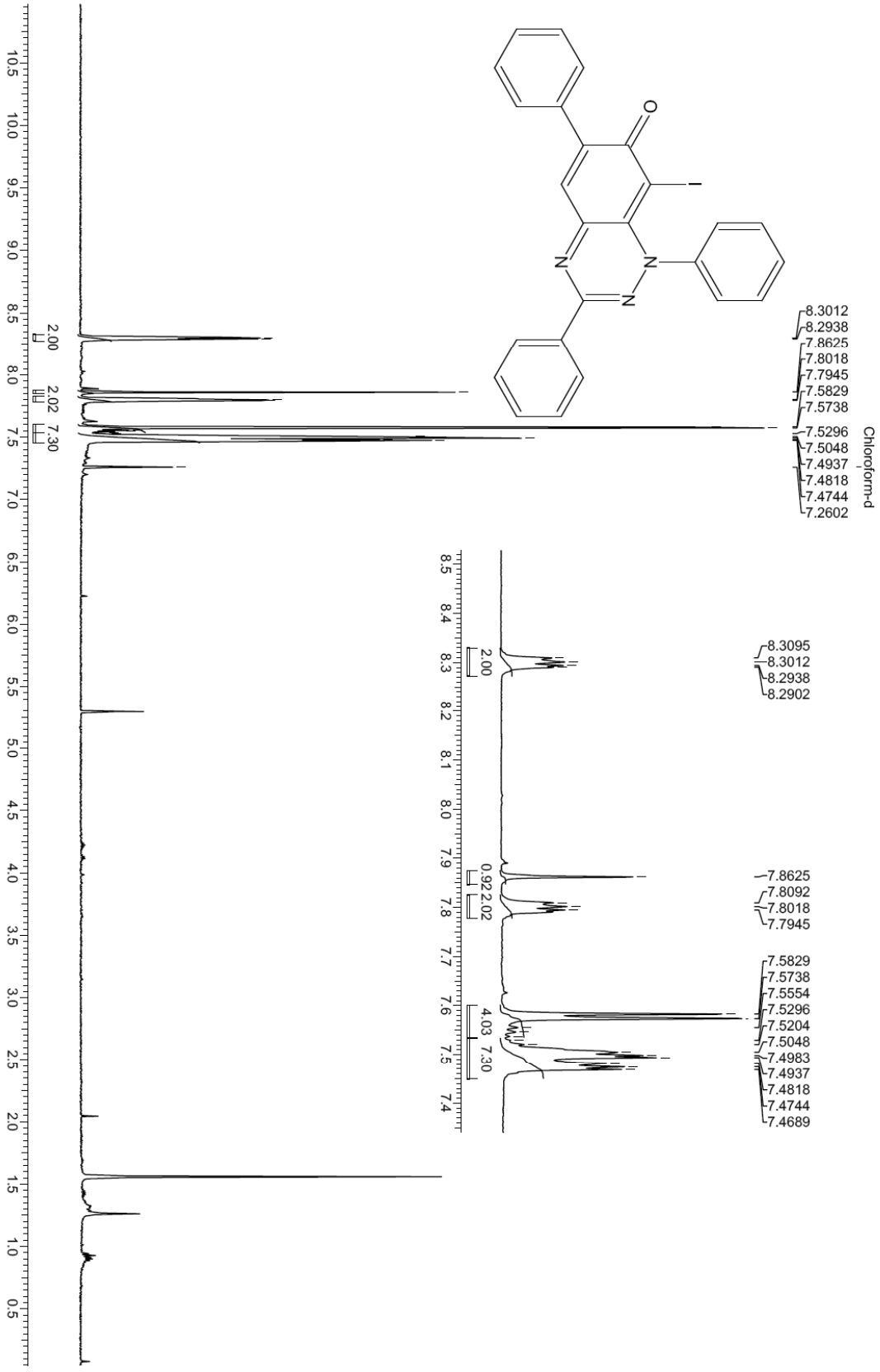


^{13}C NMR of *8-Iodo-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**32**)*



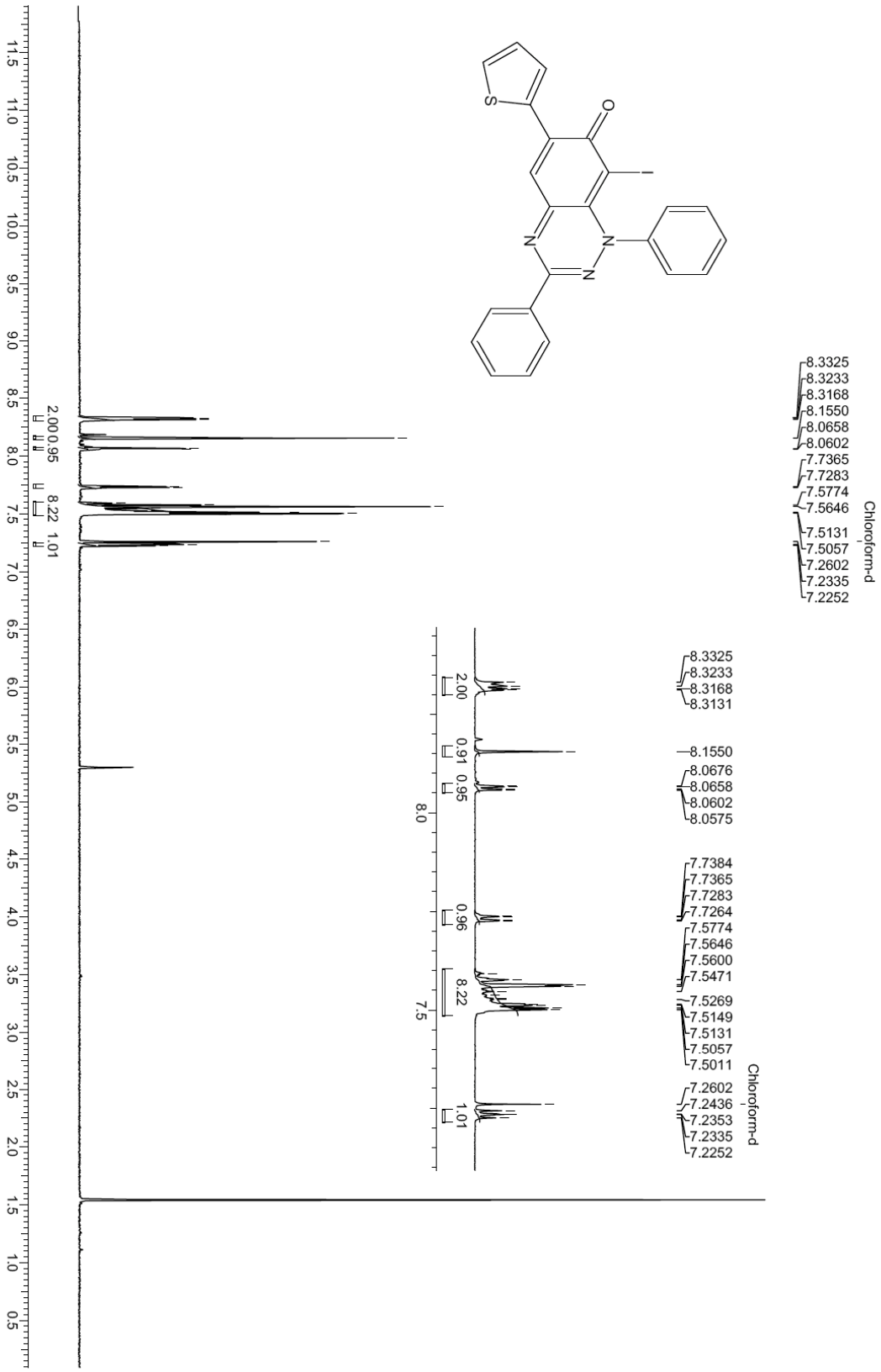


^{1}H NMR of *8-Iodo-1,3,6-triphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**33**)*

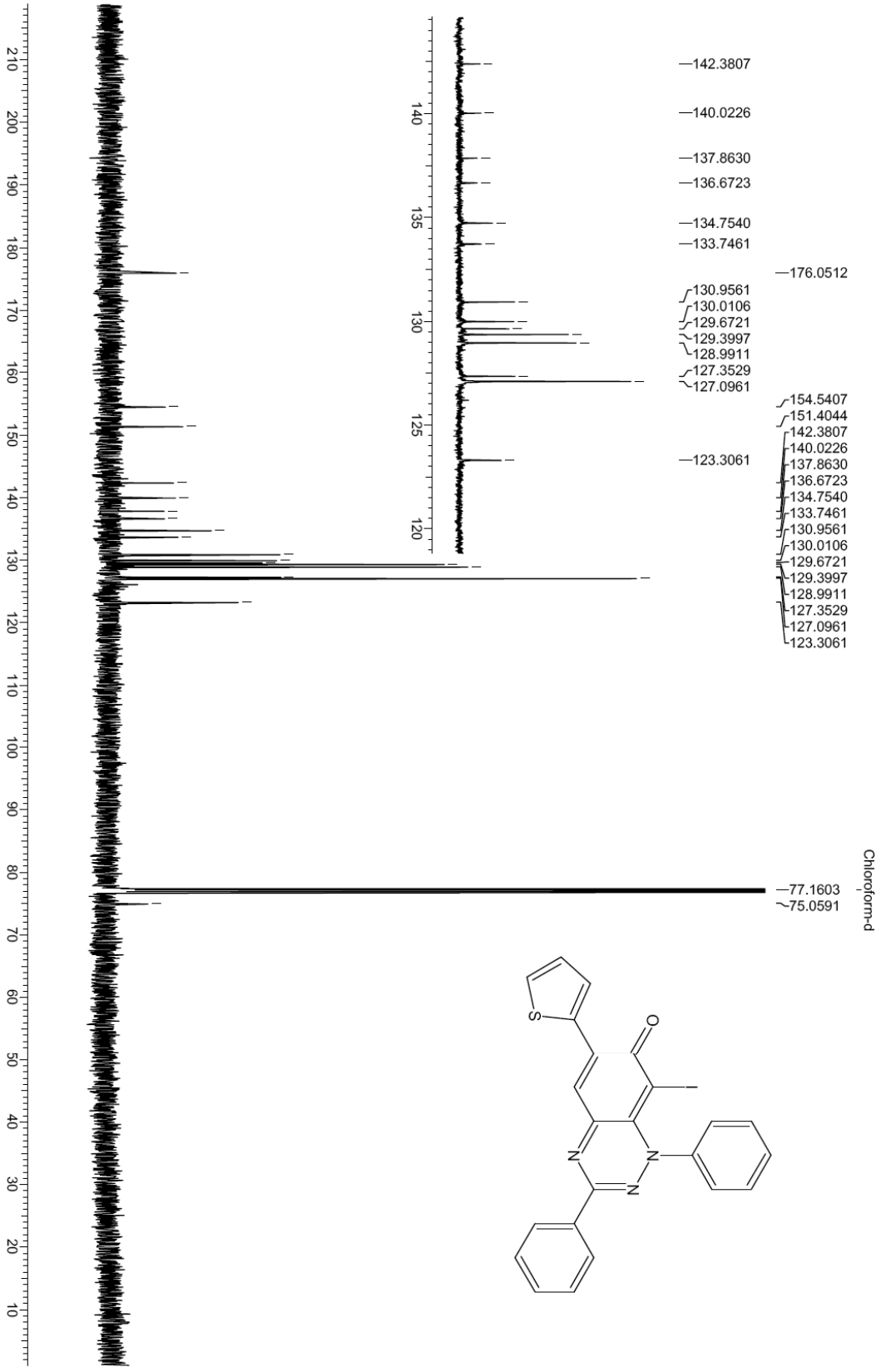


^{13}C NMR of *8-Iodo-1,3,6-triphenylbenzo*[e]*[1,2,4]triazin-7(1*H*)-one* (***33***)

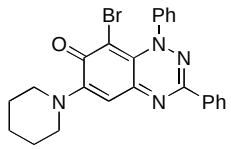
^{1}H NMR of *8-Iodo-1,3-diphenyl-6-(thien-2-yl)benzo*[e]*[1,2,4]triazin-7(1*H*)-one (**34**)*

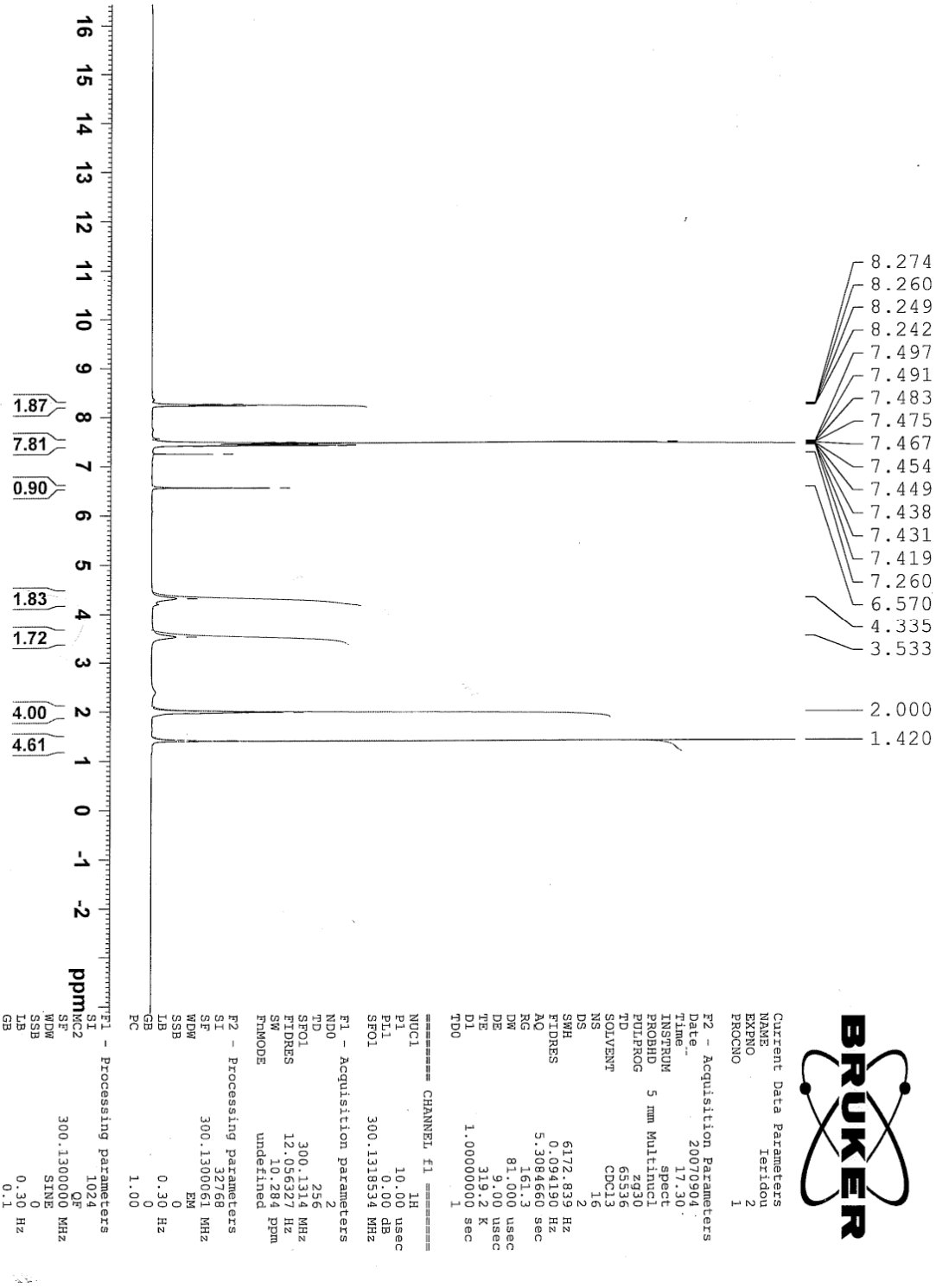


^{13}C NMR of *8-Iodo-1,3-diphenyl-6-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**34**)*

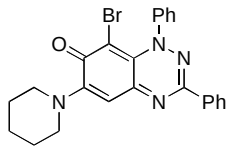


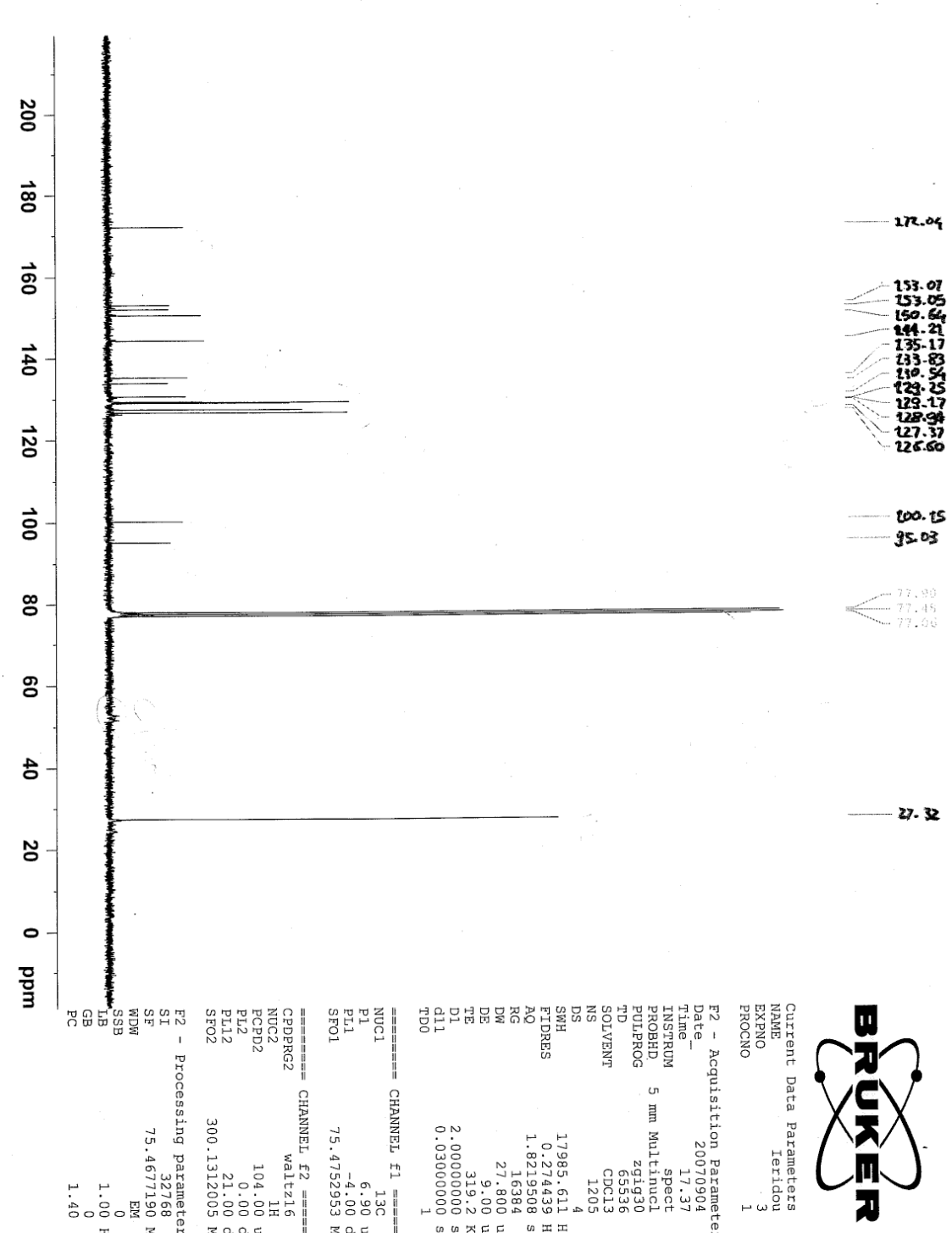
^{1}H NMR of *8-bromo-1,3-diphenyl-6-(pyrrolidin-1-yl)benzo[e][1,2,4]triazin-7(1H)-one* ***(35)***



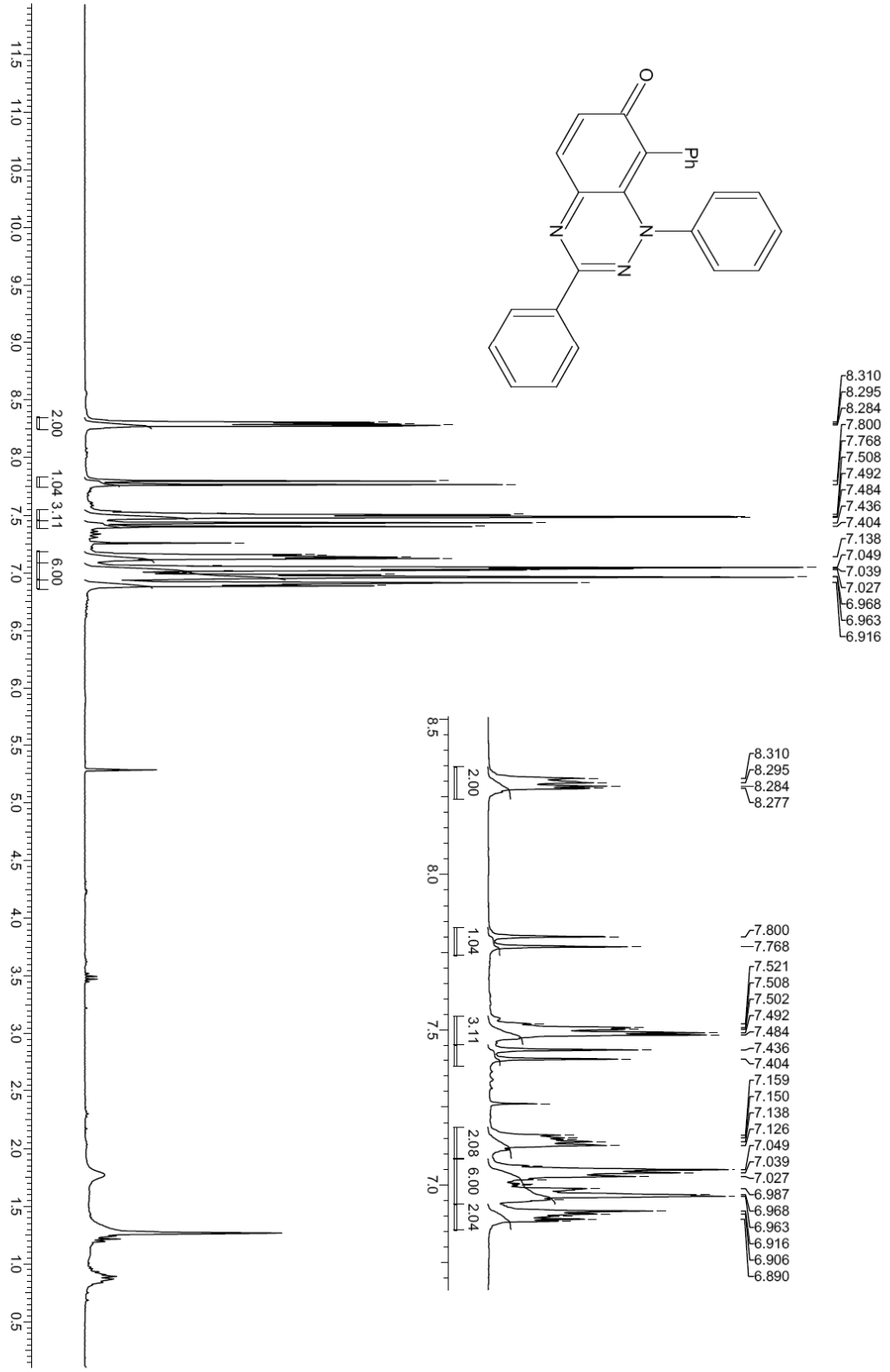


^{13}C NMR of *8-bromo-1,3-diphenyl-6-(pyrrolidin-1-yl)benzo[e][1,2,4]triazin-7(1H)-one* ***(35)***

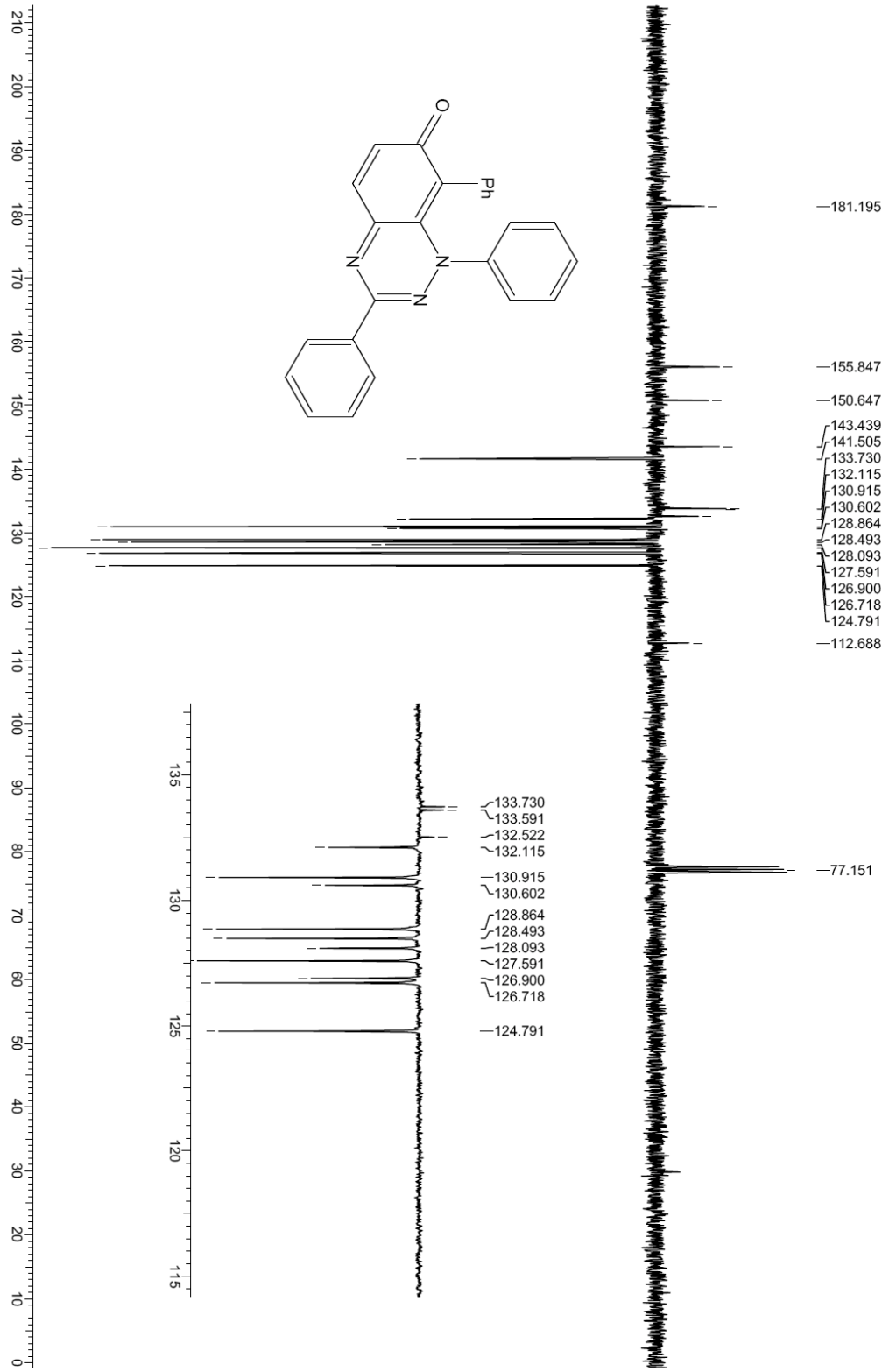




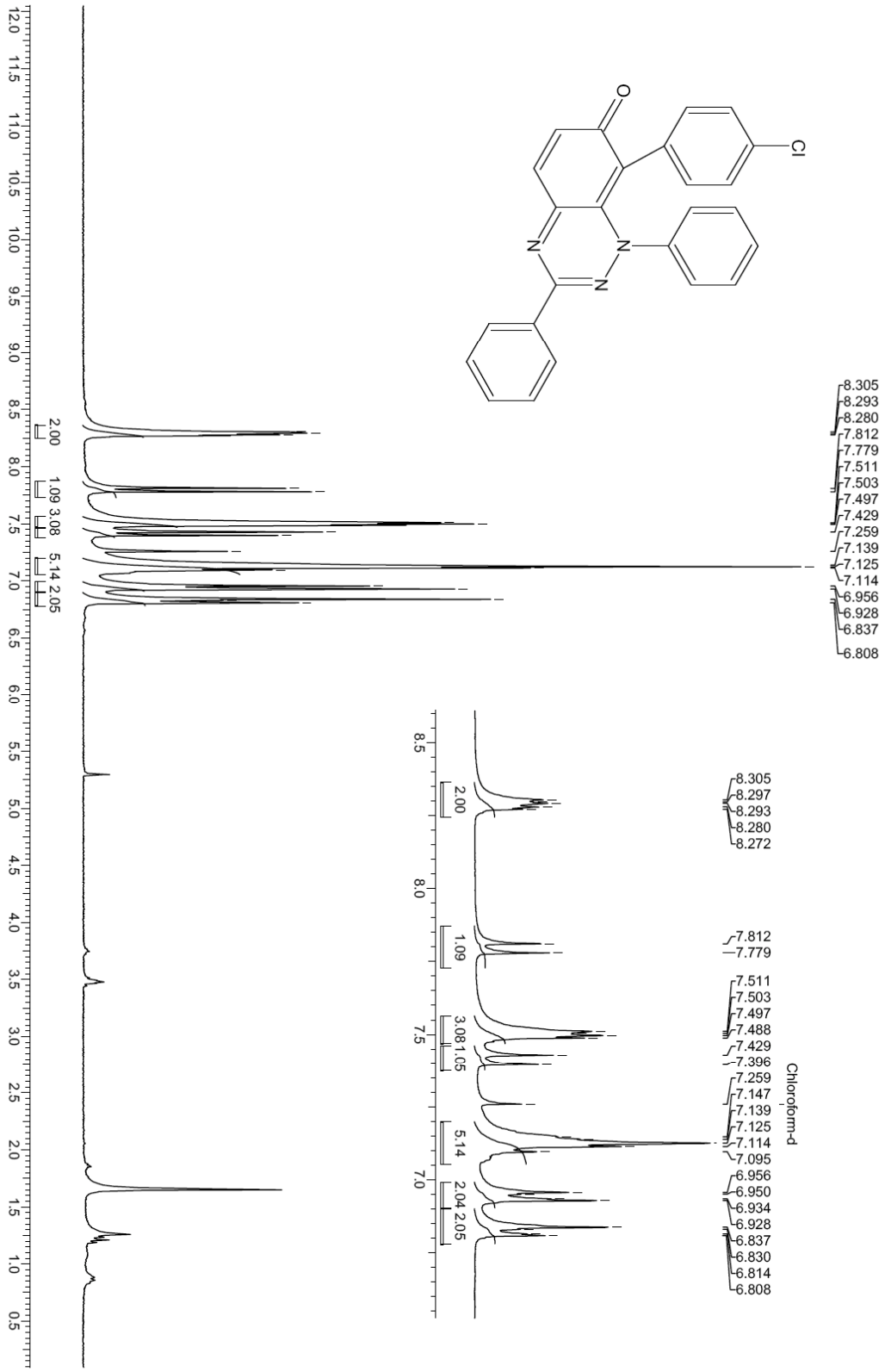
^{1}H NMR of *1,3,8-Triphenylbenzo[e][1,2,4]triazin-7(1H)-one (**36**)*



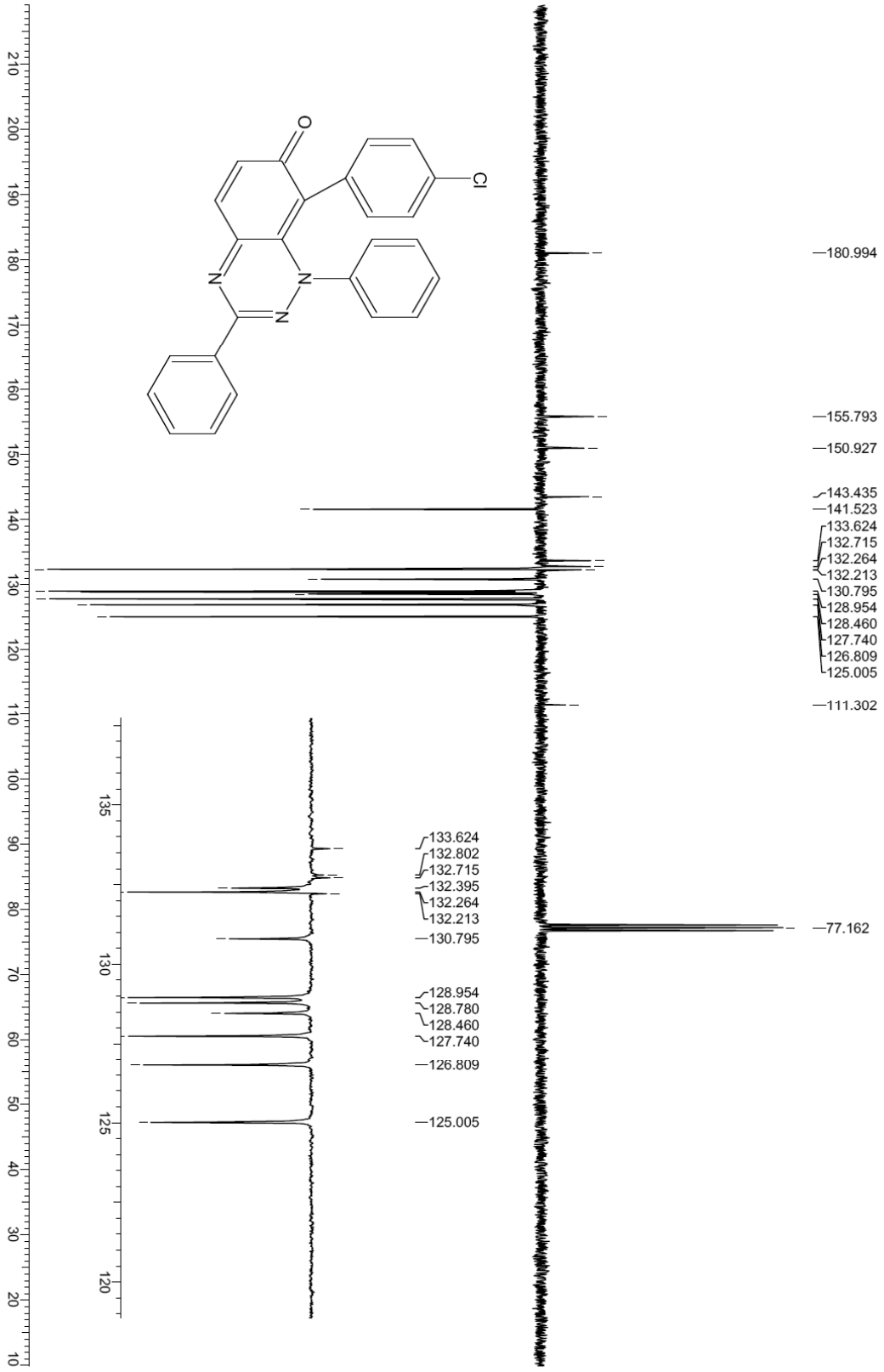
^{13}C NMR of *1,3,8-Triphenylbenzo[e][1,2,4]triazin-7(1H)-one* (***36***)



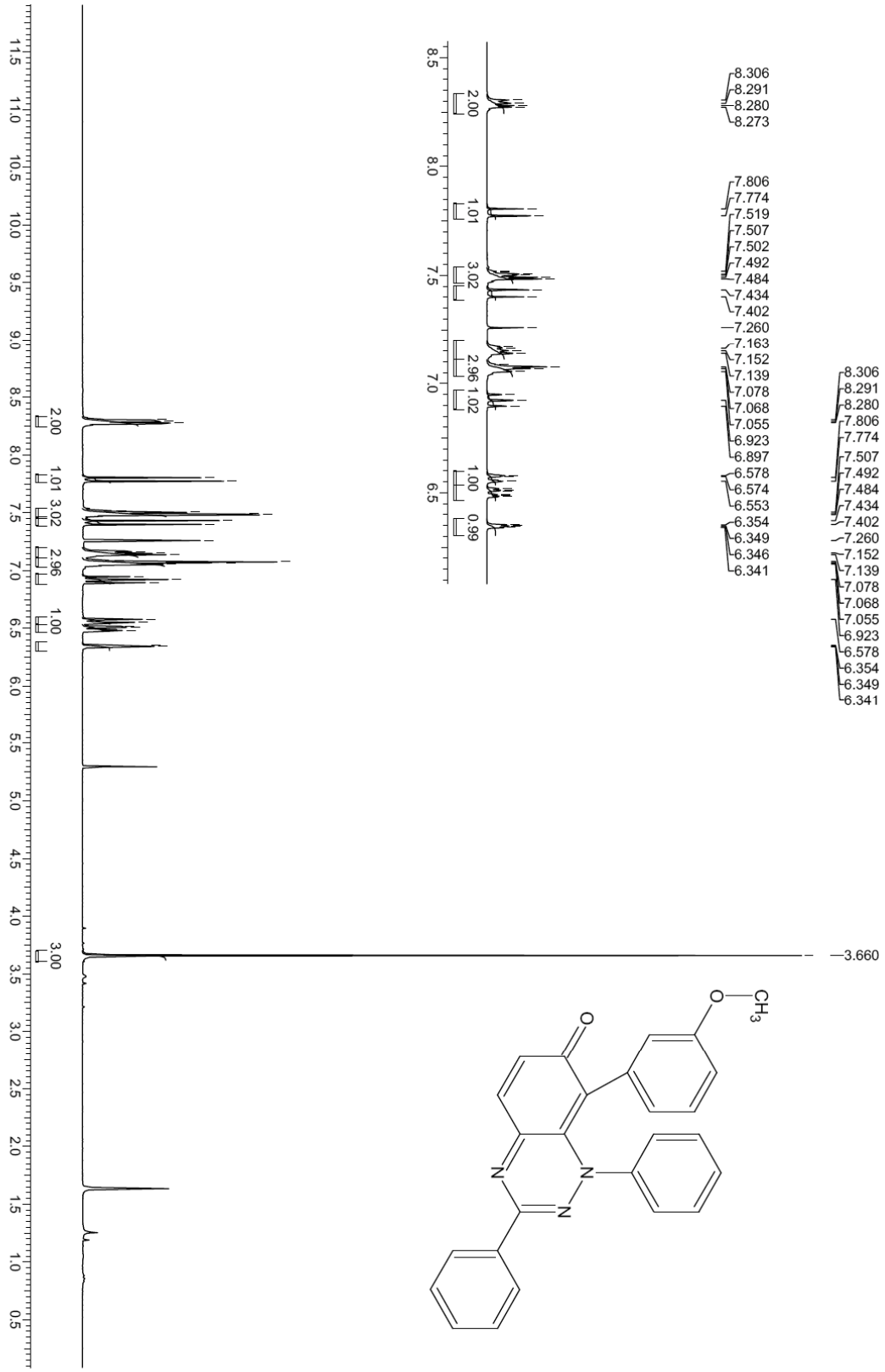
^{1}H NMR of *8-(4-Chlorophenyl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**37**)*



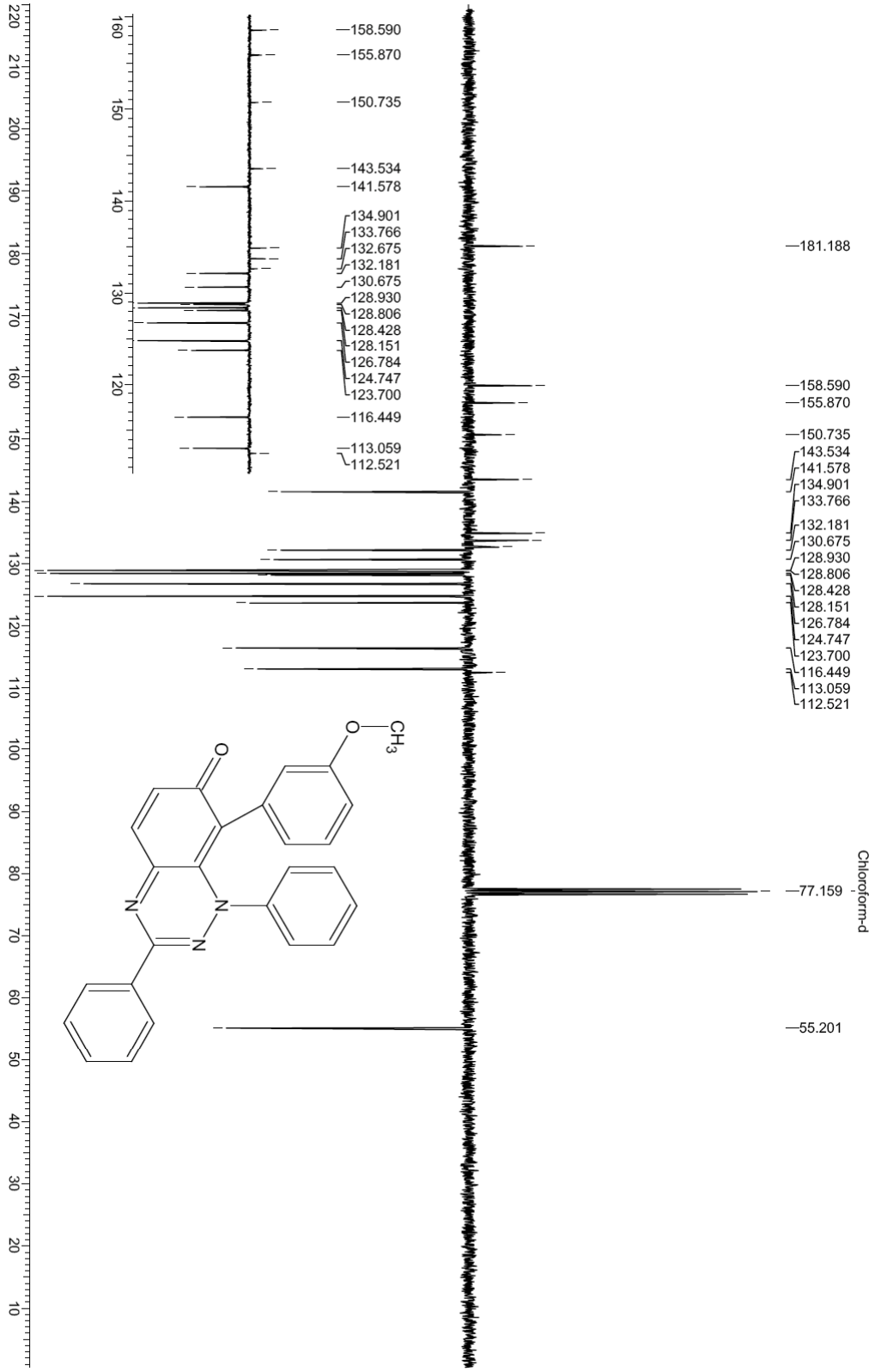
^{13}C NMR of *8-(4-Chlorophenyl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* (***37***)



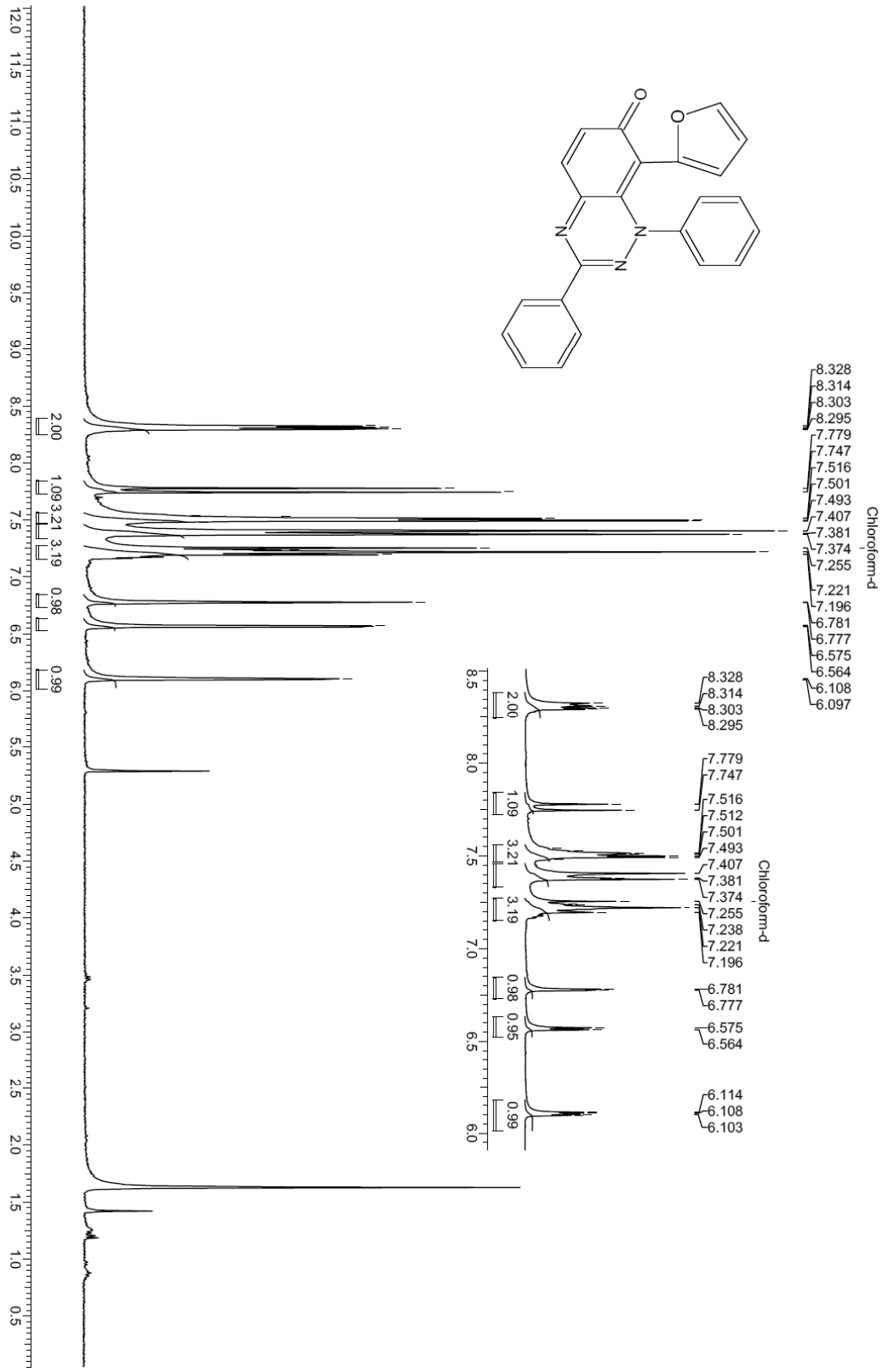
^{1}H NMR of *8-(3-Methoxyphenyl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**38**)*



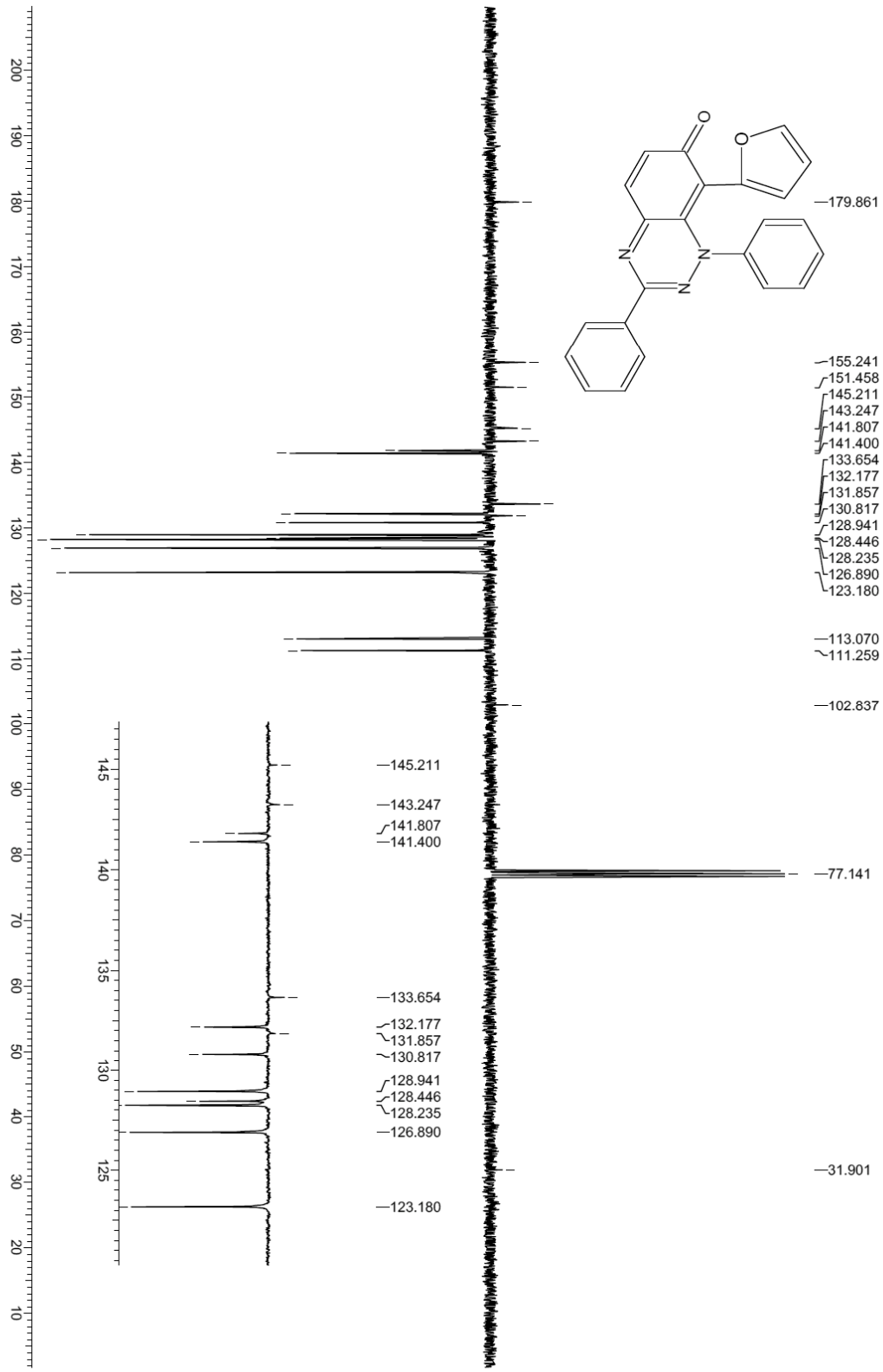
^{13}C NMR of *8-(3-Methoxyphenyl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**38**)*



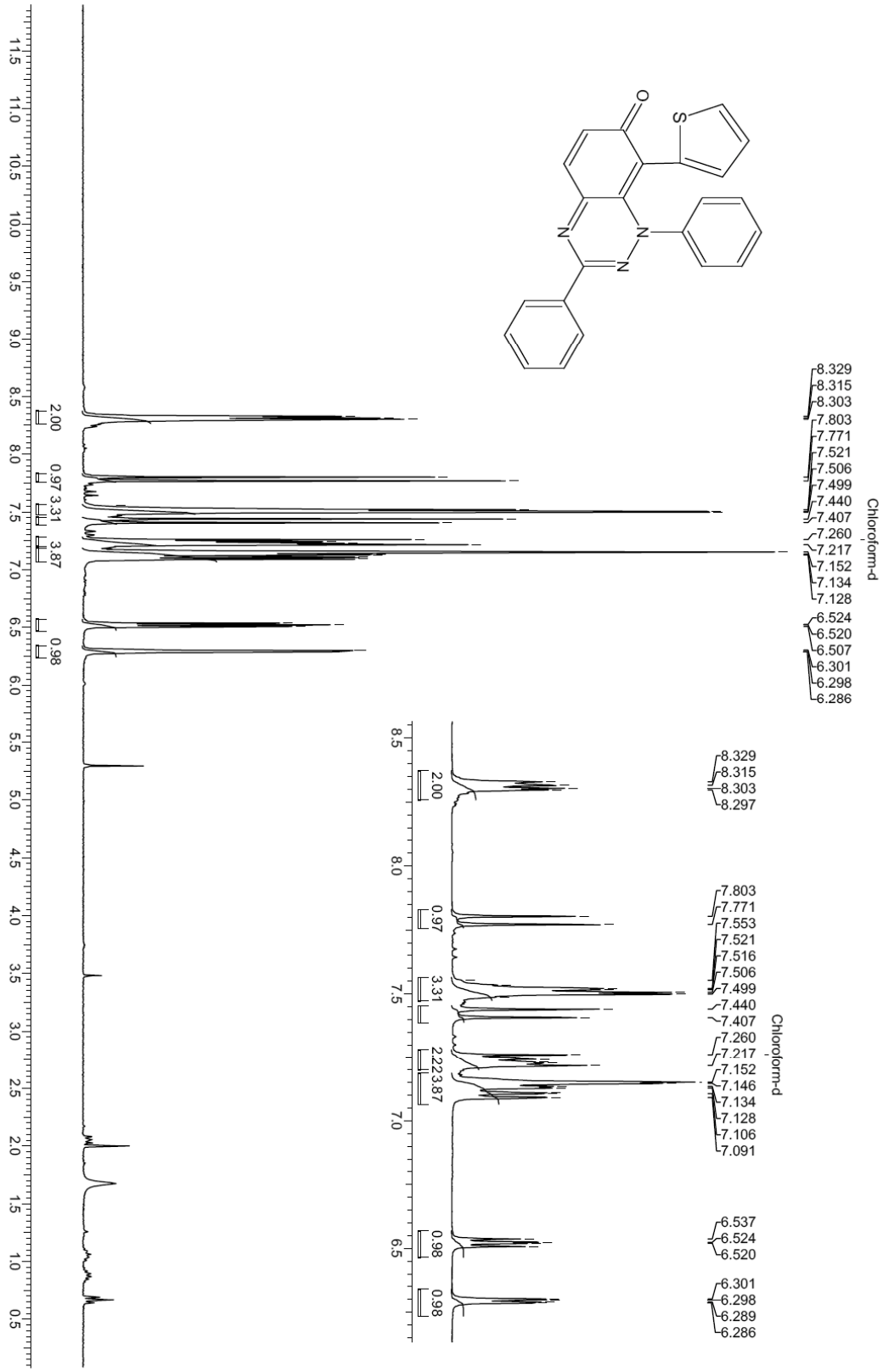
^{1}H NMR of *8-(Furan-2-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (***39***)*



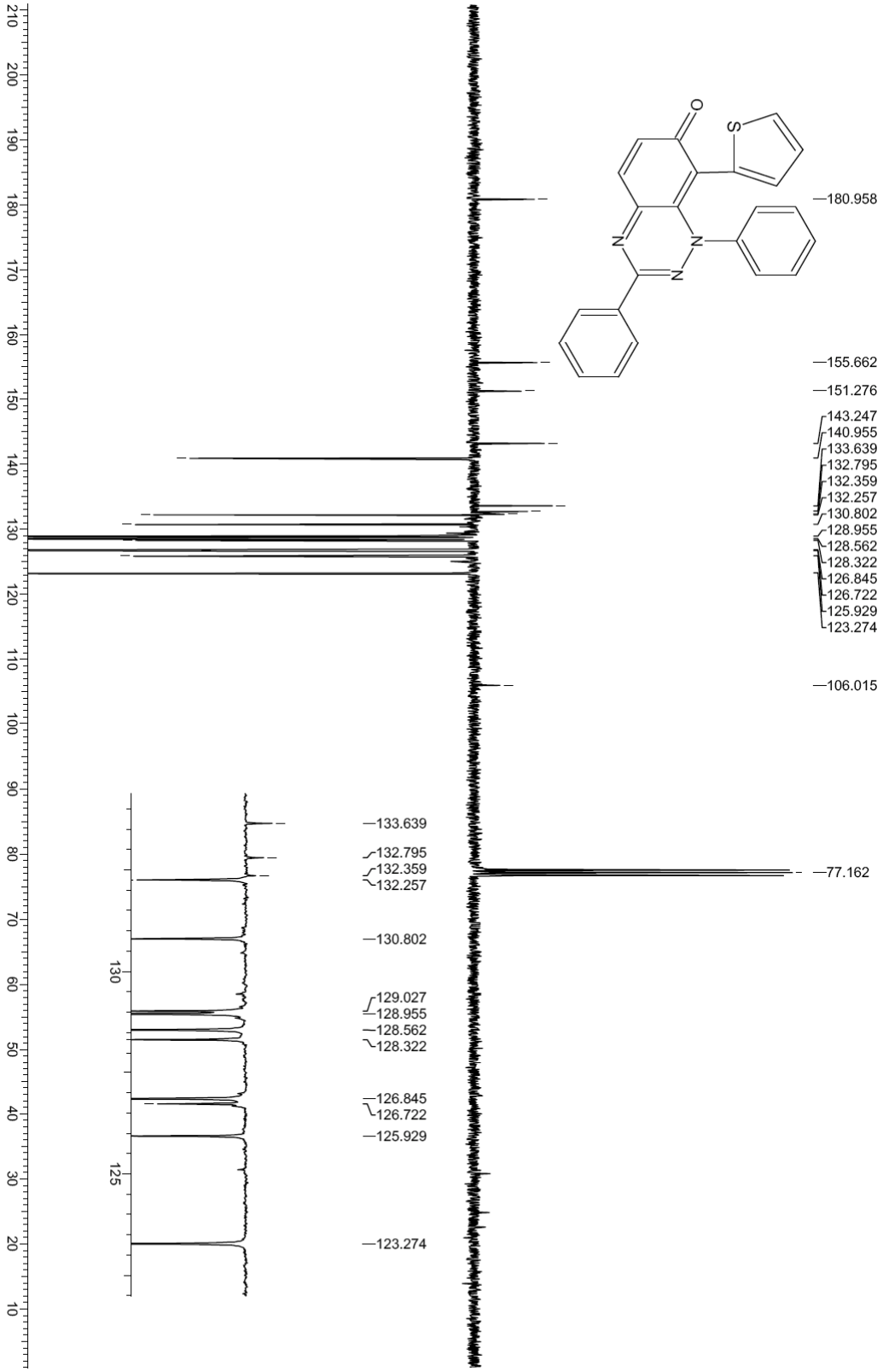
^{13}C NMR of *8-(Furan-2-yl)-1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (***39***)*



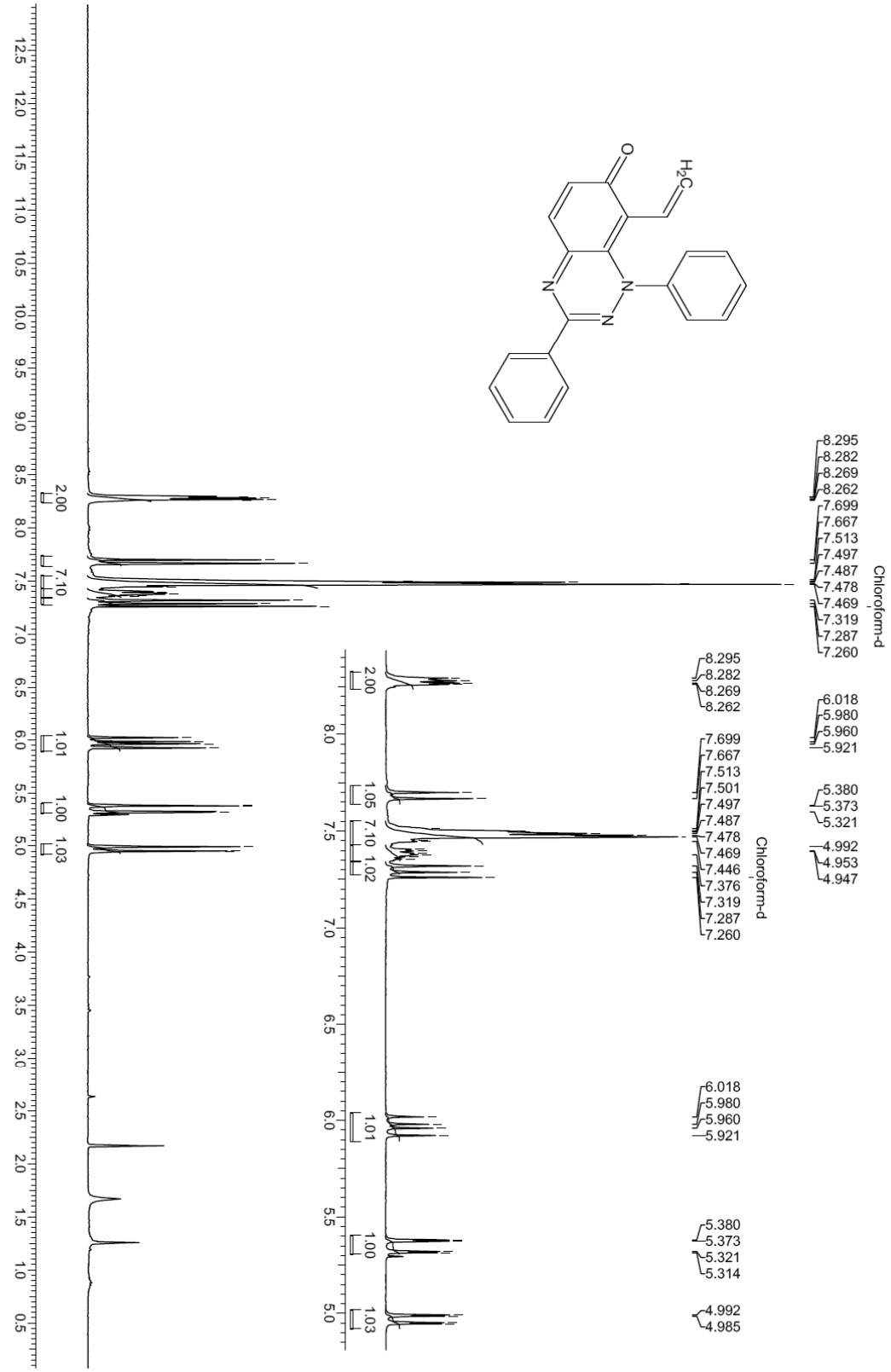
^{1}H NMR of *1,3-Diphenyl-8-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (**40**)*



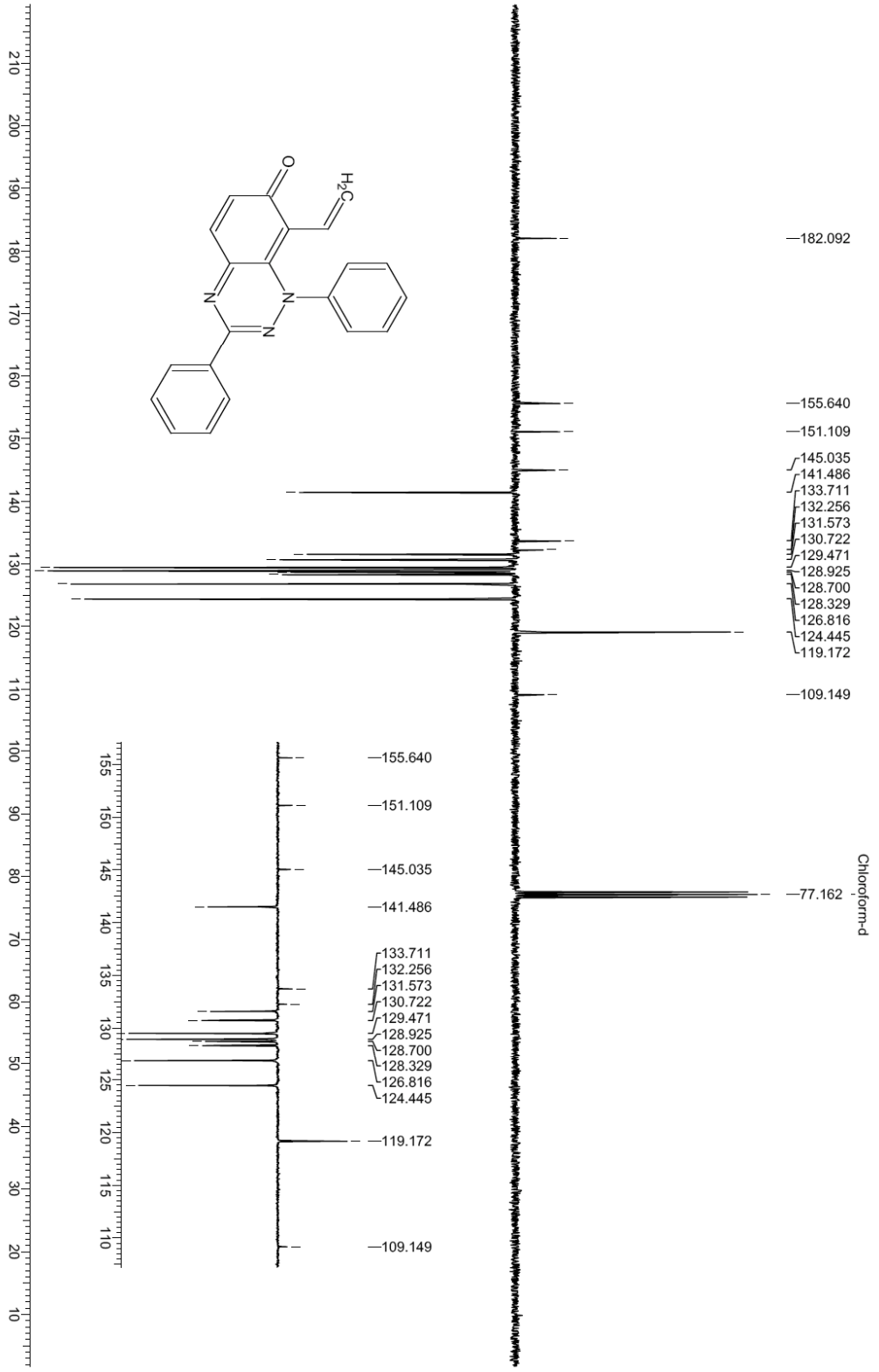
^{13}C NMR of *1,3-Diphenyl-8-(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one (***40***)*



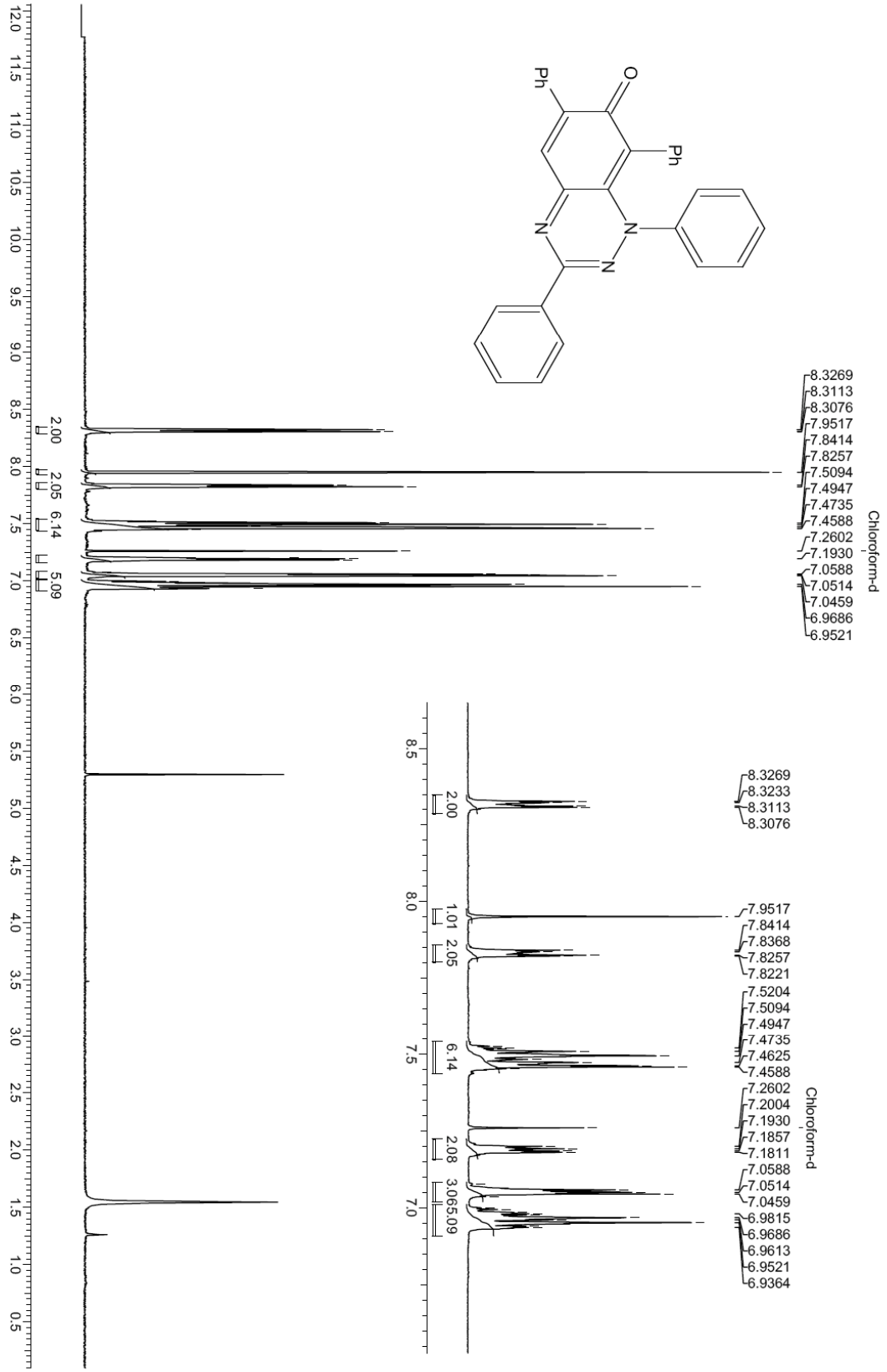
^{1}H NMR of *1,3-Diphenyl-8-vinylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* (***41***)



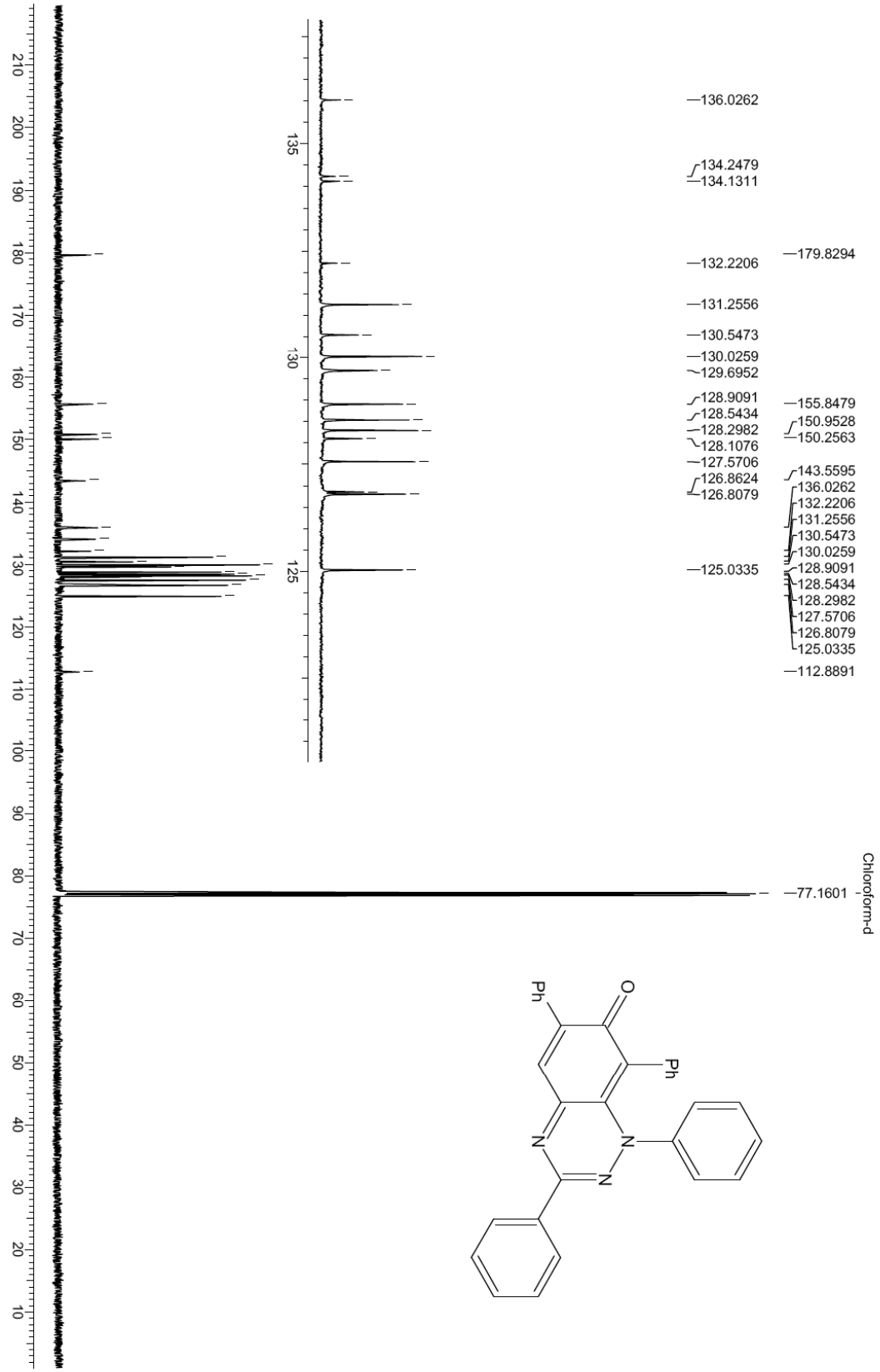
^{13}C NMR of *1,3-Diphenyl-8-vinylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* ***(41)***



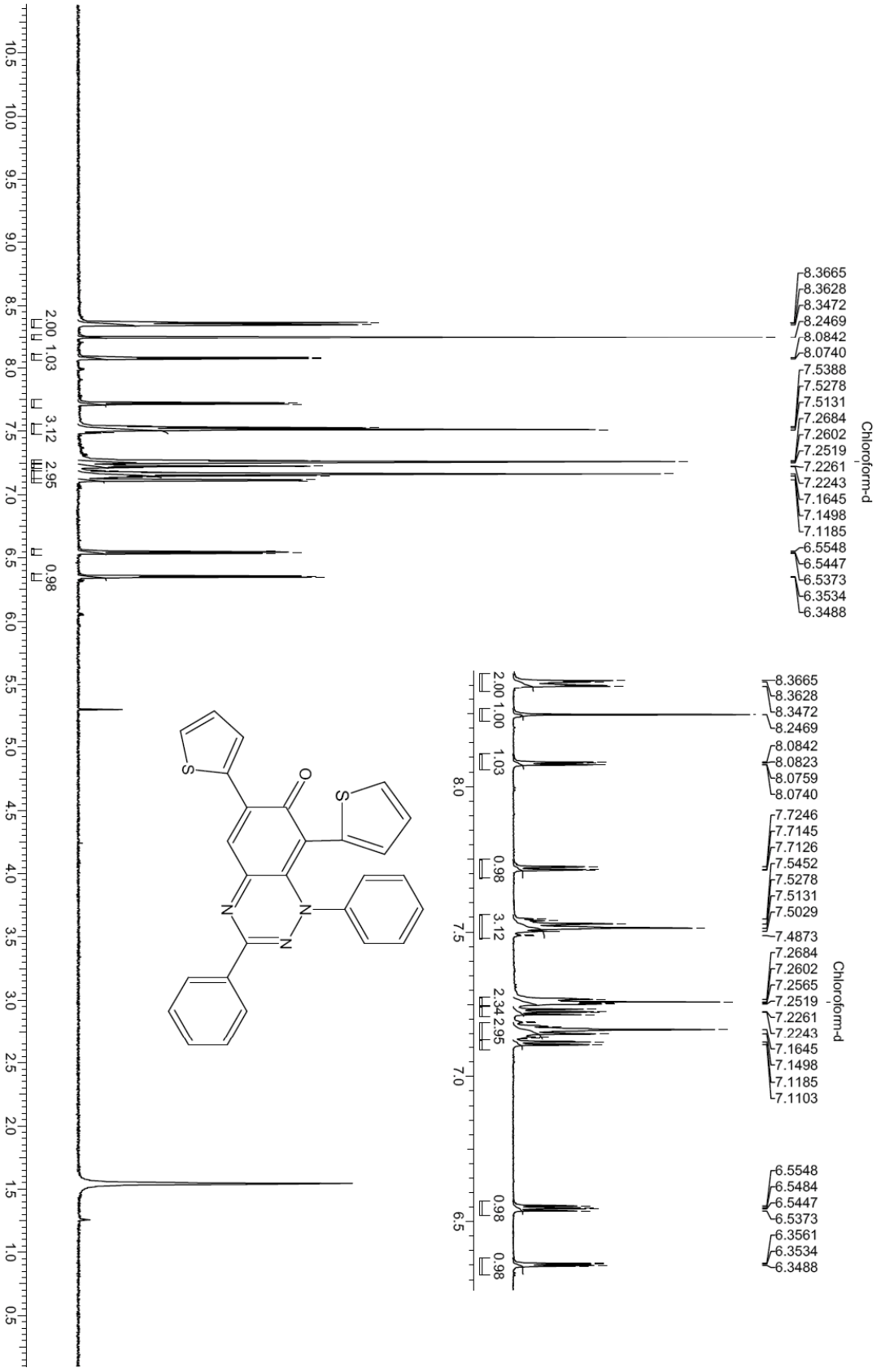
^{1}H NMR of *1,3,6,8-Tetraphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one* (***42***)



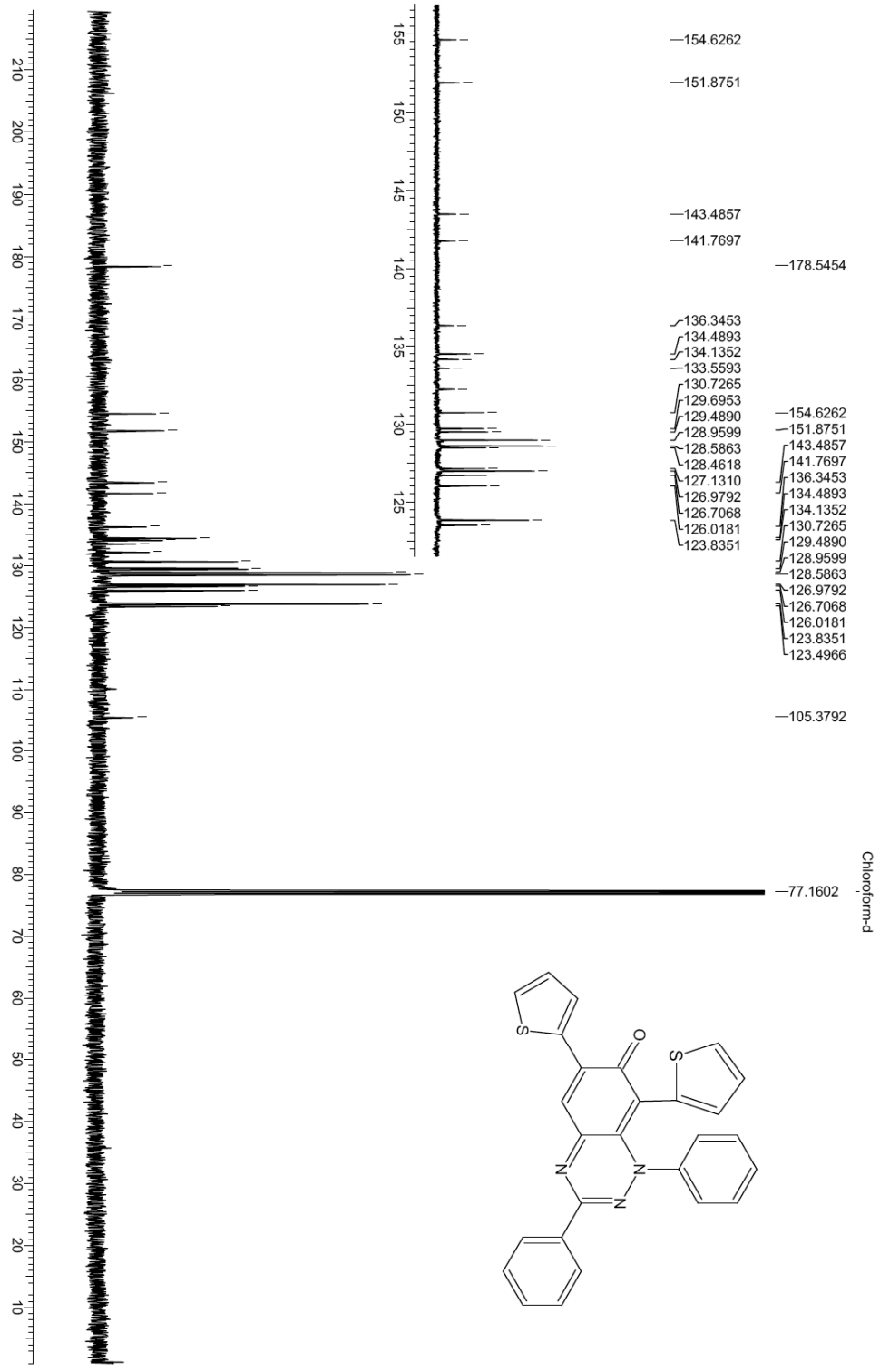
^{13}C NMR of *1,3,6,8-Tetraphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**42**)*



^{1}H NMR of *1,3-Diphenyl-6,8-di(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one* **(*43*)**



^{13}C NMR of *1,3-Diphenyl-6,8-di(thien-2-yl)benzo[*e*][1,2,4]triazin-7(1*H*)-one* **(*43*)**



3. Section C: Computational Studies

3.1. Computational Procedure

The geometry of 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**) was fully optimized, and analytical second derivatives were computed using vibrational analysis to confirm each stationary point to be a minimum by yielding zero imaginary frequencies at the RB3LYP/6-31G(d) level of theory. All the above computations were performed using the Gaussian 03 suite of programs.[1]

3.2. Computational Parameters

Table 1. Computational output parameters for 1,3-diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (**6**)

1\1\GINC-N12\FOpt\RB3LYP\6-31G(d)\C19H13N3O1\KH800\07-Apr-2011\0\\#B3LYP/6-31G* OPT FREQ\\benzotriazinone\\0,1\C,1.8813599437,-3.6891211746,-0.0520445013\C,2.9588511584,-2.6752204795,-0.1735862354\C,2.5426955126,-1.2837509686,-0.1555072871\C,1.2225886782,-0.9414164023,-0.0332221571\C,0.171484979,-1.9662317567,0.0387859668\C,0.5769644261,-3.3530990003,0.0464234465\N,0.7230053349,0.3589884645,0.0202507712\N,-0.5914356195,0.6507851429,0.0223054785\C,-1.4524991561,-0.3435917242,0.0405814932\N,-1.1026134201,-1.6714422548,0.0755290722\O,4.1385776477,-3.0276883817,-0.2826962688\C,1.5756850419,1.5179728797,0.0237695735\C,2.5681347324,1.657872541,0.9972120848\C,3.362068341,2.804185264,1.0021929147\C,3.1632015291,3.8039825695,0.0479246564\C,2.1613471043,3.6585846712,-0.9138118605\C,1.3635923007,2.5157013028,-0.9301427559\C,-2.8949920075,-0.0099316775,0.0419207943\C,-3.3276067142,1.3268877192,0.0385369191\C,-4.6868304995,1.6254519436,0.0390418123\C,-5.6351980329,0.5983672191,0.0425583378\C,-5.2119141937,-0.7313229448,0.0463309901\C,-3.8515978649,-1.0366448793,0.0464421446\H,2.205700363,-4.7259372475,-0.0587599357\H,3.3257299143,-0.5412181033,-0.2394925988\H,-0.2184527147,-4.0887746663,0.1167958162\H,2.7104412479,0.883921859,1.7439482541\H,4.1320360796,2.9168269623,1.7598241492\H,3.7851642475,4.6944193124,0.0557074568\H,2.0005573316,4.4342978213,-1.6569077103\H,0.5777324372,2.3905935463,-1.6671255818\H,-2.590639106,2.1225882568,0.0387649293\H,-5.0085271055,2.6634861338,0.0379538344\H,-6.6958779326,0.8347245671,0.0433007067\H,-5.9421476288,-1.5360875569,0.0496437889\H,-3.5170440529,-2.0677039136,0.050881768\\Version=AM64L-G03RevC.02\State=1-A\HF=-971.28953\RMSD=4.822e-09\RMSF=2.345e-06\Dipole=-1.0755908,1.3774265,0.1402156\PG=C01 [X(C19H13N3O1)]\\@

3.3. HOMO-LUMO Molecular Orbitals and Mulliken Charges for 1,3-Diphenylbenzo[*e*][1,2,4]triazin-7(1*H*)-one (6)

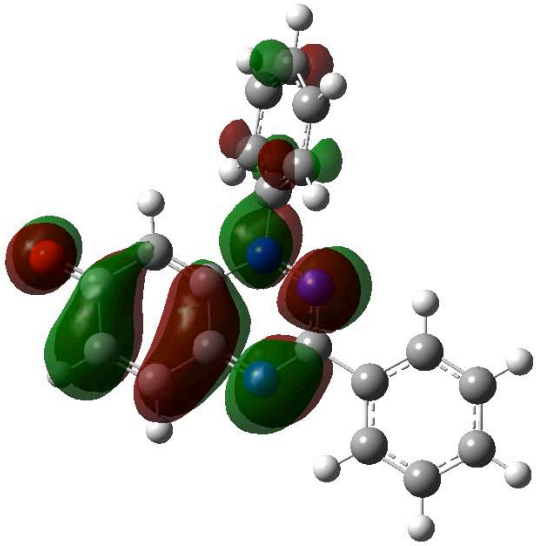


Figure 1. LUMO (-0.10654 Hartrees or -2.90 eV) orbitals of 1,3-diphenylbenzo[*e*]-[1,2,4]triazin-7(1*H*)-one (**6**) [DFT RB3LYP/6-31G(d)] generated with Gaussview03, isovalue 0.02.

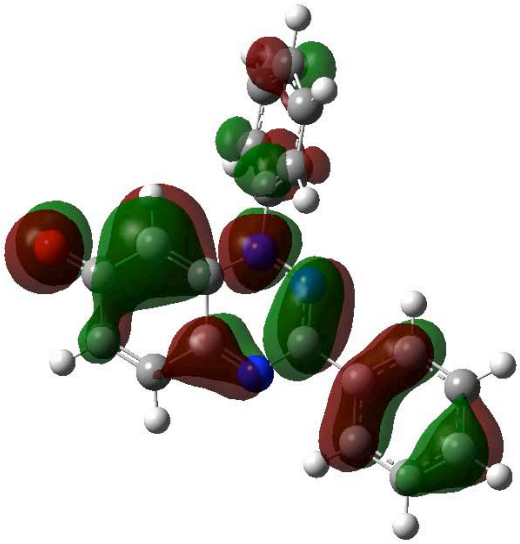


Figure 2. HOMO (-0.20427 Hartrees or -5.56 eV) orbitals of 1,3-diphenylbenzo[*e*]-[1,2,4]triazin-7(1*H*)-one (**6**) [DFT RB3LYP/6-31G(d)] generated with Gaussview03, isovalue 0.02.

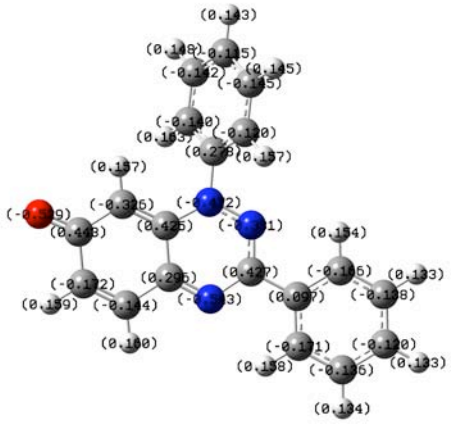


Figure 3. Charges based on Mulliken population analysis for 1,3-diphenylbenzo[*e*][1,2,4]-triazin-7(1*H*)-one (**6**) [DFT RB3LYP/6-31G(d)] generated with Gaussview03.

3.4. References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith,M. A. Al-Laham, C. Y.

Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. G. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, GAUSSIAN 03 (Revision B.02), Gaussian, Inc., Wallingford, CT, 2004.