Electronic Supplementary Material (ESI) for RSC Advances.

A green, catalyst-free, solvent-free, high yielding one step synthesis of functionalized benzo[*f*]furo[3,2-*c*]chromen-4-(5*H*)-ones and furo[3,2-*c*]quinolin-4-(5*H*)-ones

Manoj Kumar, Tanpreet Kaur, Vinod K. Gupta and **Anuj Sharma***

Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee-247667, India
(Phone: +91-1332-284751; e-mail: anujs77@gmail.com)

General Experimental Detail. NMR spectra were recorded on a BrukerAvance® 400 and Jeol Resonance ECX-400II. Chemical shifts are reported in parts per million and are referenced to TMS. Spectra were processed using Bruker Topspin® 3.0.b.8 and MestReNova[6] software. Mass spectrometry (HRMS) was performed using a BrukerdaltronicsmicroTOF-QII® spectrometer using ESI ionization, with less than 5 ppm error for all HRMS analyses. Analytical Thin layer chromatography (TLC) was performed on a silica gel plate (Merck® $60F_{254}$). IR spectra were done on Perkin Elmer FT-IR spectrometer (Spectrun Two). Melting points were performed with Ambassador®and Digital Melting point apparatus (Nutronics), Popular India. All solvent were distilled prior to use and all chemicals were purchased from sigma-Aldrich® and used without further purification.

Microwave Irradiation Experiment. All microwave experiments were carried out in a dedicated Anton PaarMonowave 300 reactor®, operating at a frequency of 2.455 GHz with continuous irradiation power of 0 to 300 W. The reactions were performed in a G10 Borosilicate glass vial sealed with Teflon septum and placed in a microwave cavity. Initially, microwave of required power was used and temperature was being ramped from room temperature to a desired temperature. Once this temperature was attained, the process vial was held at this temperature for required time. The reactions were continuously stirred. Temperature was measured by an IR sensor. After the experiments a cooling jet cooled the reaction vessel to ambient temperature.

General procedure for the microwave-assisted three component reaction. 1-Hydroxy-3*H*-benzo[*f*]chromen-3-one **1a**, or 4-Hydroxyquinolin-2(1*H*)-ones **1b** (1.0 mmol), aryl-aldehydes **2a-f** (1.0 mmol) and isonitriles **3a-f** (1.2 mmol) was mixed well in a G10 process vial capped with Teflon septum. After a pre-stirring of 1 or 2 minutes, the vial was subjected to microwave irradiation with the initial ramp time of 1 minute at 70 °C. The temperature was then raised to 120 °C with the holding time of 5 minutes. After completion of the reaction, the ethanol:water (1:4) or water:isopropanol (4:1) was added into it and the

precipitated solids were filtered. All the products were characterized through their ^{1}H, ^{13}CNMR, Mass, IR and HRMS. ^{13}C NMR for compound **4p**, **5d**, **5f**, **5g**, **5k**&**5l** could not be recorded even at higher scans due to their lower solubility in the deuterated solvents.

Preparation of 1-hydroxy-3(H)-benzo[f]chromen-3-one[1]: A mixture of 2-naphthol (2 mmol), Meldrum's acid (2 mmol) was stirred at 85 °C for 9 h. After cooling to room temperature, the reaction mixture was extracted with ethyl acetate. After acidification with conc. HCl and extraction with methylene dichloride (DCM) yielded the product. This crude intermediate (1 mmol) and Eaton's reagent (1.5 mL) was stirred at 60°C for 5 h and then water was added while stirring vigorously. The precipitate was filtered by suction and dried. The spectral data was matched with the literature data.[1]

Preparation of 4-hydroxyquinolin-2(1H)-ones[1]*:* Using the above method this starting material has also been prepared. The spectral data was matched with the literature data.[1]

[1]S. -J. Park, J. -C. Lee, K. -I. Lee, *Bull. Korean Chem. Soc.* **2007***, 28,* 1203.

2-(*tert*-Butylamino)-3-(4'-nitrophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4a). Reddish orange solid (95%), Mp decomp. 275-276 °C, IR (KBr, cm^{-1}): ν_{max} = 3381, 2977, 2345, 1704, 1603, 1508, 1202. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 1.38 (s, 9H), 6.36 (s, 1H), 7.56 -7.65 (m, 2H), 7.69-7.79 (m, 1H), 7.83 (dt, 2H, *J* = 8.8 & 2.5 Hz), 8.05 (d, 2H, *J* = 9.2 Hz), 8.23 (dt, 2H, *J* = 8.9 & 2.4 Hz), 8.89 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 30.0, 53.4, 99.6, 106.1, 109.9, 117.1, 123.0, 124.1, 125.8, 126.2, 128.4, 129.1, 130.1, 130.6, 130.7, 138.1, 145.4, 150.5, 151.5, 155.9, 156.7. HRMS (ESI) m/z calcd. for $C_{25}H_{20}N_2O_5$ $[M]^+$: 428.1366, found: 428.1361.

2-(Cyclohexylamino)-3-(4'-chlorophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4b). Pale yellow solid (75%), Mp 190-192°C, IR (KBr, cm^{-1}): ν_{max} = 3299, 2930, 2865, 1707, 1606, 1561, 1505. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H =1.12- 1.22 (m, 1H), 1.26-1.46 (m, 4H), 1.58-1.67 (m, 1H), 1.72-1.81 (m,

2H), 1.92-2.04 (m, 2H), 3.41- 3.53 (m, 1H), 6.78 (d, 1H, *J* = 7.6 Hz), 7.40-7.49 (m, 2H), 7.50-7.61 (m, 4H), 7.64-7.70 (m, 1H), 7.92 (d, 1H, *J* = 9.0 Hz), 7.98 (d, 1H, *J* = 7.9 Hz), 8.70 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 24.8, 25.2, 33.1, 53.0, 92.3, 106.2, 111.0, 116.7, 124.3, 125.6, 125.8, 127.7, 127.9, 128.7, 129.2, 129.4, 130.0, 130.5, 131.4, 149.3, 149.4, 155.2, 156.7. HRMS (ESI) m/z calcd. for $C_{27}H_{22}ClNO_3$ $[M-H]^+$: 442.1204, found: 442.1201.

3-(4'-Chlorophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4c). Yellow solid (87%), Mp 170-172 °C, IR (KBr, cm^{-1}): ν_{max} = 1709, 1613, 1562, 1494, 1439, 1209. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 1.03(s, 9H), 1.39 (s, 6H), 1.85 (s, 2H), 5.87 (s, 1H), 7.48 (d, 2H, *J* = 8.5 Hz), 7.57 -7.68 (m, 4H), 7.74 (t, 1H, *J* = 7.6 Hz), 8.08 (t, 2H, *J* = 9.3 Hz), 8.99 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 30.0, 31.3, 31.4, 53.7, 56.7, 100.9, 106.3, 110.2, 117.1, 124.1, 125.8, 126.1, 127.8, 128.0, 129.1, 129.4, 130.1, 130.2, 131.2, 131.7, 150.3, 151.0, 154.9, 156.7. HRMS (ESI) m/z calcd. for $C_{29}H_{28}ClNO_3$ $[M-H]^+$: 472.1673, found: 472.1670.

3-(4'-Chlorophenyl)-2-((2-morpholinoethyl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4d). Yellow solid (80%), Mp 198-200 °C, IR (KBr, cm^{-1}): ν_{max} = 3392, 2961, 2839, 1725, 1612, 1563, 1508. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 2.49 (t, 4H, *J* = 4.2 Hz), 2.67 (t, 2H, *J* = 6.0 Hz), 3.57 (q, 2H, *J* = 5.6 Hz), 3.66 (t, 4H, *J* = 4.3 Hz), 5.38 (t, 1H, *J* = 5.2 Hz), 7.41 (d, 2H, *J* = 8.5 Hz), 7.47-7.57 (m, 4H), 7.67 (t, 1H, *J* = 7.5 Hz), 7.80 (d, 1H, *J* = 9.0 Hz), 7.88 (d, 1H, *J* = 8.8 Hz), 8.85 (d, 1H, *J* = 8.5 Hz) . ^{13}C NMR (100 MHz, $CDCl_3$): δ_C = 40.9, 53.3, 57.0, 67.1, 95.6, 107.2, 111.3, 117.3, 125.1, 126.0, 126.6, 128.0, 128.8, 128.9, 129.1, 129.9, 130.5, 130.6, 150.6, 151.5, 155.6, 157.9. HRMS (ESI) m/z calcd. for $C_{27}H_{23}ClN_2O_4$ $[M-H]^+$: 473.1262, found: 473.1259.

2-(*tert*-Butylamino)-3-(4'-bromophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4e). Yellow solid (82%), Mpdecomp. 280-281°C, IR (KBr, cm^{-1}): ν_{max} = 3378, 2978, 1724, 1617, 1562, 1499, 1212. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H =1.36 (s, 9H), 5.87 (s, 1H), 7.57 (dt, 2H, *J* = 8.6 & 1.9 Hz), 7.60 -7.68 (m, 4H), 7.76-7.82 (m, 1H), 8.05-8.12 (m, 2H), 8.95 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 30.0, 53.4, 102.8, 106.2, 109.9, 117.1, 119.9,

124.1, 125.9, 126.1, 128.3, 129.0, 129.7, 130.1, 130.5, 130.7, 132.0, 150.6, 151.6, 154.8, 156.7. HRMS (ESI) m/z calcd. for $C_{25}H_{20}BrNO_3$ $[M]^+$: 461.0621, found: 461.0619.

2-(Cyclohexylamino)-3-(4'-bromophenyl)-4*H*-benzo[*f*]furo [3,2-*c*]chromen-4-one (4f). Brown solid (70%), Mp 175-177 °C; IR (KBr, cm^{-1}): ν_{max} = 3378, 2980, 1723, 1563, 1496, 1212. ^1H NMR (400 MHz, DMSO-d_6): δ_H = 1.09-1.24 (m, 1H), 1.27-1.48 (m, 4H), 1.57-1.68 (m, 1H), 1.71-1.84 (m, 1H), 1.90-2.07 (m, 1H), 3.44-3.56 (m, 1H), 6.81 (d, 1H, *J* =7.6 Hz), 7.48 (dt, 2H, *J* = 8.5 & 2.4 Hz), 7.53-7.62 (m, 4H), 7.70 (t, 1H, *J* = 7.7 Hz), 7.95 (d, 1H, *J* = 9.0 Hz), 8.00 (d, 1H, *J* = 8.0 Hz), 8.75 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 24.8, 25.2, 33.1, 53.0, 92.3,106.2,110.9, 116.8, 119.1, 124.3, 125.6, 125.9, 128.0, 128.8, 129.3, 129.8, 130.0, 130.7, 131.8, 149.4, 149.5, 155.2, 156.7. HRMS (ESI) m/z calcd. for $C_{27}H_{22}BrNO_3$ $[M-H]^+$: 486.0699, found: 486.0691.

3-(4'-Bromophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl) amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4g). Light yellow solid (85%); Mp 168-170 °C; IR (KBr, cm^{-1}): ν_{max} = 3379, 2963, 2900, 1728, 1612, 1558, 1496, 1216. ^1H NMR (400 MHz, DMSO-d_6): δ_H= 1.04 (s, 9H), 1.40 (s, 6H), 1.86 (s, 2H), 5.90 (s, 1H), 7.54 (dt, 2H, *J* = 8.4 & 2.4 Hz), 7.62 (dt, 2H, *J* = 9.0 & 2.3 Hz), 7.73-7.79 (m, 2H), 7.73-7.79 (m, 1 H), 8.10 (t, 2H, *J* = 9.2 Hz), 9.01 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C= 30.1, 31.3, 31.5, 53.7, 56.7, 100.7, 106.3, 110.2, 117.1, 119.7, 124.1, 125.8, 126.1, 128.0, 129.1, 129.8, 130.1, 130.2, 130.7, 132.0, 150.3, 151.0, 154.9, 156.7. HRMS (ESI) m/z calcd. for $C_{29}H_{28}BrNO_3$ $[M-H]^+$: 516.1168, found: 516.1167.

3-(4'-Bromophenyl)-2-((2-morpholinoethyl)amino)-4*H*-benzo [*f*]furo[3,2-*c*]chromen-4-one (4h). Yellow orange solid (81%), Mp 210-211°C, IR (KBr, cm^{-1}): ν_{max} = 3379, 2965, 2841, 1731, 1611, 1567, 1502, 1429. ^1H NMR (400 MHz, $CDCl_3$): δ_H = 2.35-2.55 (br m, 4H), 2.67 (t, 2H, *J* = 5.8 Hz), 3.45 (q, 2H, *J* = 5.5Hz), 3.62- 3.78 (br m, 4H), 5.38 (t, 1H, *J* = 2.2 Hz), 7.41-7.66 (m, 6H), 7.68 (t, 1H, *J* = 7.1 Hz), 7.82 (d, 1H, *J* = 8.9 Hz), 7.89 (d, 1H, *J* = 8.0 Hz), 8.87

(d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 31.2, 53.9, 58.6, 66.7, 92.5, 106.9, 111.6, 117.5, 119.6, 125.2, 126.2, 126.7, 128.7, 129.4, 130.0, 130.2, 130.7, 131.4, 132.2, 150.0, 150.1, 156.7, 157.4. HRMS (ESI) m/z calcd. for $C_{27}H_{23}BrN_2O_2$ $[M]^+$: 518.0835, found: 518.0834 .

2-(*tert*-Butylamino)-3-(2'-chloro-5'-nitrophenyl)-4*H*benzo[*f*] furo[3,2-*c*]chromen-4-one (4i). Orange solid (85%), Mpdecomp. 280-281°C, IR (KBr, cm^{-1}): ν_{max} = 3361, 3097, 2973, 1734, 1621, 1521, 1344. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H= 1.43 (s, 9H), 6.30 (s, 1H), 7.63-7.70 (m, 2H), 7.78-7.84 (m, 1H), 7.87 (d, 1H, *J* = 8.8 Hz), 8.10 (t, 2H, *J* = 9.1 Hz), 8.26 (dd, 1H, *J* = 8.8 & 2.8 Hz), 8.31 (d, 1H, *J* =2.8 Hz), 8.94 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 30.1, 53.3, 95.6, 106.4, 111.5, 117.1, 123.8, 124.1, 125.8, 126.2, 127.9, 128.3, 129.1, 130.1, 130.2, 130.5, 131.3, 141.9, 145.9, 150.2, 150.5, 155.8, 156.5. HRMS (ESI) m/z calcd. for $C_{25}H_{19}ClN_2O_5$ $[M]^+$: 462.0977, found: 462.0972.

2-(Cyclohexylamino)-3-(2'-chloro-5'-nitrophenyl)-4*H*-benzo [*f*]furo[3,2-*c*]chromen-4-one (4j). Brown solid (84%), Mp 215-220°C, IR (KBr, cm^{-1}): ν_{max} = 3403, 2932, 2852, 1723, 1628, 1527, 1345. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 1.08-1.43 (m, 5H), 1.59 (br s, 1H), 1.75 (br s, 2H), 1.97 (br s, 2H), 3.40-3.53 (m, 1H), 7.14 (s, 1H), 7.64 (br s, 2H),7.73-7.93 (m, 2H), 7.95-8.15 (m, 2H), 8.16-8.43 (m, 2H), 8.86 (br s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 24.6, 25.1, 33.1, 33.2, 52.8, 87.4, 99.4, 106.4, 116.9, 123.5, 124.4, 125.6, 126.1, 128.0, 128.1, 128.9, 129.4, 130.1, 130.4, 131.4, 141.9, 145.7, 149.5, 155.6, 156.6. HRMS (ESI) m/z calcd. for $C_{27}H_{21}ClN_2O_5$ $[M-H]^+$: 488.1133, found: 488.1129.

3-(2'-Chloro-5'-nitrophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4k). Light yellow solid (91%), Mp 194-196 °C, IR (KBr, cm^{-1}): ν_{max} = 3357, 2964, 2901, 1728, 1615, 1532, 1344, 1214. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 0.98 (s, 9H), 1.44 (d, 6H, *J* = 11.0 Hz), 1.86 (q, 2H, *J* = 7.5 Hz), 6.25 (s, 1H), 7.59-7.68 (m, 2H), 7.72 -7.79 (m, 1H), 7.87 (d, 1H, *J* = 8.8 Hz), 8.04 (d, 1H, *J* = 9.0 Hz), 8.08 (d, 1H, *J* = 7.9 Hz), 8.26 (td, 2H, *J* = 9.0 & 2.8 Hz), 8.94 (d, 1H, *J* = 8.5 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 30.1, 30.3, 31.2, 31.4, 53.2, 56.6, 94.4, 106.4, 111.7, 117.1, 123.7,

124.0, 125.6, 126.1, 127.9, 128.0, 129.0, 129.9, 130.1, 130.5, 131.5, 142.0, 145.9, 150.1, 155.7, 156.5. HRMS (ESI) m/z calcd. for $C_{29}H_{27}ClN_2O_3$ $[M-H]^+$: 518.1603, found: 518.1609.

2-(*tert*-Butylamino)-3-(4'-chlorophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4l).Yellow solid (89%), Mp 210-211°C, IR (KBr, cm^{-1}): ν_{max} = 3397, 2942, 2862, 1660, 1597, 1508, 1338. ^1H NMR (400 MHz, DMSO-d_6): δ_H = 1.36 (s, 9H), 5.85 (s, 1H), 7.50 (dt, 2H, *J* = 8.4 & 2.9 Hz), 7.60 -7.69 (m, 4H), 7.75- 7.83 (m, 1H), 8.09 (d, 2H, *J* = 9.2 Hz), 8.95 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 30.0, 53.4, 103.0, 106.2, 110.0, 117.1, 124.1, 126.0, 126.1, 127.8, 128.3, 129.0, 129.3, 130.1, 130.5, 131.3, 131.7, 150.6, 151.6, 154.89, 156.7. HRMS (ESI) m/z calcd. for $C_{25}H_{20}ClNO_3$ $[M]^+$:417.1126, found: 417.1123.

2-(Cyclohexylamino)-3-(4'-nitrophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4m). Brown solid (85%), Mpdecomp. 265-266°C, IR (KBr, cm^{-1}): ν_{max} = 2980, 1709, 1606, 1562, 1501, 1211. ^1H NMR (400 MHz, DMSO-d_6): δ_H = 1.12-1.26 (m, 1H), 1.29-1.51 (m, 4H), 1.61-1.70 (m, 1H), 1.73-1.88 (m, 2H), 1.95-2.12 (m, 2H), 3.51-3.65 (m, 1H), 7.27 (d, 1H, *J* = 7.4 Hz), 7.55 (d, 1H, *J* = 9.0 Hz), 7.59 (t, 1H, *J* = 7.2 Hz), 7.69 (t, 1H, *J* = 7.3 Hz), 7.79 (dt, 2H, *J* = 8.8 & 2.0 Hz), 7.96 (d, 1H, *J* = 8.0 Hz), 8.00 (d, 1H, *J* = 4.0 Hz), 8.24 (d, 2H, *J* = 8.9 Hz), 8.66 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 24.8, 25.2, 32.9, 53.1, 91.1, 105.9, 110.4, 116.7, 122.9, 124.1, 125.5, 125.9, 128.0, 128.8, 129.6, 130.0, 138.2, 144.5, 149.6, 149.8, 156.1, 156.6. HRMS (ESI) m/z calcd. for $C_{27}H_{22}N_2O_5$ $[M]^+$: 453.1444, found: 453.1440.

3-(4'-Nitrophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl) amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4n). Red solid (92%), Mp 192-193°C, IR (KBr, cm^{-1}): ν_{max} = 3397, 2974, 1714, 1616, 1553, 1494. ^1H NMR (400 MHz, DMSO-d_6): δ_H = 1.04 (s, 9H), 1.49 (s, 6H), 1.95 (s, 2H), 6.48 (s, 1H), 7.64-7.70 (m, 2H), 7.74-7.80 (m, 1H), 7.88 (dt, 1 H, *J* = 8.2 & 1.8 Hz), 8.11 (t, 2H, *J* = 8.8 Hz), 8.27 (dt, 2H, *J* = 8.8 & 2.4 Hz), 9.0 (d, 1H, *J* = 8.4 Hz). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 30.1, 31.3, 31.5, 53.3, 56.7, 97.8, 106.2, 110.1, 117.1, 123.0, 124.1, 125.7, 126.2, 128.1, 129.2, 130.1, 130.3, 130.6, 138.2, 145.2,

150.3, 151.0, 155.9, 156.7. HRMS (ESI) m/z calcd. for $C_{29}H_{28}N_2O_5$ $[M-H]^+$: 483.1914, found: 483.1905.

2-((Ethoxymethyl)amino)-3-(4'-nitrophenyl)-4*H*-benzo[*f*]furo [3,2-*c*]chromen-4-one (4o). Brown solid (89%), Mp 219-220°C, IR (KBr, cm^{-1}): ν_{max} = 3373, 2960, 2855, 2821, 1657, 1603, 1414. ^{1}H NMR(400 MHz, DMSO-d_6): δ_H = 1.17 (t, 3H, *J* = 7.1 Hz), 4.13 (q, 2H, *J* = 7.1 Hz), 4.25 (d, 2H, *J* = 6.2 Hz), 7.56-7.61(m, 2H), 7.64- 7.69 (m, 1H), 7.79 (dt, 2H, *J* = 9.0 & 2.5 Hz), 7.92-8.03 (m, 3H), 8.24 (dt, 2H, *J* = 9.0 & 2.5 Hz), 8.61 (d, 1H, *J* = 8.6 Hz).^{13}C NMR(100 MHz, DMSO-d_6): δ_C= 14.7, 45.1, 61.5, 92.1, 106.5, 111.1, 117.4, 123.7, 124.9, 126.1, 126.7, 128.7, 129.5, 130.5, 130.6, 138.3, 145.4, 150.4, 150.6, 156.6, 157.2, 171.1. HRMS (ESI) m/z calcd. for $C_{24}H_{18}N_2O_6$ $[M]^+$: 430.1165, found: 430.1161.

2-(*tert*-Butylamino)-3-(3,4-dimethoxyphenyl)-4*H*-benzo[*f*]furo [3,2-*c*]chromen-4-one (4p). Yellow solid (70%), IR (KBr, cm^{-1}): ν_{max} = 3290, 2363, 1713, 1649, 1619, 1585, 1218, 1091, 813. ^{1}H NMR(400 MHz, $CDCl_3$): δ_H = 1.45 (s, 9H), 3.92 (s, 3H), 3.93 (s, 3H), 4.21 (br s, 1H), 6.96 (d, 1H, *J* = 8.3 Hz), 7.08 (dd, 1H, *J* = 8.2 & 2.0 Hz), 7.14 (d, 1H, *J* = 2.0 Hz), 7.53-7.60 (m, 2H), 7.67-7.73 (m, 1H), 7.86 (d, 1H, *J* = 9.0 Hz), 7.92 (d, 1H, *J* = 7.6 Hz), 9.03 (d, 1H, *J* = 8.8 Hz). HRMS (ESI) m/z calcd. for $C_{27}H_{25}NO_5$ $[M]^+$: 443.1733, found: 443.1721.

3-(4'-Chlorophenyl)-2,6-(Dimethylphenylamino)-4H-benzo[*f*]furo[3,2-*c*]chromen-4-one (4q). Yellow-greenish solid (89%), Mp 195-196°C, IR (KBr, cm^{-1}): ν_{max}= 3372, 2959, 2854, 1654, 1602, 1412. ^{1}H NMR(400 MHz, DMSO-d_6):δ_H = 2.19 (s, 6H), 4.01 (s, 1H), 7.01-7.06 (m, 3H), 7.27-7.33 (m, 4H), 7.44 (dt, 2H, *J* = 8.8 & 2.0 Hz), 7.51-7.54 (m, 1H), 7.58-7.61 (m, 2H), 7.64 (d, 1H, J =11.6 Hz).). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 18.7, 126.3, 126.7, 127.8, 128.6, 128.7, 128.8, 129.0, 130.4, 130.6, 131.1, 131.3, 131.7, 134.4, 136.8, 139.1, 150.6, 150.7, 153.2, 153.5, 157.3, 162.8.HRMS (ESI) m/z calcd.for $C_{29}H_{20}ClNO_3$ $[M]^+$: 465.1126, found: 465.1107.

2-(Cyclohexylamino)-3-(4'-nitrophenyl)-furo[3,2-*c*]quinolin-4(5*H*)-one (5a). Dark red solid (85%), Mpdecomp. 200-210°C, IR (KBr, cm^{-1}): ν_{max} = 3397, 2942, 2862, 1660, 1597, 1508, 1338. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 1.06-1.21 (m, 1H), 1.23-1.48 (m, 4H), 1.49-1.66 (m, 1H), 1.66-1.84 (m, 2H), 1.84-2.06 (m, 2H), 3.54-3.75 (m, 1H), 6.84 (d, 1H, *J* = 7.8 Hz), 7.21-7.27 (m, 1H), 7.31-7.51 (m, 2H), 7.79 (d, 1H, *J* = 7.8 Hz), 7.85 (dt, 2H, *J* = 7.4 & 2.5 Hz), 8.19 (dt, 2H, *J* = 8.9 & 2.5 Hz), 11.67 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 24.8, 25.2, 33.1, 52.6, 93.1, 110.7, 114.8, 115.4, 118.7, 122.1, 122.7, 127.6, 130.1, 135.1, 139.5, 144.1, 147.8, 155.8, 158.5. HRMS (ESI) m/z calcd. for $C_{23}H_{21}N_3O_4$ $[M-H]^+$: 402.1448, found: 402.1442.

3-(4'-Chlorophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl) amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5b). Dark red solid (89%), Mpdecomp. 200-210°C, IR (KBr, cm^{-1}): ν_{max} = 3373, 2865, 2862, 1657, 1609, 1503, 1414. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 0.99 (s, 9H), 1.44 (s, 6H), 1.82 (s, 2H), 6.21 (s, 1H), 7.24-7.35 (m, 1H), 7.38 -7.48 (m, 2H), 7.78 (d, 1H, *J* = 7.8 Hz), 7.89 (dt, 2H, *J* = 8.9 & 2.4 Hz), 8.21 (dt, 2H, *J* = 8.9 & 1.8 Hz), 11.69 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C= 30.3, 31.3, 31.4, 53.0, 56.6, 97.6, 110.7, 114.2, 115.6, 118.7, 122.3, 122.8, 127.9, 130.4, 135.4, 139.5, 144.5, 148.6, 155.7, 158.5. HRMS (ESI) m/z calcd. for $C_{25}H_{27}N_3O_4$ $[M-H]^+$: 432.1917, found: 432.1911.

2-(Cyclohexylamino)-3-(4'-chlorophenyl)-furo[3,2-*c*]quinolin-4(5*H*)-one (5c). Light yellow solid (81%), Mpdecomp. 212-214°C, IR (KBr, cm^{-1}): ν_{max} = 3096, 2896, 1711, 1211, 1003. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 1.02-1.18 (m, 1H), 1.19-1.42 (m, 4H), 1.53-1.61 (m, 1H), 1.63-1.76 (m, 2H), 1.83-1.99 (m, 2H), 3.41-3.58 (m, 1H), 3.41-3.53 (m, 1H), 6.26 (d, 1H, *J* = 8.0 Hz) 7.22 (td, 1H, *J* = 6.7 & 1.6 Hz), 7.34-7.44 (m, 4H), 7.58 (dt, 2H, *J* = 8.5 & 2.6 Hz), 7.77 (d, 1H, *J* = 7.8 Hz), 11.57 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 24.8, 25.2, 33.2, 52.8, 94.7, 110.9, 115.3, 115.4, 118.6, 121.9, 127.3, 127.5, 130.0, 130.5, 131.6, 135.0, 147.4, 154.7, 158.6. HRMS (ESI) m/z calcd. for $C_{23}H_{21}ClN_2O_2$ $[M-H]^+$: 391.1207, found: 391.1201.

3-(4'-Chlorophenyl)-2-((2-morpholinoethyl)amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5d). Light yellow solid (84%), Mpdecomp. 263°C, IR (KBr, cm^{-1}):

ν_{max} = 3367, 2962, 2864, 2825, 1664, 1592, 1506, 1419. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 2.47 (s, 4H), 2.62 (s, 2H), 3.42- 3.52 (m, 2H), 3.66 (s, 4H), 5.26 (s, 1H), 7.21-7.30 (m, 3H), 7.35- 7.42 (m, 3H), 7.61 (dt, 2H, *J* = 7.8 & 2.6 Hz), 7.82 (d, 1H, *J* = 7.2 Hz), 10.53 (s, 1H). HRMS (ESI) m/z calcd. for $C_{23}H_{22}ClN_3O_3$ $[M]^+$: 423.1344, found: 423.1341.

2-((2-Morpholinoethylamino)-3-(4'-nitrophenyl)furo[3,2-*c*] quinolin-4(5*H*)-one (5e). Orange solid (89%); Mpdecomp. 262-263°C, IR (KBr, cm^{-1}): ν_{max} = 3363, 3164, 2959, 2860, 1661, 1603, 1569, 1508. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 2.51 (s, 4H), 2.61-2.71 (m, 2H), 3.52-3.60 (m, 2H), 3.64-3.70 (m, 4H), 5.61 (br s, 1H), 7.21-7.31 (m, 2H), 7.37-7.43 (m, 1H), 7.84 (dt, 3H, *J* = 9.3 & 2.4 Hz), 8.27 (d, 2H, *J* = 8.8 Hz), 9.51 (s, 1H). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C = 49.1, 53.7, 58.6, 66.8, 93.0, 111.2, 115.3, 116.0, 119.3, 122.7, 123.5, 128.2, 130.4, 135.6, 140.1, 144.5, 148.2, 157.3, 159.1. HRMS (ESI) m/z calcd. for $C_{23}H_{24}N_4O_5$ $[M-H]^+$: 433.1506, found: 433.1501.

3-(4'-Bromophenyl)-2-((2-morpholinoethyl)amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5f).Yellow solid (81%), Mpdecomp. 258-259°C, IR (KBr, cm^{-1}): ν_{max} = 3369, 2963, 2864, 2821, 1655, 1602, 1498. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 2.47 (s, 4H), 2.61 (s, 2H), 3.42-3.51 (m, 2H), 3.66 (s, 4H), 5.25 (br s, 1H), 7.21-7.30 (m, 3H), 7.35- 7.41 (m, 1H), 7.54 (s, 4H), 7.82 (d, 1H, *J* = 7.8 Hz), 10.49 (s, 1H). HRMS (ESI) m/z calcd. for $C_{23}H_{22}BrN_3O_3$ $[M-H]^+$: 466.0760, found: 466.0765.

3-(4'-Chlorophenyl)-2-(pentylamino)furo[3,2-*c*]quinolin-4(5*H*) -one (5g).Yellow solid (78%), Mp 218-220 °C, IR (KBr, cm^{-1}): ν_{max} = 3369, 2956, 2863, 2827, 1661, 1606, 1500, 1416. ^{1}H NMR (400 MHz, $CDCl_3$): δ_H = 0.85-0.95 (m, 3H), 1.30-1.43 (m, 4H), 1.55-1.70 (m, 2H), 3.40 (t, 2H, *J* = 7.8 Hz), 4.40 (br s, 1H), 7.15-7.25 (m, 2H), 7.27-7.35 (m, 2H), 7.41 (dt, 2H, *J* = 8.5 & 1.8 Hz), 7.58 (dt, 2H, *J* = 8.5 & 1.8 Hz), 7.82 (d, 1H, *J* = 7.8 Hz), 11.17 (s, 1H). HRMS (ESI) m/z calcd. for $C_{22}H_{21}ClN_2O_2$ $[M-H]^+$: 379.1207, found: 379.1207.

3-(2',6'-Dichlorophenyl)-2-((2-morpholinoethyl)amino) furo [3,2-*c*]quinolin-4(5*H*)-one (5h).Yellow solid (87%), Mpdecomp. 271-272 °C, IR (KBr, cm^{-1}): ν_{max} = 3433, 2938, 2856, 1661, 1602, 1491, 1350. ^{1}H NMR(400 MHz, $CDCl_3$): δ_H = 2.41 (s, 4H), 2.54 (t, 2H, *J* = 5.7 Hz), 3.36 (q, 2H, *J* = 5.7 Hz), 3.60 (t, 4H, *J* = 4.4 Hz), 4.77 (t, 1H, *J* = 5.4 Hz),7.19-7.34 (m, 4H), 7.42-7.47 (m, 2H), 7.81(dd, 1H, *J* = 7.8 Hz), 11.31 (s, 1H). ^{13}C NMR(100 MHz, DMSO-d_6): δ_C = 40.3, 53.2, 57.0, 67.1, 92.0, 112.2, 116.4, 117.2, 119.2, 122.4, 127.5, 127.8, 129.5, 130.0, 135.3, 137.4, 149.2, 155.0, 160.3. HRMS (ESI) m/z calcd. for $C_{23}H_{21}Cl_2N_3O_3$ $[M-H]^+$: 456.0876, found 456.0871.

3-(4'-Bromophenyl)-2-(cyclohexylamino)furo[3,2-*c*]quinolin-4(5*H*)-one (5i).Yellow solid (82%), Mpdecomp. 271-272 °C, IR (KBr, cm^{-1}): ν_{max} = 3433, 2938, 2856, 1661, 1602, 1491, 1350. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H = 1.11-1.30 (m, 3H), 1.31-1.45 (m, 2H), 1.60-1.70 (m, 1H), 1.70-1.82 (m, 2H), 2.02-2.10 (m, 2H), 3.50-3.66 (m, 1H), 4.20 (br s, 1H), 7.15-7.26 (m, 1H), 7.30-7.35 (m, 2H), 7.50-7.60 (m, 3H), 7.83 (d, 1H, *J* = 7.8 Hz), 11.36 (s, 1H). ^{13}C NMR(100 MHz, DMSO-d_6): δ_C = 25.4, 25.8, 33.7, 53.3, 95.0, 111.5, 115.8, 115.9, 119.0, 119.1, 122.5, 127.8, 130.9, 131.4, 132.5, 135.6, 148.0, 155.2, 159.2. HRMS (ESI) m/z calcd. for $C_{23}H_{21}BrN_2O_2$ $[M-H]^+$: 435.0702, found 435.0701.

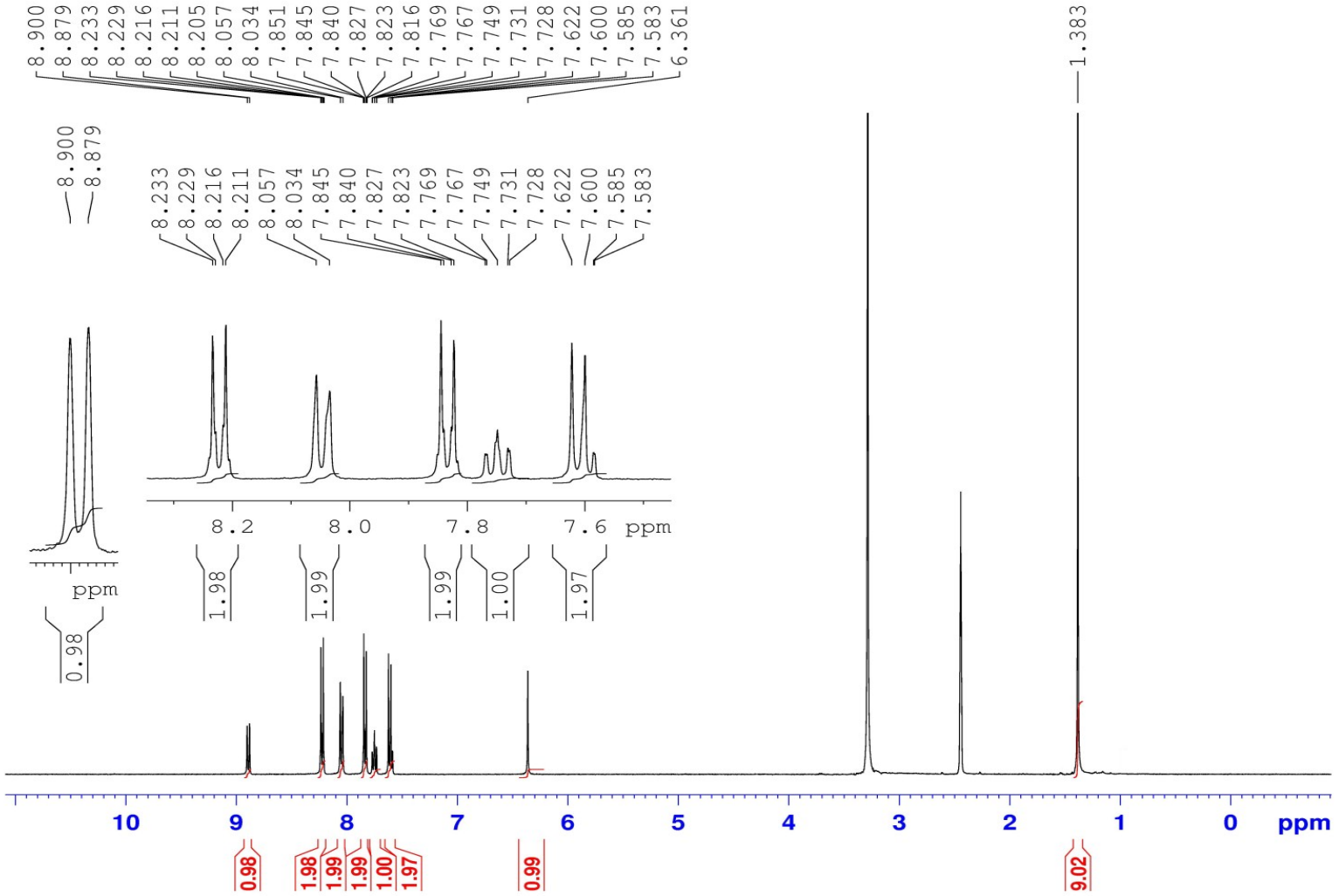
2-(Cyclohexylamino)-3-(2',6'-dichlorophenyl)furo[3,2-*c*] quinolin-4(5*H*)-one (5j).White solid (84%), Mp 265-266°C, IR (KBr, cm^{-1}): ν_{max} = 3433, 2938, 2856, 1661, 1602, 1491, 1350. ^{1}H NMR(400 MHz, $CDCl_3$): δ_H = 1.10-1.35 (m, 8H), 1.52-1.65 (m, 2H), 1.67-1.77 (m, 1H), 1.97-2.11 (m, 2H), 3.38 – 3.57 (m, 1H), 3.74 (d, 1H, *J* = 8.0 Hz), 7.18-7.34 (m, 4H), 7.45 (d, 2H, *J* = 8.0 Hz), 7.83 (d, 1H, *J* = 7.8 Hz), 10.78 (s, 1H). ^{13}C NMR(100 MHz, $CDCl_3$): δ_C = 25.0, 25.4, 25.6, 34.3, 53.7, 92.4, 112.2, 116.2, 117.1, 119.3, 122.4, 127.4, 127.9, 129.5, 130.0, 135.2, 137.4, 149.0, 154.3, 160.0. HRMS (ESI) m/z calcd. for $C_{23}H_{20}Cl_2N_2O_2$ $[M-H]^+$: 425.0818, found 425.0814.

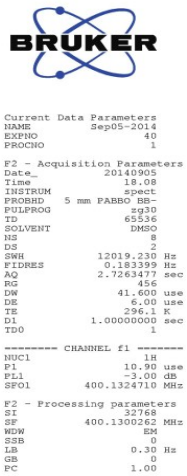
2-(*tert*-Butylamino)-3-(3',4'-dimethoxyphenyl)furo[3,2-*c*] quinolin-4(5*H*)-one (5k). Yellow solid (71%), IR (KBr, cm^{-1}): ν_{max} = 3432, 2935, 2852, 1657, 1487, 1343. ^{1}H NMR(400 MHz, $CDCl_3$): δ_H = 1.39 (s, 9H), 3.92 (s, 3H), 3.93 (s, 3H), 6.95 (d, 1H, *J* = 8.2 Hz), 7.10 (dd, 1H, *J* = 8.2 & 2.0 Hz), 7.20-7.28 (m,

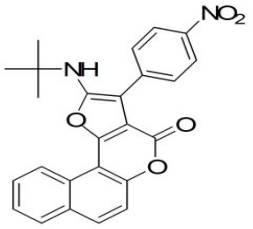
2H), 7.29-7.40 (m, 2H), 7.85 (d, 1H, *J* = 7.8 Hz), 11.2 (s, 1H). HRMS (ESI) m/z calcd. for $C_{23}H_{24}N_2O_4$ $[M]^+$: 392.1736, found 392.1729.

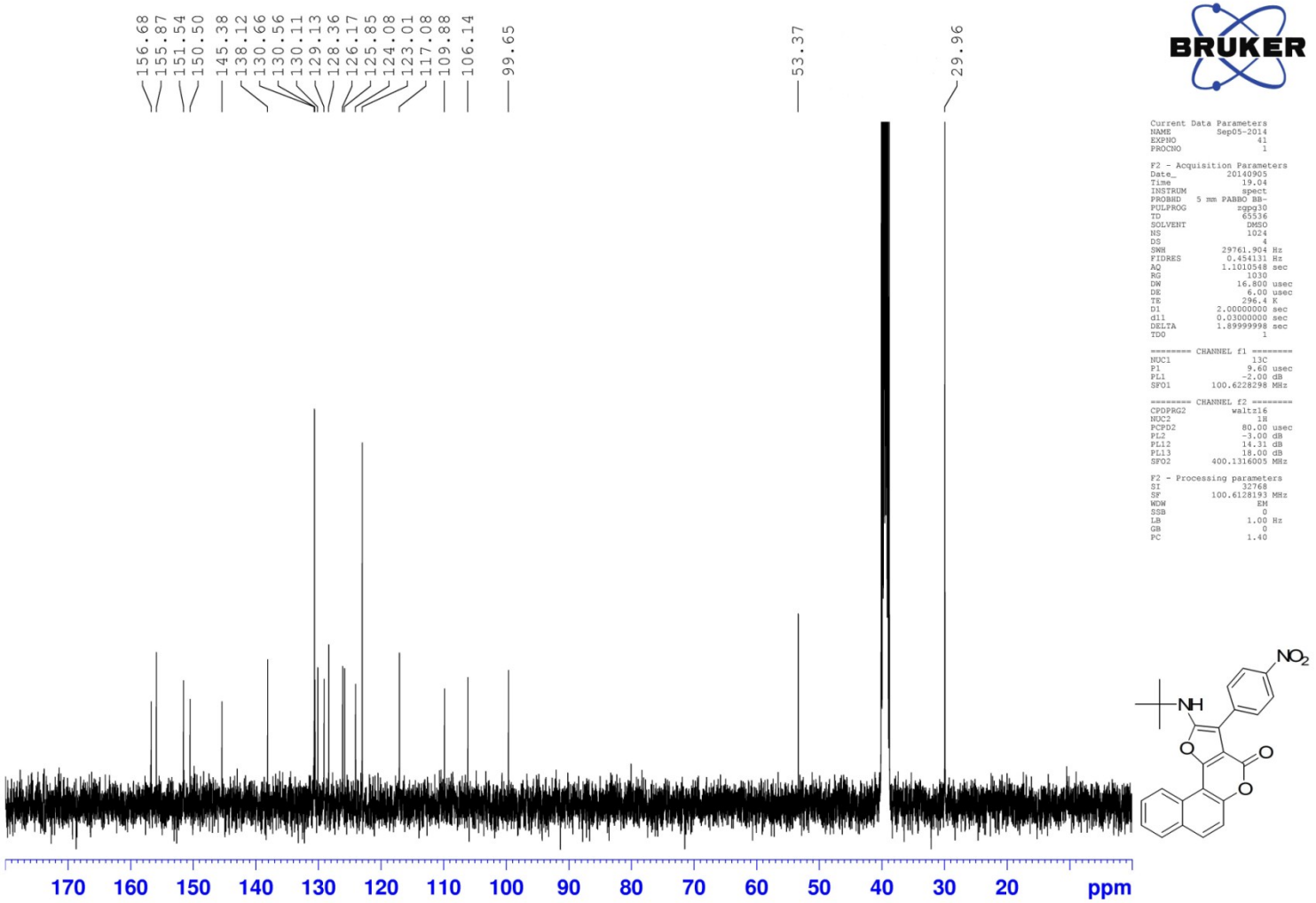
3-(4'-methoxyphenyl)-2-(2-morpholinoethyl)amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5l). Yellow solid (69%), IR (KBr, cm^{-1}): ν_{max} = 3430, 2930, 2852, 1648, 1485, 1341.^{1}H NMR(400 MHz, $CDCl_3$): δ_H = 2.45 (s, 4H), 2.59 (t, 2H, *J* = 5.6 Hz), 3.44 (q, 2H, *J* = 5.8 Hz), 3.63 (t, 4H, *J* = 4.5 Hz), 5.17 (s, 1H), 6.98 (dt, 2H, *J* = 8.8 & 3.0 Hz), 7.20-7.29 (m, 3H), 7.32-7.38 (m, 1H), 7.56 (dt, 2H, *J* = 8.0 & 3.8 Hz), 7.82 (dd, 1H, *J* = 8.0 & 1.0 Hz), 10.33 (s, 1H). HRMS (ESI) m/z calcd. for $C_{24}H_{25}N_3O_4$ $[M]^+$: 419.1845, found 419.1839.

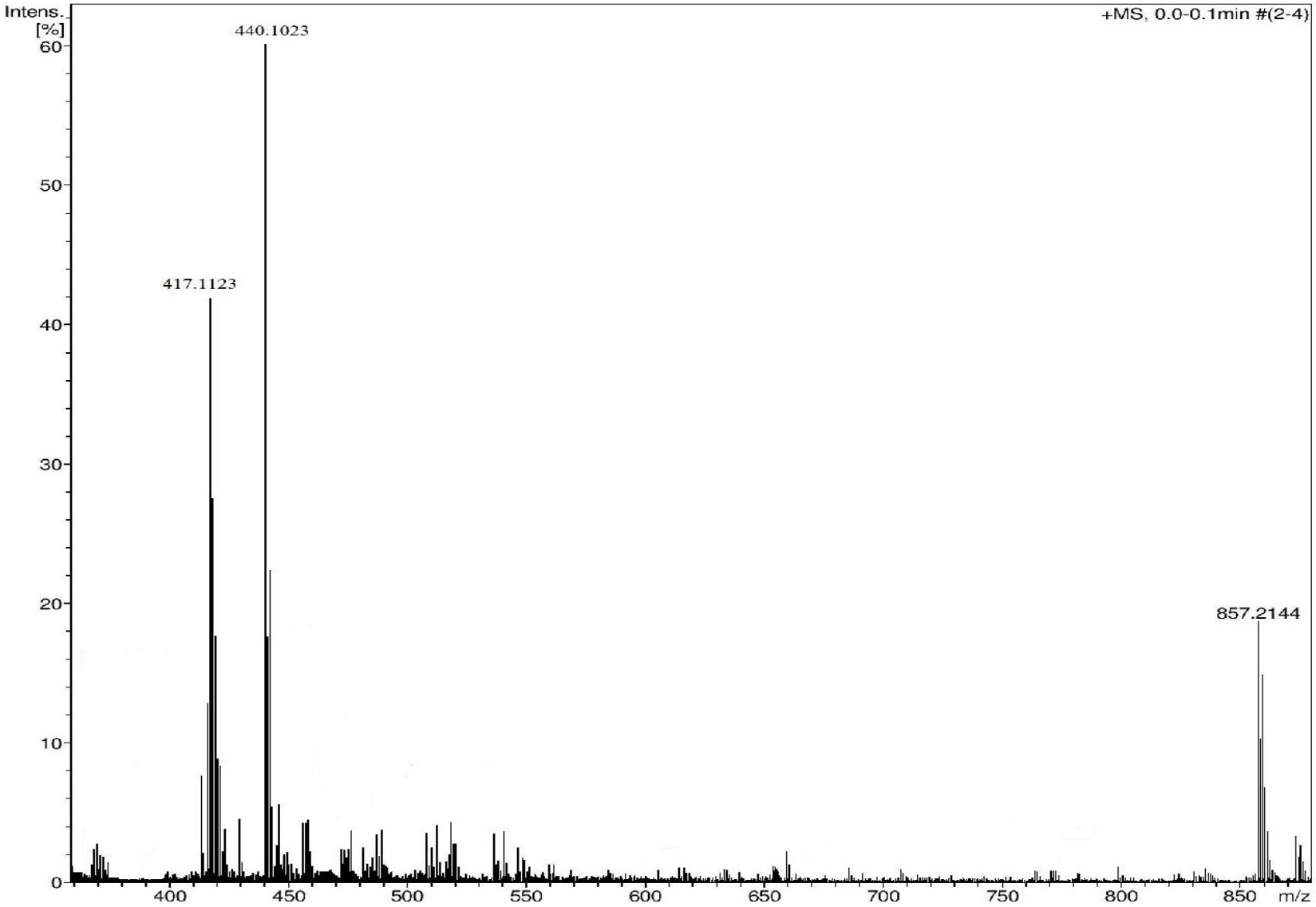
2-(*tert*-Butylamino)-3-(4'-nitrophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one(4a).



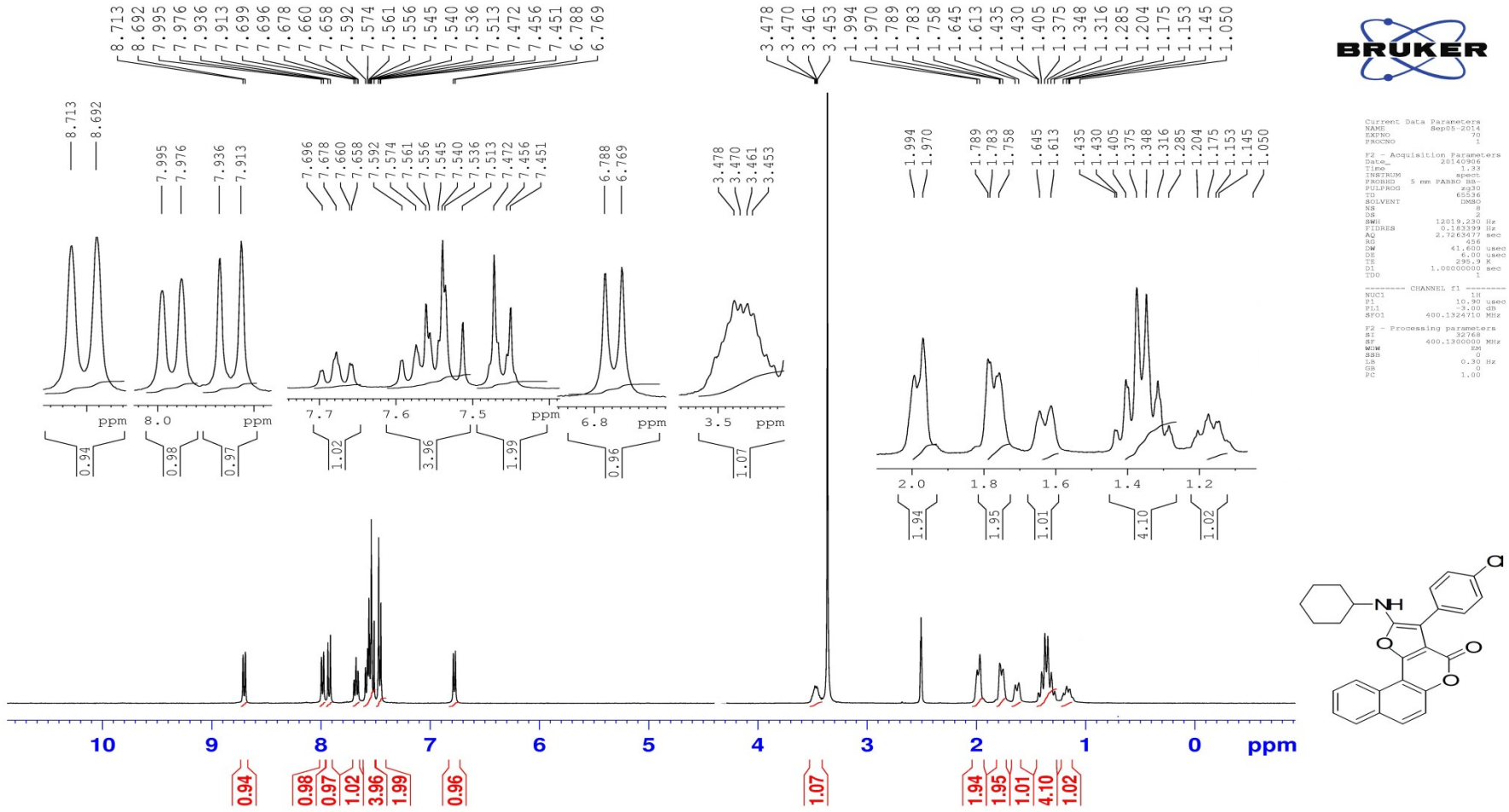


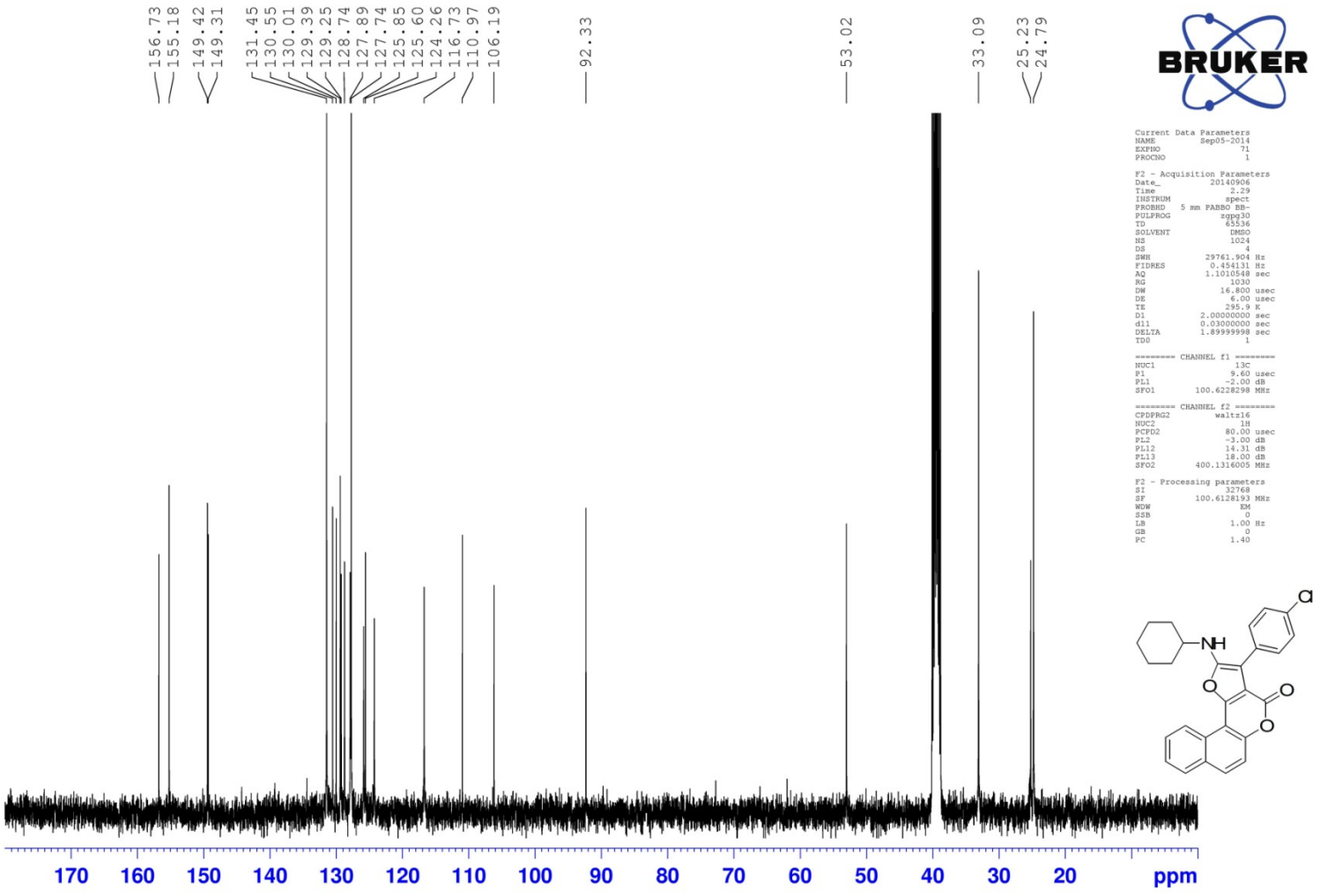


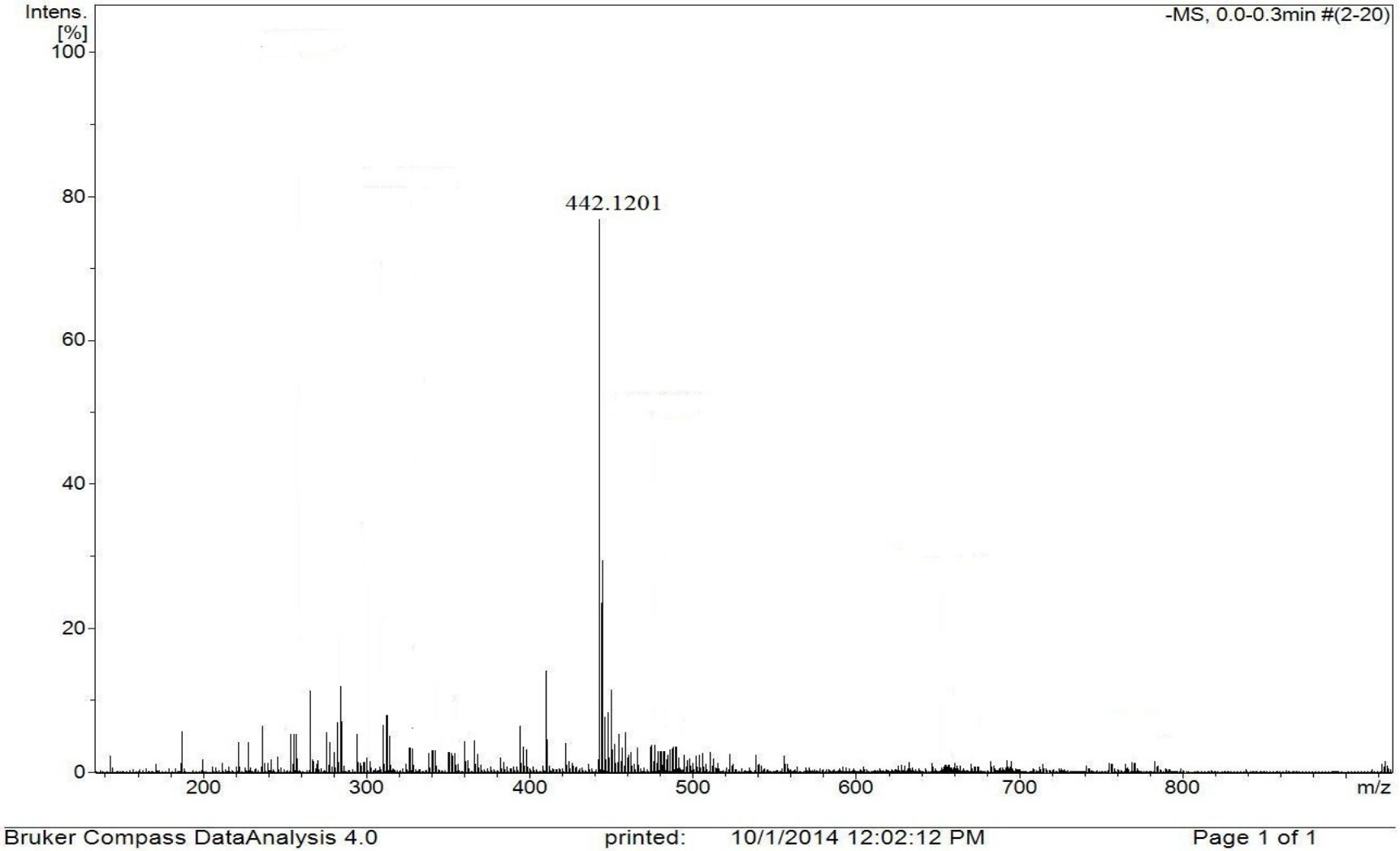

156.68
155.87
151.54
150.50
145.38
138.12
130.66
130.56
130.11
129.13
128.36
126.17
125.85
124.08
123.01
117.08
109.88
106.14
99.65
53.37
29.96
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
BRUKER
Current Data Parameters
NAME Sep05-2014
EXPNO 41
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140905
Time 19.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 296.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
NO2
NH
O
O
O


Intens.
[%]
+MS, 0.0-0.1min #(2-4)
440.1023
417.1123
857.2144
60
50
40
30
20
10
0
400
450
500
550
600
650
700
750
800
850
m/z

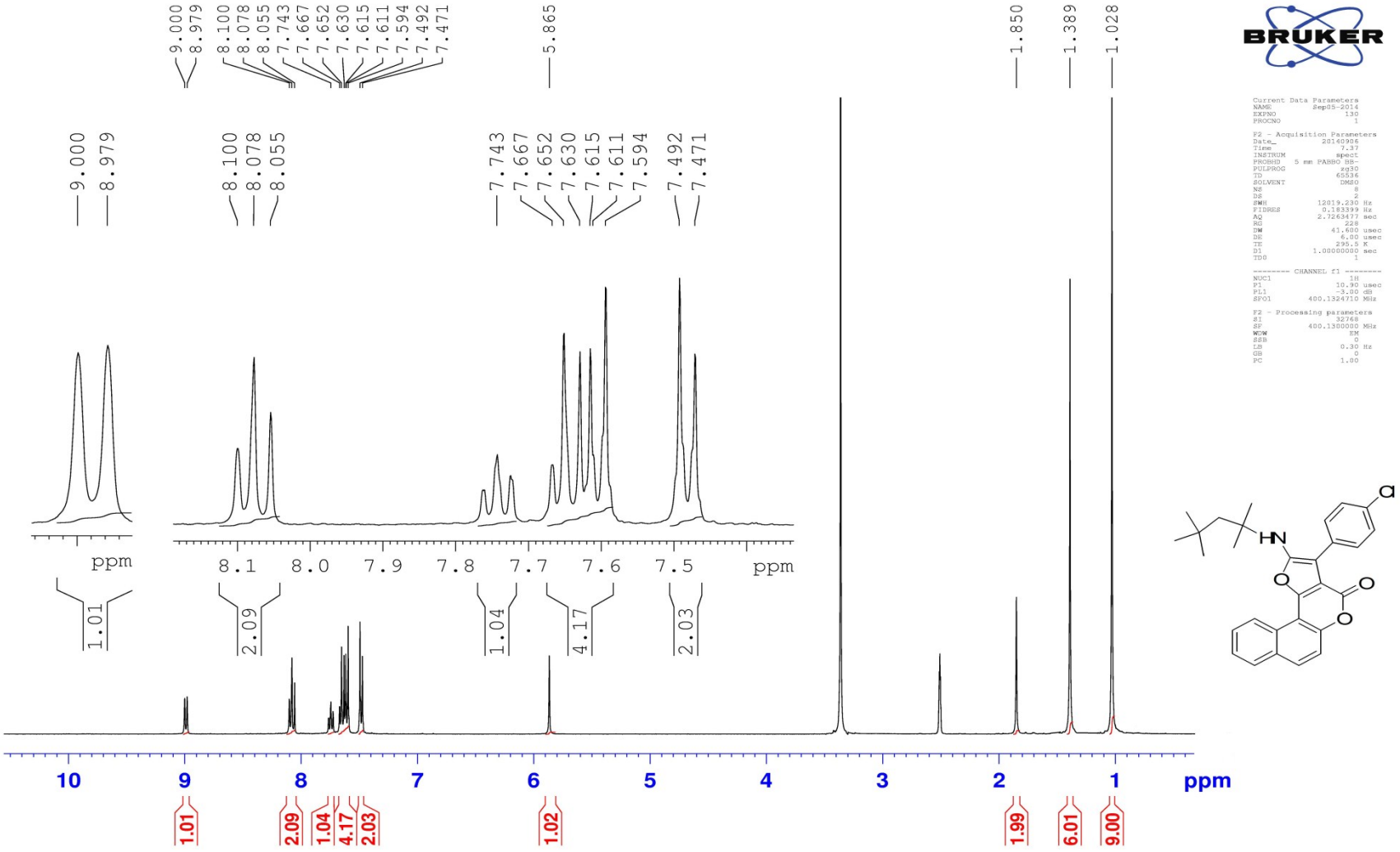
2-(Cyclohexylamino)-3-(4'-chlorophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4b).

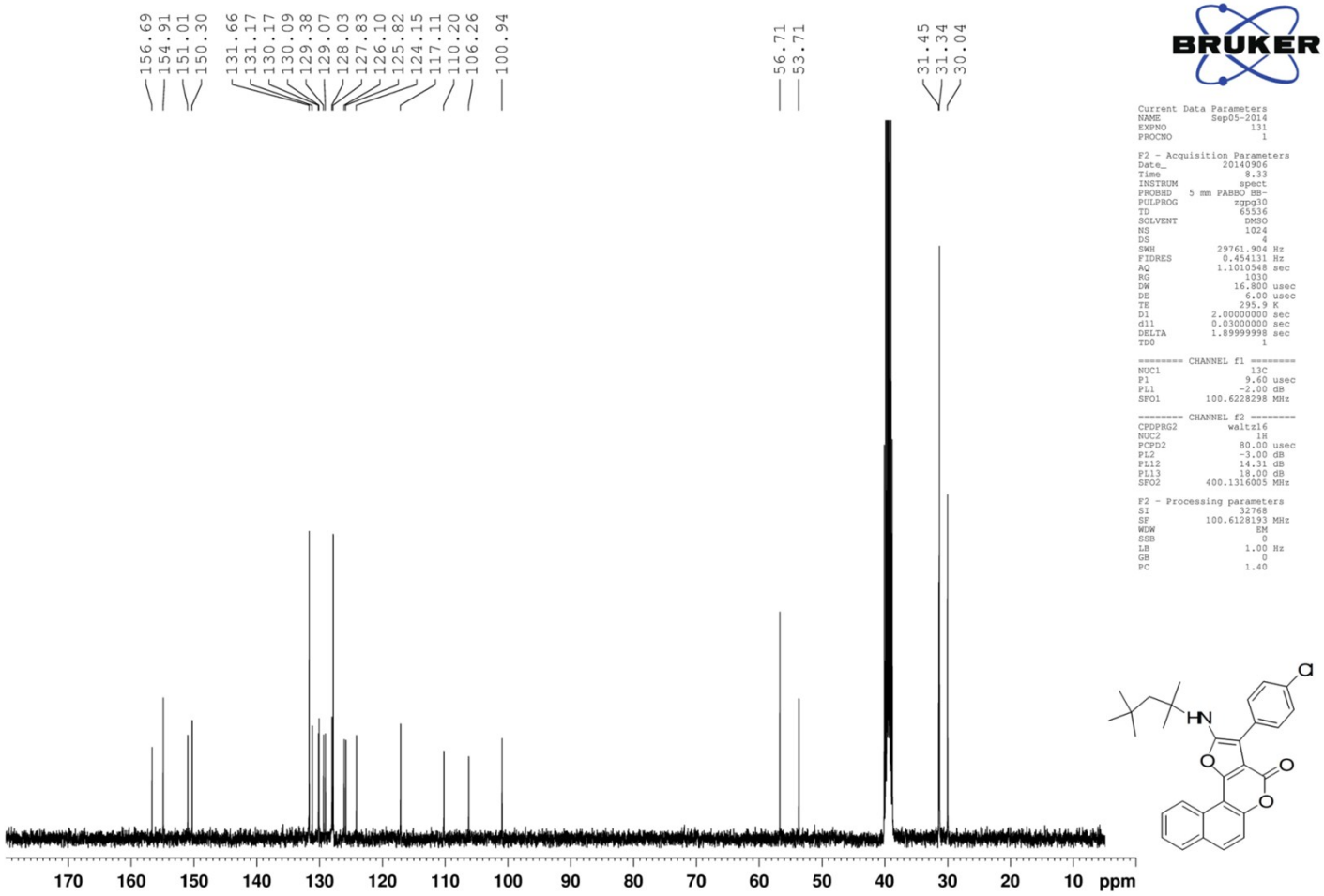



156.73
155.18
149.42
149.31
131.45
130.55
130.01
129.39
129.25
128.74
127.89
127.74
125.85
125.60
124.26
116.73
110.97
106.19
92.33
53.02
33.09
25.23
24.79
BRUKER
Current Data Parameters
NAME Sep05-2014
EXPNO 71
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140906
Time 2.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13c
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
NH
O
O
O
O
Cl
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Intens.
[%]
100
80
60
40
20
0
-MS, 0.0-0.3min #(2-20)
442.1201
200
300
400
500
600
700
800
m/z
Bruker Compass DataAnalysis 4.0
printed: 10/1/2014 12:02:12 PM
Page 1 of 1

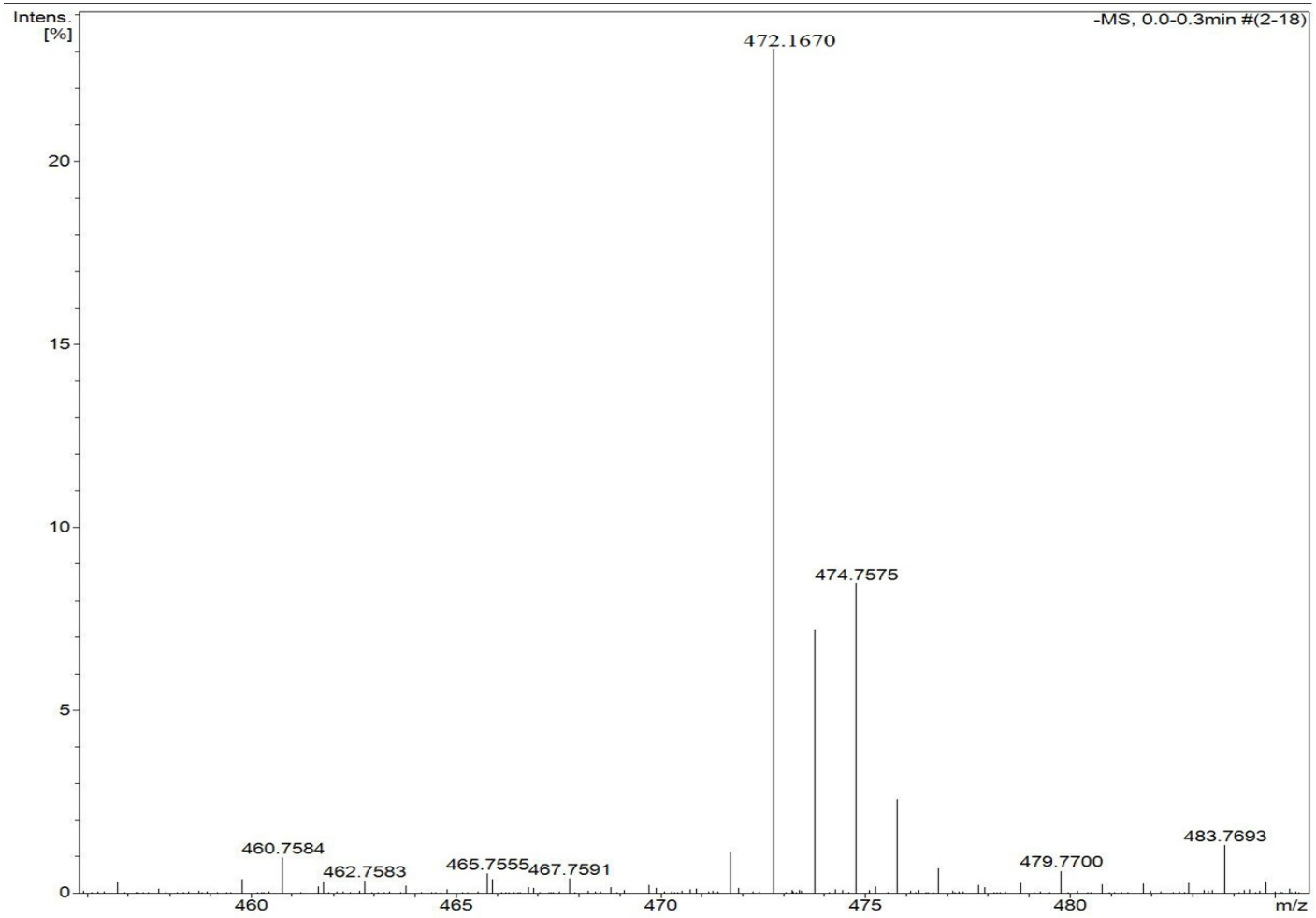
3-(4'-Chlorophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4c).



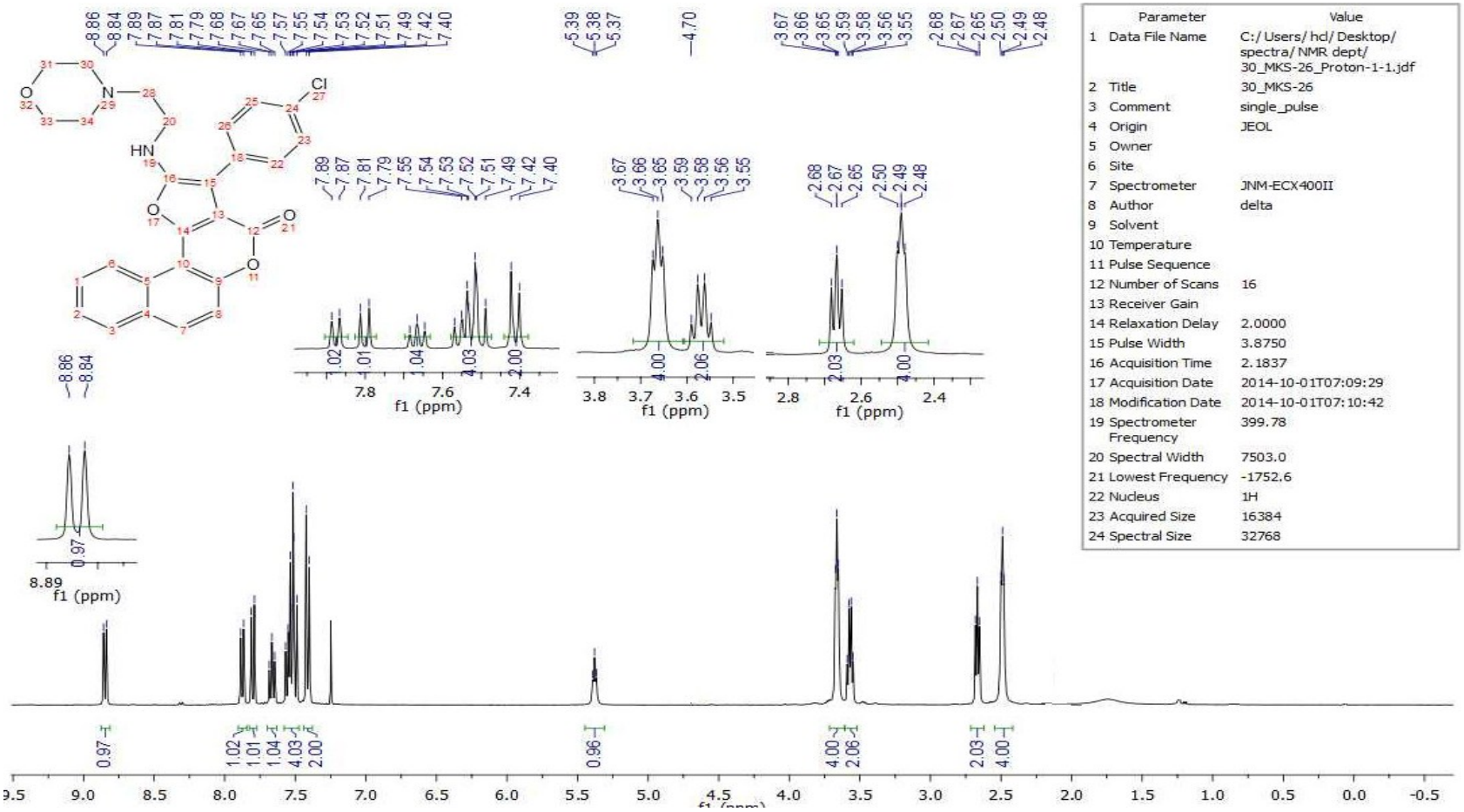


BRUKER

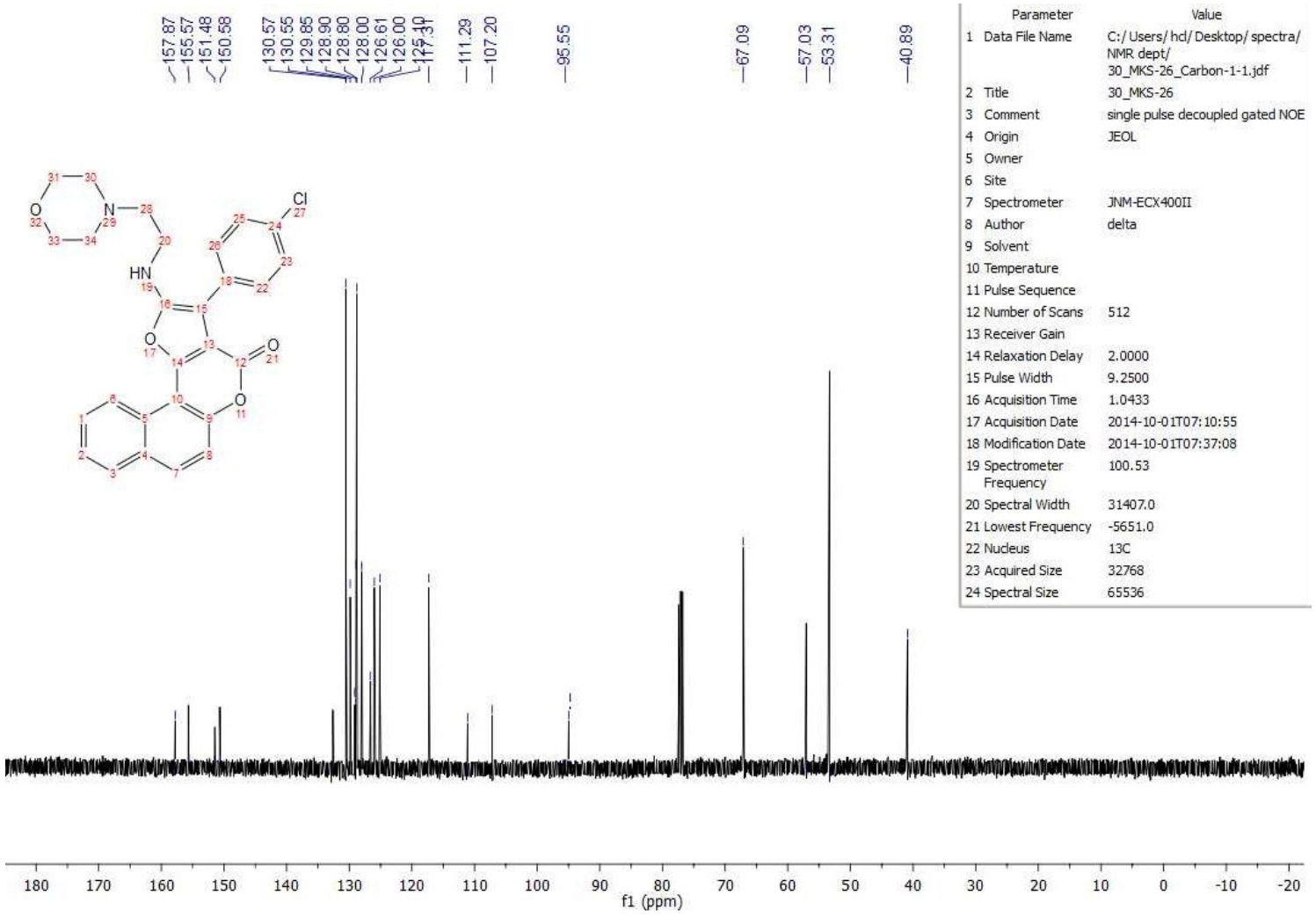
```
Current Data Parameters
NAME                  Sep05-2014
EXPNO                        131
PROCNO                         1

F2 - Acquisition Parameters
Date_               20140906
Time                     8.33
INSTRUM                 spect
PROBHD     5 mm PABBO BB-
PULPROG                 zgpg30
TD                       65536
SOLVENT                  DMSO
NS                       1024
DS                          4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010548 sec
RG                       1030
DW                   16.800 usec
DE                    6.00 usec
TE                    295.9 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                       9.60 usec
PL1                     -2.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                   80.00 usec
PL2                     -3.00 dB
PL12                    14.31 dB
PL13                    18.00 dB
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                 100.6128193 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```


Intens.
[%]
-MS, 0.0-0.3min #(2-18)
472.1670
474.7575
460.7584
462.7583
465.7555
467.7591
479.7700
483.7693
20
15
10
5
0
460
465
470
475
480
m/z

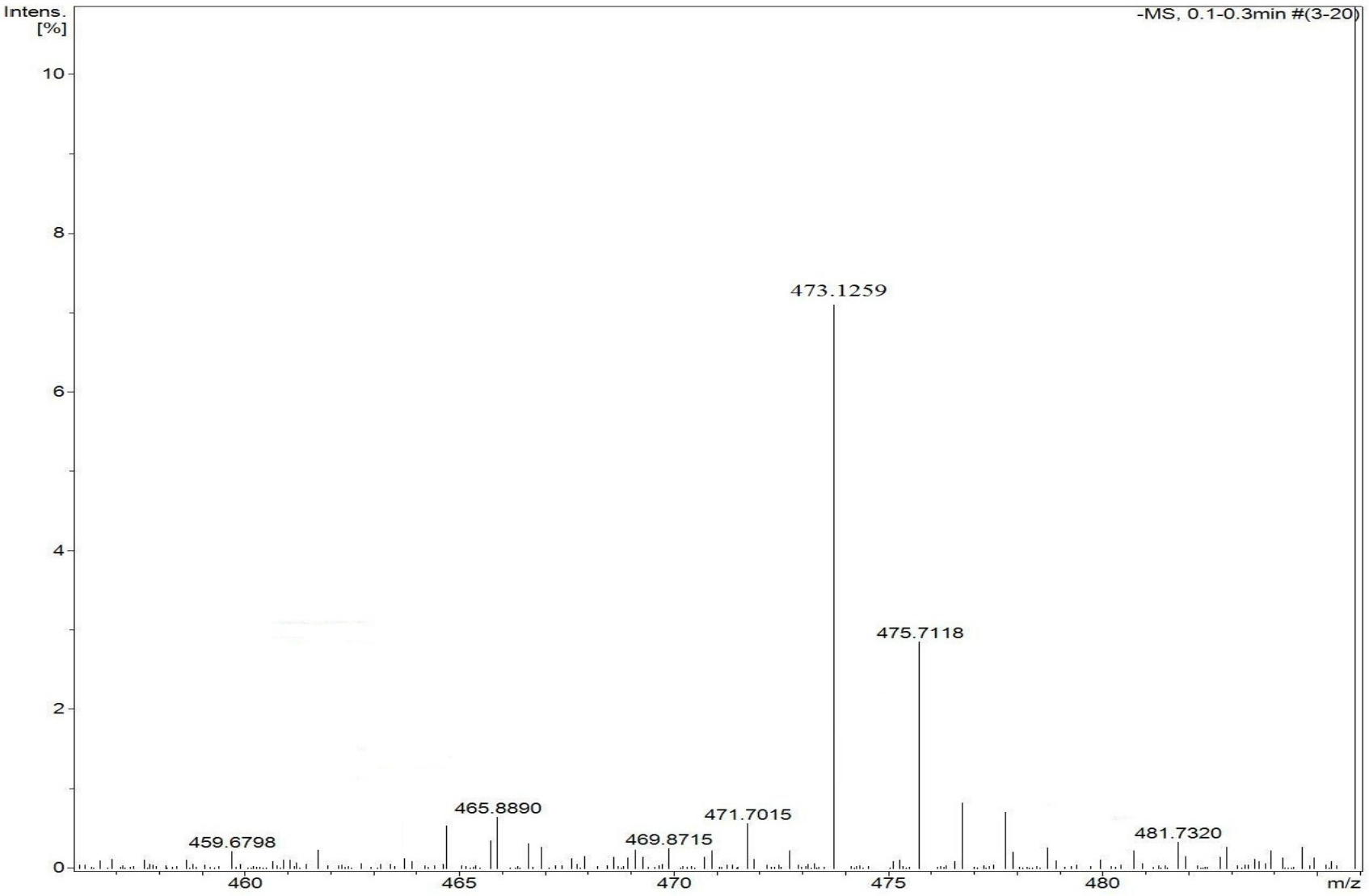
3-(4'-Chlorophenyl)-2-((2-morpholinoethyl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one(4d).



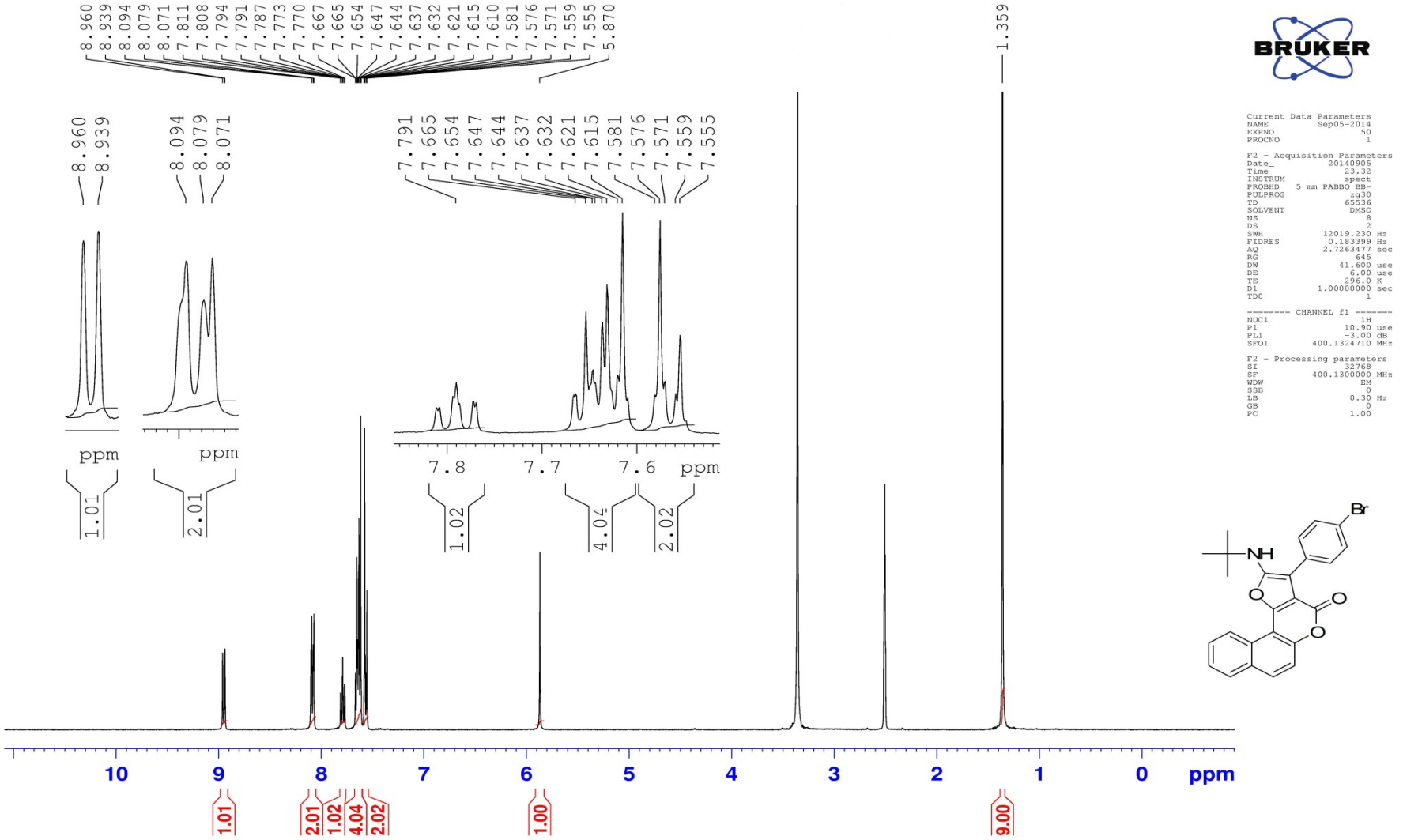
	Parameter	Value
1	Data File Name	C:/ Users/ hcl/ Desktop/ spectra/ NMR dept/ 30_MKS-26_Proton-1-1.jdf
2	Title	30_MKS-26
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	JNM-ECX400II
8	Author	delta
9	Solvent	
10	Temperature	
11	Pulse Sequence	
12	Number of Scans	16
13	Receiver Gain	
14	Relaxation Delay	2.0000
15	Pulse Width	3.8750
16	Acquisition Time	2.1837
17	Acquisition Date	2014-10-01T07:09:29
18	Modification Date	2014-10-01T07:10:42
19	Spectrometer Frequency	399.78
20	Spectral Width	7503.0
21	Lowest Frequency	-1752.6
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

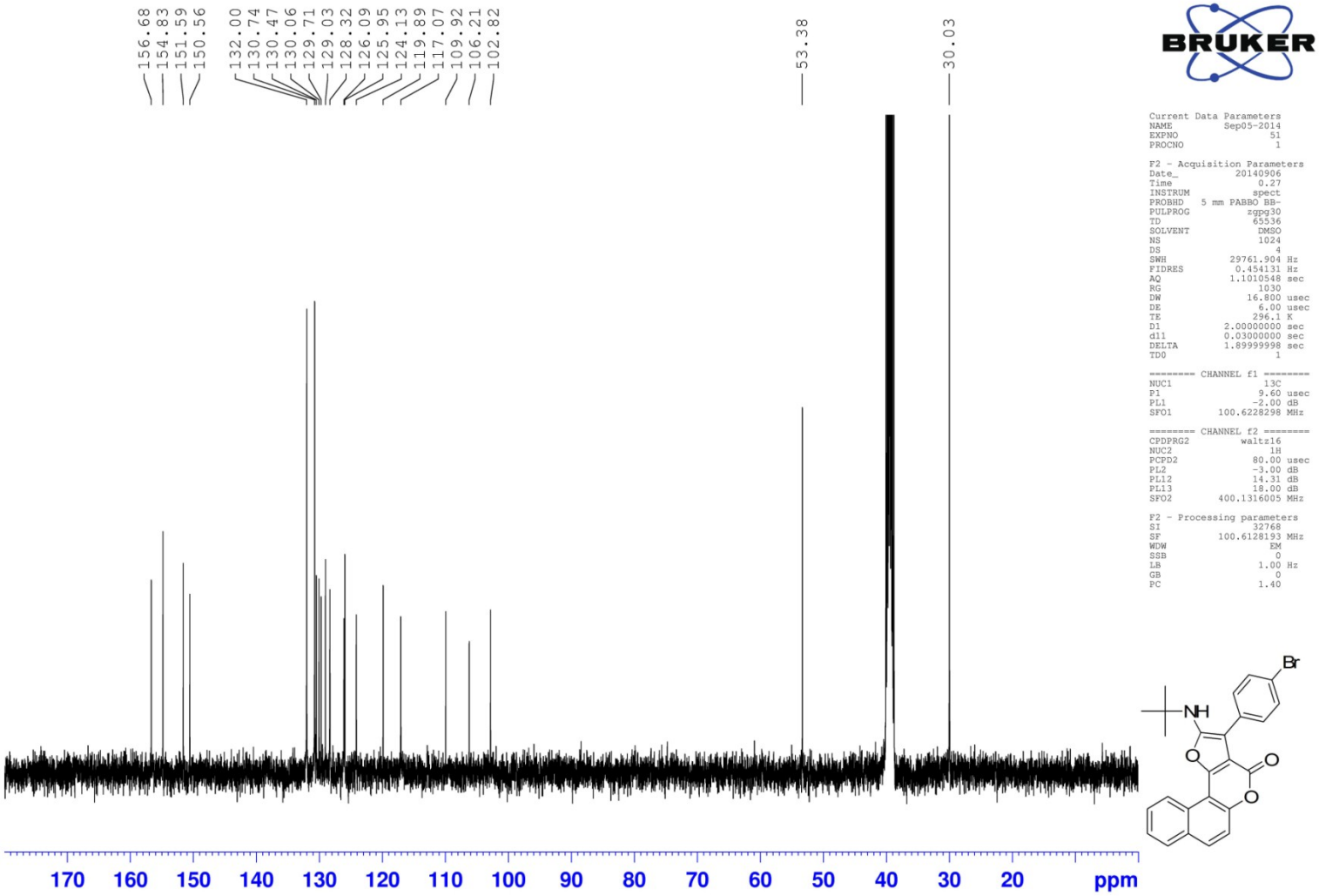


	Parameter	Value
1	Data File Name	C:/ Users/ hcl/ Desktop/ spectra/ NMR dept/ 30_MKS-26_Carbon-1-1.jdf
2	Title	30_MKS-26
3	Comment	single pulse decoupled gated NOE
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	JNM-ECX400II
8	Author	delta
9	Solvent	
10	Temperature	
11	Pulse Sequence	
12	Number of Scans	512
13	Receiver Gain	
14	Relaxation Delay	2.0000
15	Pulse Width	9.2500
16	Acquisition Time	1.0433
17	Acquisition Date	2014-10-01T07:10:55
18	Modification Date	2014-10-01T07:37:08
19	Spectrometer Frequency	100.53
20	Spectral Width	31407.0
21	Lowest Frequency	-5651.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536


Intens.
[%]
-MS, 0.1-0.3min #(3-20)
10
8
6
4
2
0
473.1259
475.7118
465.8890
471.7015
459.6798
469.8715
481.7320
460
465
470
475
480
m/z

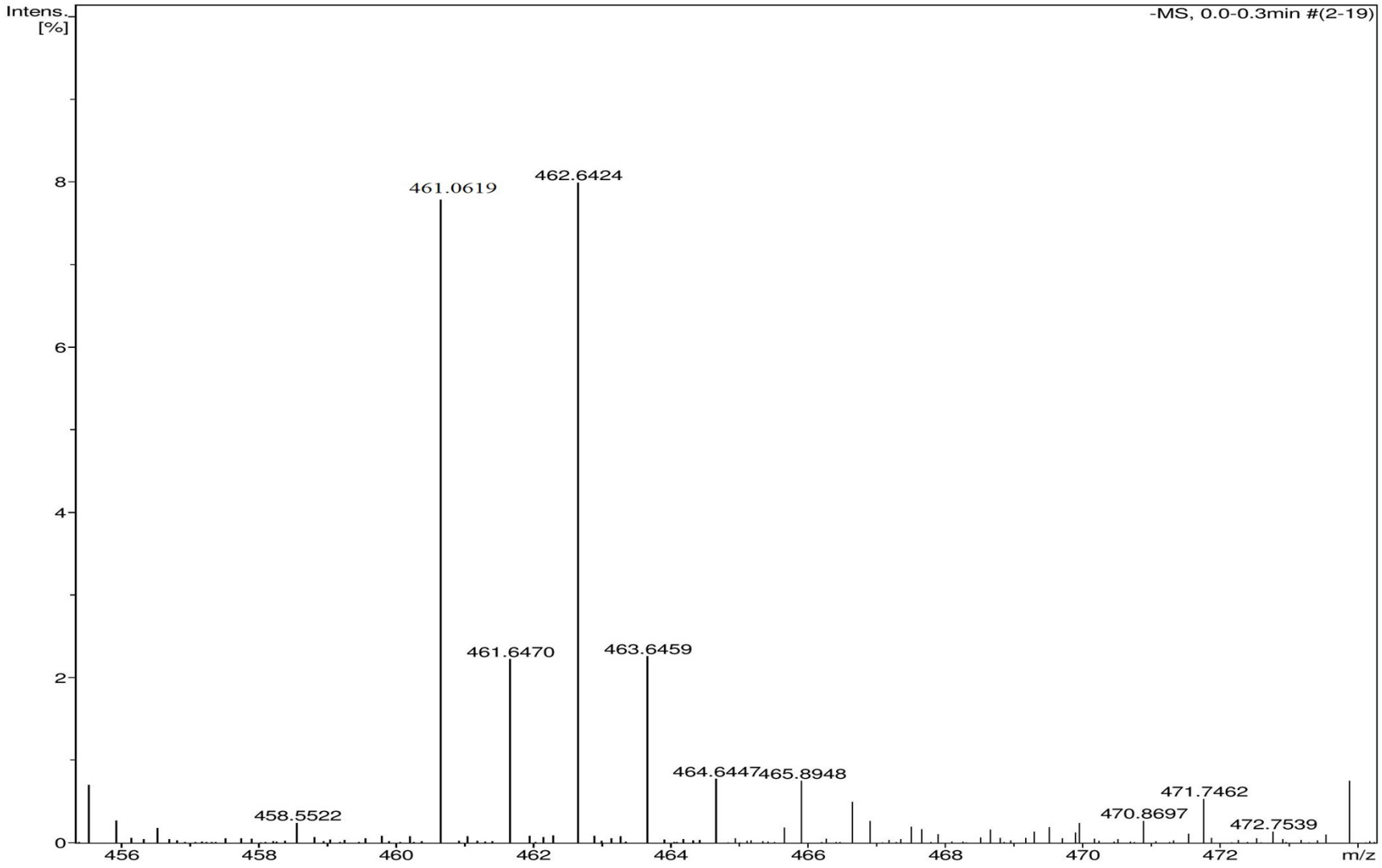
2-(*tert*-Butylamino)-3-(4'-bromophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one(4e).



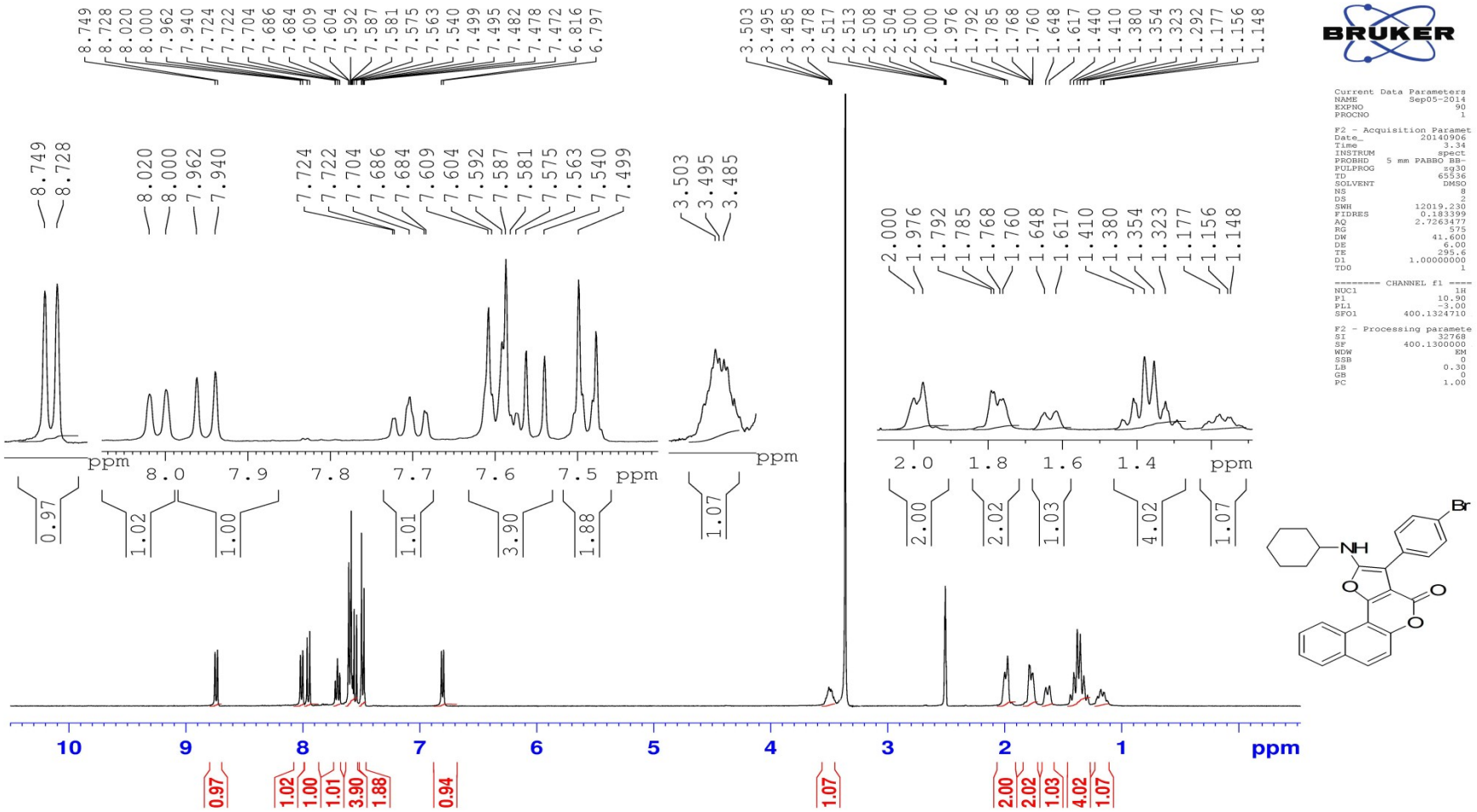


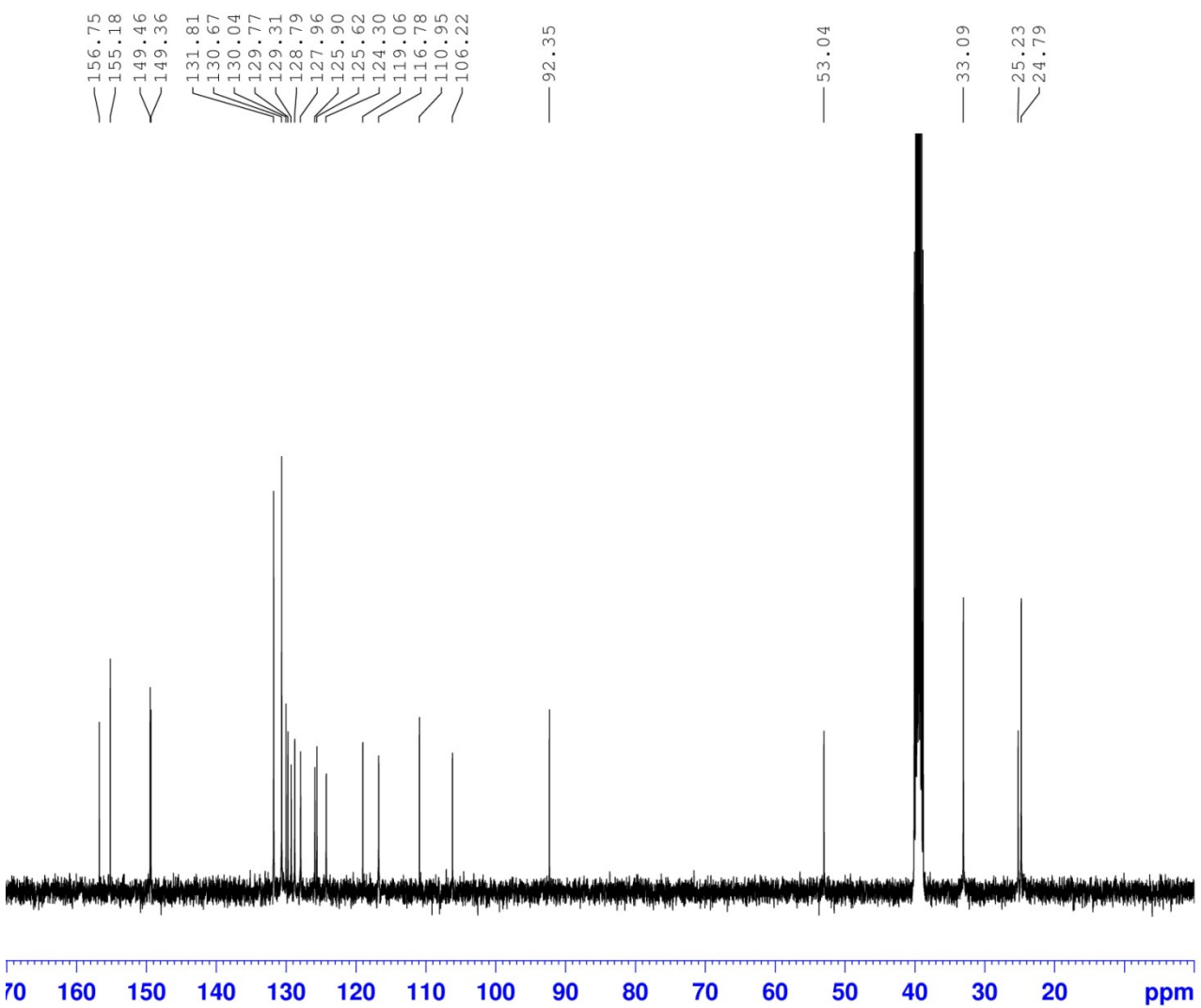
BRUKER

```
Current Data Parameters
NAME                 Sep05-2014
EXPNO                        51
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140906
Time                     0.27
INSTRUM                 spect
PROBHD     5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                  DMSO
NS                       1024
DS                          4
SWH                 29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010548 sec
RG                       1030
DW                     16.800 usec
DE                      6.00 usec
TE                      296.1 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                        9.60 usec
PL1                      -2.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL2                      -3.00 dB
PL12                     14.31 dB
PL13                     18.00 dB
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                 100.6128193 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

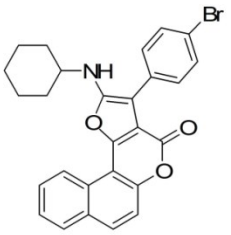

Intens.
[%]
-MS, 0.0-0.3min #(2-19)
461.0619
462.6424
461.6470
463.6459
464.6447
465.8948
458.5522
471.7462
470.8697
472.7539
0
2
4
6
8
456
458
460
462
464
466
468
470
472
m/z

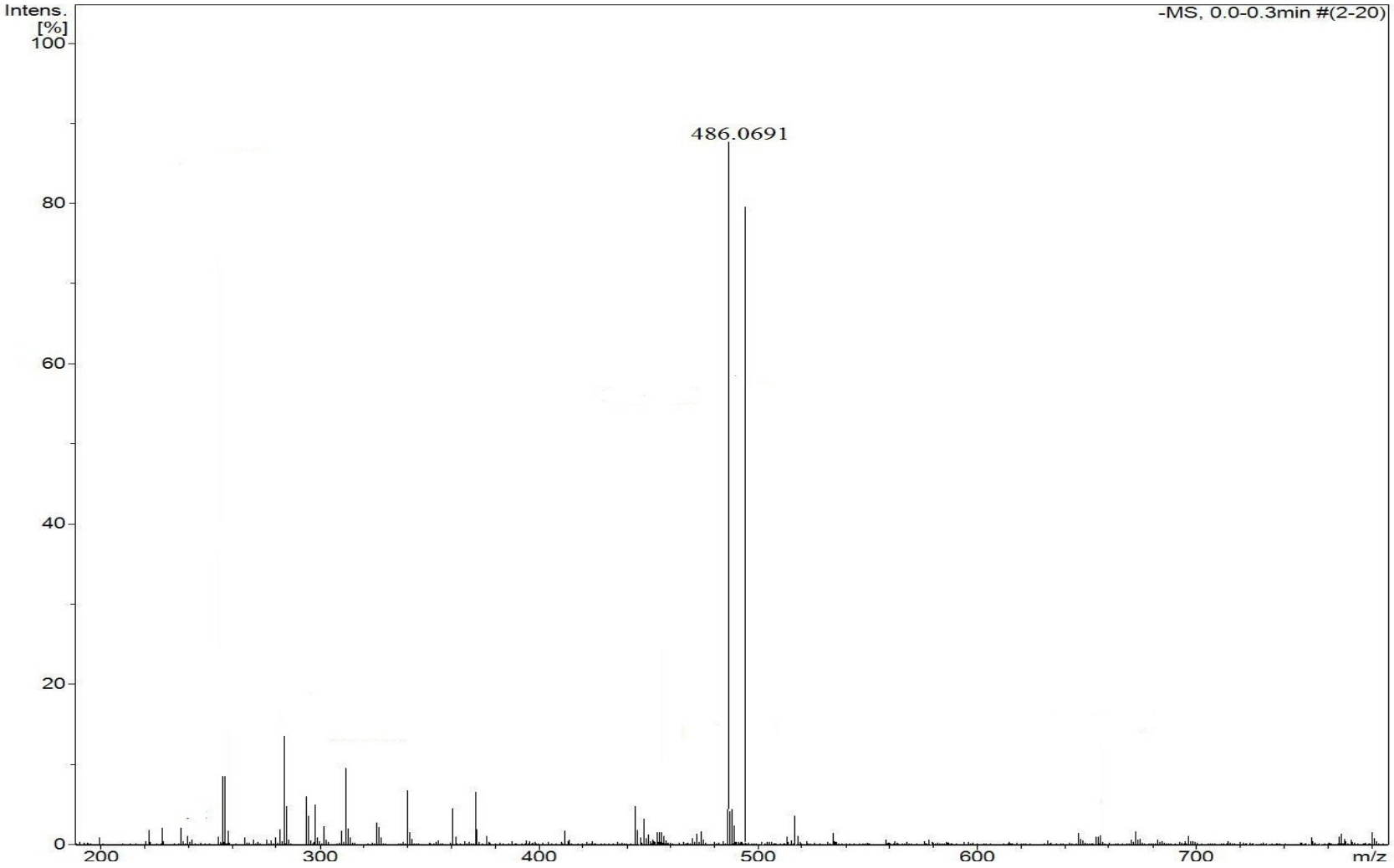
2-(Cyclohexylamino)-3-(4'-bromophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one(4f).



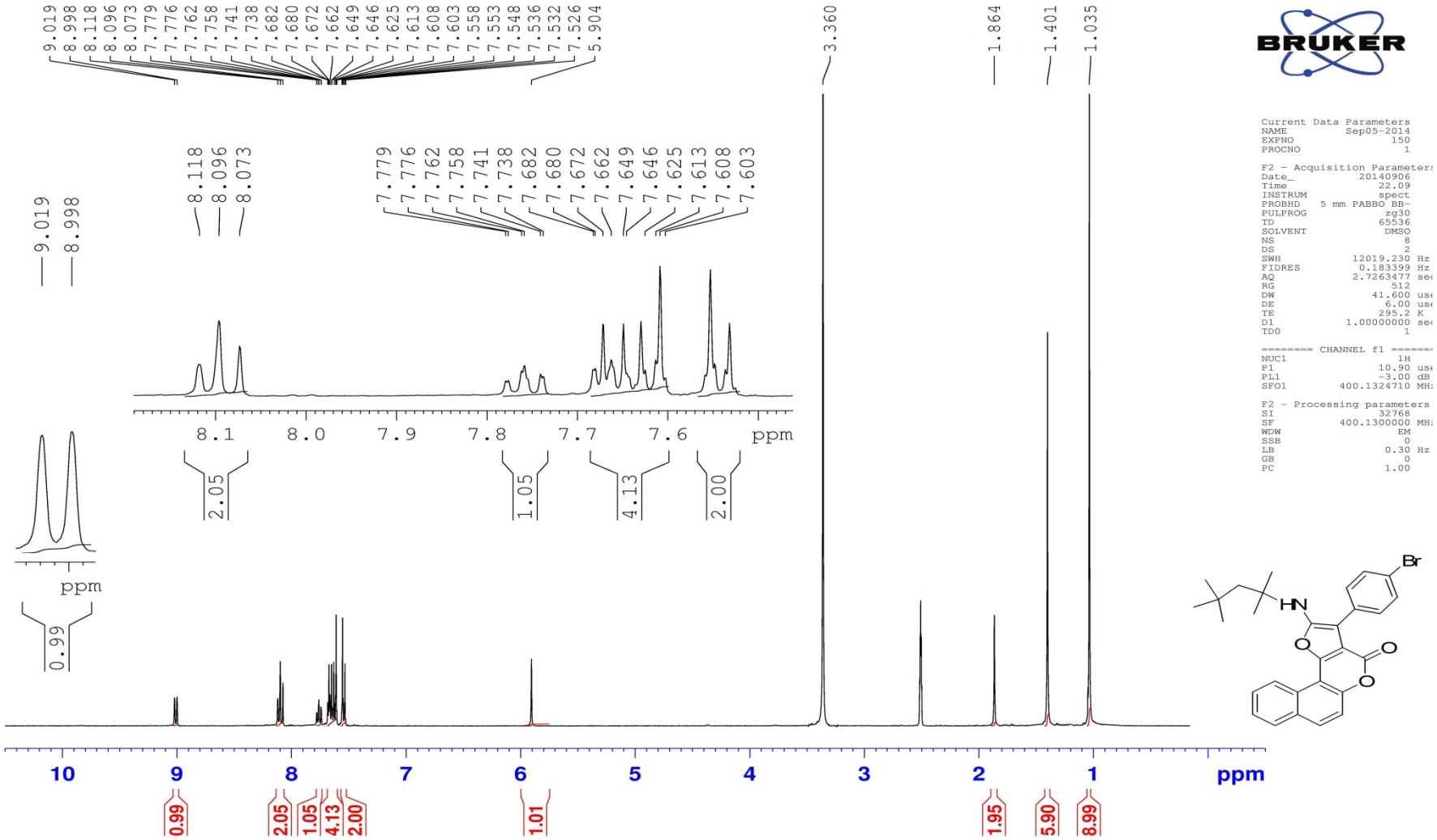


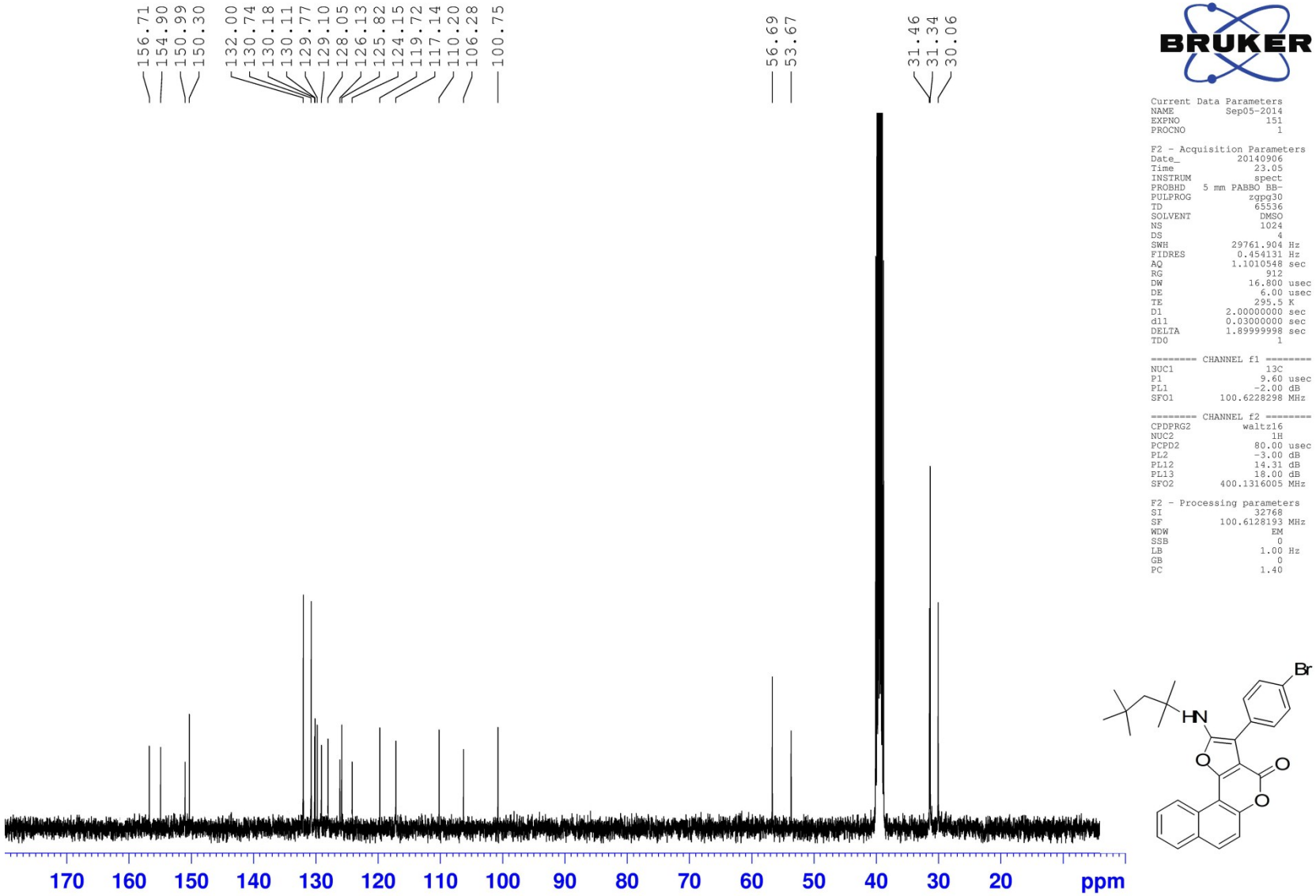

```
Current Data Parameters
NAME          Sep05-2014
EXPNO                 91
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140906
Time                4.30
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  1024
DS                     4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010548 sec
RG                   912
DW                16.800 usec
DE                 6.00 usec
TE                295.7 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.60 usec
PL1                -2.00 dB
SFO1         100.6228298 MHz

========= CHANNEL f2 =========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              14.31 dB
PL13              18.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6128193 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

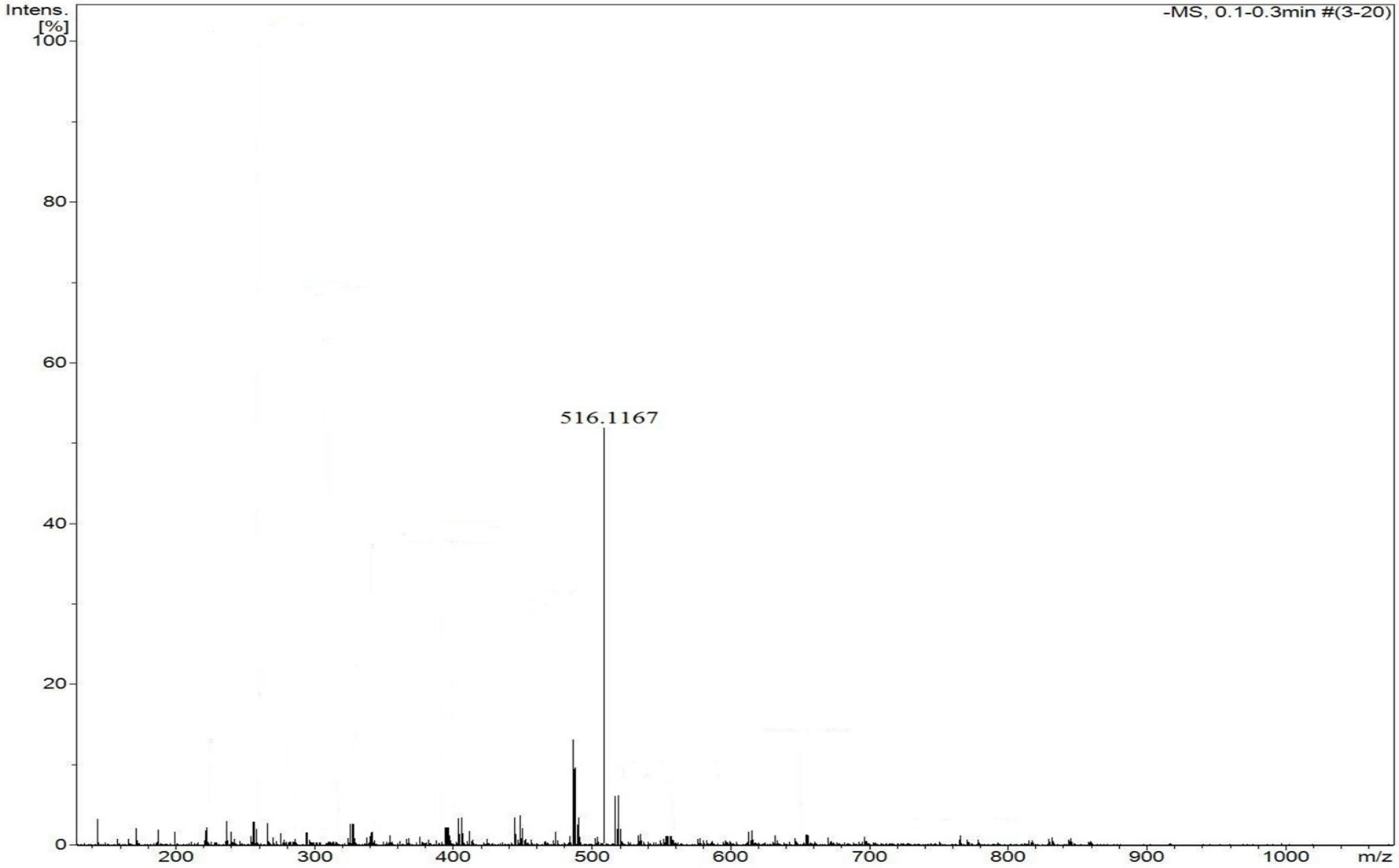



Intens.
[%]
100
80
60
40
20
0
-MS, 0.0-0.3min #(2-20)
486.0691
200
300
400
500
600
700
m/z

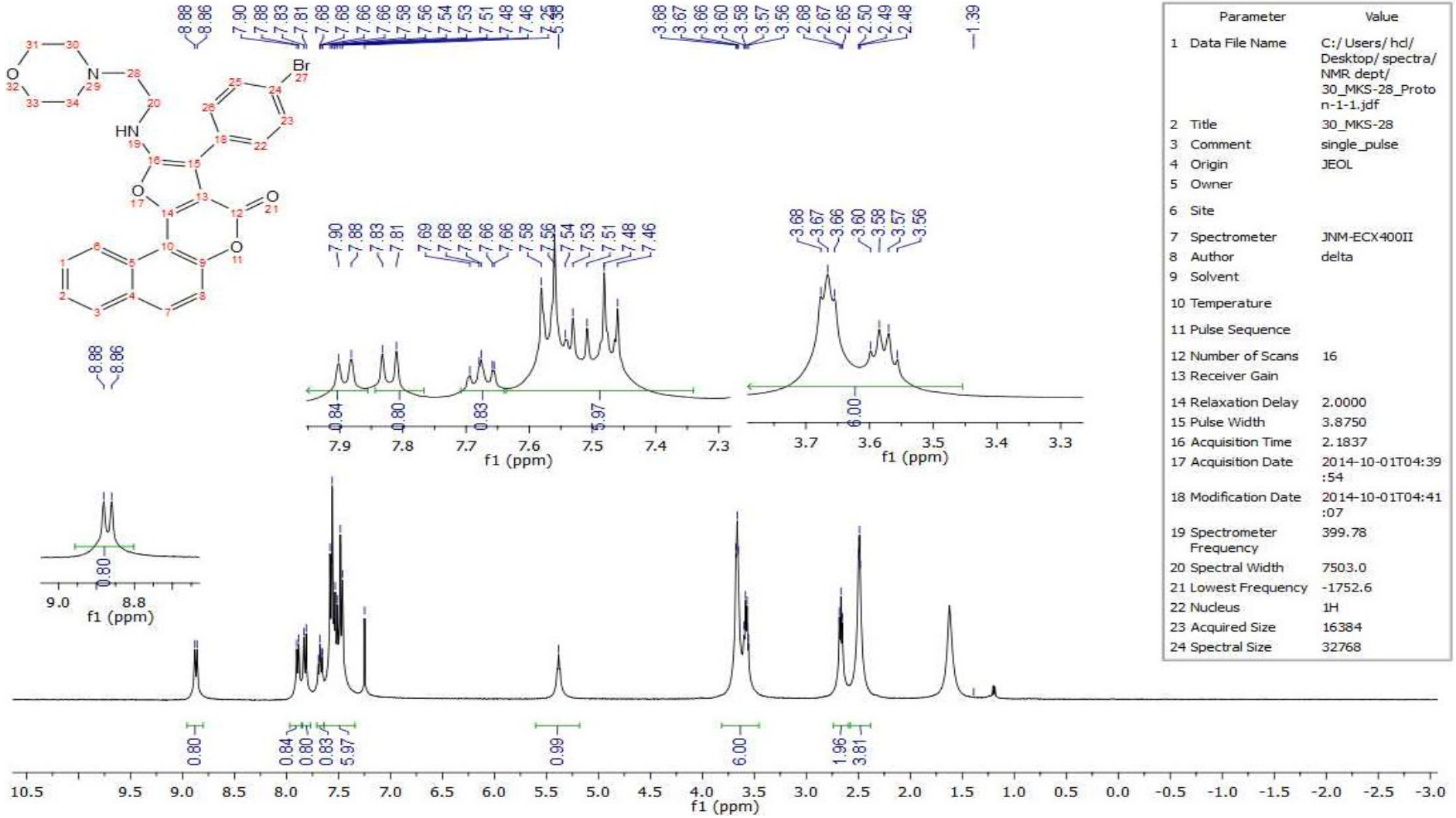
3-(4'-Bromophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one(4g).



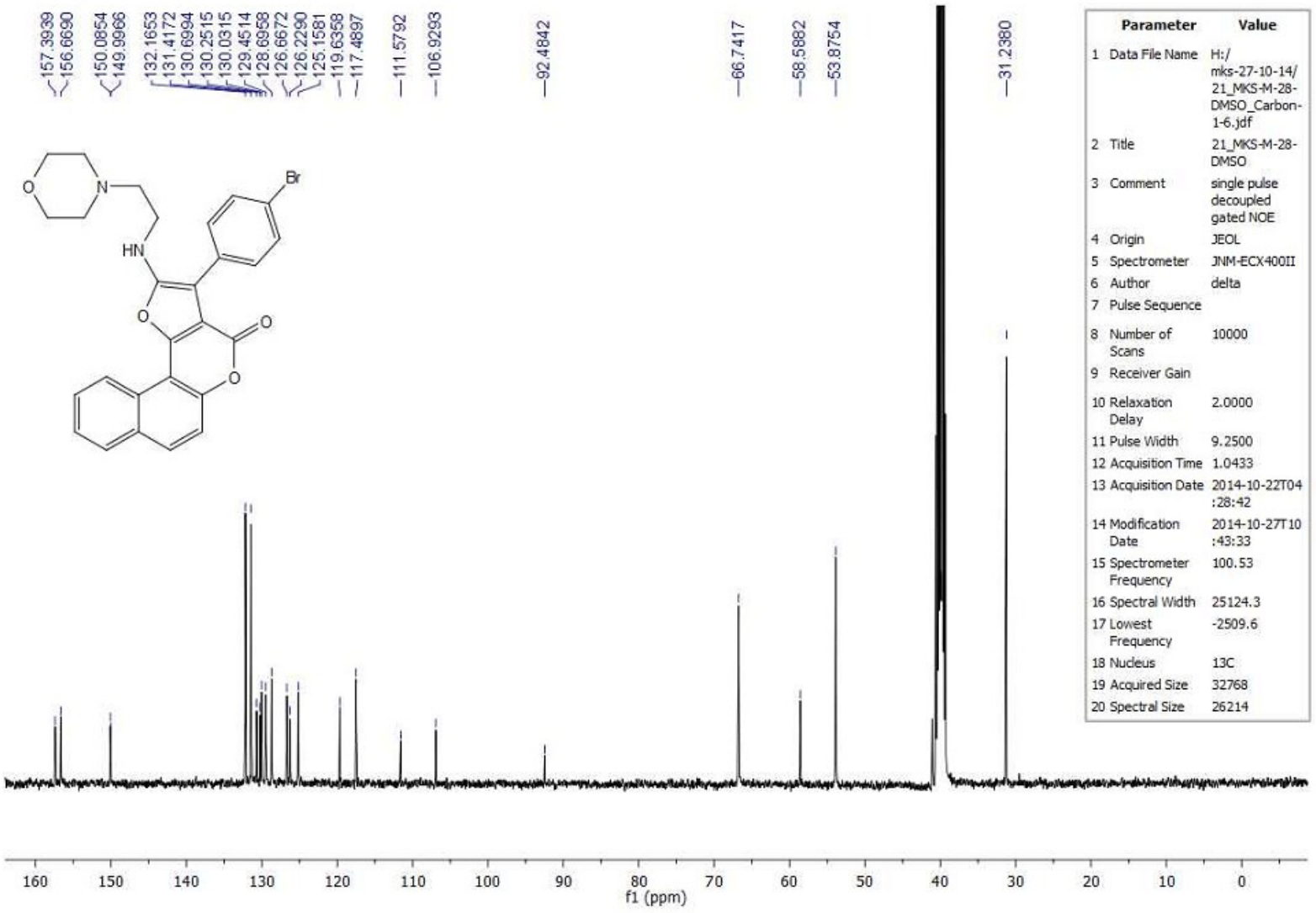

156.71
154.90
150.99
150.30
132.00
130.74
130.18
130.11
129.77
129.10
128.05
126.13
125.82
124.15
119.72
117.14
110.20
106.28
100.75
56.69
53.67
31.46
31.34
30.06
BRUKER
Current Data Parameters
NAME Sep05-2014
EXPNO 151
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140906
Time 23.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 912
DW 16.800 usec
DE 6.00 usec
TE 295.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Br
HN
O
O
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


Intens.
[%]
-MS, 0.1-0.3min #(3-20)
100
80
60
40
20
0
516.1167
200
300
400
500
600
700
800
900
1000
m/z

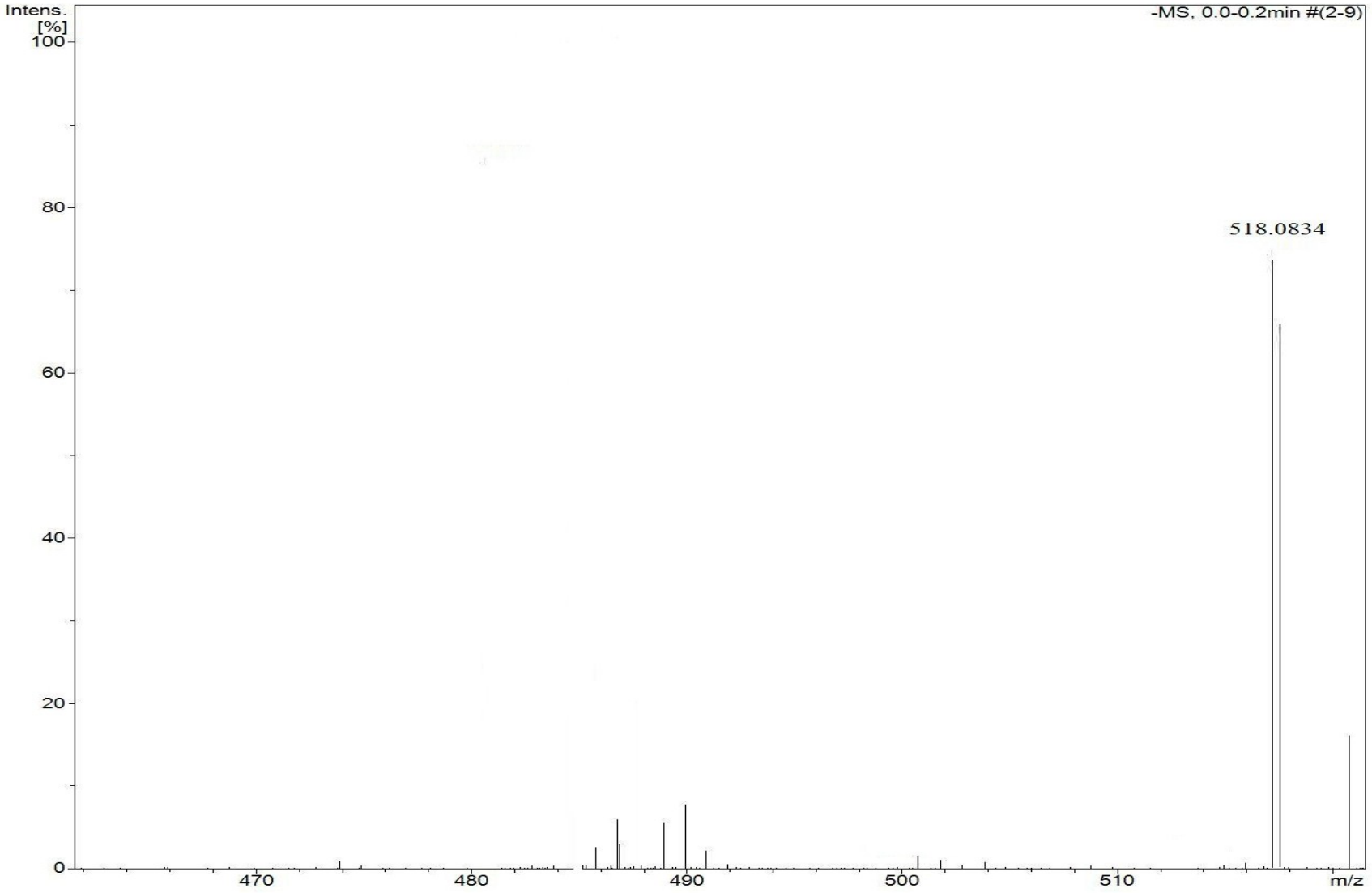
3-(4'-Bromophenyl)-2-((2-morpholinoethyl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one(4h).



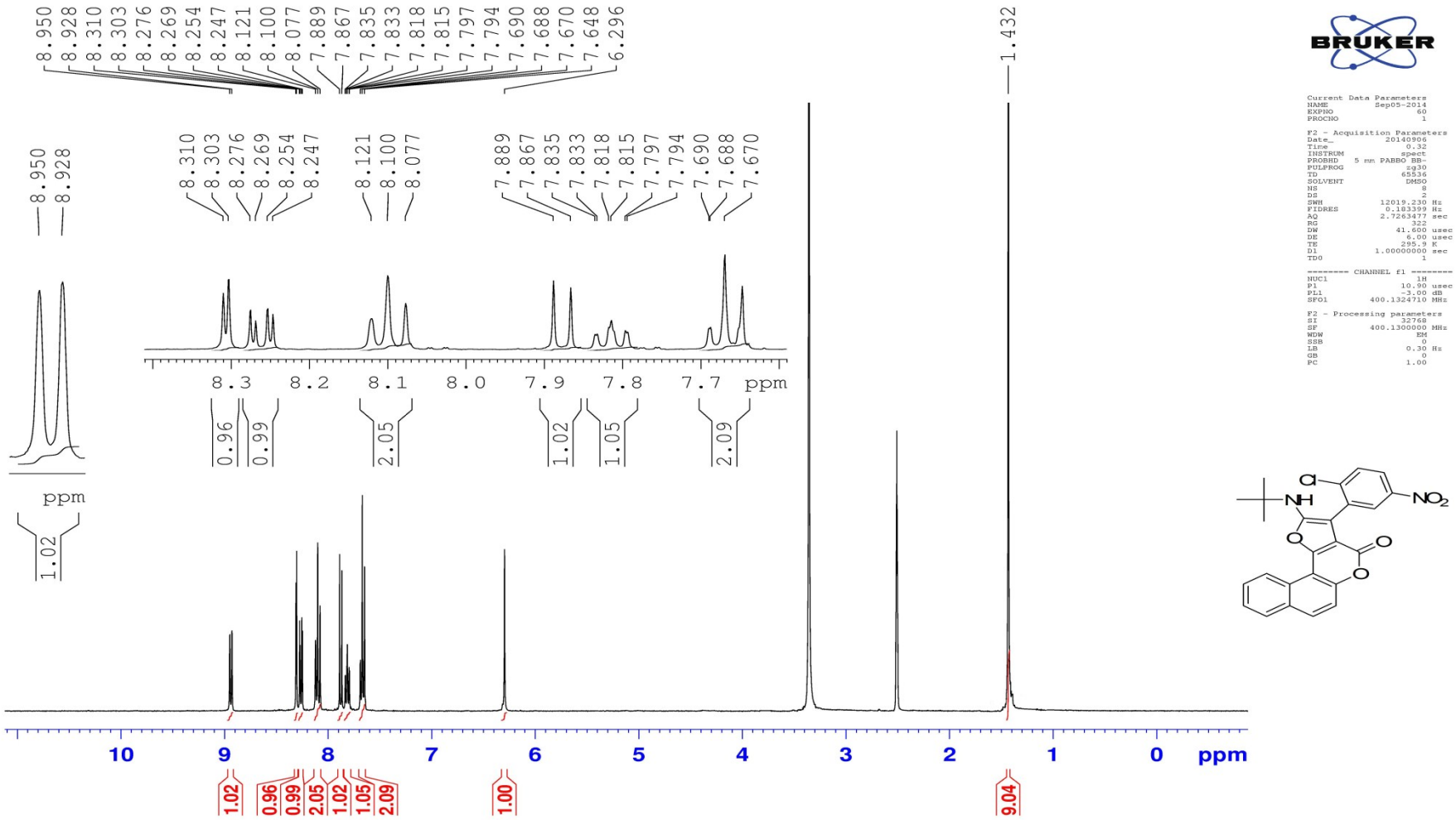
	Parameter	Value
1	Data File Name	C:/ Users/ hcl/ Desktop/ spectra/ NMR dept/ 30_MKS-28_Proton-1-1.jdf
2	Title	30_MKS-28
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	JNM-ECX400II
8	Author	delta
9	Solvent	
10	Temperature	
11	Pulse Sequence	
12	Number of Scans	16
13	Receiver Gain	
14	Relaxation Delay	2.0000
15	Pulse Width	3.8750
16	Acquisition Time	2.1837
17	Acquisition Date	2014-10-01T04:39:54
18	Modification Date	2014-10-01T04:41:07
19	Spectrometer Frequency	399.78
20	Spectral Width	7503.0
21	Lowest Frequency	-1752.6
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

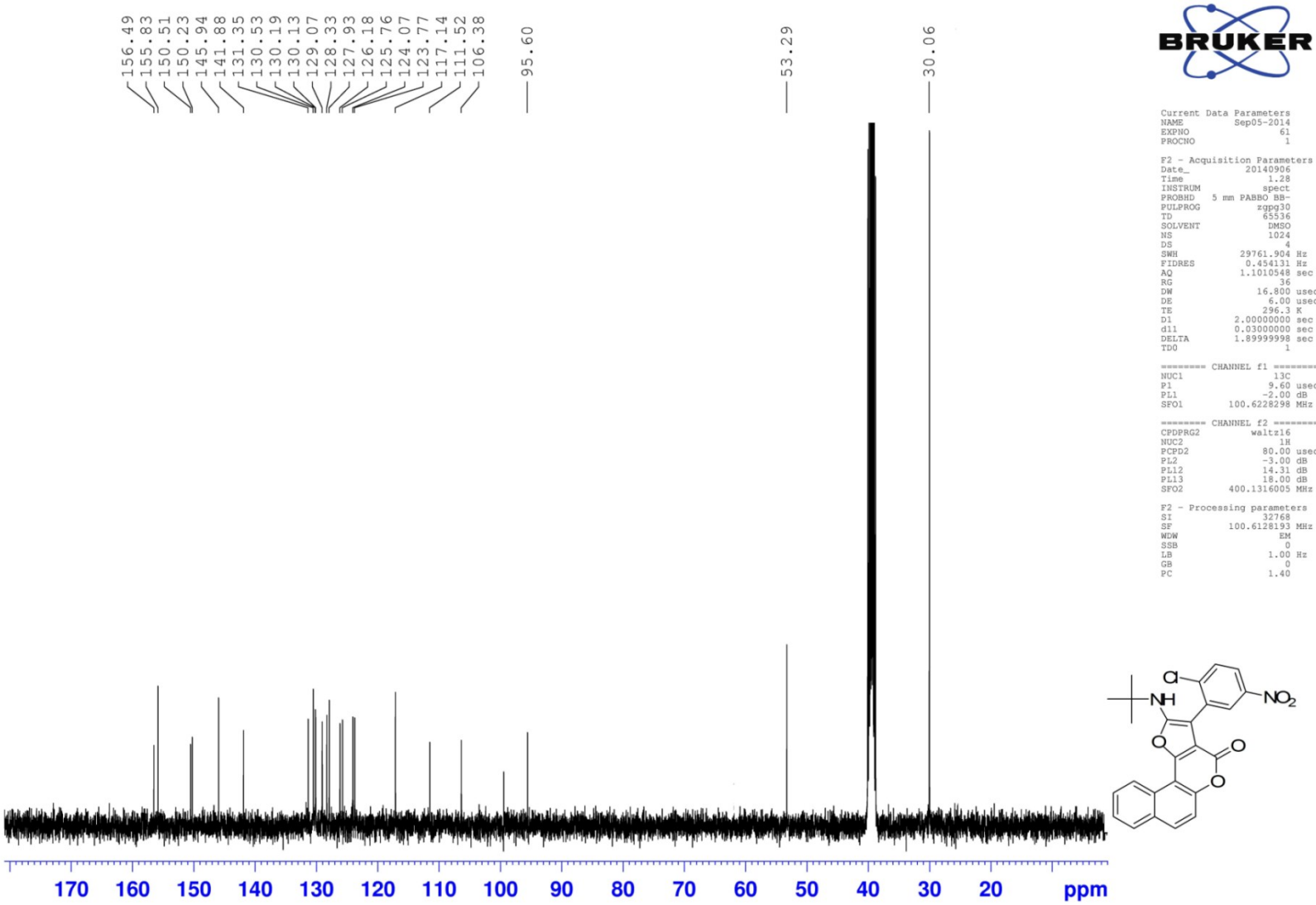


	Parameter	Value
1	Data File Name	H:/mks-27-10-14/21_MKS-M-28-DMSO_Carbon-1-6.jdf
2	Title	21_MKS-M-28-DMSO
3	Comment	single pulse decoupled gated NOE
4	Origin	JEOL
5	Spectrometer	JNM-ECX400II
6	Author	delta
7	Pulse Sequence	
8	Number of Scans	10000
9	Receiver Gain	
10	Relaxation Delay	2.0000
11	Pulse Width	9.2500
12	Acquisition Time	1.0433
13	Acquisition Date	2014-10-22T04:28:42
14	Modification Date	2014-10-27T10:43:33
15	Spectrometer Frequency	100.53
16	Spectral Width	25124.3
17	Lowest Frequency	-2509.6
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	26214


Intens.
[%]
-MS, 0.0-0.2min #(2-9)
518.0834
100
80
60
40
20
0
470
480
490
500
510
m/z

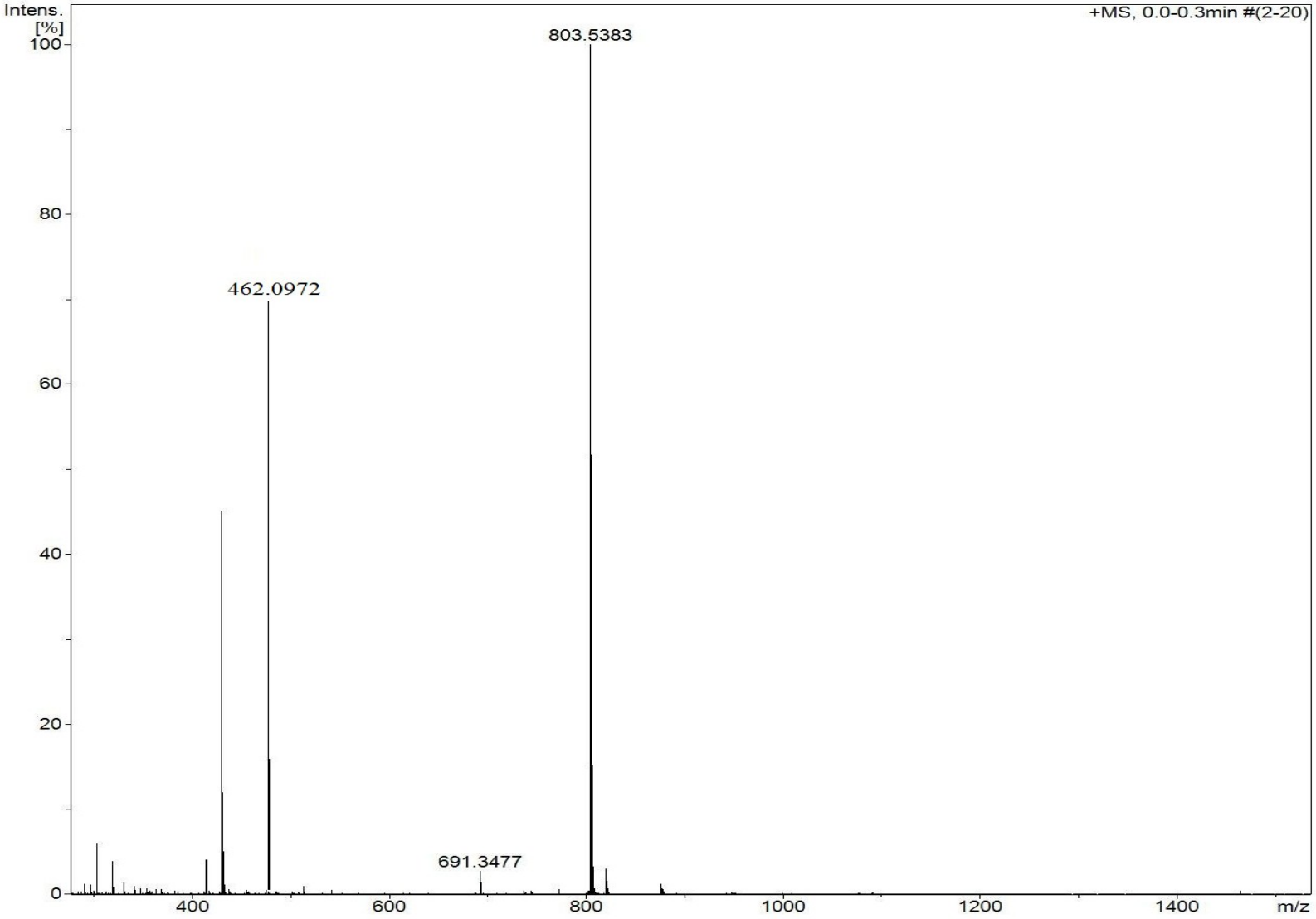
2-(*tert*-Butylamino)-3-(2'-chloro-5'-nitrophenyl)-4*H*benzo[*f*]furo[3,2-*c*]chromen-4-one(4i).



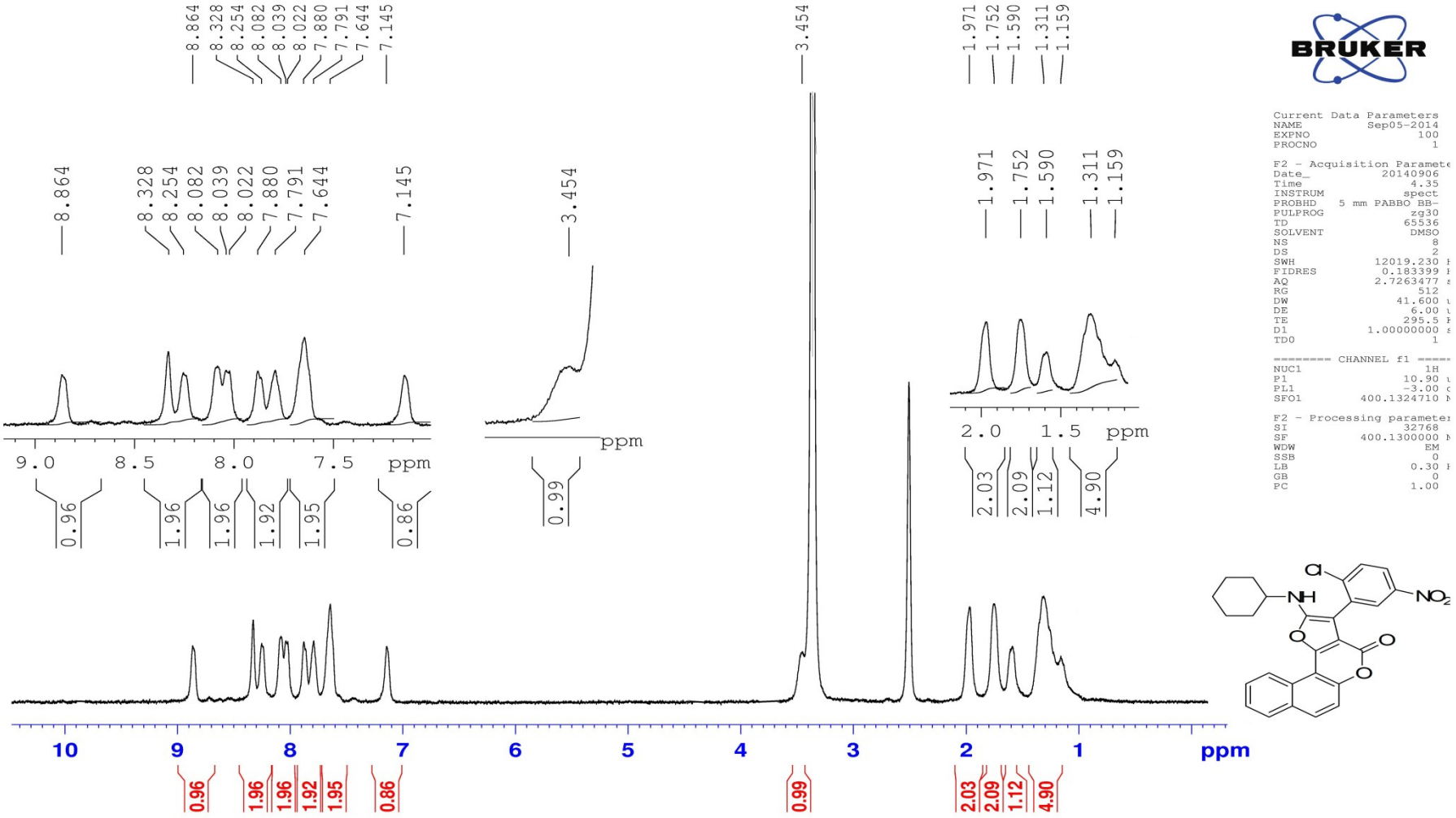


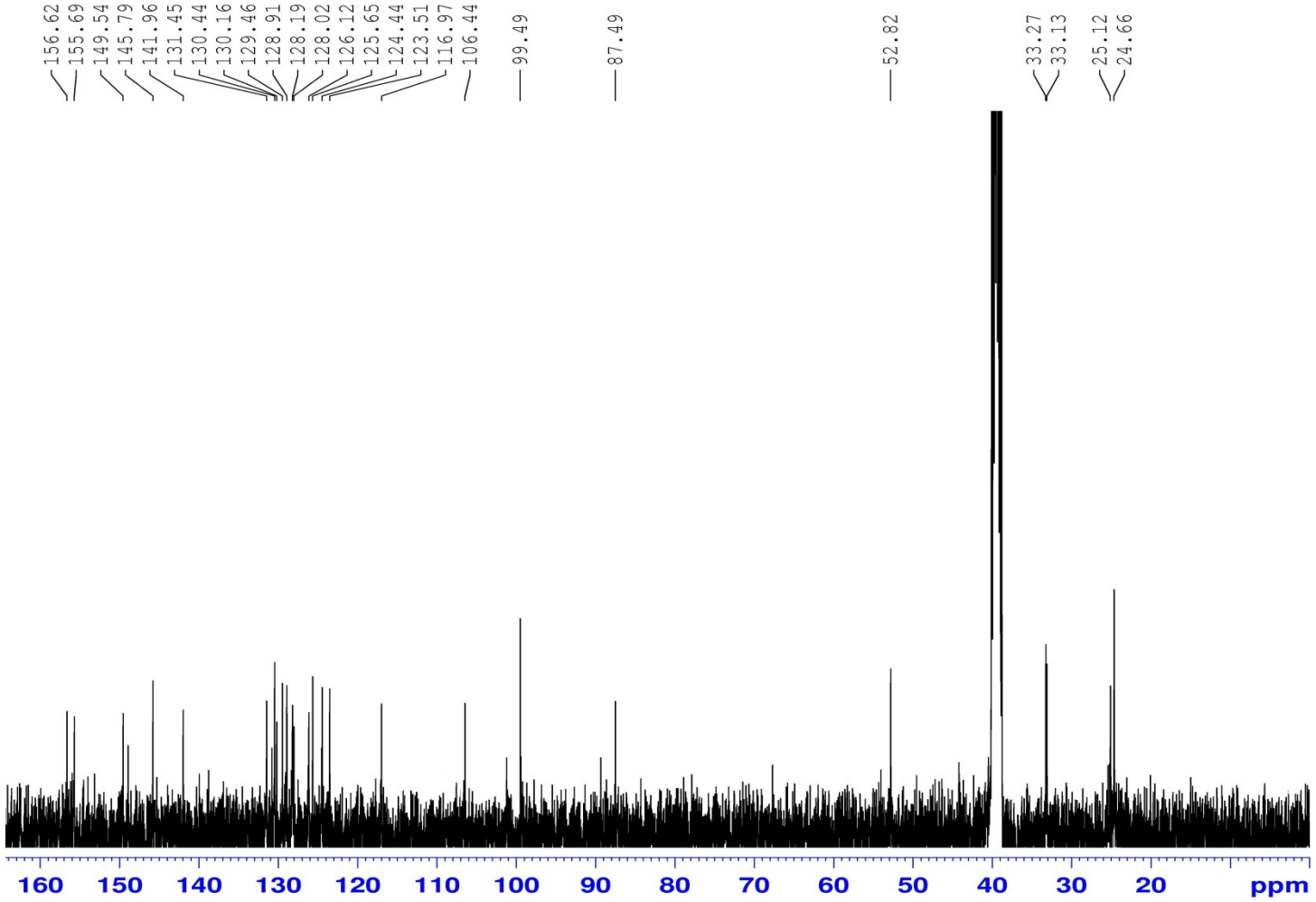
BRUKER

```
Current Data Parameters
NAME          Sep05-2014
EXPNO                 61
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140906
Time                1.28
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  1024
DS                     4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010548 sec
RG                    36
DW               16.800 usec
DE                6.00 usec
TE                296.3 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.60 usec
PL1                -2.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              14.31 dB
PL13              18.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6128193 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```


Intens.
[%]
+MS, 0.0-0.3min #(2-20)
803.5383
462.0972
691.3477
100
80
60
40
20
0
400
600
800
1000
1200
1400
m/z

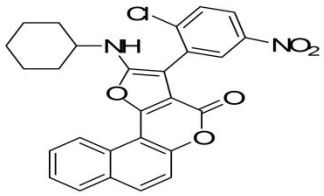
2-(Cyclohexylamino)-3-(2'-chloro-5'-nitrophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4j).

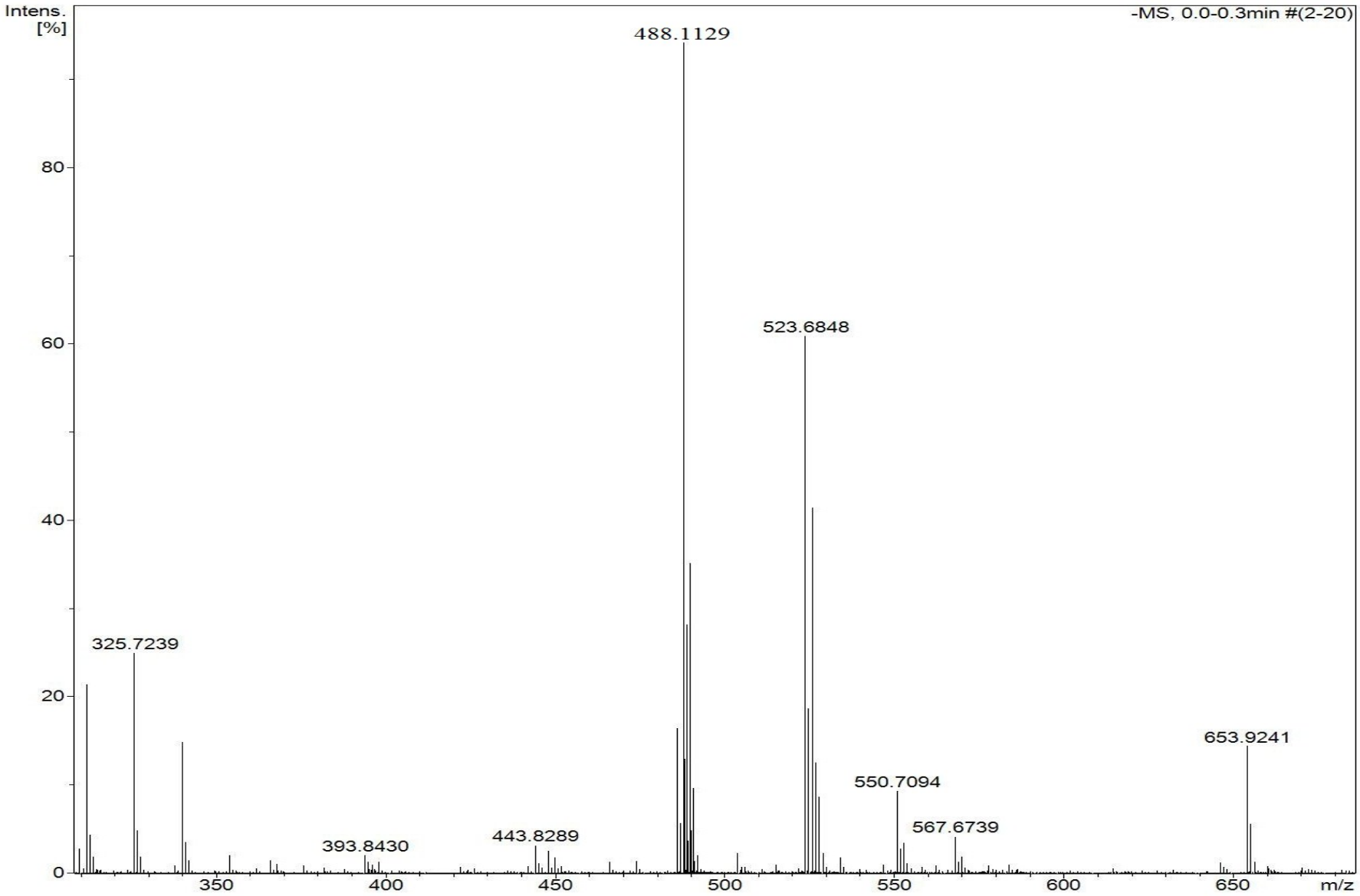




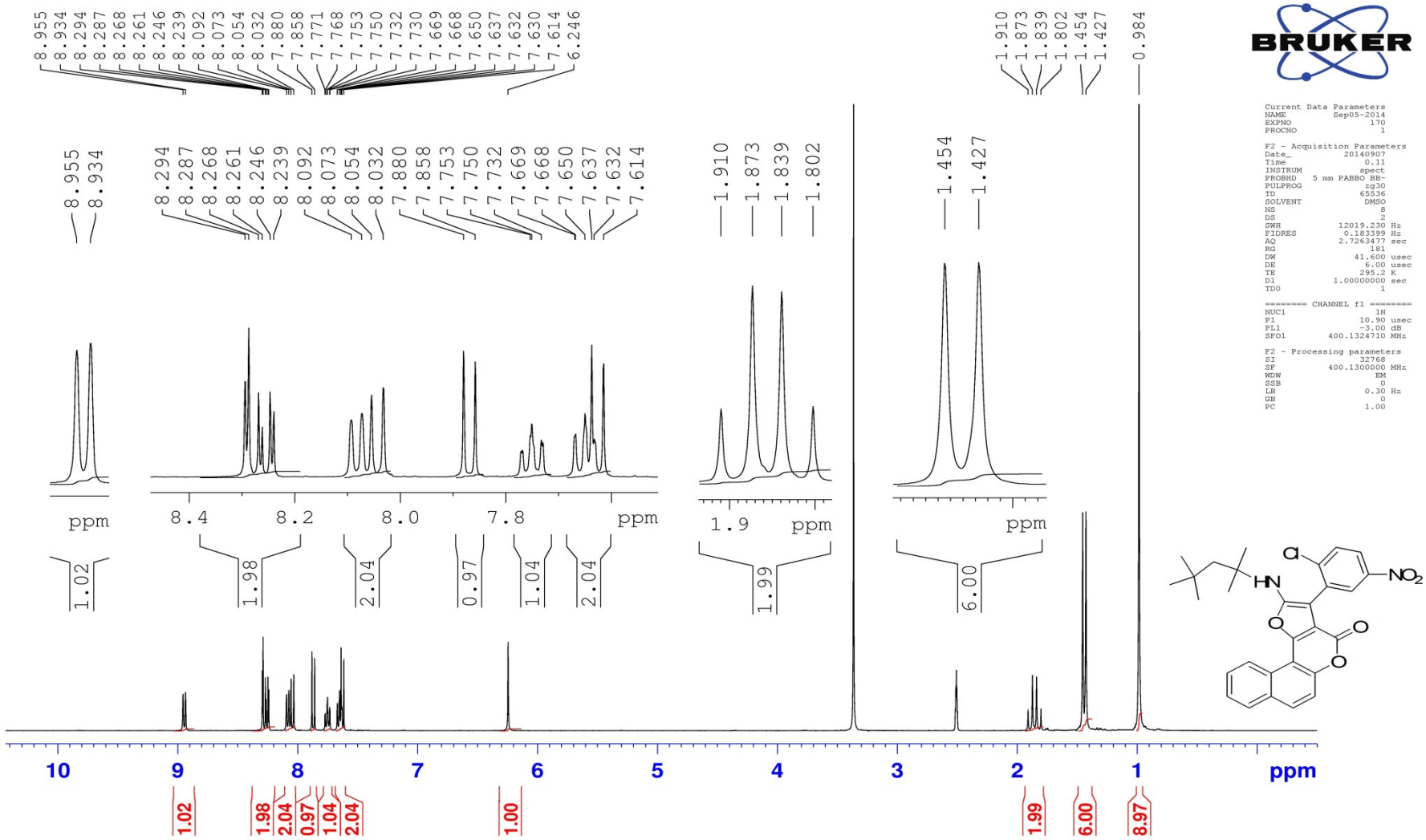
BRUKER

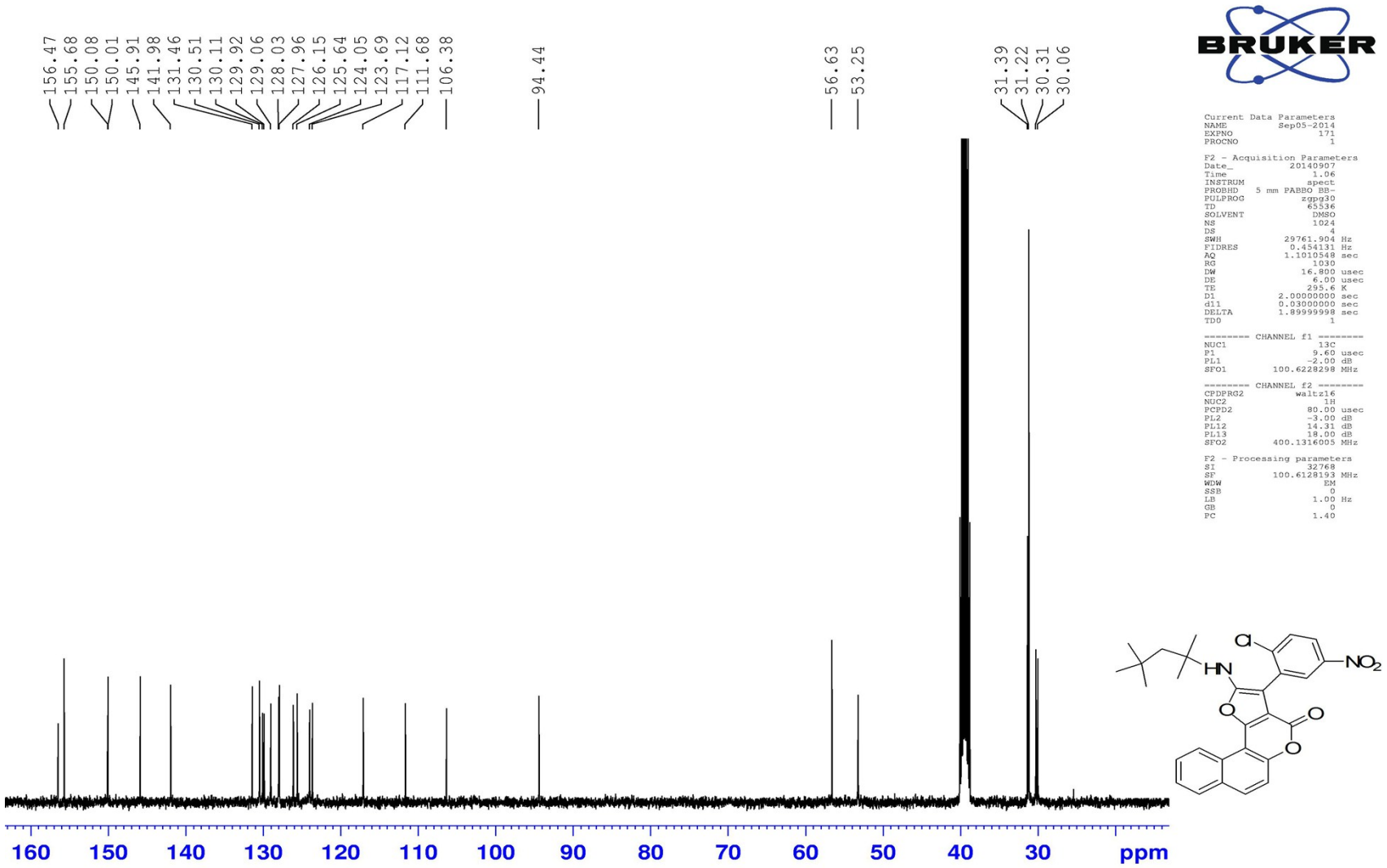
```
Current Data Parameters
NAME                  Sep05-2014
EXPNO                        101
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20140906
Time                        5.31
INSTRUM                    spect
PROBHD     5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                     DMSO
NS                          1024
DS                             4
SWH                  29761.904 Hz
FIDRES                0.454131 Hz
AQ                    1.1010548 sec
RG                            36
DW                       16.800 usec
DE                        6.00 usec
TE                        295.6 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                          9.60 usec
PL1                        -2.00 dB
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                          1H
PCPD2                      80.00 usec
PL2                        -3.00 dB
PL12                       14.31 dB
PL13                       18.00 dB
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                 100.6128193 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

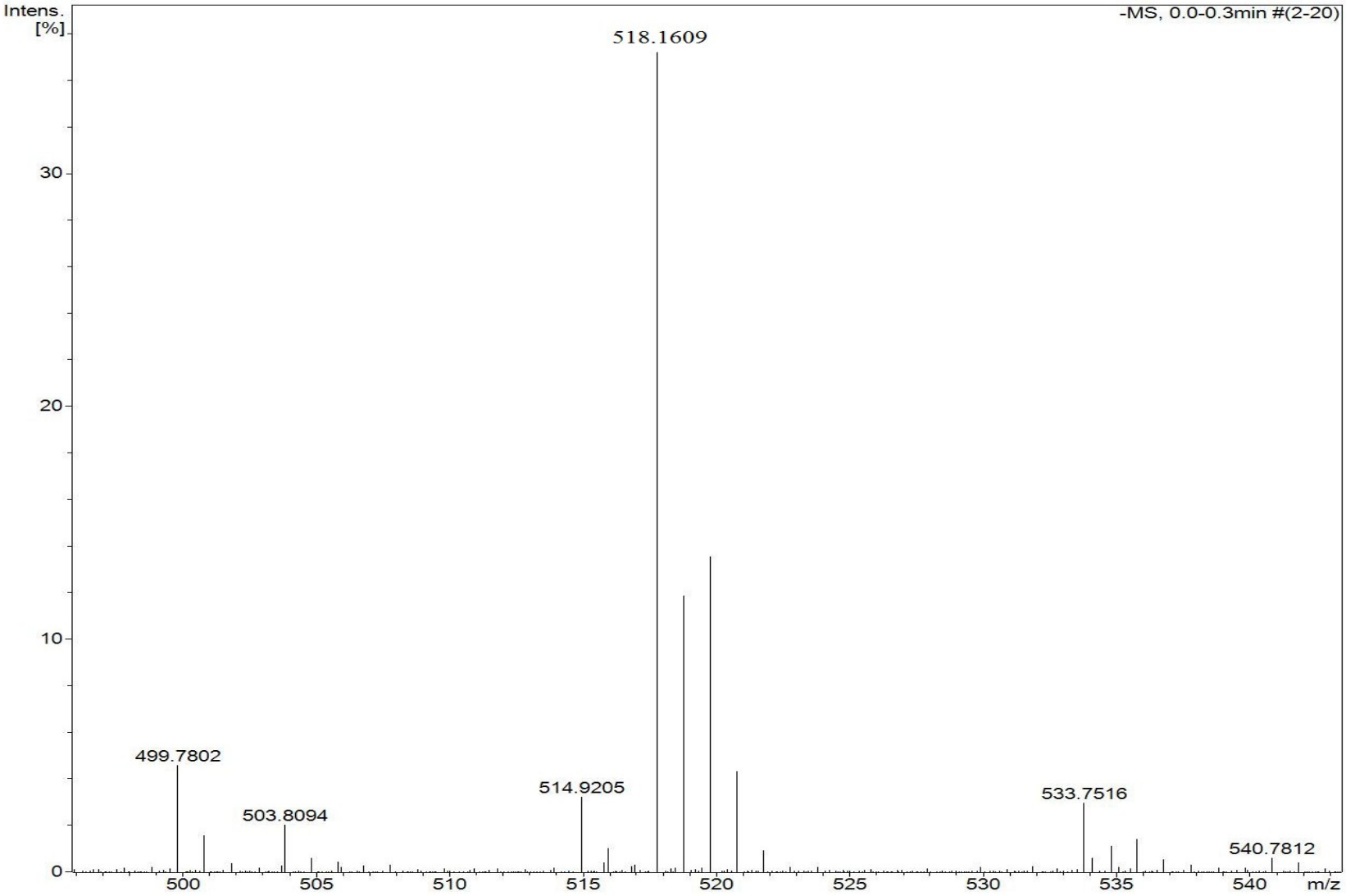



Intens.
[%]
-MS, 0.0-0.3min #(2-20)
488.1129
523.6848
325.7239
653.9241
550.7094
567.6739
393.8430
443.8289
0
20
40
60
80
350
400
450
500
550
600
650
m/z

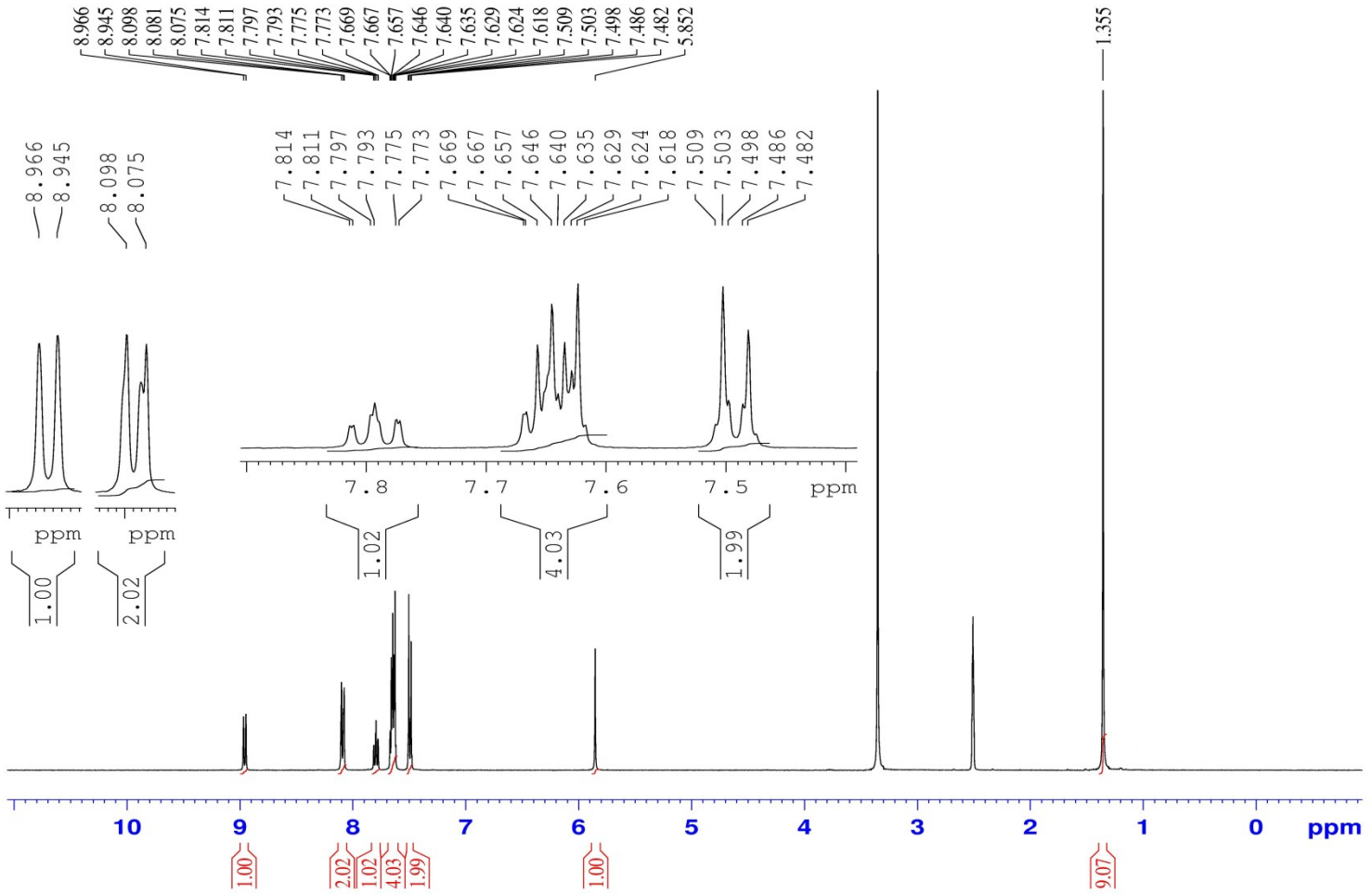
3-(2'-Chloro-5'-nitrophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4k).

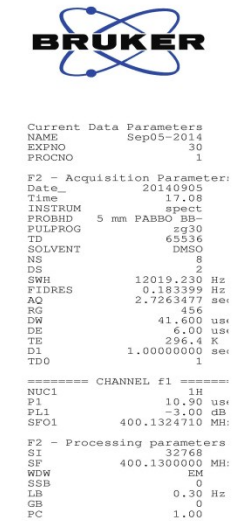


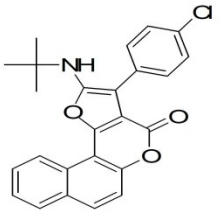

156.47
155.68
150.08
150.01
145.91
141.98
131.46
130.51
130.11
129.92
129.06
128.03
127.96
126.15
125.64
124.05
123.69
117.12
111.68
106.38
94.44
56.63
53.25
31.39
31.22
30.31
30.06
BRUKER
Current Data Parameters
NAME Sep05-2014
EXPNO 171
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140907
Time 1.06
INSTRUM apect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 295.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
NO2
HN
O
O
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
ppm

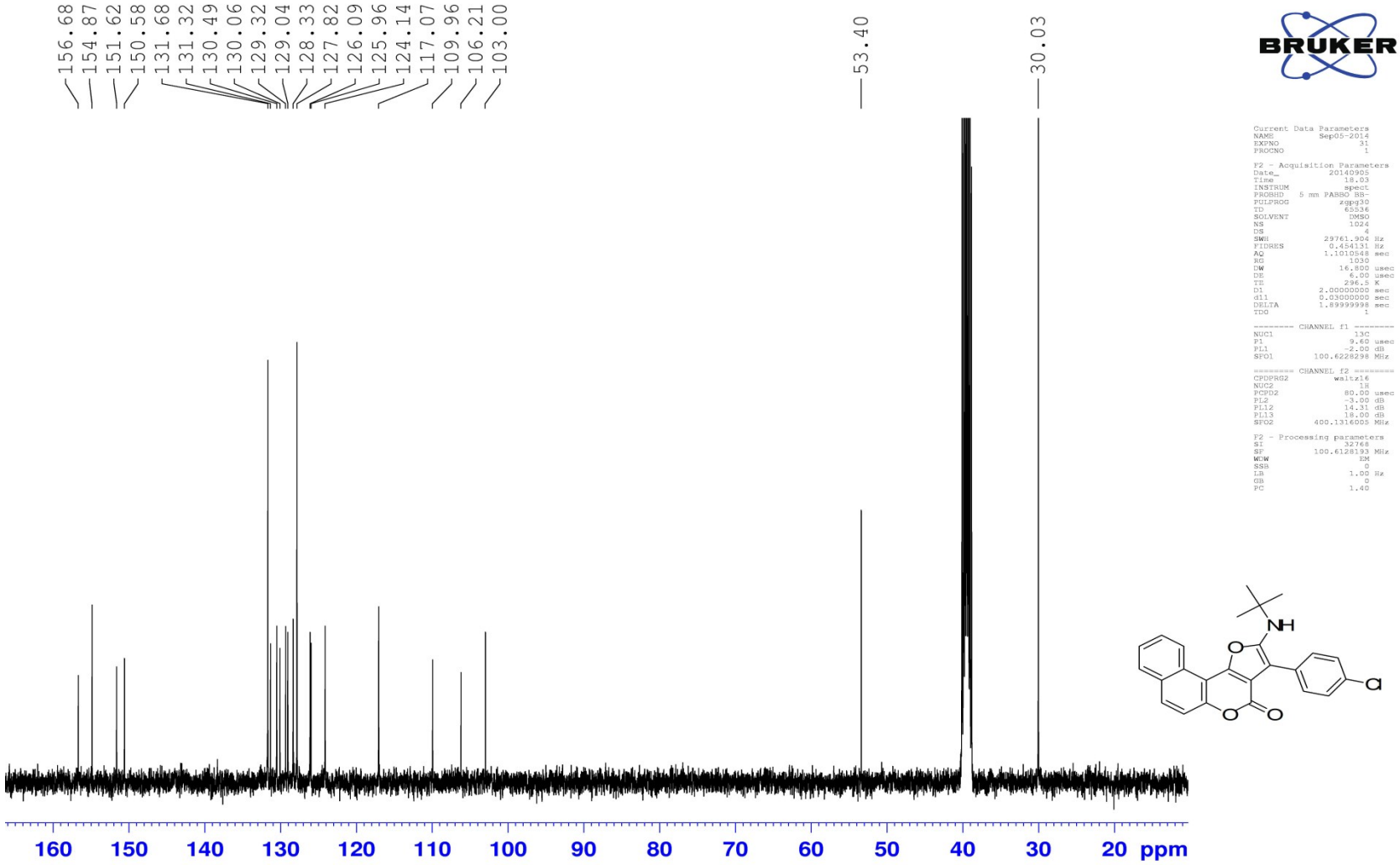

Intens.
[%]
-MS, 0.0-0.3min #(2-20)
518.1609
30
20
10
0
499.7802
503.8094
514.9205
533.7516
540.7812
500
505
510
515
520
525
530
535
540
m/z

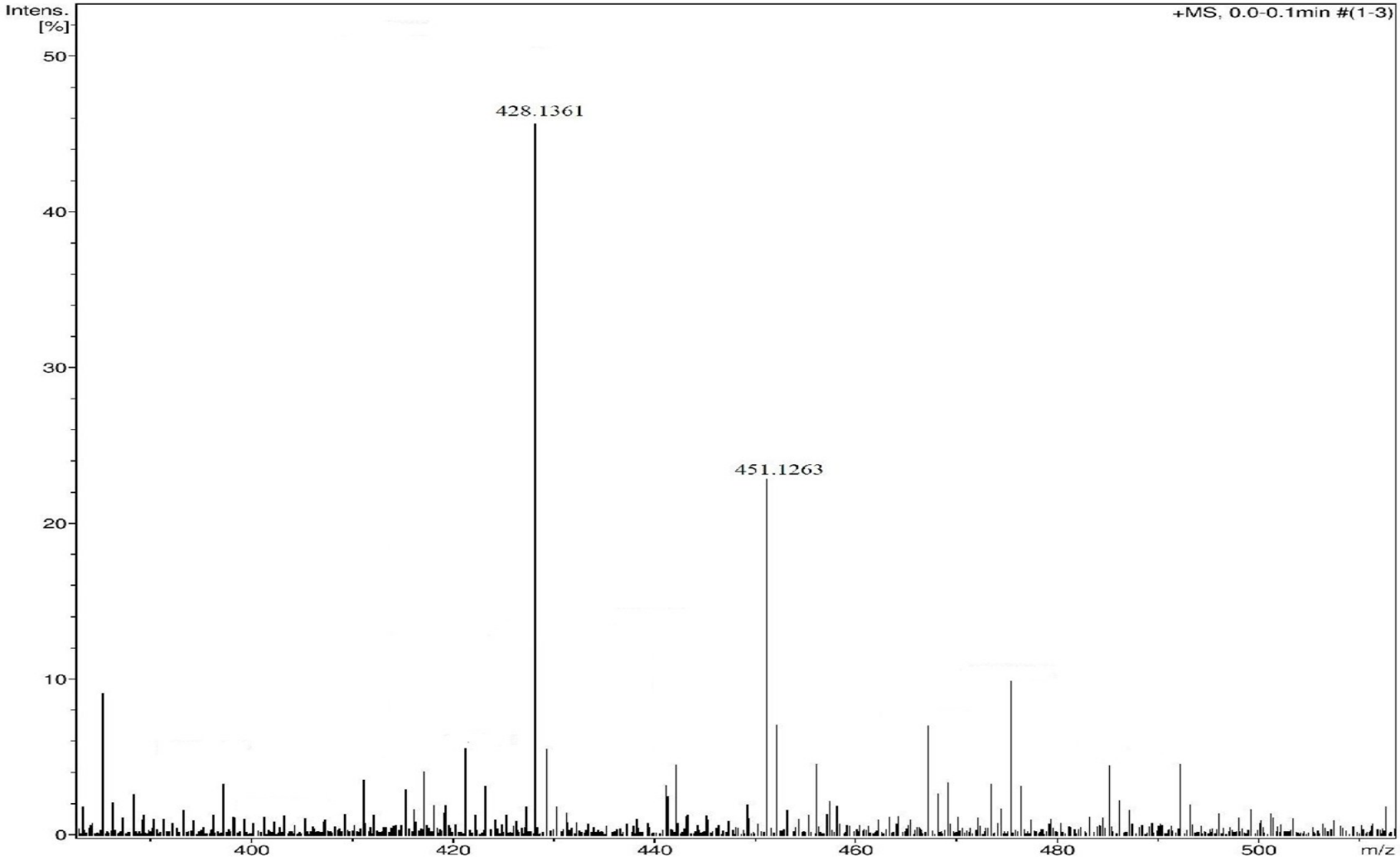
2-(*tert*-Butylamino)-3-(4'-chlorophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4l).



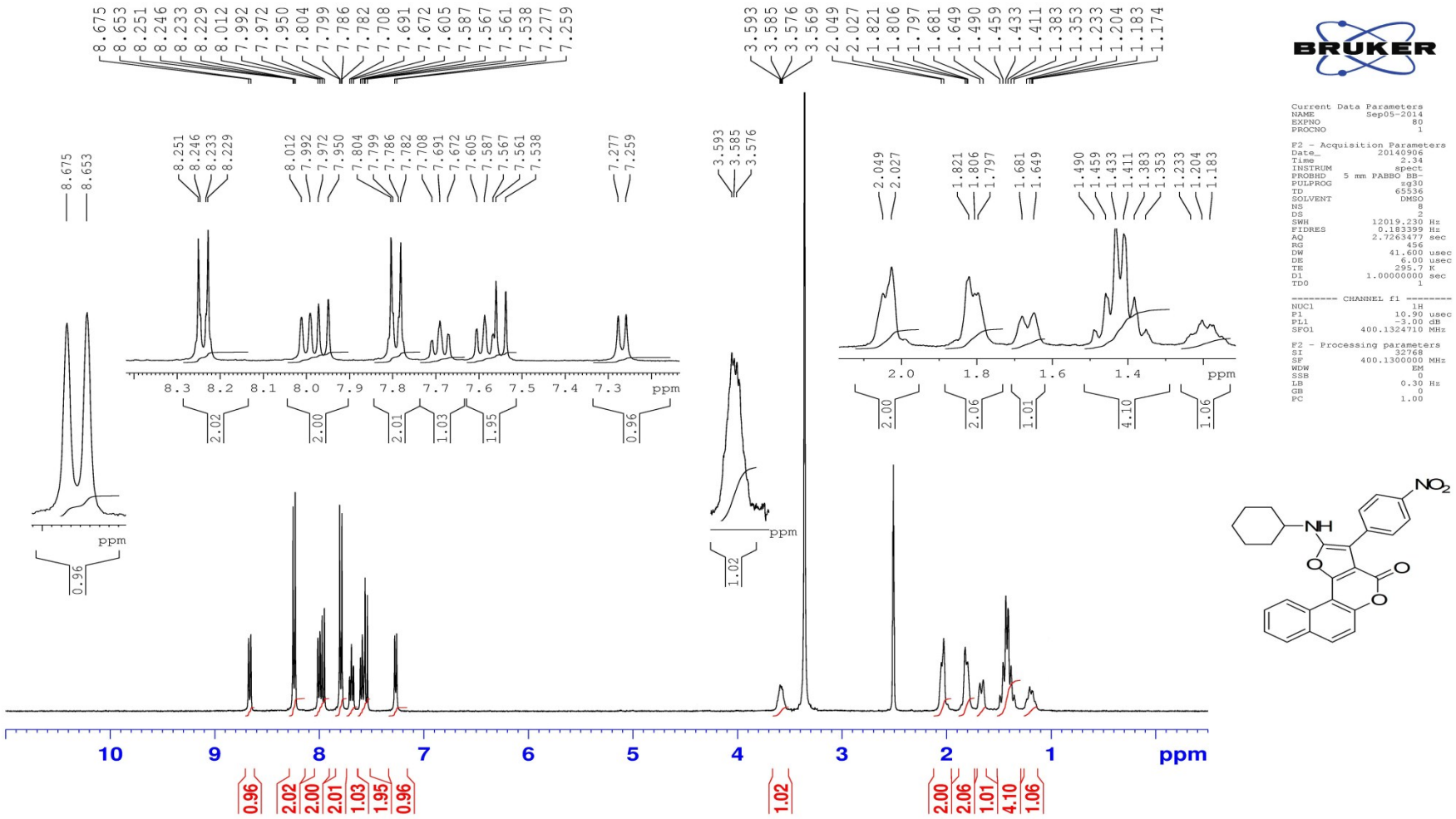


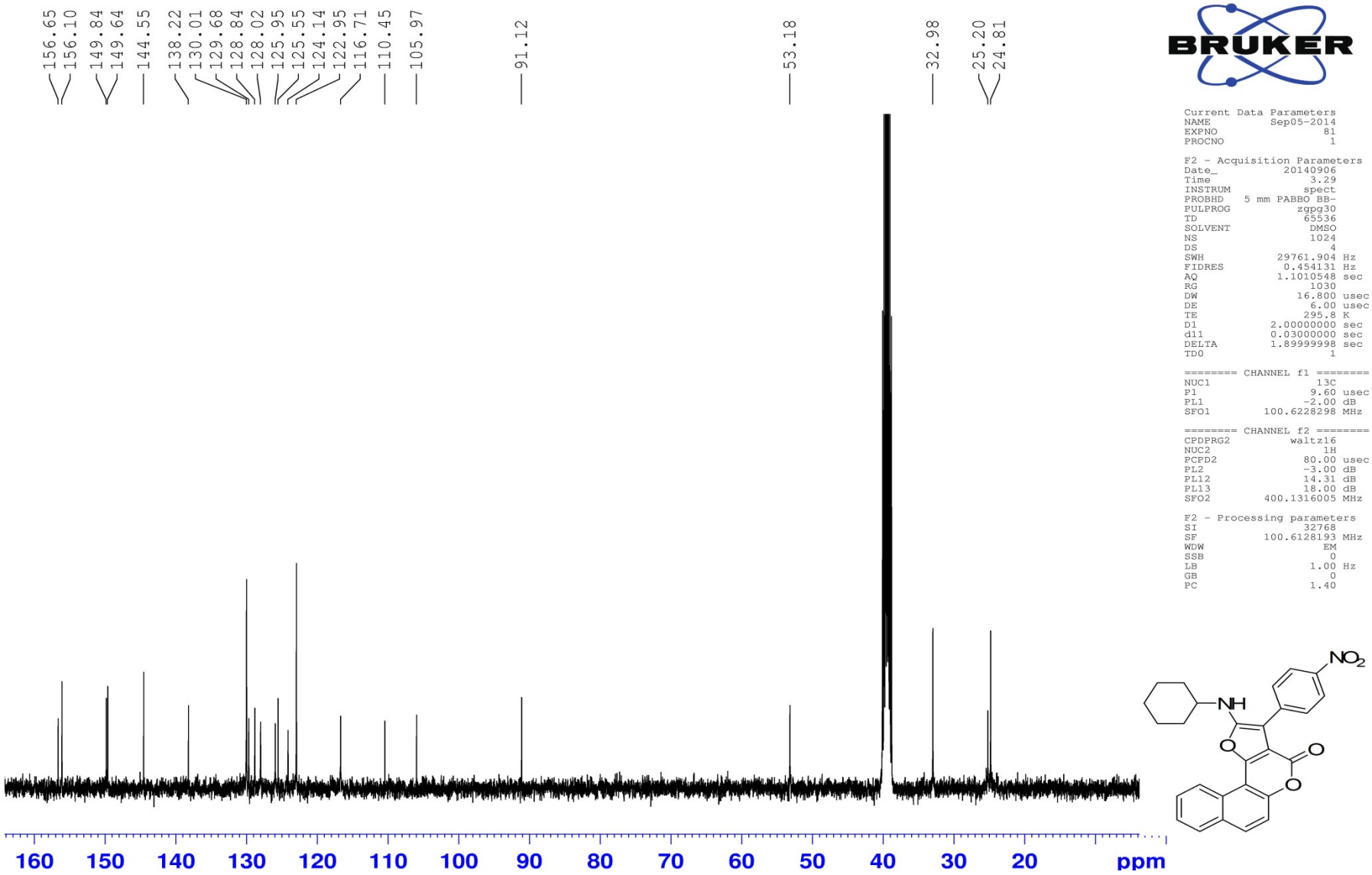


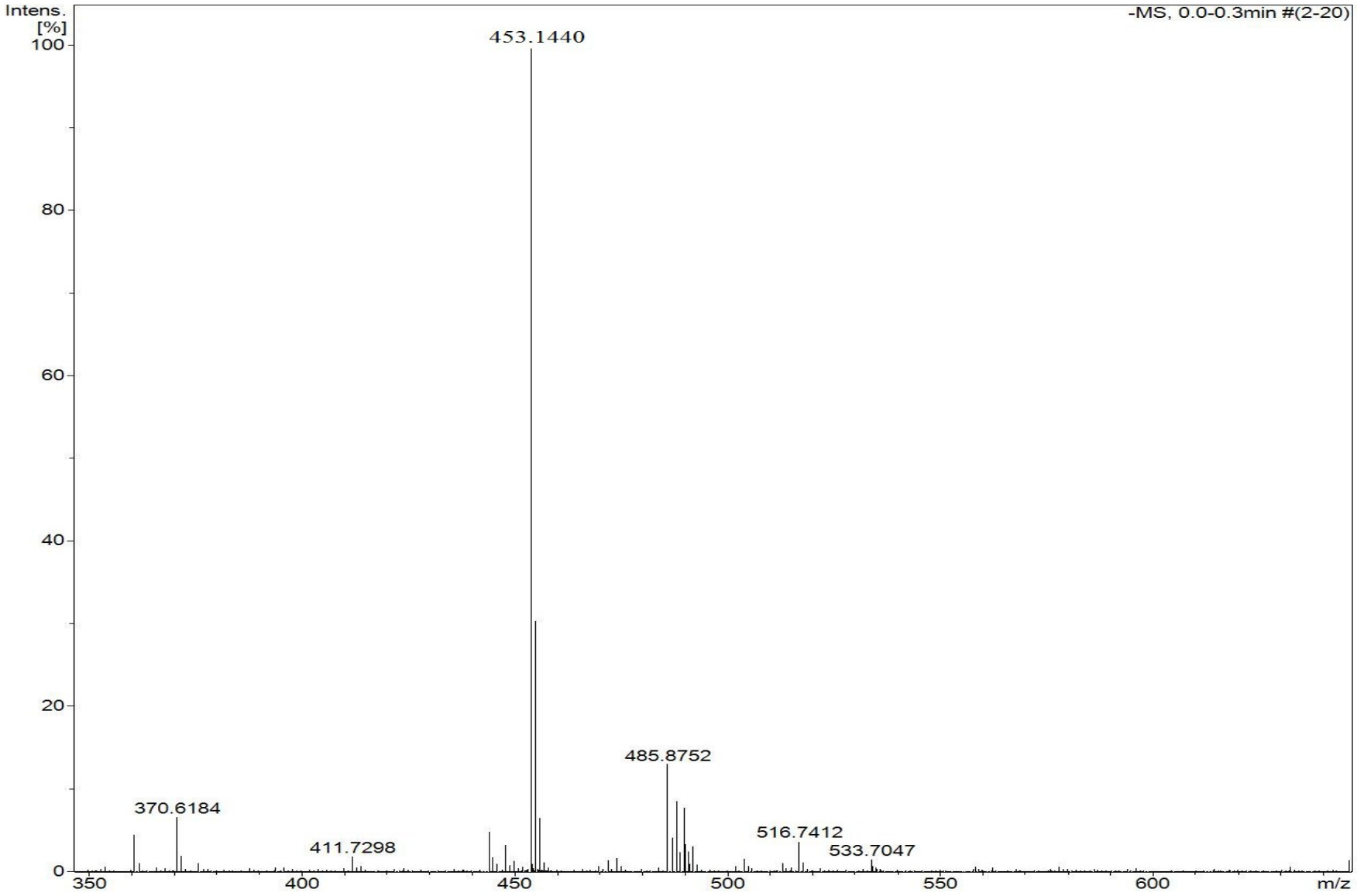

156.68
154.87
151.62
150.58
131.68
131.32
130.49
130.06
129.32
129.04
128.33
127.82
126.09
125.96
124.14
117.07
109.96
106.21
103.00
53.40
30.03
BRUKER
Current Data Parameters
NAME Sep05-2014
EXPNO 31
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140905
Time 18.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454151 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
NH
O
O
O
Cl
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Intens.
[%]
+MS, 0.0-0.1min #(1-3)
428.1361
451.1263
50
40
30
20
10
0
400
420
440
460
480
500
m/z

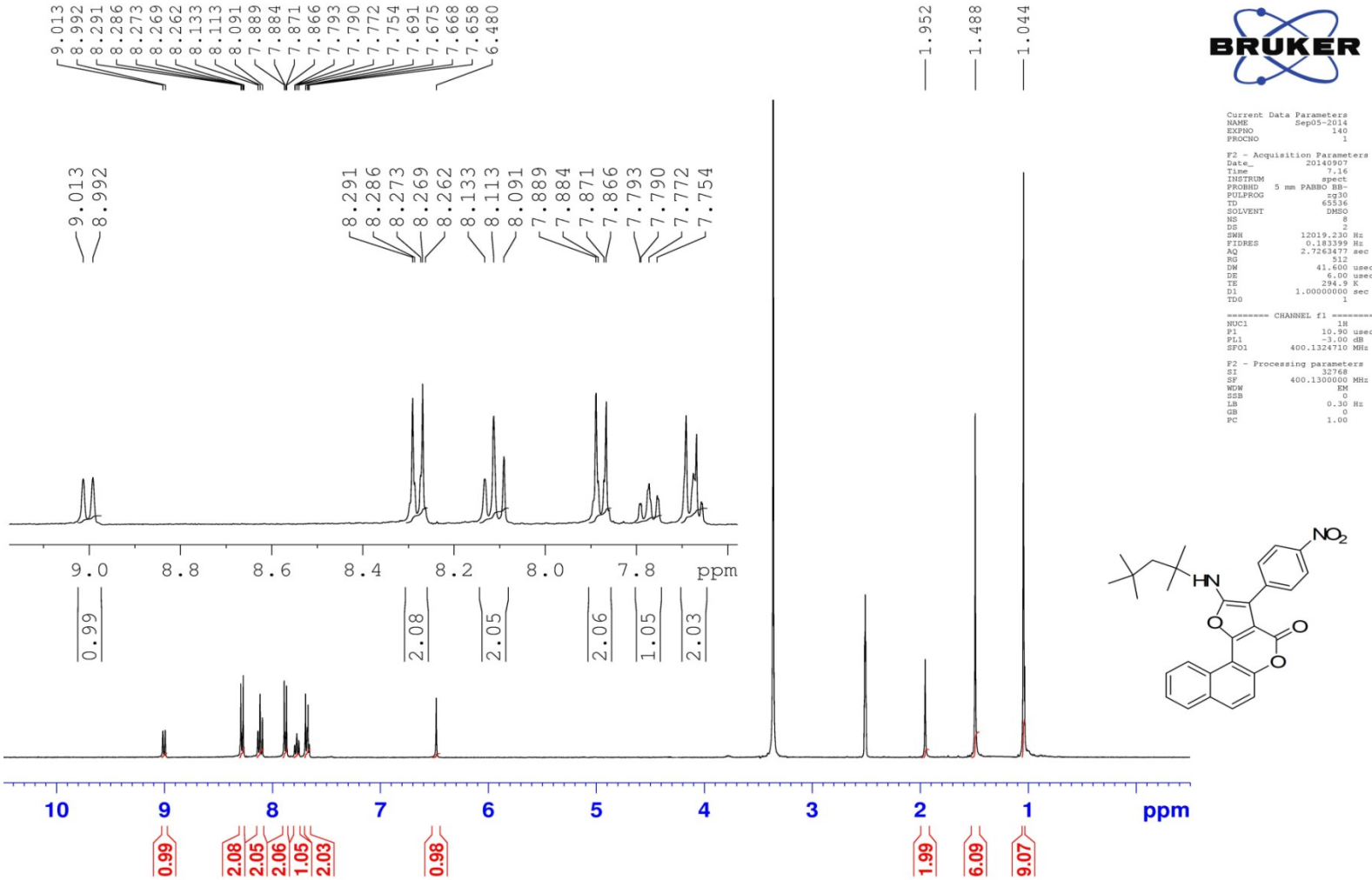
2-(Cyclohexylamino)-3-(4'-nitrophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4m).

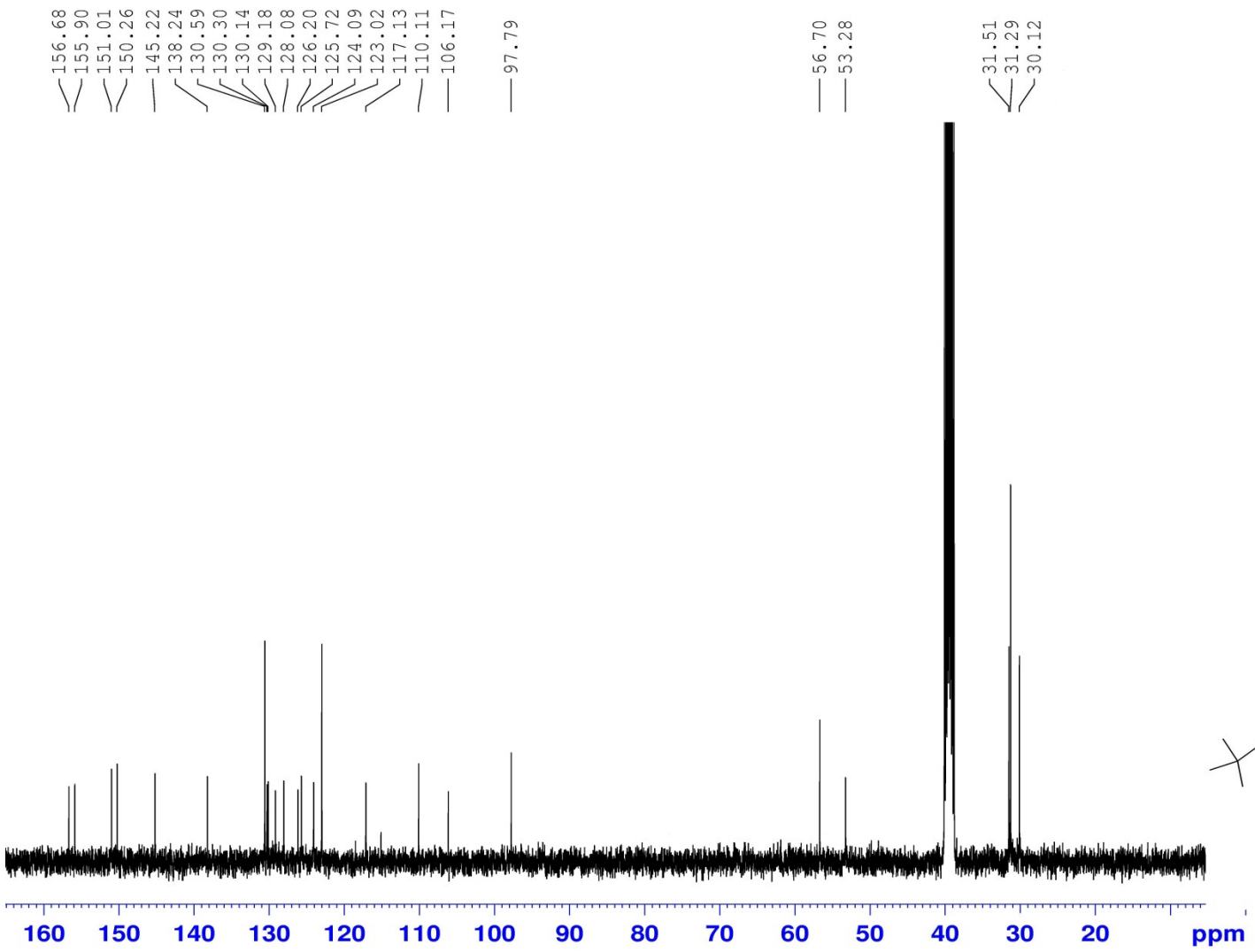



156.65
156.10
149.84
149.64
144.55
138.22
130.01
129.68
128.84
128.02
125.95
125.55
124.14
122.95
116.71
110.45
105.97
91.12
53.18
32.98
25.20
24.81
BRUKER
Current Data Parameters
NAME Sep05-2014
EXPNO 81
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140906
Time 3.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
NO2
NH
O
O
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Intens.
[%]
-MS, 0.0-0.3min #(2-20)
453.1440
485.8752
370.6184
411.7298
516.7412
533.7047
100
80
60
40
20
0
350
400
450
500
550
600
m/z

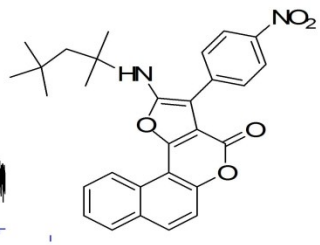
3-(4'-Nitrophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl)amino)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4n).

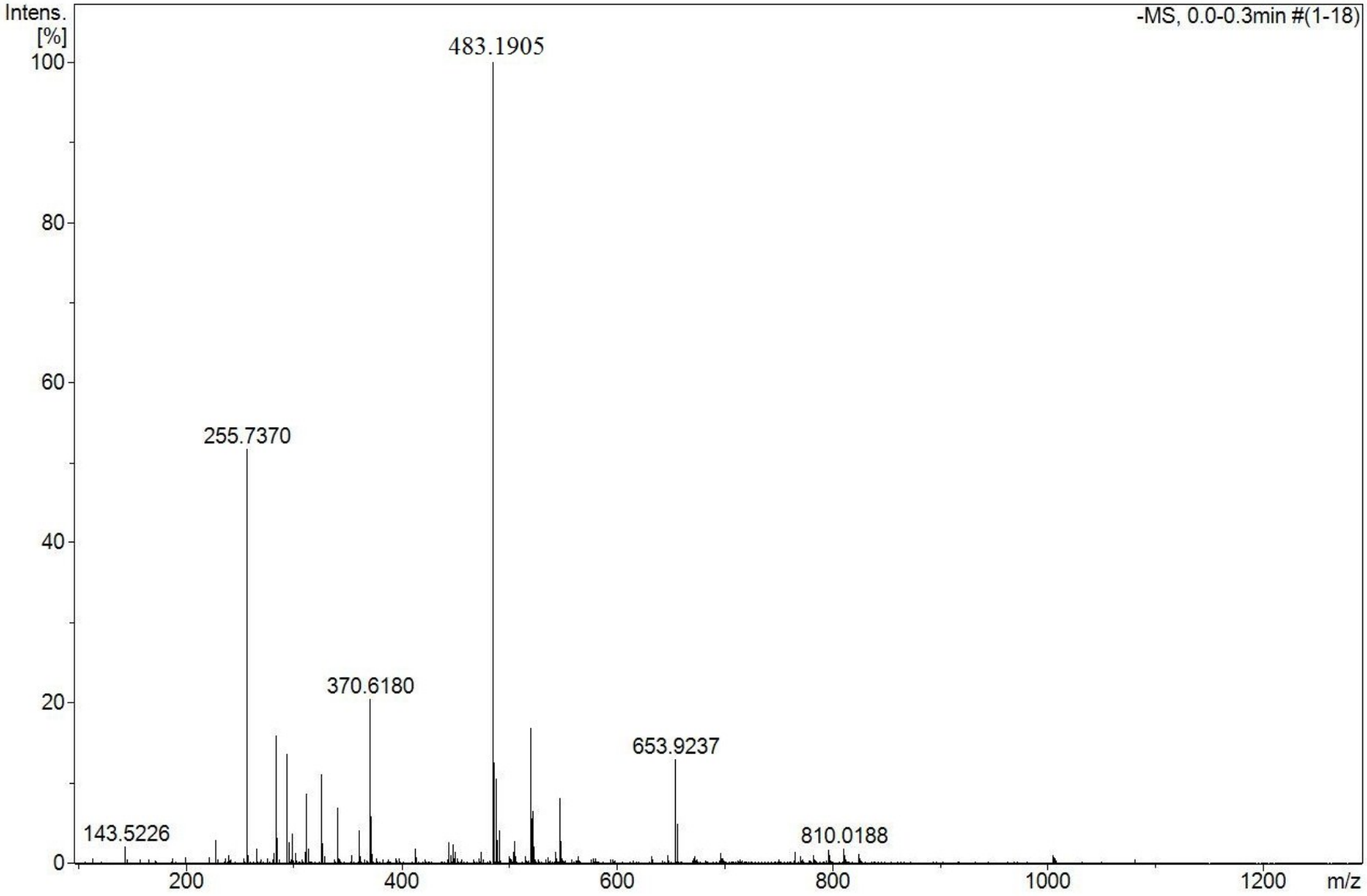




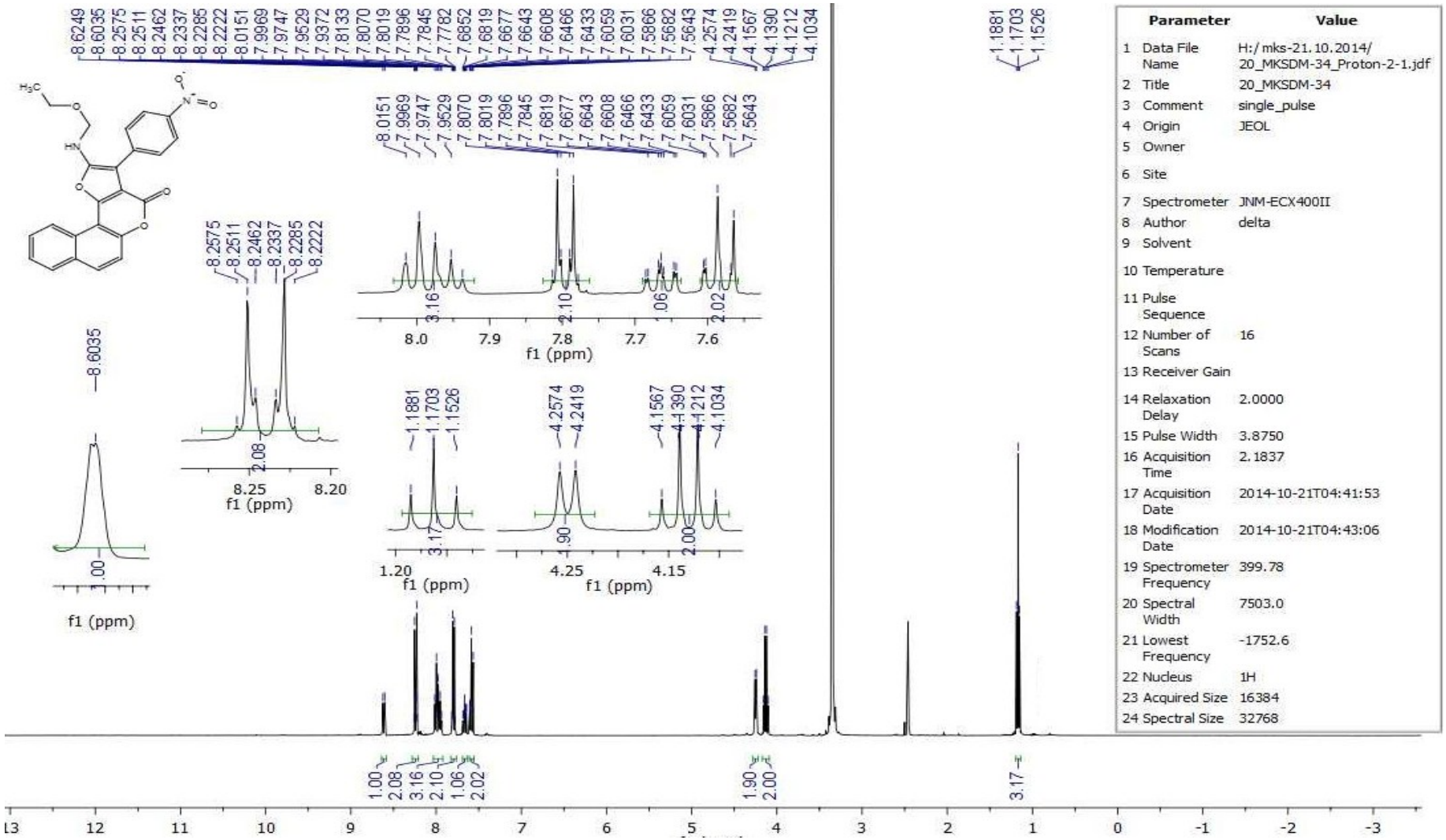
BRUKER

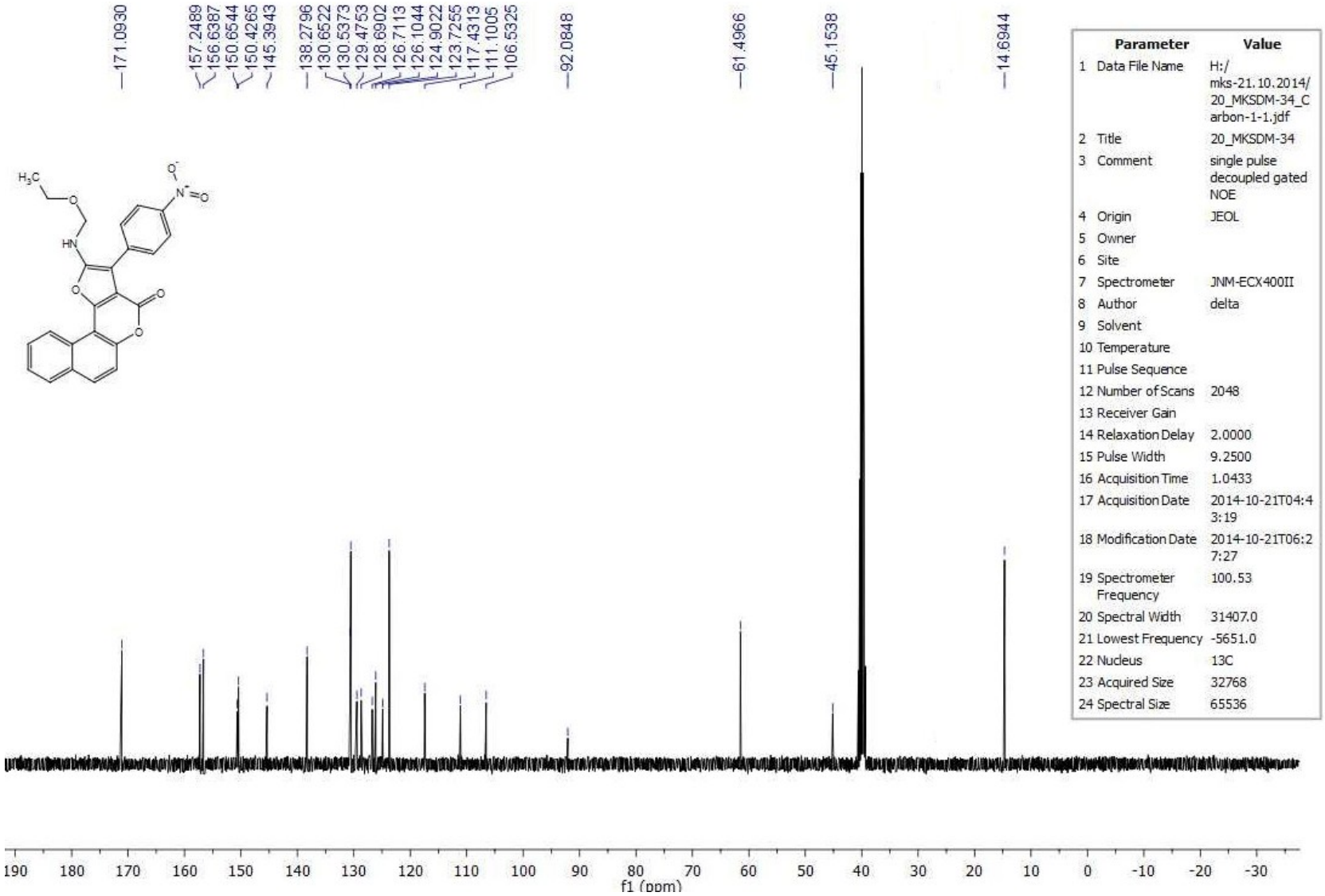
```
Current Data Parameters
NAME            Sep05-2014
EXPNO                  141
PROCNO                   1

F2 - Acquisition Parameters
Date_            20140907
Time                 8.12
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010548 sec
RG                 1030
DW               16.800 usec
DE                6.00 usec
TE                295.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                 9.60 usec
PL1               -2.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -3.00 dB
PL12              14.31 dB
PL13              18.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6128193 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



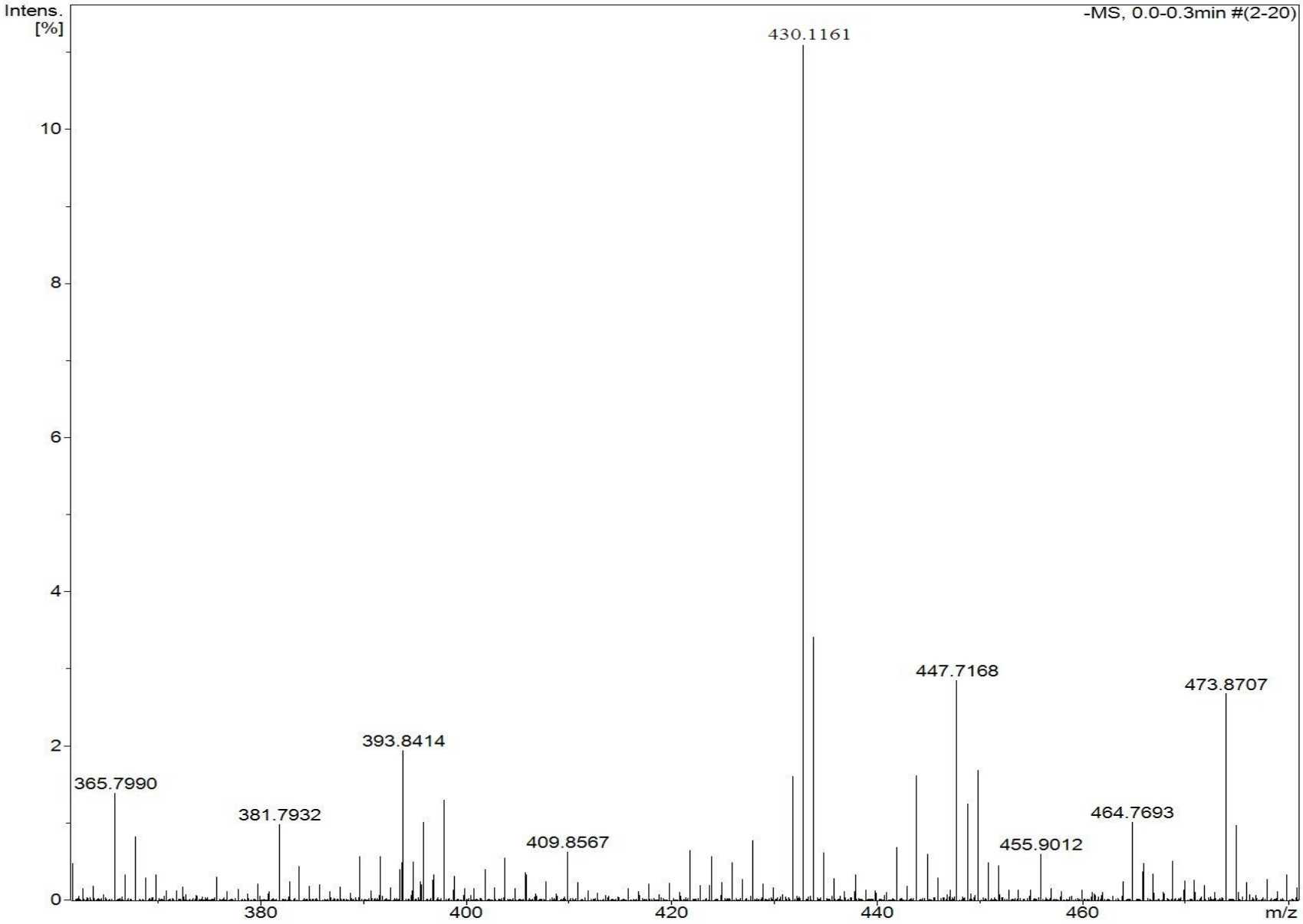

Intens.
[%]
-MS, 0.0-0.3min #(1-18)
483.1905
255.7370
370.6180
653.9237
143.5226
810.0188
100
80
60
40
20
0
200
400
600
800
1000
1200
m/z

2-((Ethoxymethyl)amino)-3-(4'-nitrophenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4o).

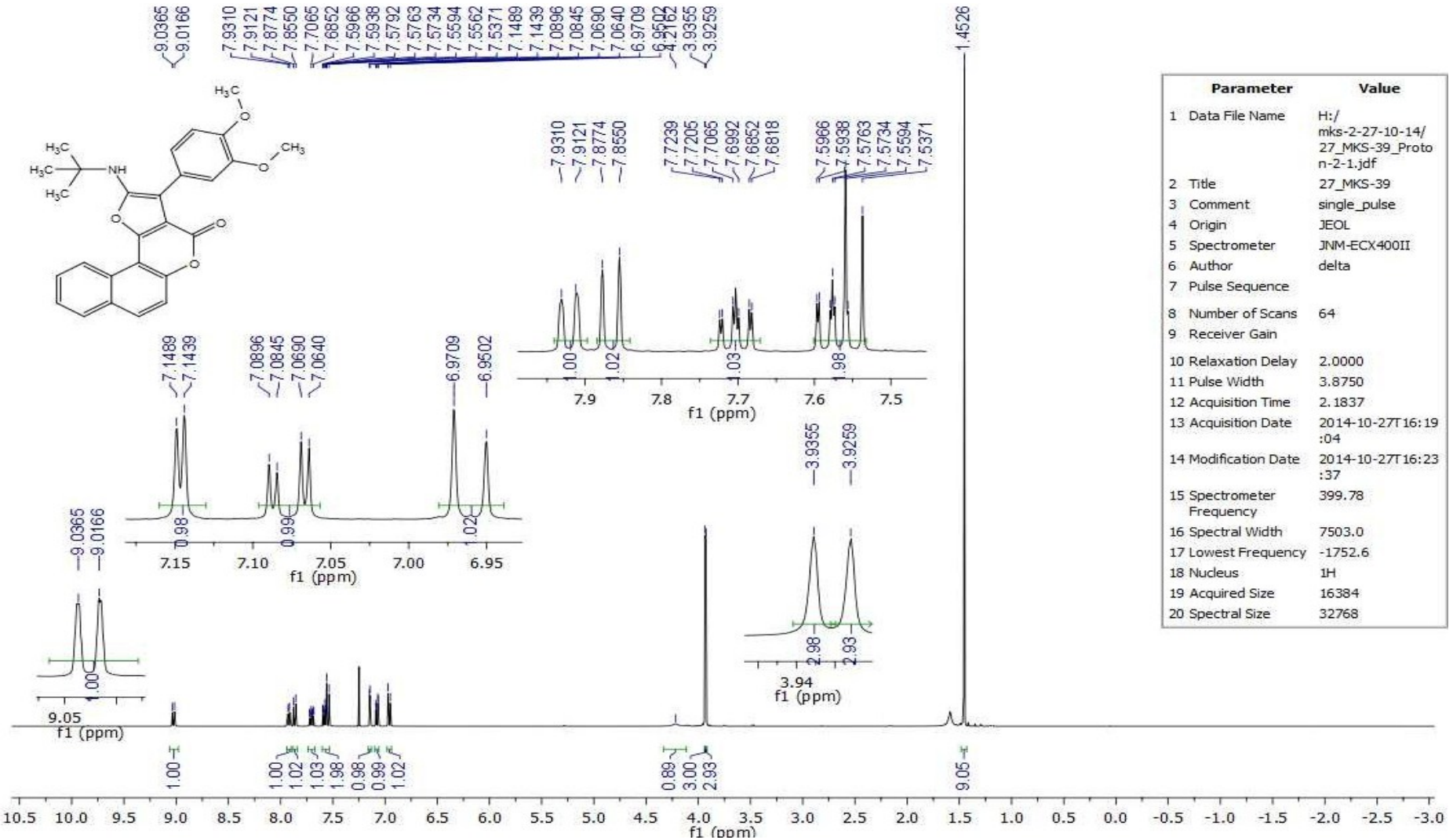




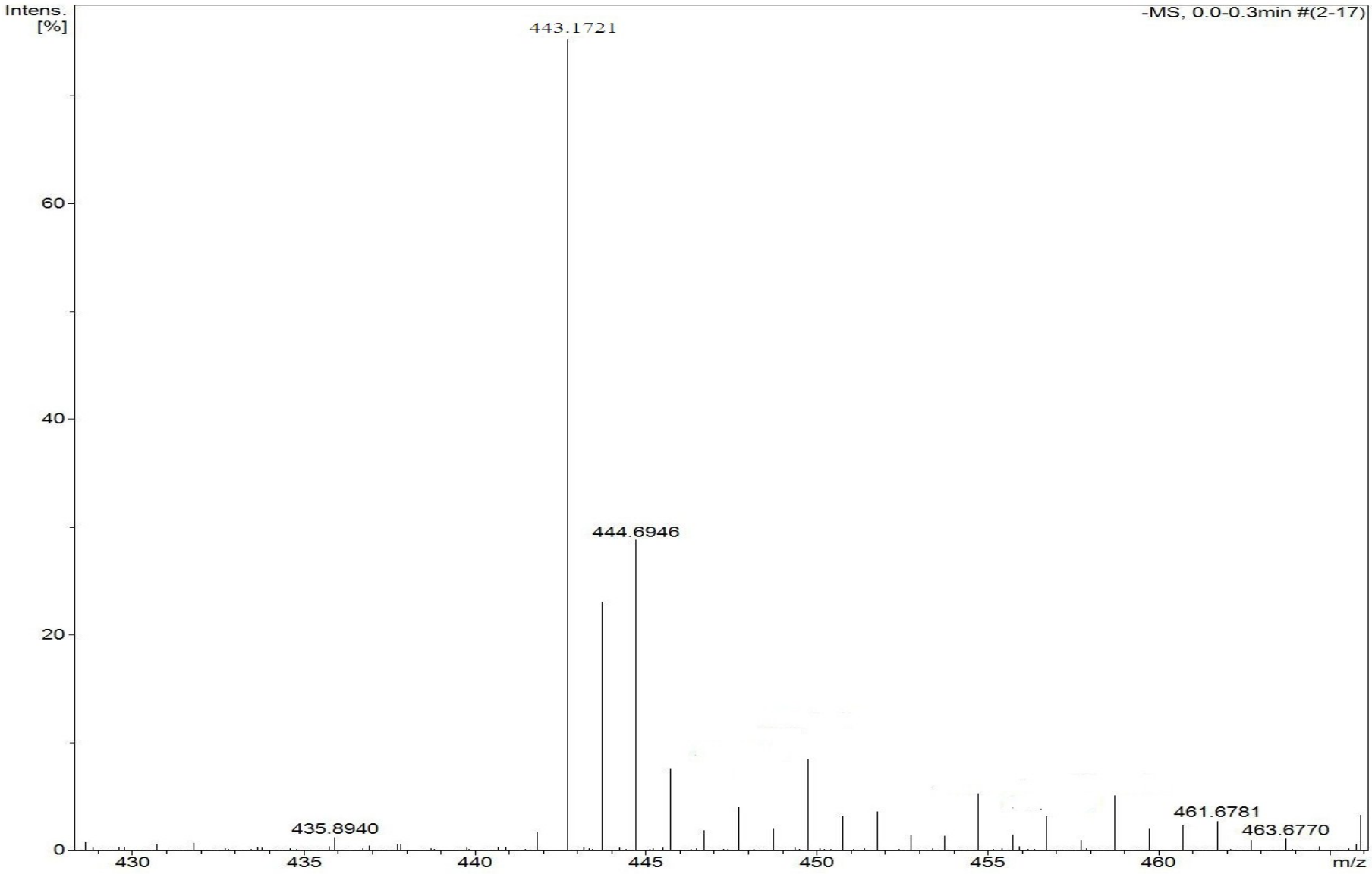
	Parameter	Value
1	Data File Name	H:/mks-21.10.2014/20_MKSDM-34_Carbon-1-1.jdf
2	Title	20_MKSDM-34
3	Comment	single pulse decoupled gated NOE
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	JNM-ECX400II
8	Author	delta
9	Solvent	
10	Temperature	
11	Pulse Sequence	
12	Number of Scans	2048
13	Receiver Gain	
14	Relaxation Delay	2.0000
15	Pulse Width	9.2500
16	Acquisition Time	1.0433
17	Acquisition Date	2014-10-21T04:43:19
18	Modification Date	2014-10-21T06:27:27
19	Spectrometer Frequency	100.53
20	Spectral Width	31407.0
21	Lowest Frequency	-5651.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536


Intens.
[%]
-MS, 0.0-0.3min #(2-20)
430.1161
447.7168
473.8707
393.8414
365.7990
381.7932
409.8567
455.9012
464.7693
10
8
6
4
2
0
380
400
420
440
460
m/z

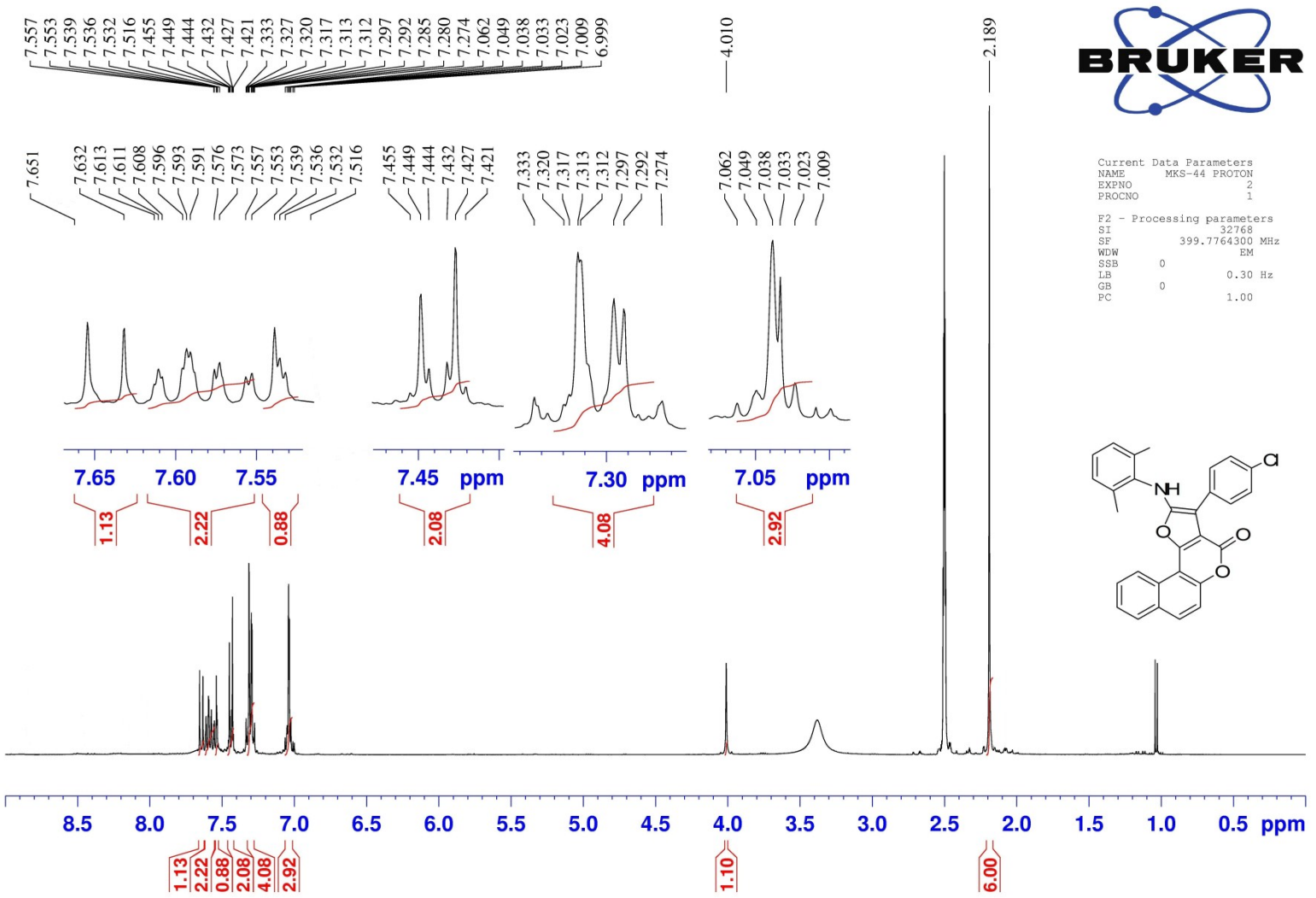
2-(*tert*-Butylamino)-3-(3',4'-dimethoxyphenyl)-4*H*-benzo[*f*]furo[3,2-*c*]chromen-4-one (4p).

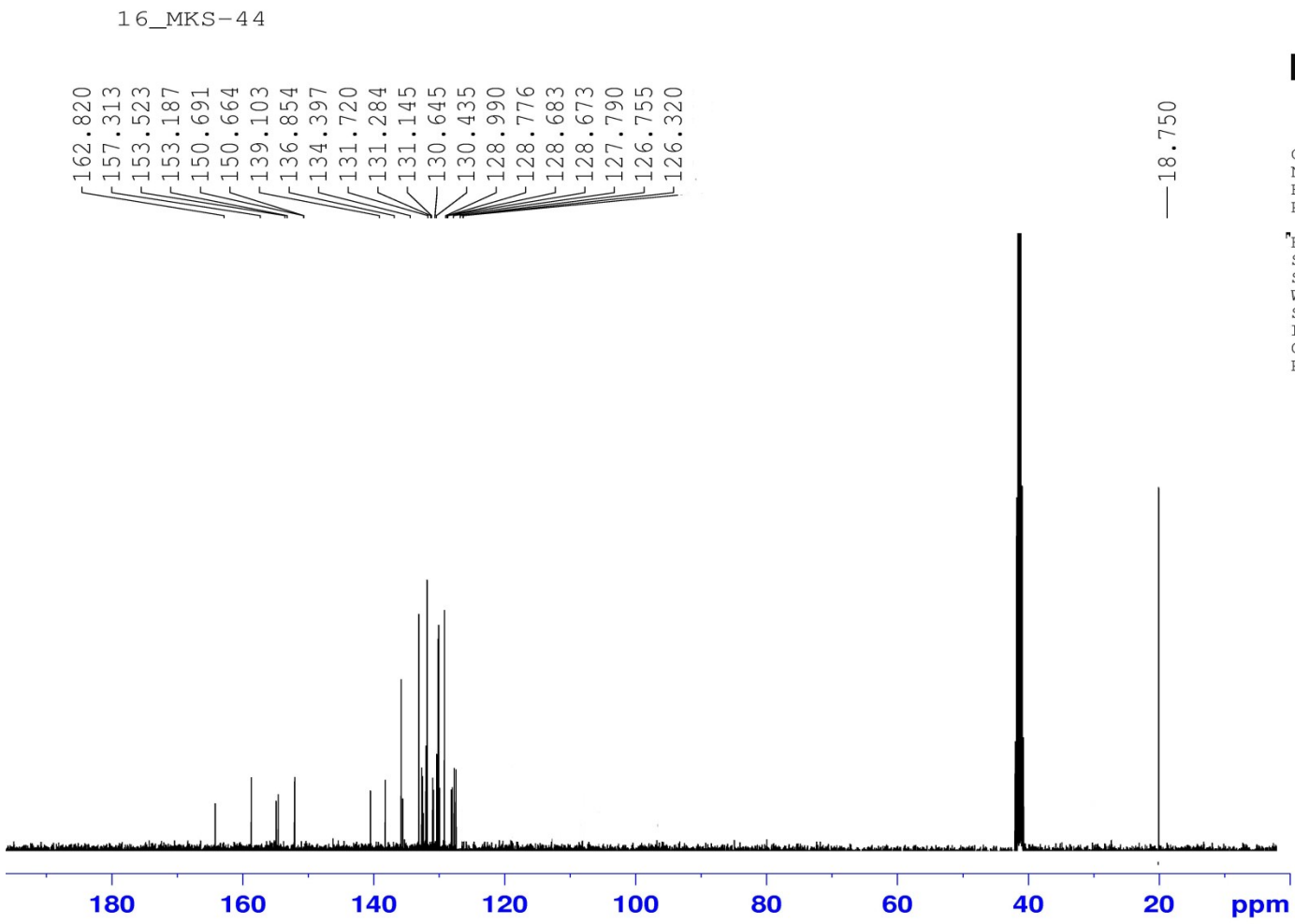


	Parameter	Value
1	Data File Name	H:/mks-2-27-10-14/27_MKS-39_Proton-2-1.jdf
2	Title	27_MKS-39
3	Comment	single_pulse
4	Origin	JEOL
5	Spectrometer	JNM-ECX400II
6	Author	delta
7	Pulse Sequence	
8	Number of Scans	64
9	Receiver Gain	
10	Relaxation Delay	2.0000
11	Pulse Width	3.8750
12	Acquisition Time	2.1837
13	Acquisition Date	2014-10-27T16:19:04
14	Modification Date	2014-10-27T16:23:37
15	Spectrometer Frequency	399.78
16	Spectral Width	7503.0
17	Lowest Frequency	-1752.6
18	Nucleus	1H
19	Acquired Size	16384
20	Spectral Size	32768


Intens.
[%]
-MS, 0.0-0.3min #(2-17)
443.1721
444.6946
435.8940
461.6781
463.6770
60
40
20
0
430
435
440
445
450
455
460
m/z

3-(4'-Chlorophenyl)-2,6-(Dimethylphenylamino)-4H-benzo[*f*]furo[3,2-*c*]chromen-4-one (4q).

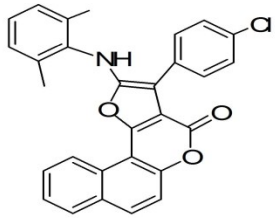


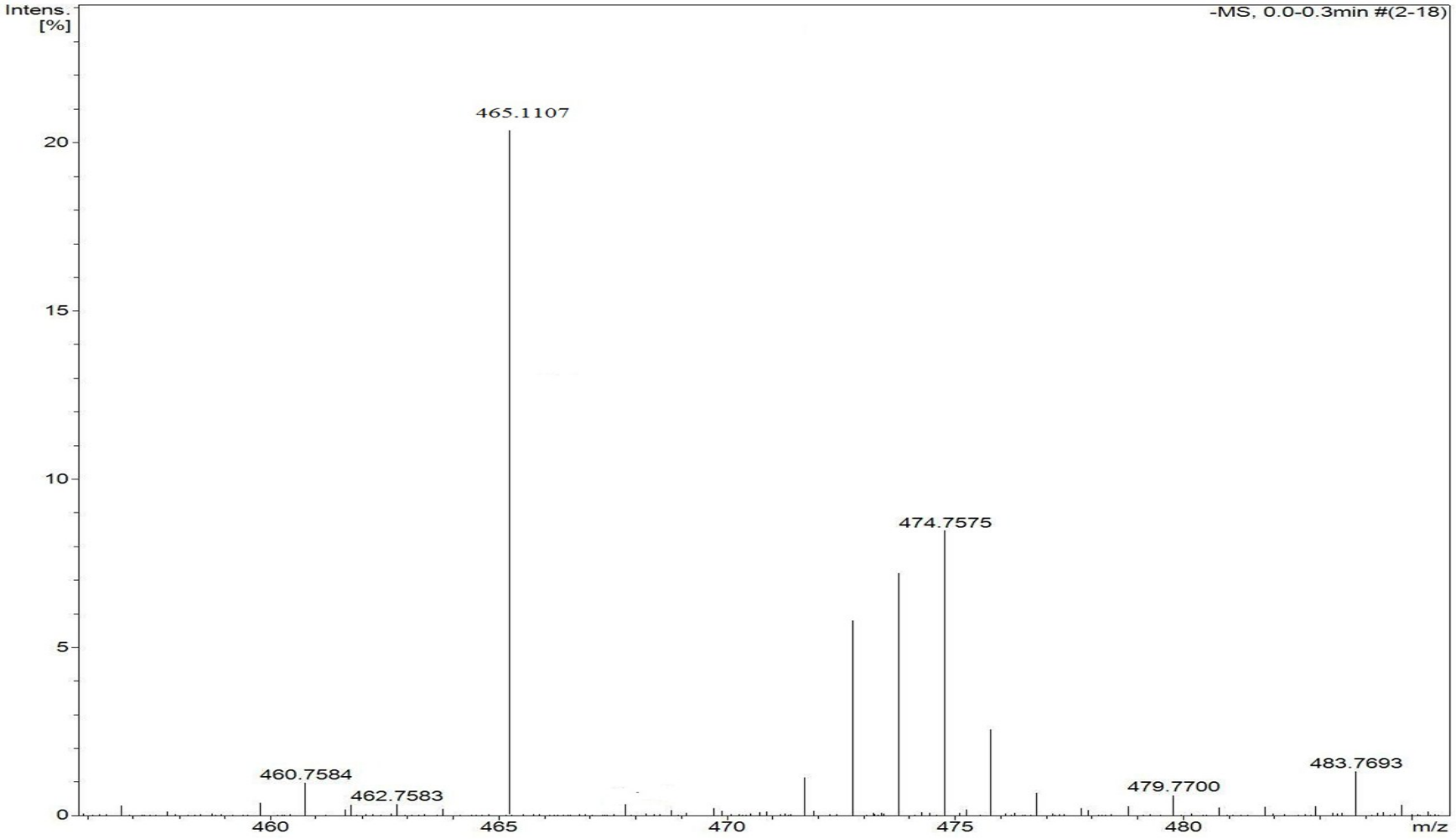


BRUKER

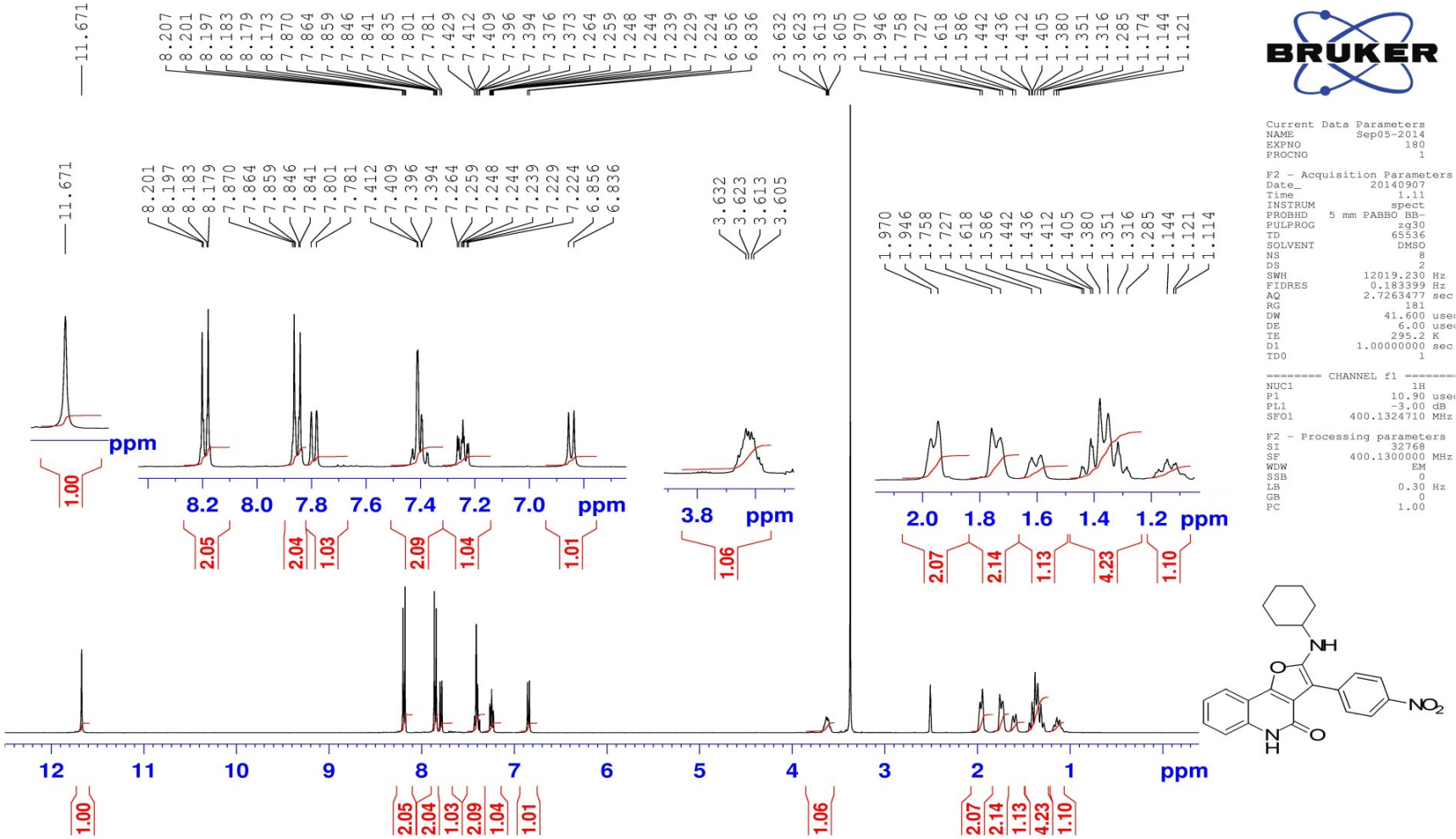
Current Data Parameters
NAME MKS-44c
EXPNO 2
PROCNO 1

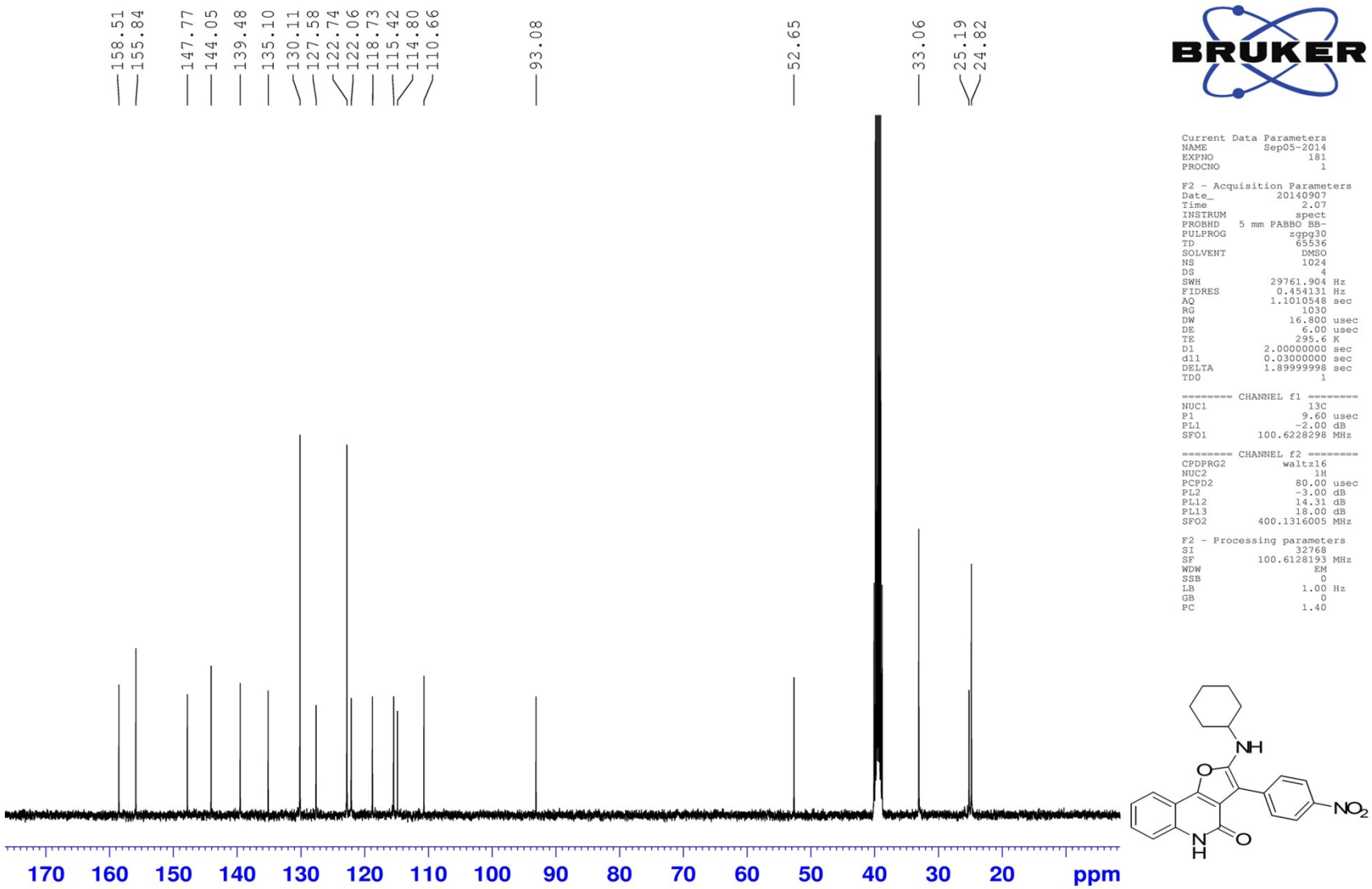
F2 - Processing parameters
SI 65536
SF 100.5253067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

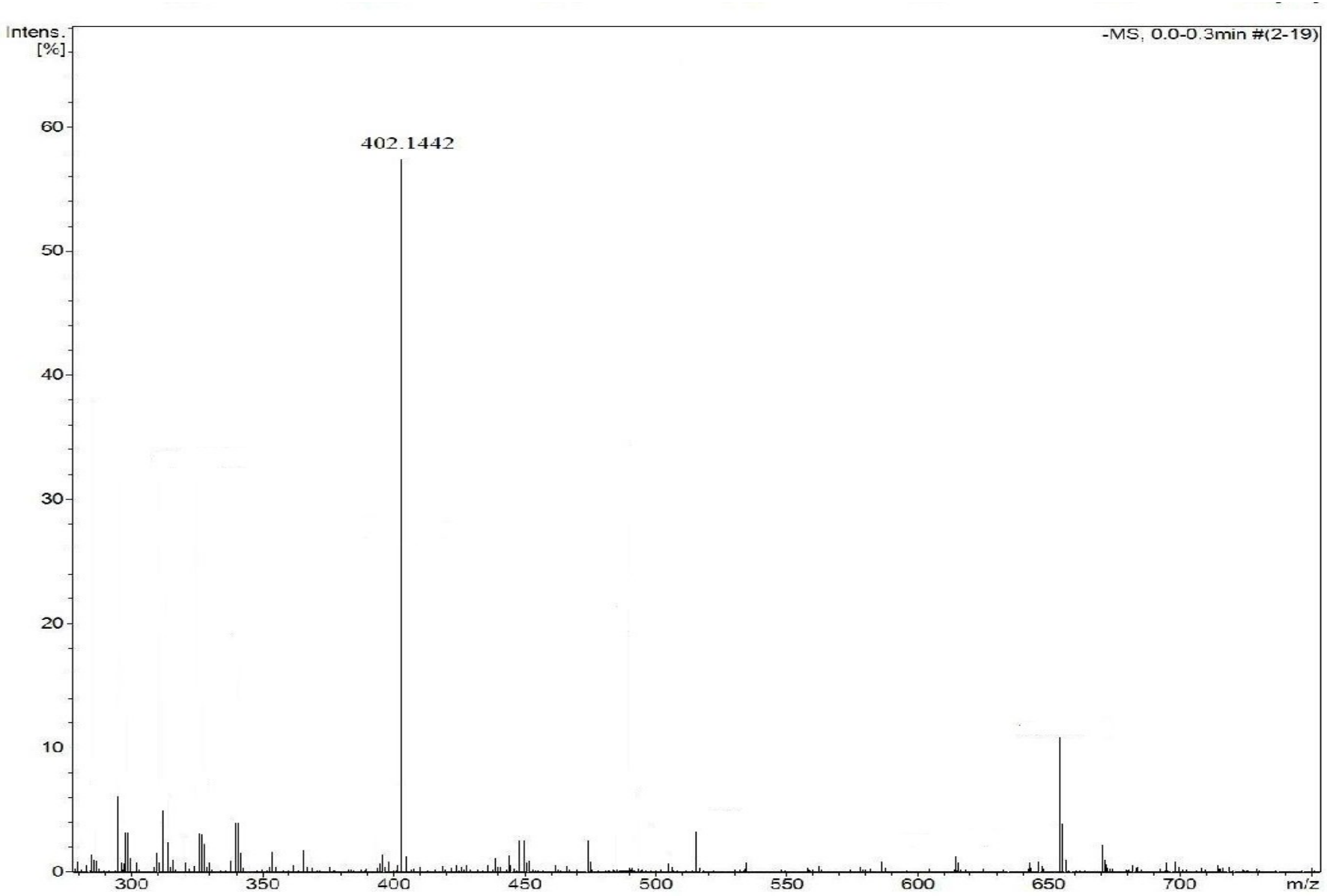



Intens.
[%]
-MS, 0.0-0.3min #(2-18)
465.1107
474.7575
460.7584
462.7583
479.7700
483.7693
20
15
10
5
0
460
465
470
475
480
m/z

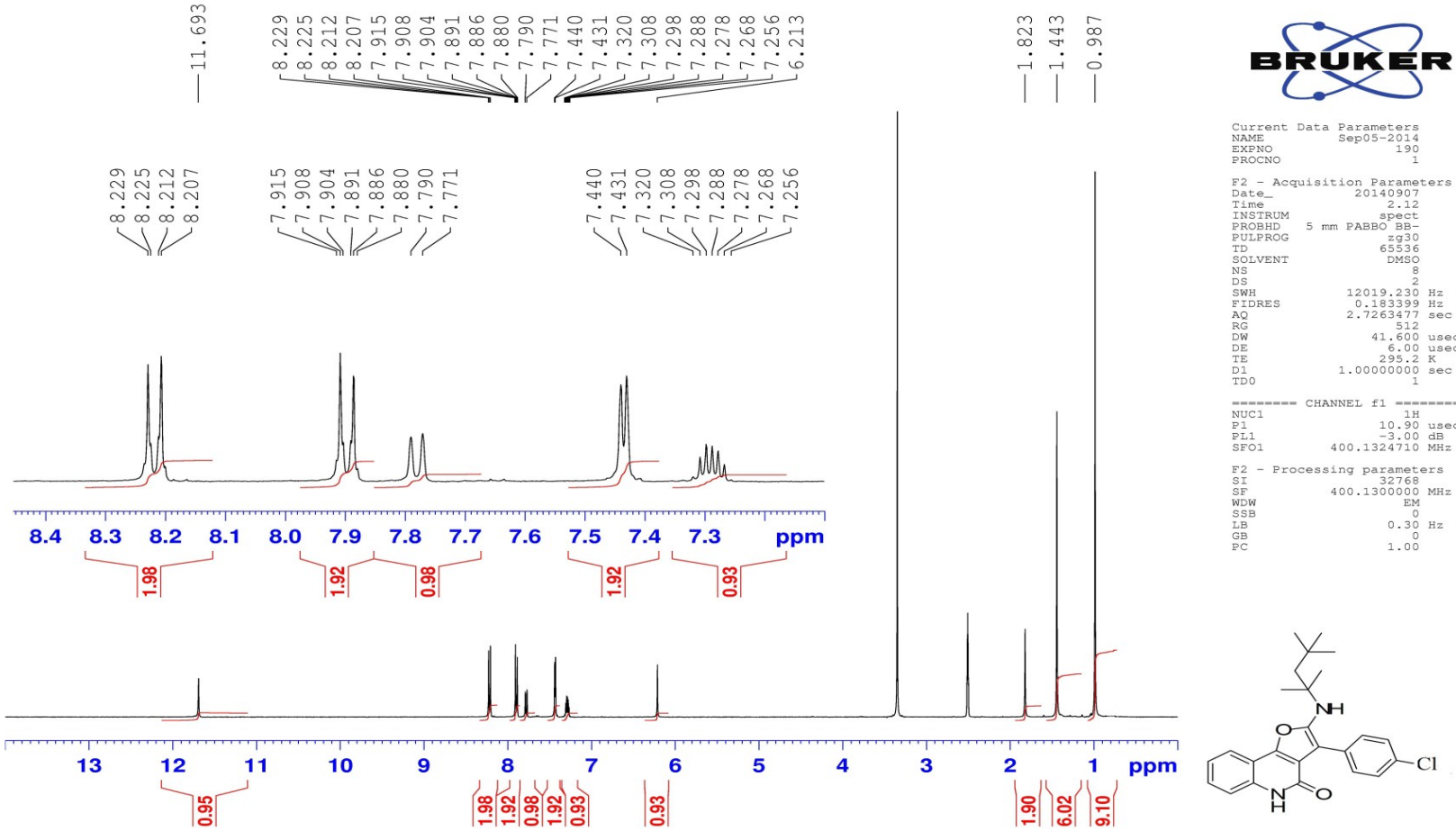
2-(Cyclohexylamino)-3-(4'-nitrophenyl)-furo[3,2-*c*]quinolin-4(5*H*)-one (5a).

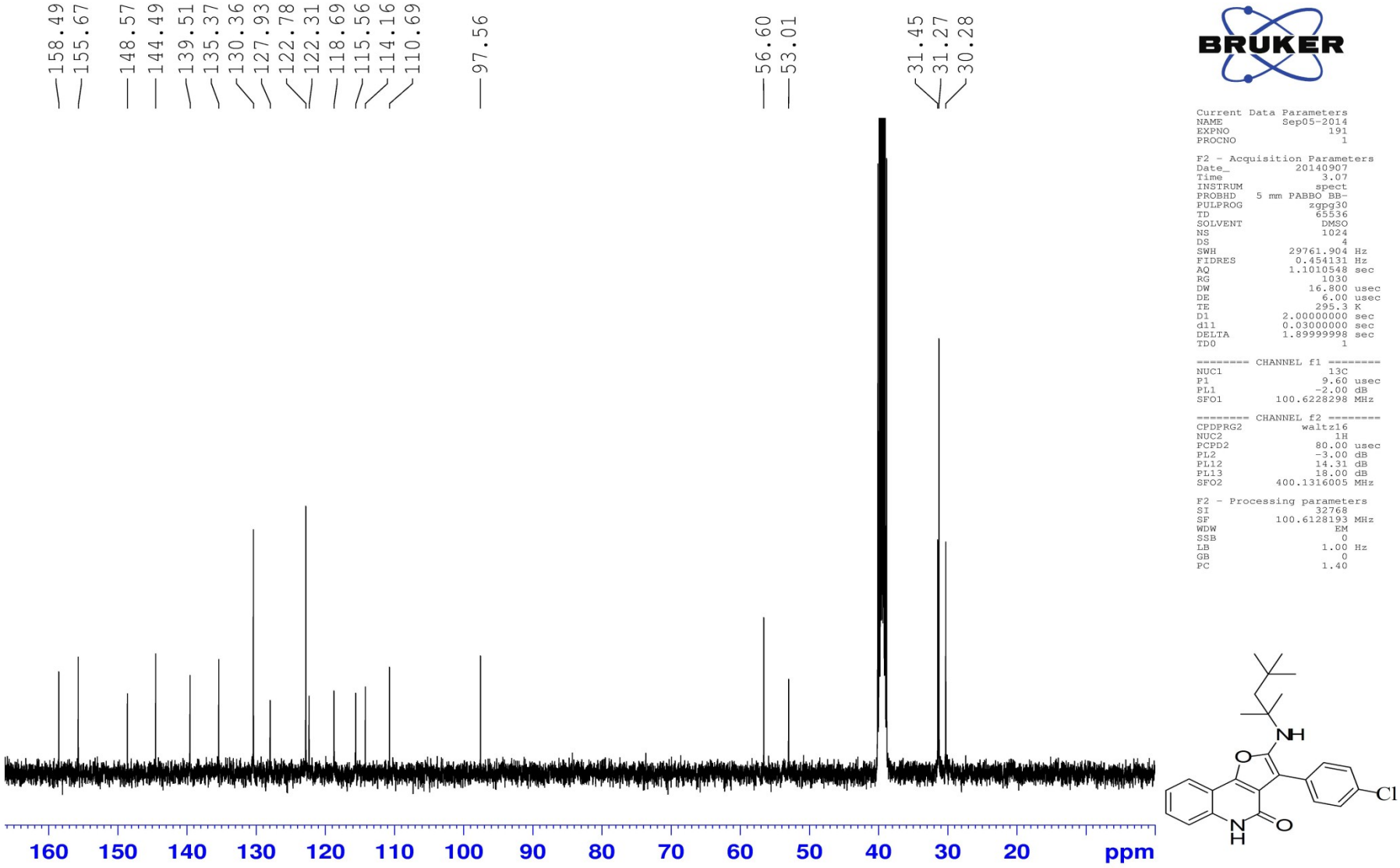


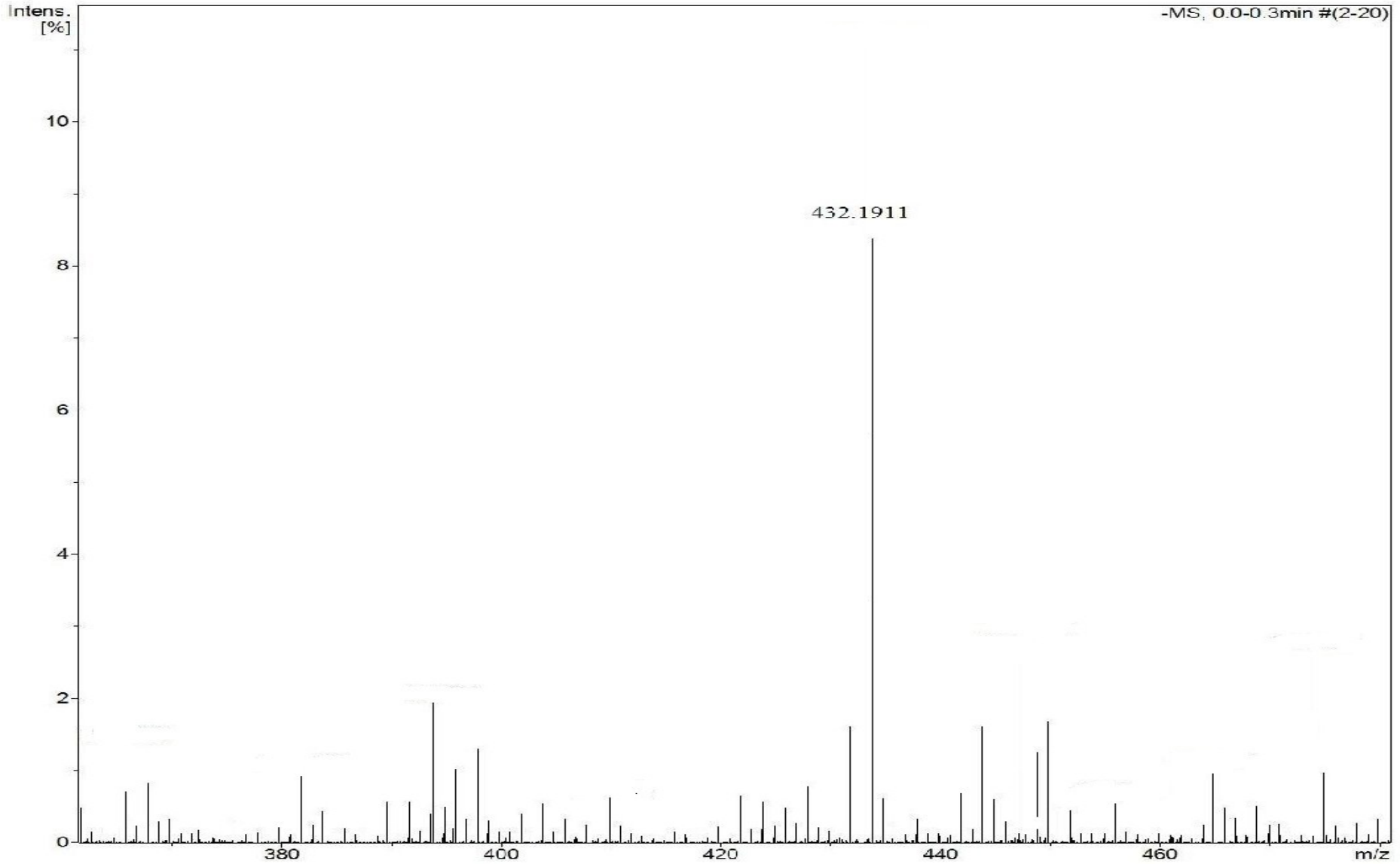

158.51
155.84
147.77
144.05
139.48
135.10
130.11
127.58
122.74
122.06
118.73
115.42
114.80
110.66
93.08
52.65
33.06
25.19
24.82
BRUKER
Current Data Parameters
NAME Sep05-2014
EXPNO 181
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140907
Time 2.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 295.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
NH
O
N
H
O
NO2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Intens.
[%]
-MS, 0.0-0.3min #(2-19)
402.1442
60
50
40
30
20
10
0
300
350
400
450
500
550
600
650
700
m/z

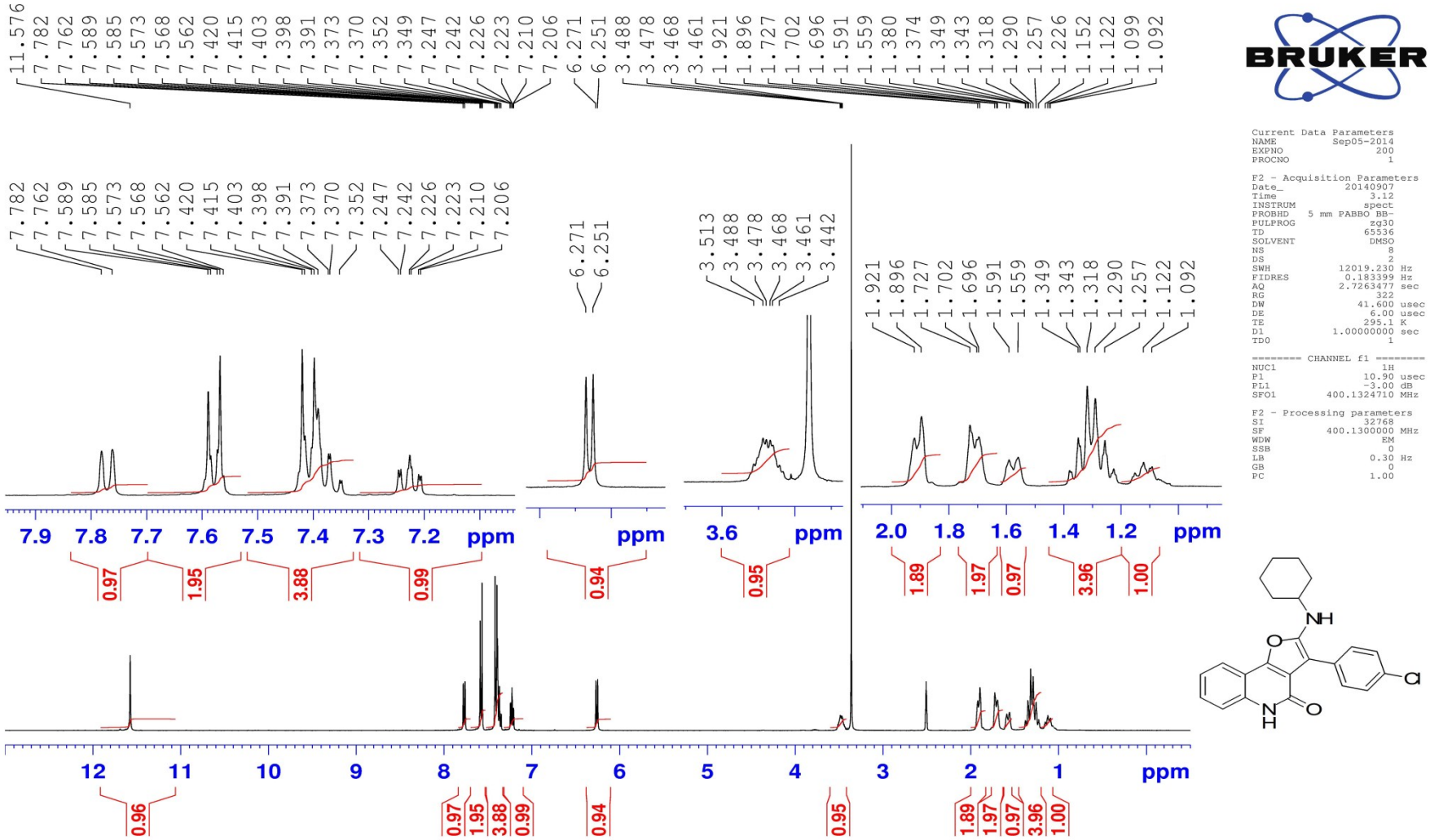
3-(4'-Chlorophenyl)-2-((2'',4'',4''-trimethylpentan-2-yl)amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5b).

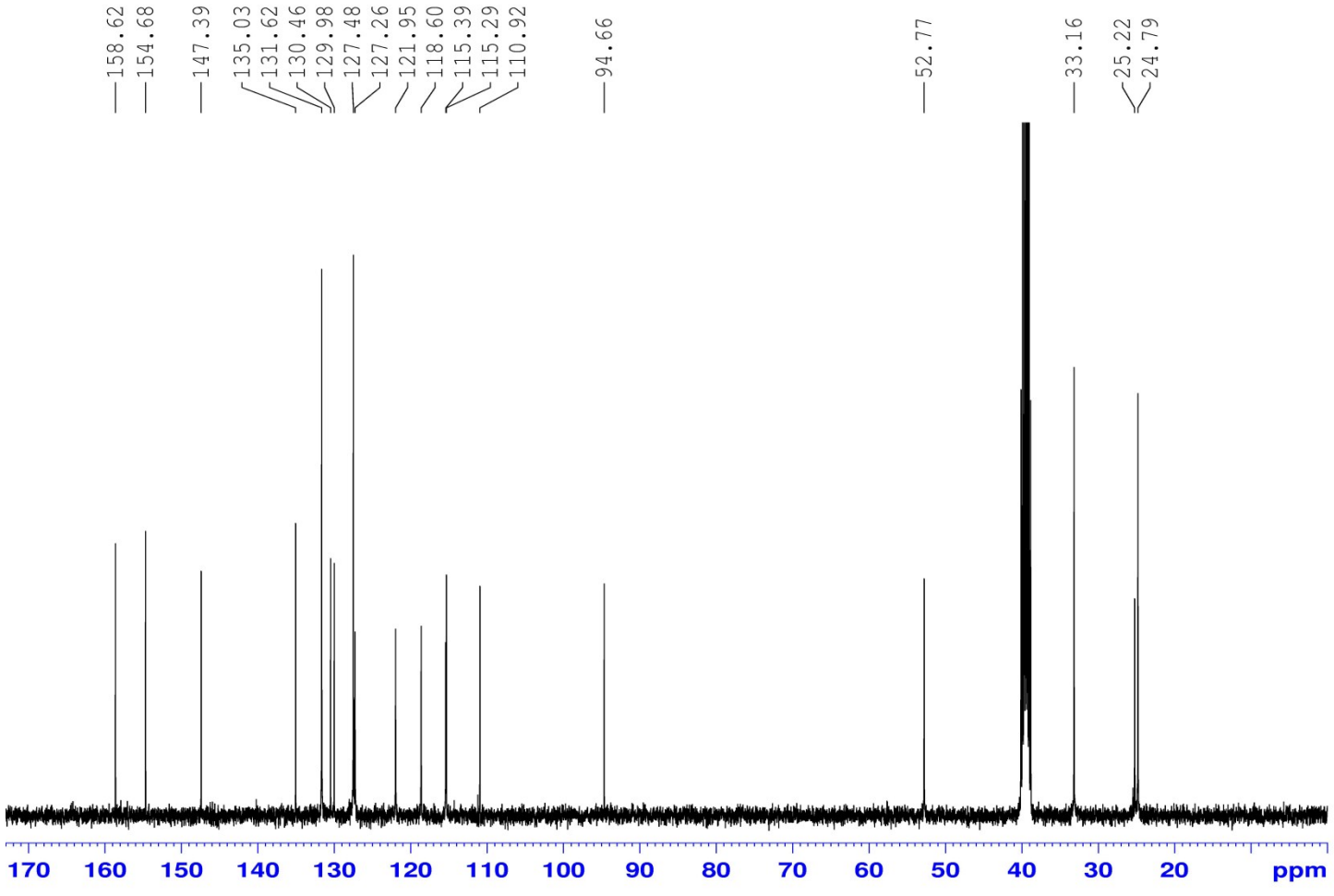



158.49
155.67
148.57
144.49
139.51
135.37
130.36
127.93
122.78
122.31
118.69
115.56
114.16
110.69
97.56
56.60
53.01
31.45
31.27
30.28
BRUKER
Current Data Parameters
NAME Sep05-2014
EXPNO 191
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140907
Time 3.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 295.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
NH
O
N
H
O
Cl


Intens.
[%]
-MS, 0.0-0.3min #(2-20)
432.1911
10
8
6
4
2
0
380
400
420
440
460
m/z

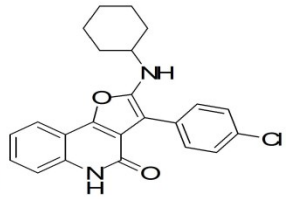
2-(Cyclohexylamino)-3-(4'-chlorophenyl)-furo[3,2-*c*]quinolin-4(5*H*)-one (5c).

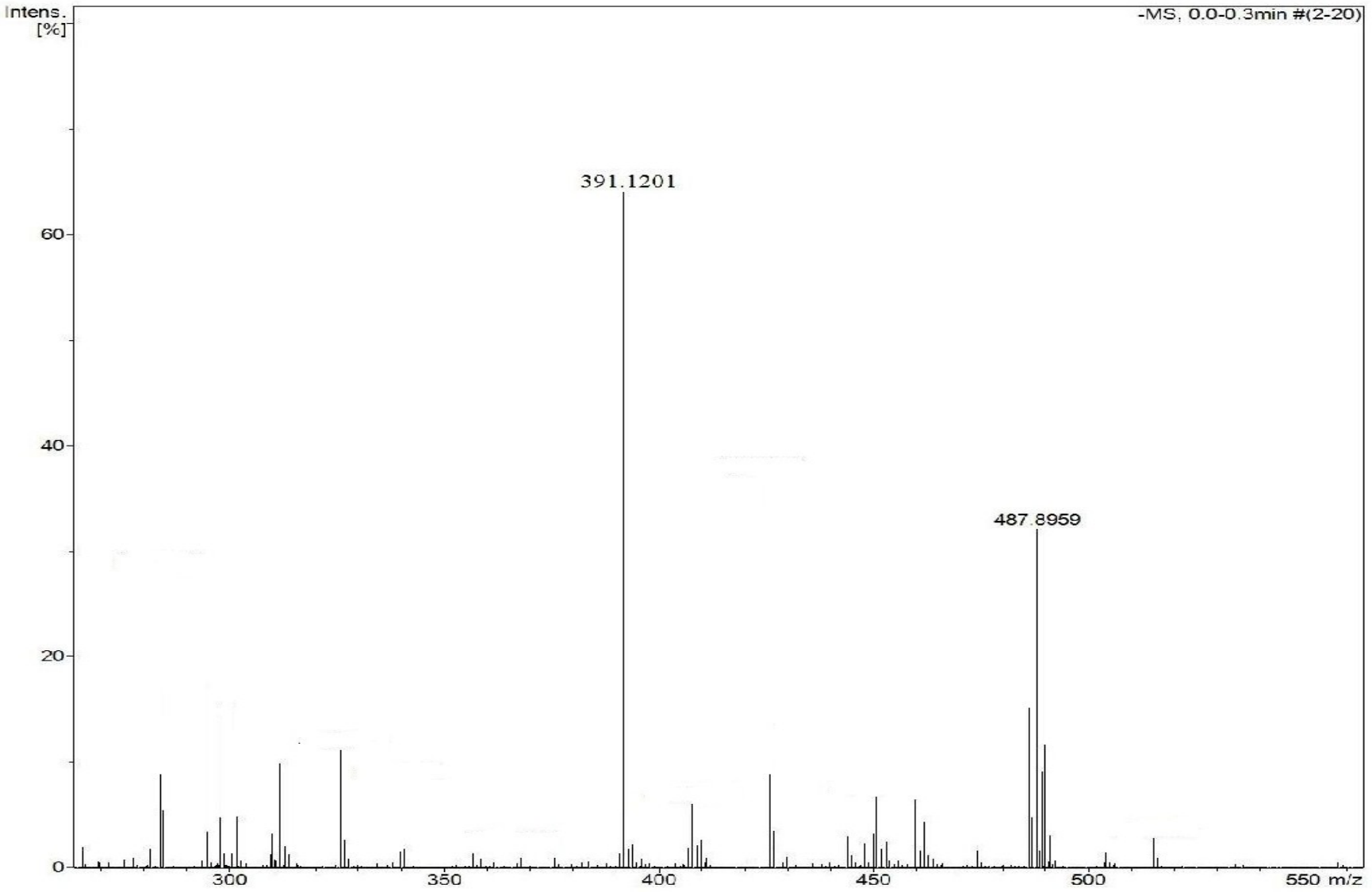




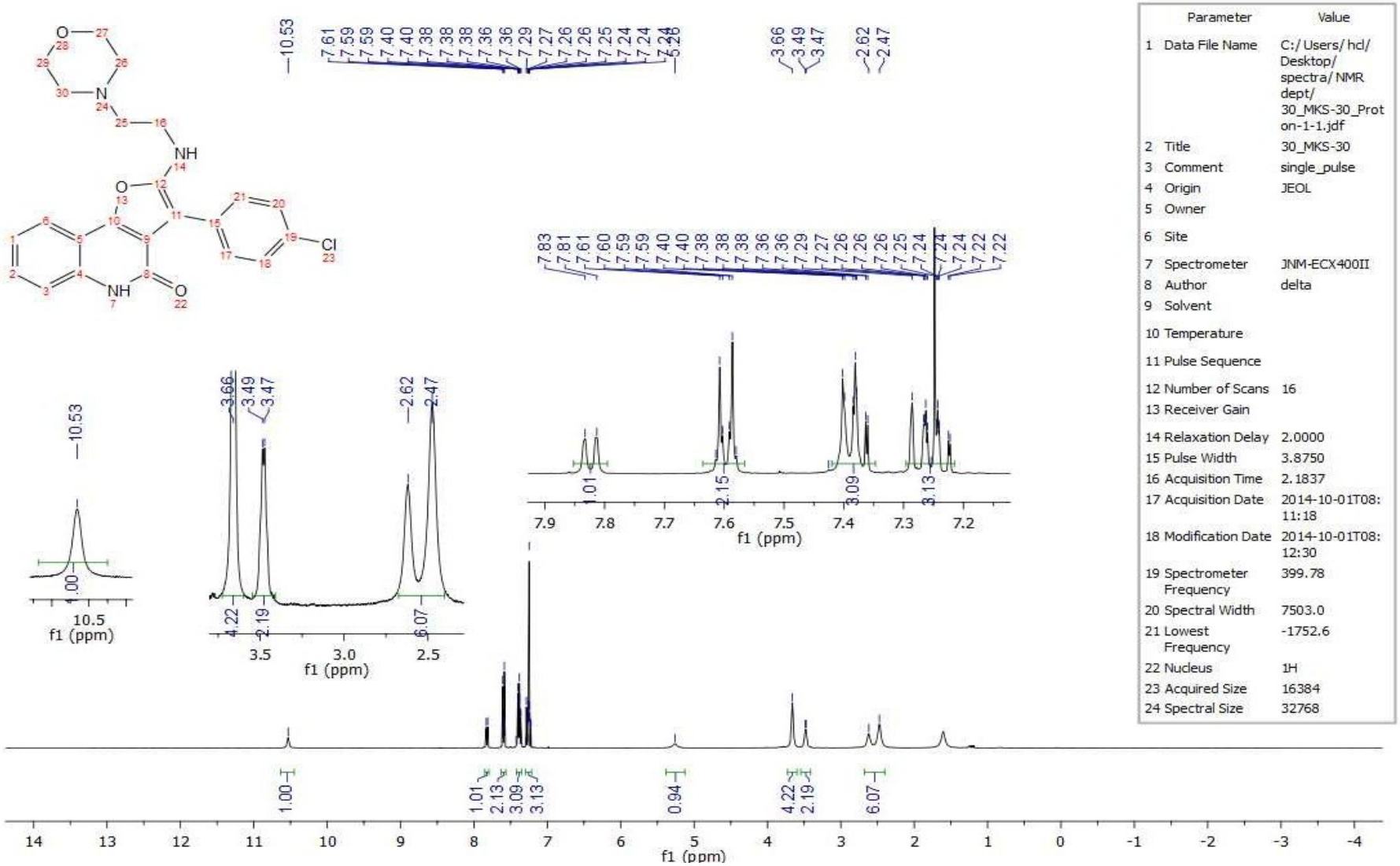
BRUKER

```
Current Data Parameters
NAME            Sep05-2014
EXPNO                  201
PROCNO                   1

F2 - Acquisition Parameters
Date_              20140907
Time                   4.08
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT               DMSO
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010548 sec
RG                    1030
DW                 16.800 usec
DE                  6.00 usec
TE                  295.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.60 usec
PL1                  -2.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2                80.00 usec
PL2                  -3.00 dB
PL12                 14.31 dB
PL13                 18.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6128193 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

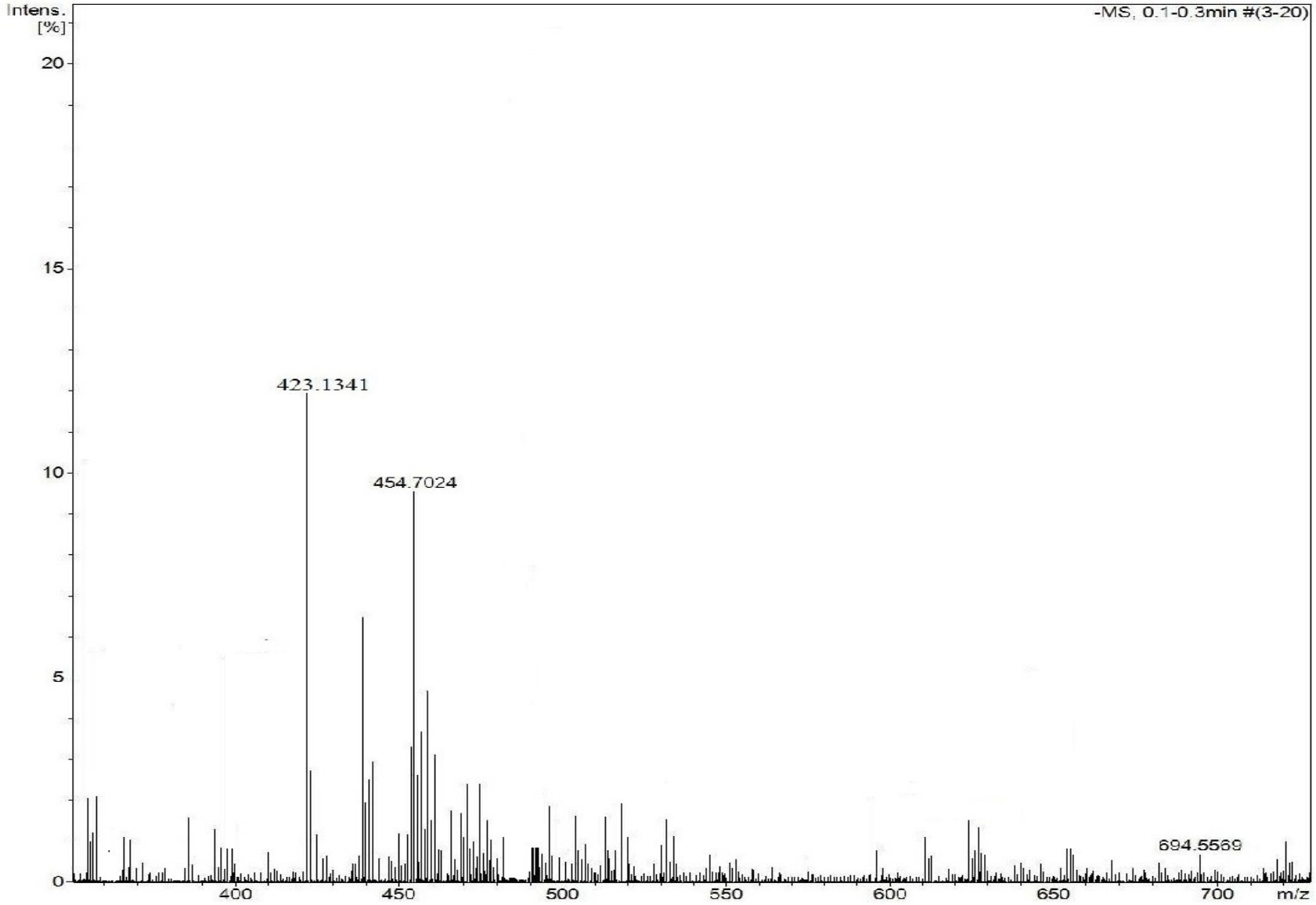



Intens.
[%]
-MS, 0.0-0.3min #(2-20)
391.1201
487.8959
60
40
20
0
300
350
400
450
500
550 m/z

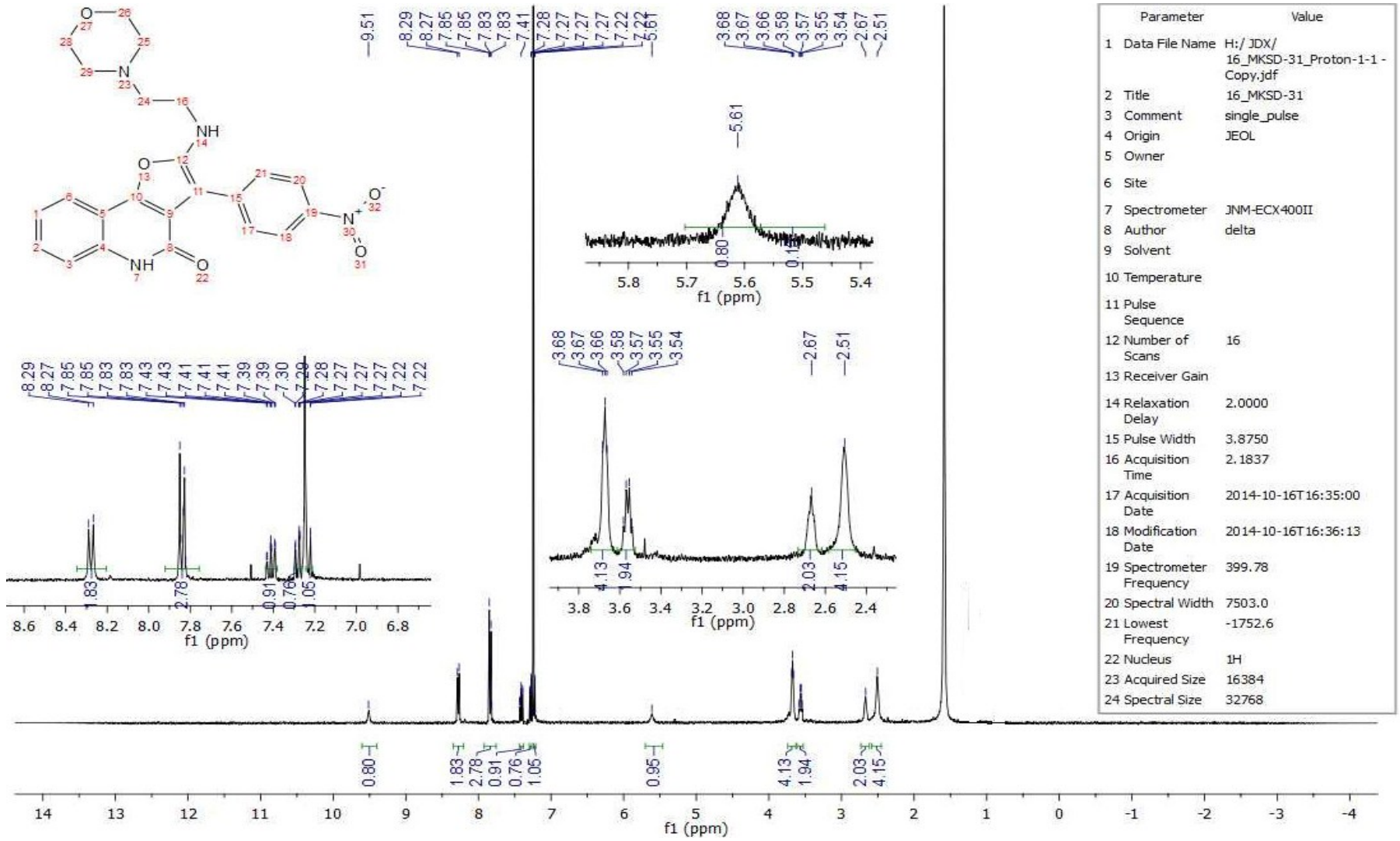
3-(4'-Chlorophenyl)-2-((2-morpholinoethyl)amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5d).



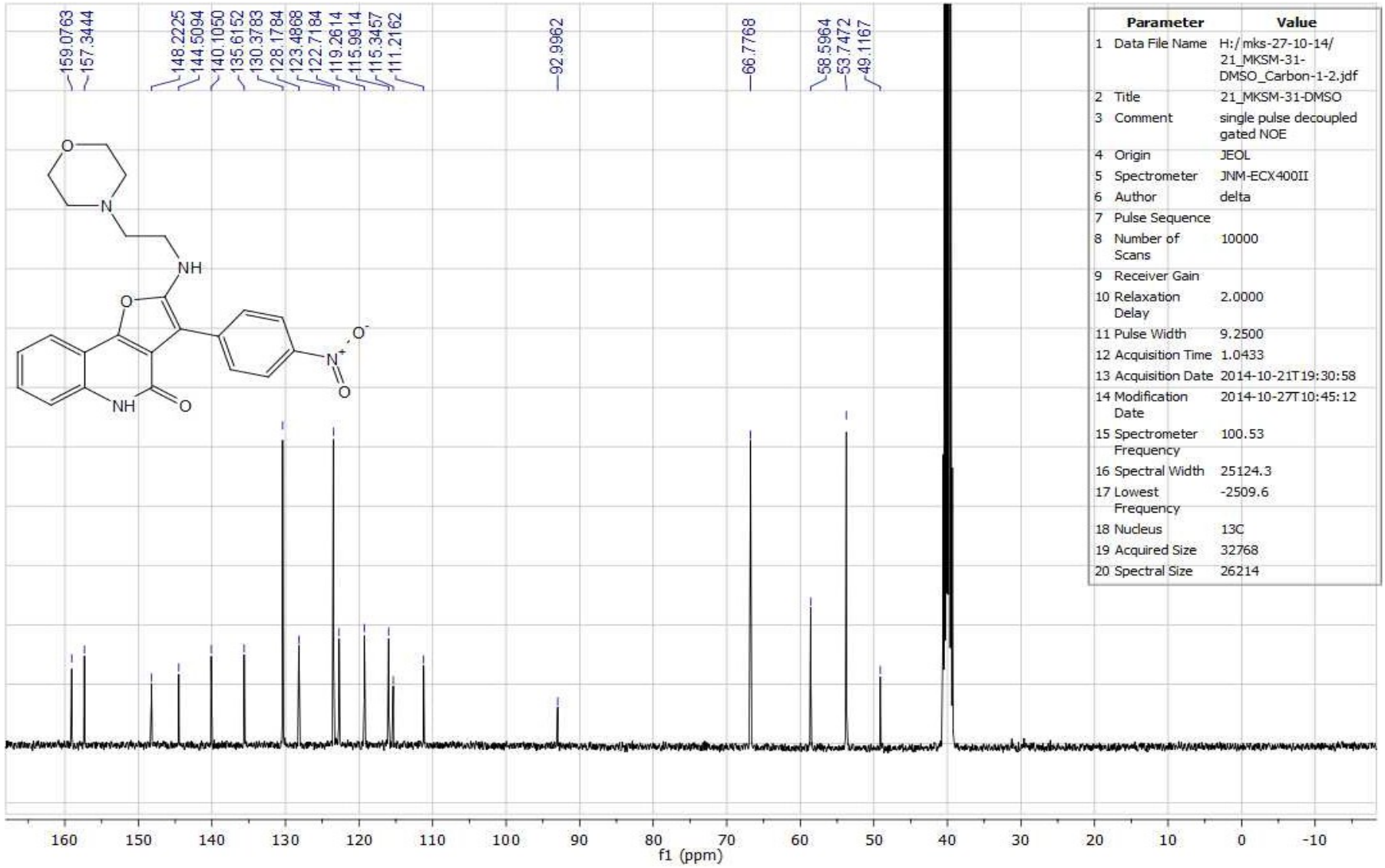
	Parameter	Value
1	Data File Name	C:/Users/hcl/Desktop/spectra/NMR dept/30_MKS-30_Proton-1-1.jdf
2	Title	30_MKS-30
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	JNM-ECX400II
8	Author	delta
9	Solvent	
10	Temperature	
11	Pulse Sequence	
12	Number of Scans	16
13	Receiver Gain	
14	Relaxation Delay	2.0000
15	Pulse Width	3.8750
16	Acquisition Time	2.1837
17	Acquisition Date	2014-10-01T08:11:18
18	Modification Date	2014-10-01T08:12:30
19	Spectrometer Frequency	399.78
20	Spectral Width	7503.0
21	Lowest Frequency	-1752.6
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768


Intens.
[%]
-MS, 0.1-0.3min #(3-20)
20
15
10
5
0
423.1341
454.7024
694.5569
400
450
500
550
600
650
700
m/z

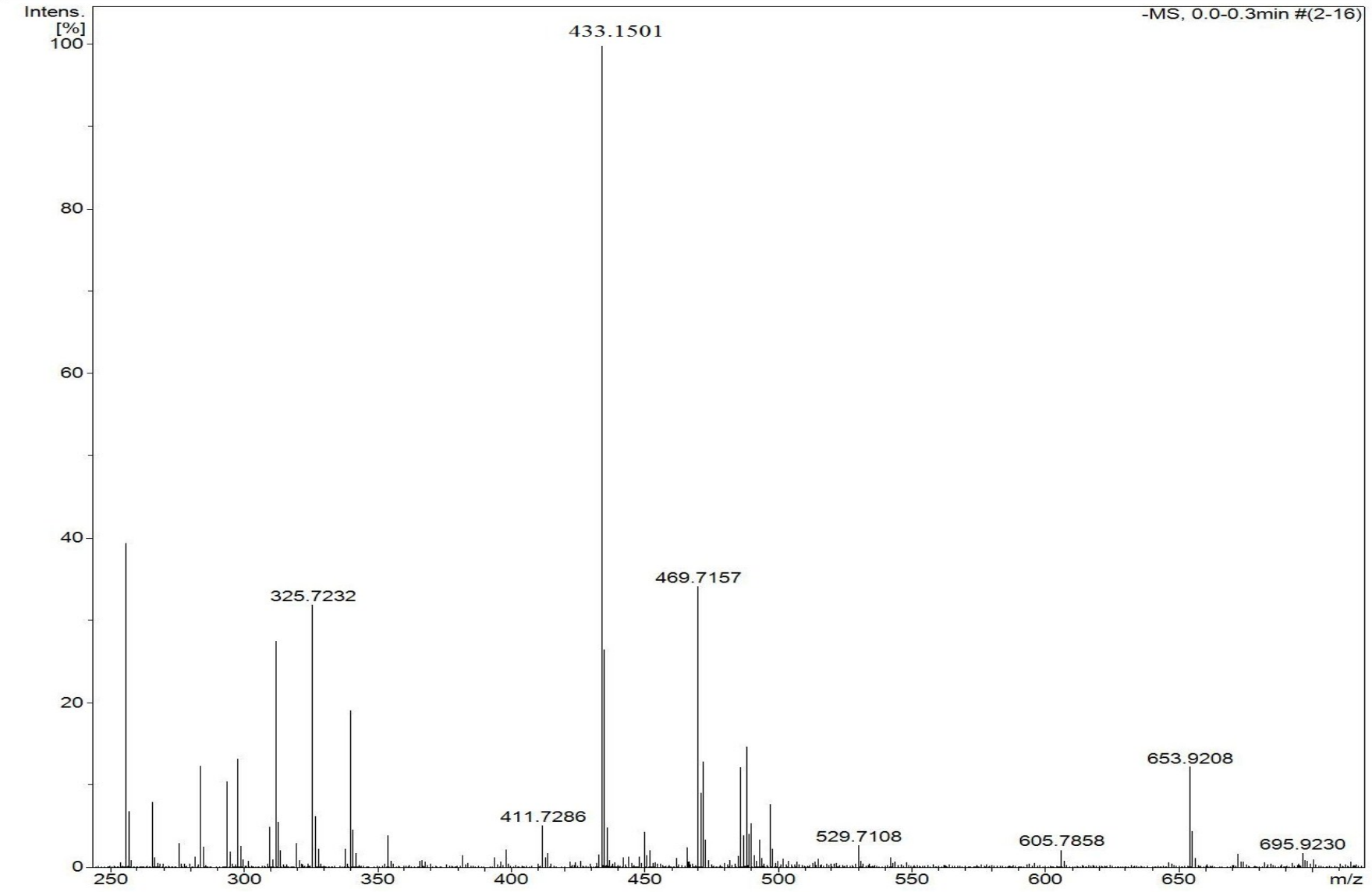
2-((2-Morpholinoethylamino)-3-(4'-nitrophenyl)furo[3,2-*c*]quinolin-4(5*H*)-one (5e).



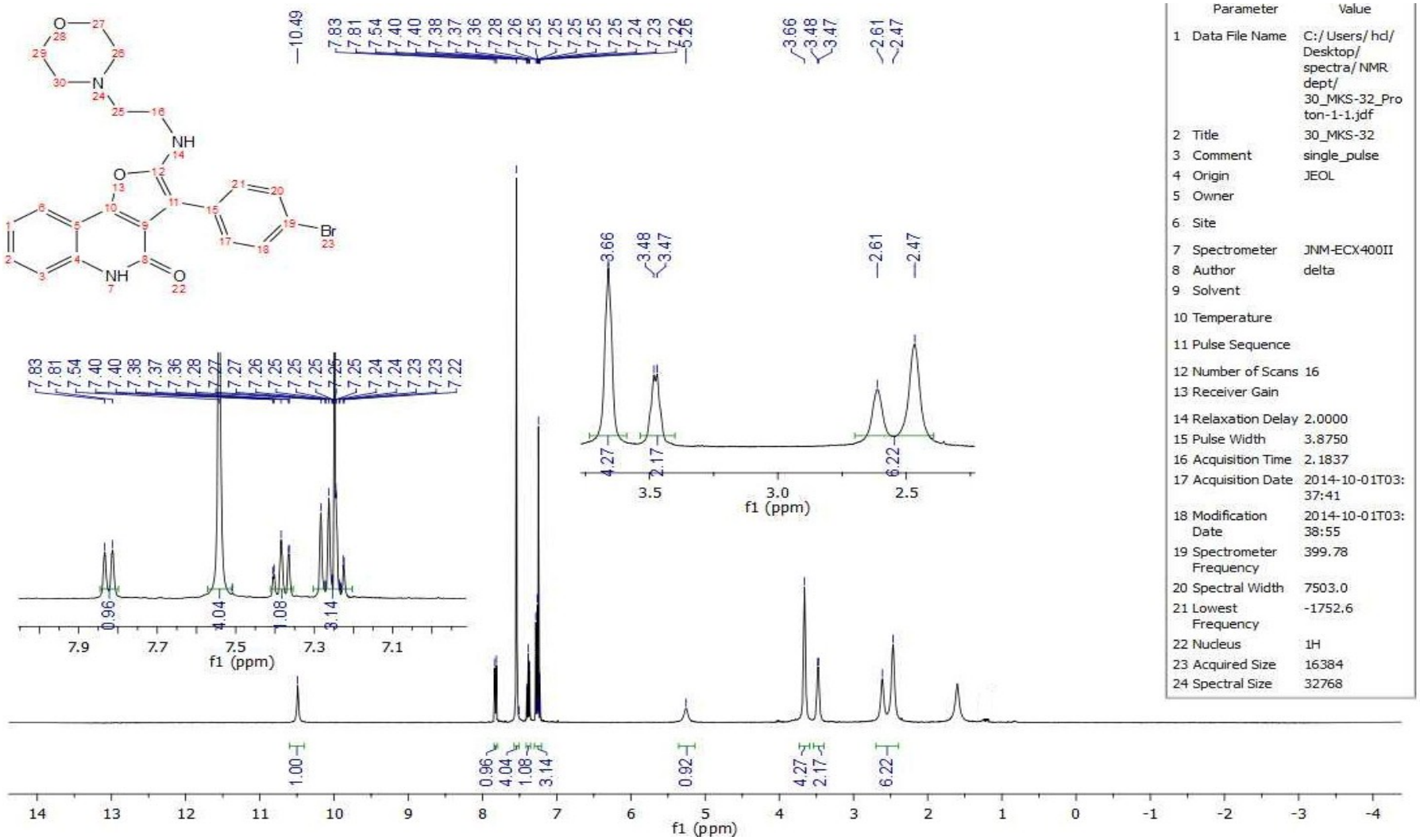
	Parameter	Value
1	Data File Name	H:/ JDX/ 16_MKSD-31_Proton-1-1 - Copy.jdf
2	Title	16_MKSD-31
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	JNM-ECX400II
8	Author	delta
9	Solvent	
10	Temperature	
11	Pulse Sequence	
12	Number of Scans	16
13	Receiver Gain	
14	Relaxation Delay	2.0000
15	Pulse Width	3.8750
16	Acquisition Time	2.1837
17	Acquisition Date	2014-10-16T16:35:00
18	Modification Date	2014-10-16T16:36:13
19	Spectrometer Frequency	399.78
20	Spectral Width	7503.0
21	Lowest Frequency	-1752.6
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

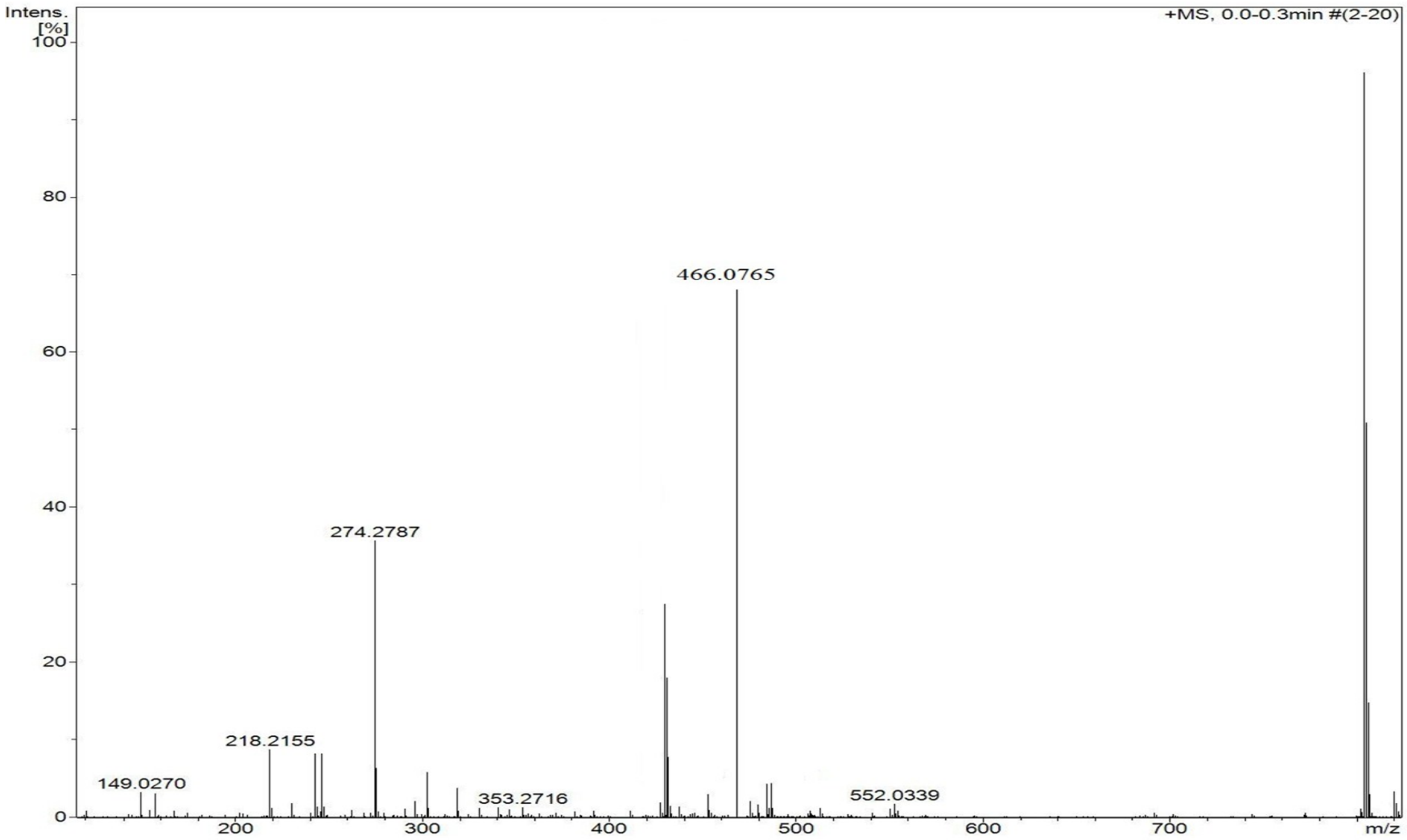


Parameter		Value
1	Data File Name	H:/mks-27-10-14/21_MKSM-31-DMSO_Carbon-1-2.jdf
2	Title	21_MKSM-31-DMSO
3	Comment	single pulse decoupled gated NOE
4	Origin	JEOL
5	Spectrometer	JNM-ECX400II
6	Author	delta
7	Pulse Sequence	
8	Number of Scans	10000
9	Receiver Gain	
10	Relaxation Delay	2.0000
11	Pulse Width	9.2500
12	Acquisition Time	1.0433
13	Acquisition Date	2014-10-21T19:30:58
14	Modification Date	2014-10-27T10:45:12
15	Spectrometer Frequency	100.53
16	Spectral Width	25124.3
17	Lowest Frequency	-2509.6
18	Nucleus	13C
19	Acquired Size	32768
20	Spectral Size	26214

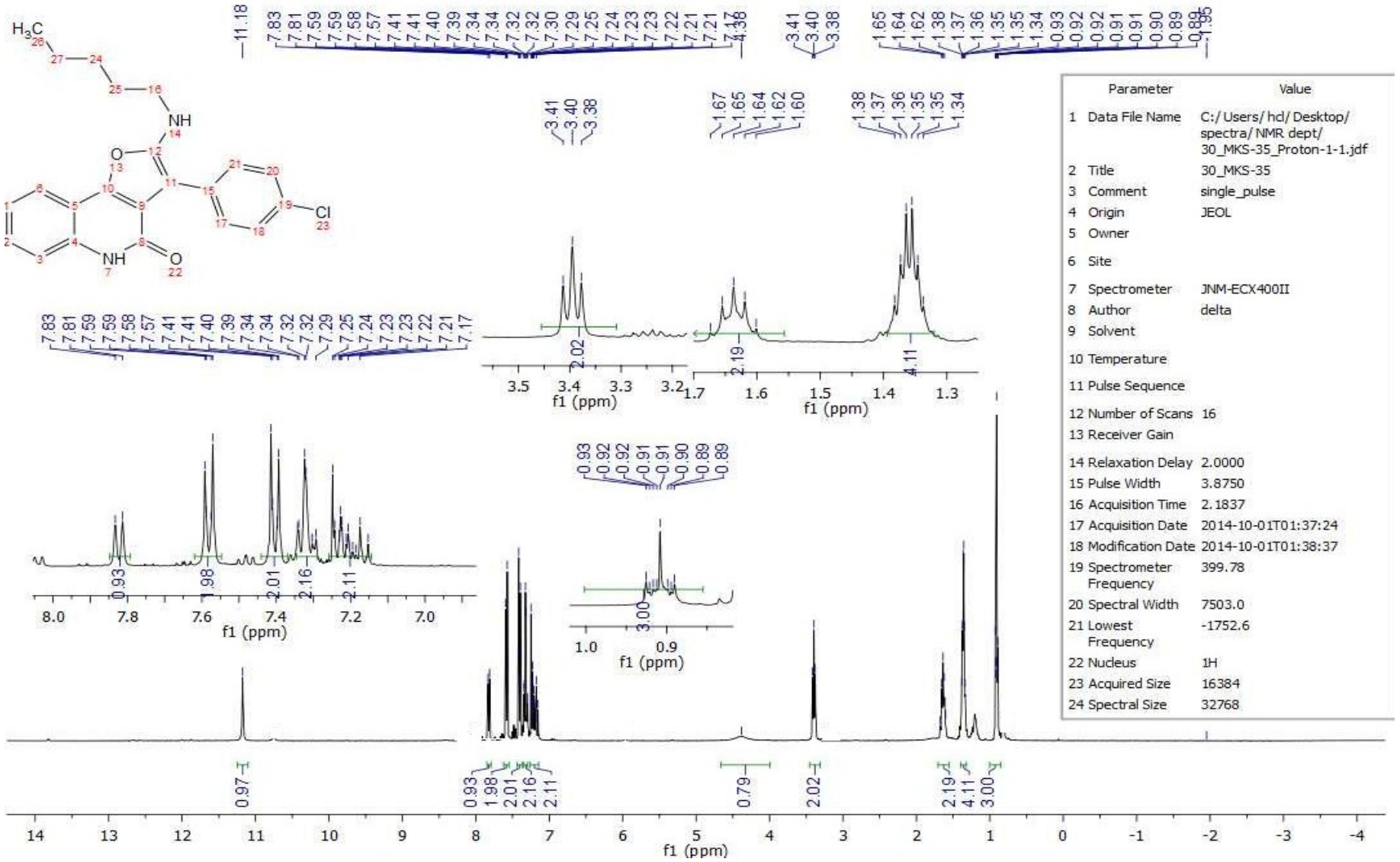

Intens.
[%]
-MS, 0.0-0.3min #(2-16)
433.1501
469.7157
325.7232
411.7286
529.7108
605.7858
653.9208
695.9230
100
80
60
40
20
0
250
300
350
400
450
500
550
600
650
m/z

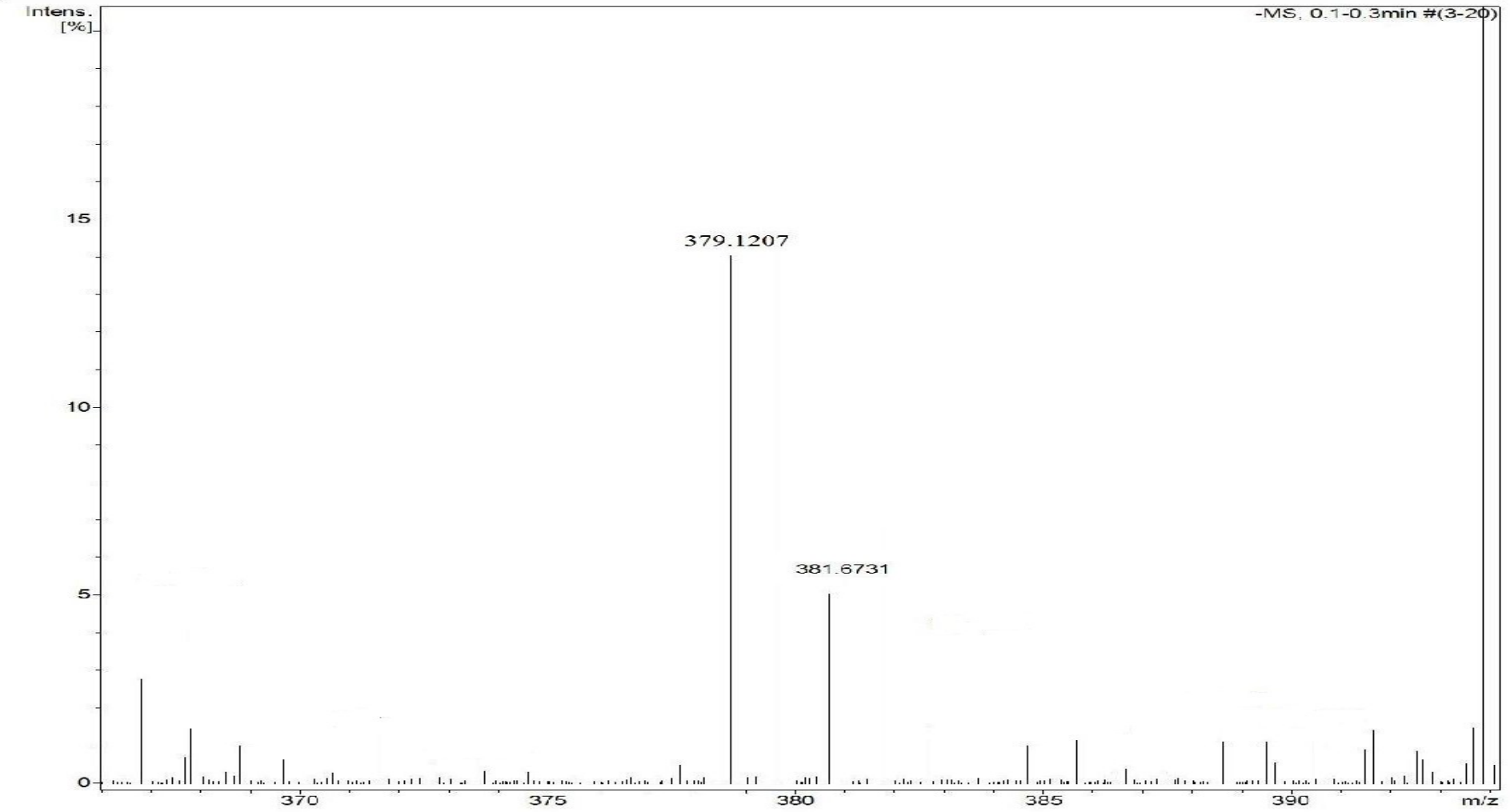
3-(4'-Bromophenyl)-2-((2-morpholinoethyl)amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5f).



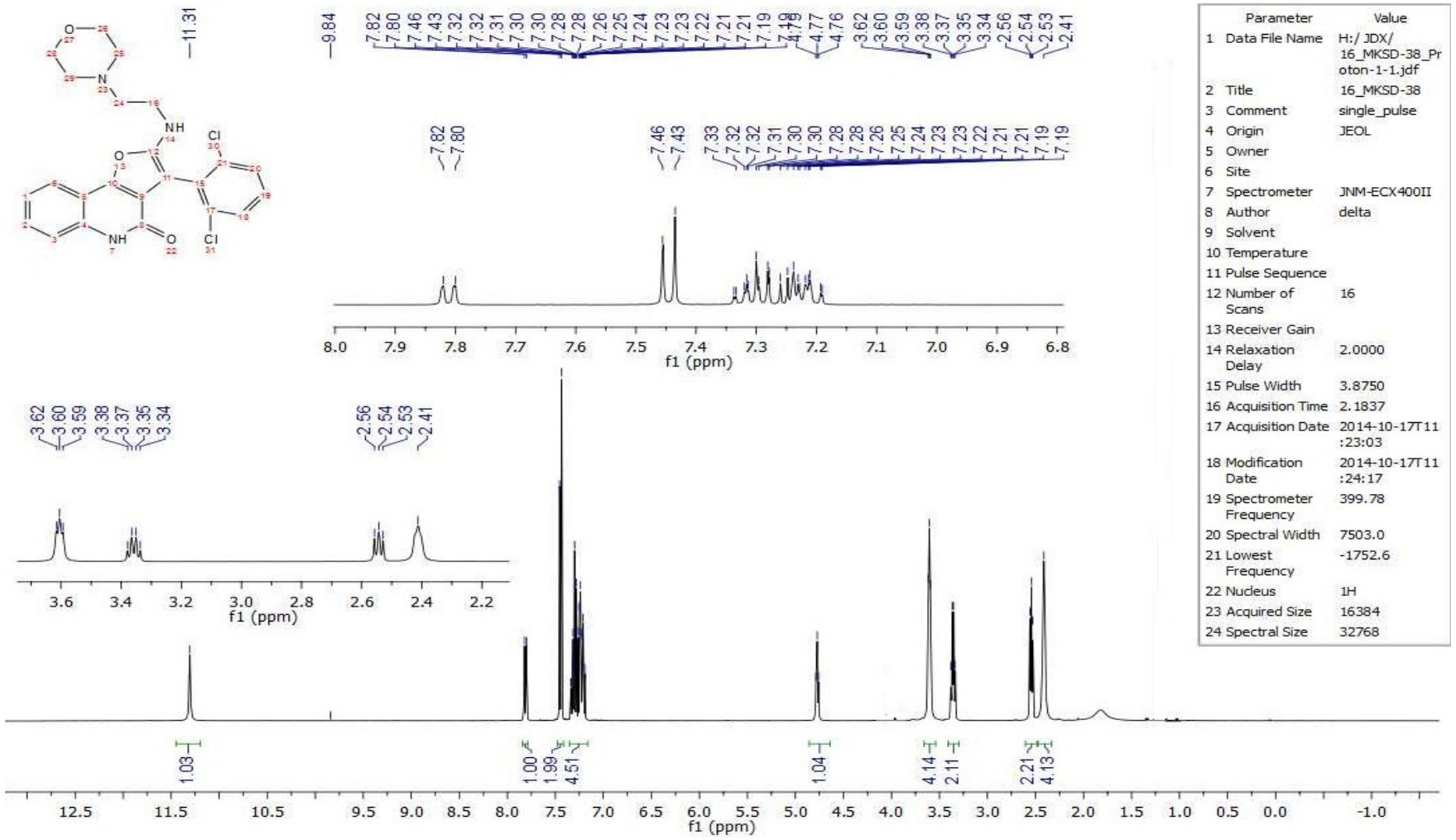

Intens.
[%]
+MS, 0.0-0.3min #(2-20)
100
80
60
40
20
0
466.0765
274.2787
218.2155
149.0270
353.2716
552.0339
200
300
400
500
600
700
m/z

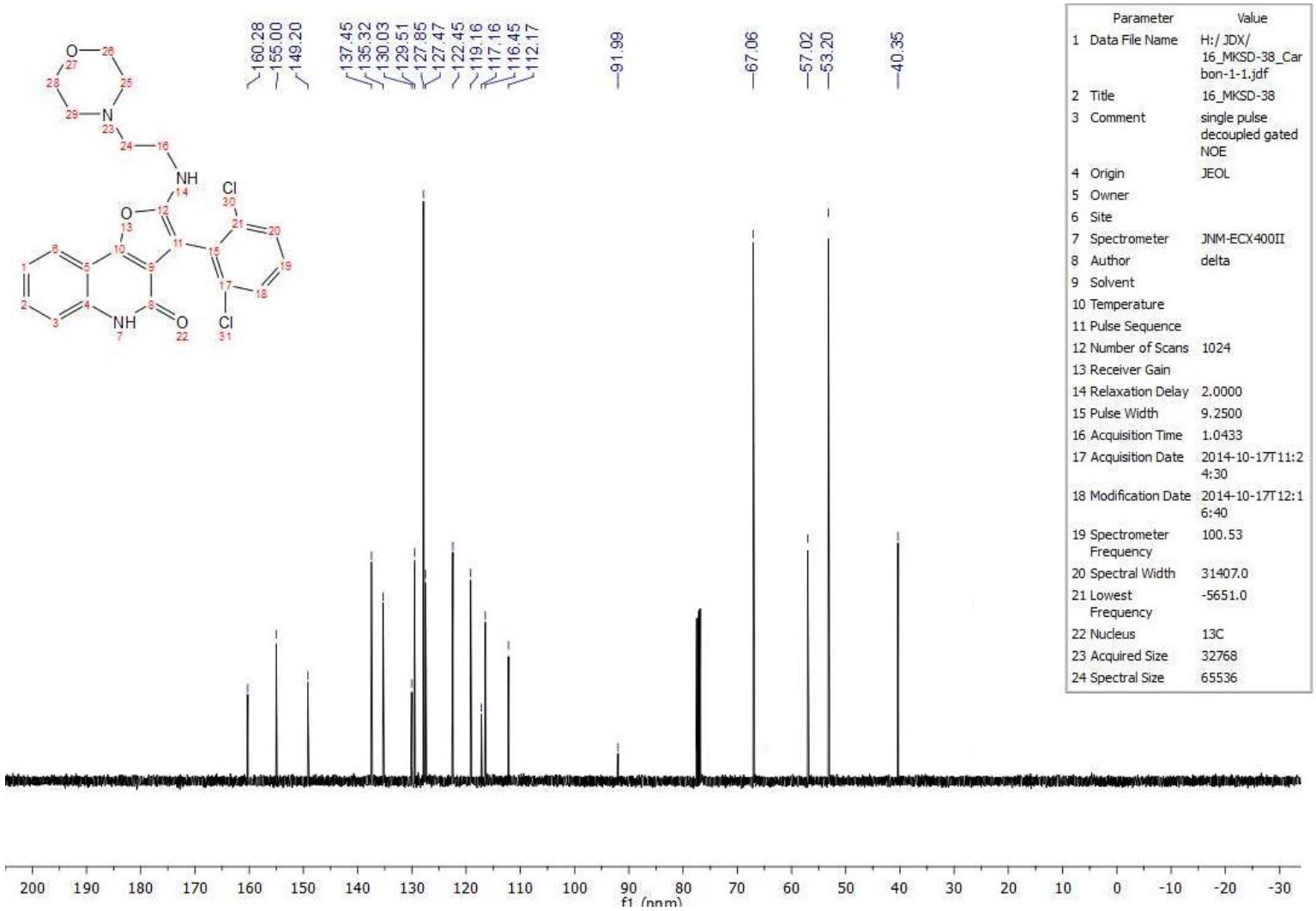
3-(4'-Chlorophenyl)-2-(pentylamino)furo[3,2-*c*]quinolin-4(5*H*)-one (5g).



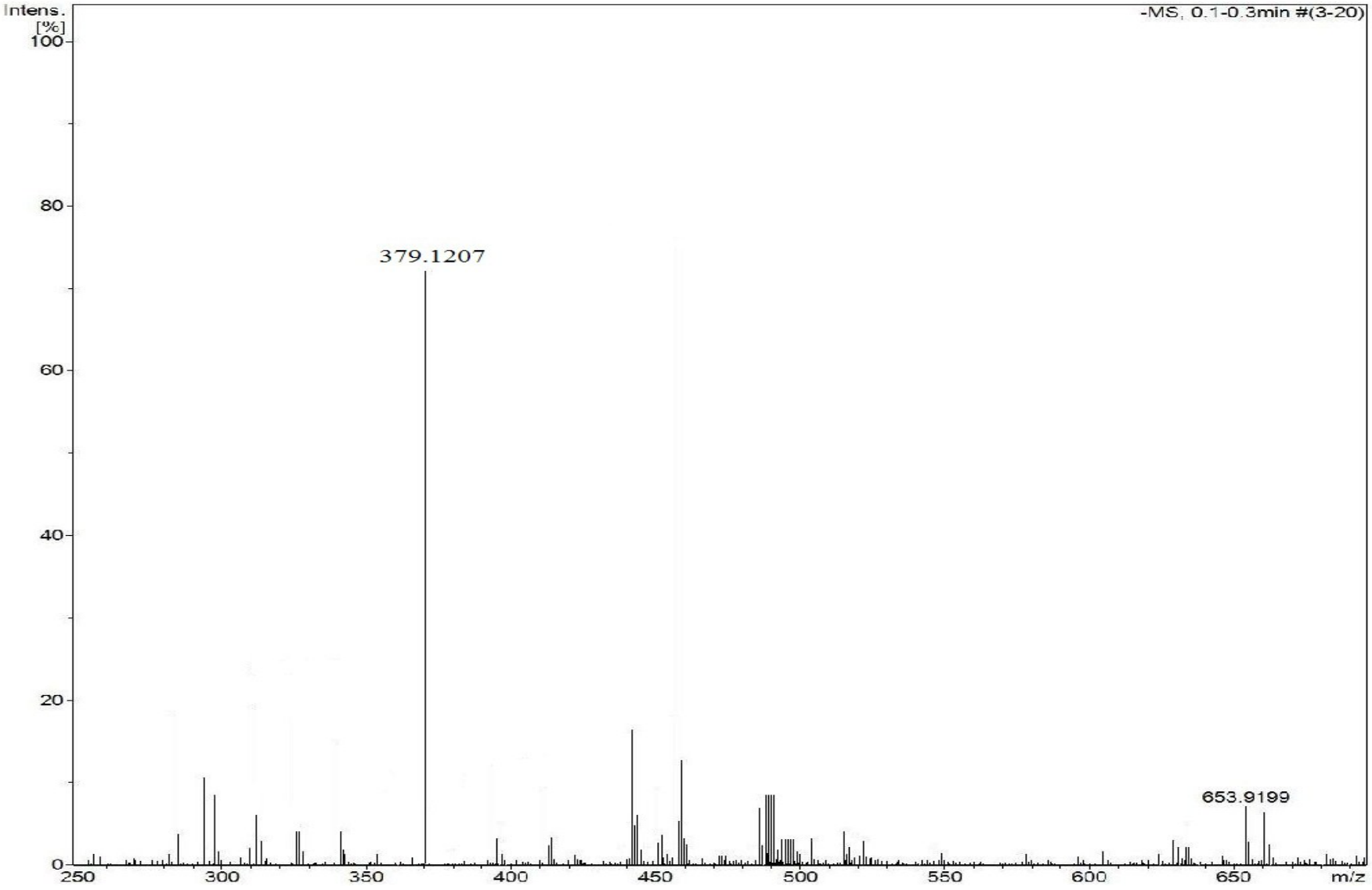

Intens.
[%]
-MS, 0.1-0.3min #(3-20)
379.1207
381.6731
15
10
5
0
370
375
380
385
390
m/z

3-(2',6'-Dichlorophenyl)-2-((2-morpholinoethyl)amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5h).

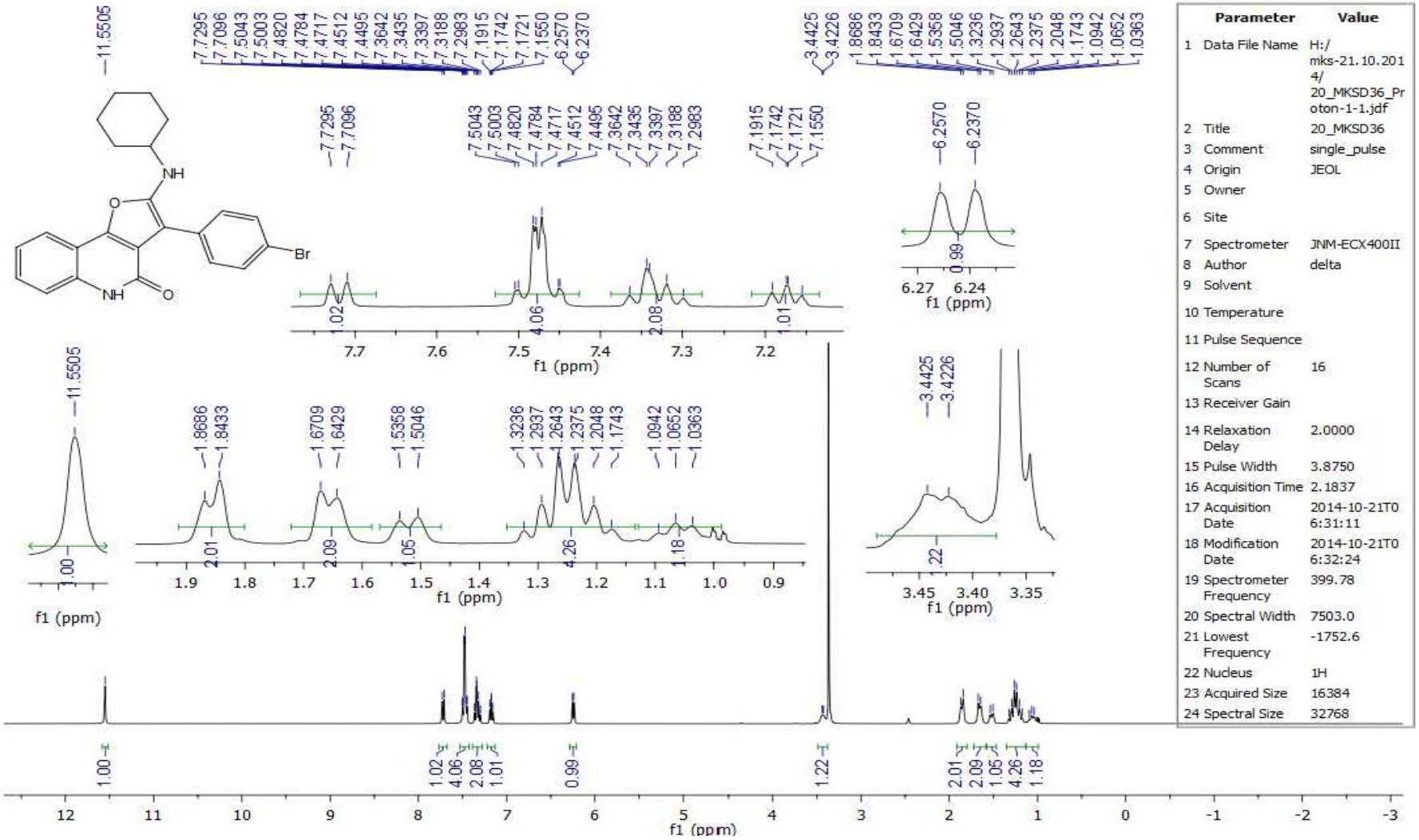


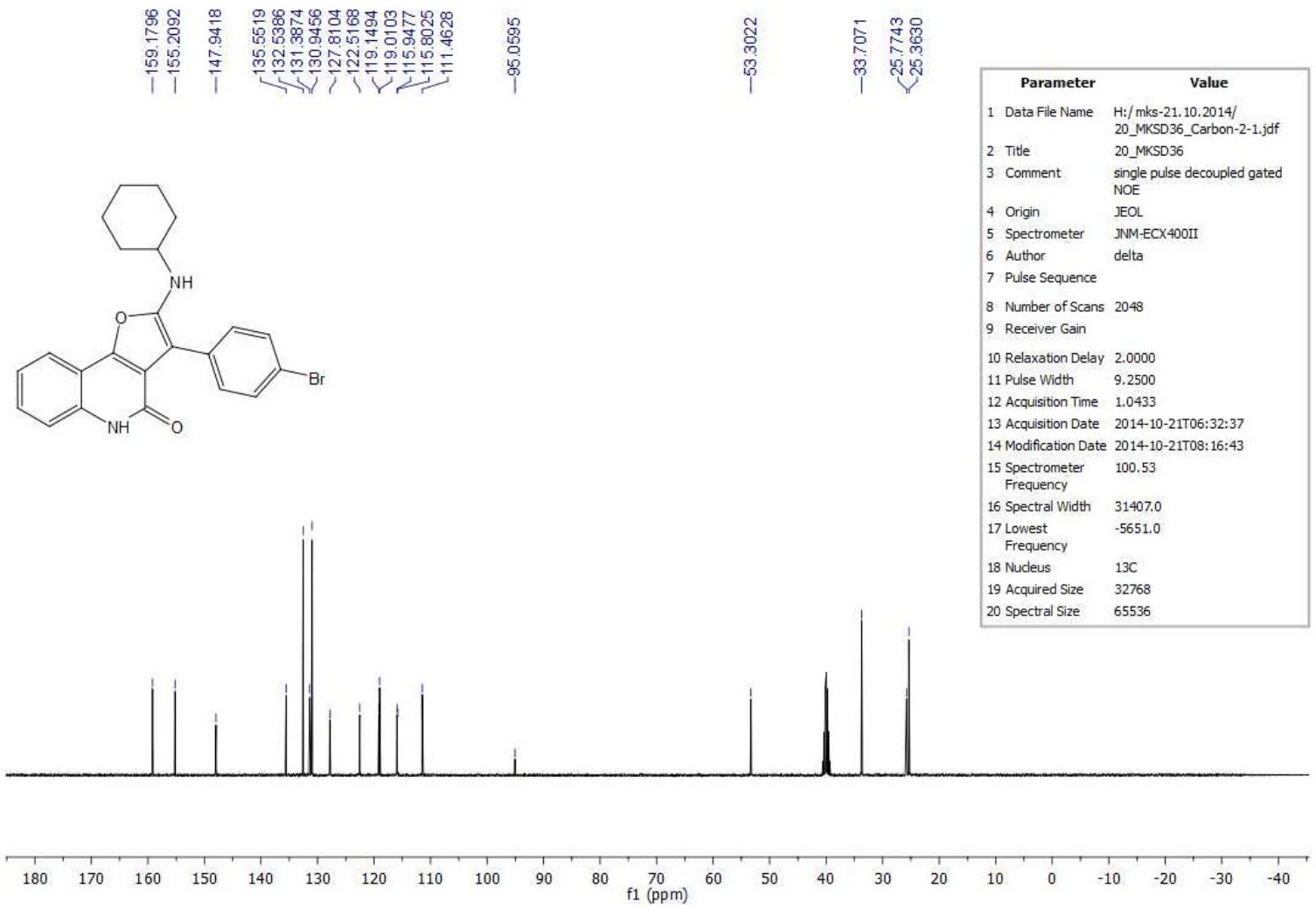


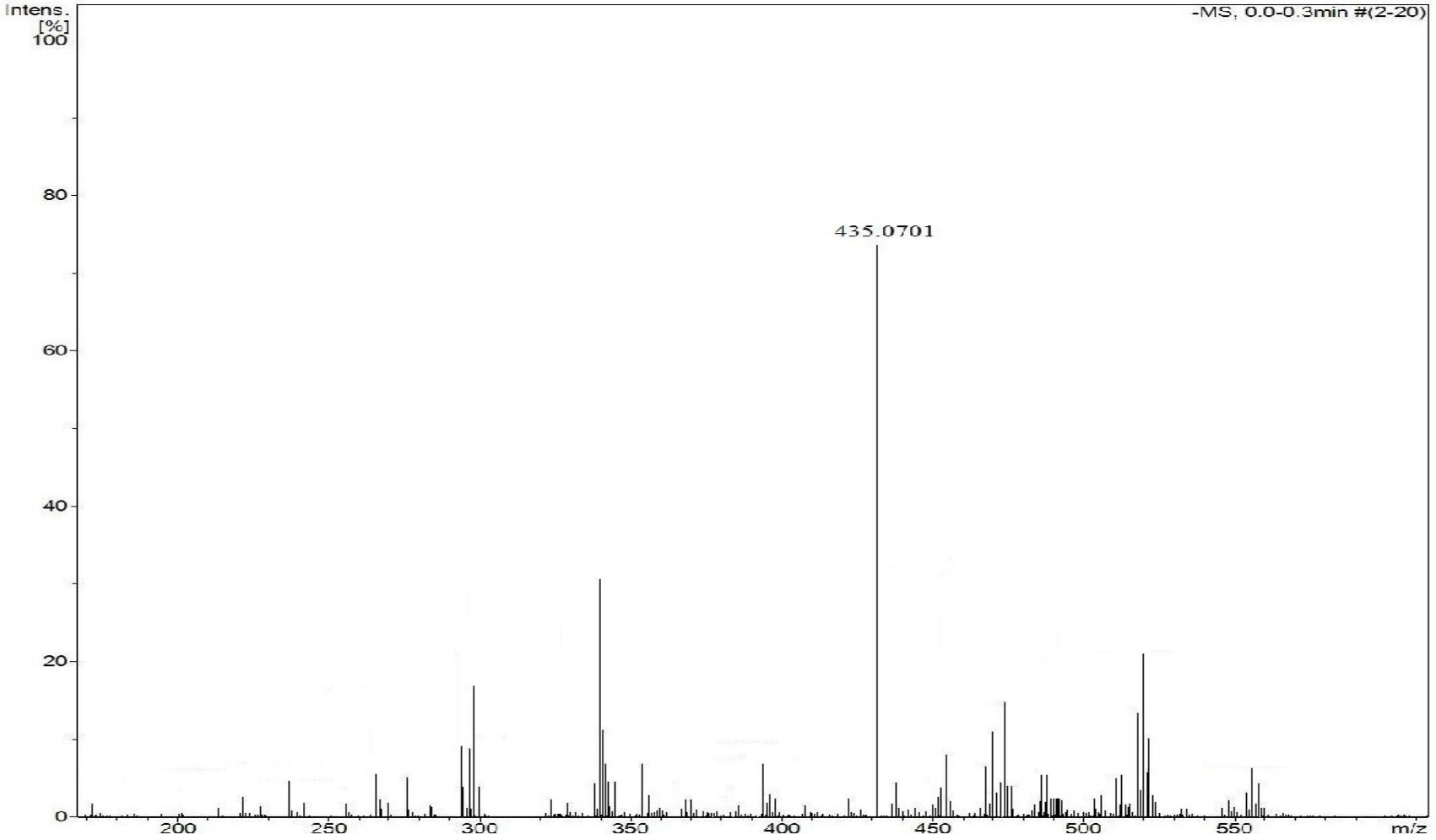
	Parameter	Value
1	Data File Name	H:/ JDX/ 16_MKSD-38_Carbon-1-1.jdf
2	Title	16_MKSD-38
3	Comment	single pulse decoupled gated NOE
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	JNM-ECX400II
8	Author	delta
9	Solvent	
10	Temperature	
11	Pulse Sequence	
12	Number of Scans	1024
13	Receiver Gain	
14	Relaxation Delay	2.0000
15	Pulse Width	9.2500
16	Acquisition Time	1.0433
17	Acquisition Date	2014-10-17T11:24:30
18	Modification Date	2014-10-17T12:16:40
19	Spectrometer Frequency	100.53
20	Spectral Width	31407.0
21	Lowest Frequency	-5651.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536


Intens.
[%]
-MS, 0.1-0.3min #(3-20)
100
80
60
40
20
0
379.1207
653.9199
250
300
350
400
450
500
550
600
650
m/z

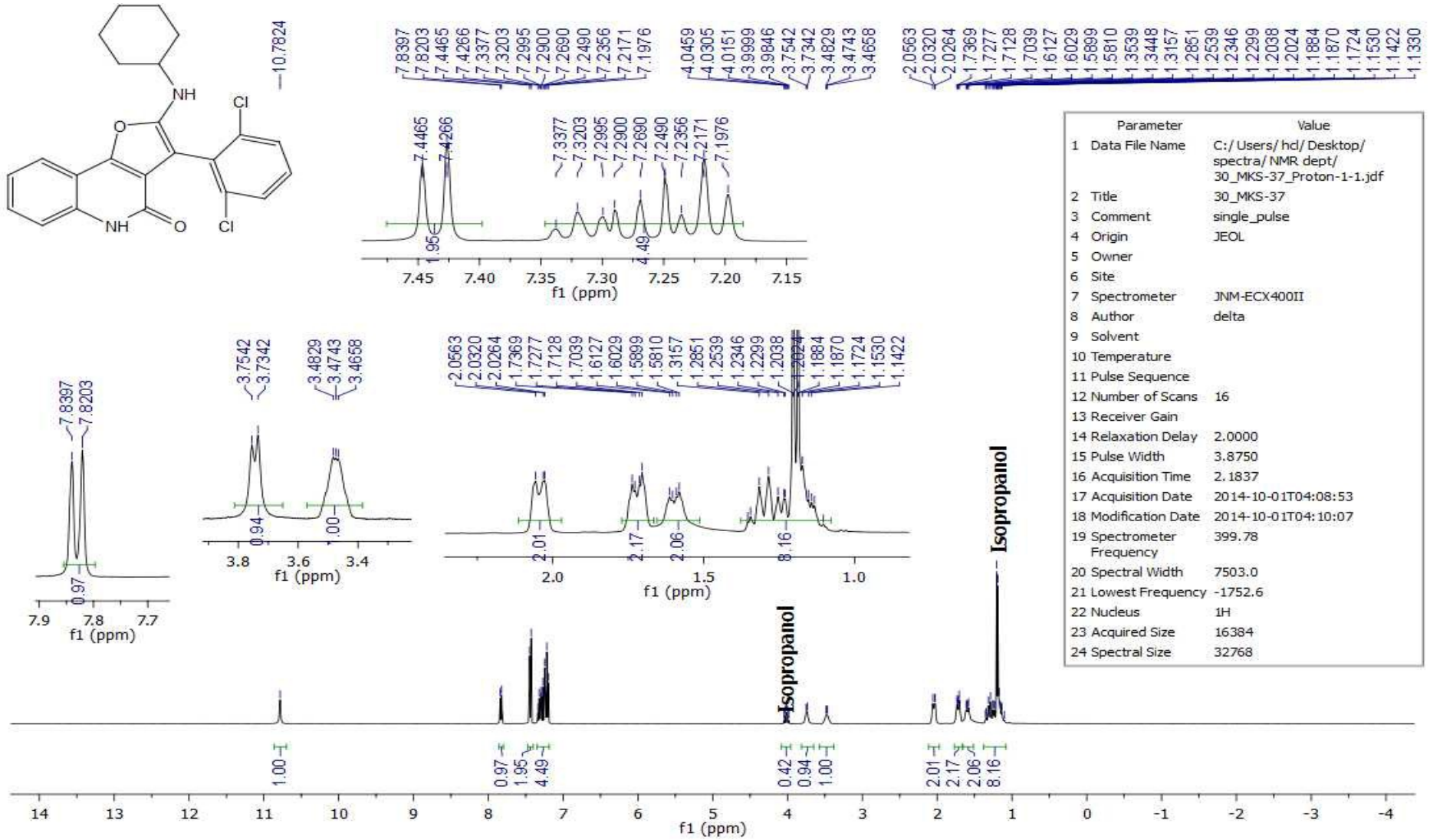
3-(4'-Bromophenyl)-2-(cyclohexylamino)furo[3,2-*c*]quinolin-4(5*H*)-one (5i).



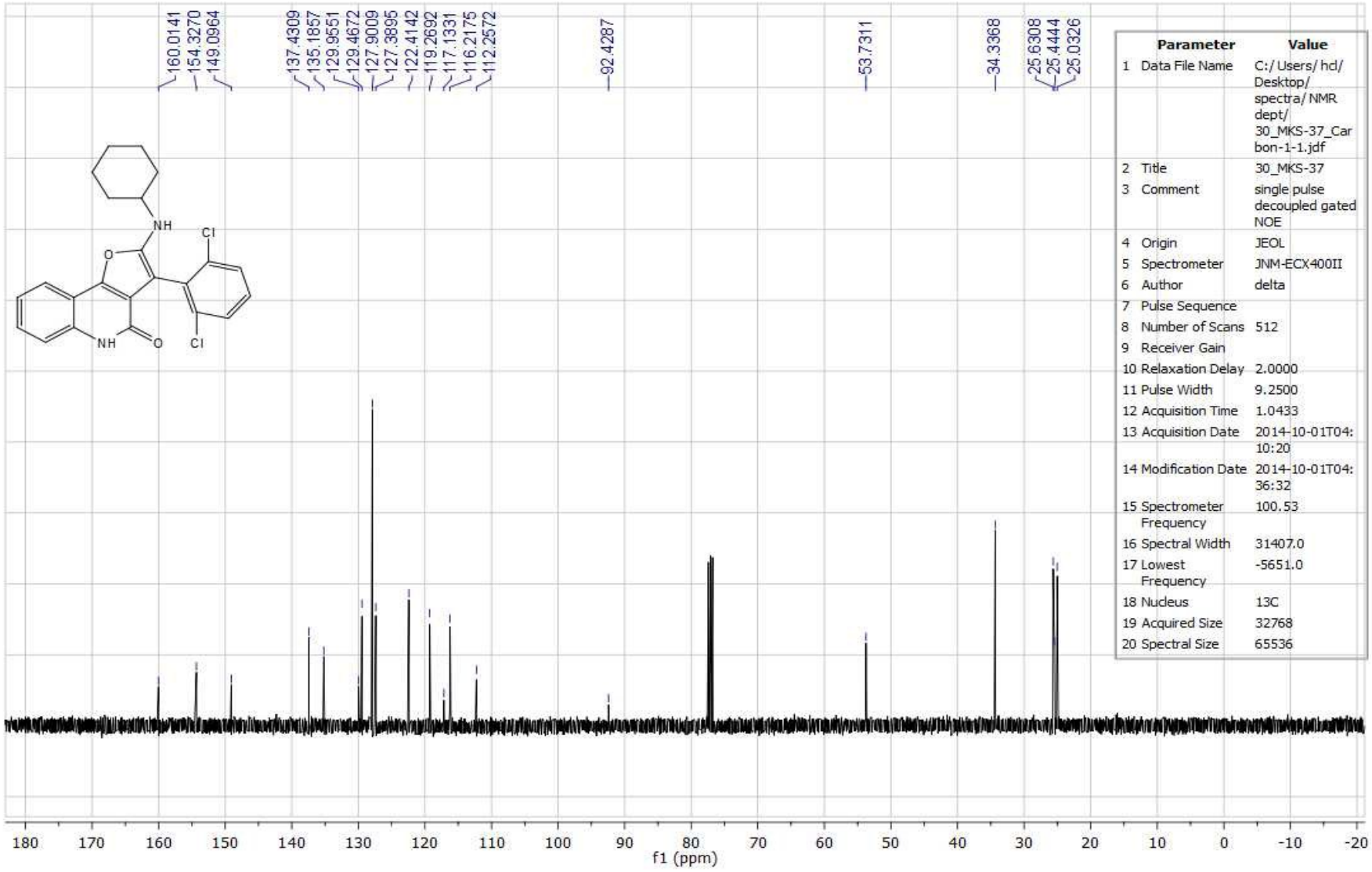

159.1796
155.2092
147.9418
135.5519
132.5386
131.3874
130.9456
127.8104
122.5168
119.1494
119.0103
115.9477
115.8025
111.4628
95.0595
53.3022
33.7071
25.7743
25.3630
NH
O
Br
NH
O
Parameter
Value
1 Data File Name
H:/ mks-21.10.2014/ 20_MKSD36_Carbon-2-1.jdf
2 Title
20_MKSD36
3 Comment
single pulse decoupled gated NOE
4 Origin
JEOL
5 Spectrometer
JNM-ECX400II
6 Author
delta
7 Pulse Sequence
8 Number of Scans
2048
9 Receiver Gain
10 Relaxation Delay
2.0000
11 Pulse Width
9.2500
12 Acquisition Time
1.0433
13 Acquisition Date
2014-10-21T06:32:37
14 Modification Date
2014-10-21T08:16:43
15 Spectrometer Frequency
100.53
16 Spectral Width
31407.0
17 Lowest Frequency
-5651.0
18 Nucleus
13C
19 Acquired Size
32768
20 Spectral Size
65536
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)

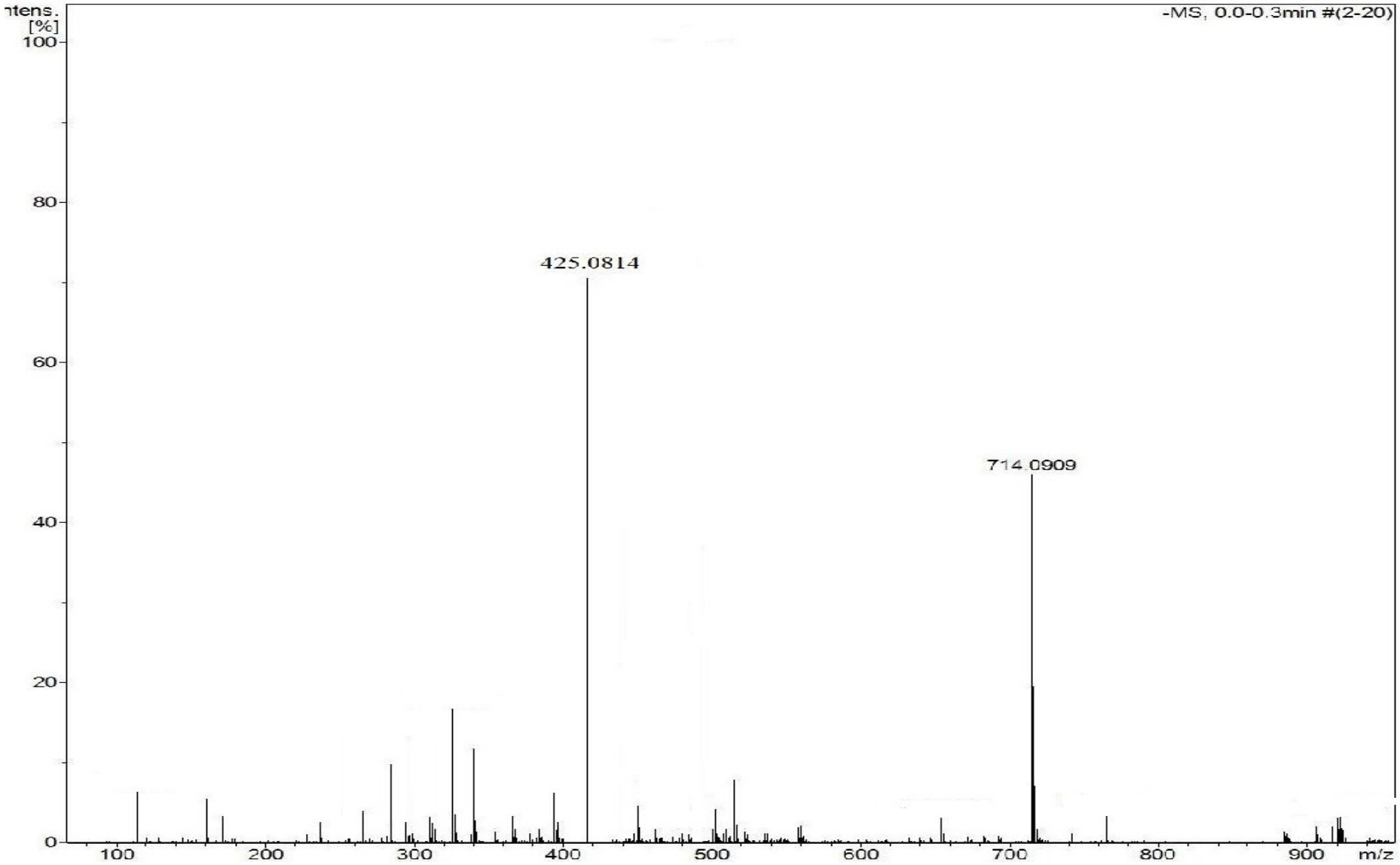

Intens.
[%]
100
80
60
40
20
0
-MS, 0.0-0.3min #(2-20)
435.0701
200
250
300
350
400
450
500
550
m/z

2-(Cyclohexylamino)3-(2',6'-dichlorophenyl)furo[3,2-*c*]quinolin-4(5*H*)-one (5j).

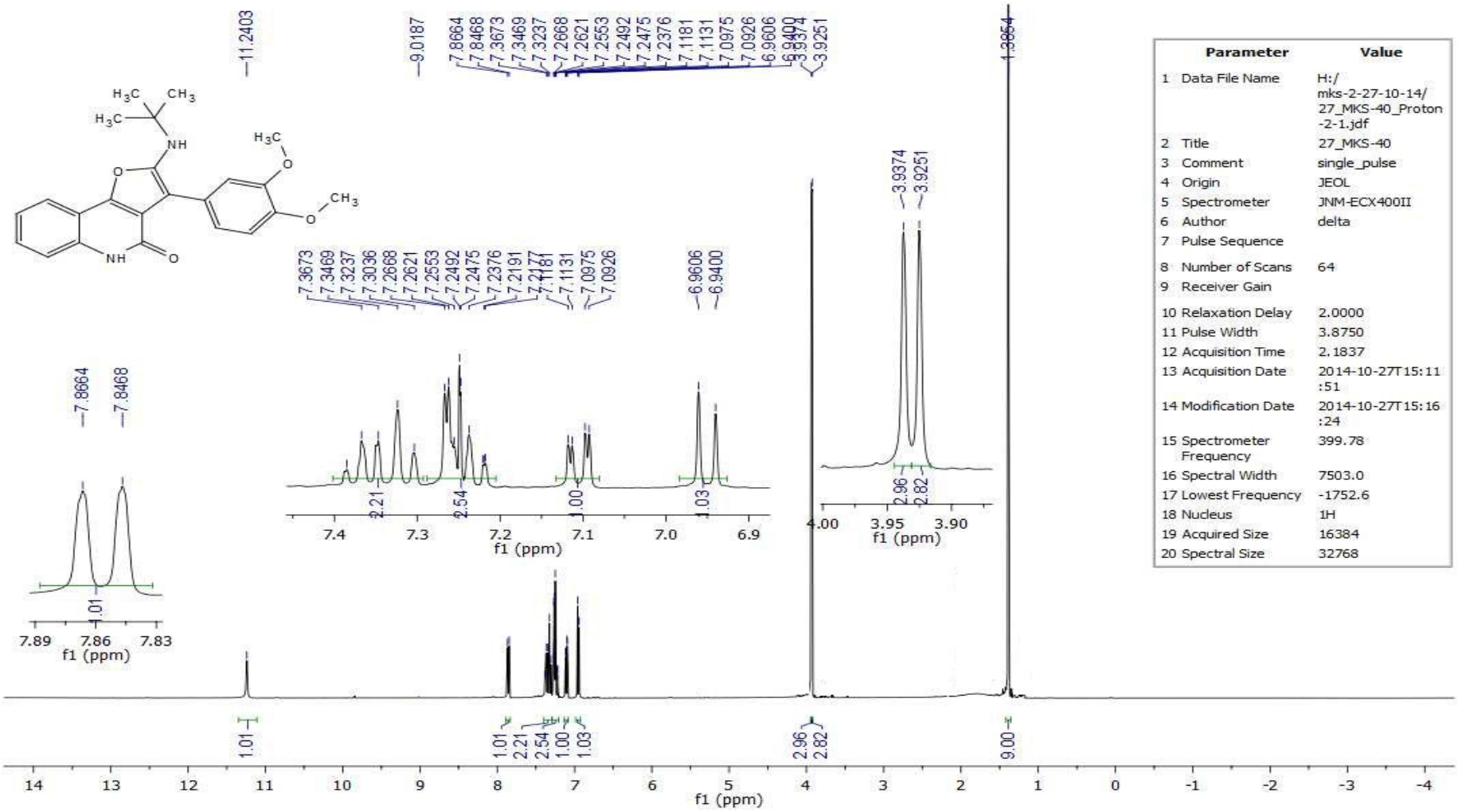


	Parameter	Value
1	Data File Name	C:/Users/hcl/Desktop/spectra/NMR dept/30_MKS-37_Proton-1-1.jdf
2	Title	30_MKS-37
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	JNM-ECX400II
8	Author	delta
9	Solvent	
10	Temperature	
11	Pulse Sequence	
12	Number of Scans	16
13	Receiver Gain	
14	Relaxation Delay	2.0000
15	Pulse Width	3.8750
16	Acquisition Time	2.1837
17	Acquisition Date	2014-10-01T04:08:53
18	Modification Date	2014-10-01T04:10:07
19	Spectrometer Frequency	399.78
20	Spectral Width	7503.0
21	Lowest Frequency	-1752.6
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

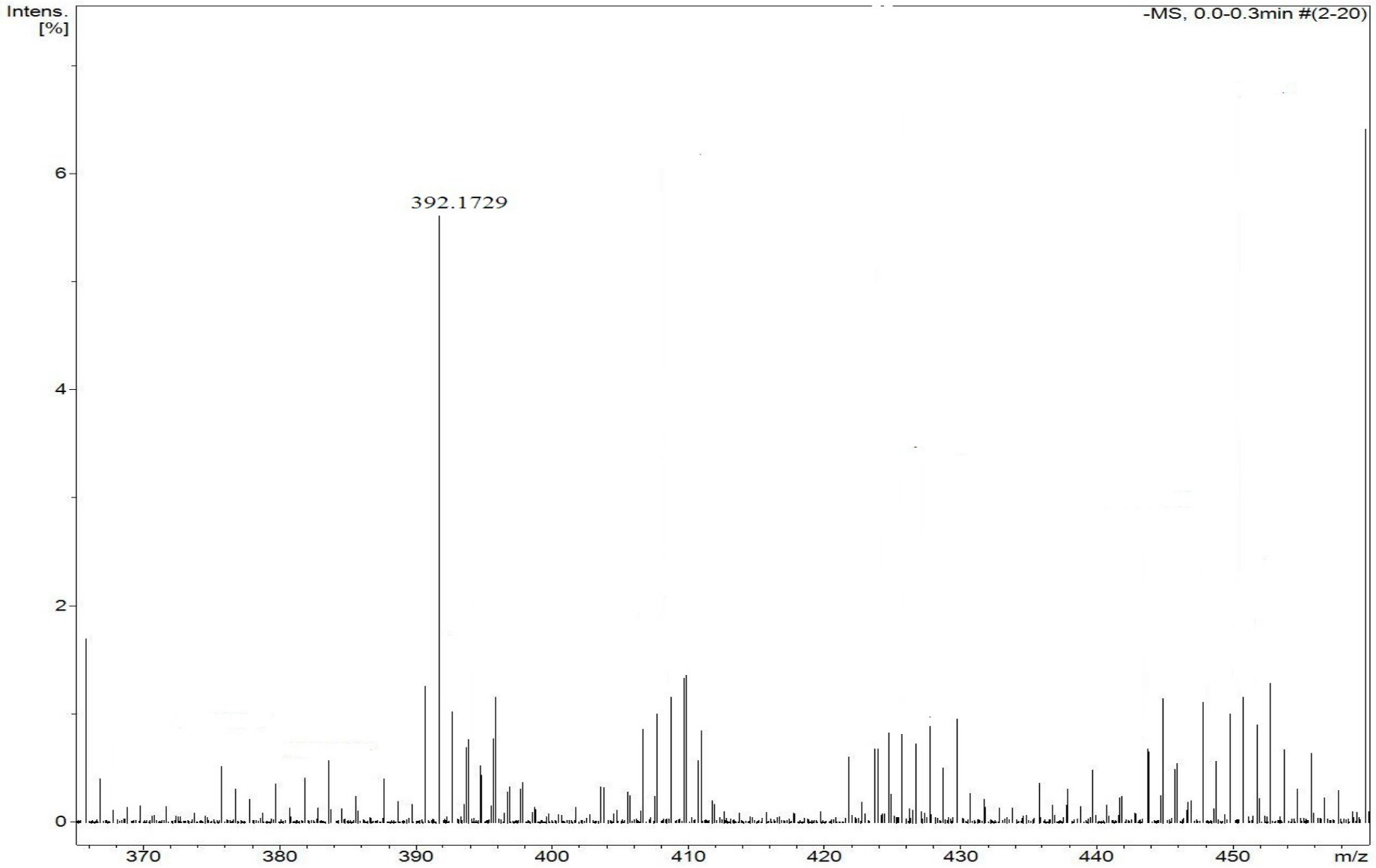

160.0141
154.3270
149.0964
137.4309
135.1857
129.9551
129.4672
127.9009
127.3895
122.4142
119.2692
117.1331
116.2175
112.2572
92.4287
53.7311
34.3368
25.6308
25.4444
25.0326
NH
O
Cl
NH
O
Cl
Parameter Value
1 Data File Name C:/Users/hcl/Desktop/spectra/NMR dept/30_MKS-37_Carbon-1-1.jdf
2 Title 30_MKS-37
3 Comment single pulse decoupled gated NOE
4 Origin JEOL
5 Spectrometer JNM-ECX400II
6 Author delta
7 Pulse Sequence
8 Number of Scans 512
9 Receiver Gain
10 Relaxation Delay 2.0000
11 Pulse Width 9.2500
12 Acquisition Time 1.0433
13 Acquisition Date 2014-10-01T04:10:20
14 Modification Date 2014-10-01T04:36:32
15 Spectrometer Frequency 100.53
16 Spectral Width 31407.0
17 Lowest Frequency -5651.0
18 Nucleus 13C
19 Acquired Size 32768
20 Spectral Size 65536
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


ntens.
[%]
-MS, 0.0-0.3min #(2-20)
425.0814
714.0909
100
80
60
40
20
0
100
200
300
400
500
600
700
800
900
m/z

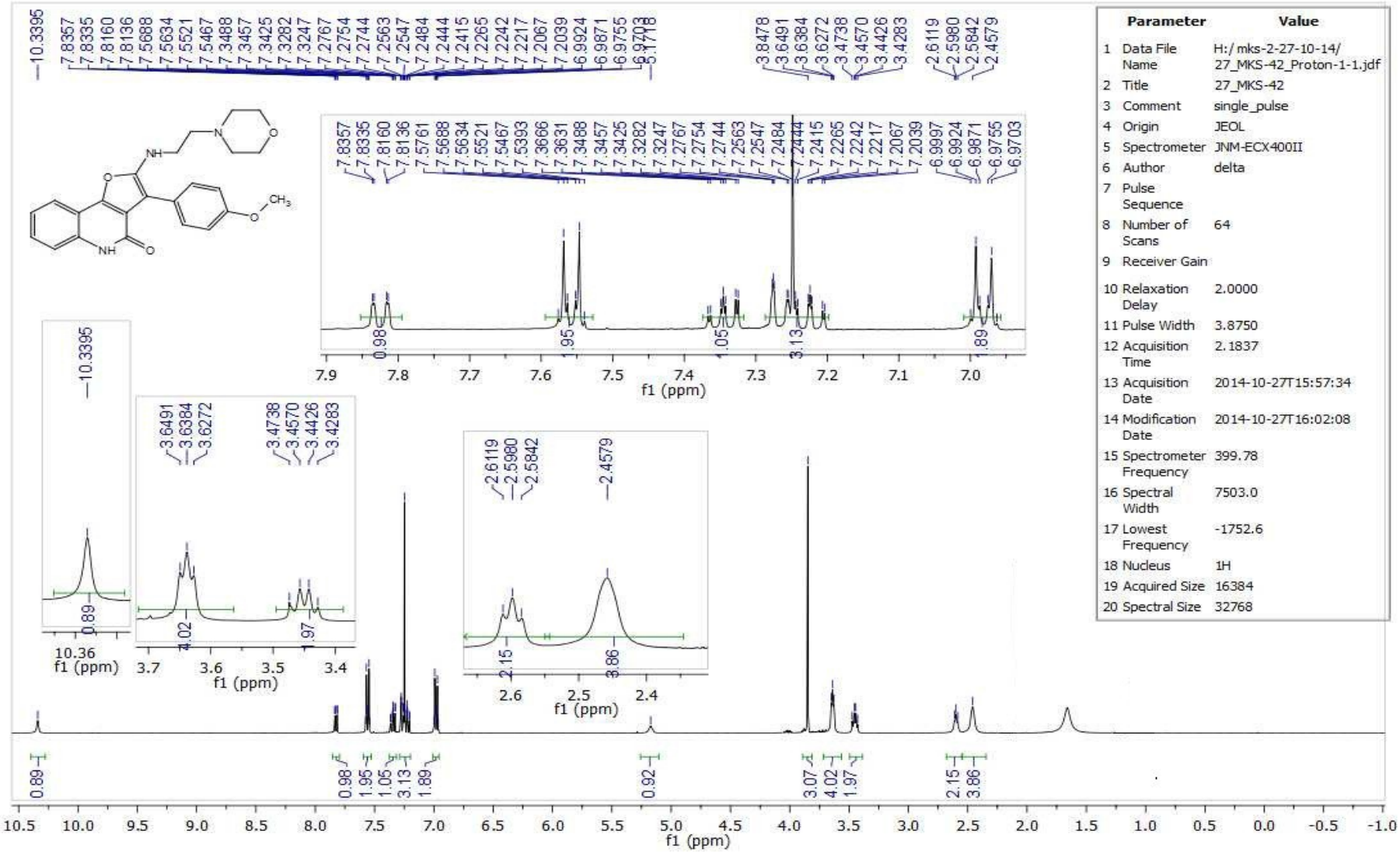
2-(*tert*-Butylamino)-3-(3',4'-dimethoxyphenyl)furo[3,2-*c*]quinolin-4(5*H*)-one (5k).

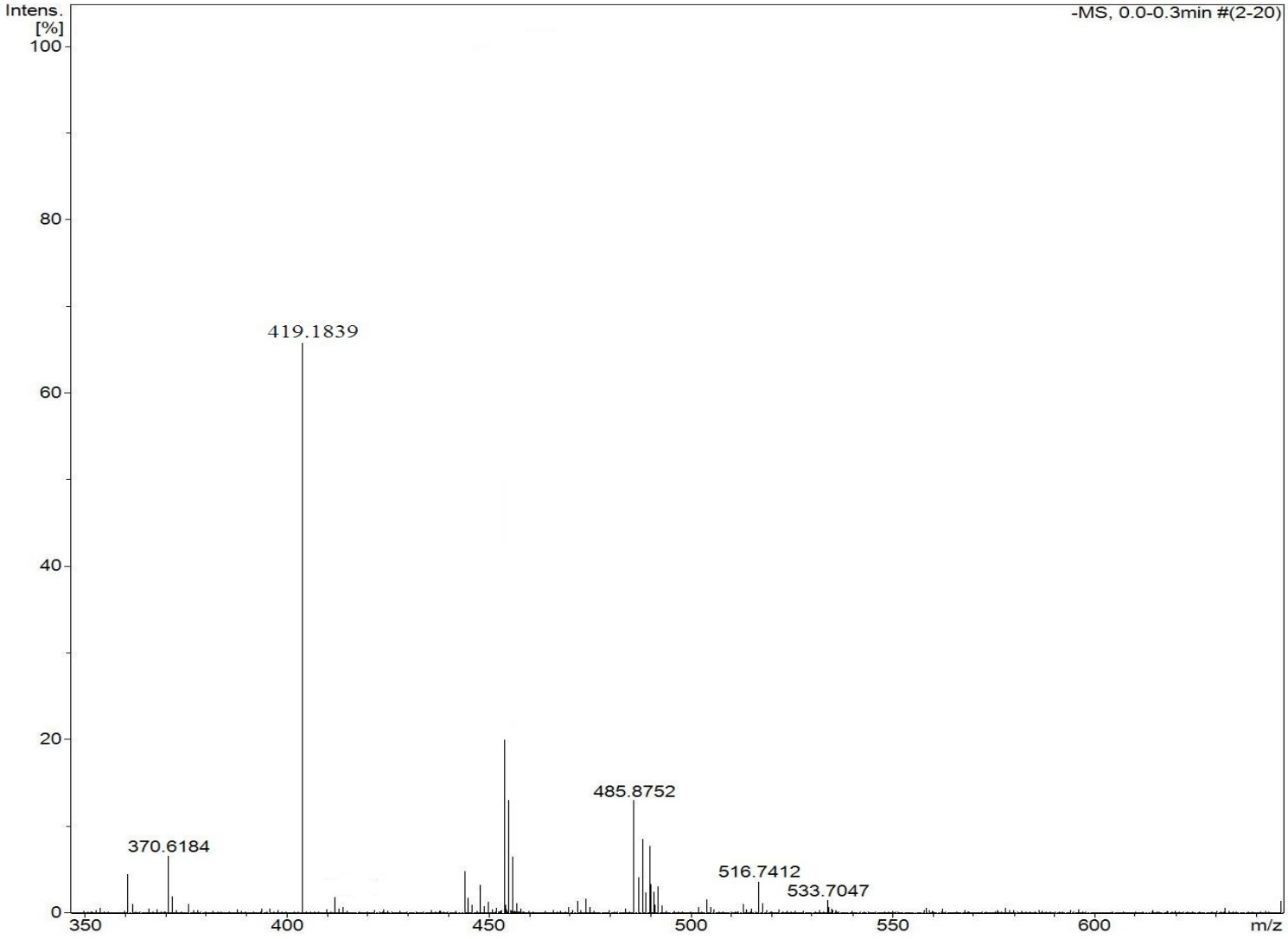


	Parameter	Value
1	Data File Name	H:/mks-2-27-10-14/27_MKS-40_Proton-2-1.jdf
2	Title	27_MKS-40
3	Comment	single_pulse
4	Origin	JEOL
5	Spectrometer	JNM-ECX400II
6	Author	delta
7	Pulse Sequence	
8	Number of Scans	64
9	Receiver Gain	
10	Relaxation Delay	2.0000
11	Pulse Width	3.8750
12	Acquisition Time	2.1837
13	Acquisition Date	2014-10-27T15:11:51
14	Modification Date	2014-10-27T15:16:24
15	Spectrometer Frequency	399.78
16	Spectral Width	7503.0
17	Lowest Frequency	-1752.6
18	Nucleus	1H
19	Acquired Size	16384
20	Spectral Size	32768


Intens.
[%]
-MS, 0.0-0.3min #(2-20)
392.1729
6
4
2
0
370
380
390
400
410
420
430
440
450
m/z

3-(4'-methoxyphenyl)-2-(2-morpholinoethyl)amino)furo[3,2-*c*]quinolin-4(5*H*)-one (5l).




Intens.
[%]
-MS, 0.0-0.3min #(2-20)
100
80
60
40
20
0
419.1839
485.8752
370.6184
516.7412
533.7047
350
400
450
500
550
600
m/z

Virtual Screening

To explore the role of these natural products like scaffolds and to predict their biological spectrum, we performed an "*in-silico* target fishing experiment" using ChemMapper server.[16]In target navigator SHAFTS based 3D similarities method was selected to explore Protein Data Bank (PDB) with similarity threshold 1.2. The top ten scorers are included in the Table S1 and S2.

The prevailed scaffold benzo[*f*]furo[3,2-*c*]chromen-4-(5*H*)-ones are predicted to be the potential binder of Cyclin-dependent Kinase 2 (CDK2, rank 1) involves in the regulation of cell cycle, Estrogen receptor beta (ESR2, rank 2) a nuclear hormone receptor binds with estrogen, serine/threonine–protein kinase (check 1, rank 3) require for checkpoint mediated cell cycle arrest and activation of DNA repair, Higher affinity *c*AMP-specific 3',5'-cyclic phosphodiesterase 7A (PDE7A, rank 5) hydrolyzes the secondary messenger *c*AMP and mitogen- activated protein kinase (MAPK10, rank 7) involves in the various processsuch as neuronal proliferation, differentiation, migration and programmed cell death (Table S1).

Table S1. Potential biological targets for the benzo[*f*]furo[3,2-*c*]naphthochromen-4-(5*H*)-ones

Target Name	Species	Score	Rank
Cell division Protein Kinase 2	*Homo sapiens*	1.0	1
Estrogen receptor beta	*Homo sapiens*	0.64	2
Serine/ Threonine protein kinase Chk1	*Homo sapiens*	0.315	3
PDE7A catalytic domain	*Homo sapiens*	0.309	4
cAMP and cAMP- inhibited cGMP 3,5-	Not available	0.304	5

cyclic phosphodiesterase 10A			
Mitogen-activated protein kinase 10	*Homo sapiens*	0.297	6
Transcriptional regulatory repressor protein (TETR-family) ETHR	*Mycobacterium* tuberculosis	0.296	7
PDK-1	*Homo sapiens*	0.296	7
Dipeptidyl peptidase 4 soluble form	*Homo sapiens*	0.293	8
Isoflavone o-methyl-transferase	*Medicago sativa*	0.29	9
NAD(P)H dehydrogenase [quinone] 1	*Homo sapiens*	0.289	10
p-38 Map kinase	*Homo sapiens*	0.289	10
Tyrosine-protein kinase Lck	*Homo Sapiens*	0.289	10

In our investigation,furo[3,2-*c*]quinolin-4-(5*H*)-ones have been shown to be the potential inhibitors of Biotin-Carboxylase (BC, rank 1), an essential component of acetyl Co enzyme A Carboxylase, Hematopoietic prostaglandin D synthase (HPGDS, rank 2),modulator of platelet aggregation, Serine/ Threonine- Protein Kinase chk1 (Check 1, rank 3) required for checkpoint mediated cell cycle arrest and activation of DNA repair, trankyrase (TNKS2, rank 6) involved in various processes such as Wnt signaling pathway, Telomere length and vesicle trafficking. In conclusion, this primary investigation suggested the potential role of these scaffolds in hypolipidemic, anticoagulation and cancer chemotherapeutic domains (Table S2).

Table S2. Potential biological targets for the furo[3,2-*c*]quinolin-4-(5*H*)-ones

Target name	Species	Score	Rank
Biotin Carboxylase (BC)	Not mentioned	1.0	1
PGDS	*Homo sapiens*	0.679	2
Serine/ Threonine-protein kinase Chk1	Not mentioned	0.677	3
RebC	*Lechevallieriaaerocolonigens*	0.675	4
Serine/ Threonine-protein kinase Chk1	*Homo sapiens*	0.672	5
Tankyrase-2	*Homo sapiens*	0.667	6
proto-oncogene serine/threonine-protein kinase Pim-1	*Homo sapiens*	0.667	6
Heat shock protein HSP 90-alpha	*Homo sapiens*	0.660	7
serine/ threonine-protein kinase chk1	not mentioned	0.651	8
proto-oncogene serine/threonine-protein kinase RET	*Homo sapiens*	0.647	9
Cell division protein kinase 2	*Homo sapiens*	0.644	10