One-pot synthesis of 4-substituted isoquinolinium zwitterionic salts by Metal-free C-H bond activation

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Supporting Information

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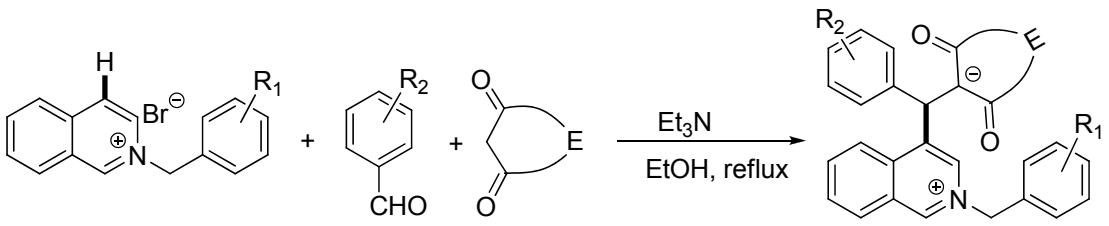
Experiment Procedure

Reagents and solvents were commercial available with analytical grade. Melting points were determined on a hot-plate microscope apparatus and were uncorrected. Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminium plates with GF-254 indicator, visualized by irradiation with UV light. IR spectra were obtained on a Bruker Tensor27 spectrometer (KBr disc). ^{1}H NMR and ^{13}C NMR spectra were measured with a Bruker AV-600 spectrover in DMSO-d_6 with chemical shift (δ) given in ppm relative to TMS as interstandard [(s = singlet, d = doublet, t = triplet, m = multiplet), coupling constant (Hz)]. High-resolution mass (ESI) were obtained with a Bruker MicroTOF spectrometer. X-ray data were collected on a Bruker Smart APEX-2 CCD diffractometer.

General procedure

One-pot reaction for the synthesis of 4a-4s, 5a-5f.

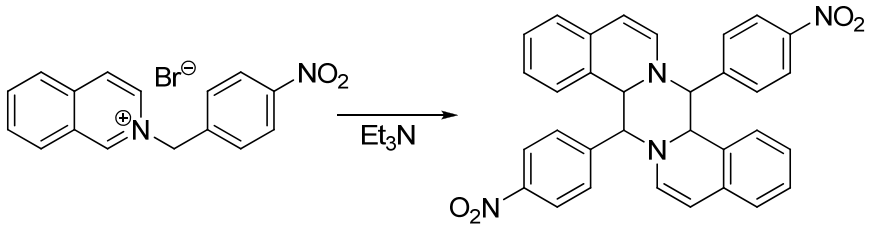
Isoquinoline (3.0 mmol, 0.388 g) and benzyl bromide (2.2mmol) were stirred in ethanol (10 mL) at 50 ^{o}C for about three hours. Aromatic aldehyde **3** (2.0 mmol) and 1,3-dicarbonyl compound **4** (2.0 mmol) and triethylamine (3.0 mmol, 0.303 g) were then added to the solution, and the mixture was stirred at reflux for overnight (TLC monitoring). The resulting precipitates were collected by filtration, washed with alcohol and chloroform and dried to give the corresponding product **4a-4s, 5a-5f**.



1a **2** **3** **4a-4s, 5a-5f**

Reaction of isoquinoline and *p*-nitrobenzyl bromide yields the dimer of the isoquinoline ylide (**F**).

Isoquinoline (3.0 mmol, 0.388 g) and *p*-nitrobenzyl bromide (2.2mmol) were stirred in ethanol (10 mL) at 50 ^{o}C for about three hours. Triethylamine (3.0 mmol, 0.303 g) were then added to the solution, and the mixture was stirred at reflux for one hour (TLC monitoring). The resulting precipitates were collected by filtration, washed with alcohol and dried to give the corresponding product **F**.



Crystal Data:

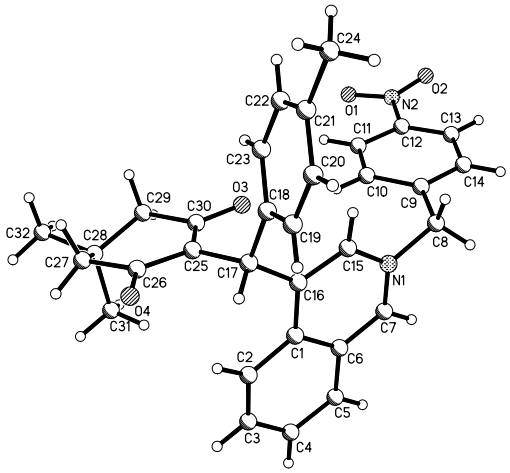


Fig. 1 X-ray structure of **4a**

Crystal data for **4a**: $C_{32}H_{30}N_2O_4$, *Mr* = 506.58, monoclinic, α = 9.822(3) Å, *b* = 12.203(4) Å, *c* = 12.763(4) Å, *U* = 1476.6(8) Å^3, *T* = 296(2) K, space group P -1, *Z* = 2, 12504 reflections measured, 6409 unique (R_{int} = 0.0671) which were used in all calculations. The final w*R* (F^2) was 0.2677 (all data). CCDC 856821.

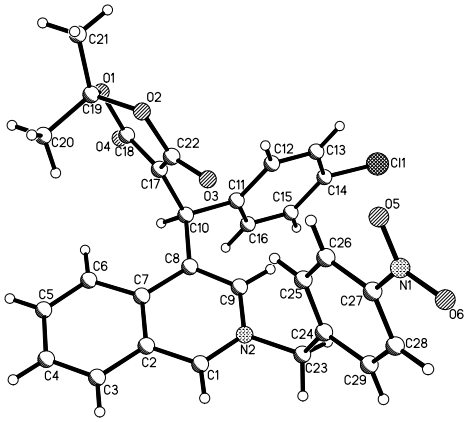


Fig. 2 X-ray structure of **4j**

Crystal data for **4j**: $C_{29}H_{23}ClN_2O_6$, *Mr* = 530.94, monoclinic, α = 14.6580(19) Å, *b* = 10.0334(13) Å, *c* = 22.667(3) Å, *U* = 3323.5(7) Å^3, *T* = 296(2) K, space group *P* 21/c, *Z* = 4, 28869 reflections measured, 7785 unique (R_{int} = 0.0468) which were used in all calculations. The final w*R* (F^2) was 0.1016 (all data). CCDC 856822.

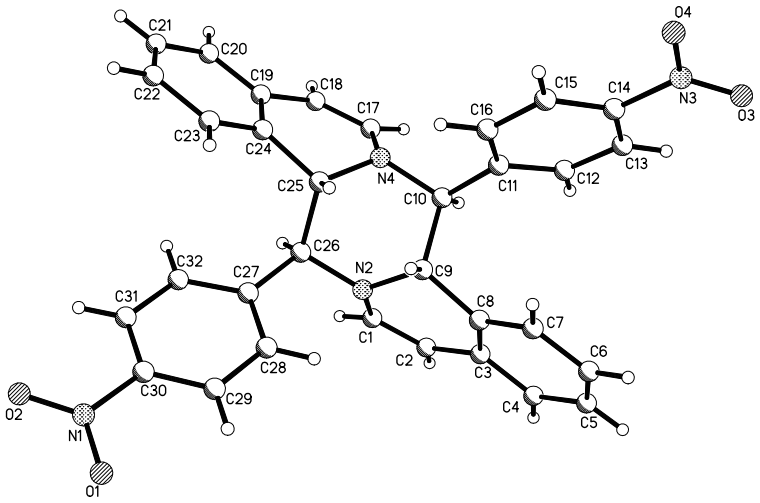


Fig 3 X-ray structure of **F**

Crystal data for **F**: $C_{32}H_{26}N_4O_4$, *Mr* = 530.57, orthorhombic, α = 24.754(4) Å, *b* = 7.9738(13) Å, *c* = 13.336(2) Å, *U* = 2632.4(7) Å^3, *T* = 296(2) K, space group *P* n a 21, *Z* = 4, 22296 reflections measured, 3162 unique (R_{int} = 0.1396) which were used in all calculations. The final w*R* (F^2) was 0.1396 (all data) CCDC 856823.

Characterization data of the 4a-4s:

4,4-dimethyl-1-((2-(4-nitrobenzyl)isoquinolinium-4-yl)(p-tolyl)methyl)-2,6-dioxocyclohexan-1-ide (4a): Yellow solid, yield: 70%, m.p. 208-210 °C, IR (KBr) ν = 3047, 2959, 2867, 1638, 1606, 1522, 1479, 1431, 1401, 1346, 1051, 995, 795 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.91 (s, 1H, ArH), 8.41 (d, *J* = 8.5 Hz, 2H, ArH), 8.20 (d, *J* = 8.5 Hz, 2H, ArH), 8.14 (t, *J* = 7.5 Hz, 1H, ArH), 7.99-7.96 (m, 2H, ArH), 7.62 (d, *J* = 8.5 Hz, 2H, ArH), 7.08 (d, *J* = 7.8 Hz, 2H, ArH), 6.98 (d, *J* = 7.8 Hz, 2H, ArH), 6.29 (s, 1H, CH), 6.09 (d, *J* = 13.0 Hz, 1H, CH), 6.05 (d, *J* = 13.0 Hz, 1H, CH), 2.23 (s, 3H, CH_3), 1.99 (d, *J* = 15.9 Hz, 2H, CH_2), 1.92 (d, *J* = 15.9 Hz, 2H, CH_2), 0.81 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 147.5, 146.3, 144.9, 141.6, 138.9, 136.6, 136.0, 135.5, 134.6, 130.6, 130.4, 129.6, 129.1, 128.4, 126.9, 124.5, 123.9, 110.6, 62.0, 49.4, 44.6, 31.2, 28.5, 20.6; MS (*m*/*z*): 505.47 ($[M-H]^-$, 100%); HRMS (ESI) Calcd. for $C_{32}H_{29}N_2O_4$ ($[M-H]^-$): 505.2127. Found: 505.2129.

1-((4-methoxyphenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (4b): Yellow solid, yield: 76%, m.p. 196-198 °C, IR (KBr) ν = 3418, 2951, 1639, 1607, 1479, 1401, 1347, 1245, 1178, 1145, 1029, 839, 796, 759 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.79 (s, 1H, ArH), 8.52 (d, *J* = 8.7 Hz, 1H, ArH), 8.35 (d, *J* = 8.3 Hz, 1H, ArH), 8.21 (d, *J* = 8.5Hz, 2H, ArH), 8.11 （t, *J* = 7.7Hz, 1H, ArH), 8.00 (s, 1H, ArH), 7.94 (t, *J* = 7.6 Hz, 1H, ArH), 7.65 (d, *J* = 8.5 Hz, 2H, ArH), 7.15 (d, *J* = 8.4 Hz, 2H, ArH), 6.74 (d, *J* = 8.4 Hz, 2H, ArH), 6.30 (s, 1H, CH), 6.07 (d, *J* = 15.0 Hz, 1H, CH), 6.01 (d, *J* = 15.0 Hz, 1H, CH), 3.70 (s, 3H, OCH_3), 1.93 (d, *J* = 15.7 Hz, 2H, CH_2), 1.84 (d, *J* = 15.7 Hz, 2H, CH_2), 0.81 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 157.3, 147.5, 145.5, 141.7, 136.7, 135.8, 135.7, 134.4, 130.4, 130.3, 130.2, 129.6, 126.9, 124.8, 123.9, 123.0, 65.0, 55.9, 54.8, 50.4, 31.1, 28.7, 18.5; MS (*m*/*z*): 521.33 ($[M-H]^-$, 100%); HRMS (ESI) Calcd. for $C_{32}H_{29}N_2O_5$ ($[M-H]^-$): 521.2076. Found: 521.2080.

1-((4-isopropylphenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (4c): Yellow solid, yield: 71%, m.p. 220-222 °C, IR (KBr) ν = 3413, 2956, 1638, 1605, 1480, 1399, 1347, 1264, 1144, 1053, 841, 793, 736 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.81 (s, 1H, ArH), 8.54 (d, *J* = 8.7 Hz, 1H, ArH), 8.38 (d, *J* = 8.3 Hz, 1H, ArH), 8.20 (d, *J* = 8.7 Hz, 2H, ArH), 8.13 (t, *J* = 7.6 Hz, 1H, ArH), 8.00 (s, 1H, ArH), 7.95 (t, *J* = 7.6 Hz, 1H, ArH), 7.63 (d, *J* = 8.6 Hz, 2H, ArH), 7.09 (d, *J* = 8.0 Hz, 2H, ArH), 7.00 (d, *J* = 8.0 Hz, 2H, ArH), 6.32 (s, 1H, CH), 6.06 (d, *J* = 15.1 Hz, 1H, CH), 6.02 (d, *J* = 15.1 Hz, 1H, CH), 2.82-2.76 (m, 1H, CH), 1.93 (d, *J* = 15.7 Hz, 2H, CH_2), 1.85 (d, *J* = 15.7 Hz, 2H, CH_2), 1.85-1.14 (m, 6H, CH_3), 0.82 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 147.5, 145.7, 145.4, 141.6, 139.8, 136.8, 135.9, 135.7, 130.4, 130.3, 129.7, 129.1, 126.9, 125.4, 124.8, 123.9, 62.1, 50.3, 32.9, 31.1, 28.7, 23.9, 23.8; MS (*m*/*z*): 533.40 ($[M-H]^-$, 100%); HRMS (ESI) Calcd. for $C_{34}H_{33}N_2O_4$ ($[M-H]^-$): 533.2440. Found: 533.2446.

1-((4-tert-butylphenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (4d): Yellow solid, yield: 55%, m.p. 220 °C, IR (KBr) ν = 3442, 2959, 1638, 1606, 1521, 1476, 1431, 1402, 1345, 1266, 1172, 1145, 854, 794,

760, 735 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.82 (s, 1H, ArH), 8.57 (d, J = 8.7 Hz, 1H, ArH), 8.38 (d, J = 8.3 Hz, 1H, ArH), 8.21 (d, J = 8.3 Hz, 2H, ArH), 8.12 (t, J = 7.5 Hz, 1H, ArH), 8.00 (s, 1H, ArH), 7.96 (t, J = 7.6 Hz, 1H, ArH), 7.63 (d, J = 8.4 Hz, 2H, ArH), 7.13 (d, J = 8.1 Hz, 2H, ArH), 7.08 (d, J = 8.1 Hz, 2H, ArH), 6.32 (s, 1H, CH), 6.05 (d, J = 15.0 Hz, 1H, CH), 6.01 (d, J = 15.0 Hz, 1H, CH), 1.94 (d, J = 15.7 Hz, 2H, CH_2), 1.85 (d, J = 15.7 Hz, 2H, CH_2), 1.23 (s, 9H, CH_3), 0.82 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 188.0, 147.6, 147.5, 145.7, 145.5, 141.4, 139.3, 136.7, 135.9, 135.6, 130.5, 130.3, 129.8, 128.8, 126.9, 124.7, 124.3, 123.9, 109.6, 62.1, 56.0, 50.2, 38.8, 33.8, 31.1, 31.0, 28.7, 18.4; MS (*m*/*z*): 547.47 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{35}H_{35}N_2O_4$ ([M-H]$^-$): 547.2597. Found: 547.2601.

1-((3-chlorophenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (4e): Yellow solid, yield: 60%, m.p. 218 °C, IR (KBr) ν = 3443, 3004, 2945, 1637, 1603, 1567, 1522, 1398, 1345, 1288, 1194, 1145, 1045, 998, 792 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.84 (s, 1H, ArH), 8.53 (d, J = 8.7 Hz, 1H, ArH), 8.38 (d, J = 8.3 Hz, 1H, ArH), 8.22 (d, J = 8.7 Hz, 2H, ArH), 8.13 (t, J = 7.7 Hz, 1H, ArH), 8.09 (s, 1H, ArH), 7.96 (t, J = 7.6 Hz, 1H, ArH), 7.67 (d, J = 8.6 Hz, 2H, ArH), 7.23-7.14 (m, 4H, ArH), 6.37 (s, 1H, CH), 6.09 (d, J = 14.9 Hz, 1H, CH), 6.04 (d, J = 14.9 Hz, 1H, CH), 1.94 (d, J = 15.7 Hz, 2H, CH_2), 1.87 (d, J = 15.7 Hz, 2H, CH_2), 0.81 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 147.6, 145.9, 145.6, 144.7, 141.7, 136.7, 135.9, 135.6, 132.4, 130.5, 130.4, 129.7, 129.4, 129.1, 127.9, 126.9, 125.5, 124.8, 123.9, 108.7, 62.0, 50.4, 31.2, 28.7; MS (*m*/*z*): 525.40 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{31}H_{26}ClN_2O_4$ ([M-H]$^-$): 525.1581. Found: 525.1577.

1-((4-fluorophenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (4f): Yellow solid, yield: 59%, m.p. 242-244 °C, IR (KBr) ν = 3428, 2946, 1637, 1603, 1476, 1397, 1344, 1265, 855, 798, 764 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.80 (s, 1H, ArH), 8.52 (d, J = 8.7 Hz, 1H, ArH), 8.37 (d, J = 8.3 Hz, 1H, ArH), 8.22 (d, J = 8.3 Hz, 2H, ArH), 8.13 (t, J = 7.8 Hz, 1H, ArH), 8.03 (s, 1H, ArH), 7.95 (t, J = 7.6 Hz, 1H, ArH), 7.66 (d, J = 8.3 Hz, 2H, ArH), 7.26 (t, J = 6.6 Hz, 2H, ArH), 7.00 (t, J = 8.5 Hz, 2H, ArH), 6.35 (s, 1H, CH), 6.12 (d, J = 15.0 Hz, 1H, CH), 6.04 (d, J = 15.0 Hz, 1H, CH), 1.94 (d, J = 15.7 Hz, 2H, CH_2), 1.85 (d, J = 15.7 Hz, 2H, CH_2), 0.81 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 187.2, 160.6 (d, J = 241.3 Hz), 147.6, 145.6, 141.8, 138.9, 136.7, 135.7 (d, J = 3.4 Hz), 131.2 (d, J = 7.6 Hz), 130.3 (d, J = 7.6 Hz), 129.6, 127.0, 124.9, 123.9, 114.2 (d, J = 20.7 Hz), 109.4, 62.0, 50.6, 31.1, 28.8; MS (*m*/*z*): 509.40 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{31}H_{26}FN_2O_4$ ([M-H]$^-$): 509.1877. Found: 509.1874.

4,4-dimethyl-1-((2-(4-nitrobenzyl)isoquinolinium-4-yl)(phenyl)methyl)-2,6-dioxocyclohexan-1-ide (4g): Yellow solid, yield: 81%, m.p. 219-221 °C, IR (KBr) ν = 3441, 2992, 1638, 1577, 1521, 1435, 1392, 1344, 1258, 1107, 796 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.91 (s, 1H, ArH), 8.59 (d, J = 8.7 Hz, 1H, ArH), 8.44 (d, J = 8.3 Hz, 1H, ArH), 8.24 (t, J = 7.8 Hz, 1H, ArH), 8.20 (d, J = 8.5 Hz, 2H, ArH), 8.02 (t, J = 7.7 Hz, 1H, ArH), 7.95 (s, 1H, ArH), 7.62 (d, J = 8.4 Hz, 2H, ArH), 7.29 (d, J = 7.6

Hz, 2H, ArH), 7.25 (t, *J* = 7.4 Hz, 2H, ArH), 7.18 (t, *J* = 7.1 Hz, 1H, ArH), 6.14-6.03 (m, 3H, CH, CH_2), 1.36 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.7, 147.6, 146.8, 144.3, 142.2, 141.5, 136.7, 136.5, 135.4, 130.9, 130.5, 129.5, 129.0, 127.9, 127.2, 125.9, 124.5, 123.9, 99.4, 75.5, 62.2, 41.3, 25.9; MS (*m*/*z*): 495.27 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{29}H_{23}N_2O_6$ ([M-H]$^-$): 495.1556. Found: 495.1561.

4,4-dimethyl-1-((2-(4-nitrobenzyl)isoquinolinium-4-yl)(p-tolyl)methyl)-2,6-dioxocyclohexan-1-ide (4h): Yellow solid, yield: 73%, m.p. 222-224 °C, IR (KBr) ν = 3442, 2990, 1639, 1580, 1525, 1437, 1388, 1343, 1256, 1212, 857, 797 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.89 (s, 1H, ArH), 8.58 (d, *J* = 8.7 Hz, 1H, ArH), 8.43 (d, *J* = 8.3 Hz, 1H, ArH), 8.24-8.19 (m, 3H, ArH), 8.00 (t, *J* = 7.7 Hz, 1H, ArH), 7.92 (s, 1H, ArH), 7.62 (d, *J* = 8.7 Hz, 2H, ArH), 7.16 (d, *J* = 8.0 Hz, 2H, ArH), 7.04 (d, *J* = 8.0 Hz, 2H, ArH), 6.10-1.01 (m, 3H, CH, CH_2), 2.26 (s, 3H, CH_3), 1.36 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.7, 147.6, 146.7, 144.5, 141.6, 139.2, 136.7, 136.4, 135.4, 134.8, 130.8, 130.5, 129.6, 128.9, 128.5, 127.1, 124.5, 123.8, 99.4, 75.6, 62.1, 40.9, 25.9, 20.6; MS (*m*/*z*): 509.33 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{30}H_{25}N_2O_6$ ([M-H]$^-$): 509.1713. Found: 509.1730.

1-((4-methoxyphenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (4i): Yellow solid, yield: 85%, m.p. 197-199 °C, IR (KBr) ν = 3425, 2994, 1581, 1514, 1391, 1347, 1253, 1204, 927, 794, 750 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.80 (s, 1H, ArH), 8.50 (d, *J* = 8.7 Hz, 1H, ArH), 8.34 (d, *J* = 8.3 Hz, 1H, ArH), 8.15-8.10 (m, 3H, ArH), 7.92 (t, *J* = 7.6 Hz, 1H, ArH), 7.82 (s, 1H, ArH), 7.53 (d, *J* = 8.6 Hz, 2H, ArH), 7.12 (d, *J* = 8.5 Hz, 2H, ArH), 6.73 (d, *J* = 8.6 Hz, 2H, ArH), 6.00 (d, *J* = 16.0 Hz, 1H, CH), 5.94 (d, *J* = 16.0 Hz, 1H, CH), 5.90 (s, 1H, CH), 3.63 (s, 3H, OCH_3), 1.27 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.8, 157.6, 147.6, 146.7, 144.8, 141.6, 136.7, 136.4, 135.4, 133.9, 130.8, 130.5, 130.0, 129.6, 127.2, 124.5 123.8, 113.3, 99.4, 75.9, 62.1, 54.9, 40.6, 25.9; MS (*m*/*z*): 525.33 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{30}H_{25}N_2O_7$ ([M-H]$^-$): 525.1662. Found: 525.1662.

1-((4-chlorophenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (4j): Yellow solid, yield: 77%, m.p. 196-198 °C, IR (KBr) ν = 3440, 2991, 1577, 1391, 1346, 1257, 1206, 1095, 1016, 919, 794, 751 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.92 (s, 1H, ArH), 8.55 (d, *J* = 8.7 Hz, 1H, ArH), 8.44 (d, *J* = 8.3 Hz, 1H, ArH), 8.24-8.20 (m, 3H, ArH), 8.01 (t, *J* = 7.7 Hz, 1H, ArH), 7.99 (s, 1H, ArH), 7.64 (d, *J* = 8.7 Hz, 2H, ArH), 7.32 (s, 4H, ArH), 6.12 (d, *J* = 15.0 Hz, 1H, CH), 6.07-6.04 (m, 2H, CH), 1.35 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.7, 147.6, 147.1, 143.7, 141.6, 141.3, 136.6, 136.5, 135.4, 130.9, 130.6, 130.5, 129.6, 127.8, 127.2, 124.4, 123.9, 99.4, 75.3, 62.1, 40.8, 25.9; MS (*m*/*z*): 529.33 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{29}H_{22}ClN_2O_6$ ([M-H]$^-$): 529.1166. Found: 529.1167.

1-((3-chlorophenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (4k): Yellow solid, yield: 71%, m.p. 204-206 °C, IR (KBr)

ν = 3447, 2990, 1639, 1578, 1521, 1390, 1347, 1258, 1201, 1112, 999, 791 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.94 (s, 1H, ArH), 8.55 (d, *J* = 8.7 Hz, 1H, ArH), 8.45 (d, *J* = 8.3 Hz, 1H, ArH), 8.23 (t, *J* = 8.2 Hz, 1H, ArH), 8.22 (d, *J* = 8.8 Hz, 2H, ArH), 8.02 (t, *J* = 7.7 Hz, 1H, ArH), 7.98 (s, 1H, ArH), 7.64 (d, *J* = 8.7 Hz, 2H, ArH), 7.30-7.22 (m, 4H, ArH), 6.13-6.03 (m, 3H, CH, CH_2), 1.35 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.7, 152.2, 147.2, 142.8, 136.5, 135.2, 132.7, 131.1, 130.5, 129.7, 129.6, 128.8, 127.7, 127.5, 127.4, 127.2, 126.0, 124.4, 123.9, 122.9, 99.5, 75.0, 62.1, 41.1, 25.9; MS (*m*/*z*): 529.33 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{29}H_{22}ClN_2O_6$ ([M-H]$^-$): 529.1166. Found: 529.1167.

5-((2-(4-nitrobenzyl)isoquinolinium-4-yl)(phenyl)methyl)-2,4,6-trioxohexahydropyrimidin-5-ide (4l): Yellow solid, yield: 88%, m.p. 297-299 °C, IR (KBr) ν = 3429, 1686, 1569, 1523, 1448, 1378, 1347, 1201, 1172, 776 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.96 (s, 1H, ArH), 9.24 (s, 2H, NH), 8.68 (d, *J* = 8.7 Hz, 1H, ArH), 8.41 (d, *J* = 8.3 Hz, 1H, ArH), 8.21-8.17 (m, 4H, ArH), 7.99-7.95 (m, 1H, ArH), 7.68 (d, *J* = 8.6 Hz, 2H, ArH), 7.29 (d, *J* = 7.6 Hz, 2H, ArH), 7.22 (t, *J* = 7.4 Hz, 2H, ArH), 7.16 (t, *J* = 7.2 Hz, 1H, ArH), 6.25 (s, 1H, CH), 6.09 (d, *J* = 15.0 Hz, 1H, CH), 6.04 (d, *J* = 15.0 Hz, 1H, CH); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 163.9, 152.1, 147.6, 146.3, 143.8, 141.9, 141.7, 135.9, 136.4, 135.9, 130.7, 130.4, 129.6, 129.0, 127.8, 127.2, 125.8, 124.5, 123.9, 85.4, 62.2, 40.2, 35.7, 30.7; MS (*m*/*z*): 479.33 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{27}H_{19}N_4O_5$ ([M-H]$^-$): 479.1355. Found: 479.1368.

5-((2-(4-nitrobenzyl)isoquinolinium-4-yl)(p-tolyl)methyl)-2,4,6-trioxohexahydropyrimidin-5-ide (4m): Yellow solid, yield: 96%, m.p. 298-300 °C, IR (KBr) ν = 3424, 1684, 1572, 1521, 1449, 1378, 1348, 1220, 1174, 791 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.84 (s, 1H, ArH), 9.22 (s, 1H, NH), 9.20 (s, 1H, NH), 8.67 (d, *J* = 8.7 Hz, 1H, ArH), 8.40 (d, *J* = 8.3 Hz, 1H, ArH), 8.20-8.15 (m, 4H, ArH), 7.97 (t, *J* = 7.6 Hz, 1H, ArH), 7.68 (d, *J* = 8.7 Hz, 2H, ArH), 7.16 (d, *J* = 7.9 Hz, 2H, ArH), 7.01 (d, *J* = 7.9 Hz, 2H, ArH), 6.19 (s, 1H, CH), 6.10 (d, *J* = 15.0 Hz, 1H, CH), 6.03 (d, *J* = 15.0 Hz, 1H, CH), 2.24 (s, 3H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.4, 152.6, 148.1, 146.7, 144.4, 142.2, 139.4, 137.5, 136.9, 136.4, 135.2, 131.2, 130.9, 130.2, 129.4, 128.9, 127.7, 124.9, 124.4, 86.0, 62.7, 40.6, 21.0; MS (*m*/*z*): 493.27 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{28}H_{21}N_4O_5$ ([M-H]$^-$): 493.1512. Found: 493.1514.

5-((4-chlorophenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-2,4,6-trioxohexahydropyrimidin-5-ide (4n): Yellow solid, yield: 96%, m.p. 289-291 °C, IR (KBr) ν = 3426, 1686, 1572, 1523, 1488, 1449, 1380, 1349, 1221, 852 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.87 (s, 1H, ArH), 9.24 (s, 2H, NH), 8.67 (d, *J* = 8.7 Hz, 1H, ArH), 8.41 (d, *J* = 8.3 Hz, 1H, ArH), 8.22-8.17 (m, 4H, ArH), 7.98 (t, *J* = 7.6 Hz, 1H, ArH), 7.70 (d, *J* = 8.7 Hz, 2H, ArH), 7.32 (d, *J* = 8.5 Hz, 2H, ArH), 7.28 (d, *J* = 8.5 Hz, 2H, ArH), 6.23 (s, 1H, CH), 6.13 (d, *J* = 14.9 Hz, 1H, CH), 6.03 (d, *J* = 14.9 Hz, 1H, CH); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.1, 162.3, 152.1, 147.6, 146.5, 143.1, 141.7, 141.0, 136.9, 136.5, 135.9, 130.9, 130.8, 130.5, 130.4, 129.7, 127.7, 127.2, 124.4, 123.9, 85.2, 62.1, 35.7, 30.7; MS (*m*/*z*): 513.27 ([M-H]$^-$, 100%);

HRMS (ESI) Calcd. for $C_{27}H_{18}ClN_4O_5$ ([M-H]$^-$): 513.0966. Found: 513.0967.

5-((4-fluorophenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-2,4,6-trioxohexahydropyrimidin-5-ide (4o): Yellow solid, yield: 90%, m.p. 263-265 °C, IR (KBr) ν = 3422, 1686, 1572, 1521, 1447, 1377, 1220, 1159, 1047, 797 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.87 (s, 1H, ArH), 9.24 (s, 2H, NH), 8.66 (d, J = 8.7 Hz, 1H, ArH), 8.41 (d, J = 8.3 Hz, 1H, ArH), 8.22-8.16 (m, 4H, ArH), 7.98 (t, J = 7.6 Hz, 1H, ArH), 7.69 (d, J = 8.6 Hz, 2H, ArH), 7.33 (q, J = 8.0 Hz, 2H, ArH), 7.04 (t, J = 8.8 Hz, 2H, ArH), 6.23 (s, 1H, CH), 6.12 (d, J = 14.9 Hz, 1H, CH), 6.03 (d, J = 14.9 Hz, 1H, CH); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.0, 160.6 (d, J = 239.8 Hz), 152.1, 147.6, 146.4, 143.6, 141.7, 138.0 (d, J = 2.6 Hz), 136.9, 136.4, 135.8, 130.9 (d, J = 7.9 Hz), 130.7, 130.4, 129.6, 127.2, 124.4, 123.9, 114.4 (d, J = 21.0 Hz), 104.3, 85.6, 62.1; MS (*m*/*z*): 497.33 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{27}H_{18}FN_4O_5$ ([M-H]$^-$): 497.1261. Found: 497.1259.

5-((2-(4-nitrobenzyl)isoquinolinium-4-yl)(3-nitrophenyl)methyl)-2,4,6-trioxohexahydropyrimidin-5-ide (4p): Yellow solid, yield: 92%, m.p. 270-272 °C, IR (KBr) ν = 3419, 1681, 1573, 1525, 1449, 1379, 1349, 1251, 1171, 780 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.91 (s, 1H, ArH), 9.31 (s, 2H, NH), 8.70 (d, J = 8.7 Hz, 1H, ArH), 8.43 (d, J = 8.3 Hz, 1H, ArH), 8.24-8.18 (m, 4H, ArH), 8.08 (d, J = 8.0 Hz, 1H, ArH), 8.00 (t, J = 7.6 Hz, 1H, ArH), 7.95 (s, 1H, ArH), 7.73 (d, J = 7.7 Hz, 1H, ArH), 7.70 (d, J = 8.7 Hz, 2H, ArH), 7.55 (t, J = 7.9 Hz, 1H, ArH), 6.37 (s, 1H, CH), 6.11 (d, J = 14.8 Hz, 1H, CH), 6.03 (d, J = 14.9 Hz, 1H, CH); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.0, 162.3, 152.1, 147.7, 147.6, 146.9, 144.5, 142.6, 141.7, 136.5, 136.0, 135.7, 130.8, 130.5, 129.6, 129.2, 127.3, 124.5, 123.8, 121.1, 84.6, 62.1, 35.7, 30.7; MS (*m*/*z*): 524.33 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{27}H_{18}N_5O_7$ ([M-H]$^-$): 524.1206. Found: 524.1205.

1,3-dimethyl-5-((2-(4-nitrobenzyl)isoquinolinium-4-yl)(phenyl)methyl)-2,4,6-trioxohexahydropyrimidin-5-ide (4q): Yellow solid, yield: 89%, m.p. 267-269 °C, IR (KBr) ν = 3056, 2997, 1674, 1638, 1600, 1567, 1519, 1428, 1325, 1263, 1110, 997, 798 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.89 (s, 1H, ArH), 8.63 (d, J = 8.6 Hz, 1H, ArH), 8.43 (d, J = 8.3 Hz, 1H, ArH), 8.22-8.20 (m, 4H, ArH), 7.98 (t, J = 7.5 Hz, 1H, ArH), 7.67 (d, J = 8.2Hz, 2H, ArH), 7.24-7.09 (m, 4H, ArH), 7.15 (t, J = 6.7 Hz, 1H, ArH), 6.36 (s, 1H, CH), 6.09 (q, J = 14.9 Hz, 2H, CH), 3.02 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 161.8, 152.8, 147.6, 146.5, 143.4, 141.9, 141.6, 136.9, 136.6, 136.0, 130.8, 130.4, 129.7, 128.9, 127.8, 127.2, 125.8, 124.3, 123.8, 85.6, 62.2, 40.9, 26.9; MS (*m*/*z*): 507.39 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{29}H_{23}N_4O_5$ ([M-H]$^-$): 507.1668. Found: 507.1675.

1,3-dimethyl-5-((2-(4-nitrobenzyl)isoquinolinium-4-yl)(p-tolyl)methyl)-2,4,6-trioxohexahydropyrimidin-5-ide (4r): Yellow solid, yield: 92%, m.p. 284 °C, IR (KBr) ν = 3007, 1670, 1638, 1575, 1518, 1429, 1305, 1265, 1111, 787 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.88 (s, 1H, ArH), 8.61 (d, J = 8.7 Hz, 1H, ArH), 8.42 (d, J = 8.3 Hz, 1H, ArH), 8.22-8.17 (m, 4H, ArH), 7.98 (t, J = 7.8 Hz, 1H, ArH), 7.67 (d, J = 8.4 Hz, 2H, ArH), 7.10 (d, J = 7.7 Hz, 2H, ArH), 7.00 (d, J = 7.7 Hz, 2H, ArH), 6.31

(s, 1H, CH), 6.12 (d, J = 15.0 Hz, 1H, CH), 6.05 (d, J = 14.9 Hz, 1H, CH), 3.01 (s, 6H, CH_3), 2.24 (s, 3H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 161.8, 152.8, 147.6, 146.4, 143.6, 141.6, 138.8, 136.9, 136.5, 136.0, 134.6, 130.8, 130.4, 129.8, 128.8, 128.4, 127.1, 124.2, 123.8, 85.8, 62.1, 55.9, 40.6, 26.9, 20.5, 18.5; MS (*m*/*z*): 521.39 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{30}H_{25}N_4O_5$ ([M-H]$^-$): 521.1825. Found: 521.1833.

5-((4-chlorophenyl)(2-(4-nitrobenzyl)isoquinolinium-4-yl)methyl)-1,3-dimethyl-2, 4,6-trioxohexahydropyrimidin-5-ide (**4s**)**:** Yellow solid, yield: 83%, m.p. 272-274 ^{o}C, IR (KBr) ν = 2984, 1672, 1638, 1574, 152, 1430, 1346, 1304, 1181, 1090, 855, 779 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.90 (s, 1H, ArH), 8.60 (d, J = 8.6 Hz, 1H, ArH), 8.43 (d, J = 8.3 Hz, 1H, ArH), 8.23-8.19 (m, 4H, ArH), 7.99 (t, J = 7.6 Hz, 1H, ArH), 7.68 (d, J = 8.3 Hz, 2H, ArH), 7.26 (t, J = 9.7 Hz, 4H, ArH), 6.34 (s, 1H, CH), 6.14 (d, J = 14.8 Hz, 1H, CH), 6.07 (d, J = 14.8 Hz, 1H, CH), 3.02 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 161.8, 152.8, 147.6, 146.7, 142.9, 141.7, 141.0, 136.9, 136.6, 136.0, 130.8, 130.5, 130.4, 129.7, 127.7, 127.2, 124.3, 123.8, 85.4, 62.1, 40.5, 26.9; MS (*m*/*z*): 541.34 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{29}H_{22}ClN_4O_5$ ([M-H]$^-$): 541.1279. Found: 541.1283.

Characterization data of the 5a-5f:

5-((2-benzylisoquinolinium-4-yl)(p-tolyl)methyl)-2,2-dimethyl-4,6-dioxo-1,3-dioxan-5-ide (5a): yellow solid, yield: 78%, m.p. 294 °C, IR (KBr) ν = 3448, 2991, 1639, 1588, 1509, 1446, 1389, 1257, 1201, 1101, 792, 749 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.88 (s, 1H, ArH), 8.55 (d, *J* = 8.7 Hz, 1H, ArH), 8.43 (d, *J* = 8.3 Hz, 1H, ArH), 8.19 (t, *J* = 7.8 Hz, 1H, ArH), 8.00-7.97 (m, 2H, ArH), 7.38-7.35 (m, 5H, ArH), 7.16 (d, *J* = 7.9 Hz, 2H, ArH), 7.05 (d, *J* = 7.9 Hz, 2H, ArH), 6.00 (s, 1H, CH), 5.88 (d, *J* = 14.4 Hz, 1H, CH), 5.84 (d, *J* = 14.4 Hz, 1H, CH), 2.29 (s, 3H, CH_3), 1.36 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.7, 146.2, 144.3, 139.3, 136.6, 136.2, 135.4, 134.8, 134.4, 130.7, 130.4, 128.9, 128.8, 128.5, 128.3, 127.1, 99.3, 79.1, 75.7, 63.3, 40.9, 25.9, 20.6; MS (*m*/*z*): 464.40 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{30}H_{26}NO_4$ ([M-H]$^-$): 464.1862. Found: 464.1872.

5-((2-benzylisoquinolinium-4-yl)(p-tolyl)methyl)-2,4,6-trioxohexahydropyrimidin-5-ide (5b): Yellow solid, yield: 89%, m.p.296-298 °C, IR (KBr) ν = 3451, 2821, 1567, 1460, 1382, 1298, 1123, 881, 831, 792 cm^{-1}; ^1H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.84 (s, 1H, ArH), 9.01 (s, 2H, NH), 8.62 (d, *J* = 8.7 Hz, 1H, ArH), 8.41 (d, *J* = 8.3 Hz, 1H, ArH), 8.19 (s, 1H, ArH), 8.16 (t, *J* = 7.7 Hz, 1H, ArH), 7.97 (t, *J* = 7.7 Hz, 1H, ArH), 7.39-7.37 (m, 5H, ArH), 7.16 (d, *J* = 7.9 Hz, 2H, ArH), 7.03 (d, *J* = 7.9 Hz, 2H, ArH), 6.16 (s, 1H, CH), 5.89 (d, *J* = 14.4 Hz, 1H, CH), 5.83 (d, *J* = 14.3 Hz, 1H, CH), 2.28 (s, 3H, CH_3); The ^{13}C NMR spectroscopy of product can't be obtained due to it's bad solubility. MS (*m*/*z*): 448.17 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{28}H_{22}N_3O_3$ ([M-H]$^-$): 448.1661. Found: 448.1671.

5-((2-benzylisoquinolinium-4-yl)(p-tolyl)methyl)-1,3-dimethyl-2,4,6-trioxohexahydropyrimidin-5-ide (5c): Yellow solid, yield: 70%, m.p. 306-308 °C, IR (KBr) ν = 3425, 3237, 1670, 1578, 1508, 1426, 1264, 1171, 1040, 797, 783, 760 cm^{-1}; ^1H NMR (600MHz, DMSO-d_6) δ (ppm): 9.87 (s, 1H, ArH), 8.58 (d, *J* = 8.7 Hz, 1H, ArH), 8.41 (d, *J* = 8.3Hz, 1H, ArH), 8.27 (s, 1H, ArH), 8.17 (t, *J* = 7.7 Hz, 1H, ArH), 7.96 (t, *J* = 7.6 Hz, 1H, ArH), 7.42-7.40 (m, 2H, ArH), 7.37-7.36 (m, 3H, ArH), 7.10 (d, *J* = 7.9 Hz, 2H, ArH), 7.02 (d, *J* = 7.9 Hz, 2H, ArH), 6.29 (s, 1H, CH), 5.91 (d, *J* = 14.3 Hz, 1H, CH), 5.85 (d, *J* = 14.3 Hz, 1H, CH), 3.02 (s, 6H, CH_3), 2.27 (s, 3H, CH_3); The ^{13}C NMR spectroscopy of product can't be obtained due to it's bad solubility; MS (*m*/*z*): 476.13 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{30}H_{26}N_3O_3$ ([M-H]$^-$): 476.1974. Found: 476.1985.

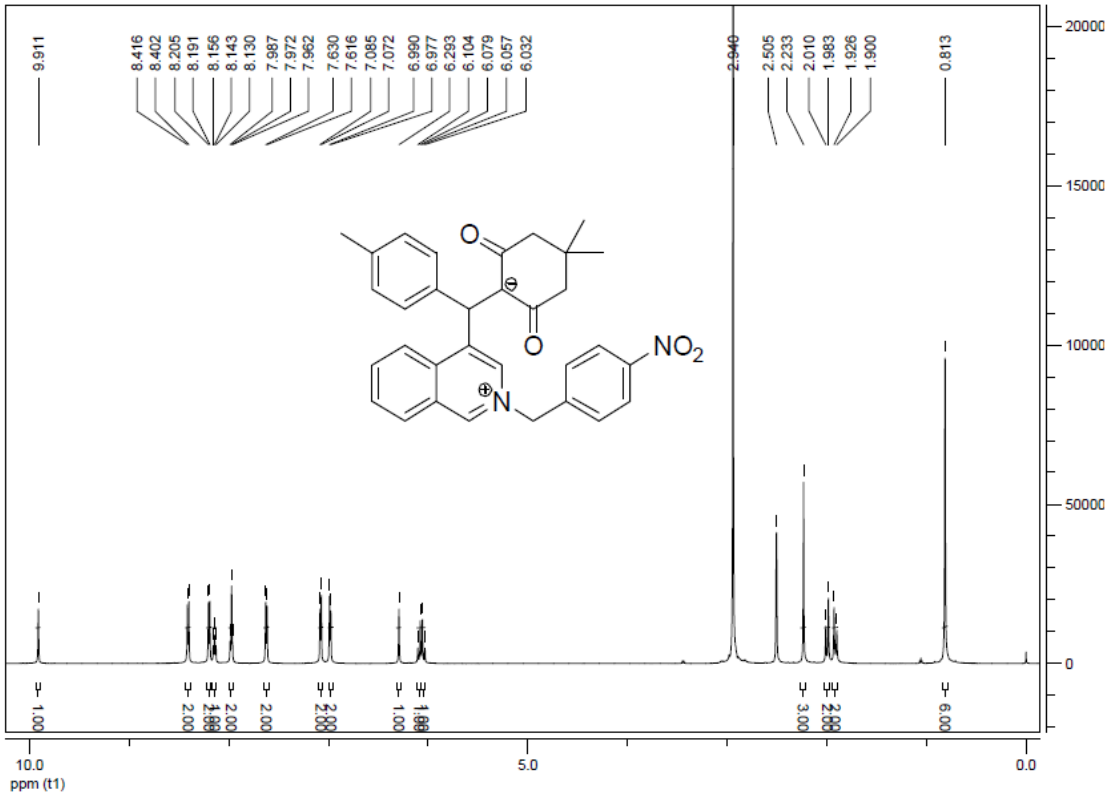
4,4-dimethyl-1-((2-(4-methylbenzyl)isoquinolinium-4-yl)(p-tolyl)methyl)-2,6-dioxocyclohexan-1-ide (5d): Yellow solid, yield: 64%, m.p. 246-248°C, IR (KBr) ν = 3461, 2951, 1638, 1608, 1567, 1477, 1398, 1268, 1172, 1147, 816, 790 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ (ppm): 9.29 (s, 1H, ArH), 8.63 (d, *J* = 8.0 Hz, 1H, ArH), 8.07 (d, *J* = 7.7 Hz, 1H, ArH), 8.00 (s, 1H, ArH), 7.95 (d, *J* = 7.7 Hz 1H, ArH), 7.70 (t, *J* = 7.6 Hz 1H, ArH), 7.13-7.08 (m, 6H, ArH), 6.98 (d, *J* = 7.6 Hz, 2H, ArH), 6.44 (s, 1H, CH), 5.56 (d, *J* = 14.0 Hz, 1H, CH), 5.37 (d, *J* = 14.0 Hz, 1H, CH), 2.31 (s, 3H, CH_3), 2.30 (s, 3H, CH_3), 2.21 (d, *J* = 16.2Hz, 2H, CH_2), 2.13 (d, *J* = 16.1Hz, 2H, CH_2), 0.94 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 140.1, 137.6,

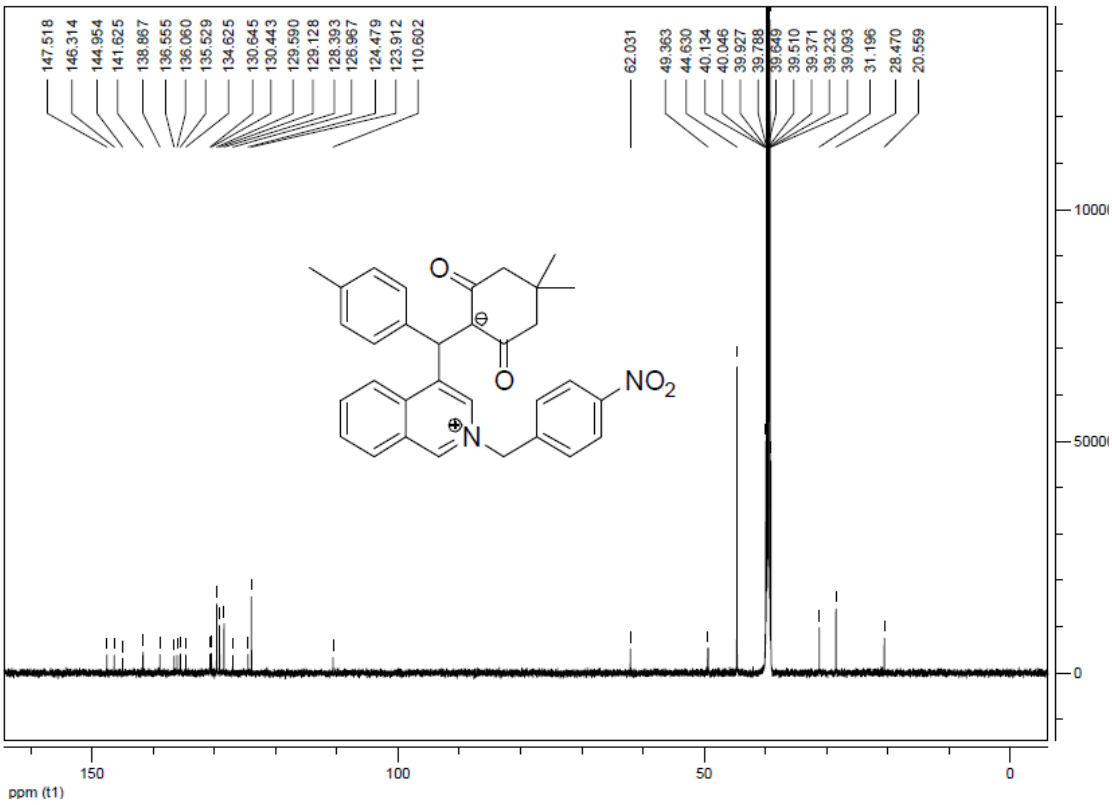
136.2, 135.9, 135.6, 130.4, 130.2, 129.4, 129.1, 129.0, 128.9, 127.4, 125.9, 111.7, 64.1, 58.3, 40.7, 31.6, 28.8, 21.2, 21.0, 18.4; MS (*m*/*z*): 474.44 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{33}H_{32}NO_2$ ([M-H]$^-$): 474.2433. Found: 474.2434.

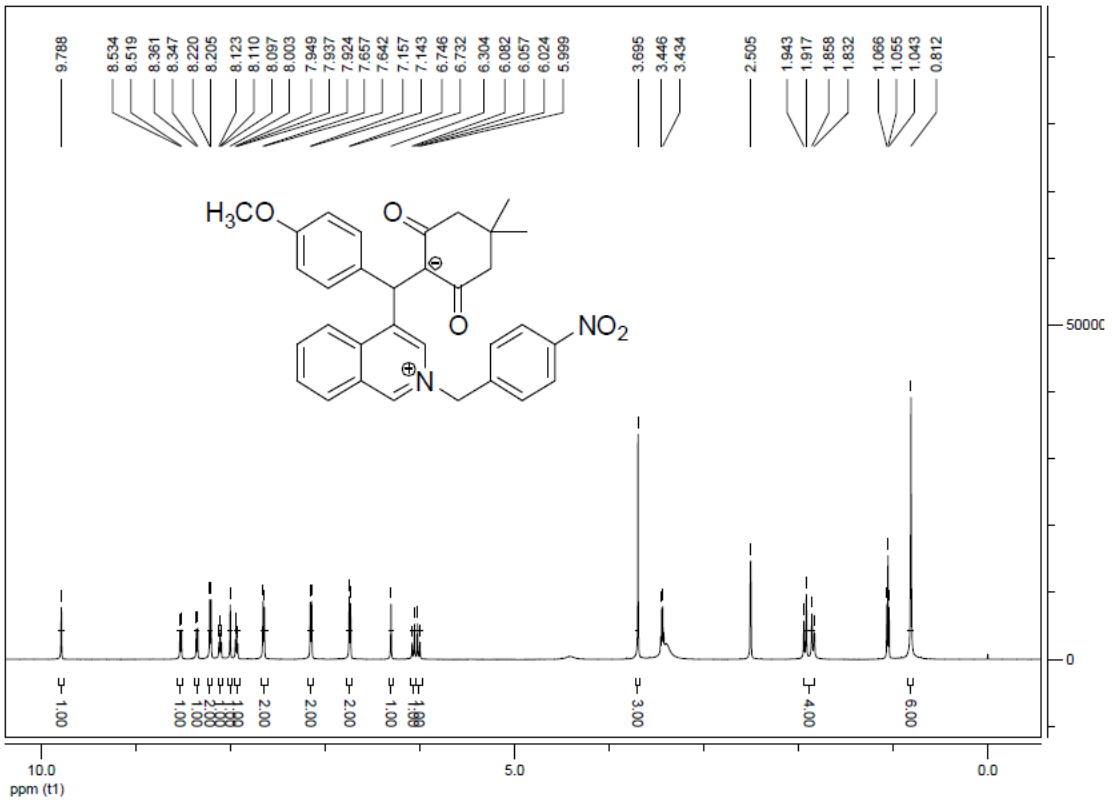
4,4-dimethyl-1-((2-(4-methylbenzyl)isoquinolinium-4-yl)(p-tolyl)methyl)-2,6-dioxocyclohexan-1-ide (5e): Yellow solid, yield: 88%, m.p. 220-222 ^oC, IR (KBr) ν = 3451, 2987, 1584, 1511, 1440, 1386, 1257, 1206, 1168, 1097, 817, 790 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.88 (s, 1H, ArH), 8.50 (d, *J* = 8.6 Hz, 1H, ArH), 8.44 (d, *J* = 8.3 Hz, 1H, ArH), 8.19 (t, *J* = 7.6 Hz, 1H, ArH), 7.99-7.97 (m, 2H, ArH), 7.31-7.26 (m, 6H, ArH), 7.17 (d, *J* = 7.8 Hz, 2H, ArH), 6.02 (s, 1H, CH), 5.85 (d, *J* = 14.2 Hz, 1H, CH), 5.80 (d, *J* = 14.1 Hz, 1H, CH), 2.29 (s, 3H, CH_3), 1.35 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.7, 146.0, 144.2, 139.3, 138.4, 136.5, 136.1, 135.3, 134.7, 131.4, 130.7, 130.5, 129.4, 128.9, 128.5, 127.1, 124.4, 99.3, 75.6, 63.2, 41.0, 25.9, 20.7, 20.6; MS (*m*/*z*): 478.39 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{31}H_{28}NO_4$ ([M-H]$^-$): 478.2018. Found: 478.2021.

1-((4-chlorophenyl)(2-(4-methylbenzyl)isoquinolinium-4-yl)methyl)-4,4-dimethyl-2,6-dioxocyclohexan-1-ide (5f): Yellow solid, yield: 81%, m.p. 226-228 ^oC, IR (KBr) ν = 3450, 2987, 1639, 1582, 1492, 1287, 1257, 1203, 1170, 1093, 917, 793 cm^{-1}; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm): 9.88 (s, 1H, ArH), 8.50 (d, *J* = 8.6 Hz, 1H, ArH), 8.44 (d, *J* = 8.3 Hz, 1H, ArH), 8.19 (t, *J* = 7.6 Hz, 1H, ArH), 7.99-7.97 (m, 2H, ArH), 7.31-7.26 (m, 6H, ArH), 7.17 (d, *J* = 7.8 Hz, 2H, ArH), 6.02 (s, 1H, CH), 5.85 (d, *J* = 14.2 Hz, 1H, CH), 5.80 (d, *J* = 14.1 Hz, 1H, CH), 2.29 (s, 3H, CH_3), 1.35 (s, 6H, CH_3); ^{13}C NMR (150 MHz, DMSO-d_6) δ(ppm): 164.6, 146.3, 143.4, 141.5, 138.5, 136.4, 136.2, 135.1, 131.4, 130.8, 130.7, 130.5, 129.5, 128.5, 127.8, 127.1, 124.4, 90.4, 75.3, 63.1, 40.8, 25.9, 20.7; MS (*m*/*z*): 498.28 ([M-H]$^-$, 100%); HRMS (ESI) Calcd. for $C_{30}H_{25}ClNO_4$ ([M-H]$^-$): 498.1472. Found: 498.1456.

Copies of NMR spectra of products



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8.123
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8.097
8.003
7.949
7.937
7.924
7.657
7.642
7.157
7.143
6.746
6.732
6.304
6.082
6.057
6.024
5.999
3.695
3.446
3.434
2.505
1.943
1.917
1.858
1.832
1.066
1.055
1.043
0.812
H3CO
O
O
NO2
N
50000
0
1.00
1.00
2.00
2.00
2.00
1.00
3.00
4.00
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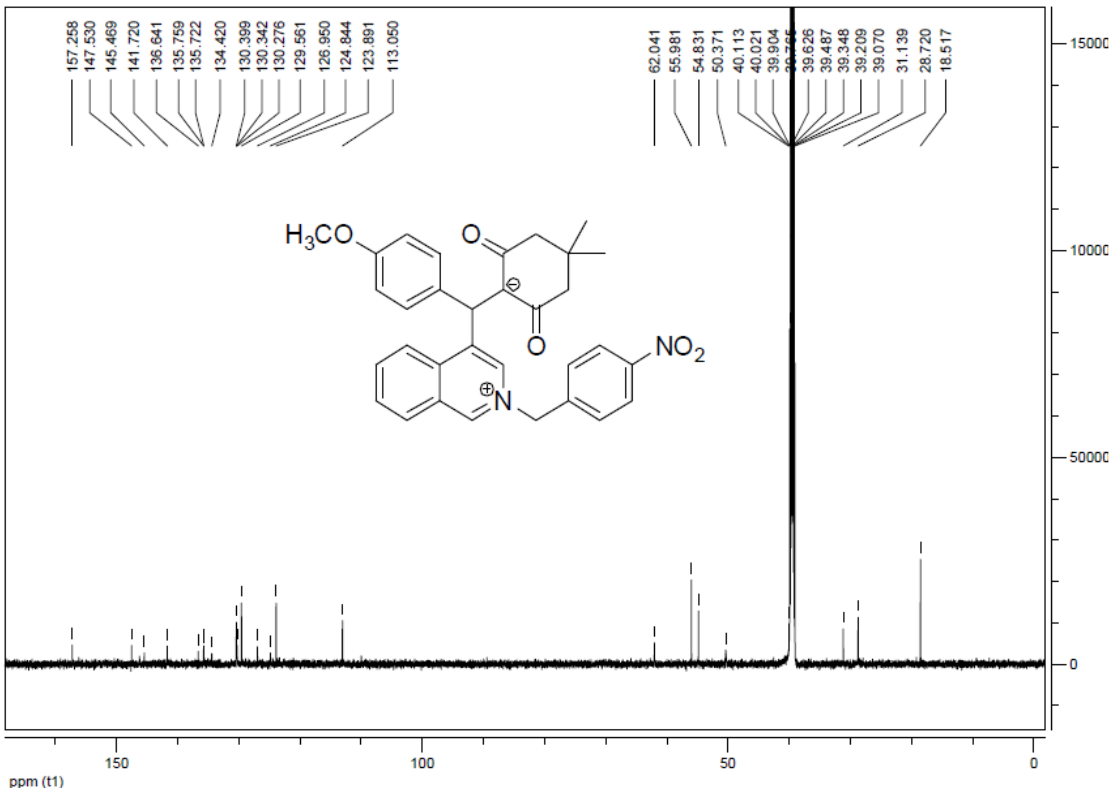
10.0
5.0
0.0
ppm (t1)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135.722
134.420
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129.561
126.950
124.844
123.891
113.050
62.041
55.981
54.831
50.371
40.113
40.021
39.904
39.626
39.487
39.348
39.209
39.070
31.139
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O
O
NO2
N
15000
10000
50000
0
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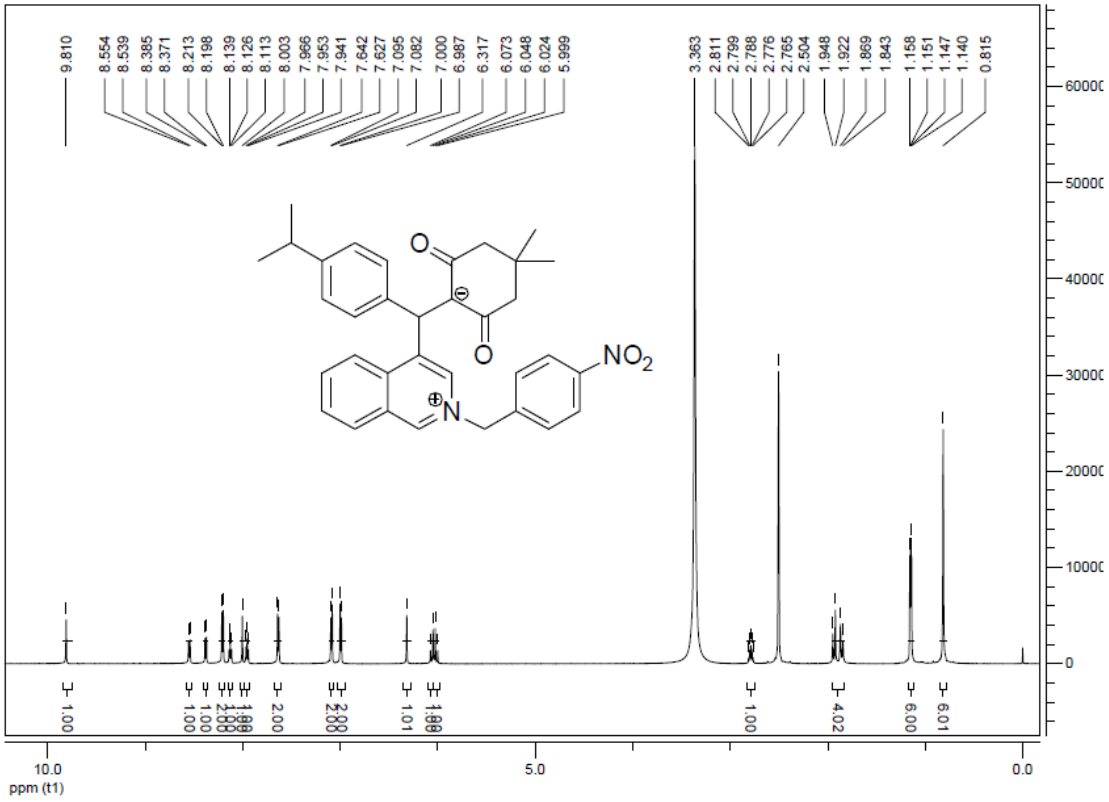
100
50
0
ppm (t1)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8.198
8.139
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8.113
8.003
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7.953
7.941
7.642
7.627
7.095
7.082
7.000
6.987
6.317
6.073
6.048
6.024
5.999
3.363
2.811
2.799
2.788
2.776
2.765
2.504
1.948
1.922
1.869
1.843
1.158
1.151
1.147
1.140
0.815
O
O
NO2
N
1.00
1.00
1.00
2.00
2.00
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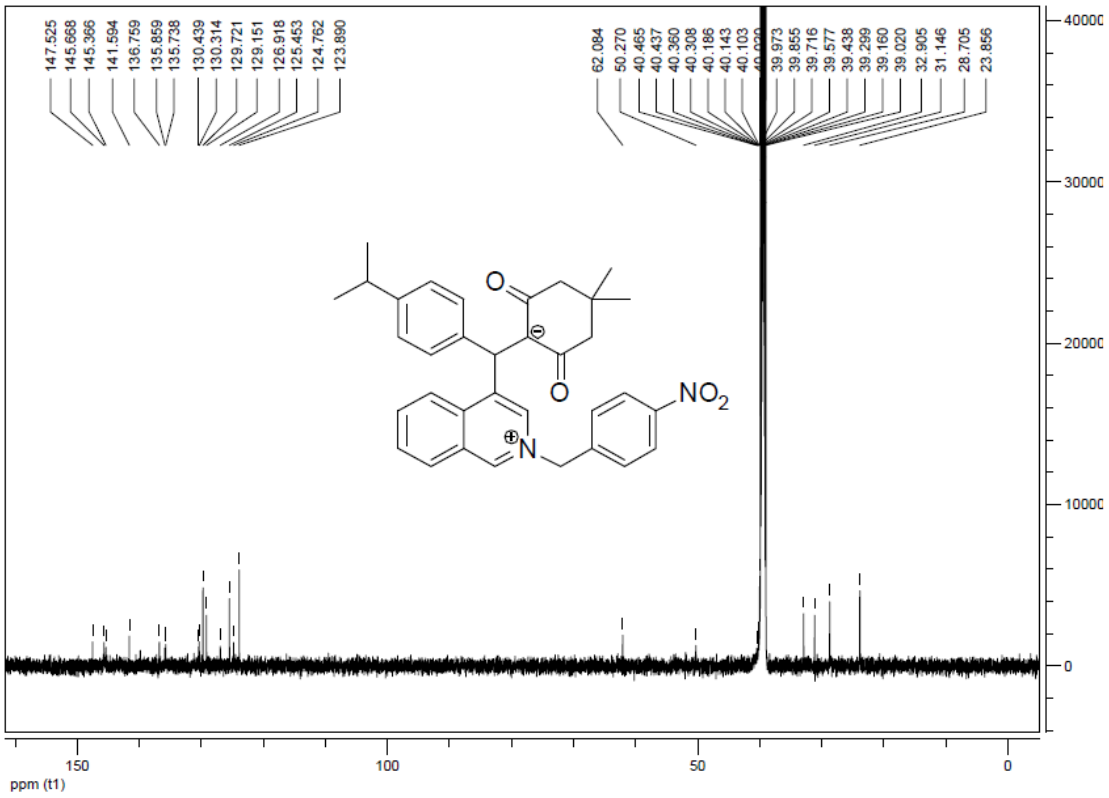
1.00
1.00
4.02
6.00
6.01
10.0
5.0
0.0
ppm (t1)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145.366
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129.151
126.918
125.453
124.762
123.890
62.084
50.270
40.465
40.437
40.360
40.308
40.186
40.143
40.103
39.973
39.855
39.716
39.577
39.438
39.299
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31.146
28.705
23.856
O
O
NO2
N
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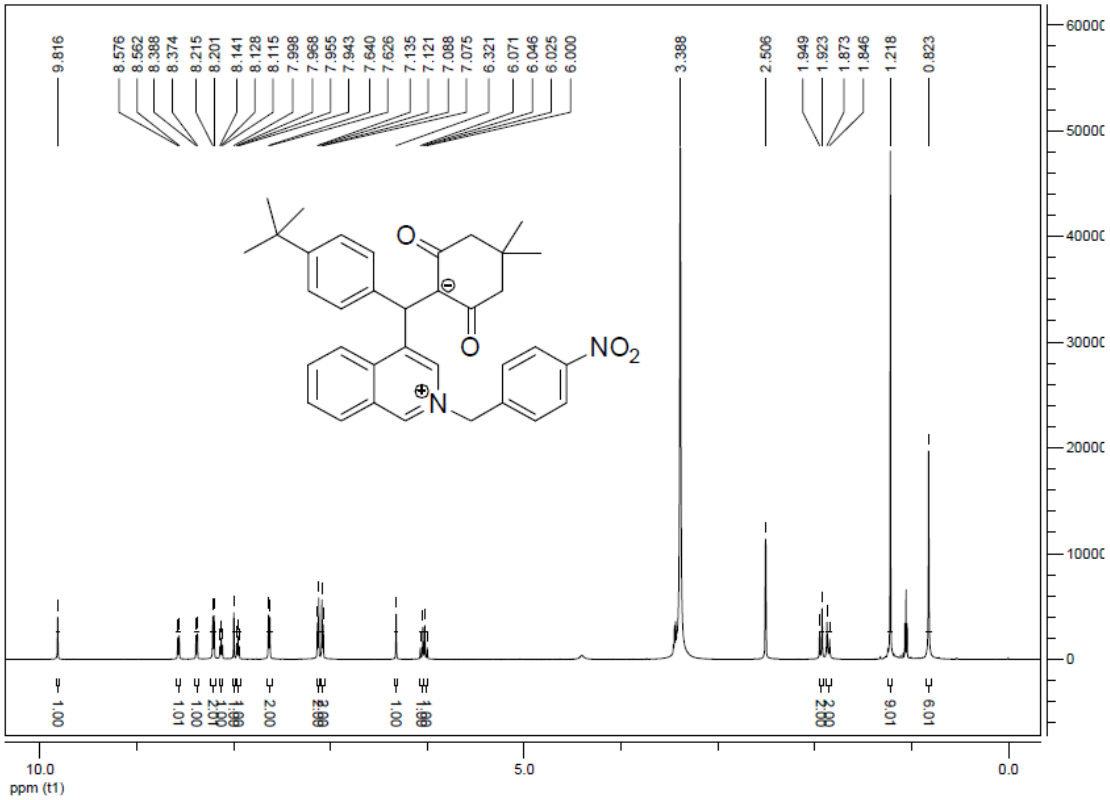
100
50
0
ppm (t1)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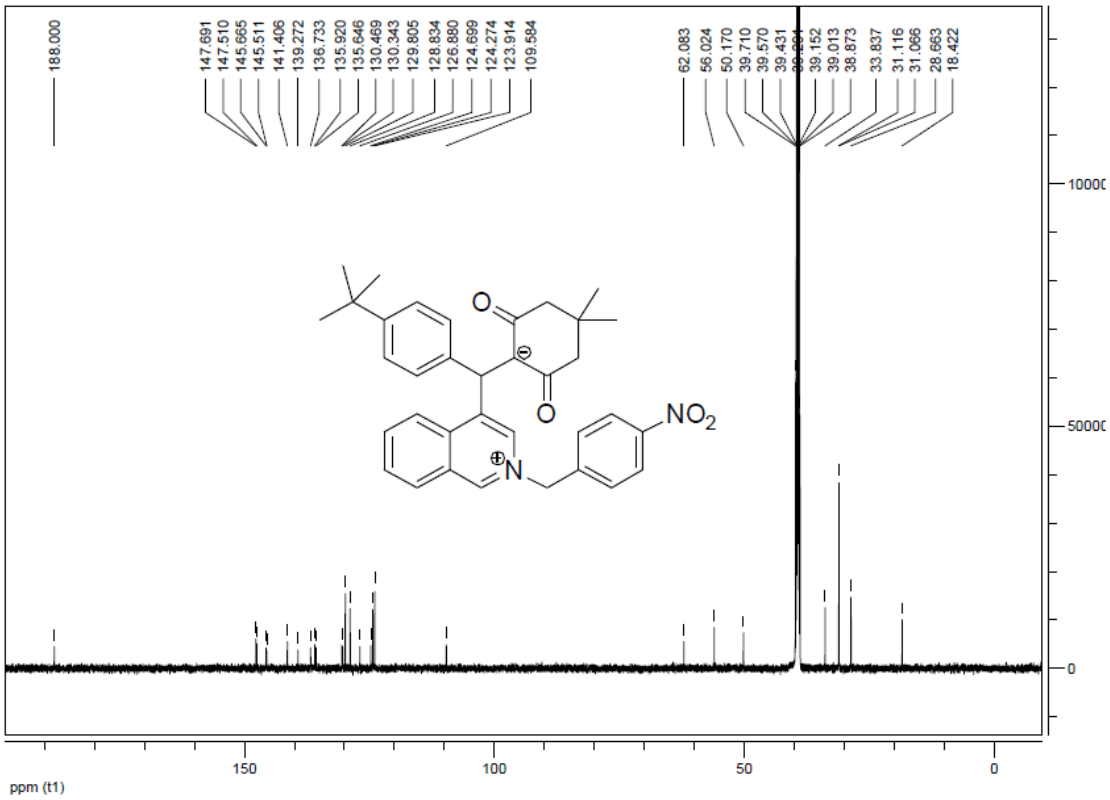
8.215
8.201
8.141
8.128
8.115
7.998
7.968
7.955
7.943
7.640
7.626
7.135
7.121
7.088
7.075
6.321
6.071
6.046
6.025
6.000
3.388
2.506
1.949
1.923
1.873
1.846
1.218
0.823
O
O
N
NO2
10.0
5.0
0.0
ppm (t1)


188.000
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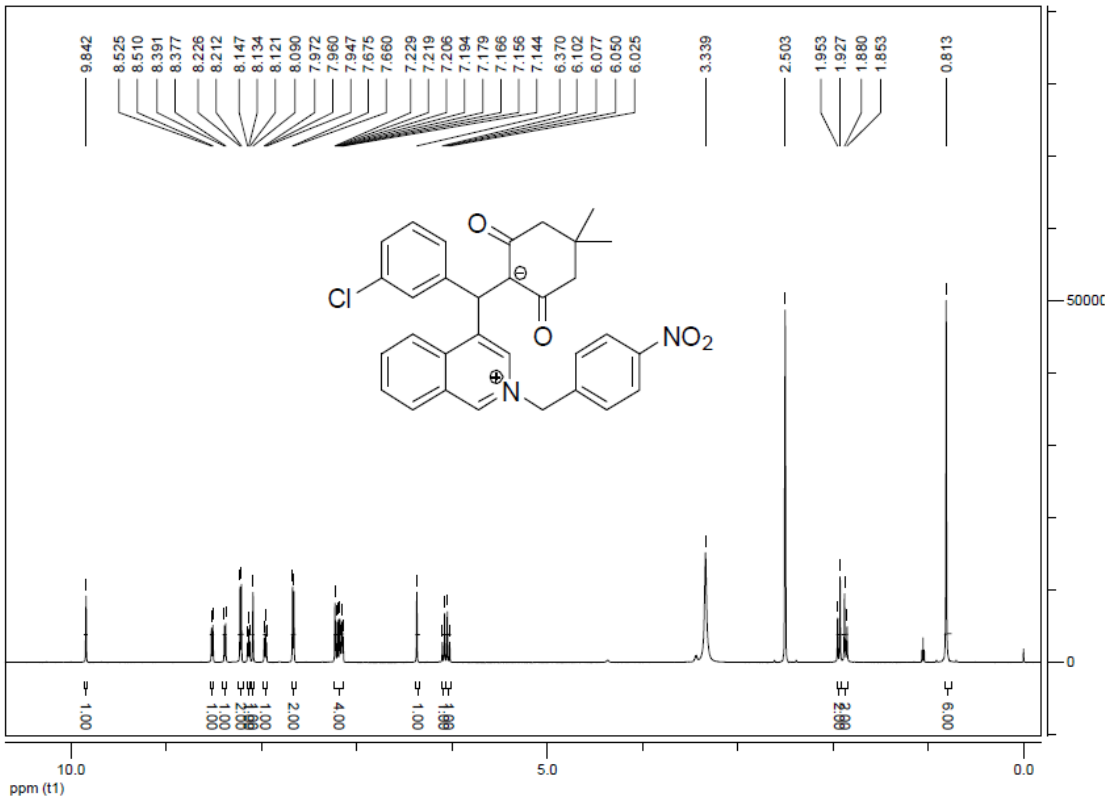
147.510
145.665
145.511
141.406
139.272
136.733
135.920
135.646
130.469
130.343
129.805
128.834
126.880
124.699
124.274
123.914
109.584
62.083
56.024
50.170
39.710
39.570
39.431
39.152
39.013
38.873
33.837
31.116
31.066
28.663
18.422
O
O
N
NO2
150
100
50
0
ppm (t1)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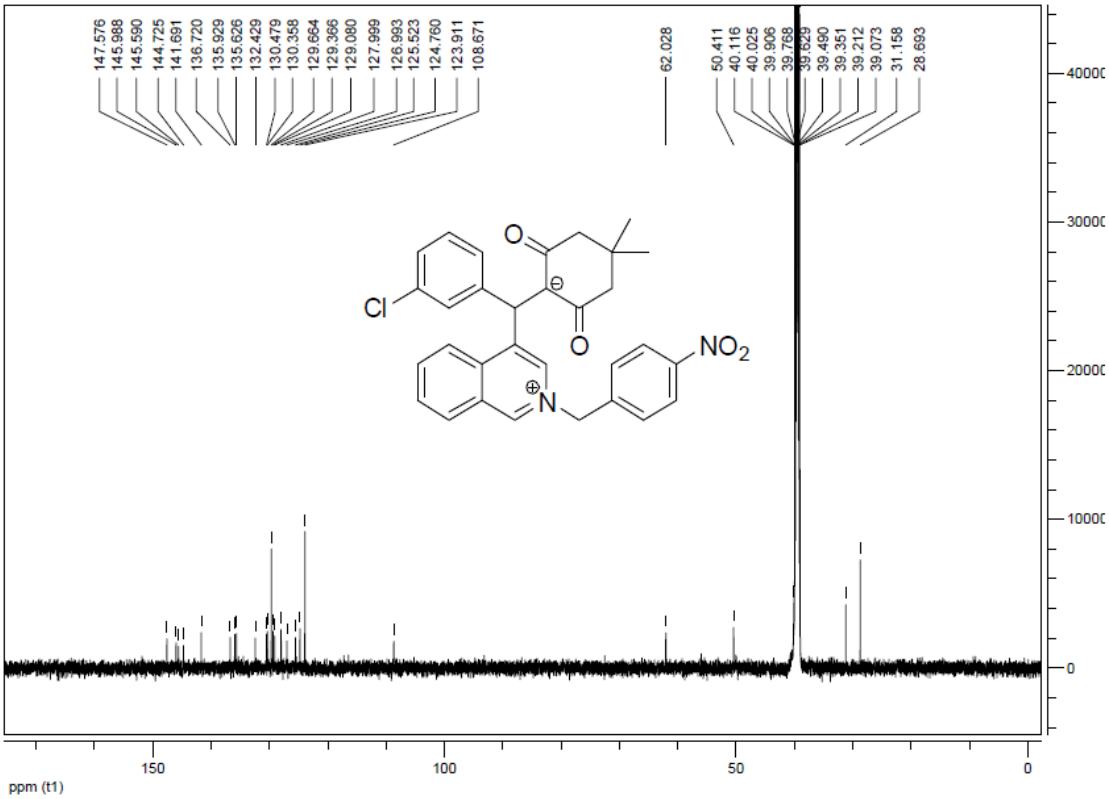
8.510
8.391
8.377
8.226
8.212
8.147
8.134
8.121
8.090
7.972
7.960
7.947
7.675
7.660
7.229
7.219
7.206
7.194
7.179
7.166
7.156
7.144
6.370
6.102
6.077
6.050
6.025
3.339
2.503
1.953
1.927
1.880
1.853
0.813
Cl
O
O
NO2
N
1.00
1.00
2.00
4.00
1.00
2.00
6.00
50000
0
10.0
5.0
0.0
ppm (t1)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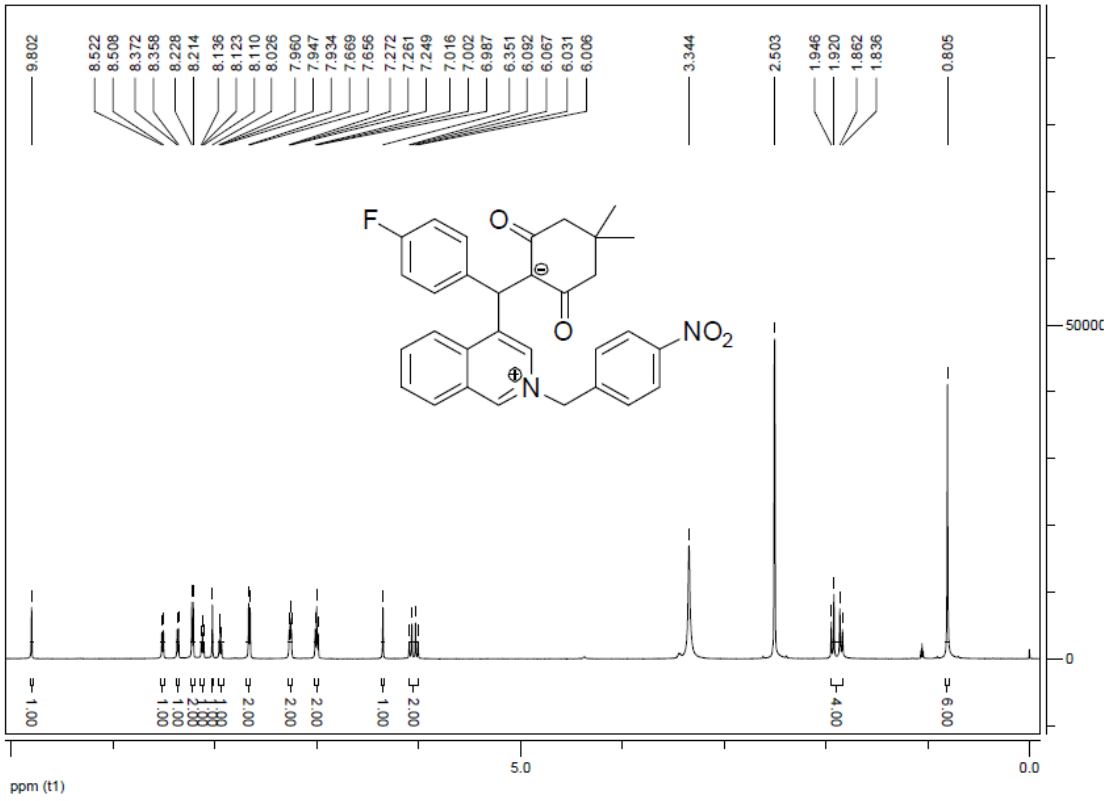
145.590
144.725
141.691
136.720
135.929
135.626
132.429
130.479
130.358
129.664
129.366
129.080
127.999
126.993
125.523
124.760
123.911
108.671
62.028
50.411
40.116
40.025
39.906
39.768
39.629
39.490
39.351
39.212
39.073
31.158
28.693
Cl
O
O
NO2
N
40000
30000
20000
10000
0
150
100
50
0
ppm (t1)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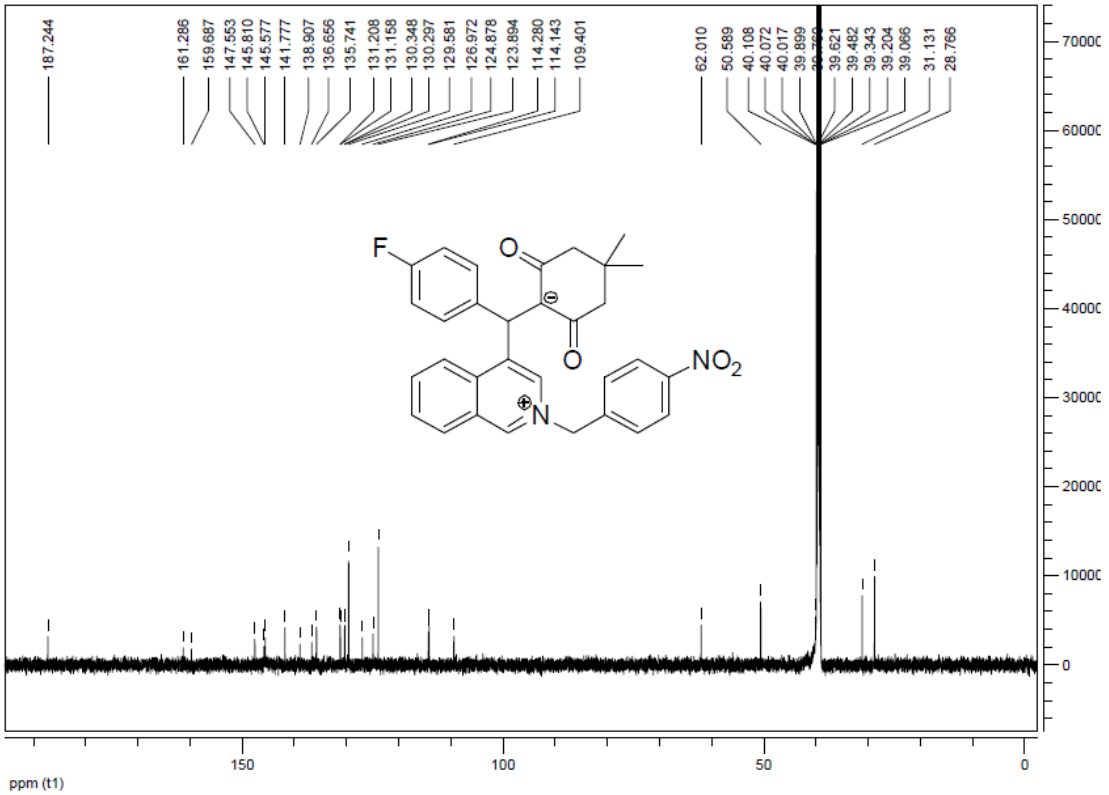
8.228
8.214
8.136
8.123
8.110
8.026
7.960
7.947
7.934
7.669
7.656
7.272
7.261
7.249
7.016
7.002
6.987
6.351
6.092
6.067
6.031
6.006
3.344
2.503
1.946
1.920
1.862
1.836
0.805
F
O
O
NO2
N
50000
0
1.00
1.00
1.00
2.00
2.00
2.00
1.00
2.00
4.00
6.00
5.0
0.0
ppm (t1)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138.907
136.656
135.741
131.208
131.158
130.348
130.297
129.581
126.972
124.878
123.894
114.280
114.143
109.401
62.010
50.589
40.108
40.072
40.017
39.899
39.621
39.482
39.343
39.204
39.066
31.131
28.766
F
O
O
NO2
N
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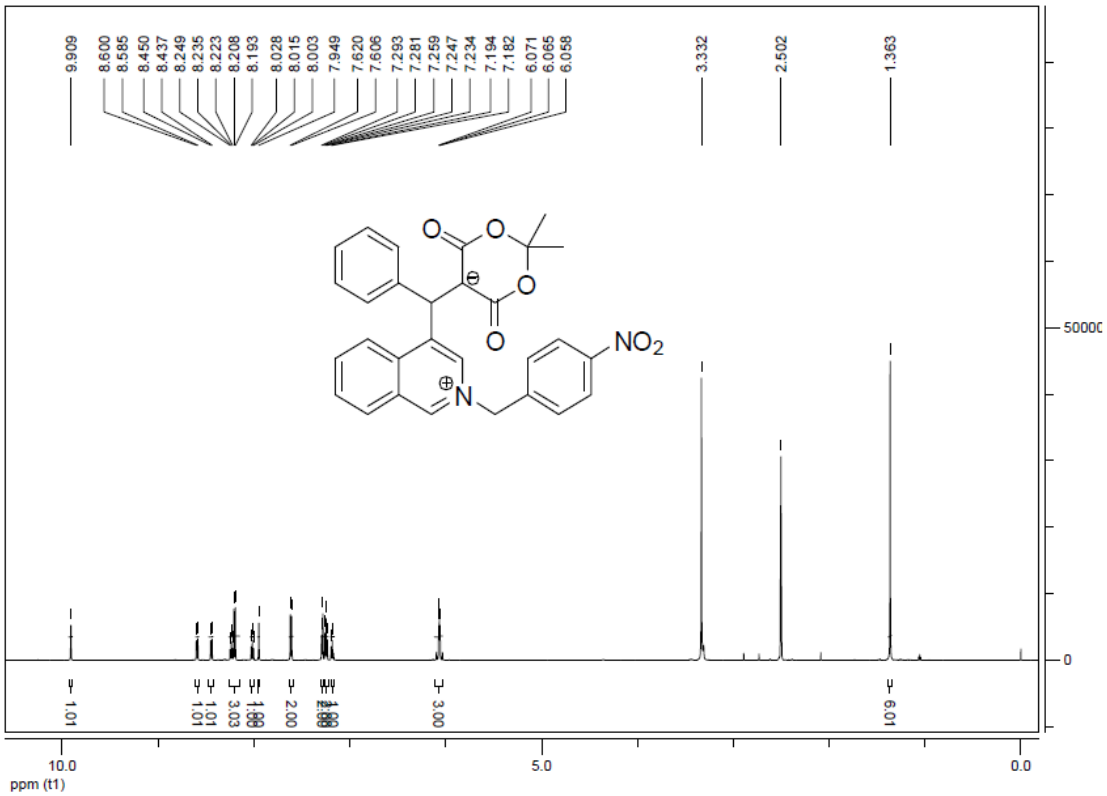
60000
50000
40000
30000
20000
10000
0
150
100
50
0
ppm (t1)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8.450
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8.249
8.235
8.223
8.208
8.193
8.028
8.015
8.003
7.949
7.620
7.606
7.293
7.281
7.259
7.247
7.234
7.194
7.182
6.071
6.065
6.058
3.332
2.502
1.363
NO2
50000
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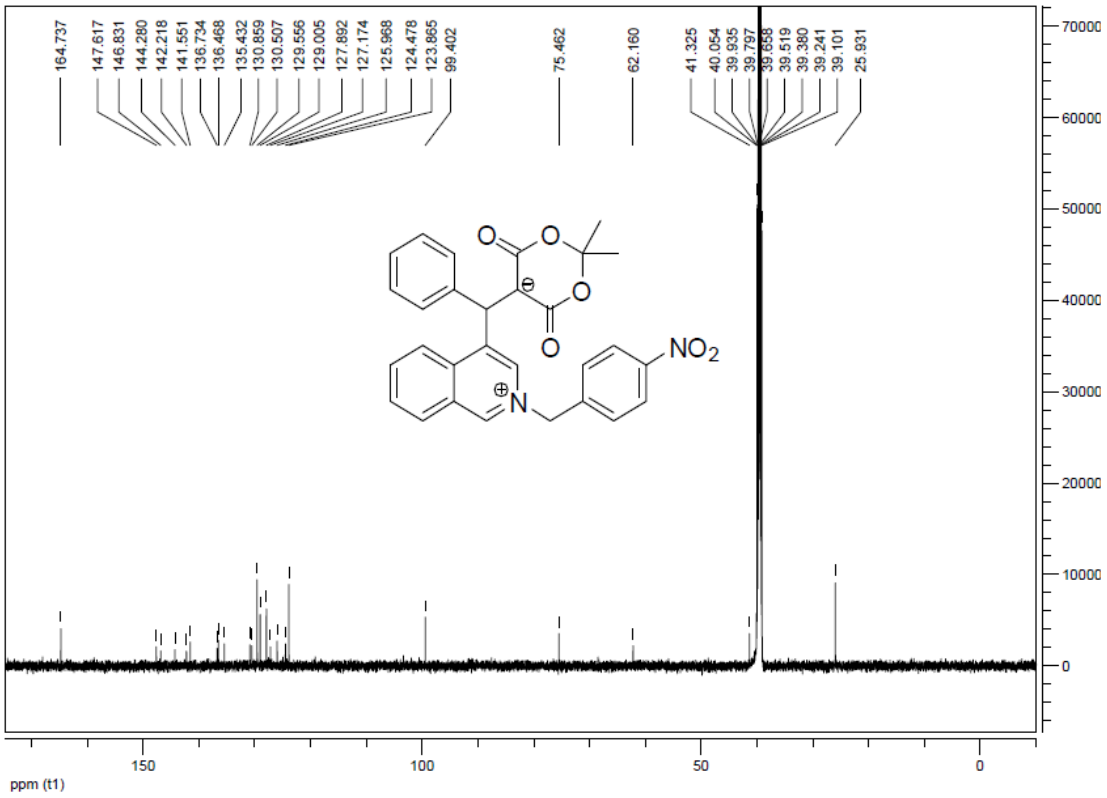
1.01
1.01
3.03
2.00
3.00
6.01
10.0
5.0
0.0
ppm (t1)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144.280
142.218
141.551
136.734
136.468
135.432
130.859
130.507
129.556
129.005
127.892
127.174
125.968
124.478
123.865
99.402
75.462
62.160
41.325
40.054
39.935
39.797
39.658
39.519
39.380
39.241
39.101
25.931
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60000
50000
40000
30000
20000
10000
0
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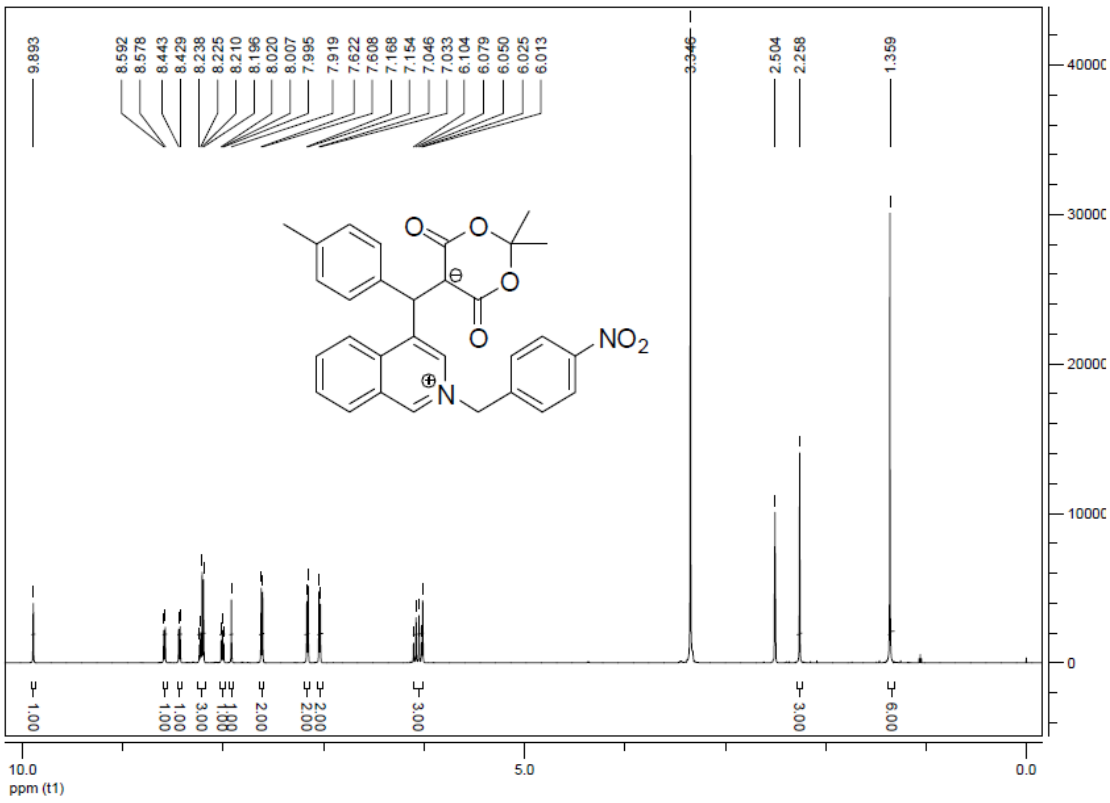
100
50
0
ppm (t1)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8.238
8.225
8.210
8.196
8.020
8.007
7.995
7.919
7.622
7.608
7.168
7.154
7.046
7.033
6.104
6.079
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6.025
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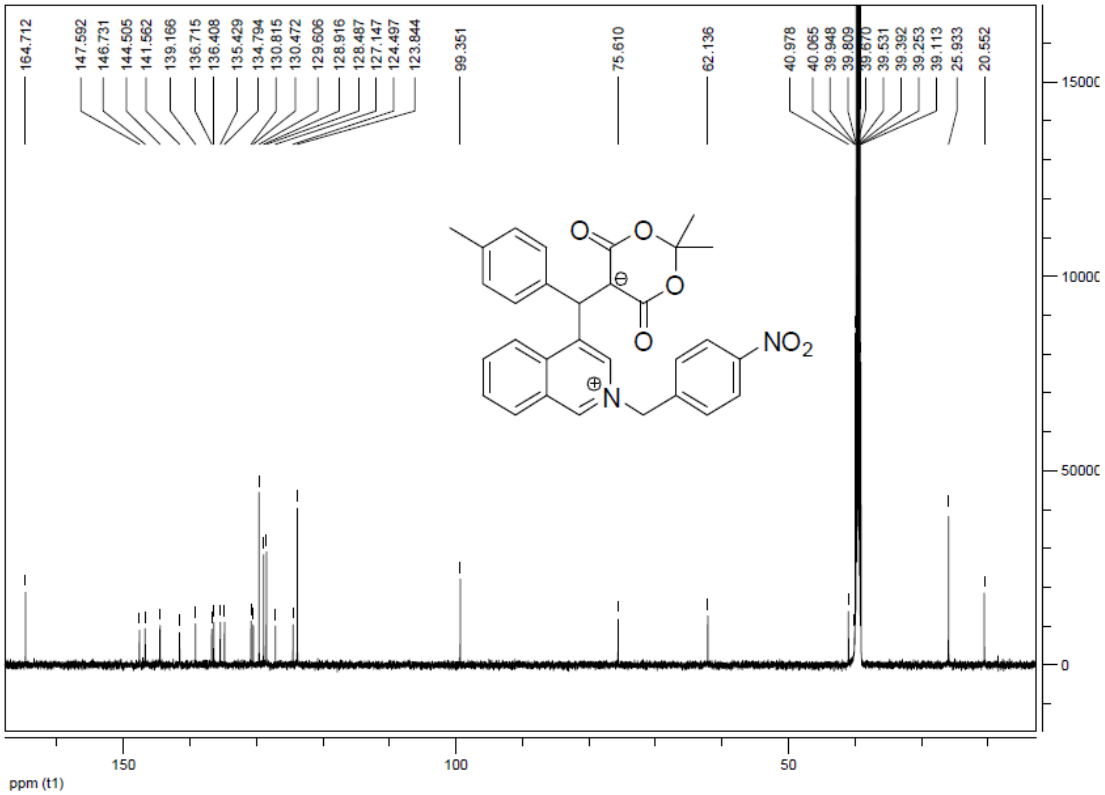
3.346
2.504
2.258
1.359
NO2
10.0
ppm (t1)
5.0
0.0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139.166
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136.408
135.429
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130.815
130.472
129.606
128.916
128.487
127.147
124.497
123.844
99.351
75.610
62.136
40.978
40.065
39.948
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39.113
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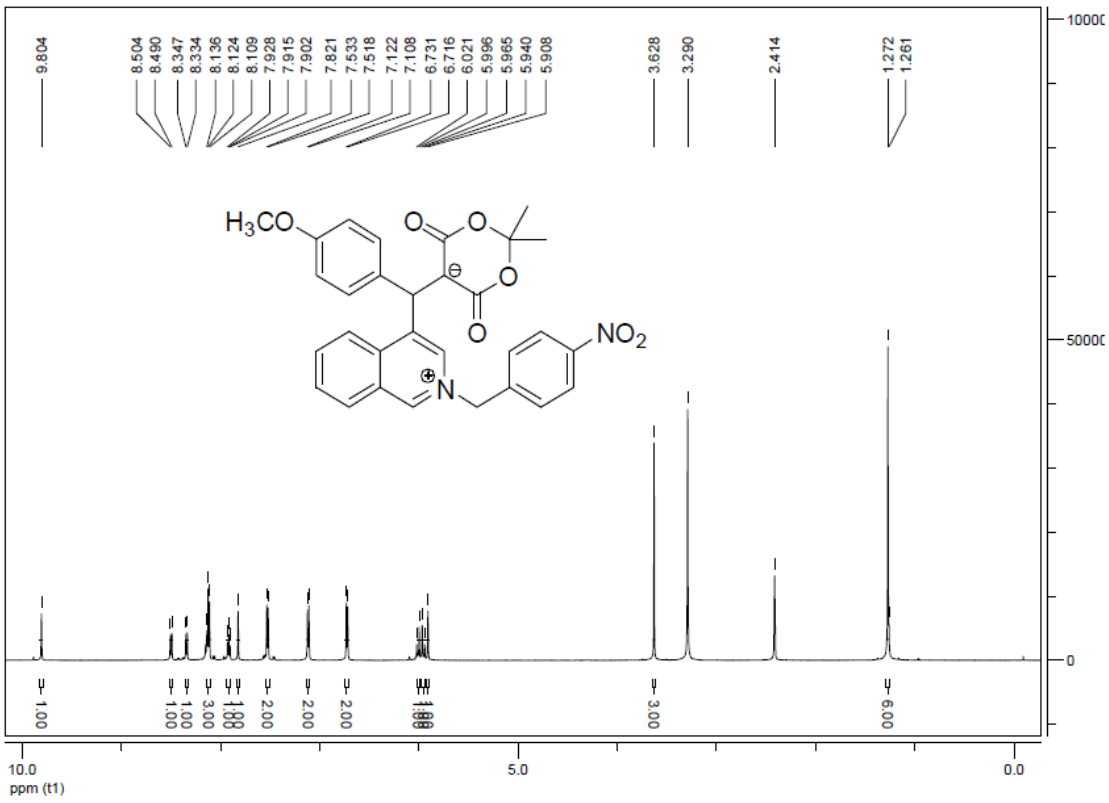
100
50
ppm (t1)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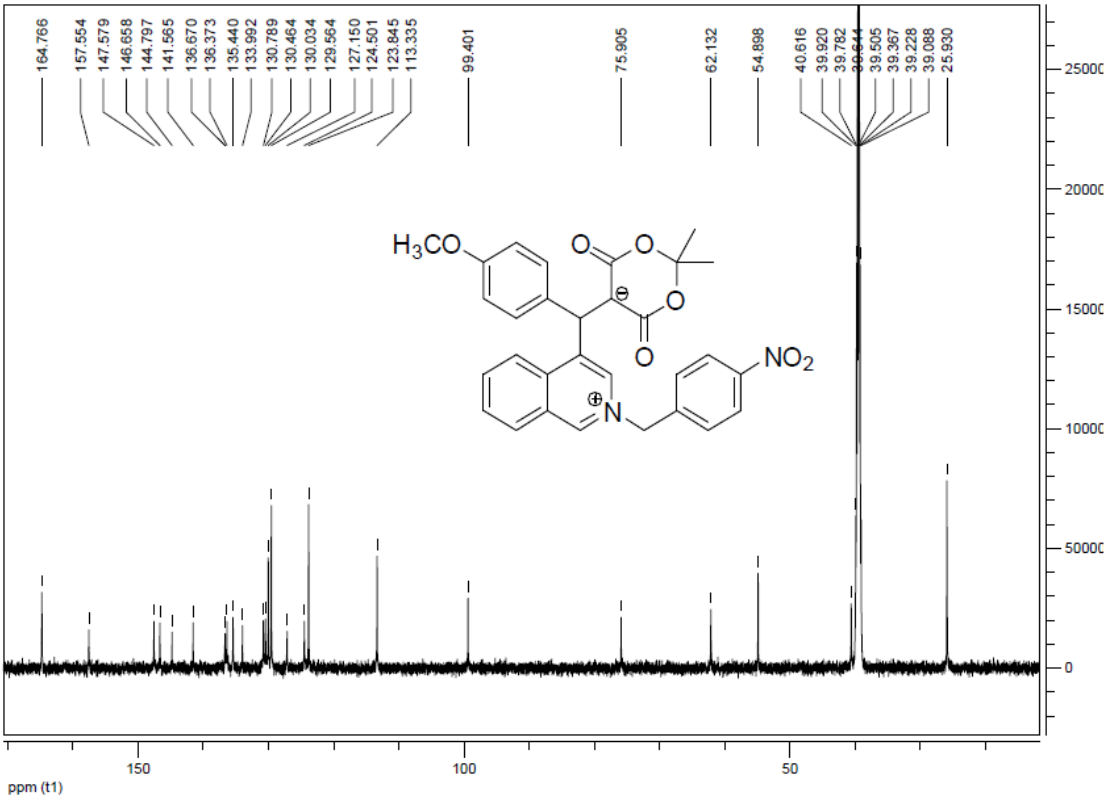
7.902
7.821
7.533
7.518
7.122
7.108
6.731
6.716
6.021
5.996
5.965
5.940
5.908
3.628
3.290
2.414
1.272
1.261
H3CO
O
O
O
O
O
NO2
N
10000
50000
0
1.00
1.00
3.00
1.00
2.00
2.00
2.00
3.00
6.00
10.0
5.0
0.0
ppm (t1)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136.373
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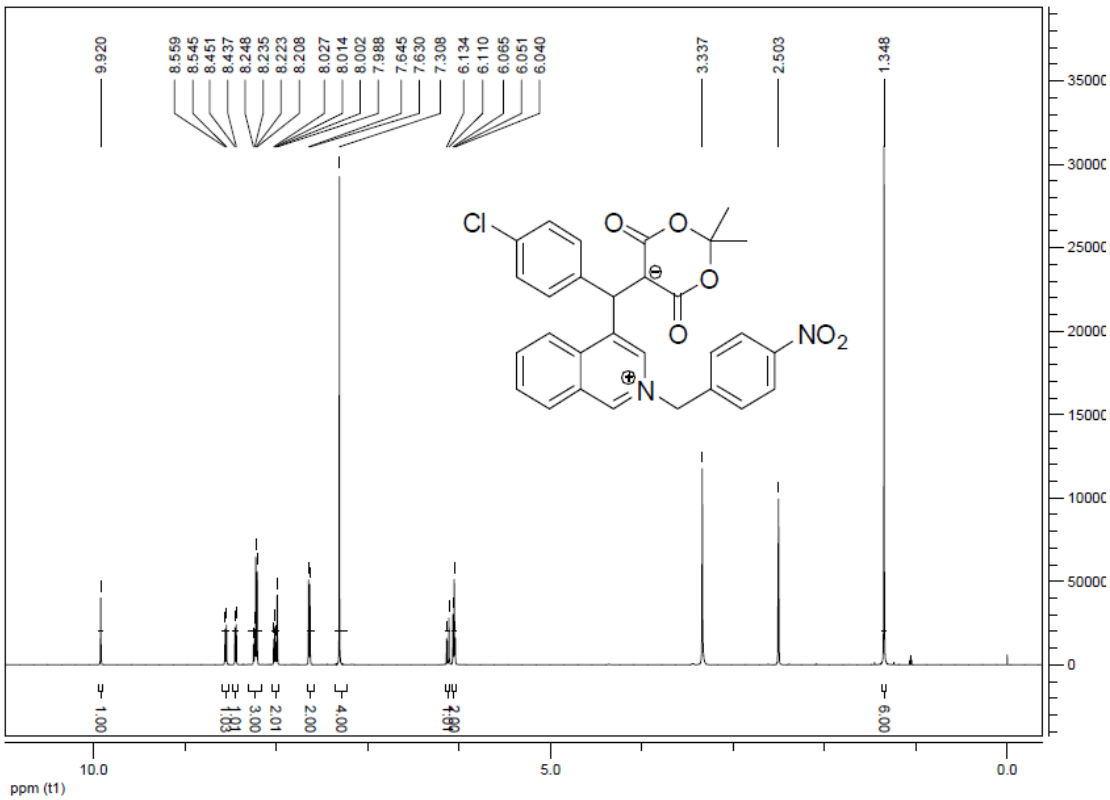
133.992
130.789
130.464
130.034
129.564
127.150
124.501
123.845
113.335
99.401
75.905
62.132
54.898
40.616
39.920
39.782
39.644
39.505
39.367
39.228
39.088
25.930
H3CO
O
O
O
O
O
NO2
N
25000
20000
15000
10000
50000
0
150
100
50
ppm (t1)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8.437
8.248
8.235
8.223
8.208
8.027
8.014
8.002
7.988
7.645
7.630
7.308
6.134
6.110
6.065
6.051
6.040
3.337
2.503
1.348
Cl
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O
O
O
O
NO2
N
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2.00
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2.00
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10.0
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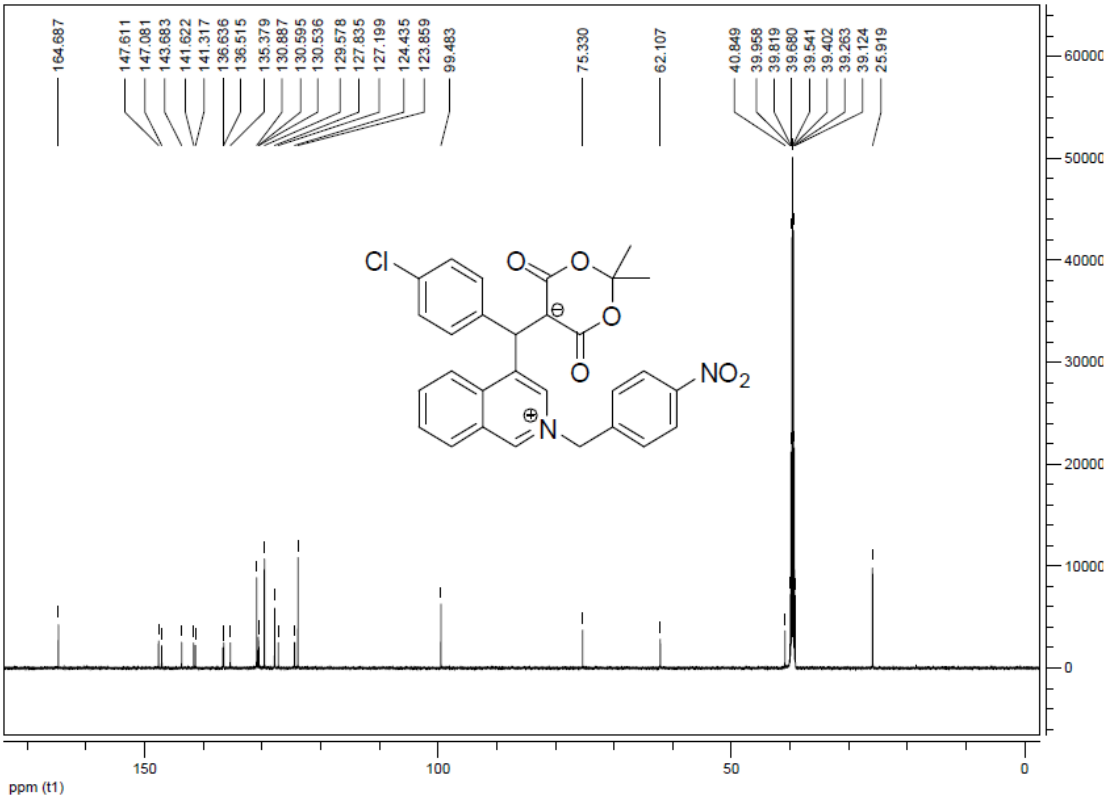
ppm (t1)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141.317
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136.515
135.379
130.887
130.595
130.536
129.578
127.835
127.199
124.435
123.859
99.483
75.330
62.107
40.849
39.958
39.819
39.680
39.541
39.402
39.263
39.124
25.919
Cl
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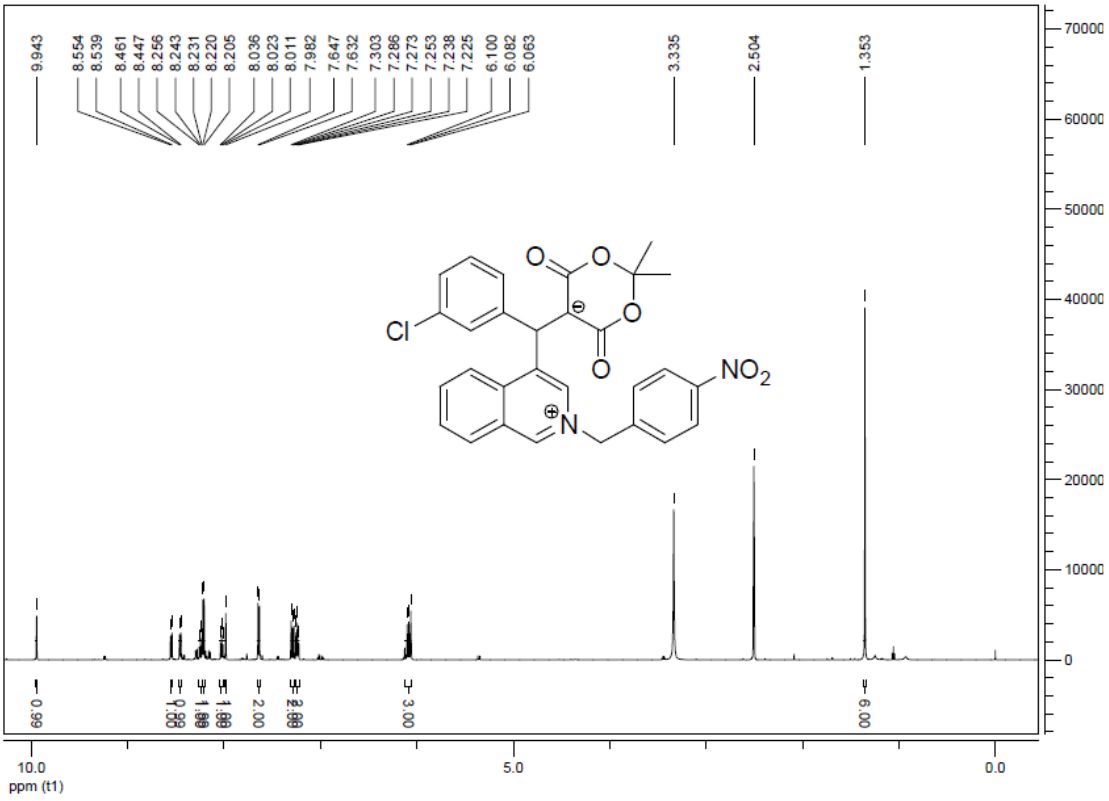
O
O
O
O
NO2
N
150
100
50
0
ppm (t1)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8.256
8.243
8.231
8.220
8.205
8.036
8.023
8.011
7.982
7.647
7.632
7.303
7.286
7.273
7.253
7.238
7.225
6.100
6.082
6.063
3.335
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NO2
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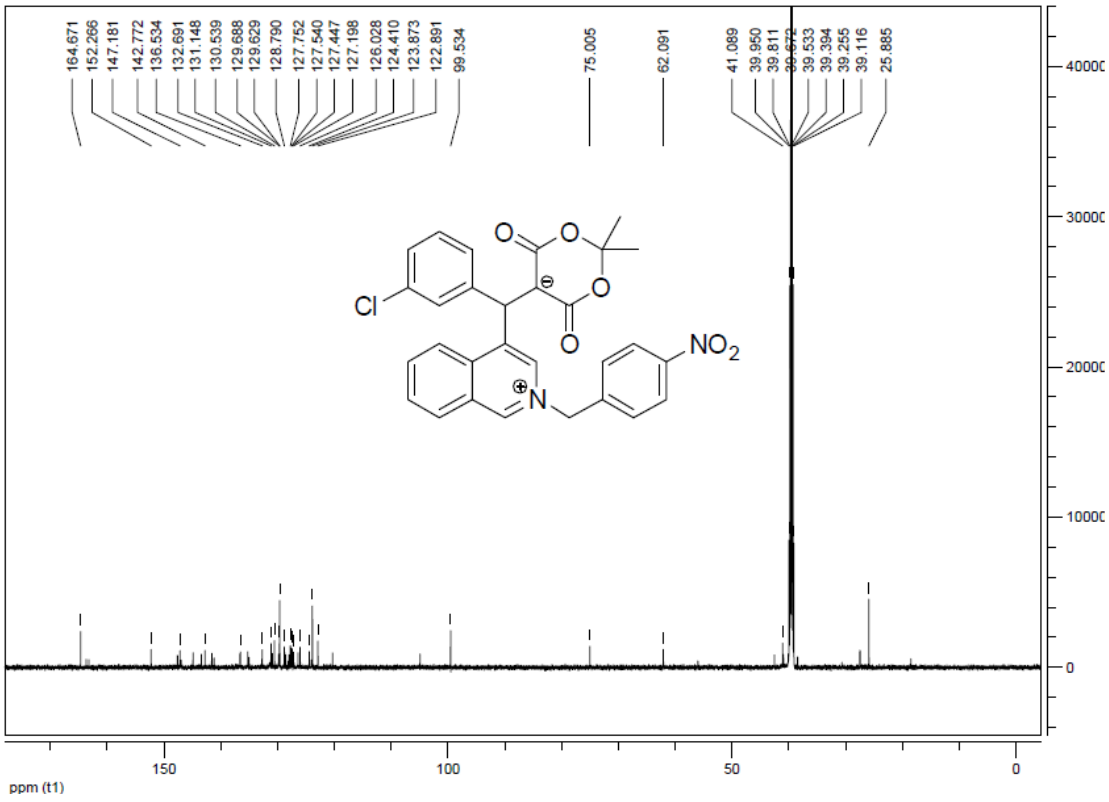
3.00
6.00
10.0
5.0
0.0
ppm (t1)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130.539
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127.540
127.447
127.198
126.028
124.410
123.873
122.891
99.534
75.005
62.091
41.089
39.950
39.811
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39.394
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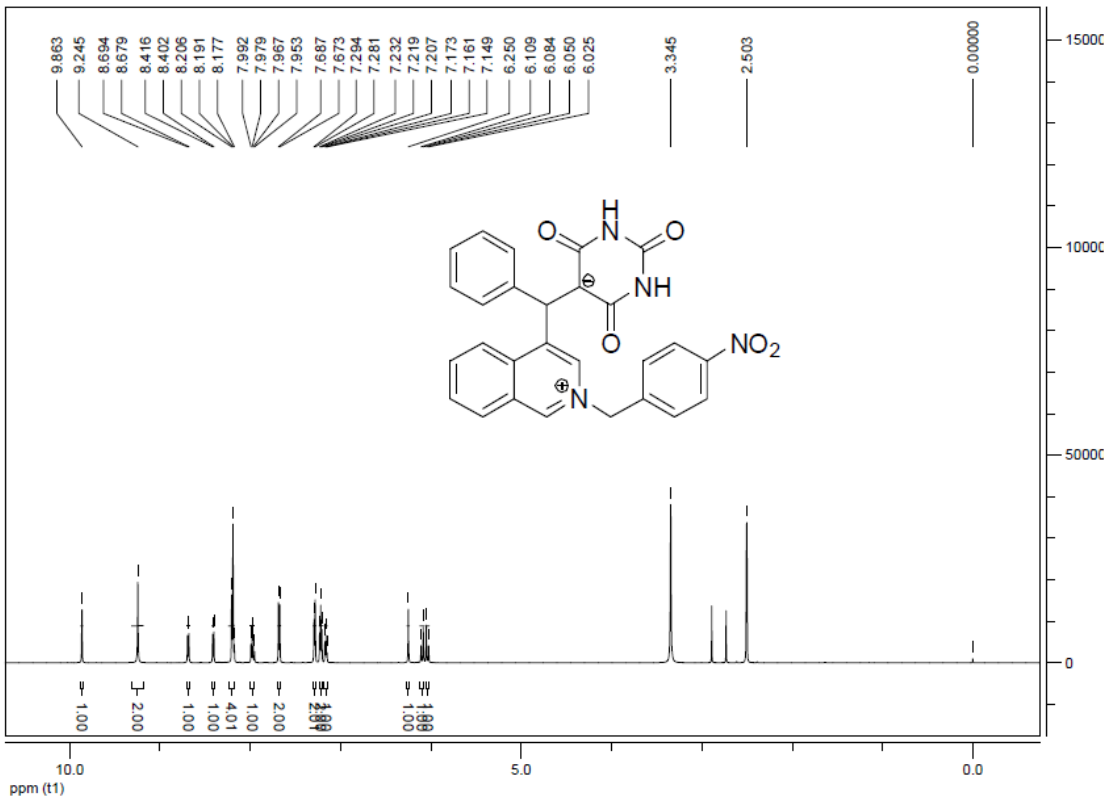
ppm (t1)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7.953
7.687
7.673
7.294
7.281
7.232
7.219
7.207
7.173
7.161
7.149
6.250
6.109
6.084
6.050
6.025
3.345
2.503
0.00000
NO2
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2.00
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1.00
4.01
1.00
2.00
1.00
10.0
5.0
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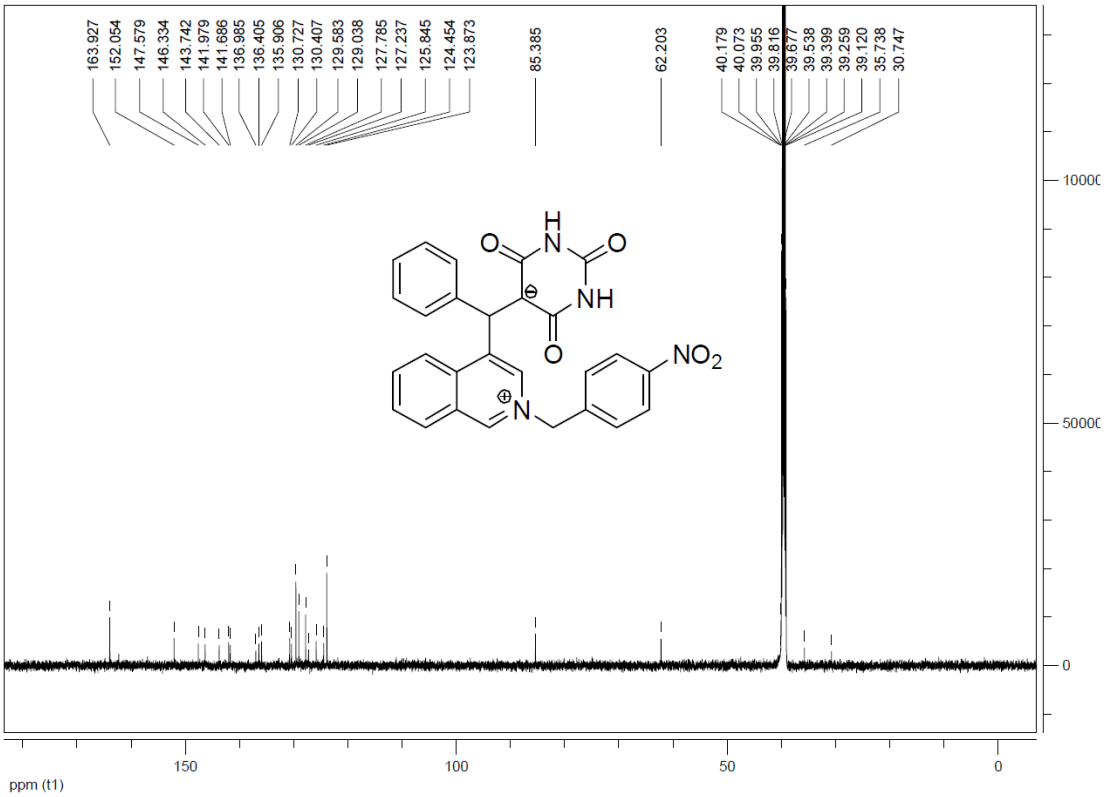
ppm (t1)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129.038
127.785
127.237
125.845
124.454
123.873
85.385
62.203
40.179
40.073
39.955
39.816
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39.259
39.120
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30.747
NO2
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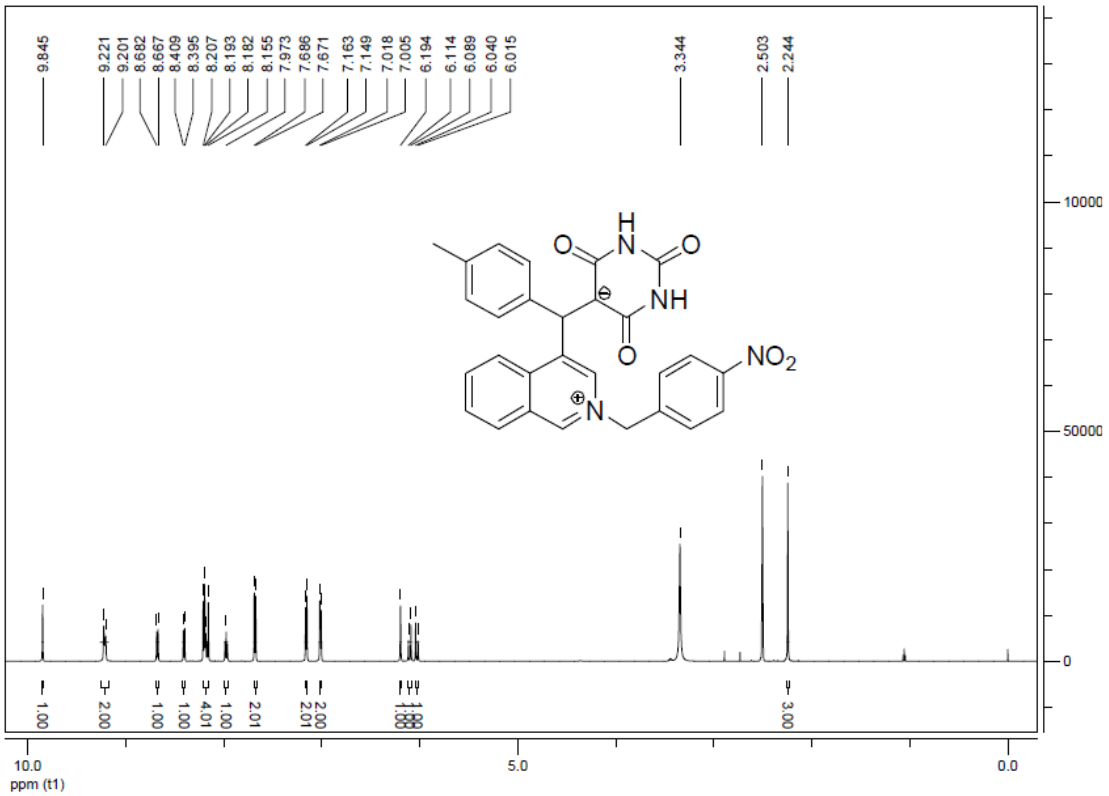
100
50
0
ppm (t1)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9.201
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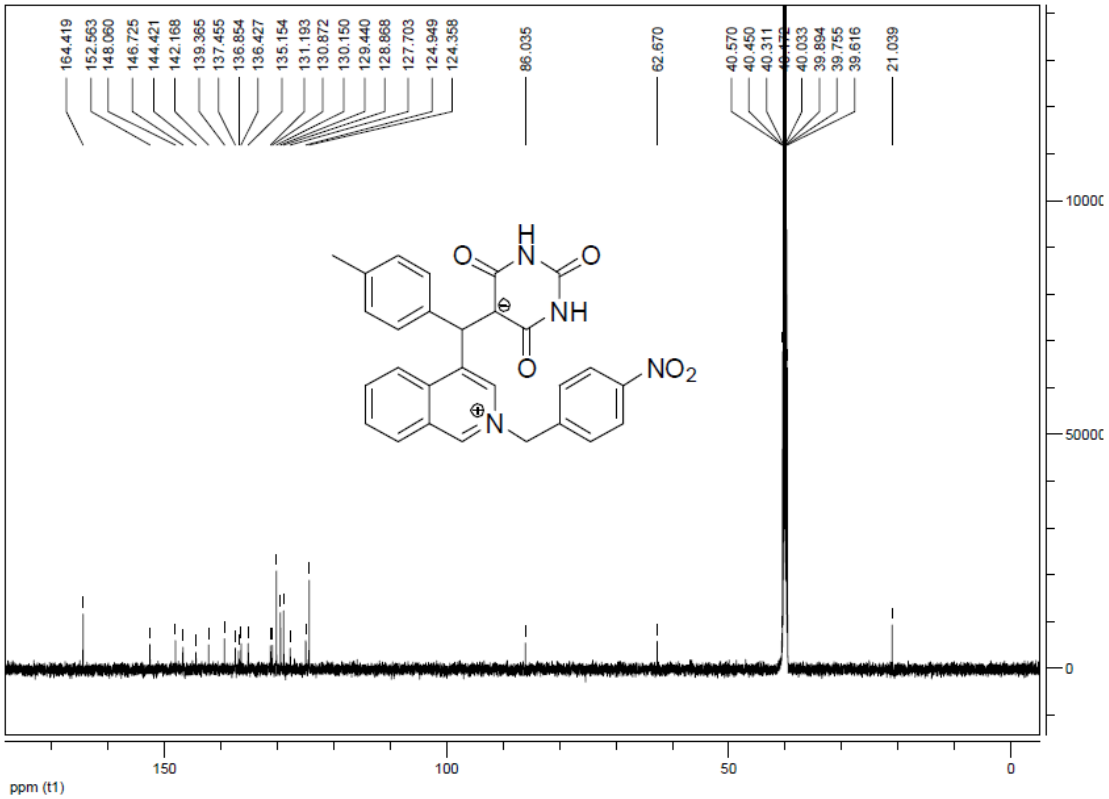
8.182
8.155
7.973
7.686
7.671
7.163
7.149
7.018
7.005
6.194
6.114
6.089
6.040
6.015
3.344
2.503
2.244
10000
50000
0
1.00
2.00
1.00
1.00
4.01
1.00
2.01
2.00
2.01
1.00
1.00
3.00
10.0
5.0
0.0
ppm (t1)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152.563
148.060
146.725
144.421
142.168
139.365
137.455
136.854
136.427
135.154
131.193
130.872
130.150
129.440
128.868
127.703
124.949
124.358
86.035
62.670
40.570
40.450
40.311
40.033
39.894
39.755
39.616
21.039
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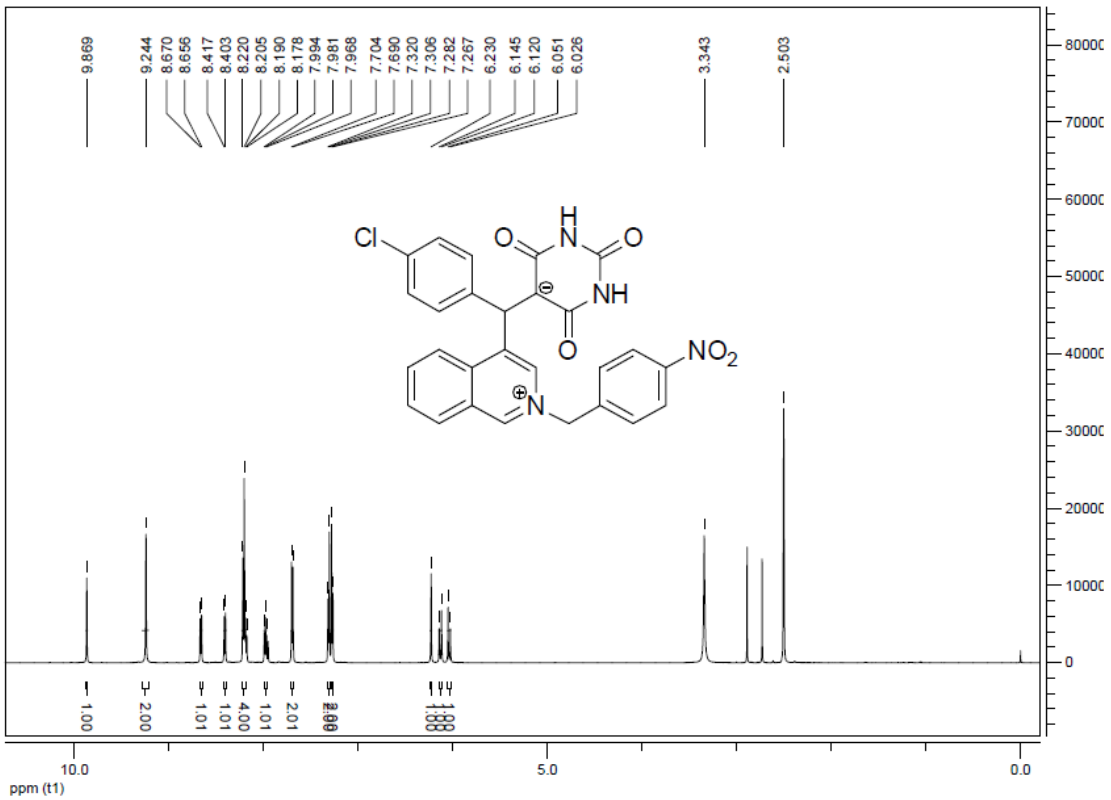
100
50
0
ppm (t1)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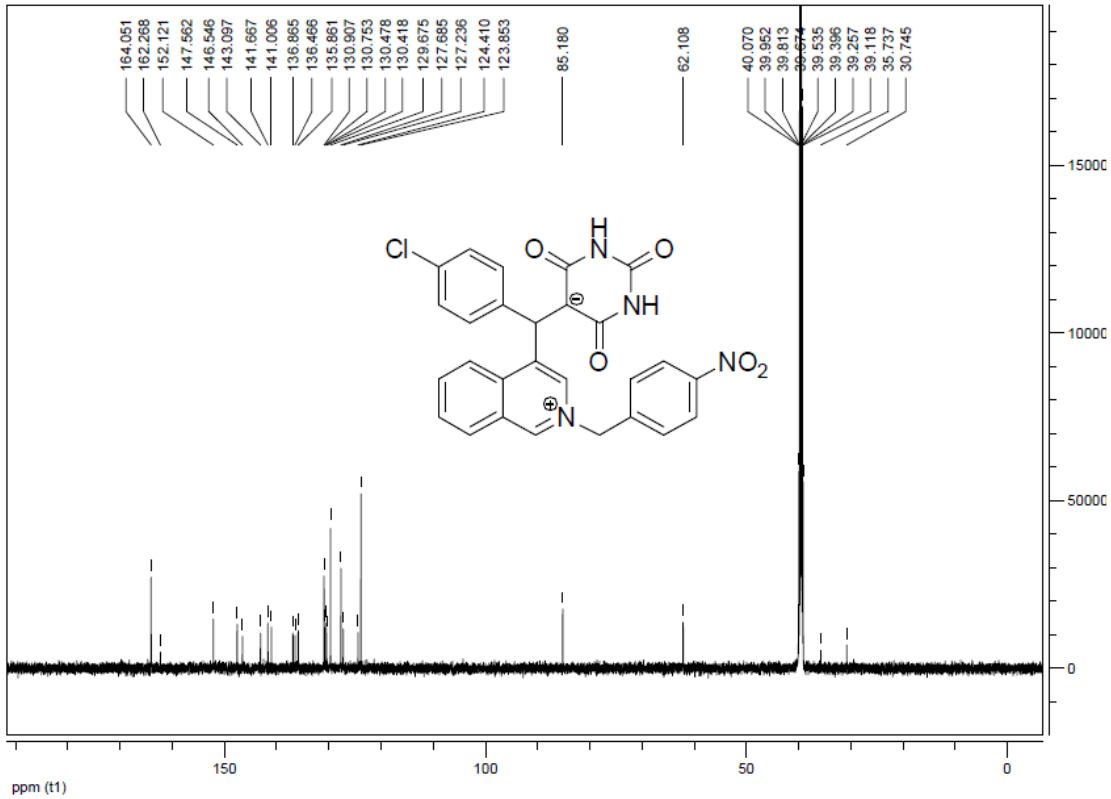
8.656
8.417
8.403
8.220
8.205
8.190
8.178
7.994
7.981
7.968
7.704
7.690
7.320
7.306
7.282
7.267
6.230
6.145
6.120
6.051
6.026
3.343
2.503
Cl
O
H
N
O
NH
O
NO2
N
1.00
2.00
1.01
1.01
4.00
1.01
2.01
10.0
5.0
0.0
ppm (t1)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162.268
152.121
147.562
146.546
143.097
141.667
141.006
136.865
136.466
135.861
130.907
130.753
130.478
130.418
129.675
127.685
127.236
124.410
123.853
85.180
62.108
40.070
39.952
39.813
39.535
39.396
39.257
39.118
35.737
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Cl
O
H
N
O
NH
O
NO2
N
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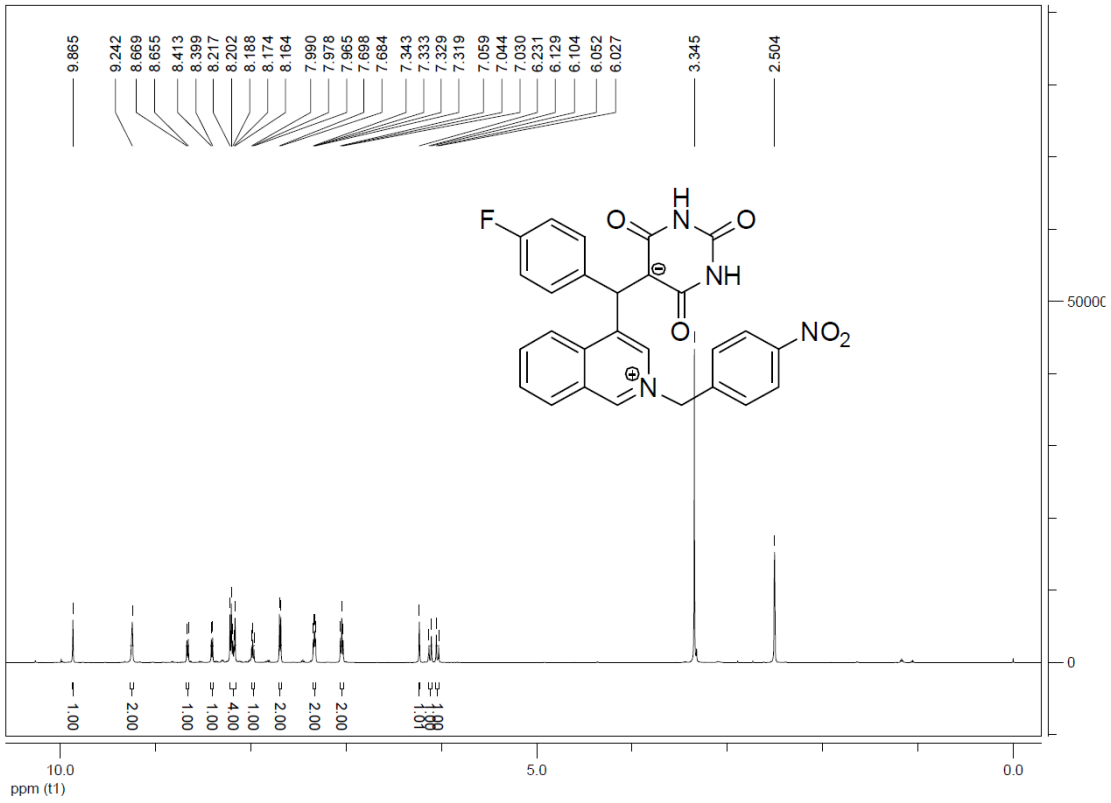
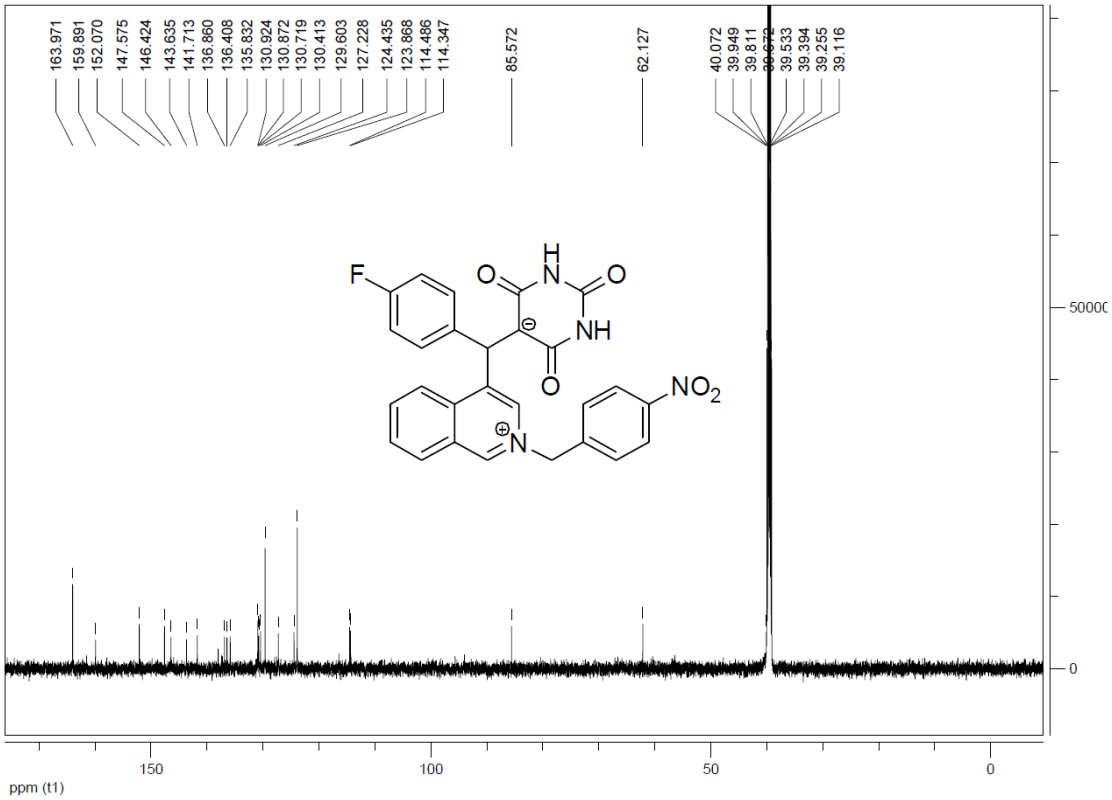
100
50
0
ppm (t1)


9.865
9.242
8.669
8.655
8.413
8.399
8.217
8.202
8.188
8.174
8.164
7.990
7.978
7.965
7.698
7.684
7.343
7.333
7.329
7.319
7.059
7.044
7.030
6.231
6.129
6.104
6.052
6.027
3.345
2.504
F
O
H
N
O
NH
O
NO2
N
1.00
2.00
1.00
1.00
4.00
1.00
2.00
2.00
2.00
50000
0
10.0
5.0
0.0
ppm (t1)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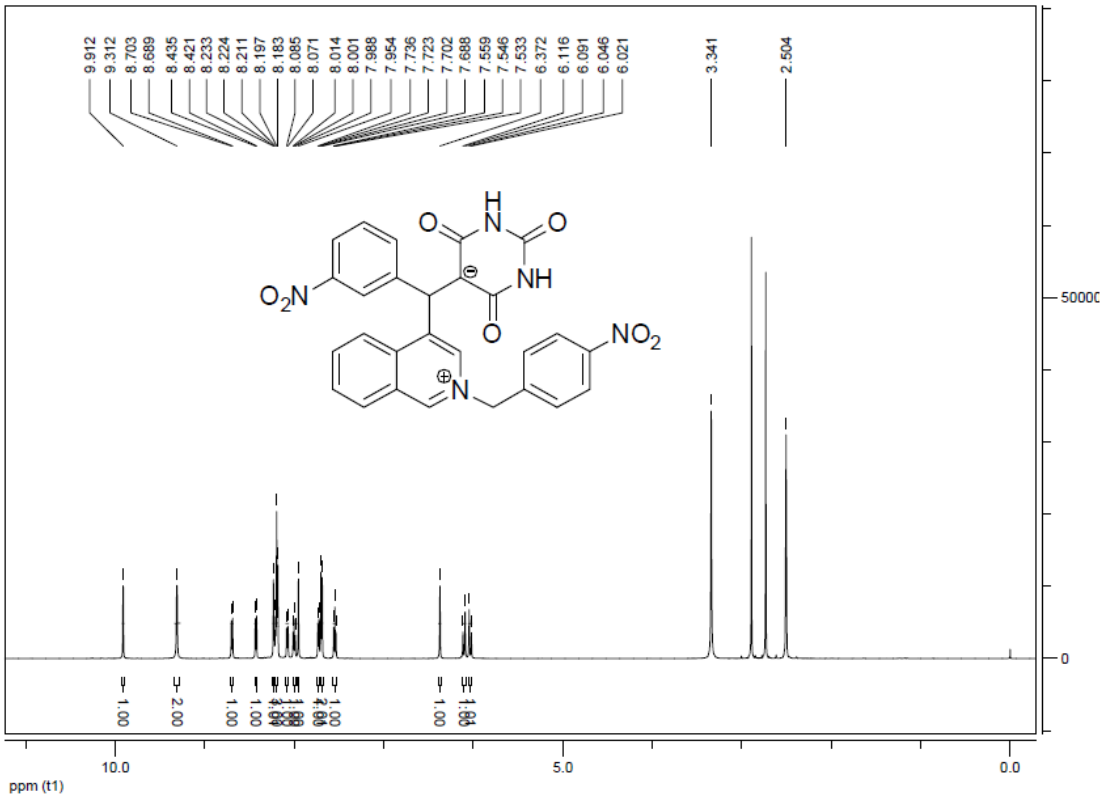
152.070
147.575
146.424
143.635
141.713
136.860
136.408
135.832
130.924
130.872
130.719
130.413
129.603
127.228
124.435
123.868
114.486
114.347
85.572
62.127
40.072
39.949
39.811
39.533
39.394
39.255
39.116
F
O
H
N
O
NH
O
NO2
N
50000
0
150
100
50
0
ppm (t1)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9.312
8.703
8.689
8.435
8.421
8.233
8.224
8.211
8.197
8.183
8.085
8.071
8.014
8.001
7.988
7.954
7.736
7.723
7.702
7.688
7.559
7.546
7.533
6.372
6.116
6.091
6.046
6.021
3.341
2.504
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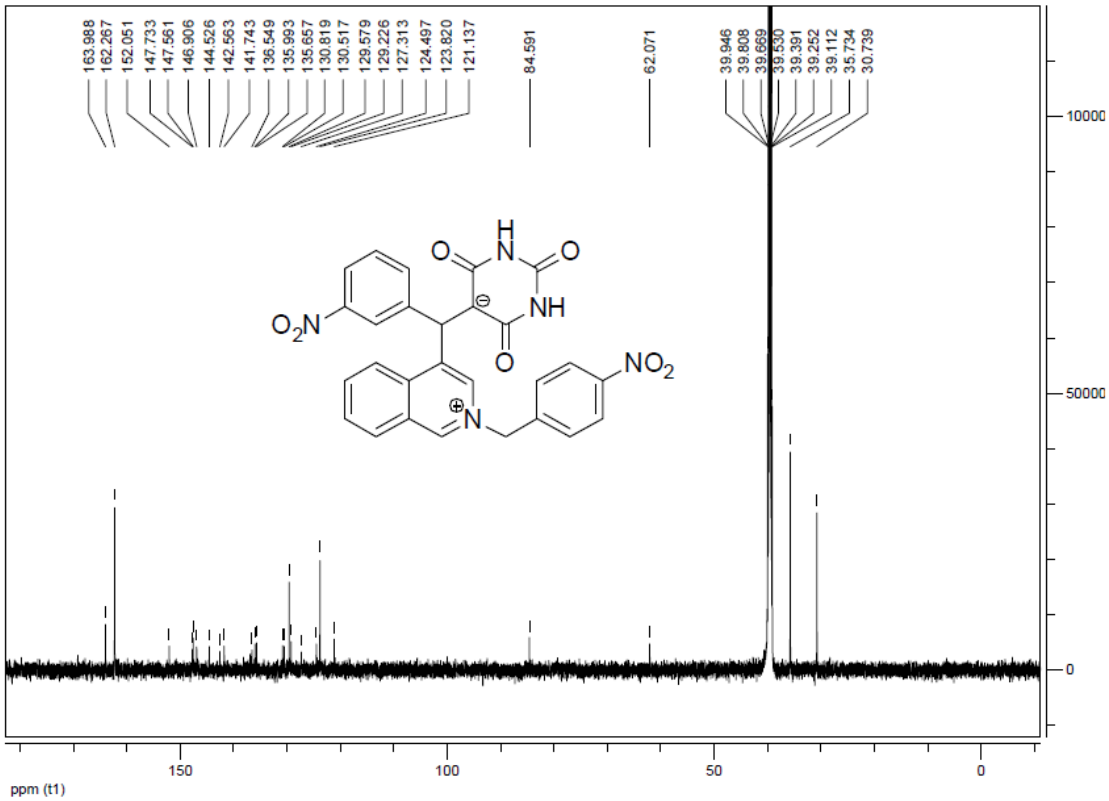
2.00
1.00
1.00
1.00
1.00
10.0
5.0
0.0
ppm (t1)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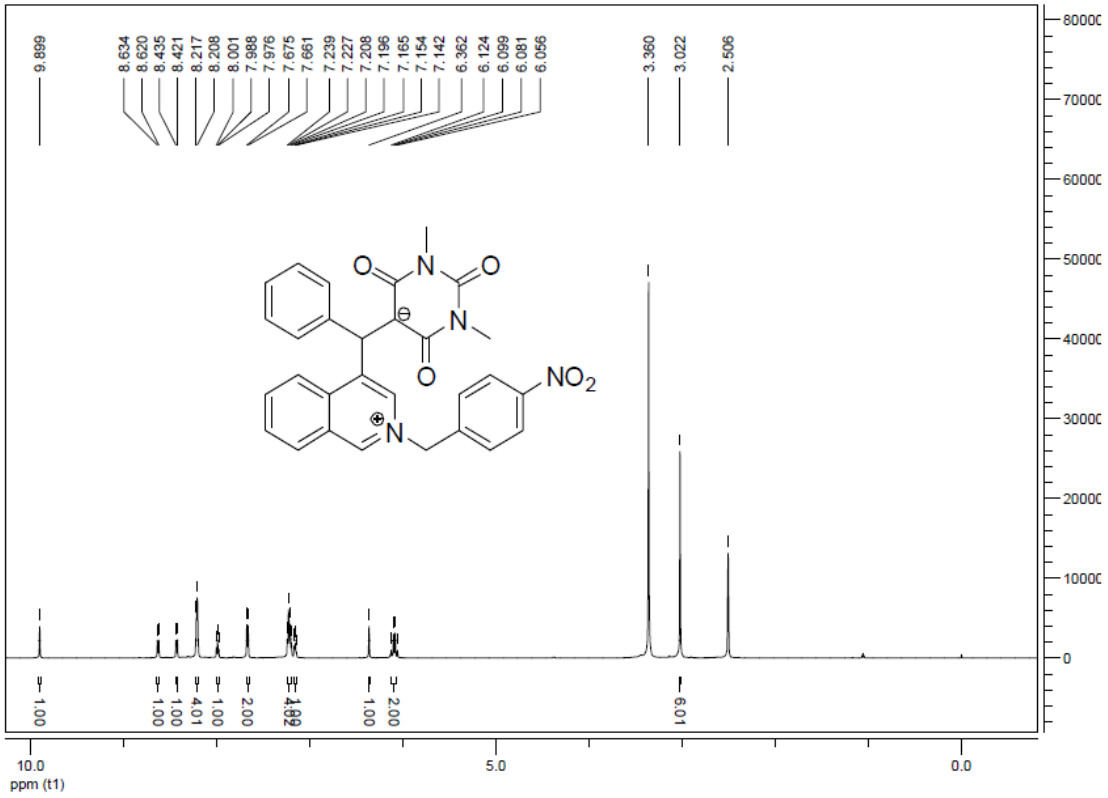
162.267
152.051
147.733
147.561
146.906
144.526
142.563
141.743
136.549
135.993
135.657
130.819
130.517
129.579
129.226
127.313
124.497
123.820
121.137
84.591
62.071
39.946
39.808
39.669
39.530
39.391
39.252
39.112
35.734
30.739
10000
50000
0
150
100
50
0
ppm (t1)


9.899
8.634
8.620
8.435
8.421
8.217
8.208
8.001
7.988
7.976
7.675
7.661
7.239
7.227
7.208
7.196
7.165
7.154
7.142
6.362
6.124
6.099
6.081
6.056
3.360
3.022
2.506
O
N
O
N
O
NO2
N
1.00
1.00
1.00
4.01
1.00
2.00
4.00
1.00
2.00
6.01
80000
70000
60000
50000
40000
30000
20000
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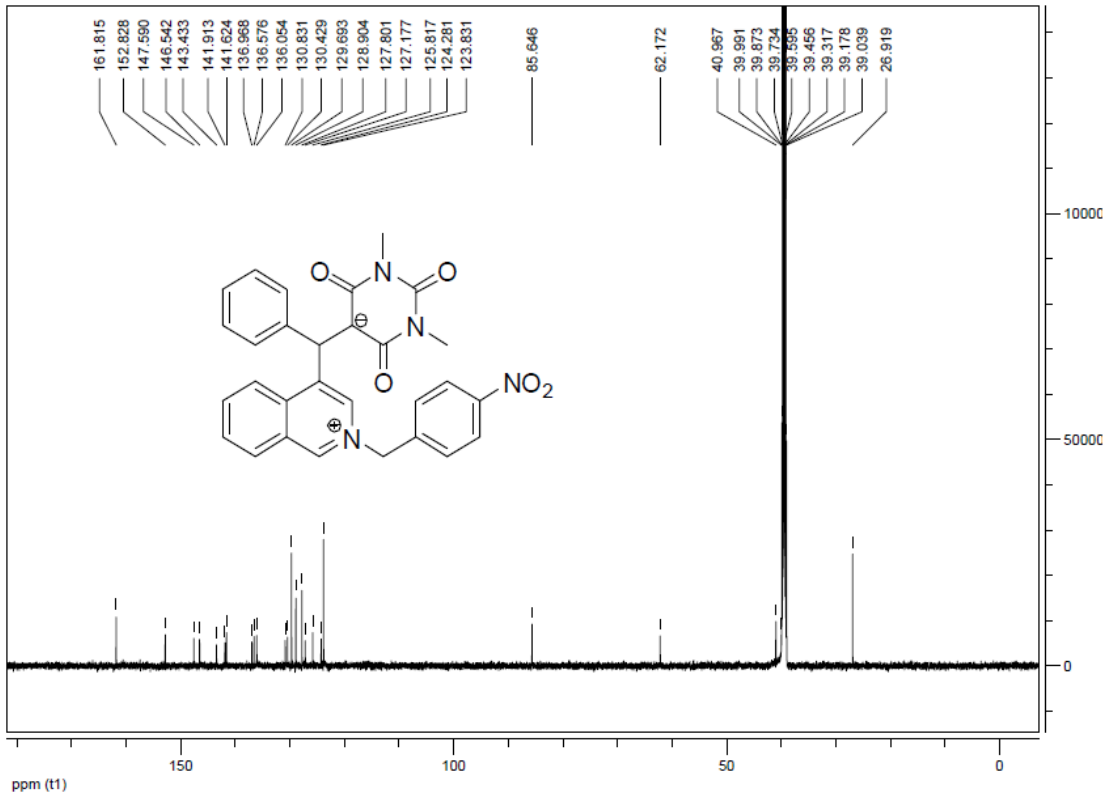
0
10.0
5.0
0.0
ppm (t1)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152.828
147.590
146.542
143.433
141.913
141.624
136.968
136.576
136.054
130.831
130.429
129.693
128.904
127.801
127.177
125.817
124.281
123.831
85.646
62.172
40.967
39.991
39.873
39.734
39.595
39.456
39.317
39.178
39.039
26.919
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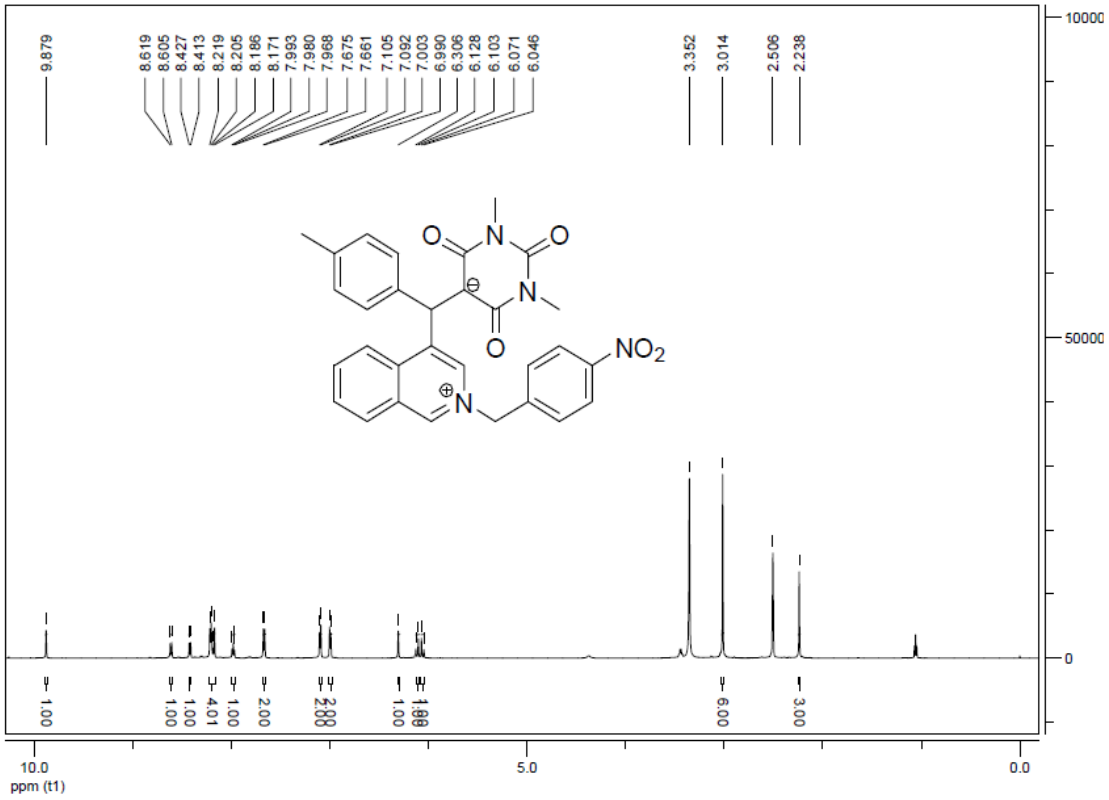
N
O
N
O
NO2
N
10000
50000
0
150
100
50
0
ppm (t1)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8.605
8.427
8.413
8.219
8.205
8.186
8.171
7.993
7.980
7.968
7.675
7.661
7.105
7.092
7.003
6.990
6.306
6.128
6.103
6.071
6.046
3.352
3.014
2.506
2.238
NO2
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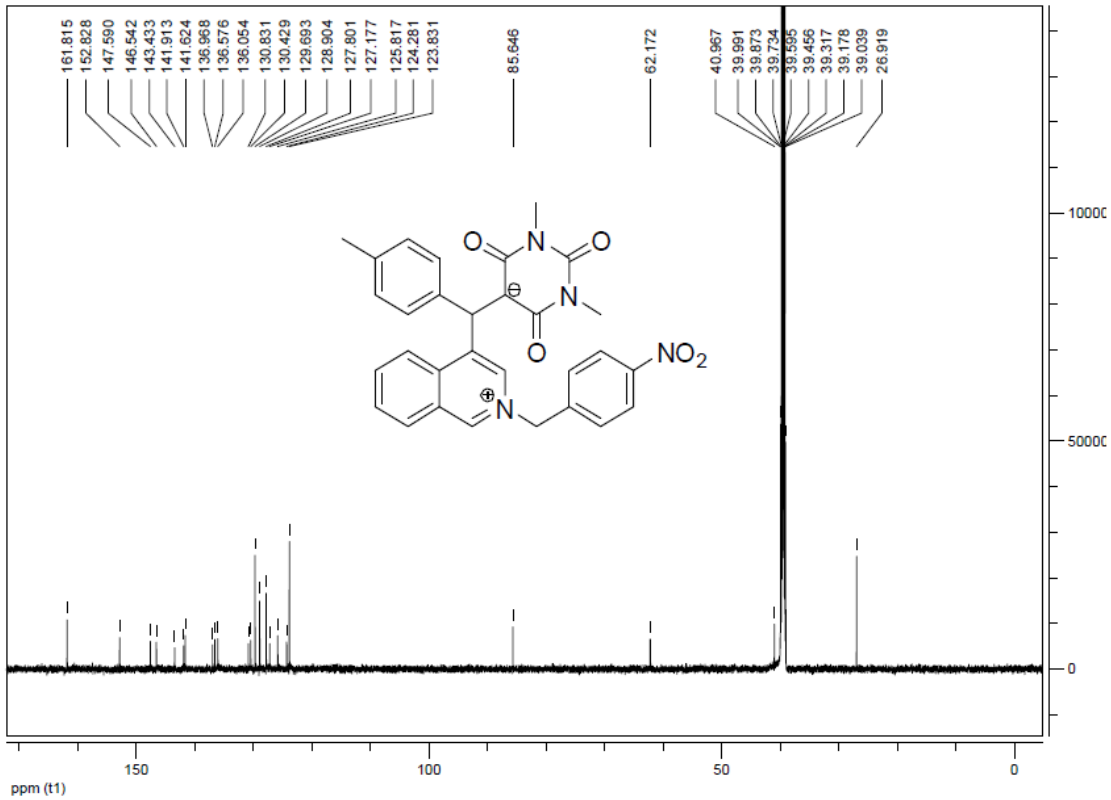
0
10.0
5.0
0.0
ppm (t1)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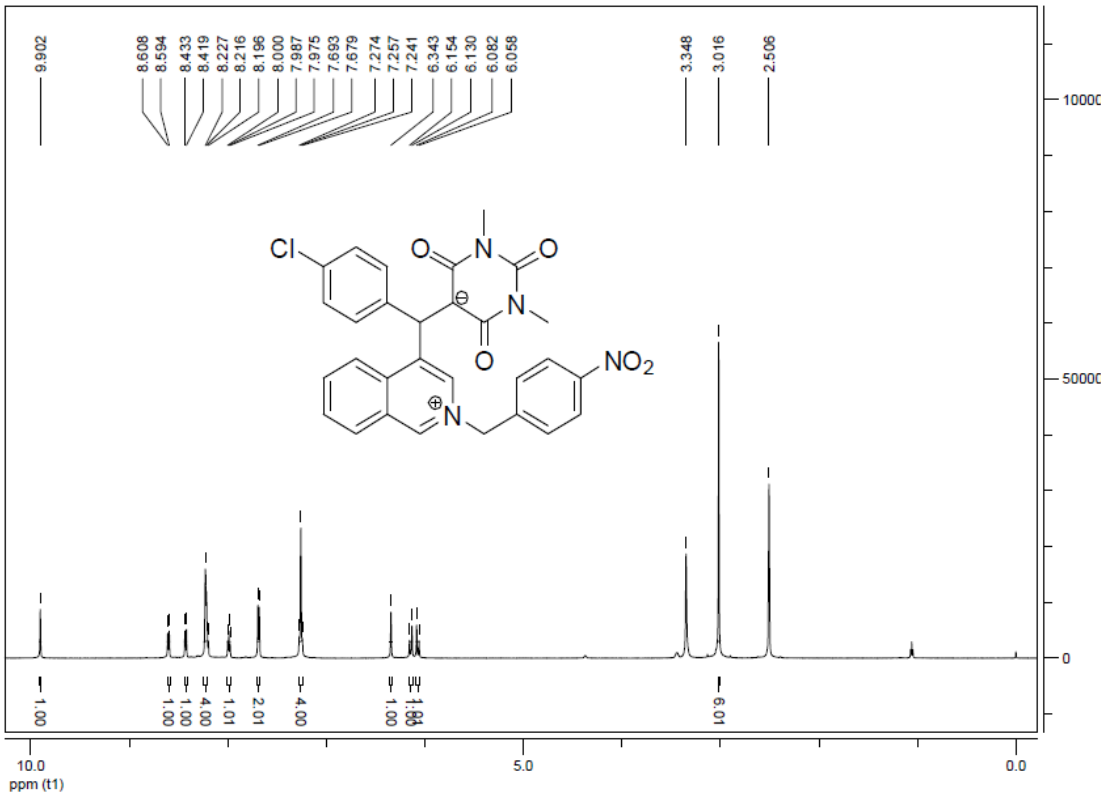
152.828
147.590
146.542
143.433
141.913
141.624
136.968
136.576
136.054
130.831
130.429
129.693
128.904
127.801
127.177
125.817
124.281
123.831
85.646
62.172
40.967
39.991
39.873
39.734
39.595
39.456
39.317
39.178
39.039
26.919
NO2
10000
50000
0
150
100
50
0
ppm (t1)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8.227
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8.196
8.000
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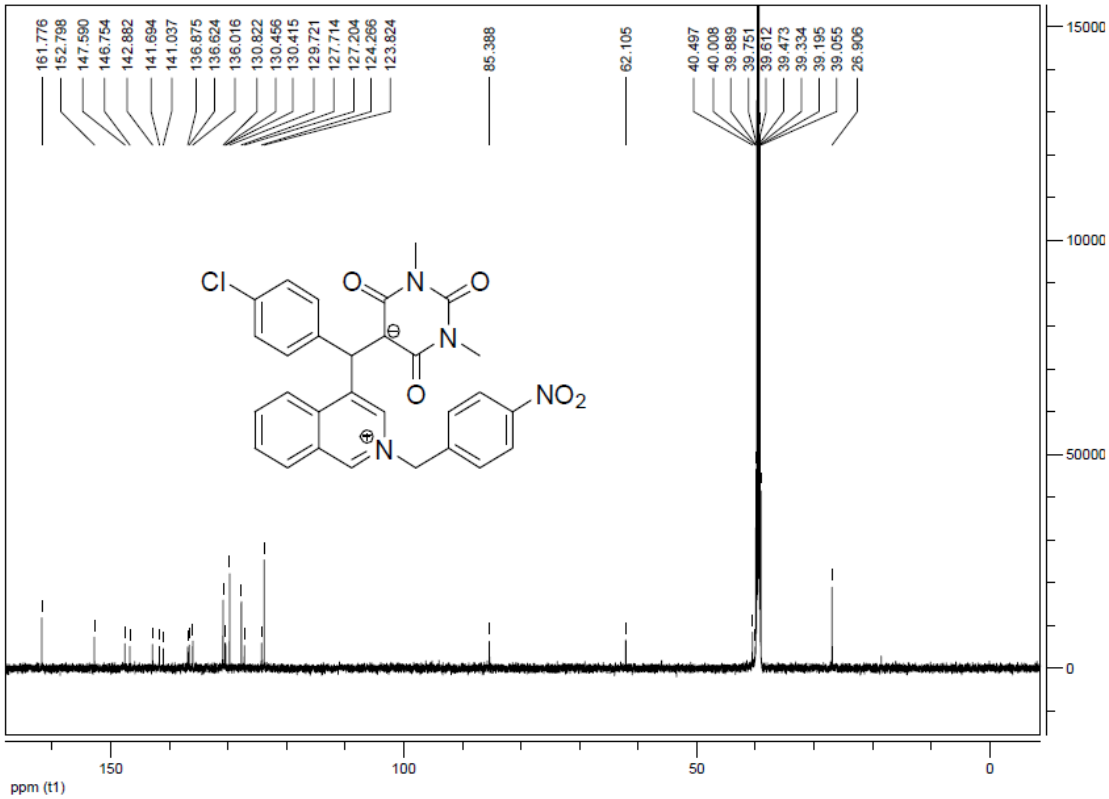
7.975
7.693
7.679
7.274
7.257
7.241
6.343
6.154
6.130
6.082
6.058
3.348
3.016
2.506
Cl
O
N
O
N
O
NO2
N
10000
50000
0
1.00
1.00
1.00
4.00
1.01
2.01
4.00
1.00
6.01
10.0
5.0
0.0
ppm (t1)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142.882
141.694
141.037
136.875
136.624
136.016
130.822
130.456
130.415
129.721
127.714
127.204
124.266
123.824
85.388
62.105
40.497
40.008
39.889
39.751
39.612
39.473
39.334
39.195
39.055
26.906
Cl
O
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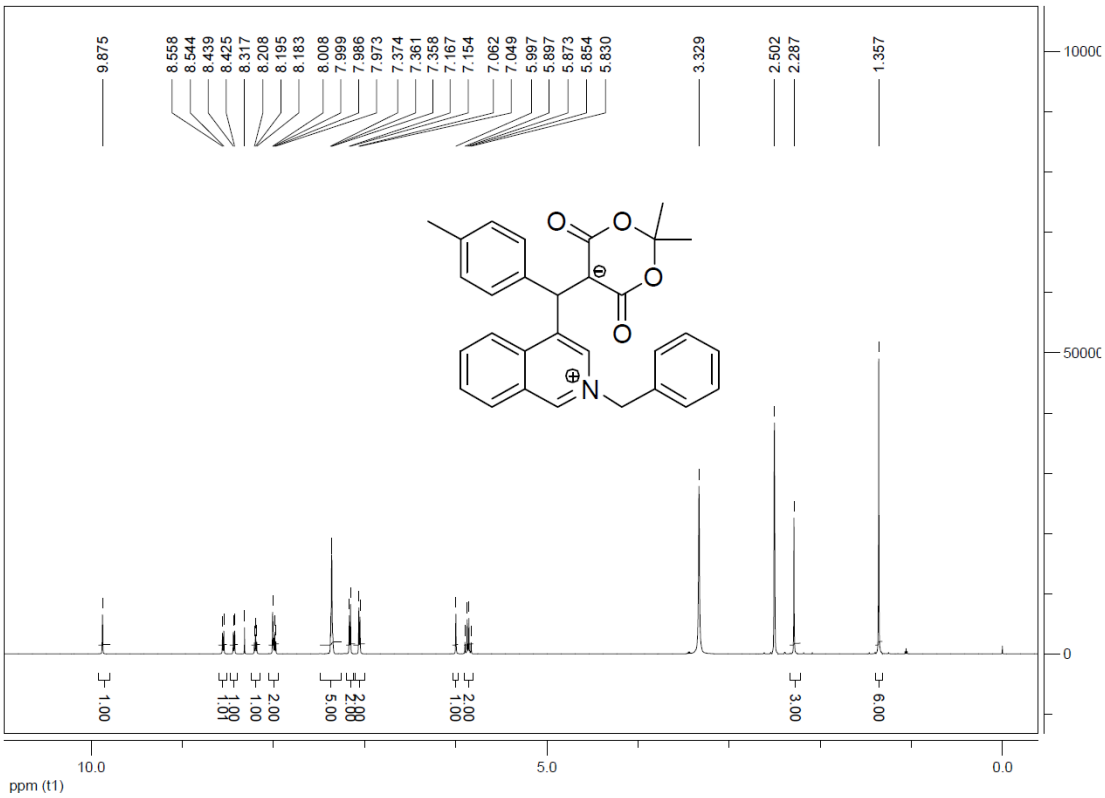
O
N
O
NO2
N
15000
10000
50000
0
150
100
50
0
ppm (t1)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8.317
8.208
8.195
8.183
8.008
7.999
7.986
7.973
7.374
7.361
7.358
7.167
7.154
7.062
7.049
5.997
5.897
5.873
5.854
5.830
3.329
2.502
2.287
1.357
10000
50000
0
1.00
1.01
1.00
2.00
5.00
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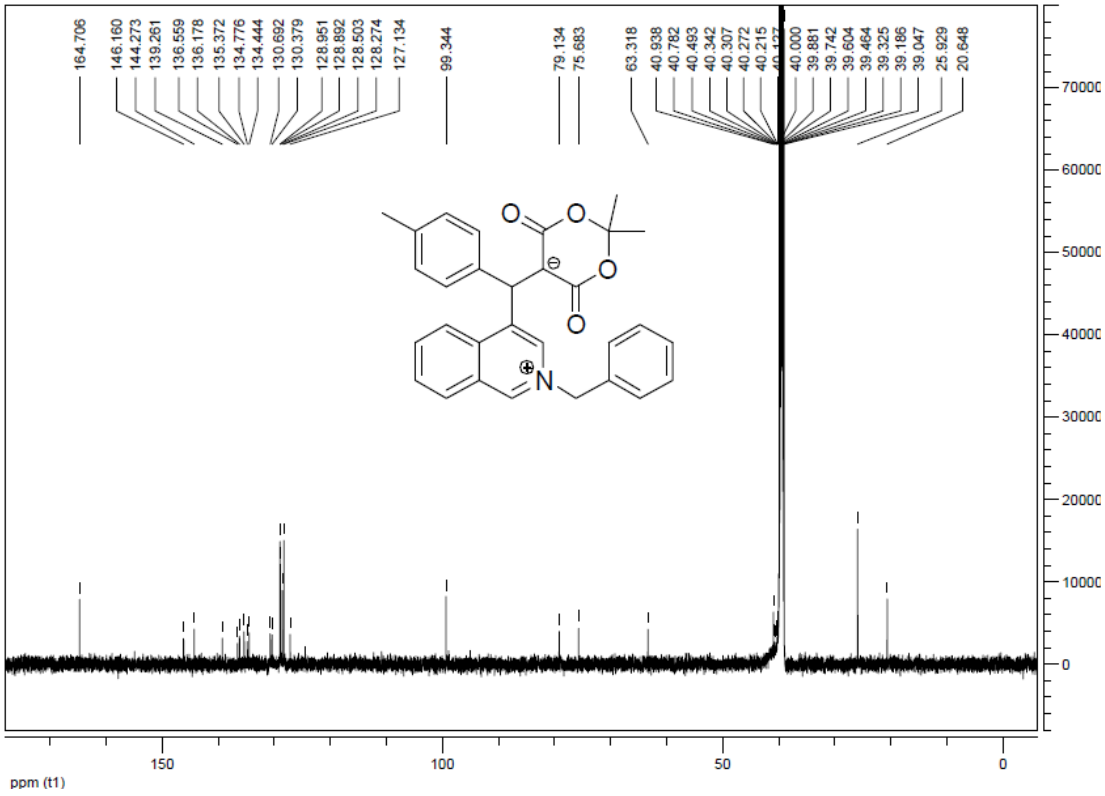
2.88
1.00
2.00
3.00
6.00
10.0
5.0
0.0
ppm (t1)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139.261
136.559
136.178
135.372
134.776
134.444
130.692
130.379
128.951
128.892
128.503
128.274
127.134
99.344
79.134
75.683
63.318
40.938
40.782
40.493
40.342
40.307
40.272
40.215
40.137
40.000
39.881
39.742
39.604
39.464
39.325
39.186
39.047
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70000
60000
50000
40000
30000
20000
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0
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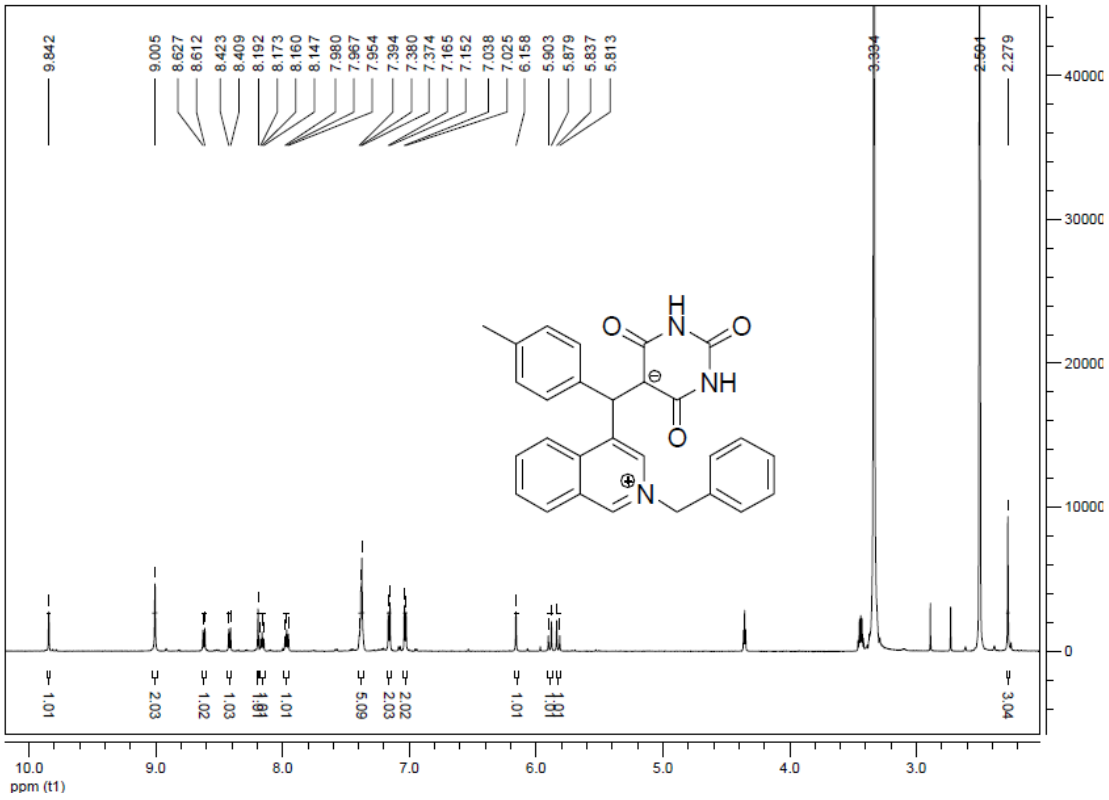
100
50
0
ppm (t1)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8.423
8.409
8.192
8.173
8.160
8.147
7.980
7.967
7.954
7.394
7.380
7.374
7.165
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7.038
7.025
6.158
5.903
5.879
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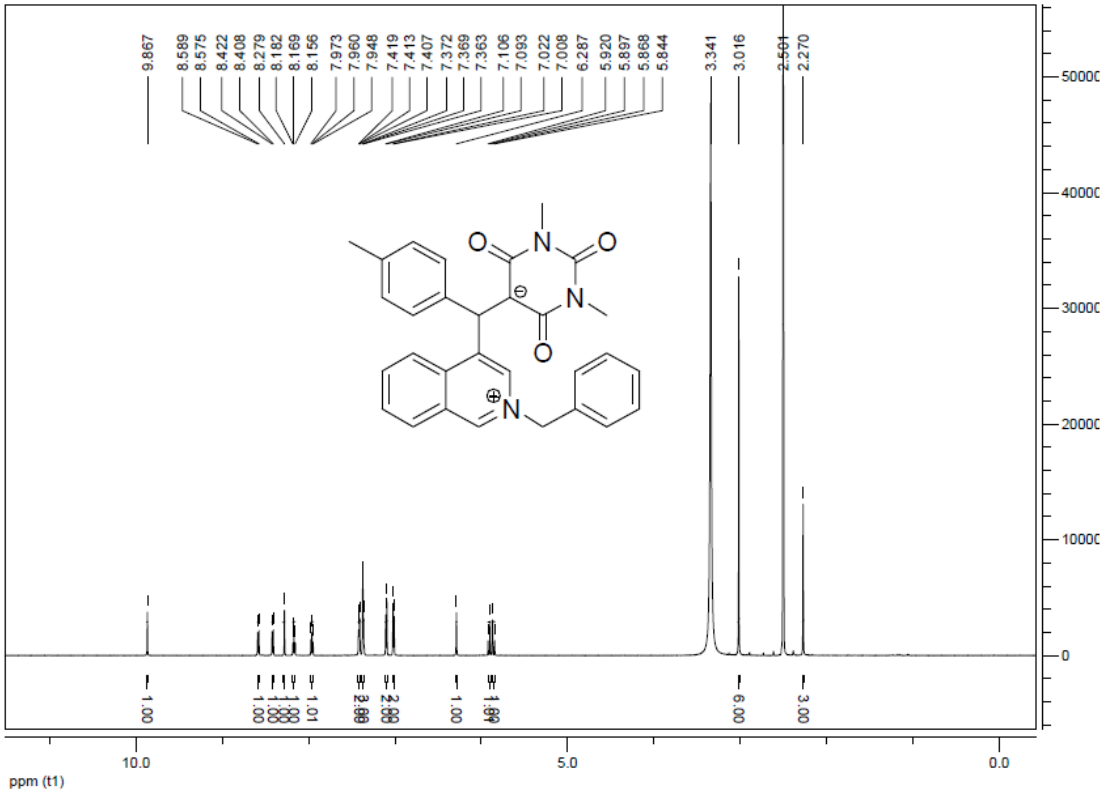
3.334
2.501
2.279
ppm (t1)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8.408
8.279
8.182
8.169
8.156
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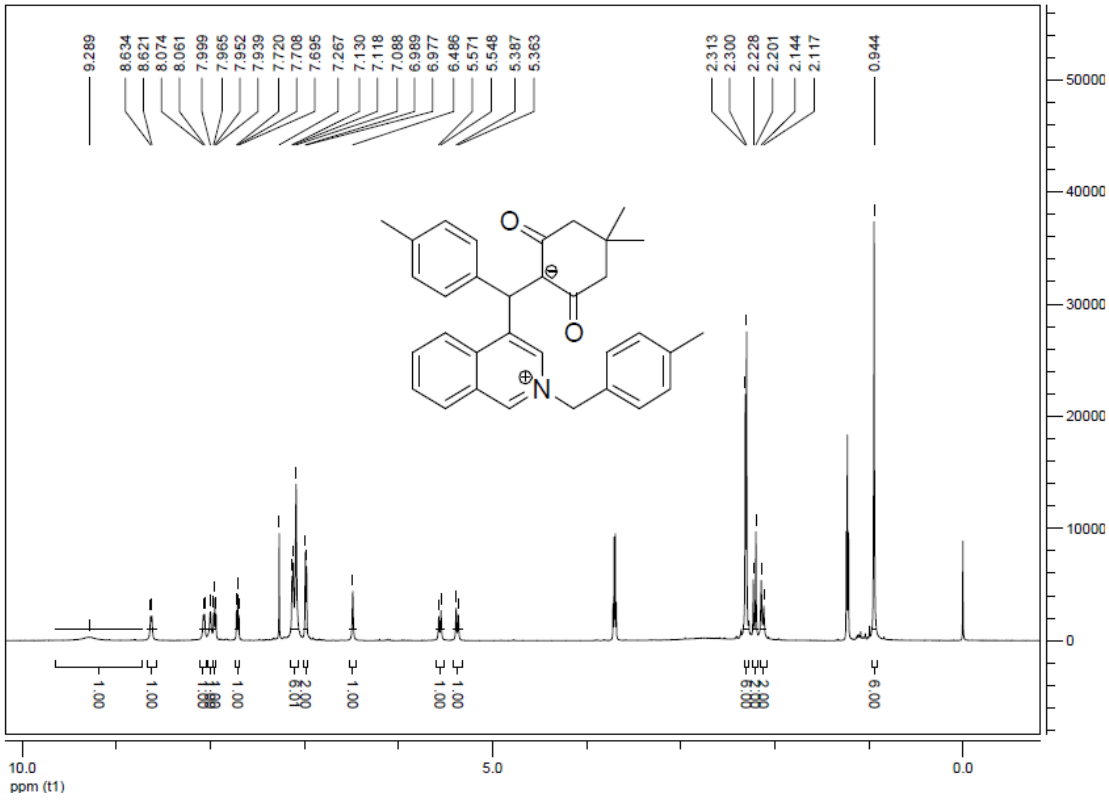
7.960
7.948
7.419
7.413
7.407
7.372
7.369
7.363
7.106
7.093
7.022
7.008
6.287
5.920
5.897
5.868
5.844
3.341
3.016
2.501
2.270
ppm (t1)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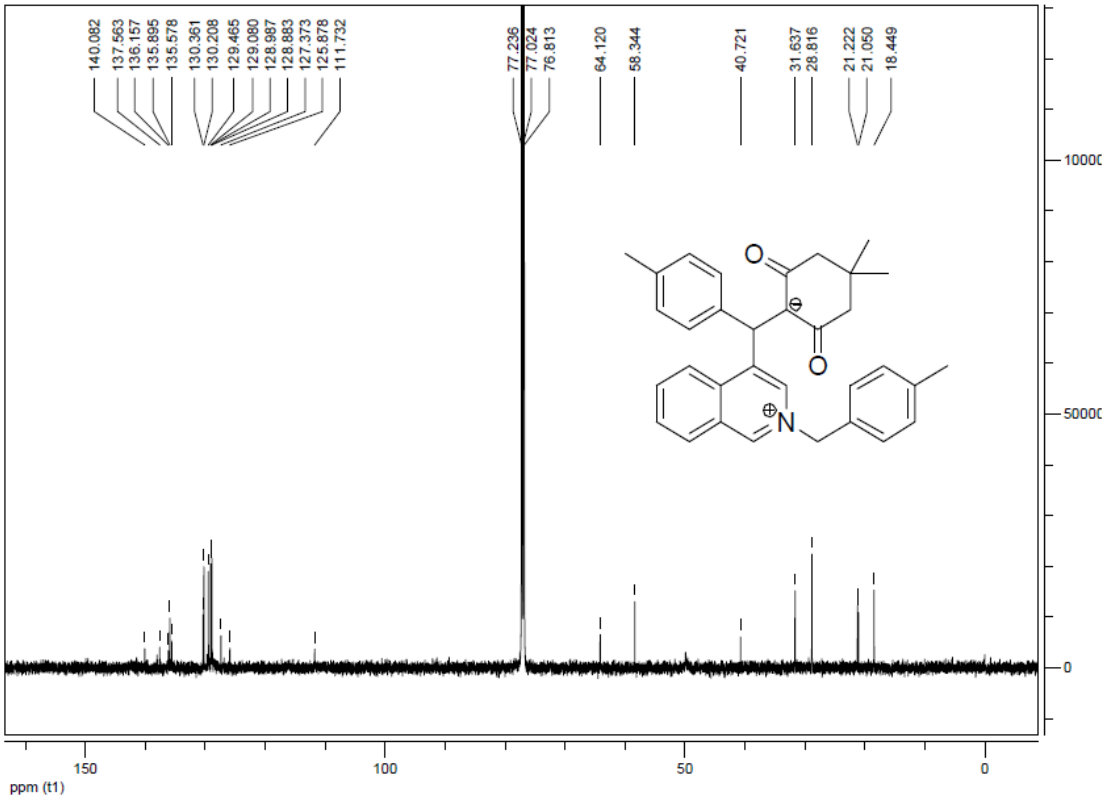
7.965
7.952
7.939
7.720
7.708
7.695
7.267
7.130
7.118
7.088
6.989
6.977
6.486
5.571
5.548
5.387
5.363
2.313
2.300
2.228
2.201
2.144
2.117
0.944
O
O
N
50000
40000
30000
20000
10000
0
1.00
1.00
1.00
2.01
1.00
1.00
1.00
6.00
10.0
5.0
0.0
ppm (t1)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135.895
135.578
130.361
130.208
129.465
129.080
128.987
128.883
127.373
125.878
111.732
77.236
77.024
76.813
64.120
58.344
40.721
31.637
28.816
21.222
21.050
18.449
O
O
N
10000
50000
0
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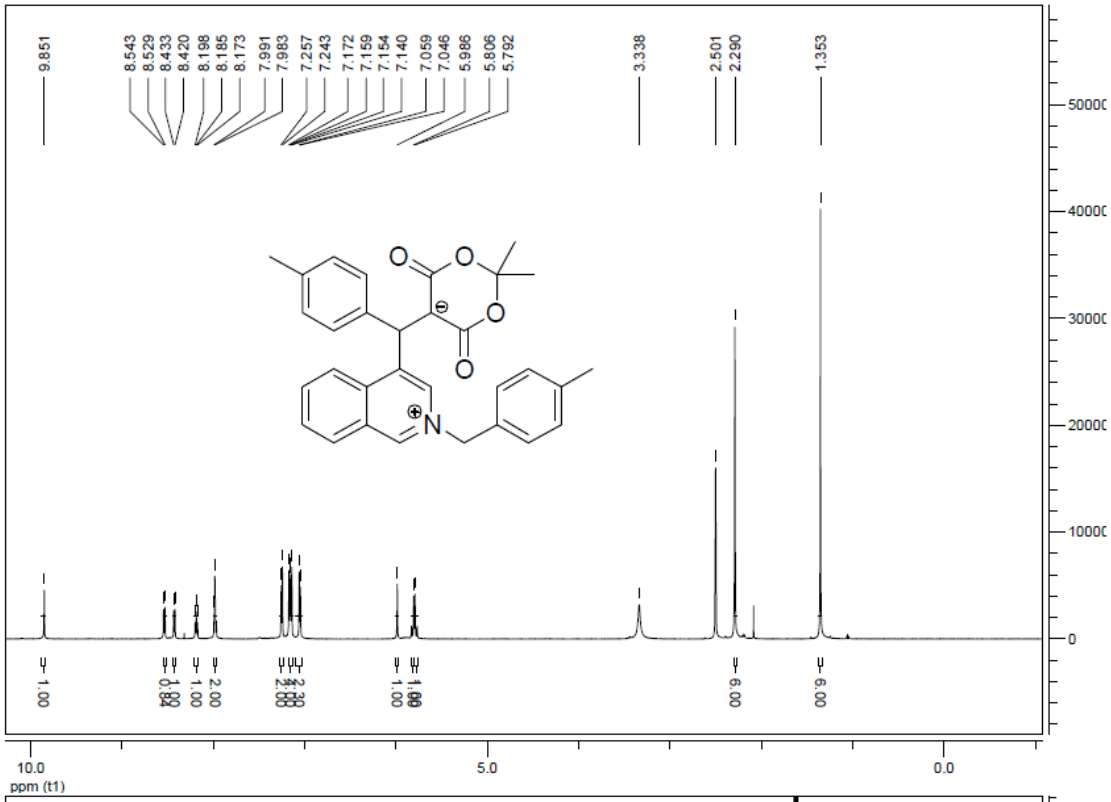
100
50
0
ppm (t1)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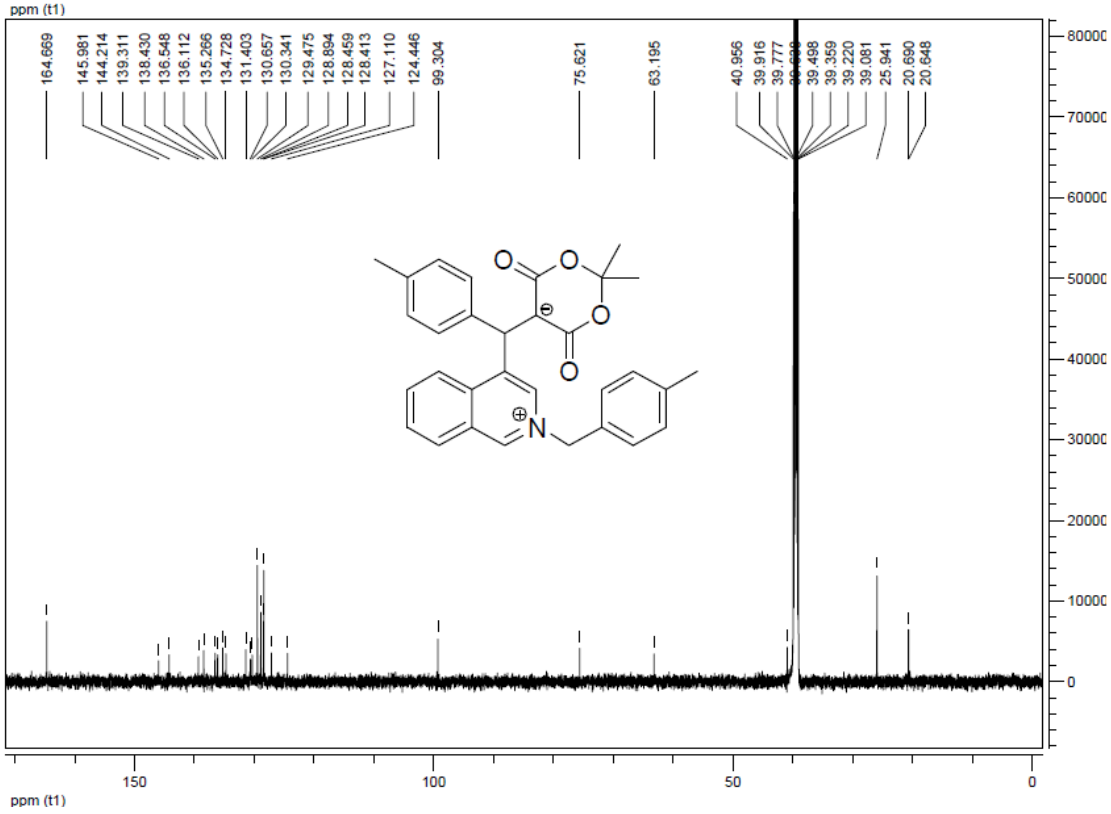
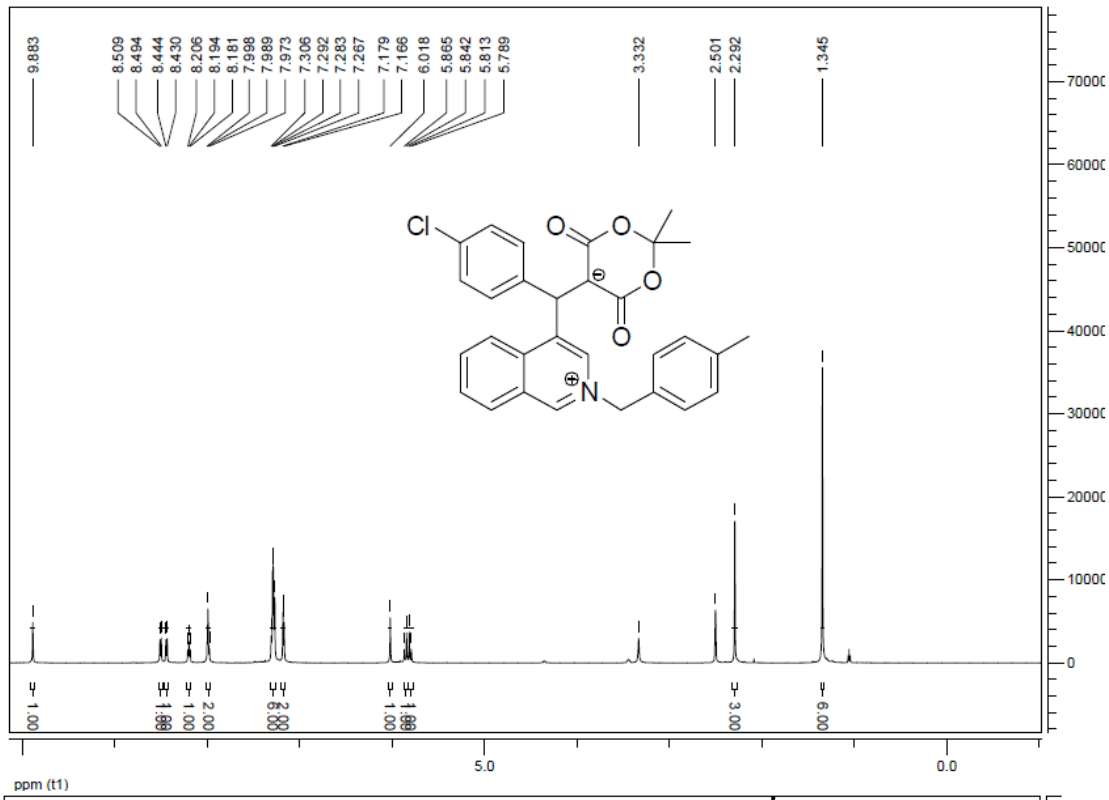
8.433
8.420
8.198
8.185
8.173
7.991
7.983
7.257
7.243
7.172
7.159
7.154
7.140
7.059
7.046
5.986
5.806
5.792
3.338
2.501
2.290
1.353
1.00
1.00
2.00
6.00
6.00
10.0
5.0
0.0
ppm (t1)


164.669
145.981
144.214
139.311
138.430
136.548
136.112
135.266
134.728
131.403
130.657
130.341
129.475
128.894
128.459
128.413
127.110
124.446
99.304
75.621
63.195
40.956
39.916
39.777
39.498
39.359
39.220
39.081
25.941
20.690
20.648
150
100
50
0
ppm (t1)


9.883
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8.430
8.206
8.194
8.181
7.998
7.989
7.973
7.306
7.292
7.283
7.267
7.179
7.166
6.018
5.865
5.842
5.813
5.789
3.332
2.501
2.292
1.345
Cl
O
O
O
O
O
⊖
⊕N
70000
60000
50000
40000
30000
20000
10000
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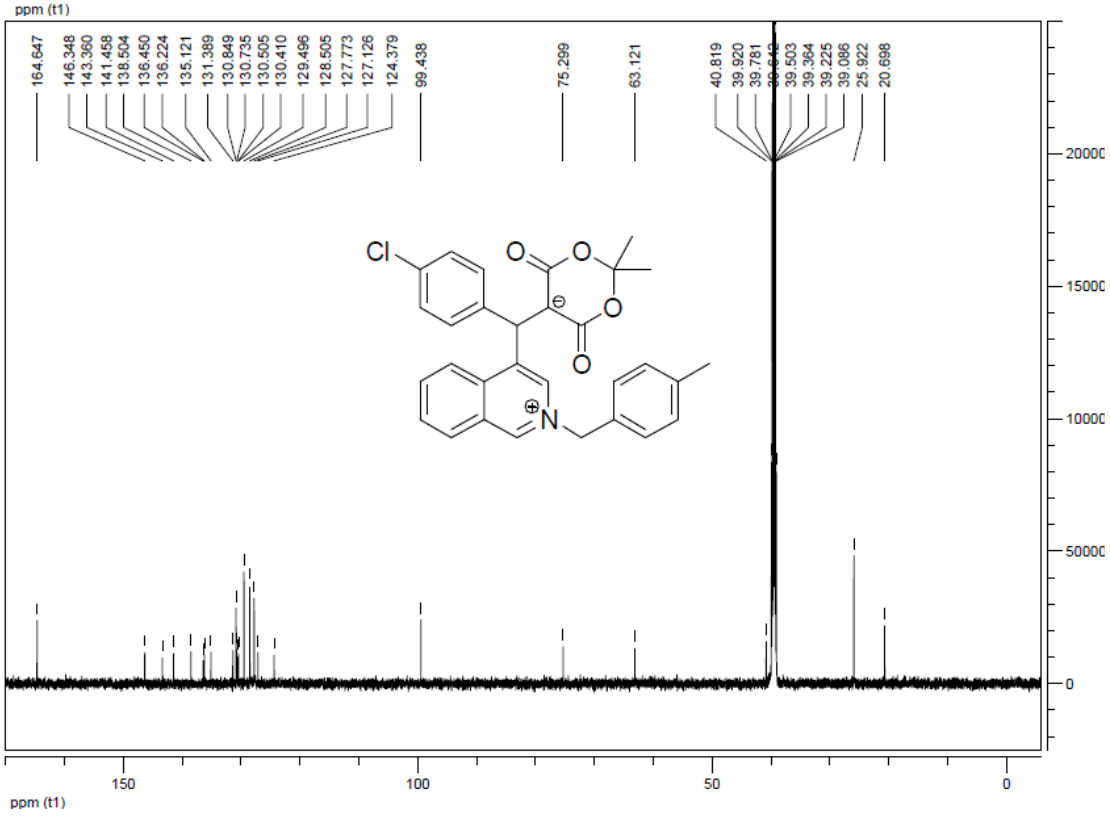
1.00
2.00
6.00
1.00
3.00
6.00
5.0
0.0
ppm (t1)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136.450
136.224
135.121
131.389
130.849
130.735
130.505
130.410
129.496
128.505
127.773
127.126
124.379
99.438
75.299
63.121
40.819
39.920
39.781
39.503
39.364
39.225
39.086
25.922
20.698
Cl
O
O
O
O
O
⊖
⊕N
200000
150000
100000
50000
0
150
100
50
0
ppm (t1)

The optimized structure of intermediates at B3LYP/6-31G(d) level

Intermediate A				Intermediate B				Intermediate G			
C	-5.970550	0.575734	-0.439798	C	4.431838	-2.149563	-0.525447	C	-4.911563	-1.762877	-0.453414
C	-4.762772	1.237110	-0.461526	C	3.144315	-1.674592	-0.788097	C	-3.788313	-1.269142	-1.088751
C	-3.561280	0.546452	-0.131181	C	2.775229	-0.383590	-0.411100	C	-3.005392	-0.246149	-0.499078
C	-3.643163	-0.839498	0.221428	C	3.717944	0.464835	0.210605	C	-3.402721	0.266815	0.773662
C	-4.895914	-1.487199	0.237270	C	5.006749	-0.022171	0.466250	C	-4.555856	-0.246452	1.409541
C	-6.045990	-0.793942	-0.088302	C	5.361209	-1.322599	0.107827	C	-5.294909	-1.244912	0.802597
H	-2.207925	2.211507	-0.472533	H	4.706281	-3.159515	-0.816614	H	-5.504215	-2.547966	-0.914753
H	-6.880629	1.111704	-0.694849	H	2.419514	-2.315472	-1.285191	H	-3.469804	-1.645506	-2.056387
H	-4.712831	2.288349	-0.732677	C	3.326028	1.837020	0.529748	C	-1.849057	0.223109	-1.230441
C	-2.311512	1.176301	-0.172174	H	5.734477	0.629028	0.944767	H	-4.854032	0.149396	2.377883
H	-4.942254	-2.538453	0.510788	H	6.363716	-1.686828	0.314634	H	-6.180434	-1.636252	1.296965
H	-7.009053	-1.295007	-0.074905	C	2.097017	2.304471	0.254801	C	-1.499810	1.732574	0.672590
C	-1.230026	-0.807551	0.532730	H	4.067302	2.499182	0.968771	H	-0.838755	2.500911	1.059188
H	-0.305443	-1.250142	0.866877	H	1.805998	3.329577	0.466247	N	-1.179206	1.203876	-0.573563
N	-1.139742	0.537854	0.142259	N	1.080601	1.538204	-0.373132	C	1.303115	1.009407	-0.753157
C	1.375121	0.711209	0.074305	C	-1.023225	0.282301	0.304404	C	1.402607	-0.383928	-0.891083
C	1.760950	-0.592409	-0.358599	C	-1.742879	0.861005	-0.753174	C	2.375000	1.722692	-0.204124
C	2.434790	1.614462	0.393921	C	-1.703831	-0.516402	1.237582	C	2.551211	-1.054093	-0.486212
C	3.091049	-0.968149	-0.425748	C	-3.109573	0.642413	-0.883889	H	0.562856	-0.928197	-1.314796
H	1.014719	-1.299794	-0.701951	H	-1.218141	1.501200	-1.454888	C	3.534977	1.066991	0.204397
C	3.761153	1.242597	0.328979	C	-3.07008	-0.74485	1.119273	H	2.308221	2.802454	-0.09656

			7	7					0
H	2.181457	2.622602	0.711224	H -1.156345	-0.963246	2.063444	C 3.603019	-0.315392	0.057349
C	4.092822	-0.059842	-0.070196	C -3.756213	-0.162295	0.054201	H 2.648361	-2.128220	-0.585088
H	3.375056	-1.956070	-0.768006	H -3.681408	1.085064	-1.690245	H 4.373645	1.602205	0.632111
H	4.554161	1.933842	0.587346	H -3.609371	-1.357771	1.830805	N 4.822113	-1.017583	0.488990
N	5.481619	-0.462477	-0.131417	N -5.198987	-0.397680	-0.078694	O 5.732431	-0.341622	0.968862
O	6.343167	0.375208	0.164478	O -5.745245	-1.105768	0.768660	O 4.859676	-2.239273	0.345449
O	5.736877	-1.623594	-0.476290	O -5.780643	0.125601	-1.030040	C 0.048534	1.724522	-1.218101
C	0.051144	1.224325	0.152760	C 0.442676	0.477383	0.436619	H 0.127219	2.799028	-1.022475
H	-0.079363	2.299162	0.174090	H 0.846159	0.337187	1.438891	H -0.101075	1.573608	-2.288285
C	-2.414401	-1.472759	0.560735	C 1.405487	0.136478	-0.680568	C -2.589562	1.291238	1.349515
H	-2.409924	-2.509285	0.885563	H 0.941530	-0.219755	-1.601015	H -2.836879	1.715231	2.317972

The total energy (E), zero point energy (ZPE) , sum of electronic and zero-point energy(E_0) and relative energy (△E) of intermediate at B3LYP/6-31G(d) level

species	E/ Hartree	ZPE/Hartree	E_0/Hartree	△E/kJ • mol^{-1}
A	-876.747888	0.247716	-876.500172	0.00
B	-876.741810	0.247753	-876.494057	16.06
G	-876.725534	0.247854	-876.477680	59.05

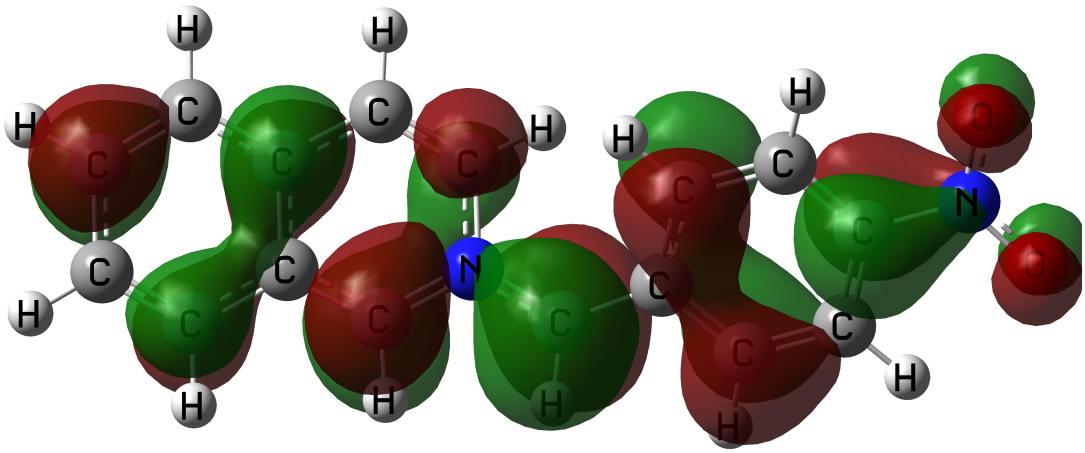
$E_0 = E + ZPE$

Mulliken atomic charges: Atomic charges with hydrogens summed into heavy atoms

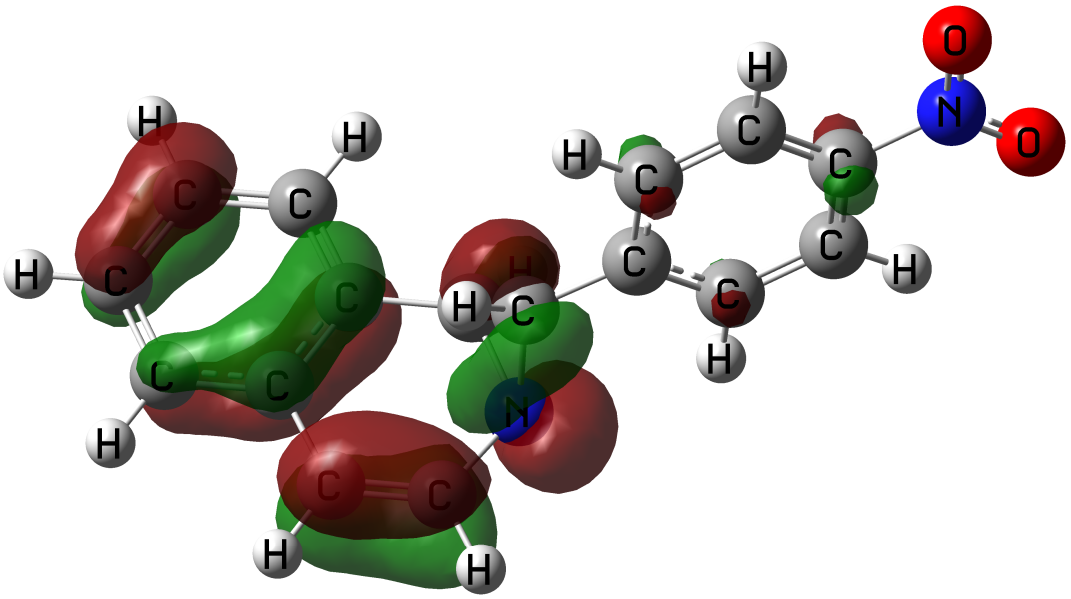
A		B		G	
C	-0.129953	C	-0.132766	C	-0.133335
C	-0.191413	C	-0.198090	C	-0.145909
C	0.091624	C	0.160147	C	-0.039376
C	0.160490	C	0.106195	C	0.159479
C	-0.182349	C	-0.199608	C	-0.184965
C	-0.139532	C	-0.127063	C	-0.128103
H	0.168341	H	0.136289	H	0.135971
H	0.142279	H	0.134864	H	0.143198
H	0.138921	C	-0.154441	C	-0.003959

A		B		G	
C	0.012326	C	0.003523	C	0.002636
C	-0.052492	C	-0.063226	C	-0.002711
C	0.091624	C	0.160147	C	-0.039376
C	0.160490	C	0.106195	C	0.159479
C	-0.041780	C	-0.065700	C	-0.053200
C	0.001336	C	0.008688	C	0.009752
H	0.000000	H	0.000000	H	0.000000
H	0.000000	H	0.000000	H	0.000000
H	0.000000	C	-0.017709	C	-0.003959
C	0.157950	H	0.000000	H	0.000000
H	0.000000	H	0.000000	H	0.000000
H	0.000000	C	0.144639	C	0.221319
C	0.249485	H	0.000000	H	0.000000
H	0.000000	H	0.000000	N	-0.388674

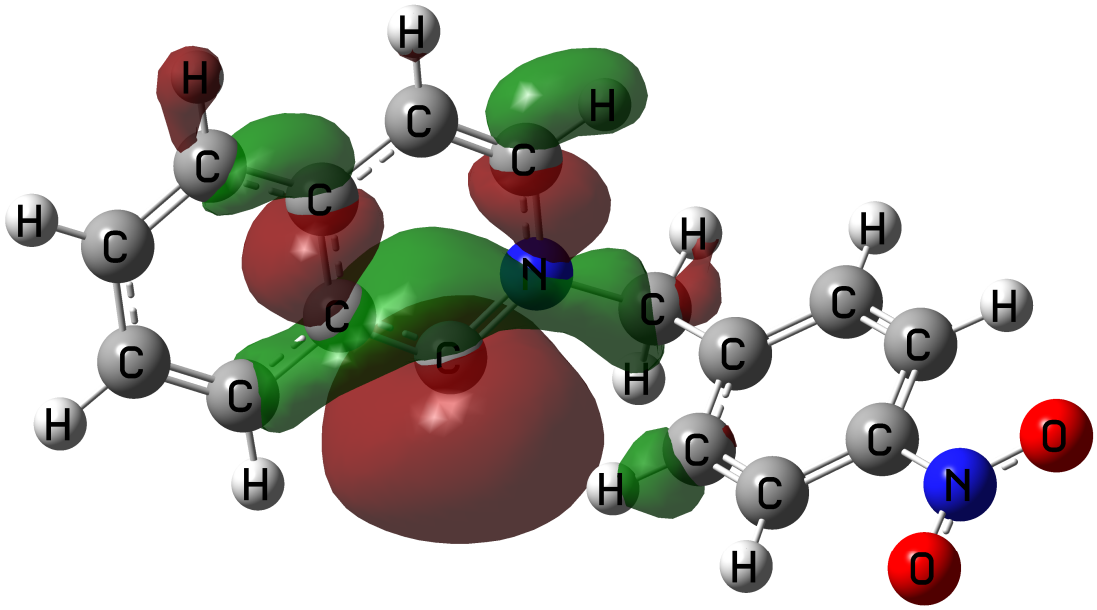
C	-0.010391	H	0.133908	H	0.131766
H	0.140569	H	0.135751	H	0.137855
H	0.140868	C	-0.007423	C	0.065591
C	0.053724	H	0.136732	H	0.155729
H	0.195761	H	0.152062	N	-0.388674
N	-0.390048	N	-0.412821	C	0.173013
C	0.204354	C	0.215358	C	-0.182020
C	-0.227518	C	-0.205573	C	-0.200223
C	-0.208623	C	-0.199321	C	-0.148746
C	-0.151527	C	-0.149076	H	0.175393
H	0.135838	H	0.169333	C	-0.147759
C	-0.150418	C	-0.155754	H	0.140633
H	0.130746	H	0.142910	C	0.275485
C	0.267592	C	0.275838	H	0.185696
H	0.173813	H	0.182405	H	0.183337
H	0.174255	H	0.182110	N	0.379840
N	0.359367	N	0.376839	O	-0.396315
O	-0.420046	O	-0.399531	O	-0.393214
O	-0.422613	O	-0.398377	C	-0.227685
C	-0.129651	C	-0.113093	H	0.155018
H	0.144865	H	0.158794	H	0.197673
C	-0.229706	C	-0.108436	C	-0.220506
H	0.160380	H	0.161837	H	0.145113



HOMO of intermediate A

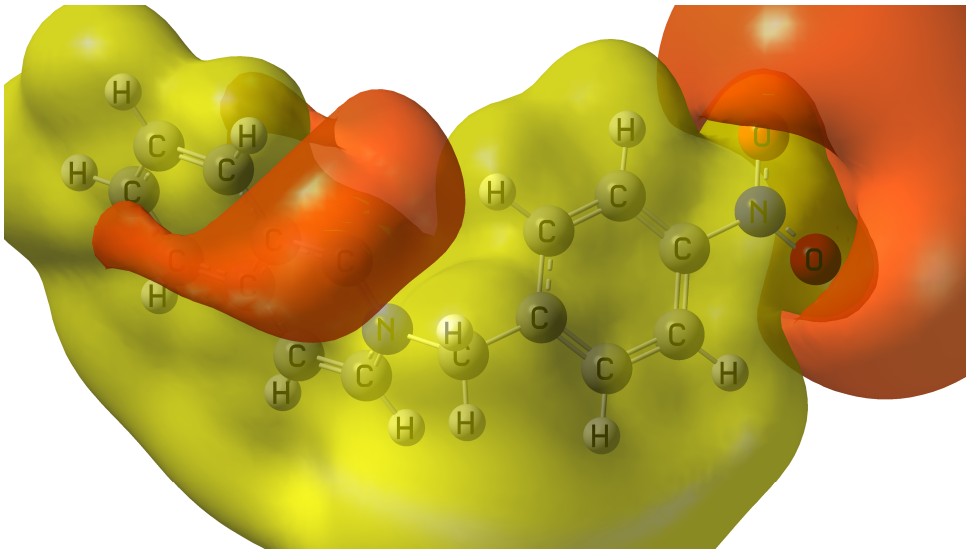


HOMO of intermediate B



HOMO of intermediate G

The highest occupied molecular orbital (HOMO) of intermediates



The ESP of intermediate G