Supporting Information

Three-Component, One-Pot Sequential Synthesis of *N*-Aryl, *N'*-Alkyl Barbiturates

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General Methods: Commercially available reagent-grade solvents were employed without purification. ^{1}H NMR spectra were run on spectrometers 400 or 500 MHz. Chemical shifts are expressed in ppm (δ), using tetramethylsilane (TMS) as internal standard for ^{1}H and ^{13}C nuclei (δ_H and $\delta_C = 0.00$), while C_6F_6 was used as external standard (δ_F 162.90) for ^{19}F.

Materials: carbodiimides **4a-c** were prepared according to the literature.[1] ^{1}H NMR and ^{13}C NMR spectral data of malonic acid mono-esteres **3b**[2] and **3c**[3] and carbodiimide **4b**[4] were in agreement with those previously reported.

General procedure for the synthesis of malonic acid monoesters 3a,b starting from benzyl ethylmalonate 5. To a stirred solution of **5** (1 equiv.) in dry DMF (0.1 M solution) 1.1 equiv. of NaH (60% in weight oil dispersion) was added at 0 °C under nitrogen atmosphere and the mixture stirred for 30'. Neat alkyl bromide (1.2 equiv.) was added, the temperature left to reach rt and the mixture stirred over-night. Water was added and the resulting mixture was extracted with Et_2O. The combined organic layers were dried over anhydrous $NaSO_4$, filtered and concentrated under vacuum. The crude was dissolved in a 1:1 mixture of AcOEt/MeOH (0.1 M solution), a catalytic amount of $Pd(OH)_2/C$ was added and the mixture was stirred under dihydrogen atmosphere until total consumption of the starting material (TLC monitoring). The catalyst was filtered through a Celite pad, the organic solvent evaporated and the crude purified by flash chromatography.

General procedure for the synthesis of 2-phenyl malonic acid mono-ethylester 3c starting from ethyl phenylacetate 6. To a LDA (2.1 equiv.) solution in dry THF (0.25M solution) a solution of **6** (1 equiv.) in dry THF (0.3M solution) was added drop wise at – 60 °C under nitrogen atmosphere. After 1 h. at the same temperature an excess of solid CO_2 was added and the mixture left to reach slowly rt. Most of the organic solvent was evaporated, the mixture acidified until pH 1 with a 1N aqueous HCl solution, extracted with AcOEt, the combined organic layers dried over anhydrous Na_2SO_4, filtered, concentrated under vacuum and the crude purified by flash chromatography.

General procedure for the synthesis of barbiturates 1a-e under NaOH\dioxane protocol. To a stirred solution of malonic acid mono-esteres **3** (1 equiv.) in dioxane (0.1M solution) carbodiimide **4** (1.1 equiv.) was added and the mixtures stirred at rt over-night. A 2N aqueous NaOH solution was added followed by neat benzyl halide **7** (4 equiv.) when the cyclization is

[1] Palomo, C.; Mestres, R. *Synthesis*, **1981**, 373-374.
[2] Ambrosie, L.; Chassagnard, C.; Revial, G.; D'Angelo, J. *Tetrahedron: Asymmetry* **1991**, *6*, 407-410.
[3] Niwayama, S. *J. Org. Chem.* **2000**, *65*, 5834-5836.
[4] Barvian, M. R.; Hollis Showalter, H. D.; Doherty, A. *Tetrahedron Lett.* **1997**, *38*, 6799-6702.

complete (typically 10', TLC monitoring). After 1 h the solution was acidified with a 1N aqueous HCl solution, extracted with AcOEt, the combined organic layers dried over anhydrous Na_2SO_4, filtered, concentrated under vacuum and the crude purified by flash chromatography.

General procedure for the synthesis of barbiturates 1f-o under K_2CO_3\CH_3CN protocol. In a sealed tube, carbodiimide **4** (1.1 equiv.) was added to a stirred solution of malonic acid mono-esteres **3** (1 equiv.) in dioxane (0.1M solution) and the mixtures stirred at rt over-night. Solid anhydrous K_2CO_3 (2.1 equiv.) followed by alkyl halide **7** (4 equiv.) were added and the mixture was heated at 120 °C. After the reaction is complete (typically 30' for highly reactive benzyl or allyl halides **7a-d,g** and 12 h for less reactive alkyl halides **7e**,**f**,**h,i**, TLC monitoring), the mixture was cooled to rt and water was added. The mixture was extracted with AcOEt, the combined organic layers dried over anhydrous Na_2SO_4, filtered, concentrated under vacuum and the crude purified by flash chromatography.

2-Octyl-malonic acid monoethyl ester 3a: R_f = 0.22 (Hexane/AcOEt = 80:20); ^{1}H NMR (400 MHz, CD_3OD) δ 4.23 (q, *J* = 7.2 Hz, 2H), 3.37 (t, *J* = 7.2 Hz, 1H), 1.92 (m, 2H), 1.31 (m, 12H), 1.29 (t, *J* = 7.2 Hz, 3H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, CD_3OD) δ 172.8, 171.5, 62.3, 53.2, 32.9, 30.4, 30.29, 30.23, 29.9, 28.35, 28.31, 23.6, 14.3; ESI (*m/z)* 267.1 [M^++Na, (100)], 245.1 [M^++1, (68)].

(4-Methoxy-benzyl)-(4-methoxyphenyl)-carbodiimide 4a: R_f = 0.56 (Hexane/AcOEt = 80:20); FTIR (nujol) ν 2118, 1512 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, *J* = 8.7 Hz, 2H), 6.93 (d, *J* = 9.0 Hz, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 6.79 (d, *J* = 9.0 Hz, 2H), 4.47 (s, 2H), 3.80 (s, 3H), 3.76 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 159.2, 156.9, 138.3, 132.5, 130.3, 128.7, 124.4, 114.6, 114.1, 55.4, 55.2, 50.1.

Methyl-(4-trifluoromethylphenyl)-carbodiimide 4c: R_f = 0.63 (Hexane/AcOEt = 80:20); FTIR (nujol) ν 2150, 1323 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 3.20 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 144.6, 126.4 (q, *J* = 3.8 Hz), 123.7, 121.5, 32.1, the corresponding resonances of CF_3 group and of C_α to the CF_3 group are obscured; ^{19}F NMR (470.6 MHz, $CDCl_3$) δ -63.1;.

1-(Methoxy-benzyl)-3-(4-methoxyphenyl)-5-octyl-pyrimidine-2,4,6-trione 1a: R_f = 0.40 (Hexane/AcOEt = 70:30); FTIR (nujol) ν 1703, 1691 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.7 Hz, 2H), 7.05 (d, *J* = 9.0 Hz, 2H), 6.97 (d, *J* = 9.0 Hz, 2H), 6.83 (d, *J* = 8.7 Hz, 2H), 5.05 (d, *J* = 13.9 Hz, 1H), 4.98 (d, *J* = 13.9 Hz, 1H), 3.83 (s, 3H), 3.79 (s, 3H), 3.60 (t, *J* = 5.5 Hz, 1H), 2.15 (m, 2H), 1.23 (m, 12H), 0.89 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 168.7, 168.6, 159.9, 159.4, 151.5, 130.9, 129.3, 128.5, 126.9, 114.8, 113.9, 55.5, 55.2, 49.7, 44.8, 32.0, 31.8, 29.2, 29.1, 29.0, 25.9, 22.6, 14.0; ESI (*m/z)* 489.1 [M^++Na, (48)], 467.1 [M^++1, (100)].

5-Benzyl-5-ethyl-1-(4-methoxybenzyl)-3-phenyl-pyrimidine-2,4,6-trione 1b: R_f = 0.45 (Hexane/AcOEt = 80:20); FTIR (nujol) ν 1698, 1687 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (m, 4H), 7.33 (d, *J* = 7.6 Hz, 2H), 7.22 (m, 1H), 7.11 (m, 2H), 6.95 (d, *J* = 7.9 Hz, 2H), 6.83 (d, *J* = 7.6 Hz, 2H), 6.81 (m, 1H), 4.98 (d, *J* = 13.7 Hz, 1H), 4.86 (d, *J* = 13.7 Hz, 1H), 3.81 (s, 3H), 3.38 (d, *J* = 12.7 Hz, 1H), 3.24 (d, *J* = 12.7 Hz, 1H), 2.28 (m, 2H), 0.89 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.5, 171.0, 159.3, 135.0, 134.5, 131.0, 129.5, 129.3, 129.0, 128.6, 128.3, 128.2, 127.6, 113.8, 59.7, 55.3, 46.1, 44.8, 33.3, 9.7; ESI (*m/z)* 465.2 [M^++Na, (100)], 443.1 [M^++1, (87)].

5-(4-Bromo-benzyl)-5-ethyl-1-(4-methoxybenzyl)-3-(4-methoxyphenyl)-pyrimidine-2,4,6-trione 1c: R_f = 0.50 (Hexane/AcOEt = 70:30); FTIR (nujol) ν 1700, 1695, 1683 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.5 Hz, 2H), 7.17 (d, *J* = 8.5 Hz, 2H) ,6.96 (d, *J* = 7.5 Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 6.80 (d, *J* = 8.5 Hz, 2H), 6.78 (m, 2H), 4.97 (d, *J* = 14.1 Hz, 1H), 4.90 (d, *J*

= 14.1 Hz, 1H), 3.85 (s, 3H), 3.84 (s, 3H), 3.28 (d, *J* = 12.7 Hz, 1H), 3.21 (d, *J* = 12.7 Hz, 1H), 2.25 (m, 2H), 0.90 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125.7 MHz, $CDCl_3$) δ 171.2, 171.1, 159.9, 159.4, 150.5, 133.9, 131.6, 131.2, 130.9, 129.1, 128.2, 126.8, 121.6, 114.8, 113.8, 59.4, 55.9, 55.3, 44.8, 33.7, 9.63; ESI (*m/z)* 573.2 [M^++Na, (45)], 551.1 [M^++1, (100)].

5-Ethyl-5-(9*H*-fluoren-9-yl)-1-(4-methoxybenzyl)-3-(4-methoxyphenyl)-pyrimidine-2,4,6-trione 1d: R_f = 0.35 (Hexane/AcOEt = 70:30); FTIR (nujol) ν 1700, 1683 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.43-7.34 (m, 4H), 7.24 (m, 1H), 7.01 (m, 2H), 6.86 (d, *J* = 8.7 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 6.84 (m, 2H), 5.06 (d, *J* = 13.5 Hz, 1H), 5.01 (d, *J* = 13.5 Hz, 1H), 4.71 (s, 1H), 3.82 (s, 3H), 3.76 (s, 3H), 2.67 (q, *J* = 7.3 Hz, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.1, 168.9, 159.7, 159.4, 150.8, 142.2, 142.1, 141.9, 141.7, 131.3, 128.9, 128.2, 128.0, 126.9, 126.8, 126.6, 125.7, 124.7, 120.3, 120.2, 114.6, 113.8, 60.4, 55.4, 55.3, 54.2, 45.0, 32.6, 9.7; ESI (*m/z)* 569.2 [M^++Na, (100)], 547.2 [M^++1, (82)].

1-(4-Methoxybenzyl)-3-(4-methoxyphenyl)-5-octyl-5-(4-trifluoromethyl-benzyl)-pyrimidine-2,4,6-trione 1e: R_f = 0.44 (Hexane/AcOEt = 80:20); FTIR (nujol) ν 1701, 1697, 1684 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (d, *J* = 8.9 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 6.94 (d, *J* = 8.4 Hz, 2H), 6.83 (d, *J* = 8.9 Hz, 2H), 6.70 (m, 2H), 4.96 (d, *J* = 13.6 Hz, 1H), 4.91 (d, *J* = 13.6 Hz, 1H), 3.83 (s, 3H), 3.82 (s, 3H), 3.40 (d, *J* = 12.7 Hz, 1H), 3.28 (d, *J* = 12.7 Hz, 1H), 2.21 (m, 2H), 1.24 (m, 12H), 0.90 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (125.7 MHz, $CDCl_3$) δ 171.2, 171.1, 159.9, 159.5, 150.4, 139.1, 131.1, 130.0, 129.0, 128.1, 126.7, 125.4 (q, *J* = 3.3 Hz), 124.0 (q, *J* = 271.7 Hz), 114.8, 113.8, 58.6, 55.5, 52.2, 45.2, 44.8, 40.6, 31.8, 29.4, 29.1, 29.0, 25.2, 22.6, 14.1, the corresponding resonance of C_α to the CF_3 group is obscured; ^{19}F NMR (470.6 MHz, $CDCl_3$) δ -63.6; ESI (*m/z)* 647.3 [M^++Na, (100)], 625.3 [M^++1, (45)].

1-(4-Methoxybenzyl)-3-(4-methoxyphenyl)-5-octyl-5-propyl-pyrimidine-2,4,6-trione 1f: R_f = 0.60 (Hexane/AcOEt = 80:20); FTIR (nujol) ν 1699, 1688 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.9 Hz, 2H), 7.05 (d, *J* = 8.9 Hz, 2H), 6.99 (d, *J* = 8.9 Hz, 2H), 6.84 (d, *J* = 8.9 Hz, 2H), 5.07 (s, 2H), 3.84 (s, 3H), 3.79 (s, 3H), 2.02 (m, 2H), 1.18 (m, 14H), 0.89 (t, *J* = 7.0 Hz, 3H), 0.86 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (125.7 MHz, $CDCl_3$) δ 172.1, 172.0, 159.8, 159.3, 151.0, 130.8, 129.3, 128.6, 127.2, 114.7, 113.8, 57.0, 55.5, 55.2, 44.7, 42.3, 40.6, 31.7, 29.4, 29.1, 29.0, 25.0, 22.6, 18.5, 14.0, 13.9; ESI (*m/z)* 531.3 [M^++Na, (100)], 509.3 [M^++1, (98)].

1-(4-Methoxybenzyl)-5,5-dioctyl-3-phenyl-pyrimidine-2,4,6-trione 1g: R_f = 0.47 (Hexane/AcOEt = 90:10); FTIR (nujol) ν 1700, 1685 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (m, 3H), 7.40 (d, *J* = 8.6 Hz, 2H), 7.13 (d, *J* = 6.8 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 5.06 (s, 2H), 3.78 (s, 3H), 2.01 (m, 2H), 1,18 (m, 24H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ

172.0, 171.9, 159.4, 150.9, 134.7, 130.8, 129.4, 129.0, 128.6, 128.3, 113.8, 57.0, 55.2, 44.7, 40.4, 31.8, 29.4, 29.2, 29.1, 25.1, 22.6, 14.1; ESI (*m/z)* 571.4 [M^++Na, (100)], 549.4 [M^++1, (31)].

5-Allyl-1-methyl-5-octyl-3-(4-trifluoromethyl-phenyl)-pyrimidine-2,4,6-trione 1h: R_f = 0.62 (Hexane/AcOEt = 80:20); FTIR (nujol) ν 1701, 1695 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 5.69 (m, 1H), 5.20 (m, 2H), 3.36 (s, 3H), 2.77 (m, 2H), 2.08 (m, 2H), 1.25 (m, 12H), 0.88 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.3, 171.1, 150.5, 137.6, 130.8, 129.1, 126.6, (q, *J* = 3.2 Hz), 121.0, 57.5, 44.4, 30.3, 31.7, 29.5, 29.2, 29.1, 28.6, 25.4, 22.6, 14.0, the corresponding resonances of CF_3 group and of C_α to the CF_3 group are obscured; ESI (*m/z)* 461.2 [M^++Na, (78)], 439.2 [M^++1, (34)], 307 (100).

1-Methyl-5-octyl-5-propyl-3-(4-trifluoromethyl-phenyl)-pyrimidine-2,4,6-trione 1i: R_f = 0.48 (Hexane/AcOEt = 90:10); FTIR (nujol) ν 1700, 1695 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 3.38 (s, 3H), 2.04 (m, 4H), 1.25 (m, 14H), 0.92 (t, *J* = 6.8 Hz, 3H), 0.88 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.9, 171.2, 150.6, 137.8, 131.4 (q, *J* = 32.6 Hz), 129.1, 126.6 (q, *J* = 3.0 Hz), 123.6 (q, *J* = 270.7 Hz), 57.4, 42.3, 40.2, 31.7, 29.5, 29.2, 29.1, 28.6, 25.4, 22.6, 18.8, 14.0, 13.9; ESI (*m/z)* 463.2 [M^++Na, (92)], 441.2 [M^++1, (100)].

1-Methyl-5-octyl-5-(3-phenyl-propyl)-3-(4-trifluoromethyl-phenyl)-pyrimidine-2,4,6-trione 1j: R_f = 0.27 (Hexane/Et_2O = 90:10); FTIR (nujol) ν 1708, 1698 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.4 Hz, 2H), 7.27 (m, 5H), 7.13 (d, *J* = 8.4 Hz, 2H), 3.37 (s, 3H), 2.61 (m, 2H), 2.13 (m, 2H), 2.05 (m, 2H), 1.56 (m, 2H), 1.24 (m, 12H), 0.89 (t, *J* = 6.4 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.7, 171.6, 150.5, 141.0, 137.7, 129.1, 128.4, 128.3, 126.6 (q, *J* = 2.8 Hz), 126.2, 57.2, 40.4, 39.5, 35.7, 31.7, 29.4, 29.15, 29.10, 28.7, 27.3, 25.3, 22.6, 14.0, the corresponding resonances of CF_3 group and of C_α to the CF_3 group are obscured; ESI (*m/z)* 539.2 [M^++Na, (37)], 517.2 [M^++1, (33)], 280 (100).

5-Benzyl-1-(4-methoxybenzyl)-3-(4-methoxyphenyl)-5-phenyl-pyrimidine-2,4,6-trione 1k: R_f = 0.46 (Hexane/AcOEt = 70:30); FTIR (nujol) ν 1699, 1695 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (m, 5H), 7.27 (d, *J* = 8.8 Hz, 2H), 7.24 (m, 1H), 7.16 (m, 4H), 6.92 (d, *J* = 9.2 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 6.80 (m, 2H), 5.01 (d, *J* = 13.6 Hz, 1H), 4.92 (d, *J* = 13.6 Hz, 1H), 3.90 (d, *J* = 12.8 Hz, 1H), 3.82 (s, 3H), 3.80 (s, 3H), 3.79 (d, *J* = 12.8 Hz, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 170.0, 169.9, 159.8, 159.3, 150.5, 138.3, 135.1, 130.8, 130.4, 129.2, 128.6, 128.5, 128.1, 127.5, 126.9, 126.5, 114.7, 113.8, 62.4, 55.5, 55.3, 45.2, 43.0; ESI (*m/z)* 543.1 [M^++Na, (100)], 521.2 [M^++1, (47)].

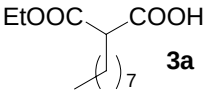
5-Allyl-1-(4-methox-benzyl)-3-(4-methoxyphenyl)-5-phenyl-pyrimidine-2,4,6-trione 1l: R_f = 0.45 (Hexane/AcOEt = 70:30); FTIR (nujol) ν 1699, 1695 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ

7.36 (d, *J* = 8.4 Hz, 2H), 7.31 (m, 3H), 7.25 (m, 2H), 7.01 (d, *J* = 8.8 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 2H), 5.74 (m, 1H), 5.24 (d, *J* = 17.2 Hz, 1H), 5.14 (d, *J* = 10.4 Hz, 1H), 5.08 (s, 2H), 3.82 (s, 3H), 3.80 (s, 3H), 3.19 (d, *J* = 6.8 Hz, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 169.5, 169.4, 159.9, 159.4, 150.9, 137.5, 131.9, 130.8, 129.3, 129.2, 128.6, 128.3, 127.1, 126.0, 114.7, 113.8, 61.4, 55.5, 55.3, 45.3, 40.8; ESI (*m/z)* 493.2 [M^++Na, (75)], 471.1 [M^++1, (87)], 459.2 (100).

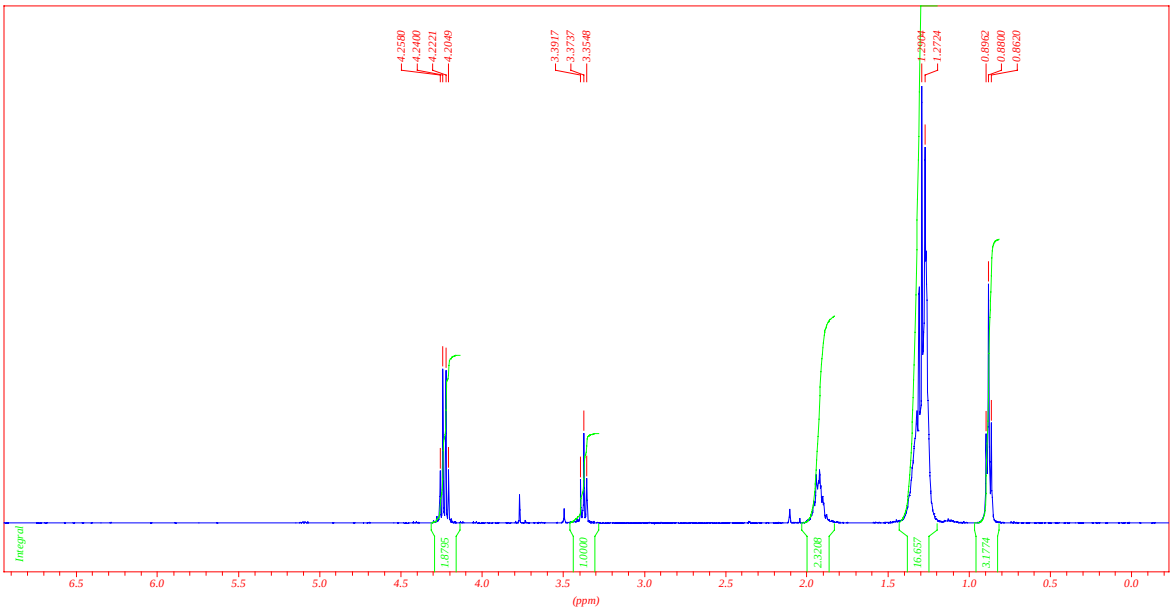
1-(4-Methoxybenzyl)-3-(4-methoxyphenyl)-5-phenyl-5-propyl-pyrimidine-2,4,6-trione 1m: R_f = 0.34 (Hexane/Et_2O = 90:10); FTIR (nujol) ν 1700, 1696, 1685 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, *J* = 8.4 Hz, 2H), 7.29 (m, 3H), 7.22 (m, 2H), 7.02 (d, *J* = 8.8 Hz, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.8 Hz, 2H), 5.08 (s, 2H), 3.82 (s, 3H), 3.80 (s, 3H), 2.41 (m, 2H), 1.36 (m, 2H), 0.96 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (125.6 MHz, $CDCl_3$) δ 170.0, 169.8, 159.9, 159.4, 150.9, 138.2, 130.8, 129.3, 129.2, 128.4, 128.3, 127.1, 125.8, 114.7, 113.8, 61.6, 55.5, 55.3, 45.3, 39.3, 19.3, 14.2; ESI (*m/z)* 495.2 [M^++Na, (21)], 473.2 [M^++1, (100)].

5-Hexyl-1-(4-methoxybenzyl)-3,5-diphenyl-pyrimidine-2,4,6-trione 1n: R_f = 0.54 (Hexane/AcOEt = 80:20); FTIR (nujol) ν 1700, 1699, 1696 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (m, 3H), 7.37 (d, *J* = 8.9 Hz, 2H), 7.30 (m, 3H), 7.23 (m, 2H), 7.11 (m, 2H), 6.82 (d, *J* = 8.9 Hz, 2H), 5.10 (s, 2H), 3.80 (s, 3H), 2.43 (m, 2H), 1.27 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 169.8, 159.4, 150.8, 138.2, 134.7, 130.8, 129.4, 129.2, 129.1, 128.5, 128.3, 125.9, 113.9, 61.6, 55.3, 45.3, 37.3, 31.4, 29.4, 25.8, 22.6, 14.0; ESI (*m/z)* 507.1 [M^++Na, (65)], 485.1 [M^++1, (32)], 296 (100).

5-Allyl-1-methyl-5-phenyl-3-(4-trifluoromethyl-phenyl)-pyrimidine-2,4,6-trione 1o: R_f = 0.41 (Hexane/AcOEt = 80:20); FTIR (nujol) ν 1704, 1699, 1695 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.4 Hz, 2H), 7.38 (m, 5H), 7.26 (d, *J* = 8.4 Hz, 2H), 5.80 (m, 1H), 5.29 (d, *J* = 17.2 Hz, 1H), 5.22 (d, *J* = 10.0 Hz, 1H), 3.41 (s, 3H), 3.22 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 169.4, 169.2, 150.4, 137.7, 137.2, 131.8, 131.5 (q, *J* = 32.8 Hz), 129.5, 129.1, 128.9, 126.6 (q, *J* = 3.7 Hz), 126.0, 123.7 (q, *J* = 273.1 Hz), 121.4, 61.8, 41.0, 29.2; ESI (*m/z)* 425.1 [M^++Na, (100)], 403.1 [M^++1, (97)].


EtOOC
COOH
7

3a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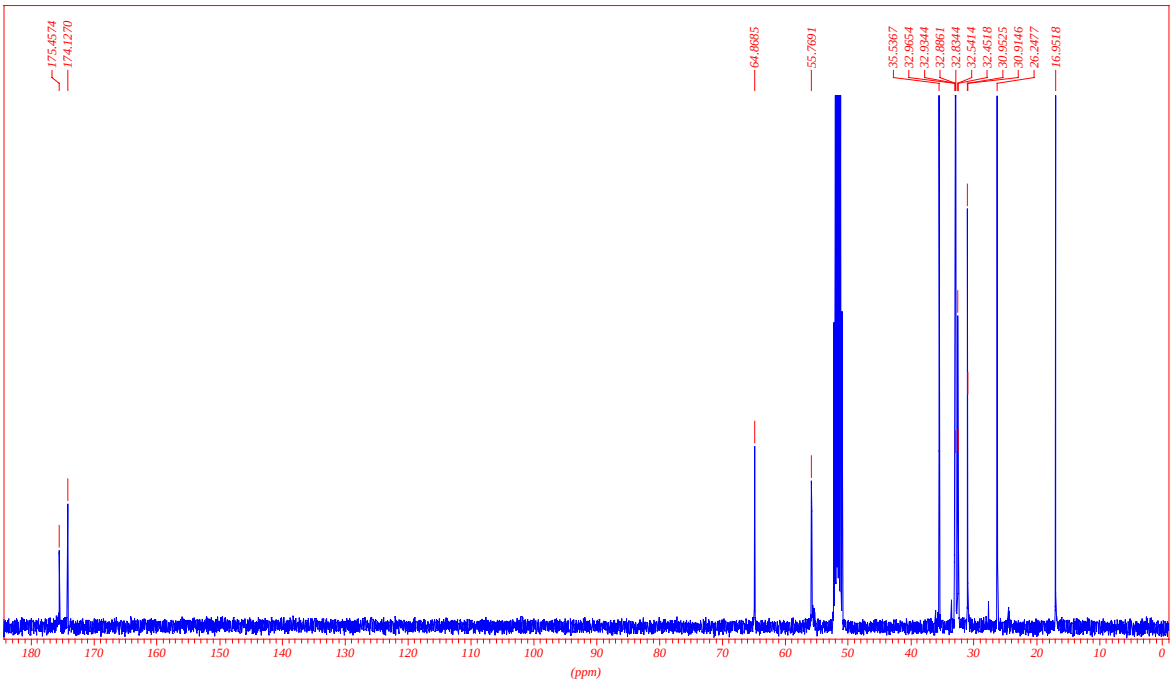
4.2400
4.2221
4.2049
3.3917
3.3737
3.3548
1.2964
1.2724
0.8962
0.8800
0.8620
Integral
1.8795
1.0000
2.3208
16.657
3.1774
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)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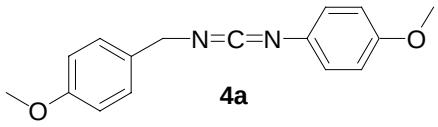
174.1270
64.8685
55.7691
35.5367
32.9654
32.9344
32.8861
32.8344
32.5414
32.4518
30.9525
30.9146
26.2477
16.9518
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)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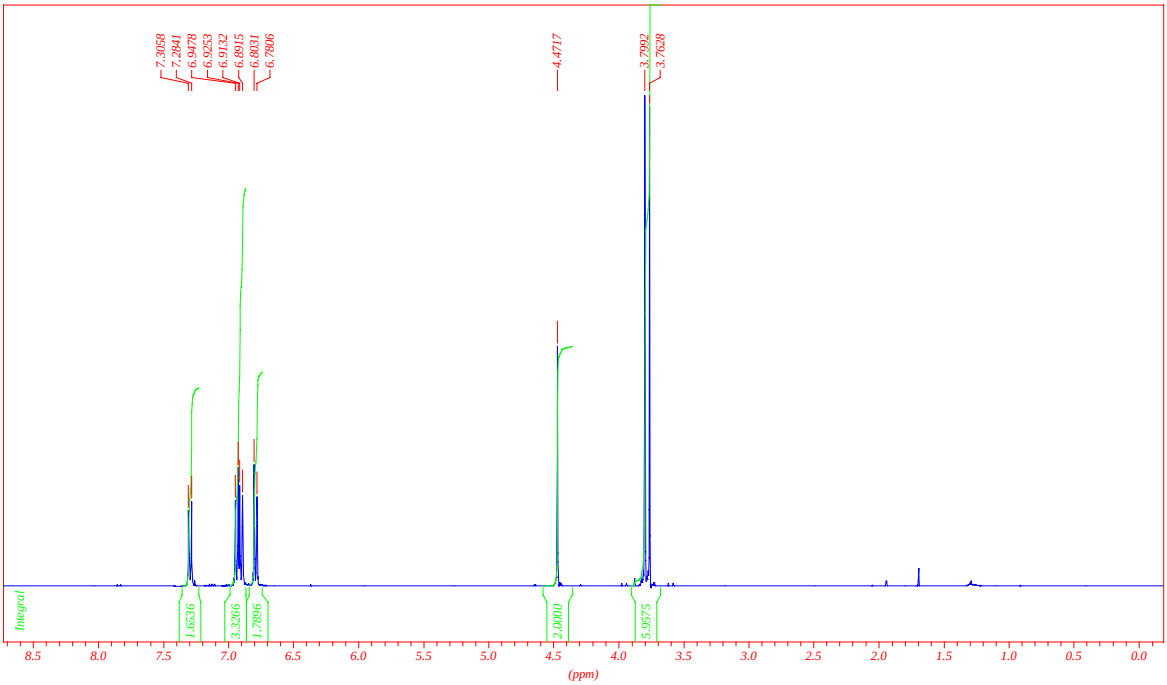
O
O

4a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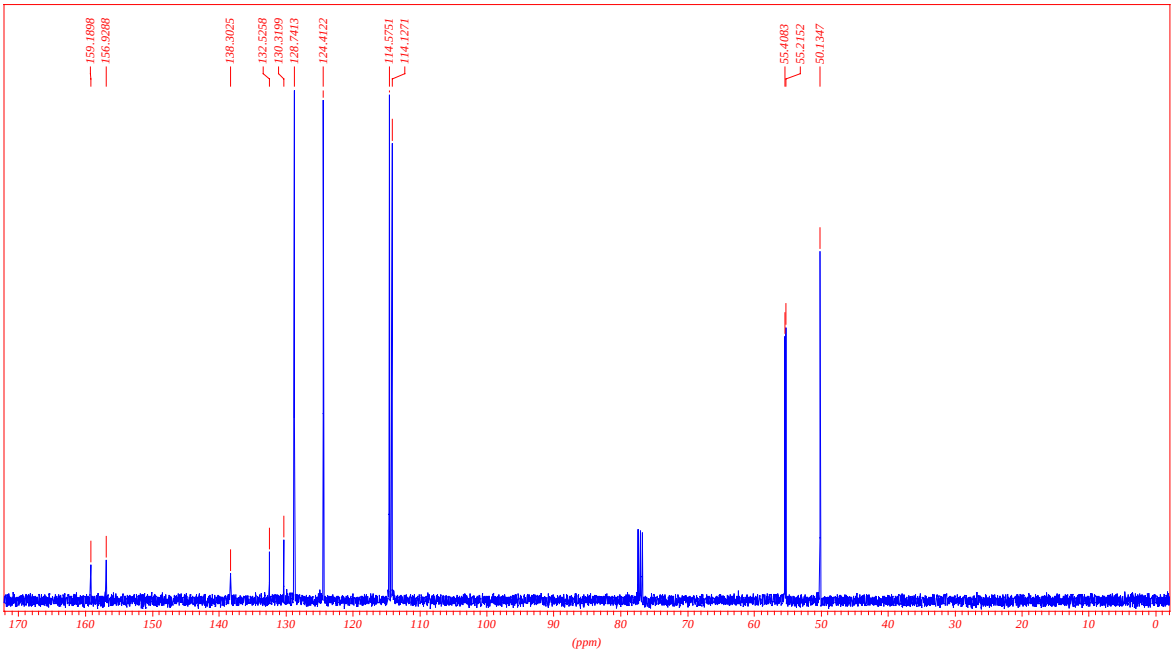
7.2841
6.9478
6.9253
6.9132
6.8915
6.8031
6.7806
4.4717
3.7992
3.7628
Integral
1.6536
3.3266
1.7896
2.0000
5.9575
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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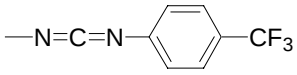
156.9288
138.3025
132.5258
130.3199
128.7413
124.4122
114.5751
114.1271
55.4083
55.2152
50.1347
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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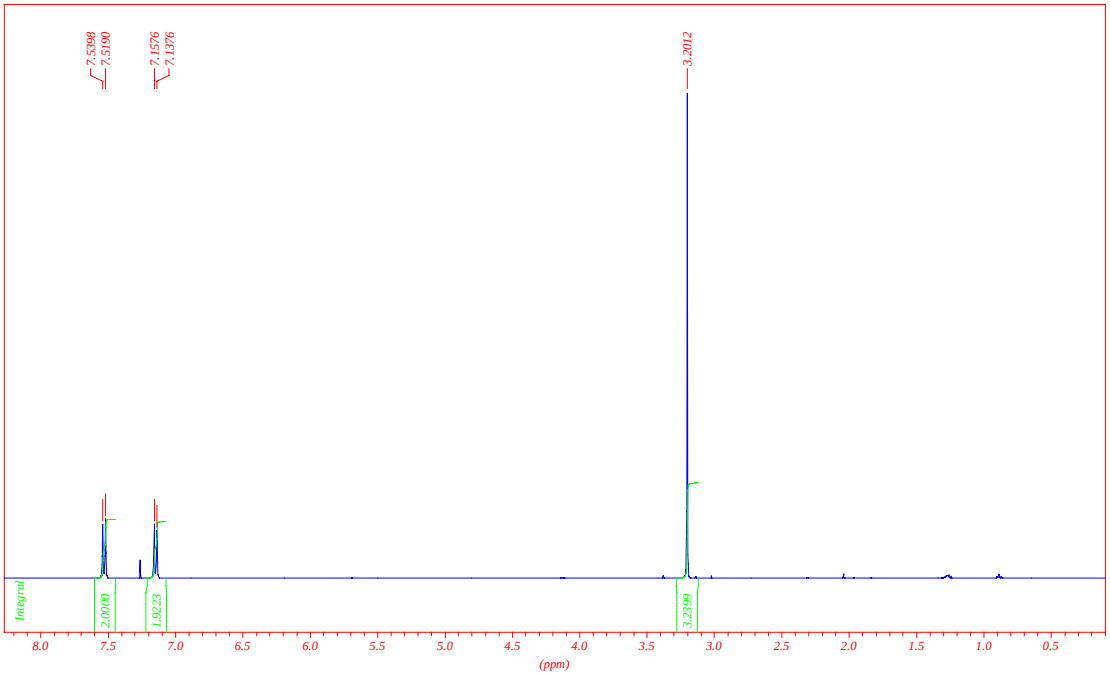
CF3

4c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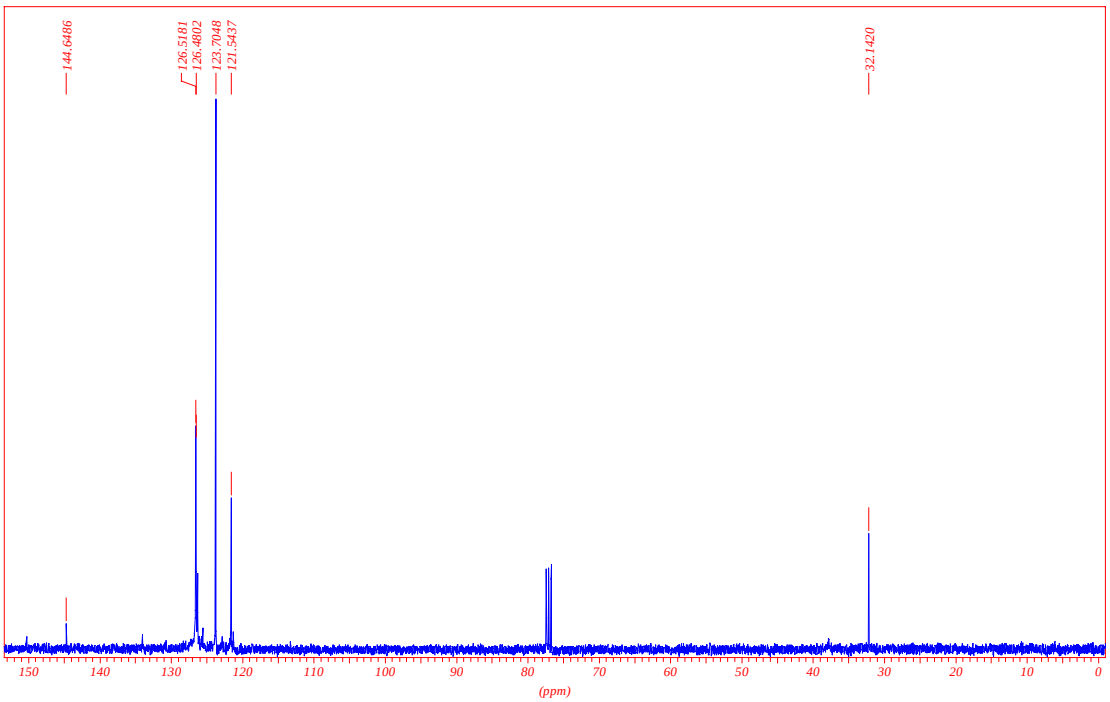
7.5190
7.1576
7.1376
3.2012
Integral
2.0000
1.9223
3.2399
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)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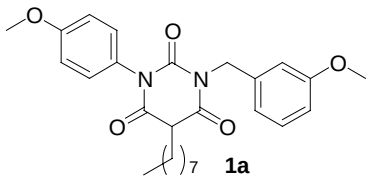
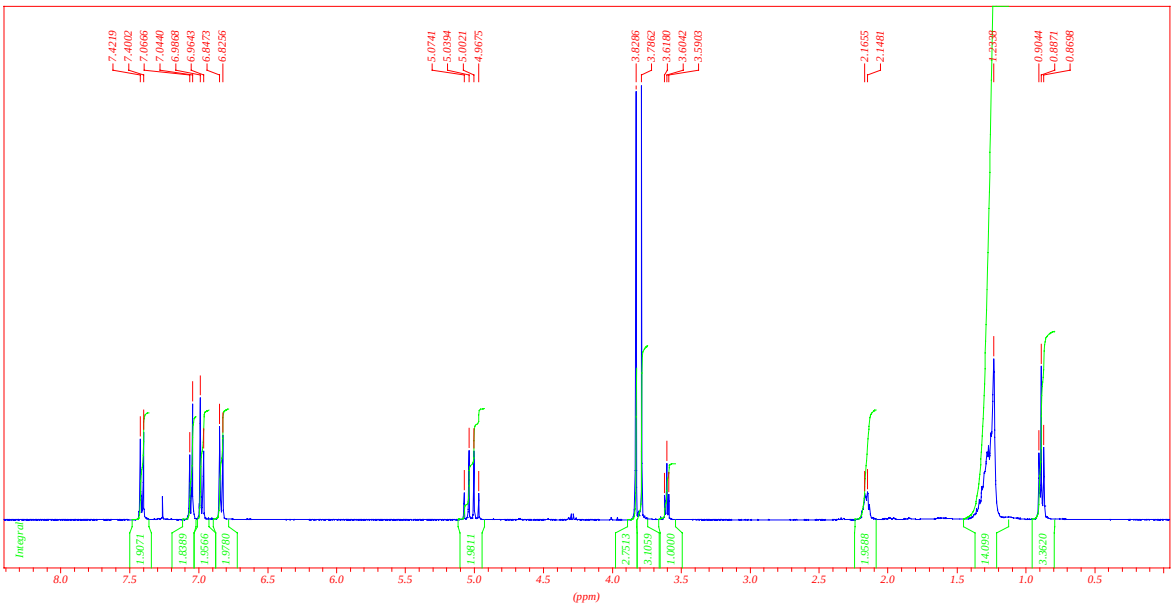
126.5181
126.4802
123.7048
121.5437
32.1420
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


O
O
N
N
O
O
O
7

1a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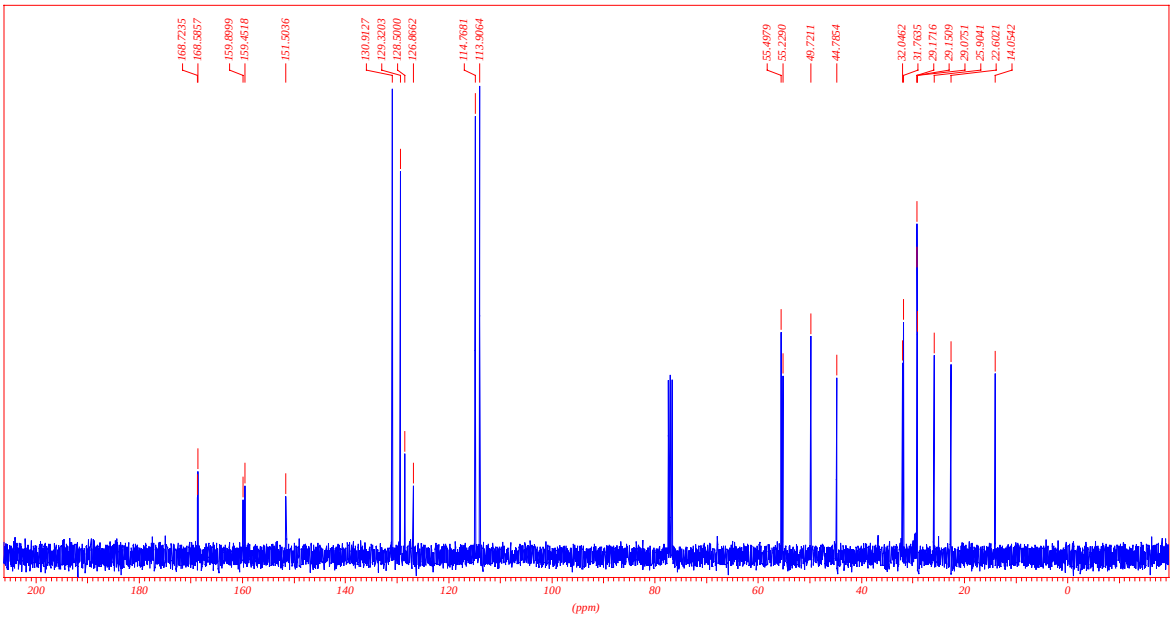
7.4002
7.0666
7.0440
6.9868
6.9643
6.8473
6.8256
5.0741
5.0394
5.0021
4.9675
3.8286
3.7862
3.6180
3.6042
3.5903
2.1655
2.1481
1.2339
0.9044
0.8871
0.8698
Integral
1.9071
1.8380
1.5566
1.5780
1.9811
2.7513
3.1059
1.0000
1.9588
14.0399
3.3620
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)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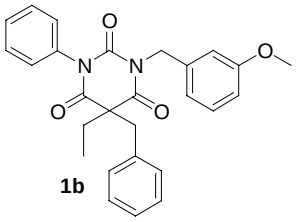
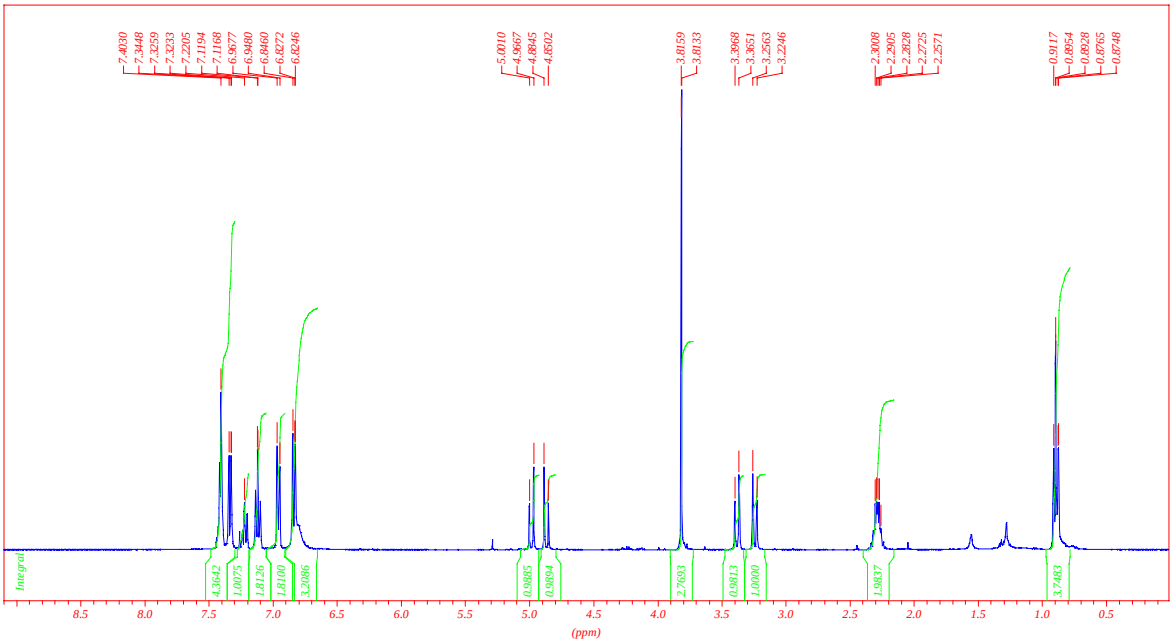
168.5857
159.8899
159.4518
151.5036
130.9127
129.3203
128.3000
126.8662
114.7681
113.9064
55.4979
55.2290
49.7211
44.7654
32.0462
31.7635
29.1716
29.1509
29.0751
25.9041
22.6021
14.0542
200
180
160
140
120
100
80
60
40
20
0
(ppm)


O
N
N
O
O
O
O

1b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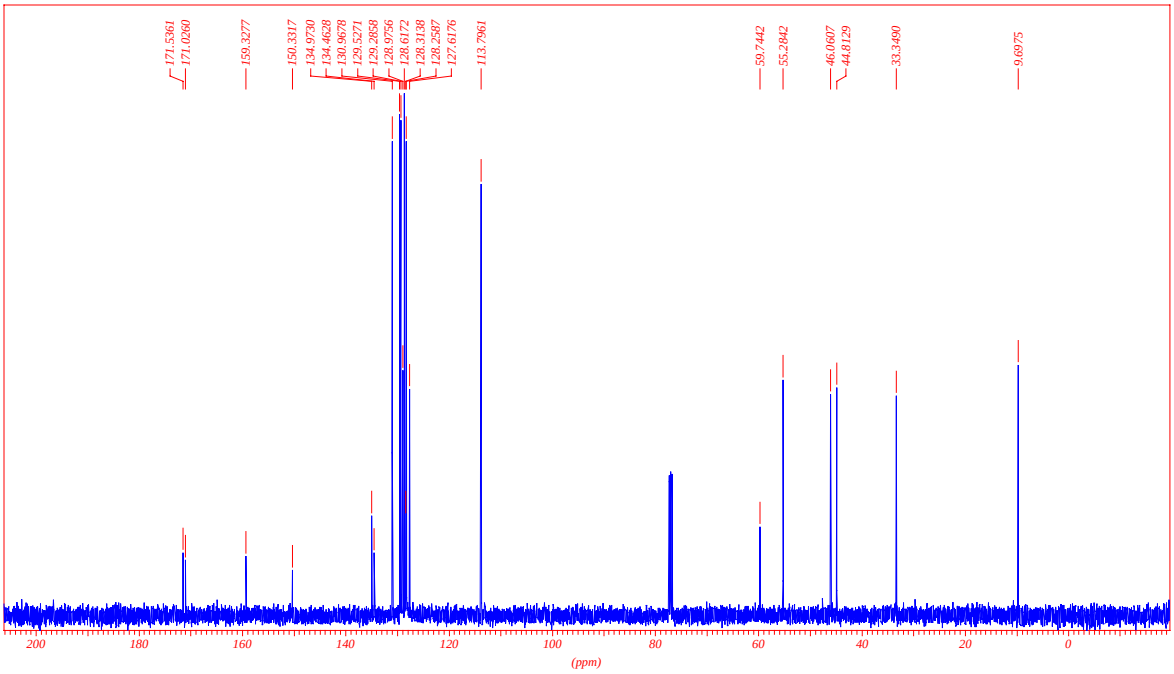
7.3259
7.3233
7.2205
7.1194
7.1168
6.9677
6.9480
6.9460
6.8272
6.8246
5.0010
4.9667
4.8845
4.8502
3.8159
3.8133
3.3968
3.3651
3.2563
3.2246
2.3008
2.2905
2.2828
2.2725
2.2571
0.9117
0.8854
0.8928
0.8765
0.8748
Integral
4.3642
1.0075
1.8126
1.8100
3.2086
0.9885
0.9894
2.7693
0.9813
1.0000
1.9837
3.7483
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)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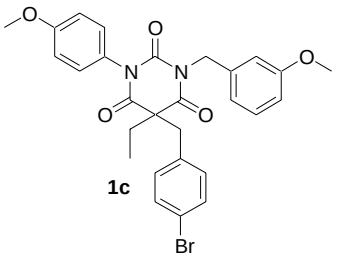
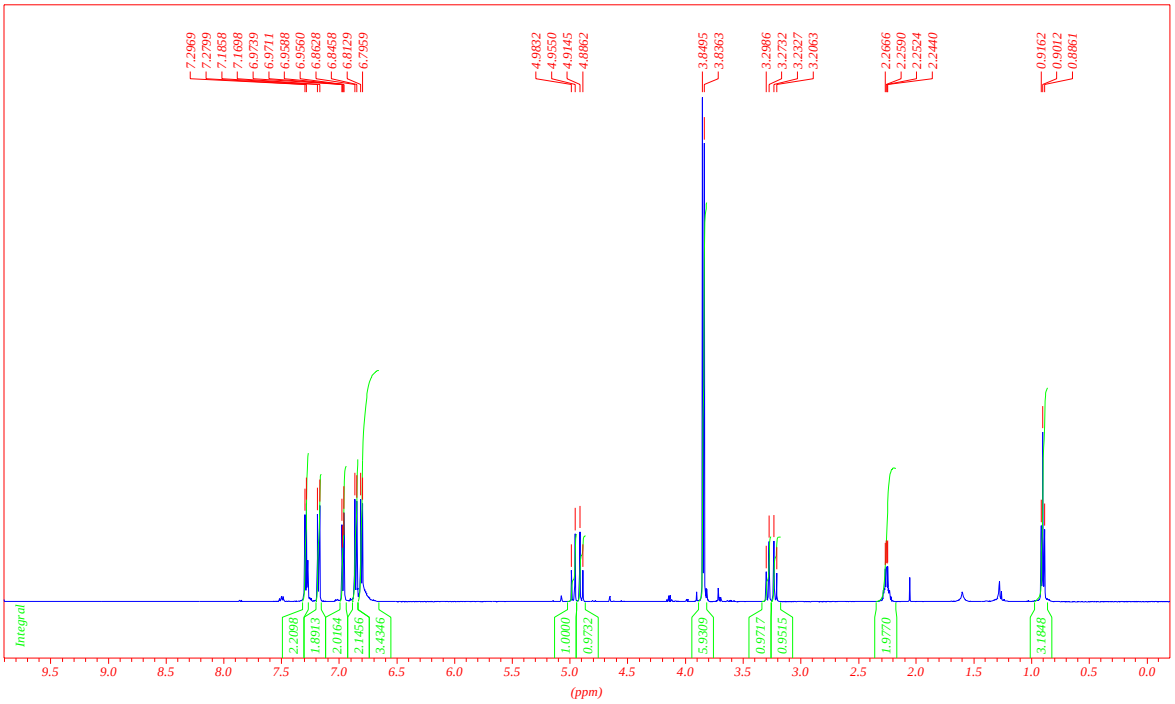
171.0260
159.3277
150.3317
134.9730
134.4628
130.9678
129.5271
129.2858
128.9756
128.6172
128.3138
128.2587
127.6176
113.7961
59.7442
55.2842
46.0607
44.8129
33.3490
9.6975
200
180
160
140
120
100
80
60
40
20
0
(ppm)


O
O
N
N
O
O
O
Br

1c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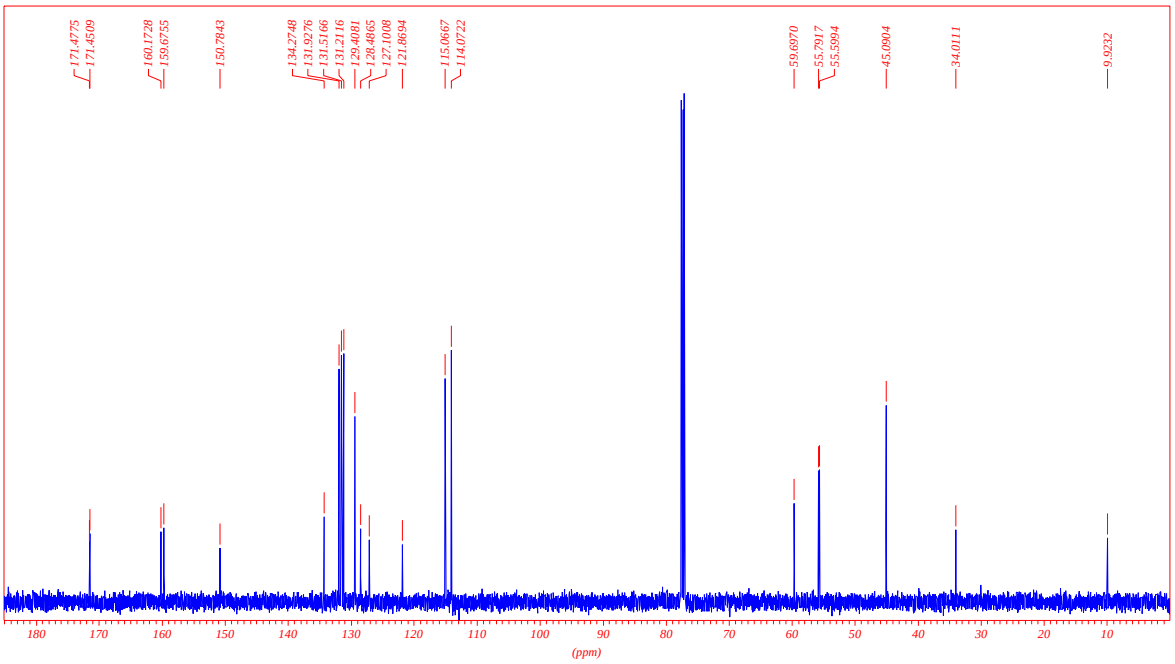
7.2799
7.1858
7.1698
6.9739
6.9711
6.9588
6.9560
6.8628
6.8458
6.8129
6.7959
4.9832
4.9550
4.9145
4.8862
3.8495
3.8363
3.2986
3.2732
3.2327
3.2063
2.2666
2.2390
2.2524
2.2440
0.9162
0.9012
0.8861
Integral
2.2098
1.8913
2.0164
2.1456
3.4346
1.0000
0.9732
5.9309
0.9717
0.9515
1.9770
3.1848
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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134.2748
131.9276
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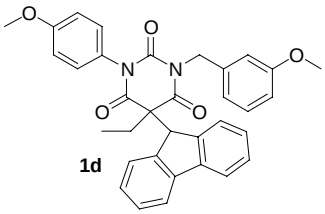
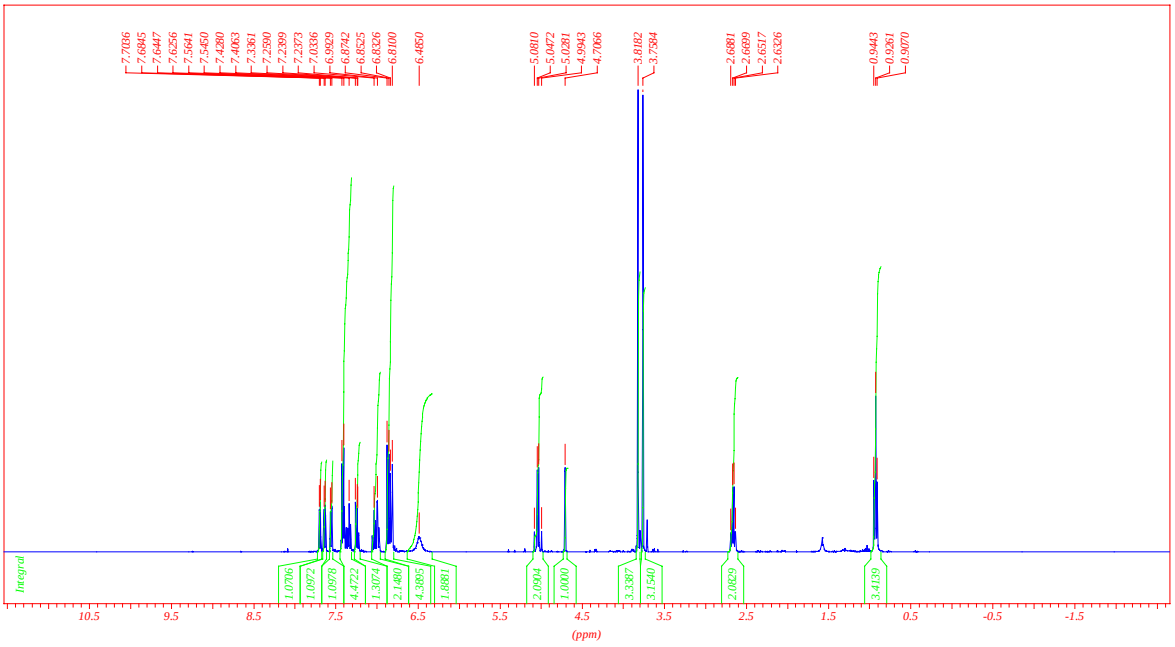
131.2116
129.4081
128.4865
127.1008
121.8694
115.0667
114.0722
59.6970
55.7917
55.5994
45.0904
34.0111
9.9232
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)



1d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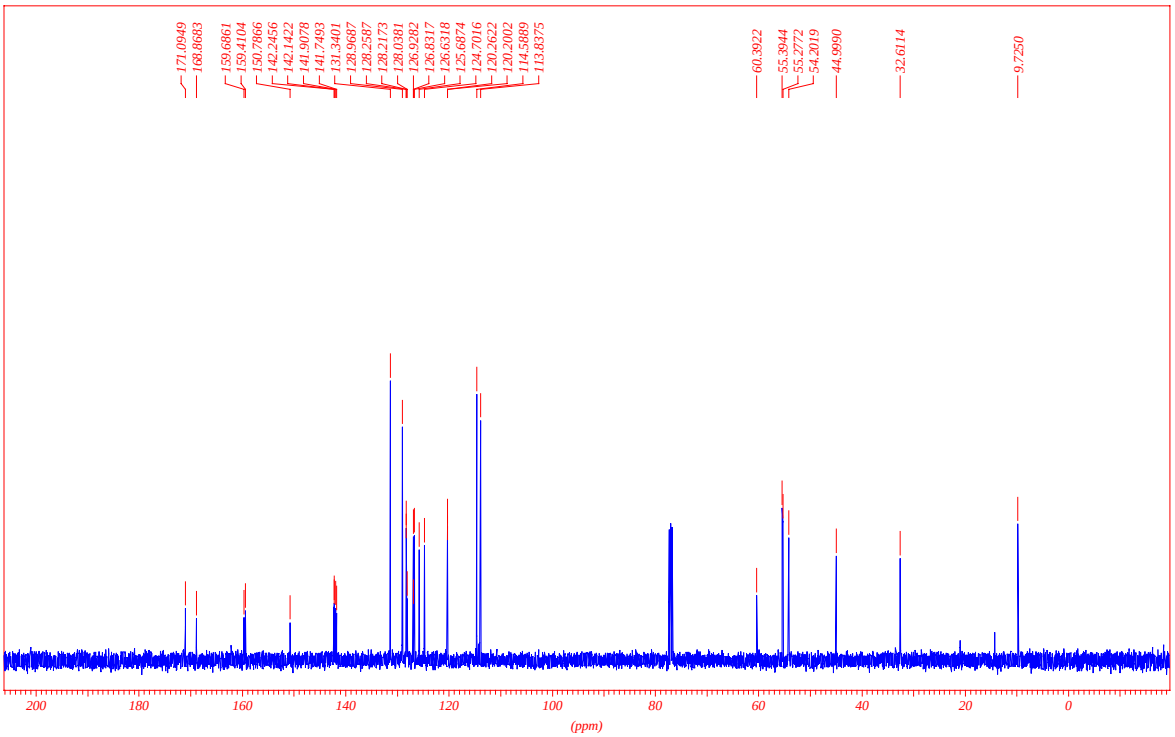
7.6256
7.5641
7.5450
7.4280
7.4063
7.3361
7.2990
7.2399
7.2373
7.0336
6.9929
6.8742
6.8525
6.8326
6.8100
6.4850
5.0810
5.0472
5.0281
4.9943
4.7066
3.8182
3.7584
2.6881
2.6699
2.6517
2.6326
0.9443
0.9261
0.9070
Integral
1.0706
1.0072
1.0978
4.4722
1.3074
2.1480
4.3895
1.8881
2.0934
1.0000
3.3387
3.1540
2.0829
3.4139
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
(ppm)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128.2587
128.2173
128.0381
126.9282
126.8317
126.6318
125.6874
124.7016
120.2622
120.2002
114.5889
113.8375
60.3922
55.3944
55.2772
54.2019
44.9990
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9.7250
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180
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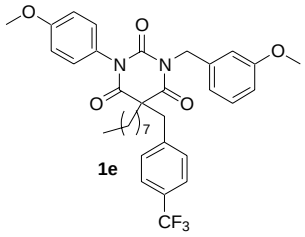
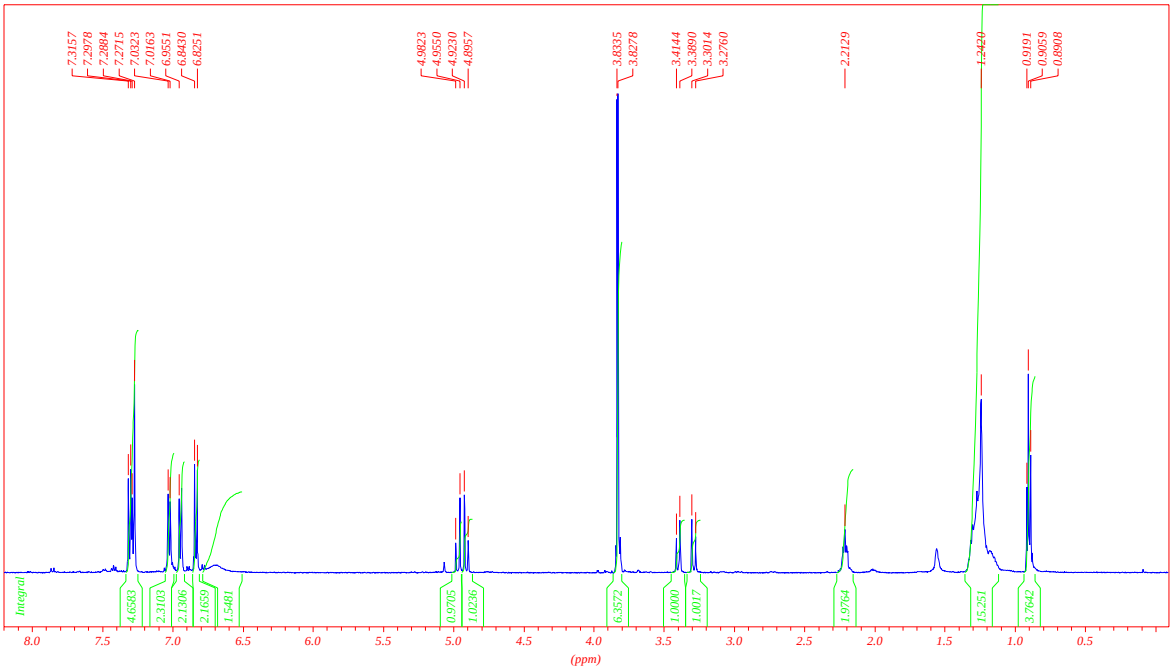
120
100
80
60
40
20
0
(ppm)


O
O
N
N
O
O
O
7
CF3

1e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6.8251
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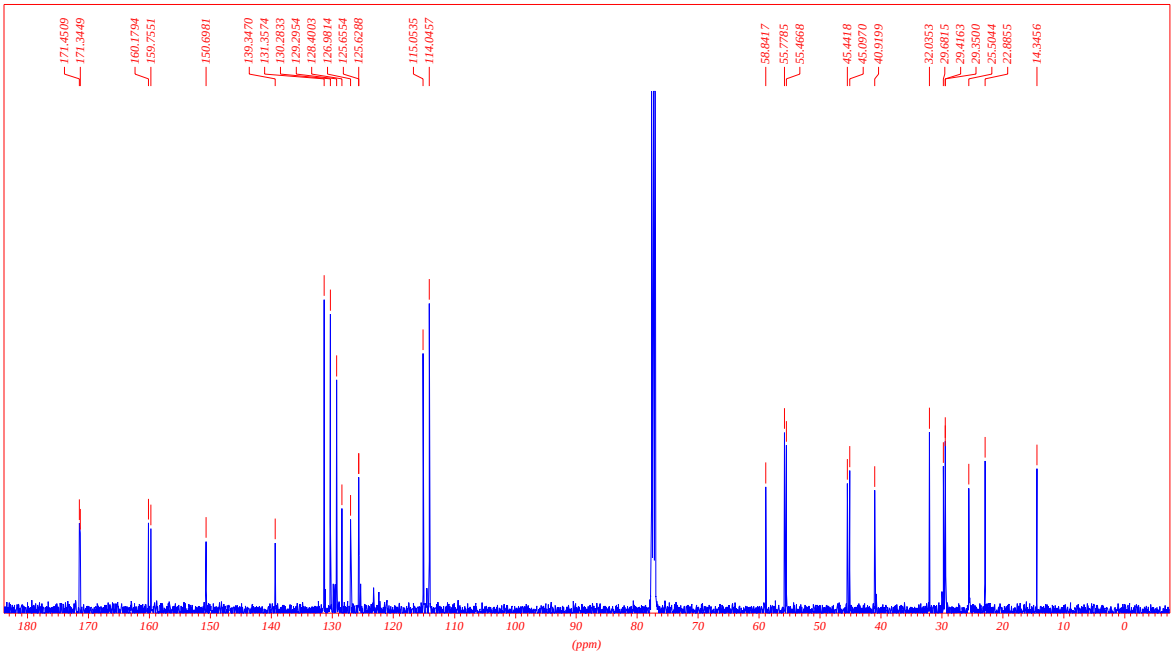
4.9550
4.9230
4.8957
3.8335
3.8278
3.4144
3.3890
3.3014
3.2760
2.2129
1.2420
0.9191
0.9059
0.8908
Integral
4.6583
2.3103
2.1306
2.1659
1.5481
0.9735
1.0236
6.3572
1.0000
1.0017
1.9764
15.251
3.7642
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)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129.2954
128.4003
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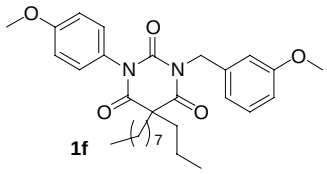
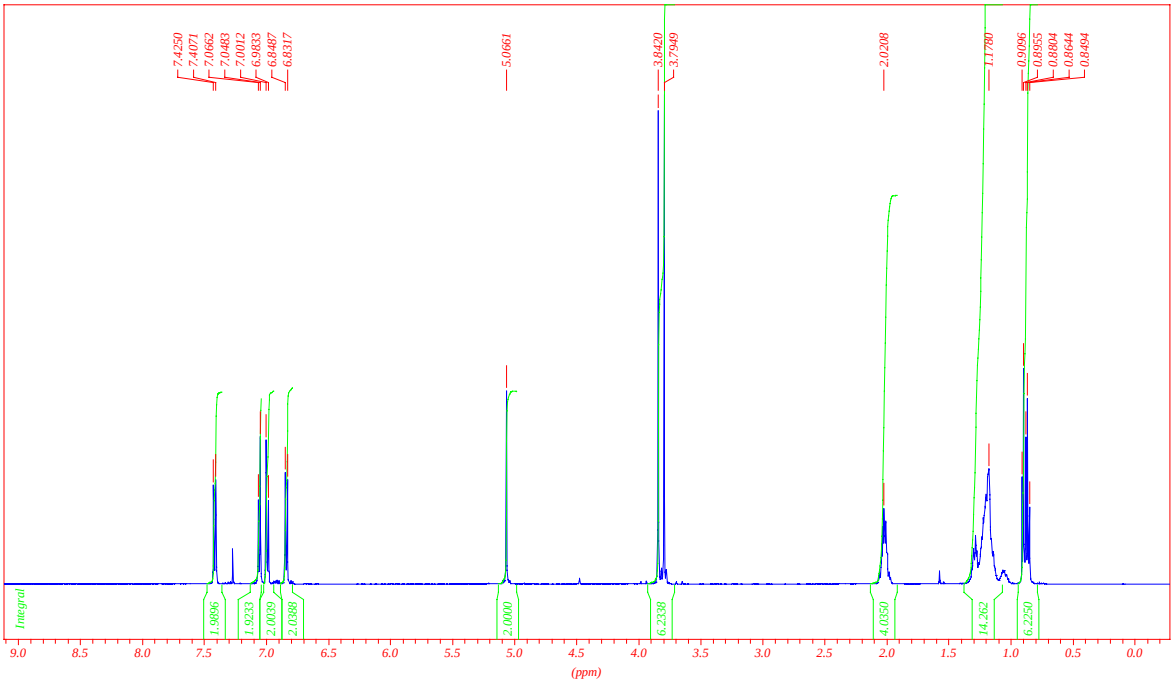
125.6554
125.6288
115.0535
114.0457
58.8417
55.7785
55.4668
45.4418
45.0970
40.9199
32.0353
29.6815
29.4163
29.3500
25.5044
22.8855
14.3456
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
(ppm)


O
O
N
N
O
O
O
7

1f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7.0483
7.0012
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6.8487
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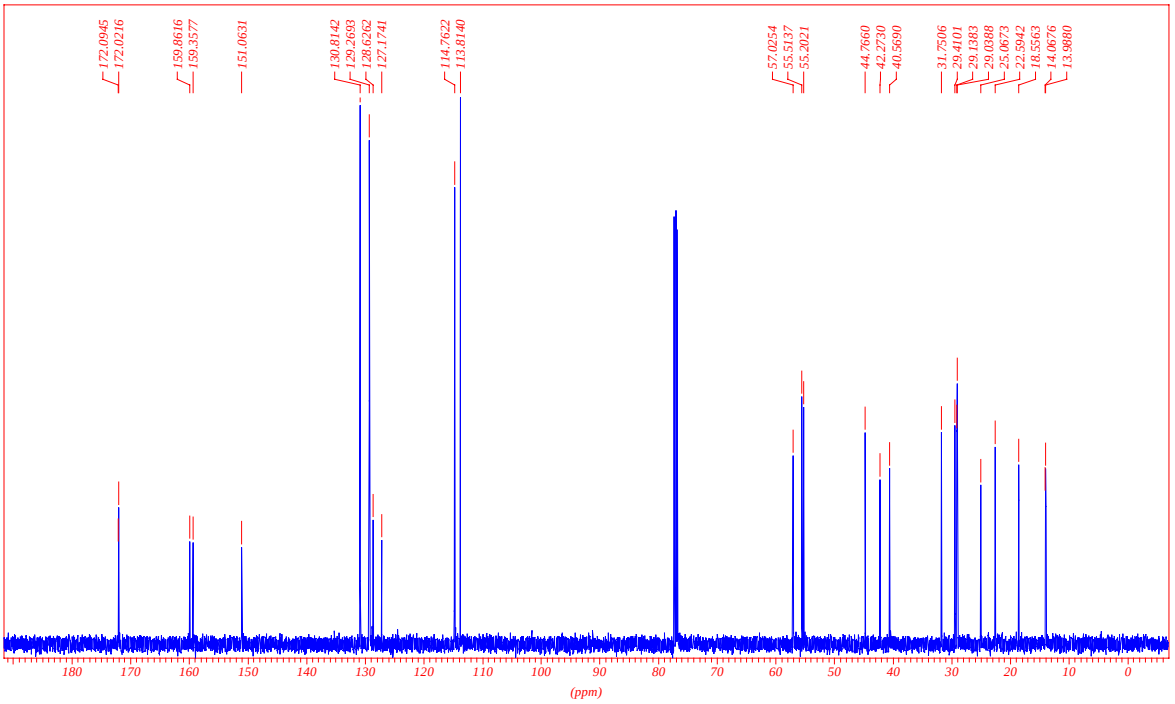
5.0661
3.8420
3.7949
2.0208
1.1780
0.9096
0.8955
0.8804
0.8644
0.8494
Integral
1.9896
1.9233
2.0039
2.0388
2.0000
6.2338
4.0350
14.262
6.2250
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)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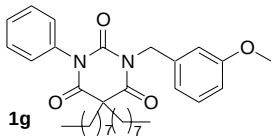
159.3577
151.0631
130.8142
129.2693
128.6262
127.1741
114.7622
113.8140
57.0254
55.5137
55.2021
44.7660
42.2730
40.5690
31.7506
29.4101
29.1383
29.0388
25.0673
22.5942
18.5563
14.0676
13.9880
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)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N
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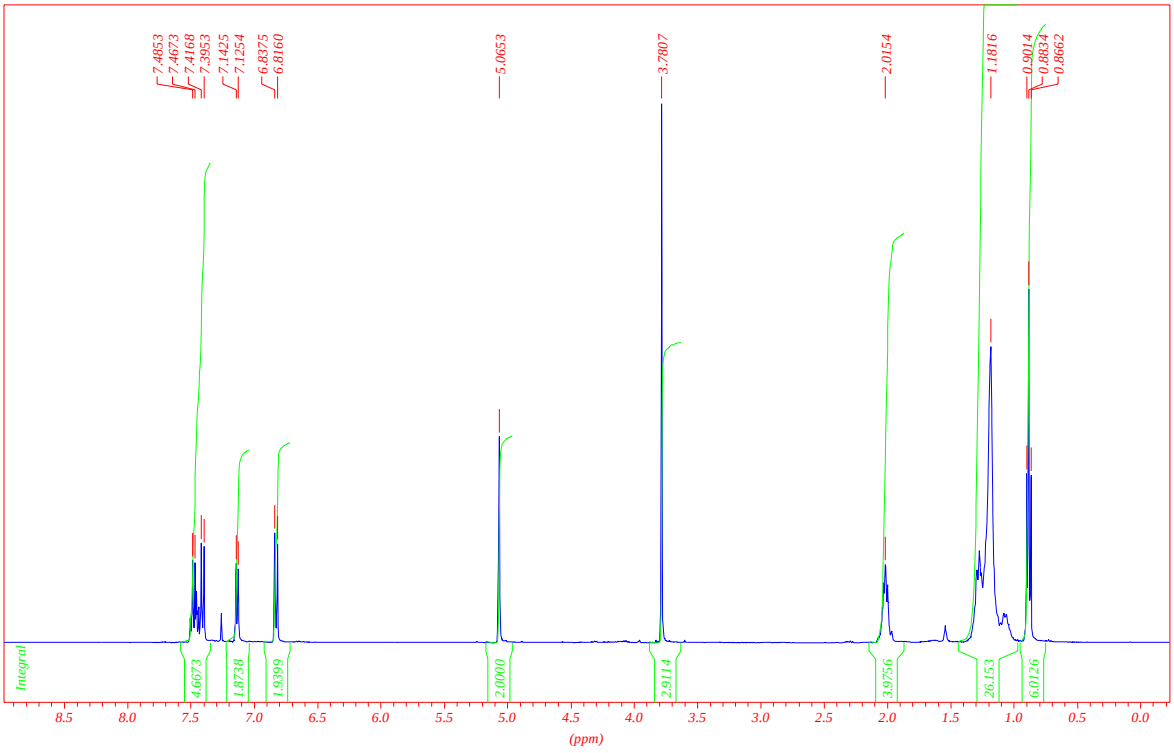
O
O
O
7
7

1g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7.4168
7.3953
7.1425
7.1254
6.8375
6.8160
5.0653
3.7807
2.0154
1.1816
0.9014
0.8834
0.8662
Integral
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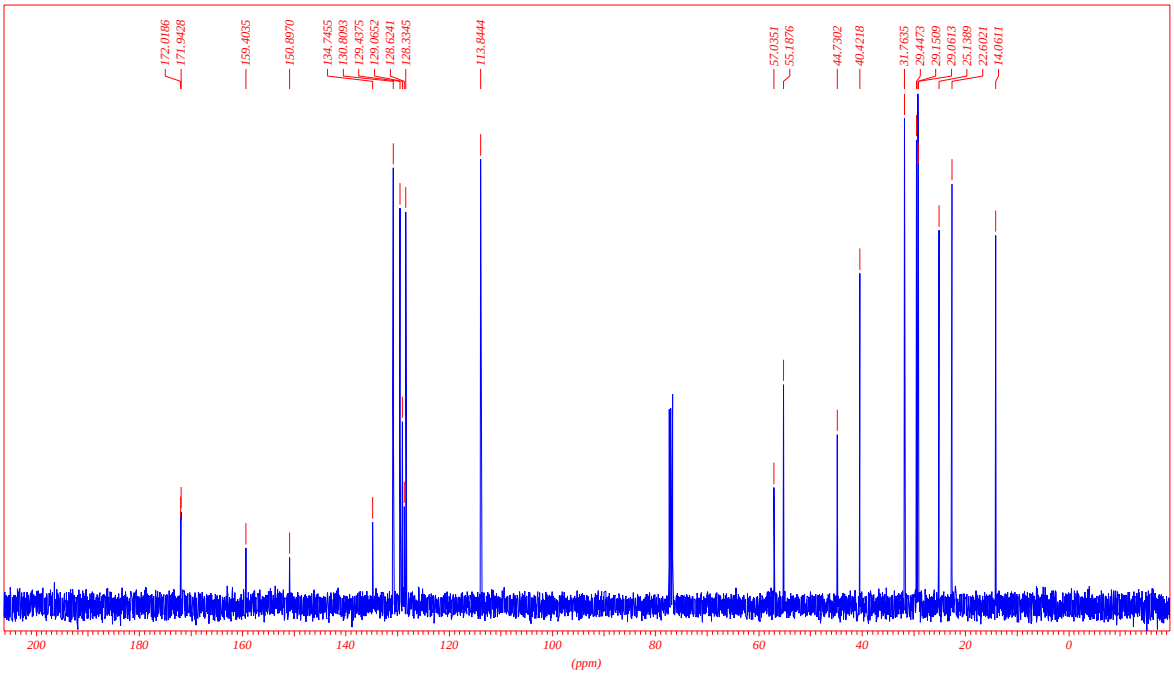
1.8738
1.9399
2.0000
2.9114
3.9756
26.153
6.0126
(ppm)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57.0351
55.1876
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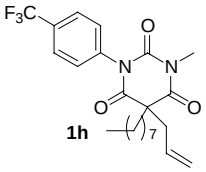
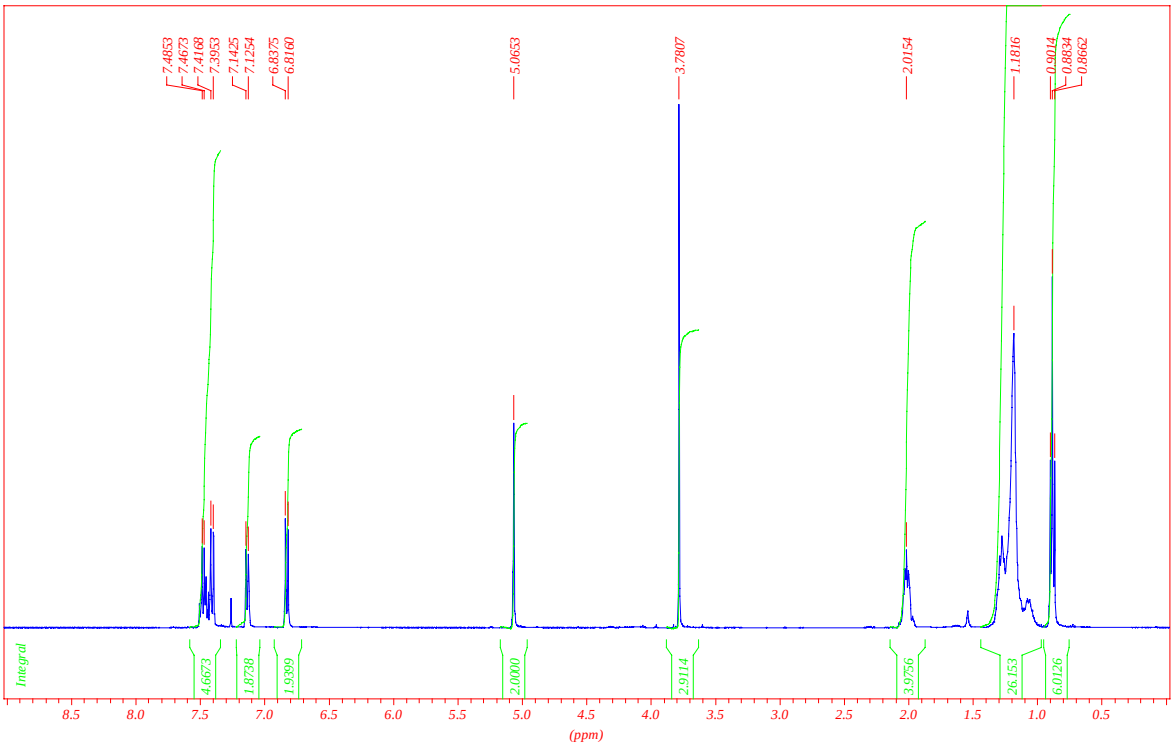
29.4473
29.1509
29.0613
25.1389
22.6021
14.0611
(ppm)


F3C
O
N
N
O
O
1h
7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7.4168
7.3933
7.1425
7.1254
6.8375
6.8160
5.0653
3.7807
2.0154
1.1816
0.9014
0.8834
0.8662
Integral
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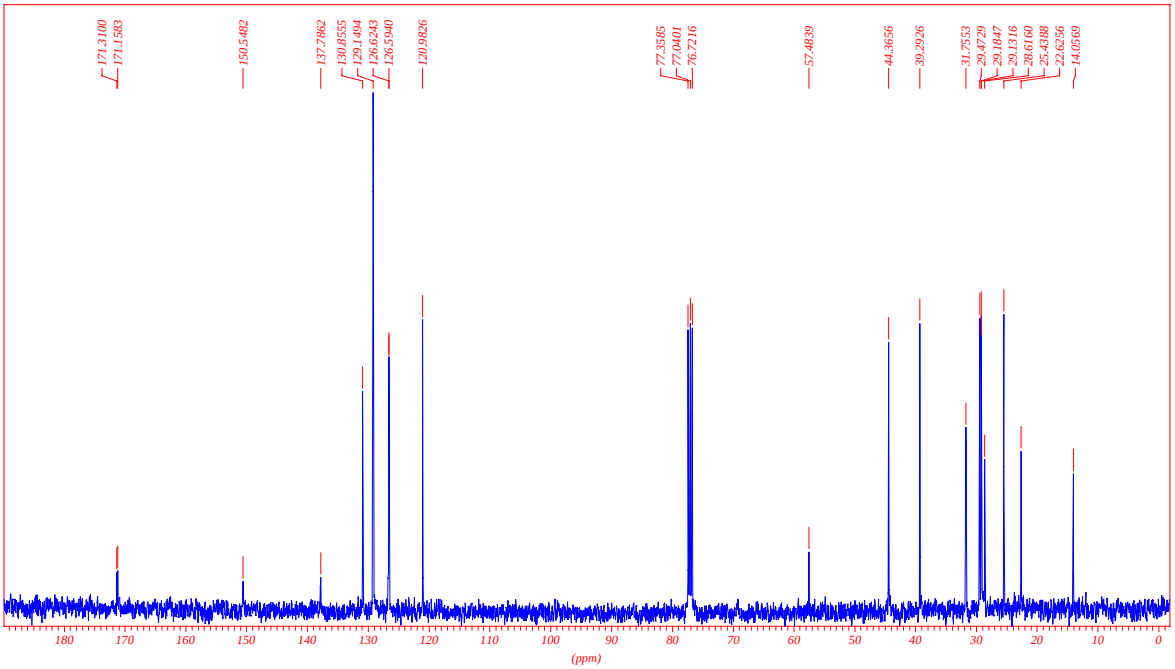
1.8738
1.9399
2.0000
2.9114
3.9756
26.153
6.0126
(ppm)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150.5482
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130.8555
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126.6243
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76.7216
57.4839
44.3656
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29.1316
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25.4388
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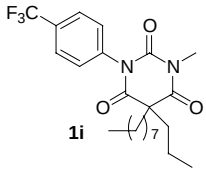
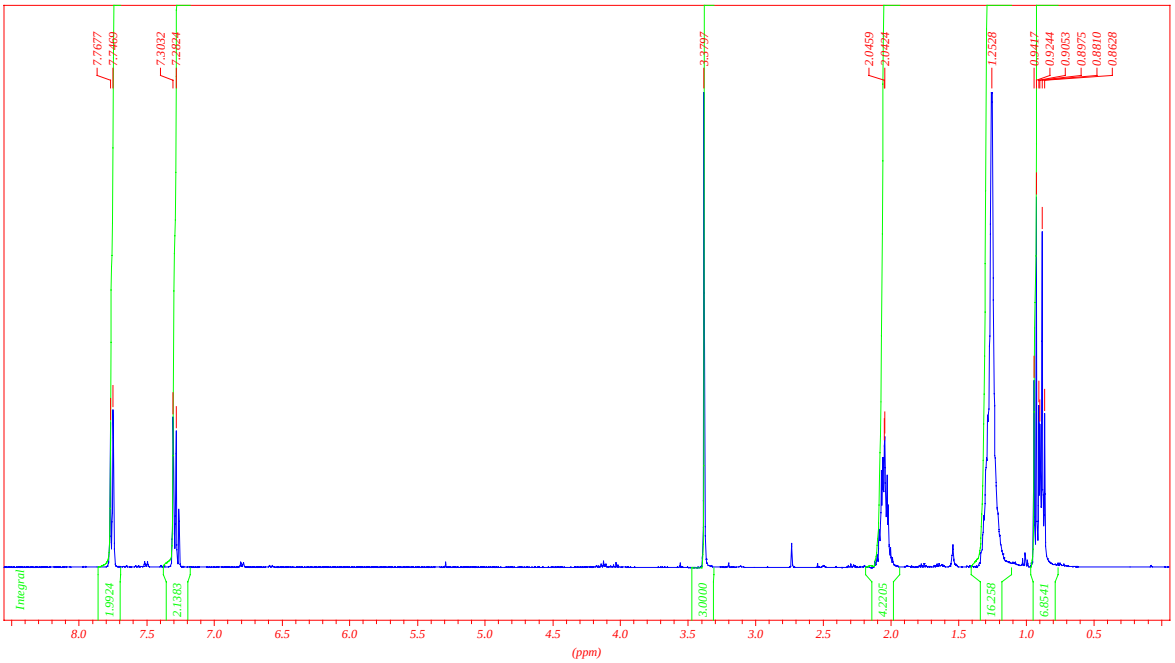
14.0569
(ppm)


F3C
O
N
N
O
O
7

1i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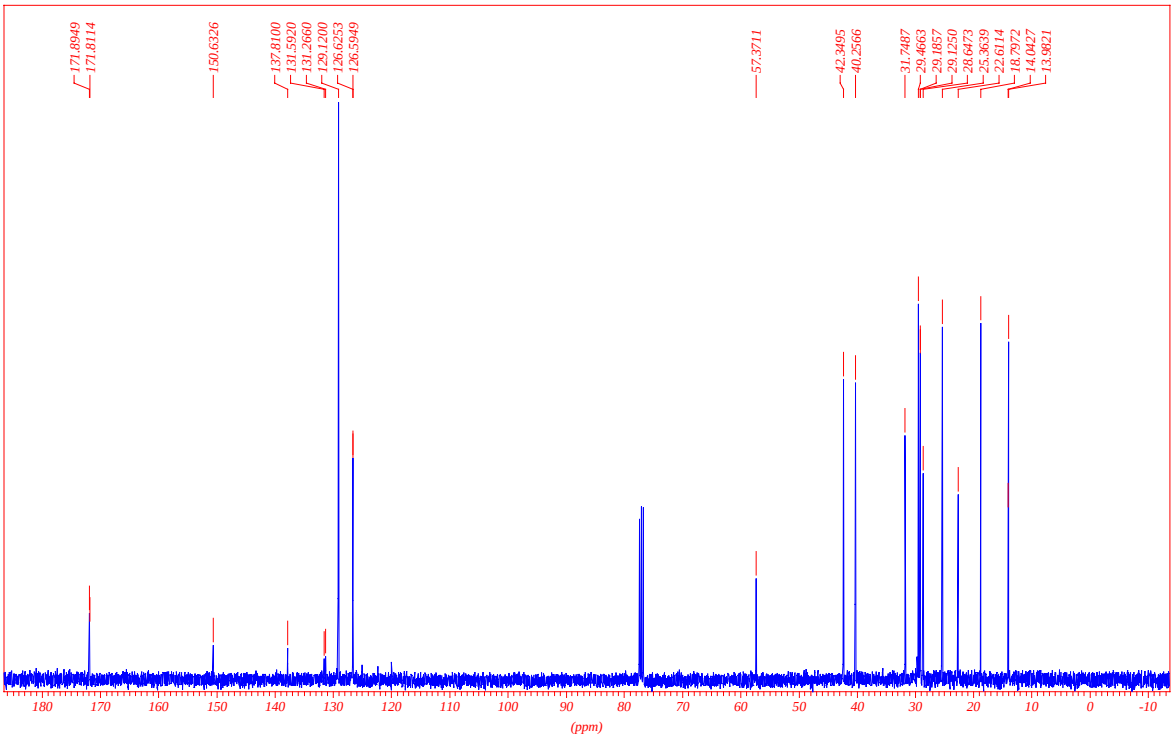
7.7469
7.3032
7.2824
3.3797
2.0459
2.0424
1.2528
0.9417
0.9244
0.9053
0.8975
0.8810
0.8628
Integral
1.9924
2.1383
3.0000
4.2205
16.258
6.8541
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
(ppm)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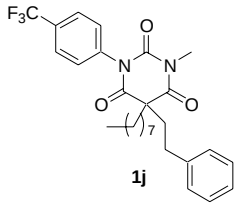
171.8114
150.6326
137.8100
131.5920
131.2660
129.1200
126.6253
126.5949
57.3711
42.3495
40.2566
31.7487
29.4663
29.1857
29.1250
28.6473
25.3639
22.6114
18.7972
14.0427
13.9821
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)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O
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N
O
O
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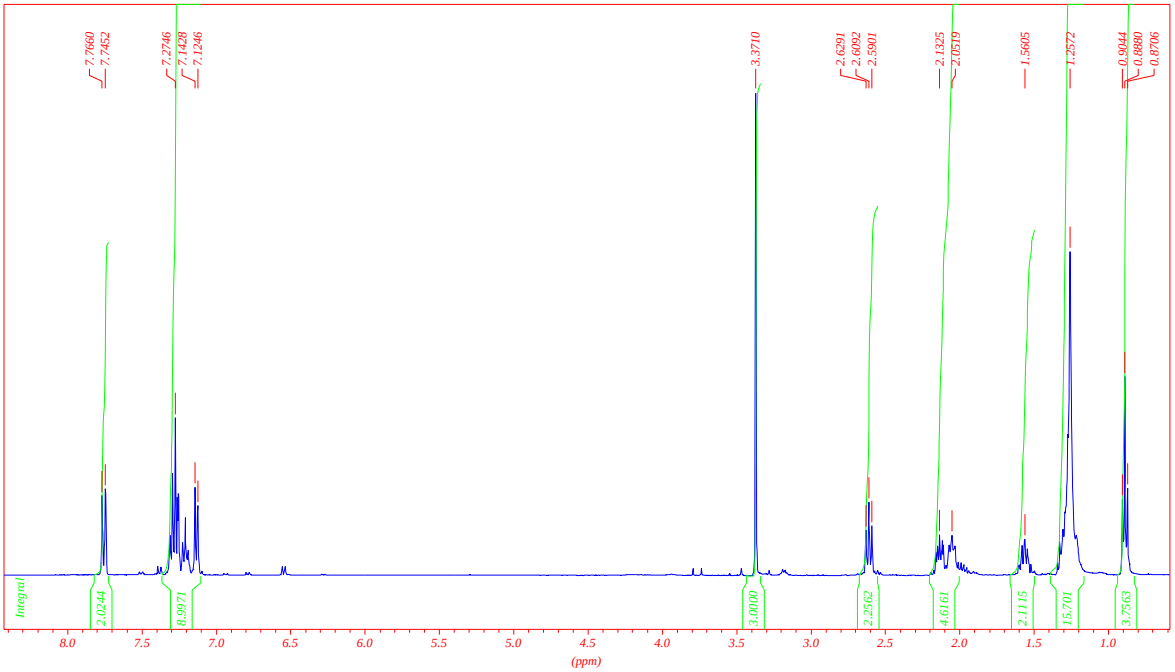
1j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7.2746
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7.1246
3.3710
2.6291
2.6092
2.5901
2.1325
2.0519
1.5605
1.2572
0.9044
0.8880
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Integral
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8.9971
3.0000
2.2562
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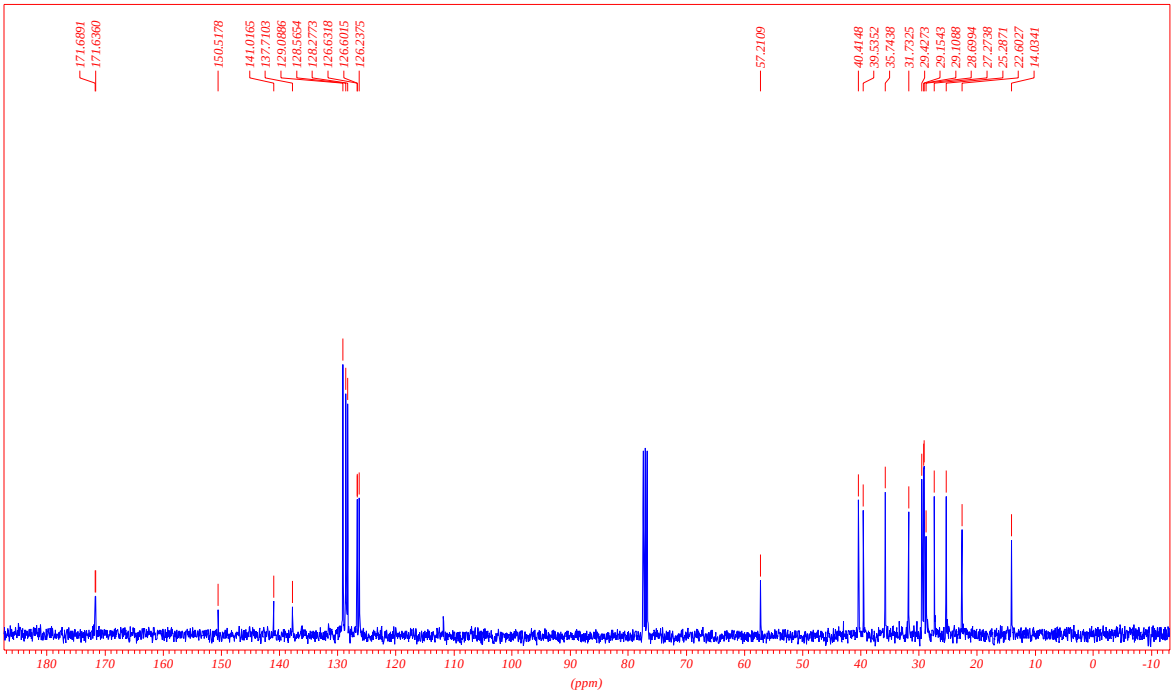
2.1115
15.701
3.7563
(ppm)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137.7103
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128.5654
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126.2375
57.2109
40.4148
39.5352
35.7438
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28.6994
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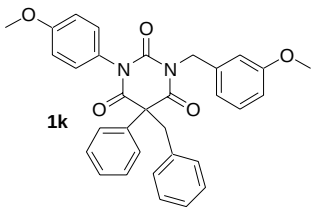
25.2871
22.6027
14.0341
(ppm)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O
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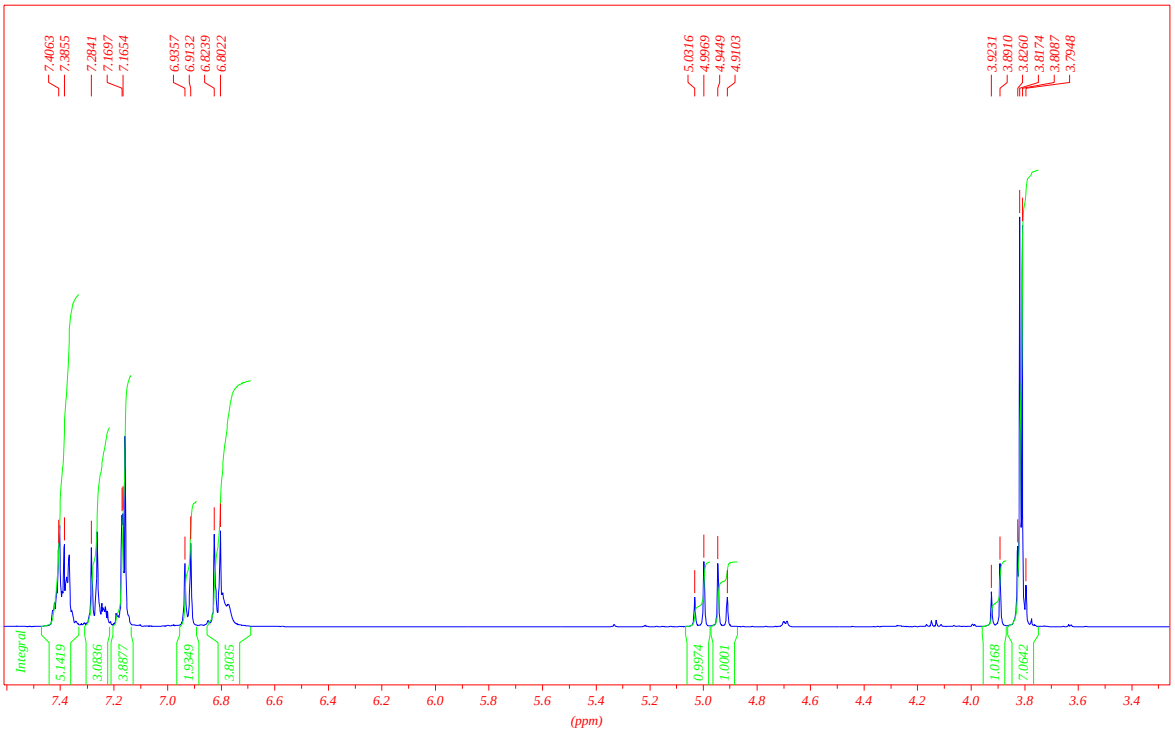
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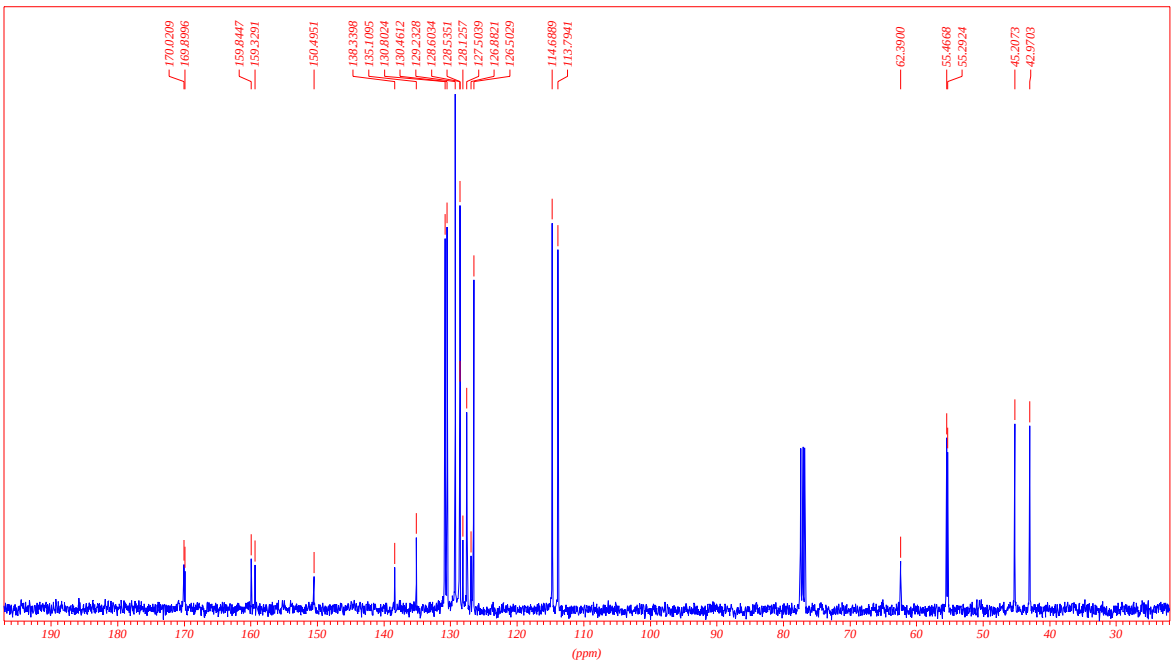
7.2841
7.1697
7.1654
6.9357
6.9132
6.8239
6.8022
5.0316
4.9969
4.9449
4.9103
3.9231
3.8910
3.8260
3.8174
3.8087
3.7948
Integral
5.1419
3.0836
3.8877
1.9349
3.8035
0.9974
1.0001
1.0168
7.0642
7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4
(ppm)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135.1095
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130.4612
129.2328
128.6034
128.5351
128.1257
127.5039
126.8821
126.5029
114.6889
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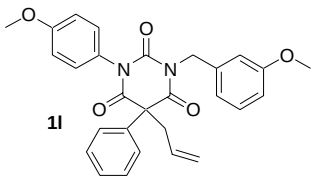
55.4668
55.2924
45.2073
42.9703
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30
(ppm)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O
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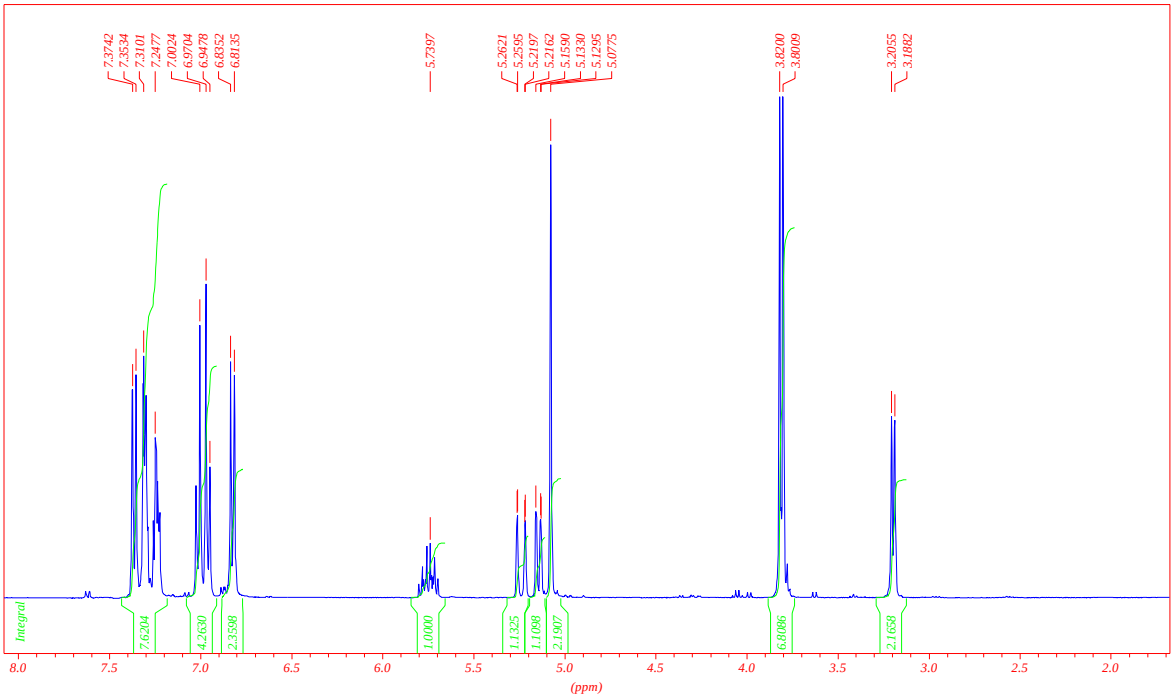
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7.2477
7.0024
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6.9478
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6.8135
5.7397
5.2621
5.2595
5.2197
5.2162
5.1530
5.1330
5.1295
5.0775
3.8200
3.8009
3.2055
3.1882
Integral
7.6204
4.2630
2.3598
1.0000
1.1325
1.1090
2.1907
6.8086
2.1658
8.0
7.5
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5.5
5.0
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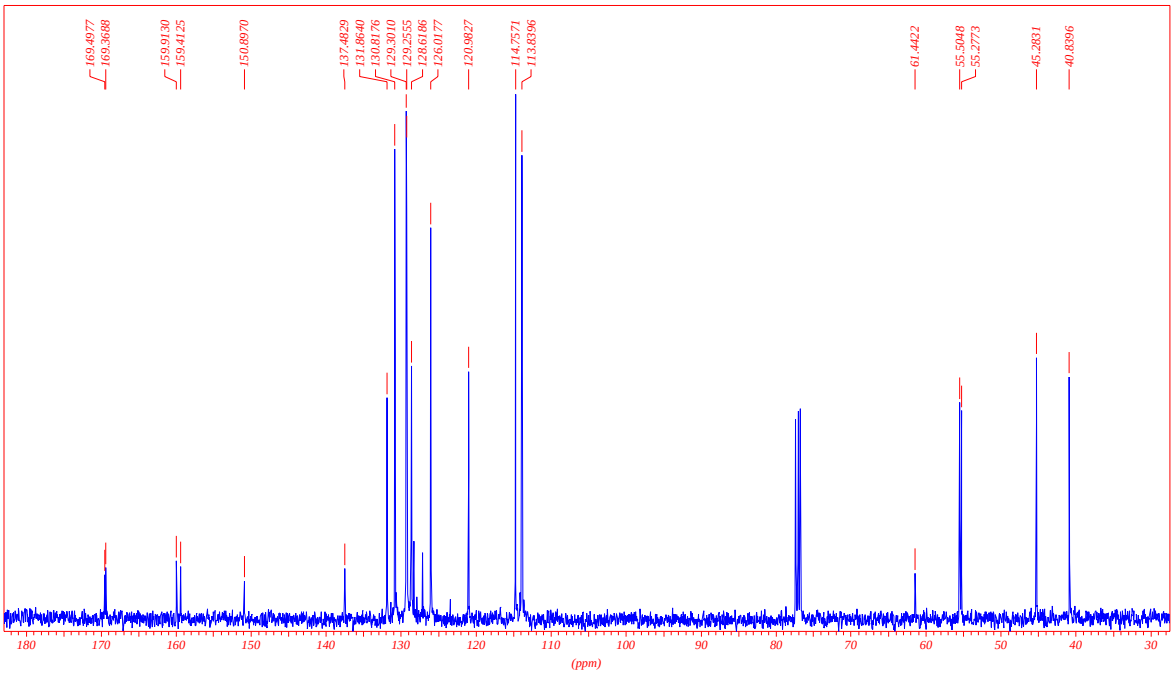
3.5
3.0
2.5
2.0
(ppm)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131.8640
130.8176
129.3010
129.2555
128.6186
126.0177
120.9827
114.7571
113.8396
61.4422
55.5048
55.2773
45.2831
40.8396
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170
160
150
140
130
120
110
100
90
80
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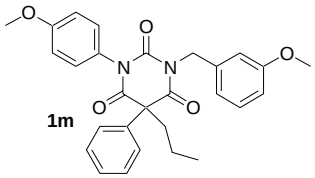
50
40
30
(ppm)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O
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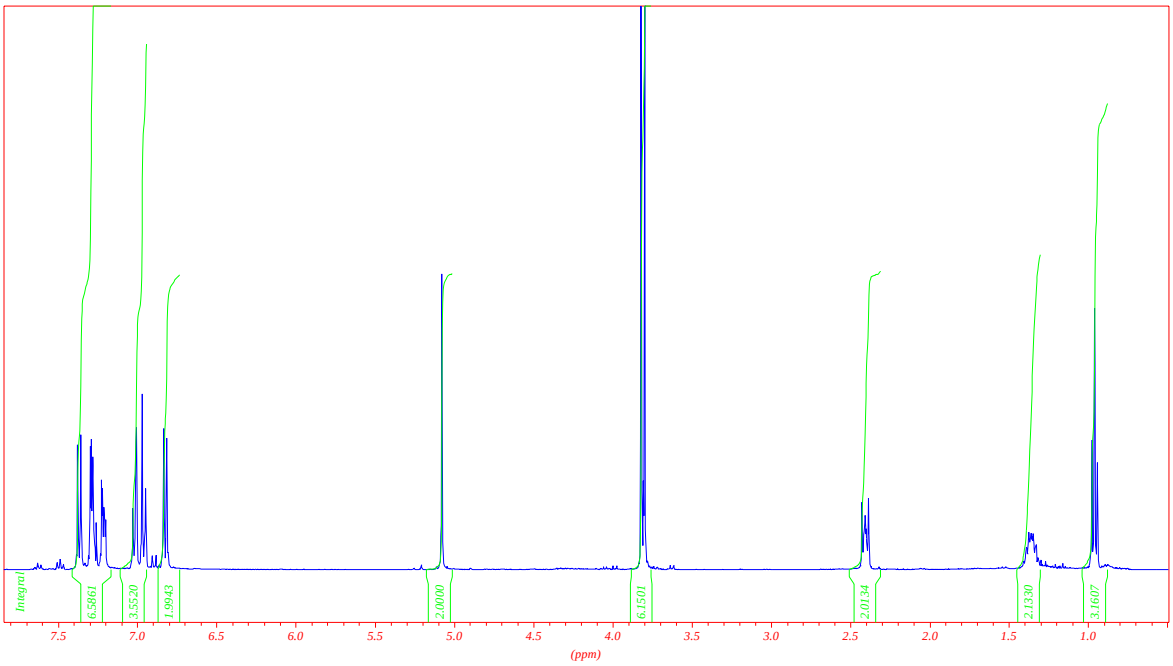
1m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2.0134
2.1330
3.1607
7.5
7.0
6.5
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3.5
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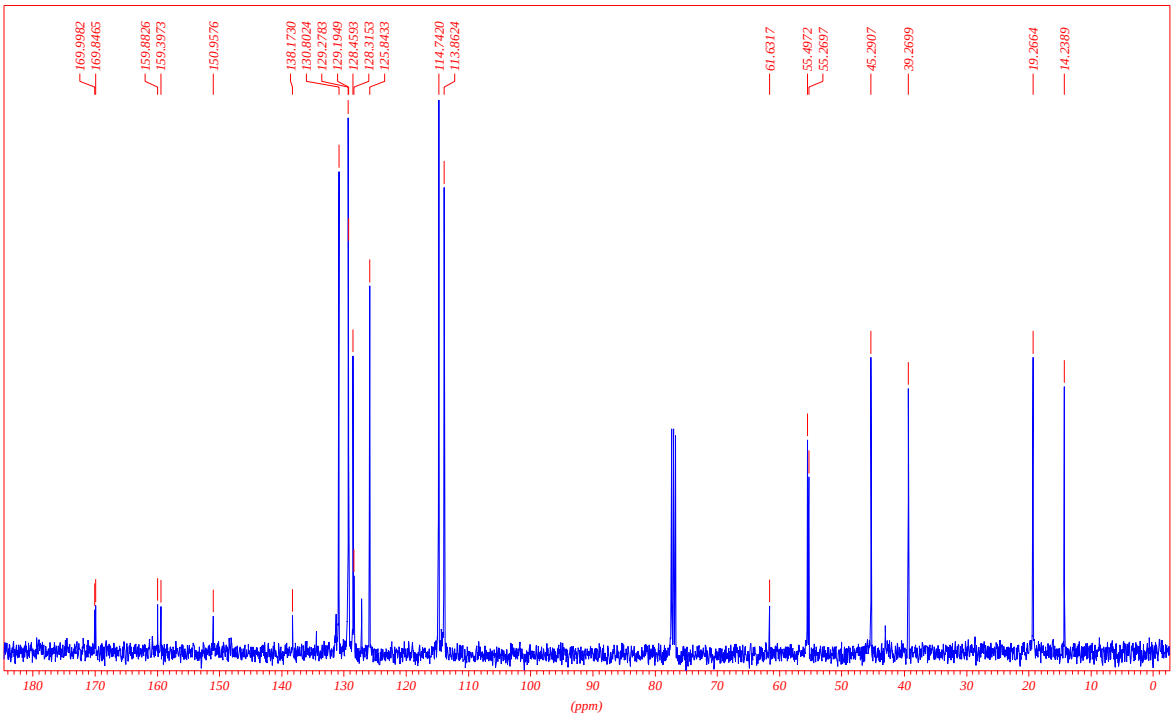
2.5
2.0
1.5
1.0
(ppm)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130.8024
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129.1949
128.4593
128.3153
125.8433
114.7420
113.8624
61.6317
55.4972
55.2697
45.2907
39.2699
19.2664
14.2389
180
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160
150
140
130
120
110
100
90
80
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60
50
40
30
20
10
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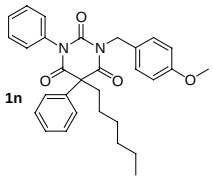
(ppm)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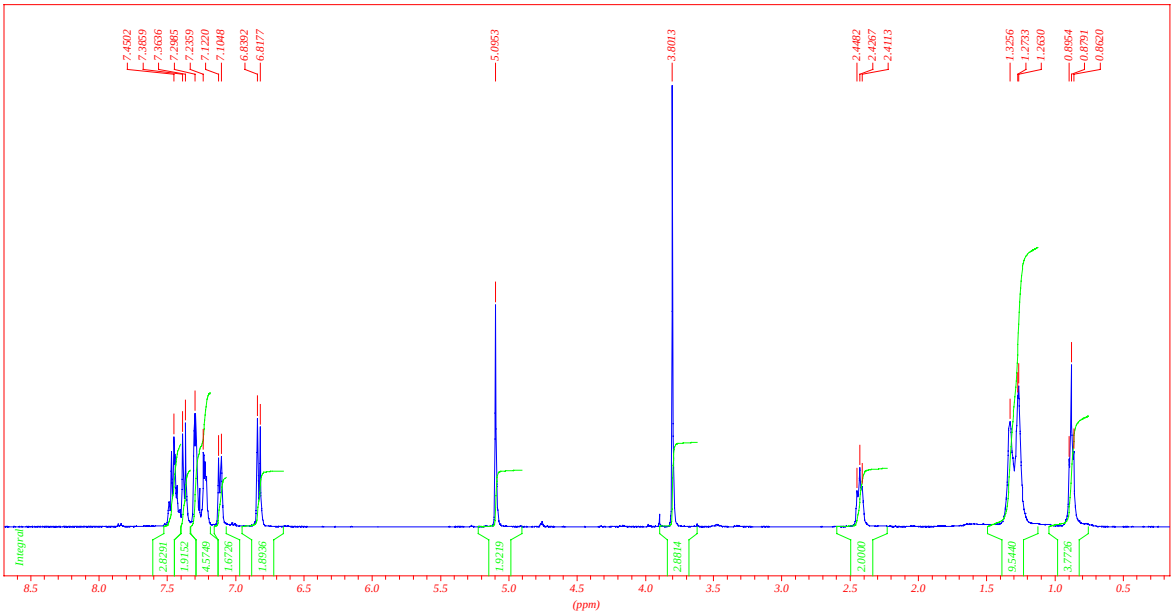
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7.2359
7.1220
7.1048
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6.8177
5.0053
3.8013
2.4482
2.4267
2.4113
1.3256
1.2733
1.2630
0.8954
0.8791
0.8620
Integral
2.8291
1.9153
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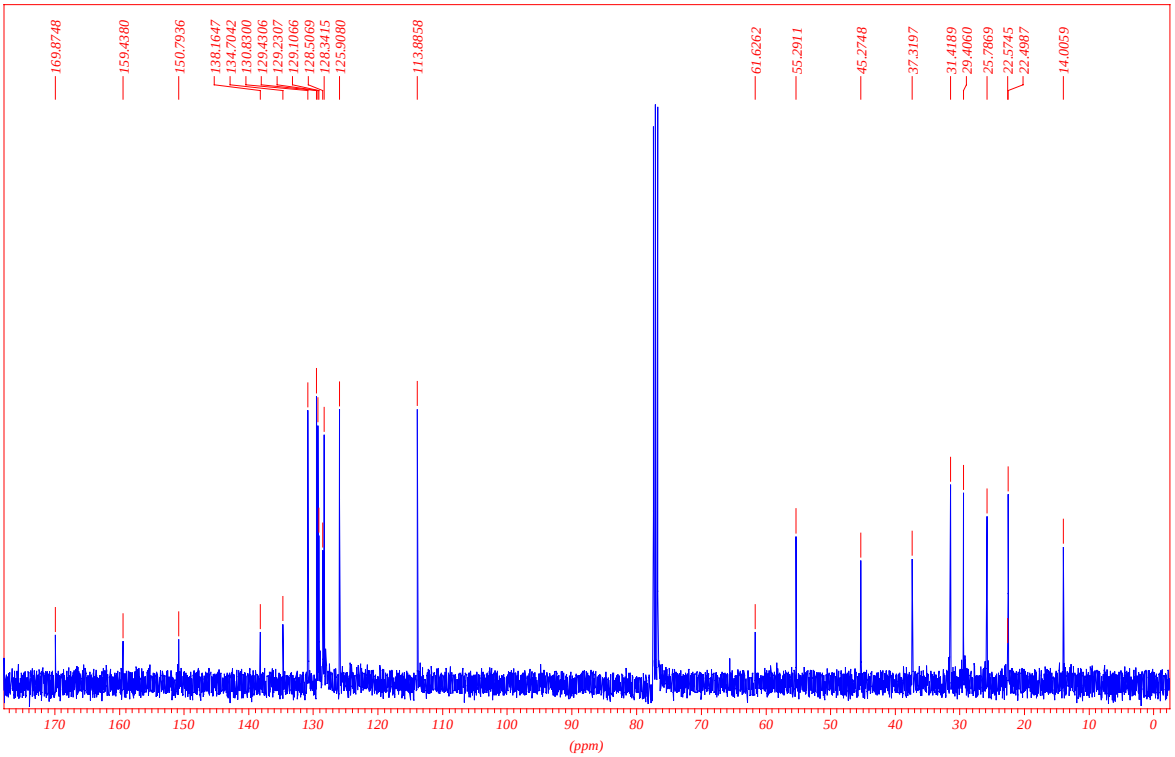
1.6758
1.8936
1.9219
2.8814
2.0000
9.5440
3.7726
(ppm)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125.9080
113.8858
61.6262
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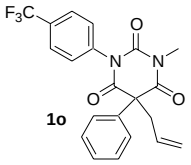
(ppm)


F3C
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O
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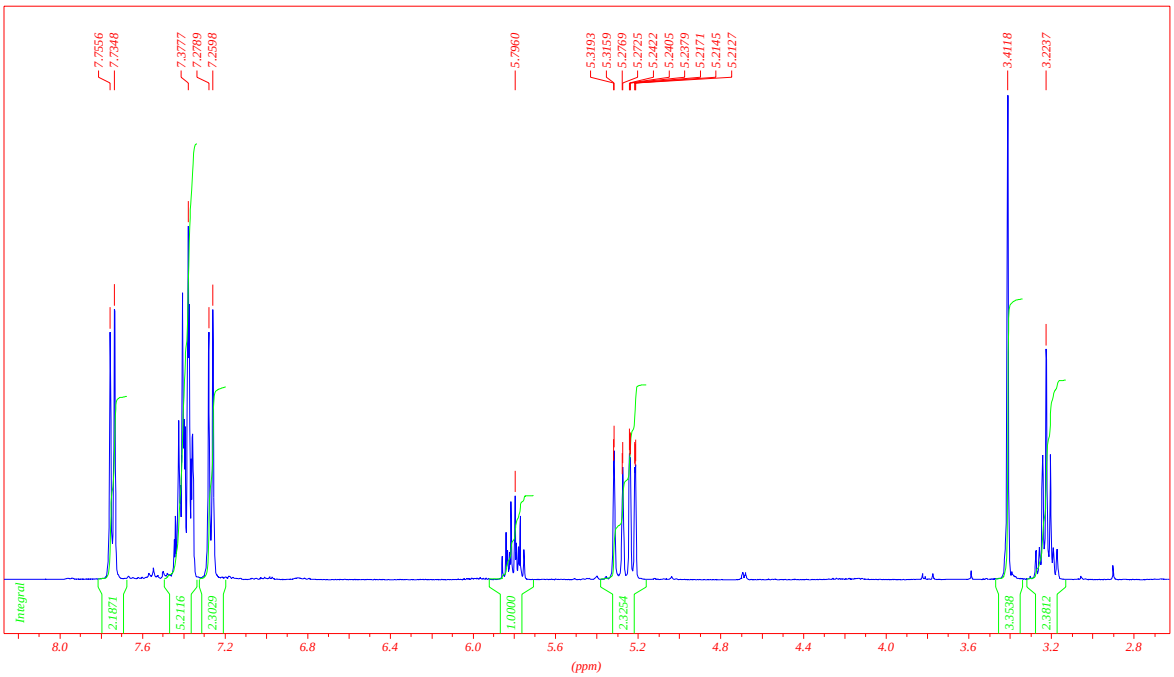
O

1o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5.2769
5.2725
5.2422
5.2405
5.2379
5.2171
5.2145
5.2127
3.4118
3.2237
Integral
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5.2116
2.3029
1.0000
2.3254
3.3538
2.3812
8.0
7.6
7.2
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5.6
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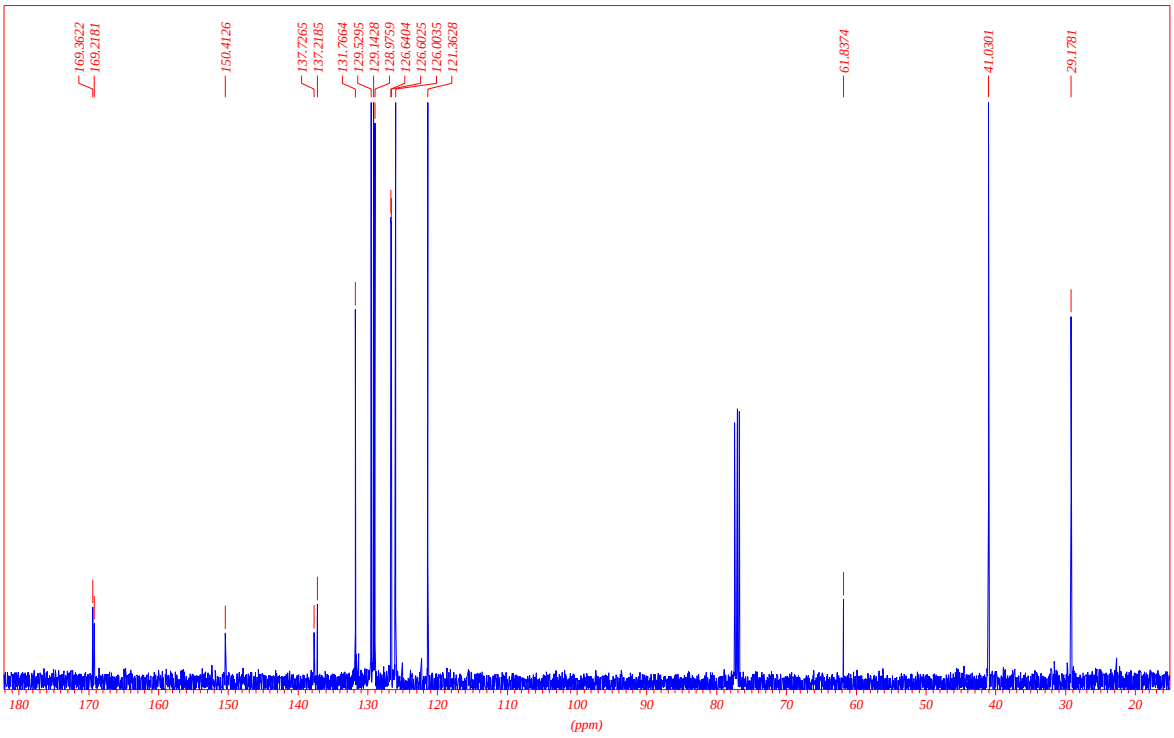
4.8
4.4
4.0
3.6
3.2
2.8
(ppm)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126.6025
126.0035
121.3628
61.8374
41.0301
29.1781
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
(ppm)