Electronic Supplementary Material for

Regioselective synthesis of 3,4,5-trisubstituted 2-aminofurans

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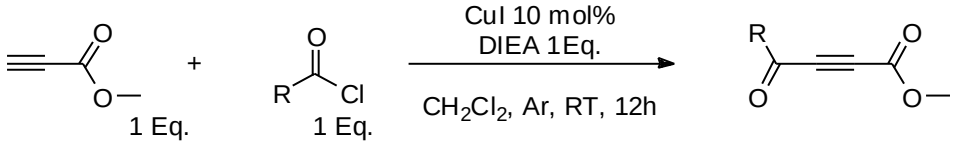
Synthesis

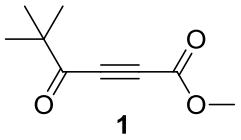
All reagents were purchased from Sigma-Aldrich and Alfa-Aesar. Analytical thin-layer chromatography (TLC) was carried out on pre-coated silica gel aluminum plate (Merck silica gel 60, F254, 0.25 mm). Silica gel CHROMAGEL® 60 (35-70 μm, Merck) was used for flash column chromatography. NMR spectra were recorded on BRUKER DPX 300 using TMS as internal reference. FT-IR spectra were recorded on SPECTRUM BX / RX PERKIN ELMER FT-IR spectrometer at 4000-400 cm-1 of wave numbers. High resolution mass spectra (HRMS) were acquired using a MSQ THERMOFINNIGAN spectrometer (ThermoFisher scientific Inc.).

A. General procedure for the synthesis of 4-oxo-2-butynoates



1, R = t-Bu
2, R = Ph
3, R = C_4H_3S

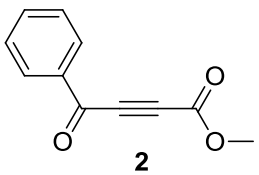
4-Oxo-2-butynoates derivatives **1**, **2** and **3** were prepared using modified Norman's procedure.[1] To a magnetically stirred suspension of CuI (190 mg, 1mM), methyl propiolate (888 μL, 10 mM) and DIEA (1.741 mL, 10 mM) in anhydrous CH_2Cl_2 under an argon atmosphere, appropriate acyl chloride (1 Eq.) was added. The mixture was then stirred at RT for 12 h. Reactive suspension was then filtered through a pad of Celite™ and concentrated under reduce pressure. The residue was then column chromatographied over silica gel using mixture of petroleum ether and ethyl acetate (95:5) as eluent to give pure 4-oxo-2-butynoates derivatives **1**, **2** and **3**.



1

Methyl 5,5-dimethyl-4-oxohex-2-ynoate, **1**.

Yield 95%.
^{1}H NMR (300 MHz, $CDCl_3$) δ 3.86 (s, 3H), 1.24 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 192.09, 152.61, 79.64, 79.58, 53.28, 44.99, 25.41.
HRMS ESI-TOF: *m/z*: 169.0863 ([M]+H, $C_9H_{13}O_3$, calc. 169.0865)
IR (film): 2971, 1726, 1682, 1434, 1248 cm^{-1}.

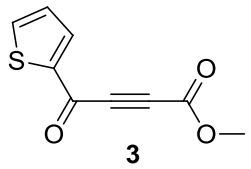


2

[1] J.F. Normant, M. Bourgain *Tetrahedron Letters* 1970, **31**, 2659-2662.

Methyl 4-oxo-4-phenylbut-2-ynoate, **2**.

Yield 65%.
^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.65 (tt, *J* = 7.0, 1.3 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 2H), 3.88 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 175.43, 152.10, 134.99, 134.83, 129.19, 128.53, 79.61, 79.41, 52.98.
HRMS ESI-TOF: *m/z*: 211.0369 ([M]+Na, $C_{11}H_8ONa$, calc. 211.0371)
IR (film): 1723, 1651, 1449, 1434, 1261 cm^{-1}.

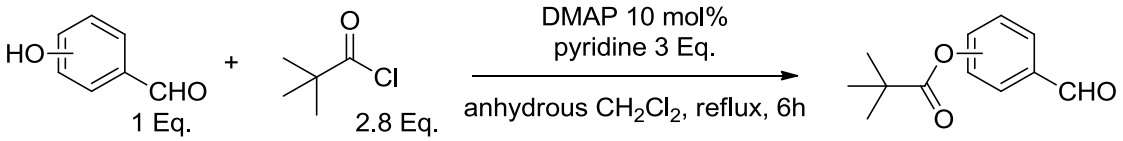


3

Methyl 4-oxo-4-(thiophen-2-yl)but-2-ynoate, **3**.

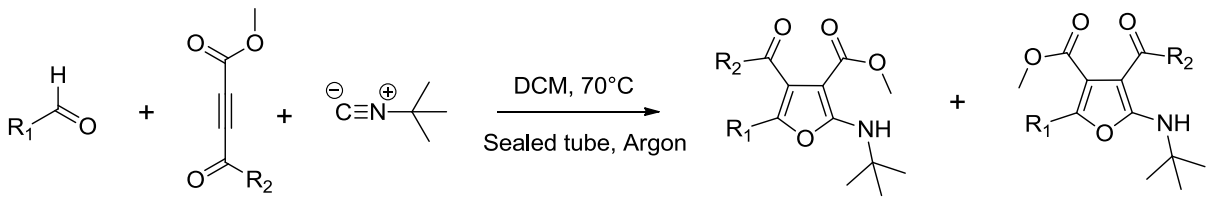
Yield 55%.
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 3.9, 1.3 Hz, 1H), 7.82 (dd, *J* = 4.9, 1.4 Hz, 1H), 7.21 (dd, *J* = 4.8, 4.0 Hz, 1H), 3.89 (s, 3H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 167.38, 152.42, 143.15, 136.98, 136.81, 128.66, 79.17, 78.32, 53.36.
HRMS ESI-TOF: *m/z*: 195.0119 ([M]+H, $C_9H_7O_3S$, calc. 195.0116)
IR (film): 1708, 1615, 1431, 1248, 935 cm^{-1}.

B. General procedure for the synthesis of tert-butyloxy aromatic aldehydes



The pivaloyl esters of 2-, 3- or 4-hydroxybenzaldehyde were prepared using the procedure described by Jiménez-González *et al.*[2]

C. General procedure for the synthesis of 3,4,5-trisubstituted-2-aminofurans

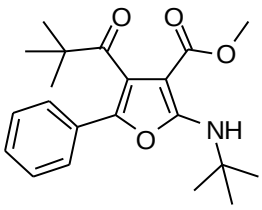


Major regioisomer **Minor regioisomer**

To a magnetically stirred solution of aromatic aldehyde (1 mmol) and alkyne (1 mmol) in anhydrous CH_2Cl_2 (5 mL) under an argon atmosphere *tert*-butyl isocyanide (1 mmol) was

[2] L. Jiménez-González, S. García-Muñoz, M. Álvarez-Corral, M. Muñoz-Dorado and I. Rodríguez-García, *Chemistry* 2007, **13**, 557-568.

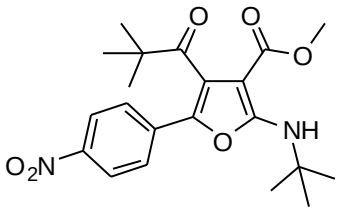
added. The mixture was then stirred for 24 h at 70°C in a sealed tube. After cooling, the solvent was removed under reduced pressure and the residue was subjected to column chromatography over silica gel using petroleum ether / ethyl acetate (80:20) as eluent.



5a

Methyl 2-(tert-butylamino)-5-phenyl-4-pivaloylfuran-3-carboxylate, **5a**

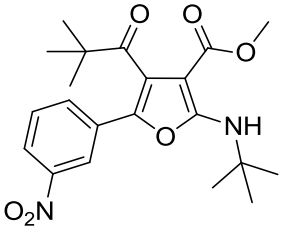
Yield 72%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 – 7.28 (m, 5H), 6.86 (s, 1H), 3.73 (s, 3H), 1.49 (s, 9H), 1.10 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 210.54, 165.13, 161.79, 138.11, 130.13, 128.47, 127.40, 125.15, 119.29, 89.27, 52.69, 50.71, 46.32, 29.85, 27.08.
HRMS EI-TOF: *m/z*: 357.1947 ([M]$^+$, $C_{21}H_{27}NO_4^+$, calc. 357.1940)
IR (film): 3338, 2966, 1767, 1604, 1470, 1217, 1095 cm^{-1}.



5b

Methyl 2-(tert-butylamino)-5-(4-nitrophényl)-4-pivaloylfuran-3-carboxylate, **5b**

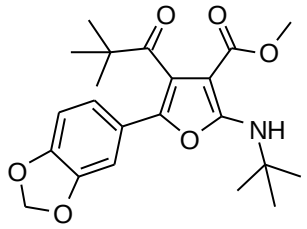
Yield 93%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.18 (d, *J* = 9.0 Hz, 2H), 7.53 (d, *J* = 9.3 Hz, 2H), 7.02 (s, 1H), 3.76 (s, 3H), 1.52 (s, 9H), 1.15 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 209.92, 164.60, 161.97, 147.40, 145.74, 135.75, 135.30, 124.43, 124.06, 90.20, 52.97, 50.94, 46.45, 29.69, 27.02.
HRMS EI-TOF: *m/z*: 402.1803 ([M]$^+$, $C_{21}H_{26}N_2O_6^+$, calc. 402.1791)
IR (film): 3331, 2971, 2355, 1682, 1592, 1330, 1216, 1105 cm^{-1}.



5c

Methyl 4-benzoyl-2-(tert-butylamino)-5-(3-nitrophenyl)furan-3-carboxylate, **5c**

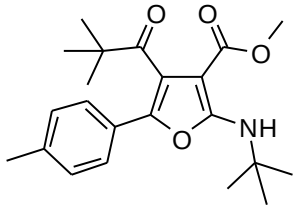
Yield 92%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 (t, *J* = 2.3 Hz, 1H), 8.05 (ddd, *J* = 8.1, 2.4, 1.0 Hz, 1H), 7.70 (dt, *J* = 8.0, 1.0 Hz, 1H), 7.49 (t, *J* = 8.1 Hz, 1H), 6.96 (s, 1H), 3.76 (s, 3H), 1.52 (s, 9H), 1.15 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 210.06, 164.84, 161.88, 148.49, 135.47, 131.57, 130.10, 129.60, 122.10, 121.53, 119.20, 89.67, 52.99, 50.96, 46.44, 29.86, 27.08.
HRMS EI-TOF: m/z: 402.1802 ([M]$^+$, $C_{21}H_{26}N_2O_6^+$, calc. 402.1791)
IR (film): 3344, 2966, 2360, 1680, 1607, 1531, 1346, 1214 cm^{-1}.



5d

Methyl 5-(benzo[d][1,3]dioxol-5-yl)-2-(tert-butylamino)-4-pivaloylfuran-3-carboxylate, **5d**

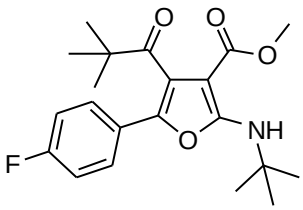
Yield 53%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.00 – 6.86 (m, 2H), 6.82 (s, 1H), 6.77 (d, *J* = 8.6 Hz, 1H), 5.97 (s, 2H), 3.72 (s, 3H), 1.47 (s, 9H), 1.10 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 210.42, 165.06, 161.50, 147.69, 147.08, 138.07, 124.30, 119.53, 118.20, 108.39, 105.95, 101.12, 89.07, 52.62, 50.61, 46.21, 29.84, 27.00.
HRMS EI-TOF: *m/z*: 401.1846 ($[M]^+$, $C_{22}H_{27}NO_6^+$, calc. 401.1838)
IR (film): 3341, 2966, 1673, 1602, 1457, 1211, 1091 cm^{-1}.



5e

Methyl 2-(tert-butylamino)-4-pivaloyl-5-(*p*-tolyl)furan-3-carboxylate, **5e**

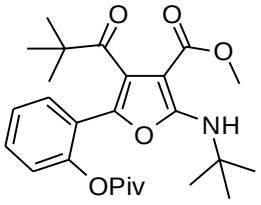
Yield 61%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.2 Hz, 2H), 7.13 (d, *J* = 8.2 Hz, 2H), 6.83 (s, 1H), 3.73 (s, 3H), 2.33 (s, 3H), 1.48 (s, 9H), 1.10 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 210.79, 166.20, 161.89, 138.61, 137.54, 129.34, 127.57, 125.38, 65.68, 52.81, 50.81, 46.44, 30.02, 27.24, 21.37.
HRMS EI-TOF: *m/z*: 371.2102 ($[M]^+$, $C_{22}H_{29}NO_4^+$, calc. 371.2097)
IR (film): 3336, 2962, 1675, 1607, 1469, 1216, 1091 cm^{-1}.



5f

Methyl 2-(tert-butylamino)-5-(4-fluorophenyl)-4-pivaloylfuran-3-carboxylate, **5f**

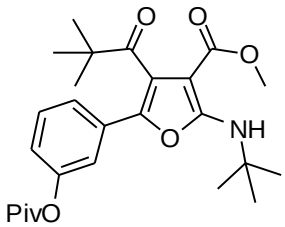
Yield 50%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.41 (dd, J = 8.9, 5.2 Hz, 2H), 7.02 (t, J = 8.8 Hz, 2H), 6.84 (S, 1H), 3.73 (s, 3H), 1.48 (s, 9H), 1.09 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 210.47, 165.09, 163.69, 161.74, 160.41, 137.33, 127.14, 127.04, 126.45, 119.18, 115.76, 115.47, 89.25, 52.74, 50.75, 46.31, 29.89, 27.02.
HRMS EI-TOF: *m/z*: 357.1849 ($[M]^+$, $C_{21}H_{26}NO_4F^+$, calc. 357.1846)
IR (film): 3336, 2966, 1673, 1607, 1469, 1216, 1088 cm^{-1}.



5g

Methyl 2-(tert-butylamino)-4-pivaloyl-5-(2-(pivaloyloxy)phenyl)furan-3-carboxylate, **5g**

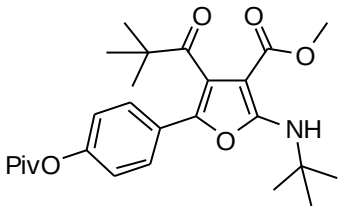
Yield 60%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.46 – 7.32 (m, 2H), 7.20 (td, *J* = 7.7, 1.3 Hz, 1H), 7.09 (d, *J* = 8.2 Hz, 1H), 6.76 (s, 1H), 3.73 (s, 3H), 1.41 (s, 9H), 1.28 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 209.45, 176.48, 165.04, 162.47, 149.94, 134.54, 132.38, 130.35, 125.64, 123.33, 122.93, 122.55, 89.15, 53.02, 50.72, 45.35, 38.96, 30.07, 26.85, 26.36.
HRMS EI-TOF: *m/z*: 4457.2450 ($[M]^+$, $C_{26}H_{35}NO_6{}^+$, calc. 457.246)
IR (film): 3331, 2966, 2360, 1751, 1678, 1604, 1453, 1214, 1110cm^{-1}.



5h

Methyl 2-(tert-butylamino)-4-pivaloyl-5-(3-(pivaloyloxy)phenyl)furan-3-carboxylate, **5h**

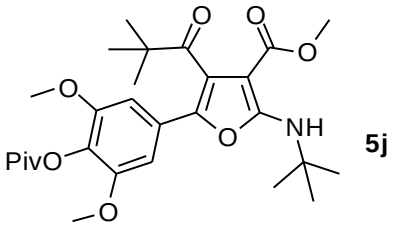
Yield 53%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 – 7.28 (m, 2H), 7.07 (t, *J* = 2.0 Hz, 1H), 6.93 (dt, *J* = 7.4, 2.0 Hz, 1H), 6.87(s, 1H), 3.73 (s, 3H), 1.48 (s, 9H), 1.36 (s, 9H), 1.11 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 210.18, 176.73, 164.90, 161.65, 151.16, 137.03, 131.32, 129.37, 122.14, 120.45, 120.11, 117.91, 89.29, 52.63, 50.61, 46.19, 38.92, 29.74, 26.96.
HRMS EI-TOF: *m/z*: 457.2457 ($[M]^+$, $C_{26}H_{35}NO_6{}^+$, calc. 457.2464)
IR (film) : 3336, 2966, 1753, 1675, 1609, 1474, 1216, 1110 cm^{-1}.



5i

Methyl 2-(tert-butylamino)-4-pivaloyl-5-(4-(pivaloyloxy)phenyl)furan-3-carboxylate, **5i**

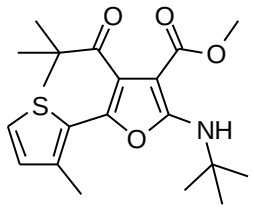
Yield 62%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.43 (d, *J* = 8.8 Hz, 2H), 7.02 (d, *J* = 8.8 Hz, 2H), 6.85 (s, 1H), 3.73 (s, 3H), 1.48 (s, 9H), 1.35 (s, 9H), 1.10 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 210.51, 176.90, 165.10, 161.79, 150.30, 137.54, 132.15, 127.68, 126.26, 121.67, 89.31, 52.75, 50.73, 46.33, 39.08, 29.88, 27.08.
HRMS EI-TOF: *m/z*: 457.2454 ($[M]^+$, $C_{26}H_{35}NO_6{}^+$, calc. 457.2464)
IR (film): 3341, 2966, 2360, 1753, 1680, 1609, 1472, 1218, 1112 cm^{-1}.



5j

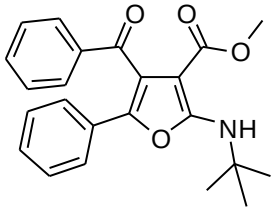
Methyl 2-(tert-butylamino)-5-(3,5-dimethoxy-4-(pivaloyloxy)phenyl)-4-pivaloylfuran-3-carboxylate, **5j**

Yield 70%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.83 (s, 1H), 6.70 (s, 2H), 3.79 (s, 6H), 3.74 (s, 3H), 1.48 (s, 9H), 1.37 (s, 9H), 1.11 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 210.77, 176.38, 165.16, 161.71, 152.39, 138.11, 128.69, 128.10, 119.52, 102.44, 89.46, 56.20, 52.86, 50.84, 46.40, 39.20, 29.97, 27.31.
HRMS EI-TOF: *m/z*: 517.2663 ($[M]^+$, $C_{28}H_{39}NO_8^+$, calc. 517.2676)
IR (film): 3334, 2962, 2350, 1682, 1595, 1460, 1211, 1112 cm^{-1}.



Methyl 2-(tert-butylamino)-5-(3-methylthiophen-2-yl)-4-pivaloylfuran-3-carboxylate, **5k**

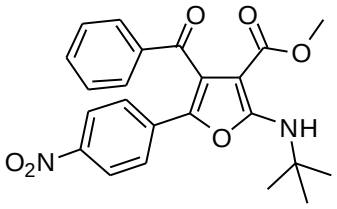
Yield 59%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.21 (d, *J* = 5.2 Hz, 1H), 6.87 (s, 1H), 6.85 (d, *J* = 5.2 Hz, 1H), 3.72 (s, 3H), 2.29 (s, 3H), 1.44 (s, 9H), 1.03 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 208.88, 165.01, 162.15, 137.57, 131.70, 130.09, 126.25, 125.73, 122.63, 88.68, 52.69, 50.67, 45.59, 29.80, 26.60, 15.02.
HRMS EI-TOF: *m/z*: 377.1665 ($[M]^+$, $C_{20}H_{27}NO_4S^+$, calc. 377.1661)
IR (film): 3331, 2971, 2355, 1675, 1602, 1469, 1211cm^{-1}.



6a

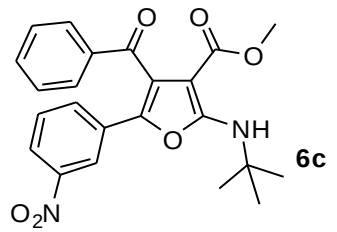
Methyl 4-benzoyl-2-(tert-butylamino)-5-phenylfuran-3-carboxylate, **6a**

Yield 52%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.1 Hz, 2H), 7.54 (d, *J* = 7.4 Hz, 1H), 7.48 – 7.36 (m, 4H), 7.25 (t, *J* = 7.2 Hz, 2H), 7.17 (d, *J* = 7.2 Hz, 1H), 6.88 (s, 1H), 3.42 (s, 3H), 1.55 (s, 10H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 193.56, 165.26, 161.68, 140.71, 137.61, 133.53, 129.46, 128.79, 128.63, 127.31, 124.30, 119.33, 90.03, 52.90, 50.70, 29.99.
HRMS EI-TOF: *m/z*: 377.1624 ($[M]^+$, $C_{23}H_{23}NO_4^+$, calc. 377.1627)
IR (film): 3336, 2966, 1673, 1607, 1472, 1214, 1095 cm^{-1}.



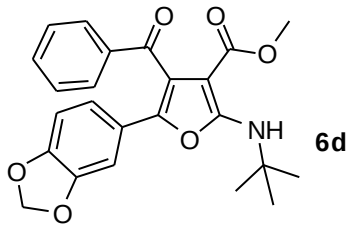
Methyl 4-benzoyl-2-(tert-butylamino)-5-(4-nitrophenyl)furan-3-carboxylate, **6b**

Yield 79%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, *J* = 9.1 Hz, 2H), 7.96 (, *J* = 8.8 Hz, 2H), 7.54 – 7.39 (m,5), 7.05 (s, 1H), 3.45 (s, 3H), 1.57 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 192.83, 164.67, 163.00, 161.97, 145.55, 137.89, 136.80, 135.10, 134.08, 129.32, 128.82, 124.36, 123.58, 91.05, 53.17, 50.91, 29.80.
HRMS EI-TOF: *m/z*: 422.1466 ($[M]^+$, $C_{23}H_{22}N_2O_6^+$, calc. 422.1478)
IR (film): 3331, 2919, 2360, 1675, 1590, 1332, 1216, 1110 cm^{-1}.



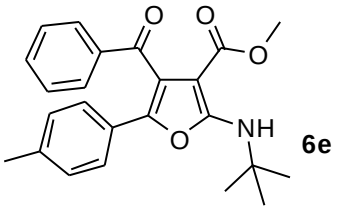
Methyl 4-benzoyl-2-(tert-butylamino)-5-(3-nitrophenyl)furan-3-carboxylate, **6c**

Yield 78%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 (t, *J* = 2.0 Hz, 1H), 8.01 – 7.92 (m, 3H), 7.64 (dt, *J* = 8.3, 1.3 Hz, 1H), 7.58 (d, *J* = 7.3 Hz, 1H), 7.46 (dd, *J* = 8.3, 6.9 Hz, 2H), 7.38 (t, *J* = 8.1 Hz, 1H), 6.99 (s, 1H), 3.44 (s, 3H), 1.57 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 192.75, 164.77, 161.69, 148.57, 137.98, 137.06, 133.86, 130.87, 129.79, 129.28, 128.70, 122.07, 121.26, 118.53, 90.31, 53.05, 50.76, 29.85.
HRMS EI-TOF: *m/z*: 422.1466 ($[M]^+$, $C_{23}H_{22}N_2O_6^+$, calc. 422.1478)
IR (film): 3331, 2914, 2355, 1573, 1609, 1528, 1346, 1214, 1095 cm^{-1}.



Methyl 5-(benzo[d][1,3]dioxol-5-yl)-4-benzoyl-2-(tert-butylamino)furan-3-carboxylate, **6d**

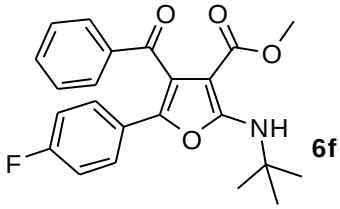
Yield 45%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 – 7.89 (m, 2H), 7.58 – 7.50 (m, 1H), 7.43 (dd, *J* = 8.3, 6.8 Hz, 2H), 6.94 (d, *J* = 8.0 Hz, 2H), 6.84 (s, 1H), 6.70 (d, *J* = 8.1 Hz, 1H), 5.92 (s, 2H), 3.40 (s, 3H), 1.53 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 193.37, 165.14, 161.31, 147.81, 146.97, 140.82, 137.60, 133.32, 129.28, 128.46, 123.53, 118.70, 117.95, 108.62, 105.17, 101.10, 89.71, 52.73, 50.50, 29.88.
HRMS EI-TOF: *m/z*: 421.1524 ($[M]^+$, $C_{24}H_{23}NO_6^+$, calc. 421.1525)
IR (film): 3341, 2914, 2355, 1668, 1602, 1453, 1216, 1093 cm^{-1}.



6e

Methyl 4-benzoyl-2-(tert-butylamino)-5-(*p*-tolyl)furan-3-carboxylate, **6e**

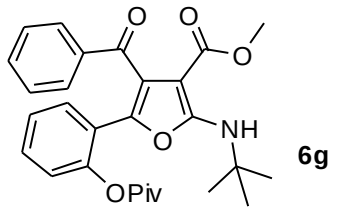
Yield 57%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.2 Hz, 2H), 7.59 – 7.46 (m, 1H), 7.41 (dd, *J* = 8.3, 6.8 Hz, 2H), 7.33 (d, *J* = 8.2 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.86 (s, 1H), 3.41 (s, 3H), 2.27 (s, 3H), 1.54 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 193.53, 165.25, 161.56, 141.13, 137.68, 137.27, 133.38, 129.42, 129.40, 128.54, 126.64, 124.38, 118.46, 89.88, 52.82, 50.61, 29.98, 21.25.
HRMS EI-TOF: *m/z*: 391.1780 ($[M]^+$, $C_{24}H_{25}NO_4^+$, calc. 391.1784)
IR (film): 3336, 2914, 2360, 1673, 1611, 1475, 1214, 1093 cm^{-1}.



6f

Methyl 4-benzoyl-2-(tert-butylamino)-5-(4-fluorophenyl)furan-3-carboxylate, **6f**

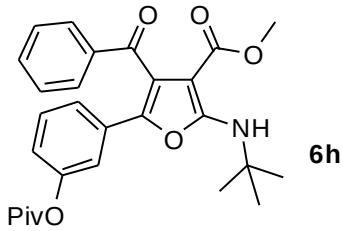
Yield 52%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (d, *J* = 7.1 Hz, 2H), 7.42 (ddd, *J* = 8.9, 7.5, 5.8 Hz, 5H), 6.96 (t, *J* = 8.7 Hz, 2H), 6.87 (s, 1H), 3.41 (s, 3H), 1.54 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 193.40, 165.23, 163.65, 161.65, 160.36, 140.19, 137.61, 133.60, 129.42, 128.66, 126.35, 126.25, 119.06, 116.05, 115.76, 89.96, 52.94, 50.71, 30.03.
HRMS EI-TOF: *m/z*: 395.1524 ($[M]^+$, $C_{23}H_{22}NO_4F^+$, calc. 395.1533)
IR (film): 3336, 2957, 2355, 1673, 1614, 1472, 1211, 1095 cm^{-1}.



6g

Methyl 4-benzoyl-2-(tert-butylamino)-5-(2-(pivaloyloxy)phényl)furan-3-carboxylate, **6g**

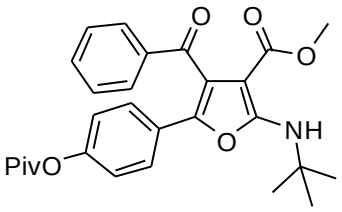
Yield 58%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.0 Hz, 2H), 7.52 – 7.40 (m, 2H), 7.32 (dd, *J* = 8.6, 6.9 Hz, 3H), 7.15 (td, *J* = 7.6, 1.2 Hz, 1H), 6.99 (dd, *J* = 8.2, 1.1 Hz, 1H), 6.85 (s, 1H), 3.44 (s, 3H), 1.44 (s, 9H), 1.30 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 191.32, 176.55, 165.55, 162.70, 150.12, 139.48, 137.74, 133.05, 132.81, 130.63, 129.37, 128.19, 125.56, 122.77, 122.68, 122.01, 89.40, 53.21, 50.72, 30.24, 27.12.
HRMS EI-TOF: *m/z*: 477.2148 ($[M]^+$, $C_{28}H_{31}NO_6^+$, calc. 477.2151)
IR (film): 3336, 2966, 2355, 1751, 1671, 1604, 1455, 1414, 1095cm^{-1}.



6h

Methyl 4-benzoyl-2-(tert-butylamino)-5-(3-(pivaloyloxy)phenyl)furan-3-carboxylate, **6h**

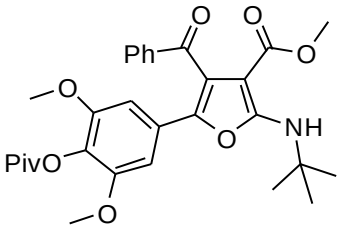
Yield 50%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 – 7.87 (m, 2H), 7.59 – 7.47 (m, 2H), 7.48 – 7.37 (m, 2H), 7.23 (dd, *J* = 4.9, 1.8 Hz, 2H), 7.07 – 7.00 (m, 1H), 6.89 (s, 1H), 3.43 (s, 3H), 1.54 (s, 9H), 1.31 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 193.24, 176.93, 165.19, 161.68, 151.46, 139.68, 137.47, 133.61, 130.81, 129.75, 129.44, 128.67, 121.49, 120.47, 117.23, 90.18, 52.96, 50.78, 39.13, 30.01, 27.15.
HRMS EI-TOF: *m/z*: 477.2150 ($[M]^+$, $C_{28}H_{31}NO_6^+$, calc. 477.2151)
IR (film): 3336, 2971, 2355, 1753, 1673, 1611, 1469, 1214, 1098 cm^{-1}.



6i

Methyl 4-benzoyl-2-(tert-butylamino)-5-(4-(pivaloyloxy)phenyl)furan-3-carboxylate, **6i**

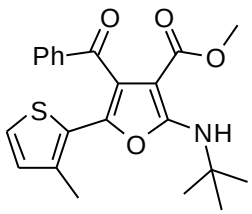
Yield 52%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.8 Hz, 2H), 7.46 – 7.39 (m, 5H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.87 (s, 1H), 3.42 (s, 3H), 1.54 (s, 9H), 1.32 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 193.46, 177.04, 165.24, 161.67, 150.22, 140.18, 137.53, 133.61, 129.44, 128.67, 127.00, 125.44, 121.96, 119.30, 90.03, 52.93, 50.73, 30.00, 27.18.
HRMS EI-TOF: *m/z*: 477.2143 ($[M]^+$, $C_{28}H_{31}NO_6^+$, calc. 477.2151)
IR (film): 3341, 2966, 2355, 1749, 1675, 1611, 1472, 1209, 1110 cm^{-1}.



6j

Methyl 4-benzoyl-2-(tert-butylamino)-5-(3,5-dimethoxy-4-(pivaloyloxy)phenyl)furan-3-carboxylate, **6j**

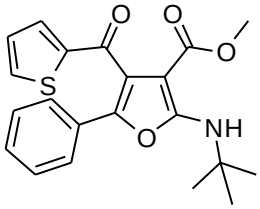
Yield 63%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 – 7.88 (m, 2H), 7.61 – 7.50 (m, 1H), 7.43 (dd, *J* = 8.4, 6.9 Hz, 2H), 6.86 (s, 1H), 6.66 (s, 2H), 3.63 (s, 6H), 3.46 (s, 3H), 1.54 (s, 9H), 1.33 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 193.32, 176.39, 165.23, 161.55, 152.42, 140.28, 137.49, 133.67, 129.40, 128.74, 127.21, 119.45, 101.53, 90.19, 56.04, 52.92, 50.84, 39.19, 30.00, 27.30.
HRMS EI-TOF: *m/z*: 537.2344 ($[M]^+$, $C_{30}H_{35}NO_8^+$, calc. 537.2363)
IR (film): 3336, 2966, 2355, 1753, 1675, 1595, 1462, 1211, 1102 cm^{-1}.



6k

Methyl 4-benzoyl-2-(tert-butylamino)-5-(3-methylthiophen-2-yl)furan-3-carboxylate**, 6k**

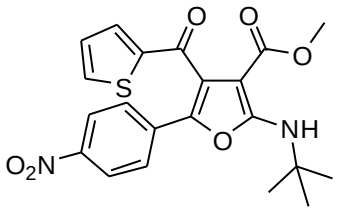
Yield 53%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 – 7.80 (m, 2H), 7.56 – 7.48 (m, 1H), 7.41 (dd, *J* = 8.3, 6.7 Hz, 2H), 7.09 (d, *J* = 5.0 Hz, 1H), 6.96 (s, 1H), 6.76 (d, *J* = 5.3 Hz, 1H), 3.41 (s, 3H), 2.27 (s, 3H), 1.50 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 192.06, 165.34, 162.02, 138.00, 136.86, 136.58, 133.20, 130.67, 129.44, 128.39, 125.25, 121.05, 89.31, 52.91, 50.68, 29.84, 15.82.
HRMS EI-TOF: *m/z*: 397.1351 ($[M]^+$, $C_{22}H_{23}NO_4S^+$, calc. 397.1348)
IR (film): 3327, 2924, 2360, 1675, 1611, 1455, 1214, 1095 cm^{-1}.



7a

Methyl 2-(tert-butylamino)-5-phenyl-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7a**

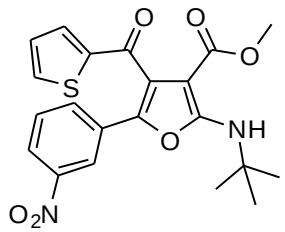
Yield 40%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 5.0, 0.9 Hz, 1H), 7.59 (dd, *J* = 3.6, 0.8 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.7 Hz, 2H), 7.31 – 7.24 (m, 2H), 7.19 (d, *J* = 7.4 Hz, 1H), 6.89 (s, 1H), 3.54 (s, 3H), 1.54 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 185.23, 165.19, 161.58, 144.82, 140.66, 134.67, 130.36, 129.19, 128.69, 128.12, 127.29, 124.33, 87.70, 52.80, 50.83, 29.87.
HRMS EI-TOF: *m/z*: 383.1185 ($[M]^+$, $C_{21}H_{21}NO_4S^+$, calc. 383.1191)
IR (film): 3345, 2962, 2355, 1673, 1607, 1469, 1408, 1216, 1095 cm^{-1}.



7b

Methyl 2-(tert-butylamino)-5-(4-nitrophenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7b**

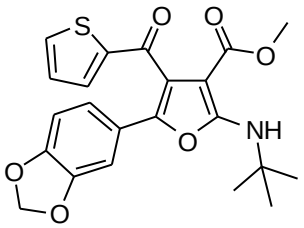
Yield 62%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, *J* = 9.0 Hz, 1H), 7.75 (dd, *J* = 4.9, 1.3 Hz, 1H), 7.61 (dd, *J* = 3.8, 1.3 Hz, 1H), 7.53 (d, *J* = 9.2 Hz, 1H), 7.09 (dd, *J* = 4.9, 3.8 Hz, 1H), 7.06 (s, 1H), 3.56 (s, 3H), 1.56 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 184.65, 164.90, 162.11, 145.81, 144.21, 138.09, 135.73, 135.15, 135.10, 128.57, 124.53, 123.88, 123.66, 91.02, 53.31, 51.28, 29.95.
HRMS EI-TOF: *m/z*: 428.1036 ($[M]^+$, $C_{21}H_{20}N_2O_6S^+$, calc. 428.1042)
IR (film): 3327, 2919, 2355, 1678, 1590, 1330, 1216, 1098 cm^{-1}.



7c

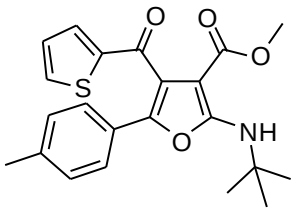
Methyl 2-(tert-butylamino)-5-(3-nitrophenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7c**

Yield 61%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 (t, *J* = 2.0 Hz, 1H), 8.00 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.77 – 7.66 (m, 2H), 7.61 (d, *J* = 3.5 Hz, 1H), 7.42 (t, *J* = 8.1 Hz, 1H), 7.12 – 7.04 (m, 1H), 7.00 (s, 1H), 3.55 (s, 3H), 1.57 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 184.40, 164.83, 161.70, 148.59, 144.27, 137.99, 135.30, 134.82, 130.75, 129.77, 129.34, 128.28, 121.70, 121.35, 118.63, 90.15, 53.05, 50.99, 29.85.
HRMS EI-TOF: *m/z*: 428.1035 ($[M]^+$, $C_{21}H_{20}N_2O_6S^+$, calc. 428.1042)
IR (film): 3336, 2924, 2360, 1678, 1609, 1408, 1349, 1216, 1095cm^{-1}.



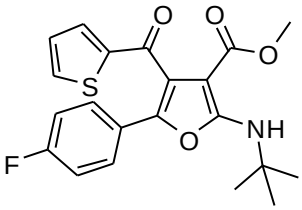
7d

Methyl 5-(benzo[d][1,3]dioxol-5-yl)-2-(tert-butylamino)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7d**
Yield 23%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 4.9, 1.3 Hz, 1H), 7.58 (dd, *J* = 3.7, 1.1 Hz, 1H), 7.05 (dd, *J* = 4.9, 3.8 Hz, 1H), 7.01 – 6.95 (m, 2H), 6.86 (s, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.93 (s, 2H), 3.52 (s, 3H), 1.52 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 185.31, 165.35, 161.49, 148.01, 147.21, 145.07, 141.02, 134.69, 128.24, 123.60, 119.03, 117.89, 108.82, 105.44, 101.31, 89.79, 52.93, 50.94, 29.85.
HRMS EI-TOF: *m/z*: 427.1089 ($[M]^+$, $C_{22}H_{21}NO_6S^+$, calc. 427.1090)
IR (film): 3336, 2919, 2360, 1671, 1607, 1469, 1408, 1214, 1093 cm^{-1}.



Methyl 2-(tert-butylamino)-4-(thiophene-2-carbonyl)-5-(p-tolyl)furan-3-carboxylate, **7e**

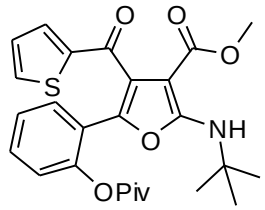
Yield 32%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, *J* = 4.4 Hz, 1H), 7.58 (d, *J* = 3.6 Hz, 1H), 7.37 (d, *J* = 8.3 Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.05 – 7.02 (m, 1H), 6.86 (s, 1H), 3.53 (s, 3H), 2.29 (s, 3H), 1.53 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 185.25, 165.20, 161.48, 144.89, 141.08, 137.30, 134.56, 130.52, 129.35, 128.06, 126.43, 124.41, 118.10, 89.67, 52.73, 50.75, 29.86, 21.16.
HRMS EI-TOF: *m/z*: 397.1349 ($[M]^+$, $C_{22}H_{23}NO_4S^+$, calc. 397.1348)
IR (film): 3336, 2962, 2355, 1673, 1607, 1467, 1048, 1214, 1095 cm^{-1}.



7f

Methyl 2-(tert-butylamino)-5-(4-fluorophenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7f**

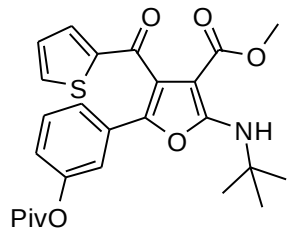
Yield 42%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 5.0, 1.2 Hz, 1H), 7.58 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.45 (dd, *J* = 9.0, 5.2 Hz, 2H), 7.05 (dd, *J* = 5.1, 3.7 Hz, 1H), 6.98 (t, *J* = 8.8 Hz, 2H), 6.88 (s, 1H), 3.53 (s, 3H), 1.53 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 185.05, 165.13, 163.54, 161.51, 144.71, 140.04, 134.75, 134.65, 128.14, 126.31, 126.21, 125.53, 118.63, 115.94, 115.65, 89.68, 52.81, 50.85, 29.88.
HRMS EI-TOF: *m/z*: 401.1090 ($[M]^+$, $C_{21}H_{20}NO_4FS^+$, calc. 401.1097)
IR (film): 3350, 2919, 2360, 1732, 1671, 1597, 1410, 1216, 1095 cm^{-1}.



7g

Methyl 2-(tert-butylamino)-5-(2-(pivaloyloxy)phenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7g**

Yield 47%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.55 (dd, *J* = 5.0, 1.3 Hz, 1H), 7.47 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.44 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.33 (td, *J* = 7.8, 1.8 Hz, 1H), 7.17 (td, *J* = 7.6, 1.3 Hz, 1H), 7.01 (dd, *J* = 8.1, 1.2 Hz, 1H), 6.95 (dd, *J* = 4.9, 3.8 Hz, 1H), 6.86 (s, 1H), 3.57 (s, 3H), 1.44 (s, 9H), 1.30 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 182.97, 176.43, 165.34, 162.63, 149.70, 144.57, 139.10, 134.29, 132.27, 130.36, 127.67, 125.50, 122.70, 121.69, 89.21, 53.08, 50.81, 39.02, 30.08, 26.95.
HRMS EI-TOF: *m/z*: 483.1705 ($[M]^+$, $C_{26}H_{29}NO_6S^+$, calc. 483.1716)
IR (film): 3322, 2966, 1752, 1671, 1604, 1470, 1411, 1214, 1103 cm^{-1}.

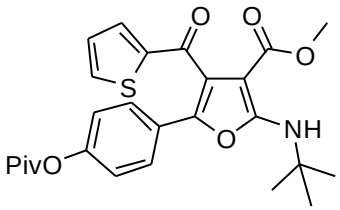


7h

Methyl 2-(tert-butylamino)-5-(3-(pivaloyloxy)phenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7h**

Yield 35%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 4.9, 1.2 Hz, 1H), 7.57 (dd, *J* = 3.7, 1.3 Hz, 1H), 7.29 (dd, *J* = 3.4, 1.9 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.08 (t, *J* = 1.9 Hz, 1H), 7.05 (dd, *J* = 4.9, 3.8 Hz, 1H), 6.90 (s, 1H), 6.89 – 6.83 (m, 1H), 3.54 (s, 3H), 1.53 (s, 9H), 1.32 (s, 9H).

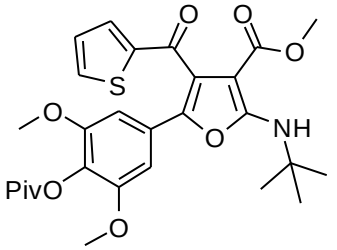
^{13}C NMR (75 MHz, $CDCl_3$) δ 184.85, 176.84, 165.08, 161.56, 151.33, 144.60, 139.64, 134.79, 130.54, 129.64, 128.20, 121.49, 120.43, 119.78, 117.21, 89.90, 52.82, 50.86, 38.99, 29.84, 27.01.
HRMS EI-TOF: *m/z*: 483.1710 ([M]$^+$, $C_{26}H_{29}NO_6S^+$, calc. 483.1716)
IR (film): 3345, 2919, 2355, 1746, 1675, 1609, 1469, 1408, 1218, 1110 cm^{-1}.



7i

Methyl 2-(tert-butylamino)-5-(4-(pivaloyloxy)phenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7i**

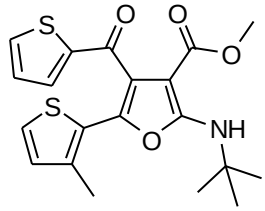
Yield 41%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 4.9, 1.2 Hz, 1H), 7.57 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.05 (dd, *J* = 4.9, 3.8 Hz, 1H), 6.97 (d, *J* = 8.7 Hz, 2H), 6.88 (s, 1H), 3.54 (s, 3H), 1.53 (s, 9H), 1.32 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 185.06, 176.90, 165.12, 161.54, 150.15, 144.68, 140.10, 134.72, 128.16, 126.75, 125.43, 121.84, 118.89, 89.77, 52.80, 50.83, 39.02, 29.85, 27.04.
HRMS EI-TOF: *m/z*: 483.1705 ([M]$^+$, $C_{26}H_{29}NO_6S^+$, calc. 483.1716)
IR (film): 3341, 2971, 2360, 1751, 1673, 1611, 1472, 1211, 1112 cm^{-1}.



7j

Methyl 2-(tert-butylamino)-5-(3,5-dimethoxy-4-(pivaloyloxy)phenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **7j**

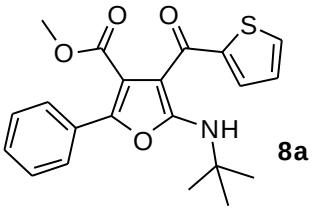
Yield 40%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.68 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.59 (dd, *J* = 3.9, 1.2 Hz, 1H), 7.11 (dd, *J* = 4.9, 3.9 Hz, 1H), 6.89 (s, 1H), 6.73 (s, 2H), 3.70 (s, 6H), 3.58 (s, 3H), 1.55 (s, 9H), 1.36 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 185.04, 176.29, 165.12, 161.43, 152.32, 144.75, 140.37, 134.85, 134.76, 128.42, 128.31, 126.95, 119.03, 101.49, 89.87, 55.97, 52.81, 50.92, 39.08, 29.87, 27.17.
HRMS EI-TOF: *m/z*: 543.1922 ([M]$^+$, $C_{28}H_{33}NO_8S^+$, calc. 543.1927)
IR (film): 3341, 2962, 2360, 1753, 1675, 1579, 1460, 1410, 1216, 1095 cm^{-1}.



7k

Methyl 2-(tert-butylamino)-5-(3-methylthiophen-2-yl)-4-(thiophene-2-carbonyl)furan-3-carboxylate**, 7k**

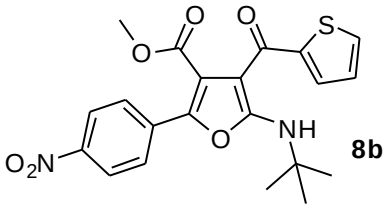
Yield 26%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.63 (dd, *J* = 4.9, 1.2 Hz, 2H), 7.56 (dd, *J* = 3.8, 1.2 Hz, 1H), 7.12 (d, *J* = 5.1 Hz, 1H), 7.03 (dd, *J* = 4.9, 3.8 Hz, 1H), 6.96 (s, 1H), 6.77 (d, *J* = 5.0 Hz, 1H), 3.55 (s, 3H), 2.29 (s, 3H), 1.49 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 183.77, 165.26, 161.98, 145.07, 136.60, 134.40, 134.32, 130.58, 128.69, 127.93, 125.32, 124.83, 102.11, 88.99, 52.79, 50.85, 29.92, 15.59.
HRMS EI-TOF: *m/z*: 403.0912 ($[M]^+$, $C_{20}H_{21}NO_4S_2^+$, calc. 403.0912)
IR (film): 3336, 2966, 2360, 1671, 1609, 1410, 1214, 1098 cm^{-1}.



8a

Methyl 5-(tert-butylamino)-2-phenyl-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8a**

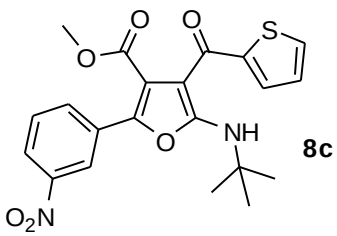
Yield 10%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.35 (s, 1H), 7.83 (d, *J* = 7.0 Hz, 2H), 7.51 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.42 (dd, *J* = 8.4, 6.4 Hz, 2H), 7.38 – 7.34 (m, 2H), 7.07 (dd, *J* = 5.0, 3.7 Hz, 1H), 3.32 (s, 3H), 1.53 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.53, 165.18, 162.63, 145.20, 130.11, 129.72, 128.88, 128.74, 128.60, 128.52, 127.11, 126.61, 113.09, 98.51, 52.94, 51.71, 29.77.
HRMS EI-TOF: *m/z*: 383.1184 ($[M]^+$, $C_{21}H_{21}NO_4S^+$, calc. 383.1191)
IR (film): 3303, 2919, 2360, 1725, 1621, 1517, 1211 cm^{-1}.



8b

Methyl 5-(tert-butylamino)-2-(4-nitrophenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8b**

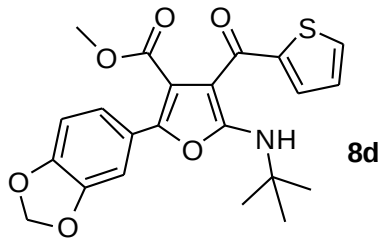
Yield 30%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (s, 1H), 8.26 (d, *J* = 9.0 Hz, 2H), 7.97 (d, *J* = 9.1 Hz, 2H), 7.56 (d, *J* = 4.9 Hz, 1H), 7.36 (d, *J* = 3.7 Hz, 1H), 7.10 (dd, *J* = 4.9, 3.6 Hz, 1H), 3.35 (s, 3H), 1.56 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.84, 164.83, 162.70, 146.56, 144.78, 141.78, 134.73, 130.70, 129.00, 127.22, 126.13, 123.97, 116.84, 99.19, 53.19, 52.05, 29.66.
HRMS EI-TOF: *m/z*: 428.1028 ($[M]^+$, $C_{21}H_{20}N_2O_6S^+$, calc. 428.1042)
IR (film): 3331, 2976, 2355, 1725, 1623, 1517, 1332, 1214cm^{-1}.



8c

Methyl 5-(tert-butylamino)-2-(3-nitrophenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8c**

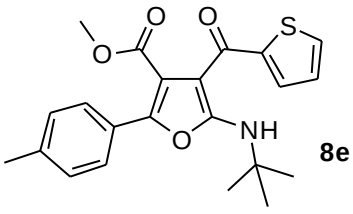
Yield 25%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.75 (t, *J* = 2.0 Hz, 1H), 8.32 (s, 1H), 8.17 (dt, *J* = 8.0, 2.2 Hz, 2H), 7.60 (t, *J* = 8.1 Hz, 1H), 7.55 (dd, *J* = 4.9, 1.1 Hz, 1H), 7.37 (dd, *J* = 3.8, 1.0 Hz, 1H), 7.09 (dd, *J* = 5.0, 3.7 Hz, 1H), 3.36 (s, 3H), 1.56 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.77, 164.74, 162.59, 148.44, 145.00, 142.31, 131.75, 130.59, 130.49, 129.60, 129.01, 127.24, 122.70, 121.27, 115.54, 98.62, 53.18, 52.02, 29.78.
HRMS EI-TOF: *m/z*: 428.1026 ($[M]^+$, $C_{21}H_{20}N_2O_6S^+$, calc. 428.1042)
IR (film): 3303, 2919, 2355, 1725, 1623, 1528, 1453, 1349, 1216 cm^{-1}.



8d

Methyl 2-(benzo[d][1,3]dioxol-5-yl)-5-(tert-butylamino)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8d**

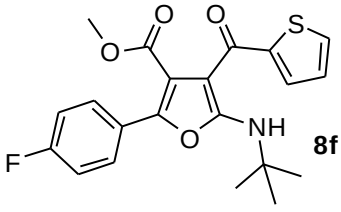
Yield 9%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.50 (dd, *J* = 4.9, 1.0 Hz, 1H), 7.40 (dd, *J* = 8.2, 1.7 Hz, 1H), 7.35 (dd, *J* = 5.0, 1.4 Hz, 2H), 7.07 (dd, *J* = 4.9, 3.7 Hz, 1H), 6.87 (d, *J* = 8.1 Hz, 1H), 6.01 (s, 2H), 3.29 (s, 3H), 1.52 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.37, 165.14, 162.31, 148.06, 147.67, 145.53, 145.35, 130.04, 128.66, 127.12, 122.83, 121.50, 111.90, 108.41, 107.36, 101.34, 98.26, 52.86, 51.63, 29.76.
HRMS EI-TOF: *m/z*: 427.1088 ($[M]^+$, $C_{22}H_{21}NO_6S^+$, calc. 427.1090)
IR (film): 3317, 2928, 2355, 1621, 1446, 1233, 1036 cm^{-1}.



8e

Methyl 5-(tert-butylamino)-4-(thiophene-2-carbonyl)-2-(*p*-tolyl)furan-3-carboxylate, **8e**

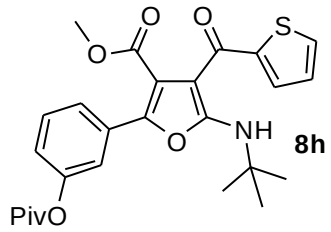
Yield 8%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.51 (d, *J* = 5.0 Hz, 1H), 7.36 (d, *J* = 3.9 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 2H), 7.07 (dd, *J* = 5.0, 3.7 Hz, 1H), 3.31 (s, 3H), 2.39 (s, 3H), 1.52 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.45, 165.20, 162.59, 145.81, 145.39, 138.86, 130.03, 129.21, 128.71, 127.10, 126.77, 126.09, 112.38, 98.40, 52.89, 51.63, 29.77, 21.38.
HRMS EI-TOF: *m/z*: 397.1344 ($[M]^+$, $C_{22}H_{23}NO_4S^+$, calc. 397.1348)
IR (film): 3734, 2919, 2355, 1621, 1512, 1209, 1042 cm^{-1}.



8f

Methyl 5-(tert-butylamino)-2-(4-fluorophenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8f**

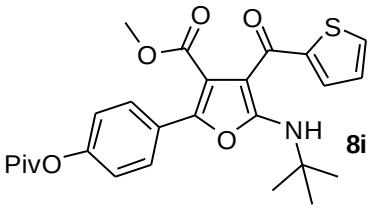
Yield 8%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.85 (dd, *J* = 9.0, 5.3 Hz, 2H), 7.61 – 7.48 (m, 1H), 7.35 (dd, *J* = 3.7, 1.1 Hz, 1H), 7.15 – 7.08 (m, 2H), 7.08 – 7.05 (m, 1H), 3.30 (s, 3H), 1.52 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.53, 165.18, 162.63, 145.20, 130.11, 129.72, 128.88, 128.74, 128.60, 128.52, 127.11, 126.61, 113.09, 98.51, 52.94, 51.71, 29.77.
HRMS EI-TOF: *m/z*: 401.1086 ($[M]^+$, $C_{21}H_{20}NO_4FS^+$, calc. 401.1097)
IR (film): 3328, 2924, 2355, 1720, 1621, 1226, 1043 cm^{-1}.



8h

Methyl 5-(tert-butylamino)-2-(3-(pivaloyloxy)phenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8h**

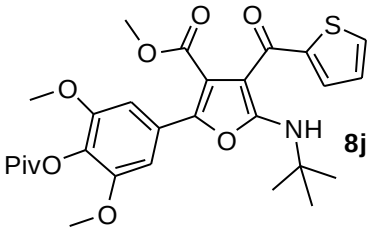
Yield 12%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.32 (s, 1H), 7.72 – 7.62 (m, 1H), 7.58 (t, *J* = 2.0 Hz, 1H), 7.51 (d, *J* = 4.9 Hz, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 3.2 Hz, 1H), 7.05 (dt, *J* = 8.2, 3.2 Hz, 2H), 3.32 (s, 3H), 1.53 (s, 9H), 1.38 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.60, 176.96, 164.94, 162.55, 151.16, 145.21, 144.13, 130.26, 130.23, 129.43, 128.83, 127.12, 123.77, 121.78, 119.78, 113.86, 98.56, 52.96, 51.76, 39.09, 29.74, 27.09.
HRMS EI-TOF: *m/z*: 483.1708 ($[M]^+$, $C_{26}H_{29}NO_6S^+$, calc. 483.1716)
IR (film): 3331, 2919, 2360, 1749, 1621, 1214, 1110 cm^{-1}.



8i

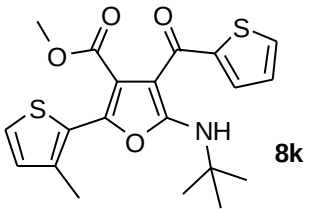
Methyl 5-(tert-butylamino)-2-(4-(pivaloyloxy)phenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8i**

Yield 12%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 (s, 1H), 7.85 (d, *J* = 8.7 Hz, 2H), 7.48 (dd, *J* = 4.9, 1.2 Hz, 1H), 7.34 (dd, *J* = 3.8, 1.1 Hz, 1H), 7.10 (d, *J* = 8.9 Hz, 2H), 7.05 (dd, *J* = 4.9, 3.8 Hz, 1H), 3.28 (s, 3H), 1.51 (s, 9H), 1.35 (s,9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.54, 176.90, 165.08, 162.58, 151.26, 145.30, 144.77, 130.16, 128.78, 127.99, 127.14, 126.40, 121.68, 112.91, 98.43, 52.96, 51.71, 29.77, 29.68, 27.10.
HRMS EI-TOF: *m/z*: 483.1709 ($[M]^+$, $C_{26}H_{29}NO_6S^+$, calc. 483.1716)
IR (film): 3312, 2966, 2355, 1751, 1621, 1453, 1209, 1110 cm^{-1}.



Methyl 5-(tert-butylamino)-2-(3,5-dimethoxy-4-(pivaloyloxy)phenyl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8j**

Yield 13%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.51 (d, *J* = 4.7 Hz, 1H), 7.38 (d, *J* = 3.7 Hz, 1H), 7.23 (s, 2H), 7.07 (dd, *J* = 4.9, 3.6 Hz, 1H), 3.85 (s, 6H), 3.27 (s, 3H), 1.53 (s, 9H), 1.39 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.52, 176.30, 165.26, 162.29, 152.19, 145.28, 144.99, 130.19, 129.57, 128.74, 127.15, 126.61, 113.26, 103.93, 98.63, 56.17, 52.92, 51.74, 39.16, 29.74, 27.22.
HRMS EI-TOF: *m/z*: 543.1912 ($[M]^+$, $C_{28}H_{33}NO_8S^+$, calc. 543.1927)
IR (film): 3269, 2919, 2360, 1751, 1623, 1457, 1207, 1112 cm^{-1}.



Methyl 5-(tert-butylamino)-2-(3-méthylthiophen-2-yl)-4-(thiophene-2-carbonyl)furan-3-carboxylate, **8k**

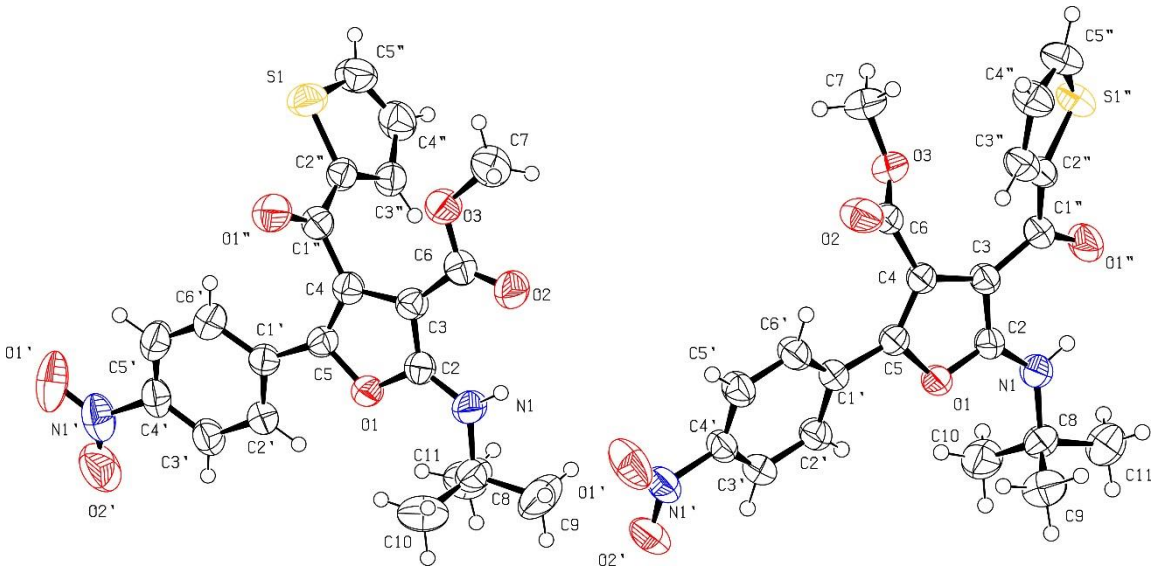
Yield 8%. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.57 – 7.44 (m, 1H), 7.36 – 7.31 (m, 2H), 7.05 (dd, *J* = 5.0, 3.6 Hz, 1H), 6.91 (d, *J* = 5.2 Hz, 1H), 3.33 (s, 3H), 2.35 (s, 3H), 1.48 (s, 9H).
^{13}C NMR (75 MHz, $CDCl_3$) δ 180.33, 164.57, 162.08, 145.48, 138.42, 130.24, 128.98, 128.88, 127.16, 122.40, 110.96, 97.80, 53.06, 51.52, 29.67, 15.76.
HRMS EI-TOF: *m/z*: 403.0911 ($[M]^+$, $C_{20}H_{21}NO_4S_2^+$, calc. 403.0912)
IR (film): 3331, 2919, 2355, 1614, 1453, 1211, 1093 cm^{-1}.

X-ray Crystallography Experiments

Single-crystal X-ray diffraction data were collected with an Enraf–Nonius Kappa-CCD diffractometer using graphite-monochromated Mo-$K\alpha$ (λ= 0.71070 Å) radiation at ambient temperature. Diffraction images were recorded according to a φ+ω scan profile data strategy derived by the COLLECT software package.[3] Intensities were reduced and merged after semi-empirical absorption correction using HKL-2000 software.[4] The structures were solved by direct methods (SHELXS-97)[5] and refined on F^2 by means of full-matrix least-squares methods (SHELXL-97).[5] All non-hydrogen atoms were refined anisotropically, whereas hydrogen atoms, located from difference Fourier maps, were refined using a riding model (except for the amine hydrogen with soft restraint on the N-H distance with sd 0.02) with U_{iso} = 1.2U_{eq} of the parent atom (1.5 for the methyl hydrogen atoms). ORTEP drawings were made using ORTEP3[6] as implemented within PLATON[7] and packing studies were carried out using MERCURY.[8]

CCDC 949882 and CCDC 949883 contain the supplementary crystallographic data. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336033; or deposit@ccdc.cam.uk).
Electronic supplementary information (ESI) available: X-ray structure data. CCDC 949882-949883.

Figure S1. ORTEP (50% ellipsoid probability) diagram of **7a** (left) and **8b** (right), showing the atom-labeling scheme.



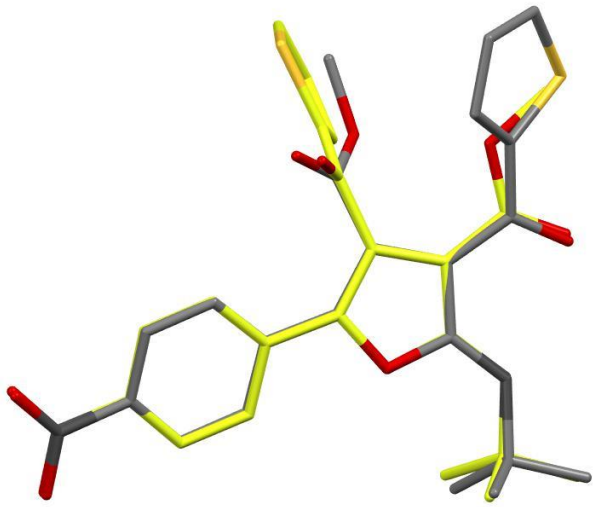
[3] Nonius (1999). COLLECT. Nonius BV, Delft, The Netherlands.
[4] Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology, Volume 276,Macromolecular Crystallography, part A, edited by C.W. Carter, Jr. & R.M. Sweet, 307-326, New York: Academic Press.*
[5] Sheldrick, G.M. (2008). *Acta Cryst.* A**64**, 112-122; Welter, R. (2006). *Acta Cryst.* **A**62, s252.
[6] Burnett, Michael N. and Johnson, Carroll K.(1996). ORTEP-III: Oak Ridge Thermal Ellipsoid Plot Program for Crystal Structure Illustrations, Oak Ridge National Laboratory Report ORNL-6895.
[7] Spek, A. L. (2003). *J.Appl. Cryst*. **36**, 7-13.
[8] Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J.Appl. Cryst*. **39**, 453-457.

Table S1. Data collection

Identification code	**7b**	**8b**
Empirical formula	$C_{21}H_{20}N_2O_6S$	$C_{21}H_{20}N_2O_6S$
Formula weight	428.45	428.45
Temperature / K	293(2)	293(2)
Wavelength / Å	0.71070	0.71070
Crystal system, space group	Trigonal, P 31	Orthorhombic, P 21 21 21
a / Å	10.104(2)	8.534(2)
b / Å	10.104(2)	15.242(4)
c / Å	17.905(4)	16.014(4)
Volume / Å^3	1583.0(6)	2083.0(9)
Z, ρ / g.cm^{-3}	3, 1.348	4, 1.366
μ (Mo Kα) / mm^{-1}	0.193	0.196
F(000)	672	896
Crystal size / mm	0.55 x 0.40 x 0.18	0.58 x 0.29 x 0.24
θ range for data collection / °	2.59 to 25.31	2.87 to 27.39
Limiting indices	$-12 \le h \le 12$, $-9 \le k \le 9$, $-21 \le l \le 21$	$-11 \le h \le 11$, $-19 \le k \le 19$, $-20 \le l \le 20$
Reflections collected / unique	9134 / 3746 [R(int) = 0.0000]	27119 / 4703 [R(int) = 0.0000]
Completeness to θ max	99.3 %	99.2 %
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.96 and 0.88	0.97 and 0.88
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3742 / 2 / 279	4692 / 1 / 279
Goodness-of-fit on F^2	1.005	1.047
Final R indices [I>2σ(I)]	R1 = 0.0438, wR2 = 0.1070	R1 = 0.0347, wR2 = 0.0800
R indices (all data)	R1 = 0.0522, wR2 = 0.1136	R1 = 0.0463, wR2 = 0.0871
Absolute structure parameter	0.07(9)	-0.04(7)
Extinction coefficient	0.053(6)	0.028(3)
Largest diff. peak and hole / e.Å^{-3}	0.143 and -0.208	0.136 and -0.155

[a] $R1 = \Sigma \big| \, |Fo| - |Fc| \, \big| / \Sigma |Fo|$. [b] $wR2 = [\Sigma\{w(Fo^2 - Fc^2)^2\}/\Sigma\{w(Fo^2)^2\}]^{1/2}$

Figure S2. An overlay of molecules **7b** (carbon atoms in yellow) and **8b** (carbon atoms in grey) generated by a least-squares fit of their common sections.



Explanation of the similar relative orientations of the nitrophenyl moiety and the trisubstituted furan moiety in both structures (19.9° and 13.2° respectively in **8b** and **7b**) can be found in the recurrent intramolecular H-bond between the N-H and the carbonyl oxygen atom. Please note that the dihedral angles between furan and thiophen groups are 73.7° and 39.1° and for **7b** and **8b**, respectively.

Table S2. Intra-molecular Hydrogen bonds [Å and °].

	D–H...A	d(D–H)	d(H...A)	d(D...A)	<(DHA)>
7b	N1–H1N … O2	0.882(19)	2.846(3)	2.263(3)	123.35
8b	N1–H1N … O1 ‘‘	0.858(16)	2.136(19)	2.775(2)	131.0(18)

Computational Details

Geometry optimizations and frequency calculations were done with the M062X/6-31G(d,p) method[9] in vacuo, were all stationary points were properly characterized by frequency analysis. NBO analysis[10] were done by single point calculation using NBO 3.0 software with IEFPCM/M062X/6-31G(d,p) method (dichloromethane continuum solvent). DFT-based reactivity indices have been determined; global electrophilicity ω,[23] which measures the stabilization in energy when the system acquires an additional electronic charge ΔN from the environment chemical hardness, chemical softness and useful Fukui[24] condensed indices f_k^+ and f_k^- using a method described elsewhere.[25] Global electrophilicity ω (ω=$\mu^2/2\eta$) was calculated in terms of the electronic chemical potential μ (μ≈ ($\varepsilon_{HOMO}+\varepsilon_{LUMO}$)/2) and the chemical hardness η (η≈($\varepsilon_{LUMO}-\varepsilon_{HOMO}$)). The chemical softness S was calculated using following expression: S = 1/η. All calculations were done with the Gaussian09 program packages.

Full reference of Gaussian09 software.

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009

Table S3. DFT-based reactivity indices of compounds **1**-**4**.

Compound	ε HOMO[a]	ε LUMO[a]	Electronic chemical potential,[a] μ	Chemical hardness,[a] η	Chemical softness,[a] S	Electrophilicity index,[b] ω
1	-0.33870	-0.02179	-0.180	0.317	3.155	1.39
2	-0.31905	-0.04797	-0.184	0.271	3.689	1.69
3	-0.30826	-0.05331	-0.181	0.255	3.922	1.74
4	-0.35223	0.09589	-0.128	0.448	2.232	0.50

[a] indices given in a.u; [b] value expressed in eV.

[9] Y. Zhao, D.G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215.

[10] F. Weinhold, "Natural Bond Orbital Methods," in *Encyclopedia of Computational Chemistry*, P. V.R. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. Schaefer III, P. R. Schreiner (Eds.), (John Wiley & Sons, Chichester, UK, 1998), Vol. 3, pp. 1792-1811.

Cartesian coordinates of compounds 1-4.

Methyl 5,5-dimethyl-4-oxohex-2-ynoate, **1**.

6	-0.075705000	0.573951000	-0.031550000
6	1.106529000	0.371057000	0.111491000
6	2.529485000	0.158303000	0.349748000
8	3.057637000	0.297684000	1.422365000
6	-1.517142000	0.823793000	-0.206506000
8	-1.899801000	1.926930000	-0.519152000
6	-2.436729000	-0.370506000	0.026574000
6	-2.062708000	-1.471152000	-0.978780000
1	-1.024732000	-1.792112000	-0.852466000
1	-2.709865000	-2.339261000	-0.821593000
1	-2.196976000	-1.126636000	-2.008417000
6	-3.882020000	0.077439000	-0.175640000
1	-4.554785000	-0.770012000	-0.015527000
1	-4.146337000	0.872461000	0.525799000
1	-4.034924000	0.462134000	-1.186691000
6	-2.221227000	-0.881755000	1.459668000
1	-2.876182000	-1.739432000	1.639685000
1	-1.187746000	-1.201598000	1.620216000
1	-2.462126000	-0.108198000	2.194856000
1	5.052039000	0.487220000	-0.295663000
1	4.739620000	-1.211164000	0.124742000
8	3.153288000	-0.210728000	-0.771739000
6	4.559035000	-0.431949000	-0.618053000
1	4.915898000	-0.739577000	-1.598438000

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# of imaginary frequency: none

Methyl 4-oxo-4-phenylbut-2-ynoate, **2**.

6	0.575775000	0.751434000	0.151614000
6	1.708131000	0.336203000	0.208761000
6	3.071509000	-0.165221000	0.344265000
8	3.523530000	-0.610739000	1.366992000
6	-0.782389000	1.306965000	0.070386000
8	-0.937238000	2.509439000	0.060973000
1	5.654071000	0.048034000	-0.019275000
1	5.114568000	-1.581552000	-0.480869000
8	3.734923000	-0.061558000	-0.809210000
6	5.087808000	-0.525397000	-0.755712000
1	5.488790000	-0.374548000	-1.755529000
6	-1.910898000	0.339664000	0.000483000

6	-1.704680000	-1.039884000	0.054302000
6	-3.204584000	0.855714000	-0.119605000
6	-2.793731000	-1.902688000	-0.011419000
1	-0.697324000	-1.433256000	0.150749000
6	-4.287770000	-0.008712000	-0.186668000
1	-3.331760000	1.932461000	-0.157929000
6	-4.081972000	-1.387710000	-0.132286000
1	-2.637609000	-2.975263000	0.032365000
1	-5.293281000	0.387587000	-0.280835000
1	-4.930371000	-2.062808000	-0.183434000

SCF Done: E(RM062X) = -649.329981982
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Methyl 4-oxo-4-(thiophen-2-yl)but-2-ynoate, **3**.

6	0.594344000	0.660755000	0.176083000
6	1.739805000	0.282225000	0.217085000
6	3.118199000	-0.184149000	0.330074000
8	3.552226000	-0.766061000	1.289957000
6	-0.789355000	1.146300000	0.115294000
8	-1.037754000	2.333824000	0.149181000
1	5.699776000	0.180280000	0.111269000
1	5.251931000	-1.375610000	-0.623132000
8	3.816316000	0.122192000	-0.764914000
6	5.186179000	-0.291039000	-0.728676000
1	5.613444000	0.033287000	-1.674914000
6	-1.816395000	0.106418000	0.009972000
6	-1.659000000	-1.257907000	-0.005606000
6	-2.896465000	-1.941750000	-0.116603000
6	-3.956677000	-1.077612000	-0.182433000
16	-3.477620000	0.566688000	-0.109273000
1	-0.689734000	-1.737612000	0.065449000
1	-2.998528000	-3.018818000	-0.145772000
1	-5.005087000	-1.327623000	-0.269460000

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Tert-butyl isocyanide, **4**.

6	-0.257107000	0.000228000	0.000102000
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6	2.357021000	-0.000370000	0.000112000
6	-0.733403000	-0.646939000	1.303409000

1	-1.826481000	-0.660198000	1.326340000
1	-0.366959000	-1.673584000	1.376643000
1	-0.369558000	-0.083352000	2.165788000
6	-0.733040000	-0.805493000	-1.211866000
1	-1.826112000	-0.820523000	-1.234299000
1	-0.367994000	-0.355455000	-2.138102000
1	-0.367928000	-1.833680000	-1.155513000
6	-0.733020000	1.452547000	-0.091641000
1	-0.367128000	1.917248000	-1.010217000
1	-1.826051000	1.479341000	-0.093908000
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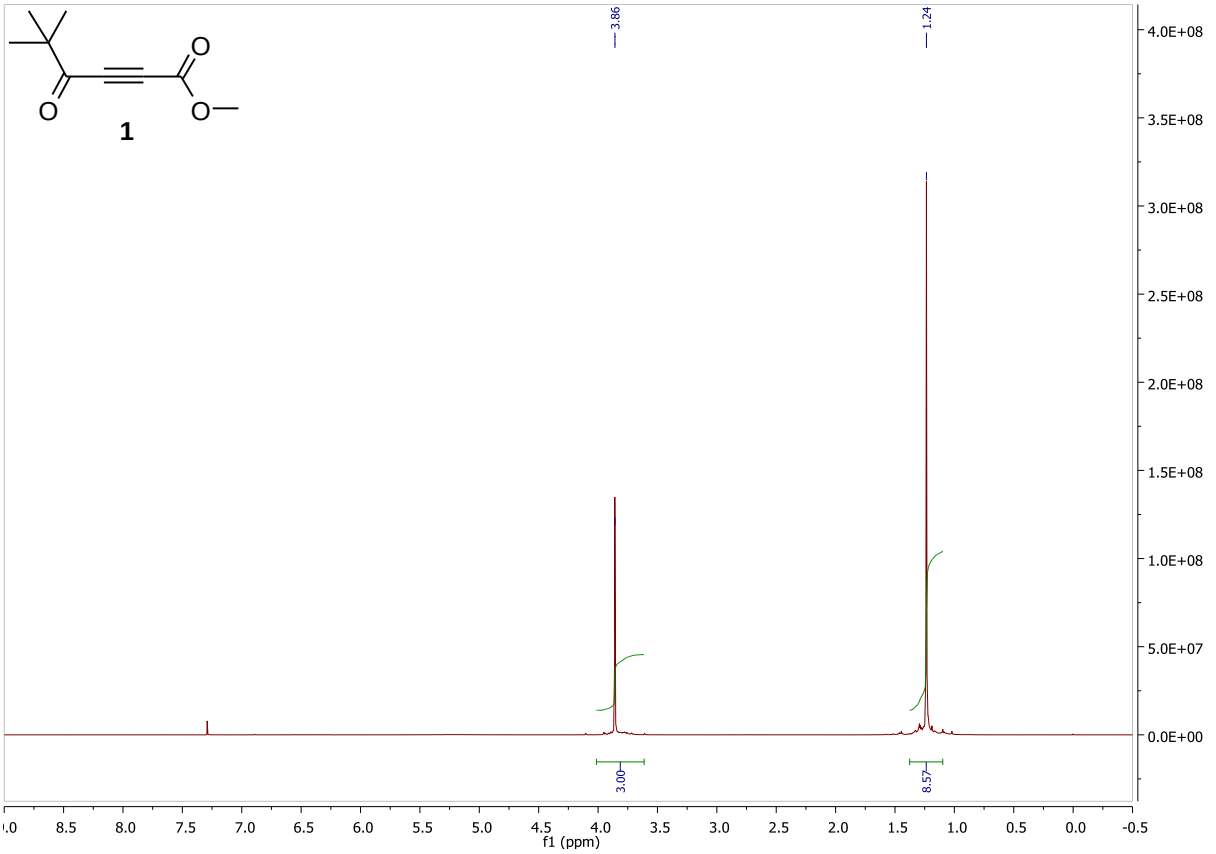
NMR Spectra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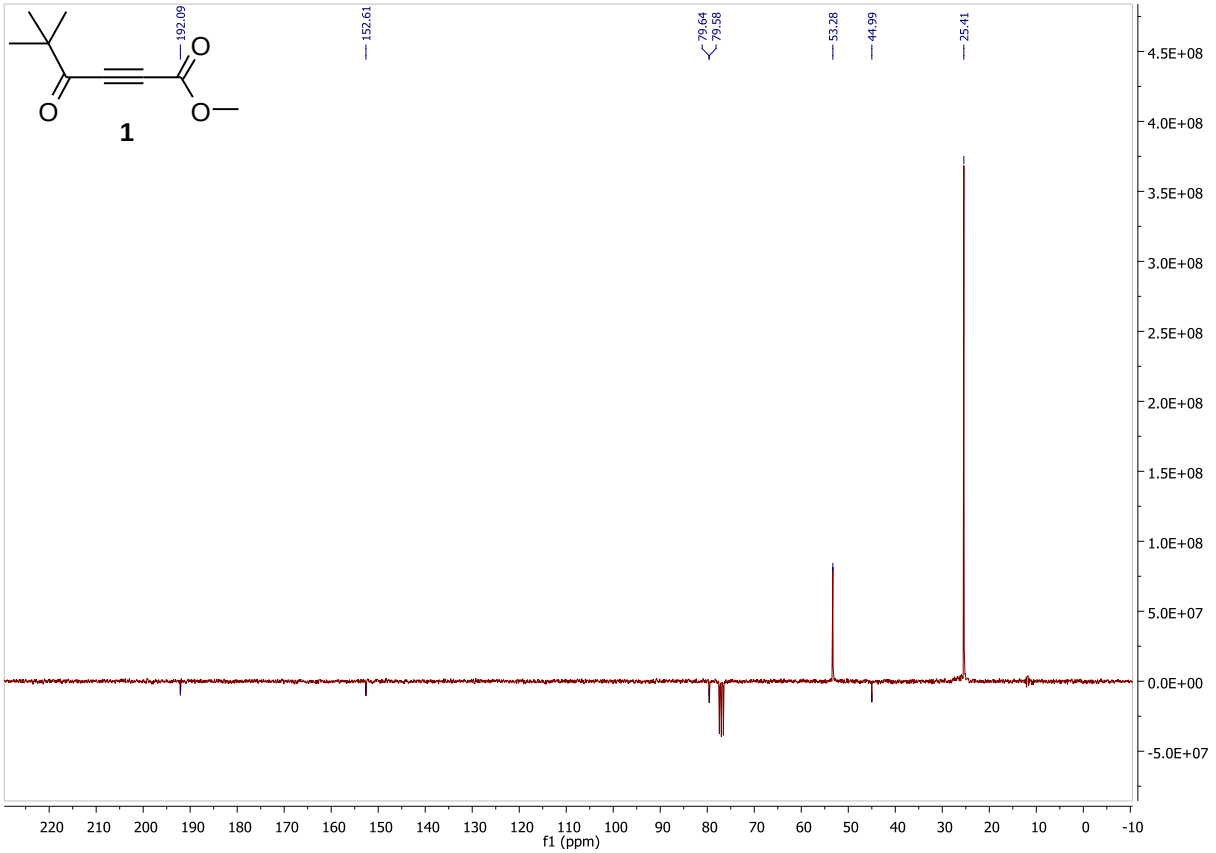
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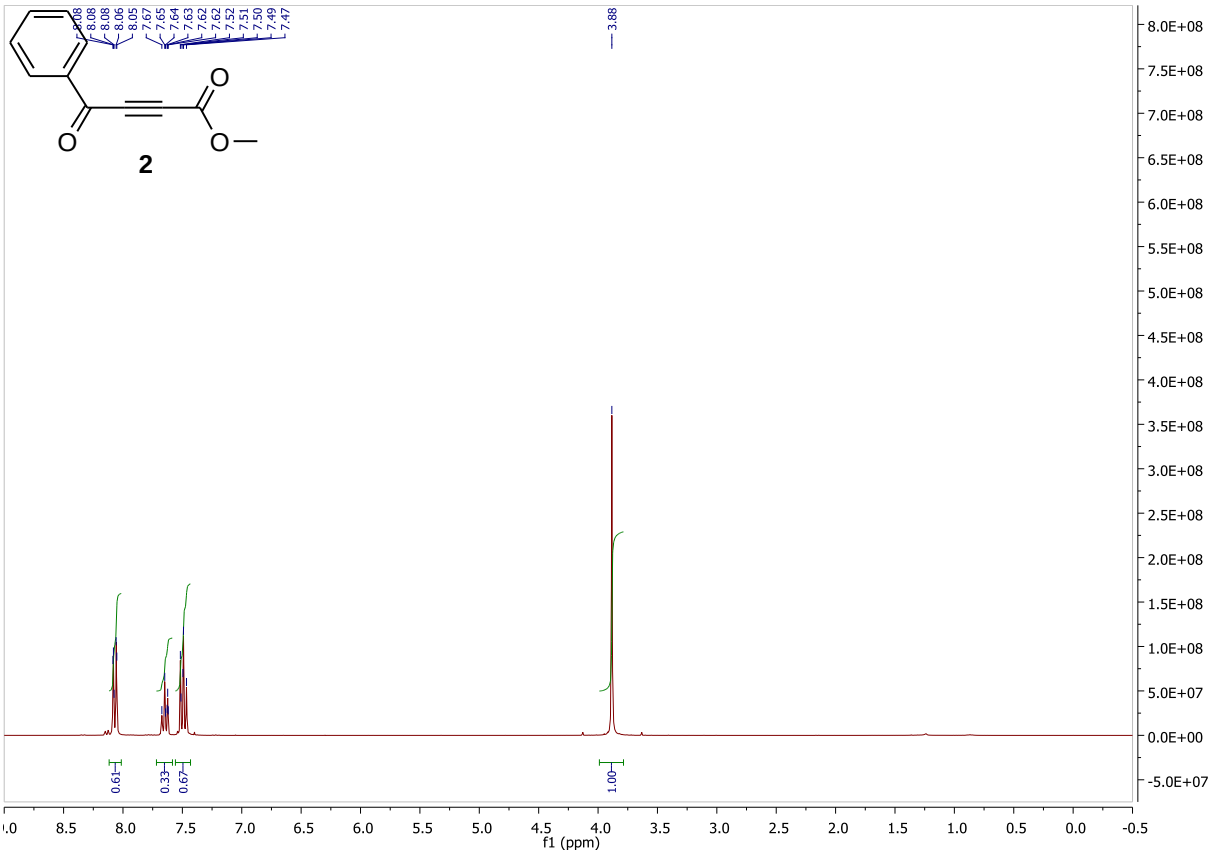
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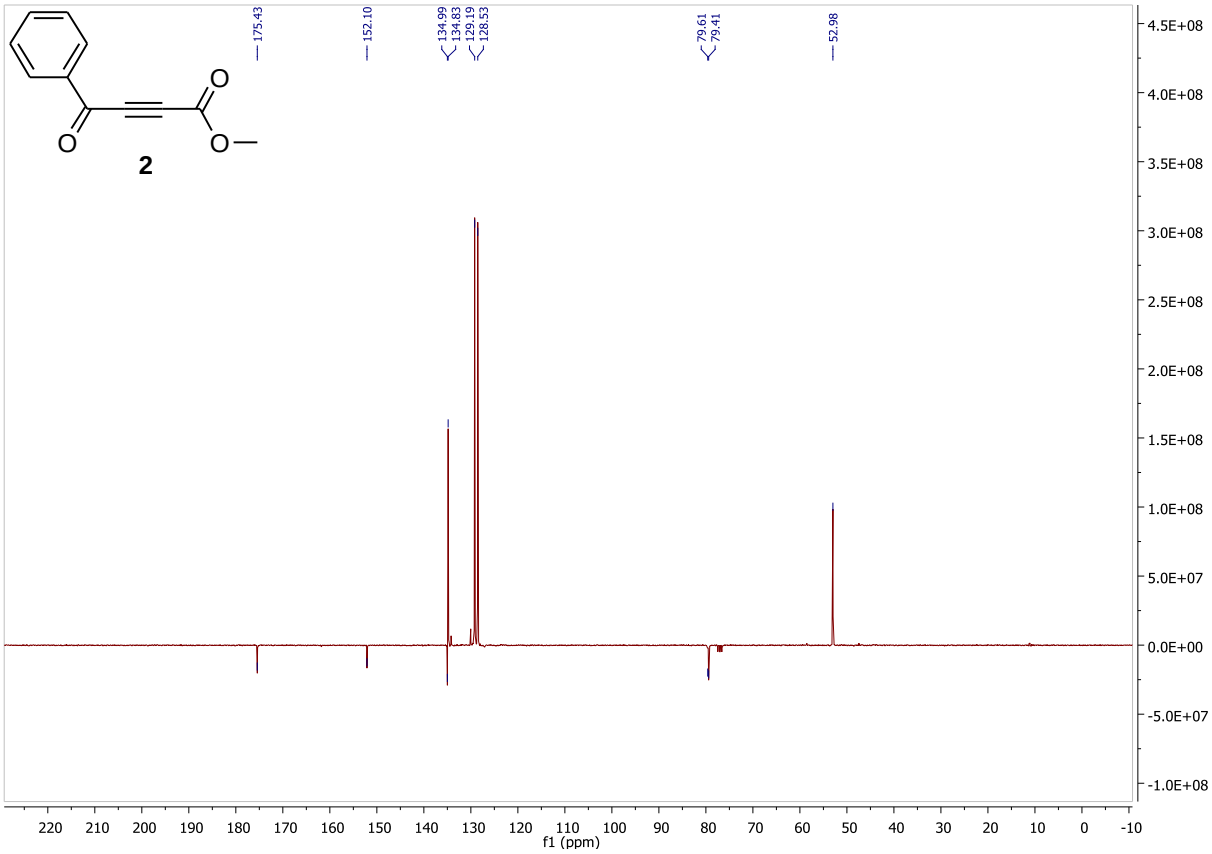
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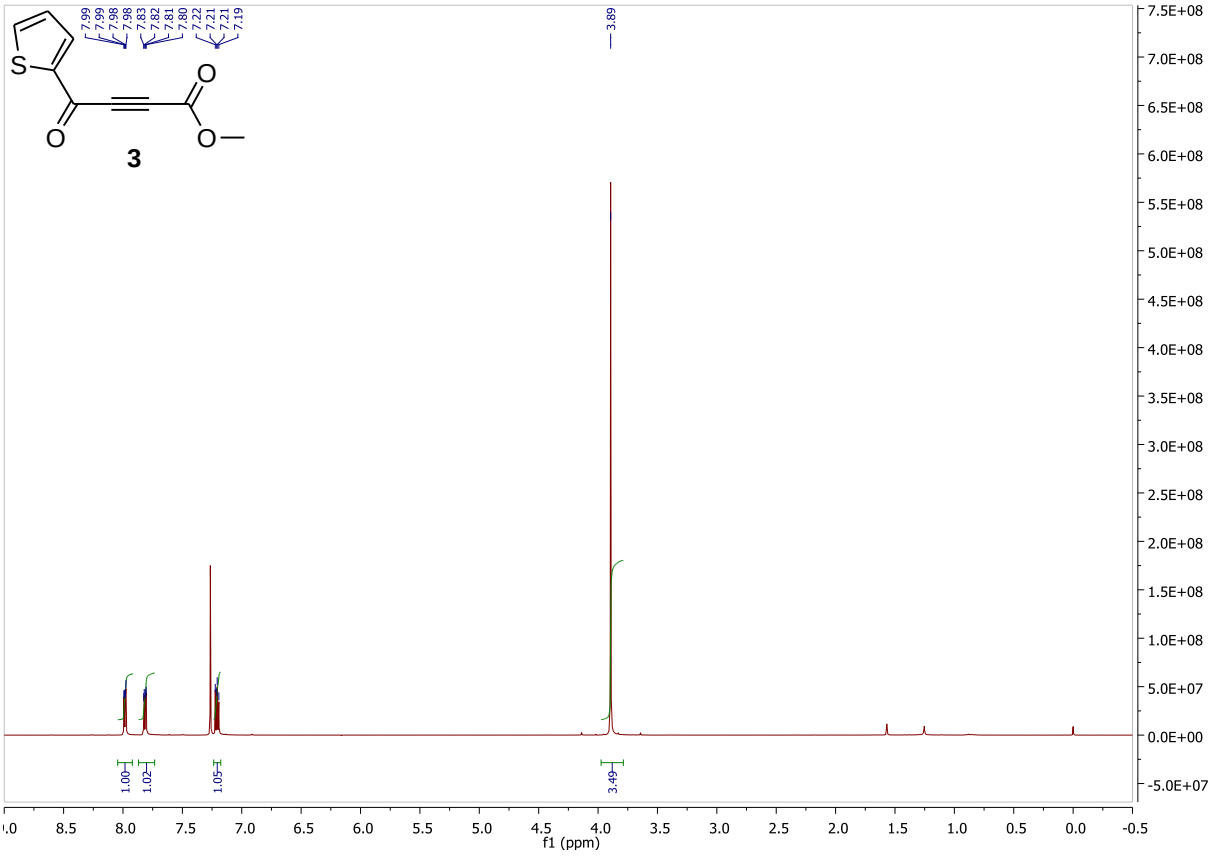
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O
O
O
O
3
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1.02
1.05
3.49
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7.0E+08
6.5E+08
6.0E+08
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5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
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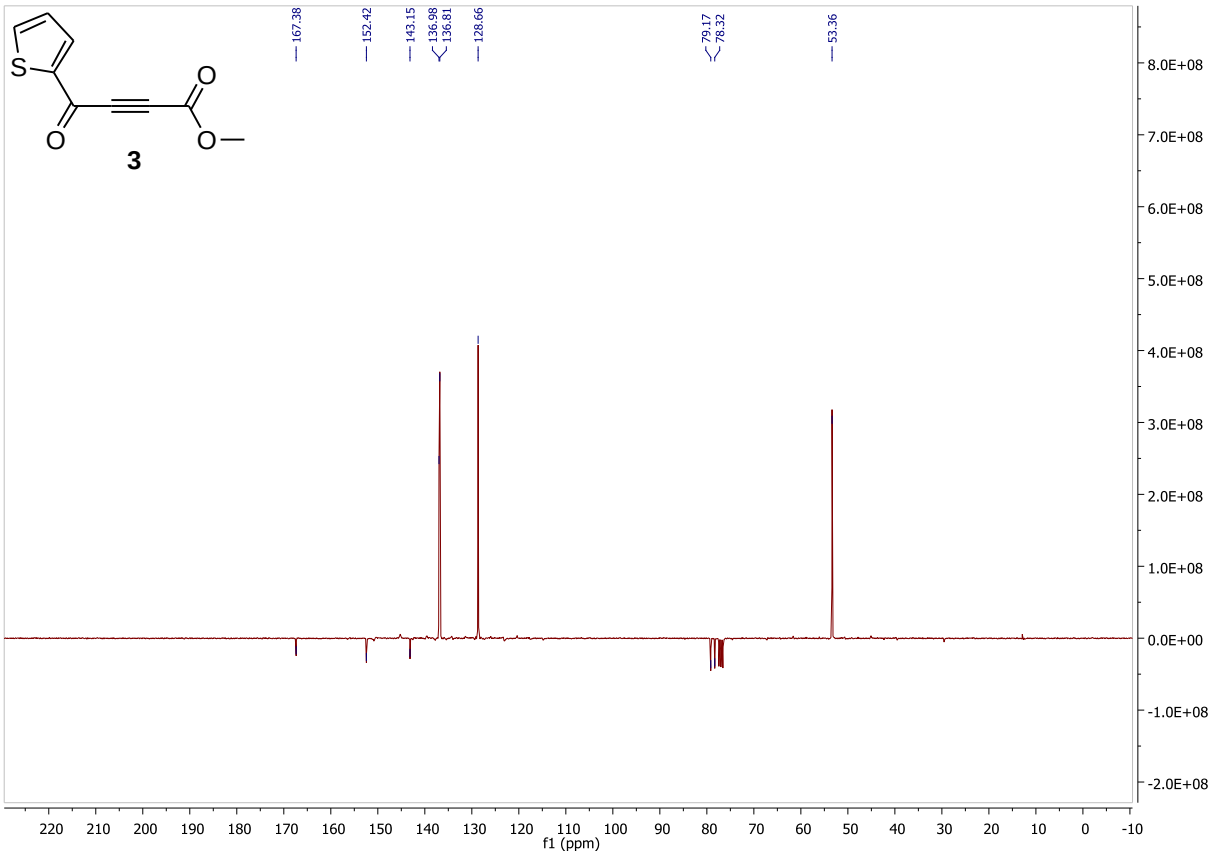
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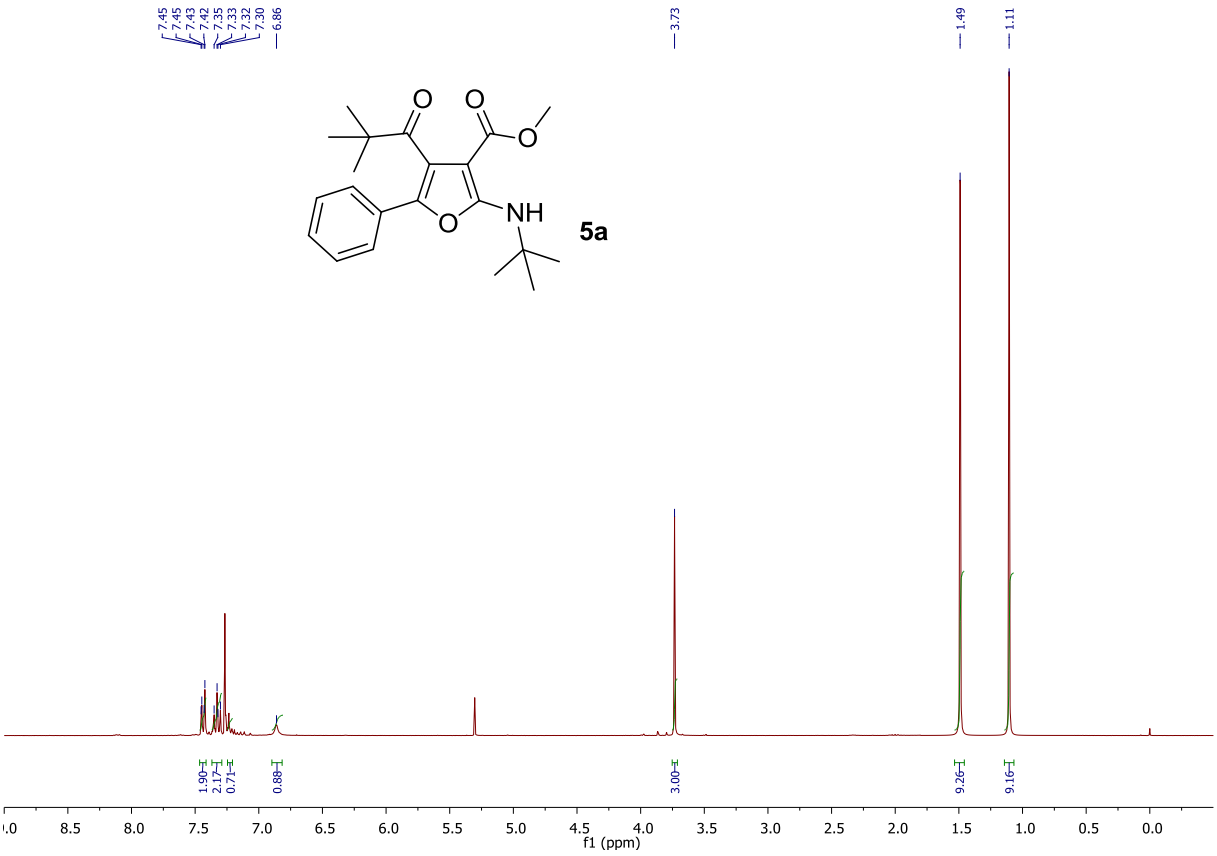
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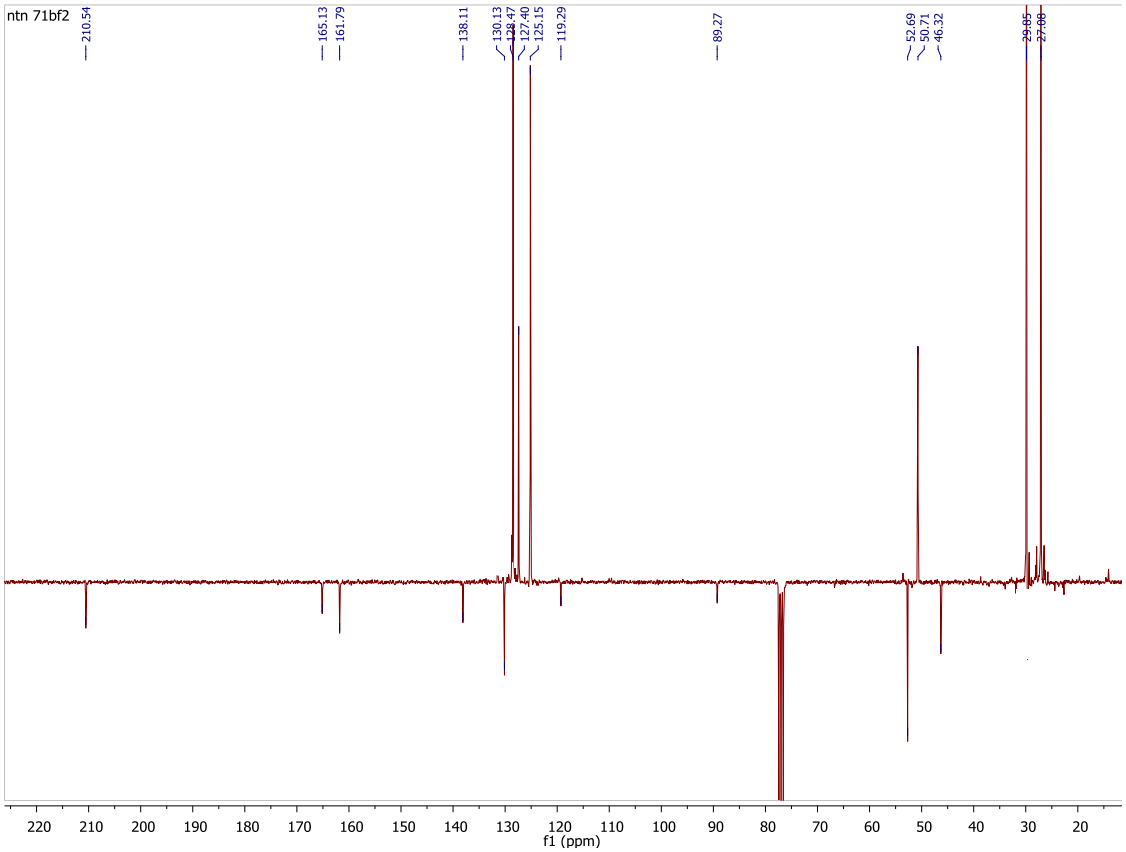
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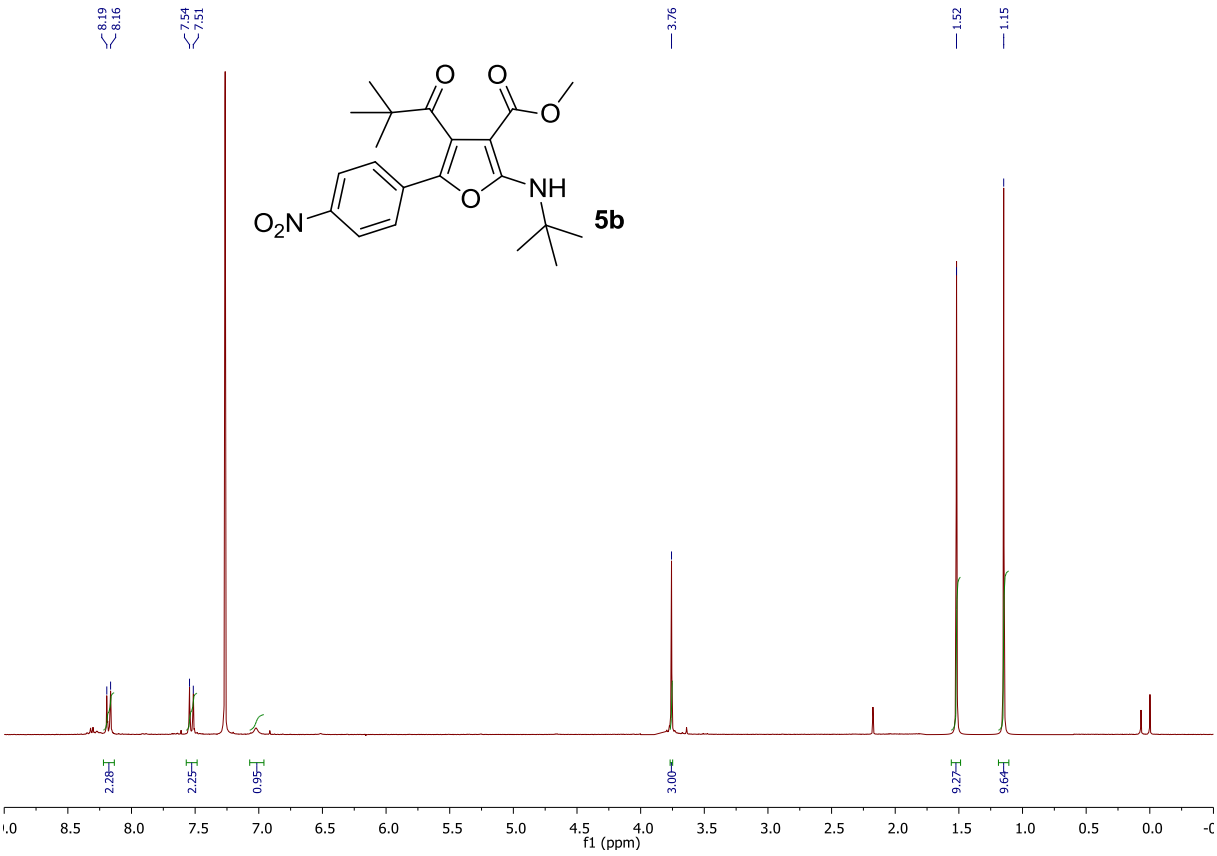
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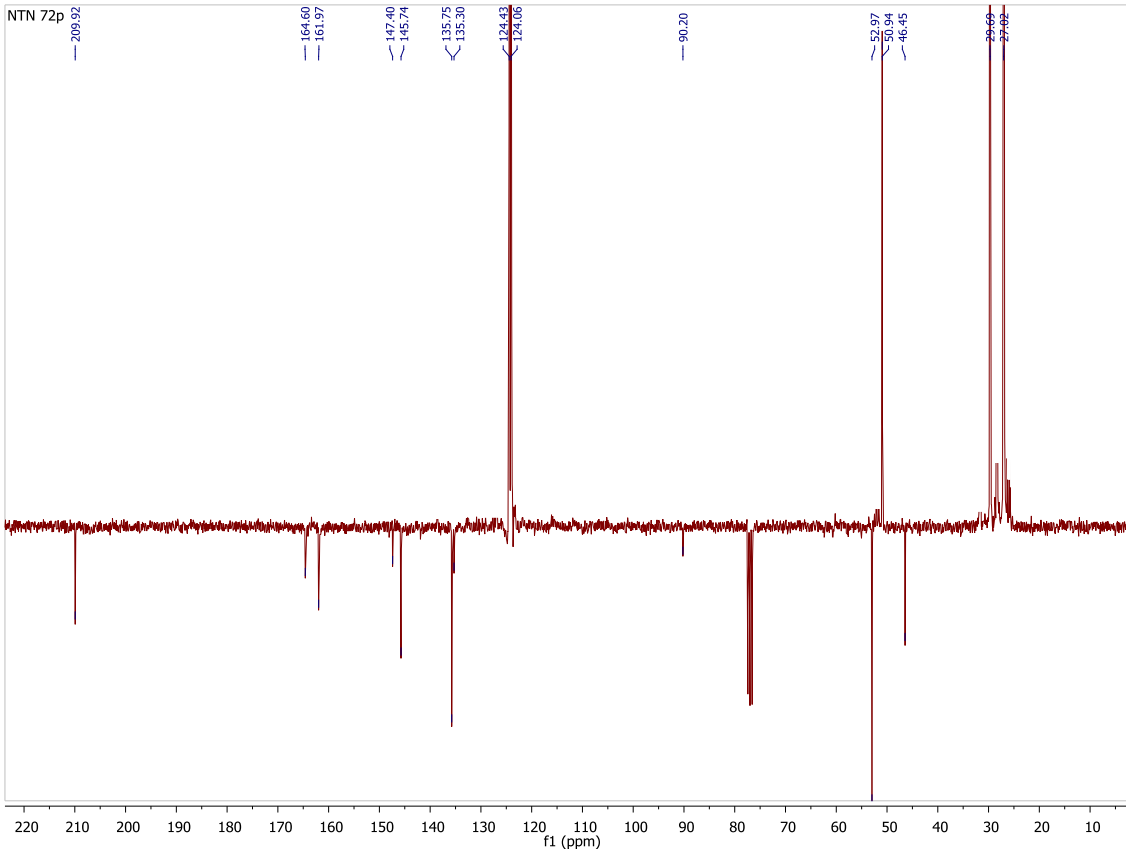
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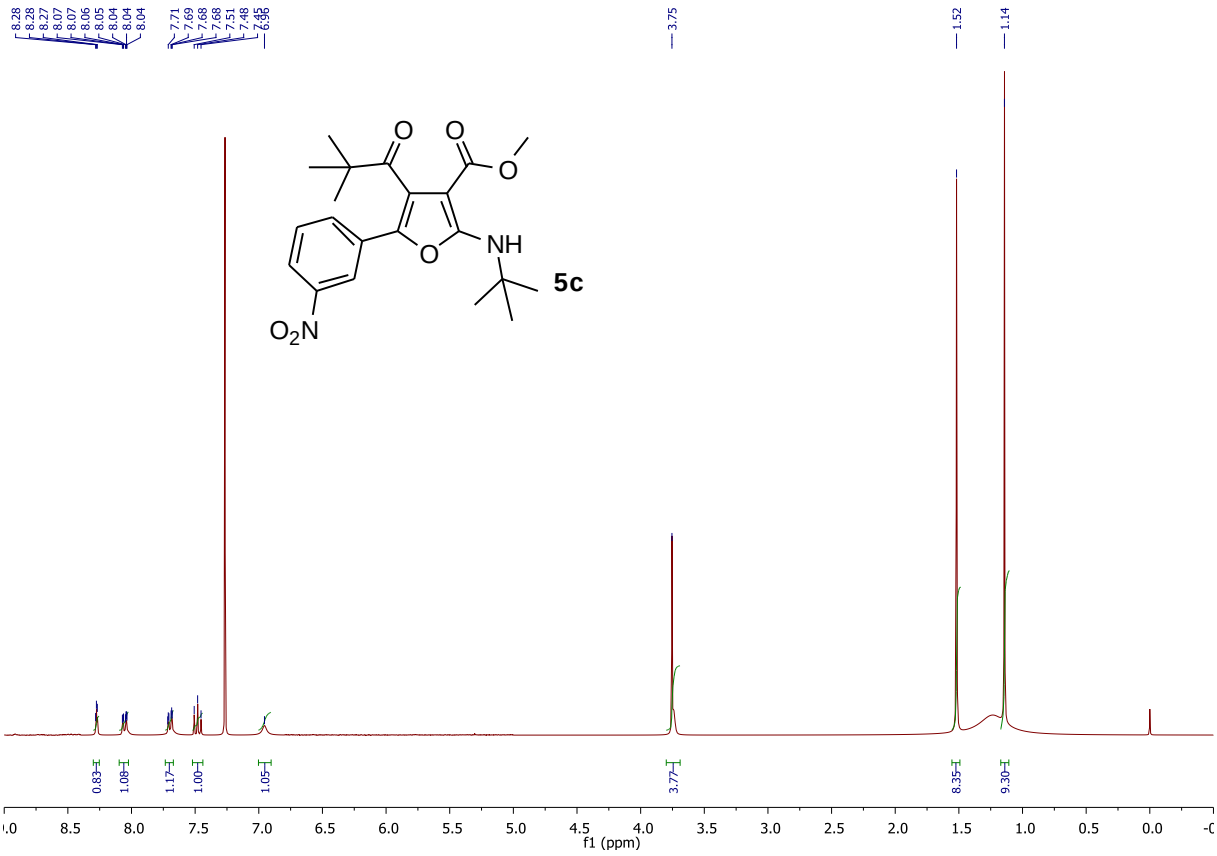
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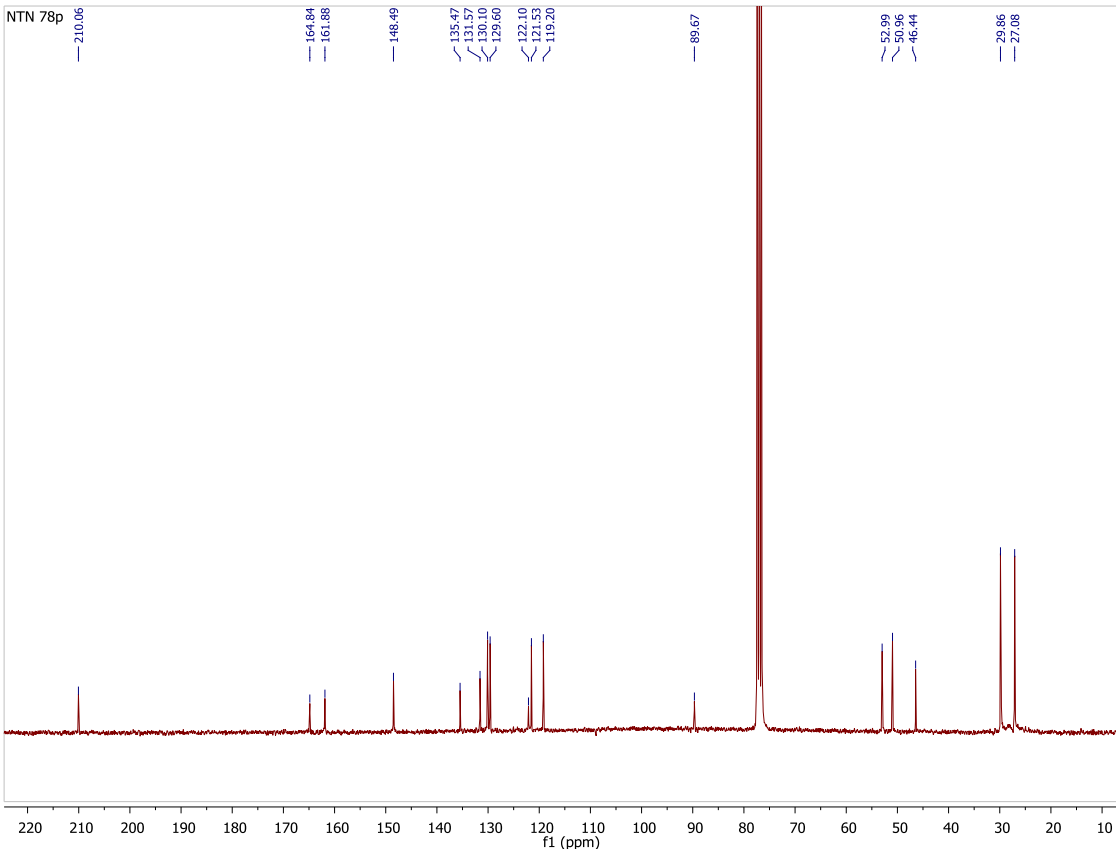
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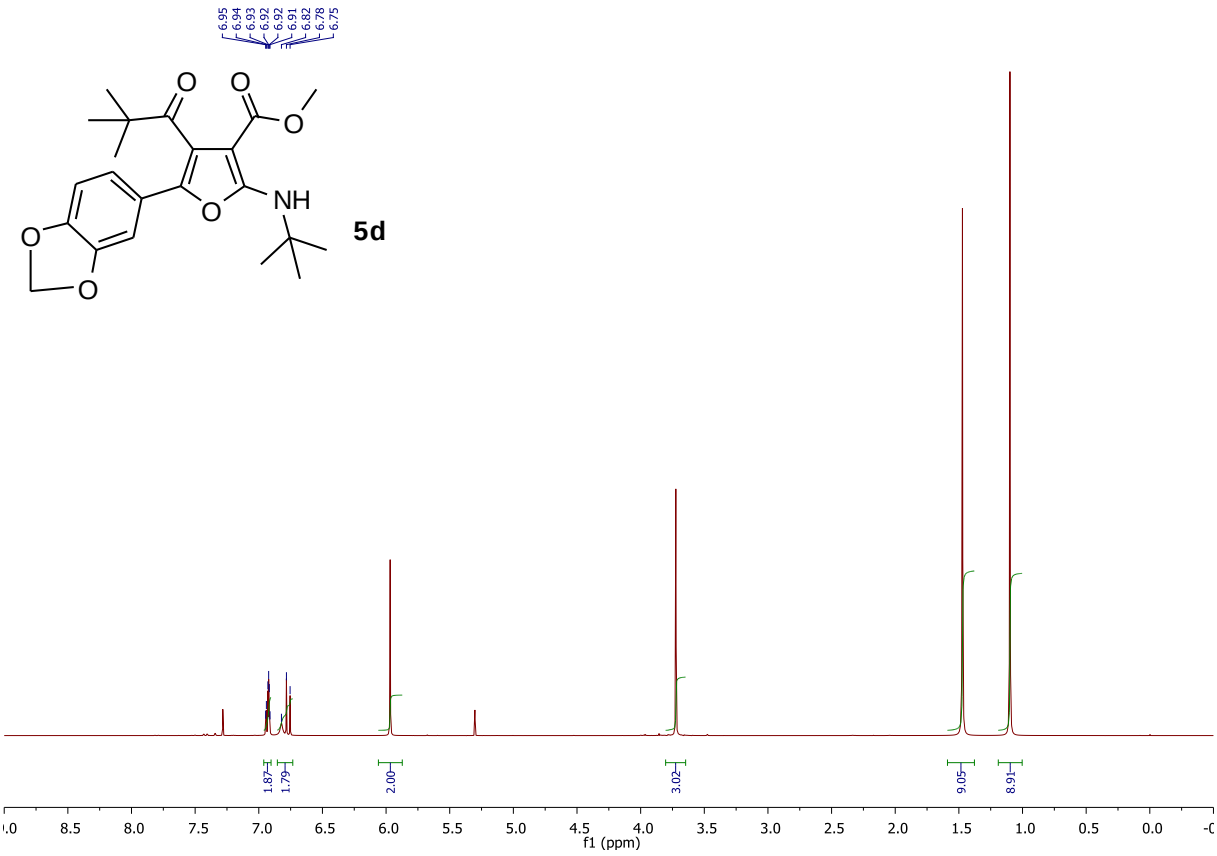
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3.02
9.05
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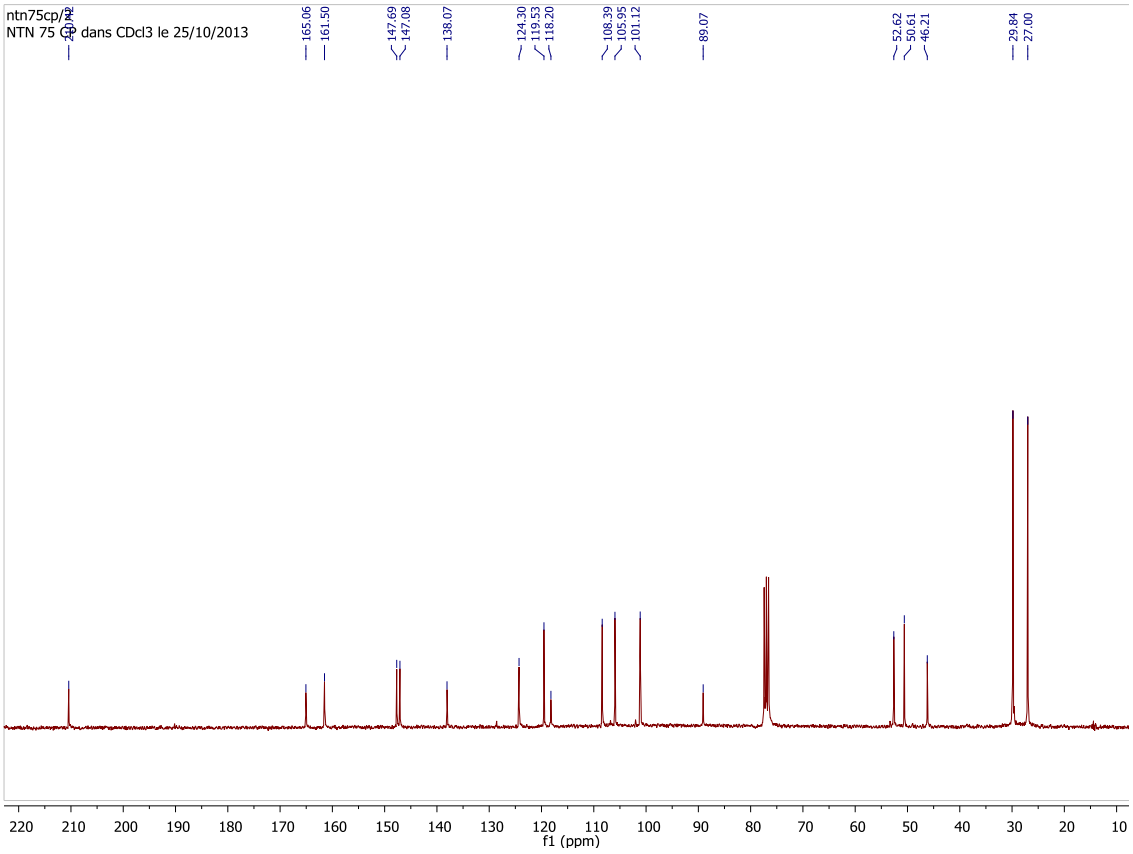
f1 (ppm)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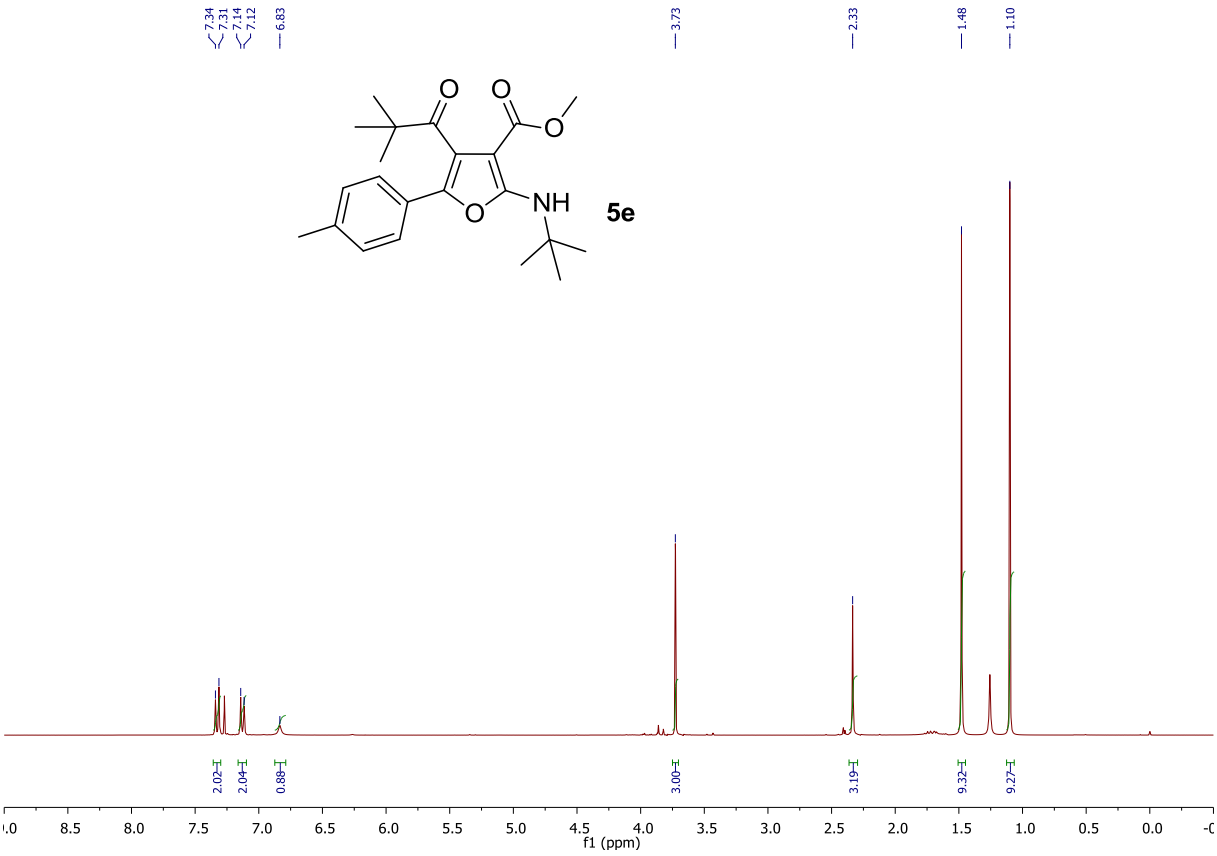
f1 (ppm)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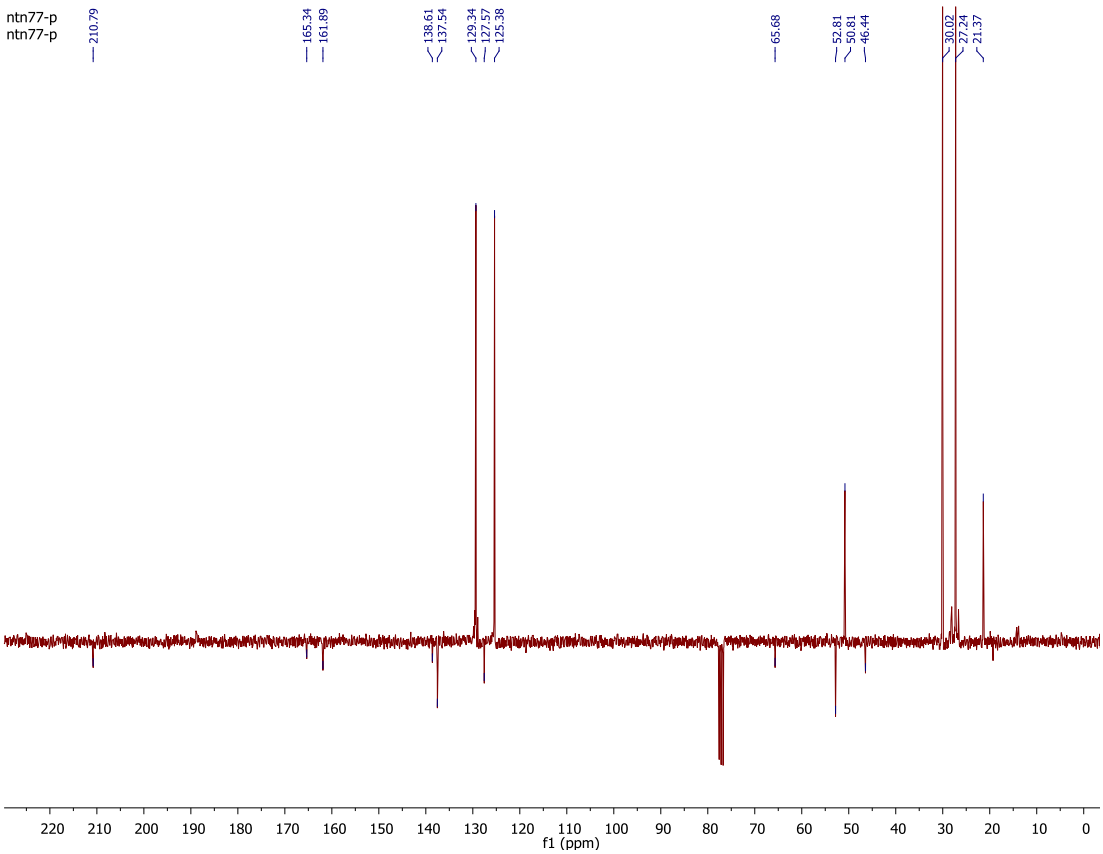
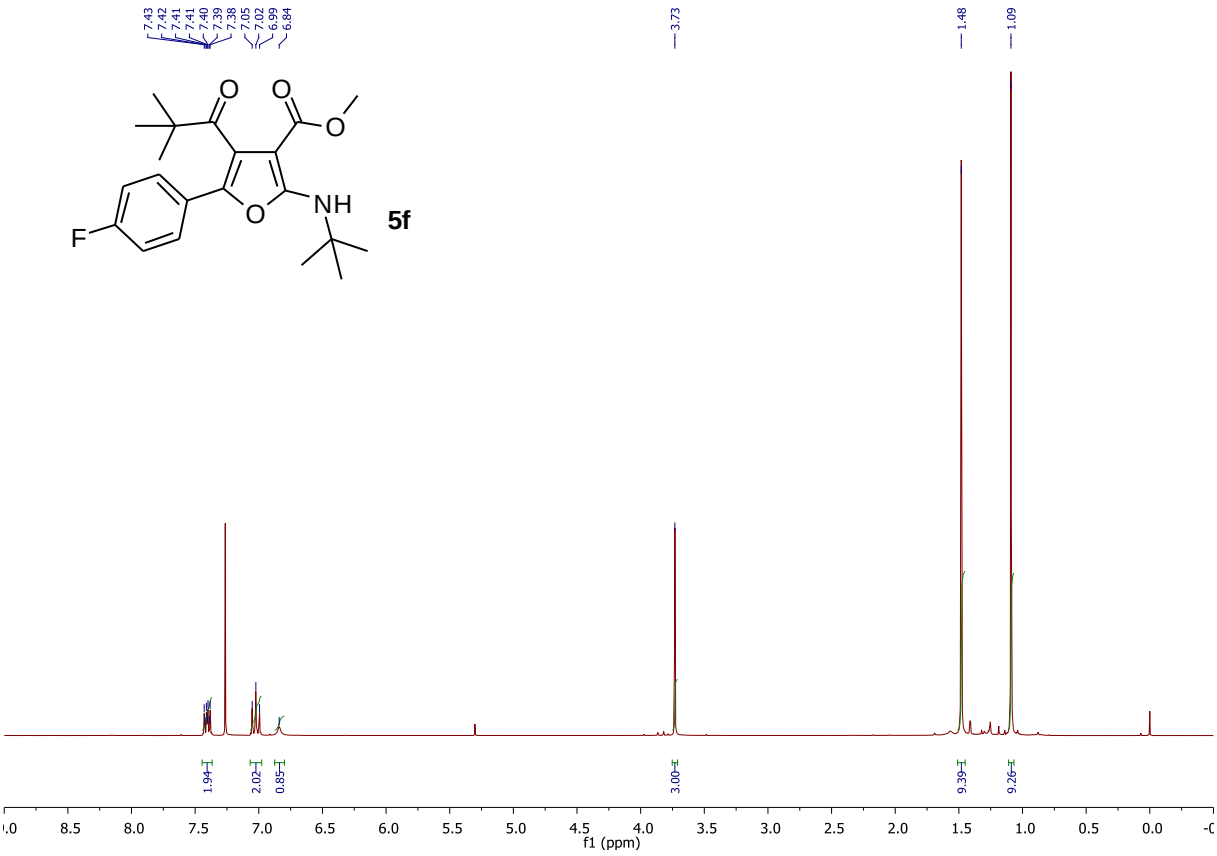
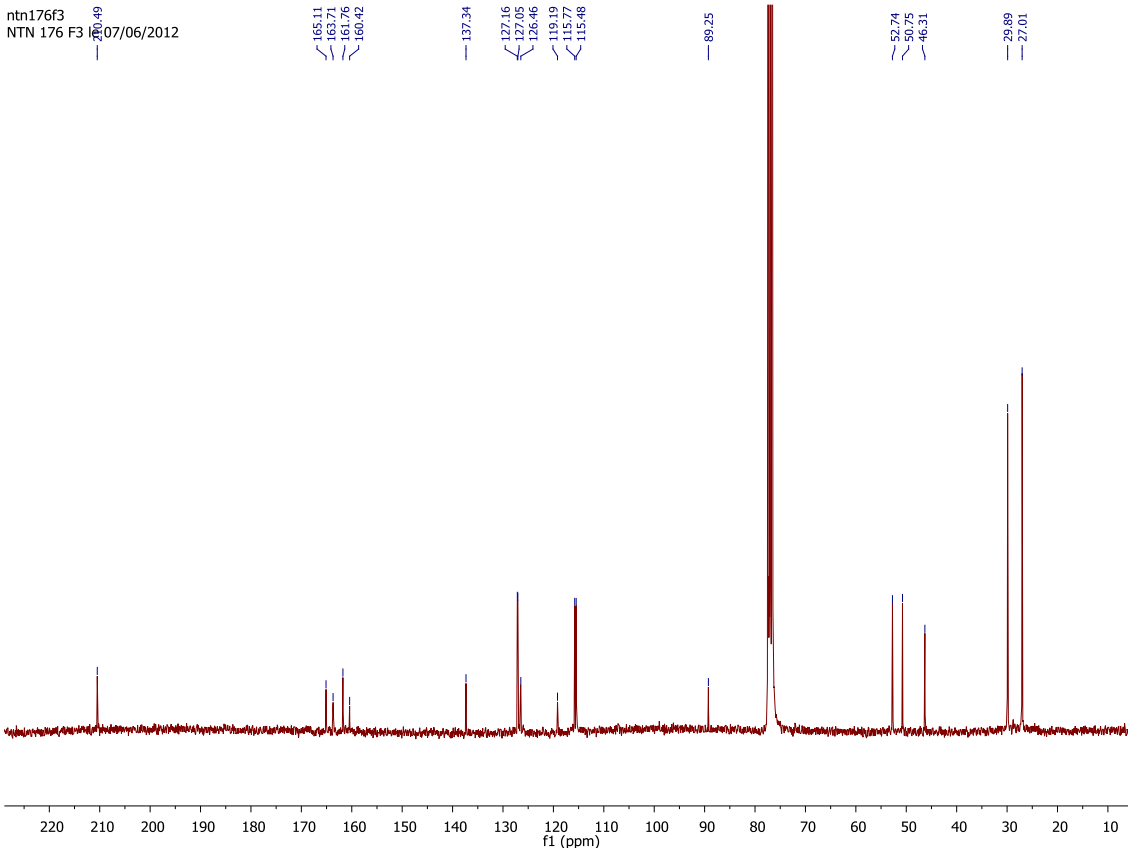
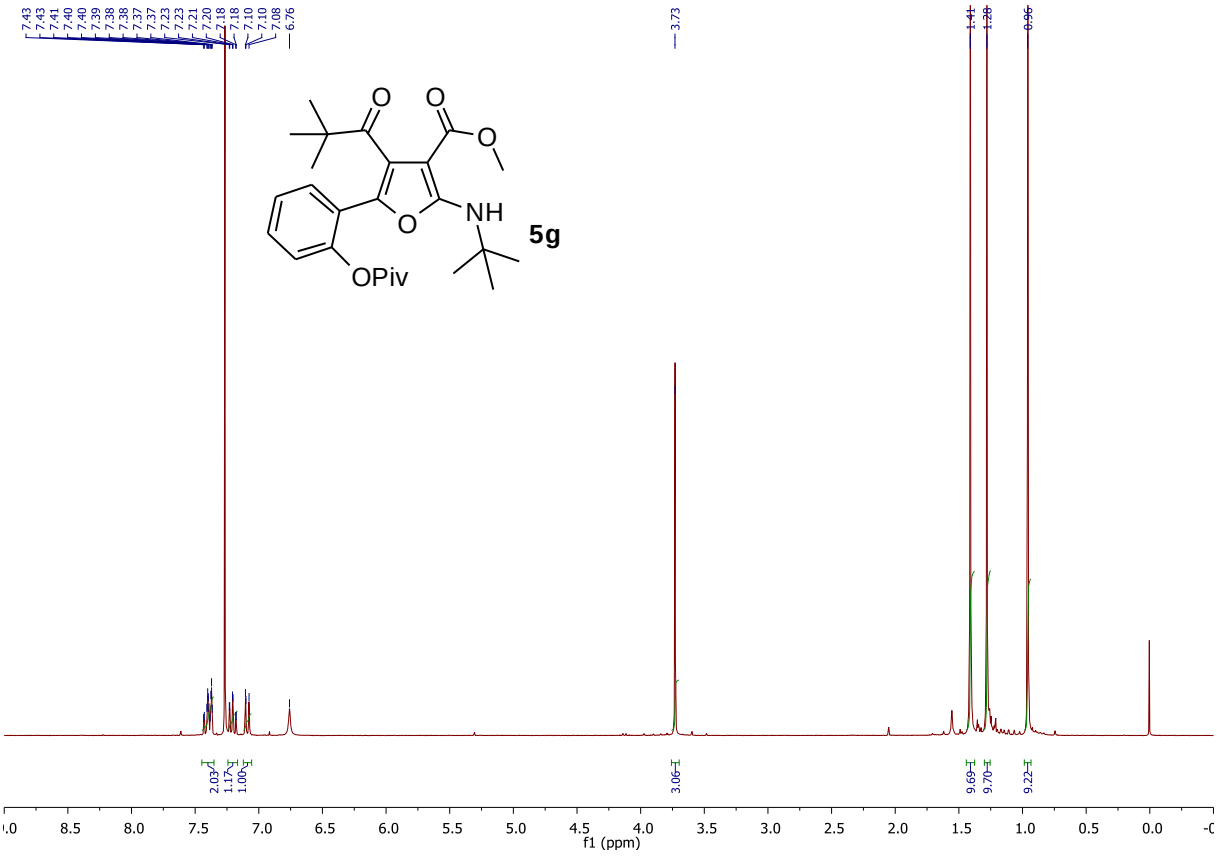
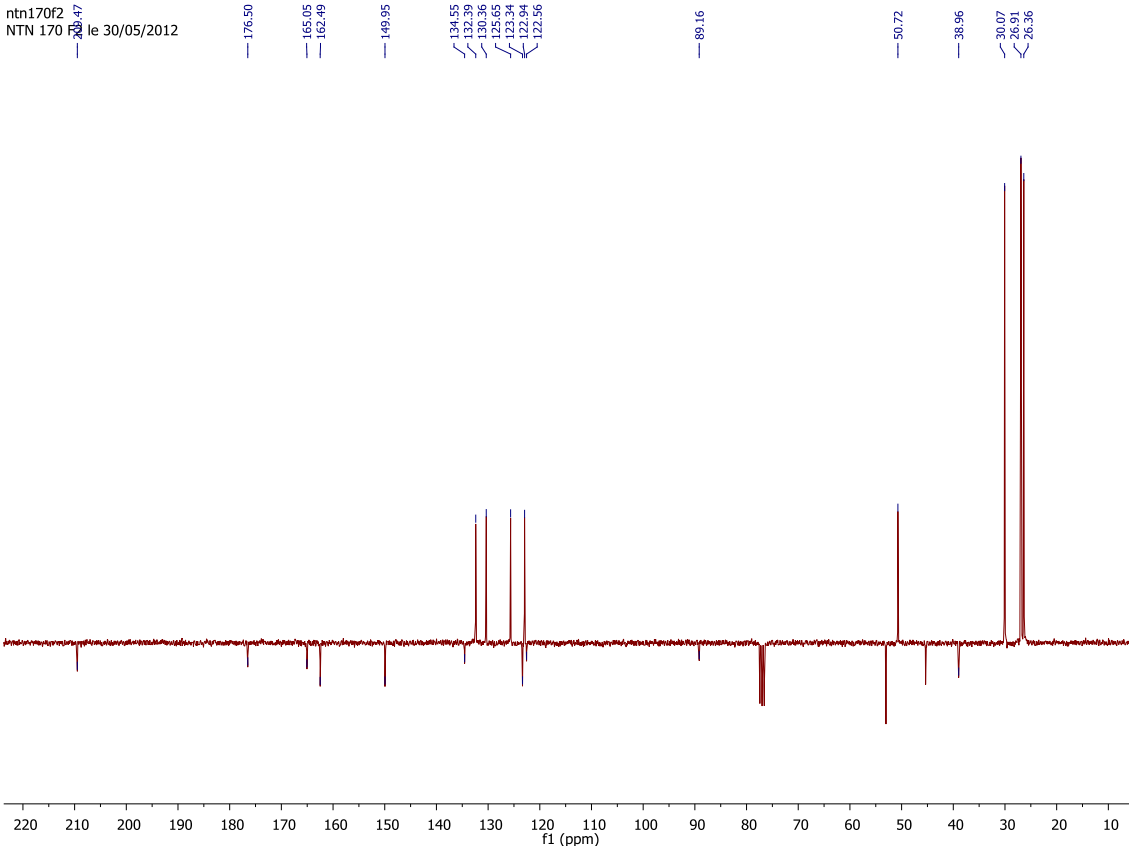
f1 (ppm)

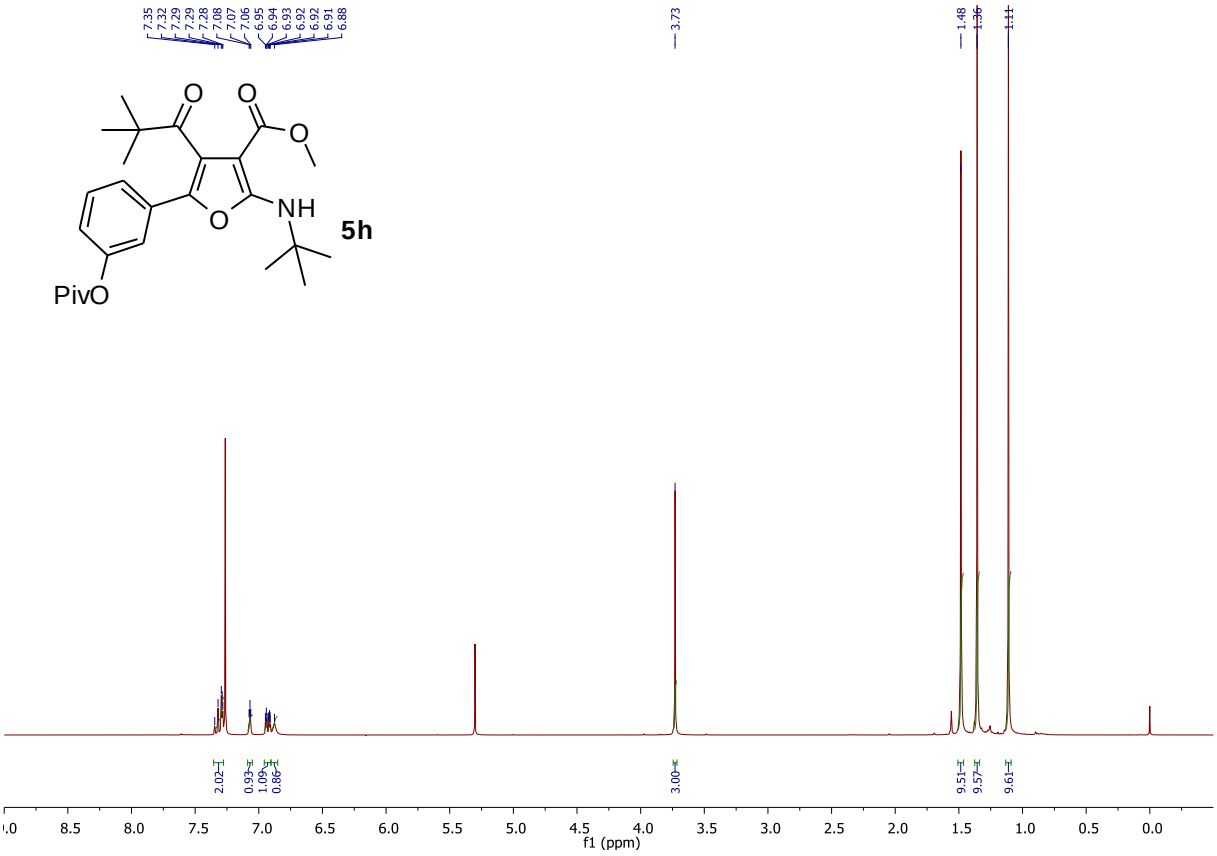

ntn77-p
ntn77-p
210.79
165.34
161.89
138.61
137.54
129.34
127.57
125.38
65.68
52.81
50.81
46.44
30.02
27.24
21.37
f1 (ppm)

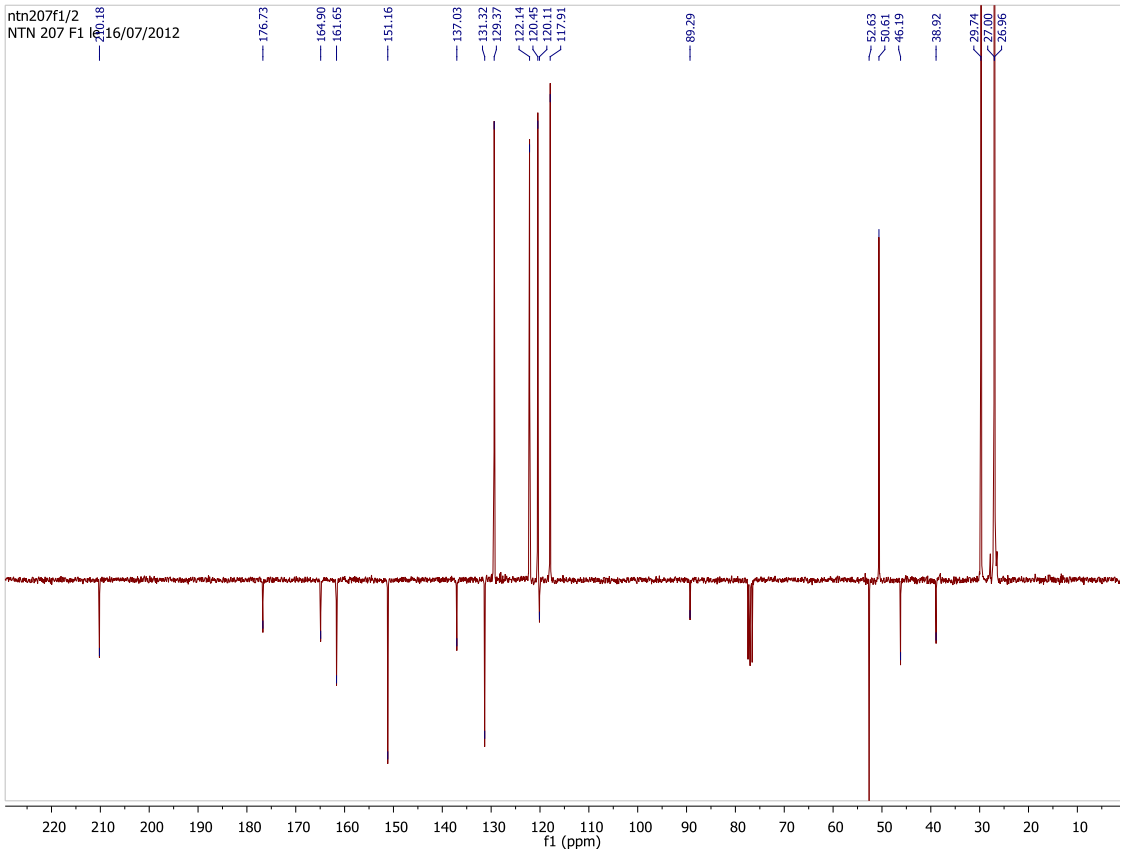

7.43
7.42
7.41
7.41
7.40
7.39
7.38
7.05
7.02
6.99
6.84
3.73
1.48
1.09
O
O
O
NH
O
F
5f
1.94
2.02
0.85
3.00
9.39
9.26
f1 (ppm)

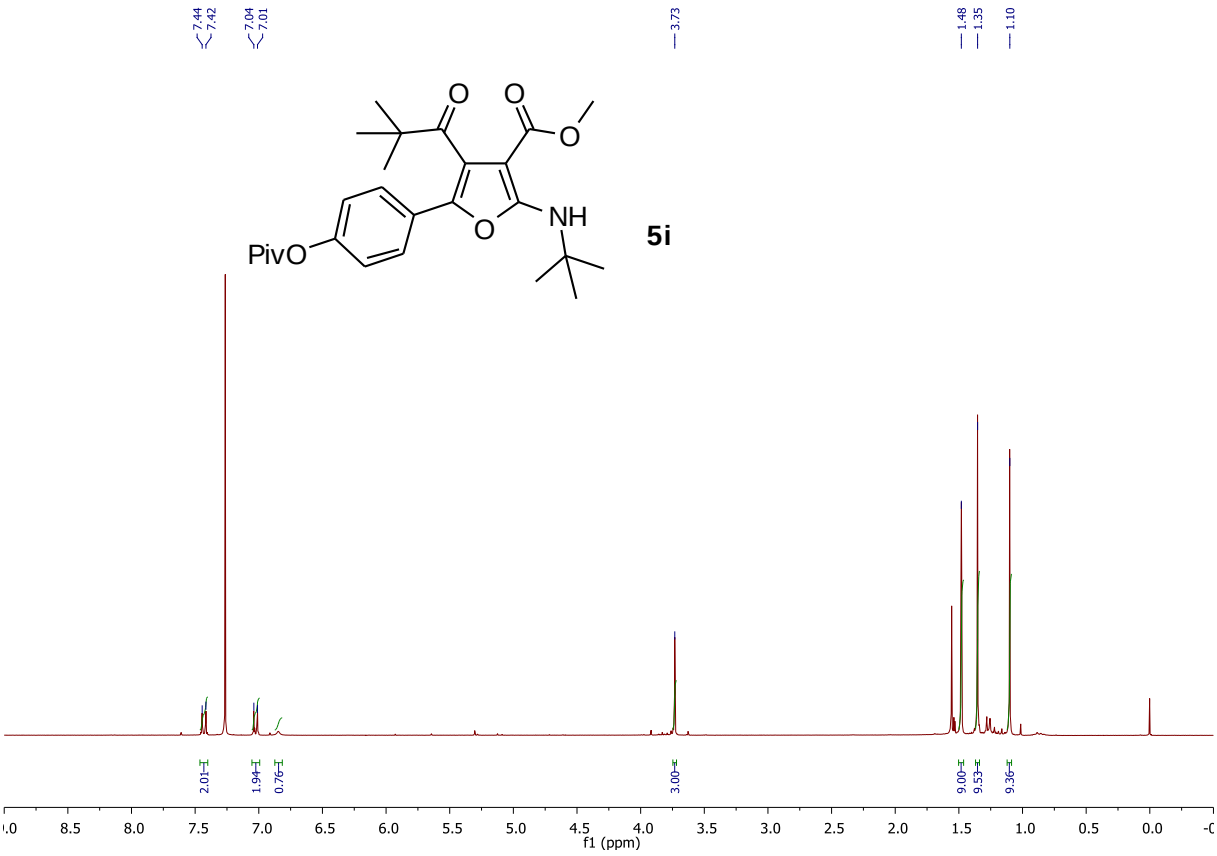

ntn176f3
NTN 176 F3 I 07/06/2012
200.49
165.11
163.71
161.76
160.42
137.34
127.16
127.05
126.46
119.19
115.77
115.48
89.25
52.74
50.75
46.31
29.89
27.01
f1 (ppm)

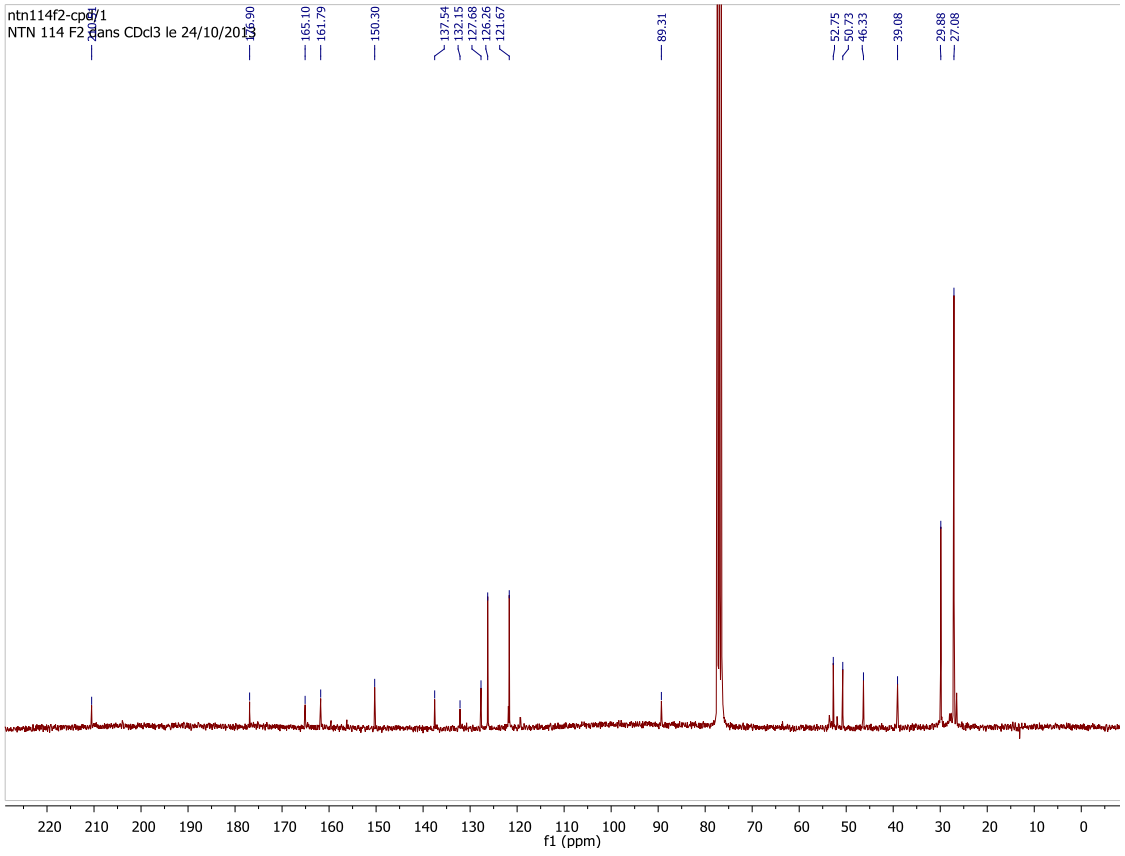

7.43
7.43
7.41
7.40
7.40
7.39
7.38
7.38
7.37
7.37
7.23
7.21
7.20
7.18
7.18
7.10
7.10
7.08
6.76
3.73
1.41
1.39
0.96
O
O
O
NH
O
OPiv
5g
2.03
1.17
1.00
3.06
9.69
9.70
9.22
f1 (ppm)

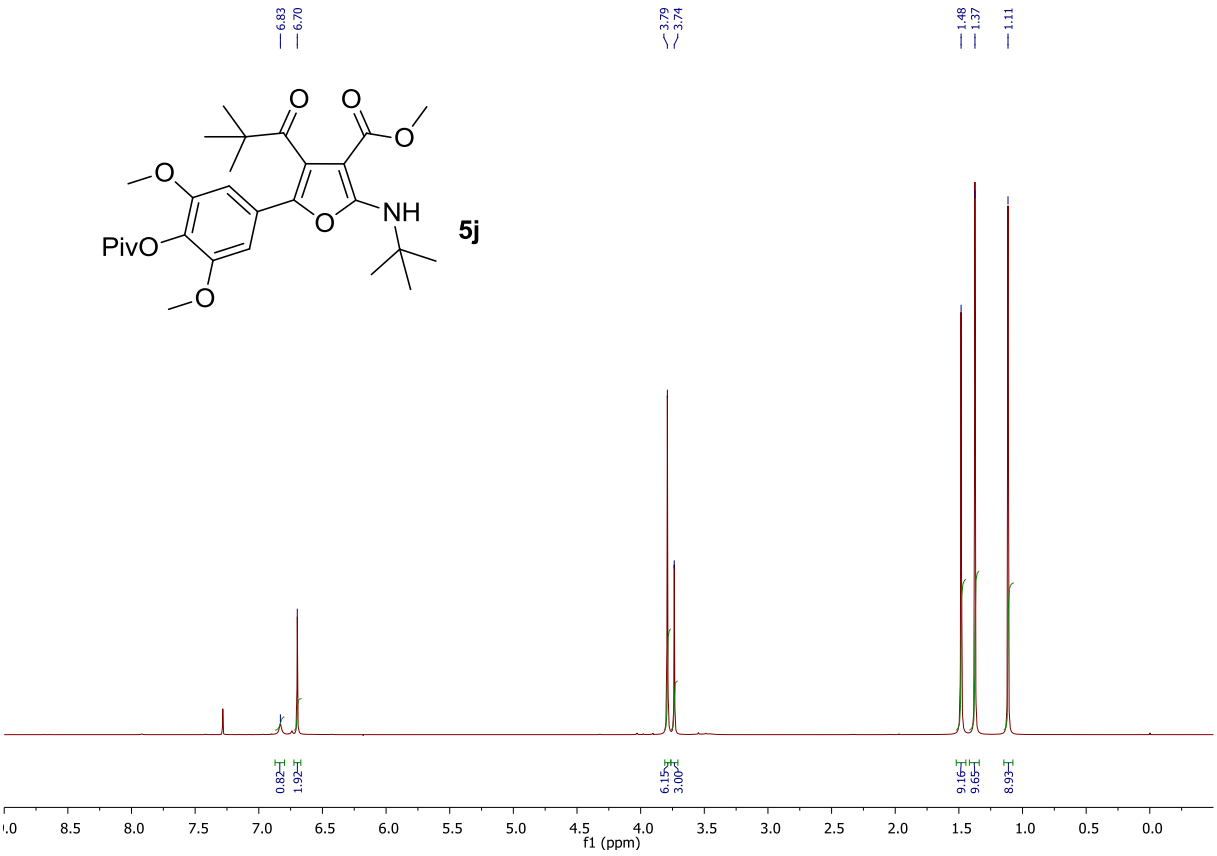

ntn170f2
NTN 170 File 30/05/2012
176.50
165.05
162.49
149.95
134.55
132.39
130.36
125.65
123.34
122.94
122.56
89.16
50.72
38.96
30.07
26.91
26.36
f1 (ppm)

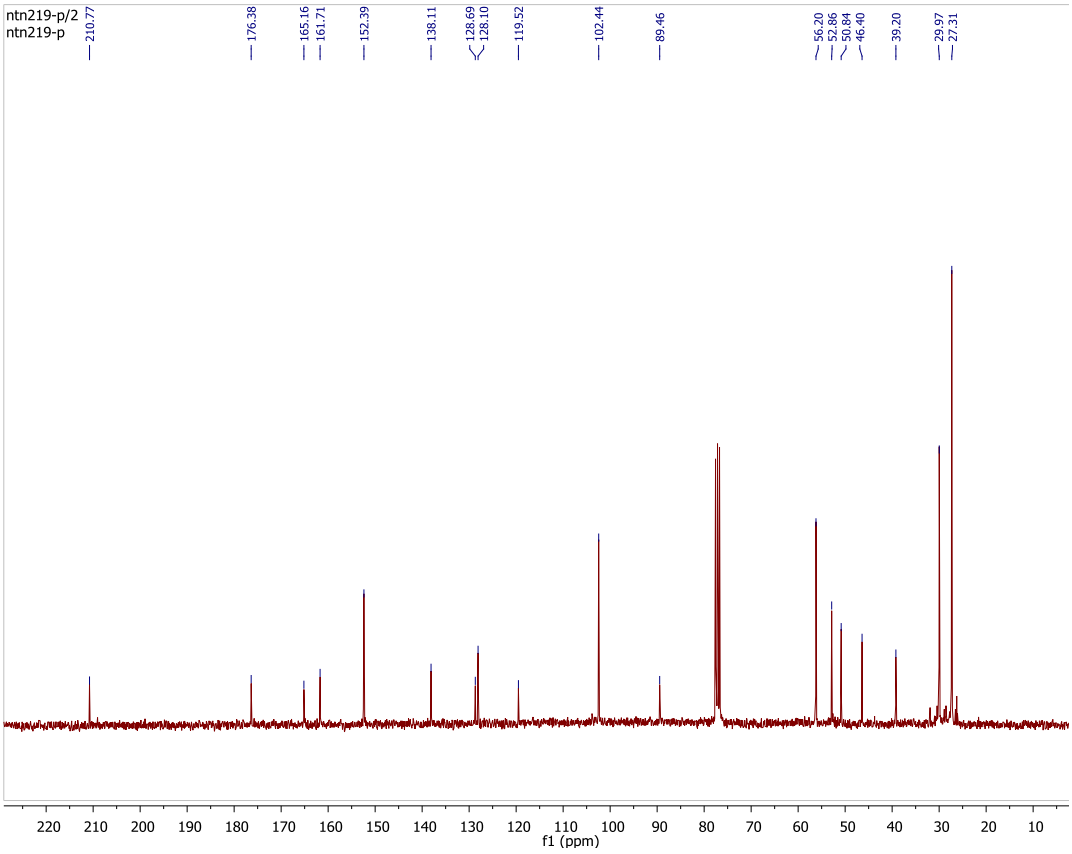

7.35
7.32
7.29
7.28
7.08
7.07
7.06
6.95
6.94
6.93
6.92
6.92
6.91
6.88
3.73
1.48
1.36
1.11
O
O
O
NH
O
PivO
5h
2.02
0.93
1.09
0.86
3.00
9.51
9.57
9.61
f1 (ppm)

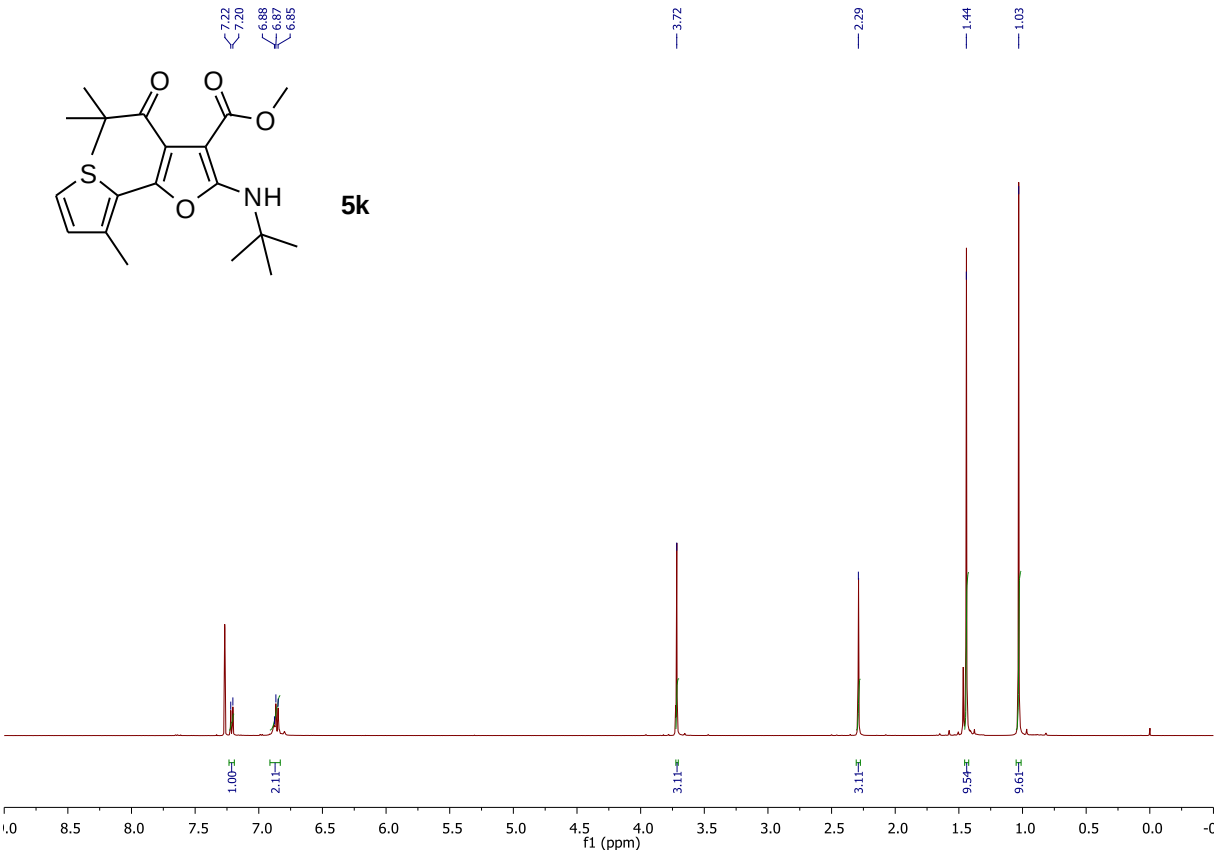

ntn207f1/2
NTN 207 F1 16/07/2012
176.73
164.90
161.65
151.16
137.03
131.32
129.37
122.14
120.45
120.11
117.91
89.29
52.63
50.61
46.19
38.92
29.74
27.00
26.96
f1 (ppm)


7.44
7.42
7.04
7.01
3.73
1.48
1.35
1.10
O
O
O
NH
O
PivO
5i
2.01
1.94
0.76
3.00
9.00
9.53
9.36
f1 (ppm)

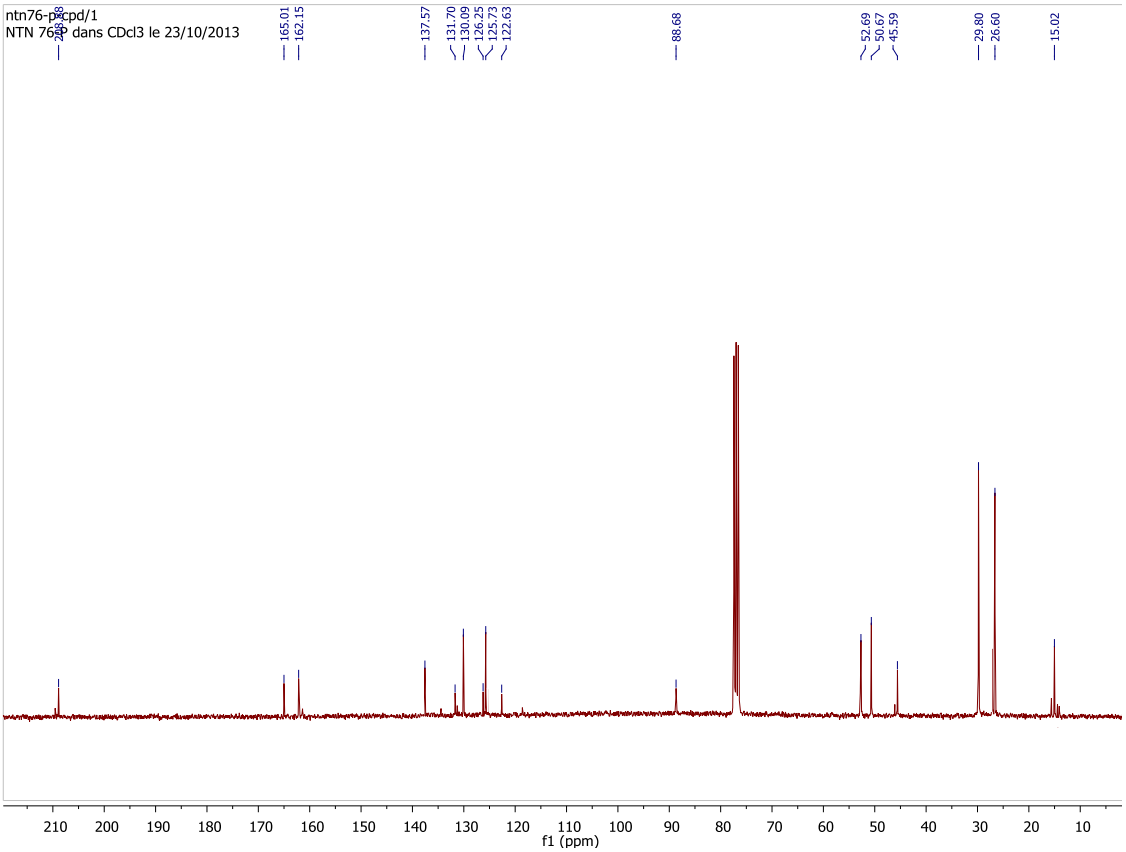

ntn114f2-cpd/1
NTN 114 F2 dans CDcl3 le 24/10/2012
176.90
165.10
161.79
150.30
137.54
132.15
127.68
126.26
121.67
89.31
52.75
50.73
46.33
39.08
29.88
27.08
f1 (ppm)

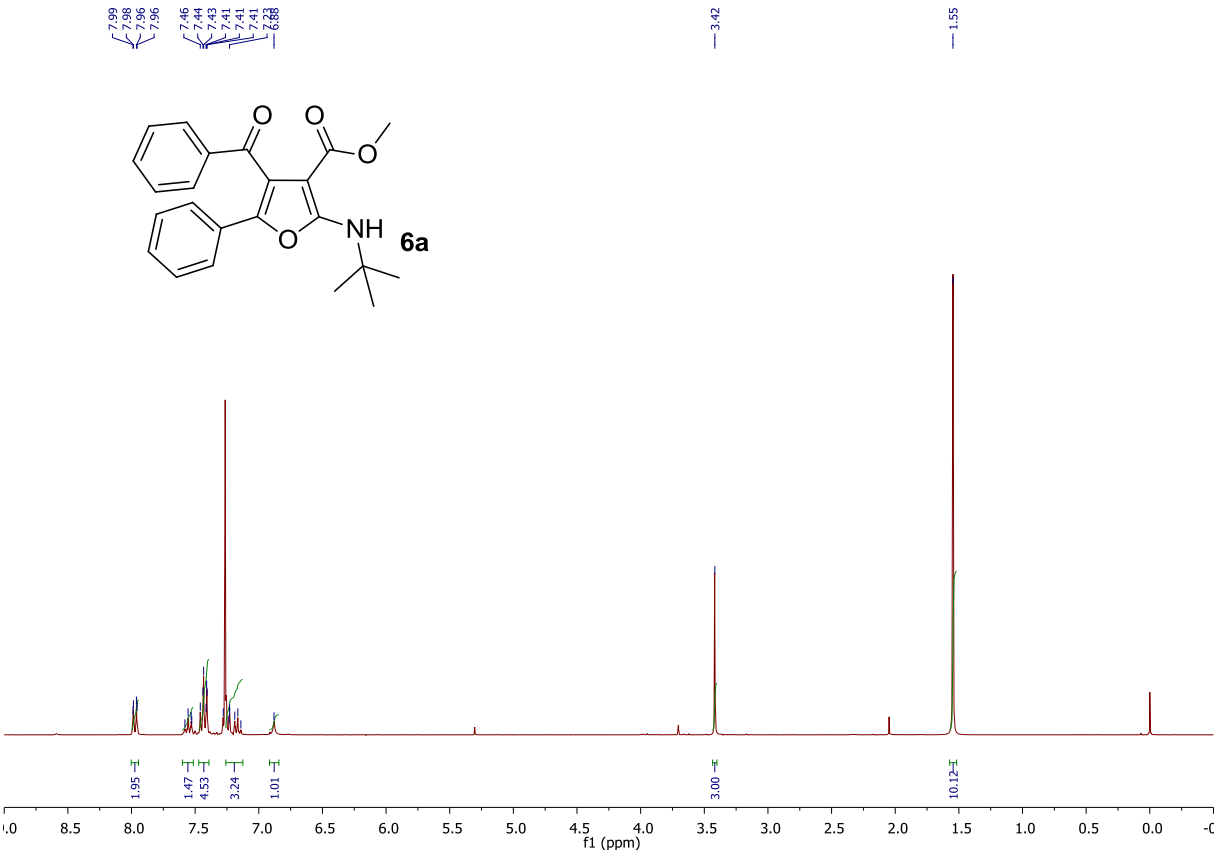

6.83
6.70
3.79
3.74
1.48
1.37
1.11
O
O
O
O
NH
PivO
O
5j
0.82
1.92
6.15
3.00
9.16
9.65
8.93
f1 (ppm)

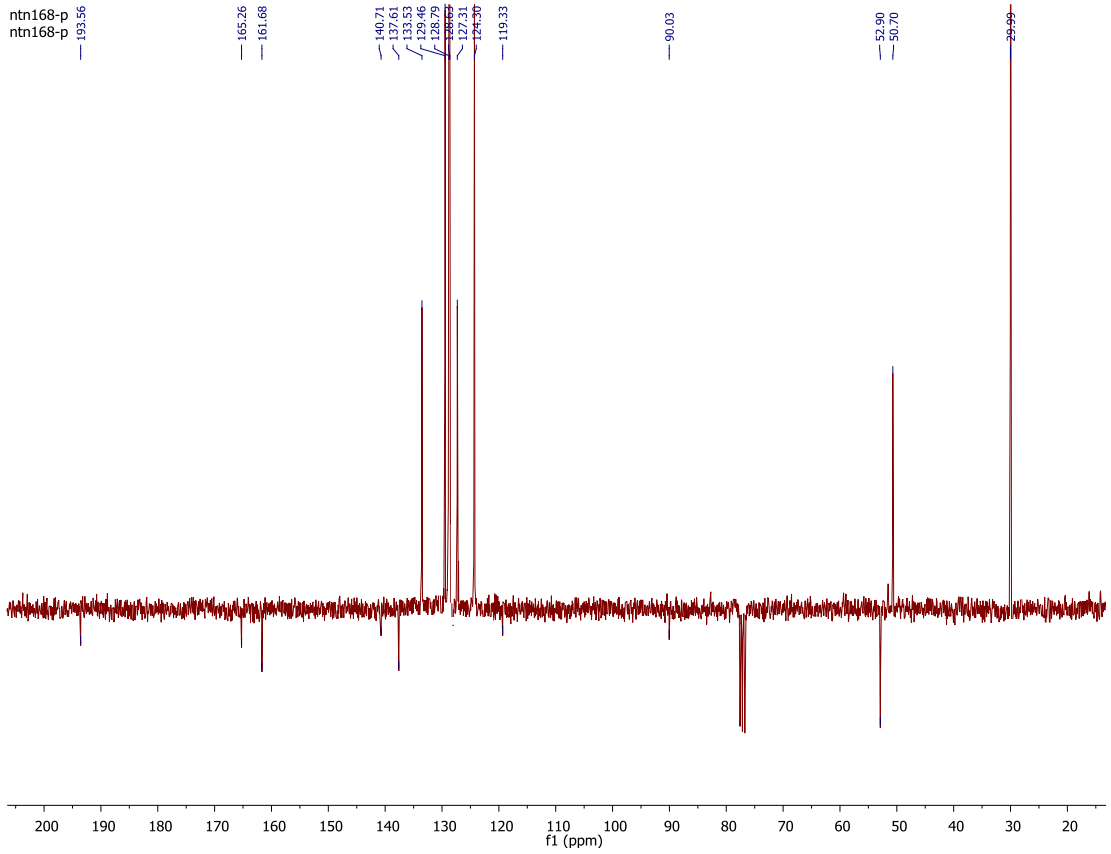

ntn219-p/2
ntn219-p
210.77
176.38
165.16
161.71
152.39
138.11
128.69
128.10
119.52
102.44
89.46
56.20
52.86
50.84
46.40
39.20
29.97
27.31
f1 (ppm)

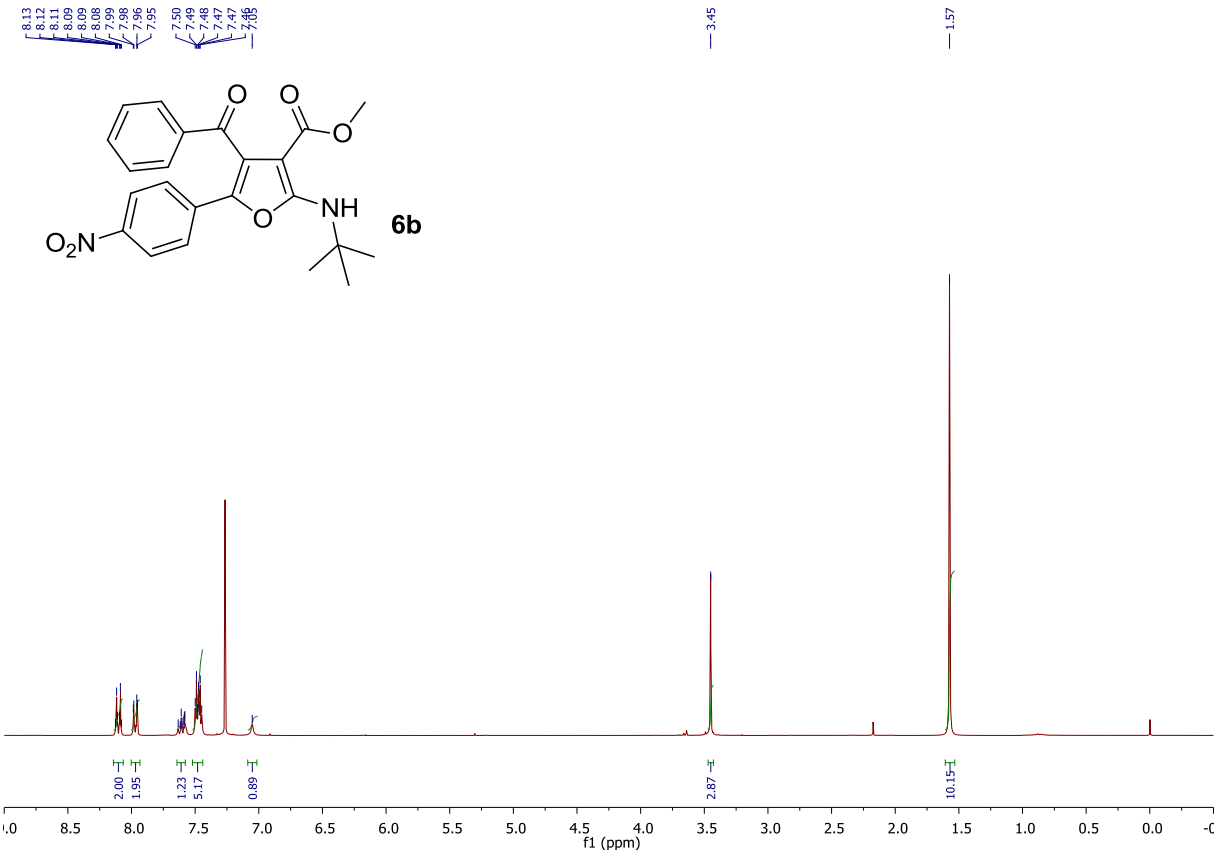

7.22
7.20
6.88
6.87
6.85
3.72
2.29
1.44
1.03
O
O
O
S
O
NH
1.00
2.11
3.11
3.11
9.54
9.61
f1 (ppm)

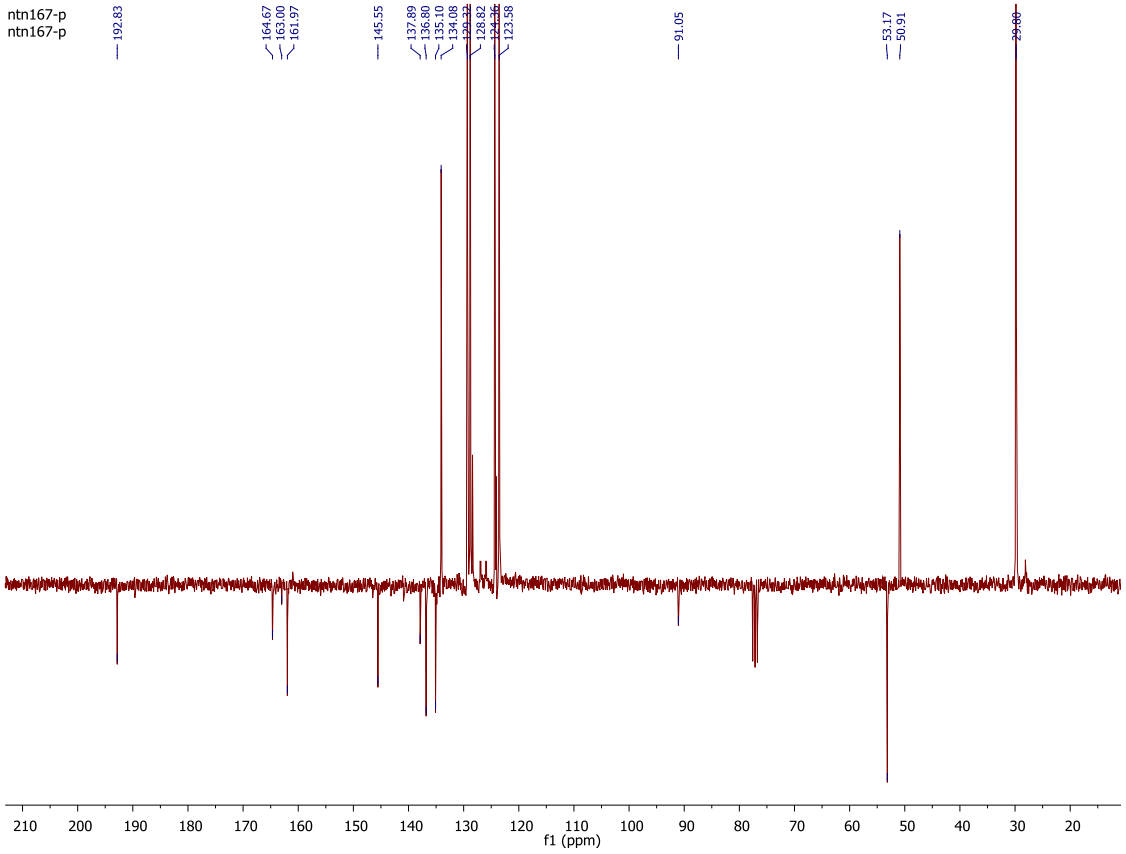
5k

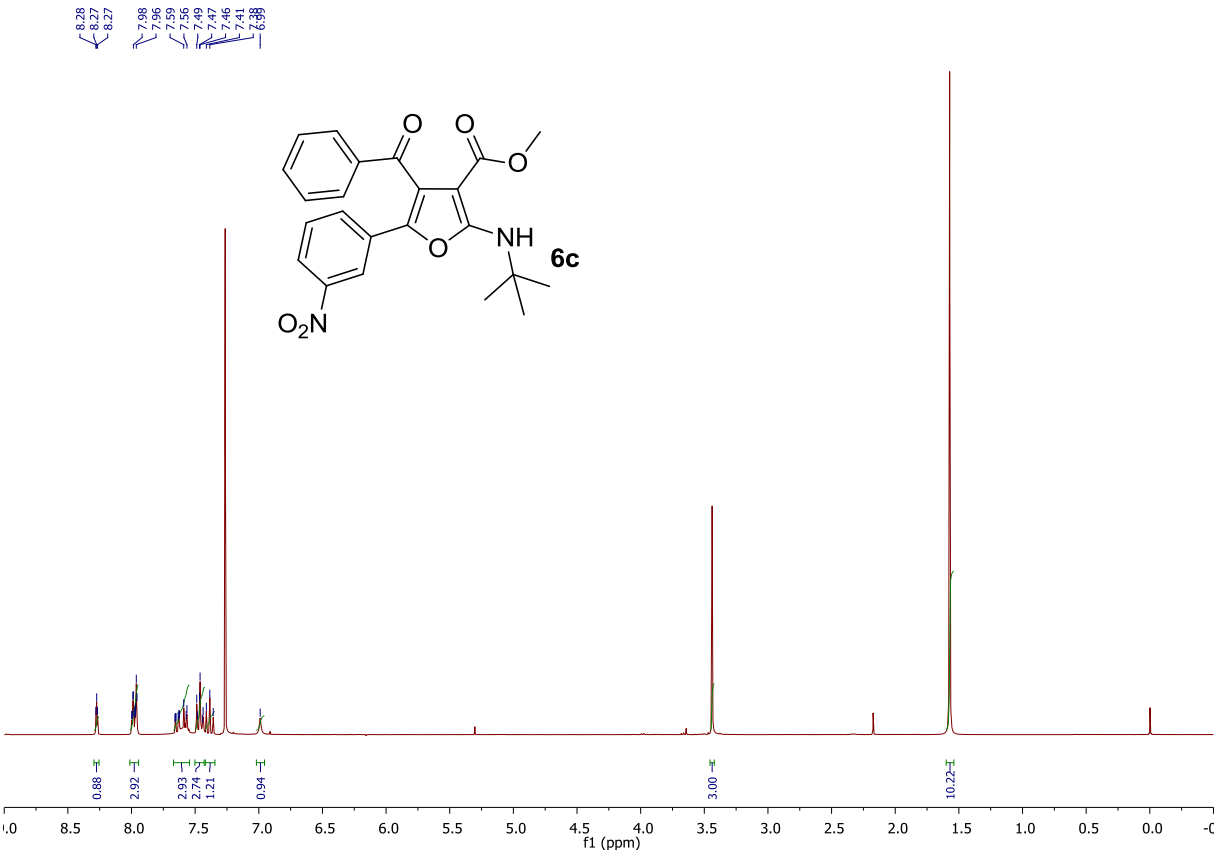

ntn76-Dccpd/1
NTN 76 P dans CDcl3 le 23/10/2013
165.01
162.15
137.57
131.70
130.09
126.25
125.73
122.63
88.68
52.69
50.67
45.59
29.80
26.60
15.02
f1 (ppm)

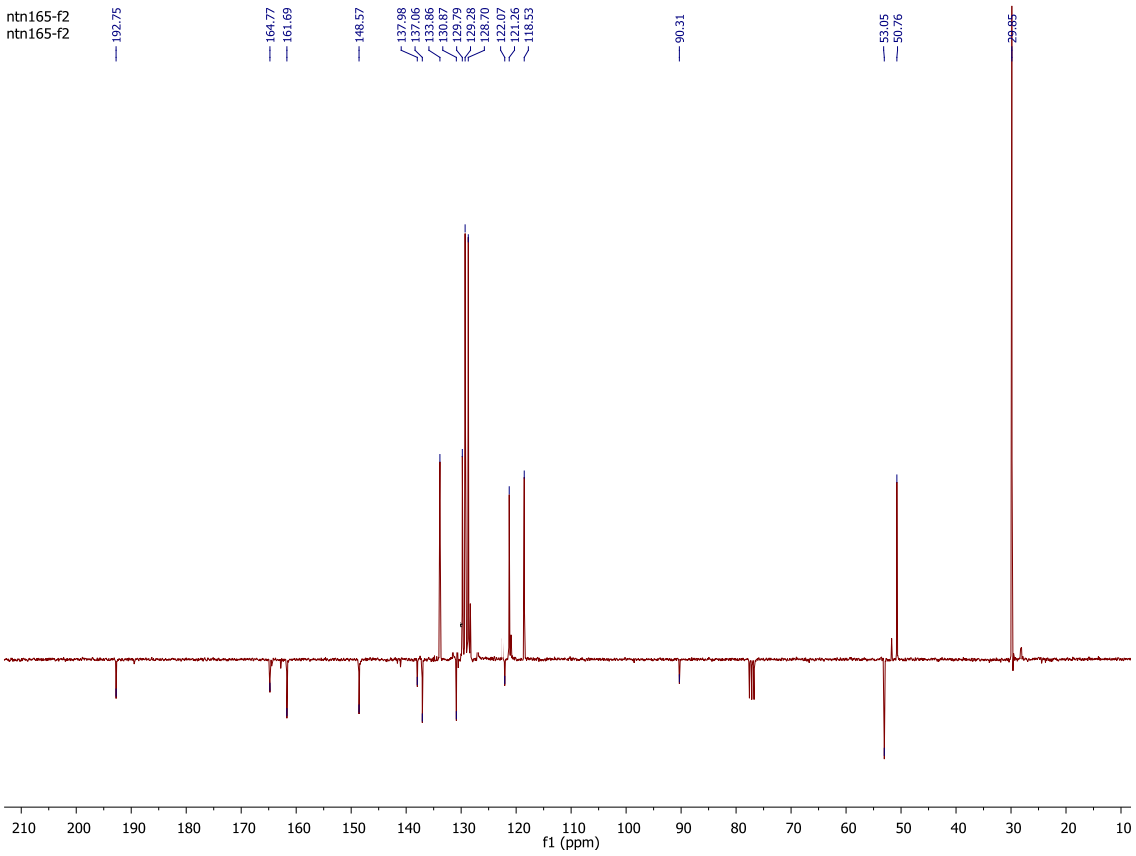

7.99
7.98
7.96
7.96
7.46
7.44
7.43
7.41
7.41
7.41
6.88
3.42
1.55
O
O
O
NH
O
6a
1.95
1.47
4.53
3.24
1.01
3.00
10.12
f1 (ppm)

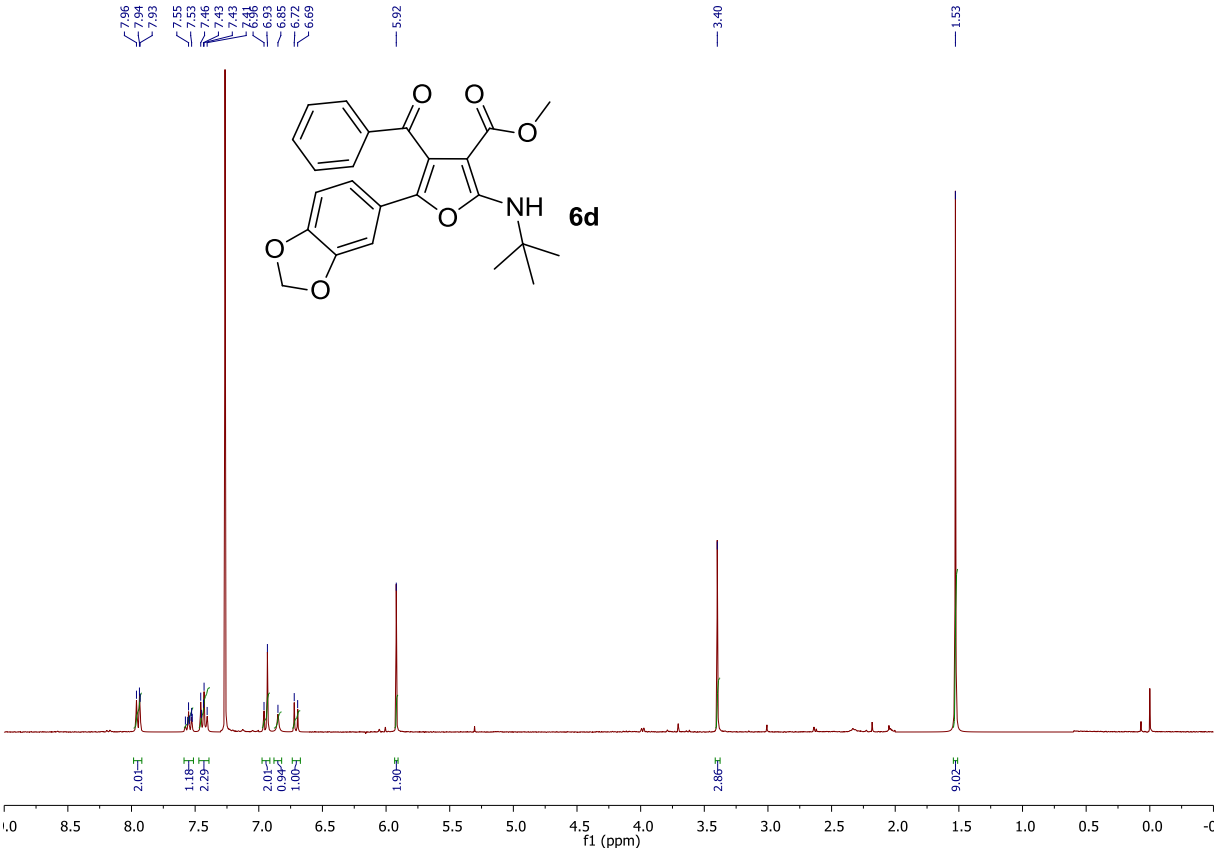

ntn168-p
ntn168-p
193.56
165.26
161.68
140.71
137.61
133.53
129.46
128.79
127.31
124.30
119.33
90.03
52.90
50.70
29.99
f1 (ppm)

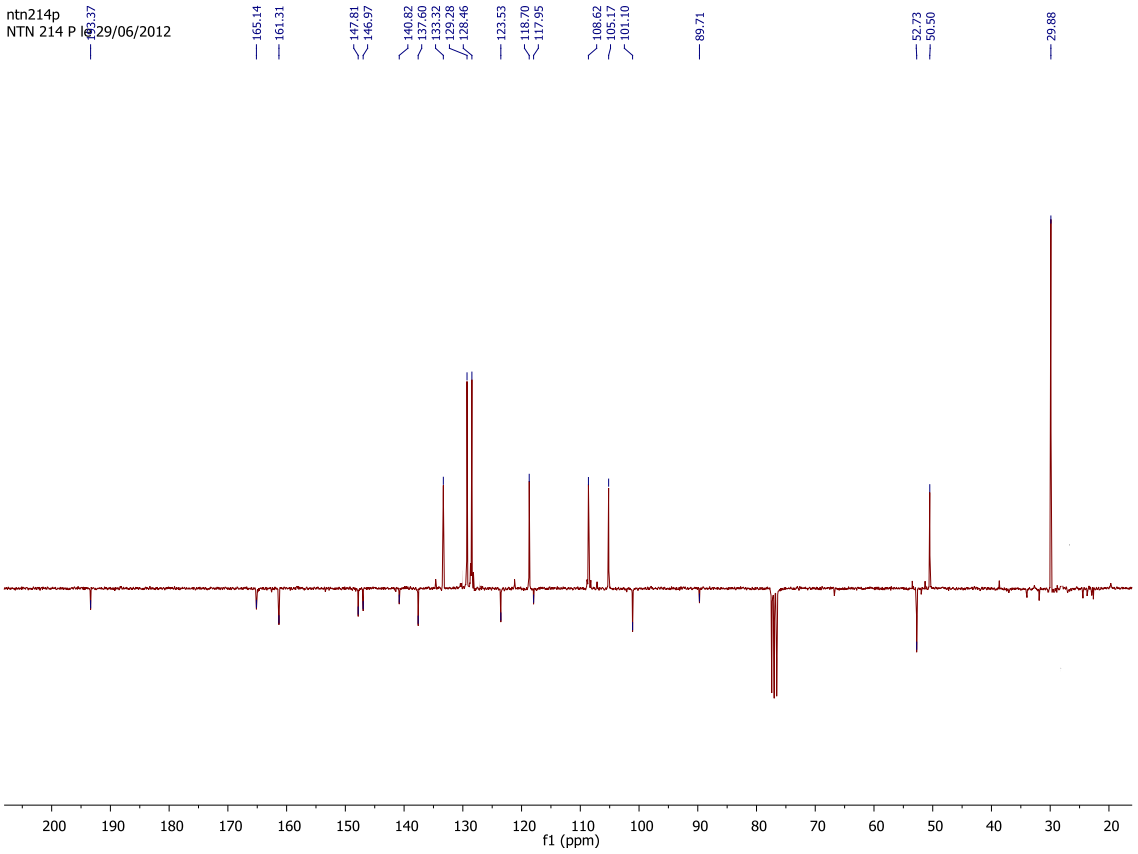

8.13
8.12
8.11
8.09
8.09
8.08
7.99
7.98
7.96
7.95
7.50
7.49
7.48
7.47
7.47
7.46
7.45
3.45
1.57
O
O
O
NH
O
O_2N
6b
2.00
1.95
1.23
5.17
0.89
2.87
10.15
f1 (ppm)

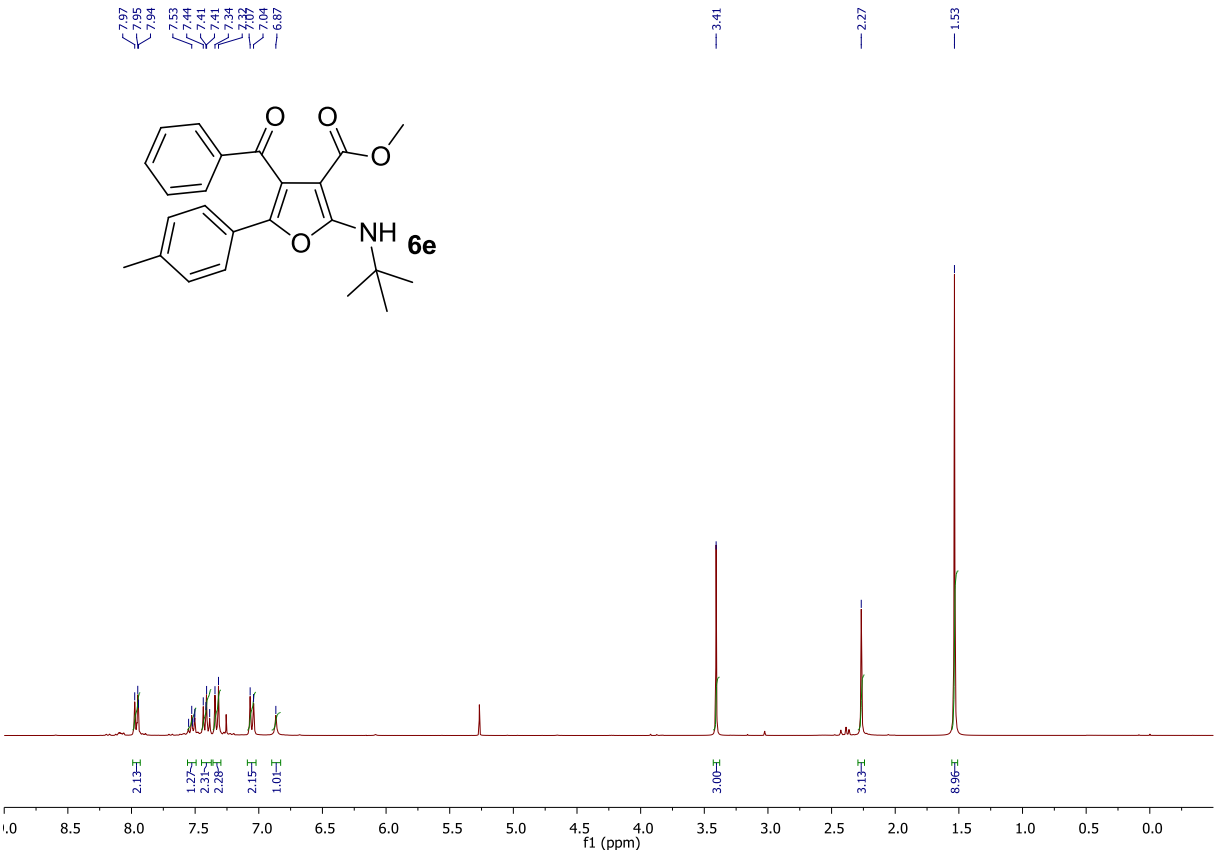

ntn167-p
ntn167-p
192.83
164.67
163.00
161.97
145.55
137.89
136.80
135.10
134.08
91.05
53.17
50.91
29.80
123.58
f1 (ppm)

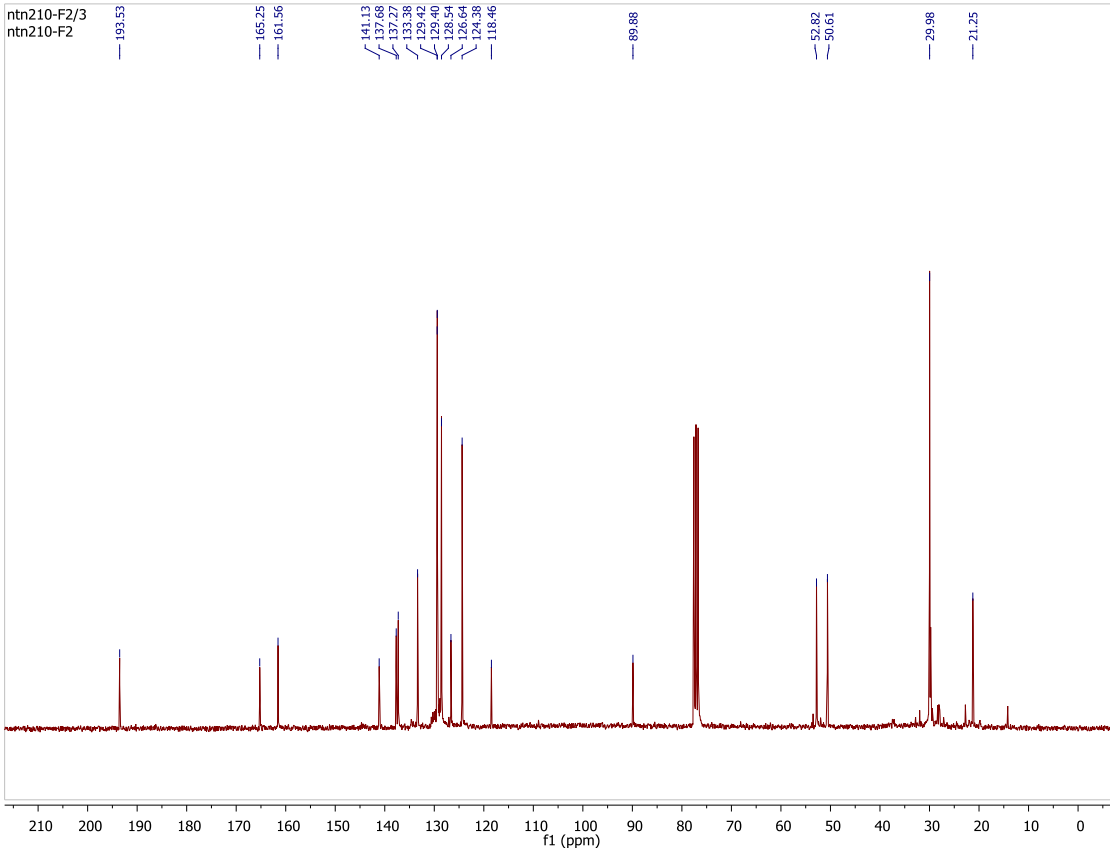

8.28
8.27
8.27
7.98
7.96
7.59
7.56
7.49
7.47
7.46
7.41
7.38
6.99
O
O
O
NH
O
6c
O2N
0.88
2.92
2.93
2.74
1.21
0.94
3.00
10.22
f1 (ppm)

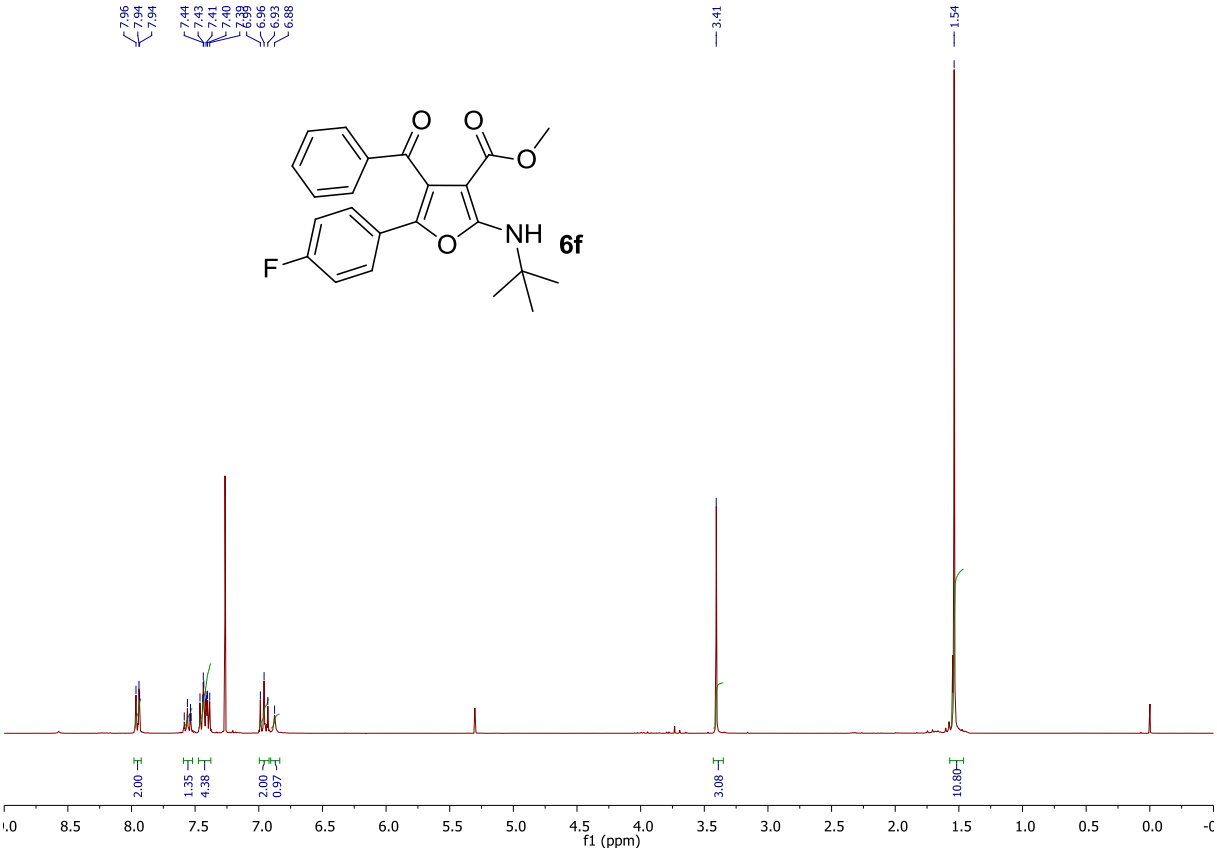

ntn165-f2
ntn165-f2
192.75
164.77
161.69
148.57
137.98
137.06
133.86
130.87
129.79
129.28
128.70
122.07
121.26
118.53
90.31
53.05
50.76
29.85
f1 (ppm)

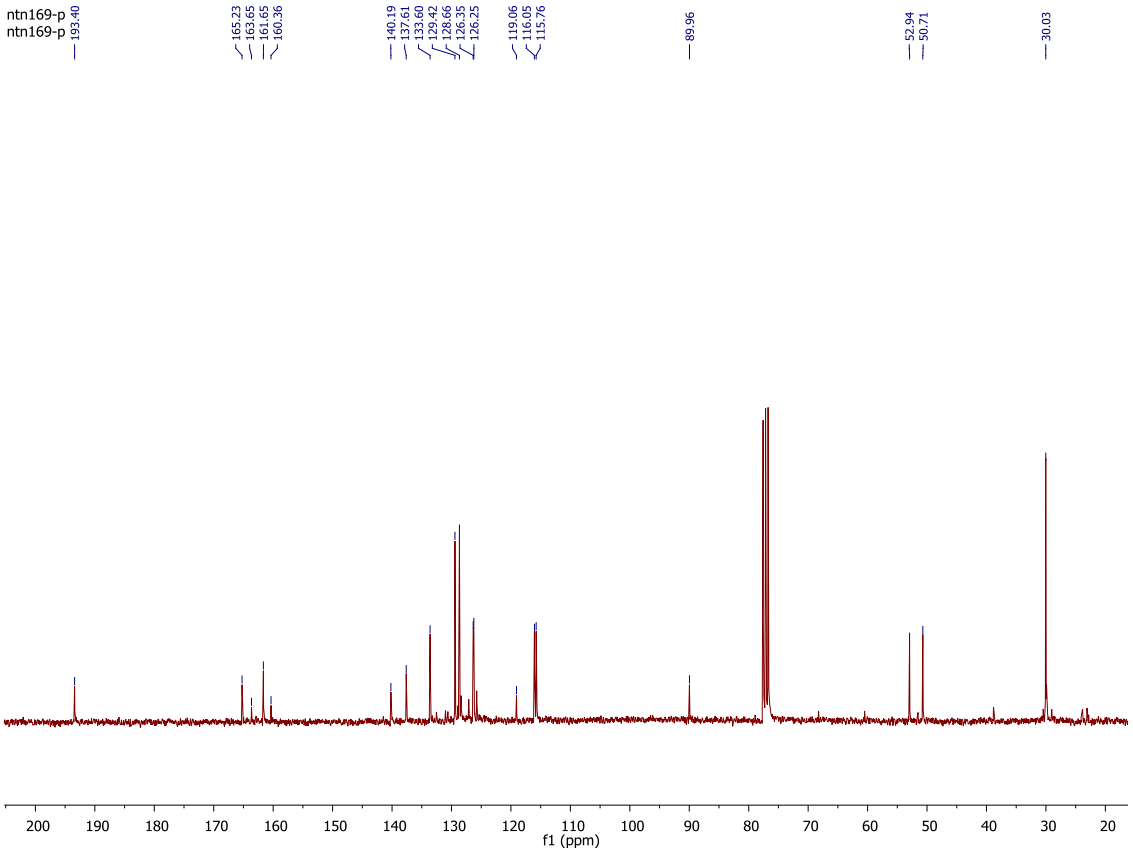

7.96
7.94
7.93
7.55
7.53
7.46
7.43
7.41
6.96
6.93
6.85
6.72
6.69
5.92
3.40
1.53
O
O
O
NH
O
O
O
6d
2.01
1.18
2.29
2.01
0.94
1.00
1.90
2.86
9.02
f1 (ppm)

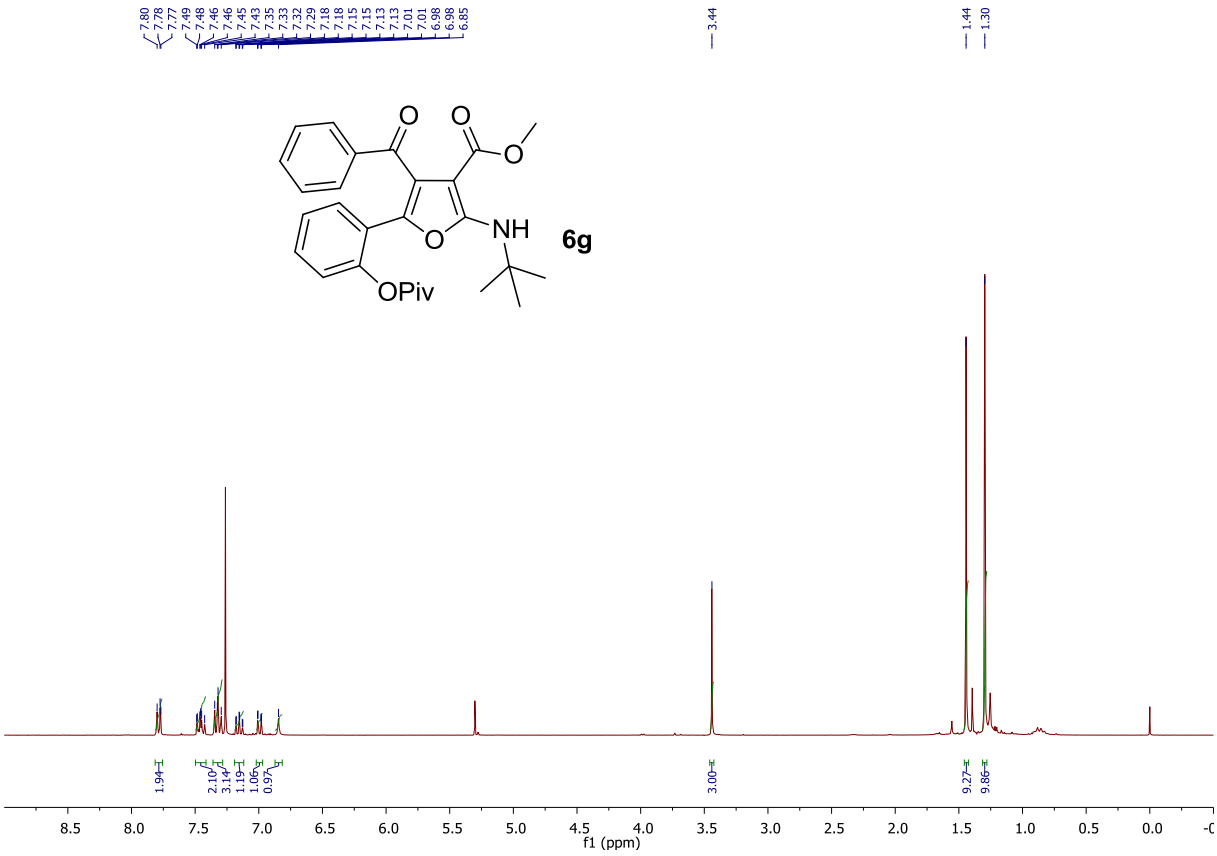

ntn214p
NTN 214 P 1 29/06/2012
165.14
161.31
147.81
146.97
140.82
137.60
133.32
129.28
128.46
123.53
118.70
117.95
108.62
105.17
101.10
89.71
52.73
50.50
29.88
f1 (ppm)

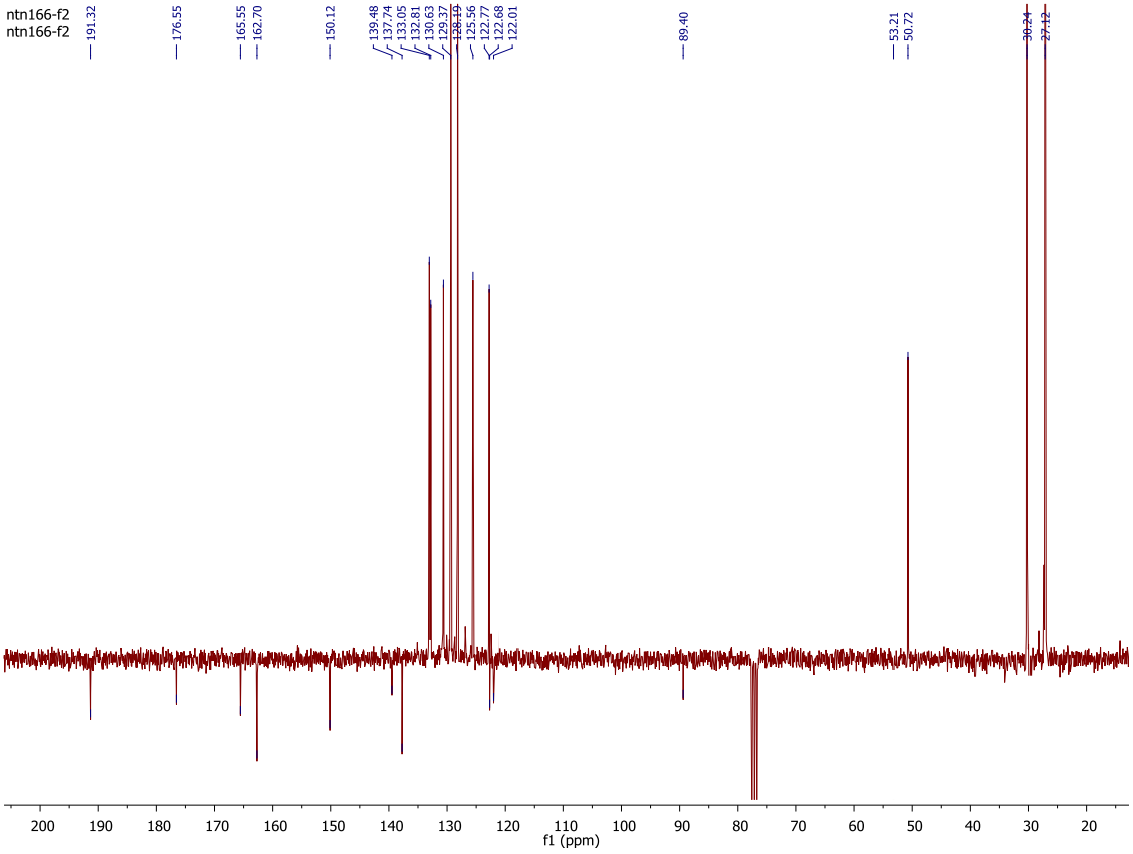

7.97
7.95
7.94
7.53
7.44
7.41
7.41
7.34
7.32
7.07
7.04
6.87
3.41
2.27
1.53
O
O
O
NH
O
6e
2.13
1.27
2.31
2.28
2.15
1.01
3.00
3.13
8.96
f1 (ppm)

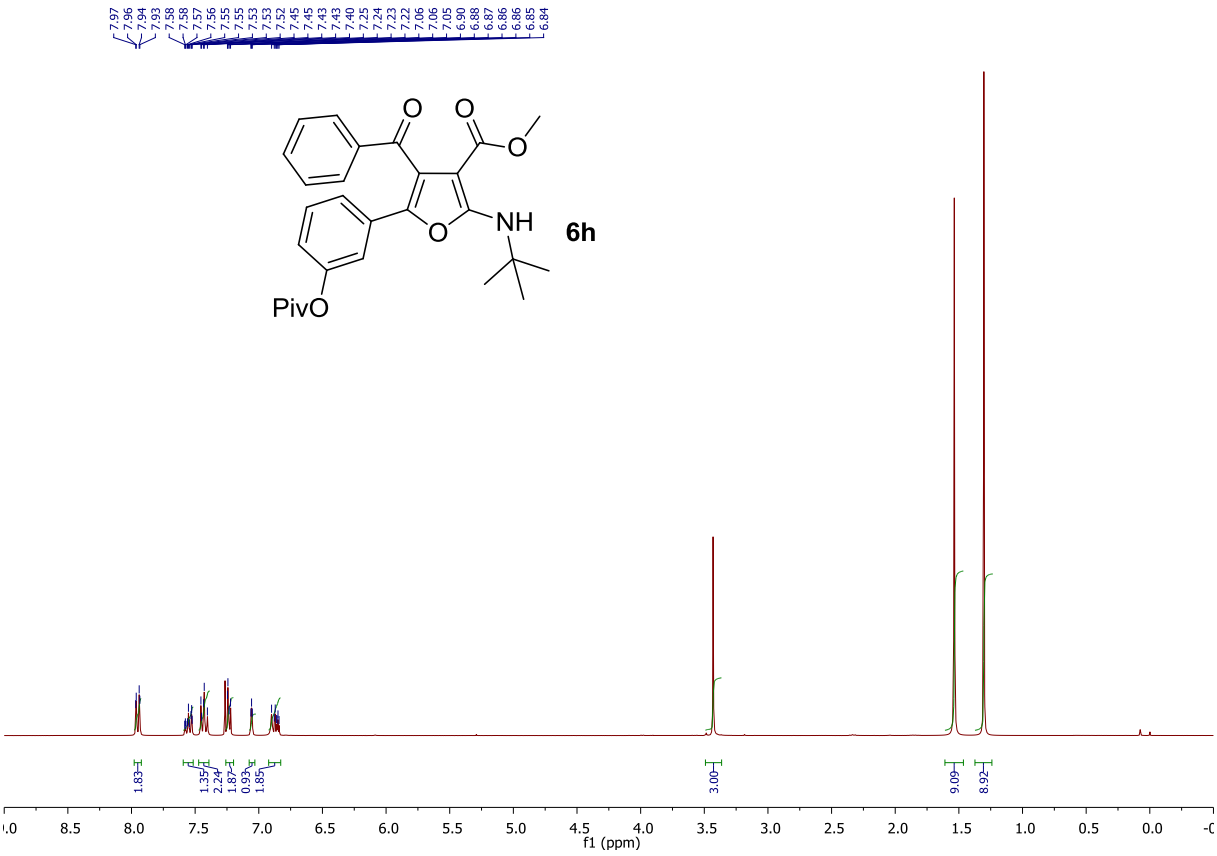

ntn210-F2/3
ntn210-F2
193.53
165.25
161.56
141.13
137.68
137.27
133.38
129.42
129.40
128.54
126.64
124.38
118.46
89.88
52.82
50.61
29.98
21.25
f1 (ppm)

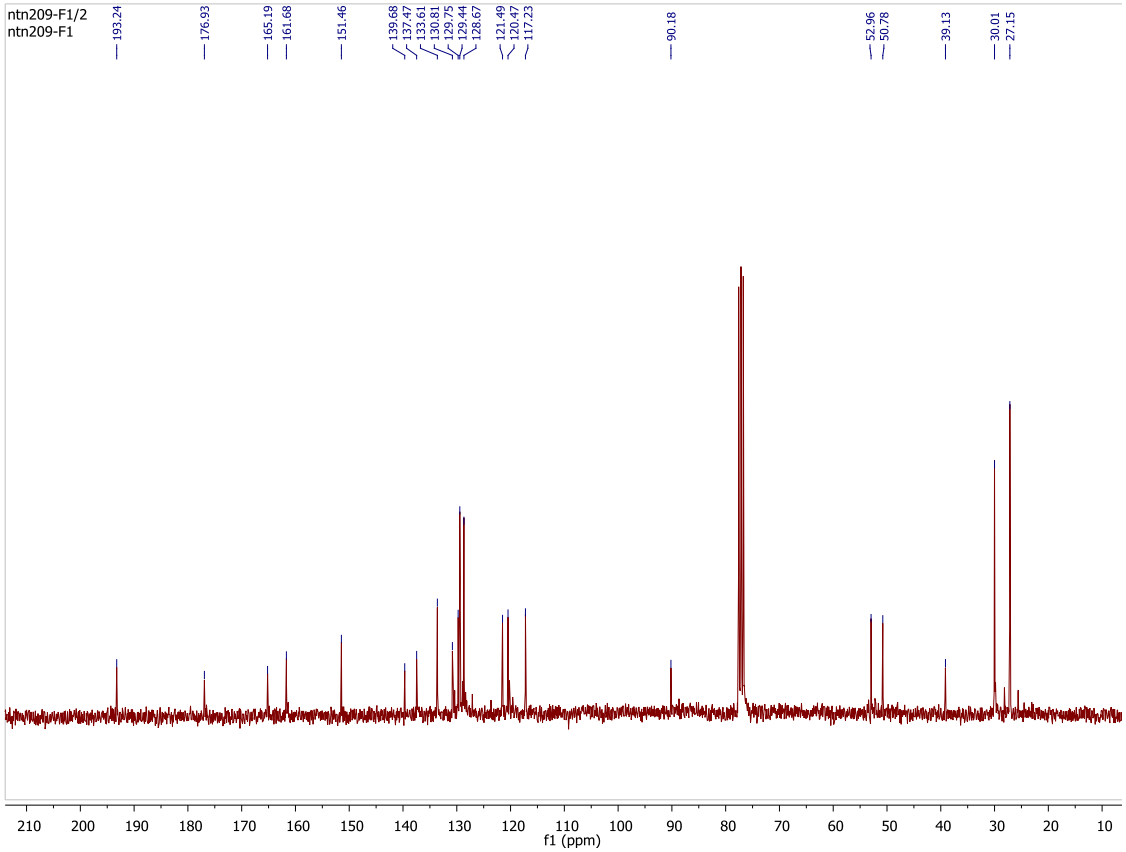

7.96
7.94
7.94
7.44
7.43
7.41
7.40
6.96
6.93
6.88
3.41
1.54
O
O
O
NH
F
6f
2.00
1.35
4.38
2.00
0.97
3.08
10.80
f1 (ppm)

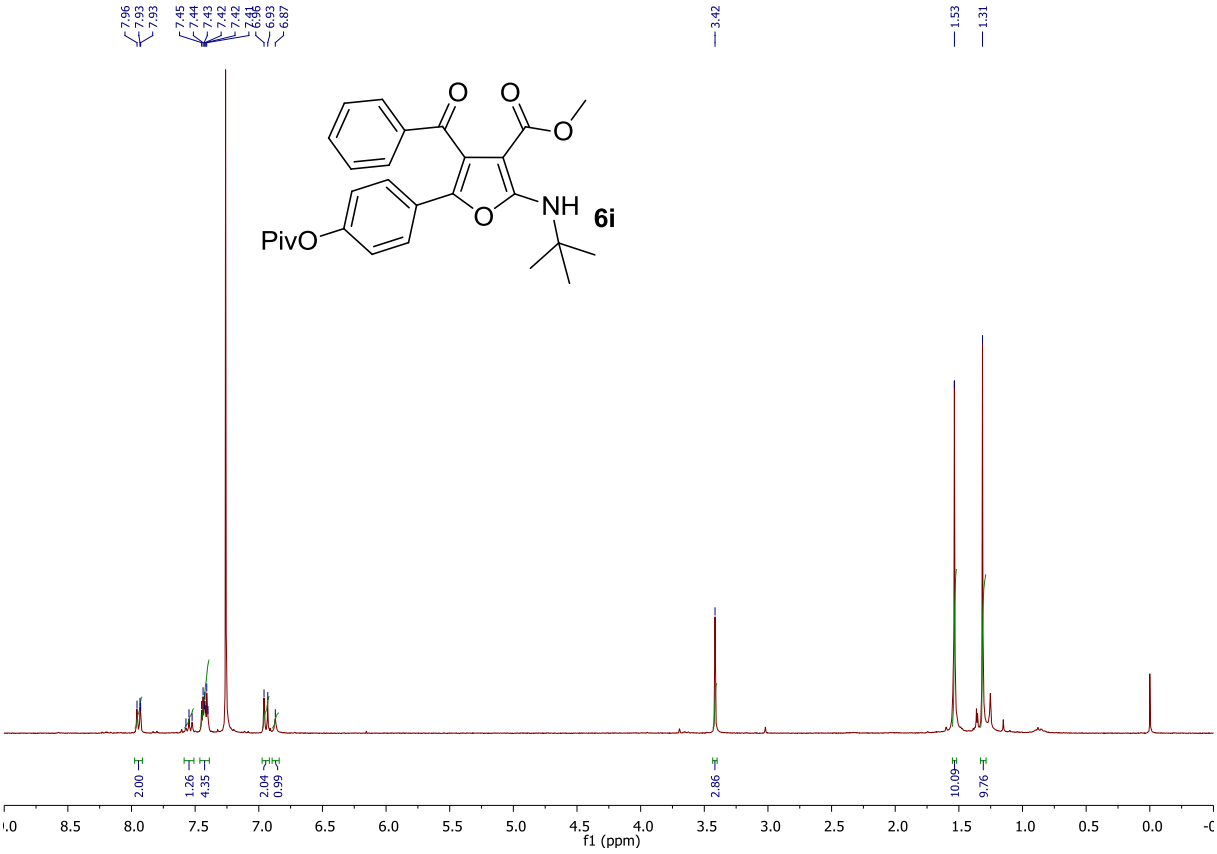

ntn169-p
ntn169-p
193.40
165.23
163.65
161.65
160.36
140.19
137.61
133.60
129.42
128.66
126.35
126.25
119.06
116.05
115.76
89.96
52.94
50.71
30.03
f1 (ppm)

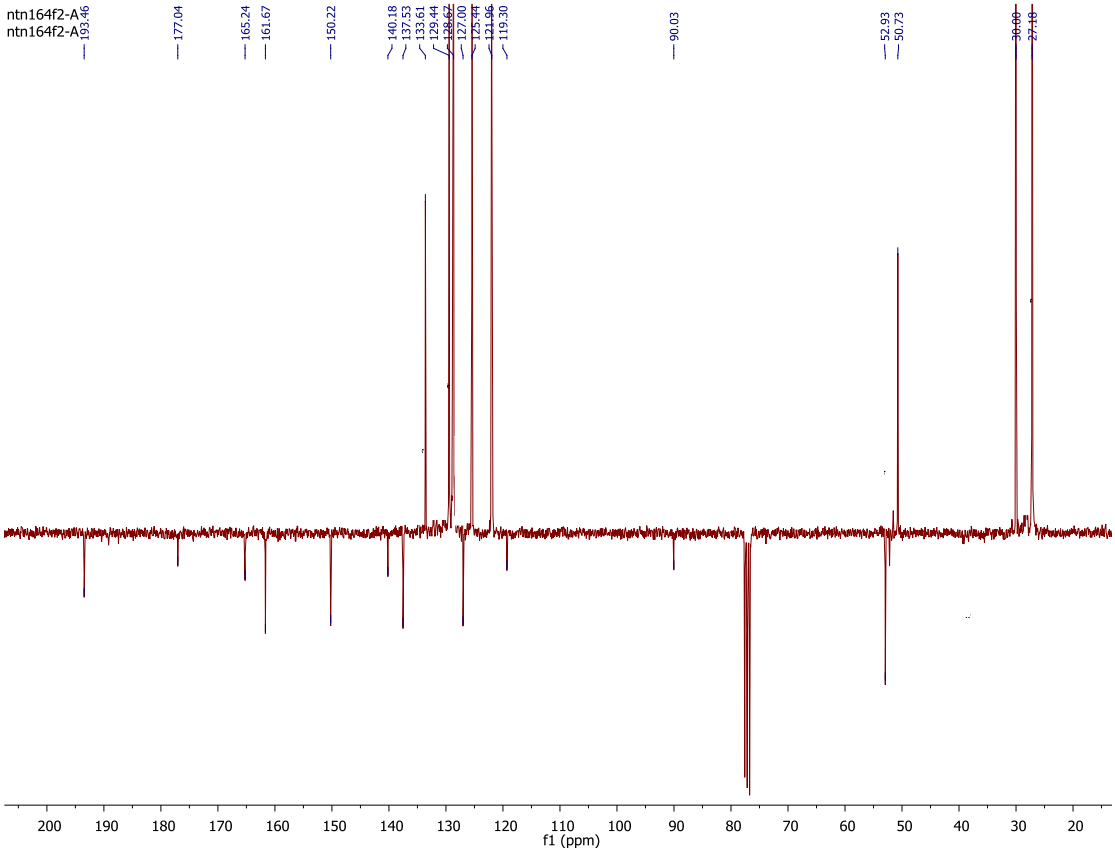

7.80
7.78
7.77
7.49
7.48
7.46
7.46
7.45
7.43
7.35
7.33
7.32
7.29
7.18
7.18
7.15
7.15
7.13
7.13
7.01
7.01
6.98
6.98
6.85
3.44
1.44
1.30
O
O
O
NH
O
OPiv
6g
1.94
2.10
3.14
1.19
1.06
0.97
3.00
9.27
9.86
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

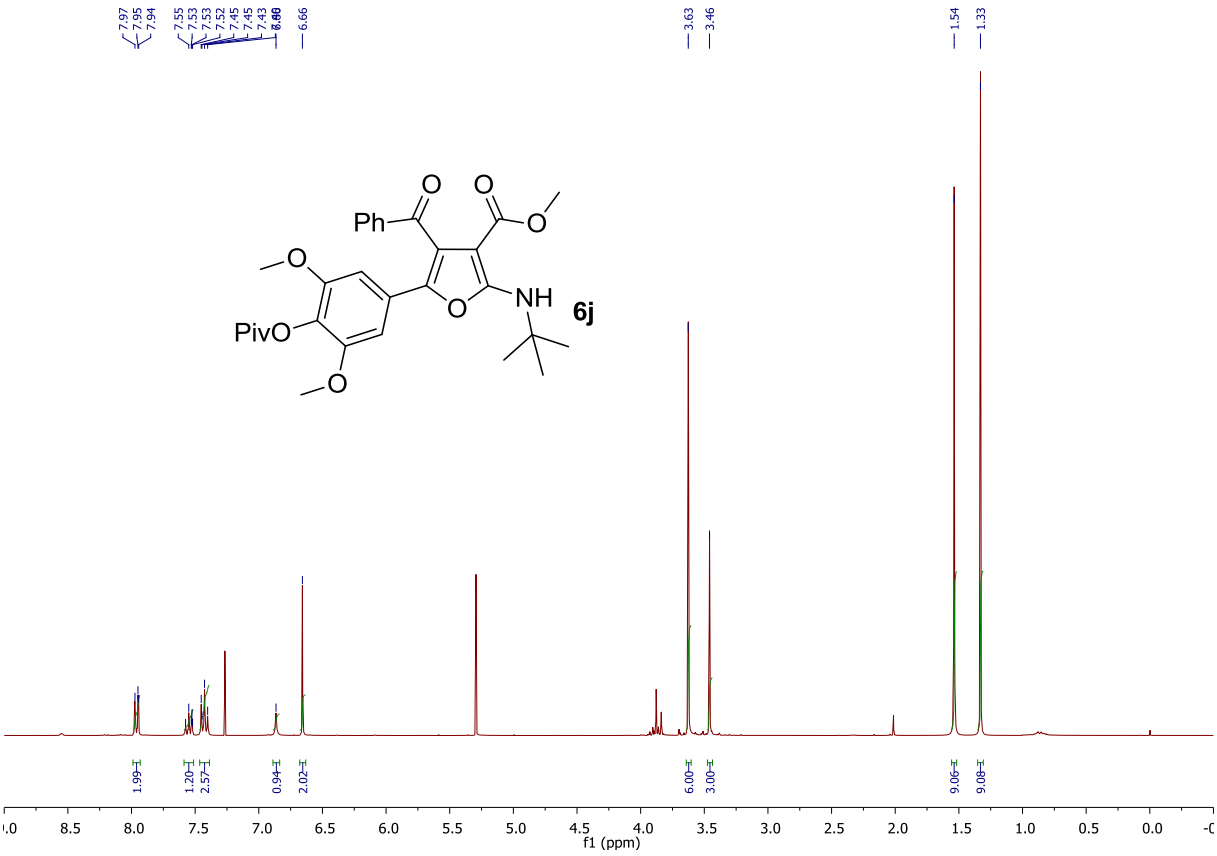

ntn166-f2
ntn166-f2
191.32
176.55
165.55
162.70
150.12
139.48
137.74
133.05
132.81
130.63
129.37
125.56
122.77
122.68
122.01
89.40
53.21
50.72
36.24
27.12
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

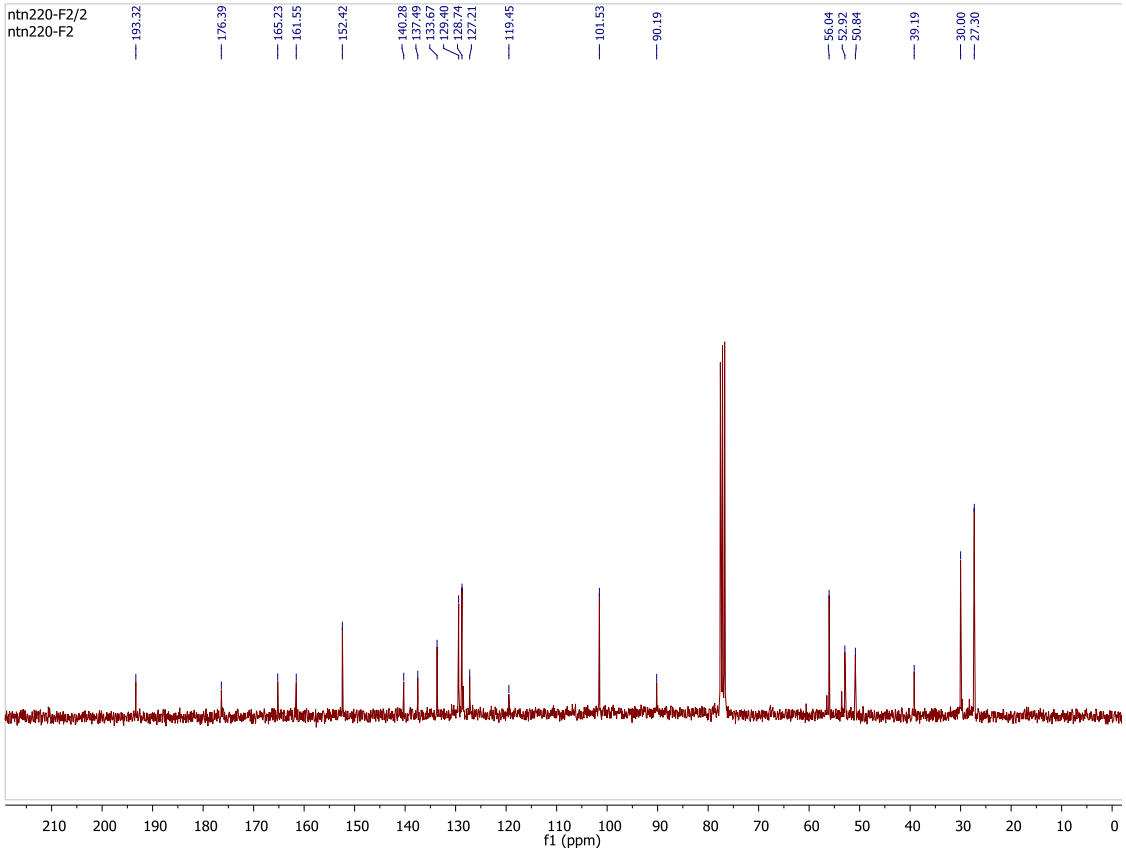

7.97
7.96
7.94
7.93
7.58
7.57
7.56
7.55
7.53
7.52
7.45
7.43
7.40
7.25
7.24
7.23
7.22
7.06
7.05
6.90
6.88
6.87
6.86
6.86
6.85
6.84
O
O
O
NH
O
PivO
6h
1.83
1.35
2.24
1.87
0.93
1.85
3.00
9.09
8.92
f1 (ppm)

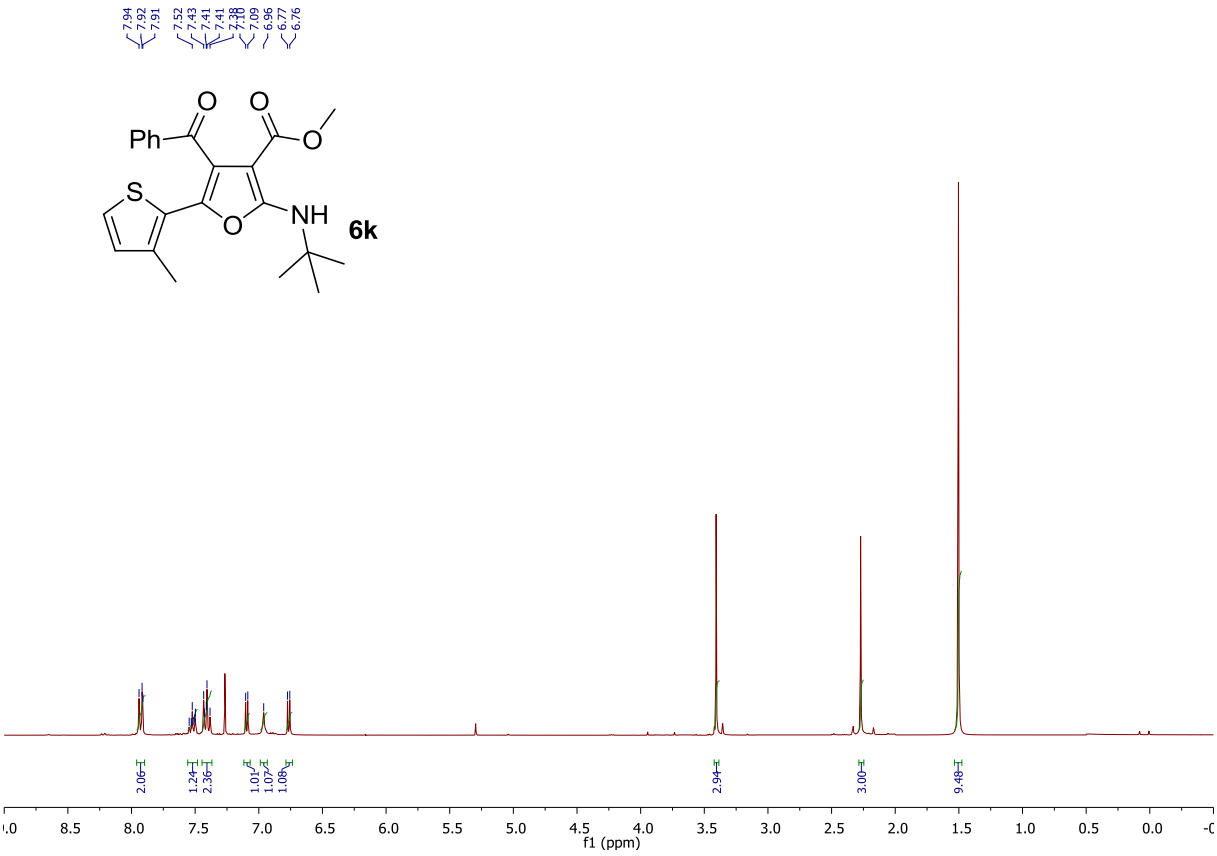

ntn209-F1/2
ntn209-F1
193.24
176.93
165.19
161.68
151.46
139.68
137.47
133.61
130.81
129.75
129.44
128.67
121.49
120.47
117.23
90.18
52.96
50.78
39.13
30.01
27.15
f1 (ppm)

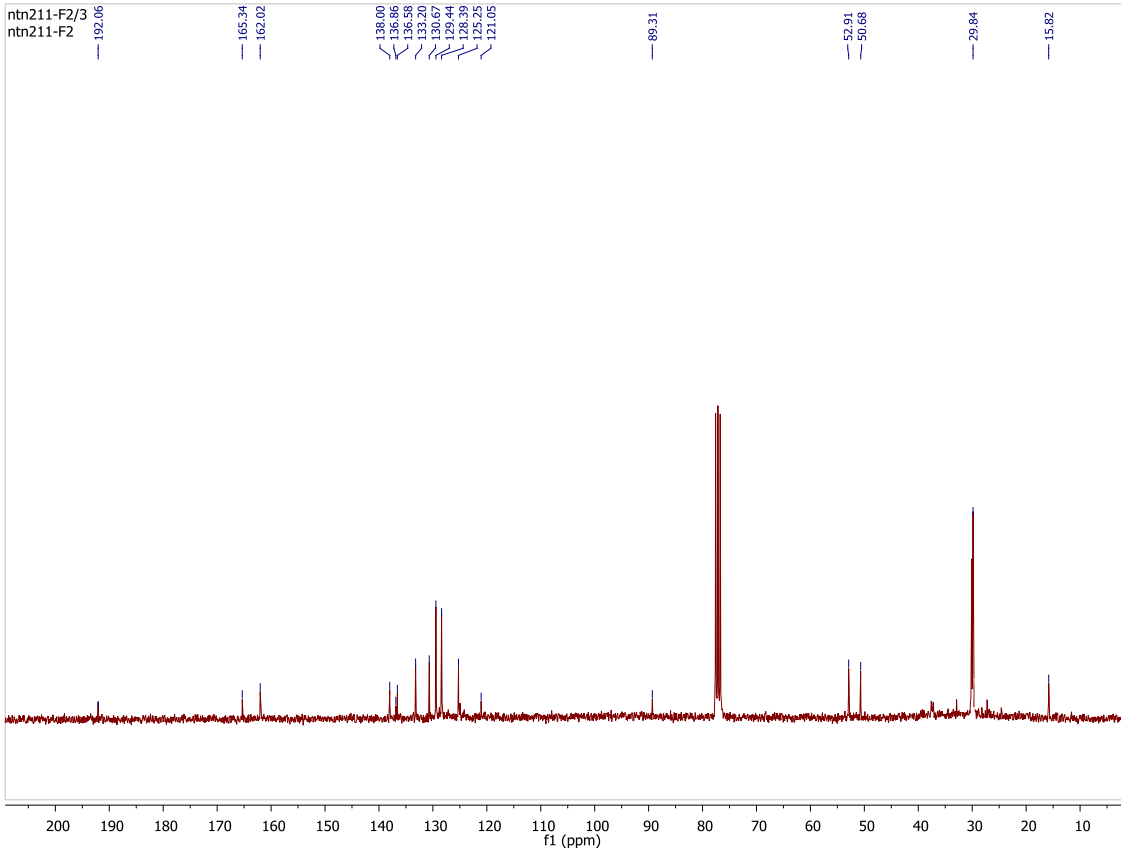

7.96
7.93
7.93
7.45
7.44
7.43
7.42
7.42
6.94
6.93
6.87
3.42
1.53
1.31
O
O
O
NH
O
PivO
6i
2.00
1.26
4.35
2.04
0.99
2.86
10.09
9.76
f1 (ppm)

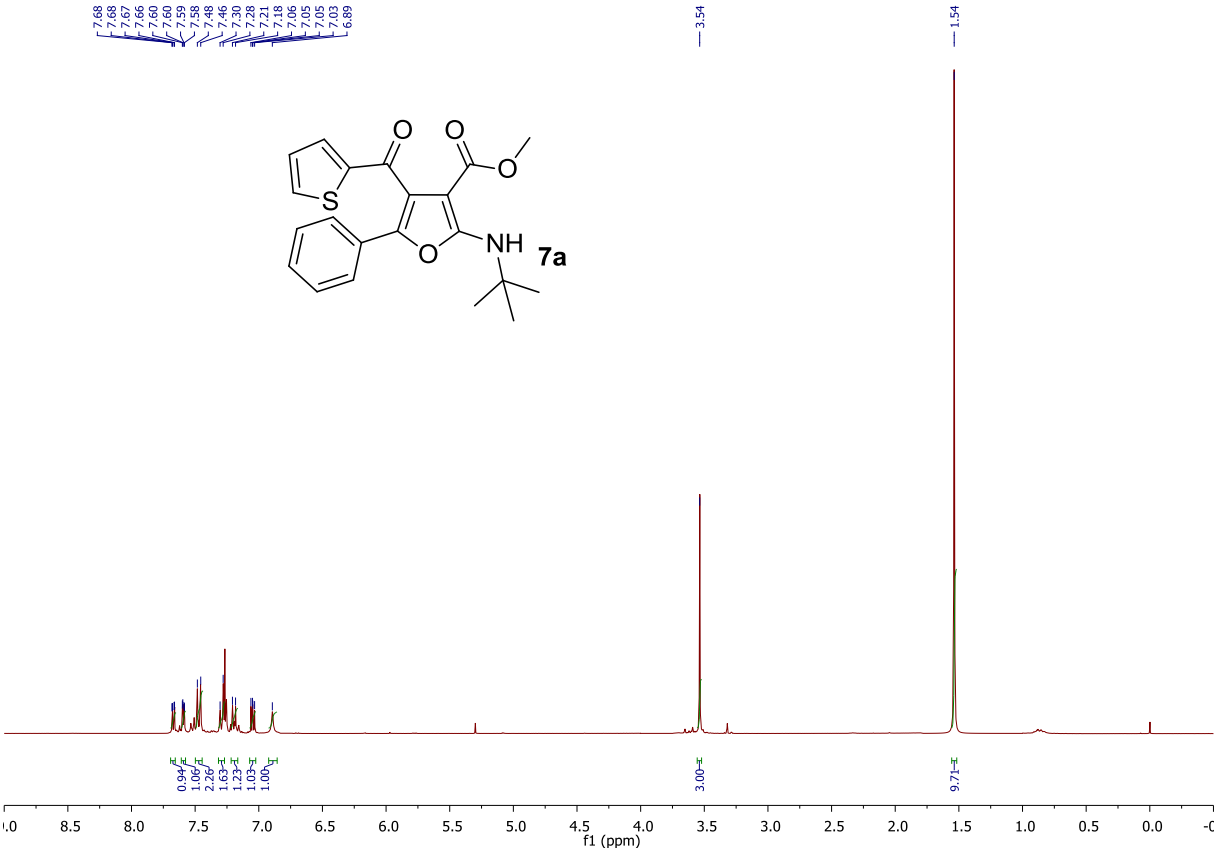

ntn164f2-A
ntn164f2-A
193.46
177.04
165.24
161.67
150.22
140.18
137.53
133.61
129.44
90.03
52.93
50.73
36.60
27.10
119.30
f1 (ppm)

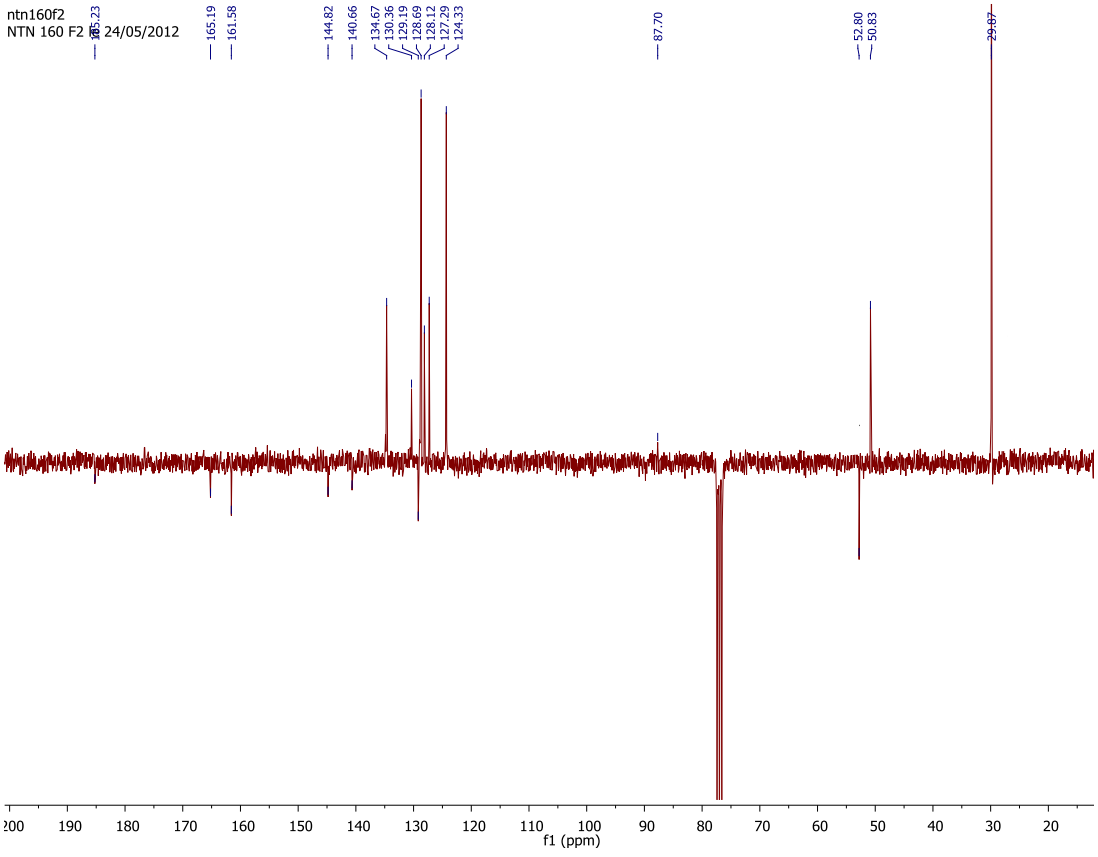

7.97
7.95
7.94
7.55
7.53
7.53
7.52
7.45
7.45
7.43
6.66
3.63
3.46
1.54
1.33
Ph
O
O
O
O
NH
PivO
O
6j
1.99
1.20
2.57
0.94
2.02
6.00
3.00
9.06
9.08
f1 (ppm)

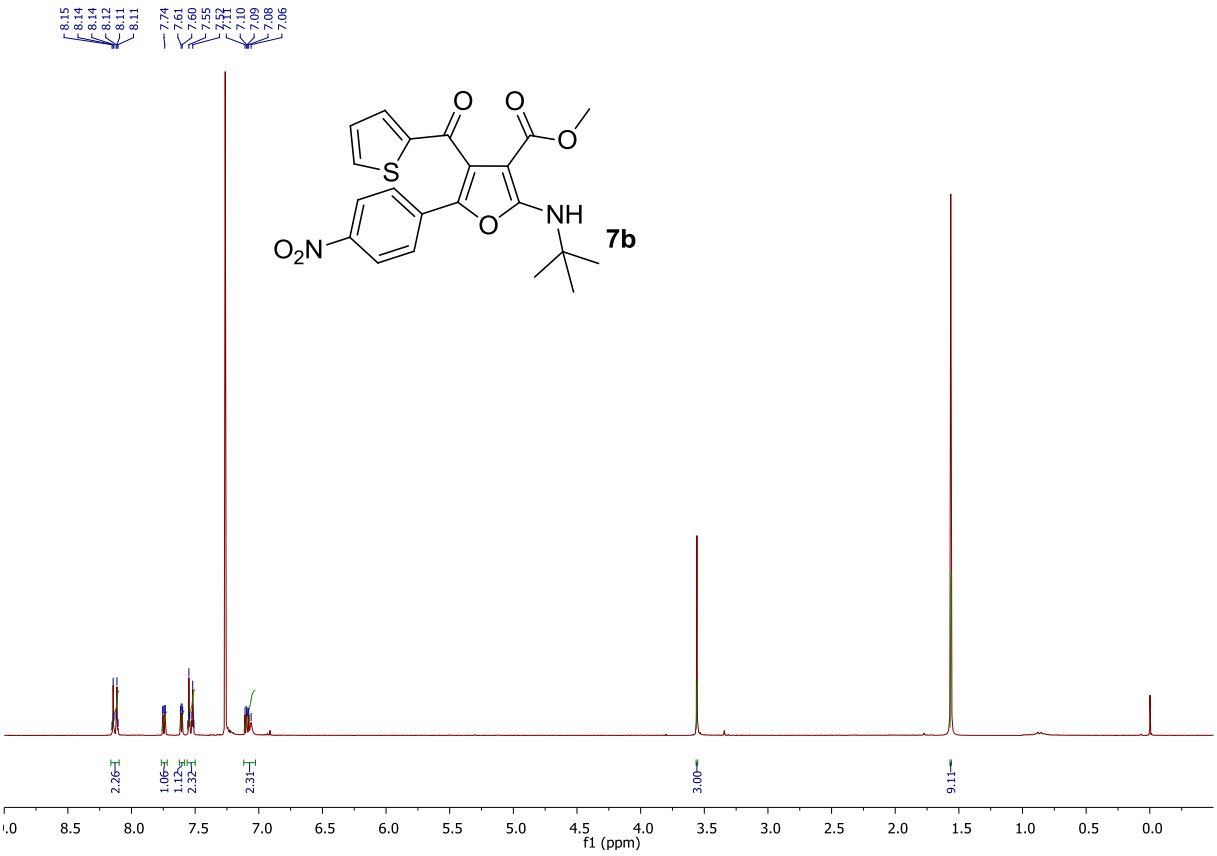

ntn220-F2/2
ntn220-F2
193.32
176.39
165.23
161.55
152.42
140.28
137.49
133.67
129.40
128.74
127.21
119.45
101.53
90.19
56.04
52.92
50.84
39.19
30.00
27.30
f1 (ppm)

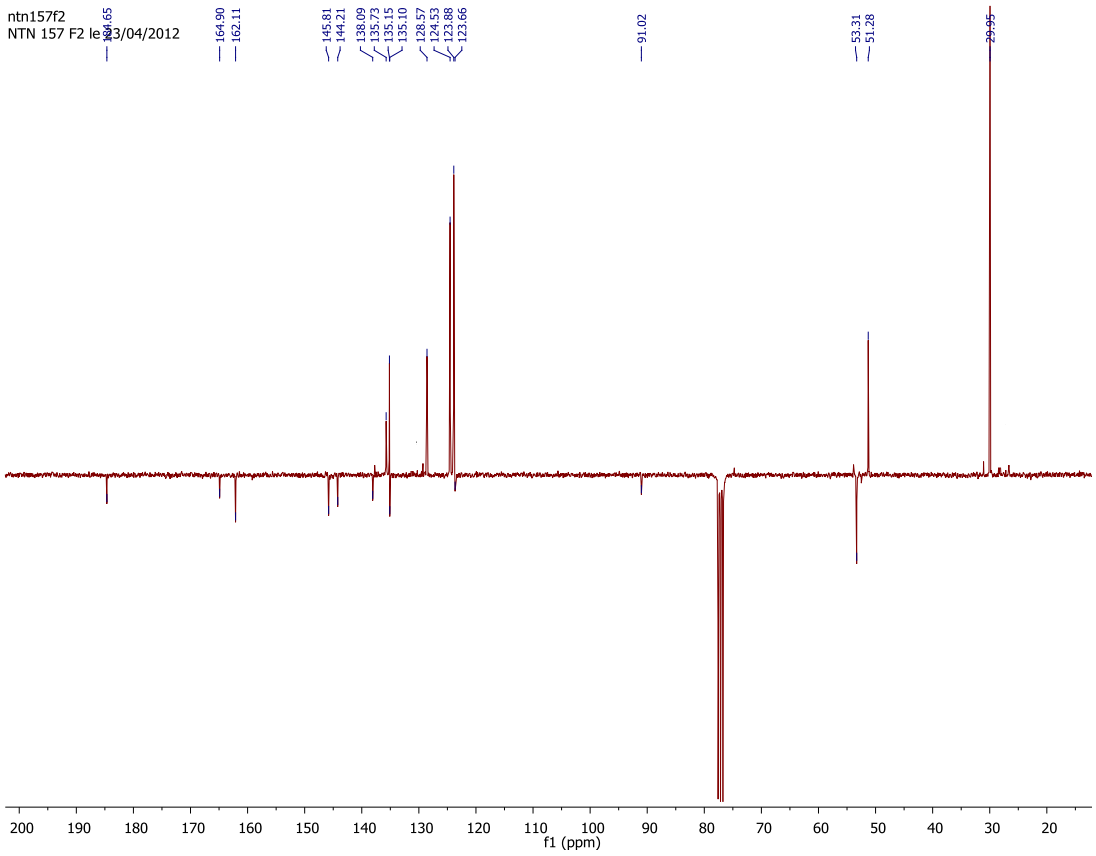

7.94
7.92
7.91
7.52
7.43
7.41
7.41
7.38
7.10
7.09
6.96
6.77
6.76
O
O
Ph
O
S
O
NH
6k
2.06
1.24
2.36
1.01
1.07
1.08
2.94
3.00
9.48
f1 (ppm)

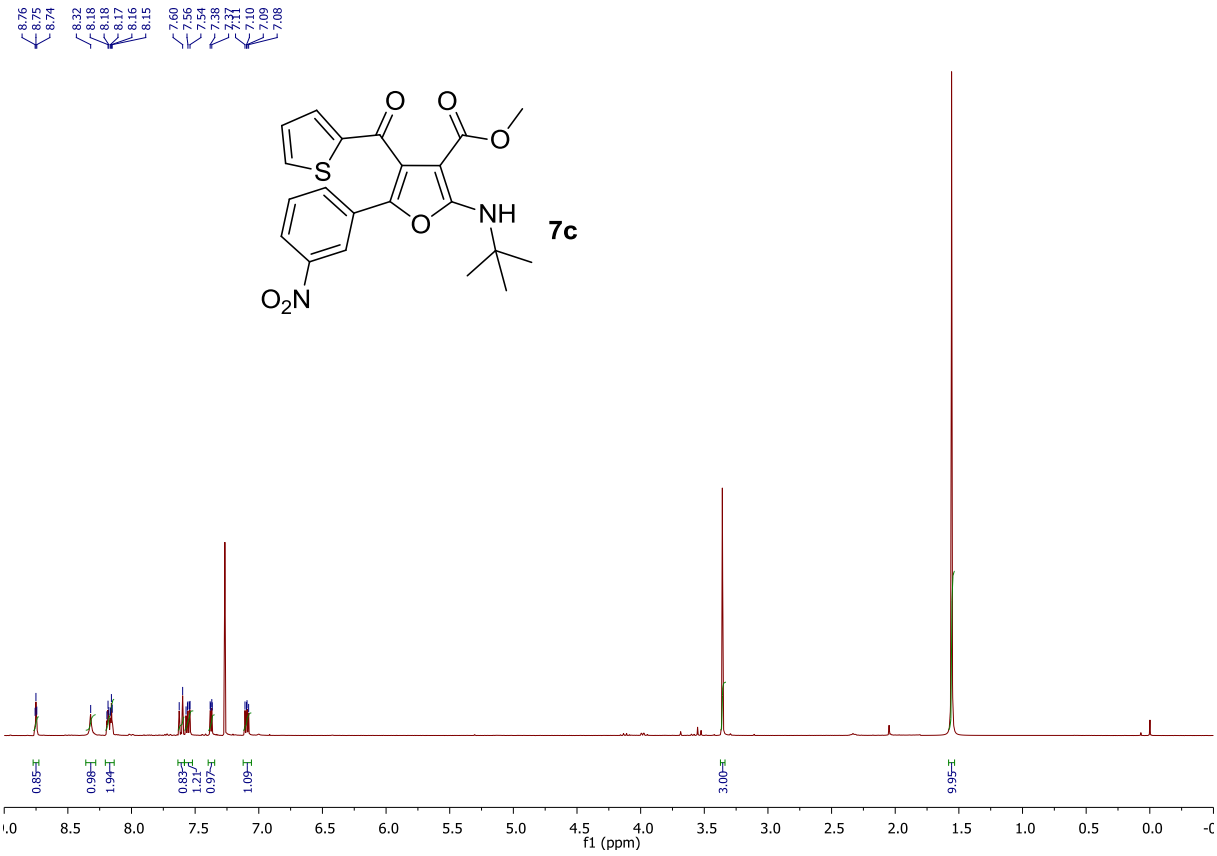

ntn211-F2/3
ntn211-F2
192.06
165.34
162.02
138.00
136.86
136.58
133.20
130.67
129.44
128.39
125.25
121.05
89.31
52.91
50.68
29.84
15.82
f1 (ppm)

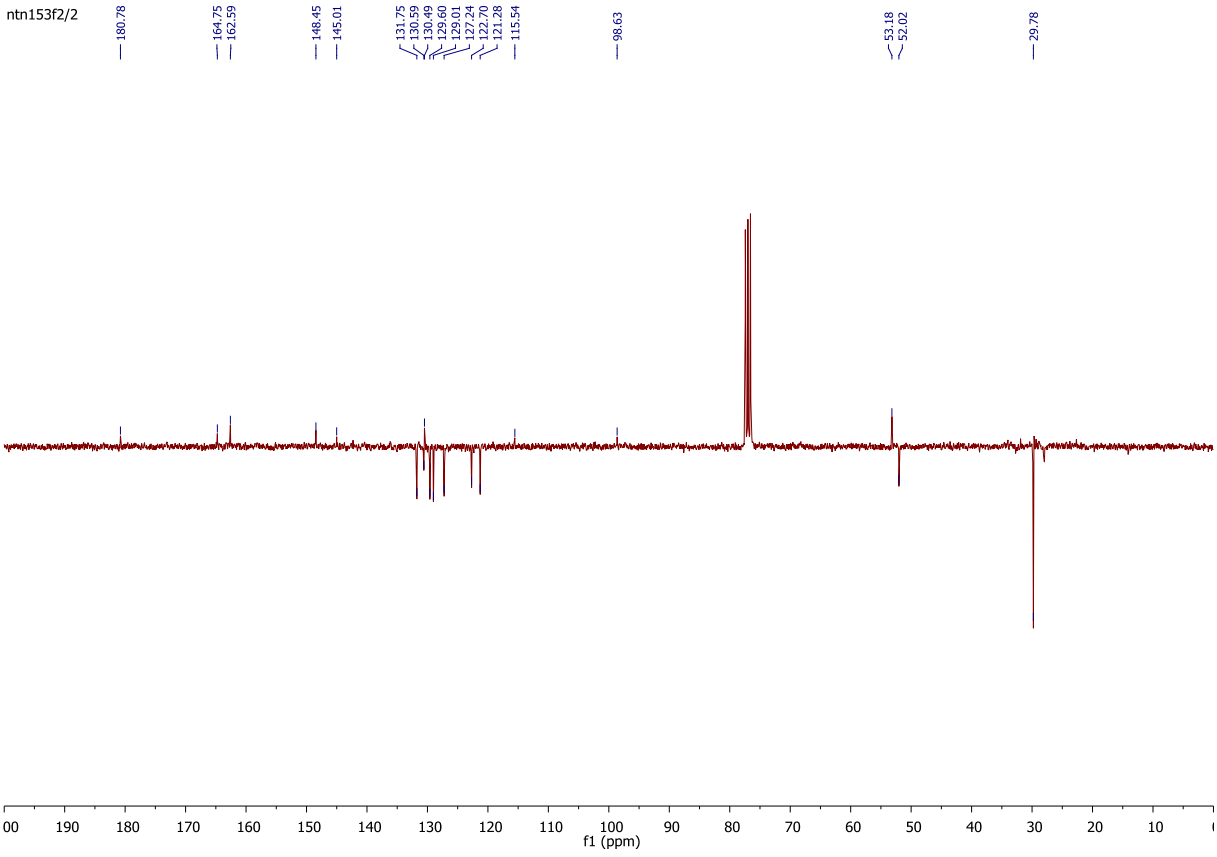

7.68
7.68
7.67
7.66
7.60
7.60
7.59
7.58
7.48
7.46
7.30
7.28
7.21
7.18
7.06
7.05
7.05
7.03
6.89
3.54
1.54
O
O
O
S
O
NH
7a
0.94
1.06
2.26
1.63
1.23
1.03
1.00
3.00
9.71
f1 (ppm)

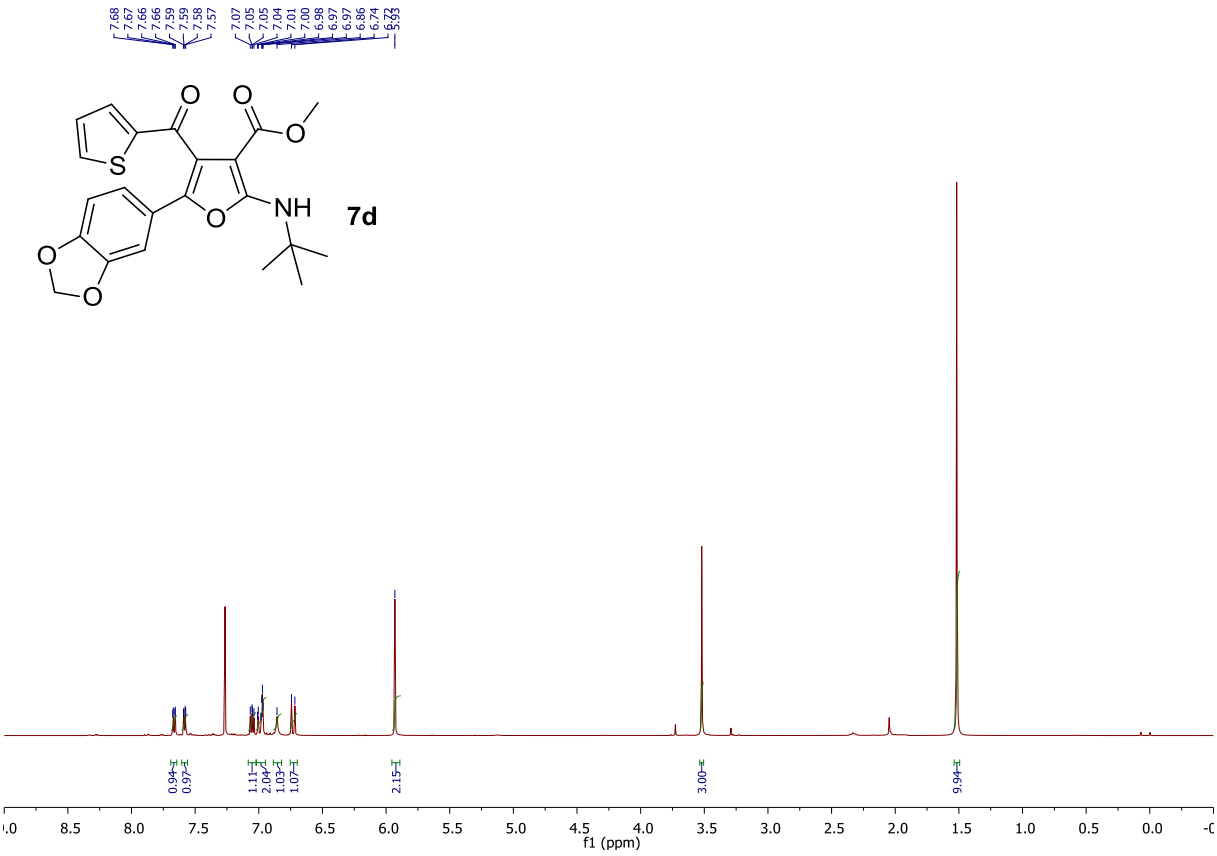

ntn160f2
NTN 160 F2 24/05/2012
165.19
161.58
144.82
140.66
134.67
130.36
129.19
128.69
128.12
127.29
124.33
87.70
52.80
50.83
29.87
f1 (ppm)

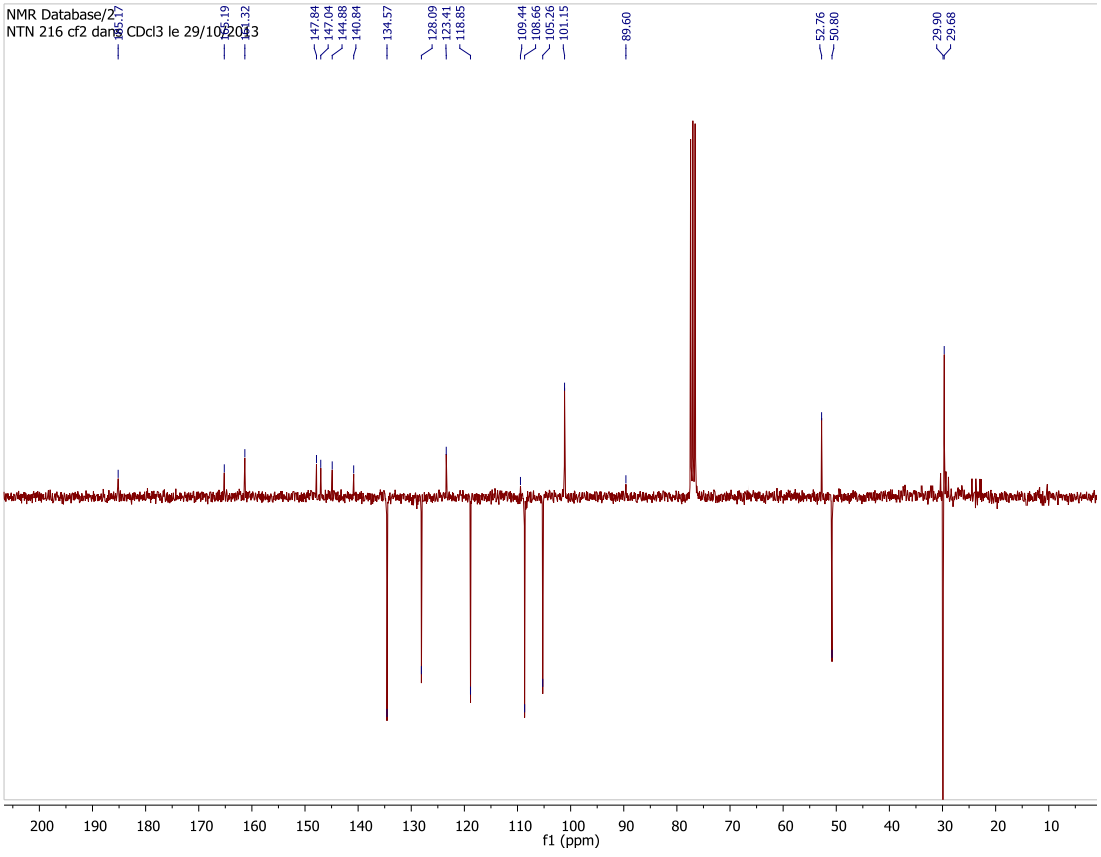

8.15
8.14
8.14
8.12
8.11
8.11
7.74
7.61
7.60
7.55
7.52
7.11
7.10
7.09
7.08
7.06
O
O
O
S
O
NH
O_2N
7b
2.26
1.06
1.12
2.32
2.31
3.00
9.11
f1 (ppm)

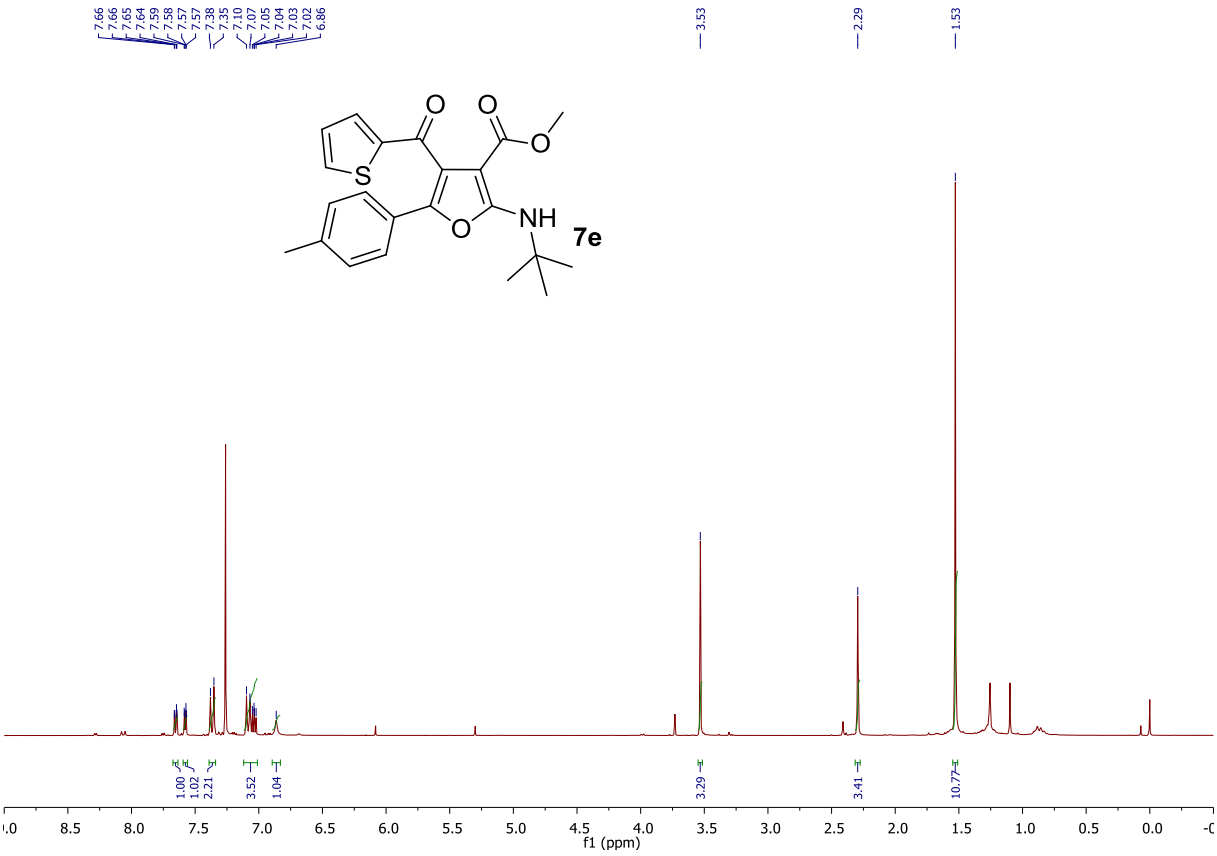

ntn157f2
NTN 157 F2 le 13/04/2012
164.90
162.11
145.81
144.21
138.09
135.73
135.15
135.10
128.57
124.53
123.88
123.66
91.02
53.31
51.28
29.95
f1 (ppm)

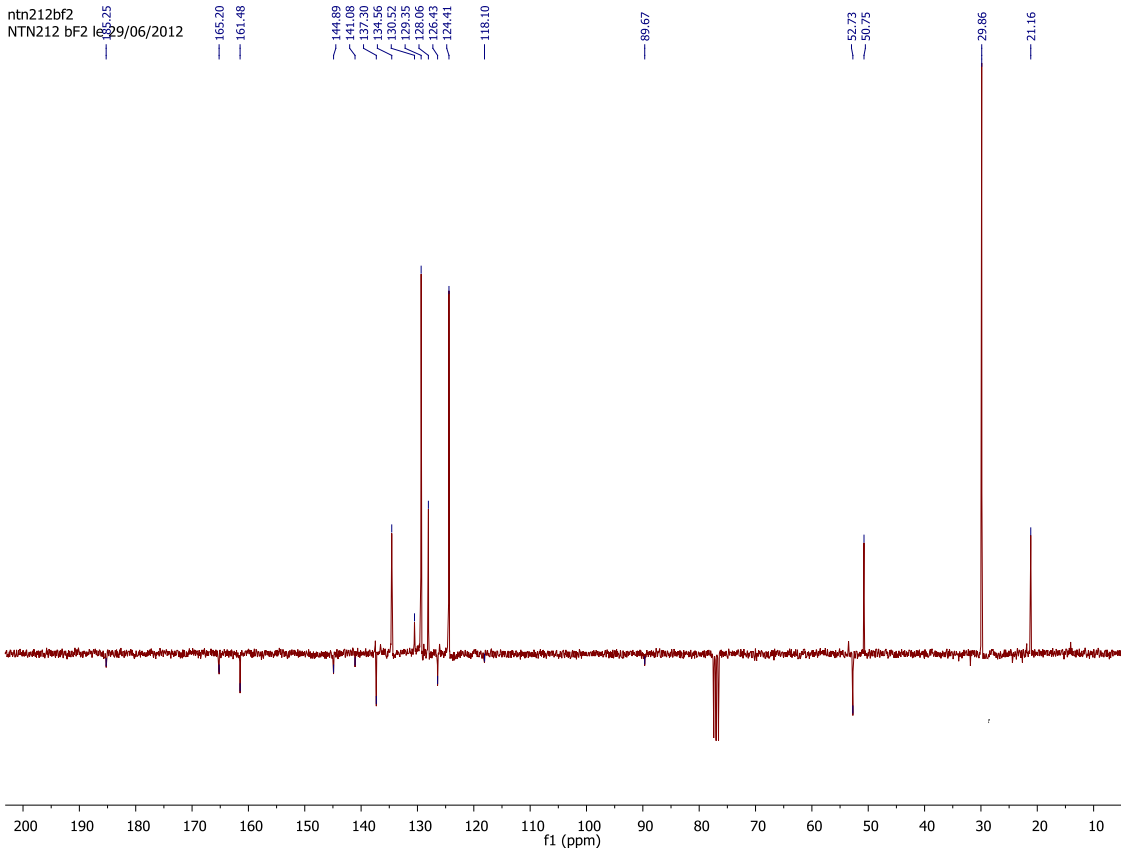

8.76
8.75
8.74
8.32
8.18
8.18
8.17
8.16
8.15
7.60
7.56
7.54
7.38
7.37
7.11
7.10
7.09
7.08
O
O
O
S
O
NH
O2N
7c
0.85
0.98
1.94
0.83
1.21
0.97
1.09
3.00
9.95
f1 (ppm)

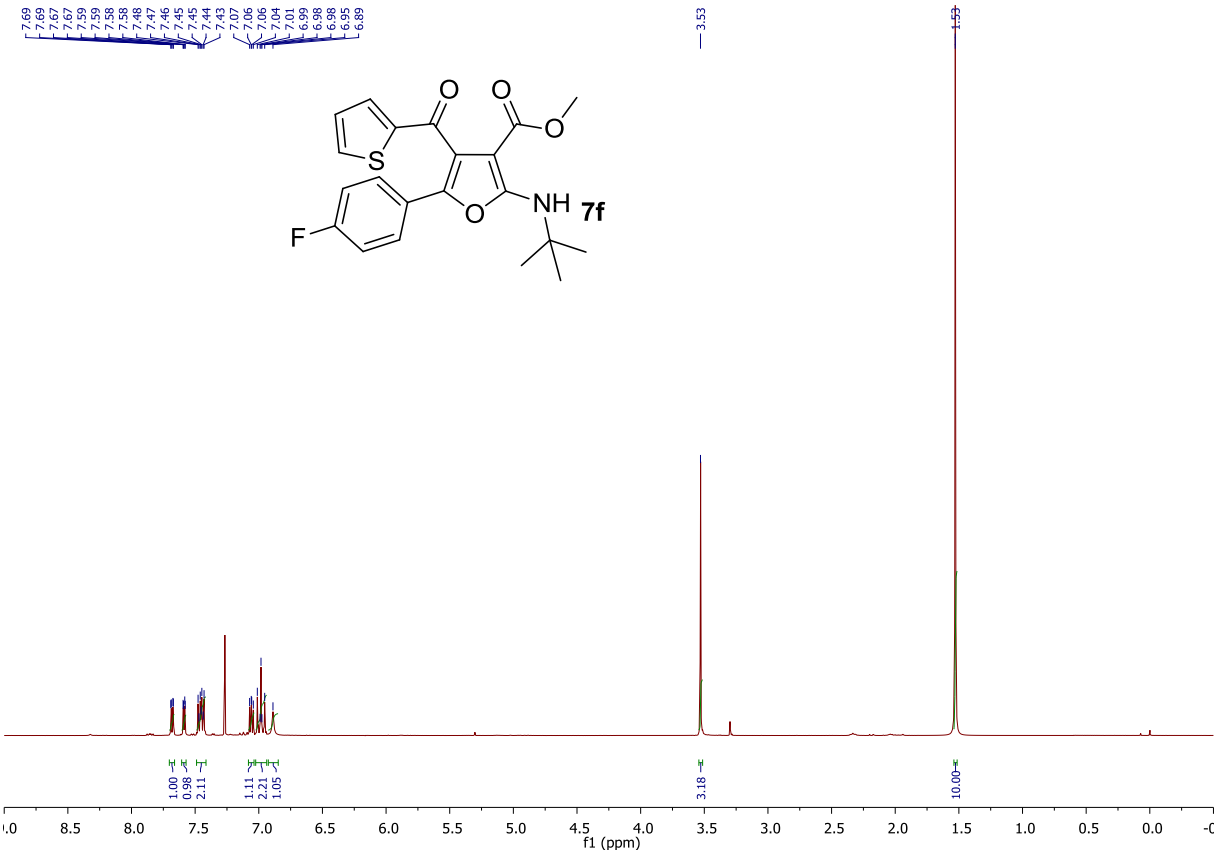

ntn153f2/2
180.78
164.75
162.59
148.45
145.01
131.75
130.59
130.49
129.60
129.01
127.24
122.70
121.28
115.54
98.63
53.18
52.02
29.78
f1 (ppm)

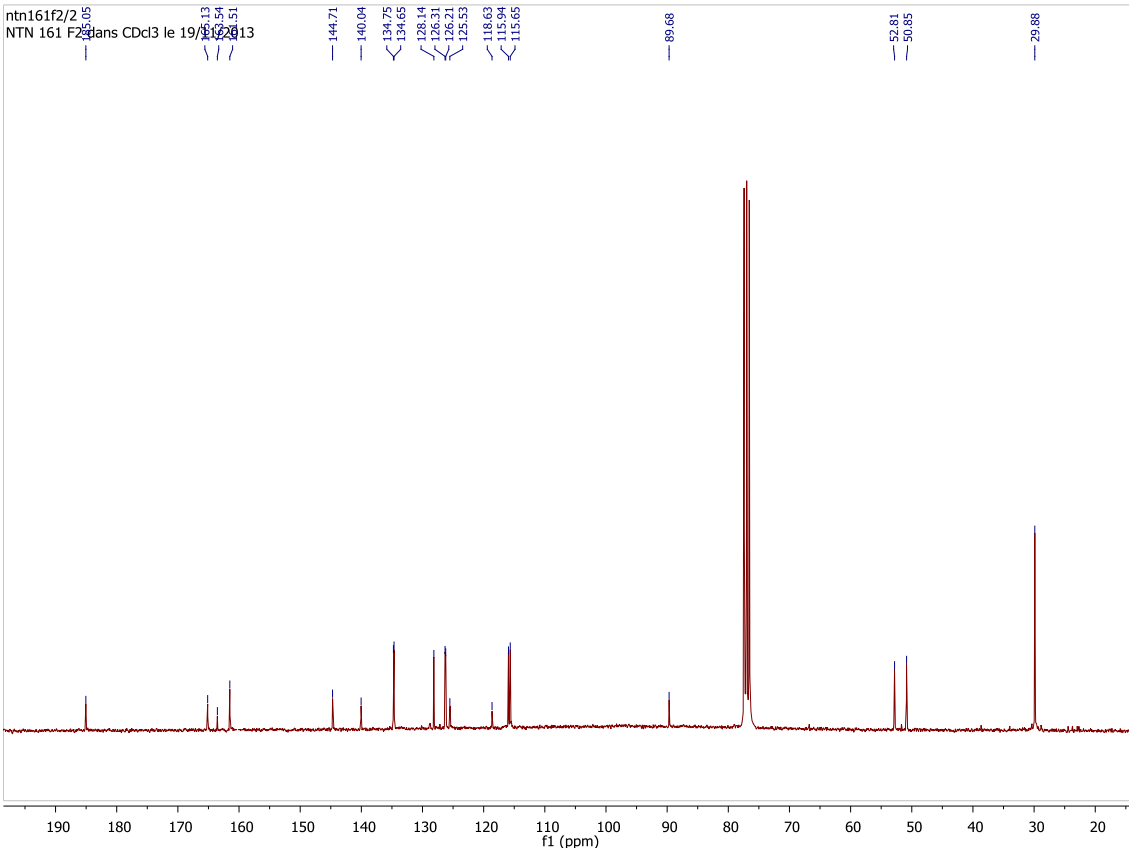

7.68
7.67
7.66
7.66
7.59
7.59
7.58
7.57
7.07
7.05
7.05
7.04
7.01
7.00
6.98
6.97
6.97
6.86
6.74
6.73
5.93
O
O
O
S
NH
O
O
O
7d
0.94
0.97
1.11
2.04
1.03
1.07
2.15
3.00
9.94
f1 (ppm)

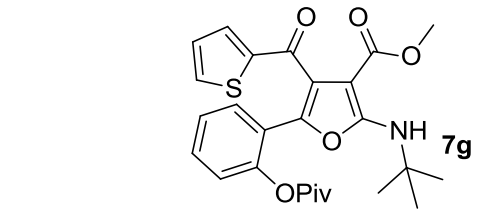

NMR Database/2
NTN 216 cf2 dans CDcl3 le 29/10/2013
85.17
68.19
64.32
147.84
147.04
144.88
140.84
134.57
128.09
123.41
118.85
109.44
108.66
105.26
101.15
89.60
52.76
50.80
29.90
29.68
f1 (ppm)


7.66
7.66
7.65
7.64
7.59
7.58
7.57
7.57
7.38
7.35
7.10
7.07
7.05
7.04
7.03
7.02
6.86
3.53
2.29
1.53
O
O
O
S
O
NH
7e
1.00
1.02
2.21
3.52
1.04
3.29
3.41
10.77
f1 (ppm)


ntn212bf2
NTN212 bF2 le 29/06/2012
165.25
165.20
161.48
144.89
141.08
137.30
134.56
130.52
129.35
128.06
126.43
124.41
118.10
89.67
52.73
50.75
29.86
21.16
f1 (ppm)

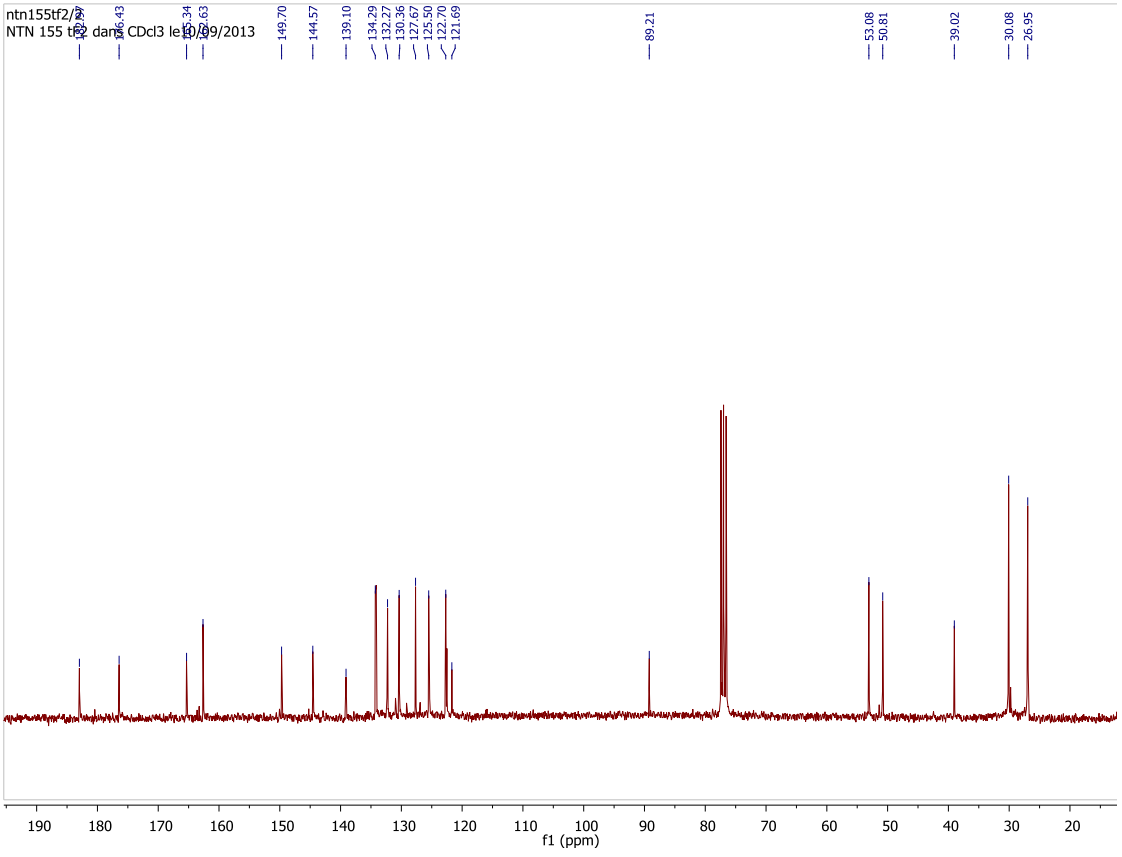

7.69
7.69
7.67
7.67
7.59
7.59
7.58
7.58
7.48
7.47
7.46
7.45
7.45
7.44
7.43
7.07
7.06
7.06
7.04
7.01
6.99
6.98
6.98
6.95
6.89
3.53
1.53
O
O
O
S
NH
7f
F
O
1.00
0.98
2.11
1.11
2.21
1.05
3.18
10.00
f1 (ppm)

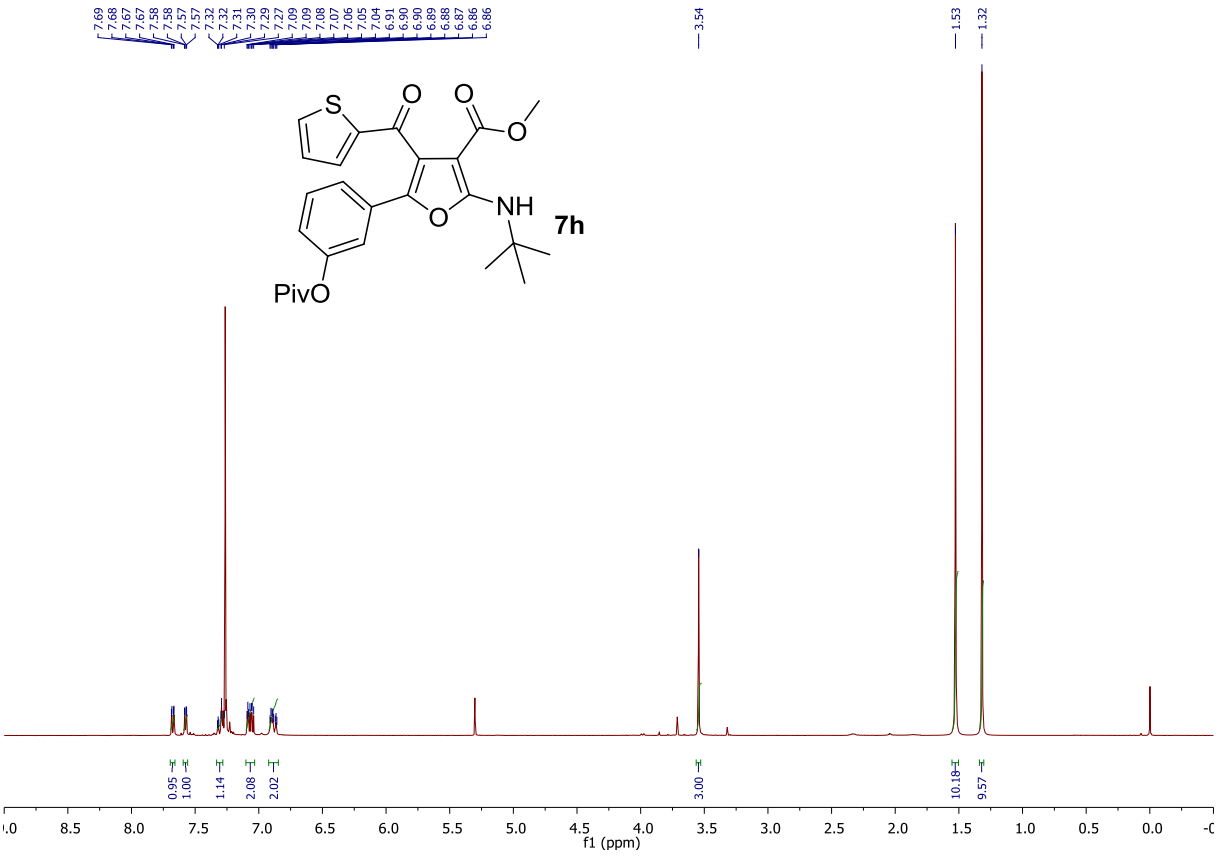

ntn161f2/2
NTN 161 F2 dans CDcl3 le 19/12/2013
165.05
161.13
159.54
158.51
144.71
140.04
134.75
134.65
128.14
126.31
126.21
125.53
118.63
115.94
115.65
89.68
52.81
50.85
29.88
f1 (ppm)

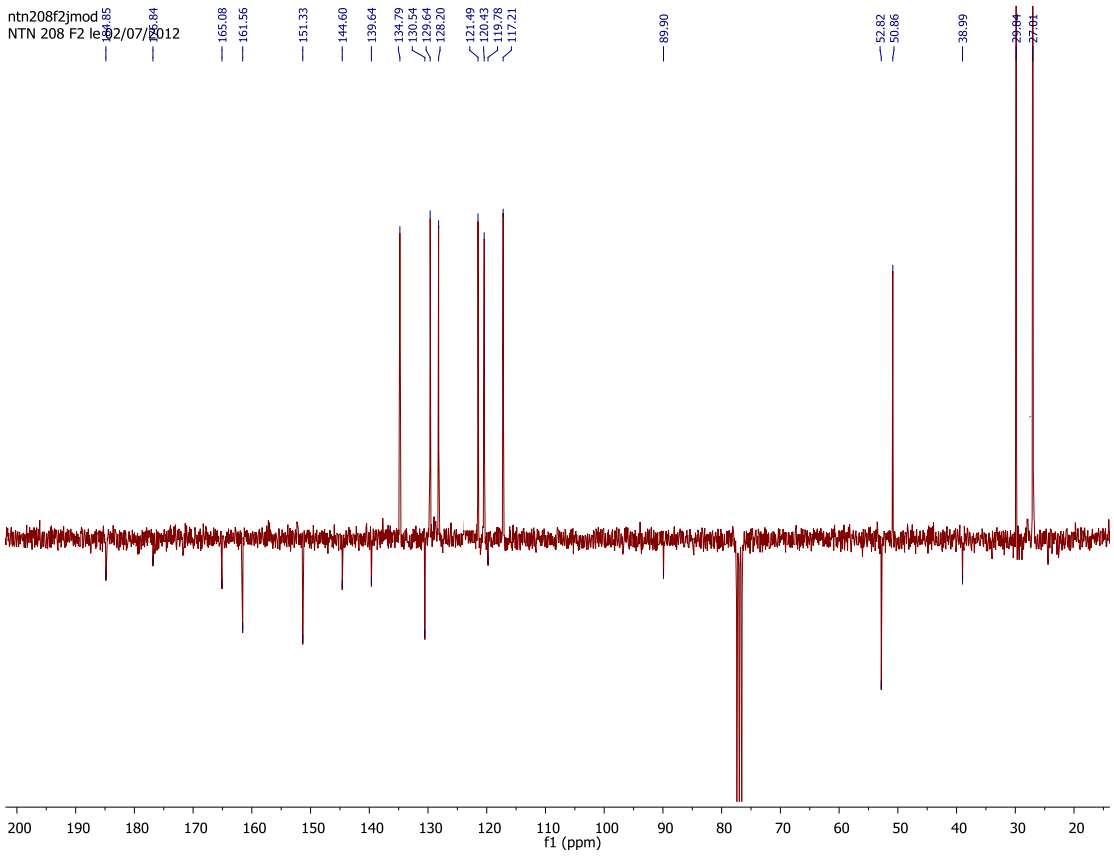

O
O
O
S
NH
O
OPiv

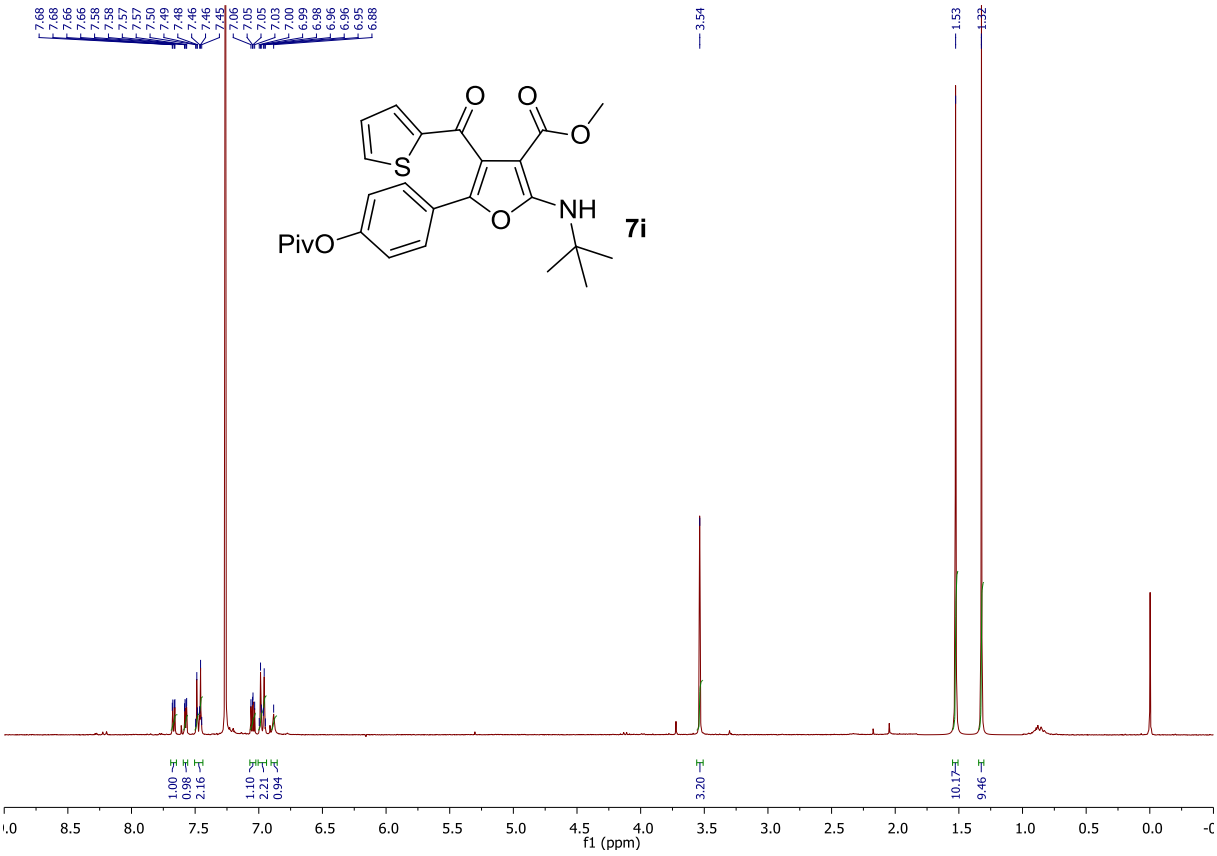
7g

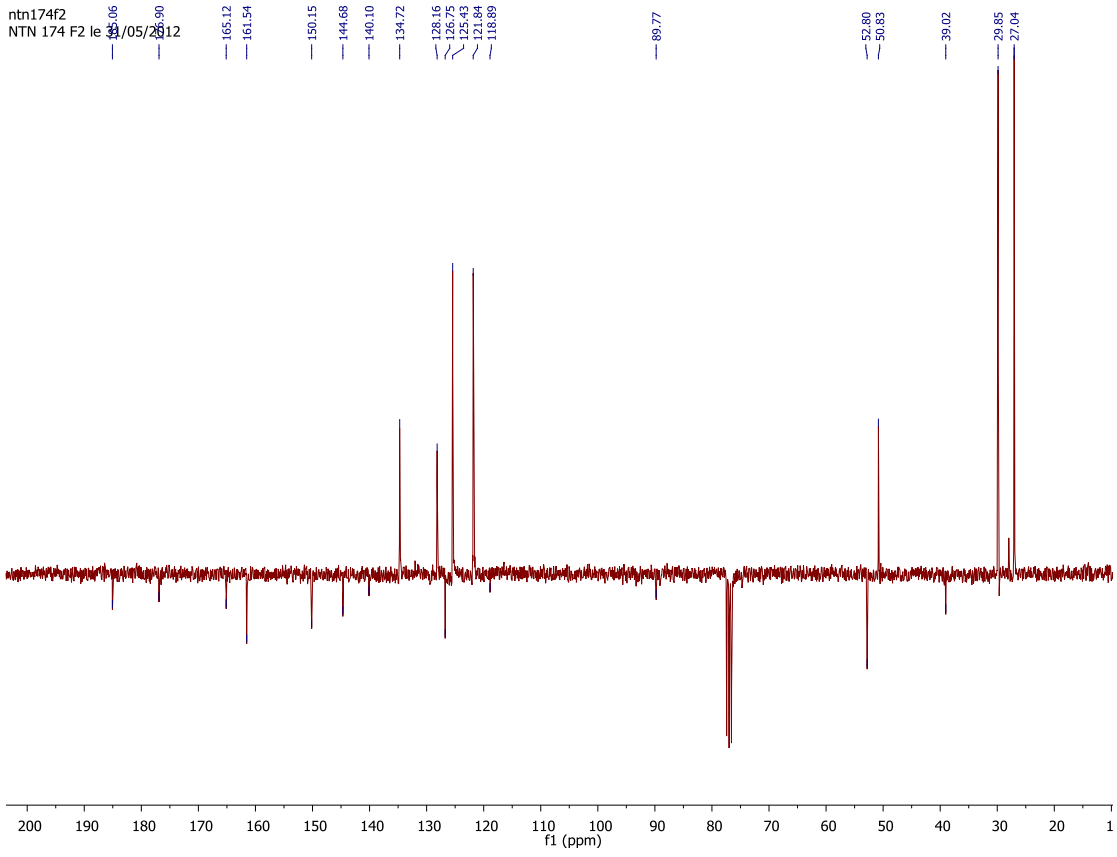
1.02
2.17
1.25
1.20
1.06
1.06
0.97
3.00
10.40
8.94
f1 (ppm)

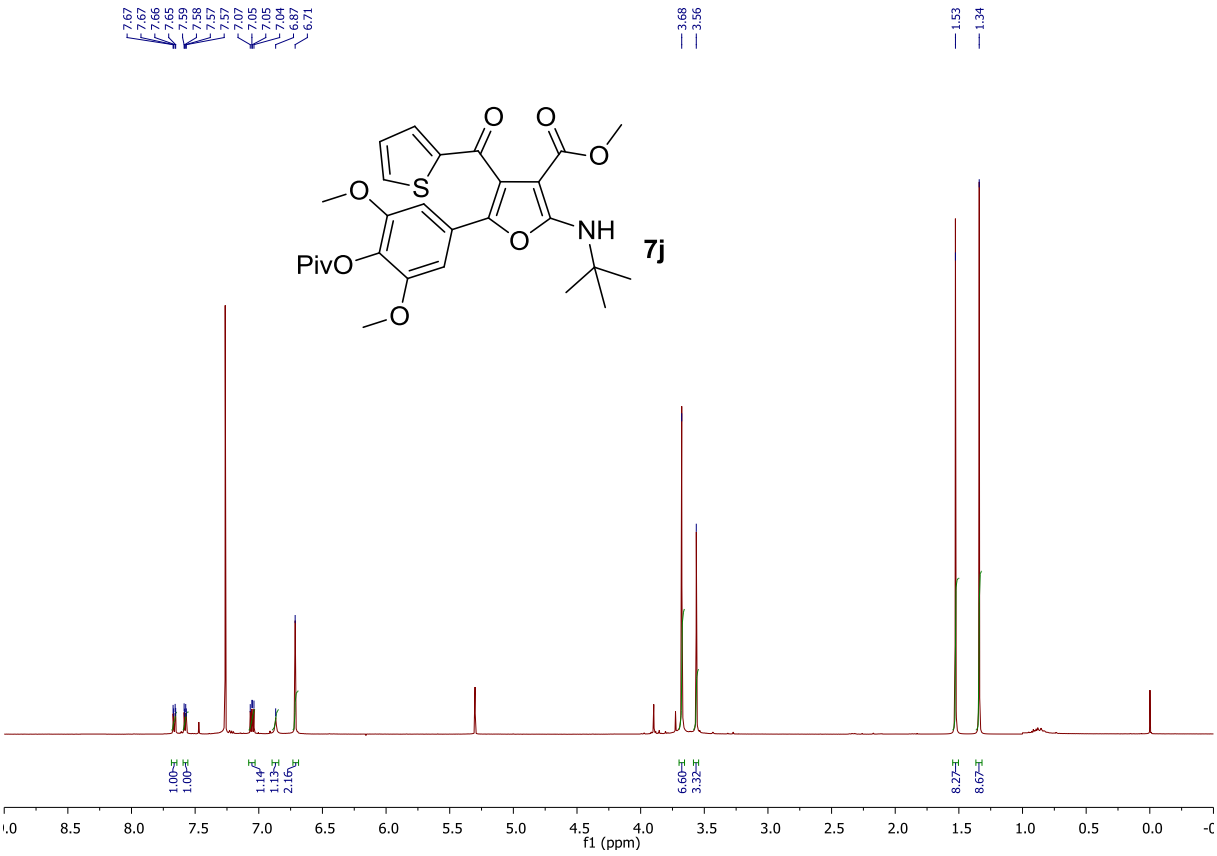

ntn155tf2/2
NTN 155 tf2 dans CDcl3 le 10/09/2013
149.70
144.57
139.10
134.29
132.27
130.36
127.67
125.50
122.70
121.69
89.21
53.08
50.81
39.02
30.08
26.95
f1 (ppm)

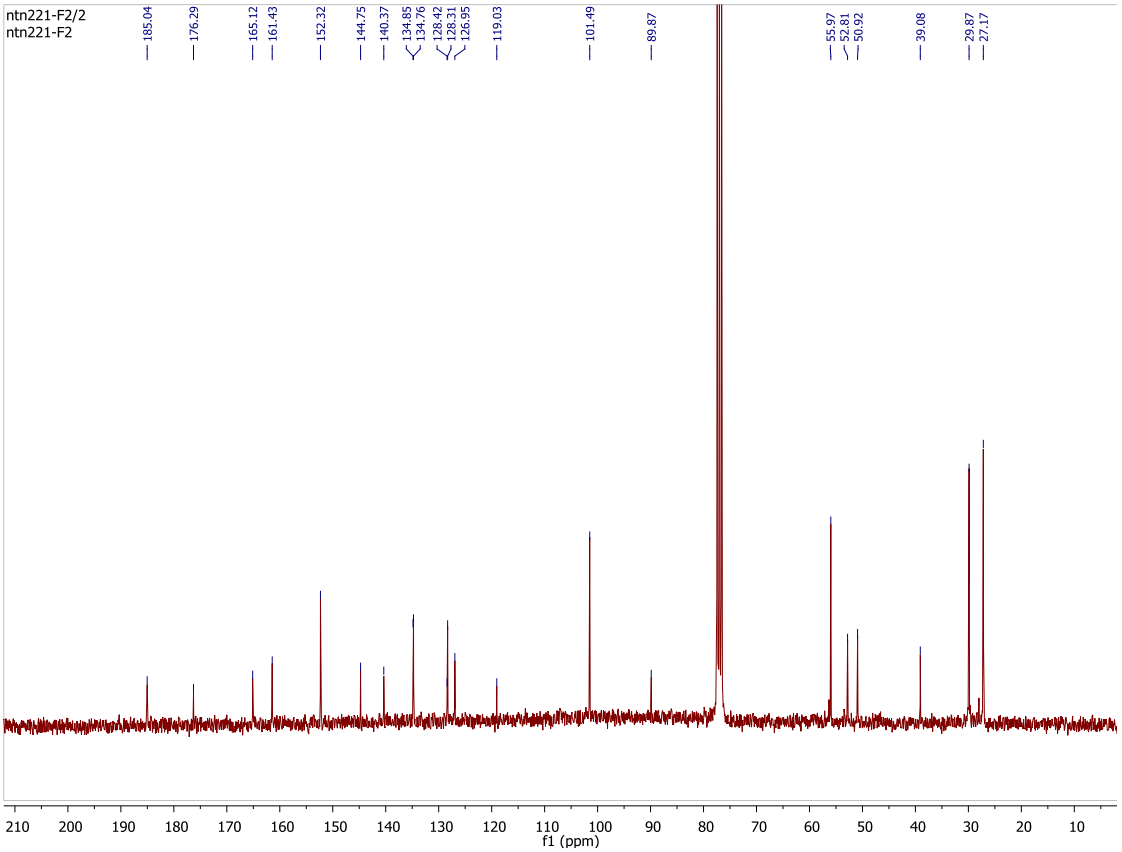

7.69
7.68
7.67
7.67
7.58
7.58
7.57
7.57
7.32
7.32
7.31
7.30
7.29
7.27
7.09
7.09
7.08
7.07
7.06
7.05
7.04
6.91
6.90
6.90
6.89
6.88
6.87
6.86
6.86
3.54
1.53
1.32
S
O
O
O
NH
O
7h
PivO
0.95
1.00
1.14
2.08
2.02
3.00
10.18
9.57
f1 (ppm)

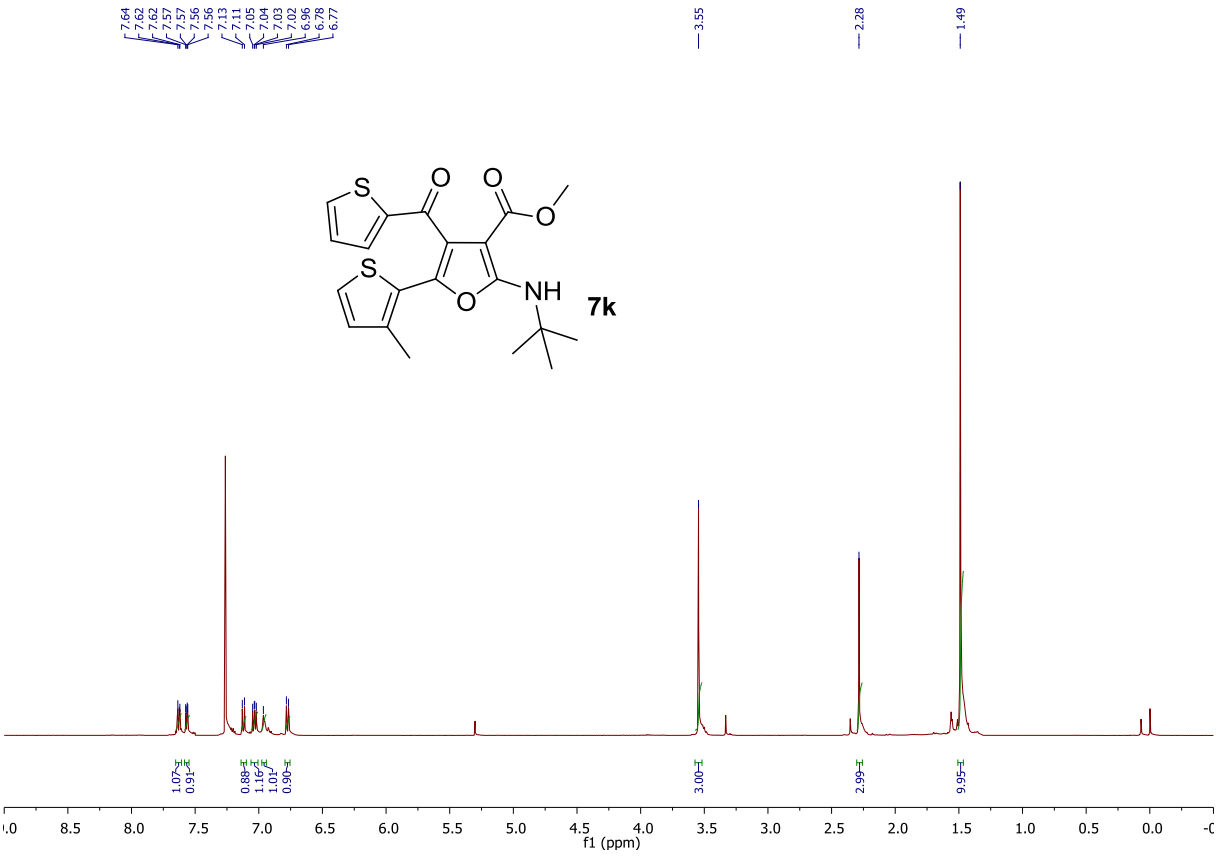

ntn208f2jmod
NTN 208 F2 le
2012
184.85
178.84
165.08
161.56
151.33
144.60
139.64
134.79
130.54
129.64
128.20
121.49
120.43
119.78
117.21
89.90
52.82
50.86
38.99
29.04
27.01
f1 (ppm)

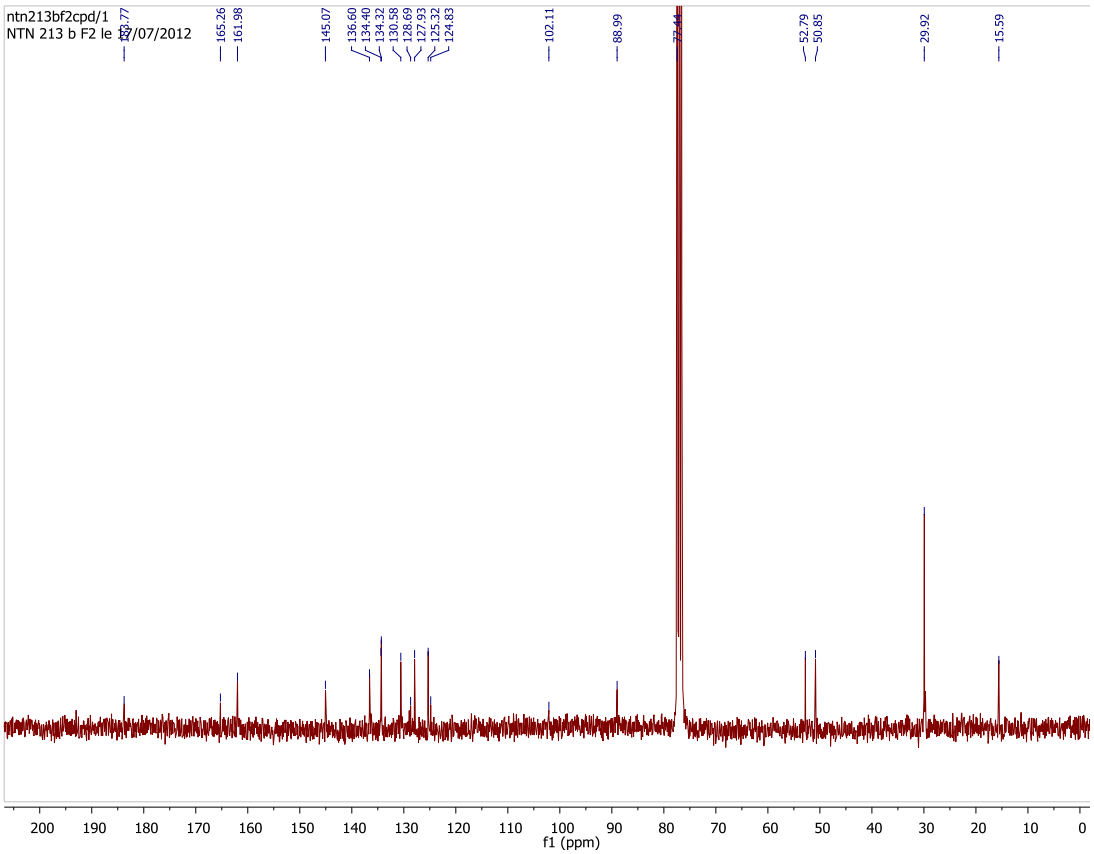

7.68
7.68
7.66
7.66
7.58
7.58
7.57
7.57
7.50
7.49
7.48
7.46
7.46
7.45
7.06
7.05
7.05
7.03
7.00
6.99
6.98
6.96
6.96
6.95
6.88
3.54
1.53
1.32
O
O
O
S
NH
O
PivO
7i
1.00
0.98
2.16
1.10
2.21
0.94
3.20
10.17
9.46
f1 (ppm)

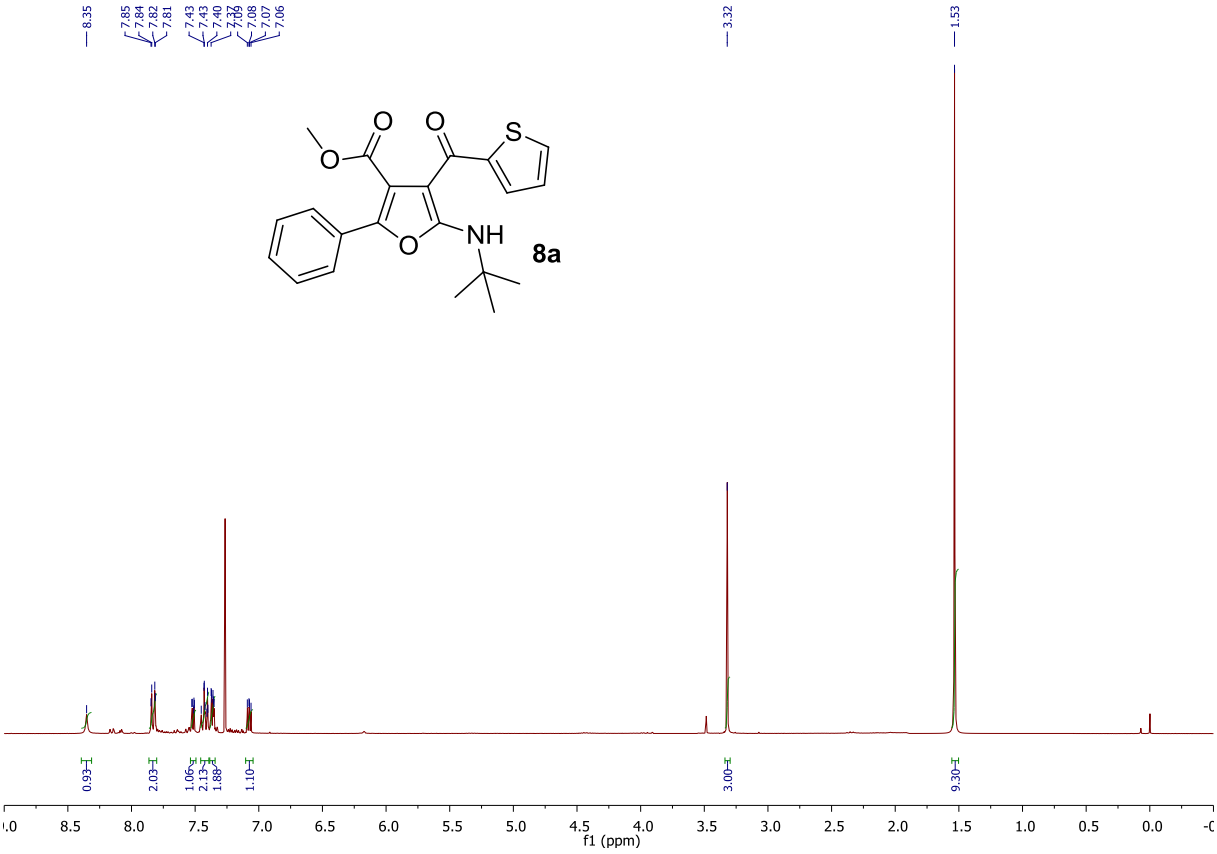

ntn174f2
NTN 174 F2 le 21/05/2012
175.06
166.90
165.12
161.54
150.15
144.68
140.10
134.72
128.16
126.75
125.43
121.84
118.89
89.77
52.80
50.83
39.02
29.85
27.04
f1 (ppm)

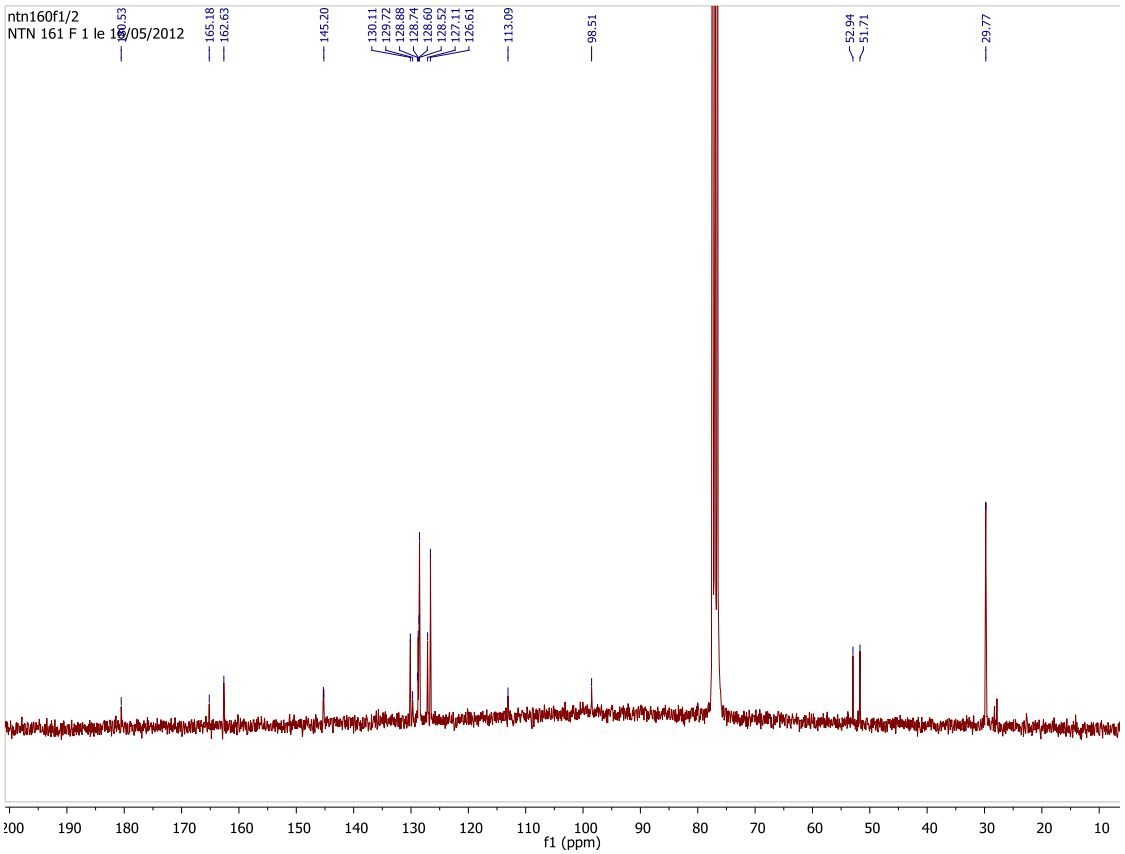

7.67
7.67
7.66
7.65
7.59
7.58
7.57
7.57
7.07
7.05
7.05
7.04
6.87
6.71
3.68
3.56
1.53
1.34
O
O
O
S
O
NH
PivO
O
7j
1.00
1.00
1.14
1.13
2.16
6.60
3.32
8.27
8.67
f1 (ppm)

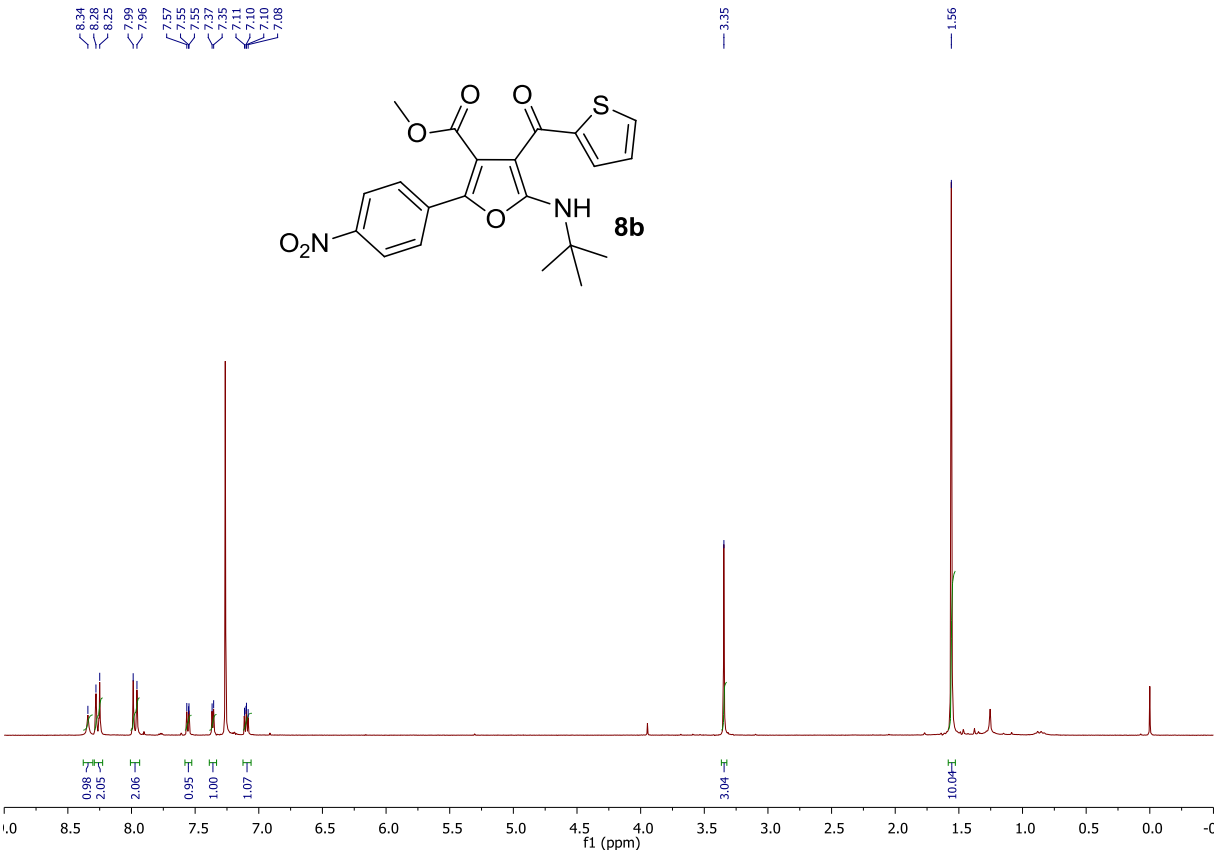

ntn221-F2/2
ntn221-F2
185.04
176.29
165.12
161.43
152.32
144.75
140.37
134.85
134.76
128.42
128.31
126.95
119.03
101.49
89.87
55.97
52.81
50.92
39.08
29.87
27.17
f1 (ppm)

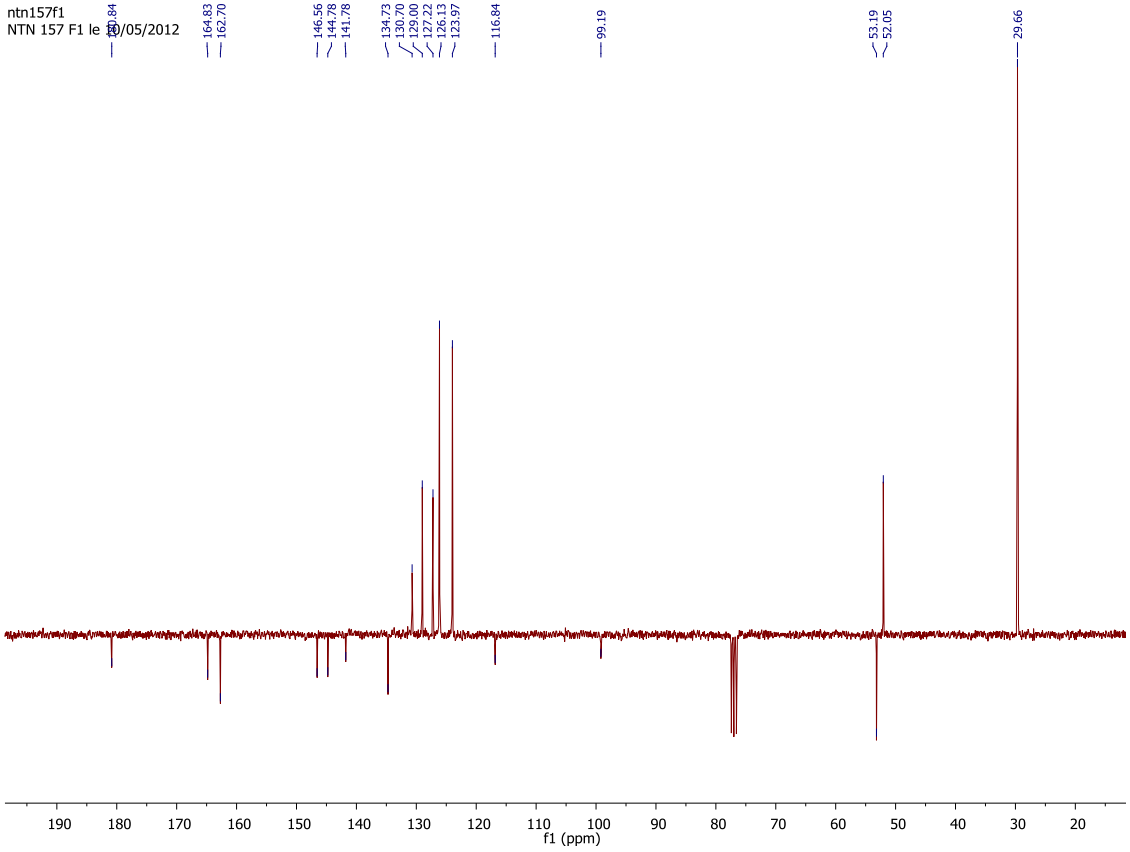

7.64
7.62
7.62
7.57
7.57
7.56
7.56
7.13
7.11
7.05
7.04
7.03
7.02
6.96
6.78
6.77
3.55
2.28
1.49
S
O
O
O
S
O
NH
7k
1.07
0.91
0.88
1.16
1.01
0.90
3.00
2.99
9.95
f1 (ppm)

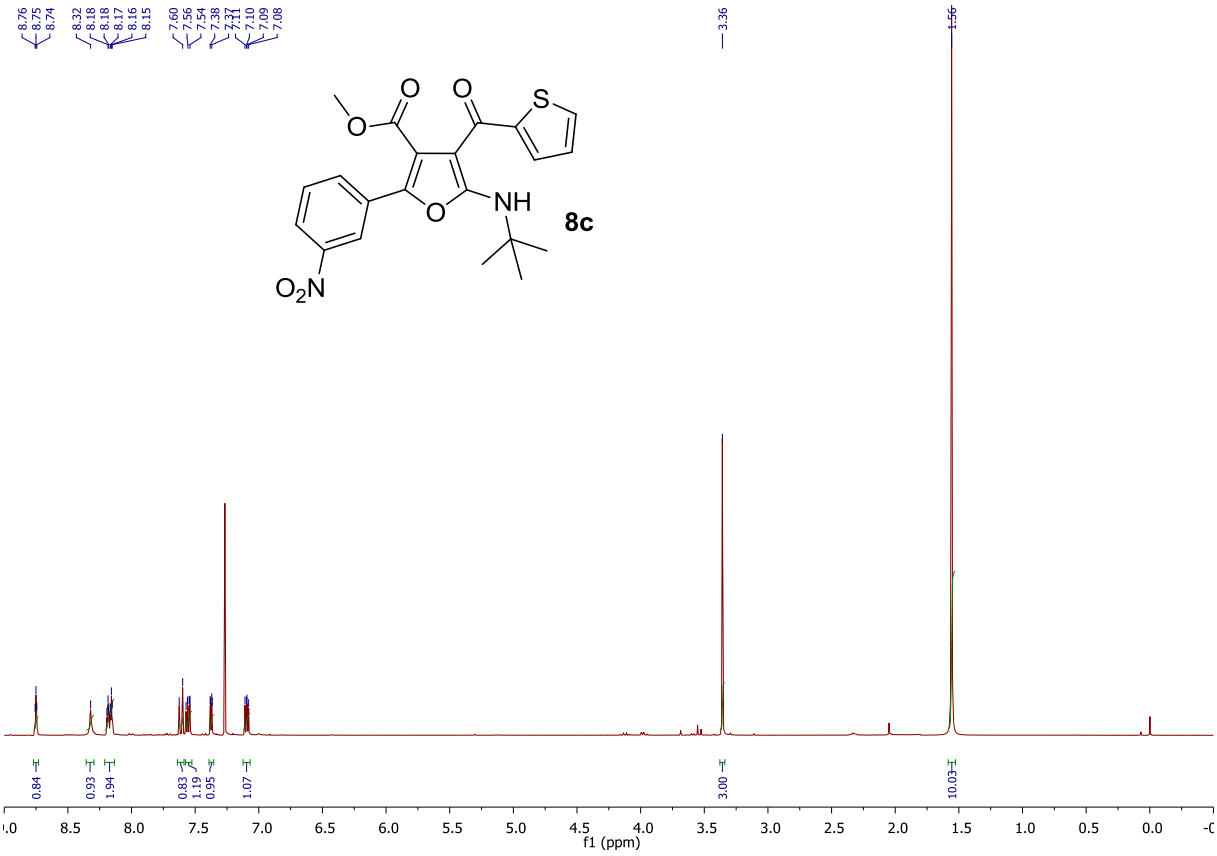

ntn213bf2cpd/1
NTN 213 b F2 le 27/07/2012
165.26
161.98
145.07
136.60
134.40
134.32
130.58
128.69
127.93
125.32
124.83
102.11
88.99
52.79
50.85
29.92
15.59
f1 (ppm)

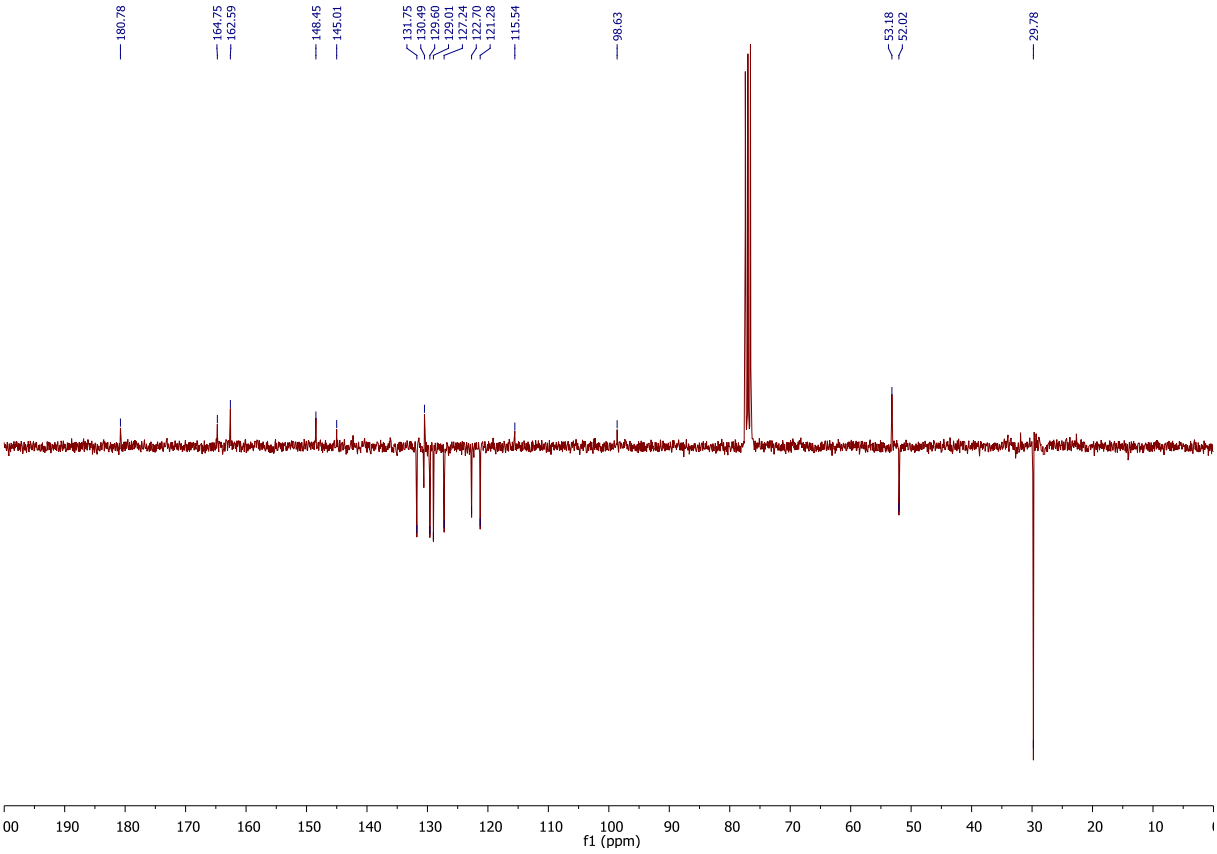

8.35
7.85
7.84
7.82
7.81
7.43
7.43
7.40
7.37
7.09
7.08
7.07
7.06
3.32
1.53
O
O
O
S
NH
O
8a
0.93
2.03
1.06
2.13
1.88
1.10
3.00
9.30
f1 (ppm)

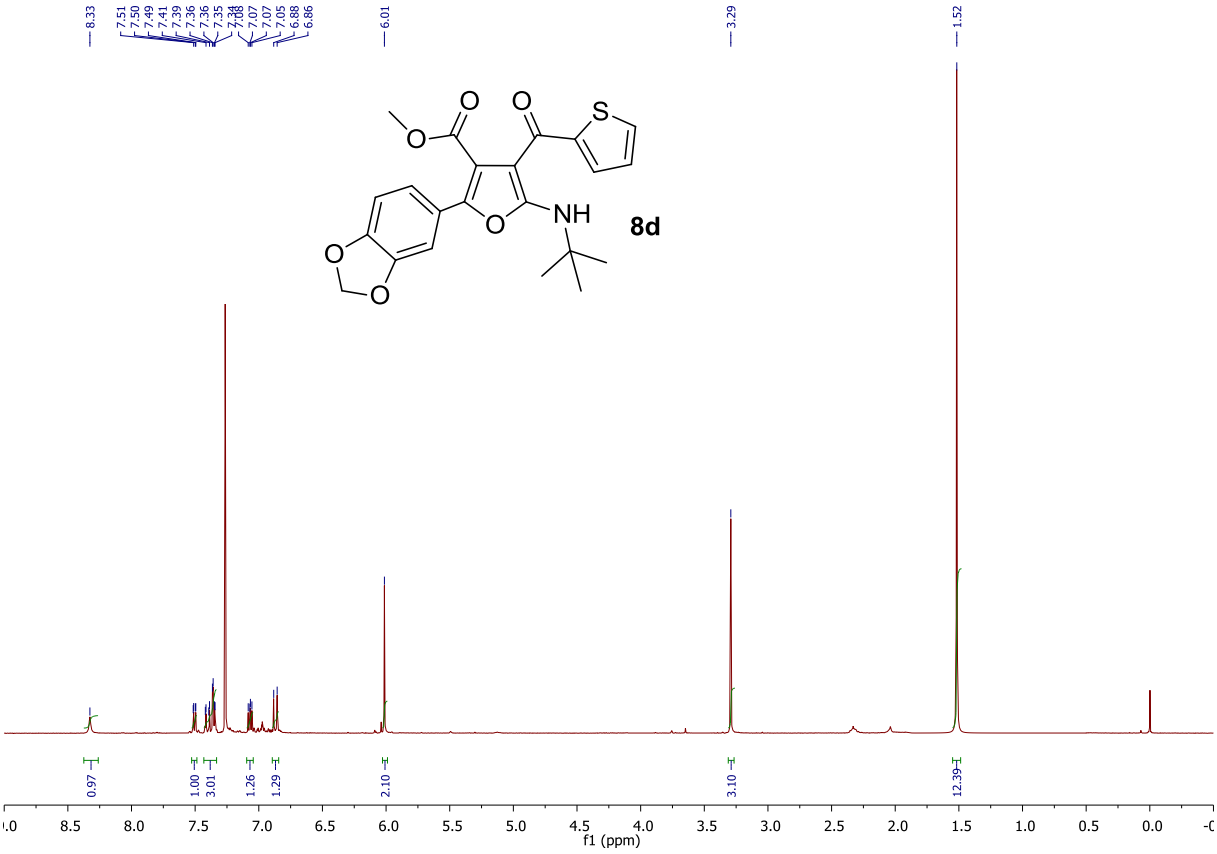

ntn160f1/2
NTN 161 F 1 le 16/05/2012
165.18
162.63
145.20
130.11
129.72
128.88
128.74
128.60
128.52
127.11
126.61
113.09
98.51
52.94
51.71
29.77
f1 (ppm)

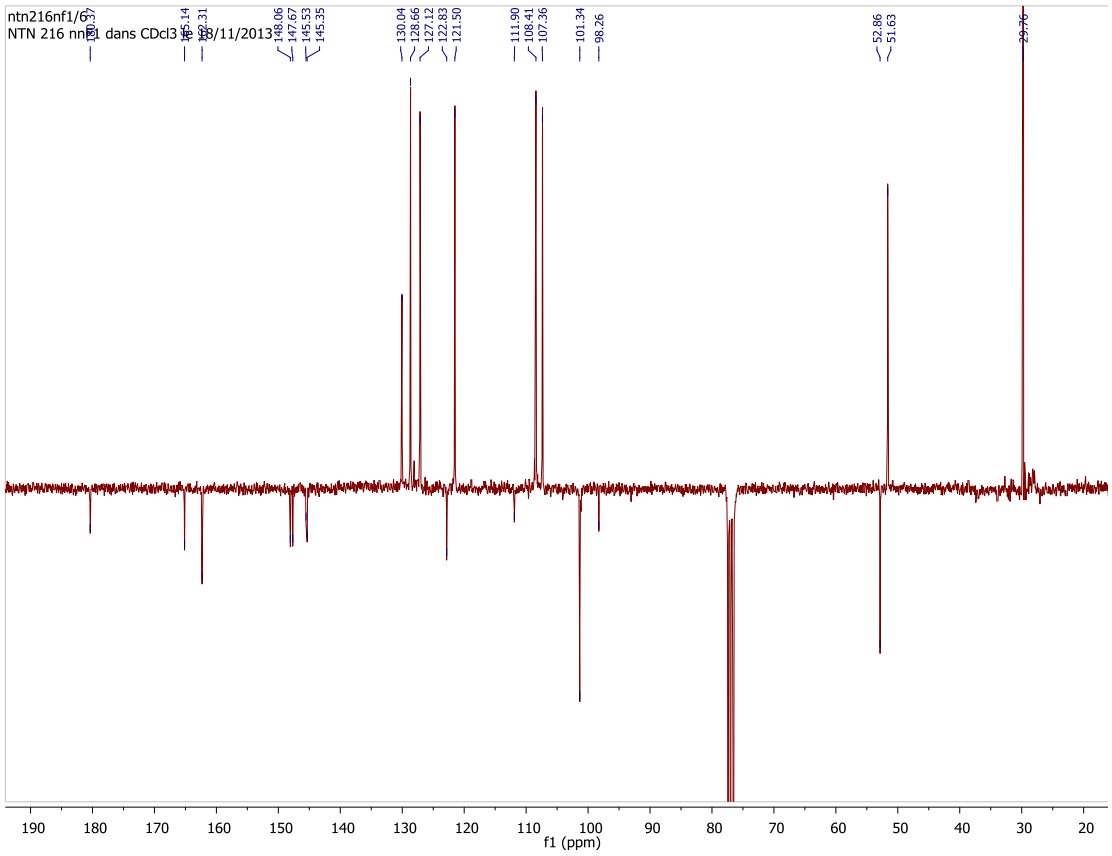

8.34
8.28
8.25
7.99
7.96
7.57
7.55
7.55
7.37
7.35
7.11
7.10
7.08
3.35
1.56
O
O
O
S
NH
O
O_2N
8b
0.98
2.05
2.06
0.95
1.00
1.07
3.04
10.04
f1 (ppm)

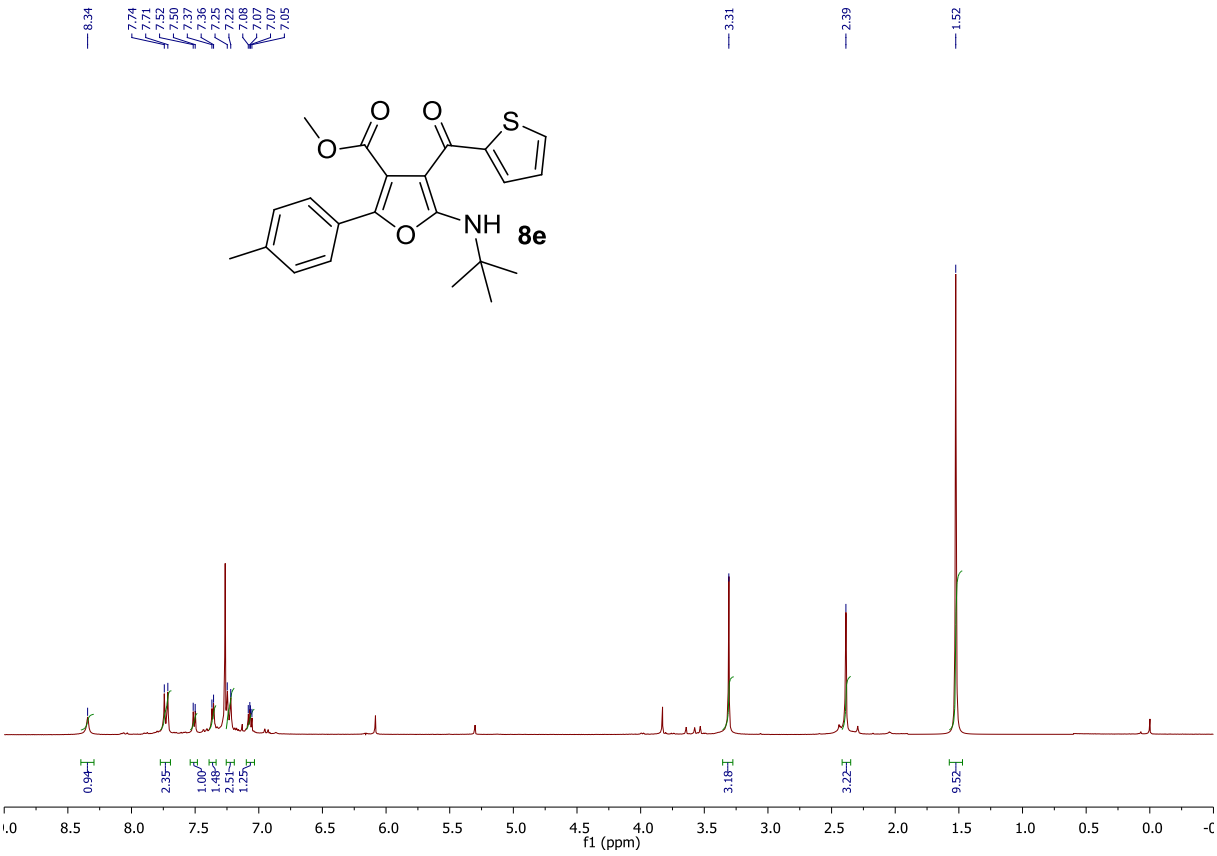

ntn157f1
NTN 157 F1 le 30/05/2012
164.83
162.70
146.56
144.78
141.78
134.73
130.70
129.00
127.22
126.13
123.97
116.84
99.19
53.19
52.05
29.66
f1 (ppm)

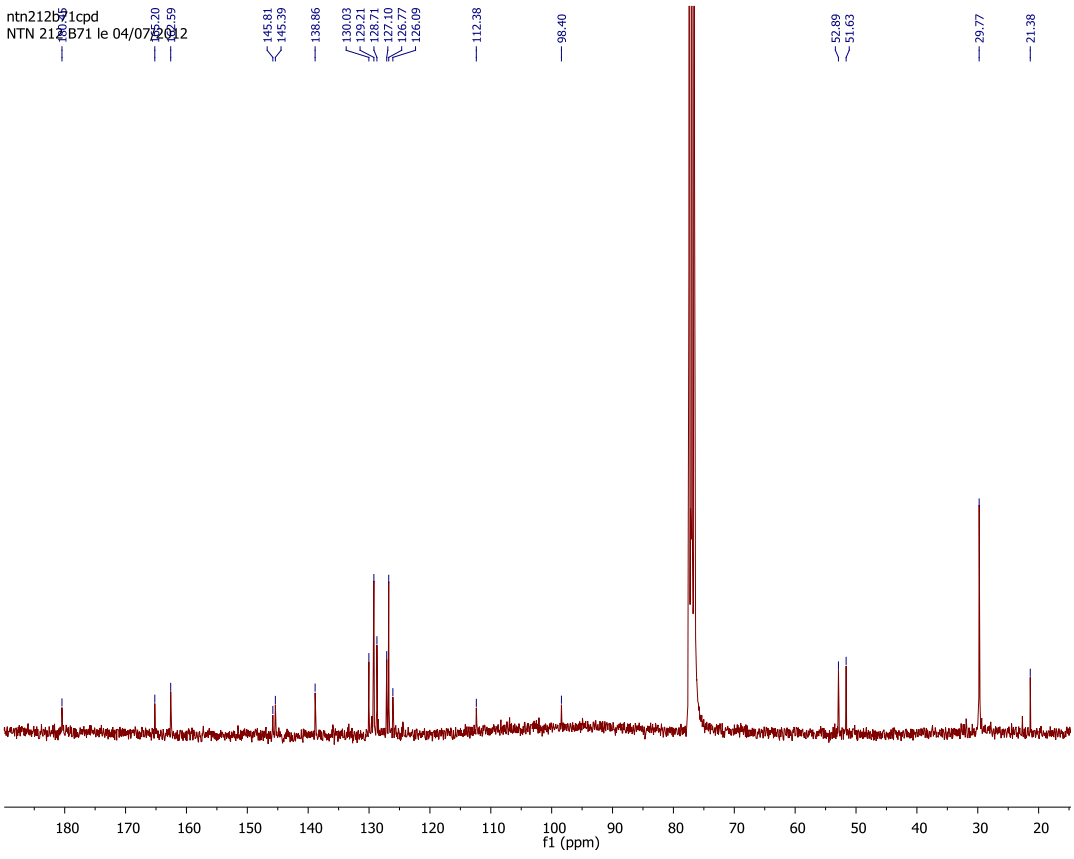

8.76
8.75
8.74
8.32
8.18
8.18
8.17
8.16
8.15
7.60
7.56
7.54
7.38
7.37
7.11
7.09
7.08
3.36
1.56
O
O
O
S
NH
O
O2N
8c
0.84
0.93
1.94
0.83
1.19
0.95
1.07
3.00
10.03
f1 (ppm)

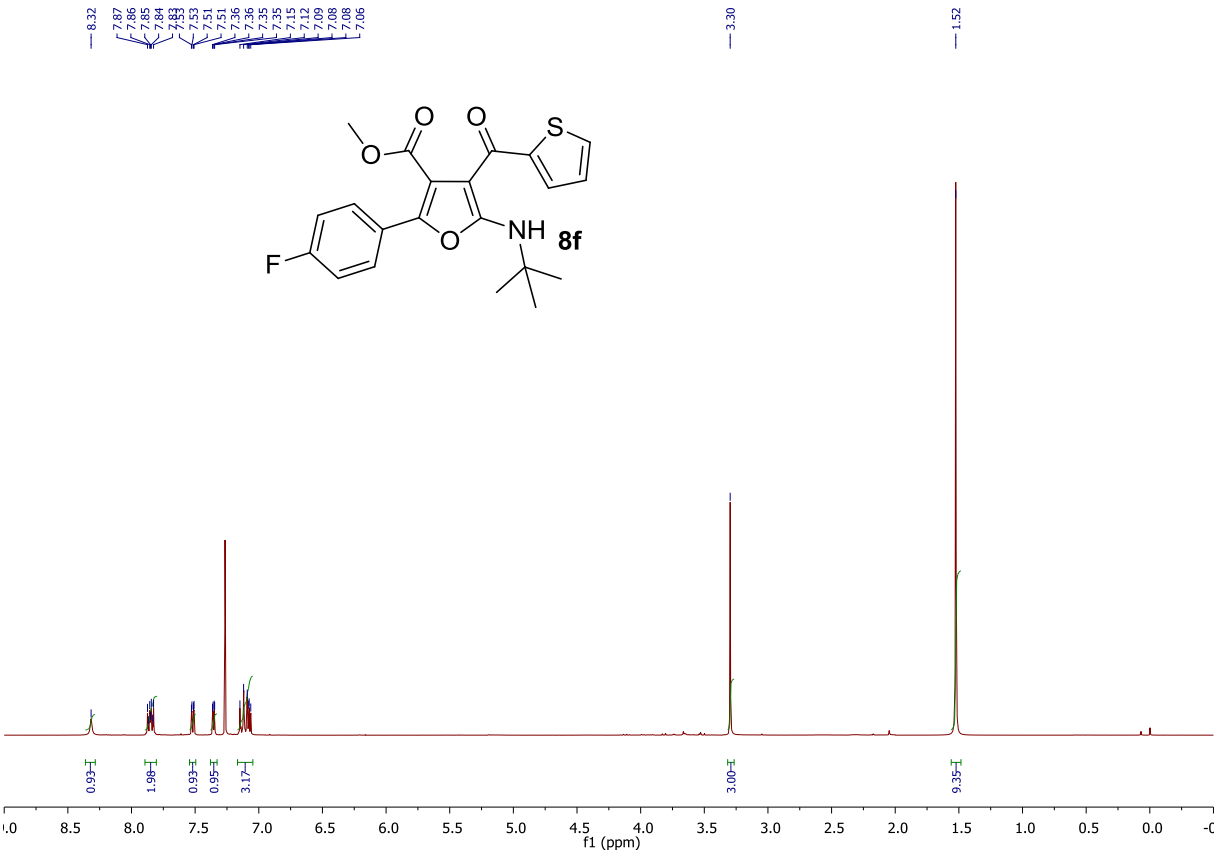

180.78
164.75
162.59
148.45
145.01
131.75
130.49
129.60
129.01
127.24
122.70
121.28
115.54
98.63
53.18
52.02
29.78
f1 (ppm)

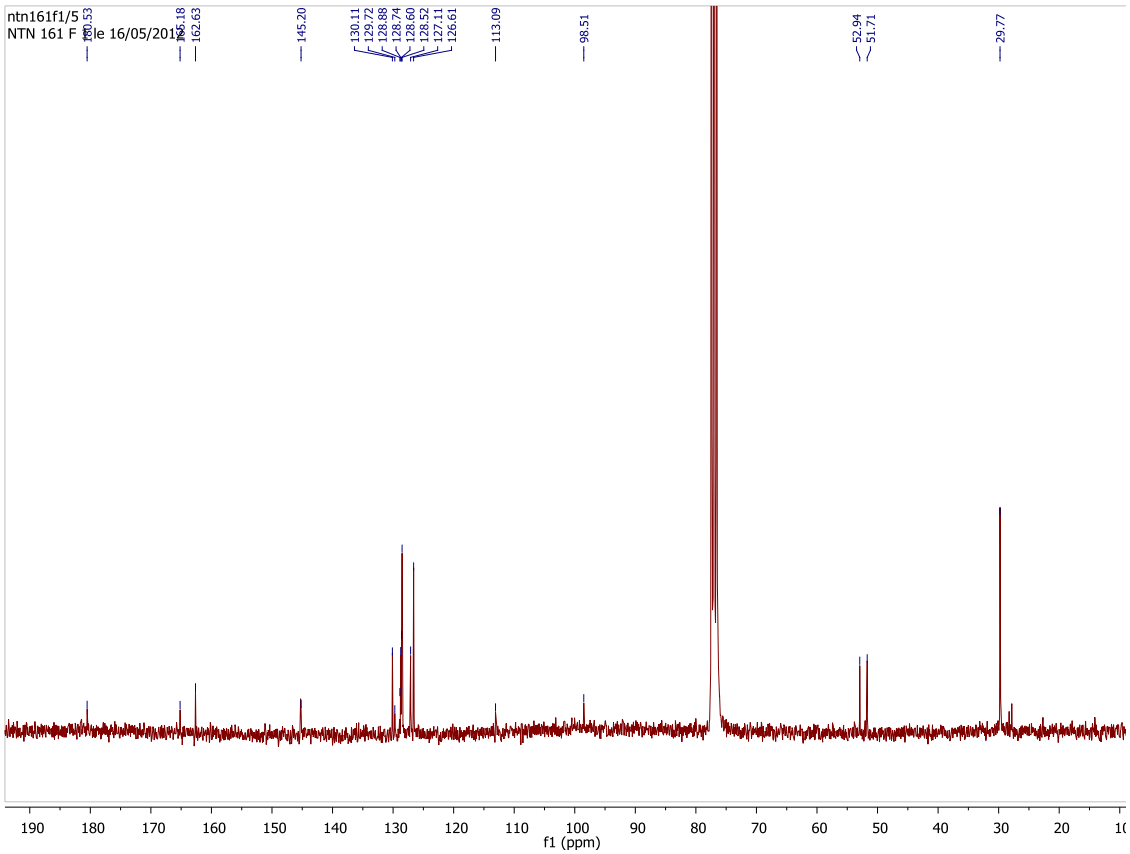

8.33
7.51
7.50
7.49
7.41
7.39
7.36
7.36
7.35
7.34
7.08
7.07
7.07
7.05
6.88
6.86
6.01
3.29
1.52
O
O
S
O
O
NH
O
O
8d
0.97
1.00
3.01
1.26
1.29
2.10
3.10
12.39
f1 (ppm)

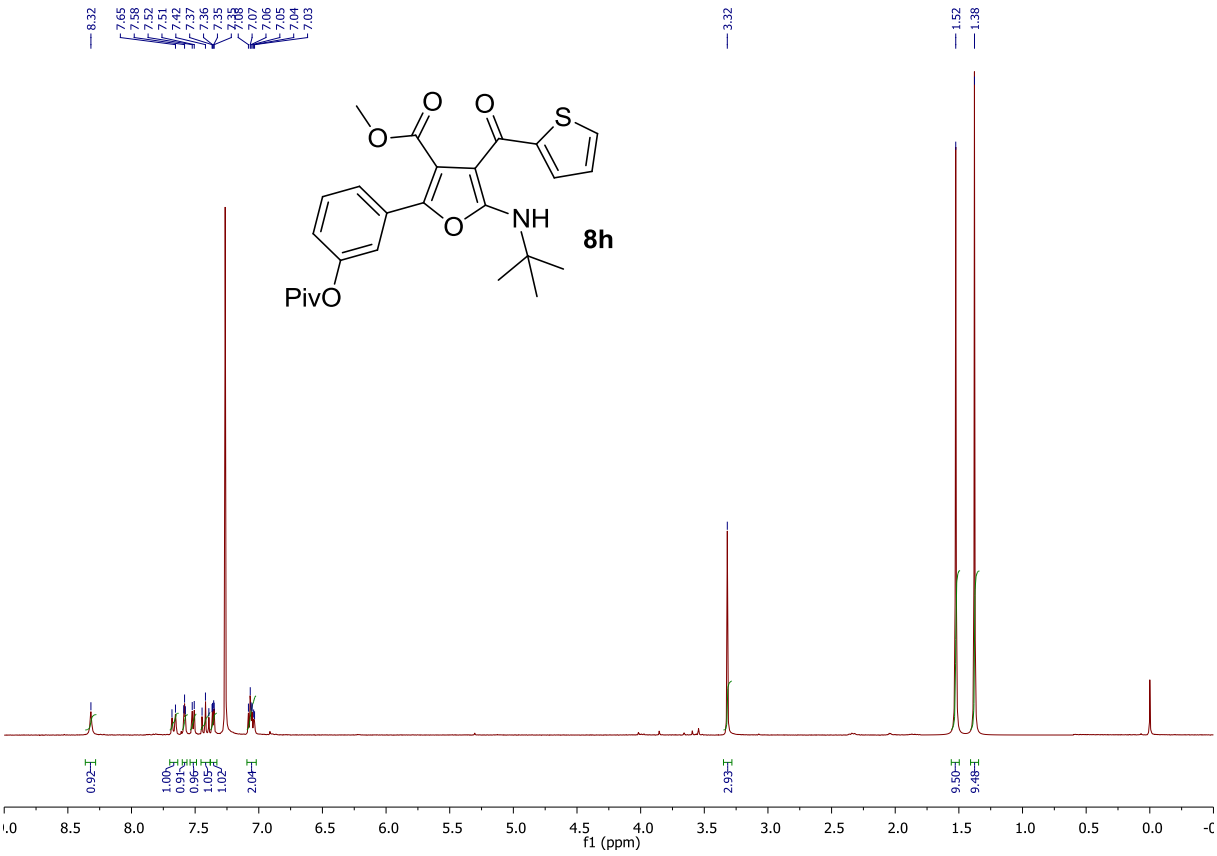

ntn216nf1/6
NTN 216 nmr1 dans CDcl3 le 28/11/2013
180.37
165.14
162.31
149.06
147.67
145.53
145.35
130.04
128.66
127.12
122.83
121.50
111.90
108.41
107.36
101.34
98.26
52.86
51.63
29.76
f1 (ppm)

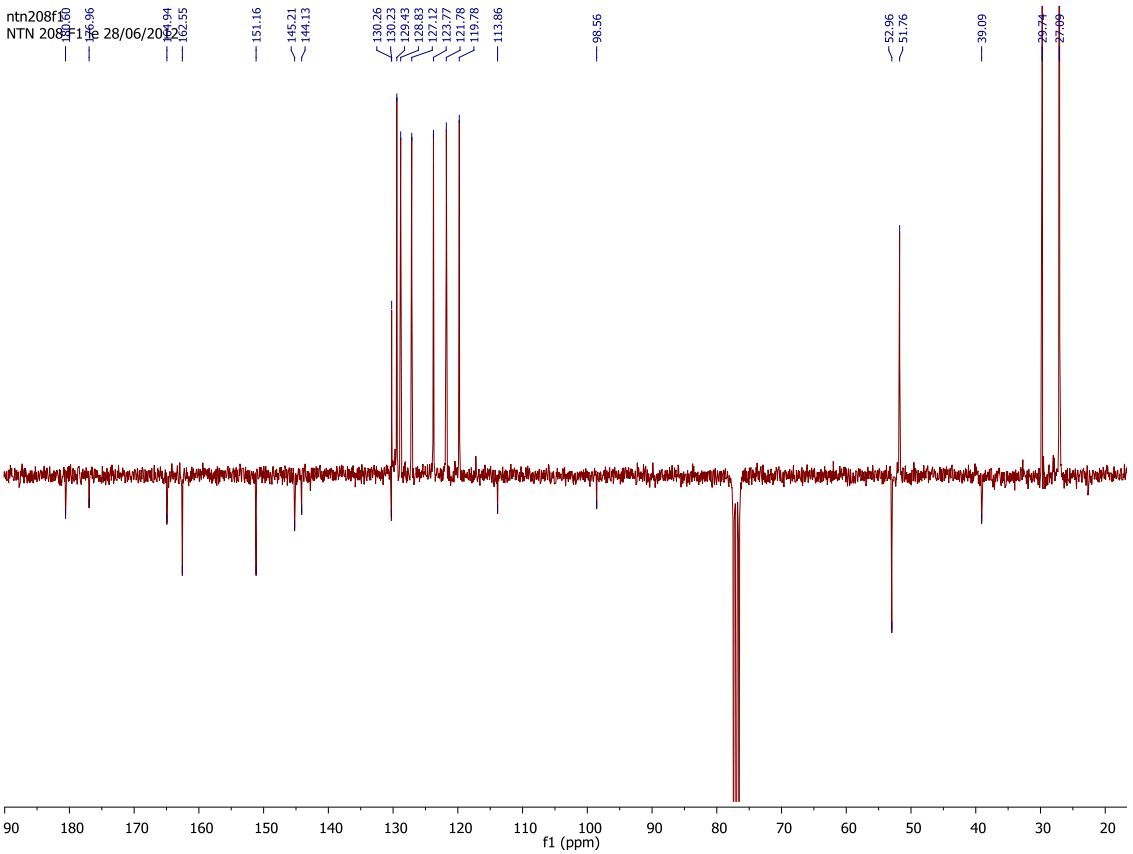

8.34
7.74
7.71
7.52
7.50
7.37
7.36
7.25
7.22
7.08
7.07
7.07
7.05
3.31
2.39
1.52
O
O
O
S
NH
O
8e
0.94
2.35
1.00
1.48
2.51
1.25
3.18
3.22
9.52
f1 (ppm)

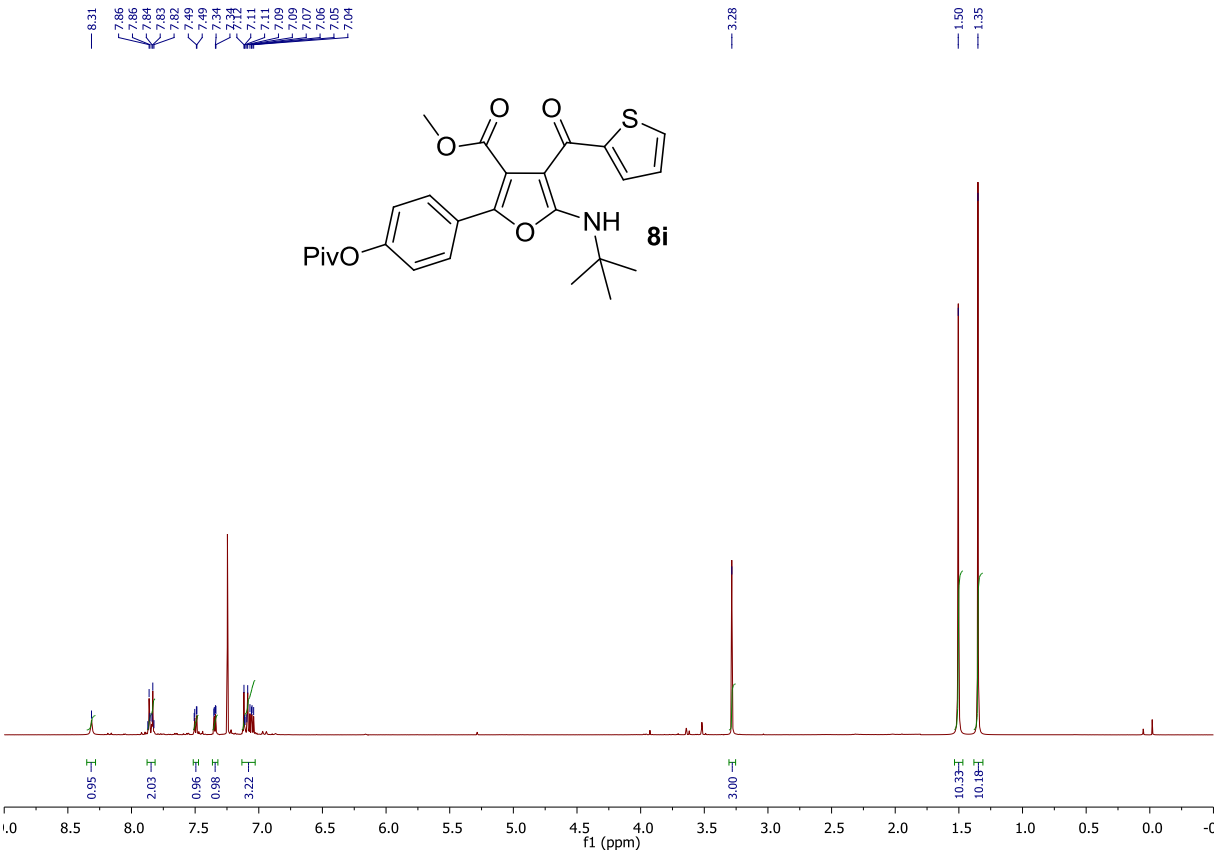

ntn212b71cpd
NTN 212B71 le 04/07/2012
145.81
145.39
138.86
130.03
129.21
128.71
127.10
126.77
126.09
112.38
98.40
52.89
51.63
29.77
21.38
f1 (ppm)

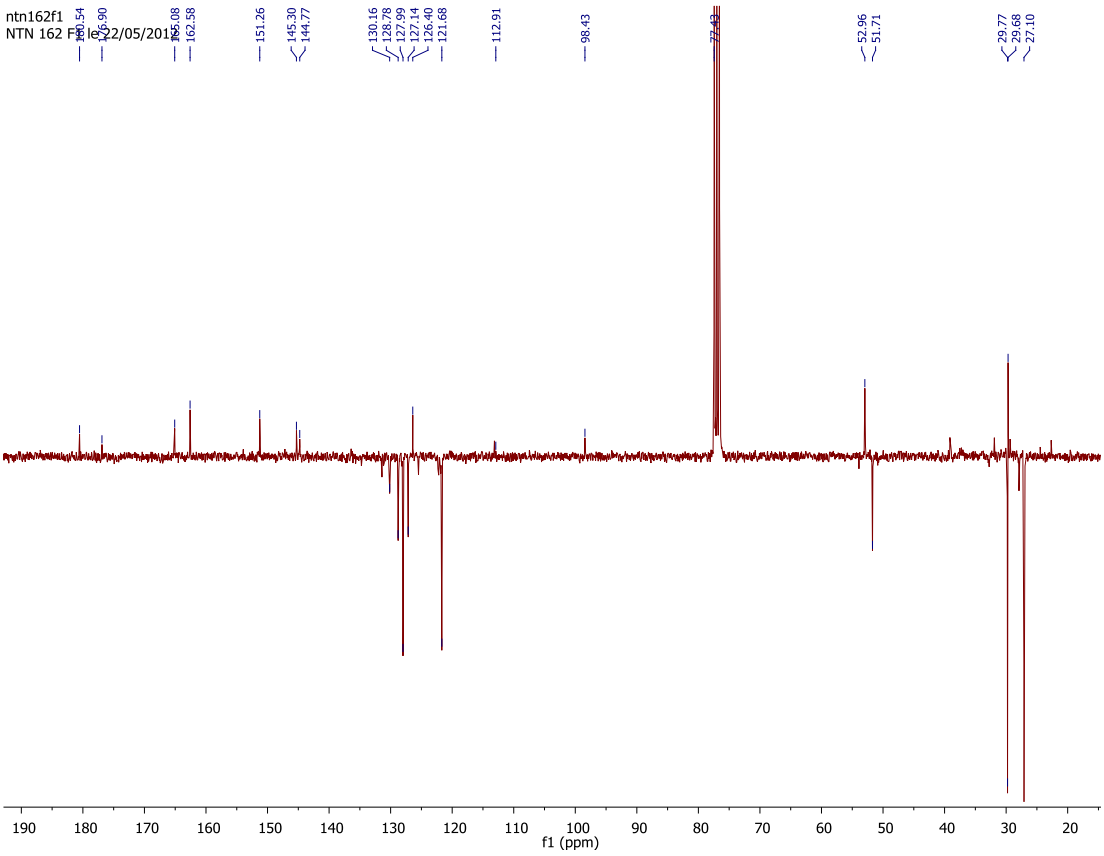

8.32
7.87
7.86
7.85
7.84
7.83
7.53
7.51
7.51
7.36
7.36
7.35
7.35
7.15
7.12
7.09
7.08
7.08
7.06
3.30
1.52
O
O
O
S
NH
O
F
8f
0.93
1.98
0.93
0.95
3.17
3.00
9.35
f1 (ppm)

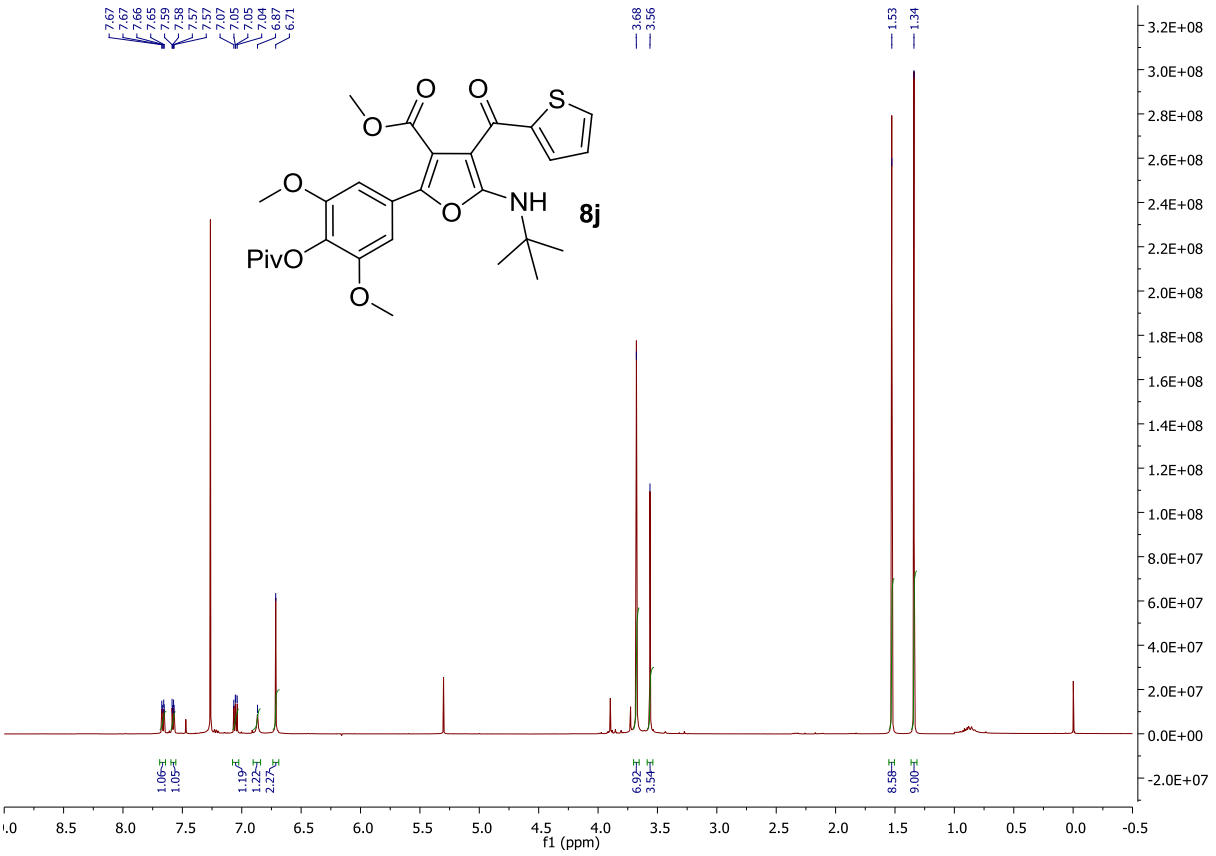

ntn161f1/5
NTN 161 F
162.63
145.20
130.11
129.72
128.88
128.74
128.60
128.52
127.11
126.61
113.09
98.51
52.94
51.71
29.77
f1 (ppm)

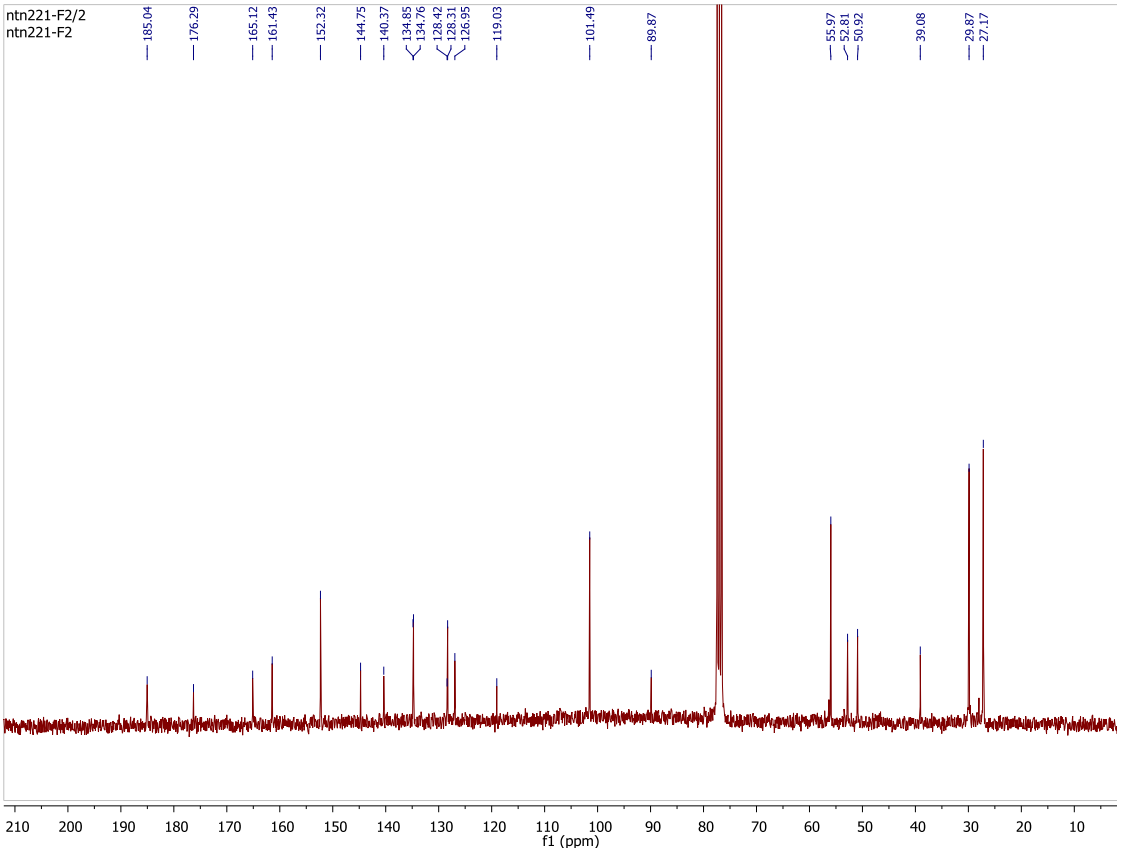

8.32
7.65
7.58
7.52
7.51
7.42
7.37
7.36
7.35
7.08
7.07
7.06
7.05
7.04
7.03
3.32
1.52
1.38
O
O
O
S
NH
PivO
8h
0.92
1.00
0.91
0.96
1.05
1.02
2.04
2.93
9.50
9.48
f1 (ppm)

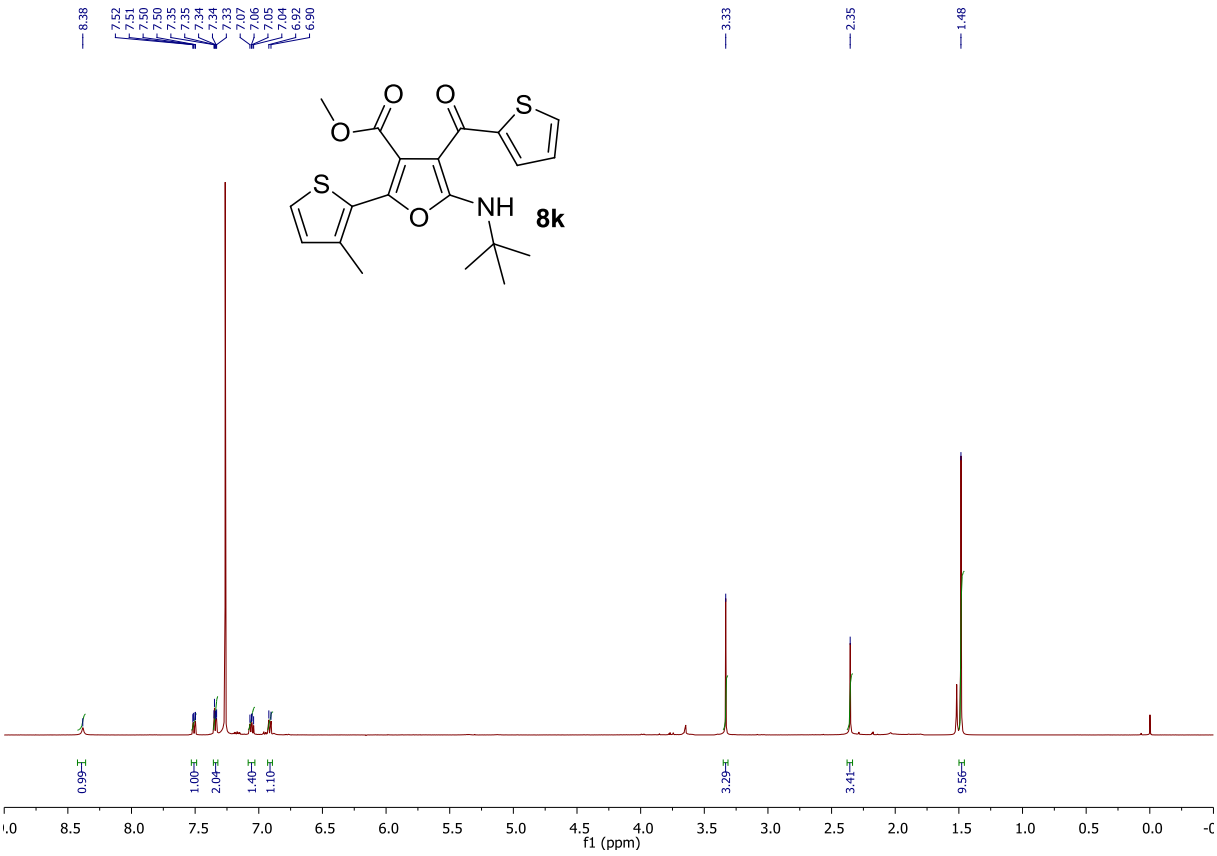

ntn208f1
NTN 208-1 1e 28/06/2017
176.96
162.55
151.16
145.21
144.13
130.26
130.23
129.43
128.83
127.12
123.77
121.78
119.78
113.86
98.56
52.96
51.76
39.09
29.74
27.09
f1 (ppm)

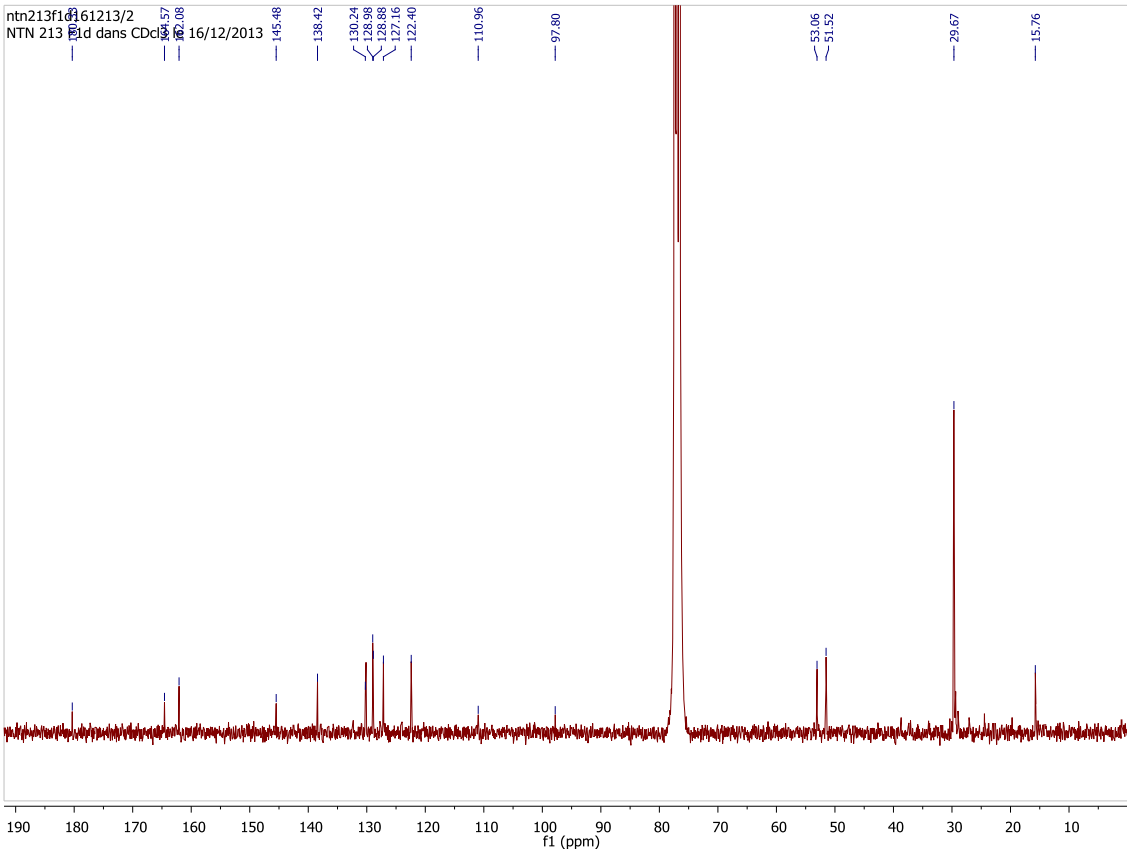

8.31
7.86
7.86
7.84
7.83
7.82
7.49
7.49
7.34
7.34
7.12
7.11
7.09
7.09
7.07
7.06
7.05
7.04
3.28
1.50
1.35
O
O
O
S
NH
PivO
8i
0.95
2.03
0.96
0.98
3.22
3.00
10.33
10.18
f1 (ppm)


ntn162f1
NTN 162 FIE 22/05/2015
160.54
156.90
163.08
162.58
151.26
145.30
144.77
130.16
128.78
127.99
127.14
126.40
121.68
112.91
98.43
77.43
52.96
51.71
29.77
29.68
27.10
f1 (ppm)


7.67
7.67
7.66
7.65
7.59
7.58
7.57
7.57
7.07
7.05
7.05
7.04
6.87
6.71
3.68
3.56
1.53
1.34
O
O
O
S
O
NH
8j
PivO
O
1.06
1.05
1.19
1.22
2.27
6.92
3.54
8.58
9.00
3.2E+08
3.0E+08
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
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
-0.5
f1 (ppm)


ntn221-F2/2
ntn221-F2
185.04
176.29
165.12
161.43
152.32
144.75
140.37
134.85
134.76
128.42
128.31
126.95
119.03
101.49
89.87
55.97
52.81
50.92
39.08
29.87
27.17
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


8.38
7.52
7.51
7.50
7.50
7.35
7.34
7.34
7.33
7.07
7.06
7.05
7.04
6.92
6.90
3.33
2.35
1.48
O
O
S
O
S
NH
8k
0.99
1.00
2.04
1.40
1.10
3.29
3.41
9.56
f1 (ppm)


ntn213f1d161213/2
NTN 213 f1d dans CDcl3 16/12/2013
145.48
138.42
130.24
128.98
128.88
127.16
122.40
110.96
97.80
53.06
51.52
29.67
15.76
f1 (ppm)