Chemoselective Synthesis of Tetrasubstituted Furans via Intramolecular Wittig Reactions: Mechanism and Theoretical Analysis

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Supporting Information

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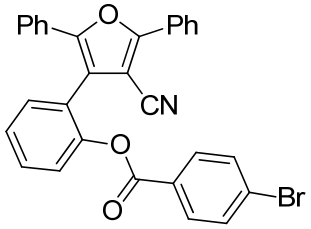
TP : Typical procedure for the preparation of compounds **3** and **14**:

A dry and nitrogen-flushed 10-mL Schlenk tube, equipped with a magnetic stirring bar and a septum, was charged with a solution of **1** (0.5 mmol) or **12** (0.3 mmol) and **4** (1.1 equiv) in dry THF (1.0 mL or 0.6 mL). Bu_3P (1.2 equiv) and Et_3N (1.3 equiv) were sequentially added, and the resulting mixture was stirred for 15 minutes to 3 hours at room temperature (27-30 ^oC). Thereafter, the solvent was removed by evaporation *in vacuo*. Purification by flash chromatography furnished **3** and **14.**

Synthesis of 2-(4-cyano-2,5-diphenylfuran-3-yl)phenyl 4-bromobenzoate (3a):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate **1a** (215.5 mg, 0.5 mmol), benzoyl chloride **4a** (64.0 μL, 1.1 equiv), Bu_3P (150.0 μL, 1.2 equiv) and Et_3N (91.0 μL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3a** as white solid (228.4 mg, 88%).

mp: 158.8-159.3 °C

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.04 (*pseudo* d, 2H, J = 7.2 Hz), 7.73 (*pseudo* d, 2H, J = 8.5 Hz), 7.59-7.36 (m, 11H), 7.36-7.30 (m, 3H).

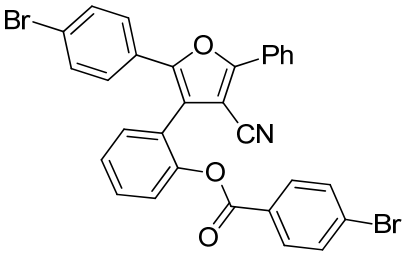
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 163.5, 158.2, 149.4, 148.6, 131.6, 131.5, 131.4, 130.3,130.1, 128.9, 128.8, 128.7, 128.5, 127.6, 127.5, 126.7, 126.0, 125.2, 123.6, 123.3, 118.9, 114.2, 95.7.

MS (70 eV, EI) *m/z* (%): 521 $[M+2]^+$ (100), 519 $[M]^+$ (80), 183 (85), 155 (30), 105 (70), 77 (30) ;

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3063 (w), 2221 (m), 1738 (s), 1587 (m), 1491 (m), 1259 (s), 1063 (s), 750 (m).

HRMS (ESI) for **$C_{30}H_{18}BrNO_3Na$**, **$[M+Na]^+$** (542.0368) found: 542.0369.

Synthesis of 2-(2-(4-bromophenyl)-4-cyano-5-phenylfuran-3-yl)phenyl 4-bromobenzoate (3b):



Prepared according to **TP** from starting material (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate **1a** (215.5 mg, 0.5 mmol), 4-bromobenzoyl chloride **4b** (120.7 mg, 1.1 equiv), Bu_3P (150.0 µL, 1.2 equiv) and Et_3N (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3b** as white solid (256.7 mg, 86%).

mp: 180.5-181.3 °C

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.02 (*pseudo* d, 2H, J = 6.8 Hz), 7.77 (*pseudo* d, 2H, J = 8.8 Hz), 7.60-7.32 (m, 13H).

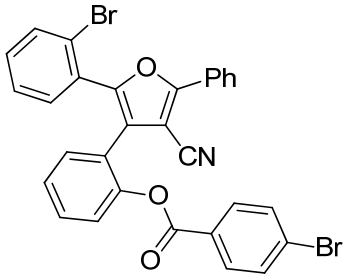
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 163.7, 158.7, 148.9, 148.6, 132.2, 131.9, 131.8, 131.6, 131.5, 130.7, 130.4, 129.2, 129.0, 127.8, 127.7, 127.6, 127.5, 127.0, 125.5, 123.5, 123.2, 119.8, 114.1, 96.0.

MS (70 eV, EI) *m/z* (%): 598 $[M+1]^+$ (25), 596 $[M-1]^+$ (17), 185(65), 183 (100), 157 (17), 155 (20), 105 (53), 77 (22).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3063 (w), 2229 (m), 1738 (s), 1591 (m), 1491(m), 1255 (s), 1067 (s), 750 (m).

HRMS (ESI) for **$C_{30}H_{17}Br_2NO_3Na$**, **$[M+Na]^+$** (619.9473) found: 619.9468.

Synthesis of 2-(2-(2-bromophenyl)-4-cyano-5-phenylfuran-3-yl)phenyl 4-bromobenzoate (3c):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate **1a** (215.5 mg, 0.5 mmol), 2-bromobenzoyl chloride **4c** (72.0 µL, 1.1 equiv), Bu_3P (150.0 µL, 1.2 equiv) and Et_3N (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3c** as white solid (274.6 mg, 92%).

mp: 160.3-160.9 °C

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.04 (*pseudo* dd, 2H, J = 8.2, 1.4 Hz), 7.97 (*pseudo* d, 2H, J = 8.6 Hz), 7.66-7.56(m, 3H), 7.53-7.41 (m, 4H), 7.34-7.18 (m, 6H).

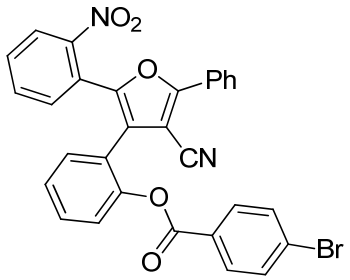
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 163.8, 159.4, 149.1, 148.8, 133.7, 132.4, 131.9, 131.8, 131.6, 130.9, 130.4, 130.2, 129.1, 127.9, 127.8, 127.5, 126.6, 125.6, 123.3, 123.2, 123.1, 122.0, 114.5, 94.7.

MS (20 eV, EI) *m/z* (%): 601 $[M+4]^+$ (25), 599 $[M+2]^+$ (88), 597 $[M]^+$ (46), 185 (100), 183 (100), 105 (3).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3063 (w), 2229 (m), 1738 (s), 1587 (m), 1488 (m), 1259 (s), 1067 (s), 750 (m).

HRMS (EI) for **$C_{30}H_{17}Br_2NO_3$**, **$[M]^+$** (596.9575) found: 596.9581.

Synthesis of 2-(4-cyano-2-(2-nitrophenyl)-5-phenylfuran-3-yl)phenyl 4-bromobenzoate (3d):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate **1a** (215.5 mg, 0.5 mmol), 2-nitrobenzoyl chloride **4d** (73.0 µL, 1.1 equiv), Bu_3P (150.0 µL, 1.2 equiv) and Et_3N (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3d** as yellow solid (248.2 mg, 88%).

mp: 201.3-202.2 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.97 (*pseudo* d, 2H, J = 8.4 Hz), 7.93-7.85 (m, 3H), 7.58 (*pseudo* d, 2H, J = 8.4 Hz), 7.55-7.28 (m, 10H).

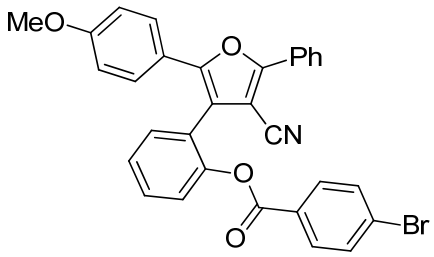
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 164.1, 160.1, 148.9, 148.5, 145.7, 132.9, 131.9, 131.8, 131.7, 131.6, 130.7, 130.1, 129.2, 129.1, 127.6, 127.3, 126.9, 125.6, 124.6, 123.4, 122.9, 122.8, 114.1, 95.0.

MS (20 eV, EI) *m/z* (%): 564 $[M]^+$ (2), 365 (30), 260 (14), 185 (36), 183 (38), 105 (100).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3063 (w), 2229 (m), 1738 (s), 1587 (m), 1528 (s), 1491 (m), 1347 (m), 1255 (s), 1067 (s), 750 (s).

HRMS (EI) for **$C_{30}H_{17}BrN_2O_5$**, **$[M]^+$** (564.0321) found: 564.0317.

Synthesis of 2-(4-cyano-2-(4-methoxyphenyl)-5-phenylfuran-3-yl)phenyl 4-bromobenzoate (3e):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate **1a** (215.5 mg, 0.5 mmol), 4-methoxybenzoyl chloride **4e** (75.0 µL, 1.1 equiv), Bu_3P (150.0 µL, 1.2 equiv) and Et_3N (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 30 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3e** as white solid (222.4 mg, 81%).

mp: 93.2-94.0 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.01 (*pseudo* d, 2H, J = 7.2 Hz), 7.77 (*pseudo* d, 2H, J = 8.4 Hz), 7.59-7.33 (m, 11H), 6.83 (*pseudo* d, 2H, J = 8.8 Hz), 3.81 (s, 3H).

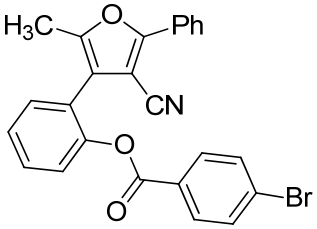
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 163.8, 160.1, 157.9, 149.8, 148.9, 131.8,131.7, 131.6, 130.2, 130.0, 129.1, 128.8, 127.9, 127.8, 127.7, 126.8, 125.3, 124.0, 123.4, 121.5, 117.5, 114.5, 114.1, 95.7, 55.3.

MS (70 eV, EI) *m/z* (%): 550 $[M+2]^+$ (70), 548 (70), 185 (74), 183 (100), 155 (18), 135 (48), 105 (48), 77 (18).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3077 (w), 2221 (m), 1735 (s), 1613 (m), 1513 (m), 1255 (s), 1071 (s), 750 (m).

HRMS (ESI) for **$C_{30}H_{21}BrNO_4$**, **$[M+H]^+$** (550.0654) found: 550.0634.

Synthesis of 2-(4-cyano-2-methyl-5-phenylfuran-3-yl)phenyl 4-bromobenzoate (3f):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate **1a** (215.5 mg, 0.5 mmol), acetyl chloride **4f** (40.0 µL, 1.1 equiv),

Bu_3P (150.0 µL, 1.2 equiv) and EtN_3 (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3f** as white solid (102.8 mg, 45%).

mp:130.0-130.8 °C

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.02 (d, 2H, J = 8.4 Hz), 7.92 (*pseudo* d, 2H, J = 7.2 Hz), 7.59 (d, 2H, J = 8.4 Hz), 7.54-7.33 (m, 7H), 2.31 (s, 3H).

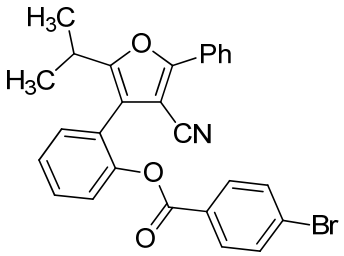
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 163.9, 158.1, 149.8, 148.9, 132.0, 131.6, 131.4, 130.0, 129.8, 129.0, 128.0, 127.9, 126.6, 125.1, 123.5, 123.1, 119.2, 114.8, 93.8, 12.1.

MS (70 eV, EI) *m/z* (%): 459 $[M+2]^+$ (27), 457 $[M]^+$ (36), 185 (64), 183 (100), 105 (35).

IR (KBr) $\tilde{\nu}$ (cm^{-1}):2915 (w), 2221 (m), 1738 (s), 1587 (m), 1491 (m), 1255 (s), 1067 (s), 750 (m).

HRMS (ESI) for **$C_{25}H_{16}BrNO_3Na$**, **$[M+Na]^+$** (480.0211) found: 480.0216.

Synthesis of 2-(4-cyano-2-isopropyl-5-phenylfuran-3-yl)phenyl 4-bromobenzoate (3g):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate **1a** (215.5 mg, 0.5 mmol), isobutyryl chloride **4g** (58.0 µL, 1.1 equiv), Bu_3P (150.0 µL, 1.2 equiv) and Et_3N (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3g** as white solid (179.5 mg, 74%).

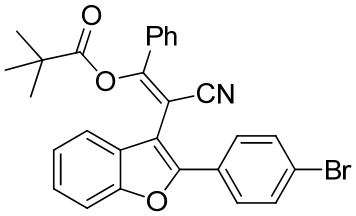
mp: 180.5-181.2 °C

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.01 (*pseudo* d, 2H, J = 8.3 Hz), 7.91 (*pseudo* d, 2H, J = 7.5 Hz), 7.61-7.28 (m, 9H), 3.02 (hept, 1H, J = 6.9 Hz), 1.48-0.97 (brs, 6H), 7.51-7.39 (m, 3H), 7.33-7.24 (m, 2H), 7.03 (*pseudo* t, 1H, J = 7.5 Hz), 6.96 (*pseudo* d, 1H, J = 8.0 Hz), 5.50-5.09 (brs, 1H), 2.36 (s, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 163.9, 158.0, 157.7, 149.2, 132.0, 131.6, 131.5, 130.1, 129.8, 129.0, 128.2, 128.0, 126.5, 125.1, 123.7, 123.1, 117.4, 114.8, 93.9, 26.5, 21.3.

MS (70 eV, EI) *m/z* (%): 487 $[M+2]^+$ (20), 485 $[M]^+$ (20), 302 (18), 272 (10), 183 (100), 155 (35), 105 (58), 77 (53).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3063 (w), 2967 (w), 2214 (m), 1738 (s), 1587 (m), 1488 (m), 1255 (s), 1067 (s), 750 (m).
HRMS (ESI) for **$C_{27}H_{20}BrNO_3Na$**, **$[M+Na]^+$** (508.0524) found: 508.0527.

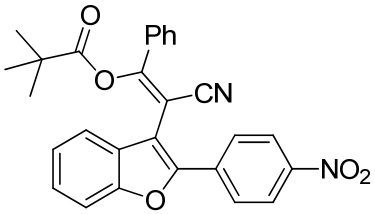
Synthesis of (*E*)-2-(2-(4-bromophenyl)benzofuran-3-yl)-2-cyano-1-phenylvinyl pivalate (3'h):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate **1a** (215.5 mg, 0.5 mmol), trimethylacetyl chloride **4h** (68.0 µL, 1.1 equiv), Bu_3P (150.0 µL, 1.2 equiv) and Et_3N (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3'h** as yellow solid (222.1 mg, 89%).

mp: 142.1-142.9 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.93-7.80 (m, 4H), 7.63 (*pseudo* d, 2H, *J* = 8.6 Hz), 7.59-7.49 (m, 5H), 7.39-7.27 (m, 2H), 94 0.81 (s, 9H).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 174.6, 163.1, 153.8, 152.1, 132.3, 132.1, 131.7, 128.9, 128.4, 128.3, 127.9, 127.8, 125.5, 123.9, 123.5, 120.4, 116.5, 111.3, 107.6, 95.4, 39.0, 26.3.
MS (70 eV, EI) *m/z* (%): 501 $[M+2]^+$ (12), 499 $[M]^+$ (12), 417 (40), 415 (60), 105 (70), 85 (25), 57 (100).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 2967 (m), 2214 (m), 1760 (s), 1480 (m), 1451 (s), 1093 (s), 1074 (s), 743 (s).
HRMS (ESI) for **$C_{28}H_{22}BrNO_3Na$**, **$[M+Na]^+$** (522.0681) found: 522.0683.

Synthesis of (*E*)-2-cyano-2-(2-(4-nitrophenyl)benzofuran-3-yl)-1-phenylvinyl pivalate (3'i):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-nitrobenzoate **1b** (199.0 mg, 0.5 mmol), trimethylacetyl chloride **4h** (68.0 μL, 1.1 equiv), Bu_3P (150.0 μL, 1.2 equiv) and Et_3N (91.0 μL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3'i** as yellow solid (202.8 mg, 87%).

mp: 171.5-172.5 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.36 (d, 2H, J = 8.8 Hz), 8.15 (d, 2H, J = 8.8 Hz), 7.90 (*pseudo* dd, 2H, J = 7.8, 1.8 Hz), 7.64-7.52 (m, 5H), 7.43 (*pseudo* t, 1H, J = 7.2 Hz), 7.36 (*pseudo* t, 1H, J = 7.2 Hz), 0.81 (s, 9H).

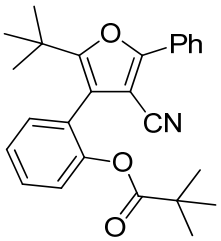
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 174.6, 163.6, 154.2, 150.4, 147.7, 135.2, 132.0, 131.9, 129.0, 127.8, 127.5, 126.6, 124.1, 123.9, 120.8, 116.3, 111.6, 110.4, 94.7, 39.0, 26.3.

MS (70 eV, EI) *m/z* (%): 382 $[M-84]^+$ (5), 105 (100), 77 (40).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 2967 (w), 2214 (w), 1760 (m), 1598 (m), 1517 (s), 1340 (s), 1097 (s), 1074 (s).

HRMS (ESI) for **$C_{28}H_{22}N_2O_5Na$**, **$[M+Na]^+$** (489.1426) found: 489.1421.

Synthesis of 2-(2-*tert*-butyl-4-cyano-5-phenylfuran-3-yl)phenyl pivalate (3j):



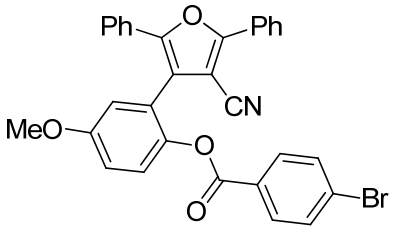
Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl pivalate **1c** (166.6 mg, 0.5 mmol), trimethylacetyl chloride **4h** (68.0 μL, 1.1 equiv), Bu_3P (150.0 μL, 1.2 equiv) and Et_3N (91.0 μL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3j** as colorless oil (154.5 mg, 77%).

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.98 (*pseudo* d, 2H, J = 7.6 Hz), 7.52-7.39 (m, 4H), 7.34 (*pseudo* dd, 1H, J = 7.6, 1.6 Hz), 7.28 (*pseudo* t, 1H, J = 7.2 Hz), 7.18 (*pseudo* d, 1H, J = 8.0), 1.24 (s, 9H), 1.15 (s, 9H).

^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 176.2, 159.0, 156.4, 149.6, 132.4, 130.0, 129.8, 129.0, 128.2, 125.4, 125.1, 124.5, 122.8, 117.2, 114.2, 95.8, 38.9, 34.5, 29.5, 26.8.

MS (70 eV, EI) *m/z* (%): 401 $[M]^+$ (25), 343 (76), 302 (88), 105 (30), 85 (30), 57 (100).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3395 (brs), 2959 (s), 2229 (s), 1620 (m), 1513 (s), 1451 (s), 1262 (s).
HRMS (ESI) for **$C_{26}H_{27}NO_3Na$**, **$[M+Na]^+$** (424.1889) found: 424.1895.

Synthesis of 2-(4-cyano-2,5-diphenylfuran-3-yl)-4-methoxyphenyl 4-bromo benzoate (3k):

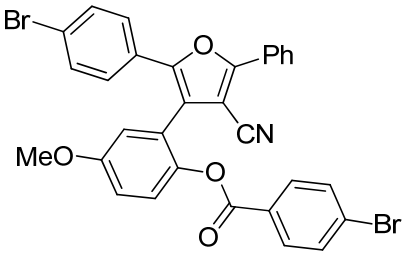


Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)-4-methoxyphenyl 4-bromobenzoate **1d** (230.5 mg, 0.5 mmol), benzoyl chloride **4a** (64.0 µL, 1.1 equiv), Bu_3P (150.0 µL, 1.2 equiv) and Et_3N (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3k** as white solid (258.1 mg, 94%).

mp: 153.0-153.8 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.03 (*pseudo* d, 2H, J = 7.2 Hz), 7.68 (*pseudo* d, 2H, J = 8.8 Hz), 7.56-7.40 (m, 7H), 7.36-7.24 (m, 4H), 7.06 (*pseudo* dd, 1H, J = 9.0, 3.0 Hz), 7.00 (d, 1H, J = 3.2 Hz), 3.82 (s, 3H).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 164.0, 158.4, 157.8, 149.6, 142.2, 131.7, 131.5, 130.3, 129.1, 128.9, 128.8, 128.7, 128.6, 127.9, 127.8, 126.1, 125.5, 124.4, 124.2, 119.1, 116.2, 115.9, 114.3, 95.9, 55.8.
MS (70 eV, EI) *m/z* (%): 551 $[M+2]^+$ (40), 549 $[M]^+$ (40), 185 (75), 183 (100), 155 (20), 105 (55), 77 (15).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3063 (w), 2827 (w), 2229 (m), 1735 (s), 1587 (m), 1488 (m), 1252 (s), 1193 (s), 1067 (s), 688 (m).
HRMS (ESI) for **$C_{31}H_{20}BrNO_4Na$**, **$[M+Na]^+$** (572.0473) found: 572.0490.

Synthesis of 2-(2-(4-bromophenyl)-4-cyano-5-phenylfuran-3-yl)-4-methoxyphenyl 4-bromobenzoate (3l):



Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)-4-methoxyphenyl 4-bromobenzoate **1d** (230.5 mg, 0.5 mmol), 4-bromobenzoyl chloride **4b** (120.7 µL, 1.1 equiv), Bu_3P (150.0 µL, 1.2 equiv) and Et_3N (91.0 µL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3l** as white solid 282.1 mg, 90%).

mp: 148.3-149.1 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.02 (*pseudo* d, 2H, J = 6.8 Hz), 7.73 (*pseudo* d, 2H, J = 8.4 Hz), 7.53-7.42 (m, 7H), 7.38 (*pseudo* d, 2H, J = 8.8 Hz), 7.29 (*pseudo* d, 1H, J = 8.8 Hz), 7.07 (*pseudo* dd, 1H, J = 9.0, 3.0 Hz), 6.97 (*pseudo* d, 1H, J = 3.2 Hz), 3.82 (s, 3H).

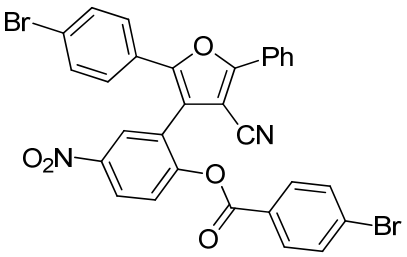
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 164.0, 158.6, 157.8, 148.4, 142.0, 131.9, 131.8, 131.5, 130.4, 129.1, 128.8, 127.8, 127.7, 127.6, 127.5, 125.4, 124.3, 124.1, 123.1, 119.6, 116.1, 115.9, 114.1, 95.9, 55.8.

MS (70 eV, EI) *m/z* (%): 183 $[M-444]^+$ (100), 155 (12), 105 (24), 77 (5).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3070 (w), 2930 (w), 2229 (m), 1738 (s), 1587 (m), 1488 (m), 1252 (s), 1189 (s), 1067 (s), 728 (m).

HRMS (ESI) for **$C_{31}H_{19}Br_2NO_4Na$**, **$[M+Na]^+$** (649.9579) found: 649.9579.

Synthesis of 2-(2-(4-bromophenyl)-4-cyano-5-phenylfuran-3-yl)-4-nitrophenyl 4-bromobenzoate (3m):



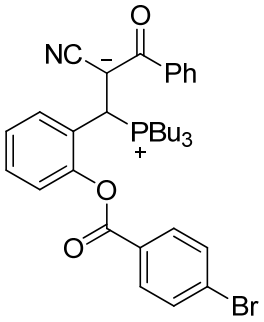
Prepared according to **TP** from (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)-4-nitrophenyl 4-bromobenzoate **1e** (230.5 mg, 0.5 mmol), 4-bromobenzoyl chloride **4b** (120.7 µL, 1.1 equiv), Bu_3P

(150.0 μL, 1.2 equiv) and Et_3N (91.0 μL, 1.3 equiv) in THF (1.0 mL) [reaction condition: 27-30 °C for 15 min]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **3m** as white solid (250.4 mg, 78%).

mp: 157.0-158.0 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.44 (*pseudo* dd, 1H, J = 8.8, 2.8 Hz), 8.37 (*pseudo* d, 1H, J = 2.8 Hz), 8.02 (*pseudo* d, 2H, J = 7.6 Hz), 7.77 (*pseudo* d, 2H, J = 7.77 Hz), 7.64-7.43 (m, 8H), 7.32 (*pseudo* d, 2H, J = 8.4 Hz).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 163.0, 159.3, 153.7, 149.4, 146.1, 132.3, 132.1, 131.7, 130.9, 129.8, 129.3, 127.6, 127.3, 127.1, 127.0, 126.7, 125.8, 125.6, 125.3, 124.8, 124.0, 117.6, 113.6, 95.5.
MS (70 eV, EI) *m/z* (%): 183 $[M-459]^+$ (100), 155 (16), 105 (45), 77 (15).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3077 (w), 2229 (m), 1742 (s), 1587 (m), 1528 (s), 1488 (m), 1347 (s), 1211 (s), 1048 (s), 743 (m).
HRMS (FAB) for **$C_{30}H_{16}Br_2N_2O_5$**, **$[M]^+$** (641.9426) found: 641.9419.

Synthesis of 1-(2-(4-bromobenzoyloxy)phenyl)-2-cyano-3-oxo-3-phenyl-1-(tributylphosphonio)propan-2-ide (5a):



A dry and nitrogen-flushed 10-mL Schlenk tube, equipped with a magnetic stirring bar and a septum, was sequentially charged with a solution of **1a** (0.5 mmol) and Bu_3P (150.0 μL, 1.2 equiv) in THF (1.0 mL). The reaction mixture was stirred for one minute at room temperature (27-30 °C). Thereafter, the solvent was removed by evaporation *in vacuo* and washed by *n*-pentane yielded **5a** as white solid (284.9 mg, 90%)**.**

mp: 93.3-94.0 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.20 (*pseudo* d, 2H, J = 6.8 Hz), 8.02 (*pseudo* d, 1H, J = 6.3 Hz),7.79-7.68 (m, 4H), 7.43-7.24 (m, 6H), 5.54 (d, 1H, J =

13.2 Hz), 2.30-2.13 (m, 3H), 2.13-1.97 (m, 3H), 1.49-1.16 (m, 12H), 0.87-0.75 (m, 9H).

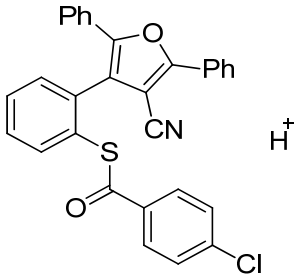
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 164.6, 147.9 (J = 6.0 Hz), 132.4, 131.9, 131.0 (J = 2.0 Hz), 129.7, 129.2, 128.8, 127.7, 127.6, 126.8 (J = 2.0 Hz), 122.9, 31.5 (J = 38.0 Hz), 24.2 (J = 4.0 Hz), 24.0 (J = 11.0 Hz), 20.1 (J = 36.0 Hz), 13.2.

^{31}P (200 MHz, CDCl3, 25 °C) δ/ppm: 34.4.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 2959 (m), 2915 (m), 2148 (m), 1735 (m), 1484 (s), 1207 (m)；

HRMS (ESI) for **$C_{35}H_{42}BrNO_3P$**, **[M]$^+$** (634.2086) found: 634.2096.

Synthesis of *S*-(2-(4-cyano-2,5-diphenylfuran-3-yl)phenyl) 4-chlorobenzothioate (14a):



Prepared according to **TP 1** from (*E*)-S-(2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl) 4-chlorobenzothioate **12** (120.9 mg, 0.3 mmol), benzoyl chloride **4a** (38.3 μL, 1.1 equiv), Bu_3P (92.0 μL, 1.2 equiv) and Et_3N (54.2 μL, 1.3 equiv) in THF (0.6 mL) [reaction condition: 27-30 °C for 1.5 h. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **14a** as white solid (120.8 mg, 82%).

R_f 0.4 (ethyl acetate/hexanes: 1/20); **mp**: 164.8-165.1 °C.

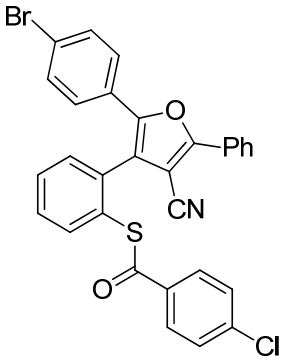
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.1(t, 2H, J =7.2 Hz), 7.70-7.85 (m, 3H), 7.54-7.63 (m, 2H), 7.42-7.53 (m, 6H), 7.34 (d, 2H, J = 8.4 Hz), 7.28-7.32 (m, 3H).

^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 187.7, 157.9, 148.3, 139.9, 137.9, 134.7, 131.7, 130.7, 130.2, 129.9, 129.1, 128.9, 128.8, 128.7, 128.6, 127.9, 127.4, 127.1, 125.9, 125.5, 125.4, 122.3, 114.3, 96.6.

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3042 (w), 1754 (s), 1624(w), 1215 (s), 1163 (s).

HRMS (EI) for **$C_{29}H_{20}BrO_3$**, **[M]$^+$** (492.0819) found: 492.0825

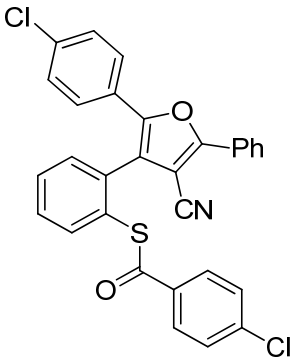
Synthesis of *S*-(2-(2-(4-bromophenyl)-4-cyano-5-phenylfuran-3-yl)phenyl) 4-chlorobenzothioate (14b):



Prepared according to **TP 1** from (*E*)-S-(2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl) 4-chlorobenzothioate **12** (121.16 mg, 0.3 mmol), 4-bromobenzoyl chloride **4b** (72.5 µL, 1.1 equiv), Bu_3P (92.0 µL, 1.2 equiv) and Et_3N (54.2 µL, 1.3 equiv) in THF (0.6 mL) [reaction condition: 27-30 °C for 1 h]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furished **14b** as yellow solid (131.4 mg, 77%).

R_f 0.4 (ethyl acetate/hexanes: 1/10); **mp**: 154.8-155.3 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.10 (d, 2H, J = 7.3 Hz), 7.8 (d, 2H, J = 8.4 Hz), 7.76-7.77 (m, 1H), 7.59-7.64 (m, 2H), 7.45-7.56 (m, 4H), 7.45-7.56 (m, 4H), 7.42 (d, 2H J = 8.5 Hz), 7.36 (t, 3H J = 8.5 Hz).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 187.8, 158.1, 148.4, 140.1, 138.0, 135.1, 134.6, 131.9, 131.8, 131.6, 130.9, 130.4, 130.2, 129.2, 128.9, 128.8, 127.8, 127.7, 127.6, 127.4, 127.2, 125.5, 122.9, 114.1, 96.7.
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3002 (w), 1760 (s), 1644 (w), 1323 (s), 1065 (s).
HRMS (EI) for **$C_{29}H_{19}BrO_3$**, **$[M]^+$** (568.9852) found: 568.9954.

Synthesis of *S*-(2-(2-(4-chlorophenyl)-4-cyano-5-phenylfuran-3-yl)phenyl) 4-chlorobenzothioate (14c):

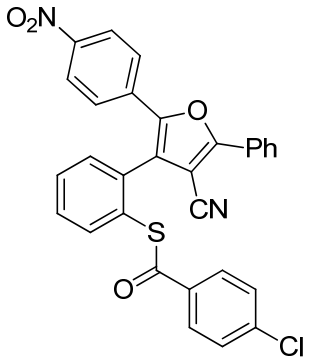


Prepared according to **TP 1** from (*E*)-S-(2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl) 4-chlorobenzothioate **12** (121.16 mg, 0.3 mmol), 4-Chlorobenzoyl chloride **4i** (42.3 µL, 1.1 equiv), Bu_3P (92.0

μL, 1.2 equiv) and Et_3N (54.2 μL, 1.3 equiv) in THF (0.6 mL) [reaction condition: 27-30 °C for 3 h]. Purification by flash chromatography (ethyl acetate/hexanes: 1/50) furnished **14c** as white solid (147.9 mg, 90%).

R_f 0.3 (ethyl acetate/hexanes: 1/50); **mp**: 149.8-151.3 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.1(d, 2H, J = 7.2 Hz), 7.75 (d, 2H, J = 8.5 Hz), 7.75 (d, 1H, J = 6.6 Hz), 7.60-7.64 (m, 2H), 7.48-7.56 (m, 4H), 7.4 (d, 2H, J = 8.5 Hz) , 7.37 (d, 2H, J = 8.5 Hz), 7.23 (d, 2H, J = 8.5 Hz).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 187.6, 157.9, 148.3, 139.9, 137.9, 134.9, 134.5, 131.5, 130.8, 130.1, 129.1, 128.9, 128.8, 128.7, 127.8, 127.7, 127.1, 125.3, 122.7, 114.1, 96.6.
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3011 (w), 1724 (s), 1651 (w), 1203 (s), 1112 (s).
HRMS (ESI) for **$C_{30}H_{17}Cl_2NO_2SNa$**, **$[M+Na]^+$** (548.0254) found: 548.0250

Synthesis of *S*-(2-(4-cyano-2-(4-nitrophenyl)-5-phenylfuran-3-yl)phenyl) 4-chlorobenzothioate (14d):

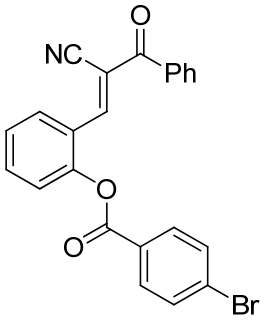


Prepared according to **TP 1** from (*E*)-S-(2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl) 4-chlorobenzothioate **12** (120.9 mg, 0.3 mmol), 4-nitrobenzoyl chloride **4d** (61.2 μL, 1.1 equiv), Bu_3P (92.0 μL, 1.2 equiv) and Et_3N (54.2 μL, 1.3 equiv) in THF (0.6 mL) [reaction condition: 27-30 °C for 1.5 h]. Purification by flash chromatography (ethyl acetate/hexanes: 1/20) furnished **14d** as white solid (120.8 mg, 82%).

R_f 0.4 (ethyl acetate/hexanes: 1/15); **mp**: 176.8-77.3 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.10 (dd, 4H, J = 7.2 Hz, J = 7.2 Hz), 7.64-7.70 (m, 3H), 7.50-7.60 (m, 4H), 7.25 (d, 2H , J = 7.2 Hz).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 187.6,159.2, 147.1, 146.9, 140.3, 138.2, 134.7, 134.4, 134.3, 131.4, 131.1, 130.9, 130.6, 129.2, 128.9, 128.8, 127.8, 127.3, 126.2, 125.9, 125.7, 123.9, 113.7, 97.2.
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3047 (w), 1734 (s), 1653 (w), 1233 (s), 1063 (s), 683 (s).

HRMS (ESI) for $\mathbf{C_{30}H_{17}ClN_2O_4SNa}$, $\mathbf{[M+Na]^+}$ (559.0495) found: 559.0499.

Synthesis of (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate (1a) [1]:



According to reported literature, compound **1a** was furnished as pale yellow solid (353.4 mg, 82%).

mp: 157.9-158.8 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 ^{o}C) δ/ppm: 8.49 (dd, 1H, J = 8.0, 1.2 Hz), 8.17 (s, 1H), 7.97 (d, 2H, J = 8.8 Hz), 7.75 (dd, 2H, J = 8.2, 1.0 Hz), 7.70-7.62 (m, 3H), 7.54-7.44 (m, 2H), 7.38-7.28 (m, 3H).

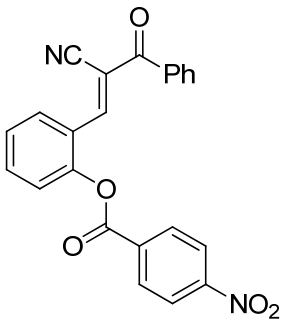
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.9, 163.8, 150.5, 148.3, 135.4, 134.2, 133.3, 132.2, 131.6, 129.6, 129.2, 129.1, 128.5, 127.2, 127.0, 124.9, 123.2, 116.0, 112.7.

MS (70 eV, EI) *m/z* (%): 432 $[M+1]^+$ (13), 430 $[M-1]^+$ (13), 326 (7), 248 (16), 183 (100), 155 (34), 105 (40), 77 (65).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3077(w), 2214 (w), 1738 (s), 1665 (m), 1587 (m), 1258 (s), 1215 (s), 746 (m).

HRMS (ESI) for $\mathbf{C_{23}H_{14}BrNO_3Na}$, $\mathbf{[M+Na]^+}$ (454.0055) found: 454.0060.

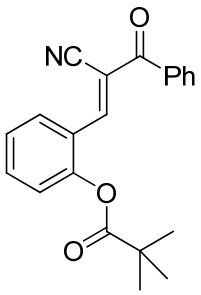
Synthesis of (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-nitrobenzoate (1b) [1]:



According to reported literature, compound **1b** was furnished as white solid (167.2 mg, 42%).

mp: 151.6-152.0 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.50 (d, 1H, J = 8.0 Hz), 8.36-8.27 (m, 4H), 8.18 (s, 1H), 7.78 (d, 2H, J = 8.0 Hz), 7.67 (t, 1H, J = 7.8 Hz), 7.55-7.47 (m, 2H), 7.43-7.31 (m, 3H).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.5, 162.6, 151.2, 150.1, 147.9, 135.4, 134.2, 133.7, 133.4, 131.3, 129.3, 129.2, 128.6, 127.2, 124.8, 123.9, 123.0, 115.9, 112.9.
MS (70 eV, EI) *m/z* (%): 398 $[M]^+$ (30), 341 (10), 293 (14), 248 (34), 150 (100), 104 (70), 77 (50).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3070 (w), 2214 (w), 1741 (s), 1661 (m), 1598 (m), 1524 (s), 1347 (m), 1263 (s), 1215 (s), 1064 (m).
HRMS (ESI) for **$C_{23}H_{14}N_2O_5Na$**, **$[M+Na]^+$** (421.0800) found: 421.0805.

Synthesis of (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)phenyl pivalate (1c) [1]:

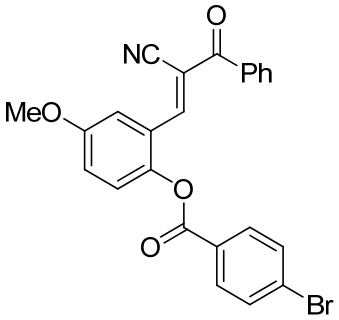


According to reported literature, compound **1c** was furnished (209.9 mg, 63%).

mp: 109.9-110.5 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.45 (dd, 1H, J = 8.0, 1.2 Hz), 8.07 (s, 1H), 7.77 (d, 2H, J = 8.4 Hz), 7.58-7.48 (m, 2H), 7.44 (t, 2H, J = 7.8 Hz), 7.34 (t, 1H, J = 7.6 Hz), 7.10 (d, 1H, J = 8.0 Hz), 1.18 (s, 9H).

^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.0, 176.3, 151.1, 148.3, 135.7, 134.3, 133.3, 129.2, 128.9, 128.7, 126.5, 124.7, 123.1, 116.3, 111.8, 39.3, 26.9.
MS (70 eV, EI) *m/z* (%): 276 $[M-57]^+$ (72), 220 (72), 105 (50), 77 (50), 57 (100).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3062 (w), 2974 (w), 2221 (w), 1757 (s), 1646 (s), 1598 (s), 1306 (m), 1259 (m), 1104 (s).
HRMS (ESI) for **$C_{21}H_{19}NO_3Na$**, **$[M+Na]^+$** (356.1263) found: 356.1225.

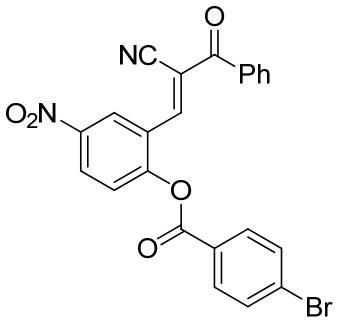
Synthesis of (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)-4-methoxyphenyl 4-bromobenzoate (1d) [1]:



According to reported literature, compound **1d** was furnished as yellow solid (355.0 mg, 77%).

mp: 169.3-169.6 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.10 (s, 1H), 8.02 (d, 1H, J = 2.8 Hz), 7.95 (d, 2H, J = 8.4 Hz), 7.73 (d, 2H, J = 8.0 Hz), 7.64 (d, 2H, J = 8.4 Hz), 7.49 (t, 1H, J = 7.8 Hz), 7.31 (t, 2H, J = 7.6 Hz), 7.25 (d, 1H, J = 9.6 Hz), 7.18 (dd, 2H, J = 8.8, 2.8 Hz), 3.92 (s, 3H).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 189.0, 164.2, 157.7, 148.3, 144.2, 135.4, 133.2, 132.2, 131.6, 129.5, 129.1, 128.5, 127.3, 125.2, 124.1, 121.5, 116.1, 112.5, 111.9, 55.9.
MS (70 eV, EI) *m/z* (%): 463 $[M+2]^+$ (10), 461 $[M]^+$ (10), 358 (5), 356 (5), 278 (7), 262 (5), 185 (100), 183 (100), 157 (12), 155 (12), 105 (10).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3063 (w), 2915 (w), 2206 (w), 1738 (s), 1587 (m), 1488 (m), 1248 (m), 1204 (s).
HRMS (ESI) for **$C_{24}H_{16}BrNO_4Na$**, **$[M+Na]^+$** (484.0160) found: 484.0165.

Synthesis of (*E*)-2-(2-cyano-3-oxo-3-phenylprop-1-en-1-yl)-4-nitrophenyl 4-bromobenzoate (1e) [1]:



According to reported literature, compound **1e** was furnished as yellow solid (166.6 mg, 35%).

mp: 196.7-197.5 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 C) δ/ppm: 9.23 (d, 1H, J = 2.8 Hz), 8.50 (dd, 1H, J = 9.0, 2.6 Hz), 8.17 (s, 1H), 8.02 (d, 2H, J = 8.4 Hz), 7.84 (dd, 2H, J = 8.2, 1.4 Hz), 7.70 (d, 2H, J = 8.8 Hz), 7.65-7.56 (s, 2H), 7.42 (t, 2H, J = 7.8 Hz).

^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 187.3, 163.0, 154.2, 146.1, 145.8, 134.9, 134.0, 132.6, 131.8, 130.4, 129.4, 128.8, 128.0, 126.5, 126.4, 124.6, 124.3, 115.9, 115.1.

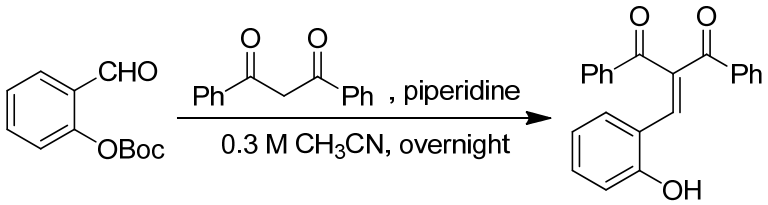
MS (70 eV, EI) *m/z* (%): 293 $[M-183]^+$ (5), 183 (100), 155 (17), 105 (28), 77 (23).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3136 (w), 2214 (w), 1742 (m), 1657 (s), 1524 (m), 1344(m), 1215 (s), 1048 (m).

HRMS (EI) for **$C_{23}H_{13}BrN_2O_5$**, **$[M]^+$** (476.0008) found: 476.0015.

Synthesis of Starting Material 1f-1h

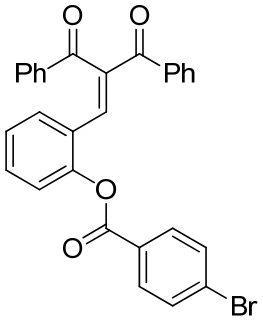
Synthesis of 2-(2-hydroxybenzylidene)-1,3-diphenylpropane-1,3-dione (15):



A 50-mL Schlenk flask, equipped with a magnetic stirring bar and a septum, was charged with a solution of *tert*-butyl 2-formylphenyl carbonate (222.0 mg，1 mmol) in acetonitrile (3.3 mL). Dibenzoylmethane (224.0 mg, 1 equiv) and piperidine (50.0 μL) was added, and the reaction mixture was stirred at room temperature overnight. Thereafter, the solvent was removed by evaporation *in vacuo*. Purification by flash chromatography (ethyl acetate/ hexanes: 1/6) furnished **15** as yellow oil (82.6 mg, 24%).

^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.78 (d, 2H, J = 6.8 Hz), 7.70 (d, 2H, J = 7.2 Hz), 7.60 (t, 1H, J = 7.4 Hz), 7.47 (t, 2H, J = 7.6 Hz), 7.42-7.28 (m, 4H), 7.22 (dd, 1H, J = 7.6, 1.6 Hz), 7.20 (s, 1H), 7.07-6.98 (m, 2H), 5.01 (s, 1H).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 195.4, 152.1, 142.7, 136.5, 135.0, 133.2, 133.1, 132.7, 129.8, 128.8, 128.7, 128.6, 128.2, 125.9, 122.1, 118.0, 117.1, 99.0.
MS (70 eV, EI) *m/z* (%):251 $[M-77]^+$ (15), 223 (18), 105 (100), 77 (45).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3328 (brs), 3055 (w), 2922 (w), 1627 (s), 1601 (s), 1572 (m), 1447 (m), 1222 (s).
HRMS (ESI) for **$C_{22}H_{16}O_3Na$**, **$[M+Na]^+$** (351.0997) found: 351.0997.

Synthesis of 2-(2-benzoyl-3-oxo-3-phenylprop-1-enyl)phenyl 4-bromobenzoate (1f):

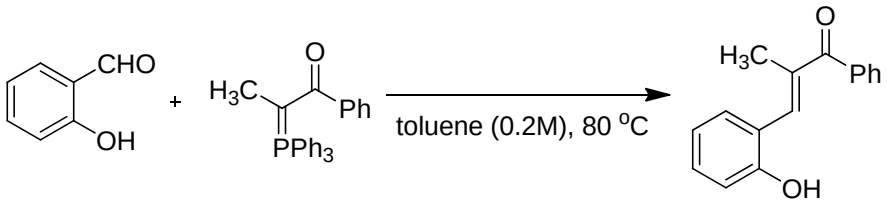


A dry and nitrogen-flushed 50-mL Schlenk flask, equipped with a magnetic stirring bar and a septum, was sequentially charged with a solution of **15** (344.1 mg, 1.0 mmol), 4-bromobenzoyl chloride **4b** (230.4 mg, 1.05 equiv) and Et_3N (210.0 µL, 1.5 equiv) in dry THF (10 mL). The reaction mixture was stirred for 30 minutes at room temperature (27-30 °C). Thereafter the resulting mixture was extracted with CH_2Cl_2. The organic phase was washed with saturated $NaHCO_3$ solution, dried over anhydrous $MgSO_4$ and then evaporated to afford **1f** white solid (1.11 g, 97%).

mp: 102.1-102.5 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 7.95 (*pseudo* d, 4H, J = 8.0 Hz), 7.73 (*pseudo* d, 2H, J = 8.0 Hz), 7.65-7.59 (m, 3H), 7.51 (*pseudo* t, 1H, J = 8.0 Hz), 7.47-7.30 (m, 5H), 7.22 (*pseudo* t, 2H, J = 8.0 Hz), 7.17 (*pseudo* d, 1H, J = 8.0 Hz), 7.08 (*pseudo* t, 1H, J = 8.0 Hz).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 195.7, 194.3, 163.9, 149.2, 140.9, 137.2, 136.9, 135.9, 133.8, 132.3, 132.0, 131.5, 131.4, 129.9, 129.3, 129.2, 129.1, 128.7, 128.2, 127.5, 126.4, 126.3, 122.6.
MS (20 eV, EI) *m/z* (%): 404 $[M-105]^+$ (50), 327 (5), 311 (50), 183 (100), 155 (25), 105 (53), 77 (50).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3062 (w), 2922 (w), 1738 (s), 1671 (m), 1642 (m), 1587 (m), 1258 (s), 1214 (s), 1067 (s).
HRMS (ESI) for **$C_{29}H_{19}BrO_4Na$**, **$[M+Na]^+$** (533.0364) found: 533.0345.

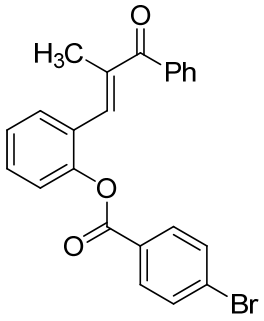
Synthesis of (*E*)-3-(2-hydroxyphenyl)-2-methyl-1-phenylprop-2-en-1-one (16):



A 50-mL Schlenk flask, equipped with a magnetic stirring bar and a septum, was sequentially charged with a solution of salicyladehyde (488.0 µL, 4.2 mmol) and 1-phenyl-2-(triphenylphosphoranylidene)propan-1-one (1576.0 mg, 4.0 mmol) in toluene (20.0 ml). The reaction mixture was stirred overnight at 80 °C . Thereafter, the solvent was removed by evaporation *in vacuo*. Purification by flash chromatography (ethyl acetate/ hexanes: 1/ 10) furnished **16** as white solid (771.1 mg, 81%).

mp: 128.2-129.0 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 C) δ/ppm: 7.75 (d, 2H, J = 7.2 Hz), 7.49 (t, 1H, J = 7.4 Hz), 7.44-7.30 (m, 4H), 7.19 (t, 1H, J = 7.4 Hz), 6.94 (d, 1H, J = 7.6 Hz), 6.87 (d, 1H, J = 8.0 Hz), 6.80-6.69 (brs, 1H), 2.16 (s, 3H).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 200.3, 154.1, 138.4, 138.1, 137.2, 131.9, 130.1, 129.9, 129.7, 128.1, 122.9, 120.1, 115.9, 14.4.
MS (70 eV, EI) *m/z* (%): 221 $[M-16]^+$ (100), 105 (18).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3269 (brs), 3062 (w), 2929 (w), 1598 (s), 1450 (s), 1258 (s), 1011 (m).
HRMS (ESI) for **$C_{16}H_{14}O_2Na$**, **$[M+Na]^+$** (261.0891) found: 261.0872.

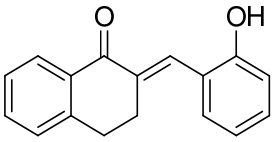
Synthesis of (*E*)-2-(2-methyl-3-oxo-3-phenylprop-1-en-1-yl)phenyl 4-bromobenzoate (1g):



A dry and nitrogen-flushed 50-mL Schlenk flask, equipped with a magnetic stirring bar and a septum, was sequentially charged with a solution of **16** (599.9 mg, 3.0 mmol), acyl chloride **4b** (686.4 mg, 1.05.equiv) and Et_3N (628.0 μL, 1.5 equiv) in dry THF (10 mL). The reaction mixture was stirred for 30 minutes at room temperature (27-30 ^oC). Thereafter the resulting mixture was extracted with CH_2Cl_2. The organic phase was washed with saturated $NaHCO_3$ solution, dried over anhydrous $MgSO_4$ and then evaporated to afford **1g** as white solid (1247.4 mg, 99%).

mp: 91.5-92.5 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 C) δ/ppm: 7.97 (d, 2H, J = 8.4 Hz), 7.65 (d, 2H, J = 8.4 Hz), 7.57-7.47 (m, 3H), 7.43 (td,1H, J = 7.6, 1.2 Hz), 7.39-7.31 (m, 2H), 7.24 (d, 1H, J = 8.0 Hz), 7.11 (s, 1H), 7.07 (t, 2H, J = 7.8 Hz), 2.16 (s, 3H).
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 198.8, 163.9, 148.8, 139.1, 137.9, 135.7, 132.1, 131.6, 131.5, 130.0, 129.7, 129.1, 129.0, 128.9, 128.0, 127.9, 126.1, 122.5, 14.3.
MS (70 eV, EI) *m/z* (%): 422 $[M+2]^+$ (13), 420 $[M]^+$ (10), 405 (32), 403 (32), 221 (100), 185 (82), 183 (82), 157 (35), 155 (35), 105 (30).
IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3062 (w), 2922 (w), 1738 (s), 1646 (m), 1587 (m), 1262 (s), 1070 (s).
HRMS (EI) for **$C_{23}H_{17}O_3Br$**, **$[M]^+$** (420.0361) found: 420.0366.

Synthesis of (*E*)-2-(2-hydroxybenzylidene)-3,4-dihydronaphthalen-1(2H)-one (17):



A dry and nitrogen-flushed 100-mL Schlenk flask, equipped with a magnetic stirring bar and a septum, was sequentially charged with a solution of salicyladehyde (2.0 g, 10.0 mmol) and 1-tetralone (1.46 mL, 1.1 equiv) in 50% KOH solution (12 ml, methane: water = 5:1). The reaction mixure was stirred overnight at room temperature (27-30 ^oC). Thereafter the resulting mixture was neutralized by adding 1N HCl solution then extracted with ethyl acetate. The organic phase was dried over anhydrous $MgSO_4$ and then evaporated to furnish **17** as brown solid (1075.0 mg, 43%).

mp: 137.5-138.5 °C.
^{1}H-NMR (400 MHz, $CDCl_3$, 25 °C) δ/ppm: 8.11 (d, 1H, J = 7.8 Hz), 7.93 (s, 1H),

7.47 (td, 1H, J = 7.4, 1.2 Hz), 7.34 (t, 1H, J = 7.4 Hz), 7.25-7.17 (m, 3H), 7.03-6.87 (m, 2H), 3.03-2.93 (m, 2H), 2.92-2.82 (m, 2H).

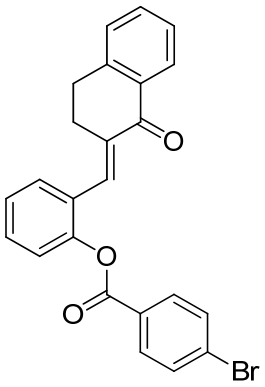
^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 188.2, 154.8, 143.7, 136.8, 133.5, 133.3, 132.1, 130.3, 129.9, 128.3, 128.2, 127.0, 122.7, 120.1, 116.2, 29.0, 27.5.

MS (70 eV, EI) *m/z* (%): 250 $[M]^+$ (20), 233 (100), 90 (30), 77 (20).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3225 (brs), 3062 (w), 2944 (w), 1658 (m), 1651 (m), 1598 (s), 1450 (s), 1299 (s), 1229 (s).

HRMS (ESI) for **$C_{17}H_{14}O_2Na$**, **$[M+Na]^+$** (273.0891) found: 273.0876.

Synthesis of (*E*)-2-((1-oxo-3,4-dihydronaphthalen-2(1H)-ylidene)methyl)phenyl 4-bromobenzoate (1h):



A dry and nitrogen-flushed 50-mL Schlenk flask, equipped with a magnetic stirring bar and a septum, was sequentially charged with a solution of **17** (750.0 mg, 3.0 mmol), 4-bromobenzoyl chloride **4b** (686.4 mg, 1.05.equiv) and Et_3N (628.0 µL, 1.5 equiv) in dry THF (10 mL). The reaction mixture was stirred for 30 minutes at room temperature (27-30 °C). Thereafter the resulting mixture was extracted with CH_2Cl_2. The organic phase was washed with saturated $NaHCO_3$ solution, dried over anhydrous $MgSO_4$ and then evaporated to afford **1h** as purple solid (1023.9 mg, 79%).

mp: 139.1-140.0 °C.

^{1}H-NMR (400 MHz, $CDCl_3$, 25 C) δ/ppm: 8.07 (d, 1H, J = 8.0 Hz), 8.02 (d, 2H, J = 8.6 Hz), 7.80 (s, 1H), 7.62 (d, 2H, J = 8.6 Hz), 7.49-7.37 (m, 3H), 7..37-7.19 (m, 4H), 3.05-2.97 (m, 2H), 2.96-2.88 (m, 2H).

^{13}C-NMR (100 MHz, $CDCl_3$, 25 °C) δ/ppm: 187.3, 164.0, 149.4, 143.5, 137.9, 133.4, 133.2, 132.0, 131.6, 130.7, 130.2, 129.7, 129.2, 129.0, 128.3, 128.2, 128.1, 127.0, 125.9, 122.7, 29.1, 27.5.

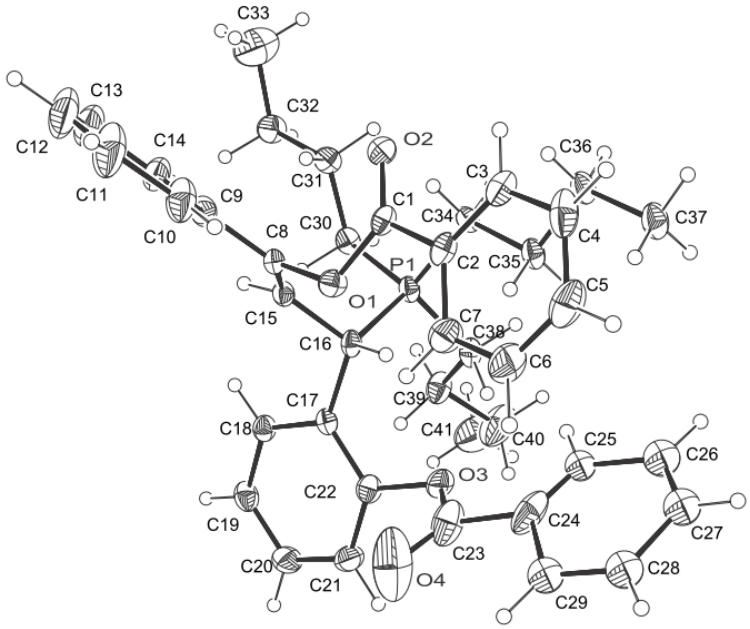
MS (70 eV, EI) *m/z* (%): 185 $[M-199]^+$ (100), 183 $[M-201]^+$ (85).

IR (KBr) $\tilde{\nu}$ (cm^{-1}): 3048 (w), 2915 (w), 1738 (s), 1668 (m), 1587 (m), 1480 (m), 1255 (s), 1211 (s), 1067 (s).

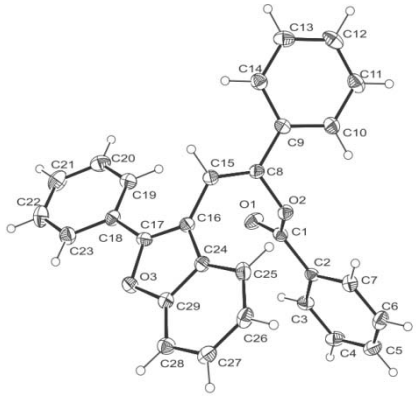
HRMS (EI) for **$C_{24}H_{17}O_3BrNa$**, **$[M+Na]^+$** (455.0259) found: 455.0254.

Reference (reported literature for synthesis of starting material **1**):

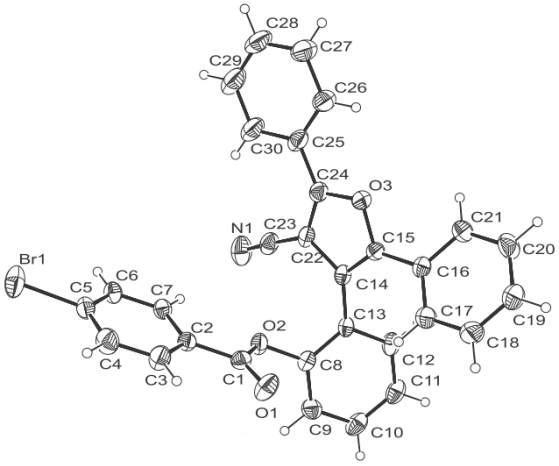
[1] P. K. Amancha, Y.-C. Lai, I-C. Chen, H.-J. Liu, J.-L. Zhu, *Tetrahedron* **2010**, *66*, 871



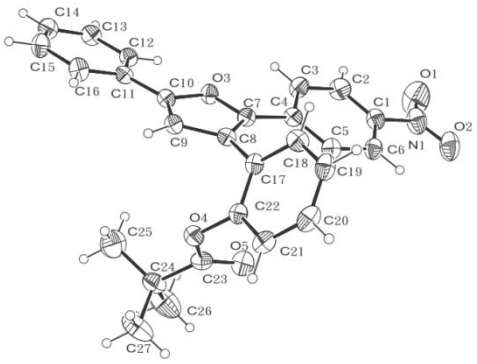
3a*



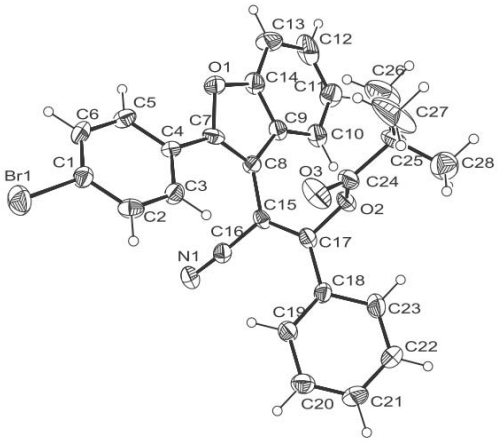
4a*



3a



4q*



3'h

Figure S1 Geometrical structures of reactants and products for intramolecular Witting reactions. The geometrical parameters of the structures are listed in Table S1. The compounds without α-substitution, denoted with *, were reported from reference 9f (Y.-T. Lee, Y.-J. Jang, S. Syu, S.-C. Chou, C.-J. Lee, W. Lin, *Chem. Commun*,. 2012, **48**, 8135-8137).

Table S1 Bond length (Å) and angle (°) comparison between DFT calculation and X-ray analysis for the structures in Figure S1.

3a*

Distance	Exp.	Theo.	Distance	Exp.	Theo.	Distance	Exp.	Theo.	Distance	Exp.	Theo.
C(1)-O(2)	1.210	1.253	C(14)-H(14)	0.950	1.086	C(27)-H(27)	0.950	1.087	C(37)-H(37A)	0.980	1.099
C(1)-O(1)	1.363	1.418	C(15)-C(16)	1.499	1.496	C(28)-C(29)	1.358	1.398	C(37)-H(37B)	0.980	1.097
C(1)-C(2)	1.483	1.471	C(15)-H(15)	0.950	1.09	C(28)-H(28)	0.950	1.088	C(37)-H(37C)	0.980	1.099
C(2)-C(3)	1.384	1.421	C(16)-C(17)	1.531	1.52	C(29)-H(29)	0.950	1.087	C(38)-C(39)	1.530	1.544
C(2)-C(7)	1.392	1.421	C(16)-P(1)	1.843	2.022	C(30)-C(31)	1.529	1.544	C(38)-P(1)	1.806	1.889
C(3)-C(4)	1.391	1.403	C(16)-H(16)	1.000	1.093	C(30)-P(1)	1.799	1.895	C(38)-H(38A)	0.990	1.092
C(3)-H(3)	0.950	1.085	C(17)-C(18)	1.390	1.416	C(30)-H(30A)	0.990	1.099	C(38)-H(38B)	0.990	1.098
C(4)-C(5)	1.394	1.412	C(17)-C(22)	1.387	1.418	C(30)-H(30B)	0.990	1.096	C(39)-C(40)	1.521	1.547
C(4)-H(4)	0.950	1.088	C(18)-C(19)	1.381	1.405	C(31)-C(32)	1.540	1.548	C(39)-H(39A)	0.990	1.097
C(5)-C(6)	1.358	1.413	C(18)-H(18)	0.950	1.088	C(31)-H(31A)	0.990	1.097	C(39)-H(39B)	0.990	1.100
C(5)-H(5)	0.950	1.087	C(19)-C(20)	1.358	1.407	C(31)-H(31B)	0.990	1.100	C(40)-C(41)	1.516	1.543
C(6)-C(7)	1.381	1.401	C(19)-H(19)	0.950	1.087	C(33)-C(32)	1.544	1.543	C(40)-H(40A)	0.990	1.100
C(6)-H(6)	0.950	1.087	C(20)-C(21)	1.386	1.404	C(32)-H(32A)	0.990	1.100	C(40)-H(40B)	0.990	1.101
C(7)-H(7)	0.950	1.086	C(20)-H(20)	0.950	1.087	C(32)-H(32B)	0.990	1.101	C(41)-H(41A)	0.980	1.098
C(8)-C(15)	1.309	1.365	C(21)-C(22)	1.379	1.406	C(33)-H(33A)	0.980	1.097	C(41)-H(41B)	0.980	1.099
C(8)-O(1)	1.426	1.427	C(21)-H(21)	0.950	1.086	C(33)-H(33B)	0.980	1.099	C(41)-H(41C)	0.980	1.098
C(8)-C(9)	1.469	1.479	C(22)-O(3)	1.420	1.411	C(33)-H(33C)	0.980	1.099			
C(9)-C(14)	1.383	1.420	C(23)-O(4)	1.202	1.438	C(34)-C(35)	1.535	1.543			
C(9)-C(10)	1.378	1.418	C(23)-O(3)	1.346	1.276	C(34)-P(1)	1.808	1.888			
C(10)-C(11)	1.394	1.405	C(23)-C(24)	1.465	1.444	C(34)-H(34A)	0.990	1.097			
C(10)-H(10)	0.950	1.085	C(24)-C(25)	1.179	1.431	C(34)-H(34B)	0.990	1.092			
C(11)-C(12)	1.363	1.411	C(24)-C(29)	1.545	1.431	C(35)-C(36)	1.532	1.548			
C(11)-H(11)	0.950	1.088	C(25)-C(26)	1.425	1.401	C(35)-H(35A)	0.990	1.099			
C(12)-C(13)	1.382	1.409	C(25)-H(25)	0.950	1.085	C(35)-H(35B)	0.990	1.100			
C(12)-H(12)	0.950	1.087	C(26)-C(27)	1.341	1.415	C(36)-C(37)	1.518	1.543			
C(13)-C(14)	1.390	1.410	C(26)-H(26)	0.950	1.088	C(36)-H(36A)	0.990	1.100			
C(13)-H(13)	0.950	1.087	C(27)-C(28)	1.421	1.416	C(36)-H(36B)	0.990	1.100			

Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.
O(1)-C(1)-O(2)	122.9	122.2	C(9)-C(10)-H(10)	119.5	120.6	C(19)-C(18)-H(18)	119.5	119.1	C(26)-C(27)-H(27)	118.5	120.4
O(2)-C(1)-C(2)	125.2	126.4	C(11)-C(10)-H(10)	119.5	118.8	C(17)-C(18)-H(18)	119.5	118.6	C(28)-C(27)-H(27)	118.8	120.4
O(1)-C(1)-C(2)	111.9	111.4	C(12)-C(11)-C(10)	120.3	120.5	C(20)-C(19)-C(18)	120.6	119.5	C(29)-C(28)-C(27)	118.7	120.8
C(7)-C(2)-C(3)	119.5	119.3	C(12)-C(11)-H(11)	119.9	120.2	C(20)-C(19)-H(19)	119.7	120.5	C(29)-C(28)-H(28)	120.7	119.5
C(3)-C(2)-C(1)	118.5	118.1	C(10)-C(11)-H(11)	119.9	119.3	C(18)-C(19)-H(19)	119.7	120.0	C(27)-C(28)-H(28)	120.6	119.7
C(7)-C(2)-C(1)	122.1	122.6	C(11)-C(12)-C(13)	119.6	119.3	C(19)-C(20)-C(21)	120.1	119.4	C(28)-C(29)-C(24)	115.8	120.3
C(4)-C(3)-C(2)	120.0	120.3	C(11)-C(12)-H(12)	120.2	120.3	C(19)-C(20)-H(20)	119.9	120.6	C(28)-C(29)-H(29)	122.2	120.6
C(2)-C(3)-H(3)	120.0	118.6	C(13)-C(12)-H(12)	120.2	120.4	C(21)-C(20)-H(20)	119.9	120.0	C(24)-C(29)-H(29)	122.3	119.1
C(4)-C(3)-H(3)	120.0	121.1	C(12)-C(13)-C(14)	119.9	120.0	C(20)-C(21)-C(22)	118.8	120.6	C(31)-C(30)-P(1)	117.2	117.4
C(5)-C(4)-C(3)	119.8	120.3	C(12)-C(13)-H(13)	120.0	119.9	C(22)-C(21)-H(21)	120.6	118.0	C(31)-C(30)-H(30A)	108.0	109.2
C(3)-C(4)-H(4)	120.1	119.8	C(14)-C(13)-H(13)	120.1	119.6	C(20)-C(21)-H(21)	120.6	121.4	P(1)-C(30)-H(30A)	108.0	105.6
C(5)-C(4)-H(4)	120.1	119.9	C(13)-C(14)-C(9)	121.0	120.8	C(21)-C(22)-C(17)	122.5	121.2	C(31)-C(30)-H(30B)	108.0	110.6
C(6)-C(5)-C(4)	119.7	119.7	C(9)-C(14)-H(14)	119.5	119.4	C(21)-C(22)-O(3)	119.4	115.2	P(1)-C(30)-H(30B)	108.0	107.0
C(6)-C(5)-H(5)	120.1	120.2	C(13)-C(14)-H(14)	119.5	119.8	C(17)-C(22)-O(3)	118.0	123.4	H(30A)-C(30)-H(30B)	107.3	106.6
C(4)-C(5)-H(5)	120.1	120.2	C(8)-C(15)-C(16)	125.2	126.2	O(4)-C(23)-O(3)	121.5	119.2	C(32)-C(31)-C(30)	111.2	111.2
C(5)-C(6)-C(7)	121.2	120.5	C(8)-C(15)-H(15)	117.4	116.8	O(4)-C(23)-C(24)	126.4	128.2	C(32)-C(31)-H(31A)	109.4	108.7
C(5)-C(6)-H(6)	119.4	119.8	C(16)-C(15)-H(15)	117.4	116.9	O(3)-C(23)-C(24)	112.0	112.6	C(30)-C(31)-H(31A)	109.4	110.4
C(7)-C(6)-H(6)	119.4	119.7	C(17)-C(16)-C(15)	113.8	116.8	C(25)-C(24)-C(23)	127.7	119.1	C(32)-C(31)-H(31B)	109.4	108.9
C(6)-C(7)-C(2)	119.8	120.0	C(15)-C(16)-P(1)	109.8	112.9	C(25)-C(24)-C(29)	121.6	118.5	C(30)-C(31)-H(31B)	109.4	110.7
C(6)-C(7)-H(7)	120.1	120.7	C(17)-C(16)-P(1)	111.4	110.4	C(23)-C(24)-C(29)	110.7	122.4	H(31A)-C(31)-H(31B)	108.0	106.8
C(2)-C(7)-H(7)	120.1	119.3	C(15)-C(16)-H(16)	107.2	108.7	C(24)-C(25)-C(26)	124.5	120.6	C(31)-C(32)-C(33)	111.9	112.4
C(15)-C(8)-O(1)	117.8	119.5	C(17)-C(16)-H(16)	107.2	107.1	C(24)-C(25)-H(25)	117.8	118.7	C(31)-C(32)-H(32A)	109.2	109.3
C(15)-C(8)-C(9)	126.1	125.3	P(1)-C(16)-H(16)	107.2	99.2	C(26)-C(25)-H(25)	117.8	120.8	C(33)-C(32)-H(32A)	109.2	109.6
O(1)-C(8)-C(9)	115.7	111.9	C(22)-C(17)-C(18)	116.9	117.0	C(27)-C(26)-C(25)	116.9	120.6	C(31)-C(32)-H(32B)	109.2	109.7
C(10)-C(9)-C(14)	118.2	118.4	C(16)-C(17)-C(18)	122.4	117.2	C(27)-C(26)-H(26)	121.7	119.7	C(33)-C(32)-H(32B)	109.2	109.6
C(14)-C(9)-C(8)	120.2	120.2	C(16)-C(17)-C(22)	120.7	125.7	C(25)-C(26)-H(26)	121.4	119.7	H(32A)-C(32)-H(32B)	107.9	106.4
C(10)-C(9)-C(8)	121.6	121.4	C(19)-C(18)-C(17)	121.1	122.3	C(26)-C(27)-C(28)	122.7	119.3	C(32)-C(33)-H(33A)	109.5	111.1

Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.
C(32)-C(33)-H(33B)	109.5	111.1	H(37C)-C(37)-H(37B)	109.5	107.8	C(30)-P(1)-C(34)	111.9	114.2
H(33A)-C(33)-H(33B)	109.5	107.7	C(39)-C(38)-P(1)	115.2	114.8	C(38)-P(1)-C(34)	109.4	105.5
C(32)-C(33)-H(33C)	109.5	111.2	C(39)-C(38)-H(38A)	108.5	109.5	C(30)-P(1)-C(16)	109.8	112.4
H(33A)-C(33)-H(33C)	109.5	107.8	P(1)-C(38)-H(38A)	108.5	105.6	C(38)-P(1)-C(16)	107.2	101.0
H(33C)-C(33)-H(33B)	109.5	107.8	C(39)-C(38)-H(38B)	108.5	111.0	C(34)-P(1)-C(16)	109.7	113.7
C(35)-C(34)-P(1)	114.1	117.5	P(1)-C(38)-H(38B)	108.5	106.5			
C(35)-C(34)-H(34A)	108.7	110.1	H(38A)-C(38)-H(38B)	107.5	109.0			
P(1)-C(34)-H(34A)	108.7	104.7	C(40)-C(39)-C(38)	111.5	111.1			
C(35)-C(34)-H(34B)	108.7	112.1	C(40)-C(39)-H(39A)	109.3	108.9			
P(1)-C(34)-H(34B)	108.7	105.1	C(38)-C(39)-H(39A)	109.3	109.0			
H(34A)-C(34)-H(34B)	107.6	106.6	C(40)-C(39)-H(39B)	109.3	108.9			
C(34)-C(35)-C(36)	110.8	110.7	C(38)-C(39)-H(39B)	109.3	111.1			
C(34)-C(35)-H(35A)	109.5	110.8	H(39A)-C(39)-H(39B)	108.0	107.7			
C(36)-C(35)-H(35A)	109.5	108.6	C(39)-C(40)-C(41)	112.4	112.4			
C(34)-C(35)-H(35B)	109.5	110.6	C(39)-C(40)-H(40A)	109.1	109.0			
C(36)-C(35)-H(35B)	109.5	108.9	C(41)-C(40)-H(40A)	109.1	109.6			
H(35A)-C(35)-H(35B)	108.1	107.2	C(39)-C(40)-H(40B)	109.1	109.5			
C(37)-C(36)-C(35)	111.8	112.5	C(41)-C(40)-H(40B)	109.1	109.5			
C(37)-C(36)-H(36A)	109.3	109.7	H(40A)-C(40)-H(40B)	107.8	106.7			
C(35)-C(36)-H(36A)	109.3	109.1	C(40)-C(41)-H(41A)	109.5	110.9			
C(37)-C(36)-H(36B)	109.3	109.6	C(40)-C(41)-H(41B)	109.5	111.2			
C(35)-C(36)-H(36B)	109.3	109.3	H(41A)-C(41)-H(41B)	109.5	107.8			
H(36A)-C(36)-H(36B)	107.9	106.4	C(40)-C(41)-H(41C)	109.5	111.2			
C(36)-C(37)-H(37A)	109.5	111.1	H(41A)-C(41)-H(41C)	109.5	107.8			
C(36)-C(37)-H(37B)	109.5	111.1	H(41C)-C(41)-H(41B)	109.5	107.8			
H(37A)-C(37)-H(37B)	109.5	107.8	C(1)-O(1)-C(8)	116.8	124.6			
C(36)-C(37)-H(37C)	109.5	111.2	C(23)-O(3)-C(22)	119.1	120.0			
H(37A)-C(37)-H(37C)	109.5	107.8	C(30)-P(1)-C(38)	108.7	108.7			

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Distance	Exp.	Theo.	Distance	Exp.	Theo.	Distance	Exp.	Theo.
C(1)-O(1)	1.201	1.238	C(14)-H(14)	0.950	1.087	C(28)-H(28)	0.950	1.085
C(1)-O(2)	1.363	1.408	C(15)-C(16)	1.464	1.467	C(29)-O(3)	1.383	1.397
C(1)-C(2)	1.477	1.486	C(15)-H(15)	0.950	1.089			
C(2)-C(7)	1.388	1.414	C(16)-C(17)	1.359	1.390			
C(2)-C(3)	1.391	1.413	C(16)-C(24)	1.360	1.462			
C(3)-C(4)	1.380	1.405	C(17)-O(3)	1.387	1.423			
C(3)-H(3)	0.950	1.084	C(17)-C(18)	1.465	1.464			
C(4)-C(5)	1.378	1.409	C(18)-C(23)	1.390	1.416			
C(4)-H(4)	0.950	1.087	C(18)-C(19)	1.393	1.418			
C(5)-C(6)	1.376	1.403	C(19)-C(20)	1.373	1.404			
C(5)-H(5)	0.950	1.088	C(19)-H(19)	0.950	1.085			
C(6)-C(7)	1.380	1.403	C(20)-C(21)	1.376	1.409			
C(6)-H(6)	0.950	1.087	C(20)-H(20)	0.950	1.087			
C(7)-H(7)	0.950	1.086	C(21)-C(22)	1.376	1.410			
C(8)-C(15)	1.331	1.354	C(21)-H(21)	0.950	1.087			
C(8)-O(2)	1.413	1.428	C(22)-C(23)	1.375	1.404			
C(8)-C(9)	1.465	1.481	C(22)-H(22)	0.950	1.087			
C(9)-C(10)	1.393	1.415	C(23)-H(23)	0.950	1.084			
C(9)-C(14)	1.402	1.416	C(24)-C(29)	1.389	1.413			
C(10)-C(11)	1.380	1.405	C(24)-C(25)	1.410	1.412			
C(10)-H(10)	0.950	1.086	C(25)-C(26)	1.382	1.405			
C(11)-C(12)	1.373	1.407	C(25)-H(25)	0.950	1.087			
C(11)-H(11)	0.950	1.087	C(26)-C(27)	1.386	1.419			
C(12)-C(13)	1.380	1.410	C(26)-H(26)	0.950	1.087			
C(12)-H(12)	0.950	1.087	C(27)-C(28)	1.372	1.408			
C(13)-C(14)	1.382	1.403	C(27)-H(27)	0.950	1.087			
C(13)-H(13)	0.950	1.087	C(28)-C(29)	1.372	1.396			

Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.
O(1)-C(1)-O(2)	122.7	122.2	C(11)-C(10)-C(9)	121.2	120.6	C(20)-C(19)-C(18)	120.8	120.6	C(29)-C(28)-C(27)	116.1	116.3
O(1)-C(1)-C(2)	125.4	126.0	C(11)-C(10)-H(10)	119.4	119.9	C(20)-C(19)-H(19)	119.6	120.3	C(29)-C(28)-H(28)	122.0	121.6
O(2)-C(1)-C(2)	111.7	111.9	C(9)-C(10)-H(10)	119.4	119.4	C(18)-C(19)-H(19)	119.6	119.1	C(27)-C(28)-H(28)	122.0	122.1
C(7)-C(2)-C(3)	119.2	120.1	C(12)-C(11)-C(10)	120.3	120.3	C(19)-C(20)-C(21)	120.4	120.3	C(28)-C(29)-O(3)	125.8	126.5
C(7)-C(2)-C(1)	121.7	117.8	C(12)-C(11)-H(11)	119.8	120.0	C(19)-C(20)-H(20)	119.8	119.6	C(28)-C(29)-C(24)	124.6	124.1
C(3)-C(2)-C(1)	118.9	122.1	C(10)-C(11)-H(11)	119.8	119.7	C(21)-C(20)-H(20)	119.8	120.1	O(3)-C(29)-C(24)	109.6	109.5
C(4)-C(3)-C(2)	119.7	119.6	C(11)-C(12)-C(13)	119.8	119.4	C(20)-C(21)-C(22)	119.4	119.4	C(1)-O(2)-C(8)	116.8	118.7
C(4)-C(3)-H(3)	120.2	120.7	C(11)-C(12)-H(12)	120.1	120.3	C(20)-C(21)-H(21)	120.3	120.3	C(29)-O(3)-C(17)	106.0	107.1
C(2)-C(3)-H(3)	120.2	119.7	C(13)-C(12)-H(12)	120.1	120.2	C(22)-C(21)-H(21)	120.3	120.3			
C(5)-C(4)-C(3)	120.8	120.2	C(12)-C(13)-C(14)	120.1	120.3	C(23)-C(22)-C(21)	120.7	120.5			
C(5)-C(4)-H(4)	119.6	120.1	C(12)-C(13)-H(13)	119.9	120.0	C(23)-C(22)-H(22)	119.6	119.5			
C(3)-C(4)-H(4)	119.6	119.7	C(14)-C(13)-H(13)	119.9	119.7	C(21)-C(22)-H(22)	119.6	120.0			
C(6)-C(5)-C(4)	119.6	120.1	C(13)-C(14)-C(9)	120.9	120.6	C(22)-C(23)-C(18)	120.5	120.5			
C(6)-C(5)-H(5)	120.2	119.9	C(13)-C(14)-H(14)	119.6	119.3	C(22)-C(23)-H(23)	119.8	119.6			
C(4)-C(5)-H(5)	120.2	120.0	C(9)-C(14)-H(14)	119.6	120.0	C(18)-C(23)-H(23)	119.8	119.9			
C(5)-C(6)-C(7)	120.3	120.0	C(8)-C(15)-C(16)	125.4	128.2	C(29)-C(24)-C(25)	118.1	118.9			
C(5)-C(6)-H(6)	119.9	121.2	C(8)-C(15)-H(15)	117.3	116.4	C(29)-C(24)-C(16)	106.87	106.8			
C(7)-C(6)-H(6)	119.9	120.0	C(16)-C(15)-H(15)	117.3	115.3	C(25)-C(24)-C(16)	134.9	134.2			
C(6)-C(7)-C(2)	120.3	120.0	C(17)-C(16)-C(24)	105.9	106.6	C(26)-C(25)-C(24)	117.8	118.3			
C(6)-C(7)-H(7)	119.8	121.2	C(17)-C(16)-C(15)	126.6	131.3	C(26)-C(25)-H(25)	121.1	120.6			
C(2)-C(7)-H(7)	119.8	118.8	C(24)-C(16)-C(15)	127.2	122.1	C(24)-C(25)-H(25)	121.1	121.1			
C(15)-C(8)-O(2)	118.2	118.4	C(16)-C(17)-O(3)	111.5	109.9	C(25)-C(26)-C(27)	121.5	121.3			
C(15)-C(8)-C(9)	128.2	126.3	C(16)-C(17)-C(18)	133.6	135.4	C(25)-C(26)-H(26)	119.3	119.6			
O(2)-C(8)-C(9)	113.4	115.1	O(3)-C(17)-C(18)	114.8	114.1	C(27)-C(26)-H(26)	119.3	119.1			
C(10)-C(9)-C(14)	117.6	118.6	C(23)-C(18)-C(19)	118.2	118.7	C(28)-C(27)-C(26)	121.9	121.2			
C(10)-C(9)-C(8)	121.5	120.0	C(23)-C(18)-C(17)	121.3	121.7	C(28)-C(27)-H(27)	119.0	119.4			
C(14)-C(9)-C(8)	120.8	121.4	C(19)-C(18)-C(17)	120.5	119.5	C(26)-C(27)-H(27)	119.0	119.4			

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Distance	Exp.	Theo.	Distance	Exp.	Theo.	Distance	Exp.	Theo.
Br(1)-C(5)	1.903	1.965	C(12)-H(12)	0.930	1.086	C(29)-C(30)	1.365	1.404
O(1)-C(1)	1.196	1.241	C(13)-C(14)	1.474	1.482	C(29)-H(29)	0.930	1.087
O(2)-C(1)	1.359	1.401	C(14)-C(15)	1.351	1.383	C(30)-H(30)	0.930	1.085
O(2)-C(8)	1.404	1.425	C(14)-C(22)	1.453	1.459			
O(3)-C(15)	1.350	1.409	C(15)-C(16)	1.465	1.465			
O(3)-C(24)	1.362	1.394	C(16)-C(17)	1.388	1.416			
N(1)-C(23)	1.146	1.184	C(16)-C(21)	1.387	1.416			
C(1)-C(2)	1.481	1.484	C(17)-C(18)	1.375	1.405			
C(2)-C(7)	1.382	1.413	C(17)-H(17)	0.930	1.085			
C(2)-C(3)	1.386	1.413	C(18)-C(19)	1.359	1.409			
C(3)-C(4)	1.379	1.403	C(18)-H(18)	0.930	1.087			
C(3)-H(3)	0.930	1.086	C(19)-C(20)	1.363	1.409			
C(4)-C(5)	1.373	1.407	C(19)-H(19)	0.93	1.087			
C(4)-H(4)	0.930	1.085	C(20)-C(21)	1.387	1.404			
C(5)-C(6)	1.363	1.406	C(20)-H(20)	0.930	1.087			
C(6)-C(7)	1.369	1.405	C(21)-H(21)	0.930	1.086			
C(6)-H(6)	0.930	1.085	C(22)-C(24)	1.368	1.395			
C(7)-H(7)	0.930	1.085	C(22)-C(23)	1.421	1.422			
C(8)-C(13)	1.386	1.410	C(24)-C(25)	1.453	1.461			
C(8)-C(9)	1.380	1.399	C(25)-C(26)	1.382	1.419			
C(9)-C(10)	1.380	1.406	C(25)-C(30)	1.389	1.418			
C(9)-H(9)	0.930	1.086	C(26)-C(27)	1.388	1.403			
C(10)-C(11)	1.369	1.409	C(26)-H(26)	0.930	1.085			
C(10)-H(10)	0.930	1.087	C(27)-C(28)	1.366	1.409			
C(11)-C(12)	1.378	1.405	C(27)-H(27)	0.930	1.087			
C(11)-H(11)	0.930	1.087	C(28)-C(29)	1.357	1.409			
C(12)-C(13)	1.404	1.414	C(28)-H(28)	0.930	1.087			

Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.
C(1)-O(2)-C(8)	118.0	119.5	C(8)-C(9)-H(9)	120.1	119.2	C(19)-C(18)-H(18)	119.6	120.0	C(29)-C(28)-C(27)	120.6	119.6
C(15)-O(3)-C(24)	108.6	109.1	C(10)-C(9)-H(9)	120.1	121.6	C(17)-C(18)-H(18)	119.6	119.4	C(29)-C(28)-H(28)	119.7	120.2
O(1)-C(1)-O(2)	122.2	122.5	C(11)-C(10)-C(9)	119.6	119.7	C(20)-C(19)-C(18)	120.3	119.7	C(27)-C(28)-H(28)	119.7	120.2
O(1)-C(1)-C(2)	126.3	126.0	C(11)-C(10)-H(10)	120.2	120.4	C(20)-C(19)-H(19)	119.8	120.1	C(28)-C(29)-C(30)	120.3	120.5
O(2)-C(1)-C(2)	111.5	111.5	C(9)-C(10)-H(10)	120.2	119.9	C(18)-C(19)-H(19)	119.8	120.2	C(28)-C(29)-H(29)	119.8	120.1
C(7)-C(2)-C(3)	119.1	120.0	C(10)-C(11)-C(12)	120.6	120.1	C(19)-C(20)-C(21)	120.2	120.2	C(30)-C(29)-H(29)	119.8	119.4
C(7)-C(2)-C(1)	123.0	121.8	C(10)-C(11)-H(11)	119.7	120.1	C(19)-C(20)-H(20)	119.9	120.1	C(29)-C(30)-C(25)	120.6	120.2
C(3)-C(2)-C(1)	117.9	118.2	C(12)-C(11)-H(11)	119.7	119.8	C(21)-C(20)-H(20)	119.9	119.8	C(29)-C(30)-H(30)	119.7	119.2
C(2)-C(3)-C(4)	120.9	120.3	C(11)-C(12)-C(13)	121.1	121.2	C(16)-C(21)-C(20)	119.7	120.3	C(25)-C(30)-H(30)	119.7	120.6
C(2)-C(3)-H(3)	119.5	119.1	C(11)-C(12)-H(12)	119.4	120.1	C(16)-C(21)-H(21)	120.1	119.4			
C(4)-C(3)-H(3)	119.5	120.6	C(13)-C(12)-H(12)	119.4	118.8	C(20)-C(21)-H(21)	120.1	120.2			
C(5)-C(4)-C(3)	118.0	118.9	C(8)-C(13)-C(12)	116.8	117.3	C(24)-C(22)-C(23)	127.3	126.7			
C(5)-C(4)-H(4)	121.0	120.6	C(8)-C(13)-C(14)	123.3	122.3	C(24)-C(22)-C(14)	107.5	108.0			
C(3)-C(4)-H(4)	121.0	120.5	C(12)-C(13)-C(14)	119.8	120.4	C(23)-C(22)-C(14)	124.9	125.3			
C(4)-C(5)-C(6)	122.3	121.6	C(15)-C(14)-C(22)	105.3	106.5	N(1)-C(23)-C(22)	177.1	179.3			
C(4)-C(5)-Br(1)	117.7	119.2	C(15)-C(14)-C(13)	126.8	127.4	C(22)-C(24)-O(3)	108.3	107.6			
C(6)-C(5)-Br(1)	119.9	119.2	C(22)-C(14)-C(13)	127.8	125.8	C(22)-C(24)-C(25)	136.4	135.5			
C(5)-C(6)-C(7)	119.3	119.2	O(3)-C(15)-C(14)	110.2	108.7	O(3)-C(24)-C(25)	115.3	116.8			
C(5)-C(6)-H(6)	120.4	120.6	O(3)-C(15)-C(16)	114.4	116.4	C(26)-C(25)-C(30)	118.7	118.9			
C(7)-C(6)-H(6)	120.4	120.2	C(14)-C(15)-C(16)	135.4	134.8	C(26)-C(25)-C(24)	120.2	119.4			
C(2)-C(7)-C(6)	120.4	120.0	C(17)-C(16)-C(21)	119.1	119.4	C(30)-C(25)-C(24)	121.2	121.6			
C(2)-C(7)-H(7)	119.8	119.8	C(17)-C(16)-C(15)	121.3	120.6	C(25)-C(26)-C(27)	120.0	120.5			
C(6)-C(7)-H(7)	119.8	120.2	C(21)-C(16)-C(15)	119.6	120.1	C(25)-C(26)-H(26)	120.0	119.2			
C(13)-C(8)-C(9)	122.0	122.5	C(16)-C(17)-C(18)	119.9	120.0	C(27)-C(26)-H(26)	120.0	120.3			
C(13)-C(8)-O(2)	117.9	119.9	C(16)-C(17)-H(17)	120.0	119.9	C(28)-C(27)-C(26)	119.9	120.3			
C(9)-C(8)-O(2)	120.0	117.6	C(18)-C(17)-H(17)	120.0	120.1	C(28)-C(27)-H(27)	120.1	120.0			
C(8)-C(9)-C(10)	119.8	119.2	C(19)-C(18)-C(17)	120.7	120.5	C(26)-C(27)-H(27)	120.1	119.7			

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Distance	Exp.	Theo.	Distance	Exp.	Theo.	Distance	Exp.	Theo.
C(1)-C(6)	1.361	1.408	C(14)-H(14)	0.950	1.087	C(27)-H(27A)	0.980	1.095
C(1)-C(2)	1.379	1.408	C(15)-C(16)	1.390	1.403	C(27)-H(27B)	0.980	1.097
C(1)-N(1)	1.468	1.469	C(15)-H(15)	0.950	1.087	C(27)-H(27C)	0.980	1.097
C(2)-C(3)	1.384	1.398	C(16)-H(16)	0.950	1.087	N(1)-O(1)	1.209	1.281
C(2)-H(2)	0.950	1.084	C(17)-C(22)	1.391	1.411	N(1)-O(2)	1.230	1.282
C(3)-C(4)	1.392	1.420	C(17)-C(18)	1.398	1.415			
C(3)-H(3)	0.950	1.085	C(18)-C(19)	1.390	1.405			
C(4)-C(5)	1.404	1.420	C(18)-H(18)	0.950	1.087			
C(4)-C(7)	1.450	1.458	C(19)-C(20)	1.371	1.408			
C(5)-C(6)	1.383	1.398	C(19)-H(19)	0.950	1.087			
C(5)-H(5)	0.950	1.084	C(20)-C(21)	1.376	1.406			
C(6)-H(6)	0.950	1.084	C(20)-H(20)	0.950	1.087			
C(7)-C(8)	1.363	1.391	C(21)-C(22)	1.383	1.401			
C(7)-O(3)	1.395	1.407	C(21)-H(21)	0.950	1.086			
C(8)-C(9)	1.433	1.441	C(22)-O(4)	1.405	1.427			
C(8)-C(17)	1.490	1.483	C(23)-O(5)	1.205	1.236			
C(9)-C(10)	1.350	1.383	C(23)-O(4)	1.351	1.41			
C(9)-H(9)	0.950	1.079	C(23)-C(24)	1.505	1.532			
C(10)-O(3)	1.362	1.403	C(24)-C(26)	1.518	1.546			
C(10)-C(11)	1.469	1.46	C(24)-C(27)	1.531	1.554			
C(11)-C(16)	1.384	1.417	C(24)-C(25)	1.524	1.557			
C(11)-C(12)	1.384	1.417	C(25)-H(25A)	0.980	1.095			
C(12)-C(13)	1.390	1.404	C(25)-H(25B)	0.980	1.097			
C(12)-H(12)	0.950	1.086	C(25)-H(25C)	0.980	1.098			
C(13)-C(14)	1.380	1.409	C(26)-H(26A)	0.980	1.096			
C(13)-H(13)	0.950	1.087	C(26)-H(26B)	0.980	1.096			
C(14)-C(15)	1.374	1.410	C(26)-H(26C)	0.980	1.097			

Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.
C(6)-C(1)-C(2)	122.7	121.7	C(9)-C(10)-O(3)	108.7	108.3	C(20)-C(19)-C(18)	120.6	120.0	C(24)-C(26)-H(26A)	109.5	109.4
C(6)-C(1)-N(1)	118.8	119.2	C(9)-C(10)-C(11)	134.7	134.1	C(20)-C(19)-H(19)	119.7	120.2	C(24)-C(26)-H(26B)	109.5	111.3
C(2)-C(1)-N(1)	118.5	118.8	O(3)-C(10)-C(11)	116.6	117.6	C(18)-C(19)-H(19)	119.7	119.8	H(26A)-C(26)-H(26B)	109.5	107.6
C(1-C(2)-C(3)	119.3	119.1	C(16)-C(11)-C(12)	118.3	119.0	C(19)-C(20)-C(21)	120.2	119.7	C(24)-C(26)-H(26C)	109.5	111.3
C(1)-C(2)-H(2)	120.4	119.6	C(16)-C(11)-C(10)	120.9	120.3	C(19)-C(20)-H(20)	119.9	120.4	H(26A)-C(26)-H(26C)	109.5	108.5
C(3)-C(2)-H(2)	120.4	121.6	C(12)-C(11)-C(10)	120.8	120.7	C(21)-C(20)-H(20)	119.9	120.2	H(26B)-C(26)-H(26C)	109.5	108.6
C(2)-C(3)-C(4)	119.8	120.8	C(11)-C(12)-C(13)	120.8	120.4	C(20)-C(21)-C(22)	119.1	119.5	C(24)-C(27)-H(27A)	109.5	109.2
C(2)-C(3)-H(3)	120.1	120.0	C(11)-C(12)-H(12)	119.6	119.3	C(20)-C(21)-H(21)	120.5	120.4	C(24)-C(27)-H(27B)	109.5	111.1
C(4)-C(3)-H(3)	120.1	119.2	C(13)-C(12)-H(12)	119.6	120.4	C(22)-C(21)-H(21)	120.5	119.1	H(27A)-C(27)-H(27B)	109.5	108.0
C(3)-C(4)-C(5)	119.0	119.2	C(14)-C(13)-C(12)	120.4	120.4	C(21)-C(22)-C(17)	122.6	122.2	C(24)-C(27)-H(27C)	109.5	111.3
C(3)-C(4)-C(7)	119.5	119.9	C(14)-C(13)-H(13)	119.8	120.0	C(21)-C(22)-O(4)	118.2	117.1	H(27A)-C(27)-H(27C)	109.5	108.7
C(5)-C(4)-C(7)	121.5	120.9	C(12)-C(13)-H(13)	119.8	119.7	C(17)-C(22)-O(4)	119.2	120.7	H(27B)-C(27)-H(27C)	109.5	108.5
C(6)-C(5)-C(4)	121.0	120.4	C(15)-C(14)-C(13)	119.1	119.5	O(5)-C(23)-O(4)	121.3	121.6	O(1)-N(1)-O(2)	123.7	123.4
C(6)-C(5)-H(5)	119.5	119.8	C(15)-C(14)-H(14)	120.5	120.2	O(5)-C(23)-C(24)	126.5	127.2	O(1)-N(1)-C(1)	118.5	118.3
C(4)-C(5)-H(5)	119.5	119.7	C(13)-C(14)-H(14)	120.5	120.3	O(4)-C(23)-C(24)	112.1	111.2	O(2)-N(1)-C(1)	117.9	123.4
C(1)-C(6)-C(5)	118.3	119.1	C(14)-C(15)-C(16)	120.6	120.3	C(23)-C(24)-C(26)	109.9	108.8	C(10)-O(3)-C(7)	108.2	108.1
C(1)-C(6)-H(6)	120.9	119.6	C(14)-C(15)-H(15)	119.7	120.0	C(23)-C(24)-C(27)	107.3	108.1	C(23)-O(4)-C(22)	117.4	119.1
C(5)-C(6)-H(6)	120.9	121.3	C(16)-C(15)-H(15)	119.7	119.7	C(26)-C(24)-C(27)	109.3	110.2			
C(8)-C(7)-O(3)	108.8	108.6	C(11)-C(16)-C(15)	120.8	120.4	C(23)-C(24)-C(25)	110.4	109.6			
C(8)-C(7)-C(4)	136.6	135.0	C(11)-C(16)-H(16)	119.6	120.0	C(26)-C(24)-C(25)	110.3	110.4			
O(3)-C(7)-C(4)	114.6	116.3	C(15)-C(16)-H(16)	119.6	119.6	C(27)-C(24)-C(25)	109.7	109.7			
C(7)-C(8)-C(9)	105.8	106.8	C(22)-C(17)-C(18)	116.9	117.3	C(24)-C(25)-H(25A)	109.5	109.1			
C(7)-C(8)-C(17)	127.9	127.9	C(22)-C(17)-C(8)	121.6	122.3	C(24)-C(25)-H(25B)	109.5	111.3			
C(9)-C(8)-C(17)	126.1	125.0	C(18)-C(17)-C(8)	121.3	120.4	H(25A)-C(25)-H(25C)	109.5	108.1			
C(10)-C(9)-C(8)	108.5	108.1	C(17)-C(18)-C(19)	120.6	121.3	C(24)-C(25)-H(25C)	109.5	111.1			
C(10)-C(9)-H(9)	125.7	126.7	C(17)-C(18)-H(18)	119.7	118.7	H(25A)-C(25)-H(25C)	109.5	108.5			
C(8)-C(9)-H(9)	125.7	125.2	C(19)-C(18)-H(18)	119.7	120.0	H(25B)-C(25)-H(25C)	109.5	108.6			

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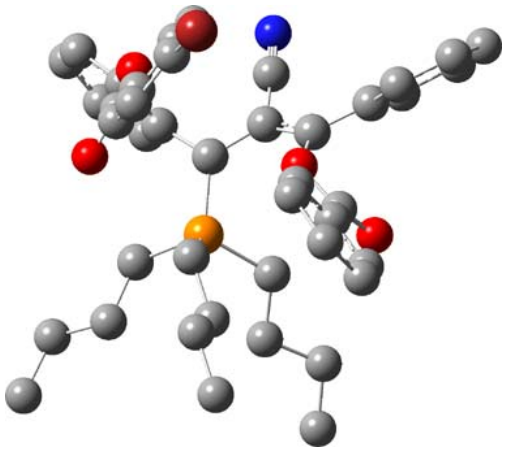
Distance	Exp.	Theo.	Distance	Exp.	Theo.	Distance	Exp.	Theo.
C(1)-C(6)	1.358	1.404	C(15)-C(17)	1.363	1.369	C(27)-H(27C)	0.98	1.097
C(1)-C(2)	1.385	1.405	C(15)-C(16)	1.435	1.438	C(28)-H(28A)	0.98	1.096
C(1)-Br(1)	1.886	1.967	C(16)-N(1)	1.158	1.184	C(28)-H(28B)	0.98	1.097
C(2)-C(3)	1.379	1.403	C(17)-O(2)	1.381	1.418	C(28)-H(28C)	0.98	1.096
C(2)-H(2)	0.950	1.085	C(17)-C(18)	1.466	1.479			
C(3)-C(4)	1.371	1.416	C(18)-C(19)	1.363	1.415			
C(3)-H(3)	0.950	1.084	C(18)-C(23)	1.405	1.417			
C(4)-C(5)	1.397	1.418	C(19)-C(20)	1.374	1.404			
C(4)-C(7)	1.477	1.463	C(19)-H(19)	0.950	1.085			
C(5)-C(6)	1.392	1.404	C(20)-C(21)	1.358	1.408			
C(5)-H(5)	0.950	1.085	C(20)-H(20)	0.950	1.087			
C(6)-H(6)	0.950	1.085	C(21)-C(22)	1.393	1.409			
C(7)-C(8)	1.37	1.385	C(21)-H(21)	0.950	1.087			
C(7)-O(1)	1.388	1.419	C(22)-C(23)	1.368	1.403			
C(8)-C(9)	1.448	1.457	C(22)-H(22)	0.950	1.087			
C(8)-C(15)	1.451	1.488	C(23)-H(23)	0.950	1.086			
C(9)-C(10)	1.384	1.412	C(24)-O(3)	1.192	1.232			
C(9)-C(14)	1.386	1.414	C(24)-O(2)	1.380	1.423			
C(10)-C(11)	1.377	1.404	C(24)-C(25)	1.507	1.531			
C(10)-H(10)	0.950	1.086	C(25)-C(28)	1.404	1.546			
C(11)-C(12)	1.403	1.420	C(25)-C(26)	1.505	1.554			
C(11)-H(11)	0.950	1.087	C(25)-C(27)	1.522	1.556			
C(12)-C(13)	1.381	1.408	C(26)-H(26A)	0.980	1.097			
C(12)-H(12)	0.950	1.087	C(26)-H(26B)	0.980	1.098			
C(13)-C(14)	1.391	1.395	C(26)-H(26C)	0.980	1.095			
C(13)-H(13)	0.950	1.085	C(27)-H(27A)	0.980	1.097			
C(14)-O(1)	1.373	1.400	C(27)-H(27B)	0.980	1.094			

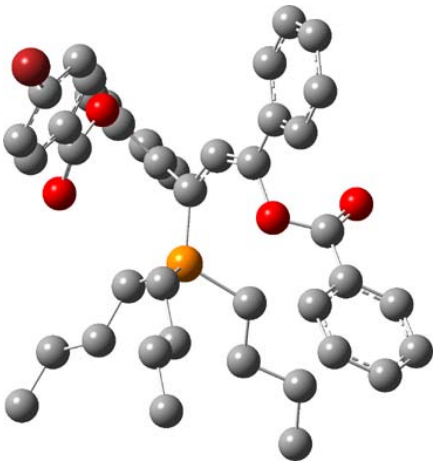
Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.	Angle	Exp.	Theo.
C(6)-C(1)-C(2)	119.7	121.0	C(11)-C(10)-C(9)	118.1	118.1	C(20)-C(19)-H(19)	118.9	119.4	H(26B)-C(26)-H(26C)	109.5	108.9
C(6)-C(1)-Br(1)	121.6	119.6	C(11)-C(10)-H(10)	120.9	120.8	C(21)-C(20)-C(19)	118.8	120.4	C(25)-C(27)-H(27A)	109.5	109.0
C(2)-C(1)-Br(1)	118.7	119.4	C(9)-C(10)-H(10)	120.9	121.1	C(21)-C(20)-H(20)	120.6	120.1	C(25)-C(27)-H(27B)	109.5	111.2
C(3)-C(2)-C(1)	119.8	119.4	C(10)-C(11)-C(12)	120.1	121.4	C(19)-C(20)-H(20)	120.6	119.5	H(27A)-C(27)-H(27B)	109.5	108.0
C(3)-C(2)-H(2)	120.1	120.0	C(10)-C(11)-H(11)	119.9	119.6	C(20)-C(21)-C(22)	120.7	119.7	C(25)-C(27)-H(27C)	109.5	111.3
C(1)-C(2)-H(2)	120.1	120.6	C(12)-C(11)-H(11)	119.9	119	C(20)-C(21)-H(21)	119.7	120.1	H(27A)-C(27)-H(27C)	109.5	108.6
C(4)-C(3)-C(2)	120.8	120.9	C(13)-C(12)-C(11)	123	121.2	C(22)-C(21)-H(21)	119.7	120.2	H(27B)-C(27)-H(27C)	109.5	108.6
C(4)-C(3)-H(3)	119.6	120.5	C(13)-C(12)-H(12)	118.5	119.4	C(23)-C(22)-C(21)	120.2	120.1	C(25)-C(28)-H(28A)	109.5	111.3
C(2)-C(3)-H(3)	119.6	118.6	C(11)-C(12)-H(12)	118.5	119.4	C(23)-C(22)-H(22)	119.9	119.8	C(25)-C(28)-H(28B)	109.5	109.4
C(3)-C(4)-C(5)	119.8	118.4	C(12)-C(13)-C(14)	115.2	116.2	C(21)-C(22)-H(22)	119.9	120.1	H(28A)-C(28)-H(28B)	109.5	108.6
C(3)-C(4)-C(7)	121.1	122.0	C(12)-C(13)-H(13)	122.4	122.1	C(22)-C(23)-C(18)	119.2	120.5	C(25)-C(28)-H(28C)	109.5	111.4
C(5)-C(4)-C(7)	119.0	119.6	C(14)-C(13)-H(13)	122.4	121.7	C(22)-C(23)-H(23)	120.4	120.0	H(28A)-C(28)-H(28C)	109.5	107.6
C(6)-C(5)-C(4)	118.6	121.0	O(1)-C(14)-C(9)	110.9	109.5	C(18)-C(23)-H(23)	120.4	119.5	H(28B)-C(28)-H(28C)	109.5	108.5
C(6)-C(5)-H(5)	120.7	119.6	O(1)-C(14)-C(13)	126.1	126.5	O(3)-C(24)-O(2)	119.9	121.1	C(14)-O(1)-C(7)	106.2	107.1
C(4)-C(5)-H(5)	120.7	119.3	C(9)-C(14)-C(13)	123	124	O(3)-C(24)-C(25)	127.1	127.9	C(24)-O(2)-C(17)	115.9	119.3
C(1)-C(6)-C(5)	121.4	119.2	C(17)-C(15)-C(16)	121.4	121.5	O(2)-C(24)-C(25)	113.0	111.0			
C(1)-C(6)-H(6)	119.3	120.6	C(17)-C(15)-C(8)	121.9	123.3	C(28)-C(25)-C(26)	122.6	110.3			
C(5)-C(6)-H(6)	119.3	120.1	C(16)-C(15)-C(8)	116.7	115.2	C(28)-C(25)-C(24)	111.0	108.5			
C(8)-C(7)-O(1)	110.9	109.8	N(1)-C(16)-C(15)	176.1	176.5	C(26)-C(25)-C(24)	108.4	109.7			
C(8)-C(7)-C(4)	133.4	135.4	C(15)-C(17)-O(2)	116	115.8	C(28)-C(25)-C(27)	99.1	110.3			
O(1)-C(7)-C(4)	115.7	114.8	C(15)-C(17)-C(18)	128.5	128.9	C(26)-C(25)-C(27)	106.3	109.7			
C(7)-C(8)-C(9)	106.3	107.2	O(2)-C(17)-C(18)	115.4	115.1	C(24)-C(25)-C(27)	108.2	108.5			
C(7)-C(8)-C(15)	126.8	128.9	C(19)-C(18)-C(23)	118.8	119	C(25)-C(26)-H(26A)	109.5	109.1			
C(9)-C(8)-C(15)	126.8	123.9	C(19)-C(18)-C(17)	123.3	122.1	C(25)-C(26)-H(26B)	109.5	111.3			
C(10)-C(9)-C(14)	120.6	119.1	C(23)-C(18)-C(17)	117.8	118.9	H(26A)-C(26)-H(26B)	109.5	107.9			
C(10)-C(9)-C(8)	133.7	134.5	C(18)-C(19)-C(20)	122.2	120.3	C(25)-C(26)-H(26C)	109.5	111.2			
C(14)-C(9)-C(8)	105.7	106.5	C(18)-C(19)-H(19)	118.9	120.3	H(26A)-C(26)-H(26C)	109.5	108.3			

Intermediate **2** (**R**^{1}, **R**^{2}, **R**^{3} = 4-BrC_6H_4, Ph, Ph)

FG = CN

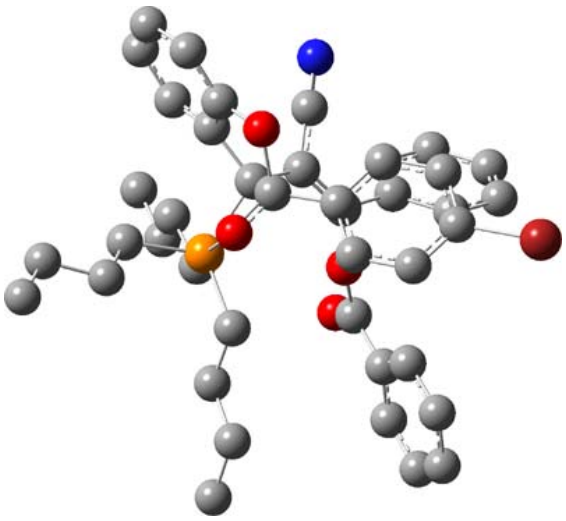


FG = H

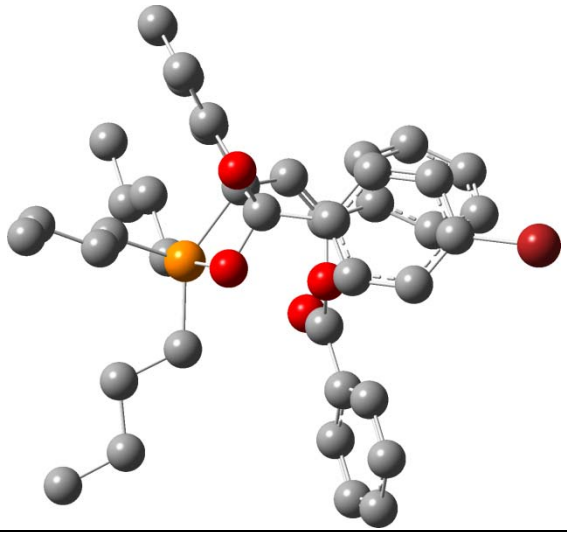


Intermediate **6** (**R**^{1}, **R**^{2}, **R**^{3} = 4-BrC_6H_4, Ph, Ph)

FG = CN

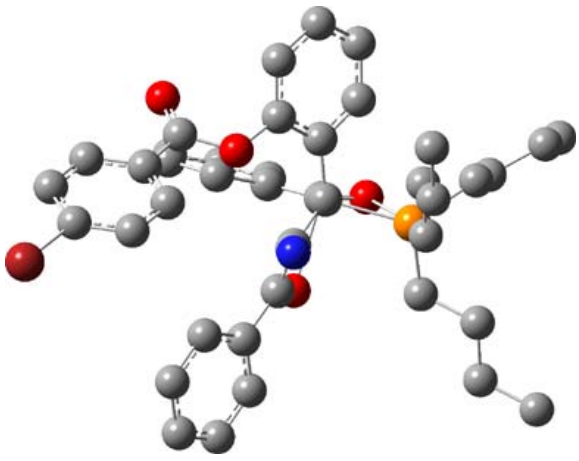


FG = H

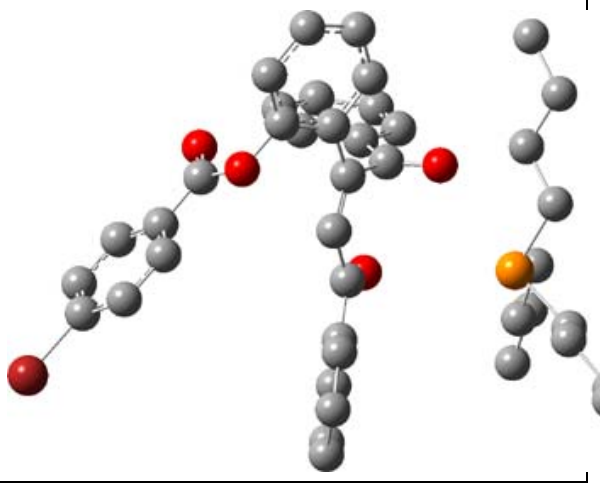


Intermediate **8** (**R**^{1}, **R**^{2}, **R**^{3} = 4-BrC_6H_4, Ph, Ph)

FG = CN



FG = H



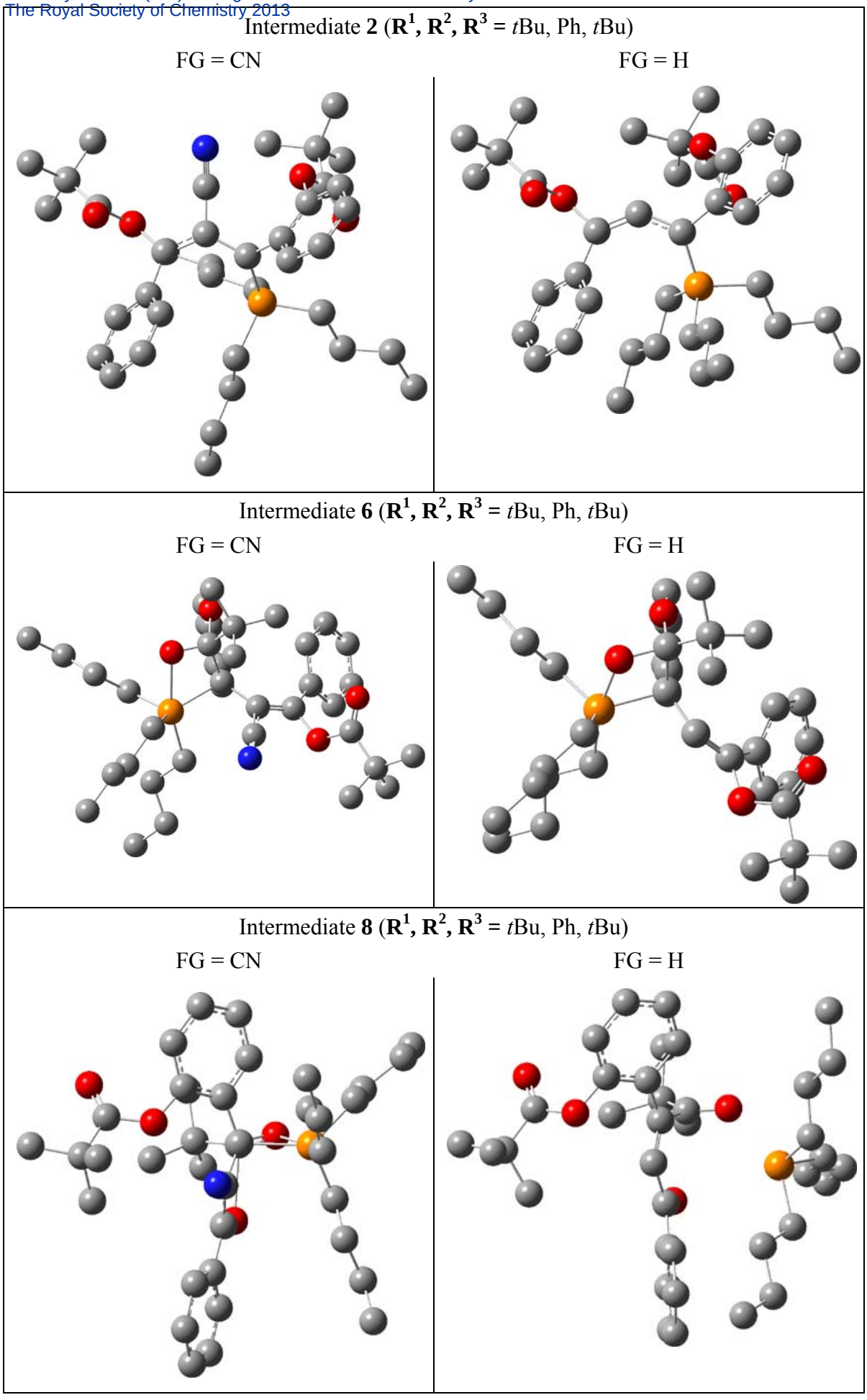


Figure S2 Optimized structures of intermediates **2**, **6** (from path **a**) and **8** (from path **b**) with and without CN substitution (FG = CN and H). The Cartesian coordinates of them are listed in Table S2.

Table S2 Optimized Geometries of Intermediates **2**, **6** and **8** (Figure S2) in Cartesian Coordinates (Å)

Intermediate **2**; FG = CN; **R¹**, **R²**, **R³** = 4-BrC_6H_4, Ph, Ph

C	1.298	-3.032	-3.726	C	-1.053	-0.216	-3.370	C	0.468	-1.163	-2.326	H	1.549	3.247	0.423
C	0.258	-2.344	-3.085	N	-1.907	-0.458	-4.115	C	-0.254	0.009	-2.674	H	3.114	4.529	1.834
C	-1.029	-2.895	-3.252	H	2.309	-2.662	-3.620	C	-0.180	1.390	-2.350	H	5.163	5.491	0.850
C	-1.254	-4.025	-4.028	H	-2.263	-4.397	-4.159	C	-1.159	2.411	-2.816	H	5.632	5.199	-1.559
C	-0.197	-4.671	-4.645	H	-0.370	-5.548	-5.254	C	-2.017	2.206	-3.905	H	4.063	3.928	-2.975
C	1.084	-4.171	-4.481	H	1.923	-4.680	-4.938	C	-2.925	3.173	-4.296	H	1.604	-3.597	-0.616
O	-2.162	-2.306	-2.638	H	-4.052	-0.834	-2.483	C	-3.010	4.380	-3.621	H	2.930	-3.100	-1.755
C	-2.178	-2.423	-1.249	H	-5.987	0.292	-1.451	C	-2.167	4.605	-2.544	H	0.478	0.321	0.674
O	-1.329	-3.019	-0.607	H	-4.877	-1.310	2.369	C	-1.261	3.639	-2.149	H	0.129	-1.434	0.993
C	-3.373	-1.705	-0.643	H	-2.943	-2.428	1.331	O	0.880	1.905	-1.539	H	3.588	-0.275	-2.209
C	-4.230	-0.933	-1.420	H	-1.973	1.271	-4.445	C	1.774	2.694	-2.266	H	2.648	1.066	-1.421
C	-5.318	-0.300	-0.840	H	-3.583	2.980	-5.134	O	1.801	2.747	-3.483	H	4.201	-2.176	0.171
C	-5.557	-0.436	0.524	H	-3.727	5.130	-3.923	C	2.707	3.497	-1.366	H	2.913	-2.659	1.277
C	-4.700	-1.209	1.305	H	-2.213	5.548	-2.014	C	2.440	3.678	-0.013	H	2.443	-1.708	1.862
C	-3.615	-1.837	0.720	H	-0.609	3.839	-1.311	C	3.320	4.398	0.780	H	2.782	-0.007	1.553
C	6.243	1.051	0.749	H	7.043	1.749	0.520	Br	-7.043	0.406	1.311	H	5.763	1.361	1.674

C	4.470	4.940	0.226	H	3.536	0.353	0.788
C	4.740	4.767	-1.125	H	4.448	-0.948	0.025
C	3.859	4.051	-1.918	H	3.253	-5.051	0.605
P	1.678	-1.147	-0.909	H	4.538	-4.567	-0.477
C	2.413	-2.856	-0.800	H	0.950	0.639	3.138
C	0.922	-0.698	0.735	H	0.616	-1.050	3.446
C	3.064	0.044	-1.281	H	5.712	0.751	-1.324
C	3.416	-2.906	0.346	H	4.818	2.035	-0.544
C	1.999	-0.716	1.812	H	4.559	-4.192	2.559
C	4.051	0.054	-0.121	H	5.472	-5.412	1.662
C	4.041	-4.316	0.458	H	5.859	-3.700	1.466
C	1.407	-0.348	3.192	H	2.917	-1.345	4.386
C	5.215	1.033	-0.398	H	3.256	0.362	4.073
C	5.053	-4.411	1.617	H	2.024	-0.090	5.254
C	2.475	-0.357	4.303	H	6.667	0.061	0.886

Intermediate **6**; FG = CN; **R¹**, **R²**, **R³** = 4-BrC_6H_4, Ph, Ph

C	-3.684	-2.341	0.627	C	-0.768	-2.618	1.799	C	-1.422	-1.110	-0.105	H	-4.536	1.242	-0.489
C	-2.570	-2.122	-0.202	N	-0.933	-3.667	2.320	C	-0.570	-1.346	1.146	H	-4.377	0.412	1.892
C	-2.357	-2.986	-1.301	H	-3.861	-1.727	1.502	C	-2.151	0.722	-0.331	H	-2.947	-0.276	2.677
C	-3.245	-4.030	-1.609	H	-3.049	-4.667	-2.466	C	-2.504	1.434	1.402	H	-2.412	3.772	-0.759
C	-4.361	-4.223	-0.778	H	-5.057	-5.030	-0.993	C	-1.083	2.073	-1.131	H	-1.086	3.647	0.400
C	-4.582	-3.385	0.338	H	-5.439	-3.554	0.984	C	-3.855	0.697	-1.157	H	-3.655	2.345	-2.581
O	-1.203	-2.740	-1.996	H	0.908	0.214	-3.089	C	-3.421	0.666	2.372	H	-3.151	0.756	-3.194
C	-0.723	-1.286	-1.612	H	3.404	0.044	-3.399	C	-1.345	3.520	-0.660	H	-2.753	1.778	4.115
O	-1.292	-0.358	-2.385	H	3.458	-3.334	-0.694	C	-3.903	1.273	-2.587	H	-4.196	2.446	3.353
C	0.797	-1.417	-1.708	H	0.995	-3.174	-0.450	O	-3.707	1.503	3.642	H	0.548	4.281	-1.411
C	1.489	-0.529	-2.551	H	-1.543	1.622	1.891	C	-0.521	4.526	-1.499	H	-0.782	4.411	-2.562
C	2.882	-0.630	-2.727	H	-2.953	2.416	1.198	O	-5.305	1.090	-3.213	H	-5.543	0.016	-3.253
C	3.579	-1.633	-2.035	H	-0.044	1.782	-0.969	C	-4.593	0.753	4.658	H	-6.067	1.558	-2.571
C	2.911	-2.545	-1.201	H	-1.272	1.959	-2.199	C	-0.754	5.987	-1.063	H	-4.112	-0.177	4.992
C	1.517	-2.436	-1.051	H	-4.170	-0.350	-1.174	C	-5.390	1.688	-4.633	H	-4.785	1.368	5.547
C	2.443	3.886	1.461	H	3.619	5.687	1.251	Br	5.538	-1.779	-2.257	H	1.915	4.215	2.351

C	0.454	-0.580	1.640	H	-5.565	0.488	4.218
C	1.329	-0.913	2.795	H	-1.811	6.268	-1.167
C	0.799	-1.271	4.052	H	-0.470	6.135	-0.012
P	1.656	-1.573	5.122	H	-0.161	6.681	-1.672
C	3.053	-1.520	4.949	H	-4.656	1.218	-5.300
C	3.588	-1.161	3.697	H	-6.387	1.538	-5.070
C	2.734	-0.853	2.626	H	-5.189	2.768	-4.620
C	0.848	0.575	0.919	H	-0.277	-1.301	4.198
C	1.166	1.769	1.632	H	1.236	-1.845	6.087
C	0.603	2.042	2.700	H	3.714	-1.756	5.779
C	2.162	2.605	0.929	H	4.665	-1.126	3.553
C	2.848	2.145	-0.217	H	3.153	-0.597	1.657
C	3.809	2.967	-0.829	H	2.635	1.161	-0.619
C	4.085	4.245	-0.302	H	4.342	2.612	-1.706
C	3.401	4.703	0.844	H	4.831	4.878	-0.778

Intermediate **8**; FG = CN; **R¹**, **R²**, **R³** = 4-BrC_6H_4, Ph, Ph

C	2.189	-2.769	-0.279	C	-0.434	0.750	-1.013	C	1.363	-0.447	0.278	H	-0.635	-1.157	2.004
C	1.077	-1.887	-0.202	N	-1.016	0.884	-2.043	C	0.325	0.610	0.174	H	-1.719	-2.016	4.050
C	-0.187	-2.469	-0.480	H	3.162	-2.394	0.015	C	0.369	1.644	1.174	H	-0.390	-2.320	6.146
C	-0.307	-3.809	-0.900	H	-1.293	-4.203	-1.121	C	-0.640	2.751	1.263	H	2.054	-1.787	6.152
C	0.819	-4.632	-1.006	H	0.710	-5.664	-1.326	C	-1.979	2.619	0.829	H	3.150	-0.964	4.055
C	2.080	-4.107	-0.669	H	2.966	-4.735	-0.702	C	-2.885	3.683	0.985	H	4.358	-1.594	-1.745
O	-1.393	-1.720	-0.398	H	-2.938	-0.300	-1.652	C	-2.467	4.891	1.574	H	5.065	-0.037	-2.165
C	-2.505	-2.218	0.309	H	-5.098	0.815	-2.170	C	-1.137	5.026	2.023	H	3.152	1.218	-3.159
O	-2.420	-3.154	1.119	H	-7.015	-1.384	1.033	C	-0.235	3.960	1.877	H	1.514	1.389	-2.518
C	-3.754	-1.488	-0.025	H	-4.842	-2.523	1.530	O	1.322	1.623	2.046	H	3.903	1.792	0.802
C	-3.823	-0.544	-1.073	H	-2.324	1.689	0.391	C	2.079	-0.543	1.675	H	2.585	2.549	-0.078
C	-5.043	0.092	-1.363	H	-3.914	3.566	0.654	O	3.341	-0.500	1.680	H	5.911	0.199	0.237
C	-6.179	-0.219	-0.598	H	-3.169	5.714	1.690	C	1.340	-1.015	2.888	H	5.280	-1.389	0.601
C	-6.128	-1.155	0.451	H	-0.811	5.952	2.490	C	-0.040	-1.305	2.896	H	2.734	-1.220	-3.631
C	-4.910	-1.790	0.732	H	0.783	4.035	2.246	C	-0.659	-1.778	4.064	H	1.114	-1.088	-2.937
C	5.875	4.967	-1.206	H	6.096	5.923	-0.714	Br	-7.884	0.673	-1.002	H	6.824	4.425	-1.324

C	0.091	-1.954	5.242	H	5.452	2.220	-1.195
C	1.470	-1.657	5.243	H	4.111	2.985	-2.057
C	2.089	-1.195	4.073	H	6.769	-2.385	-1.203
P	3.023	0.301	-0.905	H	7.408	-0.778	-1.549
C	4.641	-0.618	-1.333	H	0.466	0.576	-4.663
C	2.345	0.688	-2.633	H	2.085	0.508	-5.375
C	3.515	1.985	-0.201	H	3.936	4.721	-0.253
C	5.686	-0.778	-0.212	H	5.262	3.957	0.621
C	1.892	-0.529	-3.470	H	7.669	-2.238	1.165
C	4.520	2.788	-1.056	H	8.968	-2.046	-0.031
C	6.993	-1.409	-0.747	H	8.318	-0.626	0.814
C	1.327	-0.084	-4.838	H	1.736	-1.949	-5.922
C	4.861	4.142	-0.387	H	0.112	-1.866	-5.208
C	8.049	-1.591	0.363	H	0.485	-0.938	-6.673
C	0.891	-1.279	-5.711	H	5.487	5.189	-2.210

Intermediate **2**; FG = CN; **R¹**, **R²**, **R³** = *t*Bu, Ph, *t*Bu

C	1.895	-1.357	-2.972	H	-0.729	-2.430	2.289	C	-2.123	-0.655	-0.467	H	-5.421	3.371	1.092
C	1.445	-1.673	-1.664	H	-0.804	-3.960	3.192	C	-3.480	-1.250	-0.464	H	-3.496	4.913	0.605
C	1.989	-2.854	-1.099	H	1.142	-3.239	4.707	C	-4.044	-1.871	-1.605	H	-3.208	4.261	-1.026
C	2.907	-3.671	-1.772	H	1.211	-1.683	3.851	C	-5.341	-2.412	-1.566	H	-1.891	4.298	0.171
C	3.339	-3.315	-3.061	H	2.673	-2.673	3.993	C	-6.117	-2.327	-0.394	H	-3.423	3.306	2.629
C	2.830	-2.149	-3.662	H	1.280	-5.437	3.436	C	-5.578	-1.694	0.744	H	-1.885	2.584	2.117
O	1.532	-3.342	0.162	H	2.825	-4.946	2.710	C	-4.279	-1.163	0.708	H	-3.296	1.550	2.382
C	1.871	-2.731	1.358	H	1.471	-5.447	1.667	O	-2.096	0.648	0.183	H	3.239	-0.302	-0.403
O	2.632	-1.750	1.419	H	-3.474	-1.916	-2.527	C	-2.851	1.673	-0.431	H	3.139	0.906	-1.690
C	1.213	-3.448	2.546	H	-5.748	-2.886	-2.455	O	-3.069	1.681	-1.649	H	-0.234	0.675	1.679
C	-0.329	-3.451	2.343	H	-7.122	-2.743	-0.368	C	-3.407	2.734	0.538	H	1.477	0.322	1.989
C	1.586	-2.713	3.852	H	-6.163	-1.628	1.659	C	-4.960	2.626	0.431	H	-0.111	1.891	-2.157
C	1.735	-4.913	2.585	H	-3.861	-0.700	1.599	C	-2.969	4.138	0.036	H	-0.431	2.694	-0.628
C	0.443	-0.802	-0.961	H	-5.312	1.632	0.730	C	-2.971	2.524	2.003	H	3.552	2.727	0.086
C	-0.939	-1.234	-0.911	H	-5.290	2.811	-0.597	P	1.086	0.779	-0.353	H	3.696	1.444	1.297
H	3.263	-4.575	-1.286	H	0.760	3.906	5.270	H	4.049	-3.946	-3.589	H	2.454	5.290	-3.463
H	-0.605	-3.973	1.422	H	1.999	6.171	-1.991	H	3.138	-1.873	-4.668	H	1.084	6.417	-3.492

C	3.496	-1.549	1.665	H	-0.876	5.973	2.569
C	4.764	-1.991	2.076	H	-1.613	7.002	1.325
C	5.836	-2.012	1.163	H	-6.346	1.216	-1.348
C	5.633	-1.586	-0.163	H	-7.508	1.355	-0.013
C	4.368	-1.133	-0.573	H	-6.348	2.663	-0.321
C	1.932	0.614	-0.748	H	2.674	-1.530	2.374
C	2.595	1.746	-0.200	H	4.914	-2.318	3.101
C	2.746	1.852	1.022	H	6.816	-2.361	1.481
C	3.022	2.745	-1.283	H	6.453	-1.613	-0.876
C	4.027	2.040	-2.239	H	4.210	-0.825	-1.602
C	3.706	3.951	-0.596	H	3.543	1.230	-2.795
C	1.785	3.216	-2.105	H	4.889	1.636	-1.693
C	1.033	-2.790	0.246	H	4.399	2.777	-2.961
N	1.252	-3.927	0.489	H	3.984	4.689	-1.357
H	-1.064	-3.116	1.530	H	4.611	3.647	-0.057

Intermediate **6**; FG = CN; **R¹**, **R²**, **R³** = *t*Bu, Ph, *t*Bu

C	-1.851	-2.953	0.804	H	-0.055	-3.260	-2.229	C	-1.176	0.646	0.704	H	0.083	-1.582	2.670
C	-1.716	-1.998	-0.225	H	-0.106	-3.300	-3.994	C	-0.257	0.550	2.361	H	-2.299	3.292	1.704
C	-2.795	-1.801	-1.144	H	1.523	-1.448	-4.428	C	-0.964	2.455	0.175	H	-0.580	3.444	2.091
C	-3.965	-2.600	-1.046	H	1.855	-1.571	-2.695	C	-3.004	0.494	1.175	H	-3.832	2.253	0.178
C	-4.065	-3.558	-0.029	H	1.474	0.017	-3.416	C	-0.400	-0.744	3.187	H	-3.833	0.788	-0.814
C	-3.013	-3.737	0.901	H	-0.693	-1.282	-5.364	C	-1.308	3.491	1.270	H	1.296	-0.289	4.472
O	-2.629	-0.833	-2.052	H	-0.821	0.327	-4.600	C	-3.998	1.166	0.202	H	-0.255	0.237	5.123
C	-0.753	-0.405	-1.994	H	-2.107	-0.866	-4.352	O	0.242	-0.586	4.586	H	-0.323	5.135	0.240
O	-0.644	0.859	-2.117	H	0.799	0.771	2.165	C	-1.306	4.927	0.690	H	-2.042	4.991	-0.124
C	-0.281	-1.287	-3.220	H	-0.654	1.392	2.942	O	-5.460	0.894	0.626	H	-5.634	-0.192	0.634
C	-0.531	-2.809	-3.107	H	0.064	2.567	-0.163	C	0.155	-1.877	5.426	H	-5.622	1.249	1.657
C	1.243	-1.052	-3.443	H	-1.587	2.567	-0.714	C	-1.619	5.994	1.759	H	0.666	-2.711	4.925
C	-1.028	-0.740	-4.468	H	-3.231	-0.572	1.270	C	-6.475	1.571	-0.318	H	0.619	-1.742	6.411
C	-0.622	-0.984	-0.479	H	-3.086	0.936	2.179	C	1.947	-0.643	-0.114	H	-0.890	-2.175	5.585
C	0.802	-1.405	-0.088	H	-1.458	-1.017	3.307	P	3.287	-1.116	0.338	H	-2.608	5.828	2.207
H	-3.095	-4.485	1.684	H	1.176	3.923	-1.528	H	-4.765	-2.445	-1.765	H	3.034	4.432	0.125
H	-1.598	-3.044	-3.076	H	1.145	2.382	-2.412	H	-4.961	-4.171	0.047	H	2.140	3.741	-3.000

C	3.022	2.745	-1.283	H	6.453	-1.613	-0.876
C	4.027	2.040	-2.239	H	4.210	-0.825	-1.602
C	3.706	3.951	-0.596	H	3.543	1.230	-2.795
C	1.785	3.216	-2.105	H	4.889	1.636	-1.693
C	1.033	-2.790	0.246	H	4.399	2.777	-2.961
N	1.252	-3.927	0.489	H	3.984	4.689	-1.357
H	-1.064	-3.116	1.530	H	4.611	3.647	-0.057

Intermediate **8;** FG = CN**; R^1, R^2, R^3** = *t*Bu, Ph, *t*Bu

C	1.358	2.742	-0.204	H	-4.473	0.144	-1.448	C	-0.790	-1.748	-0.690	H	-2.107	1.024	-3.795	C	3.911	0.595	0.507	H	2.500	1.677	2.972
C	0.208	1.917	-0.088	H	-5.374	-0.447	-0.035	C	-1.687	-2.911	-0.360	H	-0.253	0.090	-5.225	C	1.864	-0.334	2.381	H	0.769	1.533	2.649
C	-1.002	2.586	0.239	H	-6.795	1.665	-0.065	C	-2.141	-3.247	0.939	H	0.073	-1.267	-4.111	C	2.526	-2.042	-0.050	H	2.763	-3.033	1.894
C	-1.016	3.963	0.549	H	-5.885	2.312	-1.452	C	-2.948	-4.382	1.141	H	1.380	-0.149	-4.553	C	4.659	0.700	-0.834	H	1.137	-3.153	1.214
C	0.152	4.728	0.478	H	-6.040	3.275	0.025	C	-3.322	-5.196	0.057	H	-0.021	2.874	-2.743	C	1.628	1.017	3.092	H	6.054	2.221	-0.139
C	1.349	4.113	0.068	H	-5.579	0.976	2.076	C	-2.871	-4.874	-1.239	H	-0.149	2.422	-4.451	C	2.204	-3.167	0.956	H	6.650	0.571	0.043
O	-2.229	1.882	0.306	H	-4.788	2.561	2.181	C	-2.057	-3.750	-1.441	H	1.408	2.249	-3.610	C	6.095	1.239	-0.635	H	0.460	0.174	4.707
C	-3.429	2.414	-0.225	H	-3.805	1.074	2.181	O	-0.130	-1.822	-1.810	H	3.790	1.582	0.967	C	1.351	0.809	4.599	H	2.193	0.266	5.058
O	-3.439	3.417	-0.948	H	-1.873	-2.644	1.796	C	0.804	0.258	-1.926	H	4.493	-0.018	1.214	C	2.552	-4.552	0.361	H	1.990	-4.692	-0.573
C	-4.643	1.588	0.209	H	-3.283	-4.625	2.147	O	2.043	0.109	-2.123	H	2.744	-0.832	2.812	C	6.861	1.368	-1.968	H	3.620	-4.577	0.093
C	-4.505	0.144	-0.351	H	-3.951	-6.069	0.218	C	-0.076	0.687	-3.138	H	1.007	-0.991	2.548	C	1.125	2.140	5.344	H	6.344	2.054	-2.654
C	-5.918	2.255	-0.358	H	-3.151	-5.499	-2.085	C	-1.600	0.620	-2.909	H	3.590	-2.065	-0.318	C	2.235	-5.707	1.334	H	7.877	1.752	-1.809
C	-4.696	1.549	1.763	H	-1.684	-3.503	-2.430	C	0.310	-0.224	-4.336	H	1.957	-2.176	-0.972	C	-1.195	-0.388	1.381	H	6.942	0.395	-2.471
C	0.377	0.417	-0.410	H	-1.916	1.215	-2.051	C	0.321	2.156	-3.496	H	4.700	-0.281	-1.325	N	-1.619	-0.241	2.483	H	2.005	2.795	5.267
C	-0.623	-0.570	0.099	H	-1.933	-0.411	-2.766	P	2.194	-0.253	0.513	H	4.112	1.348	-1.527	H	2.279	2.293	-0.555	H	0.265	2.680	4.924
H	-1.955	4.430	0.822	H	0.926	1.969	6.409	H	2.261	4.694	-0.042	H	2.489	-6.678	0.891								
H	0.121	5.787	0.718	H	1.167	-5.723	1.588	H	-3.602	-0.343	0.024	H	2.803	-5.606	2.270								

Intermediate **2;** FG = H**; R^1, R^2, R^3** = 4-BrC_6H_4, Ph, Ph

C	1.441	-3.053	-2.967	H	2.434	-2.609	-2.992	C	0.676	-1.106	-1.507	H	2.535	4.491	3.059	C	4.082	5.070	1.655	H	2.671	0.823	2.160
C	0.424	-2.375	-2.243	H	-2.155	-4.526	-3.039	C	-0.101	0.036	-1.872	H	4.626	5.674	2.379	C	4.549	4.968	0.329	H	1.899	-5.375	1.583
C	-0.861	-2.978	-2.299	H	-0.312	-5.671	-4.318	C	-0.087	1.385	-1.600	H	5.453	5.492	0.029	C	3.842	4.197	-0.607	H	3.595	-5.203	1.130
C	-1.142	-4.133	-3.037	H	2.002	-4.707	-4.241	C	-1.058	2.371	-2.090	H	4.174	4.118	-1.638	P	1.843	-1.163	-0.123	H	6.150	-0.102	-1.213
C	-0.107	-4.773	-3.743	H	-3.786	-0.786	-1.614	C	-1.936	2.090	-3.177	H	1.257	-3.499	0.019	C	2.196	-2.984	0.247	H	5.874	1.049	0.094
C	1.193	-4.231	-3.693	H	-5.736	0.453	-0.672	C	-2.871	3.035	-3.623	H	2.948	-3.329	-0.472	C	3.500	-0.273	-0.434	H	0.565	1.516	3.347
O	-1.971	-2.377	-1.619	H	-4.824	-1.114	3.260	C	-2.965	4.303	-3.012	H	3.642	-0.325	-1.521	C	1.035	-0.413	1.418	H	0.469	-0.069	4.111
C	-2.023	-2.388	-0.231	H	-2.859	-2.338	2.301	C	-2.098	4.603	-1.945	H	3.334	0.780	-0.186	C	2.631	-3.333	1.687	H	2.495	-4.950	4.010
O	-1.184	-2.972	0.480	H	-0.907	-0.233	-2.553	C	-1.163	3.657	-1.492	H	0.439	0.425	1.046	C	4.752	-0.802	0.298	H	3.396	-6.336	3.367
C	-3.203	-1.645	0.285	H	-1.867	1.139	-3.699	O	0.928	1.930	-0.706	H	0.342	-1.185	1.774	C	1.974	0.066	2.545	H	4.202	-4.767	3.558
C	-4.018	-0.859	-0.558	H	-3.517	2.789	-4.464	C	1.935	2.729	-1.262	H	3.564	-2.822	1.959	C	2.833	-4.858	1.847	H	7.198	-0.428	1.681
C	-5.117	-0.163	-0.028	H	-3.686	5.037	-3.365	O	2.192	2.764	-2.473	H	1.862	-3.006	2.401	C	6.019	-0.020	-0.123	H	7.478	-1.585	0.363
C	-5.395	-0.267	1.345	H	-2.150	5.576	-1.460	C	2.665	3.516	-0.221	H	4.627	-0.716	1.386	C	1.176	0.679	3.720	H	8.174	0.044	0.277
C	-4.595	-1.044	2.202	H	-0.519	3.912	-0.655	C	2.196	3.622	1.107	H	4.905	-1.868	0.076	C	3.256	-5.251	3.278	H	2.786	1.943	4.504
C	-3.495	-1.730	1.664	H	1.281	3.113	1.389	C	2.904	4.400	2.041	H	2.581	-0.764	2.930	C	7.291	-0.526	0.590	H	1.501	1.604	5.682
C	2.089	1.172	4.862	H	2.686	0.348	5.275	Br	-6.936	0.700	2.091												

Intermediate **6;** FG = CN**; R^1, R^2, R^3** = 4-BrC_6H_4, Ph, Ph

C	1.361	-2.364	-2.472	H	1.480	-1.583	-3.220	C	0.833	-0.676	-0.538	H	5.109	-1.982	-0.056	C	-0.086	1.524	-1.611	H	5.523	3.330	3.623
C	1.025	-2.055	-1.139	H	0.852	-5.247	0.133	C	0.679	0.407	-1.582	H	3.839	-2.500	-1.169	C	-0.113	2.492	-2.739	H	5.950	3.987	2.030
C	0.830	-3.102	-0.169	H	1.483	-5.775	-2.229	C	2.538	-0.213	0.467	H	4.257	1.352	2.480	C	1.044	2.752	-3.510	H	5.072	4.992	3.199
C	1.006	-4.454	-0.594	H	1.780	-3.939	-3.902	C	3.902	-0.342	-0.847	H	4.718	2.006	0.903	P	0.997	3.646	-4.592	H	1.173	-2.181	5.560
C	1.355	-4.738	-1.920	H	-2.096	-1.058	2.439	C	2.576	1.566	1.095	H	2.466	-0.153	3.580	C	-0.206	4.305	-4.915	H	2.660	-2.705	6.378
C	1.531	-3.702	-2.871	H	-4.451	-1.860	2.169	C	3.080	-1.364	1.865	H	1.297	-1.378	3.076	C	-1.359	4.062	-4.145	H	2.391	-0.982	6.037
O	0.497	-2.734	1.061	H	-3.808	-2.203	-2.098	C	4.589	-1.721	-0.988	H	5.092	-1.486	-3.088	C	-1.313	3.165	-3.064	H	1.988	2.281	-3.247
C	-0.233	-0.681	0.606	H	-1.478	-1.429	-1.813	C	3.932	2.026	1.673	H	6.358	-0.932	-1.987	C	-1.055	1.768	-0.599	H	1.897	3.842	-5.170
O	0.004	0.015	1.640	H	1.273	0.257	-2.478	C	2.363	-1.187	3.215	H	3.483	4.139	1.439	C	-0.904	2.883	0.245	H	-0.241	5.001	-5.750
C	-1.622	-1.187	0.343	H	3.450	-0.055	-1.804	O	5.611	-1.727	-2.147	H	3.060	3.491	3.019	C	0.136	3.562	0.244	H	-2.291	4.566	-4.387
C	-2.482	-1.311	1.457	H	4.649	0.423	-0.603	C	3.830	3.465	2.235	H	2.804	-3.192	3.913	C	-2.104	3.121	1.080	H	-2.210	2.972	-2.482
C	-3.803	-1.756	1.305	H	2.261	2.217	0.272	O	2.939	-2.160	4.269	H	4.024	-1.999	4.380	C	-3.238	2.281	1.016	H	-3.233	1.423	0.354
C	-4.268	-2.071	0.016	H	1.788	1.613	1.850	C	6.325	-3.087	-2.290	H	5.600	-3.890	-2.478	C	-4.356	2.561	1.819	H	-5.227	1.914	1.773
C	-3.438	-1.955	-1.108	H	2.926	-2.383	1.500	C	5.171	3.973	2.804	H	7.040	-3.075	-3.123	C	-4.345	3.672	2.686	H	-5.212	3.884	3.307
C	-2.113	-1.513	-0.938	H	4.161	-1.189	1.972	C	2.253	-1.998	5.642	H	6.878	-3.341	-1.376	C	-3.211	4.507	2.753	H	-3.203	5.363	3.423
C	-2.092	4.234	1.952	H	-1.209	4.865	1.986	Br	-6.129	-2.687	-0.214												

Intermediate **8;** FG = CN**; R^1, R^2, R^3** = 4-BrC_6H_4, Ph, Ph

C	-1.050	3.225	-1.930	H	-1.898	3.453	-1.293	C	-0.198	1.732	-0.098	H	2.618	5.330	2.037	C	0.793	5.797	3.111	H	-2.643	-1.385	2.206
C	-0.063	2.320	-1.459	H	1.942	2.357	-4.251	C	0.240	0.483	0.223	H	1.237	6.614	3.676	C	-0.565	5.462	3.303	H	-5.734	0.954	-3.934
C	1.010	2.041	-2.345	H	0.161	3.939	-5.050	C	0.148	-0.081	1.592	H	-1.166	6.018	4.018	C	-1.135	4.408	2.576	H	-6.563	1.669	-2.551
C	1.096	2.611	-3.620	H	-1.760	4.482	-3.532	C	0.438	-1.536	1.797	H	-2.176	4.129	2.711	P	-4.008	-1.553	-0.487	H	-5.686	-5.792	-0.078
C	0.097	3.497	-4.060	H	3.179	-0.968	-2.411	C	0.340	-2.483	0.751	H	-5.311	-1.199	-2.569	C	-5.173	-0.584	-1.668	H	-7.128	-4.959	-0.657
C	-0.979	3.801	-3.207	H	4.941	-2.717	-2.139	C	0.594	-3.843	1.002	H	-6.157	-0.482	-1.186	C	-5.156	-3.052	-0.128	H	-3.342	0.701	3.398
O	2.045	1.111	-2.015	H	7.075	-0.129	0.599	C	0.957	-4.268	2.295	H	-6.154	-2.677	0.148	C	-4.326	-0.543	1.113	H	-4.901	-0.031	3.794
C	3.111	1.505	-1.196	H	5.300	1.615	0.317	C	1.049	-3.329	3.344	H	-4.745	-3.566	0.752	C	-4.628	0.804	-2.068	H	-4.065	2.866	-3.924
O	3.163	2.623	-0.662	H	0.692	-0.133	-0.545	C	0.783	-1.974	3.097	H	-5.413	-0.416	1.241	C	-5.263	-4.050	-1.302	H	-5.728	3.464	-4.113
C	4.129	0.434	-1.062	H	0.029	-2.176	-0.243	O	-0.138	0.658	2.577	H	-3.886	0.449	0.956	C	-3.708	-1.174	2.380	H	-4.913	3.589	-2.540
C	4.026	-0.791	-1.757	H	0.502	-4.568	0.197	C	-1.004	2.568	0.899	H	-4.464	1.416	-1.169	C	-5.576	1.560	-3.028	H	-6.686	-5.818	-3.006
C	5.017	-1.774	-1.606	H	1.159	-5.319	2.485	O	-2.243	2.354	0.968	H	-3.644	0.689	-2.548	C	-6.121	-5.289	-0.955	H	-5.239	-6.660	-2.420
C	6.108	-1.521	-0.755	H	1.323	-3.656	4.343	C	-0.353	3.675	1.651	H	-5.697	-3.552	-2.182	C	-3.837	-0.256	3.617	H	-6.846	-7.158	-1.853
C	6.228	-0.308	-0.055	H	0.836	-1.237	3.894	C	1.006	4.012	1.461	H	-4.254	-4.380	-1.596	C	-5.041	2.952	-3.426	H	-2.146	-1.061	4.742
C	5.233	0.669	-0.213	H	1.622	3.467	0.753	C	1.573	5.072	2.189	H	-4.188	-2.141	2.598	C	-6.230	-6.290	-2.125	H	-3.329	-0.208	5.752
C	-3.219	-0.876	4.887	H	-3.699	-1.833	5.136	Br	7.495	-2.894	-0.542												

Intermediate **2;** FG = H**; R^1, R^2, R^3** = *t*Bu, Ph, *t*Bu

C	-1.907	1.432	-2.846	H	-1.372	0.204	2.326	C	1.345	-4.926	0.313	H	-7.009	-0.349	1.937	C	-0.847	-2.026	3.934	H	5.769	-1.827	0.874
C	-0.989	1.607	-1.774	H	-4.699	-0.859	0.862	C	0.737	-4.306	-0.798	H	-4.556	-2.913	-4.156	C	-6.601	0.623	2.247	H	5.075	-0.366	1.615
C	-0.591	2.954	-1.543	H	-3.884	0.002	2.173	C	0.855	-2.920	-0.995	H	-2.900	-3.360	-4.611	C	-3.739	-3.618	-3.951	H	6.544	1.752	-0.133
C	-1.027	4.031	-2.324	H	-3.616	-1.429	-2.230	C	3.145	-0.226	-0.083	H	-4.087	-4.622	-4.228	C	-1.228	-3.315	4.692	H	4.805	1.785	0.250
C	-1.937	3.812	-3.374	H	-1.968	-1.874	-2.685	C	4.139	-0.597	-0.994	H	-0.866	-4.204	4.158	C	-2.212	0.420	-3.095	H	5.346	1.851	-1.442
C	-2.384	2.501	-3.623	H	-2.542	-2.062	2.583	C	3.893	-1.210	-2.042	H	-0.792	-3.327	5.699	C	-0.664	5.028	-2.091	H	0.768	3.358	3.205
O	0.344	3.287	-0.506	H	-1.094	-2.856	1.952	C	-1.715	-0.441	0.016	H	-2.318	-3.406	4.796	C	-2.282	4.644	-3.981	H	1.088	3.766	1.748
C	-0.036	3.262	0.832	H	-5.141	2.094	1.583	O	-3.253	0.644	0.182	H	6.591	-0.646	-1.528	C	-3.079	2.307	-4.437	H	1.105	5.321	1.624
O	-1.174	2.928	1.198	H	-5.950	1.245	0.267	C	-2.381	-2.129	-0.569	H	5.531	-0.142	-0.522	C	1.481	1.208	-1.112	H	2.460	3.192	1.315
C	-0.488	0.458	-0.969	H	-2.519	-4.300	-2.285	O	-1.043	-0.686	1.773	H	5.809	-0.730	0.888	C	2.788	-2.153	1.716	H	0.778	2.267	3.320
C	0.935	0.313	-0.807	H	-4.163	-3.857	-1.831	C	-4.319	0.127	1.171	H	5.552	1.412	-0.457	C	2.574	-4.605	2.070	H	-0.219	3.720	3.513
C	1.770	-0.672	-0.332	H	0.248	-1.952	3.862	C	-2.815	-2.162	-2.046	H	6.392	-0.265	-2.536	C	1.261	-6.000	0.458	H	1.524	3.780	3.879
C	1.579	-2.110	-0.083	H	-1.186	-1.148	4.505	C	-1.448	-1.979	2.510	H	6.592	-1.740	-1.586	H	0.199	-4.909	-1.528	H	1.888	5.728	2.277
C	2.204	-2.752	1.020	H	-6.196	0.508	3.262	C	-5.512	1.108	1.267	H	7.588	-0.310	-1.215	H	0.436	-2.455	-1.884	H	0.144	5.755	1.931
C	2.086	-4.138	1.216	H	-7.434	1.335	2.298	P	-3.315	-3.563	-2.469	H	6.812	-0.430	1.221	H	-2.873	1.623	0.495	H	1.318	5.630	0.595
H	-3.227	-2.367	0.089	H	2.464	2.096	1.327	H	-1.603	-2.874	-0.387	H	2.721	3.516	0.303	H	-3.685	0.762	-0.817	H	3.234	3.550	2.008
H	0.046	-0.630	1.685																				

Intermediate **6;** FG = H**; R^1, R^2, R^3 =** *t*Bu, Ph, *t*Bu

C	0.849	-1.286	1.966	H	-2.895	0.322	3.204	C	-1.982	0.132	0.078	H	-4.821	5.022	-0.212
C	0.291	-1.519	0.698	H	-4.593	1.890	-0.001	C	-1.622	1.166	1.652	H	-5.686	5.068	-1.762
C	-0.061	-2.837	0.310	H	-3.261	3.012	0.299	C	-2.772	1.394	-1.098	H	-6.142	-3.032	-1.857
C	0.148	-3.927	1.180	H	-5.028	-0.533	-0.357	C	-3.188	-1.226	0.606	H	-7.043	-3.741	-0.502
C	0.701	-3.677	2.450	H	-4.005	-1.593	-1.353	C	-2.742	1.291	2.709	H	-7.129	-1.995	-0.808
C	1.053	-2.367	2.847	H	-1.423	2.085	4.243	C	-3.752	2.413	-0.481	H	2.027	0.927	-0.442
O	-0.614	-2.944	-0.929	H	-2.258	3.325	3.309	C	-4.389	-1.430	-0.341	H	2.653	2.241	-0.750
C	-0.603	-1.434	-1.666	H	-3.478	3.895	-2.049	O	-2.391	2.343	3.788	H	3.933	2.304	-1.349
O	-1.844	-1.069	-1.978	H	-4.810	2.780	-2.344	C	-4.313	3.370	-1.561	H	4.511	3.543	-1.672
C	-0.125	-0.555	-0.381	H	-4.606	-3.544	0.089	O	-5.239	-2.645	0.098	H	3.823	4.741	-1.398
C	0.709	0.671	-0.633	H	-5.580	-2.509	1.137	C	-3.469	2.447	4.887	H	2.552	4.688	-0.792
C	0.436	-0.370	-3.729	H	-3.596	1.487	5.407	C	-5.303	4.400	-0.979	H	1.975	3.449	-0.467
C	0.333	-1.680	-2.902	H	-3.200	3.201	5.637	C	-6.460	-2.867	-0.819	H	2.943	-0.114	-0.108
C	-0.363	-2.752	-3.786	H	-4.442	2.728	4.462	C	1.142	-0.285	2.271	H	3.715	-0.036	1.067
C	1.745	-2.181	-2.518	H	-6.164	3.901	-0.514	P	-0.124	-4.929	0.864	H	3.486	0.818	1.931
H	-3.524	-1.001	1.624	H	3.482	-2.813	1.401	H	-2.595	-2.145	0.639	H	3.837	-2.483	-0.302
H	-3.700	1.564	2.245												

H	-1.940	1.916	-1.589	H	5.512	-0.684	-0.962	C	-1.314	-3.103	-0.049	H	-6.293	2.492	-3.142
H	-3.248	0.786	-1.869	H	5.079	-3.223	0.735	C	-1.794	-1.802	-0.350	H	-6.513	1.434	-1.727
								C	-2.375	-1.611	-1.627	H	-6.547	0.742	-3.354
								C	-2.472	-2.650	-2.562	H	-4.140	2.386	-4.520
								C	-1.978	-3.925	-2.243	H	-4.372	0.645	-4.772
								C	-1.395	-4.149	-0.980	H	-2.845	1.246	-4.081
								O	-2.851	-0.323	-2.015	H	-1.041	0.754	-0.730
								C	-4.241	-0.090	-2.103	H	0.746	1.990	-0.765
								O	-5.065	-0.942	-1.756	H	1.984	4.064	-1.315
								C	-4.536	1.303	-2.672	H	1.636	6.133	0.036
								C	-3.887	2.381	-1.759	H	0.043	6.111	1.962
								C	-6.068	1.502	-2.726	H	-1.203	4.006	2.520
								C	-3.929	1.394	-4.102	H	-4.416	-0.763	0.958
								C	-1.648	-0.713	0.657	H	-4.006	0.660	1.958
								C	-1.252	0.542	0.312	H	-5.248	-0.490	2.493
								H	-4.276	2.321	-0.734	H	1.825	0.950	4.859
								H	-4.123	3.377	-2.154				

Intermediate **8;** FG = H**; R^1, R^2, R^3 =** *t*Bu, Ph, *t*Bu

C	-1.108	1.644	1.290	H	-4.086	-0.854	4.725	C	4.889	-1.590	-1.046	H	3.578	2.097	-1.931
C	-0.344	2.872	0.902	H	-2.849	0.340	4.244	C	4.533	1.172	-0.209	H	2.725	0.743	2.419
C	0.564	2.889	-0.183	H	-2.357	-1.282	4.773	C	3.737	-0.992	1.564	H	1.680	-0.662	2.190
C	1.279	4.061	-0.488	H	-4.594	-2.838	3.268	C	4.432	-3.050	-1.247	H	5.809	-3.505	-2.865
C	1.087	5.227	0.278	H	-2.885	-3.331	3.296	C	4.599	1.910	-1.563	H	6.425	-3.919	-1.264
C	0.187	5.214	1.365	H	-3.736	-3.126	1.742	C	2.688	-0.355	2.501	H	4.877	3.894	-0.725
C	-0.518	4.042	1.678	H	5.158	-1.151	-2.017	C	5.521	-3.938	-1.893	H	6.383	3.064	-1.110
O	-1.647	1.564	2.433	H	5.788	-1.554	-0.410	C	5.362	3.252	-1.477	H	2.868	-1.850	4.063
C	-1.820	-1.135	2.117	H	5.549	0.958	0.157	C	2.892	-0.753	3.981	H	3.894	-0.434	4.312
O	-0.799	-1.533	2.726	H	4.046	1.813	0.538	C	5.063	-5.397	-2.094	H	4.178	-5.446	-2.743
C	-3.222	-1.220	2.758	H	4.757	-0.738	1.894	C	5.428	3.995	-2.828	H	5.853	-6.005	-2.556
C	-4.280	-0.400	1.984	H	3.644	-2.087	1.602	C	1.817	-0.148	4.909	H	4.799	-5.862	-1.134
C	-3.119	-0.720	4.223	H	4.145	-3.490	-0.279	H	-0.849	-3.278	0.916	H	5.941	3.388	-3.586
C	-3.628	-2.729	2.759	H	3.529	-3.069	-1.876	H	-2.934	-2.455	-3.525	H	4.420	4.218	-3.207
P	3.535	-0.468	-0.271	H	5.086	1.272	-2.317	H	-2.048	-4.731	-2.968	H	5.970	4.946	-2.736
H	-2.799	2.272	-1.724	H	1.983	-0.439	5.956	H	-1.006	-5.130	-0.724	H	0.818	-0.490	4.611

Table S3 APT charge analysis for the ylide intermediate **2** in Scheme 6 with and without CN substitution.

	R^1, R^2, R^3 = 4-BrC_6H_4, Ph, Ph (3a)[a]		**R^1, R^2, R^3** = *t*Bu, Ph, *t*Bu (3j)	
	CN substitution	No substitution	CN substitution	No substitution
FG	-0.16	0.00	-0.14	0.00
C(-FG)	0.67	0.77	0.53	0.63
C(-PBu_3)	-0.98	-1.15	-0.80	-0.96
PBu_3	0.95	0.95	0.82	0.82
R	0.29	0.20	0.45	0.38
R^1	-0.13	-0.13	0.10	0.09
R^2	0.13	0.14	0.02	0.06
R^3	-0.06	-0.07	0.06	0.05
OCO(-R^1)	-0.38	-0.38	-0.54	-0.52
OCO(-R^3)	-0.33	-0.35	-0.50	-0.54
C(-R^1)	1.32	1.31	1.03	1.00
C(-R^3)	1.21	1.22	1.00	1.02

[a] The notation in the parentheses correspond to the final products in from Scheme 2.

Table S4 The computed activation barrier (*Ea*) and reaction energy (*ΔE*), in kcal/mol, through paths **a** and **b** (Scheme 6) for several R^1 and R^3 combinations at the B3LYP/LanL2DZ level.

R¹, **R²**, **R³**	Path **a**		Path **b**	
	Ea	*ΔH*	*Ea*	*ΔH*
4-BrC_6H_4, Ph, Ph (**a**)[a]	7.3	4.4	3.9	-11.1
4-BrC_6H_4, Ph, 4-BrC_6H_4 (**b**)	7.2	4.6	2.4	-12.5
4-BrC_6H_4, Ph, 2-BrC_6H_4 (**c**)	12.2	11.6	9.0	-5.3
4-BrC_6H_4, Ph, 4-$NO_2C_6H_4$ (**d**)	9.3	8.6	8.4	-12.6
4-BrC_6H_4, Ph, 4-$MeOC_6H_4$ (**e**)	6.1	3.6	3.6	-9.7
4-BrC_6H_4, Ph, Me (**f**)	6.9	4.4	3.6	-16.3
4-BrC_6H_4, Ph, *i*Pr (**g**)	7.8	4.9	4.2	-10.6
4-BrC_6H_4, Ph, *t*Bu (**h**)	5.8	-2.2	6.4	-11.4
4-$NO_2C_6H_4$, Ph, *t*Bu (**i**)	5.2	-5.2	6.0	-11.4
*t*Bu, Ph, *t*Bu (**j**)	12.5	8.8	8.8	-10.9

[a] The notation in the parentheses corresponds to ylide with **R¹** and **R³** combinations that give final products of **3a** – **3j**, respectively, in Scheme 2.

Table S5 Optimized Geometries of CN-substituted Intermediates **2**, **6** and **8** and related transition states in paths **a** and **b** in Cartesian Coordinates (Å)

(a) Intermediate **2;** FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Ph

C	3.406	2.544	2.088	C	1.053	-0.017	2.213	C	-1.525	-3.898	-1.627	N	1.398	0.859	4.678	H	-4.364	-3.228	-3.416	H	5.948	2.278	-2.213
C	2.104	2.211	1.636	C	0.245	-1.142	2.054	P	2.341	0.168	-0.340	H	4.152	1.755	2.120	H	-2.604	-4.983	-3.155	H	-0.687	-1.191	-3.530
C	1.159	3.264	1.671	C	-0.245	-2.058	3.098	C	3.636	1.394	-0.970	H	0.674	5.307	2.140	H	-0.760	-4.656	-1.486	H	0.265	0.008	-4.409
C	1.456	4.554	2.127	C	0.580	-2.464	4.177	C	1.073	0.011	-1.756	H	3.004	5.841	2.921	H	3.226	2.384	-0.741	H	5.284	-3.216	0.481
C	2.761	4.846	2.561	C	0.091	-3.318	5.179	C	3.160	-1.519	-0.032	H	4.747	4.041	2.887	H	4.530	1.262	-0.350	H	4.122	-4.053	-0.544
C	3.740	3.834	2.536	C	-1.226	-3.811	5.118	C	4.006	1.329	-2.468	H	-2.360	2.169	1.901	H	0.119	-0.203	-1.270	H	4.550	2.576	-4.956
O	-0.201	3.019	1.303	C	-2.052	-3.434	4.040	C	1.372	-1.031	-2.853	H	-4.765	1.578	1.553	H	0.997	1.021	-2.175	H	6.169	3.177	-4.549
C	-0.537	2.865	-0.030	C	-1.570	-2.571	3.045	C	4.309	-1.932	-0.978	H	-4.294	2.219	-2.705	H	3.531	-1.447	0.998	H	5.862	1.431	-4.606
O	0.271	3.025	-0.965	O	-0.346	-1.334	0.751	C	5.045	2.418	-2.826	H	-1.883	2.797	-2.337	H	2.376	-2.282	-0.028	H	1.555	-1.858	-5.555
C	-1.975	2.520	-0.198	C	-0.366	-2.592	0.145	C	0.302	-1.001	-3.971	H	1.610	-2.124	4.223	H	4.418	0.346	-2.733	H	0.586	-3.057	-4.672
C	-2.788	2.179	0.905	O	0.461	-3.485	0.407	C	4.915	-3.292	-0.553	H	0.744	-3.610	5.998	H	3.112	1.482	-3.086	H	-0.188	-1.994	-5.863
C	-4.139	1.845	0.708	C	-1.470	-2.723	-0.844	C	5.429	2.399	-4.320	H	-1.600	-4.480	5.890	H	2.355	-0.849	-3.309	H	6.883	-3.013	-1.481
C	-4.664	1.862	-0.596	C	-2.468	-1.732	-0.990	C	0.580	-2.037	-5.080	H	-3.072	-3.807	3.979	H	1.404	-2.041	-2.420	H	6.472	-4.709	-1.160
C	-3.870	2.204	-1.706	C	-3.507	-1.917	-1.918	C	6.061	-3.743	-1.481	H	-2.229	-2.273	2.233	H	3.950	-2.015	-2.012	H	5.711	-3.855	-2.516
C	-2.521	2.530	-1.499	C	-3.556	-3.087	-2.702	Br	-6.553	1.392	-0.879	H	-2.428	-0.838	-0.375	H	5.106	-1.174	-0.973	H	4.638	3.406	-2.562
C	1.727	0.815	1.237	C	-2.563	-4.077	-2.555	C	1.232	0.433	3.586	H	-4.278	-1.159	-2.022								

(a) Intermediate **6;** FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Ph

C	-3.684	-2.341	0.627	C	-0.768	-2.618	1.799	C	-1.422	-1.110	-0.105	H	-4.536	1.242	-0.489	C	0.454	-0.580	1.640	H	-5.565	0.488	4.218
C	-2.570	-2.122	-0.202	N	-0.933	-3.667	2.320	C	-0.570	-1.346	1.146	H	-4.377	0.412	1.892	C	1.329	-0.913	2.795	H	-1.811	6.268	-1.167
C	-2.357	-2.986	-1.301	H	-3.861	-1.727	1.502	C	-2.151	0.722	-0.331	H	-2.947	-0.276	2.677	C	0.799	-1.271	4.052	H	-0.470	6.135	-0.012
C	-3.245	-4.030	-1.609	H	-3.049	-4.667	-2.466	C	-2.504	1.434	1.402	H	-2.412	3.772	-0.759	P	1.656	-1.573	5.122	H	-0.161	6.681	-1.672
C	-4.361	-4.223	-0.778	H	-5.057	-5.030	-0.993	C	-1.083	2.073	-1.131	H	-1.086	3.647	0.400	C	3.053	-1.520	4.949	H	-4.656	1.218	-5.300
C	-4.582	-3.385	0.338	H	-5.439	-3.554	0.984	C	-3.855	0.697	-1.157	H	-3.655	2.345	-2.581	C	3.588	-1.161	3.697	H	-6.387	1.538	-5.070
O	-1.203	-2.740	-1.996	H	0.908	0.214	-3.089	C	-3.421	0.666	2.372	H	-3.151	0.756	-3.194	C	2.734	-0.853	2.626	H	-5.189	2.768	-4.620
C	-0.723	-1.286	-1.612	H	3.404	0.044	-3.399	C	-1.345	3.520	-0.660	H	-2.753	1.778	4.115	C	0.848	0.575	0.919	H	-0.277	-1.301	4.198
O	-1.292	-0.358	-2.385	H	3.458	-3.334	-0.694	C	-3.903	1.273	-2.587	H	-4.196	2.446	3.353	C	1.166	1.769	1.632	H	1.236	-1.845	6.087
C	0.797	-1.417	-1.708	H	0.995	-3.174	-0.450	O	-3.707	1.503	3.642	H	0.548	4.281	-1.411	C	0.603	2.042	2.700	H	3.714	-1.756	5.779
C	1.489	-0.529	-2.551	H	-1.543	1.622	1.891	C	-0.521	4.526	-1.499	H	-0.782	4.411	-2.562	C	2.162	2.605	0.929	H	4.665	-1.126	3.553
C	2.882	-0.630	-2.727	H	-2.953	2.416	1.198	O	-5.305	1.090	-3.213	H	-5.543	0.016	-3.253	C	2.848	2.145	-0.217	H	3.153	-0.597	1.657
C	3.579	-1.633	-2.035	H	-0.044	1.782	-0.969	C	-4.593	0.753	4.658	H	-6.067	1.558	-2.571	C	3.809	2.967	-0.829	H	2.635	1.161	-0.619
C	2.911	-2.545	-1.201	H	-1.272	1.959	-2.199	C	-0.754	5.987	-1.063	H	-4.112	-0.177	4.992	C	4.085	4.245	-0.302	H	4.342	2.612	-1.706
C	1.517	-2.436	-1.051	H	-4.170	-0.350	-1.174	C	-5.390	1.688	-4.633	H	-4.785	1.368	5.547	C	3.401	4.703	0.844	H	4.831	4.878	-0.778
C	2.443	3.886	1.461	H	3.619	5.687	1.251	Br	5.538	-1.779	-2.257	H	1.915	4.215	2.351								

(a) Intermediate **8;** FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Ph

C	2.189	-2.769	-0.279	C	-0.434	0.750	-1.013	C	1.363	-0.447	0.278	H	-0.635	-1.157	2.004	C	0.091	-1.954	5.242	H	5.452	2.220	-1.195
C	1.077	-1.887	-0.202	N	-1.016	0.884	-2.043	C	0.325	0.610	0.174	H	-1.719	-2.016	4.050	C	1.470	-1.657	5.243	H	4.111	2.985	-2.057
C	-0.187	-2.469	-0.480	H	3.162	-2.394	0.015	C	0.369	1.644	1.174	H	-0.390	-2.320	6.146	C	2.089	-1.195	4.073	H	6.769	-2.385	-1.203
C	-0.307	-3.809	-0.900	H	-1.293	-4.203	-1.121	C	-0.640	2.751	1.263	H	2.054	-1.787	6.152	P	3.023	0.301	-0.905	H	7.408	-0.778	-1.549
C	0.819	-4.632	-1.006	H	0.710	-5.664	-1.326	C	-1.979	2.619	0.829	H	3.150	-0.964	4.055	C	4.641	-0.618	-1.333	H	0.466	0.576	-4.663
C	2.080	-4.107	-0.669	H	2.966	-4.735	-0.702	C	-2.885	3.683	0.985	H	4.358	-1.594	-1.745	C	2.345	0.688	-2.633	H	2.085	0.508	-5.375
O	-1.393	-1.720	-0.398	H	-2.938	-0.300	-1.652	C	-2.467	4.891	1.574	H	5.065	-0.037	-2.165	C	3.515	1.985	-0.201	H	3.936	4.721	-0.253
C	-2.505	-2.218	0.309	H	-5.098	0.815	-2.170	C	-1.137	5.026	2.023	H	3.152	1.218	-3.159	C	5.686	-0.778	-0.212	H	5.262	3.957	0.621
O	-2.420	-3.154	1.119	H	-7.015	-1.384	1.033	C	-0.235	3.960	1.877	H	1.514	1.389	-2.518	C	1.892	-0.529	-3.470	H	7.669	-2.238	1.165
C	-3.754	-1.488	-0.025	H	-4.842	-2.523	1.530	O	1.322	1.623	2.046	H	3.903	1.792	0.802	C	4.520	2.788	-1.056	H	8.968	-2.046	-0.031
C	-3.823	-0.544	-1.073	H	-2.324	1.689	0.391	C	2.079	-0.543	1.675	H	2.585	2.549	-0.078	C	6.993	-1.409	-0.747	H	8.318	-0.626	0.814
C	-5.043	0.092	-1.363	H	-3.914	3.566	0.654	O	3.341	-0.500	1.680	H	5.911	0.199	0.237	C	1.327	-0.084	-4.838	H	1.736	-1.949	-5.922
C	-6.179	-0.219	-0.598	H	-3.169	5.714	1.690	C	1.340	-1.015	2.888	H	5.280	-1.389	0.601	C	4.861	4.142	-0.387	H	0.112	-1.866	-5.208
C	-6.128	-1.155	0.451	H	-0.811	5.952	2.490	C	-0.040	-1.305	2.896	H	2.734	-1.220	-3.631	C	8.049	-1.591	0.363	H	0.485	-0.938	-6.673
C	-4.910	-1.790	0.732	H	0.783	4.035	2.246	C	-0.659	-1.778	4.064	H	1.114	-1.088	-2.937	C	0.891	-1.279	-5.711	H	5.487	5.189	-2.210
C	5.875	4.967	-1.206	H	6.096	5.923	-0.714	Br	-7.884	0.673	-1.002	H	6.824	4.425	-1.324								

(a) Transition state in path **a;** FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Ph

C	-3.212	-2.910	1.092	C	-0.097	-2.748	1.944	C	-1.233	-1.453	0.178	H	2.477	1.450	-0.757	C	3.280	4.778	-0.700	H	-2.788	3.002	-1.183
C	-2.163	-2.649	0.188	N	0.004	-3.804	2.467	C	-0.223	-1.471	1.269	H	3.848	3.130	-1.988	C	2.528	5.174	0.427	H	-1.463	3.207	-0.034
C	-1.874	-3.625	-0.792	H	-3.436	-2.199	1.886	C	0.709	-0.528	1.654	H	3.880	5.510	-1.236	C	1.760	4.230	1.123	H	-5.454	-0.630	-3.206
C	-2.602	-4.819	-0.900	H	-2.342	-5.538	-1.670	C	1.723	-0.651	2.730	H	2.549	6.209	0.759	P	-2.195	0.137	-0.150	H	-6.442	-0.217	-1.804
C	-3.651	-5.050	0.008	H	-4.222	-5.973	-0.056	C	1.380	-1.089	4.029	H	1.187	4.510	2.002	C	-3.790	-0.353	-1.035	H	-4.318	1.408	3.674
C	-3.959	-4.099	1.003	H	-4.761	-4.292	1.711	C	2.360	-1.186	5.031	H	-3.485	-1.159	-1.711	C	-2.646	0.897	1.528	H	-3.265	2.799	3.422
O	-0.782	-3.373	-1.608	H	1.478	-3.290	-0.429	C	3.696	-0.838	4.756	H	-4.464	-0.776	-0.282	C	-1.306	1.393	-1.250	H	0.109	3.672	-1.944
C	-0.512	-1.926	-1.806	H	3.928	-2.867	-0.511	C	4.046	-0.391	3.466	H	-2.802	0.037	2.191	C	-4.497	0.759	-1.840	H	-1.214	3.451	-3.088
O	-1.289	-1.287	-2.592	H	3.282	0.256	-3.440	C	3.069	-0.295	2.463	H	-1.762	1.420	1.908	C	-3.884	1.819	1.583	H	-5.825	1.690	-4.160
C	0.978	-1.714	-1.828	H	0.811	-0.160	-3.307	O	0.850	0.649	0.853	H	-0.239	1.250	-1.072	C	-1.706	2.871	-1.053	H	-7.366	0.856	-3.884
C	1.864	-2.492	-1.054	H	0.349	-1.338	4.260	C	0.936	1.914	1.478	H	-1.507	1.050	-2.268	C	-5.752	0.202	-2.553	H	-6.822	2.109	-2.751
C	3.251	-2.267	-1.112	H	2.079	-1.525	6.025	O	0.359	2.152	2.551	H	-4.797	1.594	-1.192	C	-4.158	2.288	3.033	H	-5.228	4.132	2.522
C	3.744	-1.263	-1.960	H	4.452	-0.912	5.534	C	1.736	2.883	0.692	H	-3.816	1.165	-2.600	C	-0.977	3.784	-2.067	H	-6.291	2.731	2.773
C	2.884	-0.492	-2.760	H	5.076	-0.126	3.241	C	2.490	2.486	-0.435	H	-3.741	2.702	0.947	C	-6.484	1.277	-3.384	H	-5.551	3.545	4.165
C	1.500	-0.723	-2.684	H	3.354	0.026	1.464	C	3.260	3.436	-1.127	H	-4.773	1.293	1.207	C	-5.378	3.228	3.129	H	-1.104	5.636	-0.903
C	-1.364	5.269	-1.905	H	-0.841	5.897	-2.637	Br	5.689	-0.932	-2.044	H	-2.444	5.415	-2.048								

(a) Transition state in path **b;** FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Ph

C	-2.708	-2.105	0.862	C	0.655	1.258	0.776	C	-1.478	0.001	0.219	H	-0.679	-2.231	-2.216	C	-3.516	-3.970	-3.012	H	-1.502	4.118	1.604
C	-1.471	-1.404	0.710	N	1.293	1.703	1.674	C	-0.211	0.695	-0.211	H	-1.429	-4.518	-2.789	C	-4.452	-2.917	-2.954	H	-0.661	3.531	0.171
C	-0.320	-2.190	0.992	H	-3.619	-1.608	0.556	C	0.047	0.811	-1.566	H	-3.840	-4.975	-3.273	C	-4.028	-1.620	-2.622	H	-6.750	-0.678	1.396
C	-0.387	-3.523	1.429	H	0.542	-4.049	1.635	C	1.190	1.449	-2.265	H	-5.499	-3.105	-3.181	P	-2.562	1.199	1.179	H	-7.091	1.050	1.494
C	-1.624	-4.155	1.604	H	-1.673	-5.186	1.944	C	2.443	1.684	-1.650	H	-4.729	-0.790	-2.611	C	-4.344	0.673	1.545	H	-0.258	1.276	5.113
C	-2.794	-3.428	1.306	H	-3.769	-3.902	1.388	C	3.480	2.307	-2.363	H	-4.304	-0.267	2.104	C	-1.919	1.589	2.928	H	-1.907	1.509	5.699
O	1.000	-1.629	0.931	H	2.880	-0.568	2.015	C	3.291	2.701	-3.701	H	-4.701	1.446	2.241	C	-2.735	2.862	0.296	H	-2.073	5.025	-1.276
C	1.852	-2.005	-0.108	H	5.255	0.122	2.335	C	2.052	2.458	-4.327	H	-2.627	2.315	3.355	C	-5.306	0.568	0.346	H	-2.919	5.617	0.155
O	1.466	-2.654	-1.095	H	6.301	-1.741	-1.432	C	1.013	1.834	-3.619	H	-0.952	2.088	2.819	C	-1.769	0.362	3.853	H	-7.432	-0.682	-1.044
C	3.250	-1.552	0.121	H	3.911	-2.430	-1.738	O	-0.861	0.270	-2.438	H	-3.699	3.264	0.641	C	-1.624	3.908	0.532	H	-8.750	-0.087	-0.014
C	3.627	-0.831	1.275	H	2.625	1.379	-0.627	C	-2.270	0.043	-2.030	H	-2.836	2.616	-0.766	C	-6.747	0.256	0.813	H	-7.770	1.056	-0.953
C	4.964	-0.438	1.453	H	4.436	2.477	-1.874	O	-3.055	1.023	-2.102	H	-5.302	1.501	-0.231	C	-1.227	0.772	5.242	H	-2.022	-0.940	6.360
C	5.913	-0.775	0.472	H	4.097	3.183	-4.249	C	-2.667	-1.362	-2.345	H	-4.969	-0.210	-0.348	C	-1.952	5.229	-0.202	H	-0.365	-1.171	5.769
C	5.556	-1.491	-0.684	H	1.897	2.752	-5.362	C	-1.730	-2.416	-2.412	H	-2.733	-0.153	3.982	C	-7.733	0.129	-0.367	H	-0.669	-0.120	7.166
C	4.218	-1.878	-0.855	H	0.062	1.635	-4.099	C	-2.157	-3.713	-2.744	H	-1.080	-0.363	3.400	C	-1.061	-0.434	6.190	H	0.110	5.949	-0.379
C	-0.859	6.299	0.002	H	-1.111	7.229	-0.524	Br	7.786	-0.228	0.720	H	-0.732	6.538	1.067								

(b) Intermediate **2;** FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 4-BrC$_6$H$_4$

C	4.958	-1.970	0.436	Br	-5.866	3.027	0.394	C	2.706	-0.977	-0.261	H	-1.639	-1.277	-2.936
C	3.541	-1.960	0.502	C	2.660	-2.627	-2.043	C	2.058	-1.427	-1.475	H	-2.025	-0.245	-0.224
C	2.961	-3.003	1.263	N	3.178	-3.610	-2.448	C	0.954	-0.933	-2.167	H	-4.206	0.522	0.711
C	3.707	-3.993	1.914	H	5.447	-1.218	-0.179	C	0.462	-1.328	-3.498	H	-3.857	4.215	-1.524
C	5.110	-3.961	1.832	H	3.189	-4.772	2.466	C	1.350	-1.583	-4.573	H	-1.677	3.421	-2.469
C	5.735	-2.939	1.092	H	5.701	-4.727	2.328	C	0.868	-1.981	-5.830	H	4.099	0.060	2.128
O	1.539	-3.132	1.327	H	6.819	-2.916	1.004	C	-0.516	-2.111	-6.057	H	5.039	0.955	0.933
C	0.803	-2.264	2.116	H	-0.494	-3.772	0.223	C	-1.413	-1.841	-5.003	H	0.312	0.745	0.753
O	1.317	-1.432	2.886	H	-2.964	-4.061	-0.033	C	-0.932	-1.456	-3.743	H	1.268	0.926	2.215
C	-0.661	-2.476	1.946	H	-3.608	-1.513	3.410	O	0.068	-0.061	-1.428	H	3.963	1.327	-1.675
C	-1.176	-3.284	0.909	H	-1.130	-1.219	3.638	C	-0.414	1.119	-1.997	H	2.267	1.690	-1.961
C	-2.565	-3.445	0.766	H	2.419	-1.454	-4.429	O	0.184	1.733	-2.901	H	4.042	3.135	1.837
C	-3.426	-2.799	1.670	H	1.572	-2.175	-6.636	C	-1.701	1.550	-1.391	H	3.152	2.196	3.040
C	-2.930	-1.996	2.713	H	-0.888	-2.411	-7.033	C	-2.421	0.727	-0.496	H	1.624	3.426	1.569
C	-1.542	-1.835	2.844	H	-2.484	-1.938	-5.163	C	-3.649	1.159	0.031	H	0.508	3.169	0.226
C	4.009	5.503	-2.269	H	4.247	5.951	-3.242	Br	-5.370	-3.014	1.469	H	3.140	6.036	-1.858

(b) Intermediate **6;** FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 4-BrC$_6$H$_4$

C	-4.934	-0.887	0.111	Br	6.617	2.499	-0.129	C	-2.309	-0.599	-0.326	H	-4.386	1.399	-1.291
C	-3.752	-1.006	-0.642	C	-2.524	-2.526	1.281	C	-1.758	-1.371	0.878	H	-4.153	2.857	-0.312
C	-3.803	-1.668	-1.890	N	-3.154	-3.476	1.596	C	-2.203	1.383	-0.210	H	-4.569	1.628	1.872
C	-5.004	-2.174	-2.416	H	-4.931	-0.425	1.091	C	-2.408	1.870	1.623	H	-3.608	0.296	2.534
C	-6.177	-2.030	-1.656	H	-5.001	-2.671	-3.381	C	-0.614	2.300	-0.706	H	-1.210	4.294	-0.027
C	-6.145	-1.392	-0.396	H	-7.116	-2.422	-2.040	C	-3.683	2.204	-1.060	H	-0.130	3.459	1.095
O	-2.588	-1.807	-2.505	H	-7.055	-1.302	0.191	C	-3.640	1.387	2.410	H	-2.687	3.834	-2.126
C	-1.591	-0.792	-1.820	H	0.646	0.076	-2.973	C	-0.334	3.628	0.029	H	-2.826	2.315	-3.035
O	-1.636	0.409	-2.400	H	2.860	-1.094	-3.266	C	-3.353	2.986	-2.348	H	-2.760	1.815	4.350
C	-0.263	-1.545	-1.911	H	1.247	-4.547	-1.215	O	-3.693	2.039	3.813	H	-3.735	3.134	3.702
C	0.811	-0.918	-2.568	H	-0.936	-3.393	-0.993	C	0.877	4.358	-0.602	H	1.760	3.703	-0.556
C	2.045	-1.575	-2.733	H	-1.501	1.565	2.153	O	-4.638	3.525	-3.018	H	0.676	4.537	-1.669
C	2.193	-2.874	-2.220	H	-2.412	2.968	1.608	C	-4.900	1.557	4.644	H	-5.299	2.679	-3.261
C	1.130	-3.532	-1.580	H	0.208	1.594	-0.581	C	1.190	5.697	0.097	H	-5.190	4.164	-2.311
C	-0.100	-2.863	-1.439	H	-0.727	2.453	-1.780	C	-4.333	4.322	-4.303	H	-4.868	0.470	4.795
C	3.104	1.981	2.167	H	4.929	3.137	2.289	Br	3.926	-3.801	-2.423	H	2.696	2.355	3.102

(b) Intermediate **8;** FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 4-BrC$_6$H$_4$

C	-2.215	0.455	-2.646	Br	0.888	6.742	0.410	C	-1.427	-0.100	-0.311	H	-0.909	-0.101	4.568
C	-1.124	0.081	-1.816	C	0.310	-1.837	0.261	C	-0.406	-0.669	0.612	H	0.627	1.727	-0.271
C	0.141	0.019	-2.457	N	0.855	-2.854	-0.034	C	-0.442	-0.172	1.959	H	1.762	3.911	-0.235
C	0.278	0.231	-3.843	H	-3.185	0.603	-2.184	C	0.520	-0.586	3.030	H	-1.948	5.822	0.921
C	-0.829	0.558	-4.632	H	1.264	0.155	-4.289	C	1.840	-1.019	2.766	H	-3.097	3.601	0.822
C	-2.088	0.690	-4.019	H	-0.706	0.725	-5.699	C	2.703	-1.353	3.824	H	-4.419	-1.319	-2.232
O	1.330	-0.310	-1.749	H	-2.958	0.982	-4.601	C	2.261	-1.262	5.158	H	-5.177	-2.343	-1.016
C	2.473	0.509	-1.844	H	2.795	-2.122	-1.018	C	0.951	-0.818	5.430	H	-3.328	-3.844	-0.309
O	2.427	1.670	-2.280	H	4.917	-3.183	-0.275	C	0.092	-0.474	4.374	H	-1.675	-3.406	0.140
C	3.697	-0.174	-1.357	H	7.001	0.576	-0.821	O	-1.362	0.686	2.271	H	-3.970	-0.498	1.926
C	3.709	-1.537	-0.987	H	4.865	1.630	-1.591	C	-2.097	1.228	0.207	H	-2.689	-1.662	2.239
C	4.907	-2.136	-0.561	H	2.205	-1.078	1.747	O	-3.361	1.255	0.252	H	-5.995	-0.270	0.212
C	6.080	-1.365	-0.506	H	3.718	-1.676	3.608	C	-1.325	2.511	0.261	H	-5.278	0.742	-1.020
C	6.086	-0.006	-0.869	H	2.931	-1.523	5.974	C	0.052	2.608	-0.024	H	-2.865	-3.230	-2.704
C	4.889	0.585	-1.298	H	0.608	-0.733	6.458	C	0.708	3.849	0.012	H	-1.233	-2.710	-2.269
C	-6.063	-3.608	3.911	H	-6.303	-3.557	4.980	Br	7.754	-2.204	0.092	H	-6.998	-3.466	3.351

(b) Transition state in path **a;** FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 4-BrC$_6$H$_4$

C	-4.869	-1.323	0.555	C	-2.178	-2.803	1.545	C	-2.349	-0.928	-0.050	H	2.198	-2.075	1.651
C	-3.734	-1.506	-0.259	N	-2.653	-3.825	1.906	C	-1.601	-1.561	1.069	H	2.370	-0.165	-0.381
C	-3.845	-2.374	-1.369	Br	6.365	2.967	-0.517	C	-0.384	-1.245	1.637	H	4.511	0.712	-1.295
C	-5.040	-3.034	-1.688	H	-4.807	-0.695	1.442	C	0.315	-1.967	2.729	H	4.613	3.714	1.825
C	-6.162	-2.827	-0.865	H	-5.076	-3.690	-2.551	C	-0.342	-2.305	3.934	H	2.471	2.808	2.750
C	-6.081	-1.973	0.255	H	-7.096	-3.334	-1.094	C	0.344	-2.980	4.956	H	-3.975	0.647	-1.948
O	-2.685	-2.594	-2.095	H	-6.948	-1.830	0.895	C	1.701	-3.320	4.797	H	-4.786	1.296	-0.511
C	-1.734	-1.455	-2.048	H	-0.805	-3.765	-0.820	C	2.367	-2.980	3.603	H	-3.190	0.887	2.109
O	-2.017	-0.427	-2.751	H	1.537	-4.602	-0.756	C	1.682	-2.308	2.579	H	-1.602	1.629	2.064
C	-0.332	-2.002	-1.985	H	2.789	-1.259	-3.206	O	0.395	-0.208	1.032	H	-0.053	1.057	-0.848
C	-0.019	-3.197	-1.305	H	0.427	-0.413	-3.220	C	1.022	0.764	1.840	H	-1.124	1.660	-2.099
C	1.302	-3.682	-1.282	H	-1.382	-2.027	4.077	O	0.530	1.144	2.914	H	-3.831	3.610	-1.072
C	2.304	-2.964	-1.954	H	-0.177	-3.233	5.877	C	2.275	1.276	1.238	H	-3.061	2.912	-2.504
C	2.012	-1.783	-2.658	H	2.231	-3.842	5.590	C	2.854	0.680	0.096	H	-2.646	3.800	1.243
C	0.690	-1.308	-2.664	H	3.413	-3.246	3.467	C	4.061	1.176	-0.423	H	-4.237	3.034	1.249
C	1.009	5.173	-1.067	H	1.853	5.537	-1.666	Br	4.160	-3.636	-1.928	H	0.161	5.852	-1.236

(b) Transition state in path **b;** FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 4-BrC$_6$H$_4$

C	-2.515	-0.229	1.814	C	1.497	1.703	0.145	C	-0.916	0.942	0.253	H	0.416	-0.037	-4.331
C	-1.180	-0.042	1.335	N	-5.330	-4.889	-0.263	C	0.408	1.001	-0.461	H	-1.007	-2.284	-0.827
C	-0.224	-0.910	1.931	Br	2.324	2.320	0.733	C	0.524	0.411	-1.707	H	-2.366	-4.258	-0.225
C	-0.547	-1.840	2.932	H	-3.314	0.320	1.333	C	1.687	0.340	-2.624	H	-5.972	-2.139	-1.348
C	-1.863	-1.960	3.397	H	0.248	-2.457	3.343	C	3.027	0.494	-2.191	H	-4.586	-0.147	-1.962
C	-2.852	-1.141	2.818	H	-2.110	-2.679	4.173	C	4.083	0.433	-3.113	H	-3.521	2.364	1.994
O	1.171	-0.822	1.603	H	-3.891	-1.238	3.126	C	3.827	0.213	-4.480	H	-3.462	3.962	1.247
C	1.751	-1.817	0.817	H	3.378	0.031	2.060	C	2.499	0.045	-4.919	H	-1.155	4.602	1.986
O	1.082	-2.678	0.219	H	5.870	0.103	1.999	C	1.440	0.102	-4.000	H	0.363	3.772	1.597
C	3.234	-1.723	0.798	H	5.904	-3.393	-0.557	O	-0.581	-0.230	-2.217	H	-2.244	4.433	-0.994
C	3.930	-0.717	1.503	H	3.400	-3.453	-0.484	C	-1.942	0.151	-1.799	H	-1.575	3.051	-1.868
C	5.334	-0.674	1.465	H	3.258	0.650	-1.145	O	-2.455	1.170	-2.324	H	-4.256	2.934	-0.958
C	6.028	-1.643	0.721	H	5.105	0.549	-2.762	C	-2.712	-1.064	-1.407	H	-4.412	1.386	-0.159
C	5.352	-2.654	0.013	H	4.649	0.166	-5.191	C	-2.085	-2.237	-0.934	H	-1.713	2.740	3.638
C	3.950	-2.688	0.055	H	2.290	-0.132	-5.971	C	-2.854	-3.363	-0.596	H	-0.212	1.922	3.205
C	1.166	6.175	-2.732	H	1.107	6.775	-3.649	Br	7.993	-1.585	0.665	H	1.367	6.858	-1.895

(c) Intermediate **2**; FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 2-BrC$_6$H$_4$

C -3.482 2.638 -1.889	Br 2.623 -1.529 0.306	C -1.824 0.921 -0.991	H 1.352 -2.949 -2.008	C 1.961 -4.297 3.397	H -5.270 0.127 0.406
C -2.153 2.276 -1.550	C -1.533 0.279 -3.309	C -1.400 -0.110 -1.912	H 3.494 -2.965 2.656	C 0.655 -4.785 3.205	H -4.383 -0.608 -0.937
C -1.165 3.245 -1.844	N -1.635 0.649 -4.428	C -0.864 -1.383 -1.722	H 2.579 -4.670 4.210	C -0.115 -4.291 2.147	H -3.740 4.324 2.974
C -1.450 4.482 -2.437	H -4.268 1.906 -1.719	C -0.620 -2.417 -2.747	H 0.248 -5.545 3.866	P -2.225 0.632 0.749	H -5.237 3.469 2.604
C -2.780 4.805 -2.751	H -0.635 5.167 -2.650	C -1.583 -2.707 -3.746	H -1.117 -4.667 1.964	C -3.124 2.170 1.371	H 1.073 -0.694 3.693
C -3.801 3.876 -2.472	H -3.013 5.759 -3.216	C -1.334 -3.678 -4.729	H -2.452 3.008 1.154	C -0.756 0.404 1.939	H 0.386 0.747 4.442
O 0.219 2.959 -1.625	H -4.833 4.105 -2.728	C -0.128 -4.404 -4.727	H -4.016 2.298 0.750	C -3.394 -0.839 0.980	H -4.928 -2.893 -0.052
C 0.742 2.987 -0.345	H 2.293 2.054 -2.410	C 0.830 -4.141 -3.728	H 0.031 -0.078 1.353	C -3.515 2.166 2.864	H -5.819 -2.174 1.292
O 0.070 3.286 0.661	H 4.731 1.503 -2.325	C 0.589 -3.161 -2.753	H -0.422 1.425 2.159	C -1.029 -0.382 3.241	H -3.835 3.469 5.362
C 2.190 2.651 -0.333	H 4.832 2.639 1.853	O -0.330 -1.679 -0.408	H -2.847 -1.750 0.725	C -4.668 -0.748 0.115	H -5.300 4.380 4.949
C 2.851 2.180 -1.489	H 2.387 3.177 1.752	C -0.590 -2.906 0.180	H -3.647 -0.891 2.046	C -4.330 3.431 3.227	H -5.342 2.606 4.990
C 4.221 1.869 -1.440	H -2.534 -2.183 -3.741	O -1.569 -3.611 -0.132	H -4.114 1.277 3.112	C 0.180 -0.308 4.203	H -0.930 -0.719 6.050
C 4.918 2.041 -0.231	H -2.089 -3.878 -5.487	C 0.376 -3.297 1.258	H -2.616 2.136 3.495	C -5.534 -2.023 0.239	H -0.221 -2.162 5.297
C 4.277 2.511 0.929	H 0.060 -5.162 -5.484	C 1.699 -2.830 1.461	H -1.913 0.010 3.762	C -4.725 3.474 4.717	H 0.814 -1.022 6.178
C 2.908 2.812 0.872	H 1.769 -4.691 -3.715	C 2.480 -3.328 2.523	H -1.238 -1.436 3.012	C -0.052 -1.098 5.508	H -6.544 -1.840 -1.695
C -6.803 -1.958 -0.635	H -7.400 -2.874 -0.536	Br 6.836 1.614 -0.159	H -7.441 -1.109 -0.348		

(c) Intermediate **6**; FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 2-BrC$_6$H$_4$

C -3.407 -2.407 1.714	Br 2.857 1.496 -1.040	C -1.363 -1.346 0.357	H -4.040 -1.467 -1.029	C 0.339 0.064 1.815	H -5.552 2.664 4.447
C -2.410 -2.401 0.722	C -0.366 -2.091 2.515	C -0.470 -1.012 1.557	H -4.717 0.165 -0.906	C 1.227 0.211 3.003	H -5.992 1.133 3.665
C -2.227 -3.562 -0.064	N -0.287 -2.994 3.275	C -2.288 0.163 -0.579	H -4.577 0.312 1.618	C 0.724 0.098 4.316	H -2.826 4.895 -3.552
C -3.054 -4.691 0.071	H -3.533 -1.565 2.383	C -2.908 1.419 0.728	H -3.128 0.396 2.633	P 1.582 0.245 5.418	H -1.608 5.515 -2.417
C -4.065 -4.664 1.046	H -2.885 -5.560 -0.558	C -1.362 1.310 -1.784	H -3.009 2.699 -2.175	C 2.951 0.507 5.220	H -1.235 5.405 -4.149
C -4.237 -3.531 1.873	H -4.709 -5.530 1.175	C -3.911 -0.431 -1.356	H -1.814 3.324 -1.033	C 3.458 0.625 3.912	H -4.544 -1.439 -5.436
O -1.155 -3.513 -0.911	H -5.002 -3.533 2.645	C -3.752 0.967 1.933	H -3.874 0.674 -3.244	C 2.601 0.485 2.807	H -6.313 -1.321 -5.341
C -0.656 -2.020 -0.999	H 0.985 -1.095 -2.885	C -1.931 2.736 -1.953	H -3.115 -0.931 -3.295	C 0.481 1.101 0.845	H -5.322 0.152 -5.326
O -1.214 -1.386 -2.038	H 3.468 -1.418 -3.147	C -3.964 -0.367 -2.896	H -3.510 2.852 2.984	C 0.446 2.437 1.296	H -0.333 -0.088 4.477
C 0.862 -2.193 -1.051	H 3.502 -3.733 0.510	O -4.335 2.186 2.687	H -4.975 2.764 2.002	C -0.159 2.735 2.337	H 1.183 0.159 6.425
C 1.556 -1.643 -2.143	H 1.054 -3.446 0.714	C -1.216 3.473 -3.111	H -0.136 3.510 -2.906	C 1.095 3.445 0.408	H 3.615 0.617 6.075
C 2.944 -1.830 -2.290	H -2.046 1.976 1.100	O -5.288 -0.958 -3.434	H -1.339 2.894 -4.038	C 2.086 3.239 -0.584	H 4.515 0.818 3.750
C 3.633 -2.571 -1.318	H -3.506 2.122 0.132	C -5.147 1.782 3.934	H -5.371 -2.006 -3.110	C 2.607 4.331 -1.307	H 2.999 0.560 1.799
C 2.963 -3.143 -0.224	H -0.322 1.330 -1.452	C -1.752 4.905 -3.319	H -6.144 -0.423 -2.994	C 2.154 5.636 -1.057	H 3.370 4.156 -2.058
C 1.575 -2.956 -0.103	H -1.379 0.761 -2.726	C -5.373 -0.887 -4.974	H -4.520 1.236 4.652	C 1.177 5.863 -0.069	H 2.567 6.464 -1.627
C 0.665 4.780 0.651	H 0.825 6.869 0.139	Br 5.582 -2.839 -1.507	H -0.075 4.934 1.431		

(c) Intermediate **8;** FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 2-BrC$_6$H$_4$

C 2.245 -1.403 -2.082	Br -0.246 -3.372 0.812	C 1.310 -0.172 -0.113	H 0.841 -0.482 4.583	C 3.567 -5.123 0.591	H 3.478 4.349 0.247
C 1.083 -0.890 -1.444	C -0.711 1.374 0.299	C 0.145 0.330 0.717	H 1.476 -5.683 0.574	C 4.472 -4.049 0.679	H 1.713 4.475 0.258
C -0.141 -1.108 -2.124	N -1.363 2.299 -0.065	C 0.211 -0.151 2.021	H 3.921 -6.147 0.504	C 3.985 -2.740 0.791	H 6.893 0.328 -0.866
C -0.183 -1.737 -3.385	H 3.196 -1.309 -1.573	C -0.677 0.115 3.170	H 5.544 -4.232 0.669	P 2.510 1.469 -0.406	H 6.958 1.993 -1.447
C 0.988 -2.205 -3.990	H -1.140 -1.875 -3.875	C -2.012 0.559 3.013	H 4.658 -1.895 0.892	C 4.304 1.326 -1.030	H 0.278 3.350 -3.995
C 2.216 -2.049 -3.321	H 0.939 -2.696 -4.959	C -2.818 0.786 4.141	H 4.437 0.313 -1.418	C 1.709 2.508 -1.795	H 1.942 3.905 -4.181
O -1.375 -0.631 -1.595	H 3.136 -2.430 -3.756	C -2.307 0.570 5.436	H 4.387 2.018 -1.879	C 2.464 2.606 1.107	H 1.742 4.685 2.762
C -2.505 -1.477 -1.570	H -2.974 1.264 -1.413	C -0.983 0.114 5.598	H 2.253 3.462 -1.765	C 5.389 1.620 0.024	H 3.501 4.571 2.756
O -2.442 -2.691 -1.809	H -5.142 2.363 -0.921	C -0.175 -0.118 4.474	H 0.675 2.722 -1.508	C 1.759 1.952 -3.236	H 7.794 1.076 1.385
C -3.759 -0.751 -1.237	H -7.013 -1.517 -0.467	O 1.258 -0.965 2.260	H 3.270 2.243 1.748	C 2.576 4.121 0.838	H 8.909 1.502 0.070
C -3.849 0.657 -1.221	H -4.827 -2.615 -0.994	C 2.258 -0.944 0.973	H 1.527 2.386 1.628	C 6.806 1.378 -0.546	H 7.873 2.747 0.793
C -5.076 1.281 -0.937	H -2.429 0.711 2.024	O 3.309 -0.169 1.223	H 5.319 2.665 0.362	C 1.294 3.018 -4.257	H 2.317 2.181 -6.007
C -6.203 0.487 -0.666	H -3.843 1.122 4.009	C 2.600 -2.444 0.817	H 5.221 0.976 0.893	C 2.638 4.913 2.166	H 0.644 1.621 -5.815
C -6.134 -0.918 -0.678	H -2.935 0.746 6.306	C 1.716 -3.542 0.747	H 2.777 1.631 -3.499	C 7.911 1.693 0.484	H 0.968 3.261 -6.413
C -4.908 -1.532 -0.969	H -0.586 -0.063 6.594	C 2.187 -4.864 0.630	H 1.118 1.069 -3.330	C 1.306 2.491 -5.707	H 1.866 6.808 1.380
C 2.735 6.436 1.941	H 2.773 6.975 2.896	Br -7.920 1.359 -0.263	H 3.638 6.697 1.373		

(c) Transition state in path **a;** FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 2-BrC$_6$H$_4$

C -3.168 -2.845 1.442	C 0.037 -2.577 2.079	C -1.224 -1.556 0.239	H 3.082 0.528 1.632	C 1.345 5.929 -0.104	H -2.862 2.525 -1.854
C -2.147 -2.736 0.479	Br 2.610 1.997 -0.875	C -0.251 -1.353 1.356	H 2.667 4.837 -1.421	C 0.432 5.837 0.964	H -1.513 3.056 -0.849
C -1.863 -3.858 -0.331	N 0.264 -3.592 2.642	C 0.494 -0.271 1.767	H 1.597 6.894 -0.535	C 0.132 4.582 1.504	H -5.302 -1.348 -3.486
C -2.593 -5.053 -0.227	H -3.364 -2.017 2.120	C 1.487 -0.254 2.876	H -0.031 6.730 1.372	P -2.217 -0.072 -0.410	H -6.351 -0.870 -2.152
C -3.622 -5.132 0.727	H -2.341 -5.891 -0.869	C 1.141 -0.676 4.179	H -0.552 4.488 2.342	C -3.718 -0.768 -1.319	H -4.004 1.477 3.495
C -3.911 -4.034 1.566	H -4.192 -6.053 0.826	C 2.093 -0.652 5.212	H -3.306 -1.591 -1.911	C -2.832 0.998 1.037	H -4.453 2.780 2.398
O -0.781 -3.742 -1.178	H -4.693 -4.113 2.317	C 3.401 -0.196 4.961	H -4.392 -1.186 -0.565	C -1.273 1.026 -1.631	H -0.036 3.131 -2.892
C -0.443 -2.314 -1.524	H 1.453 -3.646 0.030	C 3.751 0.237 3.667	H -2.186 0.777 1.893	C -4.469 0.219 -2.237	H -1.399 2.626 -3.888
O -1.134 -1.791 -2.469	H 3.921 -3.408 -0.070	C 2.800 0.212 2.632	H -2.647 2.043 0.763	C -4.314 0.832 1.442	H -5.789 0.844 -4.665
C 1.066 -2.192 -1.529	H 3.511 -0.561 -3.304	O 0.428 0.951 1.012	H -0.224 0.996 -1.331	C -1.769 2.483 -1.751	H -7.284 -0.053 -4.341
C 1.893 -2.944 -0.669	H 1.019 -0.794 -3.163	C 0.276 2.152 1.720	H -1.352 0.488 -2.579	C -5.669 -0.479 -2.922	H -6.843 1.331 -3.321
C 3.293 -2.826 -0.735	H 0.129 -1.010 4.387	O -0.246 2.175 2.846	H -4.840 1.089 -1.674	C -4.663 1.730 2.652	H -6.818 1.862 2.265
C 3.859 -1.955 -1.679	H 1.812 -0.981 6.209	C 0.712 3.387 0.998	H -3.794 0.600 -3.015	C -1.131 3.181 -2.977	H -6.366 0.554 3.376
C 3.059 -1.210 -2.560	H 4.137 -0.177 5.761	C 1.638 3.502 -0.070	H -4.974 1.091 0.603	C -6.441 0.465 -3.866	H -6.364 2.236 3.939
C 1.661 -1.334 -2.475	H 4.761 0.583 3.461	C 1.948 4.766 -0.610	H -4.529 -0.213 1.699	C -6.138 1.588 3.083	H -1.285 5.237 -2.233
C -1.575 4.652 -3.116	H -1.118 5.121 -3.996	Br 5.825 -1.787 -1.784	H -2.666 4.727 -3.226		

(c) Transition state in path **b;** FG = CN; **R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, 2-BrC$_6$H$_4$

C 2.520 0.031 -2.186	C -0.943 1.059 1.015	C 1.313 0.491 -0.025	H 0.744 -2.473 3.833	C 5.295 -3.443 -1.243	H 0.502 3.534 2.723
C 1.284 0.129 -1.480	Br 1.123 -3.429 -0.822	C 0.162 0.159 0.887	H 3.538 -4.448 -1.998	C 5.775 -2.454 -0.363	H 0.623 1.838 3.187
C 0.131 -0.167 -2.260	N -1.778 1.900 1.089	C 0.244 -0.969 1.679	H 5.982 -4.032 -1.846	C 4.865 -1.716 0.402	H 5.946 2.247 -1.972
C 0.198 -0.502 -3.622	H 3.437 0.163 -1.625	C -0.765 -1.545 2.594	H 6.842 -2.273 -0.264	P 1.977 2.218 0.312	H 6.150 3.621 -0.884
C 1.434 -0.560 -4.280	H -0.719 -0.721 -4.160	C -2.156 -1.372 2.394	H 5.213 -0.980 1.119	C 3.563 2.673 -0.615	H -1.366 4.836 -1.407
C 2.605 -0.290 -3.546	H 1.480 -0.823 -5.333	C -3.077 -1.936 3.292	H 3.411 2.432 -1.671	C 0.818 3.637 -0.212	H 0.069 5.779 -1.813
O -1.176 -0.025 -1.686	H 3.580 -0.358 -4.022	C -2.628 -2.687 4.395	H 3.615 3.769 -0.537	C 2.380 2.563 2.126	H 2.400 2.417 4.868
C -2.109 -1.066 -1.794	H -3.036 1.453 -1.089	C -1.245 -2.878 4.592	H 1.352 4.563 0.048	C 4.871 2.048 -0.091	H 2.281 4.119 4.412
O -1.811 -2.208 -2.177	H -5.377 2.068 -0.518	C -0.321 -2.319 3.696	H -0.078 3.579 0.412	C 0.417 3.633 -1.702	H 7.395 0.823 -0.457
C -3.484 -0.641 -1.413	H -6.591 -2.054 -1.065	O 1.408 -1.701 1.647	H 2.999 3.472 2.098	C 1.196 2.767 3.095	H 8.268 2.268 -1.002
C -3.809 0.696 -1.098	H -4.229 -2.654 -1.649	C 2.658 -1.055 1.260	H 2.996 1.723 2.460	C 6.091 2.521 -0.916	H 7.601 2.202 0.641
C -5.131 1.042 -0.771	H -2.525 -0.818 1.538	O 3.221 -0.318 2.112	H 5.023 2.313 0.964	C -0.473 4.850 -2.049	H -0.028 4.912 -4.196
C -6.118 0.044 -0.763	H -4.142 -1.797 3.123	C 3.461 -1.922 0.323	H 4.810 0.954 -0.126	C 1.705 3.184 4.495	H -1.465 3.956 -3.785
C -5.816 -1.295 -1.075	H -3.344 -3.124 5.087	C 3.002 -2.935 -0.555	H 1.309 3.647 -2.347	C 7.416 1.920 -0.404	H -1.540 5.729 -3.751
C -4.494 -1.631 -1.400	H -0.891 -3.464 5.436	C 3.915 -3.680 -1.330	H -0.128 2.711 -1.936	C -0.901 4.864 -3.531	H -0.017 2.444 5.627
C 0.554 3.374 5.504	H 0.936 3.667 6.491	Br -7.970 0.525 -0.304	H -0.144 4.152 5.167		

(d) Intermediate **2**; FG = CN; $\mathbf{R^1}$, $\mathbf{R^2}$, $\mathbf{R^3}$ = 4-BrC$_6$H$_4$, Ph, 2-NO$_2$C$_6$H$_4$

C -0.752 2.672 -3.414	O -2.747 -1.782 2.897	C -0.323 0.958 -1.600	H 1.299 -5.603 0.436	C -6.364 -2.810 0.977	H -1.938 1.530 2.945
C 0.148 2.056 -2.505	O -1.833 -3.446 1.665	C 0.108 -0.405 -1.811	H 0.241 -3.368 0.622	C -6.308 -2.876 -0.430	H -3.780 0.355 1.554
C 1.468 2.577 -2.504	C 1.279 -0.536 -2.668	C -0.376 -1.634 -1.364	H -5.191 -2.637 2.798	C -5.075 -2.769 -1.089	H -3.887 2.110 1.487
C 1.875 3.626 -3.340	N 2.222 -0.625 -3.375	C 0.271 -2.965 -1.508	H -7.316 -2.886 1.495	P -1.351 1.480 -0.189	H -0.844 5.767 1.291
C 0.948 4.222 -4.212	H -1.763 2.275 -3.470	C 0.632 -3.492 -2.772	H -7.219 -3.004 -1.007	C -1.142 3.353 -0.008	H -1.804 6.018 -0.166
C -0.374 3.739 -4.248	H 2.908 3.957 -3.302	C 1.246 -4.750 -2.876	H -5.018 -2.806 -2.172	C -0.726 0.613 1.373	H -0.703 -0.425 3.920
O 2.506 1.963 -1.741	H 1.258 5.037 -4.860	C 1.493 -5.521 -1.723	H -0.131 3.500 0.384	C -3.223 1.189 -0.384	H 0.832 0.403 3.642
C 2.650 2.100 -0.374	H -1.097 4.176 -4.933	C 1.117 -5.018 -0.462	H -1.141 3.748 -1.030	C -2.188 4.122 0.827	H -5.869 1.946 -0.052
O 1.931 2.836 0.327	H 4.149 0.229 -1.727	C 0.514 -3.753 -0.355	H -1.223 -0.358 1.418	C -0.878 1.368 2.710	H -5.790 0.187 0.038
C 3.781 1.279 0.134	H 6.038 -1.118 -0.807	O -1.637 -1.655 -0.634	H 0.335 0.430 1.170	C -4.069 1.196 0.910	H -2.916 6.102 2.721
C 4.459 0.358 -0.695	H 5.532 0.801 3.043	C -2.638 -2.447 -1.213	H -3.565 1.977 -1.070	C -1.849 5.631 0.864	H -2.612 7.513 1.690
C 5.521 -0.402 -0.176	H 3.634 2.144 2.109	O -2.551 -2.916 -2.356	H -3.327 0.236 -0.908	C -0.233 0.566 3.866	H -3.883 6.355 1.253
C 5.895 -0.229 1.167	H 0.412 -2.926 -3.671	C -3.865 -2.614 -0.372	H -3.193 3.999 0.400	C -5.583 1.108 0.602	H 0.110 2.272 5.204
C 5.229 0.681 2.008	H 1.518 -5.134 -3.857	C -3.948 -2.594 1.038	H -2.228 3.746 1.858	C -2.874 6.447 1.678	H -1.427 1.429 5.489
C 4.167 1.433 1.484	H 1.965 -6.497 -1.806	C -5.180 -2.666 1.713	H -0.396 2.354 2.647	C -0.371 1.284 5.225	H 0.097 0.700 6.029
Br 7.385 -1.287 1.895	H -7.513 1.070 1.644	N -2.755 -2.597 1.900	H -6.191 0.299 2.545	C -6.444 1.137 1.882	H -6.283 2.067 2.445

(d) Intermediate **6**; FG = CN; $\mathbf{R^1}$, $\mathbf{R^2}$, $\mathbf{R^3}$ = 4-BrC$_6$H$_4$, Ph, 2-NO$_2$C$_6$H$_4$

C -2.065 -3.336 1.737	O 2.485 2.734 -2.288	C -0.797 -1.478 0.298	H -2.144 1.038 -2.375	C 0.746 0.207 1.592	H -3.340 -0.766 5.361
C -1.437 -2.822 0.587	O 2.812 2.557 -0.060	C 0.188 -1.021 1.371	H -3.733 -2.092 -0.314	C 1.807 0.459 2.615	H -4.764 0.232 5.706
C -1.320 -3.653 -0.554	C 0.715 -2.078 2.205	C -2.257 -0.141 -0.279	H -4.641 -0.590 -0.498	C 1.491 0.502 3.990	H -4.914 -1.197 4.664
C -1.861 -4.951 -0.591	N 1.130 -2.961 2.873	C -2.906 0.623 1.366	H -3.883 -1.117 2.258	P 2.507 0.680 4.942	H -5.627 3.839 -2.278
C -2.507 -5.432 0.560	H -2.122 -2.754 2.649	C -2.225 1.438 -1.363	H -2.320 -0.713 2.977	C 3.847 0.814 4.528	H -4.619 4.962 -1.346
C -2.601 -4.635 1.723	H -1.752 -5.556 -1.485	C -3.759 -1.141 -0.855	H -4.377 1.816 -1.230	C 4.164 0.771 3.157	H -4.687 5.087 -3.116
O -0.606 -3.109 -1.588	H -2.923 -6.437 0.560	C -3.241 -0.280 2.566	H -3.402 2.936 -0.275	C 3.149 0.597 2.200	H -4.263 -3.040 -4.622
C -0.197 -1.634 -1.213	H -3.073 -5.032 2.618	C -3.435 2.386 -1.226	H -3.949 -0.444 -2.913	C 0.403 1.298 0.728	H -6.024 -3.215 -4.465
O -0.880 -0.745 -1.964	H 1.289 0.241 -2.444	C -3.850 -1.398 -2.373	H -2.917 -1.853 -2.722	C 0.184 2.561 1.297	H -5.312 -1.620 -4.787
C 1.320 -1.620 -1.371	H 3.771 0.370 -2.705	O -3.949 0.514 3.689	H -3.315 1.364 3.986	C -0.121 2.707 2.486	H 0.457 0.409 4.308
C 1.923 -0.539 -2.037	H 4.147 -3.420 -0.639	C -3.482 3.404 -2.392	H -4.884 0.943 3.296	C 0.172 3.688 0.310	H 2.256 0.712 5.999
C 3.320 -0.477 -2.199	H 1.686 -3.519 -0.380	O -5.054 -2.303 -2.719	H -2.539 3.970 -2.420	C 0.989 3.836 -0.833	H 4.635 0.945 5.266
C 4.106 -1.519 -1.687	H -2.181 1.382 1.682	C -4.260 -0.353 4.926	H -3.544 2.857 -3.345	C 0.812 4.892 -1.741	H 5.196 0.864 2.830
C 3.529 -2.616 -1.026	H -3.815 1.160 1.067	C -4.671 4.380 -2.277	H -4.946 -3.263 -2.192	C -0.178 5.856 -1.495	H 3.401 0.548 1.146
C 2.132 -2.659 -0.872	H -1.282 1.948 -1.158	C -5.172 -2.561 -4.236	H -5.987 -1.846 -2.350	C -0.974 5.760 -0.339	H 1.462 4.956 -2.607
Br 6.069 -1.447 -1.902	H -1.728 6.514 -0.130	N 2.159 2.969 -1.075	H -1.421 4.593 1.433	C -0.803 4.683 0.546	H -0.312 6.681 -2.189

(d) Intermediate **8**; FG = CN; $\mathbf{R^1}$, $\mathbf{R^2}$, $\mathbf{R^3}$ = 4-BrC$_6$H$_4$, Ph, 2-NO$_2$C$_6$H$_4$

C 2.296 -2.065 -1.576	O -1.265 -3.209 2.930	C 1.283 -0.306 -0.104	H -1.226 2.201 5.878	C 2.398 -5.082 2.428	H 1.546 0.109 -3.472
C 1.127 -1.347 -1.212	O -0.903 -2.030 1.050	C 0.125 0.555 0.341	H 0.309 0.989 4.932	C 3.482 -4.273 2.041	H 4.200 3.779 -0.432
C -0.056 -1.695 -1.909	C -0.562 1.438 -0.522	C -0.022 0.520 1.722	H 0.249 -5.122 2.734	C 3.265 -2.941 1.657	H 2.527 4.221 -0.796
C -0.040 -2.631 -2.963	N -1.085 2.201 -1.267	C -0.964 1.244 2.595	H 2.553 -6.111 2.739	P 2.759 1.053 -0.615	H 6.957 -0.670 -0.219
C 1.143 -3.287 -3.321	H 3.208 -1.878 -1.022	C -2.199 1.750 2.124	H 4.494 -4.670 2.059	C 4.582 0.593 -0.929	H 7.334 0.836 -1.059
C 2.321 -3.016 -2.601	H -0.967 -2.855 -3.479	C -3.067 2.422 3.000	H 4.098 -2.285 1.432	C 2.265 1.805 -2.298	H 1.137 2.226 -4.774
O -1.299 -1.083 -1.601	H 1.139 -4.009 -4.133	C -2.717 2.595 4.354	H 4.623 -0.480 -1.136	C 2.706 2.524 0.572	H 2.878 2.468 -4.924
C -2.420 -1.897 -1.329	H 3.244 -3.539 -2.834	C -1.496 2.081 4.832	H 4.862 1.113 -2.366	C 5.560 0.939 0.211	H 2.234 5.050 1.562
O -2.361 -3.133 -1.287	H -2.904 0.768 -1.943	C -0.628 1.403 3.962	H 2.969 2.636 -2.442	C 2.316 0.885 -3.538	H 3.905 4.618 1.922
C -3.657 -1.100 -1.135	H -5.049 1.985 -1.647	O 0.857 -0.297 2.350	H 1.268 2.243 -2.196	C 3.194 3.876 0.005	H 7.679 0.373 1.979
C -3.758 0.254 -1.519	H -6.840 -1.576 0.049	C 1.946 -0.848 1.276	H 3.295 2.206 1.436	C 6.986 0.424 -0.098	H 8.994 0.406 0.786
C -4.970 0.945 -1.348	H -4.682 -2.801 -0.285	O 3.124 -0.260 1.449	H 1.669 2.615 0.909	C 2.098 1.695 -4.838	H 8.069 1.881 1.130
C -6.068 0.274 -0.784	H -2.498 1.600 1.093	C 1.977 -2.366 1.608	H 5.603 2.028 0.357	C 3.235 4.953 1.116	H 3.073 0.280 -6.201
C -5.985 -1.073 -0.391	H -4.017 2.798 2.630	C 0.911 -3.208 2.003	H 5.194 0.494 1.141	C 7.991 0.791 1.013	H 1.321 0.044 -6.049
C -4.775 -1.759 -0.575	H -3.394 3.114 5.029	C 1.108 -4.538 2.422	H 3.283 0.364 -3.600	C 2.113 0.804 -6.097	H 1.954 1.398 -7.006
Br -7.764 1.242 -0.537	H 3.719 7.072 1.394	N -0.500 -2.776 2.003	H 4.714 6.266 0.166	C 3.702 6.326 0.590	H 3.030 6.697 -0.196

(d) Transition state in path **a**; FG = CN; $\mathbf{R^1}$, $\mathbf{R^2}$, $\mathbf{R^3}$ = 4-BrC$_6$H$_4$, Ph, 2-NO$_2$C$_6$H$_4$

C -2.300 -3.261 1.597	N 1.715 3.029 -0.829	C -0.789 -1.640 0.193	H 5.329 0.898 2.491	C -0.401 6.049 -0.225	H -4.147 -0.959 2.009
C -1.462 -2.961 0.507	N 1.347 -3.401 2.302	C 0.270 -1.275 1.180	H 3.393 0.704 0.949	C -1.012 5.746 1.006	H -3.473 2.021 -1.558
C -1.130 -3.995 -0.397	O 1.579 2.780 -2.078	C 0.862 -0.090 1.546	H 0.955 5.332 -1.766	C -0.786 4.502 1.614	H -2.163 2.886 -0.756
C -1.648 -5.294 -0.257	O 2.701 2.650 -0.121	C 2.012 0.044 2.486	H -0.576 7.006 -0.707	P -2.104 -0.357 -0.304	H -5.156 -2.225 -3.100
C -2.500 -5.566 0.827	H -2.517 -2.497 2.341	C 1.870 -0.275 3.854	H -1.665 6.471 1.485	C -3.520 -1.335 -1.082	H -6.140 -1.987 -1.656
C -2.825 -4.557 1.759	H -1.370 -6.061 -0.973	C 2.966 -0.173 4.725	H -1.260 4.248 2.558	C -2.745 0.537 1.247	H -3.744 0.757 3.813
O -0.227 -3.685 -1.388	H -2.901 -6.569 0.954	C 4.217 0.255 4.239	H -3.012 -2.051 -1.735	C -1.556 0.942 -1.567	H -4.514 1.986 2.812
C -0.062 -2.195 -1.633	H -3.464 -4.784 2.609	C 4.364 0.579 2.877	H -4.014 -1.887 -0.277	C -4.549 -0.523 -1.898	H -1.043 3.219 -3.001
O -0.853 -1.700 -2.513	H 2.075 -3.680 -0.650	C 3.268 0.476 2.002	H -1.994 0.386 2.030	C -4.135 0.113 1.773	H -2.379 2.379 -3.779
C 1.418 -1.884 -1.662	H 4.489 -3.090 -0.728	O 0.430 1.139 0.913	H -2.756 1.608 1.015	C -2.398 2.238 -1.612	H -6.210 -0.179 -4.166
C 2.385 -2.746 -1.105	H 3.509 0.589 -2.796	C 0.153 2.229 1.744	H -0.507 1.165 -1.364	C -5.638 -1.456 -2.479	H -7.442 -1.375 -3.721
C 3.752 -2.419 -1.157	H 1.105 -0.043 -2.746	O -0.093 2.105 2.951	H -1.586 0.405 -2.517	C -4.515 0.910 3.044	H -7.202 0.065 -2.713
C 4.142 -1.216 -1.764	H 0.902 -0.591 4.233	C 0.063 3.538 1.025	H -5.034 0.247 -1.280	C -2.120 3.018 -2.921	H -6.689 0.675 2.864
C 3.202 -0.342 -2.331	H 2.846 -0.425 5.776	C 0.693 3.885 -0.190	H -4.050 -0.007 -2.729	C -6.683 -0.692 -3.318	H -5.913 -0.560 3.876
C 1.841 -0.690 -2.282	H 5.067 0.331 4.913	C 0.456 5.113 -0.827	H -4.904 0.276 1.005	C -5.894 0.504 3.604	H -6.142 1.083 4.503
Br 6.060 -0.746 -1.828	H -2.701 4.867 -3.942	C 0.874 -2.438 1.805	H -3.996 4.154 -2.963	C -2.914 4.338 -3.005	H -2.656 5.008 -2.173

(d) Transition state in path **b**; FG = CN; $\mathbf{R^1}$, $\mathbf{R^2}$, $\mathbf{R^3}$ = 4-BrC$_6$H$_4$, Ph, 2-NO$_2$C$_6$H$_4$

C 2.723 -0.258 -2.137	N 0.918 -3.713 0.048	C 1.387 0.475 -0.142	H -2.331 -3.872 4.099	C 4.418 -4.276 -1.154	H 0.605 2.703 -2.299
C 1.443 -0.052 -1.532	N -1.559 2.250 0.587	C 0.195 0.315 0.756	H -0.519 -3.195 2.555	C 5.141 -3.290 -0.456	H 0.904 3.830 2.382
C 0.336 -0.392 -2.368	O 0.604 -4.634 0.877	C 0.067 -0.733 1.645	H 2.458 -5.148 -1.485	C 4.468 -2.392 0.383	H 0.541 2.188 2.910
C 0.496 -0.810 -3.701	O 0.087 -3.056 -0.650	C -1.039 -1.087 2.565	H 4.929 -4.975 -1.810	P 2.254 2.079 0.185	H 6.408 1.465 -1.641
C 1.773 -0.939 -4.266	H 3.602 -0.128 -1.519	C -1.937 -0.126 3.094	H 6.221 -3.229 -0.560	C 3.981 2.289 -0.564	H 6.698 2.828 -0.561
C 2.896 -0.673 -3.463	H -0.380 -1.045 -4.293	C -2.960 -0.513 3.973	H 5.012 -1.645 0.953	C 1.374 3.634 -0.489	H -0.608 4.874 -1.987
O -0.990 -0.218 -1.861	H 1.882 -1.261 -5.298	C -3.112 -1.864 4.342	H 3.915 2.055 -1.631	C 2.525 2.393 2.031	H 0.901 5.765 -2.200
C -2.005 -1.148 -2.146	H 3.901 -0.810 -3.856	C -2.223 -2.826 3.825	H 4.181 3.367 -0.480	C 5.116 1.493 0.108	H 2.236 2.410 4.762
O -1.812 -2.218 -2.740	H -2.819 1.385 -1.342	C -1.193 -2.444 2.951	H 1.989 4.496 -0.190	C 1.156 3.611 -2.017	H 2.575 4.063 4.247
C -3.342 -0.690 -1.679	H -5.106 2.058 -0.651	O 1.070 -1.707 1.654	H 0.409 3.714 0.021	C 1.339 2.937 2.855	H 7.454 -0.107 0.054
C -3.610 0.648 -1.323	H -6.472 -2.015 -1.209	C 2.444 -1.436 1.459	H 3.355 3.114 2.070	C 6.476 1.750 -0.581	H 8.587 1.174 -0.416
C -4.905 1.029 -0.930	H -4.163 -2.672 -1.928	O 3.098 -0.707 2.230	H 2.878 1.444 2.448	C 0.366 4.850 -2.498	H 7.742 1.263 1.143
C -5.920 0.061 -0.893	H -1.844 0.922 2.836	C 3.065 -2.443 0.545	H 5.193 1.764 1.170	C 1.786 3.296 4.291	H 1.107 4.859 -4.562
C -5.675 -1.279 -1.245	H -3.637 0.240 4.369	C 2.373 -3.466 -0.139	H 4.891 0.420 0.084	C 7.632 0.976 0.088	H -0.408 3.961 -4.344
C -4.382 -1.647 -1.643	H -3.909 -2.161 5.019	C 3.028 -4.374 -0.981	H 2.120 3.574 -2.547	C 0.149 4.853 -4.025	H -0.420 5.736 -4.344
Br -7.734 0.589 -0.336	H 0.959 4.064 6.172	C -0.819 1.329 0.693	H 0.159 4.703 4.721	C 0.618 3.807 5.161	H -0.164 3.042 5.256

(e) Intermediate **2**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-BrC$_6$H$_4$, Ph, 4-MeOC$_6$H$_4$

C	-4.269	2.668	-0.023	C	-1.984	2.439	-2.524	C	-2.227	1.191	-0.454	H	2.338	-0.210	-0.240	C	4.086	-3.123	0.143	H	-4.868	-2.455	0.063
C	-2.879	2.420	0.105	N	-2.359	3.398	-3.109	C	-1.557	1.293	-1.735	H	4.423	-1.108	0.828	C	3.250	-3.995	-0.593	H	-5.017	0.204	4.134
C	-2.130	3.455	0.716	H	-4.875	1.920	-0.527	C	-0.560	0.509	-2.314	H	3.497	-5.045	-0.706	C	2.089	-3.487	-1.191	H	-6.141	-0.725	3.142
C	-2.694	4.656	1.164	H	-2.052	5.411	1.609	C	-0.067	0.555	-3.701	H	1.440	-4.136	-1.773	P	-2.511	-0.394	0.377	H	1.127	-2.696	1.999
C	-4.078	4.859	1.025	H	-4.527	5.789	1.363	C	-0.949	0.732	-4.797	H	-3.691	0.860	2.079	C	-3.895	-0.121	1.636	H	0.135	-2.506	3.445
C	-4.867	3.855	0.432	H	-5.936	4.008	0.301	C	-0.463	0.795	-6.113	H	-4.829	-0.032	1.068	C	-1.050	-1.098	1.378	H	-4.924	-3.123	-2.359
O	-0.710	3.339	0.830	H	1.440	3.525	-0.205	C	0.914	0.658	-6.374	H	-0.155	-0.762	0.850	C	-3.077	-1.664	-0.916	H	-3.480	-4.104	-2.127
C	-0.160	2.481	1.766	H	3.932	3.376	-0.353	C	1.800	0.459	-5.297	H	-1.077	-0.557	2.331	C	-4.046	-1.170	2.758	H	-4.463	-1.878	5.470
O	-0.835	1.862	2.611	H	4.008	1.146	3.359	C	1.318	0.408	-3.980	H	-3.627	-1.061	-1.649	C	-1.008	-2.625	1.600	H	-6.201	-1.528	5.524
C	1.322	2.422	1.651	H	1.510	1.298	3.486	O	0.220	-0.314	-1.421	H	-2.188	-2.043	-1.429	C	-3.961	-2.834	-0.432	H	-5.590	-2.818	4.471
C	2.005	3.013	0.566	H	-2.018	0.804	-4.620	C	0.514	-1.646	-1.738	H	-4.238	-2.169	2.344	C	-5.204	-0.796	3.714	H	-0.644	-4.913	3.231
C	3.405	2.927	0.483	H	-1.162	0.936	-6.935	O	-0.204	-2.334	-2.490	H	-3.118	-1.236	3.342	C	0.198	-3.032	2.480	H	0.356	-5.099	1.775
C	4.110	2.252	1.494	H	1.288	0.698	-7.395	C	1.742	-2.125	-1.064	H	-1.928	-2.977	2.086	C	-4.382	-3.732	-1.620	H	1.124	-4.819	3.350
C	3.448	1.660	2.585	H	2.867	0.351	-5.482	C	2.592	-1.261	-0.329	H	-0.936	-3.148	0.635	C	-5.375	-1.814	4.861	H	-6.188	-4.572	-0.701
C	2.049	1.747	2.657	H	2.021	0.277	-3.161	C	3.754	-1.755	0.270	H	-3.427	-3.449	0.304	C	0.262	-4.554	2.724	H	-5.544	-5.543	-2.039
Br	6.069	2.125	1.380	H	5.882	-5.176	-0.381	C	5.700	-4.900	0.667	H	6.635	-4.947	1.228	C	-5.262	-4.920	-1.180	H	-4.732	-5.560	-0.462
O	5.259	-3.513	0.775	H	4.965	-5.585	1.111																

(e) Intermediate **6**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-BrC$_6$H$_4$, Ph, 4-MeOC$_6$H$_4$

C	-4.444	-1.462	0.451	C	-1.744	-2.568	1.627	C	-1.922	-0.829	-0.183	H	-4.268	2.319	-0.430	C	-0.020	-0.923	1.608	H	-5.558	1.470	4.249
C	-3.296	-1.483	-0.361	N	-2.197	-3.564	2.079	C	-1.198	-1.360	1.058	H	-4.399	1.266	1.916	C	0.701	-1.545	2.751	H	-0.401	6.472	-0.759
C	-3.304	-2.276	-1.532	H	-4.466	-0.904	1.378	C	-2.125	1.149	-0.287	H	-3.203	0.174	2.632	C	0.061	-1.807	3.981	H	0.835	5.950	0.403
C	-4.436	-3.010	-1.926	H	-4.402	-3.602	-2.835	C	-2.320	1.807	1.492	H	-1.604	4.183	-0.505	P	0.774	-2.390	5.040	H	1.312	6.496	-1.217
C	-5.578	-2.962	-1.111	H	-6.463	-3.529	-1.392	C	-0.725	2.234	-0.976	H	-0.375	3.662	0.654	C	2.134	-2.719	4.883	H	-4.288	2.515	-5.243
C	-5.585	-2.195	0.075	H	-6.468	-2.180	0.709	C	-3.754	1.636	-1.121	H	-3.086	3.229	-2.461	C	2.780	-2.458	3.659	H	-5.871	3.288	-5.024
O	-2.114	-2.299	-2.207	H	0.799	-0.026	-3.025	C	-3.416	1.228	2.407	H	-3.016	1.593	-3.146	C	2.071	-1.868	2.599	H	-4.394	4.128	-4.510
C	-1.248	-1.081	-1.687	H	3.148	-0.896	-3.312	C	-0.634	3.669	-0.413	H	-2.505	1.986	4.227	C	0.682	0.124	0.965	H	-0.984	-1.544	4.114
O	-1.494	0.029	-2.387	H	2.122	-4.320	-0.872	C	-3.615	2.265	-2.522	H	-3.715	3.065	3.532	C	1.301	1.144	1.756	H	0.271	-2.585	5.984
C	0.170	-1.645	-1.774	H	-0.194	-3.465	-0.649	O	-3.492	2.007	3.741	H	1.406	3.983	-1.095	C	0.801	1.498	2.834	H	2.684	-3.174	5.704
C	1.120	-0.942	-2.538	H	-1.351	1.712	1.991	C	0.433	4.488	-1.180	H	0.179	4.501	-2.250	C	2.497	1.707	1.116	H	3.827	-2.718	3.527
C	2.428	-1.434	-2.701	H	-2.507	2.881	1.359	O	-4.998	2.497	-3.173	H	-5.520	1.532	-3.260	C	3.062	1.153	-0.062	H	2.568	-1.689	1.650
C	2.779	-2.641	-2.078	H	0.203	1.682	-0.816	C	-4.557	1.436	4.701	H	-5.618	3.133	-2.522	C	4.216	1.709	-0.614	H	2.598	0.294	-0.533
C	1.846	-3.373	-1.326	H	-0.901	2.235	-2.052	C	0.552	5.935	-0.658	H	-4.340	0.389	4.954	C	4.826	2.829	-0.001	H	4.669	1.297	-1.510
C	0.539	-2.872	-1.186	H	-4.349	0.720	-1.187	C	-4.883	3.145	-4.569	H	-4.593	2.006	5.638	C	4.273	3.389	1.176	H	4.733	4.244	1.660
Br	4.617	-3.340	-2.285	H	7.036	4.216	0.957	C	6.678	4.444	-0.056	H	7.527	4.610	-0.720	C	3.116	2.822	1.725	H	2.683	3.231	2.633
O	5.965	3.304	-0.628	H	6.040	5.338	-0.036																

(e) Intermediate **8**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-BrC$_6$H$_4$, Ph, 4-MeOC$_6$H$_4$

C	-2.486	-0.740	2.537	C	0.332	1.557	0.007	C	-1.545	-0.092	0.279	H	0.444	-1.967	0.030	C	-0.315	-5.136	-0.961	H	-1.817	2.572	-2.415
C	-1.328	-0.420	1.777	N	0.927	2.485	0.457	C	-0.440	0.498	-0.528	H	1.501	-4.193	-0.287	C	-1.693	-4.976	-1.227	H	-7.026	0.490	2.514
C	-0.093	-0.538	2.466	H	-3.444	-0.756	2.031	C	-0.414	0.182	-1.932	H	-2.295	-5.804	-1.590	C	-2.289	-3.725	-1.022	H	-7.573	1.459	1.144
C	-0.041	-0.852	3.840	H	0.925	-0.910	4.328	C	0.696	0.624	-2.844	H	-3.346	-3.582	-1.224	P	-3.135	1.337	0.150	H	-0.564	4.631	1.946
C	-1.209	-1.115	4.562	H	-1.151	-1.363	5.618	C	2.026	0.815	-2.409	H	-4.564	1.264	2.166	C	-4.797	1.306	1.096	H	-2.180	5.280	2.263
C	-2.446	-1.079	3.892	H	-3.366	-1.320	4.418	C	3.030	1.178	-3.324	H	-5.214	2.307	0.899	C	-2.443	3.007	0.725	H	-3.159	1.785	-4.384
O	1.152	-0.296	1.822	H	2.791	1.438	1.281	C	2.718	1.358	-4.685	H	-3.221	3.746	0.484	C	-3.605	1.562	-1.679	H	-4.463	2.891	-3.948
C	2.227	-1.194	1.969	H	5.015	2.350	0.650	C	1.395	1.157	-5.130	H	-1.568	3.241	0.113	C	-5.827	0.227	0.714	H	-7.870	-1.611	1.368
O	2.084	-2.350	2.397	H	6.764	-1.592	1.065	C	0.396	0.784	-4.217	H	-4.693	1.714	-1.686	C	-2.072	3.104	2.221	H	-9.177	-0.429	1.588
C	3.517	-0.594	1.544	H	4.526	-2.498	1.727	O	-1.373	-0.513	-2.445	H	-3.394	0.604	-2.158	C	-2.905	2.709	-2.438	H	-8.422	-0.637	-0.005
C	3.653	0.779	1.241	H	2.288	0.662	-1.368	C	-2.260	-1.336	-0.362	H	-5.983	0.215	-0.373	C	-7.181	0.468	1.423	H	-2.009	4.512	4.680
C	4.909	1.295	0.880	H	4.051	1.313	-2.977	O	-3.519	-1.282	-0.465	H	-5.448	-0.769	0.965	C	-1.469	4.489	2.553	H	-0.384	3.877	4.352
C	6.016	0.431	0.819	H	3.496	1.642	-5.391	C	-1.540	-2.621	-0.560	H	-2.956	2.933	2.853	C	-3.370	2.756	-3.912	H	-0.689	5.622	4.260
C	5.899	-0.939	1.116	H	1.150	1.281	-6.182	C	-0.160	-2.801	-0.303	H	-1.336	2.334	2.480	C	-8.224	-0.614	1.075	H	-1.591	3.748	-4.715
C	4.644	-1.447	1.483	H	-0.620	0.592	-4.550	C	0.447	-4.043	-0.496	H	-3.116	3.680	-1.967	C	-1.119	4.634	4.048	H	-3.024	3.896	-5.754
Br	7.773	1.153	0.310	H	-0.746	-7.324	-2.615	C	-0.329	-7.502	-1.614	H	0.421	-8.293	-1.663	C	-2.681	3.882	-4.711	H	-2.896	4.867	-4.274
O	0.383	-6.329	-1.125	H	-1.133	-7.795	-0.924																

(e) Transition state in path **a**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-BrC$_6$H$_4$, Ph, 4-MeOC$_6$H$_4$

C	-4.056	-2.154	0.826	O	5.257	4.618	-0.375	C	-1.747	-1.240	-0.057	H	2.657	0.809	-0.531	C	4.267	3.731	0.042	H	-0.841	3.309	0.155
C	-2.984	-2.123	-0.058	C	5.985	4.212	-1.541	C	-0.845	-1.541	1.124	H	4.445	2.195	-1.463	C	3.576	4.130	1.198	H	-5.436	0.903	-3.370
C	-2.962	-3.045	-1.109	H	-4.097	-1.465	1.661	C	0.256	-0.907	1.559	H	3.852	5.064	1.669	C	2.574	3.342	1.713	H	-6.356	1.361	-1.950
C	-3.983	-3.979	-1.278	H	-3.936	-4.686	-2.094	C	1.125	-1.386	2.700	H	2.042	3.644	2.608	P	-2.273	0.547	-0.189	H	-4.023	2.020	3.703
C	-5.041	-3.980	-0.387	H	-5.843	-4.699	-0.507	C	0.602	-1.652	3.963	H	-3.653	-0.190	-1.945	C	-3.836	0.552	-1.171	H	-2.765	3.211	3.439
C	-5.082	-3.071	0.662	H	-5.911	-3.083	1.357	C	1.428	-2.082	4.989	H	-4.633	0.187	-0.531	C	-2.554	1.267	1.493	H	0.939	3.408	-1.606
O	-1.852	-3.033	-1.929	H	0.241	-3.772	-0.722	C	2.787	-2.246	4.768	H	-2.854	0.443	2.132	C	-1.037	1.557	-1.113	H	-0.295	3.586	-2.837
C	-1.205	-1.722	-1.943	H	2.677	-4.125	-0.715	C	3.319	-1.974	3.517	H	-1.594	1.611	1.867	C	-4.256	1.877	-1.842	H	-5.261	3.317	-4.042
O	-1.681	-0.837	-2.683	H	3.190	-0.596	-3.088	C	2.495	-1.542	2.491	H	-0.063	1.170	-0.838	C	-3.599	2.398	1.615	H	-6.942	2.823	-3.880
C	0.330	-1.969	-1.879	H	0.739	-0.255	-3.081	O	0.754	0.217	0.864	H	-1.195	1.309	-2.158	C	-1.075	3.083	-0.883	H	-6.181	3.781	-2.614
C	0.887	-3.064	-1.227	H	-0.456	-1.516	4.148	C	1.137	1.288	1.697	H	-4.395	2.662	-1.103	C	-5.573	1.689	-2.631	H	-4.489	4.861	2.647
C	2.257	-3.269	-1.227	H	1.008	-2.287	5.966	O	0.582	1.503	2.761	H	-3.479	2.202	-2.529	C	-3.734	2.866	3.083	H	-5.752	3.664	2.911
C	3.094	-2.376	-1.890	H	3.431	-2.583	5.571	C	2.229	2.139	1.090	H	-3.313	3.246	0.998	C	-0.056	3.803	-1.797	H	-4.843	4.300	4.277
C	2.546	-1.285	-2.557	H	4.380	-2.099	3.339	C	2.914	1.744	-0.049	H	-4.567	2.047	1.264	C	-6.016	2.986	-3.336	H	0.208	5.569	-0.552
C	1.174	-1.091	-2.547	H	2.913	-1.333	1.515	C	3.928	2.529	-0.578	H	-2.066	3.479	-1.086	C	-4.771	3.995	3.238	H	0.666	5.804	-2.235
Br	4.959	-2.645	-1.891	H	5.341	4.117	-2.419	N	-1.358	-3.829	2.310	H	6.720	4.996	-1.731	C	-0.055	5.328	-1.578	H	-1.035	5.748	-1.786
C	-1.135	-2.817	1.796	H	6.515	3.267	-1.389																

(e) Transition state in path **b**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-BrC$_6$H$_4$, Ph, 4-MeOC$_6$H$_4$

C	2.699	0.912	1.754	O	4.268	5.522	-0.787	C	1.397	-0.471	0.093	H	0.708	2.594	-0.711	C	3.612	4.299	-0.972	H	0.251	-3.472	-1.371
C	1.450	0.457	1.293	C	3.442	6.576	-0.280	C	0.028	-0.866	-0.414	H	1.622	4.808	-0.312	C	4.416	3.275	-1.485	H	6.630	-0.796	1.199
C	0.333	1.023	1.938	H	3.589	0.571	1.252	C	-0.285	-0.337	-1.609	H	5.452	3.491	-1.709	C	3.885	2.023	-1.708	H	6.845	-2.369	0.456
C	0.478	1.925	2.994	H	-0.416	2.315	3.463	C	-1.577	-0.435	-2.383	H	4.498	1.237	-2.130	P	2.356	-2.066	0.399	H	0.118	-3.808	3.912
C	1.724	2.315	3.435	H	1.824	3.013	4.255	C	-2.390	-1.565	-2.362	H	4.230	-1.411	1.790	C	4.142	-1.950	0.854	H	1.744	-4.388	4.220
C	2.844	1.803	2.795	H	3.836	2.111	3.102	C	-3.561	-1.599	-3.103	H	4.461	-2.971	1.047	C	1.699	-3.157	1.742	H	1.383	-4.052	-3.520
O	-0.991	0.640	1.610	H	-3.090	-0.492	2.066	C	-3.934	-0.508	-3.873	H	2.320	-4.048	1.763	C	2.377	-3.084	-1.141	H	2.258	-5.340	-2.715
C	-1.735	1.656	0.999	H	-5.505	-0.970	1.910	C	-3.125	0.619	-3.908	H	0.696	-3.465	1.472	C	5.070	-1.321	-0.207	H	7.226	0.317	-0.971
O	-1.237	2.686	0.581	H	-6.057	2.584	-0.424	C	-1.953	0.653	-3.173	H	3.292	-3.668	-1.123	C	1.667	-2.510	3.144	H	8.516	-0.751	-0.430
C	-3.212	1.313	0.913	H	-3.634	3.056	-0.255	O	0.625	0.487	-2.216	H	2.456	-2.349	-1.944	C	1.181	-4.033	-1.367	H	7.435	-1.260	-1.723
C	-3.742	0.182	1.525	H	-2.111	-2.429	-1.776	C	2.006	0.337	-1.747	H	4.981	-1.864	-1.145	C	6.543	-1.342	0.261	H	2.070	-2.572	5.929
C	-5.098	-0.087	1.435	H	-4.183	-2.485	-3.080	O	2.718	-0.509	-2.311	H	4.766	-0.298	-0.404	C	1.120	-3.496	4.201	H	0.437	-1.993	5.619
C	-5.936	0.775	0.733	H	-4.850	-0.538	-4.449	C	2.549	1.748	-1.421	H	2.667	-2.193	3.435	C	1.325	-4.780	-2.713	H	0.686	-3.585	6.328
C	-5.408	1.911	0.121	H	-3.408	1.472	-4.511	C	1.753	2.772	-0.929	H	1.037	-1.624	3.123	C	7.490	-0.719	-0.783	H	-0.791	-5.200	-3.001
C	-4.053	2.175	0.215	H	-1.314	1.527	-3.203	C	2.272	4.039	-0.700	H	1.119	-4.762	-0.562	C	1.076	-2.871	5.609	H	0.279	-6.251	-3.921
Br	-7.777	0.410	0.610	H	3.033	6.346	0.708	N	-1.577	-2.425	0.934	H	4.083	7.455	-0.194	C	0.149	-5.742	-2.971	H	0.085	-6.492	-2.188
C	-0.893	-1.716	0.325	H	2.614	6.815	-0.954																

(f) Intermediate **2**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Me

C	-2.445	-0.487	3.532	H	-3.288	0.112	3.197	C	-1.213	0.235	1.417	H	-0.639	2.237	-4.176	C	-1.083	-1.114	-1.402	H	0.269	-1.675	-3.723
C	-1.290	-0.523	2.710	H	0.657	-2.453	4.801	C	-0.535	1.514	1.410	H	-2.402	-2.503	1.203	C	-3.406	0.925	-0.509	H	-0.633	-3.120	-3.273
C	-0.198	-1.261	3.227	H	-1.430	-2.375	6.203	C	-0.107	2.342	0.373	H	-3.855	-1.515	1.378	C	-3.846	-2.770	-0.403	H	-5.915	1.899	-1.135
C	-0.227	-1.920	4.462	H	-3.413	-1.087	5.372	C	0.479	3.691	0.466	H	-0.192	-0.481	-1.415	C	-1.670	-1.262	-2.822	H	-4.684	2.945	-1.850
C	-1.396	-1.872	5.240	H	3.135	-0.211	2.058	C	-0.043	4.679	1.339	H	-0.778	-2.091	-1.007	C	-4.152	0.845	-1.857	H	-4.596	-5.294	-1.449
C	-2.511	-1.151	4.769	H	5.363	0.088	0.966	C	0.540	5.954	1.418	H	-4.130	0.910	0.318	C	-4.613	-3.933	0.269	H	-5.853	-5.664	-0.253
O	1.049	-1.281	2.529	H	4.449	-3.144	-1.767	C	1.645	6.288	0.610	H	-2.872	1.879	-0.441	C	-0.739	-2.118	-3.716	H	-6.052	-4.283	-1.349
C	1.200	-2.037	1.381	H	2.217	-3.428	-0.664	C	2.163	5.323	-0.277	H	-4.555	-2.173	-0.995	C	-5.197	1.980	-1.966	H	-2.252	-2.713	-5.187
O	0.318	-2.804	0.946	H	-0.916	4.454	1.943	C	1.590	4.043	-0.348	H	-3.114	-3.194	-1.105	C	-5.319	-4.846	-0.754	H	-1.343	-1.258	-5.641
C	2.538	-1.838	0.764	H	0.121	6.691	2.099	O	-0.045	1.766	-0.957	H	-2.664	-1.726	-2.802	C	-1.259	-2.244	-5.163	H	-0.584	-2.856	-5.776
C	3.428	-0.846	1.229	H	2.089	7.278	0.668	C	-0.622	2.447	-2.039	H	-1.796	-0.277	-3.288	C	-5.958	1.956	-3.308	H	-6.495	1.007	-3.445
C	4.680	-0.677	0.614	H	3.020	5.564	-0.902	O	-1.534	3.274	-1.914	H	-3.447	0.944	-2.690	Br	6.783	-1.279	-1.324	H	-6.694	2.769	-3.359
C	5.031	-1.511	-0.462	H	2.023	3.297	-1.011	C	0.039	2.054	-3.339	H	-4.657	-0.125	-1.975	C	-0.207	1.999	2.742				
C	4.159	-2.507	-0.937	H	0.365	1.011	-3.322	P	-2.158	-0.411	0.012	H	-3.909	-4.528	0.870	N	0.056	2.342	3.843				
C	2.909	-2.665	-0.319	H	0.932	2.678	-3.475	C	-3.131	-1.898	0.651	H	-5.355	-3.523	0.971	H	-5.268	2.078	-4.154				

(f) Intermediate **6**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Me

C	2.314	0.216	-3.041	H	2.481	1.270	-2.858	C	0.744	-0.188	-0.918	H	2.298	2.657	-1.354	C	-0.975	1.545	-0.084	H	4.778	0.494	5.511
C	1.495	-0.551	-2.190	H	1.660	-3.569	-3.839	C	-0.186	1.012	-1.070	H	3.773	-1.133	3.012	C	-1.966	2.642	-0.228	H	3.935	-0.468	6.741
C	1.269	-1.912	-2.509	H	3.144	-2.192	-5.333	C	2.095	-0.011	0.605	H	3.779	0.632	3.122	C	-1.620	3.889	-0.788	H	4.529	-4.943	-0.560
C	1.860	-2.523	-3.630	H	3.529	0.223	-4.829	C	2.543	1.856	0.654	H	3.690	-2.621	1.348	C	-2.585	4.903	-0.904	H	6.289	-4.780	-0.382
C	2.683	-1.742	-4.457	H	-1.228	-2.505	1.714	C	1.854	-0.225	2.494	H	3.007	-2.849	-0.241	C	-3.905	4.679	-0.468	H	5.236	-4.689	1.045
C	2.908	-0.377	-4.169	H	-3.714	-2.782	2.036	C	3.727	-0.827	0.107	H	2.773	4.561	0.225	C	-4.257	3.434	0.088	H	-0.601	4.074	-1.115
O	0.405	-2.560	-1.670	H	-4.345	-1.337	-1.994	C	3.087	2.572	-0.595	H	4.397	3.928	0.488	C	-3.293	2.421	0.214	H	-2.307	5.863	-1.331
C	0.115	-1.623	-0.420	H	-1.895	-1.115	-2.298	C	3.169	-0.265	3.306	H	2.271	0.512	5.129	C	-0.980	0.883	1.163	H	-4.650	5.465	-0.562
O	0.844	-2.002	0.641	H	1.650	2.380	1.018	C	3.826	-2.355	0.291	H	2.270	-1.250	5.023	C	-1.030	1.607	2.386	H	-5.277	3.250	0.413
C	-1.401	-1.750	-0.280	H	3.291	1.928	1.457	O	3.587	3.996	-0.255	H	5.311	-2.640	-1.270	C	-0.591	2.754	2.482	H	-3.574	1.451	0.617
C	-1.928	-2.236	0.929	H	1.254	0.626	2.831	C	2.877	-0.354	4.824	H	6.009	-2.379	0.332	C	-1.637	0.758	3.468	H	-1.253	-0.264	3.410
C	-3.314	-2.392	1.104	H	1.285	-1.147	2.612	O	5.190	-2.888	-0.204	H	3.289	4.877	-2.241	Br	-6.126	-2.241	0.287	H	-2.722	0.704	3.314
C	-4.173	-2.047	0.048	H	3.894	-0.565	-0.944	C	4.089	4.764	-1.496	H	4.440	5.768	-1.226	C	-0.350	1.567	-2.389				
C	-3.673	-1.579	-1.177	H	4.499	-0.313	0.697	P	4.166	-0.404	5.670	H	4.922	4.235	-1.978	N	-0.475	2.014	-3.477				
C	-2.281	-1.441	-1.336	H	3.912	2.004	-1.047	C	5.321	-4.413	-0.015	H	4.778	-1.278	5.407	H	-1.433	1.197	4.446				

(f) Intermediate **8**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Me

C	-2.616	-2.719	-0.643	H	-3.549	-2.209	-0.850	C	-1.561	-0.407	-0.610	H	-1.261	0.130	-4.064	C	-2.743	0.221	2.298	H	-1.184	-0.532	4.456
C	-1.440	-1.941	-0.473	H	0.731	-4.586	-0.168	C	-0.422	0.469	-0.170	H	-4.820	-1.557	0.849	C	-3.505	2.098	0.026	H	-2.884	-0.525	4.947
C	-0.235	-2.675	-0.342	H	-1.387	-5.899	-0.386	C	-0.225	1.647	-0.953	H	-5.446	0.028	1.305	C	-5.786	-0.469	-0.786	H	-2.843	4.707	-0.552
C	-0.222	-4.081	-0.294	H	-3.547	-4.661	-0.754	C	0.855	2.662	-0.717	H	-3.561	0.736	2.821	C	-2.537	-1.187	2.900	H	-4.292	4.712	0.455
C	-1.408	-4.813	-0.420	H	2.735	-1.243	1.291	C	2.077	2.378	-0.065	H	-1.838	0.817	2.439	C	-2.863	3.149	0.958	H	-7.637	-1.577	-2.605
C	-2.616	-4.118	-0.614	H	5.011	-0.495	1.979	C	3.056	3.377	0.080	H	-4.597	2.218	0.020	C	-7.220	-0.993	-0.534	H	-9.095	-1.339	-1.620
O	1.030	-2.046	-0.195	H	6.455	-1.166	-2.049	C	2.830	4.673	-0.420	H	-3.150	2.224	-0.998	C	-2.125	-1.095	4.388	H	-8.174	0.062	-2.201
C	1.986	-2.134	-1.216	H	4.169	-1.939	-2.724	C	1.619	4.963	-1.081	H	-5.833	0.559	-1.166	C	-3.199	4.581	0.481	H	-2.875	-3.066	4.998
O	1.722	-2.574	-2.345	H	2.281	1.384	0.314	C	0.646	3.964	-1.234	H	-5.312	-1.050	-1.584	C	-8.083	-0.961	-1.813	H	-1.166	-3.058	4.513
C	3.313	-1.646	-0.762	H	3.994	3.140	0.575	O	-1.041	1.866	-1.944	H	-3.457	-1.785	2.815	C	-1.944	-2.484	5.034	H	-1.644	-2.394	6.086
C	3.546	-1.237	0.570	H	3.589	5.444	-0.304	C	-2.018	-0.137	-2.092	H	-1.751	-1.722	2.355	C	-2.568	5.664	1.381	H	-1.474	5.575	1.393
C	4.828	-0.809	0.956	H	1.442	5.959	-1.481	O	-3.249	0.035	-2.301	H	-3.217	3.026	1.992	Br	7.654	-0.188	0.545	H	-2.820	6.671	1.023
C	5.861	-0.790	0.004	H	-0.278	4.161	-1.769	C	-1.071	-0.524	-3.210	H	-1.773	3.027	0.976	C	0.223	0.230	1.066				
C	5.646	-1.190	-1.327	H	-1.272	-1.562	-3.508	P	-3.203	0.274	0.462	H	-7.173	-2.024	-0.149	N	0.716	0.025	2.130				
C	4.365	-1.620	-1.705	H	-0.022	-0.450	-2.920	C	-4.939	-0.525	0.499	H	-7.703	-0.389	0.250	H	-2.925	5.577	2.417				

(f) Transition state in path **a**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Me

C	2.282	2.142	2.381	H	2.596	1.192	2.796	C	0.698	1.047	0.583	H	-1.127	-4.676	-0.997	C	2.489	-1.396	0.997	H	4.020	-2.566	2.972
C	1.389	2.183	1.317	H	1.147	5.566	0.985	C	-0.301	0.331	1.471	H	2.946	1.933	-0.975	C	1.405	-0.808	-1.766	H	3.509	-3.813	1.851
C	0.993	3.429	0.825	H	2.756	5.455	2.870	C	-1.001	-0.795	1.264	H	3.923	1.284	0.338	C	4.444	0.527	-1.629	H	0.610	-2.611	-3.682
C	1.476	4.614	1.379	H	3.472	3.268	3.759	C	-2.065	-1.323	2.203	H	2.315	-1.004	1.994	C	3.942	-1.913	0.910	H	1.906	-1.651	-4.362
C	2.371	4.543	2.431	H	-2.198	2.656	0.593	C	-1.799	-1.583	3.545	H	1.799	-2.223	0.866	C	2.150	-2.070	-2.255	H	6.107	0.950	-3.860
C	2.777	3.312	2.933	H	-4.523	2.001	0.125	C	-2.795	-2.070	4.376	H	0.354	-1.032	-1.626	C	5.553	1.581	-1.852	H	7.350	1.883	-3.035
O	0.055	3.433	-0.186	H	-3.264	0.171	-3.538	C	-4.066	-2.308	3.875	H	1.465	-0.003	-2.492	C	4.208	-2.990	1.987	H	7.070	0.204	-2.590
C	0.078	2.181	-0.947	H	-0.934	0.845	-3.054	C	-4.338	-2.061	2.538	H	4.901	-0.404	-1.306	C	1.688	-2.468	-3.676	H	5.854	-3.978	0.959
O	0.932	2.062	-1.852	H	-0.807	-1.409	3.942	C	-3.343	-1.575	1.706	H	3.943	0.340	-2.576	C	6.585	1.124	-2.901	H	6.367	-2.725	2.084
C	-1.404	1.766	-1.189	H	-2.576	-2.268	5.418	O	-0.875	-1.503	0.048	H	4.134	-2.338	-0.072	C	5.651	-3.526	1.926	H	5.807	-4.279	2.693
C	-2.427	2.099	-0.306	H	-4.843	-2.688	4.526	C	-0.817	-2.903	0.196	H	4.638	-1.089	1.054	C	2.379	-3.753	-4.173	H	2.153	-4.590	-3.519
C	-3.737	1.736	-0.571	H	-5.329	-2.244	2.142	O	-0.337	-3.433	1.178	H	3.223	-1.903	-2.274	Br	-5.823	0.527	-2.092	H	2.039	-4.002	-5.174
C	-4.044	1.032	-1.732	H	-3.559	-1.377	0.664	C	-1.380	-3.622	-1.041	H	1.964	-2.898	-1.573	C	-0.674	1.081	2.680				
C	-3.031	0.706	-2.627	H	-0.978	-3.184	-1.948	P	1.990	-0.061	-0.185	H	5.097	2.515	-2.175	N	-0.975	1.681	3.623				
C	-1.724	1.077	-2.351	H	-2.462	-3.514	-1.059	C	3.421	1.033	-0.590	H	6.058	1.777	-0.908	H	3.457	-3.624	-4.202				

(f) Transition state in path **b**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, Me

C	-2.901	-2.501	-0.620	H	-3.825	-1.978	-0.788	C	-1.756	-0.248	-0.368	H	-2.511	-1.098	-3.246	C	-3.198	0.180	2.413	H	-4.101	-0.959	4.768
C	-1.736	-1.756	-0.357	H	0.351	-4.455	-0.190	C	-0.511	0.456	0.112	H	-5.136	-0.959	0.395	C	-3.180	2.329	0.382	H	-1.976	4.784	0.006
C	-0.560	-2.529	-0.233	H	-1.763	-5.687	-0.594	C	0.131	1.187	-0.815	H	-5.564	0.691	0.749	C	-5.308	0.308	-1.361	H	-3.372	4.994	1.046
C	-0.583	-3.921	-0.310	H	-3.859	-4.382	-0.903	C	1.425	1.954	-0.685	H	-4.055	0.700	2.832	C	-3.243	-1.311	2.811	H	-6.605	-0.415	-3.748
C	-1.757	-4.607	-0.536	H	2.537	-1.306	1.471	C	1.834	2.563	0.499	H	-2.306	0.630	2.833	C	-2.308	3.136	1.367	H	-8.244	-0.017	-3.239
C	-2.923	-3.876	-0.701	H	4.841	-0.664	2.081	C	3.028	3.263	0.553	H	-2.865	2.492	-0.648	C	-6.798	-0.016	-1.617	H	-7.029	1.251	-3.371
O	0.695	-1.936	0.053	H	6.044	-1.105	-2.011	C	3.830	3.366	-0.573	H	-5.109	1.342	-1.630	C	-3.242	-1.480	4.348	H	-4.181	-3.444	4.390
C	1.589	-1.977	-1.022	H	3.730	-1.750	-2.609	C	3.428	2.772	-1.761	H	-4.688	-0.309	-2.006	C	-2.341	4.643	1.021	H	-2.422	-3.494	4.381
O	1.261	-2.298	-2.151	H	1.219	2.501	1.386	C	2.233	2.076	-1.818	H	-4.132	-1.784	2.400	C	-7.194	0.216	-3.088	H	-3.281	-3.048	5.850
C	2.991	-1.567	-0.609	H	3.332	3.733	1.480	O	-0.362	1.250	-2.092	H	-2.378	-1.825	2.397	C	-3.285	-2.961	4.768	H	-0.452	5.167	1.966
C	3.307	-1.263	0.711	H	4.764	3.913	-0.527	C	-1.697	0.696	-2.305	H	-2.666	2.999	2.385	C	-1.491	5.481	1.995	H	-1.536	6.532	1.727
C	4.600	-0.902	1.053	H	4.047	2.852	-2.645	O	-2.633	1.496	-2.355	H	-1.280	2.787	1.334	Br	7.345	-0.352	0.537	H	-1.852	5.373	3.013
C	5.590	-0.843	0.074	H	1.912	1.617	-2.744	C	-1.578	-0.546	-3.237	H	-6.993	-1.053	-1.349	C	-0.001	0.303	1.469				
C	5.277	-1.149	-1.249	H	-0.773	-1.201	-2.925	P	-3.198	0.493	0.589	H	-7.418	0.605	-0.973	N	0.344	0.160	2.564				
C	3.983	-1.509	-1.584	H	-1.373	-0.197	-4.246	C	-4.934	0.070	0.118	H	-2.348	-1.013	4.756	H	-4.208	2.666	0.468				

(g) Intermediate **2**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *i*Pr

C	-1.982	-1.777	3.340	H	1.178	-4.013	3.650	C	-0.945	-0.407	1.468	H	-2.156	5.075	-2.888	P	-2.021	-0.723	0.045	H	-5.092	-1.385	-0.192
C	-0.887	-1.515	2.477	H	-0.806	-4.446	5.136	C	-0.171	0.803	1.676	H	-4.496	4.574	-2.008	C	-2.491	-2.556	0.097	H	-2.288	-5.211	-0.580
C	0.230	-2.376	2.631	H	-2.831	-2.981	4.926	C	-0.188	2.052	1.067	H	-4.072	5.141	-0.373	C	-1.105	-0.395	-1.581	H	-3.997	-4.832	-0.359
C	0.278	-3.410	3.574	H	3.437	-0.858	1.802	C	0.740	3.188	1.280	H	-4.733	3.516	-0.597	C	-3.666	0.253	0.044	H	-0.469	1.098	-3.822
C	-0.834	-3.645	4.402	H	5.616	-0.093	0.851	C	1.033	3.701	2.567	H	-1.622	-3.062	0.524	C	-2.837	-3.222	-1.252	H	-0.355	-0.612	-4.233
C	-1.971	-2.824	4.280	H	4.710	-2.136	-2.860	C	1.912	4.785	2.727	H	-3.322	-2.659	0.805	C	-1.958	-0.144	-2.842	H	-6.349	0.664	0.571
O	1.432	-2.149	1.897	H	2.524	-2.890	-1.894	C	2.506	5.397	1.606	H	-0.474	0.476	-1.381	C	-4.887	-0.401	-0.637	H	-5.972	1.458	-0.957
C	1.539	-2.391	0.542	H	0.557	3.265	3.439	C	2.210	4.909	0.318	H	-0.450	-1.264	-1.711	C	-3.152	-4.724	-1.056	H	-2.640	-5.374	-3.085
O	0.651	-2.951	-0.132	H	2.121	5.160	3.726	C	1.339	3.819	0.159	H	-3.875	0.436	1.105	C	-1.069	0.206	-4.059	H	-3.701	-6.500	-2.217
C	2.848	-1.927	0.012	H	3.182	6.239	1.733	O	-1.133	2.271	-0.014	H	-3.449	1.223	-0.408	C	-6.155	0.475	-0.496	H	-4.359	-4.986	-2.869
C	3.722	-1.138	0.793	H	2.667	5.368	-0.556	C	-2.022	3.363	0.113	H	-3.698	-2.739	-1.733	C	-3.483	-5.437	-2.383	H	-2.477	-0.428	-5.615
C	4.947	-0.706	0.257	H	1.139	3.431	-0.838	O	-2.219	3.946	1.183	H	-1.984	-3.131	-1.938	C	-1.889	0.458	-5.341	H	-2.588	1.295	-5.207
C	5.287	-1.074	-1.056	H	-2.642	2.846	-1.865	C	-2.638	3.741	-1.230	H	-2.564	-1.026	-3.088	C	-7.397	-0.174	-1.140	H	-1.235	0.701	-6.188
C	4.429	-1.860	-1.848	H	-0.716	4.432	-2.065	C	-1.734	4.806	-1.912	H	-2.659	0.686	-2.668	Br	7.001	-0.475	-1.810	H	-7.626	-1.141	-0.672
C	3.206	-2.282	-1.307	H	-1.677	5.712	-1.297	C	-4.074	4.273	-1.040	H	-4.689	-0.569	-1.705	C	0.836	0.681	2.718	H	-8.281	0.468	-1.031
N	1.652	0.559	3.565	H	-7.241	-0.350	-2.213	H	-2.845	-1.117	3.281												

(g) Intermediate **6**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *i*Pr

C	2.535	-0.572	-3.034	H	1.919	-4.444	-2.912	C	0.880	-0.461	-0.941	H	3.628	-0.512	3.224	P	-0.868	1.420	-0.632	H	3.702	0.990	6.695
C	1.682	-1.118	-2.055	H	3.458	-3.456	-4.639	C	-0.032	0.669	-1.417	H	3.789	1.222	2.912	C	-1.808	2.469	-1.108	H	4.566	-4.991	0.699
C	1.472	-2.518	-2.039	H	3.822	-0.985	-4.721	C	2.174	0.104	0.527	H	3.634	-2.282	1.945	C	-1.361	3.561	-1.882	H	6.310	-4.797	0.979
C	2.109	-3.376	-2.956	H	-1.256	-2.182	2.049	C	2.654	1.919	0.131	H	3.070	-2.875	0.407	C	-2.271	4.533	-2.326	H	5.149	-4.371	2.254
C	2.963	-2.811	-3.916	H	-3.752	-2.467	2.257	C	1.824	0.388	2.388	H	2.954	4.440	-0.920	C	-3.638	4.423	-2.006	H	-0.307	3.658	-2.124
C	3.175	-1.414	-3.960	H	-4.126	-1.883	-2.015	C	3.806	-0.831	0.324	H	4.553	3.874	-0.439	C	-4.090	3.333	-1.236	H	-1.916	5.373	-2.917
O	0.586	-2.956	-1.098	H	-1.665	-1.652	-2.198	C	3.264	2.309	-1.227	H	2.216	1.717	4.801	C	-3.180	2.364	-0.783	H	-4.342	5.174	-2.354
C	0.220	-1.731	-0.130	H	1.752	2.519	0.313	C	3.094	0.446	3.267	H	2.028	-0.012	5.105	C	-0.966	1.067	0.731	H	-5.146	3.234	-0.997
O	0.876	-1.835	1.030	H	3.363	2.180	0.929	C	3.857	-2.273	0.870	H	5.451	-2.920	-0.459	C	-1.060	2.055	1.753	H	-3.537	1.511	-0.213
C	-1.301	-1.853	-0.066	H	1.294	1.343	2.462	O	3.777	3.770	-1.213	H	6.029	-2.295	1.088	C	-0.655	3.206	1.574	H	-1.265	0.450	3.113
C	-1.903	-2.100	1.180	H	1.166	-0.427	2.690	C	2.736	0.748	4.742	H	3.579	4.153	-3.363	C	-1.668	1.465	3.013	H	-3.464	0.656	2.022
C	-3.296	-2.261	1.293	H	4.025	-0.831	-0.750	O	5.243	-2.911	0.622	H	4.704	5.250	-2.539	C	-3.209	1.340	2.837	H	-3.664	2.320	2.644
C	-4.084	-2.163	0.136	H	4.565	-0.202	0.811	C	4.345	4.214	-2.577	H	5.187	3.577	-2.882	C	-1.303	2.315	4.245	H	-3.641	0.941	3.762
C	-3.508	-1.934	-1.124	H	4.098	1.643	-1.491	C	3.979	0.775	5.655	H	4.500	-0.191	5.639	Br	-6.045	-2.372	0.280	H	-1.745	1.870	5.144
C	-2.112	-1.788	-1.217	H	2.511	2.216	-2.020	C	5.324	-4.351	1.170	H	4.691	1.546	5.331	C	-0.115	0.903	-2.836	H	-1.682	3.338	4.140
N	-0.178	1.084	-4.004	H	-0.218	2.374	4.391	H	2.695	0.496	-3.106												

(g) Intermediate **8**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *i*Pr

C	-2.497	-2.702	-0.656	H	0.882	-4.517	-0.234	C	-1.534	-0.372	-0.538	H	0.280	-0.831	-4.299	P	-3.082	0.145	0.774	H	-1.693	2.879	1.500
C	-1.334	-1.901	-0.487	H	-1.205	-5.856	-0.433	C	-0.421	0.566	-0.170	H	-1.907	-0.056	-5.383	C	-4.772	-0.737	0.921	H	-7.025	-2.247	0.362
C	-0.111	-2.610	-0.379	H	-3.394	-4.659	-0.784	C	-0.387	1.763	-0.937	H	-2.040	1.396	-4.358	C	-2.443	-0.070	2.548	H	-7.540	-0.729	1.099
C	-0.077	-4.019	-0.339	H	2.767	-0.943	1.268	C	0.610	2.867	-0.772	H	-3.356	0.206	-4.377	C	-3.459	1.997	0.567	H	-0.695	-0.900	4.516
C	-1.249	-4.771	-0.460	H	4.982	-0.068	1.982	C	1.911	2.673	-0.253	H	-4.569	-1.802	1.078	C	-5.803	-0.535	-0.205	H	-2.349	-1.124	5.101
C	-2.473	-4.100	-0.644	H	6.734	-1.442	-1.734	C	2.809	3.751	-0.166	H	-5.172	-0.347	1.870	C	-2.086	-1.511	2.973	H	-2.913	4.683	0.253
O	1.136	-1.938	-0.257	H	4.506	-2.347	-2.432	C	2.422	5.036	-0.592	H	-3.244	0.321	3.191	C	-2.785	2.960	1.568	H	-4.292	4.515	1.341
C	2.213	-2.286	-1.098	H	2.236	1.689	0.062	C	1.132	5.235	-1.124	H	-1.572	0.576	2.683	C	-7.163	-1.172	0.164	H	-7.877	-1.448	-1.890
O	2.074	-2.997	-2.104	H	3.809	3.586	0.227	C	0.238	4.158	-1.220	H	-4.552	2.081	0.637	C	-1.580	-1.546	4.434	H	-9.173	-1.445	-0.676
C	3.496	-1.704	-0.632	H	3.120	5.868	-0.522	O	-1.300	1.915	-1.860	H	-3.180	2.241	-0.460	C	-3.196	4.424	1.283	H	-8.393	0.078	-1.150
C	3.628	-1.060	0.618	H	0.831	6.222	-1.468	C	-2.216	-0.004	-1.921	H	-5.943	0.535	-0.405	C	-8.214	-0.987	-0.952	H	-2.092	-3.641	4.848
C	4.878	-0.560	1.020	H	-0.748	4.289	-1.657	O	-3.474	0.163	-1.875	H	-5.430	-0.959	-1.143	C	-1.221	-2.973	4.898	H	-0.431	-3.402	4.267
C	5.983	-0.703	0.164	H	-1.843	-1.494	-3.345	C	-1.575	-0.425	-3.262	H	-2.957	-2.176	2.875	C	-2.540	5.419	2.263	H	-0.858	-2.972	5.934
C	5.871	-1.340	-1.085	H	0.480	-0.791	-2.548	C	-0.042	-0.321	-3.383	H	-1.299	-1.912	2.324	Br	7.731	0.003	0.725	H	-1.445	5.372	2.195
C	4.622	-1.844	-1.477	H	0.269	0.726	-3.445	C	-2.269	0.327	-4.420	H	-3.061	2.710	2.602	C	0.333	0.374	1.010	H	-2.847	6.450	2.045
N	0.917	0.212	2.035	H	-2.822	5.197	3.302	H	-3.441	-2.201	-0.839												

(g) Transition state in path **a**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *i*Pr

C	-2.608	-2.879	1.629	C	0.964	0.041	1.554	C	-2.066	2.606	-1.527	H	1.991	-2.961	-0.204	H	-4.926	0.962	-1.203	H	-6.319	2.523	2.685
C	-1.658	-2.631	0.619	C	2.055	0.169	2.555	C	-5.756	-0.761	-2.225	H	4.351	-2.223	-0.466	H	-3.970	0.405	-2.585	H	-5.625	3.670	3.846
C	-1.292	-3.701	-0.228	C	1.820	-0.046	3.931	C	-4.131	2.438	2.821	H	3.143	0.502	-3.605	H	-3.914	2.524	0.667	H	-1.838	5.405	-1.962
C	-1.854	-4.980	-0.103	C	2.864	0.079	4.862	C	-1.577	3.384	-2.773	H	0.769	-0.249	-3.314	H	-4.709	1.060	1.250	H	-1.790	5.342	-3.735
C	-2.807	-5.200	0.908	C	4.159	0.430	4.433	C	-6.658	0.043	-3.184	H	0.820	-0.297	4.273	H	-3.162	2.553	-1.566	H	-3.242	4.806	-2.868
C	-3.187	-4.153	1.774	C	4.401	0.651	3.064	C	-5.472	3.199	2.867	H	2.666	-0.089	5.918	H	-1.809	3.176	-0.622	H	3.046	2.275	-0.636
O	-0.295	-3.441	-1.154	C	3.358	0.524	2.132	C	-2.144	4.817	-2.838	H	4.966	0.527	5.155	H	-5.383	-1.661	-2.735	H	3.403	3.460	0.647
C	-0.231	-2.014	-1.569	O	0.865	1.127	0.624	Br	5.753	-0.211	-2.246	H	5.401	0.909	2.721	H	-6.349	-1.110	-1.366	H	3.121	4.008	-1.018
O	-1.123	-1.608	-2.388	C	0.849	2.462	1.096	C	0.514	-2.205	2.182	H	3.560	0.665	1.074	H	-4.113	1.674	3.613	H	1.229	5.574	-0.385
C	1.214	-1.613	-1.709	O	0.492	2.742	2.246	N	0.802	-3.152	2.829	H	0.766	3.164	-0.904	H	-3.304	3.130	3.038	H	1.455	5.175	1.334
C	2.234	-2.184	-0.920	C	1.294	3.439	0.019	C	2.814	3.277	-0.260	H	-3.296	-1.663	-1.329	H	-0.477	3.423	-2.776	H	-0.141	5.001	0.594
C	3.571	-1.779	-1.076	P	-2.092	0.038	-0.129	C	0.934	4.885	0.415	H	-4.229	-1.135	0.084	H	-1.866	2.830	-3.678	H	-1.623	0.640	-2.407
C	3.879	-0.799	-2.033	C	-3.660	-0.786	-0.785	H	-2.881	-2.087	2.325	H	-2.512	0.272	2.246	H	-6.098	0.366	-4.073	H	-5.505	3.990	2.106
C	2.886	-0.232	-2.848	C	-2.532	1.013	1.437	H	-1.541	-5.771	-0.777	H	-1.709	1.706	1.640	H	-7.507	-0.562	-3.527	H	-3.912	-4.335	2.563
C	1.554	-0.647	-2.678	C	-1.448	1.193	-1.480	H	-3.248	-6.187	1.024	H	-0.367	1.239	-1.339	H	-7.060	0.940	-2.695	C	-3.884	1.759	1.453
C	-0.905	-1.342	0.359	C	-4.550	0.066	-1.716	C	0.159	-1.062	1.362												

(g) Transition state in path **b**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *i*Pr

C	-2.805	-2.582	-0.383	C	-0.392	0.449	0.205	C	-5.415	0.134	-0.663	H	-3.786	-4.468	-0.704	H	-5.288	1.185	-0.947	H	-2.222	-3.342	6.186
C	-1.600	-1.820	-0.233	C	0.011	1.401	-0.713	C	-2.701	-1.506	3.219	H	2.708	-1.704	1.383	H	-4.873	-0.436	-1.426	H	-0.380	5.104	2.617
C	-0.415	-2.605	-0.351	C	1.148	2.357	-0.635	C	-2.168	3.046	1.878	H	5.042	-1.179	2.091	H	-3.619	-2.030	2.912	H	-1.500	6.464	2.408
C	-0.422	-3.991	-0.575	C	2.302	2.120	0.149	C	-6.915	-0.241	-0.700	H	6.190	-0.711	-2.060	H	-1.872	-1.969	2.669	H	-1.819	5.235	3.648
C	-1.628	-4.693	-0.696	C	3.345	3.060	0.183	C	-2.479	-1.720	4.734	H	3.843	-1.253	-2.754	H	-2.526	2.853	2.900	H	0.052	0.918	-4.165
C	-2.829	-3.963	-0.597	C	3.260	4.249	-0.565	C	-2.245	4.566	1.602	H	2.404	1.207	0.722	H	-1.118	2.731	1.844	H	-1.539	1.054	-4.953
O	0.883	-2.030	-0.137	C	2.120	4.489	-1.359	C	-7.541	0.002	-2.089	H	4.226	2.857	0.786	H	-7.038	-1.299	-0.421	H	-0.553	-0.412	-5.175
C	1.759	-1.846	-1.202	C	1.078	3.550	-1.399	C	-2.388	-3.213	5.109	H	4.070	4.974	-0.537	H	-7.460	0.346	0.056	H	-2.443	-1.870	-4.430
O	1.417	-1.953	-2.392	O	-0.728	1.594	-1.851	C	-1.440	5.390	2.628	H	2.047	5.400	-1.947	H	-1.552	-1.209	5.033	H	-3.510	-0.478	-4.114
C	3.132	-1.515	-0.733	C	-1.921	0.765	-2.225	Br	7.588	-0.495	0.611	H	0.206	3.723	-2.020	H	-3.299	-1.247	5.297	H	-3.195	-1.678	-2.839
C	3.468	-1.495	0.639	O	-3.016	1.357	-2.200	C	0.281	0.273	1.456	H	-0.778	-0.978	-2.771	H	-1.866	4.767	0.590	H	-1.630	-5.765	-0.866
C	4.782	-1.196	1.037	C	-1.519	-0.316	-3.230	N	0.746	0.057	2.528	H	-4.931	-1.168	1.031	H	-3.298	4.888	1.614	H	-2.704	2.472	-0.175
C	5.748	-0.916	0.055	P	-3.002	0.369	1.016	C	-0.845	0.363	-4.457	H	-5.353	0.481	1.483	H	-7.033	-0.595	-2.858	H	-1.557	-3.699	4.580
C	5.432	-0.930	-1.315	C	-4.815	-0.120	0.734	C	-2.748	-1.133	-3.675	H	-3.630	0.472	3.386	H	-8.605	-0.270	-2.099	H	-3.311	-3.747	4.844
C	4.118	-1.232	-1.704	C	-2.784	-0.005	2.870	H	-3.752	-2.060	-0.373	H	-1.867	0.496	3.196	H	-7.458	1.057	-2.380	H	-4.064	2.551	0.935
C	-1.642	-0.352	-0.055	C	-3.009	2.255	0.853	H	0.532	-4.508	-0.639												

(h) Intermediate **2**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *t*Bu

C	-1.835	-1.826	3.368	H	1.408	-3.927	3.758	C	-0.851	-0.485	1.447	H	-4.551	4.557	-1.978	C	-2.066	3.327	-2.438	H	-2.687	0.166	-2.794
C	-0.750	-1.554	2.496	H	-0.560	-4.385	5.255	C	-0.157	0.774	1.643	H	-4.609	4.265	-0.222	P	-1.912	-0.893	0.038	H	-4.661	-0.973	-1.633
C	0.400	-2.364	2.682	H	-2.638	-3.005	4.997	C	-0.235	2.016	1.026	H	-4.588	2.896	-1.355	C	-2.298	-2.742	0.173	H	-4.923	-1.699	-0.046
C	0.485	-3.363	3.659	H	3.537	-0.731	1.818	C	0.604	3.214	1.276	H	-2.419	3.922	-3.291	C	-1.013	-0.579	-1.601	H	-2.029	-5.425	-0.356
C	-0.618	-3.611	4.494	H	5.681	0.108	0.852	C	0.824	3.735	2.575	H	-2.387	2.292	-2.594	C	-3.586	0.030	-0.015	H	-3.746	-5.078	-0.142
C	-1.785	-2.838	4.344	H	4.896	-2.092	-2.795	C	1.614	4.881	2.767	H	-0.972	3.345	-2.435	C	-2.633	-3.491	-1.134	H	-0.553	0.800	-3.959
O	1.595	-2.111	1.945	H	2.743	-2.921	-1.815	C	2.188	5.548	1.667	H	-1.399	-3.186	0.606	C	-1.866	-0.560	-2.887	H	-0.183	-0.904	-4.218
C	1.721	-2.393	0.600	H	0.364	3.253	3.431	C	1.962	5.053	0.368	H	-3.110	-2.849	0.901	C	-4.805	-0.739	-0.569	H	-6.261	0.308	0.659
O	0.867	-3.021	-0.058	H	1.769	5.260	3.775	C	1.179	3.903	0.175	H	-0.513	0.386	-1.468	C	-2.908	-4.987	-0.851	H	-6.017	1.035	-0.926
C	3.010	-1.883	0.061	H	2.797	6.436	1.820	O	-1.159	2.220	-0.080	H	-0.244	-1.358	-1.649	C	-1.012	-0.186	-4.121	H	-2.395	-5.733	-2.846
C	3.840	-1.028	0.820	H	2.405	5.555	-0.491	C	-2.177	3.181	0.136	H	-3.766	0.338	1.022	C	-6.114	0.071	-0.405	H	-3.420	-6.837	-1.910
C	5.045	-0.555	0.275	H	1.030	3.514	-0.829	O	-2.604	3.432	1.268	H	-3.418	0.945	-0.590	C	-3.230	-5.780	-2.134	H	-4.122	-5.378	-2.635
C	5.410	-0.948	-1.024	H	-1.063	5.441	-0.883	C	-2.645	3.916	-1.134	H	-3.509	-3.059	-1.636	C	-1.833	-0.166	-5.428	H	-2.282	-1.149	-5.629
C	4.597	-1.798	-1.794	H	-2.586	5.838	-0.064	C	-2.155	5.389	-0.964	H	-1.786	-3.417	-1.827	C	-7.347	-0.685	-0.943	H	-2.647	0.569	-5.371
C	3.392	-2.262	-1.245	H	-2.467	5.976	-1.838	C	-4.196	3.905	-1.171	H	-2.330	-1.539	-3.063	Br	7.099	-0.290	-1.789	H	-1.204	0.097	-6.287
N	1.672	0.648	3.540	H	-8.261	-0.091	-0.817	H	-2.721	-1.201	3.285	H	-7.238	-0.909	-2.013	C	0.852	0.719	2.691	H	-7.490	-1.637	-0.414

(h) Intermediate **6**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *t*Bu

C	-0.481	-1.981	2.895	H	0.237	-5.058	0.567	C	-0.596	0.789	1.425	H	-5.066	0.692	-1.082	C	-1.231	3.843	2.227	H	-2.318	-3.085	-6.275
C	-0.421	-1.808	1.498	H	0.083	-5.357	3.052	C	-2.394	-0.647	-0.311	H	-2.279	-0.562	-3.435	C	-1.244	5.074	2.901	H	-2.170	-1.352	-5.912
C	-0.152	-2.932	0.643	H	-0.341	-3.388	4.532	C	-3.685	-1.155	0.984	H	-0.985	-1.670	-3.000	C	-0.035	5.718	3.229	H	-2.172	3.371	1.964
C	0.026	-4.217	1.222	H	2.096	-1.323	-2.469	C	-2.918	1.084	-0.857	H	-4.644	-2.435	3.243	C	1.191	5.126	2.867	H	-2.193	5.531	3.166
C	-0.057	-4.371	2.612	H	4.540	-1.816	-2.306	C	-2.713	-1.865	-1.729	H	-5.897	-2.462	2.000	C	1.207	3.901	2.181	H	-0.048	6.669	3.756
C	-0.301	-3.260	3.454	H	4.382	-1.033	1.947	C	-3.871	-2.671	1.227	H	-4.728	3.179	-1.089	C	1.038	1.980	0.095	H	2.129	5.616	3.119
O	-0.077	-2.669	-0.666	H	1.965	-0.552	1.773	C	-4.239	1.138	-1.656	H	-3.784	3.055	-2.571	C	0.794	2.812	-1.037	H	2.152	3.444	1.904
C	0.394	-0.606	-0.568	H	-3.429	-0.661	1.925	C	-2.069	-1.587	-3.097	H	-2.370	-3.616	-3.815	C	-0.337	3.262	-1.241	H	3.316	1.477	-1.087
O	-0.010	-0.072	-1.650	H	-4.632	-0.716	0.638	O	-4.947	-2.928	2.308	H	-3.685	-2.514	-4.239	C	2.026	3.057	-1.910	H	3.528	3.054	-0.304
C	1.857	-0.897	-0.370	H	-3.009	1.690	0.053	C	-4.614	2.596	-2.015	H	-4.240	-4.913	2.899	C	3.335	2.555	-1.262	H	4.174	2.781	-1.934
C	2.605	-1.251	-1.513	H	-2.088	1.494	-1.438	O	-2.589	-2.592	-4.152	H	-5.929	-4.594	3.341	C	2.106	4.592	-2.154	H	2.927	4.802	-2.850
C	3.977	-1.531	-1.423	H	-2.375	-2.836	-1.359	C	-5.169	-4.432	2.566	H	-5.504	-4.946	1.654	C	1.771	2.329	-3.265	H	2.300	5.137	-1.222
C	4.605	-1.446	-0.168	H	-3.812	-1.878	-1.813	C	-5.912	2.684	-2.843	H	-5.813	2.139	-3.792	Br	6.534	-1.834	-0.025	H	1.174	4.970	-2.587
C	3.887	-1.094	0.983	H	-4.173	-3.177	0.300	C	-1.948	-2.361	-5.537	H	-6.763	2.254	-2.296	C	-1.462	0.864	2.576	H	2.640	2.478	-3.919
C	2.510	-0.823	0.876	H	-2.927	-3.124	1.550	C	0.071	1.952	1.121	H	-6.159	3.726	-3.081	N	-2.201	0.925	3.499	H	0.884	2.737	-3.761
C	-0.579	-0.550	0.665	H	-4.144	0.558	-2.584	P	-0.006	3.240	1.866	H	-0.856	-2.463	-5.482	H	-0.659	-1.150	3.566	H	1.613	1.257	-3.112

(h) Intermediate **8**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *t*Bu

C	-2.443	-2.710	-0.202	H	-1.428	-2.734	-2.934	C	-0.383	0.573	-0.115	H	-1.613	0.174	-5.272	C	-4.786	-0.623	1.077	H	-1.849	3.144	1.071
C	-1.279	-1.895	-0.198	H	0.957	-4.461	0.304	C	-0.348	1.778	-0.887	H	-1.746	1.472	-4.051	C	-2.465	0.339	2.582	H	-6.985	-2.267	0.779
C	-0.048	-2.588	-0.050	H	-1.131	-5.810	0.380	C	0.703	2.837	-0.731	H	-3.114	0.373	-4.331	C	-3.592	2.049	0.341	H	-7.568	-0.639	1.126
C	-0.007	-3.980	0.175	H	-3.338	-4.664	-0.024	C	2.027	2.560	-0.323	H	-1.538	-2.193	-4.617	C	-5.770	-0.690	-0.105	H	-0.635	-0.228	4.586
C	-1.180	-4.738	0.209	H	2.849	-0.790	1.333	C	2.979	3.592	-0.248	H	-2.969	-2.091	-3.566	C	-2.127	-1.019	3.234	H	-2.269	-0.248	5.266
C	-2.413	-4.094	-0.005	H	5.077	0.141	1.927	C	2.622	4.914	-0.577	H	-4.567	-1.626	1.461	C	-2.942	3.181	1.165	H	-3.210	4.671	-0.390
O	1.199	-1.909	-0.066	H	6.784	-1.646	-1.631	C	1.306	5.196	-0.998	H	-5.236	-0.055	1.907	C	-7.135	-1.271	0.334	H	-4.533	4.615	0.776
C	2.261	-2.374	-0.865	H	4.542	-2.602	-2.208	C	0.359	4.164	-1.082	H	-3.250	0.845	3.161	C	-1.554	-0.825	4.657	H	-7.738	-2.029	-1.631
O	2.103	-3.199	-1.777	H	2.326	1.545	-0.086	O	-1.267	1.971	-1.781	H	-1.583	0.984	2.595	C	-3.437	4.565	0.681	H	-9.094	-1.790	-0.510
C	3.555	-1.755	-0.481	H	3.997	3.363	0.058	C	-2.150	-0.198	-1.864	H	-4.685	2.091	0.444	C	-8.131	-1.378	-0.840	H	-8.322	-0.392	-1.285
C	3.702	-0.980	0.690	H	3.360	5.710	-0.517	O	-3.406	-0.090	-1.860	H	-3.350	2.160	-0.717	C	-1.248	-2.166	5.356	H	-2.155	-2.779	5.457
C	4.961	-0.450	1.025	H	1.027	6.213	-1.266	C	-1.451	-0.528	-3.217	H	-5.919	0.308	-0.536	C	-2.794	5.727	1.466	H	-0.512	-2.745	4.783
C	6.056	-0.697	0.181	H	-0.649	4.361	-1.435	C	0.091	-0.447	-3.218	H	-5.353	-1.297	-0.917	Br	7.815	0.049	0.646	H	-0.838	-2.003	6.361
C	5.927	-1.466	-0.991	H	0.541	-1.076	-2.448	C	-2.022	0.441	-4.288	H	-3.023	-1.656	3.289	C	0.368	0.418	1.074	H	-1.701	5.714	1.360
C	4.670	-1.997	-1.315	H	0.438	0.580	-3.088	C	-1.878	-1.985	-3.595	H	-1.385	-1.557	2.632	N	0.949	0.299	2.106	H	-3.157	6.698	1.105
C	-1.472	-0.384	-0.448	H	0.459	-0.808	-4.188	P	-3.114	0.263	0.800	H	-3.174	3.075	2.234	H	-3.397	-2.240	-0.409	H	-3.028	5.659	2.538

(h) Transition state in path **a**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *t*Bu

C	-2.635	-2.737	1.897	H	-1.671	-5.824	-0.300	C	0.132	-0.967	1.423	H	0.349	5.140	0.705	C	-3.705	-0.885	-0.707	H	-2.010	3.102	-0.871
C	-1.707	-2.582	0.848	H	-3.339	-6.071	1.567	C	0.964	0.128	1.524	H	-0.123	4.450	-0.865	C	-2.601	1.081	1.383	H	-5.387	-1.962	-2.587
C	-1.378	-3.722	0.079	H	-3.936	-4.094	2.973	C	2.060	0.293	2.517	H	2.699	3.620	-1.845	C	-1.511	1.078	-1.533	H	-6.371	-1.334	-1.265
C	-1.956	-4.978	0.318	H	1.895	-3.074	0.014	C	1.804	0.288	3.906	H	1.303	2.527	-1.906	C	-4.609	-0.136	-1.709	H	-4.229	1.847	3.493
C	-2.886	-5.104	1.364	H	4.278	-2.454	-0.328	C	2.855	0.443	4.825	H	2.787	2.006	-1.106	C	-3.948	1.835	1.336	H	-3.382	3.263	2.874
C	-3.229	-3.987	2.155	H	3.138	0.054	-3.669	C	4.177	0.612	4.369	H	-3.325	-1.798	-1.176	C	-2.216	2.438	-1.723	H	-0.669	3.257	-3.022
O	-0.402	-3.557	-0.889	H	0.740	-0.578	-3.297	C	4.441	0.625	2.985	H	-4.269	-1.170	0.188	C	-5.788	-1.036	-2.150	H	-1.987	2.469	-3.882
C	-0.303	-2.170	-1.415	H	0.785	0.171	4.262	C	3.390	0.471	2.065	H	-2.600	0.388	2.234	C	-4.216	2.576	2.669	H	-6.162	-0.066	-4.078
O	-1.187	-1.805	-2.261	H	2.644	0.435	5.891	O	0.939	1.159	0.525	H	-1.772	1.775	1.555	C	-1.761	3.129	-3.031	H	-7.541	-0.998	-3.465
C	1.153	-1.827	-1.593	H	4.990	0.729	5.082	C	0.885	2.511	0.944	H	-0.441	1.208	-1.356	C	-6.713	-0.340	-3.169	H	-7.148	0.578	-2.749
C	2.159	-2.368	-0.766	H	5.460	0.741	2.625	O	0.280	2.831	1.975	H	-1.615	0.437	-2.413	C	-5.544	3.360	2.650	H	-5.544	4.119	1.857
C	3.509	-2.030	-0.967	H	3.600	0.454	0.999	C	1.646	3.496	0.043	H	-5.012	0.789	-1.274	C	-2.440	4.497	-3.244	H	-6.398	2.690	2.474
C	3.842	-1.146	-2.004	H	3.543	3.140	1.129	C	2.874	3.972	0.884	H	-4.031	0.144	-2.600	Br	5.736	-0.653	-2.282	H	-5.713	3.873	3.605
C	2.862	-0.609	-2.854	H	2.548	4.440	1.819	C	0.730	4.720	-0.232	H	-3.956	2.566	0.518	C	0.477	-2.035	2.345	H	-2.203	5.191	-2.425
C	1.517	-0.956	-2.639	H	3.440	4.707	0.299	C	2.135	2.867	-1.279	H	-4.774	1.134	1.148	N	0.757	-2.921	3.077	H	-2.110	4.961	-4.182
C	-0.949	-1.326	0.465	H	1.306	5.494	-0.753	P	-2.149	0.009	-0.114	H	-3.305	2.311	-1.765	H	-2.880	-1.890	2.536	H	-3.533	4.393	-3.289

(h) Transition state in path **b**; FG = CN**; R^1, R^2, R^3** = 4-BrC$_6$H$_4$, Ph, *t*Bu

C	-2.683	-2.512	-0.703	H	0.674	-4.352	-1.197	C	-0.370	0.532	0.139	H	-4.335	0.126	-3.309	C	-4.653	-0.481	1.092	H	-0.992	2.340	2.408
C	-1.488	-1.753	-0.488	H	-1.463	-5.612	-1.497	C	-0.116	1.625	-0.667	H	-3.329	-1.298	-2.929	C	-2.370	-0.665	2.927	H	-7.024	-1.503	0.114
C	-0.289	-2.494	-0.703	H	-3.640	-4.374	-1.201	C	0.991	2.611	-0.568	H	-0.756	-1.107	-2.953	C	-2.956	1.952	1.526	H	-7.382	0.004	0.958
C	-0.280	-3.854	-1.055	H	2.740	-1.503	1.175	C	2.270	2.270	-0.071	H	-0.863	-0.604	-4.639	C	-5.482	0.021	-0.106	H	-0.870	-2.191	4.673
C	-1.477	-4.561	-1.224	H	5.014	-0.901	1.988	C	3.289	3.234	-0.009	H	0.006	0.408	-3.474	C	-2.199	-2.199	2.958	H	-2.575	-2.376	5.096
C	-2.690	-3.866	-1.049	H	6.458	-0.834	-2.096	C	3.051	4.552	-0.445	H	-4.663	-1.574	1.146	C	-2.047	2.552	2.619	H	-1.993	4.540	1.744
O	0.989	-1.886	-0.472	H	4.169	-1.463	-2.898	C	1.783	4.897	-0.955	H	-5.099	-0.112	2.028	C	-6.962	-0.407	0.026	H	-3.302	4.308	2.903
C	1.980	-1.914	-1.457	H	2.483	1.257	0.249	C	0.764	3.934	-1.023	H	-3.158	-0.351	3.627	C	-1.805	-2.686	4.372	H	-7.438	-0.363	-2.112
O	1.763	-2.237	-2.636	H	4.269	2.954	0.369	O	-0.965	1.920	-1.696	H	-1.437	-0.188	3.240	C	-2.241	4.084	2.714	H	-8.862	-0.245	-1.059
C	3.310	-1.520	-0.918	H	3.843	5.295	-0.396	C	-2.253	1.189	-1.942	H	-4.010	2.142	1.774	C	-7.814	0.062	-1.172	H	-7.791	1.155	-1.268
C	3.548	-1.365	0.466	H	1.593	5.910	-1.301	O	-3.291	1.726	-1.499	H	-2.781	2.414	0.552	C	-1.624	-4.217	4.436	H	-2.552	-4.738	4.163
C	4.831	-1.021	0.925	H	-0.209	4.190	-1.431	C	-2.181	0.525	-3.340	H	-5.416	1.112	-0.189	C	-1.373	4.719	3.820	H	-0.839	-4.547	3.743
C	5.865	-0.831	-0.008	H	-1.441	2.414	-4.218	C	-2.283	1.724	-4.342	H	-5.071	-0.366	-1.046	Br	7.660	-0.342	0.633	H	-1.340	-4.541	5.446
C	5.648	-0.983	-1.389	H	-3.217	2.278	-4.195	C	-3.403	-0.399	-3.547	H	-3.126	-2.705	2.649	C	0.429	0.267	1.297	H	-0.306	4.532	3.639
C	4.365	-1.332	-1.838	H	-2.263	1.333	-5.368	C	-0.868	-0.239	-3.603	H	-1.420	-2.502	2.248	N	1.002	-0.022	2.297	H	-1.521	5.806	3.865
C	-1.588	-0.312	-0.128	H	-3.444	-0.717	-4.597	P	-2.844	0.082	1.240	H	-2.270	2.106	3.599	H	-3.633	-1.998	-0.642	H	-1.623	4.305	4.807

(i) Intermediate **2**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-$NO_2C_6H_4$, Ph, *t*Bu

C	1.170	-1.774	-3.444	H	1.757	-4.074	-5.384	C	0.195	2.070	-0.822	H	3.322	3.520	2.909
C	0.169	-1.443	-2.494	H	-3.990	-2.931	-5.177	C	-0.536	3.361	-0.867	H	1.930	1.915	2.199
C	-1.065	-2.124	-2.652	H	-6.042	-0.271	-1.529	C	-0.948	3.968	-2.078	H	0.695	2.990	2.422
C	-1.309	-3.049	-3.675	H	-5.326	0.665	-0.403	C	-1.621	5.201	-2.073	H	2.421	-3.235	-0.673
C	-0.285	-3.357	-4.587	H	-3.265	-1.856	3.025	C	-1.886	5.868	-0.861	H	0.431	-3.139	-1.055
C	0.962	-2.716	-4.467	H	-0.724	-2.793	1.897	C	-1.465	5.286	0.351	H	-0.017	0.371	1.500
O	-2.190	-1.806	-1.829	H	-1.927	3.486	-3.024	C	-0.797	4.050	0.347	H	3.529	-1.330	1.710
C	-2.287	-2.168	-0.506	H	-2.406	5.647	-3.017	O	1.338	2.128	0.078	H	3.364	-0.173	-1.230
O	-1.471	-2.902	0.083	H	-1.667	6.823	-0.861	C	2.415	2.941	-0.365	H	2.925	0.553	0.364
C	-3.515	-1.592	0.121	H	-0.491	5.788	1.295	O	2.613	3.156	-1.565	H	1.183	-3.461	1.442
C	-4.290	-0.616	-0.545	H	1.758	3.599	1.288	C	3.244	3.581	0.765	H	2.151	-3.539	1.746
C	-5.431	-0.090	0.079	H	3.016	5.202	1.015	C	2.822	5.085	0.784	H	2.638	-1.741	2.958
C	-5.776	-0.557	1.359	H	3.404	5.554	-0.187	C	4.746	3.485	0.389	H	4.320	-0.068	2.681
C	-5.018	-1.527	2.039	H	5.345	5.611	1.551	C	2.990	2.959	2.154	H	4.451	-1.537	1.433
C	-3.879	-2.042	1.409	H	4.924	4.043	1.119	P	1.561	-1.049	-0.100	H	1.001	-2.293	-0.157
C	0.447	-0.457	-1.399	H	5.095	3.906	-0.606	C	1.669	-2.931	-0.284	H	2.732	-5.543	0.261
C	-0.125	0.877	-1.455	H	3.557	2.445	0.385								

C	0.831	-0.643	1.598	H	0.649	-5.474	-0.070								
C	3.359	-0.400	-0.170	H	0.156	0.733	3.987								
C	1.960	-3.741	0.997	H	6.028	-0.936	4.267								
C	1.767	-0.721	2.823	H	5.922	-0.465	-0.887								
C	4.472	-1.326	0.365	H	1.480	0.258	0.717								
C	1.970	-5.258	0.695	H	2.244	-5.935	2.720								
C	1.033	-0.290	4.115	H	3.224	-7.180	1.714								
C	5.875	-0.700	0.177	H	2.317	-5.864	2.390								
C	2.246	-6.109	1.952	H	2.811	-1.368	5.528								
C	1.942	-0.350	5.360	H	1.401	0.313	5.245								
C	7.006	-1.625	0.671	H	7.005	-0.039	6.262								
C	-1.281	0.980	-2.332	H	7.990	-2.578	0.123								
N	-2.224	1.040	-3.043	H	6.894	-1.159	0.529								
H	2.119	-1.246	-3.384	N	-6.981	-1.853	1.740								
H	-2.290	-3.510	-3.748	O	-7.271	-0.007	2.020								
H	-0.465	-4.074	-5.384	O	-7.672	-0.433	3.192								

(i) Intermediate **6**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-$NO_2C_6H_4$, Ph, *t*Bu

C	-0.883	-1.965	2.872	H	-1.174	-3.401	4.462	C	-2.290	-0.113	-0.291	H	-4.922	-1.118	3.314
C	-0.709	-1.782	1.486	H	1.896	-1.916	-2.468	C	-3.657	-0.207	1.023	H	-6.138	-0.825	2.068
C	-0.675	-2.920	0.616	H	4.189	-2.949	-2.293	C	-2.319	1.670	-0.910	H	-3.433	4.193	-1.231
C	-0.844	-4.221	1.146	H	4.193	-2.170	1.947	C	-2.930	-1.263	-1.656	H	-2.655	3.704	-2.733
C	-1.037	-4.381	2.527	H	1.924	-1.152	1.775	C	-4.252	-1.606	1.306	H	-3.064	-3.110	-3.681
C	-1.047	-3.263	3.392	H	-3.266	0.224	1.949	C	-3.608	2.069	-1.664	H	-4.107	-1.752	-4.113
O	-0.460	-2.646	-0.685	H	-4.449	0.466	0.666	C	-2.285	-1.182	-3.050	H	-5.222	-3.619	3.027
C	0.387	-0.857	-0.578	H	-2.183	2.317	-0.035	O	-5.354	-1.528	2.390	H	-6.754	-2.833	3.460
O	0.139	-0.221	-1.660	H	-1.436	1.790	-1.542	C	-3.551	3.549	-2.115	H	-6.453	-3.327	1.782
C	1.760	-1.459	-0.369	H	-2.826	-2.277	-1.262	O	-3.055	-2.074	-4.052	H	-4.930	3.364	-3.808
C	2.411	-1.968	-1.516	H	-4.003	-1.018	-1.712	C	-5.983	-2.906	2.682	H	-5.716	3.854	-2.293
C	3.681	-2.545	-1.425	H	-4.685	-2.033	0.391	C	-4.809	3.972	-2.901	H	-4.746	5.024	-3.209
C	4.305	-2.603	-0.163	H	-3.469	-2.293	1.644	C	-2.425	-2.040	-5.460	H	-1.385	-2.390	-5.430
C	3.682	-2.106	0.994	H	-3.742	1.434	-2.550	C	0.790	1.718	1.105	H	-2.976	-2.682	-6.159
C	2.405	-1.535	0.882	H	-4.496	1.929	-1.031	P	1.077	2.968	1.864	H	-2.423	-1.020	-5.868
C	-0.521	-0.516	0.665	H	-2.270	-0.148	-3.421	C	0.066	3.871	2.258	H	-0.971	3.675	2.008
C	-0.154	0.770	1.426	H	-1.245	-1.504	-2.979								

C	-2.247	0.342	2.556	H	-1.608	3.149	1.043								
C	-3.330	2.040	0.284	H	-6.725	-2.279	0.662								
C	-5.495	-0.700	-0.195	H	-7.312	-0.652	1.007								
C	-1.920	-1.011	3.223	H	-0.469	-0.204	4.611								
C	-2.702	3.178	1.117	H	-2.120	-0.232	5.247								
C	-6.867	-1.281	0.220	H	-2.952	4.663	-0.447								
C	-1.387	-0.807	4.660	H	-4.296	4.600	0.694								
C	-3.198	4.557	0.620	H	-7.441	-2.030	-1.758								
C	-7.845	-1.381	-0.970	H	-8.812	-1.794	-0.657								
C	-1.090	-2.142	5.372	H	-8.027	-0.393	-1.414								
C	-2.579	5.725	1.414	H	-1.995	-2.761	5.454								
N	7.612	-0.086	0.688	H	-0.335	-2.720	4.822								
C	0.610	0.425	1.105	H	-0.707	-1.972	6.387								
N	1.177	0.310	2.147	H	-1.484	5.721	1.327								
O	8.611	-0.343	-0.067	H	-2.943	6.693	1.045								
O	7.682	0.639	1.739	H	-2.830	5.657	2.481								

(i) Intermediate **8**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-$NO_2C_6H_4$, Ph, *t*Bu

C	-2.170	-2.719	-0.218	H	-3.117	-2.253	-0.457	C	-0.072	1.769	-0.880	H	-1.228	0.122	-5.279
C	-1.007	-1.902	-0.184	H	-1.095	-2.763	-2.910	C	0.959	2.845	-0.708	H	-1.393	1.432	-4.076
C	0.217	-2.594	0.004	H	1.215	-4.462	0.402	C	2.270	2.600	-0.240	H	-2.752	0.326	-4.378
C	0.255	-3.983	0.241	H	-0.873	-5.812	0.430	C	3.202	3.649	-0.150	H	-1.169	-2.238	-4.601
C	-0.918	-4.743	0.248	H	-3.067	-4.672	-0.052	C	2.838	4.957	-0.524	H	-2.622	-2.127	-3.582
C	-2.144	-4.101	-0.009	H	3.078	-0.768	1.430	C	1.536	5.208	-1.003	H	-4.318	-1.639	1.388
O	1.469	-1.916	0.015	H	5.314	0.194	2.047	C	0.609	4.159	-1.102	H	-4.997	-0.070	1.828
C	2.541	-2.377	-0.758	H	7.081	-1.608	-1.453	O	-0.971	1.942	-1.800	H	-3.047	0.849	3.114
O	2.418	-3.216	-1.663	H	4.837	-2.599	-2.066	C	-1.844	-0.215	-1.881	H	-1.368	0.991	2.586
C	3.829	-1.740	-0.359	H	2.574	1.596	0.033	O	-3.100	-0.109	-1.907	H	-4.425	2.078	0.363
C	3.947	-0.954	0.808	H	4.209	3.446	0.205	C	-1.113	-0.560	-3.214	H	-3.067	2.147	-0.770
C	5.193	-0.411	1.156	H	3.561	5.766	-0.451	C	0.427	-0.476	-3.183	H	-5.637	0.300	-0.626
C	6.297	-0.662	0.324	H	1.252	6.214	-1.305	C	-1.662	0.398	-4.309	H	-5.064	-1.304	-1.001
C	6.201	-1.441	-0.843	H	-0.387	4.332	-1.498	C	-1.531	-2.020	-3.588	H	-2.815	-1.652	3.258
C	4.955	-1.984	-1.179	H	0.862	-1.097	-2.396	P	-2.858	0.258	0.761	H	-1.161	-1.549	2.643
C	-1.200	-0.391	-0.446	H	0.770	0.553	-3.055	C	-4.531	-0.635	1.004	H	-2.955	3.074	2.181
C	-0.117	0.571	-0.099	H	0.817	-0.845	-4.140								

C	-2.228	1.005	1.625	H	-1.743	3.218	-0.464								
C	-1.393	1.254	-1.362	H	-5.518	-1.492	-2.344								
C	-4.549	0.191	-1.372	H	-6.327	-0.959	-0.870								
C	-3.555	1.781	1.778	H	-3.606	1.607	3.945								
C	-2.047	2.653	-1.357	H	-2.810	3.068	3.364								
C	-5.817	-0.599	-1.776	H	-0.567	3.540	-2.689								
C	-3.670	2.405	3.190	H	-1.981	2.890	-3.514								
C	-1.662	3.453	-2.624	H	-6.319	0.590	-3.547								
C	-6.794	0.248	-2.618	H	-7.684	-0.333	-2.892								
C	-4.983	3.192	3.382	H	-7.130	1.135	-2.064								
C	-2.294	4.860	-2.649	H	-5.058	4.019	2.663								
N	5.123	-0.596	-2.852	H	-5.858	2.544	3.242								
C	0.768	-2.330	1.980	H	-5.042	3.620	4.391								
N	1.063	-3.303	2.584	H	-1.966	5.460	-1.789								
O	5.331	0.286	-3.759	H	-2.015	5.403	-3.561								
O	6.062	-1.144	-2.174	H	-3.390	4.801	-2.617								

(i) Transition state in path **a**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-$NO_2C_6H_4$, Ph, *t*Bu

C	-2.393	-2.864	1.732	H	-2.552	-2.081	2.472	C	1.294	-0.112	1.347	H	0.862	4.980	1.112
C	-1.548	-2.628	0.629	H	-1.727	-5.733	-0.839	C	2.476	-0.099	2.253	H	0.210	4.477	-0.465
C	-1.329	-3.692	-0.275	H	-3.243	-6.126	1.131	C	2.337	-0.257	3.650	H	2.899	3.654	-1.792
C	-1.929	-4.949	-0.117	H	-3.651	-4.287	2.773	C	3.468	-0.248	4.483	H	1.451	2.632	-1.838
C	-2.774	-5.155	0.988	H	1.947	-3.088	-0.570	C	4.753	-0.077	3.933	H	2.974	1.970	-1.236
C	-3.009	-4.116	1.913	H	4.317	-2.432	-1.067	C	4.901	0.087	2.542	H	-3.299	-1.566	-1.142
O	-0.427	-3.454	-1.303	H	2.925	0.354	-4.052	C	3.770	0.082	1.708	H	-4.095	-1.063	0.361
C	-0.346	-2.036	-1.709	H	0.539	-0.301	-3.530	O	1.239	1.017	0.462	H	-2.160	0.237	2.406
O	-1.294	-1.569	-2.423	H	1.347	-0.377	4.080	C	1.285	2.320	1.021	H	-1.370	1.668	1.775
C	1.094	-1.692	-1.986	H	3.347	-0.371	5.556	O	0.783	2.547	2.129	H	-0.308	1.326	-1.268
C	2.159	-2.315	-1.300	H	5.628	-0.076	4.579	C	2.010	3.367	0.162	H	-1.601	0.711	-2.289
C	3.486	-1.965	-1.583	H	5.890	0.205	2.107	C	3.329	3.701	0.931	H	-4.852	1.085	-0.809
C	3.733	-0.986	-2.564	H	3.890	0.185	0.633	C	1.132	4.646	0.105	H	-4.044	0.533	-2.286
C	2.690	-0.373	-3.283	H	3.978	2.824	1.021	C	2.350	2.868	-1.259	H	-3.625	2.581	1.030
C	1.371	-0.732	-2.984	H	3.112	4.075	1.937	P	-1.957	0.070	-0.003	H	-4.412	1.113	1.614
C	-0.775	-1.361	0.322	H	3.874	4.475	0.376	C	-3.597	-0.699	-0.545	H	-3.140	2.574	-1.322
C	0.402	-1.154	1.209	H	1.691	5.449	-0.391								

C	-2.245	-0.527	2.903	H	-0.888	-2.032	4.779								
C	-2.668	2.067	1.403	H	-2.619	-2.179	5.099								
C	-5.208	0.157	-0.276	H	-1.610	4.617	1.613								
C	-2.109	-2.063	2.985	H	-2.993	4.474	2.699								
C	-1.802	2.659	2.536	H	-7.124	-0.255	-2.317								
C	-6.715	-0.176	-0.166	H	-8.569	0.014	-1.323								
C	-1.811	-2.519	4.432	H	-7.414	1.336	-1.590								
C	-1.933	4.200	2.579	H	-2.578	-4.564	4.226								
C	-7.503	0.254	-1.421	H	-0.839	-4.410	3.910								
C	-1.660	-4.051	4.544	H	-1.446	-4.354	5.577								
C	-1.103	4.829	3.717	H	-0.037	4.593	3.603								
C	0.641	0.257	1.362	H	-1.207	5.922	3.725								
N	1.166	-0.025	2.390	H	-1.427	4.454	4.698								
H	-3.409	-1.954	-0.615	N	7.410	-0.533	0.659								
H	0.843	-4.446	-0.968	O	8.352	-0.411	-0.198								
H	-1.321	-5.657	-1.270	O	7.563	-0.341	1.914								

(i) Transition state in path **b**; FG = CN; **R**^{1}, **R**^{2}, **R**^{3} = 4-$NO_2C_6H_4$, Ph, *t*Bu

C	-2.472	-2.495	-0.635	H	-3.468	-4.350	-1.081	C	0.244	1.547	-0.688	H	-0.549	-0.840	-4.622
C	-1.262	-1.760	-0.421	H	2.927	-1.538	1.326	C	1.368	2.515	-0.584	H	0.353	0.100	-3.422
C	-0.081	-2.543	-0.575	H	5.213	-0.905	2.155	C	2.578	2.220	0.087	H	-4.510	-1.395	1.098
C	-0.100	-3.916	-0.871	H	6.718	-0.992	-1.890	C	3.606	3.175	0.153	H	-4.914	0.134	1.875
C	-1.312	-4.596	-1.042	H	4.422	-1.655	-2.719	C	3.448	4.436	-0.452	H	-3.059	-0.177	3.555
C	-2.509	-3.861	-0.926	H	2.732	1.251	0.546	C	2.252	4.734	-1.133	H	-1.318	-0.060	3.249
O	1.210	-1.958	-0.341	H	4.531	2.930	0.670	C	1.223	3.782	-1.205	H	-3.725	2.310	1.577
C	2.215	-2.046	-1.298	H	4.247	5.172	-0.399	O	-0.531	1.786	-1.788	H	-2.410	2.492	0.430
O	2.031	-2.429	-2.463	H	2.123	5.703	-1.609	C	-1.862	1.126	-2.009	H	-5.074	1.234	-0.430
C	3.542	-1.631	-0.750	H	0.305	4.003	-1.738	O	-2.867	1.753	-1.607	H	-4.794	-0.319	-1.172
C	3.751	-1.426	0.632	H	-0.912	2.175	-4.331	C	-1.819	0.400	-3.378	H	-3.025	-2.559	2.633
C	5.025	-1.068	1.100	H	-2.693	2.201	-4.314	C	-1.812	1.559	-4.431	H	-1.295	-2.400	2.331
C	6.068	-0.917	0.170	H	-1.825	1.124	-5.438	C	-3.106	-0.434	-3.572	H	-2.105	2.252	3.511
C	5.883	-1.119	-1.210	H	-3.142	-0.812	-4.602	C	-0.566	-0.473	-3.587	H	-0.746	2.396	2.397
C	4.609	-1.482	-1.664	H	-3.999	0.178	-3.397	P	-2.623	0.185	1.178	H	-6.844	-1.258	-0.004
C	-1.329	-0.303	-0.128	H	-3.127	-1.298	-2.900	C	-4.449	-0.308	0.981	H	-7.138	0.324	0.720
C	-0.094	0.510	0.161	H	-0.553	-1.346	-2.933								

C	-2.228	1.005	1.625	H	-1.743	3.218	-0.464								
C	-1.393	1.254	-1.362	H	-5.518	-1.492	-2.344								
C	-4.549	0.191	-1.372	H	-6.327	-0.959	-0.870								
C	-3.555	1.781	1.778	H	-3.606	1.607	3.945								
C	-2.047	2.653	-1.357	H	-2.810	3.068	3.364								
C	-5.817	-0.599	-1.776	H	-0.567	3.540	-2.689								
C	-3.670	2.405	3.190	H	-1.981	2.890	-3.514								
C	-1.662	3.453	-2.624	H	-6.319	0.590	-3.547								
C	-6.794	0.248	-2.618	H	-7.684	-0.333	-2.892								
C	-4.983	3.192	3.382	H	-7.130	1.135	-2.064								
C	-2.294	4.860	-2.649	H	-5.058	4.019	2.663								
N	5.123	-0.596	-2.852	H	-5.858	2.544	3.242								
C	0.768	-2.330	1.980	H	-5.042	3.620	4.391								
N	1.063	-3.303	2.584	H	-1.966	5.460	-1.789								
O	5.331	0.286	-3.759	H	-2.015	5.403	-3.561								
O	6.062	-1.144	-2.174	H	-3.390	4.801	-2.617								

(j) Intermediate **2**; FG = CN**; R^1, R^2, R^3** = *t*Bu, Ph, *t*Bu

C	1.895	-1.357	-2.972	H	-0.729	-2.430	2.289	C	-2.123	-0.655	-0.467	H	-5.421	3.371	1.092
C	1.445	-1.673	-1.664	H	-0.804	-3.960	3.192	C	-3.480	-1.250	-0.464	H	-3.496	4.913	0.605
C	1.989	-2.854	-1.099	H	1.142	-3.239	4.707	C	-4.044	-1.871	-1.605	H	-3.208	4.261	-1.026
C	2.907	-3.671	-1.772	H	1.211	-1.683	3.851	C	-5.341	-2.412	-1.566	H	-1.891	4.298	0.171
C	3.339	-3.315	-3.061	H	2.673	-2.673	3.993	C	-6.117	-2.327	-0.394	H	-3.423	3.306	2.629
C	2.830	-2.149	-3.662	H	1.280	-5.437	3.436	C	-5.578	-1.694	0.744	H	-1.885	2.584	2.117
O	1.532	-3.342	0.162	H	2.825	-4.946	2.710	C	-4.279	-1.163	0.708	H	-3.296	1.550	2.382
C	1.871	-2.731	1.358	H	1.471	-5.447	1.667	O	-2.096	0.648	0.183	H	3.239	-0.302	-0.403
O	2.632	-1.750	1.419	H	-3.474	-1.916	-2.527	C	-2.851	1.673	-0.431	H	3.139	0.906	-1.690
C	1.213	-3.448	2.546	H	-5.748	-2.886	-2.455	O	-3.069	1.681	-1.649	H	-0.234	0.675	1.679
C	-0.329	-3.451	2.343	H	-7.122	-2.743	-0.368	C	-3.407	2.734	0.538	H	1.477	0.322	1.989
C	1.586	-2.713	3.852	H	-6.163	-1.628	1.659	C	-4.960	2.626	0.431	H	-0.111	1.891	-2.157
C	1.735	-4.913	2.585	H	-3.861	-0.700	1.599	C	-2.969	4.138	0.036	H	-0.431	2.694	-0.628
C	0.443	-0.802	-0.961	H	-5.312	1.632	0.730	C	-2.971	2.524	2.003	H	3.552	2.727	0.086
C	-0.939	-1.234	-0.911	H	-5.290	2.811	-0.597	P	1.086	0.779	-0.353	H	3.696	1.444	1.297
H	3.263	-4.575	-1.286	H	0.760	3.906	5.270	H	4.049	-3.946	-3.589	H	2.454	5.290	-3.463
H	-0.605	-3.973	1.422	H	1.999	6.171	-1.991	H	3.138	-1.873	-4.668	H	1.084	6.417	-3.492

(j) Intermediate **6**; FG = CN**; R^1, R^2, R^3** = *t*Bu, Ph, *t*Bu

C	-1.851	-2.953	0.804	H	-0.055	-3.260	-2.229	C	-1.176	0.646	0.704	H	0.083	-1.582	2.670
C	-1.716	-1.998	-0.225	H	-0.106	-3.300	-3.994	C	-0.257	0.550	2.361	H	-2.299	3.292	1.704
C	-2.795	-1.801	-1.144	H	1.523	-1.448	-4.428	C	-0.964	2.455	0.175	H	-0.580	3.444	2.091
C	-3.965	-2.600	-1.046	H	1.855	-1.571	-2.695	C	-3.004	0.494	1.175	H	-3.832	2.253	0.178
C	-4.065	-3.558	-0.029	H	1.474	0.017	-3.416	C	-0.400	-0.744	3.187	H	-3.833	0.788	-0.814
C	-3.013	-3.737	0.901	H	-0.693	-1.282	-5.364	C	-1.308	3.491	1.270	H	1.296	-0.289	4.472
O	-2.629	-0.833	-2.052	H	-0.821	0.327	-4.600	C	-3.998	1.166	0.202	H	-0.255	0.237	5.123
C	-0.753	-0.405	-1.994	H	-2.107	-0.866	-4.352	O	0.242	-0.586	4.586	H	-0.323	5.135	0.240
O	-0.644	0.859	-2.117	H	0.799	0.771	2.165	C	-1.306	4.927	0.690	H	-2.042	4.991	-0.124
C	-0.281	-1.287	-3.220	H	-0.654	1.392	2.942	O	-5.460	0.894	0.626	H	-5.634	-0.192	0.634
C	-0.531	-2.809	-3.107	H	0.064	2.567	-0.163	C	0.155	-1.877	5.426	H	-5.622	1.249	1.657
C	1.243	-1.052	-3.443	H	-1.587	2.567	-0.714	C	-1.619	5.994	1.759	H	0.666	-2.711	4.925
C	-1.028	-0.740	-4.468	H	-3.231	-0.572	1.270	C	-6.475	1.571	-0.318	H	0.619	-1.742	6.411
C	-0.622	-0.984	-0.479	H	-3.086	0.936	2.179	C	1.947	-0.643	-0.114	H	-0.890	-2.175	5.585
C	0.802	-1.405	-0.088	H	-1.458	-1.017	3.307	P	3.287	-1.116	0.338	H	-2.608	5.828	2.207
H	-3.095	-4.485	1.684	H	1.176	3.923	-1.528	H	-4.765	-2.445	-1.765	H	3.034	4.432	0.125
H	-1.598	-3.044	-3.076	H	1.145	2.382	-2.412	H	-4.961	-4.171	0.047	H	2.140	3.741	-3.000

(j) Intermediate **8**; FG = CN**; R^1, R^2, R^3** = *t*Bu, Ph, *t*Bu

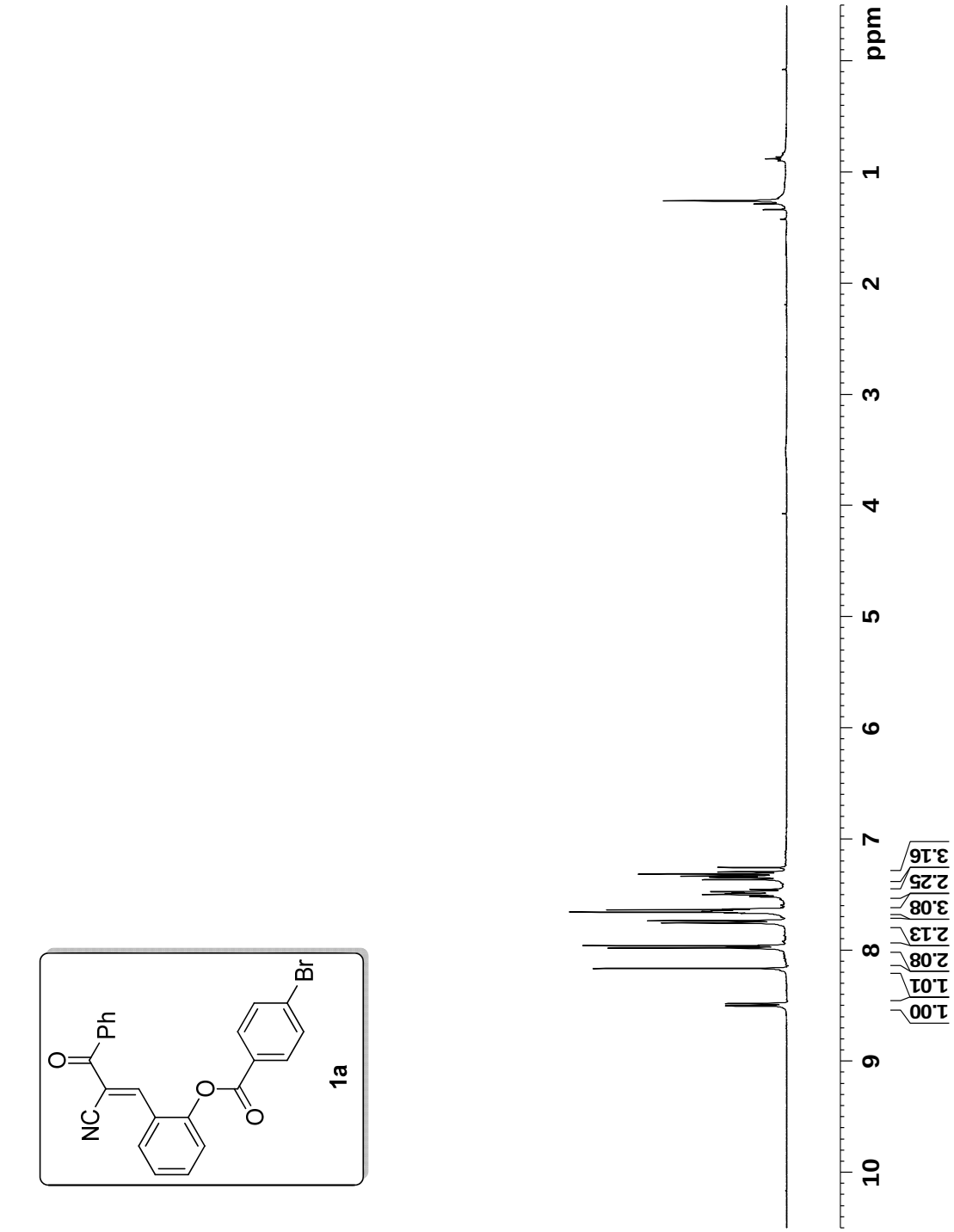
C	1.358	2.742	-0.204	H	-4.473	0.144	-1.448	C	-0.790	-1.748	-0.690	H	-2.107	1.024	-3.795
C	0.208	1.917	-0.088	H	-5.374	-0.447	-0.035	C	-1.687	-2.911	-0.360	H	-0.253	0.090	-5.225
C	-1.002	2.586	0.239	H	-6.795	1.665	-0.065	C	-2.141	-3.247	0.939	H	0.073	-1.267	-4.111
C	-1.016	3.963	0.549	H	-5.885	2.312	-1.452	C	-2.948	-4.382	1.141	H	1.380	-0.149	-4.553
C	0.152	4.728	0.478	H	-6.040	3.275	0.025	C	-3.322	-5.196	0.057	H	-0.021	2.874	-2.743
C	1.349	4.113	0.068	H	-5.579	0.976	2.076	C	-2.871	-4.874	-1.239	H	-0.149	2.422	-4.451
O	-2.229	1.882	0.306	H	-4.788	2.561	2.181	C	-2.057	-3.750	-1.441	H	1.408	2.249	-3.610
C	-3.429	2.414	-0.225	H	-3.805	1.074	2.181	O	-0.130	-1.822	-1.810	H	3.790	1.582	0.967
O	-3.439	3.417	-0.948	H	-1.873	-2.644	1.796	C	0.804	0.258	-1.926	H	4.493	-0.018	1.214
C	-4.643	1.588	0.209	H	-3.283	-4.625	2.147	O	2.043	0.109	-2.123	H	2.744	-0.832	2.812
C	-4.505	0.144	-0.351	H	-3.951	-6.069	0.218	C	-0.076	0.687	-3.138	H	1.007	-0.991	2.548
C	-5.918	2.255	-0.358	H	-3.151	-5.499	-2.085	C	-1.600	0.620	-2.909	H	3.590	-2.065	-0.318
C	-4.696	1.549	1.763	H	-1.684	-3.503	-2.430	C	0.310	-0.224	-4.336	H	1.957	-2.176	-0.972
C	0.377	0.417	-0.410	H	-1.916	1.215	-2.051	C	0.321	2.156	-3.496	H	4.700	-0.281	-1.325
C	-0.623	-0.570	0.099	H	-1.933	-0.411	-2.766	P	2.194	-0.253	0.513	H	4.112	1.348	-1.527
H	-1.955	4.430	0.822	H	0.926	1.969	6.409	H	2.261	4.694	-0.042	H	2.489	-6.678	0.891
H	0.121	5.787	0.718	H	1.167	-5.723	1.588	H	-3.602	-0.343	0.024	H	2.803	-5.606	2.270

(j) Transition state in path **a**; FG = CN**; R^1, R^2, R^3** = *t*Bu, Ph, *t*Bu

C	-1.580	-2.465	2.158	C	3.770	-1.097	2.129	C	-4.180	1.090	-0.109	H	1.783	-2.752	-1.577
C	-1.329	-2.367	0.774	C	5.098	-1.373	2.495	C	-1.784	2.173	2.478	H	1.814	-3.527	-3.165
C	-1.899	-3.340	-0.078	C	6.117	-1.373	1.523	C	-1.379	3.032	-0.955	H	1.496	-1.120	-4.119
C	-2.714	-4.374	0.419	C	5.798	-1.093	0.180	C	-5.644	0.597	-0.026	H	1.260	-0.414	-2.506
C	-2.958	-4.442	1.800	C	4.471	-0.815	-0.186	C	-1.230	2.675	3.834	H	0.000	-0.229	-3.751
C	-2.392	-3.490	2.675	O	1.920	0.667	-0.418	C	-1.303	3.866	-2.257	H	0.132	-3.060	-4.915
O	-1.587	-3.271	-1.413	C	2.440	1.874	0.112	C	-6.654	1.669	-0.483	H	-1.399	-2.237	-4.508
C	-1.063	-1.932	-1.886	O	2.440	2.085	1.331	C	-2.161	3.705	4.507	H	-1.057	-3.852	-3.849
O	-1.962	-1.075	-2.188	C	3.011	2.847	-0.932	C	-1.582	5.364	-2.018	H	2.990	-1.087	2.885
C	0.091	-2.235	-2.888	C	4.548	2.906	-0.656	C	1.342	-2.676	1.080	H	5.336	-1.585	3.534
C	1.155	-3.213	-2.344	C	2.408	4.255	-0.671	N	1.634	-3.725	1.541	H	7.143	-1.591	1.808
C	0.751	-0.912	-3.338	C	2.761	2.407	-2.390	H	-1.118	-1.760	2.845	H	6.577	-1.104	-0.579
C	-0.609	-2.890	-4.122	P	-1.359	0.351	0.203	H	-3.129	-5.102	-0.272	H	4.223	-0.624	-1.228
C	-0.462	-1.333	0.073	C	-3.209	-0.018	0.349	H	-3.581	-5.241	2.196	H	5.022	1.928	-0.792
C	0.970	-1.395	0.500	C	-0.813	1.162	1.828	H	-2.567	-3.560	3.746	H	4.746	3.245	0.367
C	2.039	-0.535	0.364	C	-1.076	1.544	-1.233	H	0.689	-4.107	-1.919	H	5.008	3.612	-1.358
C	3.440	-0.822	0.784	H	-2.381	3.156	-0.528								

(j) Transition state in path **b**; FG = CN**; R^1, R^2, R^3** = *t*Bu, Ph, *t*Bu

C	-1.979	-2.367	-0.534	C	2.369	2.244	-0.260	C	-1.942	2.420	0.823	H	3.614	-0.256	0.625
C	-0.729	-1.746	-0.211	C	2.814	2.609	1.034	C	-4.295	0.598	-1.076	H	4.420	-0.522	-0.940
C	0.355	-2.668	-0.083	C	3.935	3.440	1.196	C	-2.210	-1.450	3.012	H	5.352	-0.606	0.570
C	0.182	-4.061	-0.174	C	4.633	3.926	0.075	C	-1.175	3.096	1.978	H	6.203	-2.913	0.026
C	-1.074	-4.621	-0.436	C	4.192	3.580	-1.217	C	-5.811	0.397	-1.304	H	5.318	-2.901	-1.521
C	-2.161	-3.749	-0.637	C	3.070	2.754	-1.383	C	-2.184	-1.722	4.534	H	5.083	-4.235	-0.384
O	1.675	-2.198	0.224	O	0.684	1.565	-1.766	C	-1.162	4.634	1.804	H	4.968	-2.537	2.228
C	2.791	-2.691	-0.478	C	-0.593	1.009	-2.272	C	-6.240	0.771	-2.738	H	3.815	-3.832	1.849
O	2.682	-3.313	-1.543	O	-1.606	1.729	-2.173	C	-2.289	-3.225	4.863	H	3.220	-2.200	2.240
C	4.111	-2.362	0.235	C	-0.326	0.080	-3.477	C	-0.398	5.348	2.938	H	2.299	2.254	1.918
C	4.382	-0.838	0.111	C	0.002	1.056	-4.657	C	1.109	0.188	1.650	H	4.260	3.707	2.199
C	5.248	-3.153	-0.457	C	-1.613	-0.706	-3.820	N	1.424	-0.081	2.763	H	5.502	4.567	0.205
C	4.013	-2.758	1.733	C	0.860	-0.882	-3.272	H	-2.825	-1.730	-0.756	H	4.719	3.954	-2.091
C	-0.661	-0.268	-0.085	P	-2.085	0.530	0.866	H	1.046	-4.705	-0.048	H	2.721	2.500	-2.378
C	0.593	0.449	0.338	C	-3.890	0.218	0.360	H	-1.193	-5.698	-0.503	H	0.900	1.646	-4.444
C	1.183	1.376	-0.499	C	-2.114	0.061	2.713	H	-3.143	-4.143	-0.889	H	-0.832	1.743	-4.841
H	-0.406	6.437	2.796	H	-0.849	5.134	3.917								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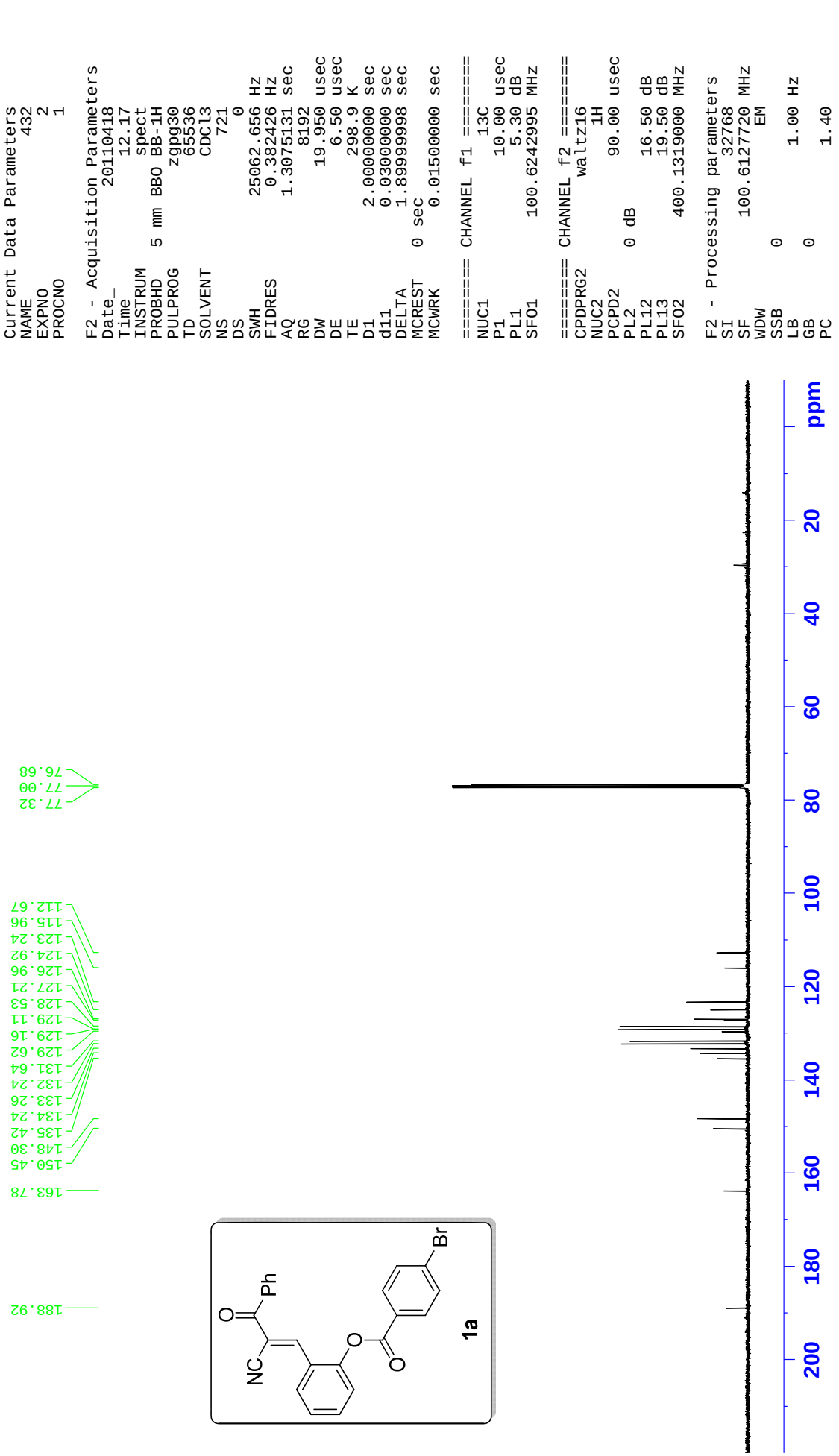
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 4
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 228.1
DW 83.200 usec
DE 6.50 usec
TE 299.5 K
D1 1.50000000 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 1H
P1 10.40 usec
PL1 -3.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
ppm
1.00
1.01
2.08
2.13
3.08
2.25
3.16
O
Ph
NC
O
O
Br
1a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PROCNO 1
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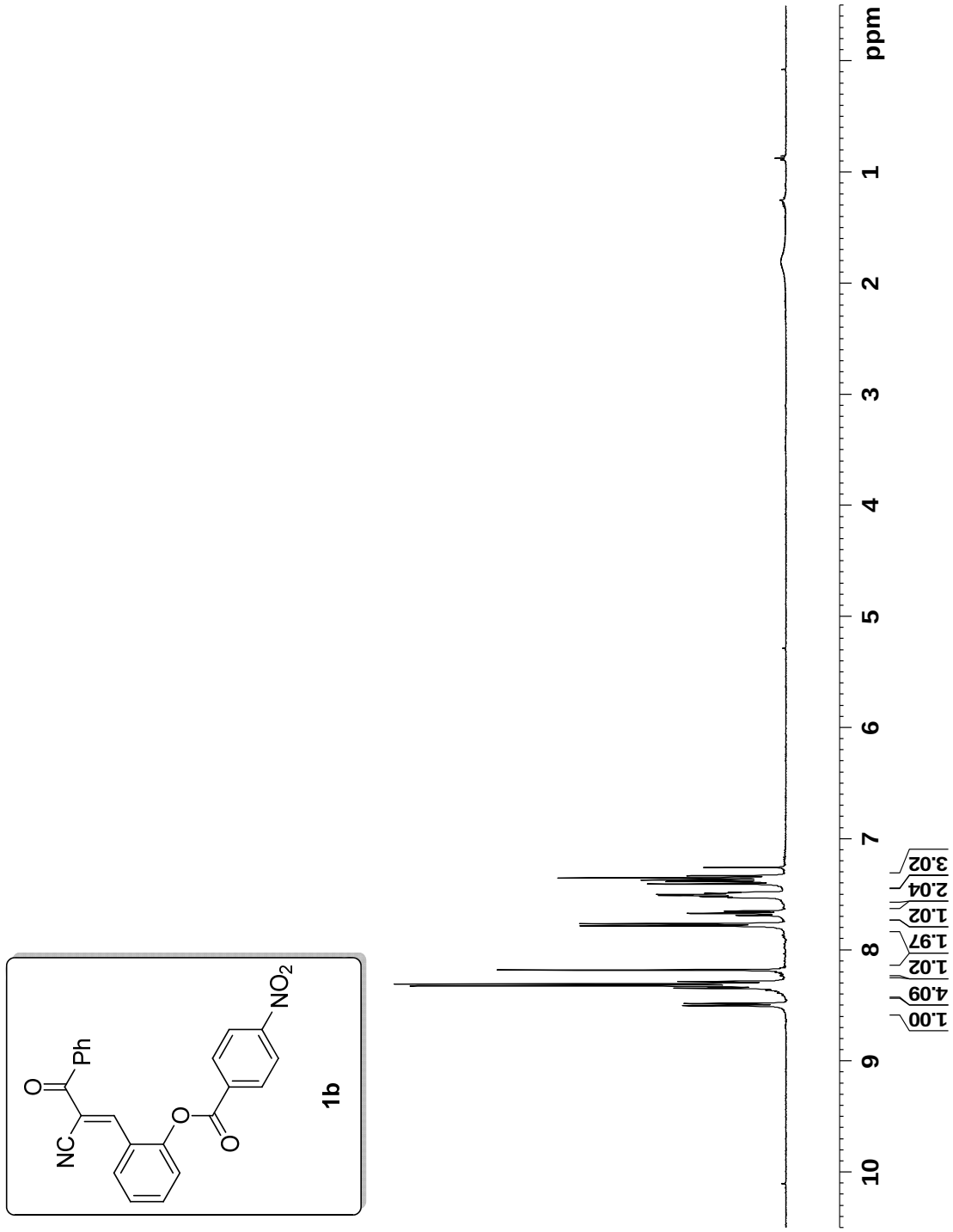
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 721
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 8192
DW 19.950 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0 dB 16.50 dB
PL12 19.50 dB
PL13 400.1319000 MHz
SFO2
F2 - Processing parameters
SI 32768
SF 100.6127720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
77.32
77.00
76.68
112.67
115.96
123.24
124.92
126.96
127.21
128.53
129.11
129.16
129.62
131.64
132.24
133.26
134.24
135.42
148.30
150.45
163.78
188.92
ppm
20
40
60
80
100
120
140
160
180
200
O
Ph
NC
O
O
Br
1a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EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110825
Time 18.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 1
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE 299.9 K
D1 1.50000000 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1.00
4.09
1.02
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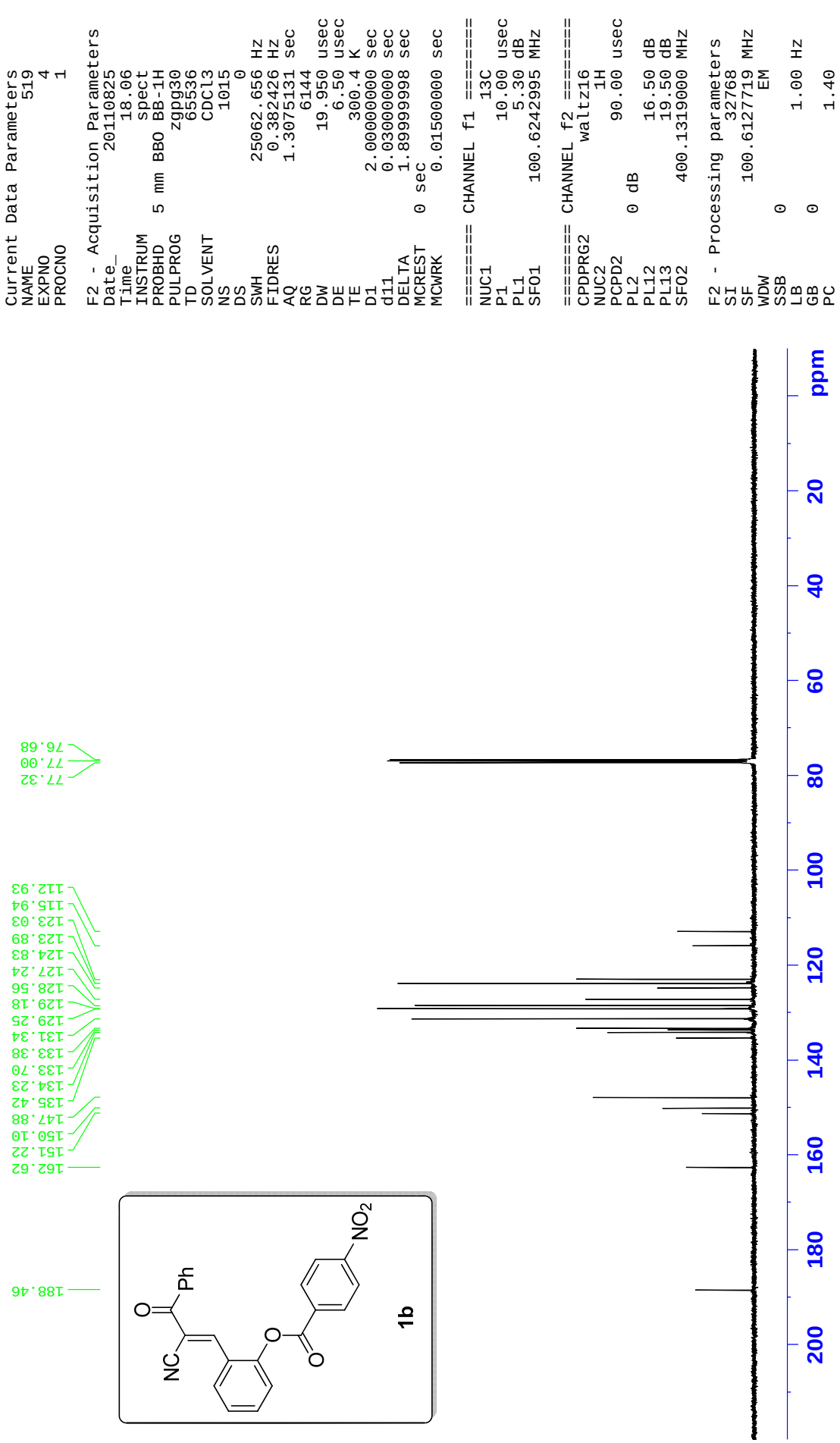
1.02
2.04
3.02
ppm
1b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PROCNO 1
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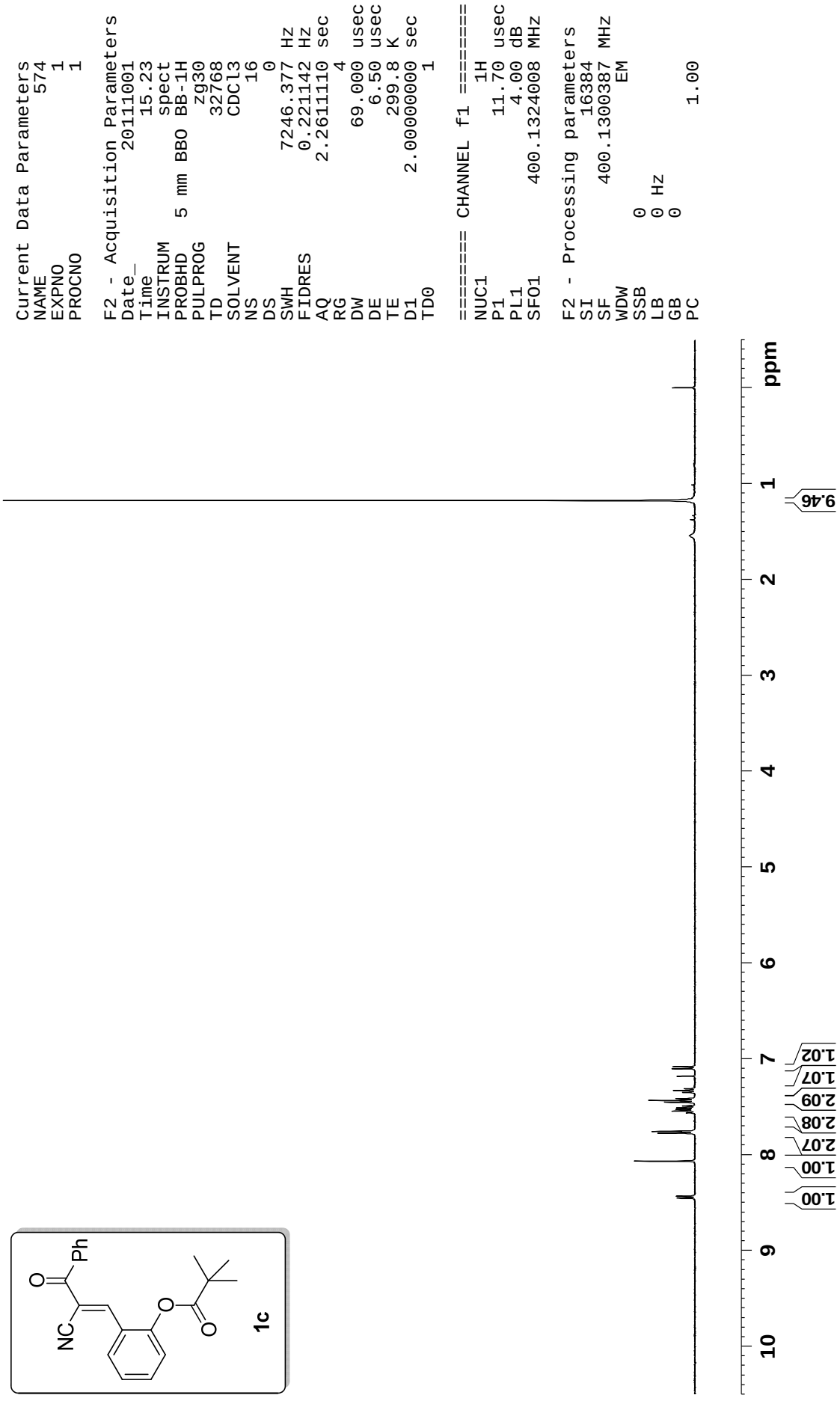
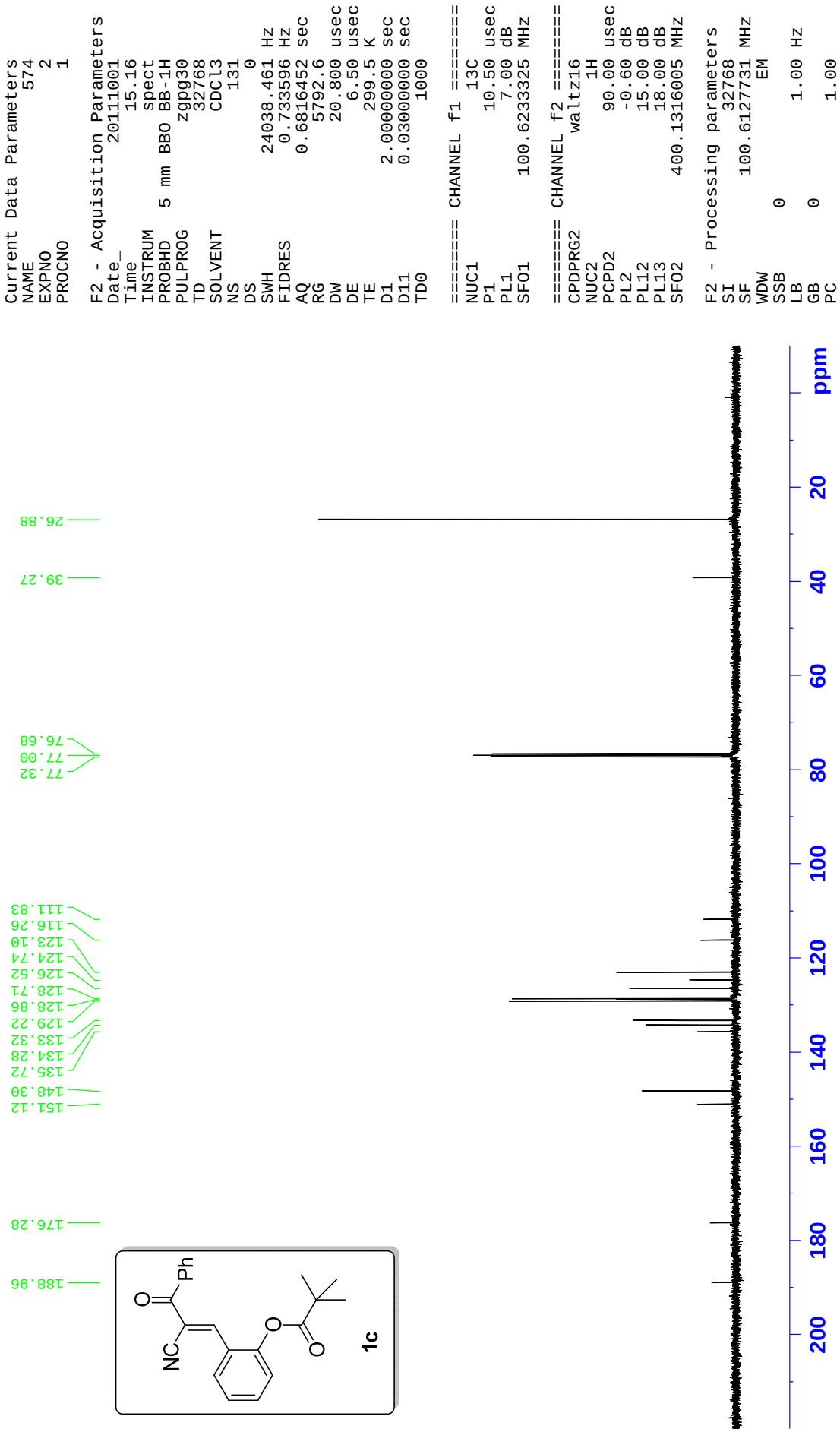
Time 18.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1015
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 6144
DW 19.950 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0 dB 16.50 dB
PL12 19.50 dB
PL13
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127719 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
188.46
162.62
151.22
150.10
147.88
135.42
134.23
133.70
133.38
131.34
129.25
129.18
128.56
127.24
124.83
123.89
123.03
115.94
112.93
77.32
77.00
76.68
O
Ph
NC
O
O
O
NO2
1b
200
180
160
140
120
100
80
60
40
20
ppm

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NAME 574
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
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Time 15.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 131
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1000
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127731 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
26.88
39.27
76.68
77.00
77.32
111.83
116.26
123.10
124.74
126.52
128.71
128.86
129.22
133.32
134.28
135.72
148.30
151.12
176.28
188.96
ppm
20
40
60
80
100
120
140
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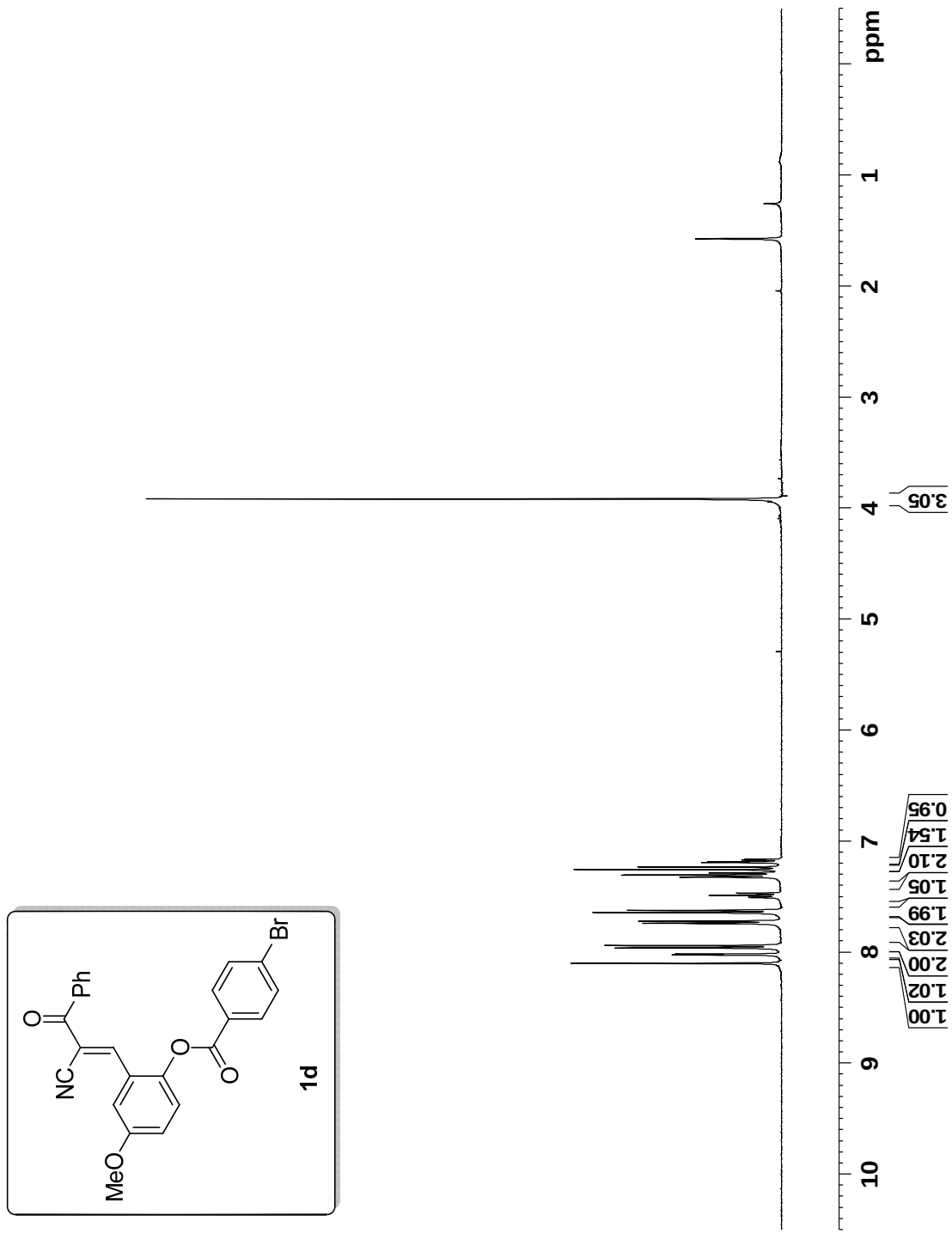
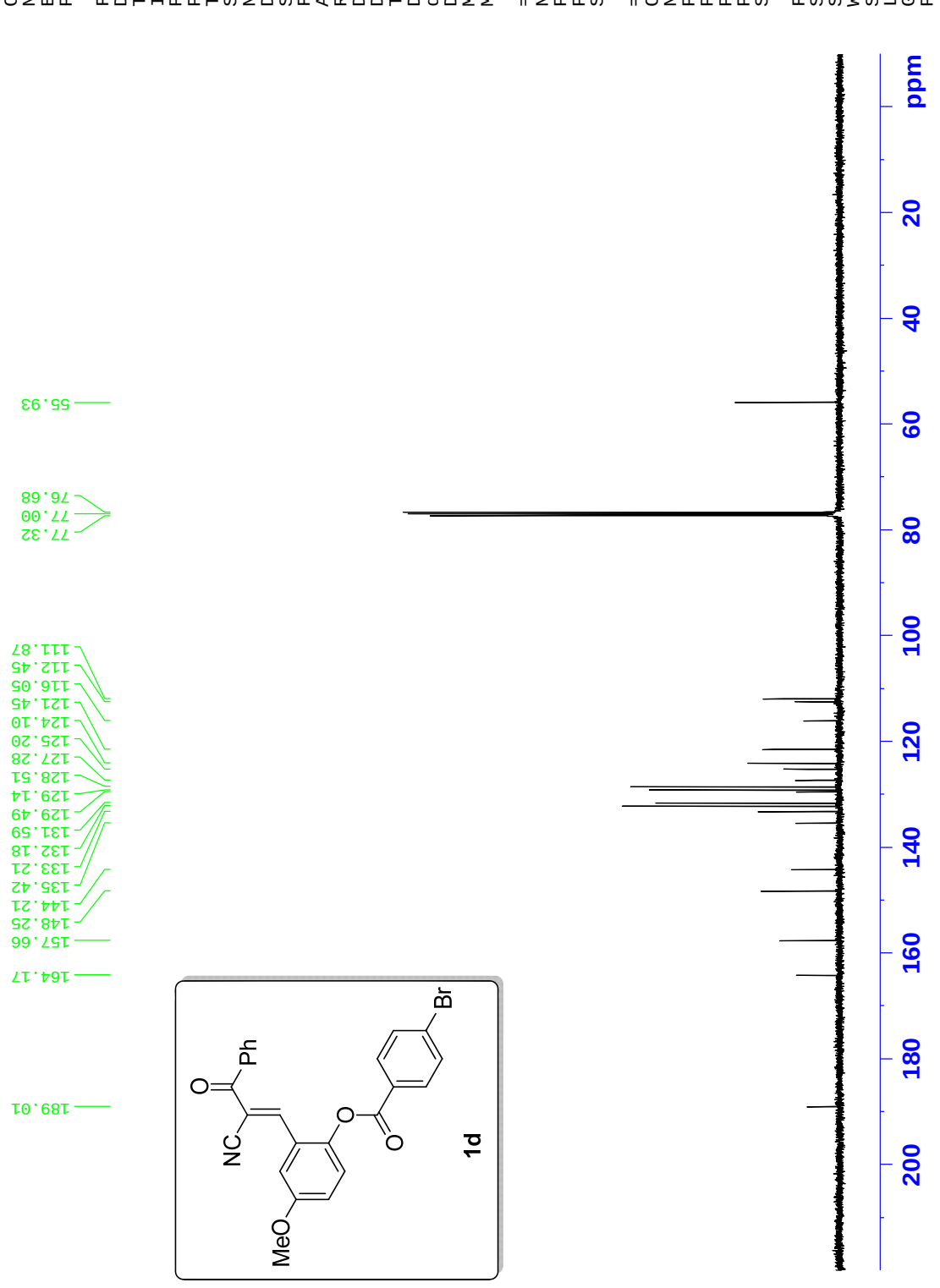
200
O
Ph
NC
O
O
1c

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PROCNO 1
F2 - Acquisition Parameters
Date_ 20110411
Time 21.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 302
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 6144
DW 19.950 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0 dB 16.50 dB
PL12 19.50 dB
PL13 400.1319000 MHz
SFO2
F2 - Processing parameters
SI 32768
SF 100.6127728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
55.93
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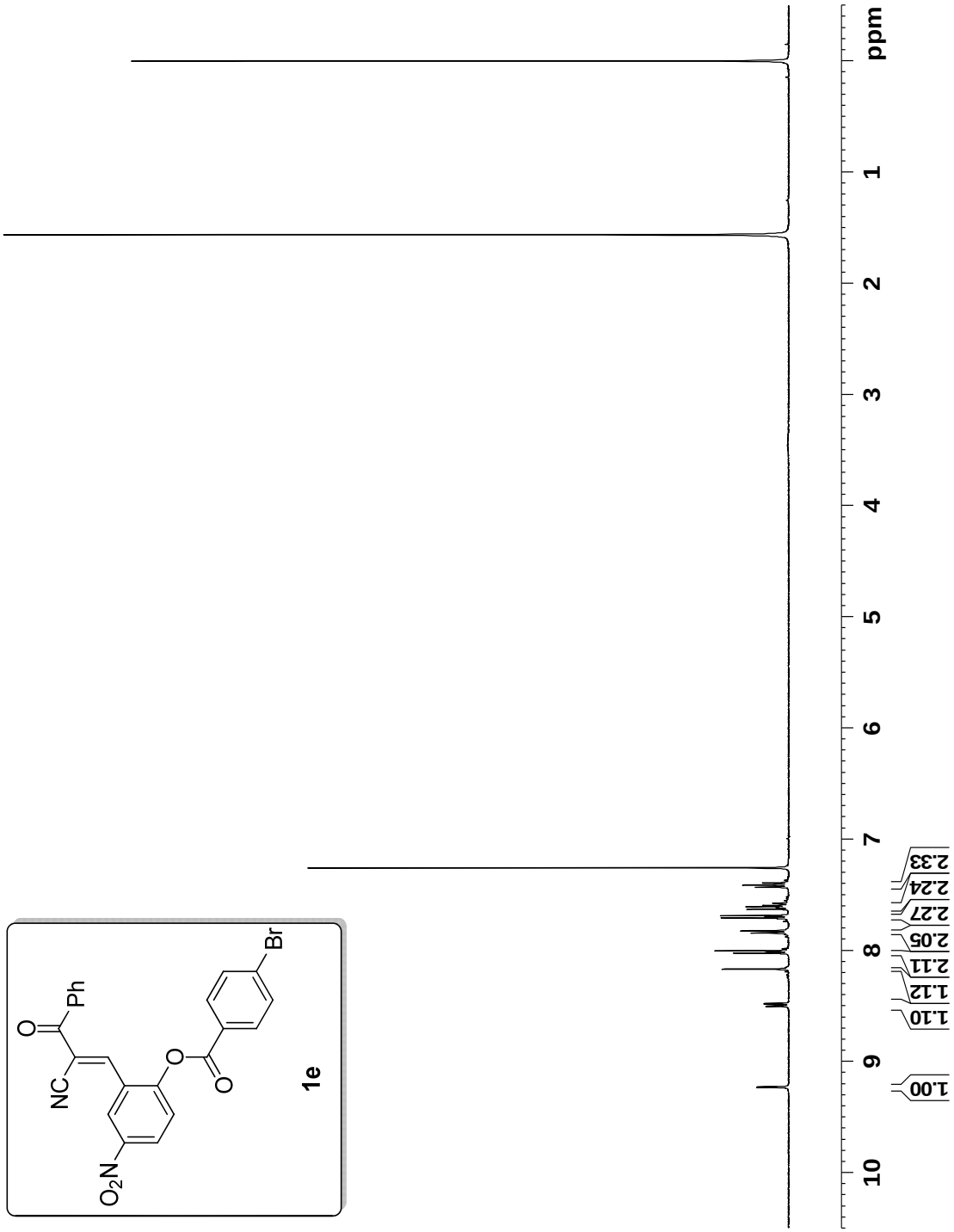
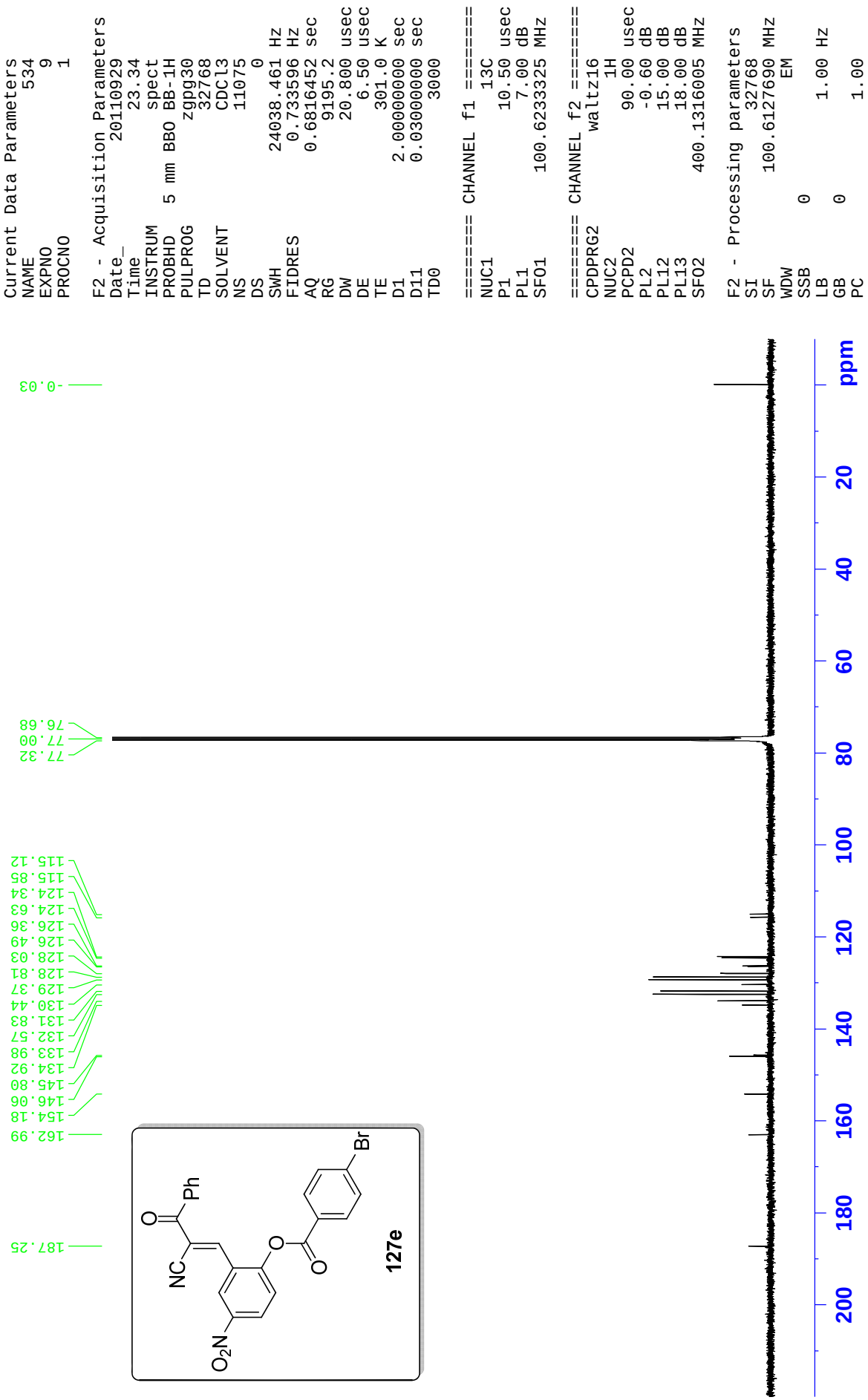
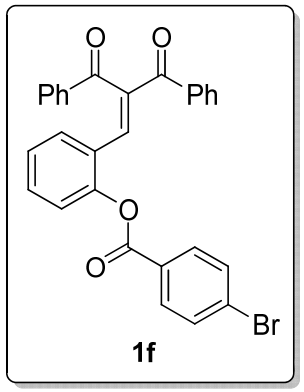
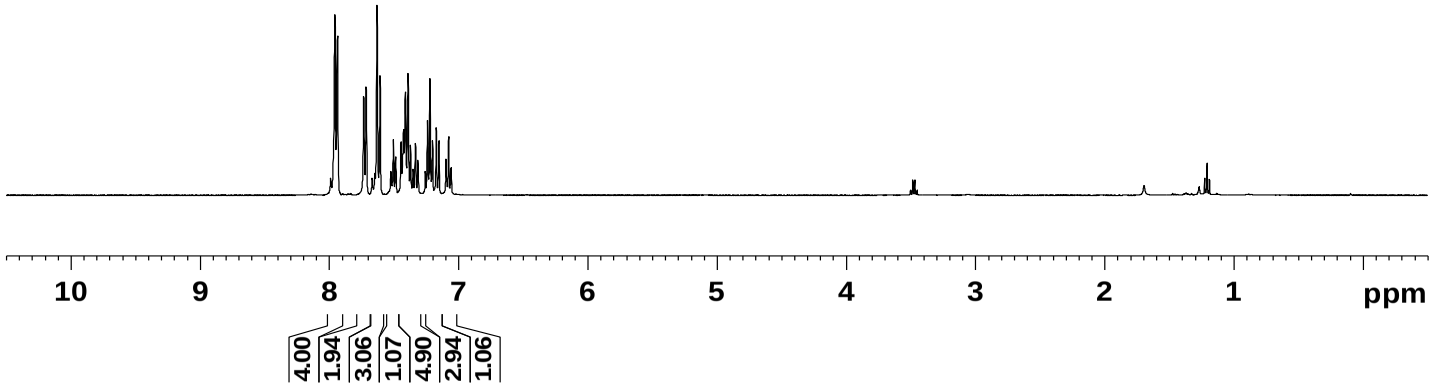
121.45
124.10
125.20
127.28
128.51
129.14
129.49
131.59
132.18
133.21
135.42
144.21
148.25
157.66
164.17
189.01
Br
O
Ph
NC
O
O
MeO
1d
ppm
200
180
160
140
120
100
80
60
40
20

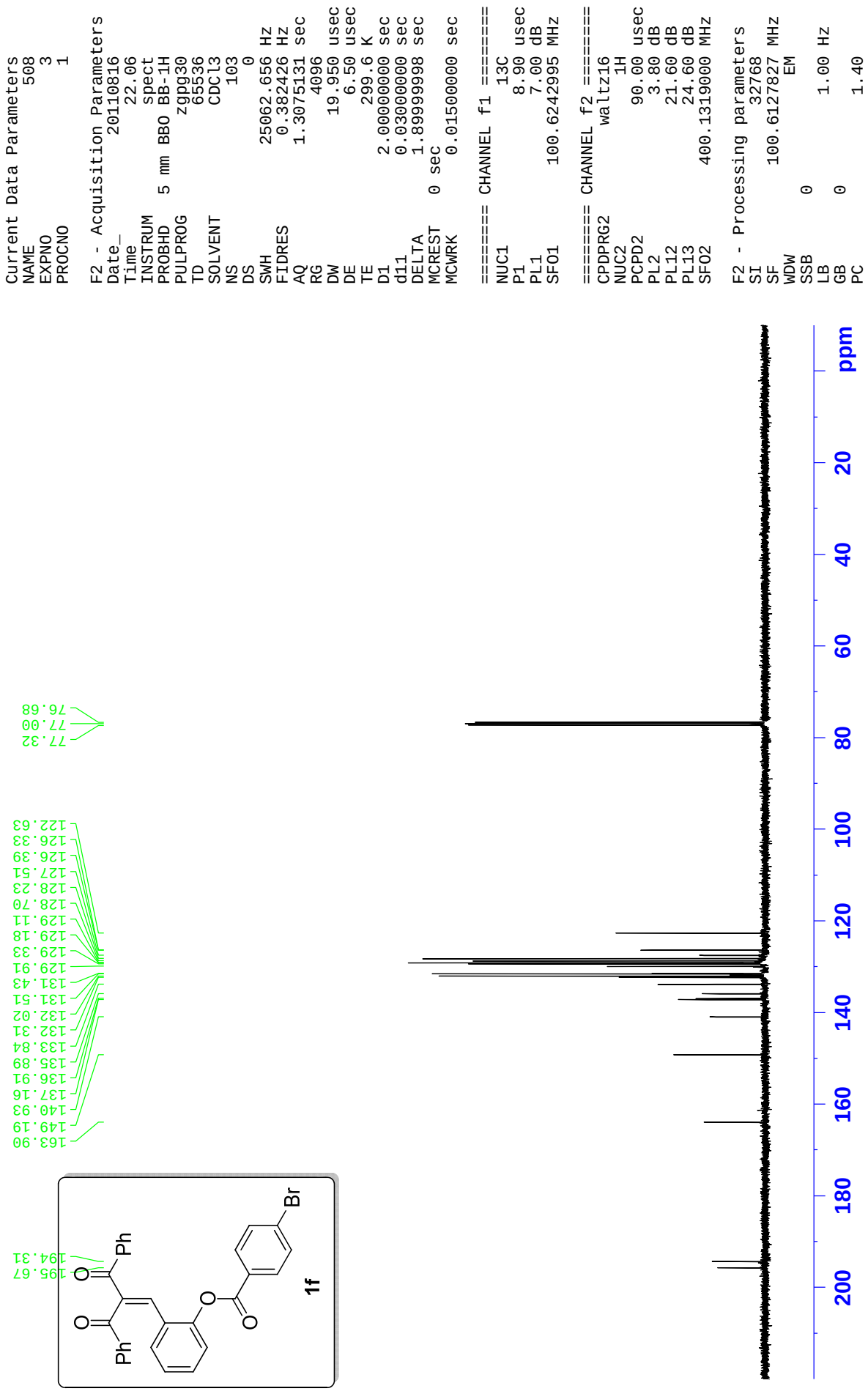

Current Data Parameters
NAME 534
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111001
Time 14.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 322.5
DW 69.000 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
1.00
1.10
1.12
2.11
2.05
2.27
2.24
2.33
ppm
1e

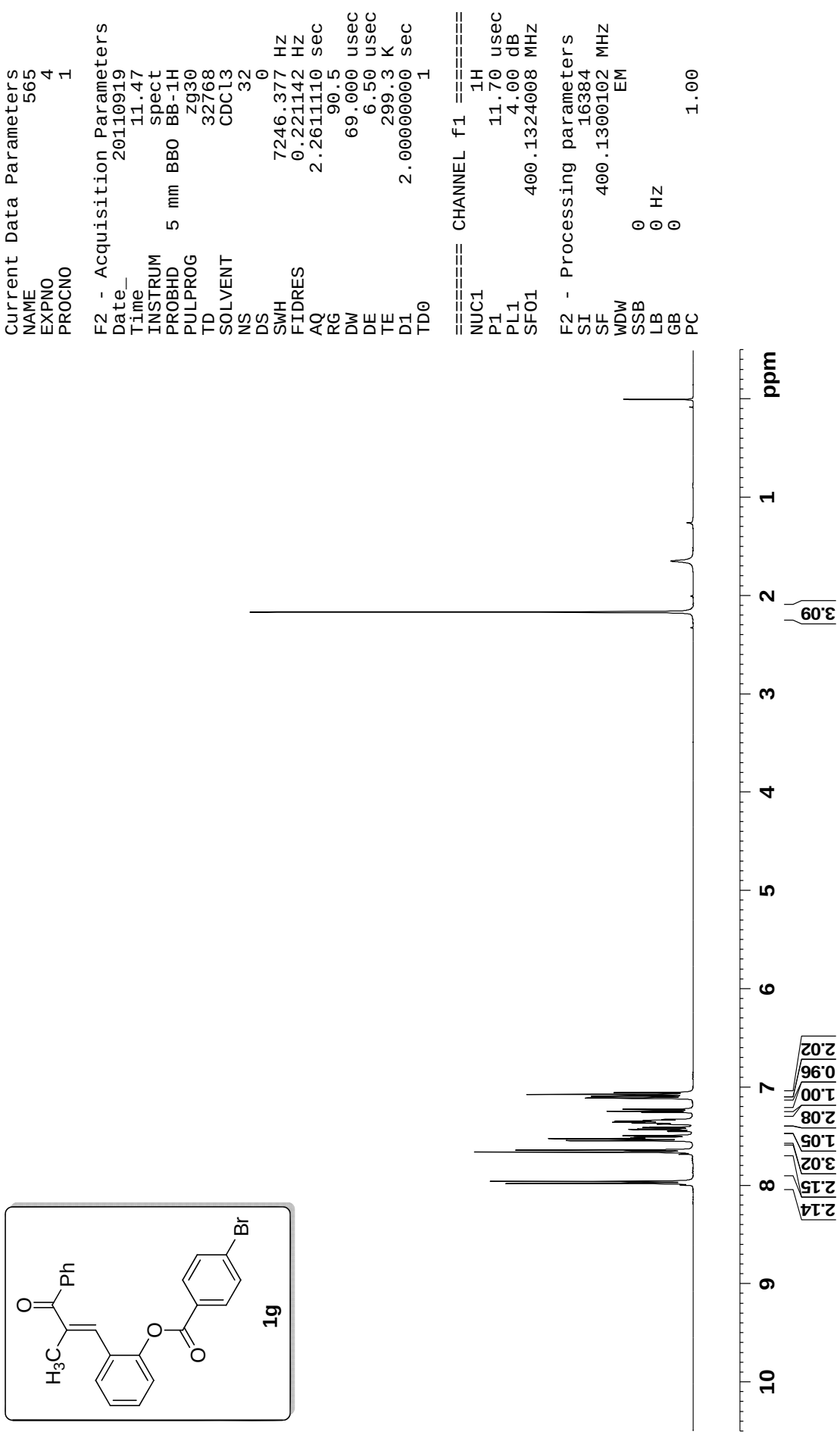

Current Data Parameters
NAME 534
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110929
Time 23.34
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 11075
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 9195.2
DW 20.800 usec
DE 6.50 usec
TE 301.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 3000
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
-0.03
76.68
77.00
77.32
115.12
115.85
124.34
124.63
126.36
126.49
128.03
128.81
129.37
130.44
131.83
132.57
133.98
134.92
145.80
146.06
154.18
162.99
187.25
ppm
20
40
60
80
100
120
140
160
180
200
Ph
O
NC
O
O
Br
O2N
127e

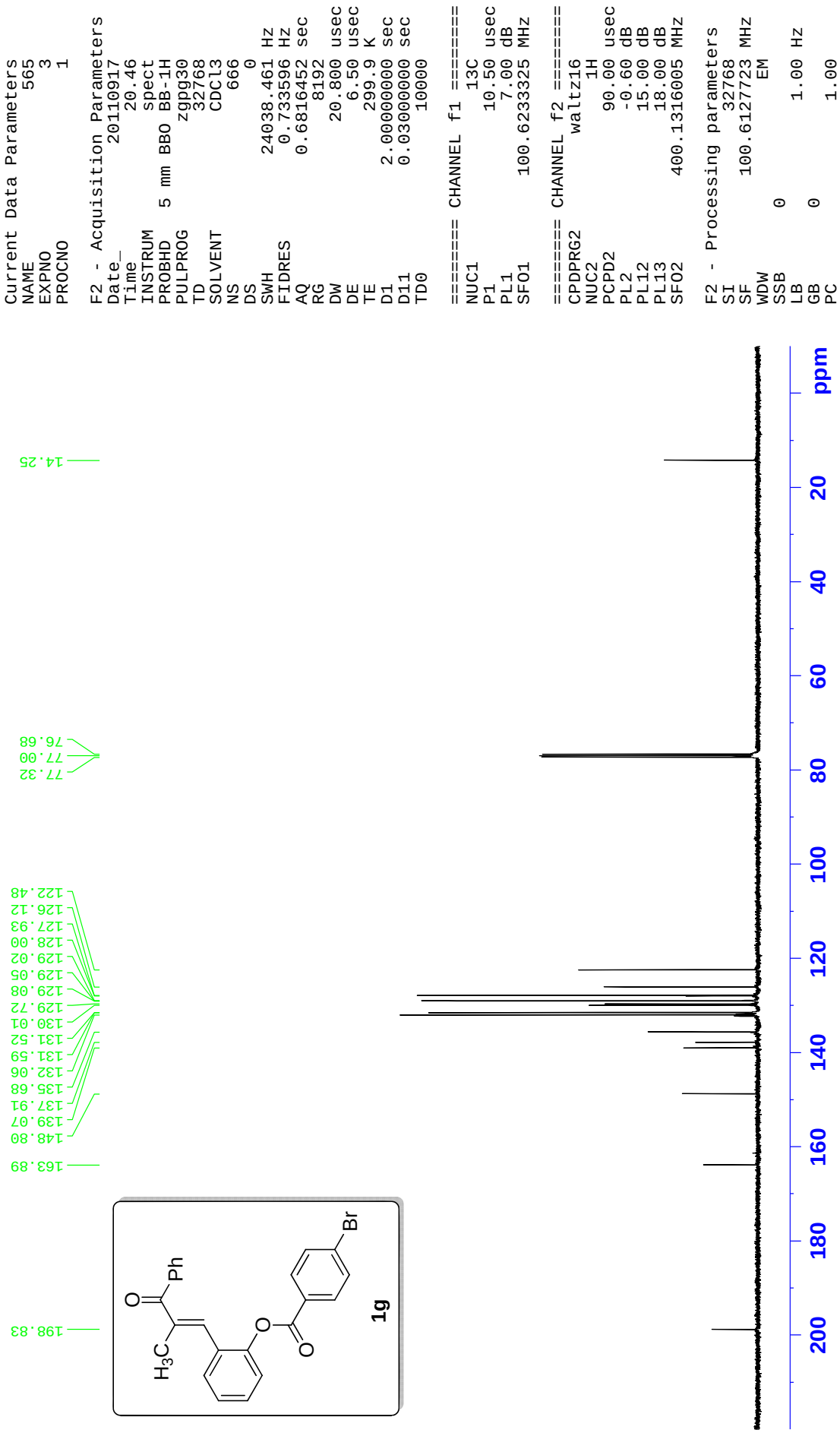


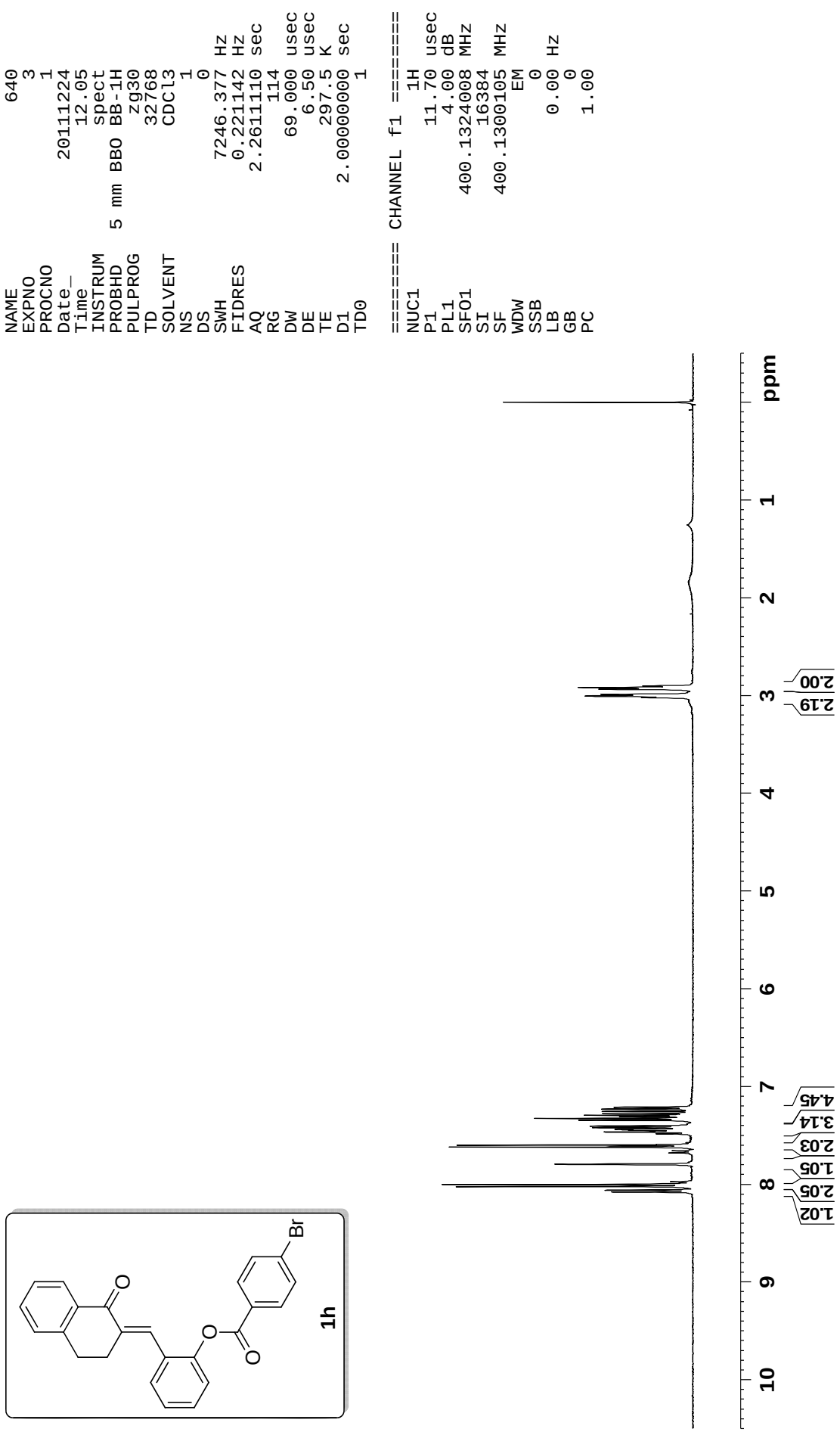


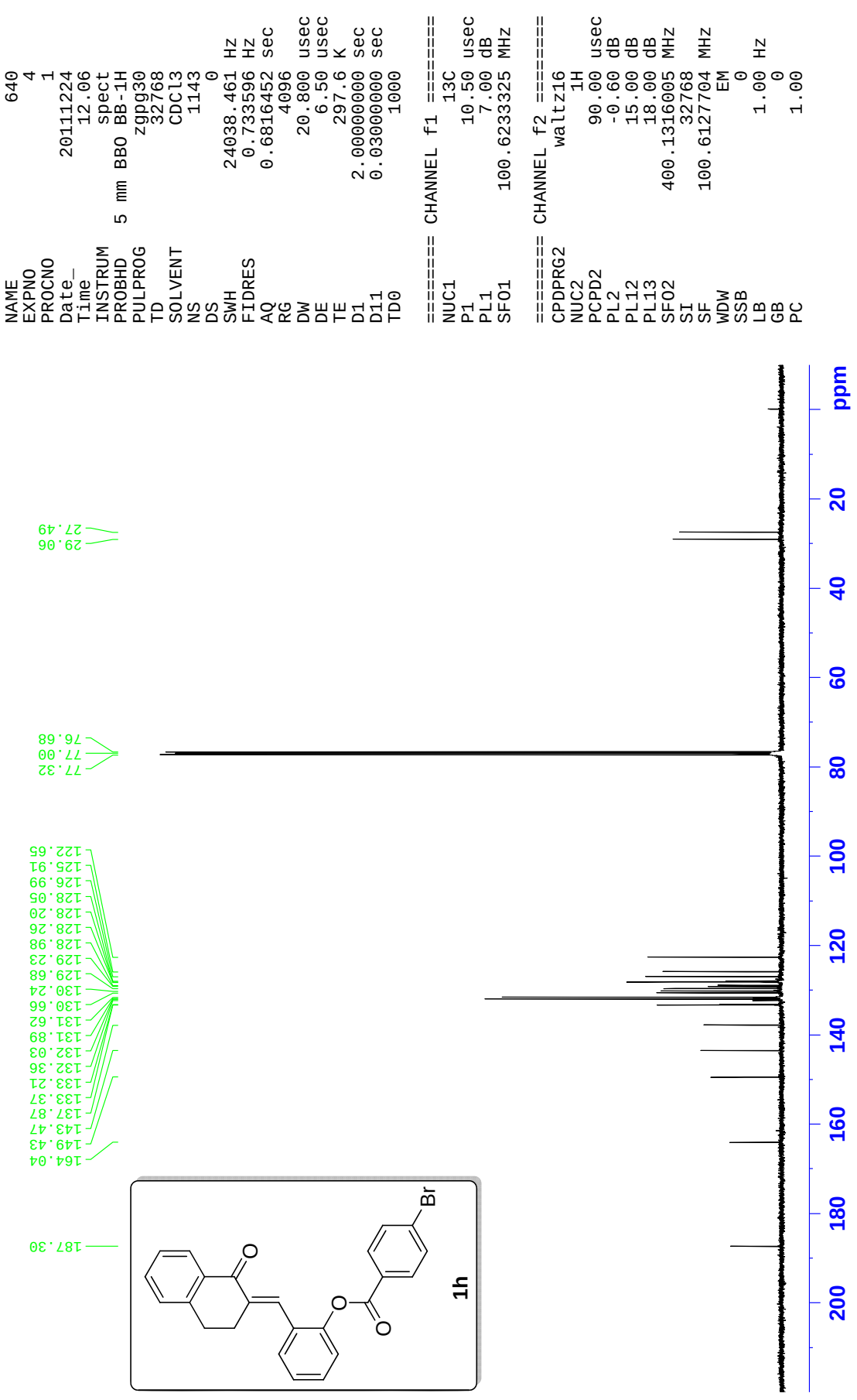

```
Current Data Parameters
NAME                   508
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20110816
Time                19.57
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  16384
SOLVENT             CDCl3
NS                      4
DS                      0
SWH              6009.615 Hz
FIDRES           0.366798 Hz
AQ              1.3632820 sec
RG                     64
DW                83.200 usec
DE                 6.50 usec
TE                299.5 K
D1             1.50000000 sec
MCREST   0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.70 usec
PL1                 4.00 dB
SFO1         400.1326008 MHz

F2 - Processing parameters
SI                  16384
SF           400.1300082 MHz
WDW                    EM
SSB      0
LB                 0.10 Hz
GB       0
PC                 1.00
```

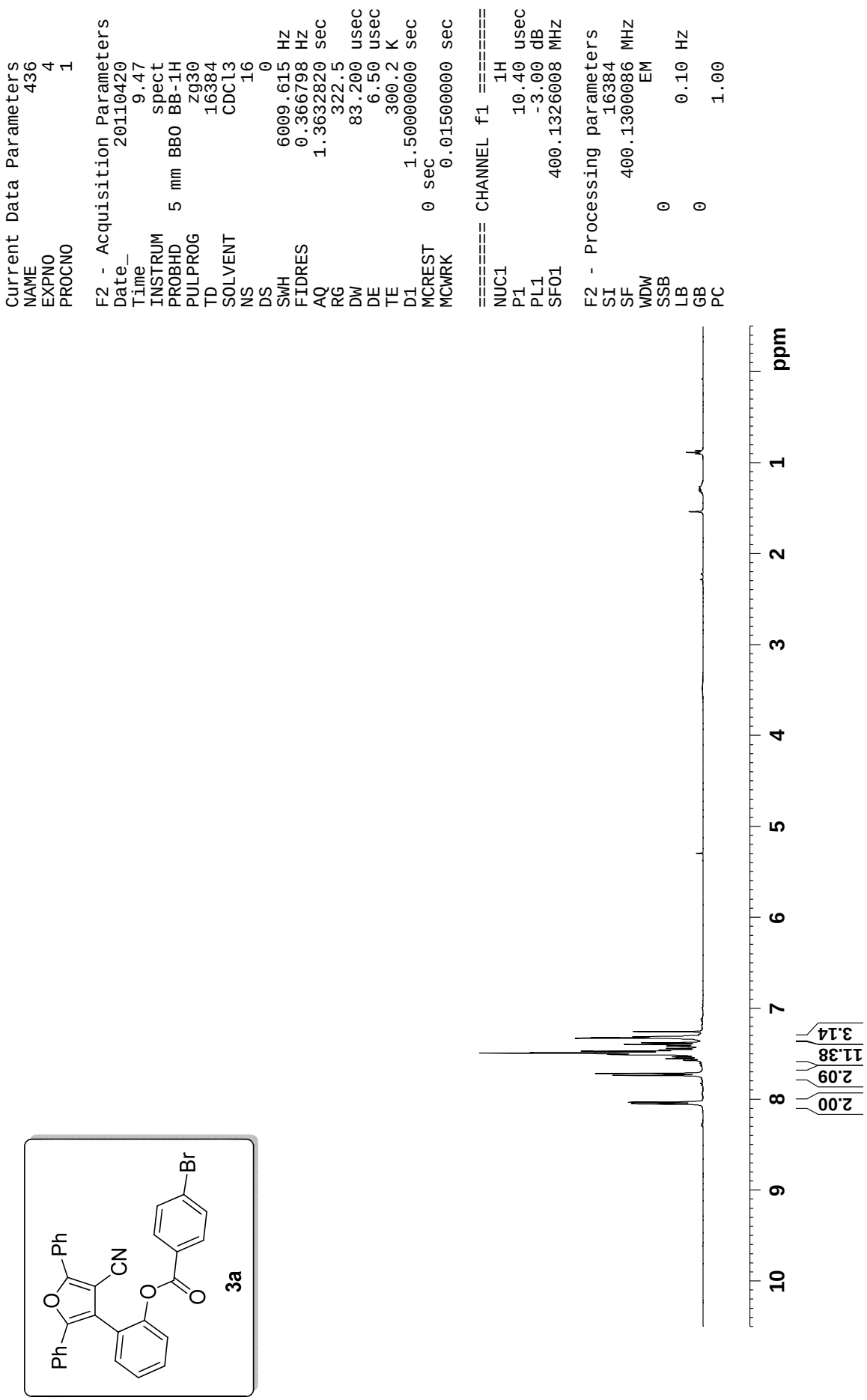

Current Data Parameters
NAME 508
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110816
Time 22.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 103
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 4096
DW 19.950 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127827 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
77.32
77.00
76.68
122.63
126.33
126.39
127.51
128.23
128.70
129.11
129.18
129.33
129.91
131.43
131.51
132.02
132.31
133.84
135.89
136.91
137.16
140.93
149.19
163.90
194.31
195.67
Ph
Ph
O
O
O
O
Br
1f
200
180
160
140
120
100
80
60
40
20
ppm

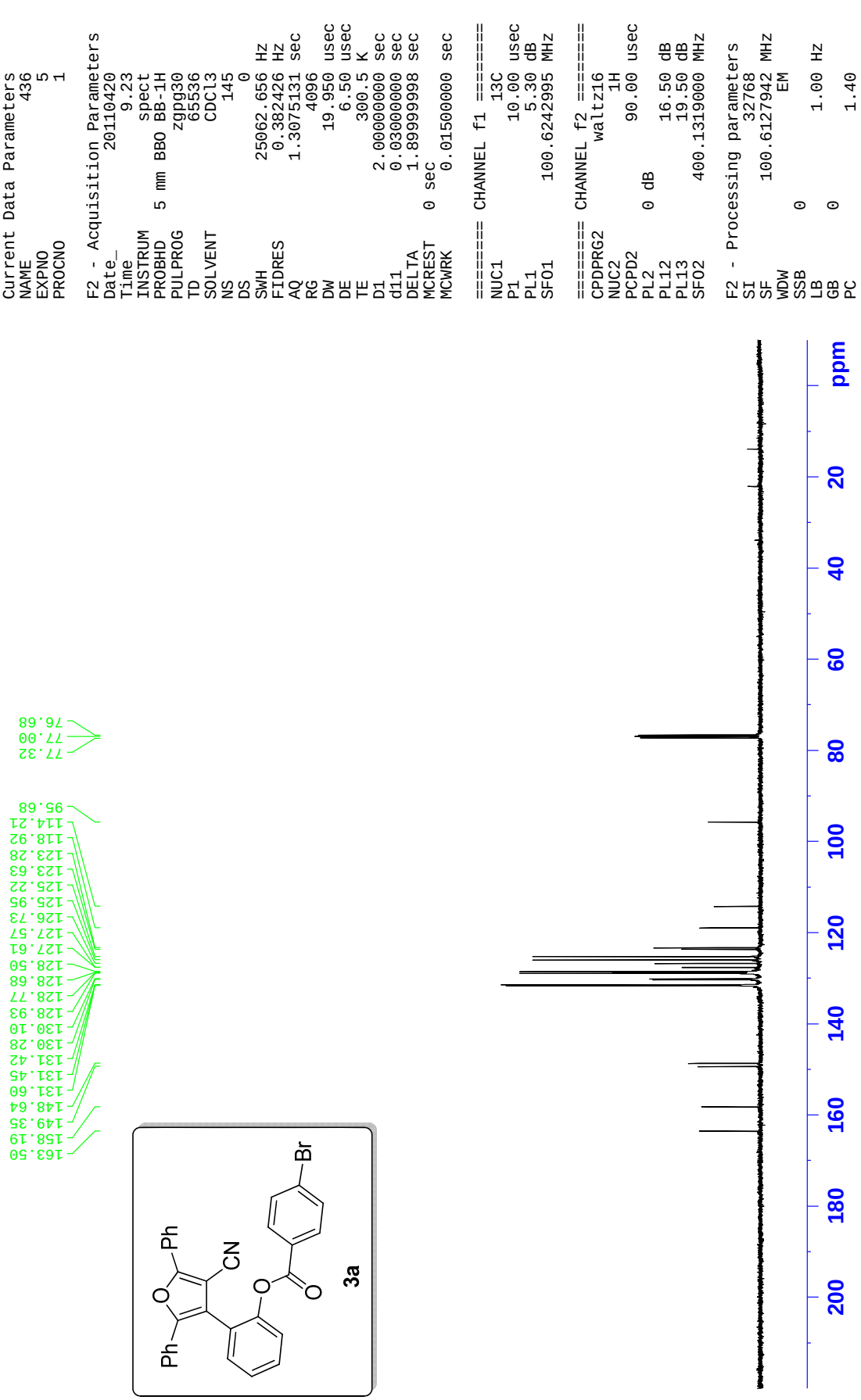


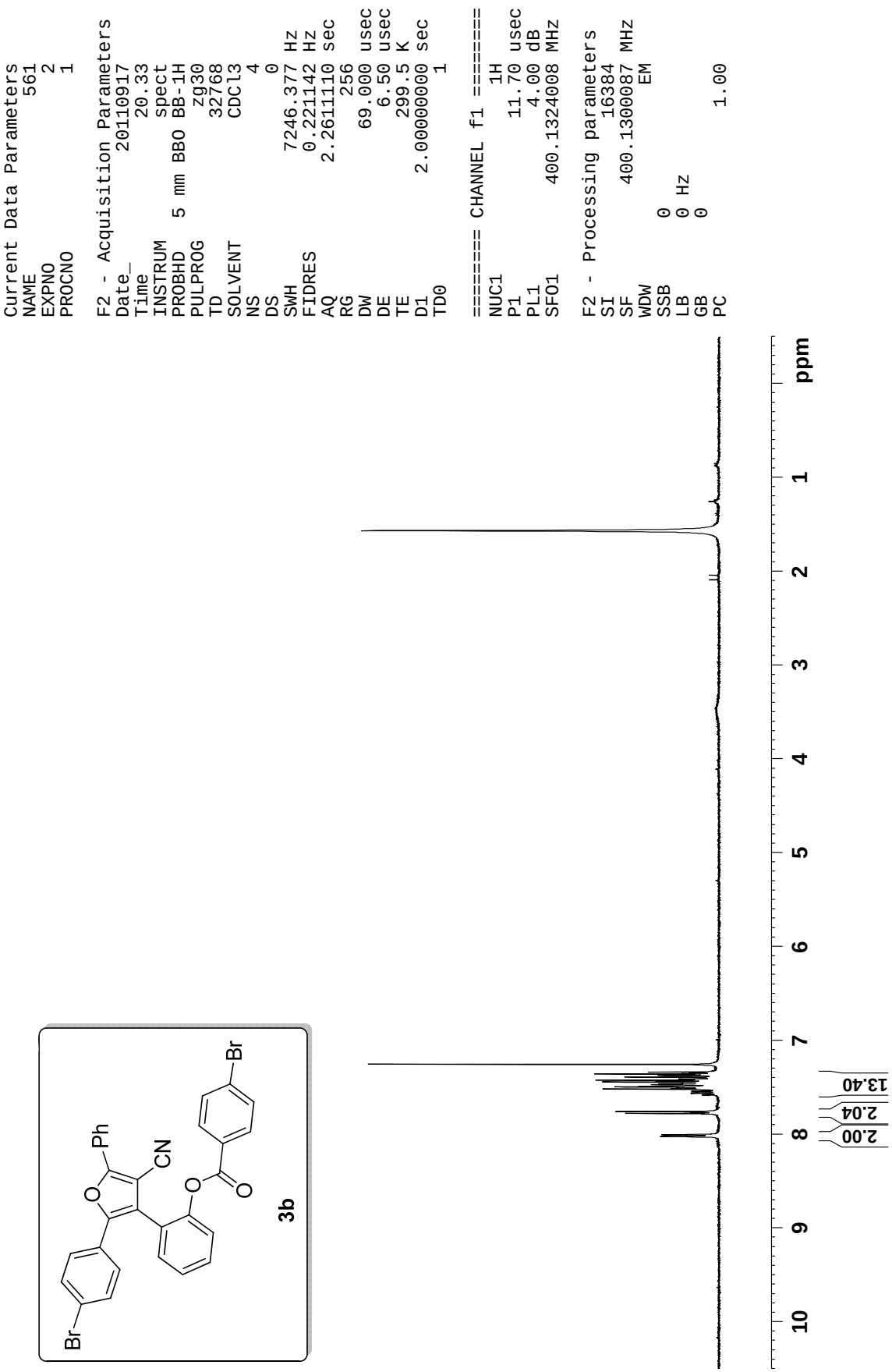

Current Data Parameters
NAME 565
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110917
Time 20.46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 666
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127723 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
14.25
77.32
77.00
76.68
122.48
126.12
127.93
128.00
129.02
129.05
129.08
129.72
130.01
131.52
131.59
132.06
135.68
137.91
139.07
148.80
163.89
198.83
O
Ph
H3C
O
O
Br
1g
200
180
160
140
120
100
80
60
40
20
ppm

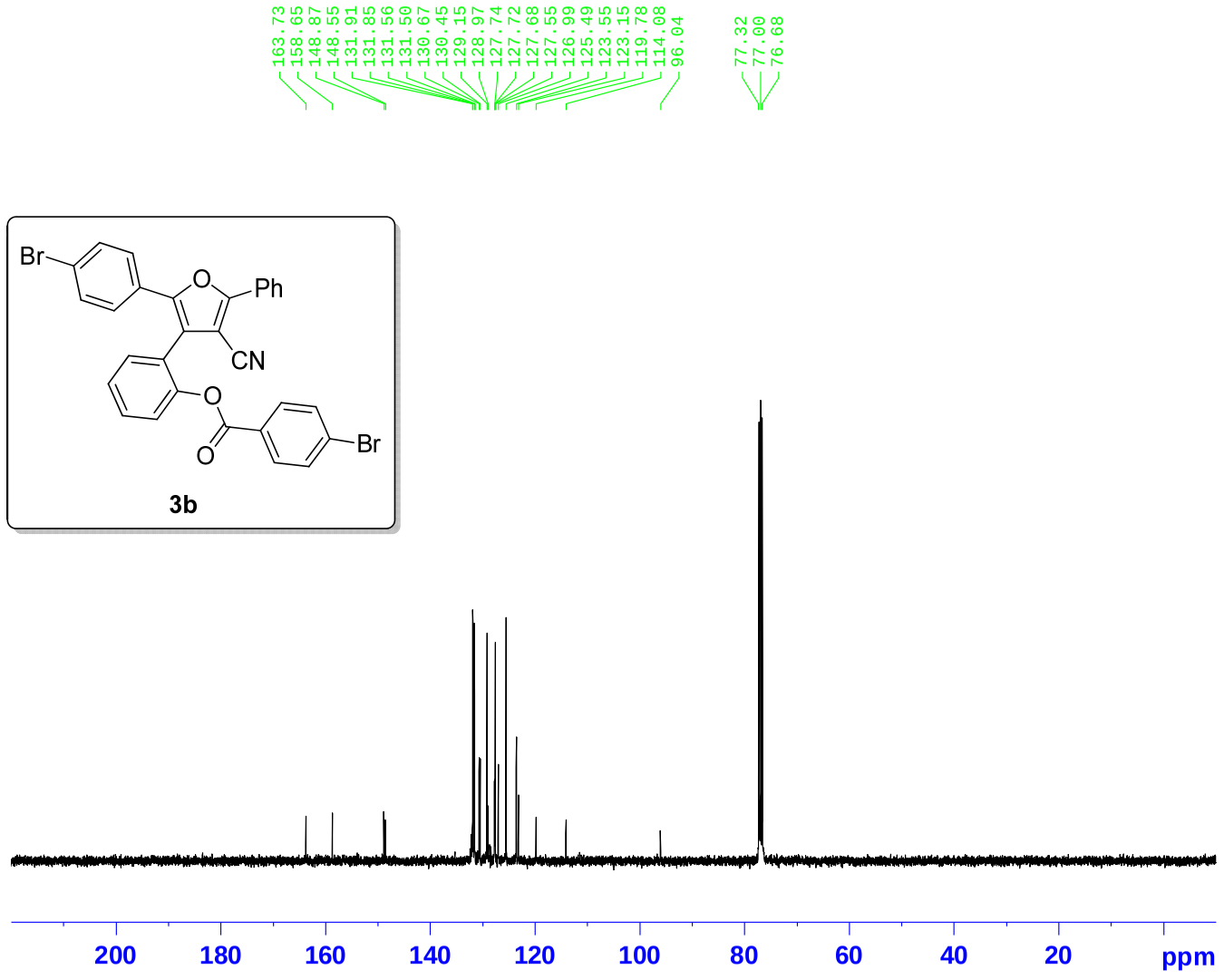




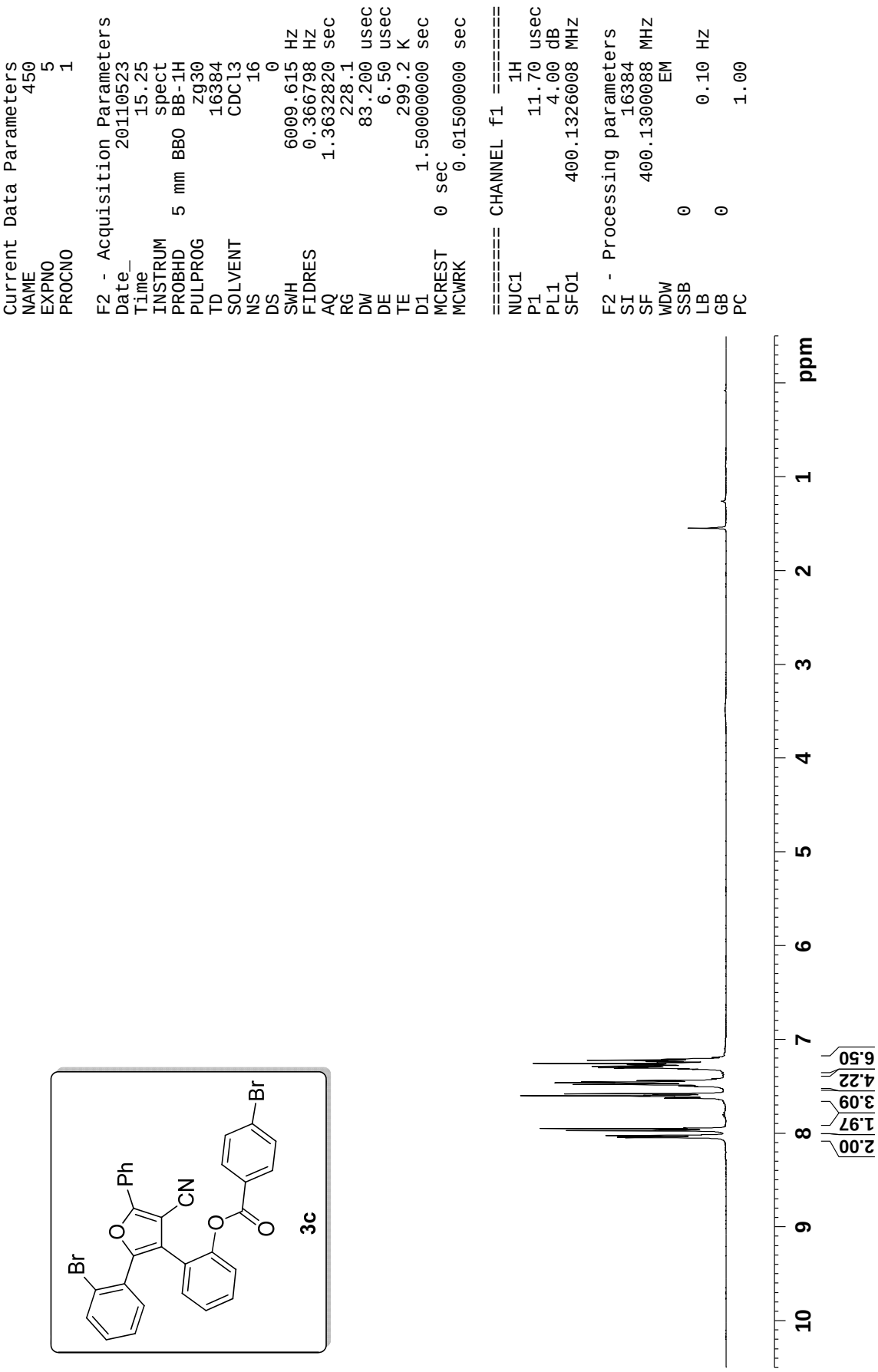

Current Data Parameters
NAME 436
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110420
Time 9.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 322.5
DW 83.200 usec
DE 6.50 usec
TE 300.2 K
D1 1.50000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.40 usec
PL1 -3.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
2.00
2.09
11.38
3.14
ppm
10
9
8
7
6
5
4
3
2
1
Ph
Ph
O
CN
O
O
Br
3a

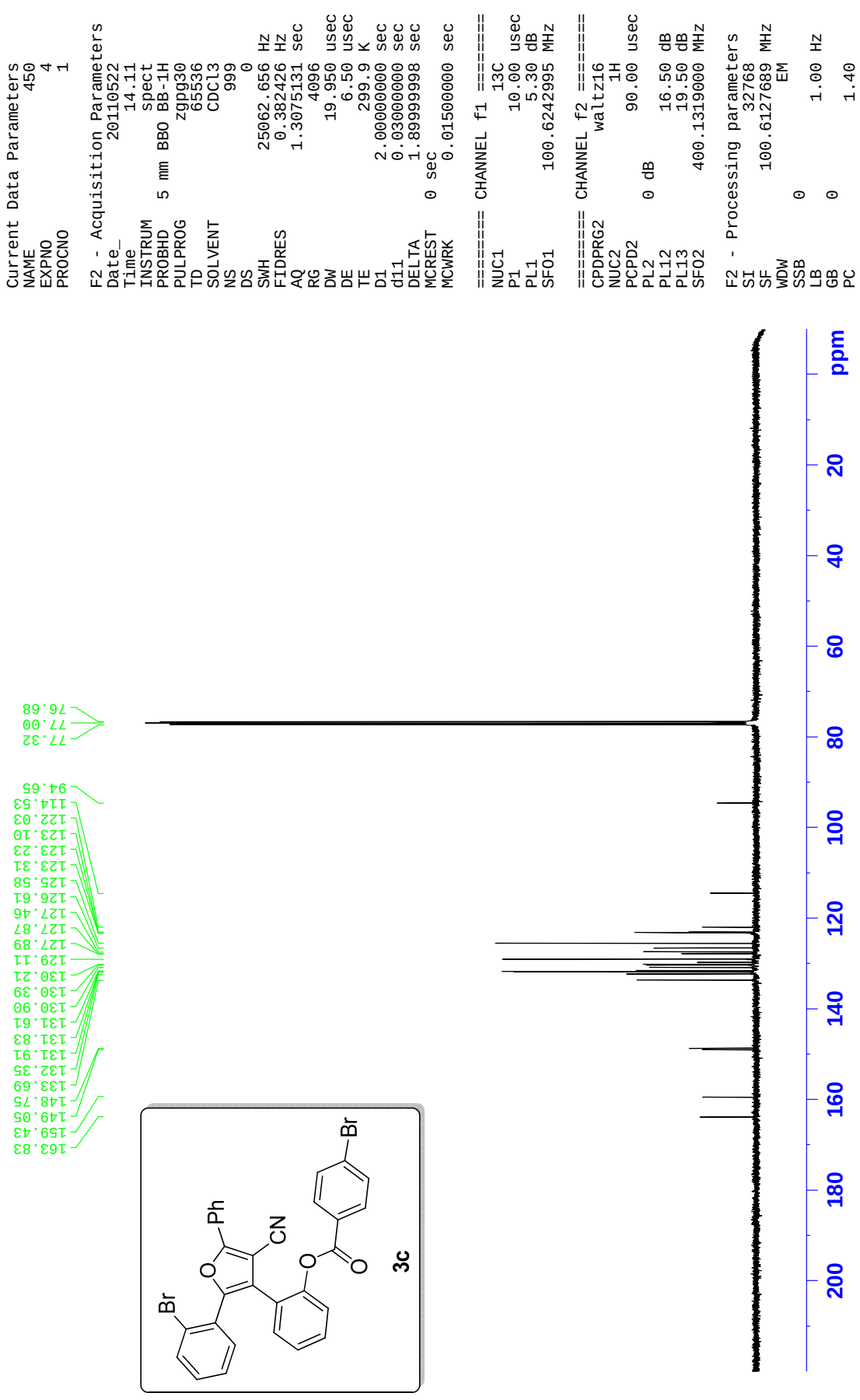

Current Data Parameters
NAME 436
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110420
Time 9.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 145
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 4096
DW 19.950 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0 dB 16.50 dB
PL12 19.50 dB
PL13
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127942 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
77.32
77.00
76.68
95.68
114.21
118.92
123.28
123.63
125.22
125.95
126.73
127.57
127.61
128.50
128.68
128.77
128.93
130.10
130.28
131.42
131.45
131.60
148.64
149.35
158.19
163.50
Ph
O
CN
Ph
O
O
Br
3a
200
180
160
140
120
100
80
60
40
20
ppm

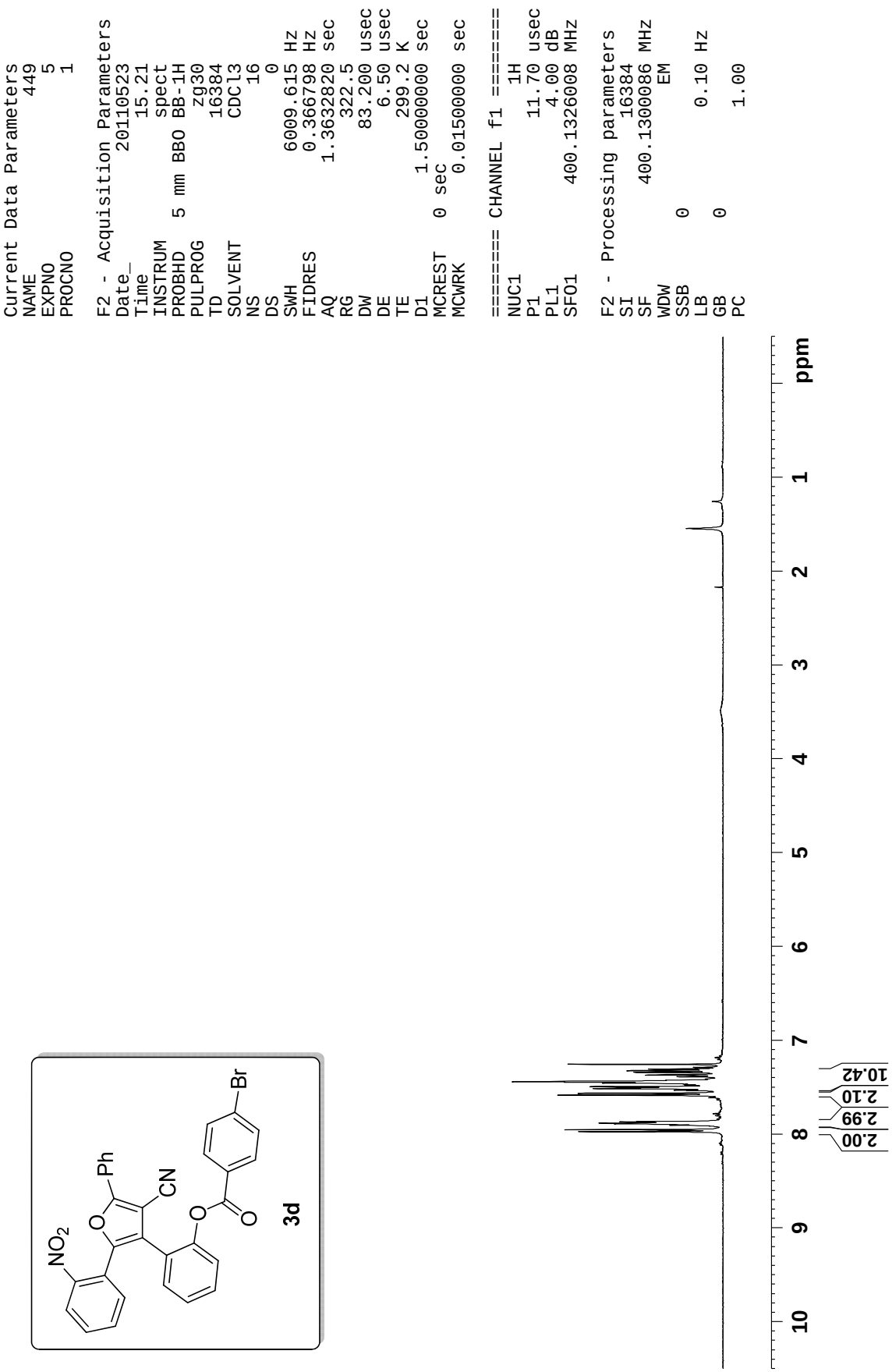

Current Data Parameters
NAME 561
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110917
Time 20.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300087 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
CN
O
O
O
Br
Br
3b
ppm
1
2
3
4
5
6
7
8
9
10
2.00
2.04
13.40

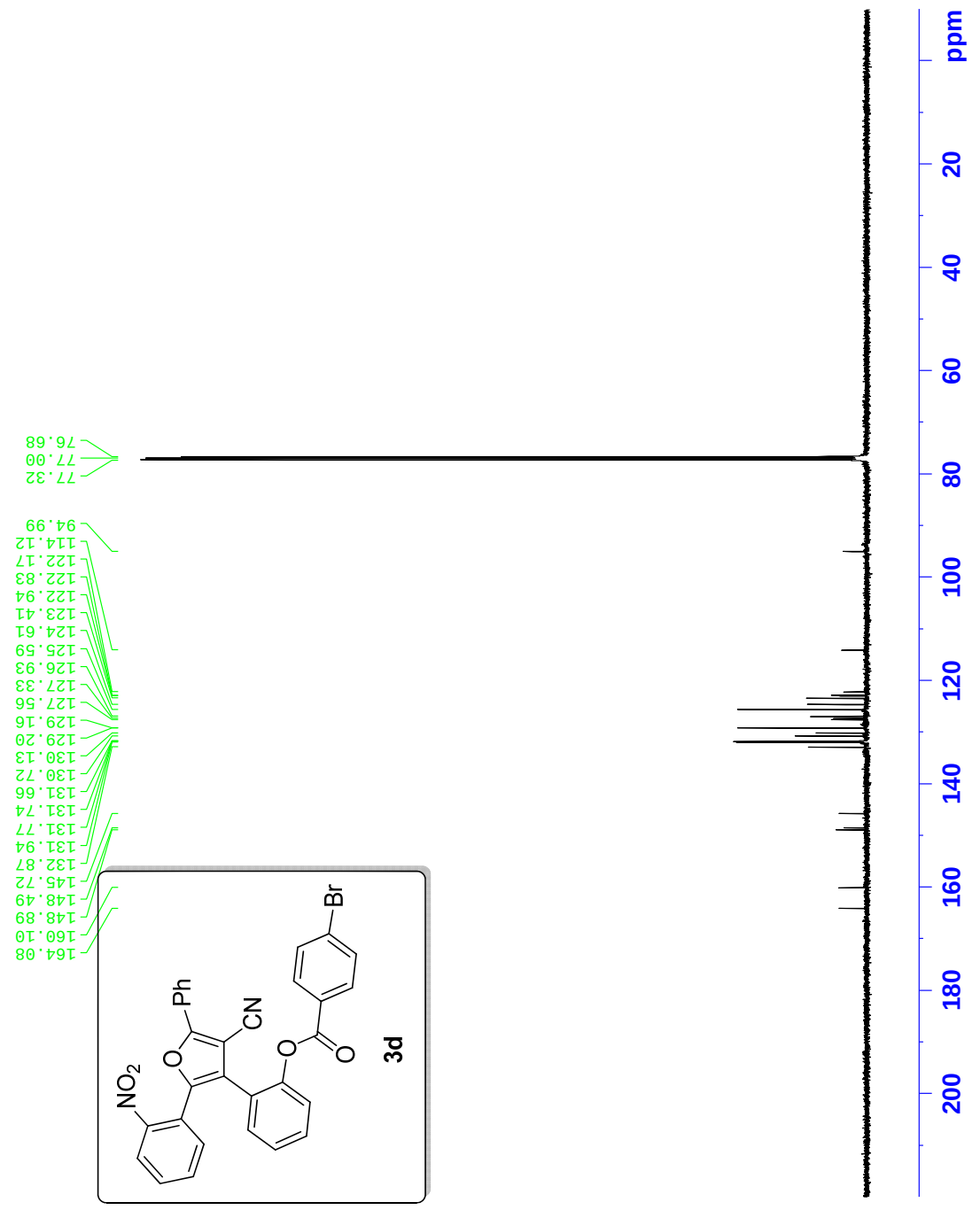


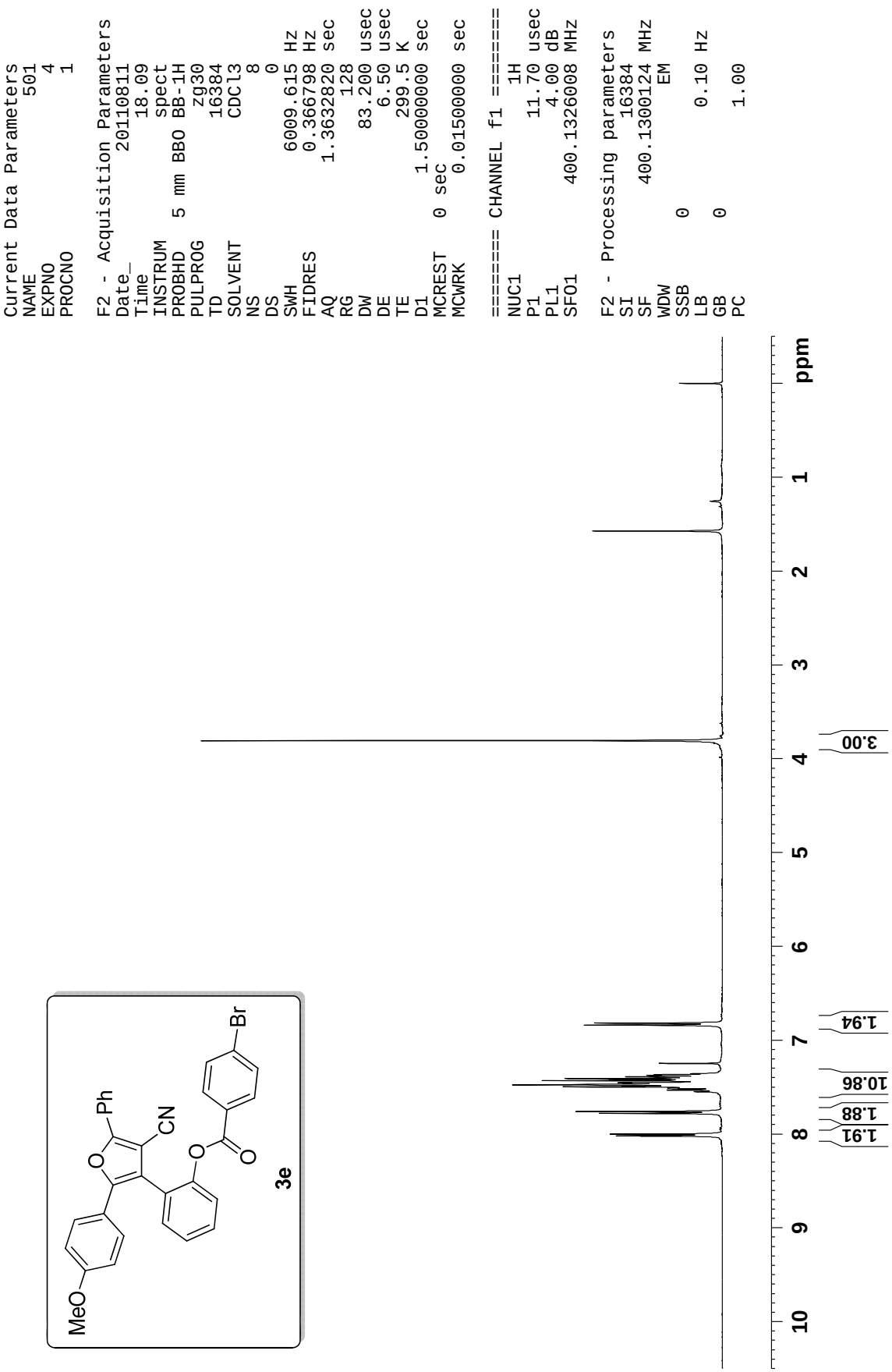

```
Current Data Parameters
NAME                   561
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_           20110917
Time               21.23
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  1000
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6816452 sec
RG                  8192
DW                20.800 usec
DE                 6.50 usec
TE                301.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                 1000

======== CHANNEL f1 ========
NUC1                13C
P1                10.50 usec
PL1                7.00 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2              90.00 usec
PL2                -0.60 dB
PL12               15.00 dB
PL13               18.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127680 MHz
WDW                EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.00
```

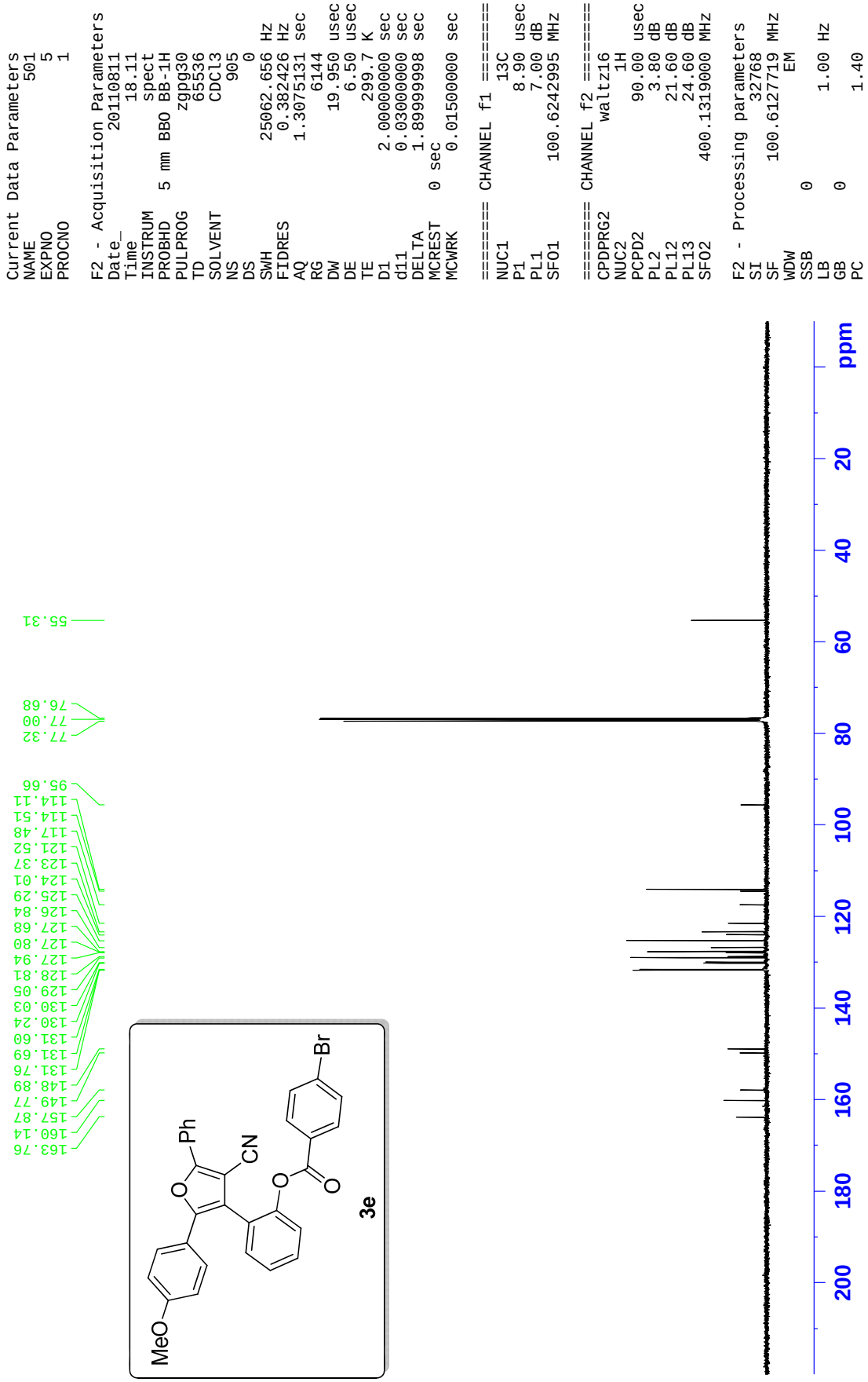

Current Data Parameters
NAME 450
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110523
Time 15.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 228.1
DW 83.200 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300088 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
Br
Ph
CN
O
O
O
Br
3c
2.00
1.97
3.09
4.22
6.50
10
9
8
7
6
5
4
3
2
1
ppm

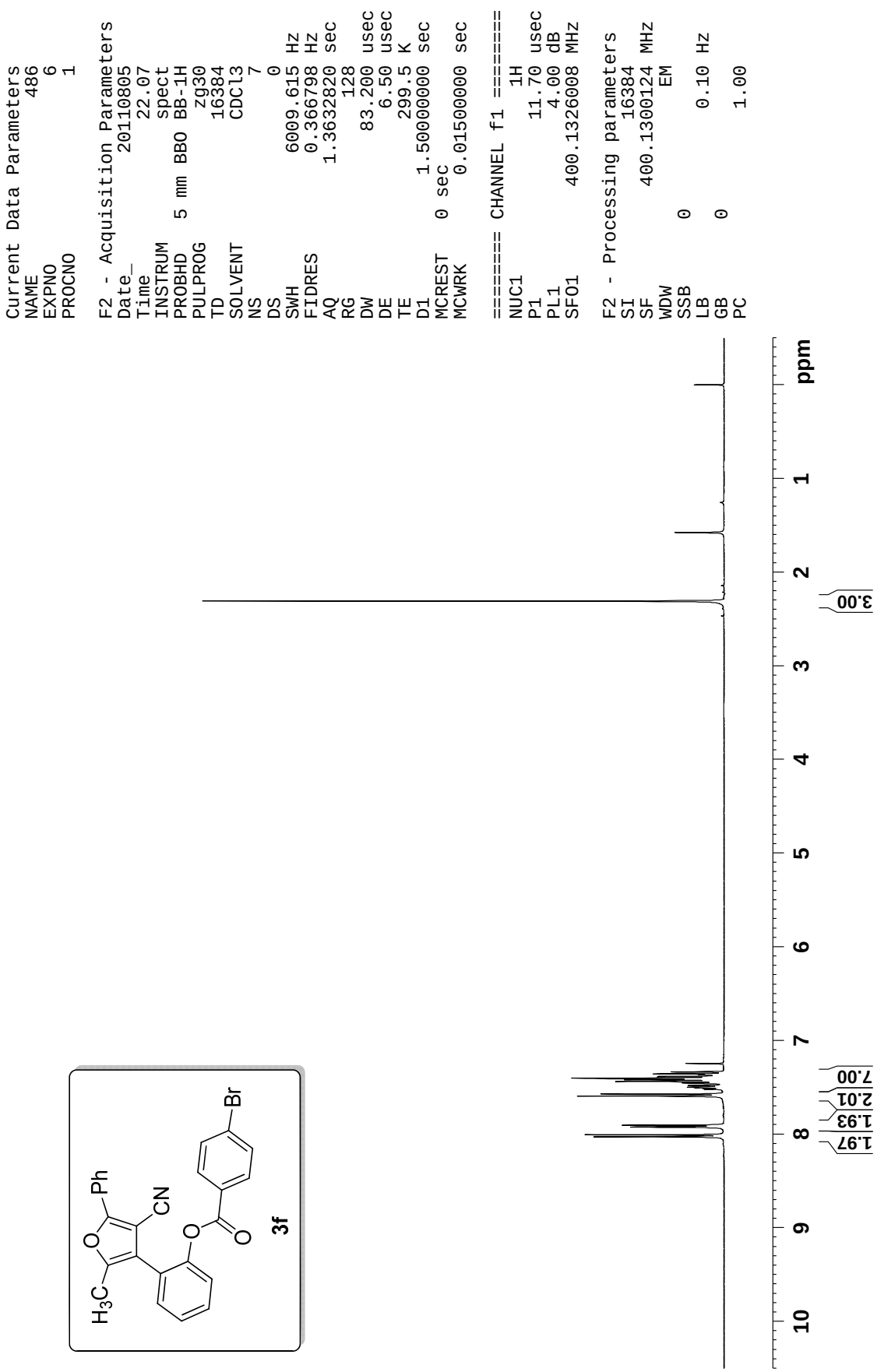

Current Data Parameters
NAME 450
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110522
Time 14.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 999
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 4096
DW 19.950 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0 dB 16.50 dB
PL12 19.50 dB
PL13
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
77.32
77.00
76.68
94.65
114.53
122.03
123.10
123.23
123.31
125.58
126.61
127.46
127.87
127.89
129.11
130.21
130.39
130.90
131.61
131.83
131.91
132.35
133.69
148.75
149.05
159.43
163.83
Br
O
Ph
CN
O
O
Br
3c
200
180
160
140
120
100
80
60
40
20
ppm

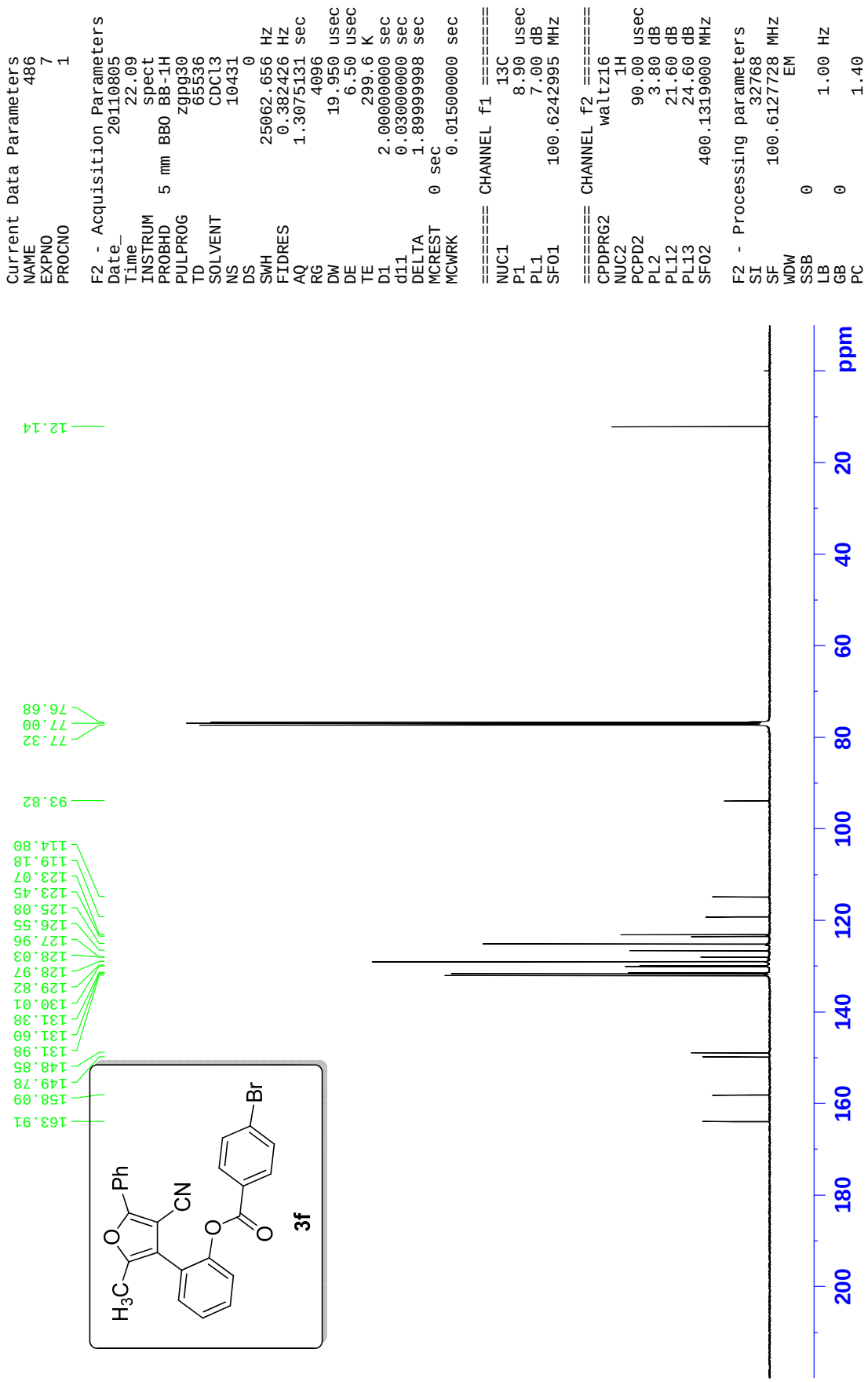

Current Data Parameters
NAME 449
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110523
Time 15.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 322.5
DW 83.200 usec
DE 6.50 usec
TE 299.2 K
D1 1.50000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
Br
O
O
CN
Ph
O
NO2
3d
2.00
2.99
2.10
10.42
10
9
8
7
6
5
4
3
2
1
ppm

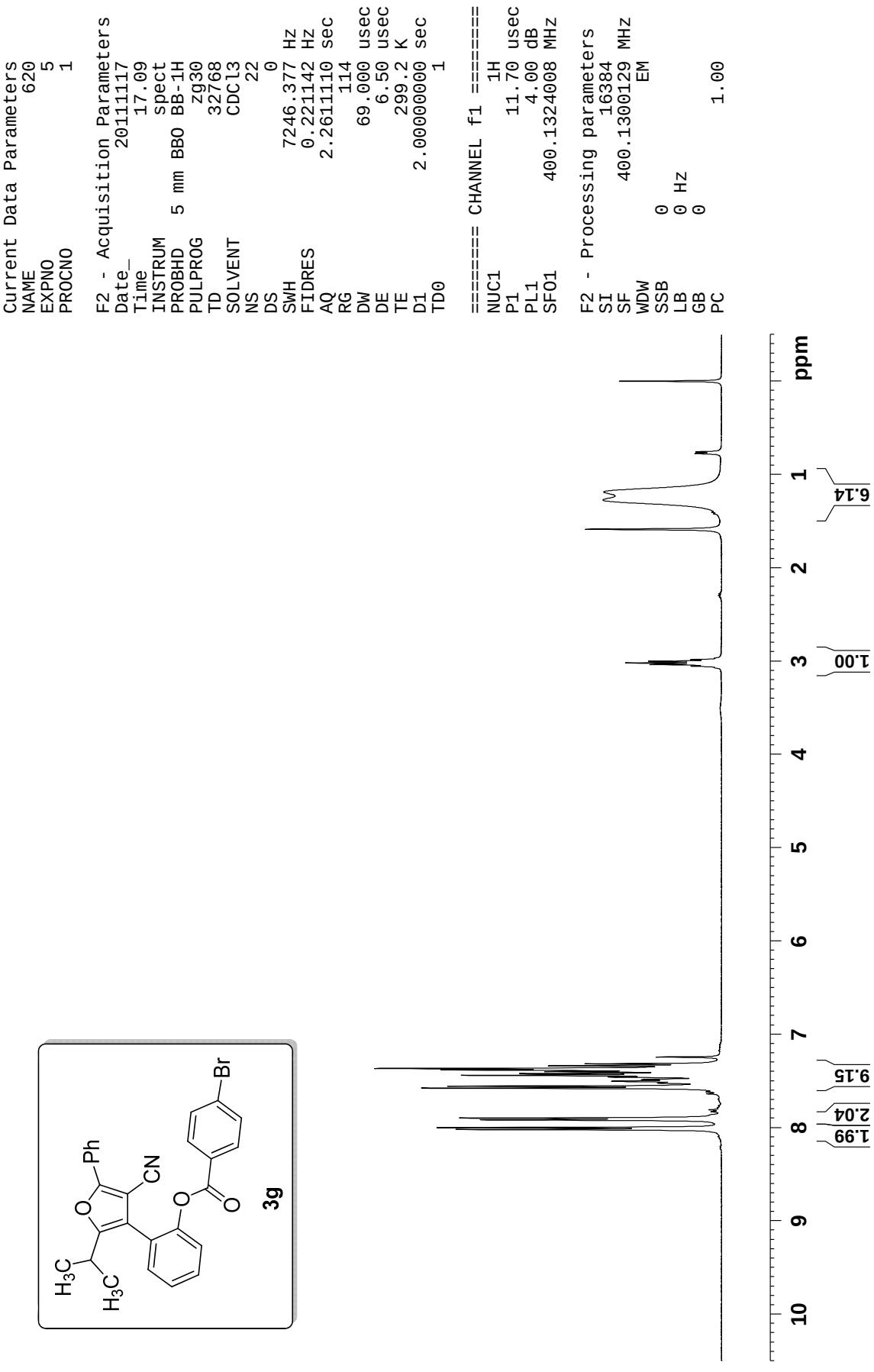

Current Data Parameters
NAME 449
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110522
Time 22.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1600
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 4096
DW 19.950 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127697 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
77.32
77.00
76.68
164.08
160.10
148.89
148.49
145.72
132.87
131.94
131.77
131.74
131.66
130.72
130.13
129.20
129.16
127.56
127.33
126.93
125.59
124.61
123.41
122.94
122.83
122.17
114.12
94.99
Ph
CN
O
O
O
Br
NO2
3d
200
180
160
140
120
100
80
60
40
20
ppm




Current Data Parameters
NAME 501
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110811
Time 18.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 905
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 6144
DW 19.950 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127719 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
55.31
76.68
77.00
77.32
95.66
114.11
114.51
117.48
121.52
123.37
124.01
125.29
126.84
127.68
127.80
127.94
128.81
129.05
130.03
130.24
131.60
131.69
131.76
148.89
149.77
157.87
160.14
163.76
MeO
Ph
O
CN
O
O
Br
3e
200
180
160
140
120
100
80
60
40
20
ppm


Current Data Parameters
NAME 486
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110805
Time 22.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 7
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE 299.5 K
D1 1.50000000 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300124 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
ppm
1 2 3 4 5 6 7 8 9 10
3.00
1.97
1.93
2.01
7.00
Ph
CN
O
O
O
Br
H3C
3f


Current Data Parameters
NAME 486
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110805
Time 22.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 10431
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 4096
DW 19.950 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127728 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
12.14
76.68
77.00
77.32
93.82
114.80
119.18
123.07
123.45
125.08
126.55
127.96
128.03
128.97
129.82
130.01
131.38
131.60
131.98
148.85
149.78
158.09
163.91
Ph
CN
O
O
O
Br
H3C
3f
ppm
200
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME 620
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111117
Time 17.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 22
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300129 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
CN
O
O
O
Br
H3C
H3C
3g
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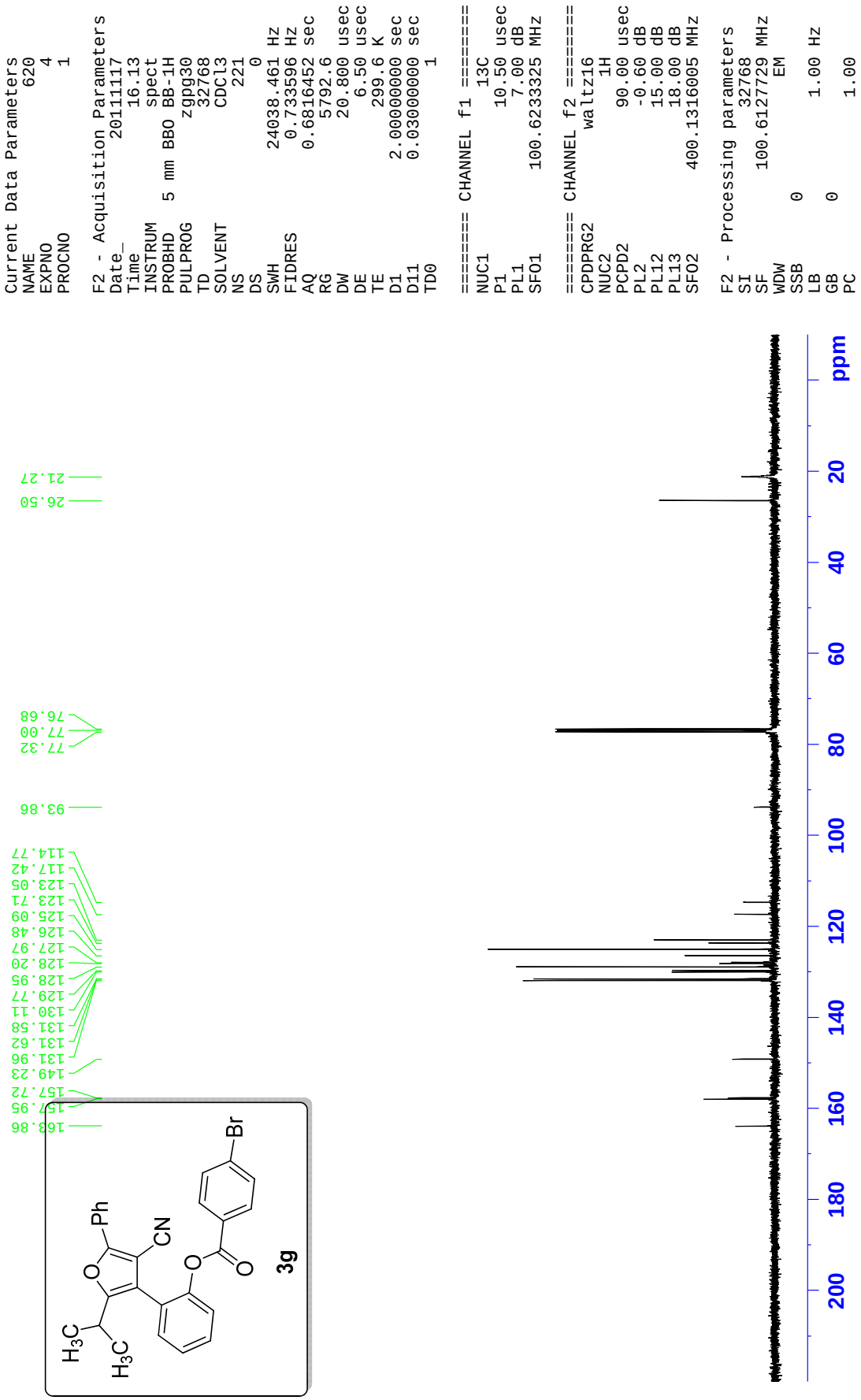
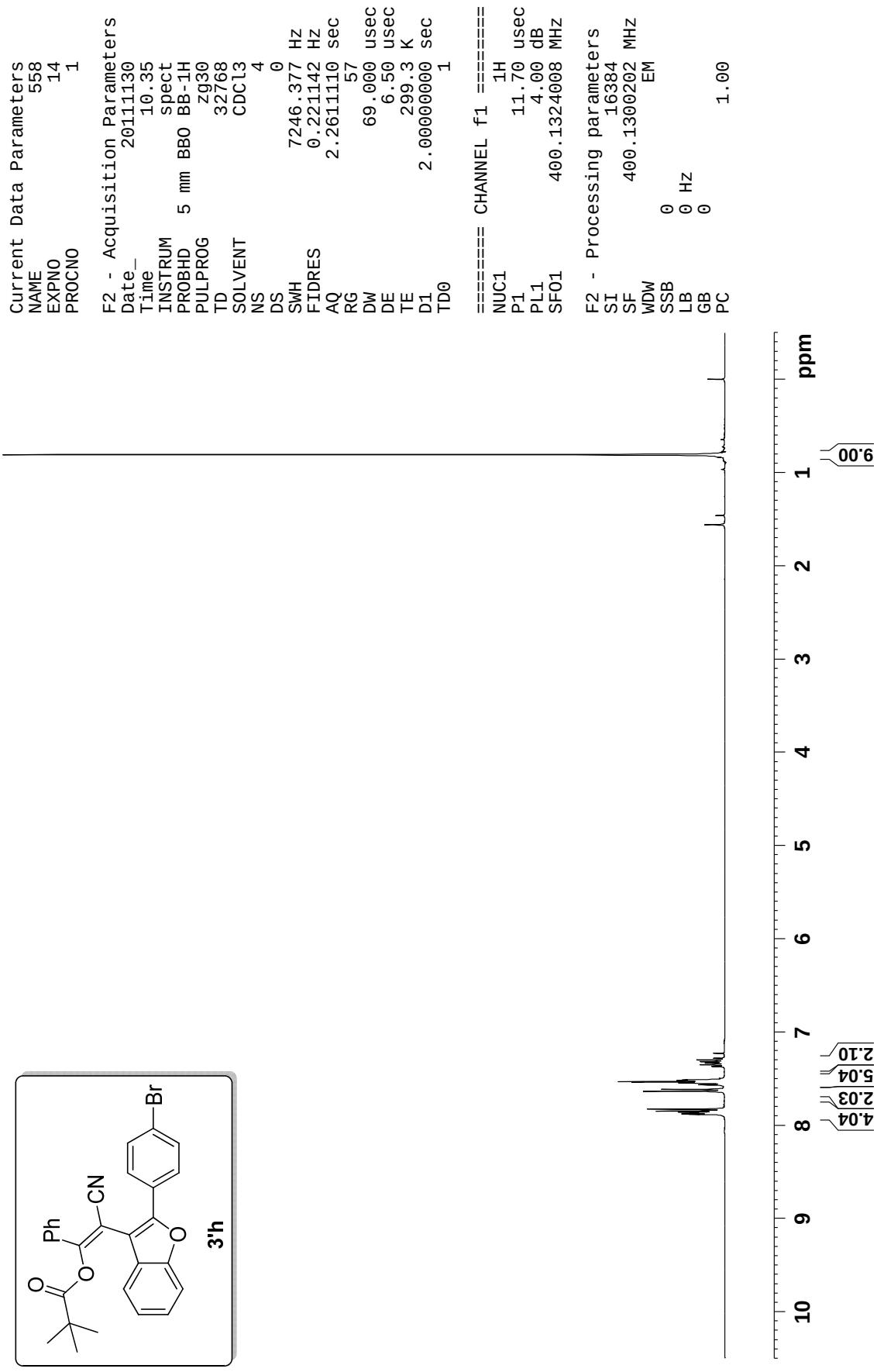
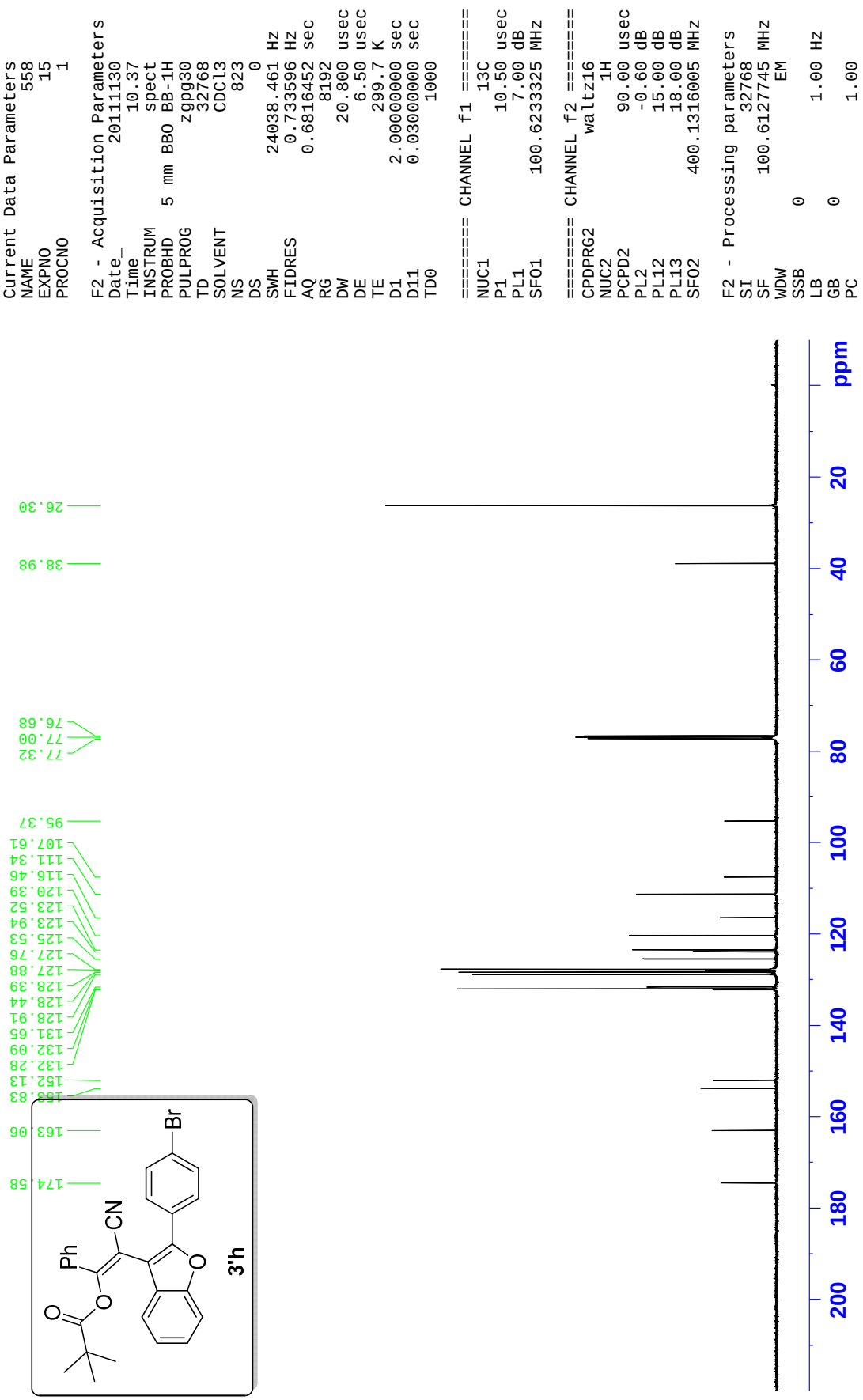
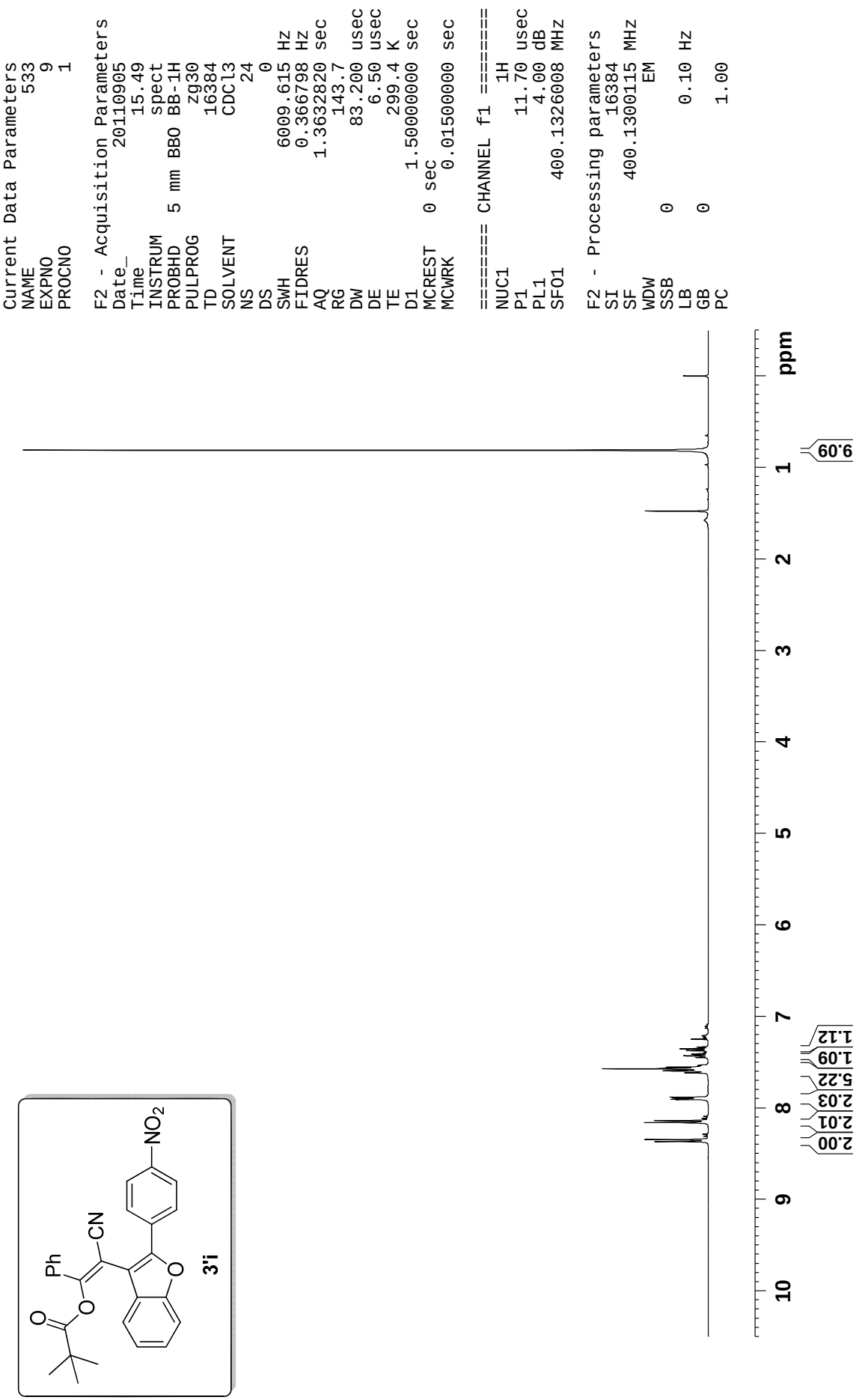
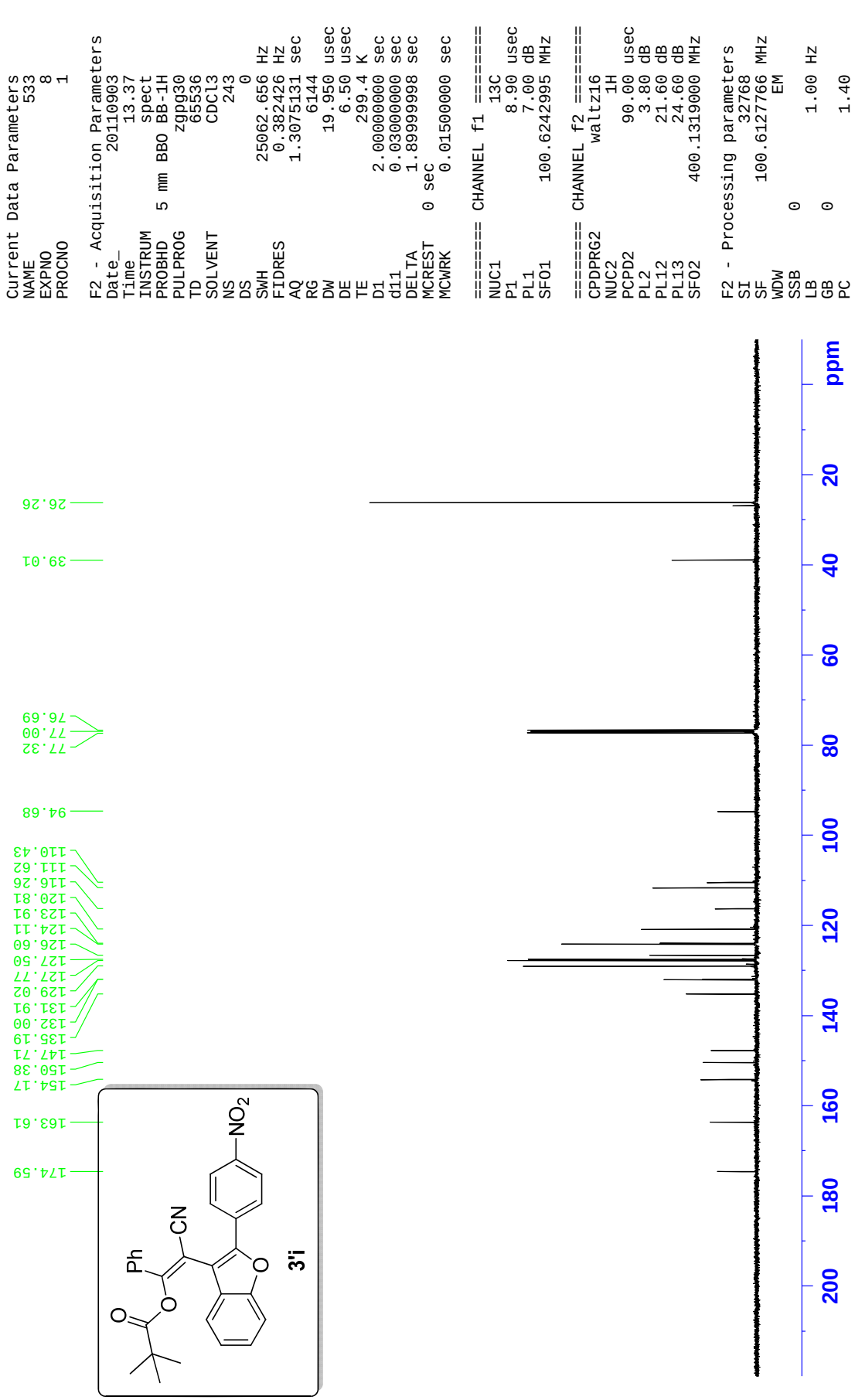
9
10
6.14
1.00
9.15
2.04
1.99

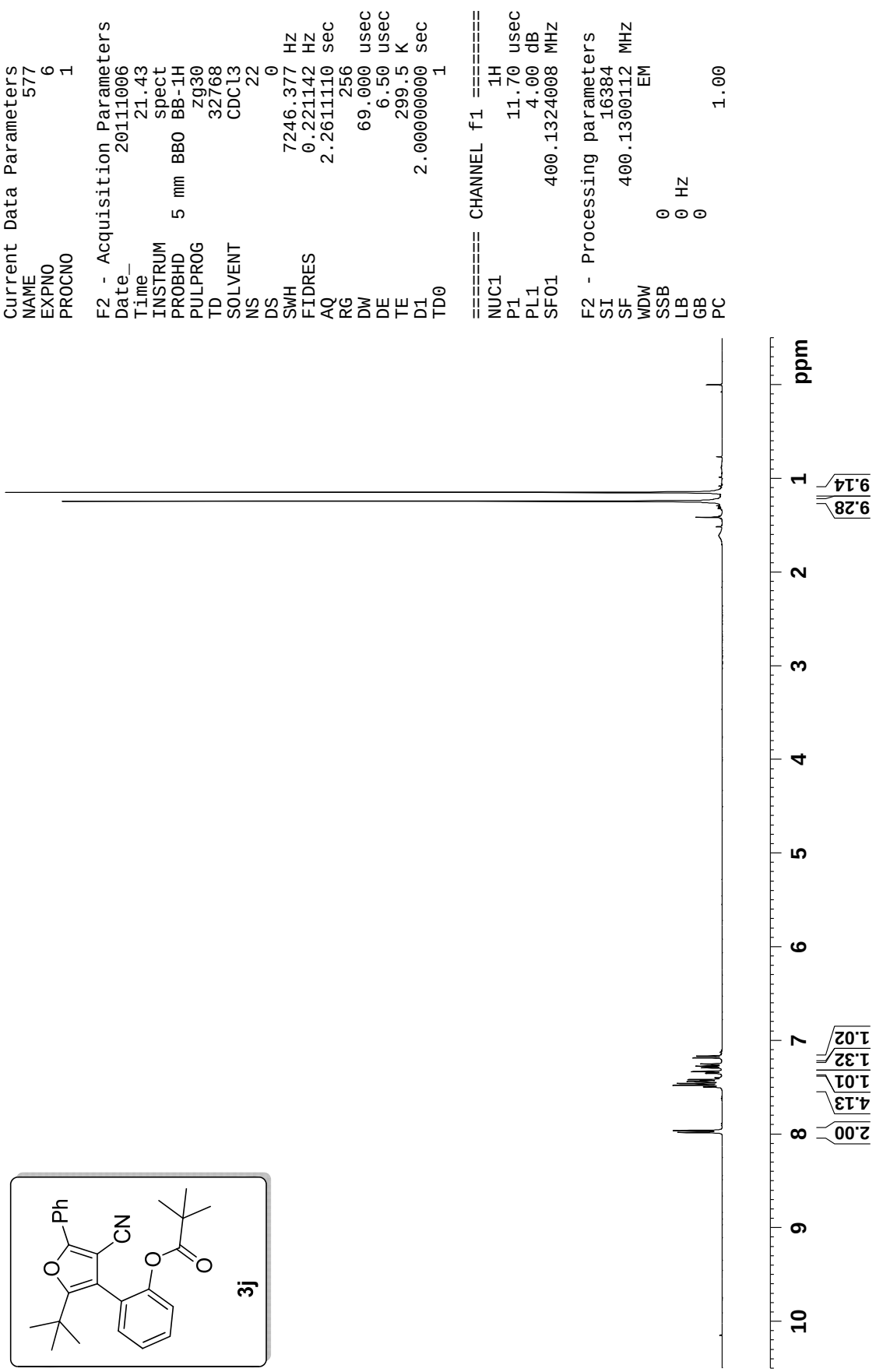

Current Data Parameters
NAME 620
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111117
Time 16.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 221
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
21.27
26.50
76.68
77.00
77.32
93.86
114.77
117.42
123.05
123.71
125.09
126.48
127.97
128.20
128.95
129.77
130.11
131.58
131.62
131.96
149.23
157.72
157.95
163.86
Ph
CN
Br
O
O
O
H3C
H3C
3g
ppm
200
180
160
140
120
100
80
60
40
20

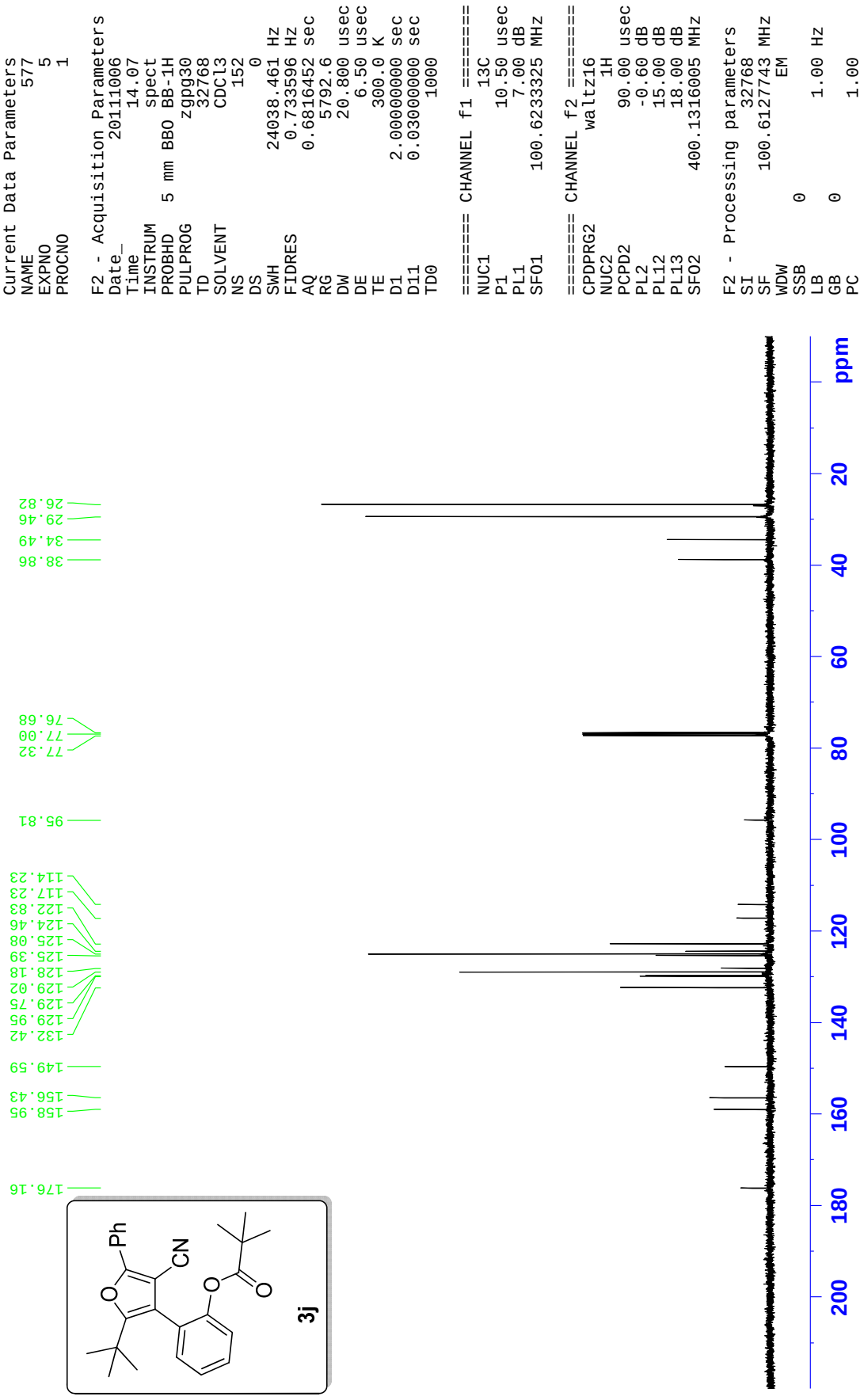


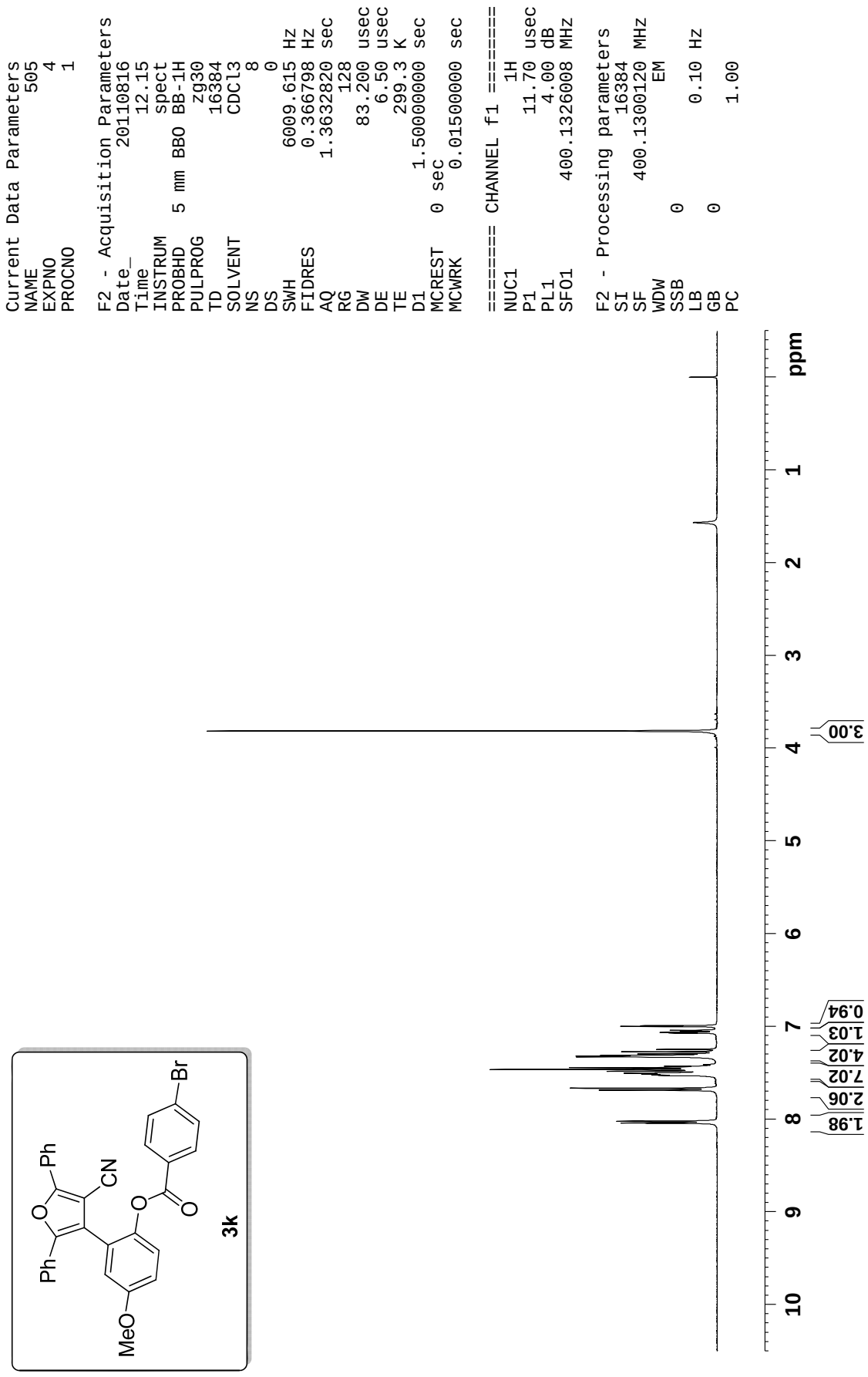


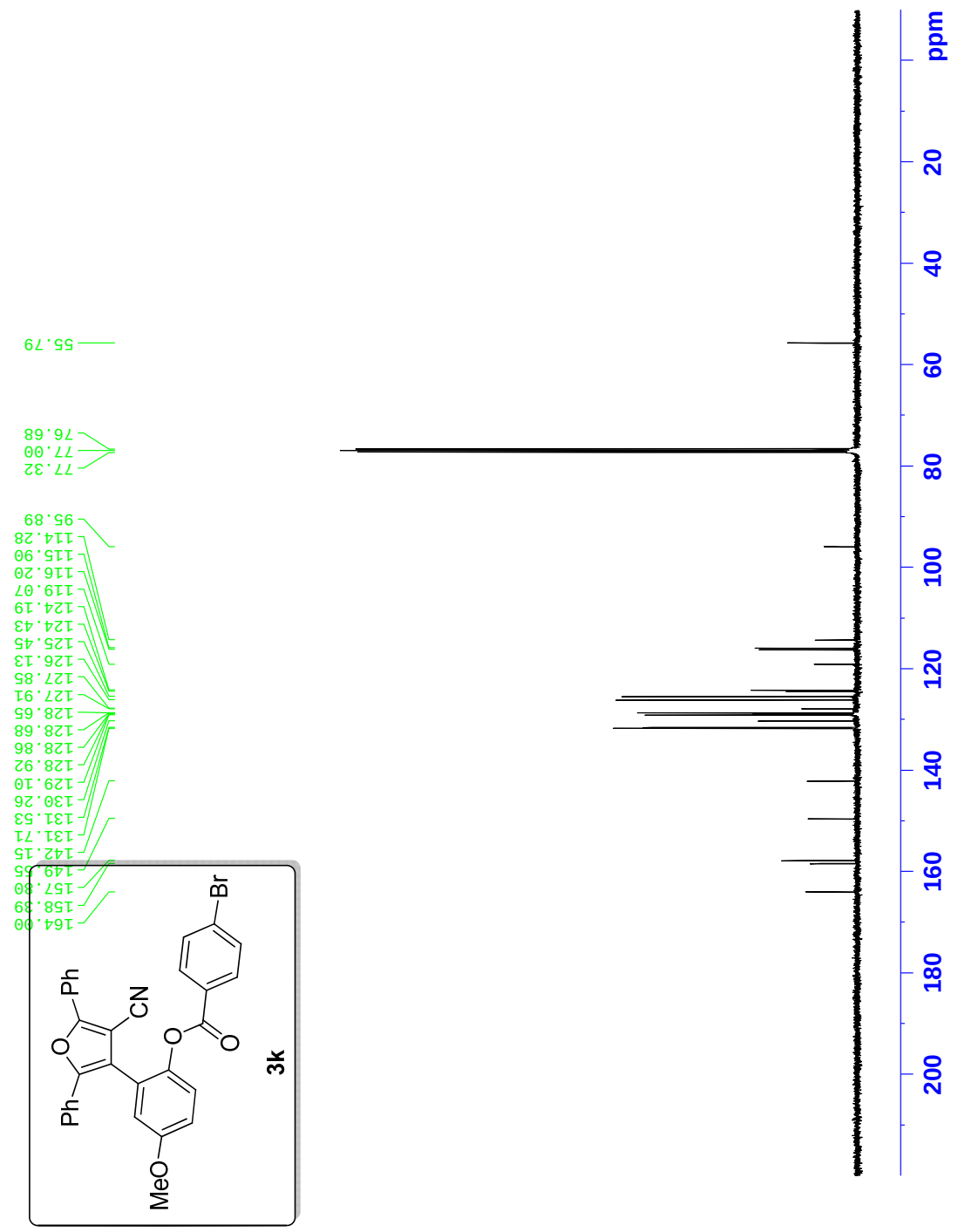

Current Data Parameters
NAME 533
EXPNO 9
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110905
Time 15.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 24
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 143.7
DW 83.200 usec
DE 6.50 usec
TE 299.4 K
D1 1.50000000 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300115 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
2.00
2.01
2.03
5.22
1.09
1.12
9.09
ppm
10
9
8
7
6
5
4
3
2
1
Ph
CN
O
O
O
NO2
3'i

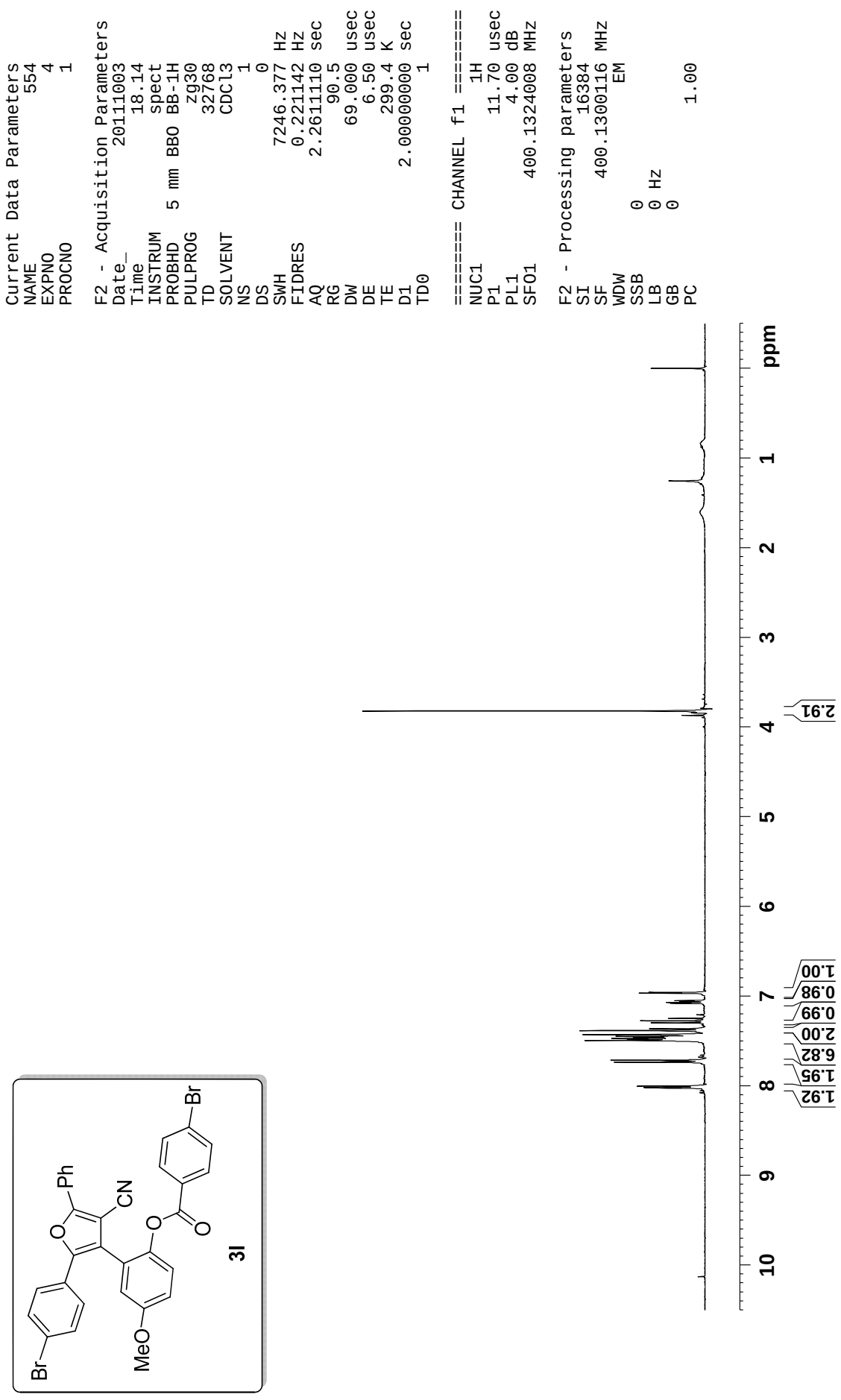

Current Data Parameters
NAME 533
EXPNO 8
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110903
Time 13.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 243
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 6144
DW 19.950 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1319000 MHz
F2 - Processing parameters
SI 32768
SF 100.6127766 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
26.26
39.01
76.69
77.00
77.32
94.68
110.43
111.62
116.26
120.81
123.91
124.11
126.60
127.50
127.77
129.02
131.91
132.00
135.19
147.71
150.38
154.17
163.61
174.59
Ph
CN
O
O
O
NO2
3'i
ppm
200
180
160
140
120
100
80
60
40
20

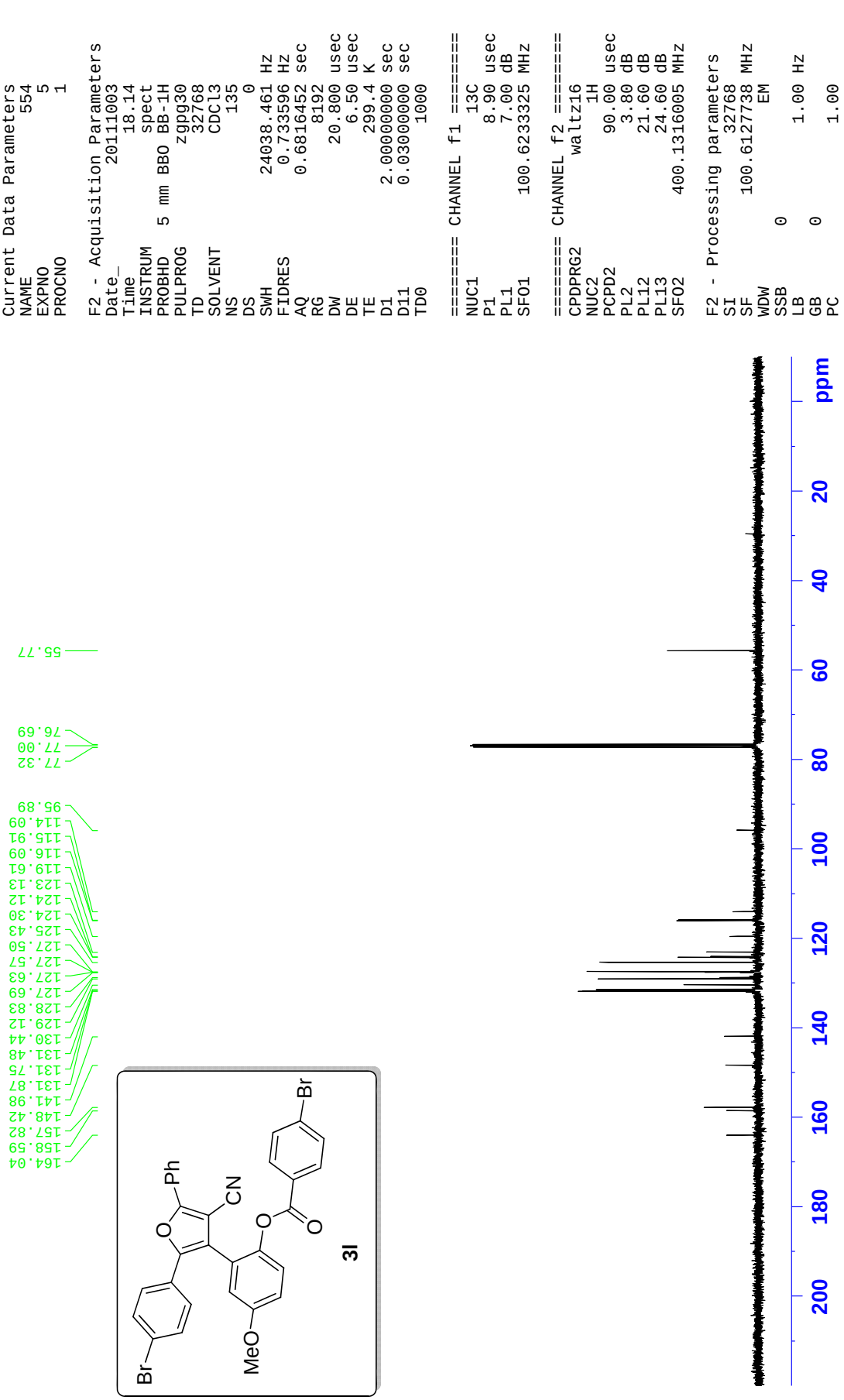

Current Data Parameters
NAME 577
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111006
Time 21.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 22
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300112 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
ppm
9.14
9.28
2.00
4.13
1.01
1.32
1.02
Ph
CN
O
O
O
3j

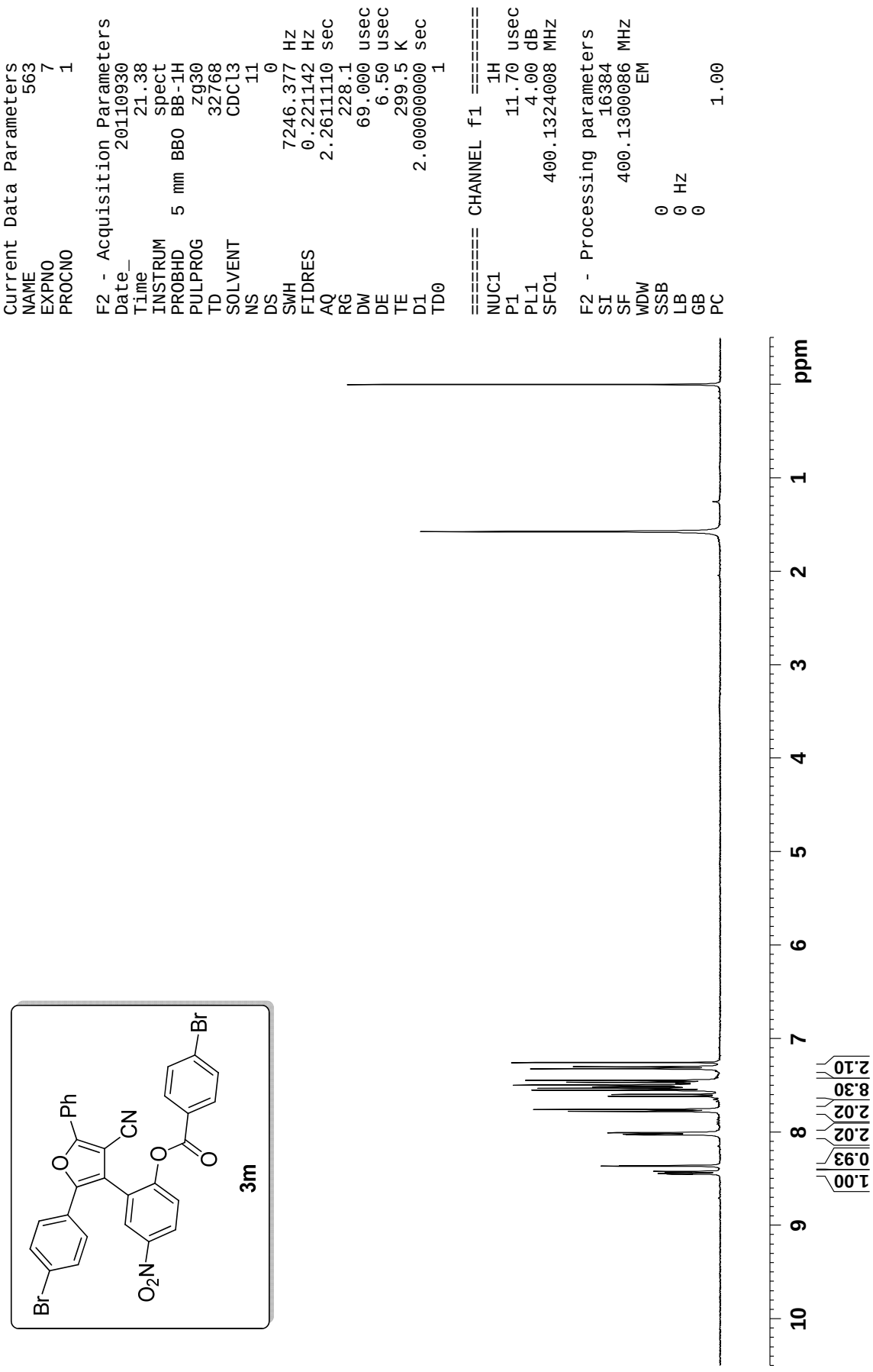

Current Data Parameters
NAME 577
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111006
Time 14.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 152
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1000
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127743 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
26.82
29.46
34.49
38.86
76.68
77.00
77.32
95.81
114.23
117.23
122.83
124.46
125.08
125.39
128.18
129.02
129.75
129.95
132.42
149.59
156.43
158.95
176.16
Ph
CN
O
O
O
3j
ppm
20
40
60
80
100
120
140
160
180
200

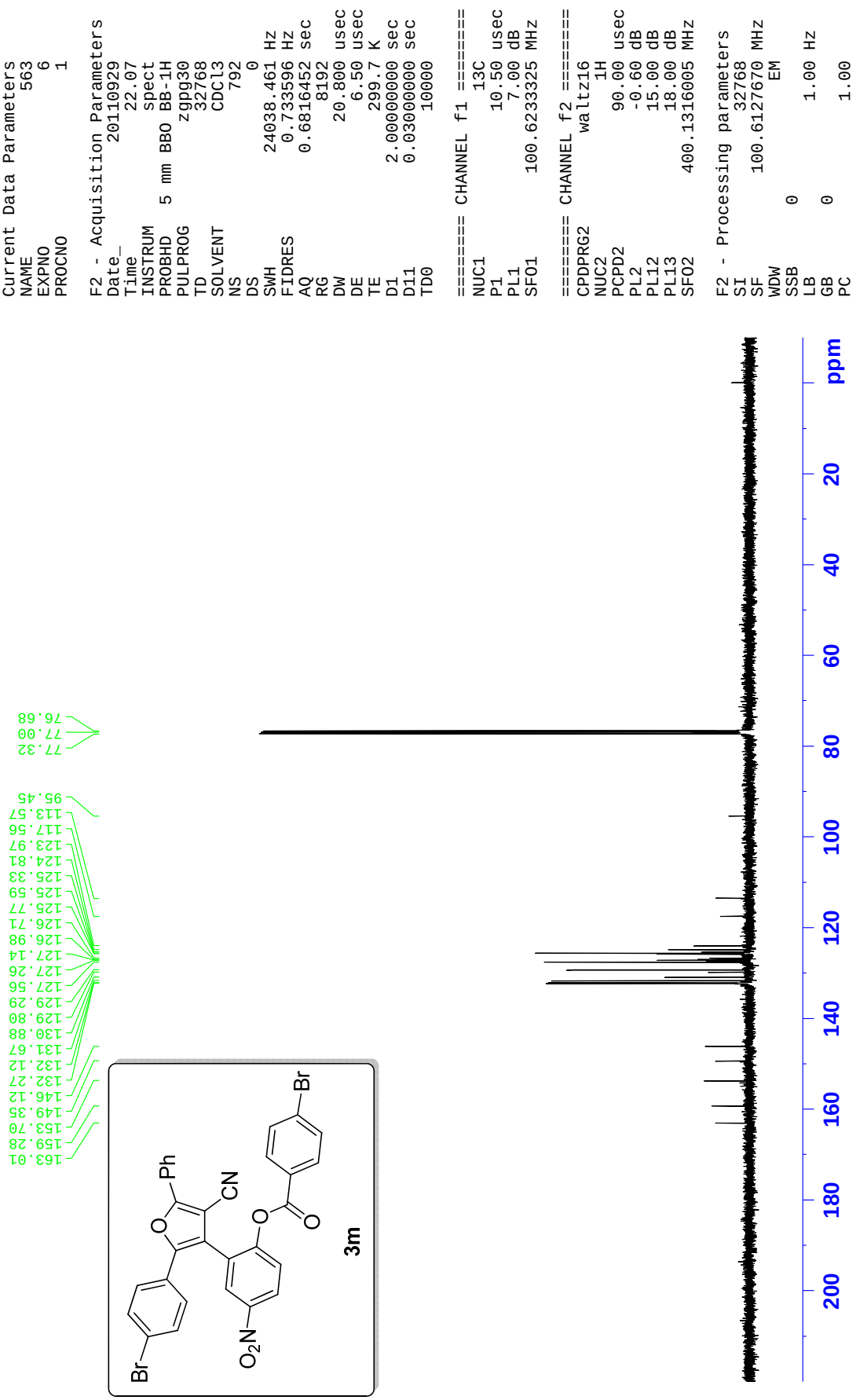

Current Data Parameters
NAME 505
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110816
Time 12.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.366798 Hz
AQ 1.3632820 sec
RG 128
DW 83.200 usec
DE 6.50 usec
TE 299.3 K
D1 1.50000000 sec
MCREST 0 sec 0.01500000 sec
MCWRK
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1326008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300120 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
3.00
0.94
1.03
4.02
7.02
2.06
1.98
ppm
Ph
CN
O
Ph
O
O
Br
MeO
3k

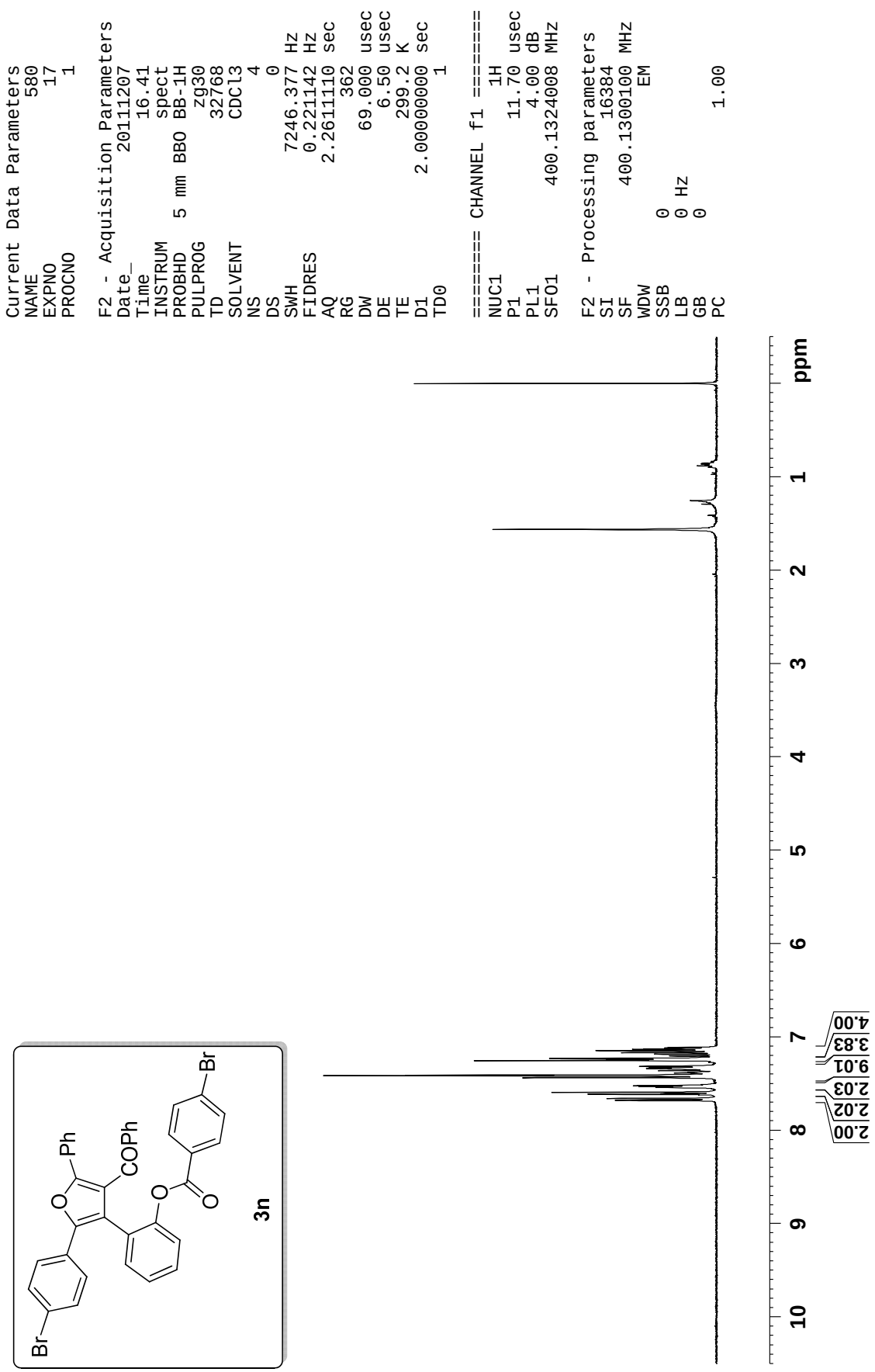

Current Data Parameters
NAME 505
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110816
Time 12.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 911
DS 0
SWH 25062.656 Hz
FIDRES 0.382426 Hz
AQ 1.3075131 sec
RG 6144
DW 19.950 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 5.30 dB
SFO1 100.6242995 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0 dB 16.50 dB
PL12 19.50 dB
PL13 400.1319000 MHz
SFO2
F2 - Processing parameters
SI 32768
SF 100.6127689 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
55.79
76.68
77.00
77.32
95.89
114.28
115.90
116.20
119.07
124.19
124.43
125.45
126.13
127.85
127.91
128.65
128.68
128.86
128.92
129.10
130.26
131.53
131.71
142.15
149.55
157.80
158.89
164.00
Ph
O
Ph
CN
O
O
Br
MeO
3k
200
180
160
140
120
100
80
60
40
20
ppm

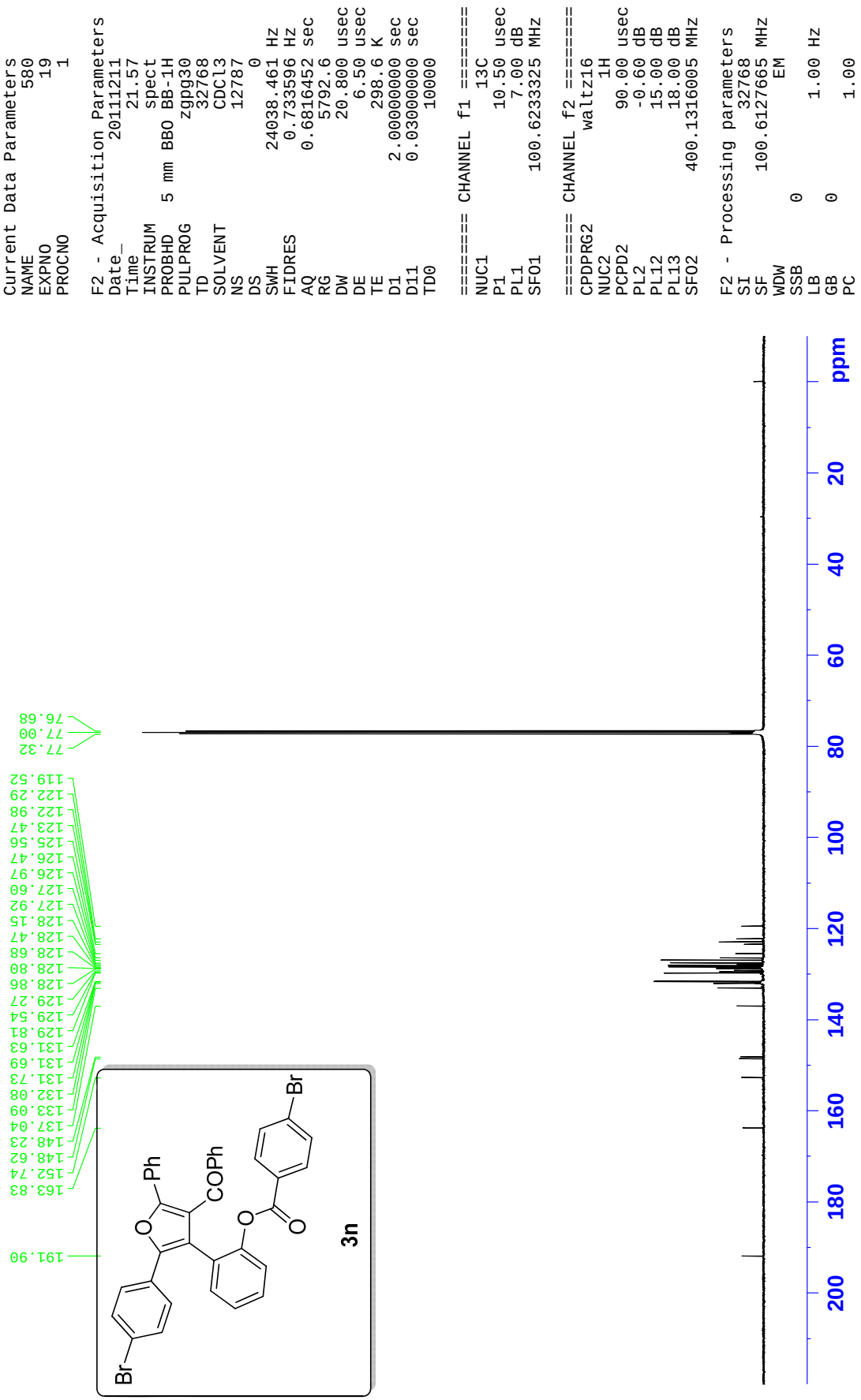

Current Data Parameters
NAME 554
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111003
Time 18.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 90.5
DW 69.000 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300116 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
2.91
1.92
1.95
6.82
2.00
0.99
0.98
1.00
ppm
Ph
CN
O
O
O
Br
Br
MeO
3l

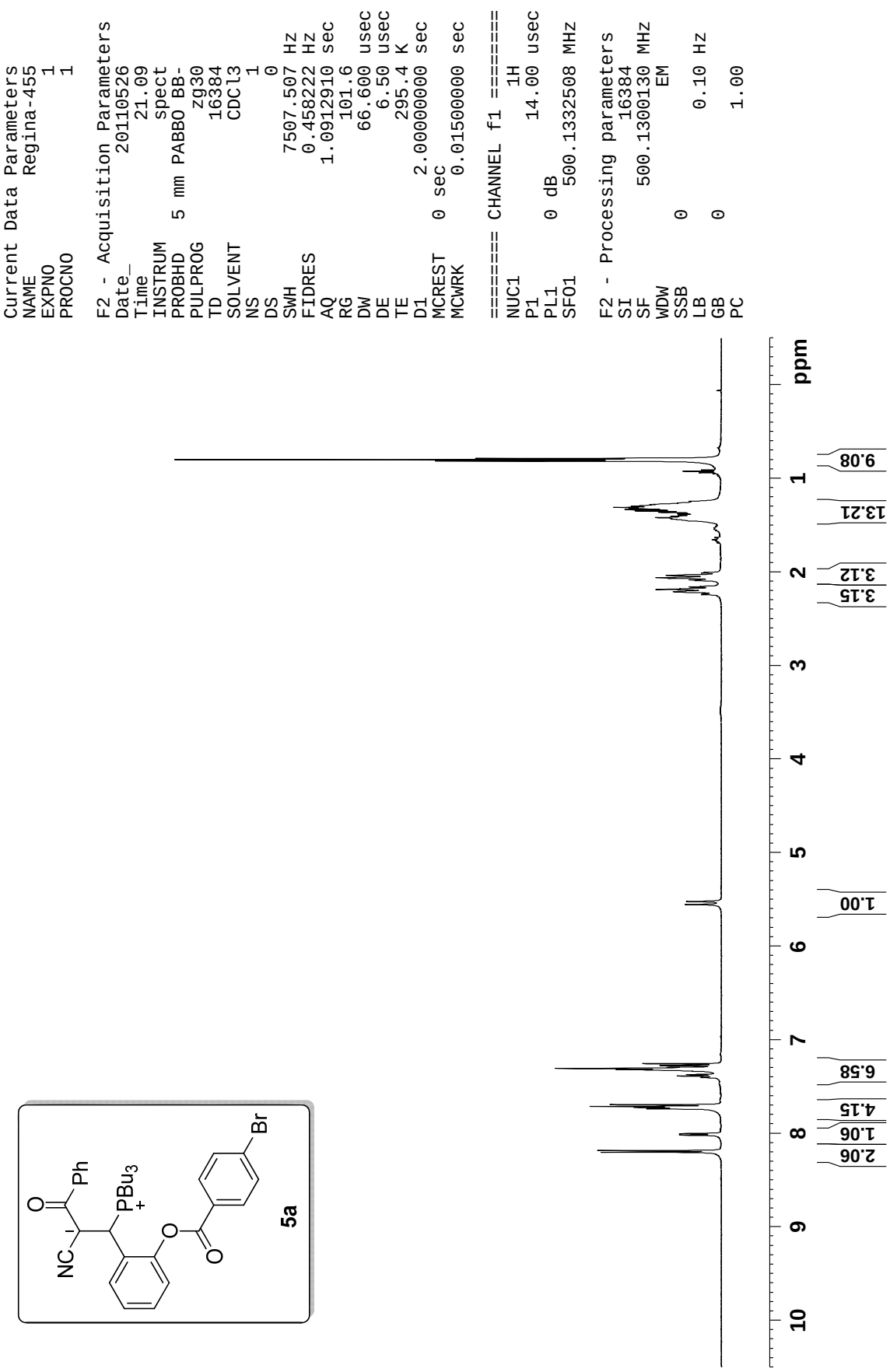

Current Data Parameters
NAME 554
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111003
Time 18.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 135
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1000
======== CHANNEL f1 ========
NUC1 13C
P1 8.90 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.80 dB
PL12 21.60 dB
PL13 24.60 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127738 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
55.77
76.69
77.00
77.32
95.89
114.09
115.91
116.09
119.61
123.13
124.12
124.30
125.43
127.50
127.57
127.63
127.69
128.83
129.12
130.44
131.48
131.75
131.87
141.98
148.42
157.82
158.59
164.04
Br
MeO
O
CN
Ph
O
O
Br
3l
200
180
160
140
120
100
80
60
40
20
ppm

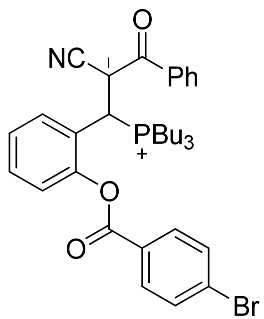

Current Data Parameters
NAME 563
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110930
Time 21.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
1.00
0.93
2.02
2.02
8.30
2.10
ppm
10
9
8
7
6
5
4
3
2
1
Ph
CN
O
O
O
Br
Br
O2N
3m


Current Data Parameters
NAME 563
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110929
Time 22.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 792
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127670 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
77.32
77.00
76.68
95.45
113.57
117.56
123.97
124.81
125.33
125.59
125.77
126.71
126.98
127.14
127.26
127.56
129.29
129.80
130.88
131.67
132.12
132.27
146.12
149.35
153.70
159.28
163.01
Ph
CN
O
O
O
Br
Br
O_2N
3m
200
180
160
140
120
100
80
60
40
20
ppm

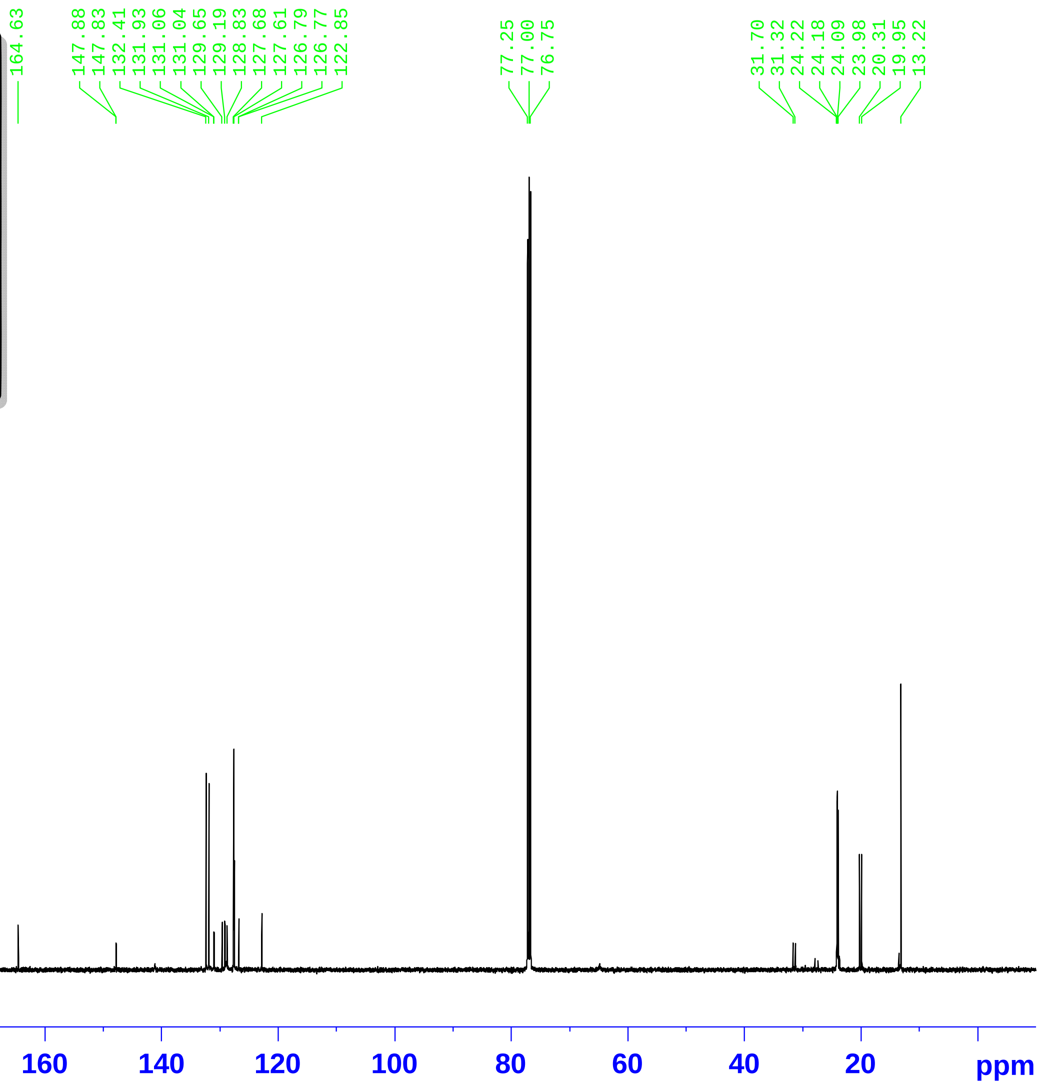

Current Data Parameters
NAME 580
EXPNO 17
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111207
Time 16.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 362
DW 69.000 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
2.00
2.02
2.03
9.01
3.83
4.00
ppm
10
9
8
7
6
5
4
3
2
1
Ph
COPh
O
O
O
Br
Br
3n


Current Data Parameters
NAME 580
EXPNO 19
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111211
Time 21.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 12787
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816452 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10000
======== CHANNEL f1 ========
NUC1 13C
P1 10.50 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -0.60 dB
PL12 15.00 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127665 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
77.32
77.00
76.68
191.90
163.83
152.74
148.62
148.23
137.04
133.09
132.08
131.73
131.69
131.63
129.81
129.54
129.27
128.86
128.80
128.68
128.47
128.15
127.92
127.60
126.97
126.47
125.56
123.47
122.98
122.29
119.52
Ph
COPh
O
O
O
Br
Br
3n
200
180
160
140
120
100
80
60
40
20
ppm

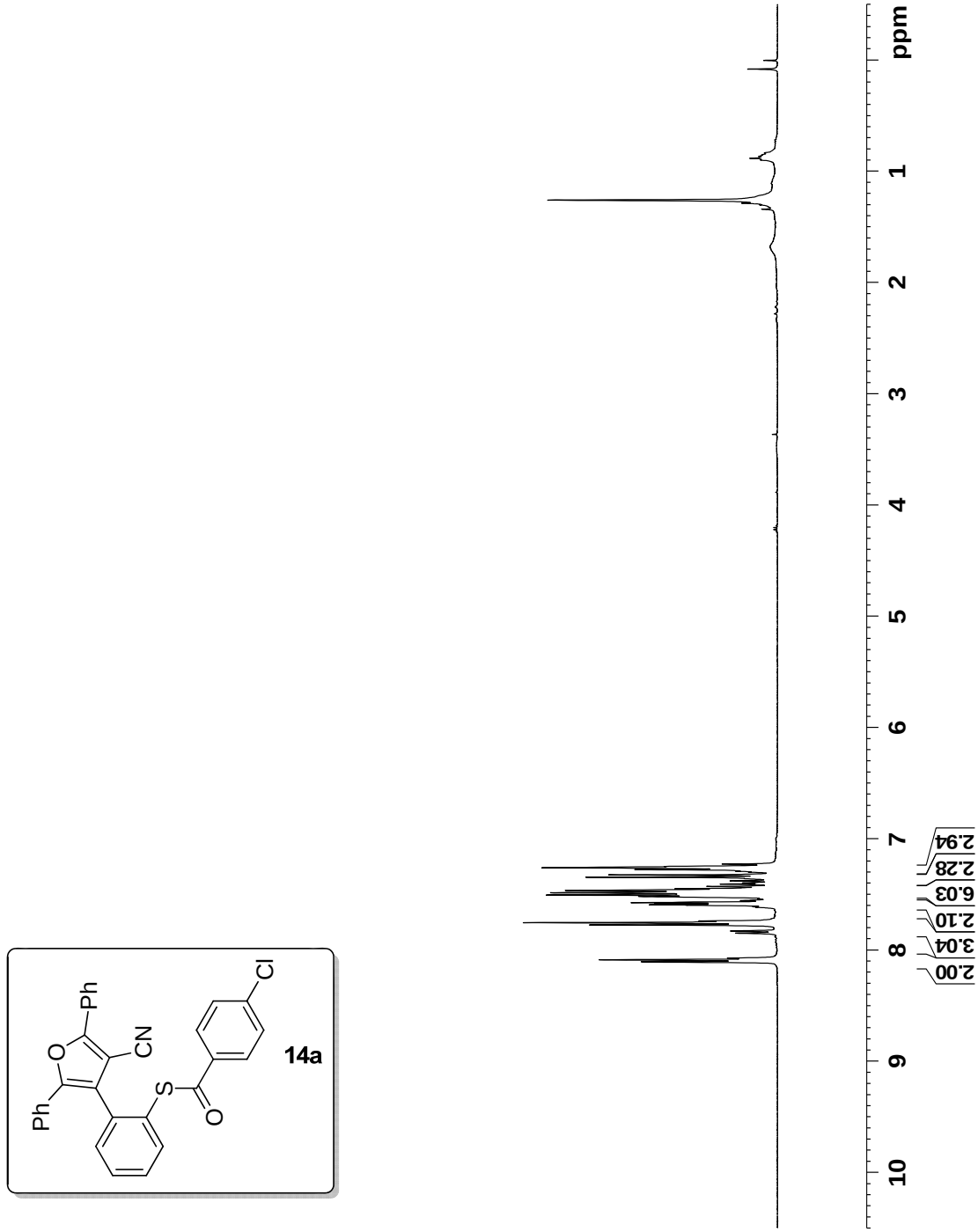

Current Data Parameters
NAME Regina-455
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110526
Time 21.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 1
DS 0
SWH 7507.507 Hz
FIDRES 0.458222 Hz
AQ 1.0912910 sec
RG 101.6
DW 66.600 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 0 dB
SFO1 500.1332508 MHz
F2 - Processing parameters
SI 16384
SF 500.1300130 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
ppm
9.08
13.21
3.12
3.15
1.00
6.58
4.15
1.06
2.06
Ph
PBu3
NC
O
O
O
Br
5a

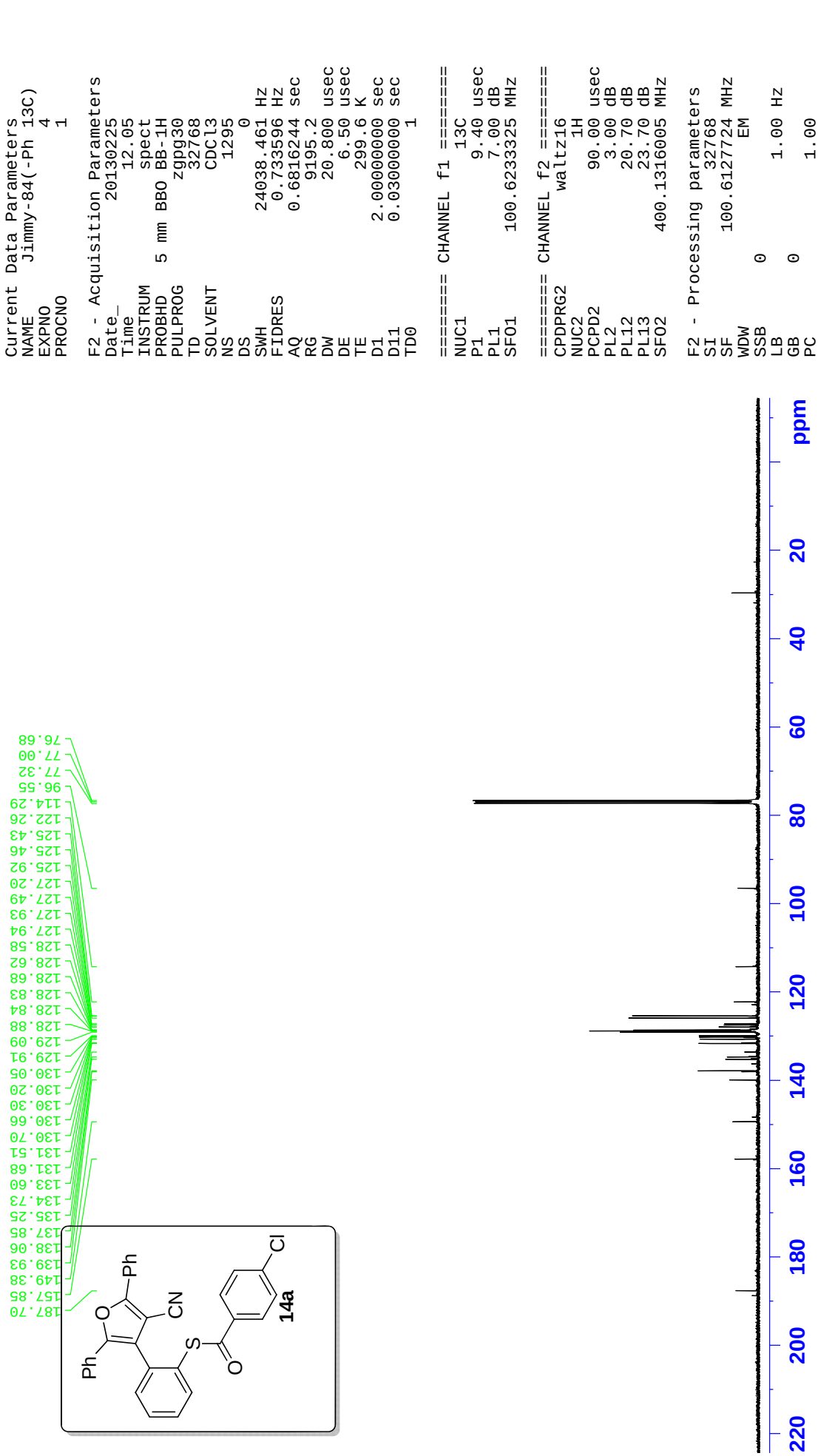


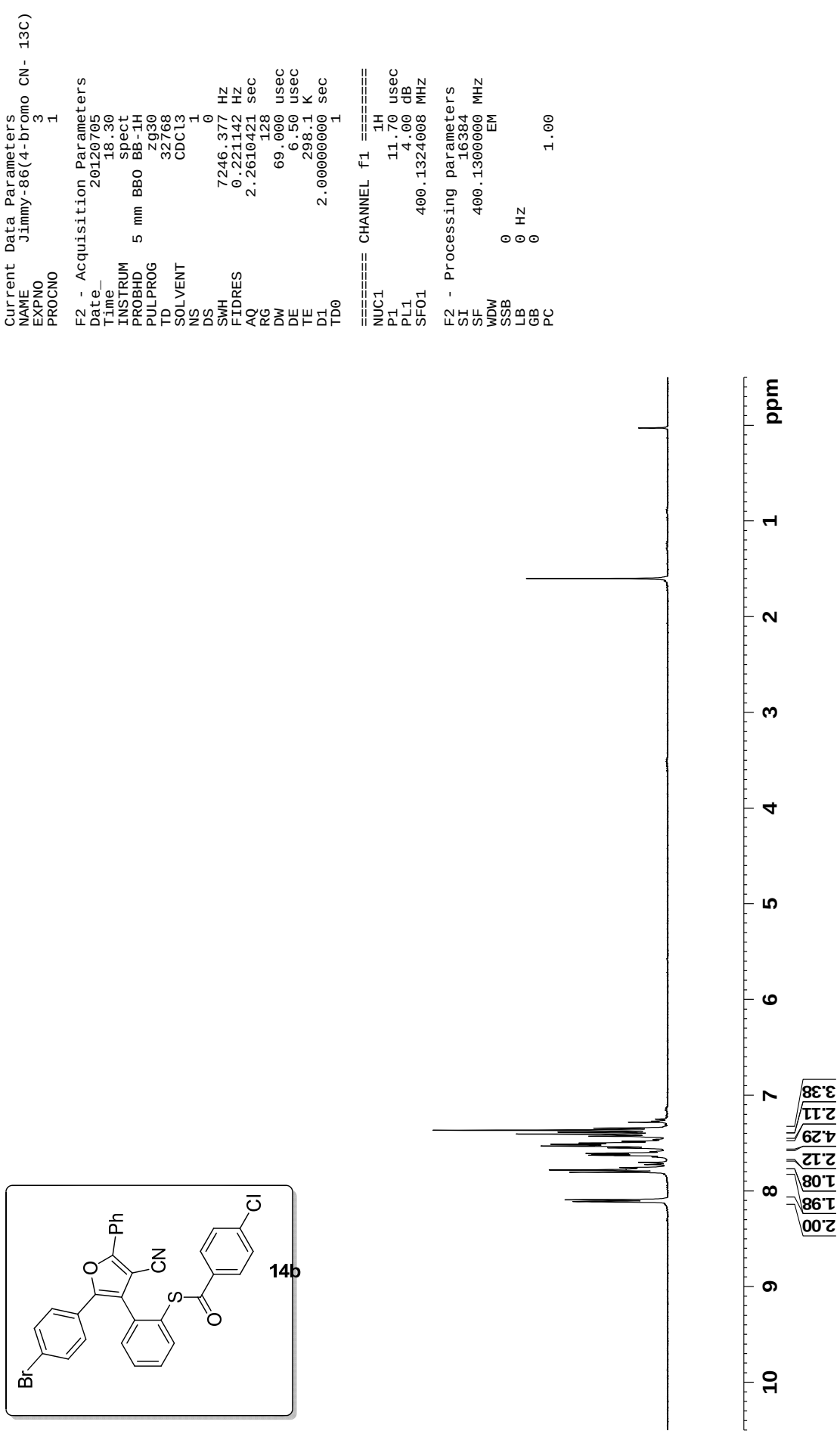
5a

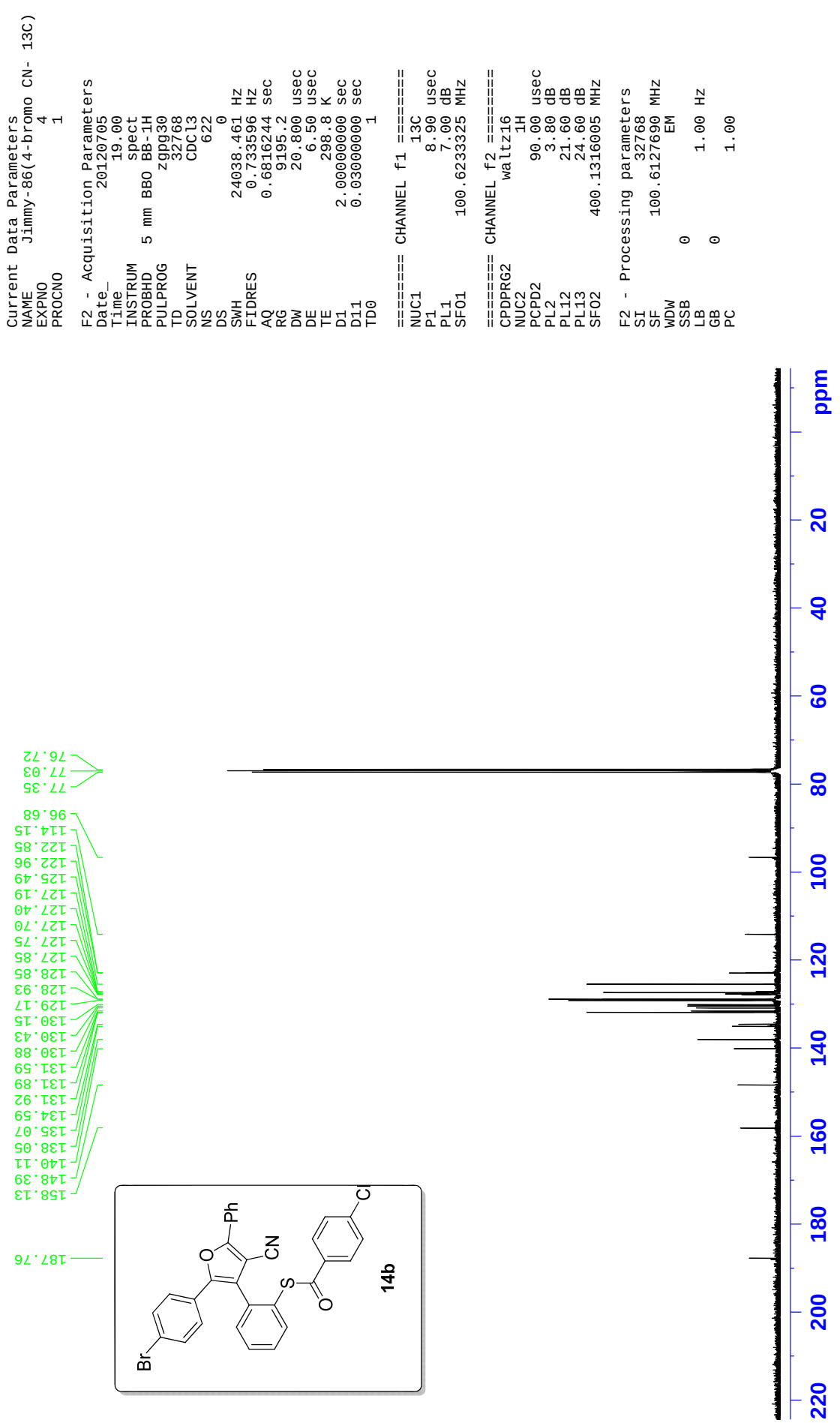


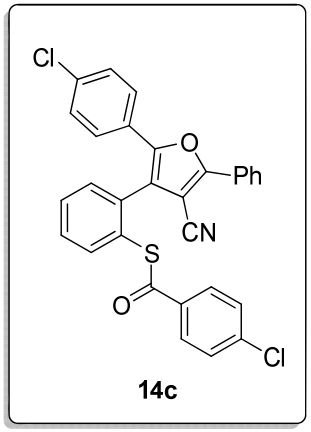

```
Current Data Parameters
NAME          Regina-455
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110526
Time               21.11
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1962
DS                     0
SWH            31446.541 Hz
FIDRES          0.479836 Hz
AQ             1.0420883 sec
RG                  4096
DW                15.900 usec
DE                  6.50 usec
TE                 296.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.50 usec
PL1                 7.00 dB
SFO1         125.7722011 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -0.60 dB
PL12               15.00 dB
PL13               18.00 dB
SFO2         500.1322506 MHz

F2 - Processing parameters
SI                 32768
SF           125.7577949 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.00
```


Current Data Parameters
NAME Jimmy-84(-Ph 13C)
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130225
Time 12.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2610421 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300118 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
ppm
1
2
3
4
5
6
7
8
9
10
2.00
3.04
2.10
6.03
2.28
2.94
14a
Ph
O
CN
Ph
S
O
Cl

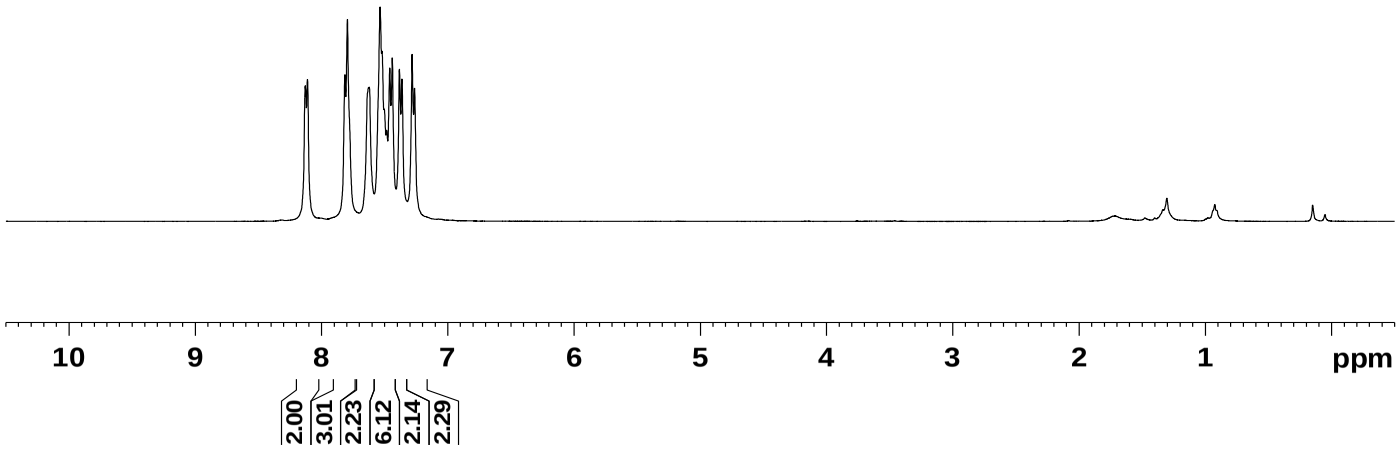

Current Data Parameters
NAME Jimmy-84(-Ph 13C)
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130225
Time 12.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1295
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 9195.2
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127724 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
187.70
157.85
149.38
139.93
138.06
137.85
135.25
134.73
133.60
131.68
131.51
130.70
130.66
130.30
130.20
130.05
129.91
129.09
128.88
128.84
128.83
128.68
128.62
128.58
127.94
127.93
127.49
127.20
125.92
125.46
125.43
122.26
114.29
96.55
77.32
77.00
76.68
Ph
O
CN
Ph
S
O
Cl
14a
ppm
220
200
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME Jimmy-86(4-bromo CN- 13C)
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120705
Time 18.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2610421 sec
RG 128
DW 69.000 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.70 usec
PL1 4.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Br
O
Ph
CN
S
O
Cl
14b
ppm
1
2
3
4
5
6
7
8
9
10
2.00
1.98
1.08
2.12
4.29
2.11
3.38

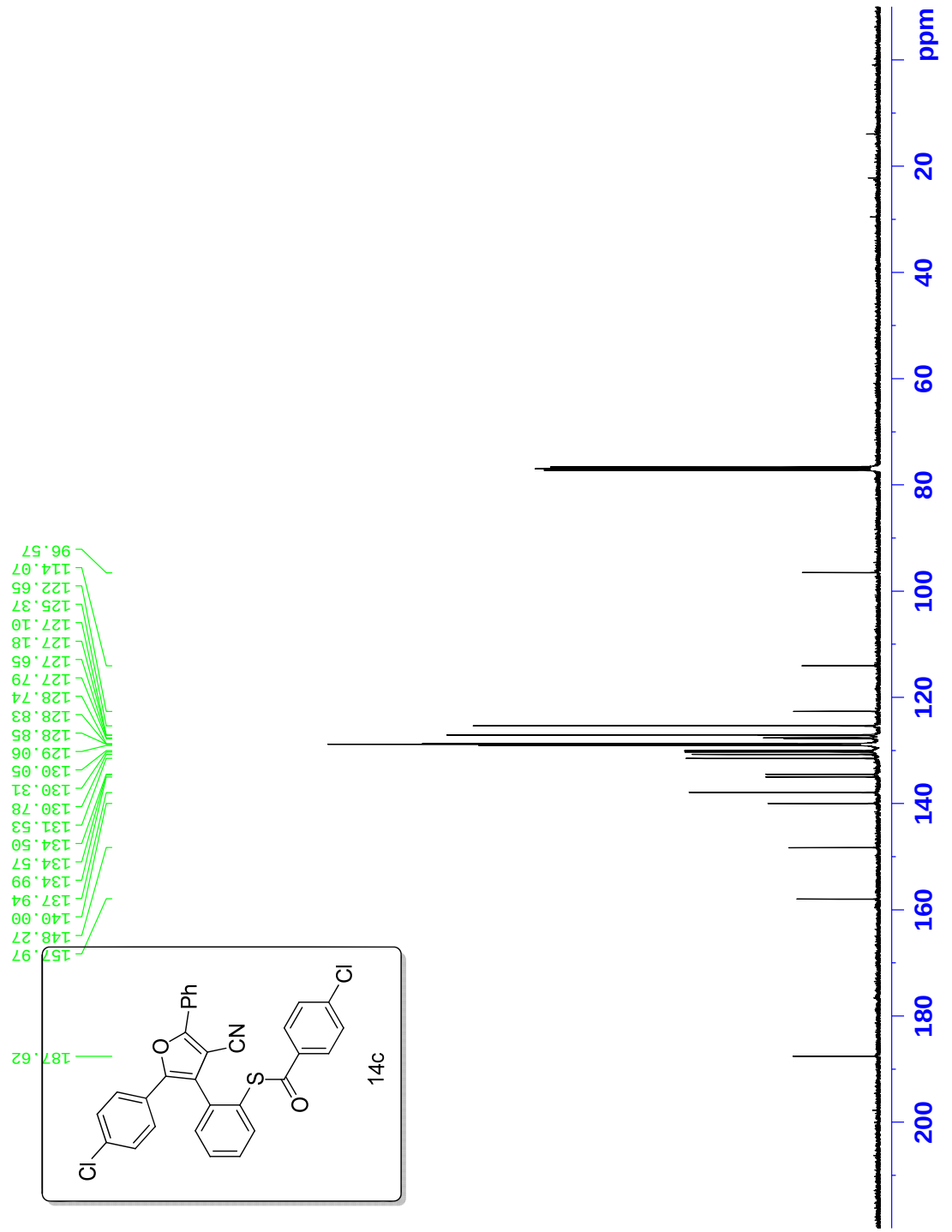


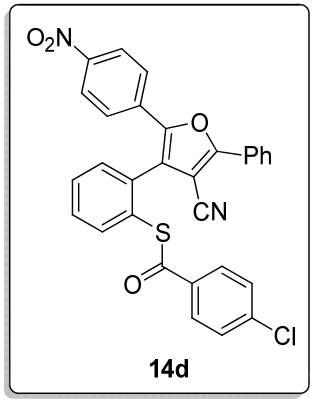


14c

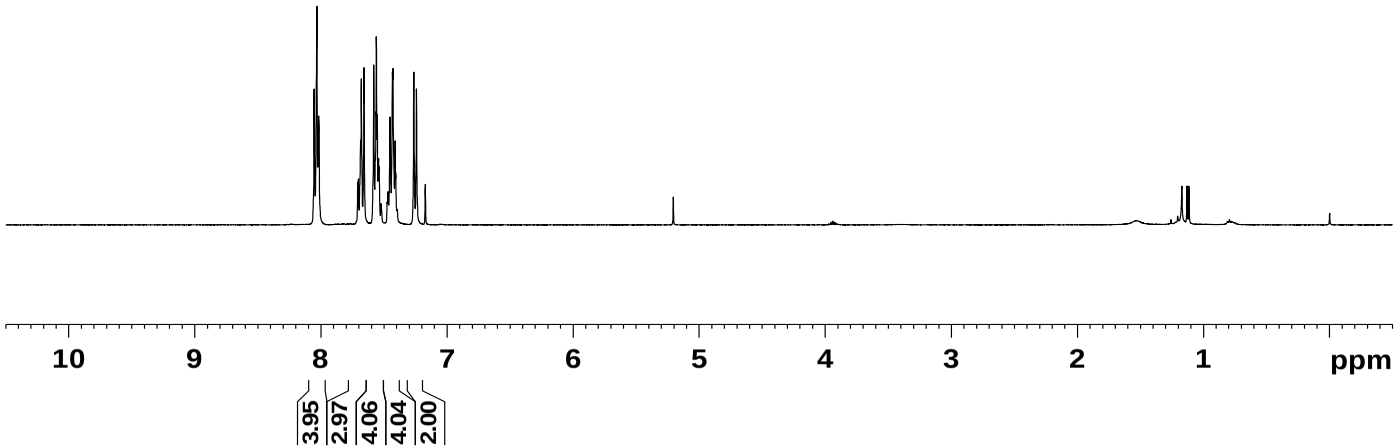



```
Current Data Parameters
NAME        Jimmy-81 13C
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20121225
Time                7.27
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ             2.2610421 sec
RG                    64
DW                69.000 usec
DE                 6.50 usec
TE                299.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF           400.1300000 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```


Current Data Parameters
NAME Jimmy-81 13C
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121225
Time 7.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 542
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6816244 sec
RG 9195.2
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127811 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
187.62
157.97
148.27
140.00
137.94
134.99
134.57
134.50
131.53
130.78
130.31
130.05
129.06
128.85
128.83
128.74
127.79
127.65
127.18
127.10
125.37
122.65
114.07
96.57
Ph
O
CN
S
O
Cl
Cl
14c
ppm
200
180
160
140
120
100
80
60
40
20



14d




```
Current Data Parameters
NAME      Jimmy-82 C13-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20130219
Time                0.22
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     4
DS                     0
SWH             7246.377 Hz
FIDRES          0.221142 Hz
AQ              2.2610421 sec
RG                   114
DW                69.000 usec
DE                 6.50 usec
TE                298.9 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.90 usec
PL1                3.00 dB
SFO1        400.1324008 MHz

F2 - Processing parameters
SI                 16384
SF          400.1300446 MHz
WDW                   EM
SSB       0
LB        0 Hz
GB        0
PC                  1.00
```