Pd-Catalyzed Thiocarbonylation with stoichiometric Carbon Monoxide: Scope and Applications

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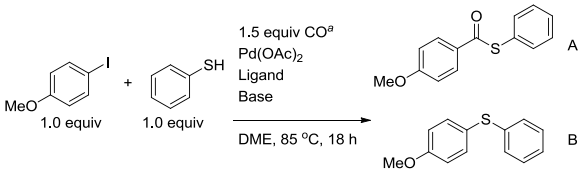
Supporting Information

I. General Methods:

Dry solvents were prepared according to standard literature procedures.[1] All other chemicals were used as received from the suppliers unless mentioned otherwise. Starting materials were made according to literature procedures. Flash column chromatography was performed on silica gel 60 (230-400 mesh). ^{1}H and ^{13}C NMR spectra were recorded at 400 MHz and 100 MHz, respectively, using a Varian Mercury 400 spectrometer. Chemical shifts are reported in ppm downfield to TMS ($\delta = 0$) and referenced to the solvent residual peak,[2] using the following peak pattern abbreviations: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; pent, pentet; sext, sextet; sept, septet; m, multiplet; dd, doublet of doublets; dt, doublet of triplets; ddd, doublet of doublet of doublets; ddt, doublet of doublet of triplets, and td, triplet of doublets. HRMS was recorded on a LC TOF (ES).

II. Optimization Tables:

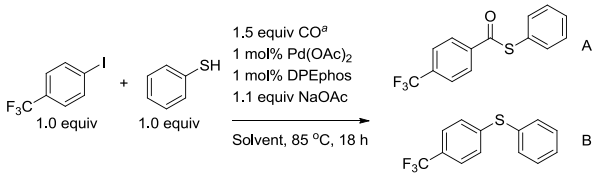


entry	ligand	base	Conv.	ratio A:B	yield
1	Josiphos	NaO^{t}Bu	>95%	B	91%
2	Josiphos	Et_3N	13%	2:1	_
3	Josiphos	K_3PO_4	30%	B	_
4	Josiphos	K_2CO_3	57%	B	_
5	Josiphos	*N*-Methyl morpholine	19%	1:1	–
6	Josiphos	Pyridine	3%	1:2	–
7	Josiphos	NaOAc	25%	1:1	_
8	Josiphos	$NaHCO_3$	16%	1:3	_
9	DPPF	NaOAc	81%	10:1	75%
10	D^{i}-PrPF	NaOAc	12%	2:1	_
11	D^{t}BuPF	NaOAc	68%	1:2	_
12	Xantphos	NaOAc	>95%	A[b]	86%
13[c]	Xantphos	NaOAc	>95%	11:1	82%
14[d]	Xantphos	NaOAc	>95%	4:1	74%
15	DPEphos	NaOAc	>95%	A[b]	93%
16[e]	DPEphos	NaOAc	>95%	A[b]	91%
17[f]	DPEphos	NaOAc	>95%	A[b]	89%
18	dcpp·2HBF_4	NaOAc	0%	_	_
19	dppe	NaOAc	0%	_	_
20	dppp	NaOAc	0%	_	_
21	dpppent	NaOAc	0%	_	_
22	P$^{t}Bu_3$·HBF_4	NaOAc	3%	1:2	_
23	CataXCiumA	NaOAc	0%	_	_
24	PPh_3	NaOAc	0%	_	_

Chamber **1:** Thiophenol (0.25 mmol), *p*-iodoanisole (0.25 mmol), $Pd(OAc)_2$ (13 μmol), bidentate ligand (13 μmol) or monodentate ligand (25μmol), base (0.28 mmol), DME (1.0 mL). [a] Chamber 2: $Pd(dba)_2$ (13 μmol), P$^{t}Bu_3$ (13 μmol), 9-methylfluorene-9-carbonyl chloride (0.38 mmol, 1.5 equiv), Cy_2NMe (0.56 mmol), DME (1.5 mL). [b] Traces of B was seen on the ^{1}H NMR. [c] The reaction was run at 75 °C. [d] The reaction was run at 65 °C. [e] Chamber 1: $Pd(OAc)_2$ (7.5 μmol), DPEphos (7.5 μmol). [f] Chamber 1: $Pd(OAc)_2$ (2.5 μmol), DPEphos (2.5 μmol).

[1] Perrin, D.; Armarego, W. *Purification of Laboratory Chemicals 3rd Ed*, Pergamon Press, **1988**
[2] Gottlieb, H. E., Kotlyar V., Nudelman A. *J. Org. Chem.* **1997**, 62, 7512-7515.

Solvent Screening



entry	solvent	Conv.	ratio A:B	yield
1	Toluene	>95%	2:3	_
2	Propionitrile	>95%	1:5	_
3	Dioxane	89%	1:4	_
4	Anisole	>95%	5:1	79%
5	CPME	>95%	1:1	–
6	Tol-CF_3	>95%	2:1	–

Chamber **1:** Thiophenol (0.25 mmol), *p*-iodoanisole (0.25 mmol), $Pd(OAc)_2$ (2.5 μmol), DPEphos (2.5 μmol), NaOAc (0.28 mmol), solvent (1.0 mL). [a] Chamber 2: $Pd(dba)_2$ (13 μmol), P^tBu_3 (13 μmol), 9-methylfluorene-9-carbonyl chloride (0.38 mmol, 1.5 eq.), Cy_2NMe (0.56 mmol), solvent (1.5 mL).

III. Equipment Used for the Thiocarbonylation:

The thiocarbonylations were performed in a two-chamber reaction vessel with a total volume of 20 mL, using 9-methylfluorene-9-carbonyl chloride as the source of carbon monoxide. The two chambers were loaded in an argon filled glovebox. **Chamber 1** was loaded with the reactants for the thiocarbonylation, all thiols were injected into chamber 1 outside the glovebox prior to heating. **Chamber 2** was loaded with 1.5 equivalents of 9-methylfluorene-9-carbonyl chloride, $Pd(dba)_2$ (3.3 mol%), $P(^tBu)_3{\cdot}HBF_4$ (3.3 mol%), DME and Cy_2NMe. The chambers were sealed with a screw cap, 2 mm stabilizing PTFE disc and a 2 mm thick PTFE-lined silicone disc before taking the two chamber vessel out of the glovebox and heating at 85°C.

IV. General Procedures for the Thiocarbonylation of Electron rich Substrates

Liquid Thiols used in the Thiocarbonylation

Chamber 1: Aryl iodide (0.25 mmol), $Pd(OAc)_2$ (0.234 mL stock solution, 2.5 μmol), DPEphos (1.3 mg, 2.5 μmol) and NaOAc (22.6 mg, 0.275 mmol) was dissolved in DME (0.766 mL). **Chamber 2:** 1.5 equivalents of CO was generated in chamber 2. The glassware was then removed from the glovebox, and the thiol (0.25 mmol) was injected into chamber 1 before mixing at 85 °C. After 18 h, the solvent was removed from chamber 1 *in vacuo* and the desired compound was purified by flash chromatography on silica gel using a pentane/CH_2Cl_2 eluent system.

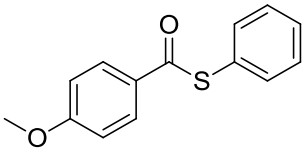
Solid Thiols used in the Thiocarbonyation.

Chamber 1: Aryl iodide (0.25 mmol), $Pd(OAc)_2$ (0.234 mL stock solution, 2.5 μmol), DPEphos (1.3 mg, 2.5 μmol) and NaOAc (22.6 mg, 0.275 mmol) was added to chamber 1. **Chamber 2:** 1.5 equivalents of CO were generated in chamber 2. The glassware was then removed from the glovebox, and the thiol (0.25 mmol) was dissolved in DME (0.766 mL) and injected into chamber 1 before mixing at 85 °C. After 18 h, the solvent was removed from chamber 1 *in vacuo* and the desired compound was purified by flash chromatography on silica gel using a pentane/CH_2Cl_2 eluent system.

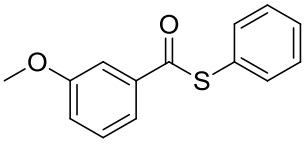
Chamber 2: 1.5 equivalents of CO: 9-methylfluorene-9-carbonyl chloride (91 mg, 0.375 mmol), $Pd(dba)_2$ (7.5 mg, 0.013 mmol), $P(^tBu)_3 \cdot HBF_4$ (3.8 mg, 0.013 mmol) was dissolved in DME (1.5 mL). Cy_2NMe (121 μL, 0.563 mmol) was added before sealing of the glassware.

Preparation of a Stock Solution: A $Pd(OAc)_2$ in DME stock solution was prepared before loading of the two chambers. $Pd(OAc)_2$ (2.4 mg) was dissolved in DME (1 mL).

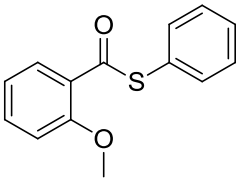
***S*-Phenyl 4-methoxybenzothioate (1):**[3] The title compound was isolated as colorless crystals (54 mg, 0.22 mmol, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.02 (d, *J* = 9.2 Hz, 2H), 7.54-7.44 (m, 5H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 188.5, 164.0, 135.2, 129.7, 129.4, 129.3, 129.1, 127.6, 113.9, 55.5. HRMS (ESI) m/z calcd for $C_{14}H_{12}O_2S$ [M+H$^+$]: 245.0631, found: 245.0632.



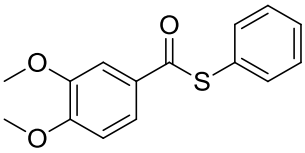
***S*-Phenyl 3-methoxybenzothioate (3):** The title compound was isolated as a colorless oil (39 mg, 0.16 mmol, 64%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.66 (d, *J* = 9.2 Hz, 1H), 7.54-7.45 (m, 6H), 7.40 (t, *J* = 8.4 Hz, 1H), 7.16 (dd, *J* = 8.4 Hz, *J* = 0.4 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.0, 159.8, 138.0, 135.0, 129.7, 129.5, 129.2, 127.4, 120.1, 120.0, 111.8, 55.5. HRMS (ESI) m/z calcd for $C_{14}H_{12}O_2S$ [M+Na$^+$]: 267.0450, found: 267.0450.



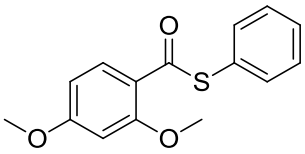
***S*-Phenyl 2-methoxybenzothioate (4):**[4] The title compound was isolated as a colorless oil (47 mg, 0.19 mmol, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.86 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1H), 7.55-7.42 (m, 6H), 7.03 (t, *J* = 7.2 Hz, 2H), 3.96 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.1, 158.2, 134.9, 134.1, 129.9, 129.3, 129.1, 128.8, 126.3, 120.5, 112.1, 56.0. HRMS (ESI) m/z calcd for $C_{14}H_{12}O_2S$ [M+Na$^+$]: 267.0450, found: 267.0451.



***S*-Phenyl 3,4-dimethoxybenzothioate (5):**[5] The title compound was isolated as colorless crystals (52 mg, 0.19 mmol, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.75 (dd, *J* = 8.4 Hz, *J* = 2.0 Hz, 1H), 7.53-7.44 (m, 6H), 6.92 (d, *J* = 8.4 Hz, 1H), 3.96 (s, 3H), 3.93 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 188.7, 153.7, 149.0, 135.1, 129.5, 129.4, 129.2, 127.6, 122.0, 110.3, 109.7, 56.1, 56.0. HRMS (ESI) m/z calcd for $C_{15}H_{14}O_3S$ [M+Na$^+$]: 297.0556, found: 297.0554.

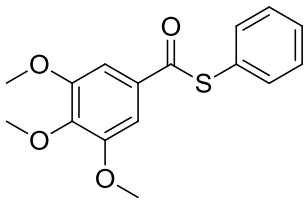


***S*-Phenyl 2,4-dimethoxybenzothioate (6):**[5] The title compound was isolated as a colorless oil (59 mg, 0.21 mmol, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.91 (d, *J* = 8.8 Hz, 1H), 7.53-7.42 (m, 5H), 6.55 (dd, *J* = 8.8 Hz, *J* = 2.0 Hz, 1H), 6.51 (d, *J* = 2.0 Hz, 1H), 3.96 (s, 3H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 187.4, 164.8, 160.5, 135.1, 132.2, 129.12, 129.07, 129.0, 119.2, 105.2, 98.7, 55.8, 55.6. HRMS (ESI) m/z calcd for $C_{15}H_{14}O_3S$ [M+Na$^+$]: 279.0556, found: 279.0553.

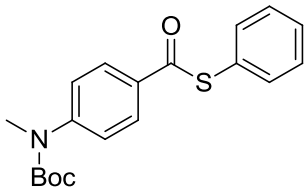


[3] Cao, H.; McNamee, L.; Alper, H. *J. Org. Chem.* **2008**, *73*, 3530.
[4] Katritzky, A. R.; Shestopalov, A. A.; Suzuki, K. *Synthesis*, **2004**, *11*, 1806.
[5] Kuhakarn, C.; Surapanich, N.; Kamtonwong, S.; Pohmakotr, M.; Reutrakul, V. *Eur. J. Org. Chem.* **2011**, *29*, 5911.

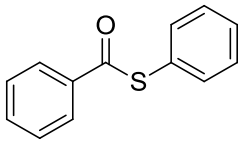
***S*-Phenyl 3,4,5-trimethoxybenzothioate (7):** The title compound was isolated as an orange oil (62 mg, 0.20 mmol, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.53-7.45 (m, 5H), 7.29 (s, 2H), 3.93 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.2, 153.2, 142.2, 134.8, 131.7, 129.5, 129.2, 127.4, 104.8, 61.0, 56.3. HRMS (ESI) m/z calcd for $C_{16}H_{16}O_4S$ [M+H$^+$]: 305.0842, found: 305.0839.



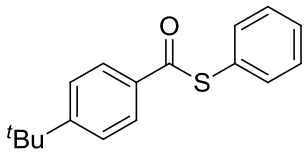
***S*-Phenyl 4-((tert-butoxycarbonyl)(methyl)amino)benzothioate (8):** The title compound was isolated as colorless crystals (66 mg, 0.19 mmol, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99 (d, *J* = 8.8 Hz, 2H), 7.53-7.51 (m, 2H), 7.47-7.44 (m, 3H), 7.39 (d, *J* = 8.8 Hz, 2H), 3.32 (s, 3H), 1.49 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.0, 154.0, 148.6, 135.1, 132.7, 129.5, 129.2, 127.9, 127.3, 124.4, 81.3, 36.8, 28.3. HRMS (ESI) m/z calcd for $C_{19}H_{21}NO_3S$ [M+H$^+$]: 344.1315, found: 344.1314.



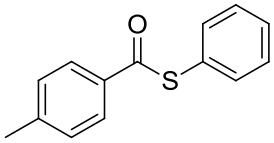
***S*-Phenyl benzothioate (9):**[3] The title compound was isolated as colorless crystals (42 mg, 0.19 mmol, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.06-8.03 (m, 2H), 7.64-7.45 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.1, 136.7, 135.1, 133.7, 129.5, 129.3, 128.8, 127.5, 127.4. HRMS (ESI) m/z calcd for $C_{13}H_{10}OS$ [M+H$^+$]: 215.0525, found: 215.0524.



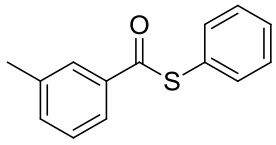
***S*-Phenyl 4-(*tert*-butyl)benzothioate (10):**[6] The title compound was isolated as colorless crystals (56 mg, 0.21 mmol, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.98 (d, *J* = 8.4 Hz, 2H), 7.54-7.44 (m, 7H), 1.37 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.6, 157.5, 135.1, 134.0, 129.4, 129.2, 127.6, 127.4, 125.7, 35.2, 31.1. HRMS (ESI) m/z calcd for $C_{17}H_{18}OS$ [M+Na$^+$]: 293.0971, found: 293.0975.



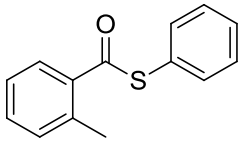
***S*-Phenyl 4-methylbenzothioate (11):**[3] The title compound was isolated as colorless crystals (48 mg, 0.21 mmol, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.94 (d, *J* = 8.4 Hz, 2H), 7.54-7.45 (m, 5H), 7.29 (d, *J* = 8.4 Hz, 2H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.7, 144.6, 135.1, 134.1, 129.4, 129.2, 127.6, 21.7. HRMS (ESI) m/z calcd for $C_{14}H_{12}OS$ [M+H$^+$]: 229.0682, found: 229.0679.



***S*-Phenyl 3-methylbenzothioate (12):**[7] The title compound was isolated as a colorless oil (47 mg, 0.21 mmol, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.86-7.84 (m, 2H), 7.54-7.36 (m, 7H), 2.44 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.2, 138.7, 136.7, 135.1, 134.4, 129.5, 129.2, 128.6, 127.7, 127.5, 124.7, 21.3. HRMS (ESI) m/z calcd for $C_{14}H_{12}OS$ [M+Na$^+$]: 251.0501, found: 251.0496.



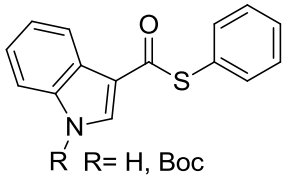
***S*-Phenyl 2-methylbenzothioate (13):**[7] The title compound was isolated as colorless crystals (35 mg, 0.15 mmol, 61%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.95 (dd, *J* = 7.6 Hz, *J* = 0.8 Hz, 1H), 7.55-7.41 (m, 6H), 7.32 (d, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 1H), 2.51 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.1, 137.4, 136.8, 134.9, 132.0, 131.7,



[6] Prangora, L.; Strelow, T.; Voss, J. *J. Chem. Res.* **1985**, *4*, 1401.
[7] Dan, W.; Deng, H.; Chen, J.; Liu, M.; Ding, J.; Wu, H. *Tetrahedron* **2010**, *66*, 7384.

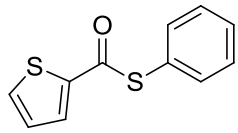
129.4, 129.2, 128.6, 128.2, 125.8, 20.8. HRMS (ESI) m/z calcd for $C_{14}H_{12}OS$ [M+H$^+$]: 229.0682, found: 229.0680.

***tert*-Butyl 3-((phenylthio)carbonyl)-indole-1-carboxylate (15):** $Pd(OAc)_2$ (0.468 mL stock solution, 0.005



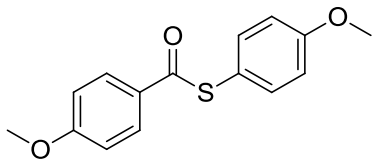
5.0 μmol), DPEphos (5.0 μmol, 2.6 mg) was used in this reaction. It yielded the carbonylation products with and without the Boc protection group. The title compound was isolated as colorless solid (37 mg, 0.10 mmol, 41%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.47 (s, 1H), 8.21 (d, *J* = 7.6 Hz, 1H), 8.17 (d, *J* = 8.4 Hz, 1H), 7.58-7.56 (m, 2H), 7.51-7.46 (m, 3H), 7.40 (dt, *J* = 8.4 Hz, *J* = 0.8 Hz, 1H), 7.34 (dt, *J* = 8.0 Hz, *J* = 1.2 Hz, 1H), 1.73 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 183.8, 148.8, 136.4, 135.2, 131.2, 129.5, 129.2, 127.1, 126.8, 125.7, 124.5, 122.0, 119.3, 115.1, 85.6, 28.1. HRMS (ESI) m/z calcd for $C_{20}H_{19}NO_3S$ [M+Na$^+$]: 376.0978, found: 376.0974. The compound without Boc protection (***S*-phenyl indole-3-carbothioate (14)**) was isolated as colorless crystals (31 mg, 0.12 mmol, 49%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.64 (br. s, 1H), 8.28-8.24 (m, 1H), 8.10 (d, *J* = 3.2 Hz, 1H), 7.59-7.56 (m, 2H), 7.49-7.41 (m, 4H), 7.32-7.28 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 183.1, 136.1, 135.3, 130.4, 129.2, 129.1, 127.7, 124.9, 123.9, 122.9, 121.9, 116.8, 111.5. HRMS (ESI) m/z calcd for $C_{15}H_{11}NOS$ [M+H$^+$]: 254.0634, found: 254.0634.

***S*-Phenyl thiophene-2-carbothioate (16):**[3] The title compound was isolated as orange crystals (45 mg, 0.20



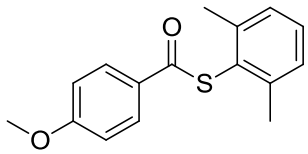
mmol, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.92 (dd, *J* = 4.0 Hz, *J* = 1.2 Hz, 1H), 7.67 (dd, *J* = 5.2 Hz, *J* = 1.2 Hz, 1H), 7.56-7.43 (m, 5H), 7.16 (dd, *J* = 4.8 Hz, *J* = 3.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 182.0, 141.4, 135.0, 133.2, 131.6, 129.6, 129.2, 128.0, 126.9. HRMS (ESI) m/z calcd for $C_{11}H_8OS_2$ [M+Na$^+$]: 242.9909, found: 242.9906.

***S*-(4-Methoxyphenyl) 4-methoxybenzothioate (17):**[8] The title compound was isolated as colorless crystals



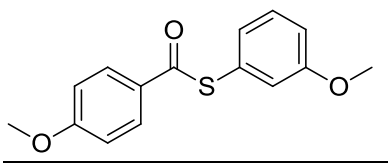
(58 mg, 0.21 mmol, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.01 (d, *J* = 8.8 Hz, 2H), 7.41 (d, *J* = 8.8 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 3.87 (s, 3H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.5, 163.9, 160.7, 136.7, 129.7, 129.4, 118.2, 114.9, 113.9, 55.5, 55.4. HRMS (ESI) m/z calcd for $C_{15}H_{14}O_3S$ [M+Na$^+$]: 297.0556, found: 297.0552.

***S*-(2,6-Dimethylphenyl) 4-methoxybenzothioate (18):** The title compound was isolated as an yellow oil (48



mg, 0.18 mmol, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.07 (d, *J* = 8.8 Hz, 2H), 7.27 (dd, *J* = 8.8 Hz, *J* = 6.4 Hz, 1H), 7.20 (d, *J* = 7.6 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 3.89 (s, 3H), 2.41 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 187.6, 163.8, 143.3, 129.83, 129.78, 128.3, 126.9, 113.8, 55.6, 22.6. HRMS (ESI) m/z calcd for $C_{16}H_{16}O_2S$ [M+H$^+$]: 273.0944, found: 273.0940.

***S*-(3-Methoxyphenyl) 4-methoxybenzothioate (19):** The title compound was isolated as colorless crystals

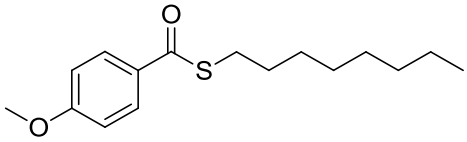


(56 mg, 0.20 mmol, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.01 (d, *J* = 9.2 Hz, 2H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.11 (ddd, *J* = 7.6 Hz, *J* = 1.6 Hz, *J* = 0.8 Hz, 1H), 7.07 (dd, *J* = 2.4 Hz, *J* = 1.6 Hz, 1H), 6.99 (ddd, , *J* = 8.0 Hz, *J* = 2.4 Hz, *J* = 0.8 Hz, 1H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H) 3.83

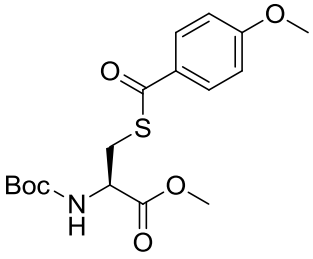
[8] Cilento, G. *J. Am. Chem. Soc.* **1953**, *75*, 3748.

(s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 188.5, 164.0, 159.9, 129.9, 129.7, 129.4, 128.5, 127.4, 120.2, 115.6, 113.9, 55.5, 55.4. HRMS (ESI) m/z calcd for $C_{15}H_{14}O_3S$ [M+Na$^+$]: 297.0556, found: 297.0558.

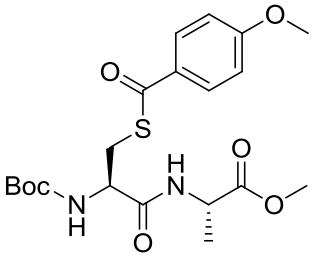
***S*-Octyl 4-methoxybenzothioate (20):**[9] The title compound was isolated as an yellow oil (50 mg, 0.18mmol, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.95 (d, *J* = 9.2 Hz, 2H), 6.91 (d, *J* = 9.2 Hz, 2H), 3.86 (s, 3H), 3.04 (t, *J* = 7.2 Hz, 2H), 1.66 (pent, *J* = 6.8 Hz 2H), 1.45-1.24 (m, 10H), 0.88 (t, *J* = 6.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.6, 163.6, 130.2, 129.3, 113.7, 55.5, 31.8, 29.7, 29.16, 29.12, 28.95, 28.91, 22.6, 14.1. HRMS (ESI) m/z calcd for $C_{16}H_{24}O_2S$ [M+Na$^+$]: 303.1389, found: 303.1389.



(*R*)-Methyl 2-((*tert*-butoxycarbonyl)amino)-3-((4-methoxybenzoyl)thio)propanoate (21): The title compound was isolated as colorless crystals (63 mg, 0.17 mmol, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.92 (d, *J* = 9.2 Hz, 2H), 6.91 (d, *J* = 8.8 Hz, 2H), 5.33 (d, *J* = 7.6 Hz, 1H), 4.59 (dd, *J* = 12.0 Hz, *J* = 6.4 Hz, 1H), 3.85 (s, 3H), 7.75 (s, 3H), 3.53 (m, 2H), 1.41 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.2, 171.1, 164.0, 155.0, 129.6, 129.3, 113.8, 80.1, 55.1, 53.4, 52.6, 30.9, 28.2. HRMS (ESI) m/z calcd for $C_{17}H_{23}NO_6S$ [M+Na$^+$]: 392.1138, found: 392.1134.



(*S*)-Methyl 2-((*R*)-2-((*tert*-butoxycarbonyl)amino)-3-((4-methoxybenzoyl)thio)propanamido) propanoate (22): The title compound was isolated as a colorless solid (79 mg, 0.18 mmol, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.93(d, *J* = 9.2 Hz, 2H), 7.05 (br s, 1H), 6.90 (d, *J* = 9.2 Hz, 2H), 5.45 (br. d, *J* = 7.2 Hz, 1H), 4.55 (pent, *J* = 7.2 Hz, 1H), 4.38 (br. s, 1H), 3.85 (s, 3H), 3.70 (s, 3H), 3.52 (dd, *J* = 14.4 Hz, *J* = 4.4 Hz, 1H), 3.36 (dd, *J* = 14.4 Hz, *J* = 8.0 Hz, 1H), 1.42 (d, *J* = 11.6 Hz, 3H), 1.39 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.7, 172.9, 169.9, 169.6, 164.1, 129.7, 129.3, 113.8, 80.4, 55.5, 55.0, 52.4, 48.2, 30.9, 28.2, 18.3. HRMS (ESI) m/z calcd for $C_{20}H_{28}N_2O_7S$ [M+H$^+$]: 441.1690, found: 441.1693.



V. General Procedure for the Thiocarbonylation of Electron poor Substrates:

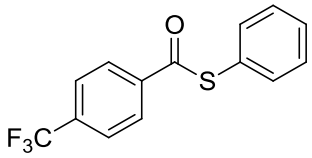
Chamber 1: Aryl iodide (0.25 mmol), $Pd(OAc)_2$ (0.234 mL stock solution, 2.5 μmol), DPEphos (1.3 mg, 2.5 μmol) and NaOAc (22.6 mg, 0.275 mmol) was dissolved in Anisole (0.766 mL). **Chamber 2:** 1.5 equivalents of CO was generated in chamber 2. The glassware was then removed from the glovebox, and the thiol (0.25 mmol) was injected into chamber 1 before mixing at 85 ^{o}C. After 18 h, the solvent was removed from chamber 1 *in vacuo* and the desired compound was purified by flash chromatography on silica gel using a pentane/CH_2Cl_2 eluent system.

Chamber 2: 1.5 equivalents of CO: 9-methylfluorene-9-carbonyl chloride (91 mg, 0.375 mmol), $Pd(dba)_2$ (7.5 mg, 0.013 mmol), $P(^tBu)_3{\cdot}HBF_4$ (3.8 mg, 0.013 mmol) was dissolved in DME (1.5 mL). Cy_2NMe (121 μL, 0.563 mmol) was added before sealing of the glassware.

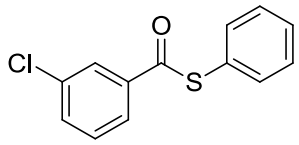
[9] Takido, T.; Toriyama, M.; Itabashi, K. *Synthesis* **1988**, *5*, 404.

Preparation of a Stock Solution: A $Pd(OAc)_2$ in anisole stock solution was prepared before loading of the two chambers. $Pd(OAc)_2$ (2.4 mg) was dissolved in anisole (1 mL).

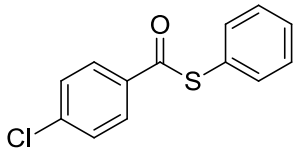
***S*-Phenyl 4-(trifluoromethyl)benzothioate (23):**[3] The title compound was isolated as colorless crystals (56 mg, 0.20 mmol, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.13 (d, J = 8.4 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H), 7.54-7.47 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.3, 139.4, 135.0, 134.9 (q, $J_{C\text{-}F}$ = 32.7 Hz), 129.9, 129.4, 127.8, 126.6, 125.9 (q, $J_{C\text{-}F}$ = 3.7 Hz), 123.5 (q, $J_{C\text{-}F}$ = 272.7 Hz). ^{19}F NMR (377 MHz, $CDCl_3$) δ (ppm) -63.14. HRMS (ESI) m/z calcd for $C_{14}H_9F_3OS$ [M+H$^+$]: 283.0399, found: 283.0402.



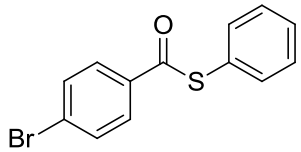
***S*-Phenyl 3-chlorobenzothioate (24):**[10] The title compound was isolated as colorless crystals (47 mg, 0.19 mmol, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99 (s, 1H), 7.92 (d, J = 7.6 Hz, 1H), 7.58 (d, J = 8.0 Hz, 1H), 7.53-7.42 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.0, 138.2, 135.03, 135.00, 133.5, 130.0, 129.7, 129.3, 127.5, 126.8, 125.6. HRMS (ESI) m/z calcd for $C_{13}H_9ClOS$ [M+Na$^+$]: 270.9955, found: 270.9957.



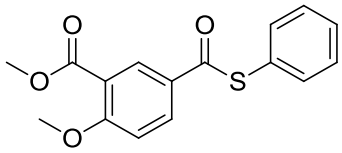
***S*-Phenyl 4-chlorobenzothioate (25):**[3] The title compound was isolated as colorless crystals (54 mg, 0.22 mmol, 86%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.97 (d, J = 8.8 Hz, 2H), 7.53-7.46 (m, 7H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.0, 140.1, 135.04, 134.96, 129.7, 129.3, 129.1, 128.8, 126.9. HRMS (ESI) m/z calcd for $C_{13}H_9ClOS$ [M+H$^+$]: 249.0135, found: 249.0141.



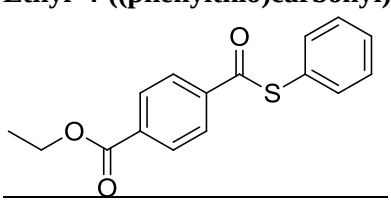
***S*-Phenyl 4-bromobenzothioate (26):**[3] The title compound was isolated as colorless crystals (62 mg, 0.21 mmol, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90 (d, J = 8.8 Hz, 2H), 7.63 (d, J = 8.4 Hz, 2H), 7.53-7.46 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.2, 135.4, 135.0, 132.0, 129.7, 129.3, 128.9, 128.7, 126.9. HRMS (ESI) m/z calcd for $C_{13}H_9BrOS$ [M+H$^+$]: 292.9630, found: 292.9629.



Methyl 2-methoxy-5-((phenylthio)carbonyl)benzoate (27): The title compound was isolated as colorless crystals (75 mg, 0.25 mmol, 99%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.50 (d, J = 2.4 Hz, 1H), 8.14 (dd, J = 8.8 Hz, J = 2.4 Hz, 1H), 7.52-7.44 (m, 5H), 7.05 (d, J = 8.8 Hz, 1H), 3.98 (s, 3H), 3.92 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 188.1, 165.5, 163.0, 135.1, 132.8, 131.6, 129.5, 129.2, 128.8, 127.1, 120.2, 111.9, 56.4, 52.3. HRMS (ESI) m/z calcd for $C_{16}H_{14}O_4S$ [M+Na$^+$]: 325.0505, found: 325.0502.



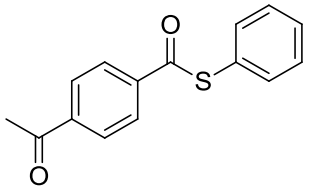
Ethyl 4-((phenylthio)carbonyl)benzoate (28): The title compound was isolated as colorless crystals (49 mg, 0.17 mmol, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.16 (d, J = 8.8 Hz, 2H), 8.07 (d, J = 8.8 Hz, 2H), 7.54-7.46 (m, 5H), 4.42 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.7, 165.6, 139.8, 135.0, 134.8, 129.9, 129.8, 129.4, 127.4, 126.8, 61.5,



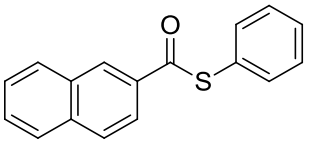
[10] Alvarez-Ibarra, C.; Mendoza, M.; Orellana, G.; Quiroga, M. L. *Synthesis*, **1989**, *7*, 560.

14.3. HRMS (ESI) m/z calcd for $C_{16}H_{14}O_3S$ [M+H$^+$]: 287.0736, found: 287.0737.

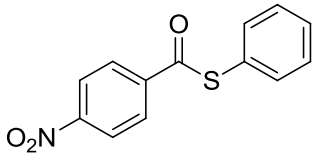
***S*-phenyl 4-acetylbenzothioate (29):** The title compound was isolated as colorless crystals (50 mg, 0.20 mmol, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.10 (d, *J* = 8.7 Hz, 2H), 8.05 (d, *J* = 8.6 Hz, 2H), 7.53-7.46 (m, 5H), 2.65 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.2, 189.6, 140.6, 139.9, 135.0, 129.8 129.4, 128.6, 127.7, 126.8, 26.9. HRMS (ESI) m/z calcd for $C_{15}H_{12}O_2S$ [M+H$^+$]: 257.0631, found: 257.0633.



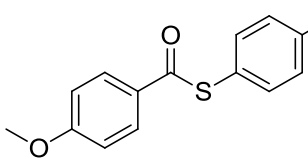
***S*-Phenyl naphthalene-2-carbothioate (30):**[3] The title compound was isolated as colorless crystals (45 mg, 0.17 mmol, 69%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.55 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 7.2 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 7.6 Hz, 1H), 7.63-7.50 (m, 8H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.2, 134.9, 134.7, 133.8, 133.3, 129.6, 129.4, 129.3, 128.4, 128.3, 128.1, 128.0, 126.7, 125.3, 124.5. HRMS (ESI) m/z calcd for $C_{17}H_{12}OS$ [M+Na$^+$]: 287.0501, found: 287.0501.



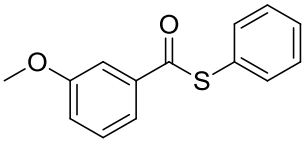
***S*-phenyl 4-nitrobenzothioate (31):**[11] 3.0 equivalents of CO was generated in Chamber 2: 9-methylfluorene-9-carbonyl chloride (0.750 mmol, 182 mg), $Pd(dba)_2$ (0.025 mmol, 14 mg), $P(^tBu)_3{\cdot}HBF_4$ (0.025 mmol, 7.3 mg) was dissolved in DME (3.0 mL). Cy_2NMe (1.13 mmol, 240 μL) was added prior before sealing the glassware. The title compound was isolated as pale yellow crystals (26 mg, 0.10 mmol, 40%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.34 (d, *J* = 8.9 Hz, 2H), 8.18 (d, *J* = 8.9 Hz, 2H), 7.54-7.48 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 188.8, 150.7, 141.3, 134.9, 130.1, 129.5, 128.5, 126.1, 124.0. HRMS (ESI) m/z calcd for $C_{13}H_9NO_3S$ [M+H$^+$]: 260.0376, found: 260.0377.



***S*-(4-fluorophenyl) 4-methoxybenzothioate (32):** The title compound was isolated as colorless crystals (40 mg, 0.15 mmol, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.00 (d, *J* = 8.8 Hz, 2H), 7.48 (dd, *J* = 8.5 Hz, *J* = 5.3 Hz, 2H), 7.15 (t, *J* = 8.6 Hz, 2H), 6.96 (d, *J* = 8.8 Hz, 2H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 188.5, 164.1, 163.5 (d, $J_{C\text{-}F}$ = 248 Hz), 137.2 (d, $J_{C\text{-}F}$ = 9.0 Hz) 129.7, 129.1, 122.9 (d, $J_{C\text{-}F}$ = 3.0 Hz), 116.4 (d, $J_{C\text{-}F}$ = 22 Hz), 114.0, 55.6. ^{19}F NMR (377 MHz, $CDCl_3$) δ (ppm) -111.36. HRMS (ESI) m/z calcd for $C_{14}H_{11}FO_2S$ [M+H$^+$]: 263.0537, found: 263.0536.



***S*-Phenyl 3-methoxybenzothioate (3):** The title compound was isolated as a colorless oil (48 mg, 0.20 mmol, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.66 (d, *J* = 9.2 Hz, 1H), 7.54-7.45 (m, 6H), 7.40 (t, *J* = 8.4 Hz, 1H), 7.16 (dd, *J* = 8.4 Hz, *J* = 0.4 Hz, 1H), 3.87 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.0, 159.8, 138.0, 135.0, 129.7, 129.5, 129.2, 127.4, 120.1, 120.0, 111.8, 55.5. HRMS (ESI) m/z calcd for $C_{14}H_{12}O_2S$ [M+Na$^+$]: 267.0450, found: 267.0450.



[11] Narayanaperumal, S.; Alberto, E.; Gul, K.; Kawasoko, C. Y.; Dornelles, L.; Rodrigues, O. E. D.; Braga, A. L. *Tetrahedron* **2011**, *67*, 4723.

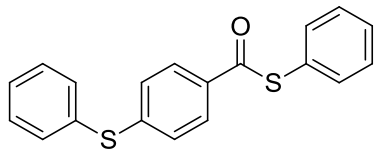
VI. Thiocarbonylation-Arylation General Procedure:

General Procedure for the Thiocarbonylation-Arylation:

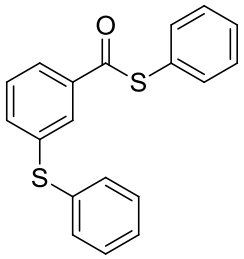
Chamber 1: Aryl diiodide (0.25 mmol), $Pd(OAc)_2$ (0.234 mL stock solution, 2.5 μmol,), DPEphos (1.3 mg, 2.5 μmol,) and NaOAc (45.1 mg, 0.55 mmol) was dissolved in DME (0.766 mL). **Chamber 2:** 3.0 equivalents of CO were generated in chamber 2. The glassware was then removed from the glovebox, and the thiol (0.50 mmol) was injected into chamber 1 before mixing at 85 °C. After 18 h, the solvent was removed from chamber 1 *in vacuo* and the desired compound was purified by flash chromatography on silica gel using a pentane/CH_2Cl_2 eluent system.

Chamber 2: 3.0 equivalents of CO: 9-methylfluorene-9-carbonyl chloride (182 mg, 0.750 mmol), $Pd(dba)_2$ (14 mg, 0.025 mmol), $P(^tBu)_3{\cdot}HBF_4$ (7.3 mg, 0.025 mmol) was dissolved in DME (3.0 mL). Cy_2NMe (240 μL, 1.13 mmol) was added prior before sealing the glassware.

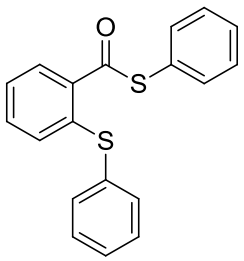
***S*-Phenyl 4-(phenylthio)benzothioate (33):**[12] The title compound was isolated as colorless crystals (57 mg, 0.18 mmol, 70%). ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.90 (d, *J* = 8.4 Hz, 2H), 7.54-7.41 (m, 10H), 7.23 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.1, 145.9, 135.1, 134.5, 134.1, 133.8, 131.8, 129.7, 129.5, 129.2, 129.0, 128.0, 127.4, 127.3. HRMS (ESI) m/z calcd for $C_{19}H_{14}OS_2$ [M+H$^+$]: 323.0564, found: 323.0557.



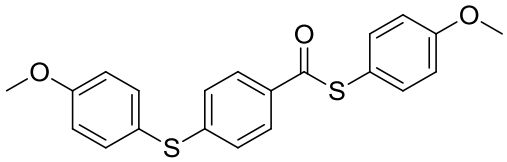
***S*-Phenyl 3-(phenylthio)benzothioate (34):** The title compound was isolated as colorless crystals (34 mg, 0.11 mmol, 43%). ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.91 (t, *J* = 2.0 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.51-7.30 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.7, 138.4, 137.4, 135.0, 134.6, 133.7, 132.4, 129.62, 129.55, 129.4, 129.3, 128.3, 128.1, 127.1, 125.5. HRMS (ESI) m/z calcd for $C_{19}H_{14}OS_2$ [M+H$^+$]: 323.0564, found: 323.0559.



***S*-Phenyl 2-(phenylthio)benzothioate (35):** The title compound was isolated as pale yellow crystals (42 mg, 0.13 mmol, 52%). ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.09 (dd, *J* = 8.0 Hz, *J* = 1.6 Hz, 1H), 7.58-7.40 (m, 10H), 7.31 (dt, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.23 (dt, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 6.95 (dd, *J* = 8.0 Hz, *J* = 1.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.1, 140.6, 135.0, 134.1, 132.8, 132.5, 129.7, 129.6, 129.5, 129.3, 128.9, 128.5, 127.5, 124.8. HRMS (ESI) m/z calcd for $C_{19}H_{14}OS_2$ [M+H$^+$]: 323.0564, found: 323.0558.



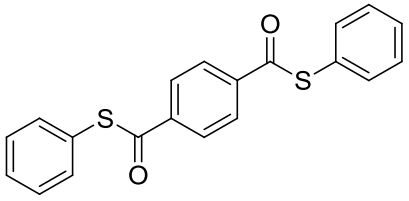
***S*-(4-Methoxyphenyl) 4-((4-methoxyphenyl)thio)benzothioate (36):** The title compound was isolated as orange crystals (64 mg, 0.17 mmol, 67%). ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.85 (d, *J* = 8.8 Hz, 2H), 7.49 (d, *J* = 8.8 Hz, 2H), 7.39 (d, *J* = 8.8 Hz, 2H), 7.10 (d, *J* = 8.4 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 9.2 Hz, 2H), 3.85 (s, 3H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.0, 160.87,



[12] Os'kina, I. A.; Vlasov, V. M. *Russ. J. Org. Chem.* **2008**, *44*, 561.

160.86, 147.7, 137.0, 136.8, 133.3, 128.0, 126.0, 121.3, 118.0, 115.6, 115.1, 55.6, 55.5. HRMS (ESI) m/z calcd for $C_{21}H_{18}O_3S_2$ [M+Na$^+$]: 405.0595, found: 405.0583.

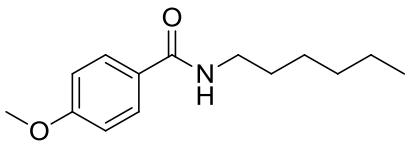
***S,S*-diphenyl benzene-1,4-bis(carbothioate) (37):**[13] Anisole was used as the solvent in both chambers. The



title compound was isolated as colorless crystals (30 mg, 0.09 mmol, 34%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.13 (s, 4H), 7.55-7.48 (m, 10H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 189.6, 163.9, 140.4, 135.0, 129.9, 129.4, 127.8, 126.7. HRMS (ESI) m/z calcd for $C_{20}H_{14}O_2S_2$ [M+H$^+$]: 351.0508, found: 351.0509.

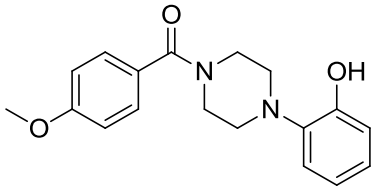
VII. Acyl Substitutions

***N*-hexyl-4-methoxybenzamide (38):**[14] General protocol for acyl transfer 1: Thioester **17** (100 mg, 0.365



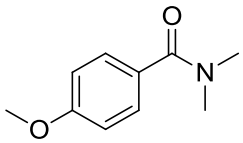
mmol) and hexylamine (36 μL, 0.27 mmol) in 1:1 TEA/pyridine (1.0 mL) was mixed in a 4 mL vial sealed with a PTFE-coated screw cap, heated to 70 ^{o}C and stirred for 26 hours. The reaction was cooled to rt, evaporated *in vacuo* and EtOAc (40 mL) was added to the reaction mixture and subsequently washed with 1 M HCl (2 x 10 mL) and brine (10 mL). The organic phase was dried over Na_2SO_4, evaporated *in vacuo* and subjected to flash column chromatography on silica gel (30% EtOAc in pentane as the eluant) to obtain the title compound **38** (42 mg, 0.18 mmol, 95%) colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.71 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.25 (br s, 1H), 3.80 (s, 3H), 3.38 (q, *J* = 6.8 Hz, 2H), 1.56 (quint, *J* = 7.2 Hz, 2H), 1.38-1.23 (m, 6H), 0.85 (t, *J* = 6.8 Hz).

(4-(2-hydroxyphenyl)piperazin-1-yl)(4-methoxyphenyl)methanone (39): According to "General protocol



for acyl transfer 1": Thioester **17** (50 mg, 0.18 mmol), 2-(piperazin-1-yl)phenol (49 mg, 0.27 mmol). Flash column chromatography on silica gel (50% EtOAc in pentane as the eluant) afforded the title compound **39** (33 mg, 0.11 mmol, 58%) as a colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.42 (d, *J* = 8.8 Hz, 2H), 7.13-7.05 (m, 2H), 6.97-6.89 (m, 1H), 6.92 (d, *J* = 8.4 Hz, 2H) 6.86 (td, *J* = 8.0, 1.6 Hz, 1H), 3.82 (s, 3H), 3.85-3.69 (m, 4H), 2.87 (br s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 170.7, 161.1, 151.5, 138.5, 129.4 (2C), 127.7, 127.1, 121.6, 120.4, 114.7, 114.0 (2C), 67.3 (2C), 55.6, 52.9 (br, 2C). HRMS (ESI) m/z calcd for $C_{18}H_{20}N_2O_3$ [M+H$^+$]: 313.1547, found: 313.1546. R_f (50% EtOAc in pentane) = 0.31.

4-methoxy-*N*,*N*-dimethylbenzamide (40):[15] According to "General protocol for acyl transfer 1": Thioester

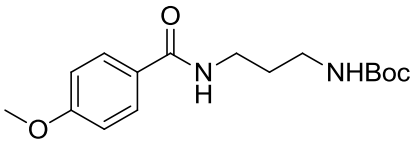


17 (50 mg, 0.18 mmol), dimethylamine hydrochloride (45 mg, 0.55 mmol). Flash column chromatography on silica gel (50% EtOAc in pentane as the eluant) afforded the title compound **40** (29 mg, 0.16 mmol, 90%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.36 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 3.79 (s, 3H), 3.01 (br s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 171.7, 160.8, 129.3 (2C), 128.6, 113.7 (2C), 55.5, 40.1

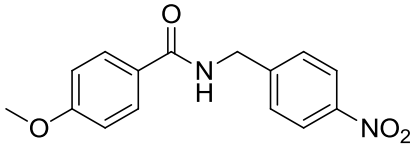
[13] Bandgar, B. P.; More, P. E.; Kamble, V. T.; Sawant, S. S. *Aust. J. Chem.* **2008**, *61*, 1006.
[14] Hermange, P.; Lindhardt, A. T.; Taaning, R. H.; Bjerglund, K.; Lupp, D.; Skrydstrup, T. *J. Am. Chem. Soc.* **2011**, *133*, 6061.
[15] Sawant, D. N.; Wagh, Y. S.; Bhatte, K. D.; Bhanage, B. M. *J. Org. Chem.*, **2011**, *76*, 5489.

(br), 35.7 (br). HRMS (ESI) m/z calcd for $C_{10}H_{13}NO_2$ [M+H$^+$]: 180.1019, found: 180.1019. R_f (50% EtOAc in pentane) = 0.21.

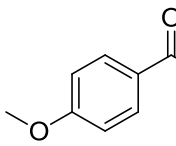
***tert*-butyl (3-(4-methoxybenzamido)propyl)carbamate (41):** According to "General protocol for acyl transfer 1": Thioester **17** (100 mg, 0.37 mmol), *tert*-butyl (3-aminopropyl)carbamate (96 mg, 0.55 mmol). Flash column chromatography on silica gel (50% EtOAc in pentane as the eluant) afforded the title compound **41** (107 mg, 0.35 mmol, 95%) as a colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.76 (d, *J* = 8.4 Hz, 2H), 7.35 (br t) 6.84 (d, *J* = 8.8 Hz, 2H), 5.22 (br t, *J* = 6.4 Hz, 1H), 3.77 (s, 3H), 3.41 (q, *J* = 6.0 Hz, 2H), 3.15 (q, *J* = 6.4 Hz, 2H), 1.62 (quint, *J* = 5.6 Hz, 2H), 1.38 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.4, 162.1, 157.0, 128.9 (2C), 126.9, 113.7 (2C), 79.3, 55.4, 37.2, 36.2, 30.2, 28.5 (3C). HRMS (ESI) m/z calcd for $C_{16}H_{24}N_2O_4$ [M+H$^+$]: 309.1809, found: 309.1813. R_f (50% EtOAc in pentane) = 0.24.



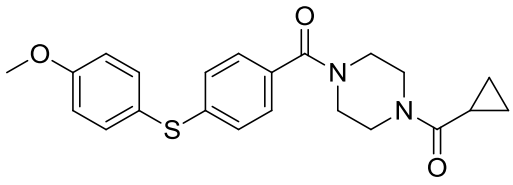
4-methoxy-*N*-(4-nitrobenzyl)benzamide (42): According to "General protocol for acyl transfer 1": Thioester **17** (100 mg, 0.37 mmol), (4-nitrophenyl)methanamine hydrochloride (103 mg, 0.55 mmol). Flash column chromatography on silica gel (50% EtOAc in pentane as the eluant) afforded the title compound **42** (53 mg, 0.18 mmol, 51%) as a light-yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.13 (d, *J* = 8.8 Hz, 2H), 7.76 (d, *J* = 9.2 Hz, 2H), 7.45 (d, *J* = 8.8 Hz, 2H), 6.90 (d, *J* = 9.2 Hz, 2H), 6.70 (br t, *J* = 4.8 Hz, 1H), 4.69 (d, *J* = 6.4 Hz, 2H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 167.3, 162.7, 147.4, 146.4, 129.1 (2C), 128.4 (2C), 126.1, 124.1 (2C), 114.1 (2C), 55.7, 43.4. HRMS (ESI) m/z calcd for $C_{15}H_{14}N_2O_4$ [M+H$^+$]: 287.1026, found: 287.1029. R_f (50% EtOAc in pentane) = 0.34.



***N*-(tert-butyl)-4-methoxybenzamide (43):**[16] According to "General protocol for acyl transfer 1": Thioester **17** (50 mg, 0.18 mmol), *tert*-butylamine (170 μL, 1.6 mmol). Flash column chromatography on silica gel (20% EtOAc in pentane as the eluant) afforded the title compound **43** (23 mg, 0.11 mmol, 60%) as a colorless solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.66 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H), 5.85 (br s, 1H), 3.81 (s, 3H), 1.44 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 166.6, 162.0, 128.6 (2C), 113.8 (2C), 55.6, 51.6, 29.1 (3C). HRMS (ESI) m/z calcd for $C_{12}H_{17}NO_2$ [M+H$^+$]: 208.1332, found: 208.1333. R_f (30% EtOAc in pentane) = 0.39.



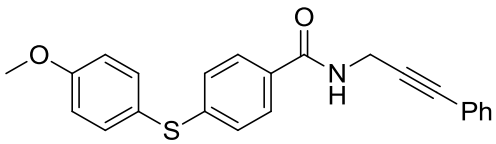
(4-(cyclopropanecarbonyl)piperazin-1-yl)(4-((4-methoxyphenyl)thio)phenyl)methanone (44): General procedure for acyl transfer 2: Thioester **36** (40 mg, 0.11 mmol), K_2CO_3 (29 mg, 0.21 mmol), cyclopropyl(piperazin-1-yl)methanone (24 mg, 0.16 mmol) and DMF (1 mL) was stirred at rt in a 4 mL vial sealed with a PTFE-coated screw cap for 69 hours (over weekend). Et_2O (100 mL) was added to the reaction mixture and washed with 1 M HCl (2 x 10 mL) and brine (10 mL). The organic phase was dried



[16] Baum, J. C.; Milne, J. E.; Murry, J. A.; Thiel, O. R. *J. Org. Chem.*, **2009**, *74*, 2207.

over Na_2SO_4, evaporated *in vacuo* and subjected to flash column chromatography on silica gel (70% EtOAc in pentane as the eluant) to obtain the title compound **44** (23 mg, 0.057 mmol, 55%) as a wax. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.43 (d, *J* = 8.8 Hz, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.4 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 3.82 (s, 3H), 3.78-3.42 (m, 8H), 1.75-1.66 (m, 1H), 1.01-0.96 (m, 2H), 0.81-0.73 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 172.5, 170.5, 160.6, 142.7, 136.6 (2C), 132.0, 128.0 (2C), 127.0 (2C), 122.5, 115.5, 55.6, 11.2, 7.9. HRMS (ESI) m/z calcd for $C_{22}H_{24}N_2O_3S$ [M+H$^+$]: 397.1582, found: 397.1580 R_f (70% EtOAc in pentane) = 0.20.

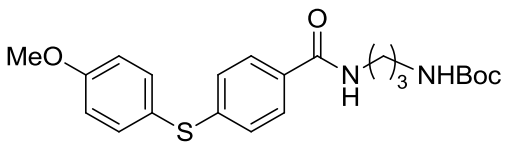
4-((4-methoxyphenyl)thio)-*N*-(3-phenylprop-2-yn-1-yl)benzamide (45): According to the "General conditions for acyl transfer 2": Thioester **36** (40 mg, 0.11 mmol), K_2CO_3 (44 mg, 0.32 mmol), 3-phenylprop-2-yn-1-amine (27 mg, 0.16 mmol) and DMF (1 mL) was stirred at rt for 25 h. Flash column chromatography on silica gel (20% EtOAc in pentane as the eluant) afforded the title compound **45** (26 mg, 0.07 mmol, 66%) as a colorless solid.



^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.65 (d, *J* = 8.8 Hz, 2H), 7.45 (d, *J* = 8.8 Hz, 2H), 7.45-7.39 (m, 2H), 7.34-7.27 (m, 3H), 7.11 (d, *J* = 8.4 Hz, 2H), 6.94 (d, *J* = 8.8 Hz, 2H), 6.37 (br t, *J* = 4.8 Hz, 1H), 4.45 (d, *J* = 4.8 Hz, 2H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 166.7, 160.7, 144.8, 136.7 (2C), 131.9 (2C), 130.7, 128.7, 128.5 (2C), 127.7 (2C), 126.7 (2C), 122.7, 122.2, 115.5 (2C), 84.9, 83.9, 55.6, 30.8. HRMS (ESI) m/z calcd for $C_{23}H_{19}NO_2S$ [M+H$^+$]: 374.1209, found: 374.1205. R_f (20% EtOAc in pentane) = 0.24.

VIII. One-pot Procedure

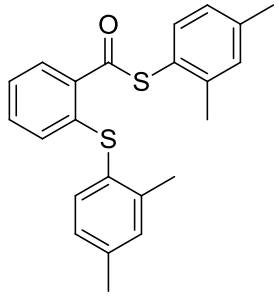
***tert*-butyl (3-(4-((4-methoxyphenyl)thio)benzamido)propyl)carbamate (46):** The title compound was prepared using the general procedure for the Thiocarbonylation-Arylation. **Chamber 1:** 1,2-diiodobenzene (83mg, 0.25 mmol), $Pd(OAc)_2$ (0.234 mL stock solution, 2.5 μmol,), DPEphos (1.3 mg, 2.5 μmol,) and NaOAc (45.1 mg, 0.55 mmol) was dissolved in DME (0.766 mL). **Chamber 2:** 3.0 equivalents of CO were generated in chamber 2. The glassware was then removed from the glovebox, and 2,4-dimehylthiophenol (68 μL, 0.50 mmol) was injected into chamber 1 before mixing at 85 ^{o}C. After 18 h, the reaction mixture from chamber 1 was transferred to a round bottomed flask and the solvent was removed *in vacuo*. The remaining solid was dissolved in 1:1TEA/pyridine (0.6 mL) and *N*-Boc-1,3-propanediamine (66 μL, 0.38 mmol) and mixed overnight at 70 ^{o}C. . The reaction was cooled to rt, evaporated *in vacuo* and the desired compound was purified by flash chromatography on silica gel using pentane/EtOAc (3:1 to 1:1) as eluent. The title compound was isolated as a yellow oil (35 mg, 0.09 mmol, 34%).



^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.68 (d, *J* = 8.2 Hz, 2H), 7.44 (d, *J* = 8.8 Hz, 2H), 7.25 (br s, 1H), 7.11 (d, *J*=8.5 Hz, 2H), 6.93 (d, *J* = 8.8 Hz, 2H), 4.95 (br s, 1H), 3.83 (s, 3H), 3.45 (q, *J*=6.2 Hz, 2H), 3.20 (q, *J*=6.2 Hz, 2H), 1.66 (pent, *J*=5.8 Hz, 2H), 1.43 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 166.9, 160.4, 157.0, 143.8, 136.3, 131.3, 127.5, 126.6, 122.4, 115.2, 79.5, 55.4, 37.0, 35.9, 30.2, 28.4. HRMS (ESI) m/z calcd for $C_{22}H_{28}N_2O_4S$ [M+Na$^+$]: 439.1667, found: 439.1669.

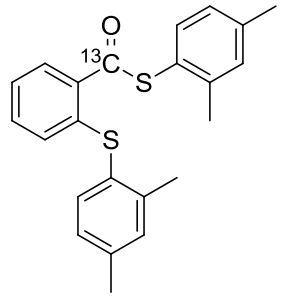
IX. Synthesis of the Vortioxetine Analog

***S*-(2,4-dimethylphenyl) 2-((2,4-dimethylphenyl)thio)benzothioate (47):** The title compound was prepared



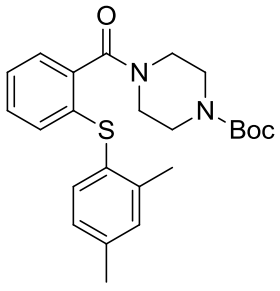
using the general procedure for the Thiocarbonylation-Arylation. **Chamber 1:** 1,2-diiodobenzene (83mg, 0.25 mmol), $Pd(OAc)_2$ (0.234 mL stock solution, 2.5 μmol,), DPEphos (1.3 mg, 2.5 μmol,) and NaOAc (45.1 mg, 0.55 mmol) was dissolved in DME (0.766 mL). **Chamber 2:** 3.0 equivalents of CO were generated in chamber 2. The glassware was then removed from the glovebox, and 2,4-dimehylthiophenol (68 μL, 0.50 mmol) was injected into chamber 1 before mixing at 85 ^{o}C. After 18 h, the solvent was removed from chamber 1 *in vacuo* and the desired compound was purified by flash chromatography on silica gel using pentane/CH_2Cl_2 (3:1) as eluent. The title compound was isolated as pale yellow crystals (60 mg, 0.16 mmol, 64%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.13 (dd, *J* = 7.7 Hz, *J* = 1.4 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 2H), 7.27-7.16 (m, 4H), 7.11-7.05 (m, 2H), 6.72 (dd, *J* = 8.1 Hz, *J* = 1.1 Hz, 1H), 2.43 (s, 3H), 2.37 (s, 3H), 2.37 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.0, 142.7, 142.3, 140.8, 140.4, 139.9, 136.7, 136.4, 133.7, 132.3, 131.8, 131.7, 129.7, 128.0, 127.9, 127.5, 126.9, 124.1, 123.6, 21.3, 21.2, 20.8, 20.5. HRMS (ESI) m/z calcd for $C_{23}H_{22}OS_2$ [M+H$^+$]: 379.1184, found: 379.1185.

***S*-(2,4-dimethylphenyl) 2-((2,4-dimethylphenyl)thio)benzo[^{13}C]thioate (^{13}C-47):** The title compound was



prepared using the general procedure for the Thiocarbonylation-Arylation. **Chamber 1:** 1,2-diiodobenzene (83mg, 0.25 mmol), $Pd(OAc)_2$ (0.234 mL stock solution, 2.5 μmol,), DPEphos (1.3 mg, 2.5 μmol,) and NaOAc (45.1 mg, 0.55 mmol) was dissolved in DME (0.766 mL). **Chamber 2:** 3.0 equivalents of ^{13}CO were generated in chamber 2. The glassware was then removed from the glovebox, and 2,4-dimehylthiophenol (68 μL, 0.50 mmol) was injected into chamber 1 before mixing at 85 ^{o}C. After 18 h, the solvent was removed from chamber 1 *in vacuo* and the desired compound was purified by flash chromatography on silica gel using pentane/CH_2Cl_2 (3:1) as eluent. The title compound was isolated as pale yellow crystals (62 mg, 0.16 mmol, 65%).^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 8.13 (ddd, *J* = 7.7 Hz, *J* = 5.5 Hz, *J* = 1.4 Hz, 1H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.27-7.16 (m, 4H), 7.11-7.05 (m, 2H), 6.72 (dd, *J* = 8.0 Hz, *J* = 1.3 Hz, 1H), 2.43 (s, 3H), 2.37 (s, 3H), 2.37 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.0 (^{13}C), 142.7, 142.4, 140.8, 140.4, 139.9, 136.7, 136.4, 133.7 (d, *J* = 62 Hz), 132.3, 131.8, 131.7, 129.7 (d, *J* = 3.8 Hz), 128.0, 127.9, 127.5, 126.9 (d, *J* = 3.7 Hz), 124.1 (d, *J* = 4.7 Hz), 123.6 (d, *J* = 1.4 Hz), 21.3, 21.2, 20.8, 20.5. HRMS (ESI) m/z calcd for [^{13}C]$C_{22}H_{22}OS_2$ [M+H$^+$]: 380.1218, found: 380.1219.

***tert*-butyl 4-(2-((2,4-dimethylphenyl)thio)benzoyl)piperazine-1-carboxylate (48):** *S*-(2,4-dimethylphenyl)



2-((2,4-dimethylphenyl)thio)benzothioate (**47**) (56 mg, 0.15 mmol), 1-Boc-piperazine (83 mg, 0.45 mmol) and K_2CO_3 (83 mg, 0.60 mmol) was dissolved in DMF (1.0 mL) and stirred at 100 ^{o}C overnight. Thereafter the reaction was cooled to rt and H_2O (20 mL) was added. The water phase was then extracted with Et_2O (3 x 20 mL) and the combined organic phase was washed with brine and dried with $MgSO_4$. The desired compound was purified by flash chromatography on silica gel using Pentane/EtOAc (3:1) as eluent. The title compound was isolated as a clear oil (45 mg, 0.10 mmol, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.29 (d, *J* = 7.8 Hz, 1H), 7.20-7.14 (m, 3H), 7.10 (br s, 1H), 6.99 (d, *J* = 7.9 Hz, 1H), 6.81-6.79 (m, 1H), 3.78 (br s, 2H), 3.53 (t, J = 5.2 Hz, 2H), 3.42 (br s, 2H), 3.26 (br s, 2H), 2.31 (s, 3H), 2.30 (s, 3H), 1.45 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 168.5, 154.5, 141.3, 139.2, 135.2 134.9, 131.8, 129.6, 128.2, 127.8, 127.6, 126.7, 125.8, 80.3, 46.8, 41.5, 28.4, 21.1, 20.6. HRMS (ESI) m/z calcd for $C_{24}H_{30}N_2O_3S$ [M+H$^+$]: 427.2050, found: 427.2051.

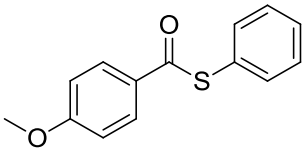
***tert*-butyl 4-(2-((2,4-dimethylphenyl)thio)[^{13}C]benzoyl)piperazine-1-carboxylate (^{13}C-48):** *S*-(2,4-dimethylphenyl) 2-((2,4-dimethylphenyl)thio)benzo[^{13}C]thioate (**^{13}C-47**) (58 mg, 0.15 mmol), 1-Boc-piperazine (86 mg, 0.45 mmol) and K_2CO_3 (85 mg, 0.60 mmol) was dissolved in DMF (1.0 mL) and stirred at 100 ^{o}C overnight. Thereafter the reaction was cooled to rt and H_2O (20 mL) was added. The water phase was then extracted with Et_2O (3 x 20 mL) and the combined organic phase was washed with brine and dried with $MgSO_4$. The desired compound was purified by flash chromatography on silica gel using Pentane/EtOAc (3:1) as eluent. The title compound was isolated as a clear oil (46 mg, 0.11 mmol, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.29 (d, *J* = 7.8 Hz, 1H), 7.20-7.14 (m, 3H), 7.10 (br s, 1H), 6.99 (dd, *J* = 7.9 Hz, *J* = 1.4 Hz, 1H), 6.81-6.79 (m, 1H), 3.78 (br s, 2H), 3.53 (t, J = 4.8 Hz, 2H), 3.43 (br s, 2H), 3.27 (br s, 2H), 2.33 (s, 3H), 2.31 (s, 3H), 1.46 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 168.6 (^{13}C), 154.5, 141.4, 139.3, 135.2 134.9, 131.8, 129.6, 128.1 (d, *J*=2.1 Hz), 127.8, 127.6, 126.7 (d, *J*=1.3 Hz), 125.8 (d, *J*=4.0 Hz), 80.3, 46.8, 41.5, 28.4, 21.1, 20.7. HRMS (ESI) m/z calcd for [^{13}C]$C_{23}H_{30}N_2O_2S$ [M+H$^+$]: 428.2083, found: 428.2087.

4-(2-((2,4-dimethylphenyl)thio)benzoyl)piperazin-1-ium trifluoroacetate (49): *tert*-butyl 4-(2-((2,4-dimethylphenyl)thio)benzoyl)piperazine-1-carboxylate (**48**) (46 mg, 0.11 mmol) was dissolved in dry CH_2Cl_2 (1.4 mL) under an argon atmosphere followed by addition of TFA (0.14 mL). The reaction mixture was stirred at rt for 3 h, where after the solvent was evaporated. TFA was removed by evaporation of the compound with CH_2Cl_2 several times giving the crude product (45 mg, 0.11 mmol, 100%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.29-7.18 (m, 4H), 7.13 (br s, 1H), 7.01 (d, *J* =7.5 Hz, 1H), 6.83 (d, *J* =8.1 Hz, 1H), 4.13 (br s, 2H), 3.66 (br s, 2H), 3.32 (br s, 2H), 3.24 (br s, 2H), 2.35 (s, 3H), 2.31 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 168.4, 141.4, 139.7, 135.2, 135.1, 133.8, 131.9, 130.2, 128.2, 128.0, 126.9, 126.8, 126.0, 43.5, 38.4, 21.1, 20.6. ^{19}F NMR (377 MHz, $CDCl_3$) δ (ppm) -75.65. HRMS (ESI) m/z calcd for $C_{19}H_{23}N_2OS$ [M$^+$]: 327.1526, found: 327.1525. The amine protons were exchanged with deuterium atoms. Grease impurities were detected in the ^{1}H NMR.

4-(2-((2,4-dimethylphenyl)thio)[^{13}C]benzoyl)piperazin-1-ium trifluoroacetate (^{13}C-49): *tert*-butyl 4-(2-((2,4-dimethylphenyl)thio)[^{13}C]benzoyl)piperazine-1-carboxylate (**^{13}C-48**) (46 mg, 0.11 mmol) was dissolved in dry CH_2Cl_2 (1.4 mL) under an argon atmosphere followed by addition of TFA (0.14 mL). The reaction mixture was stirred at rt for 3 h, where after the solvent was evaporated. TFA was removed by evaporation of the compound with CH_2Cl_2 several times giving the crude product (43 mg, 0.10 mmol, 95%). ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 9.31 (br s, 2H), 7.24-7.19 (m, 4H), 7.11 (br s, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 6.85 (d, *J* = 7.6 Hz, 1H), 4.05 (br s, 2H), 3.56 (br s, 2H), 3.29 (br s, 2H), 3.20 (br s, 2H), 2.32 (s, 3H), 2.27 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 168.8 (^{13}C), 141.2, 139.7, 135.0, 134.9, 133.5 (d, *J*=67.0 Hz), 132.0, 130.4, 128.5 (d, *J*=3.2 Hz), 128.0, 126.78, 126.76, 126.2 (d, *J*=4.0 Hz), 43.6, 38.4, 21.1, 20.5. ^{19}F NMR (377 MHz, $CDCl_3$) δ (ppm) -75.90. HRMS (ESI) m/z calcd for [^{13}C]$C_{18}H_{23}N_2OS$ [M$^+$]: 328.1559, found: 328.1568.

X. Spectral Data

S-Phenyl 4-methoxybenzothioate (1)



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4	Solvent	cdcl3
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7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
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13	Nucleus	1H
14	Acquired Size	16384
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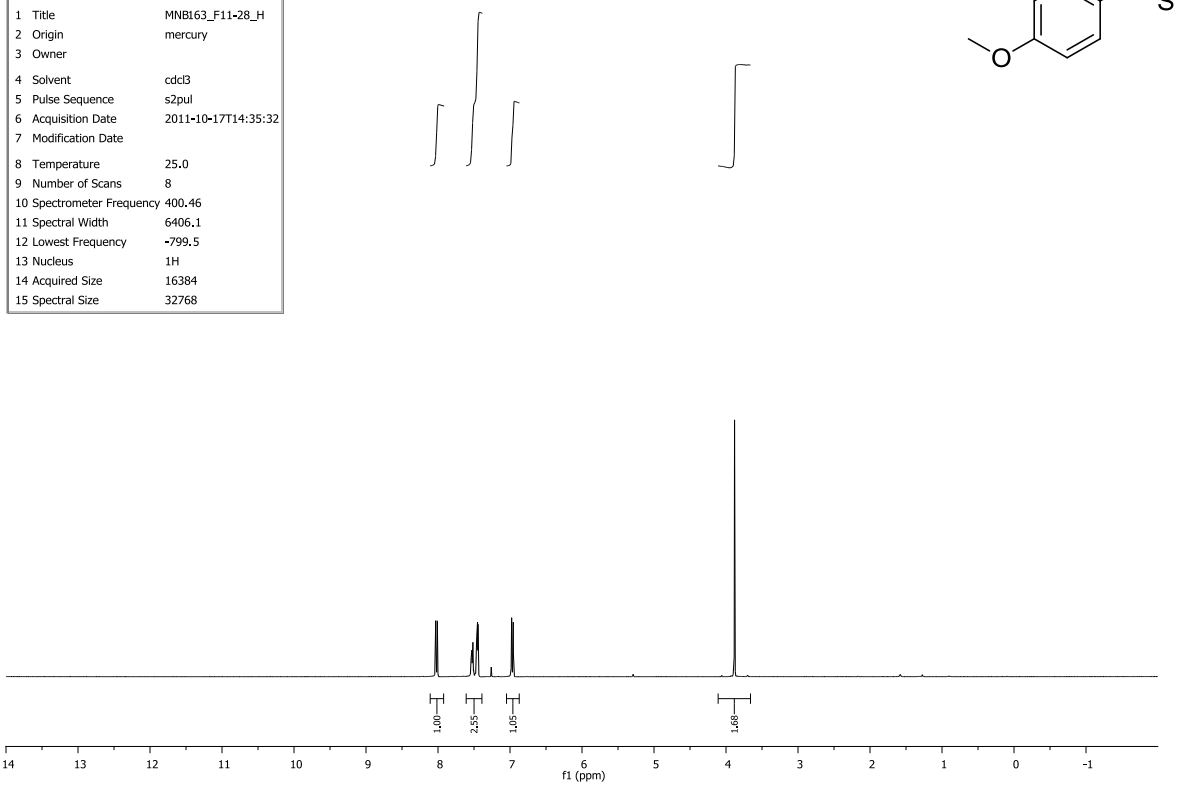

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4	Solvent	cdcl3
5	Pulse Sequence	s2pul
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7	Modification Date	
8	Temperature	25.0
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11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
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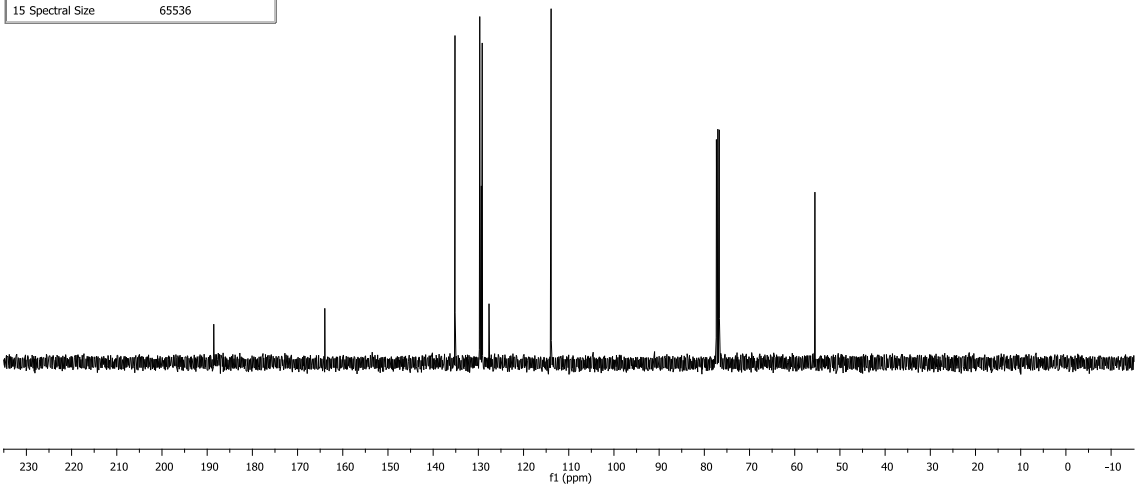

S-Phenyl 3-methoxybenzothioate (3)

	Parameter	Value
1	Title	MNB177.F9-27.H
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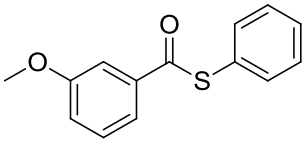
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-04T08:58:52
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



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2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-04T08:59:37
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9	Number of Scans	392
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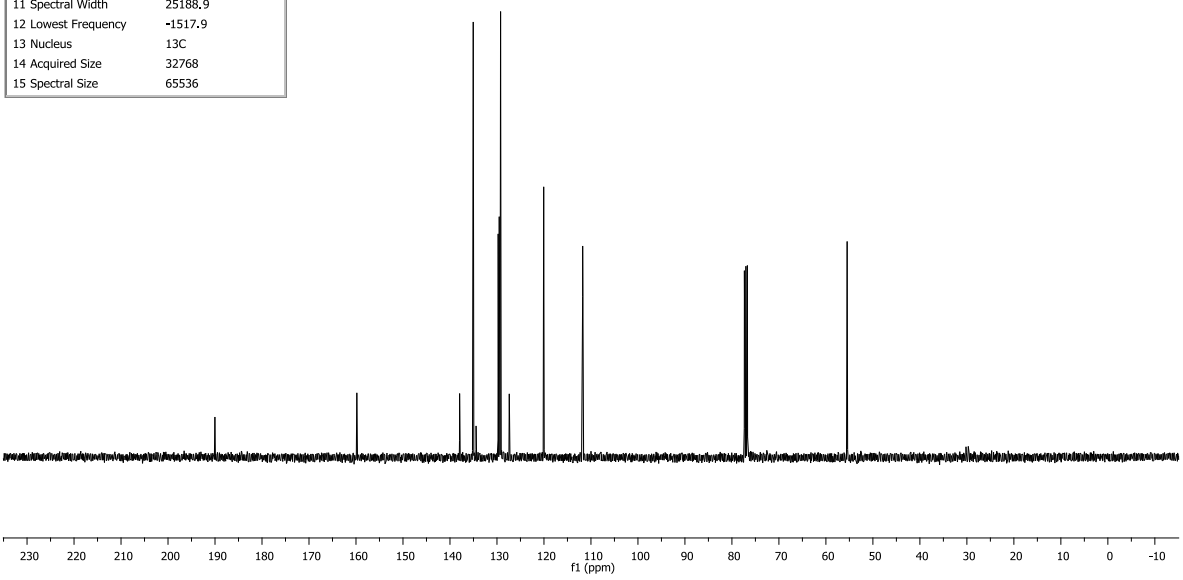
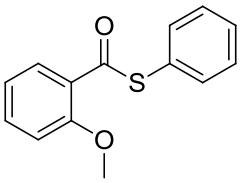
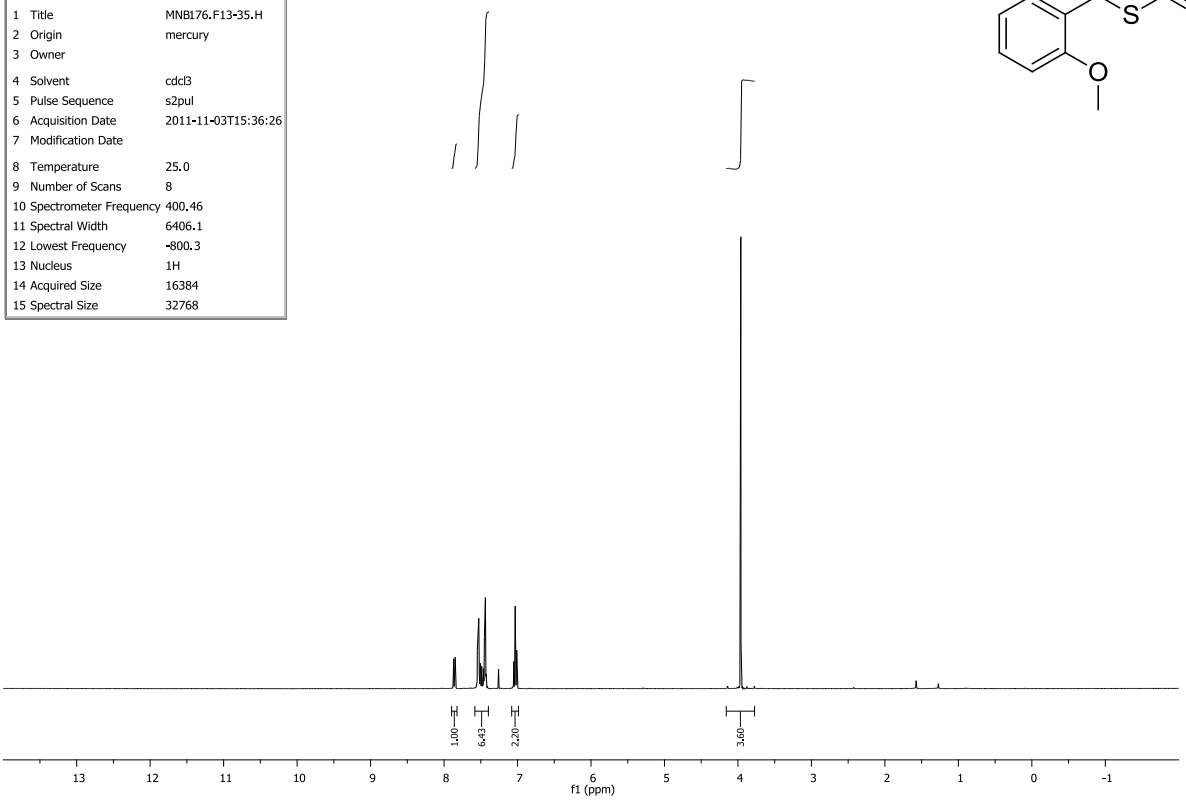
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



S-Phenyl 2-methoxybenzothioate (4)



	Parameter	Value
1	Title	MNB176.F13-35.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-03T15:36:26
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



	Parameter	Value
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3	Owner	
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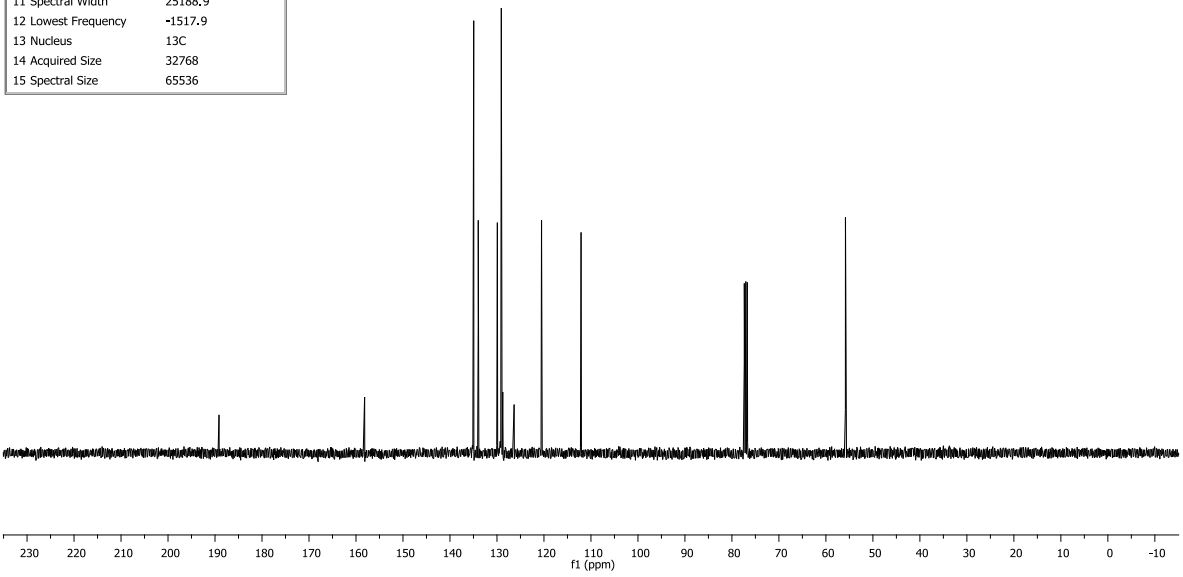
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



S-Phenyl 3,4-dimethoxybenzothioate (5)

	Parameter	Value
1	Title	MNB186.F14-28.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-22T11:26:59
7	Modification Date	
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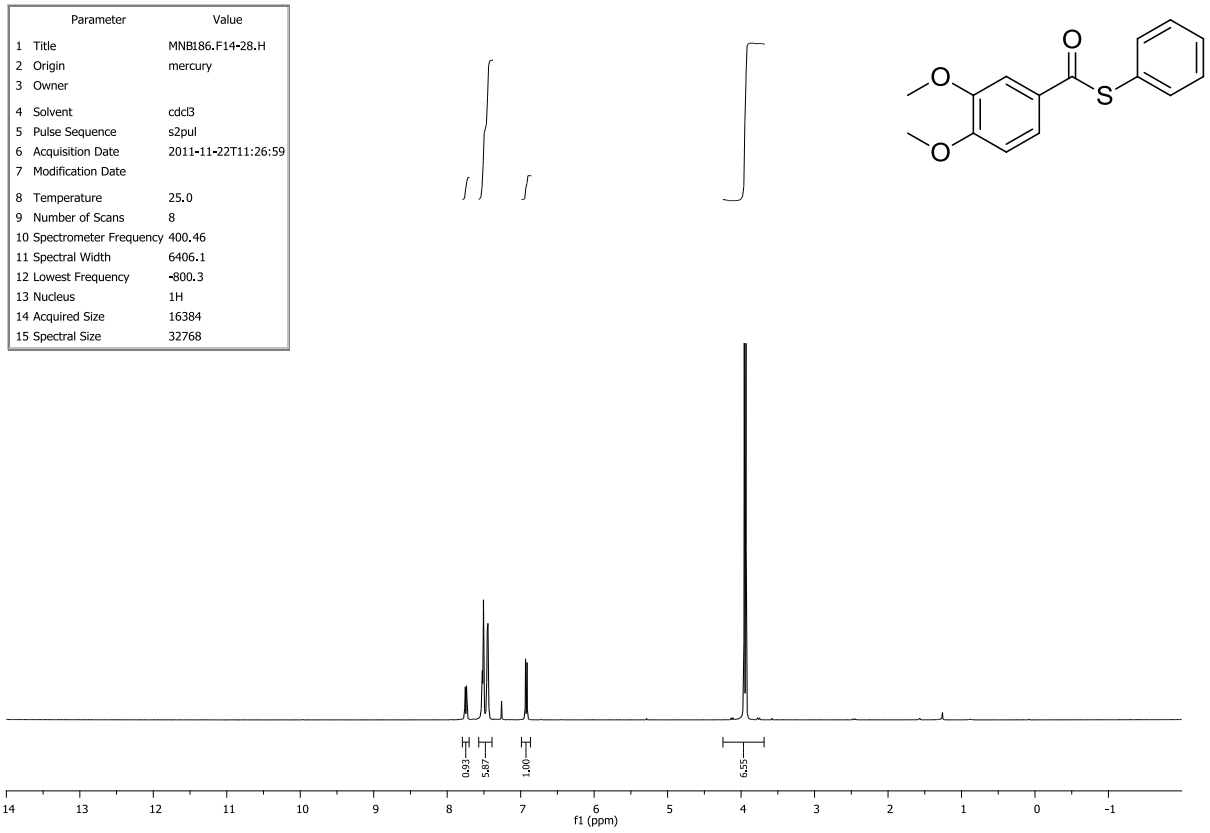
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



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3	Owner	
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5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-22T11:37:48
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
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14	Acquired Size	32768
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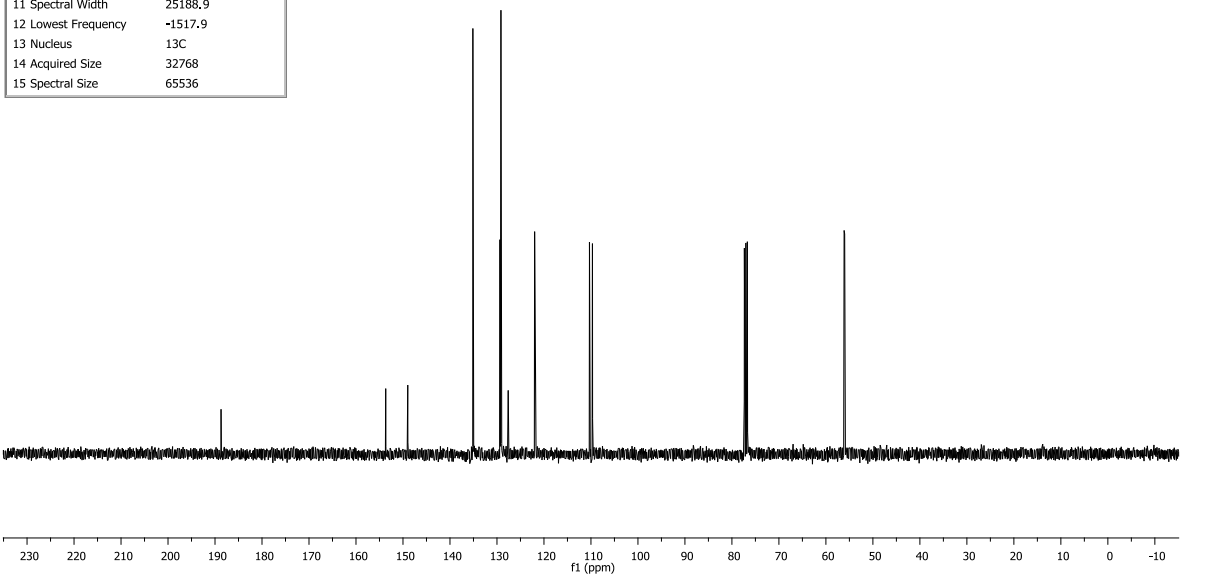

S-Phenyl 2,4-dimethoxybenzothioate (6)

	Parameter	Value
1	Title	MNB184.F7-20.H2
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7	Modification Date	
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12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
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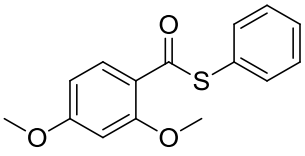

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3	Owner	
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5	Pulse Sequence	s2pul
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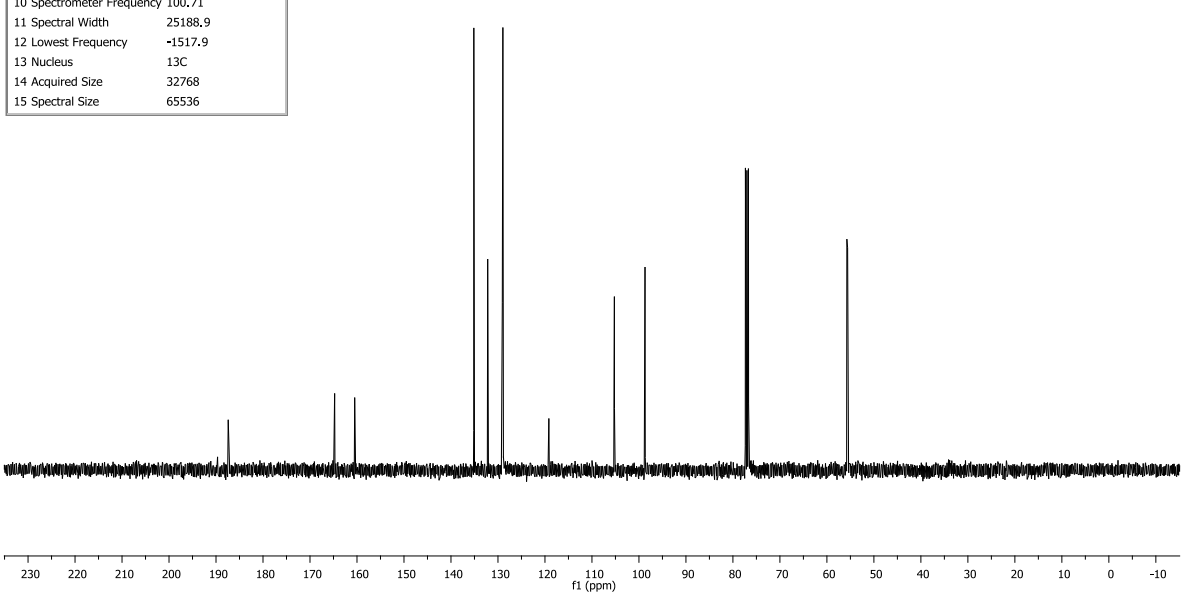
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



S-Phenyl 3,4,5-trimethoxybenzothioate (7)

	Parameter	Value
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3	Owner	
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6	Acquisition Date	2011-11-09T14:19:43
7	Modification Date	
8	Temperature	25.0
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10	Spectrometer Frequency	400.46
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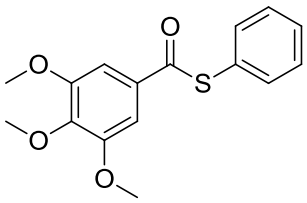
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



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3	Owner	
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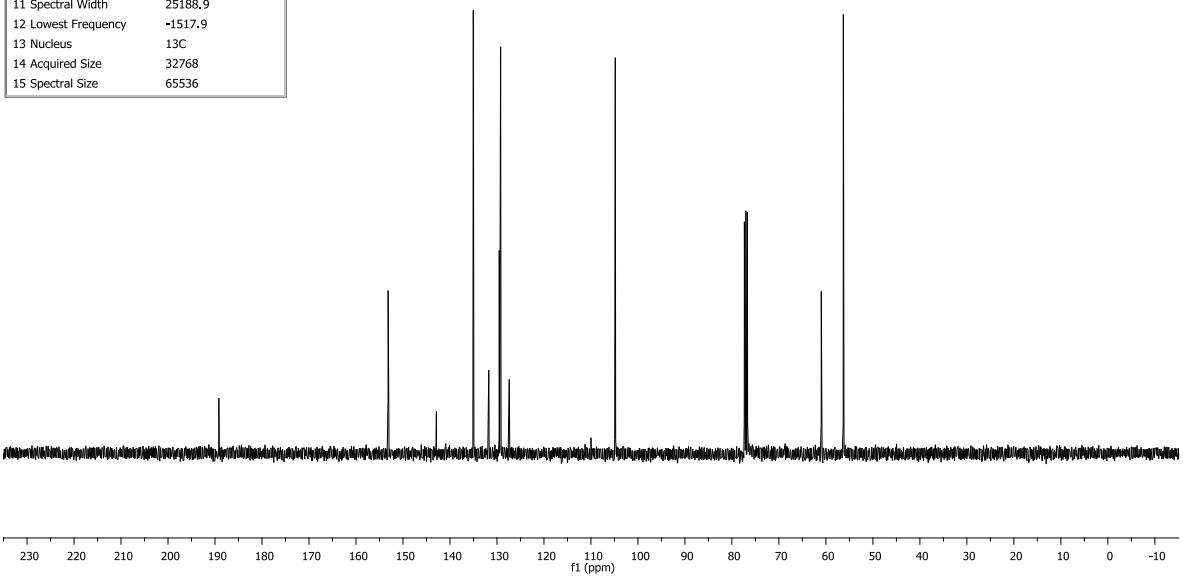
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



S-Phenyl 4-((*tert*-butoxycarbonyl)(methyl)amino)benzothioate (8)

	Parameter	Value
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7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
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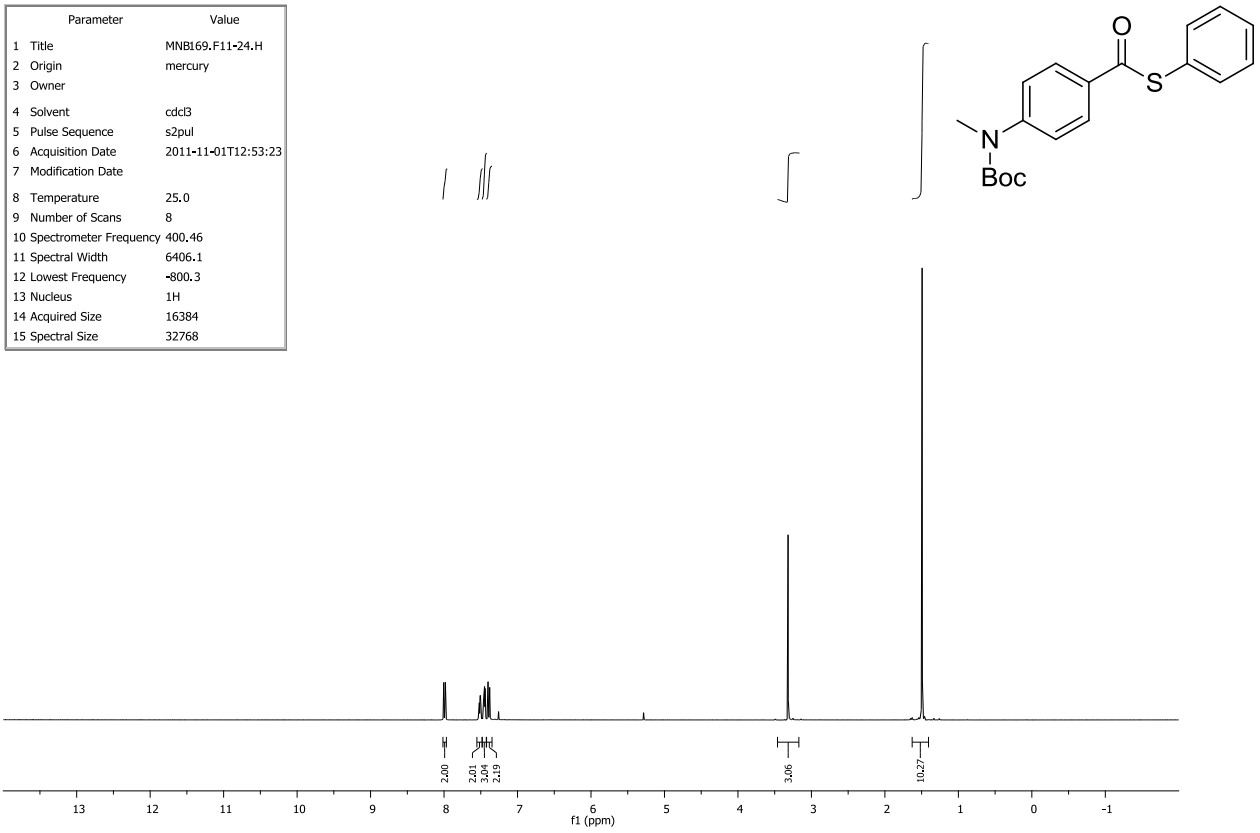
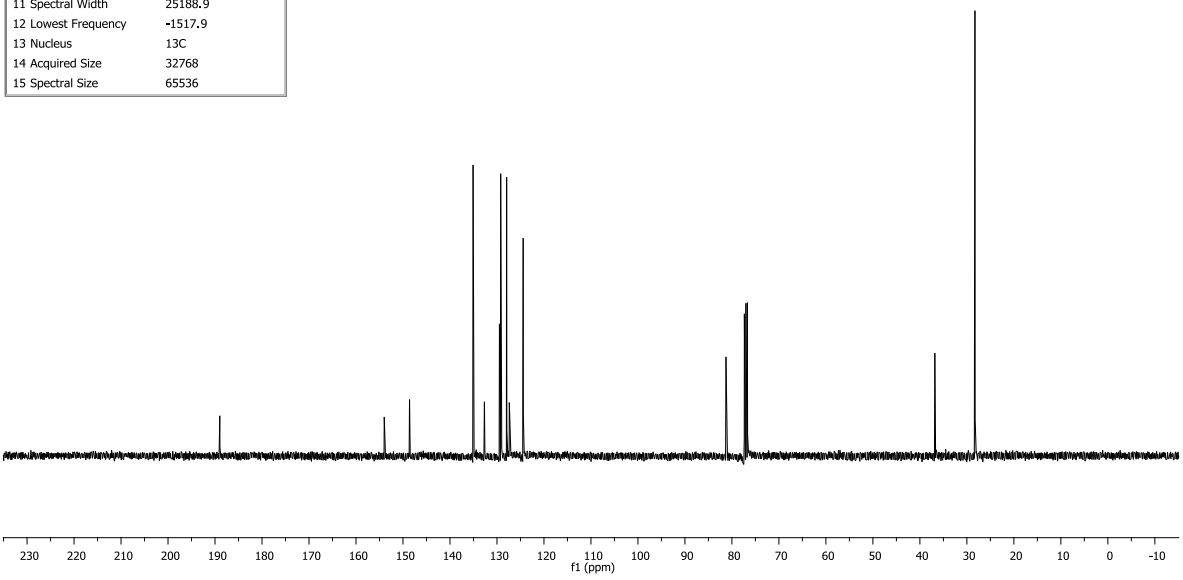
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

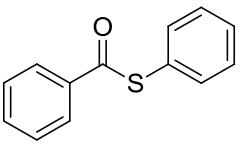


	Parameter	Value
1	Title	MNB169.F11-24.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-01T13:03:57
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536

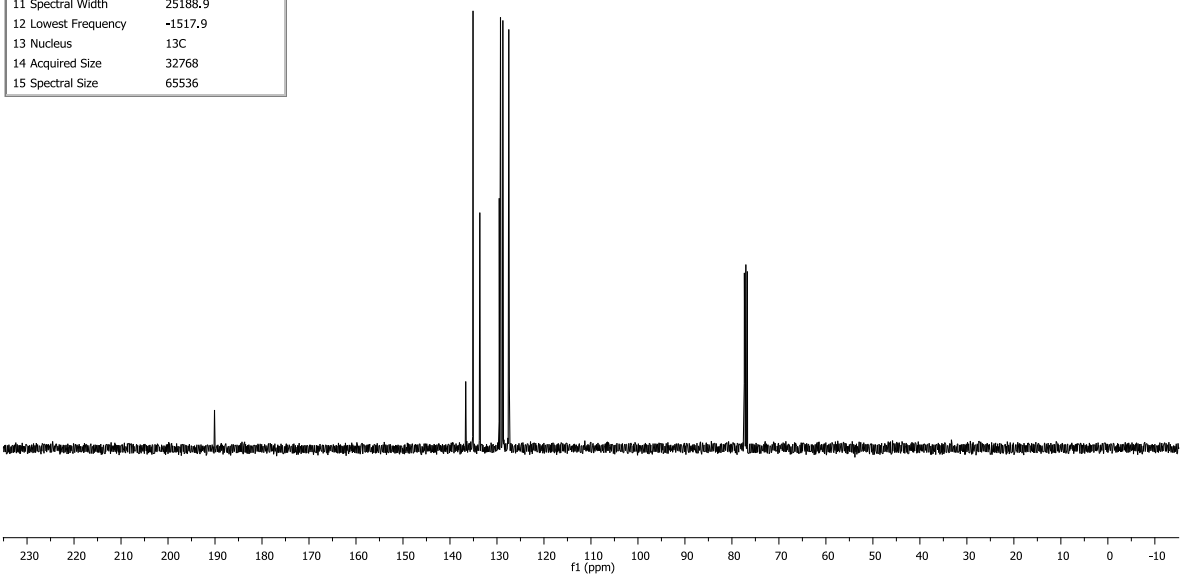


S-Phenyl benzothioate (9)

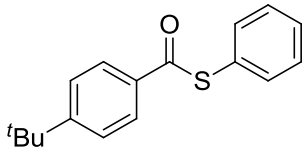
	Parameter	Value
1	Title	MNB165.F5-9.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-10-19T14:09:51
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



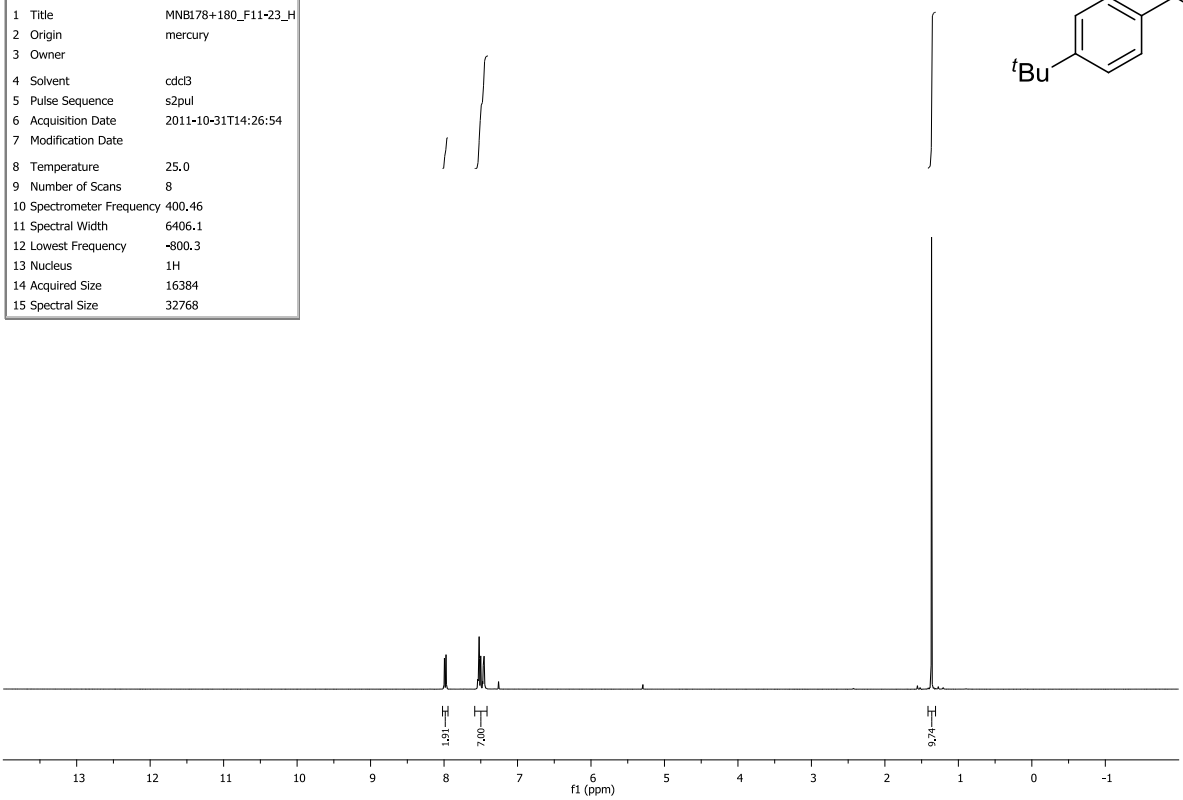
	Parameter	Value
1	Title	MNB165.F5-9.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-10-19T14:21:18
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



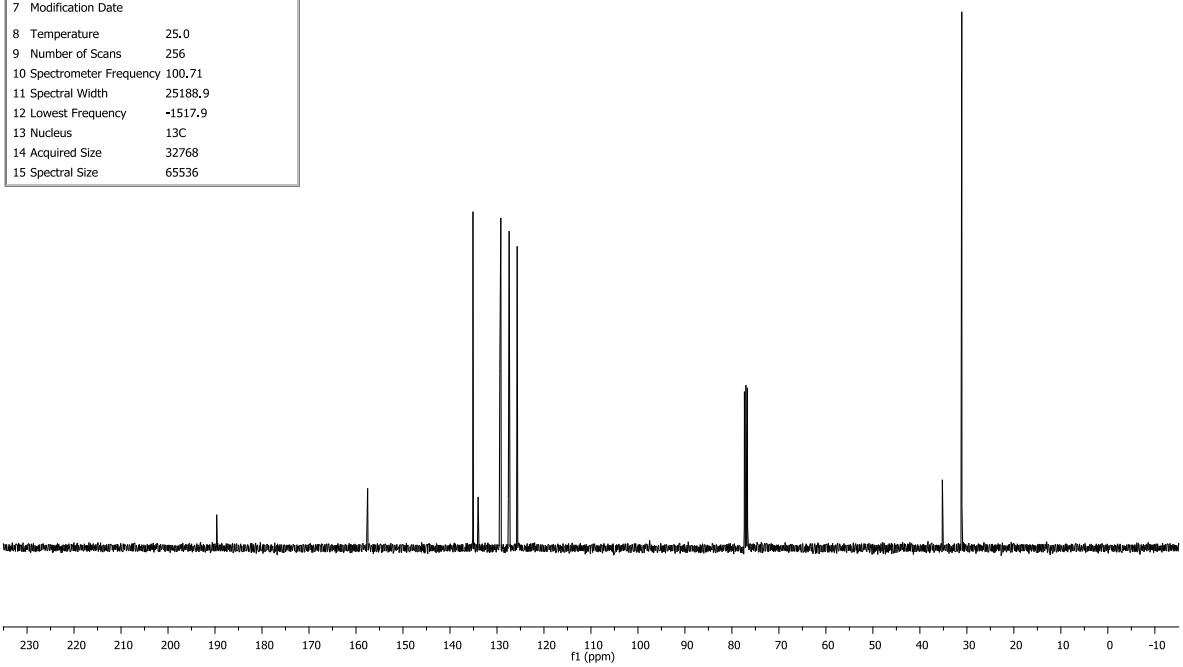
S-Phenyl 4-(*tert*-butyl)benzothioate (10)



	Parameter	Value
1	Title	MNB178+180_F11-23_H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-10-31T14:26:54
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

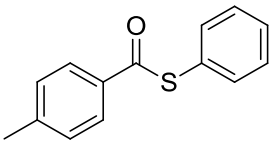


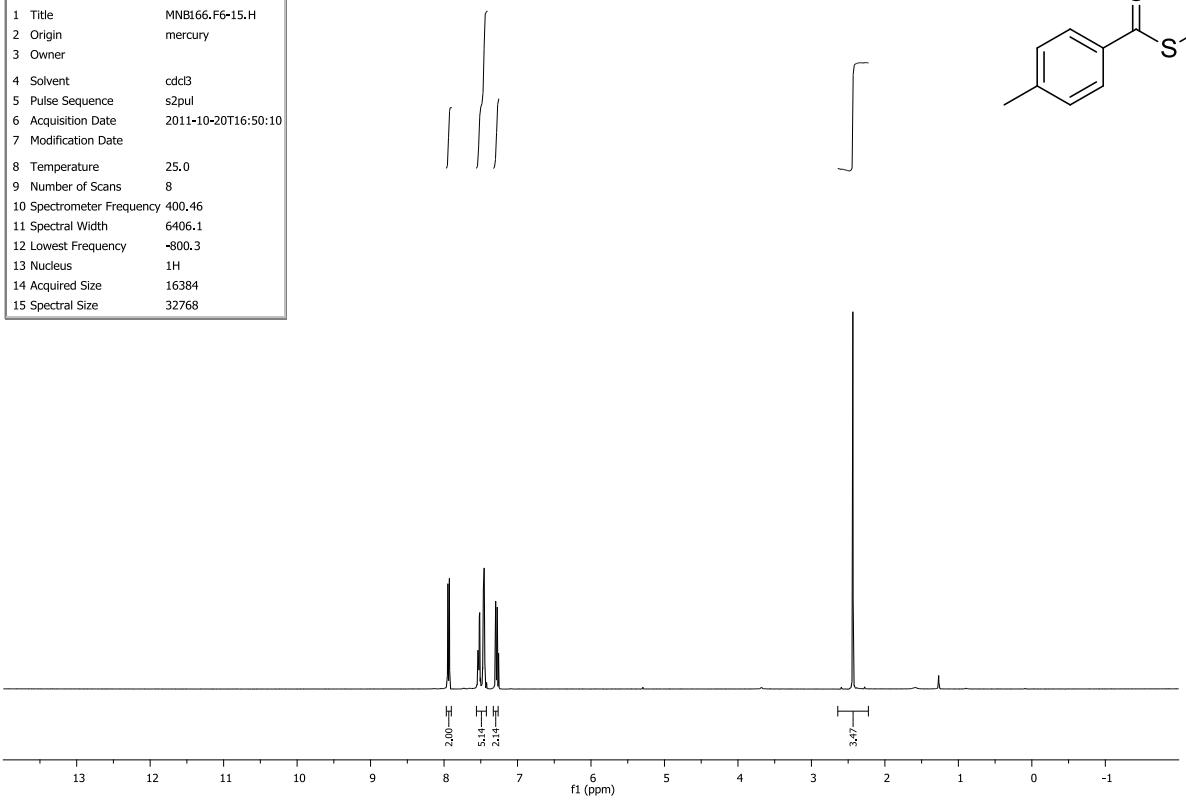
	Parameter	Value
1	Title	MNB178+180_F11-23_C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-10-31T14:38:23
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



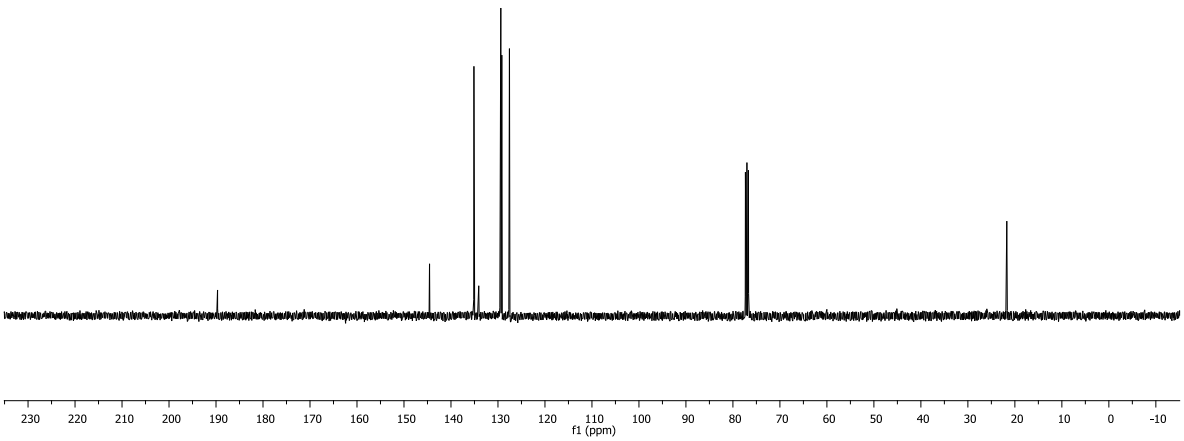
S-Phenyl 4-methylbenzothioate (11)

	Parameter	Value
1	Title	MNB166.F6-15.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-10-20T16:50:10
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



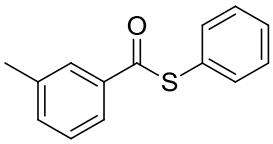


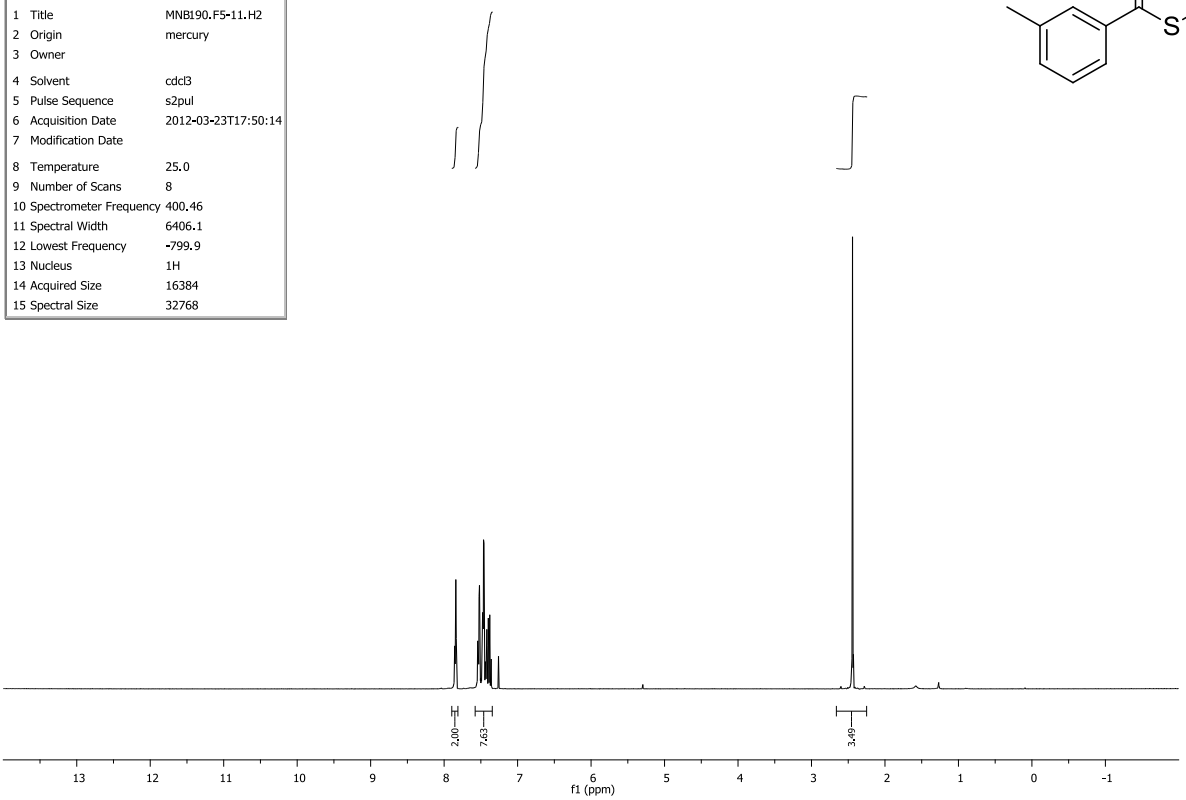
	Parameter	Value
1	Title	MNB166_F6-15_C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-10-20T17:01:17
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



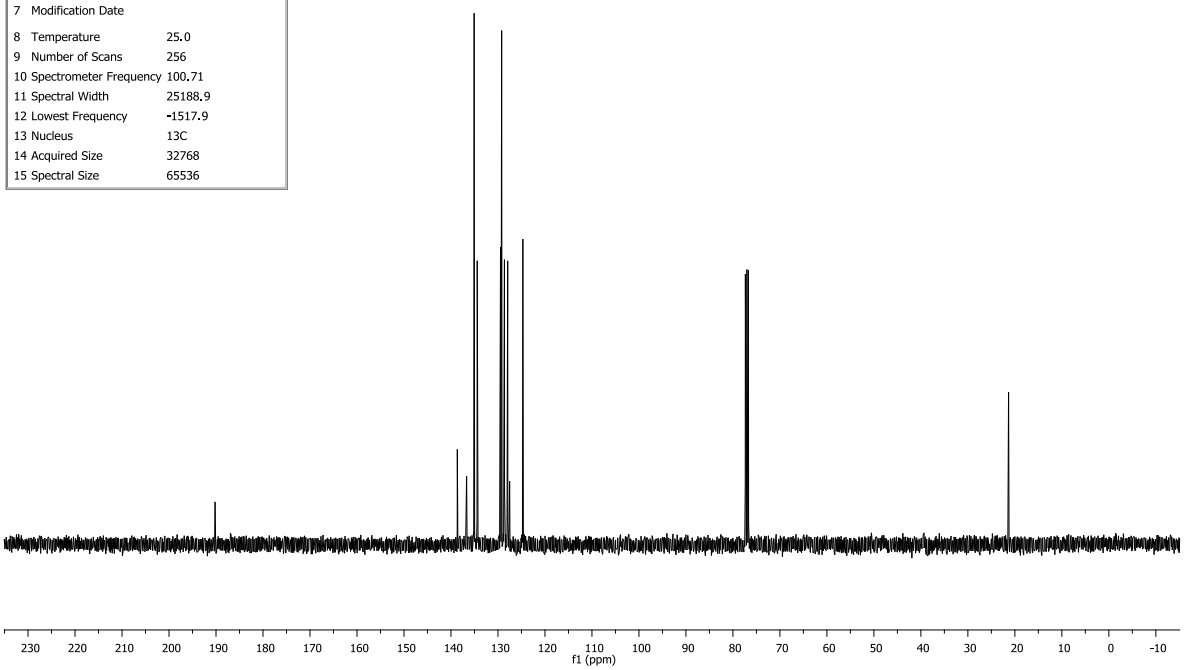
S-Phenyl 3-methylbenzothioate (12)

	Parameter	Value
1	Title	MNB190.F5-11.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-23T17:50:14
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-799.9
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

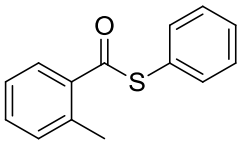




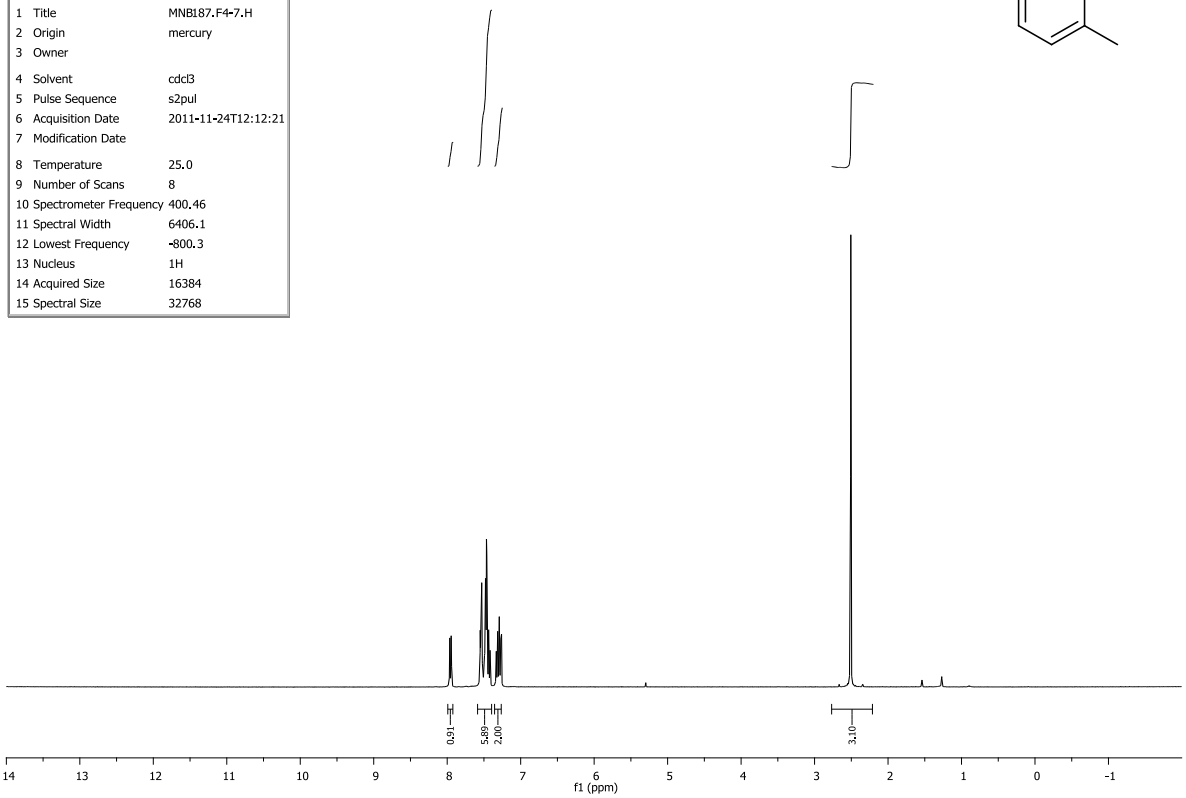
	Parameter	Value
1	Title	MNB190.F5-11.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-25T15:20:29
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



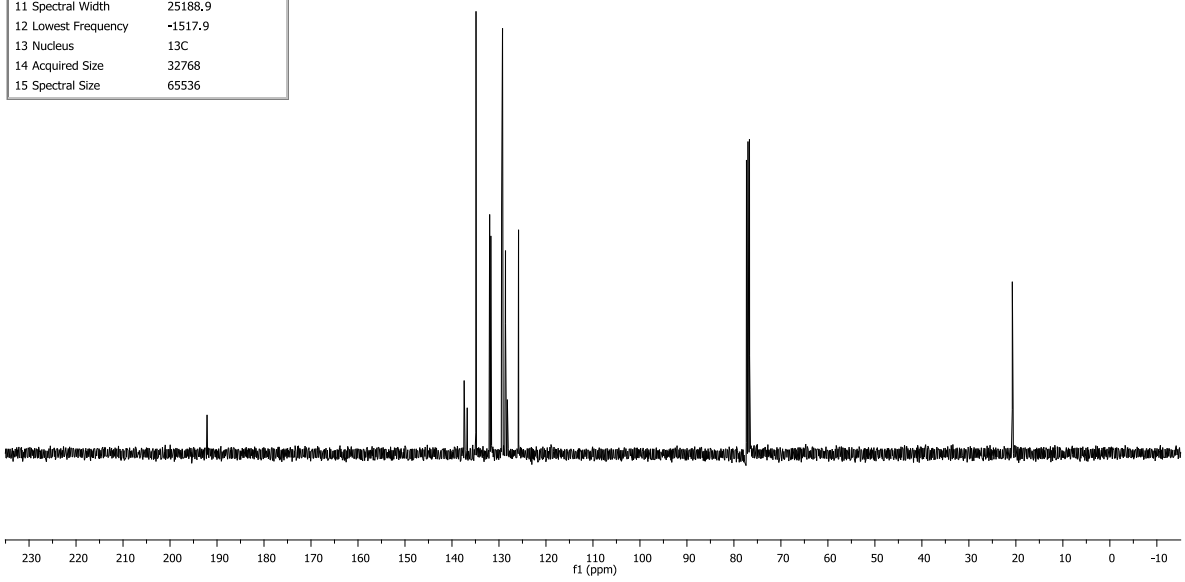
S-Phenyl 2-methylbenzothioate (13)



	Parameter	Value
1	Title	MNB187.F4-7.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-24T12:12:21
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

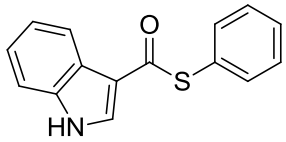


	Parameter	Value
1	Title	MNB187.F4-7.C2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-24T13:04:01
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	512
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536

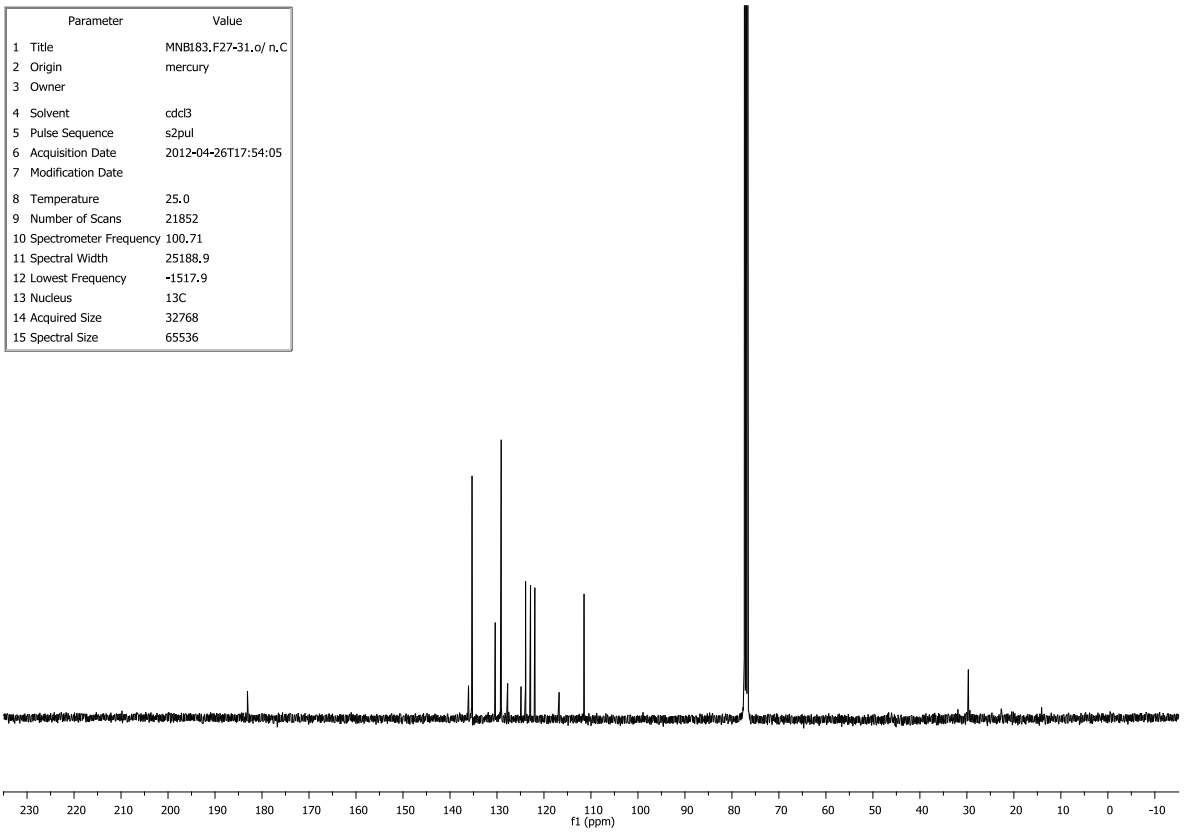


S-Phenyl-indole-3-carbothioate (14)

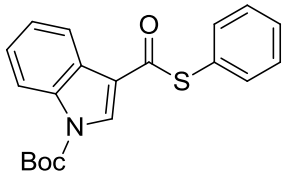
	Parameter	Value
1	Title	MNB183.F27-31.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-18T14:41:45
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-828.9
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



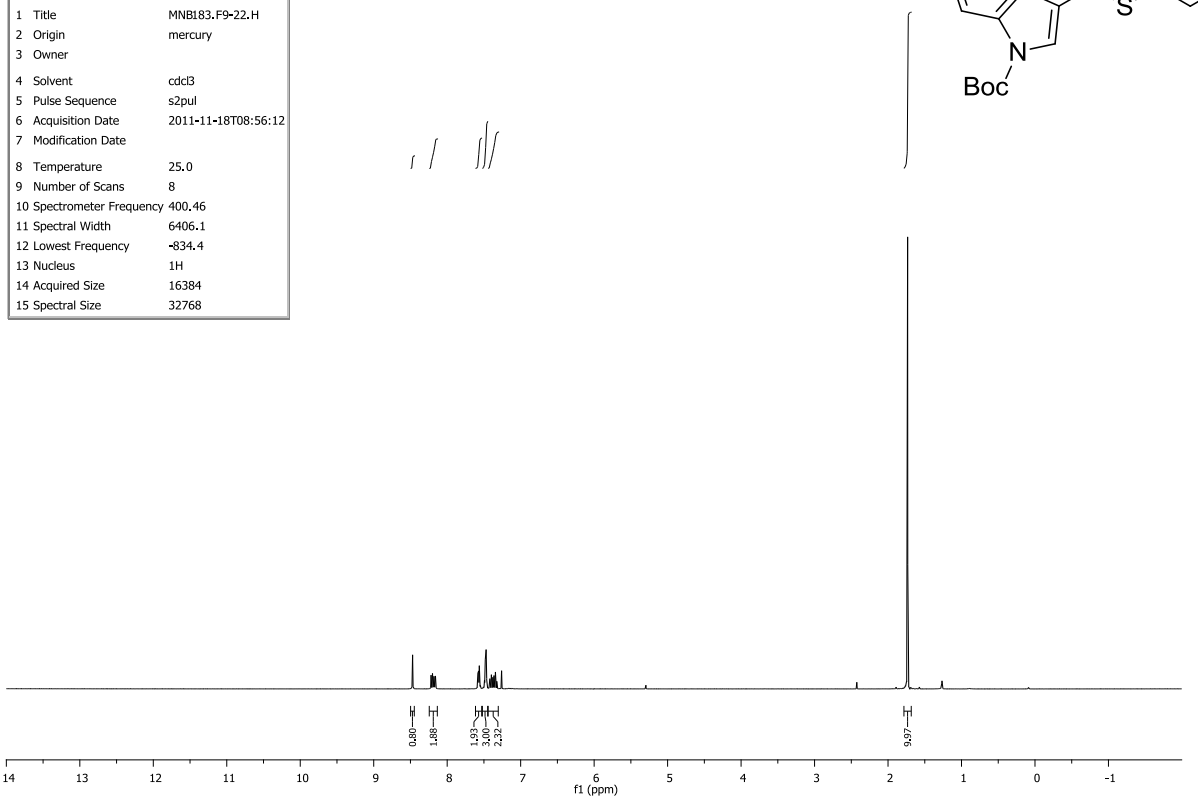
	Parameter	Value
1	Title	MNB183.F27-31.o/ n.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-04-26T17:54:05
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	21852
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



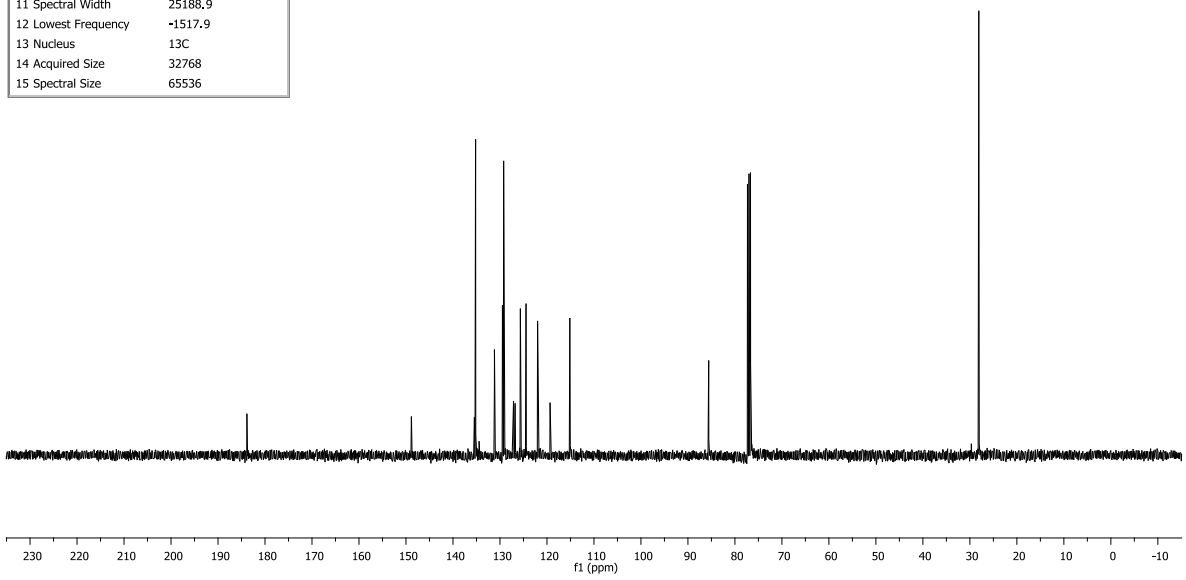
tert-Butyl 3-((phenylthio)carbonyl)-indole-1-carboxylate (15)



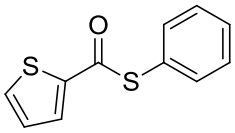
	Parameter	Value
1	Title	MNB183.F9-22.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-18T08:56:12
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-834.4
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



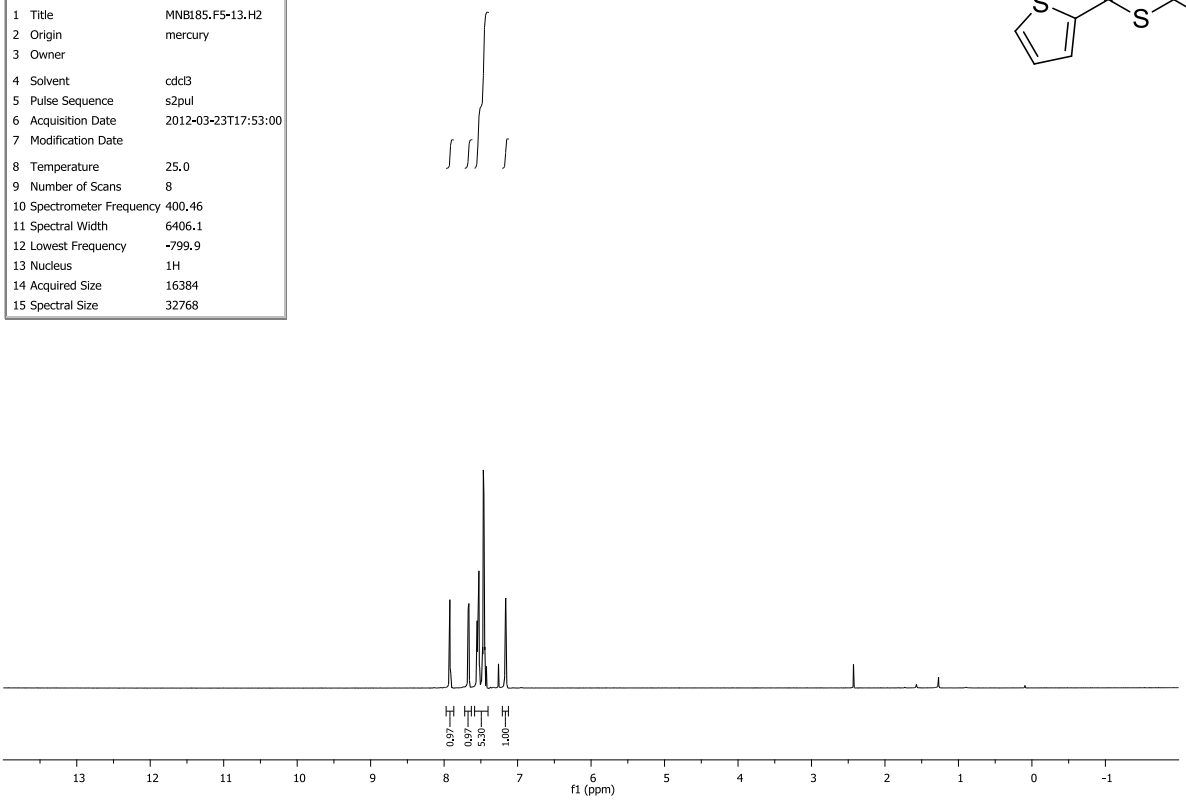
	Parameter	Value
1	Title	MNB183_F9-22_C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-18T11:45:10
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	572
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



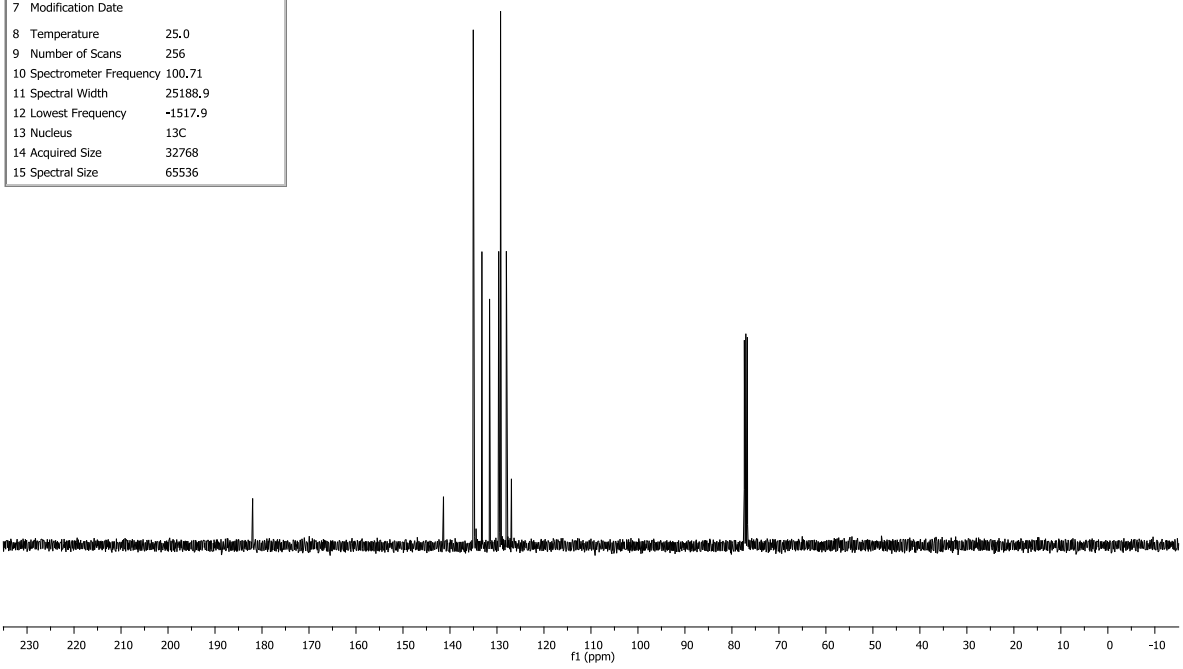
S-Phenyl thiophene-2-carbothioate (16)



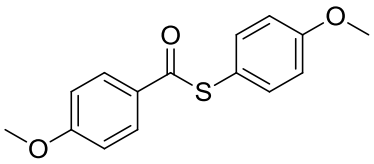
	Parameter	Value
1	Title	MNB185.F5-13.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-23T17:53:00
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-799.9
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



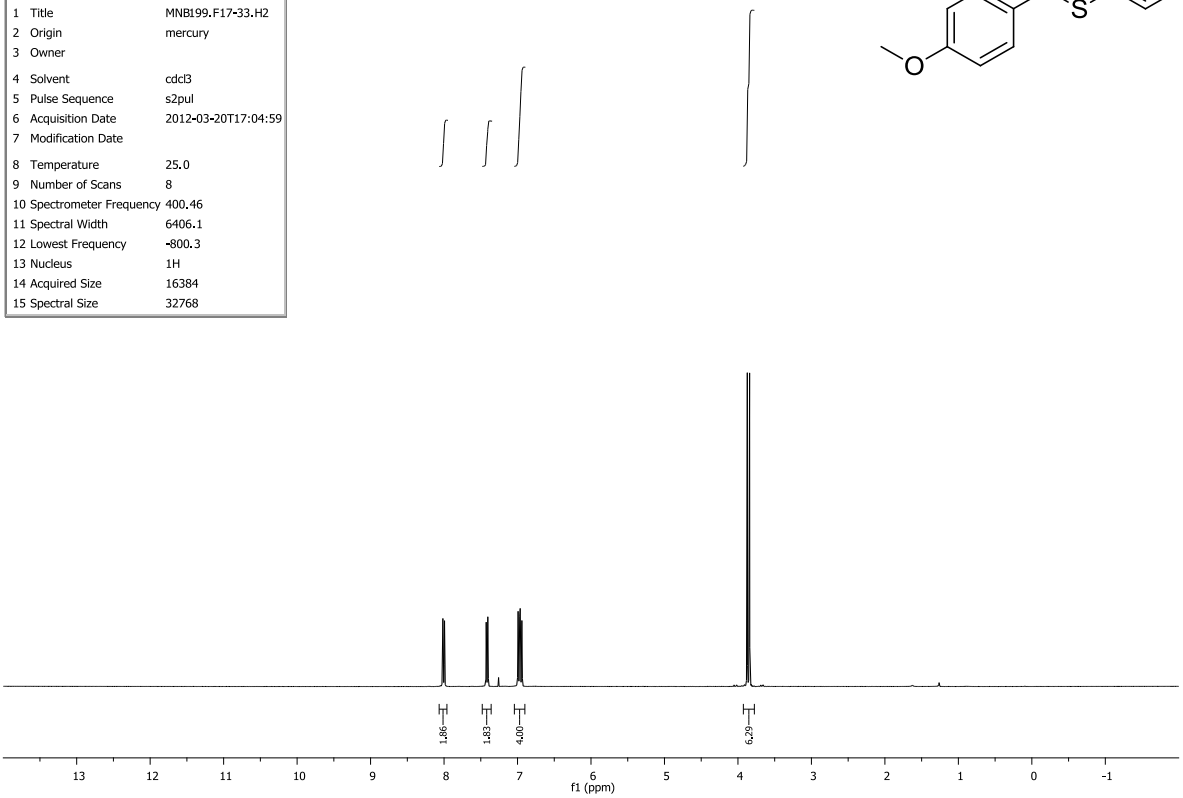
	Parameter	Value
1	Title	MNB185.F5-13.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-17T09:34:38
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



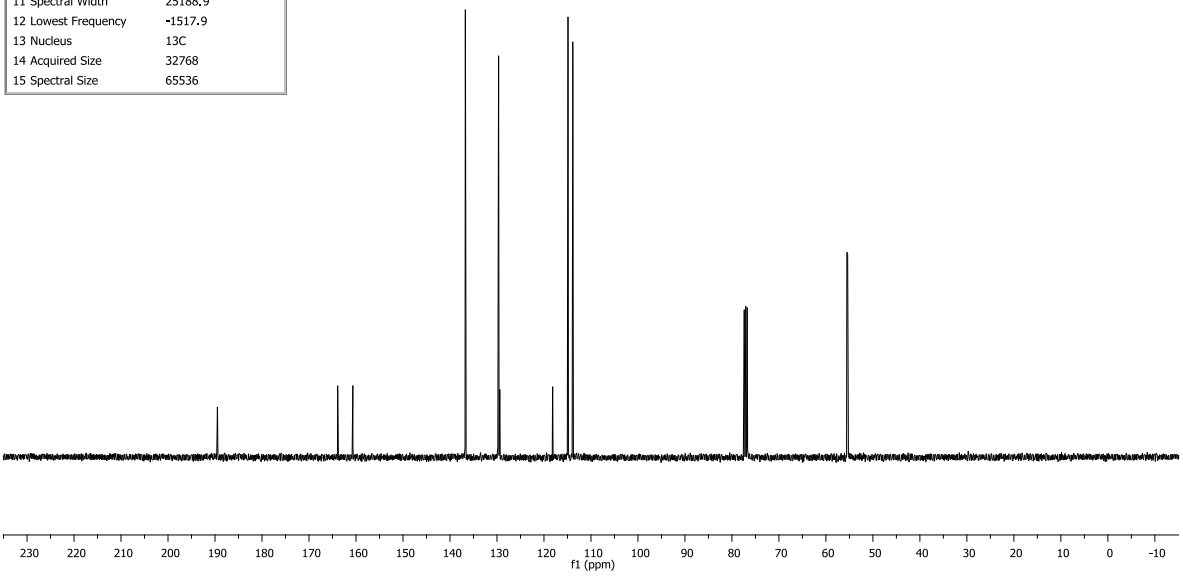
S-(4-Methoxyphenyl) 4-methoxybenzothioate (17)



	Parameter	Value
1	Title	MNB199.F17-33.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-20T17:04:59
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

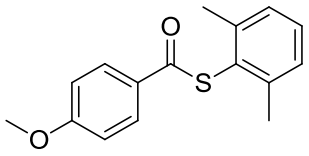


	Parameter	Value
1	Title	MNB199.F17-33.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-20T17:05:47
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536

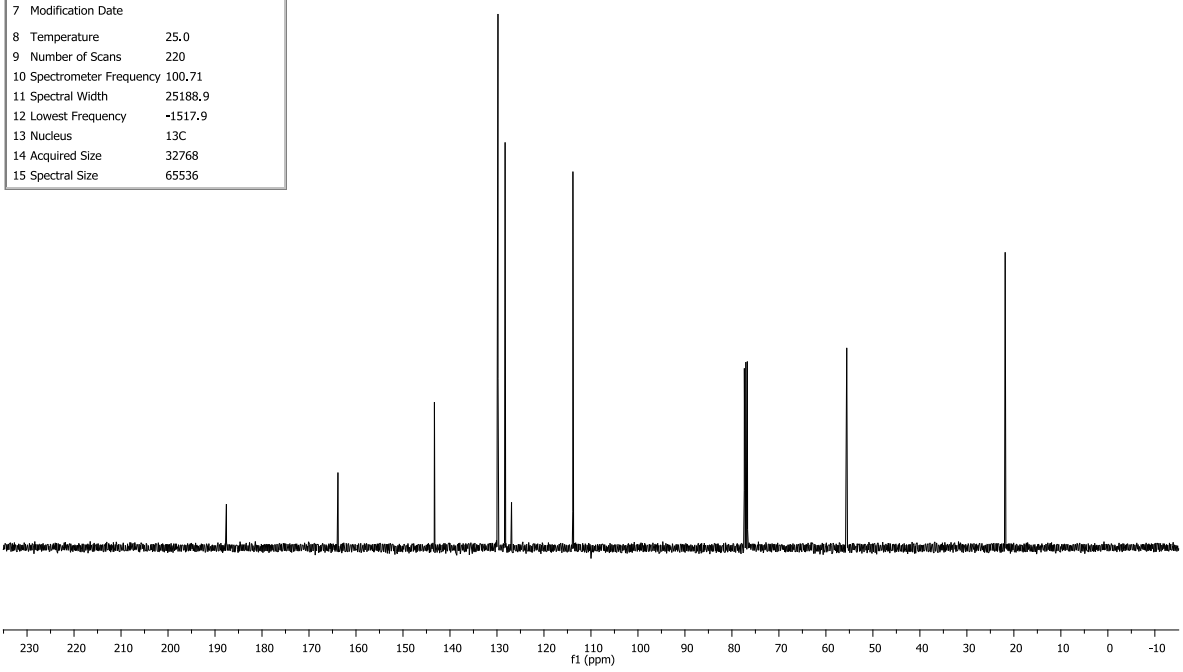


S-(2,6-Dimethylphenyl) 4-methoxybenzothioate (18)

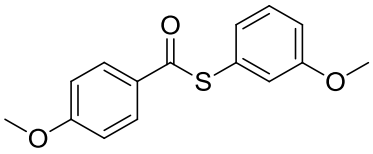
	Parameter	Value
1	Title	MNB215.F5-15.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-04-25T07:41:33
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-799.9
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



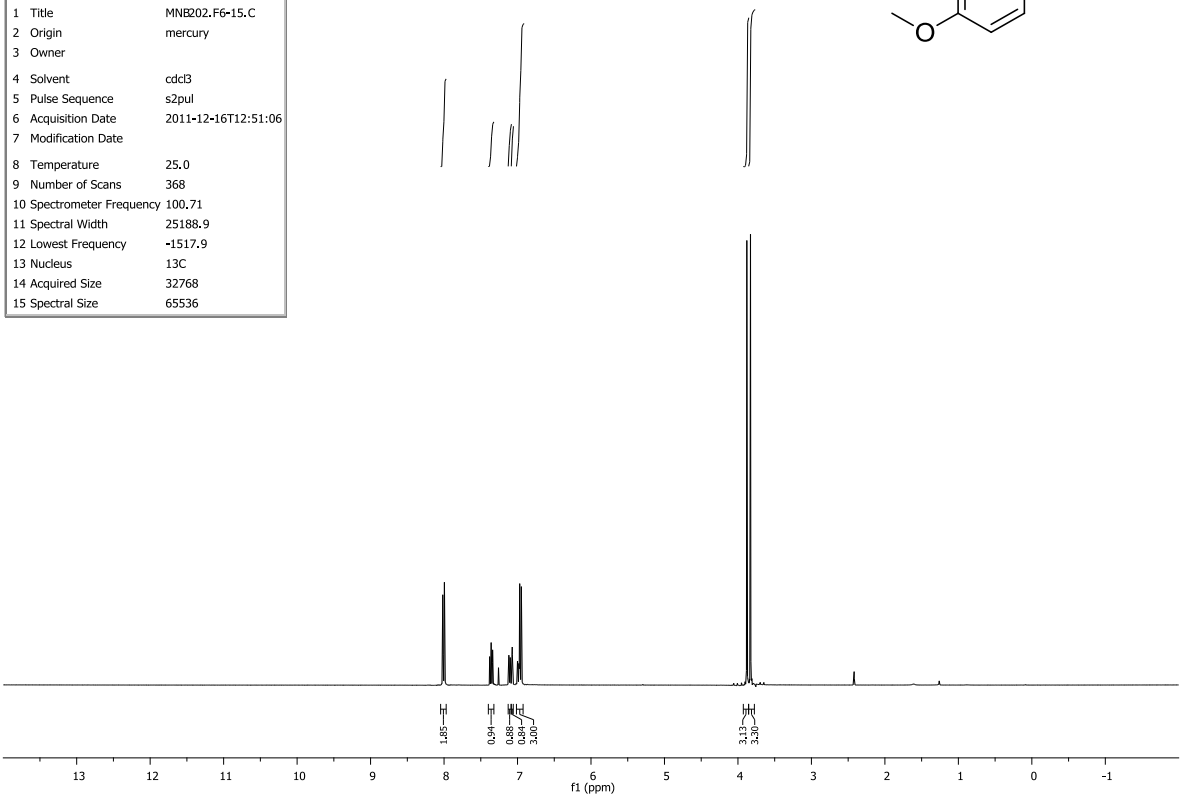
	Parameter	Value
1	Title	MNB215.F5-15.C2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-04-25T07:42:12
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	220
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



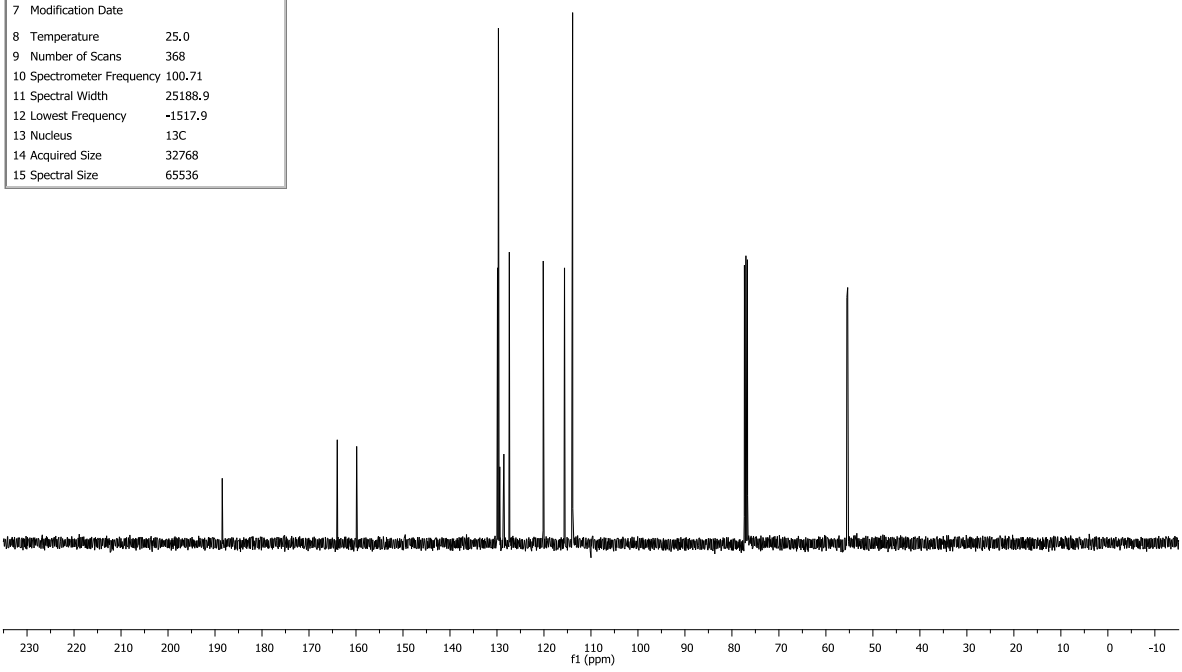
S-(3-Methoxyphenyl) 4-methoxybenzothioate (19)



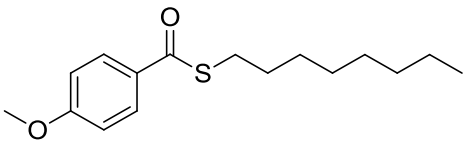
	Parameter	Value
1	Title	MNB202.F6-15.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-12-16T12:51:06
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	368
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



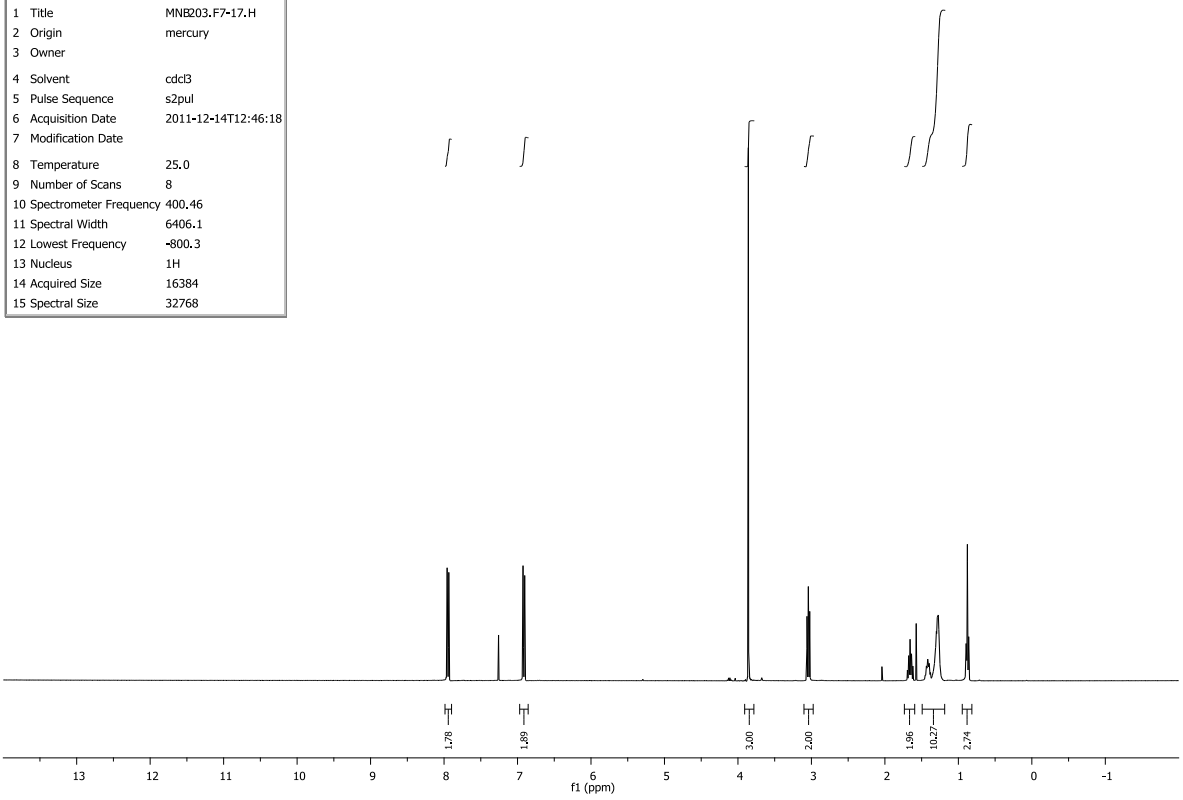
	Parameter	Value
1	Title	MNB202.F6-15.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-12-16T12:51:06
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	368
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



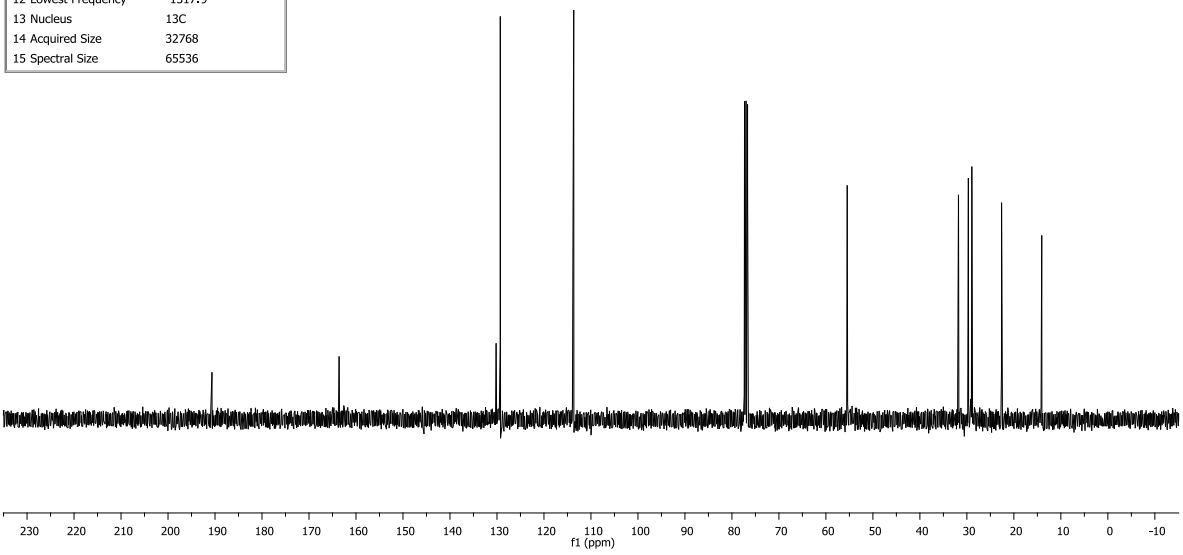
S-Octyl 4-methoxybenzothioate (20)



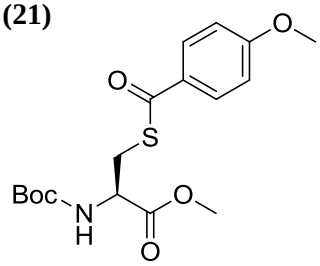
	Parameter	Value
1	Title	MNB203.F7-17.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-12-14T12:46:18
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



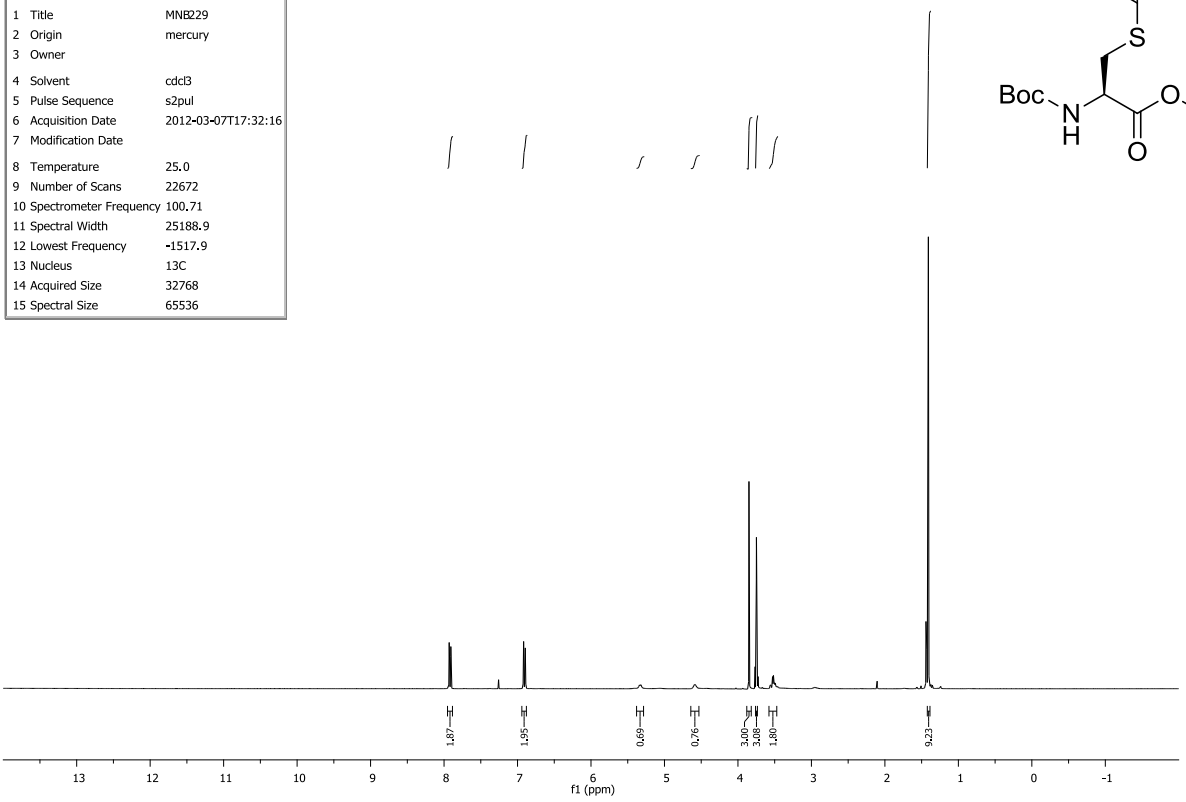
	Parameter	Value
1	Title	MNB203.F7-17.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-12-14T12:57:44
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



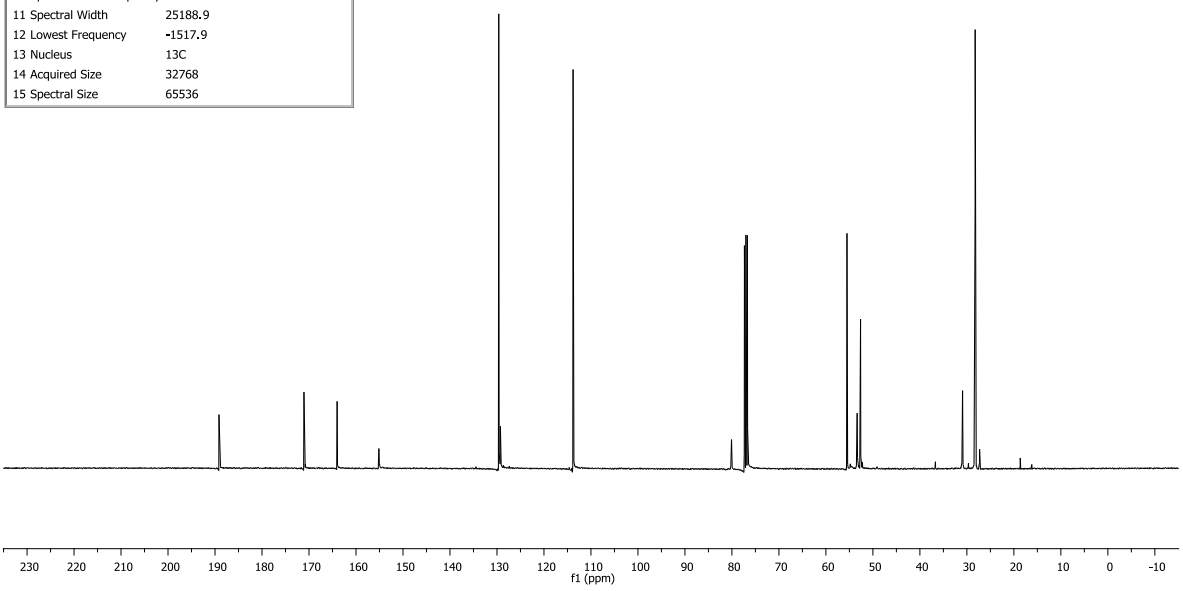
(*R*)-Methyl 2-((tert-butoxycarbonyl)amino)-3-((4-methoxybenzoyl)thio)propanoate (21)



	Parameter	Value
1	Title	MNB229
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-07T17:32:16
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	22672
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536

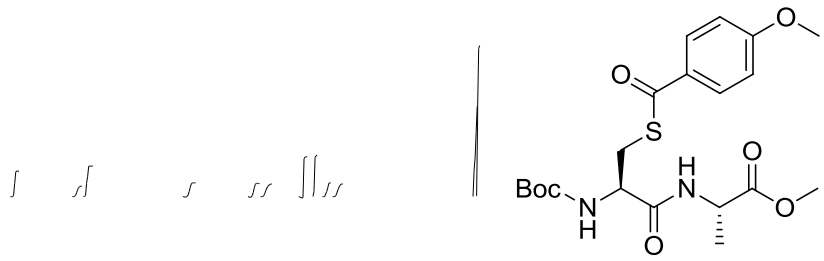


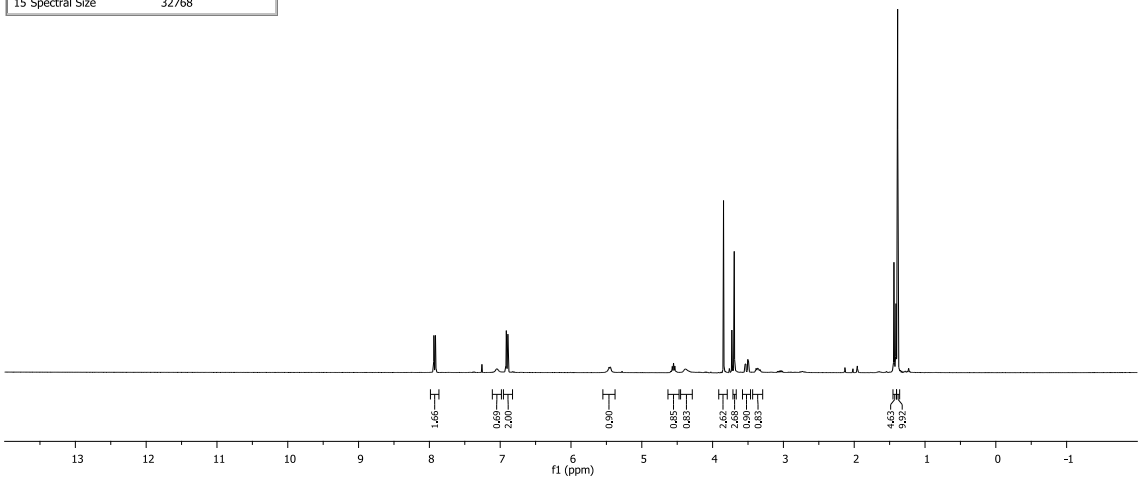
	Parameter	Value
1	Title	STANDARD CARBON PARAMETERS
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-07T17:32:16
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	22672
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



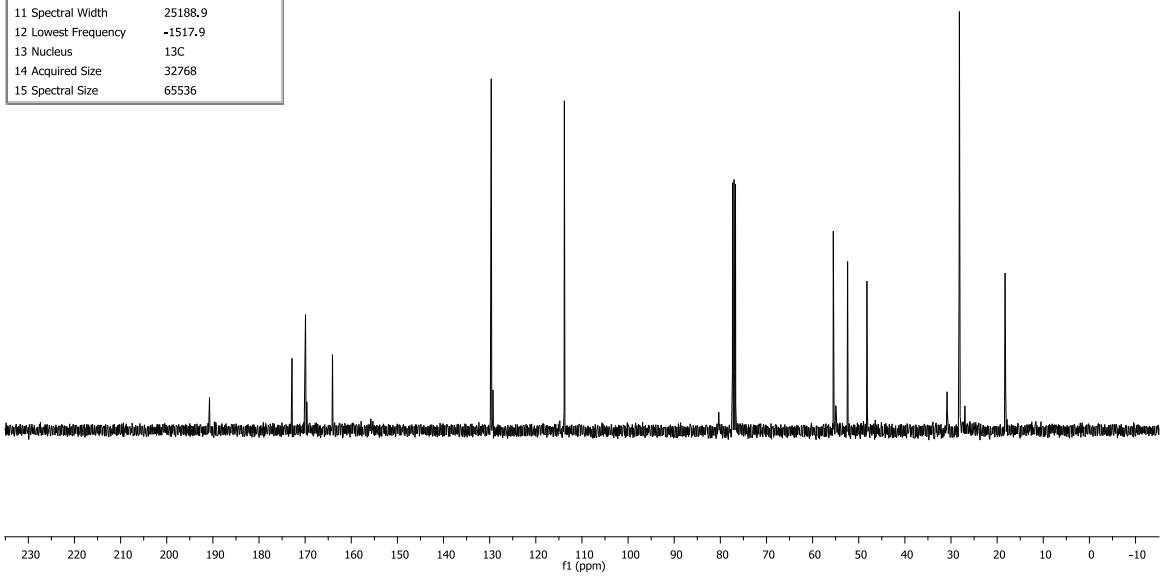
(*S*)-Methyl 2-((*R*)-2-((*tert*-butoxycarbonyl)amino)-3-((4-ethoxybenzoyl)thio)propanamido)propanoate (22)

	Parameter	Value
1	Title	MNB259.FC2.F7-17.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-14T12:57:45
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

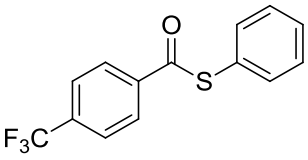




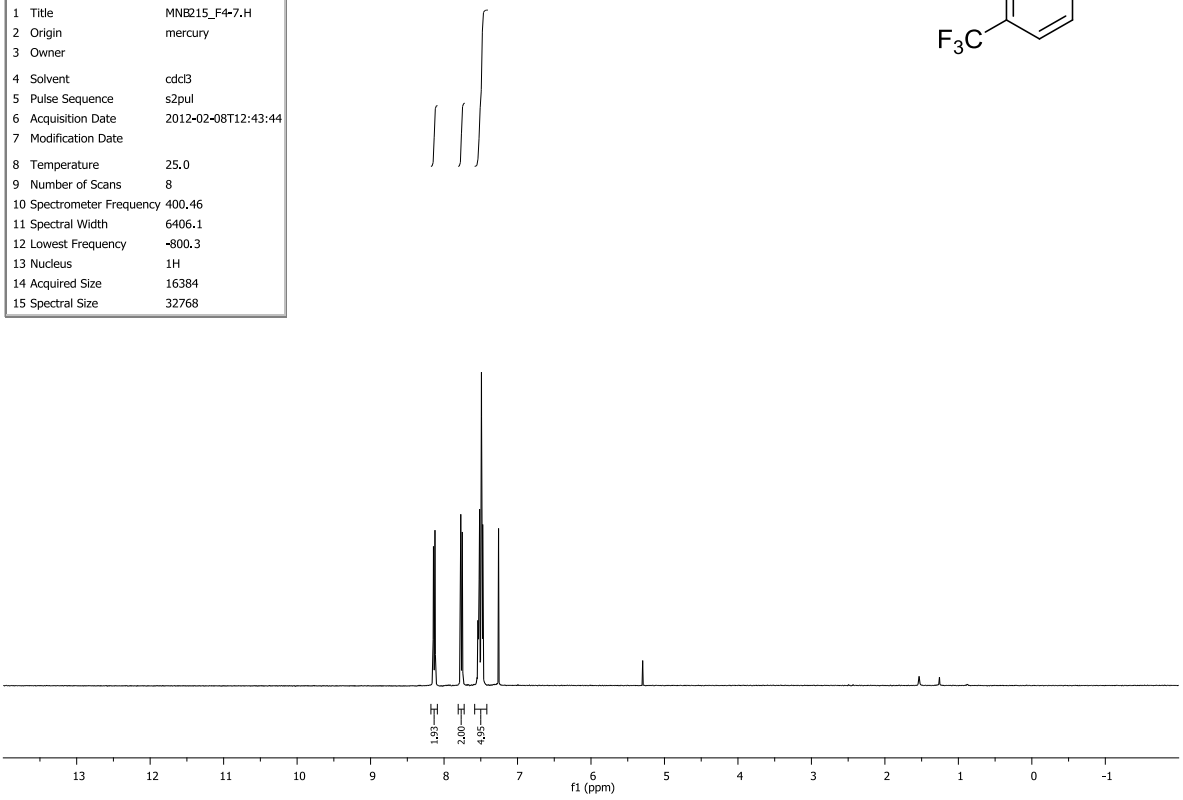
	Parameter	Value
1	Title	MNB259.FC2.F7-17.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-14T13:08:44
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



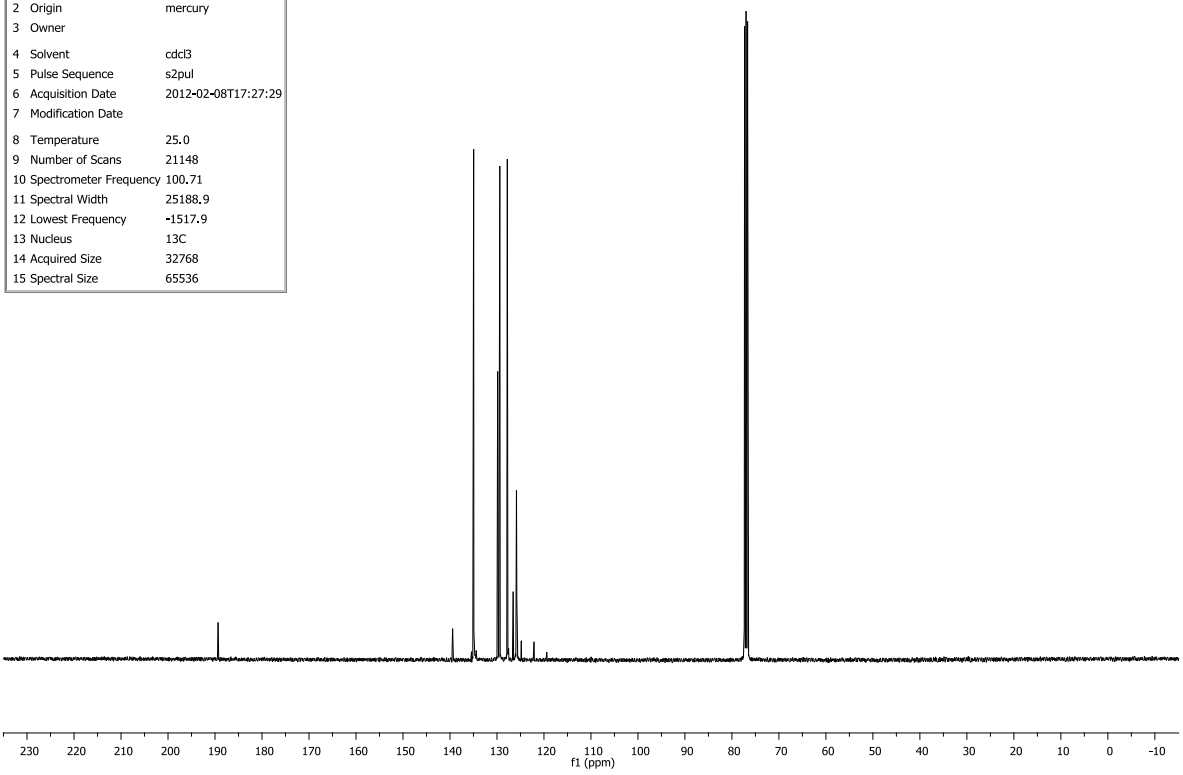
S-Phenyl 4-(trifluoromethyl)benzothioate (23)



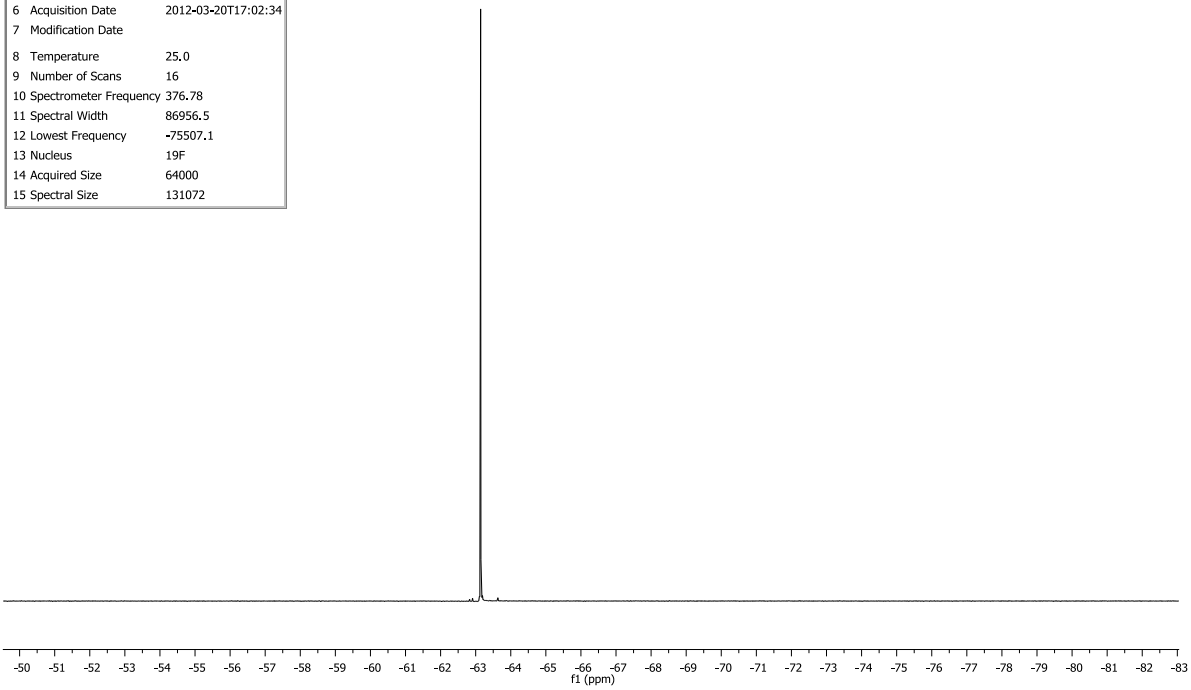
	Parameter	Value
1	Title	MNB215_F4-7.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-02-08T12:43:44
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



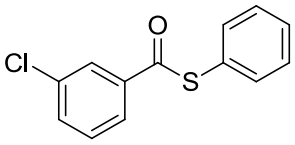
	Parameter	Value
1	Title	MNB215_F4-7_C_o/ n
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-02-08T17:27:29
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	21148
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



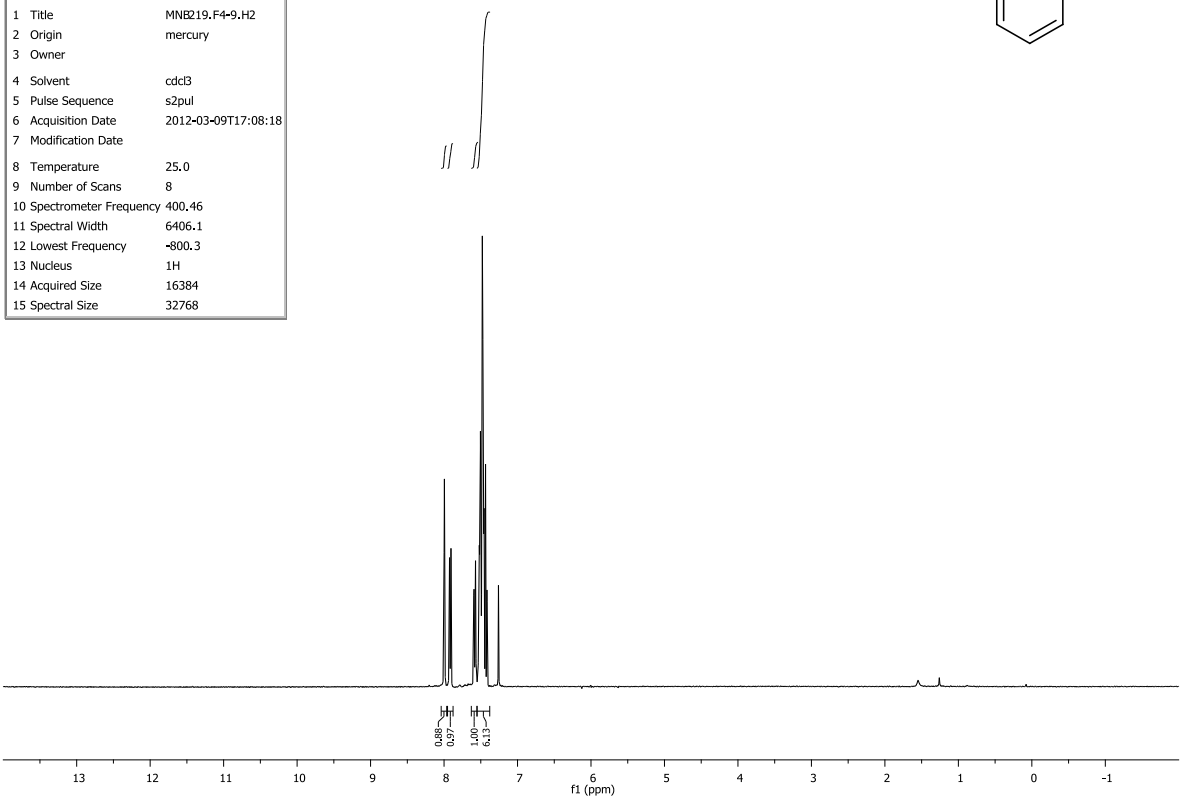
	Parameter	Value
1	Title	MNB215.F4-7.F
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-20T17:02:34
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	16
10	Spectrometer Frequency	376.78
11	Spectral Width	86956.5
12	Lowest Frequency	-75507.1
13	Nucleus	19F
14	Acquired Size	64000
15	Spectral Size	131072



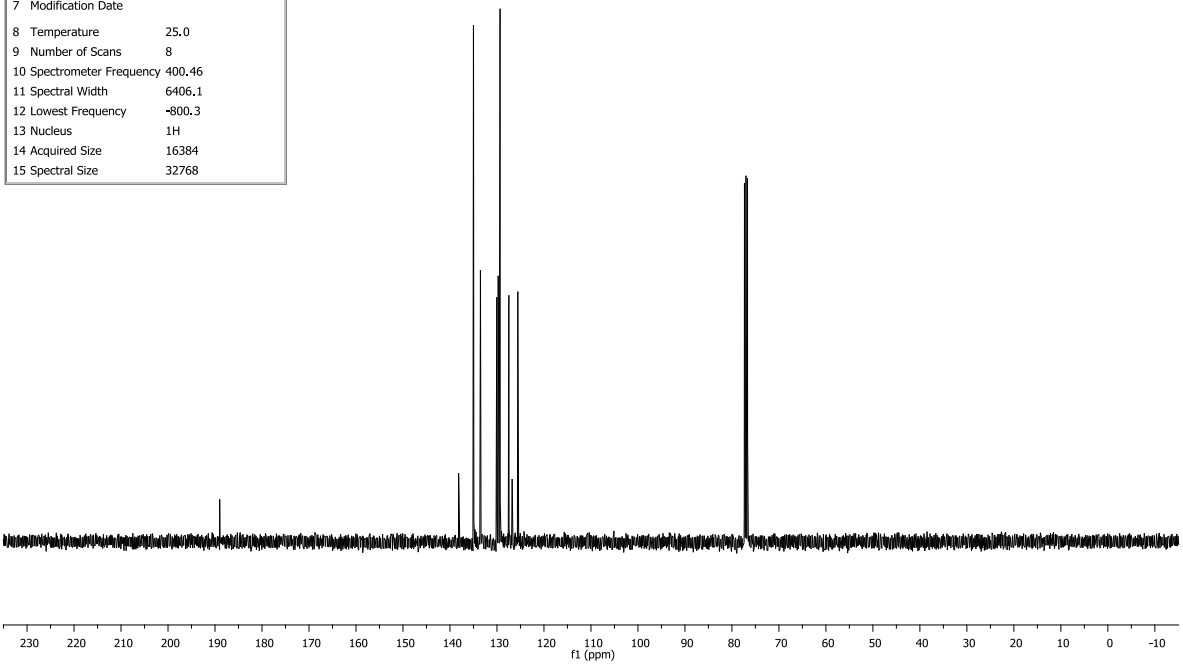
S-Phenyl 3-chlorobenzothioate (24)



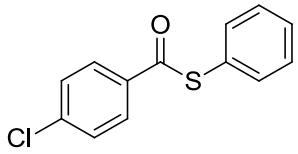
	Parameter	Value
1	Title	MNB219.F4-9.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-09T17:08:18
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



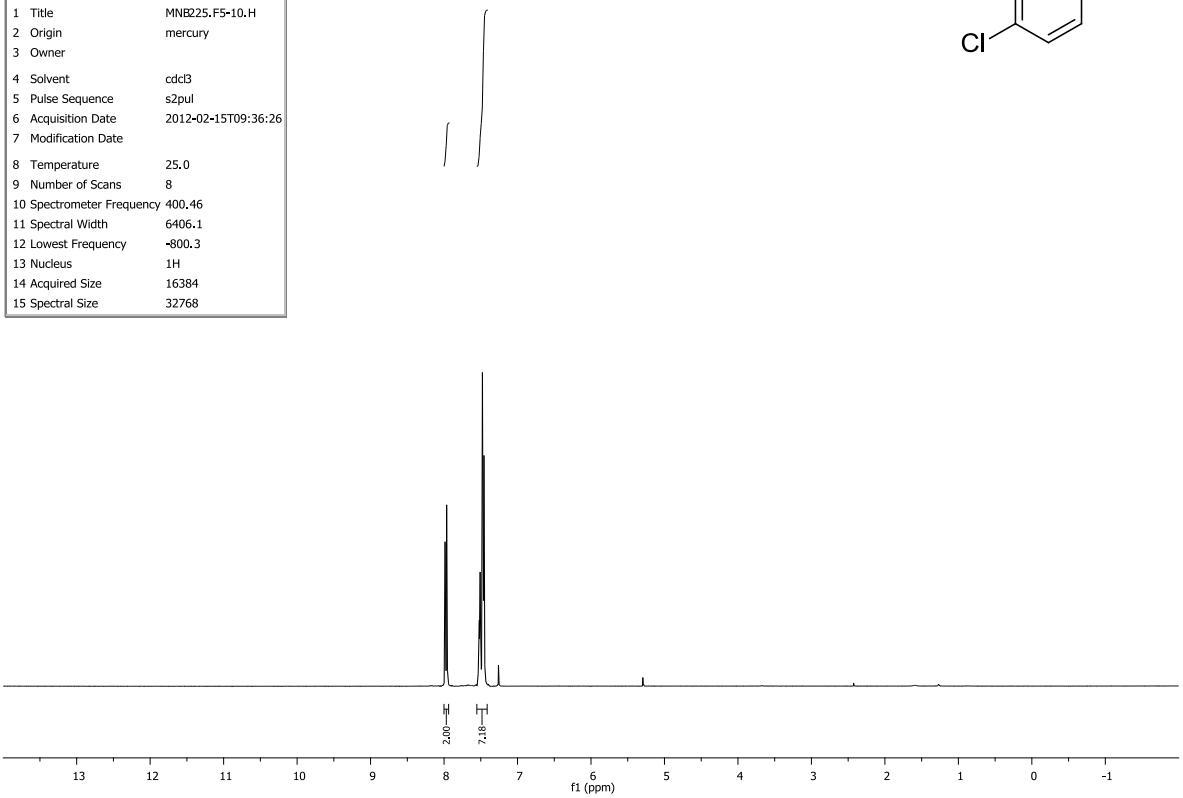
	Parameter	Value
1	Title	MNB219.F4-9.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-09T17:08:18
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



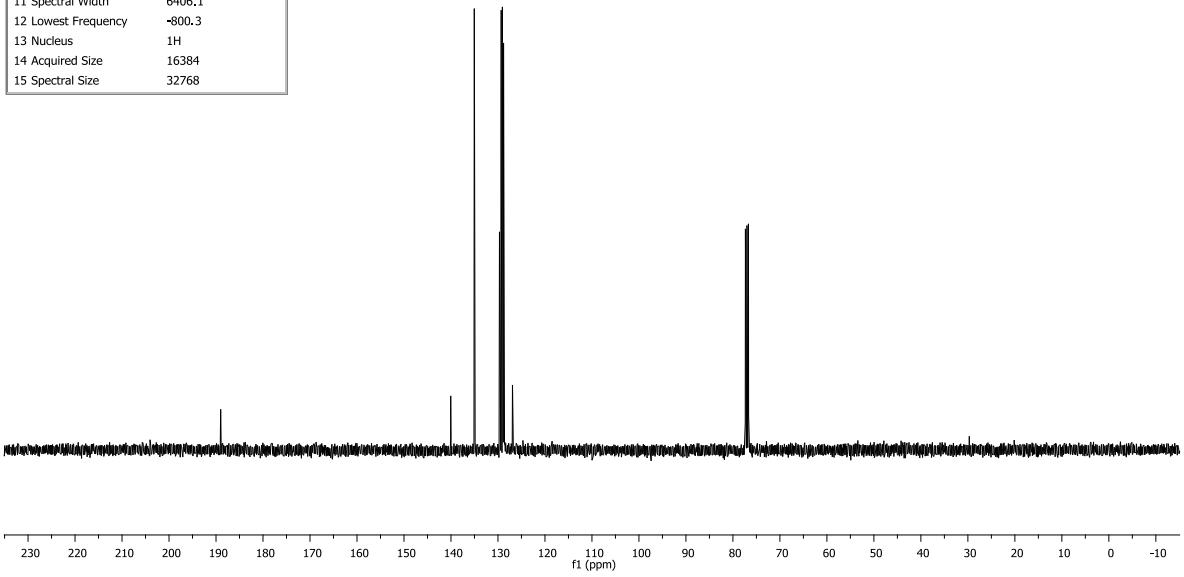
S-Phenyl 4-chlorobenzothioate (25)



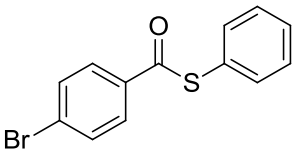
	Parameter	Value
1	Title	MNB225.F5-10.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-02-15T09:36:26
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



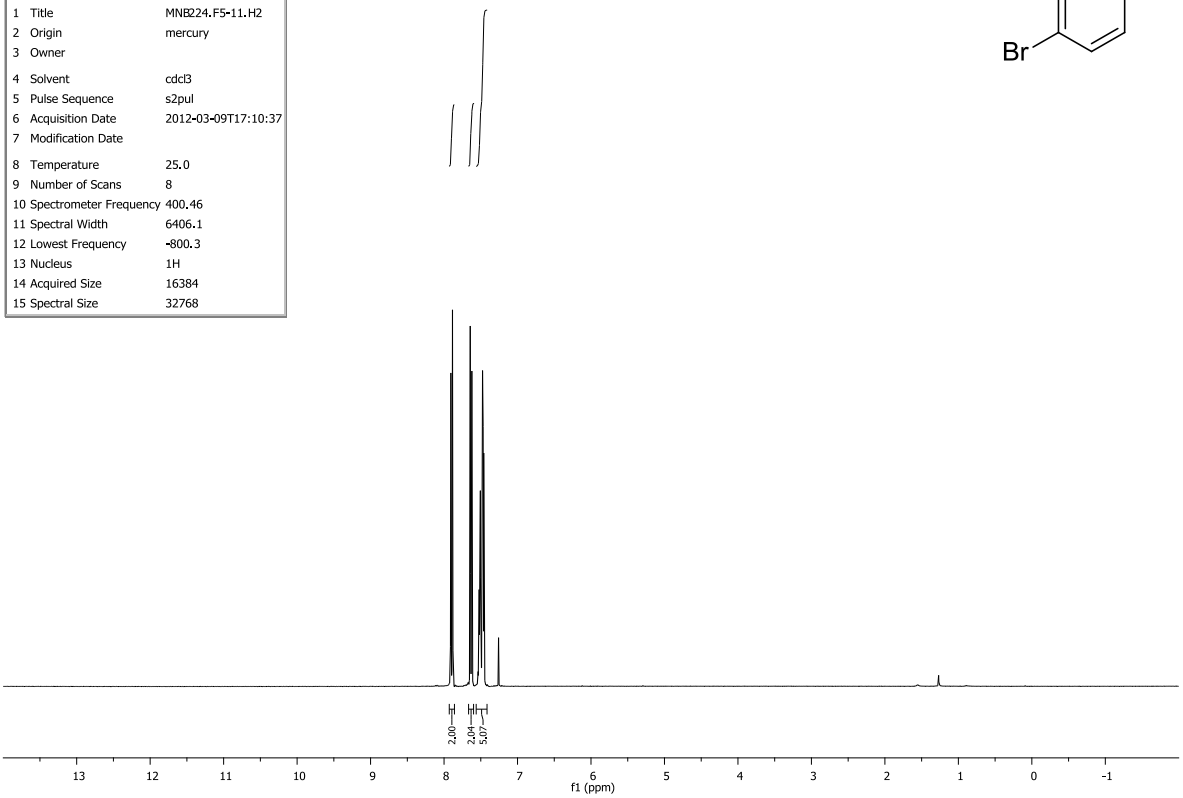
	Parameter	Value
1	Title	MNB225.F5-10.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-02-15T09:36:26
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



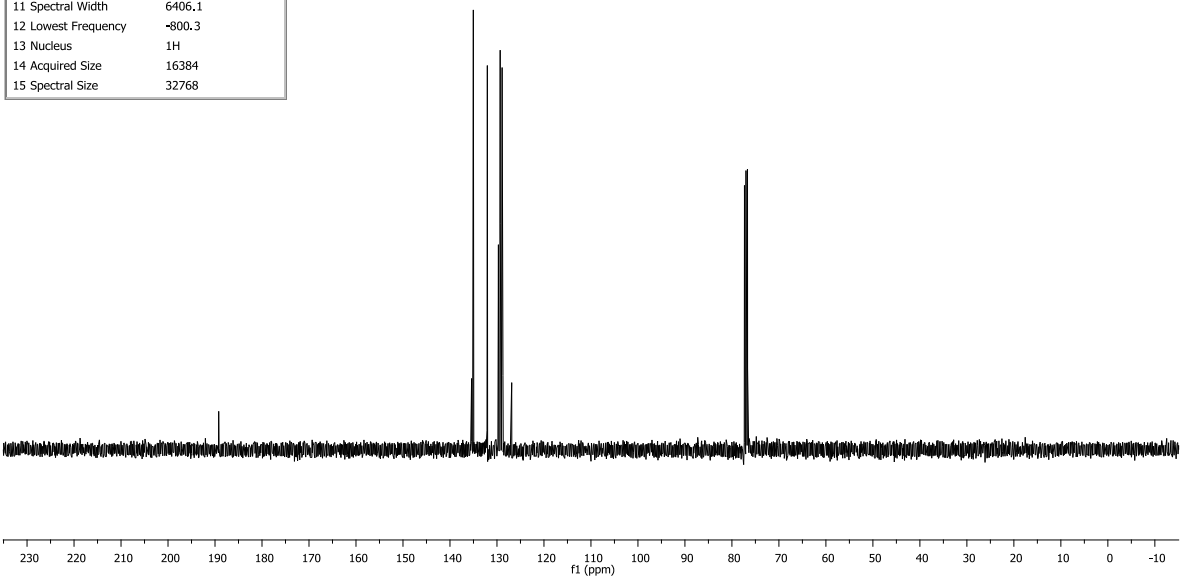
S-Phenyl 4-bromobenzothioate (26)



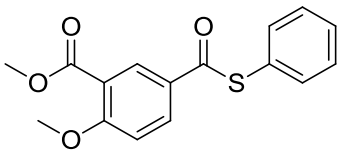
	Parameter	Value
1	Title	MNB224.F5-11.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-09T17:10:37
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



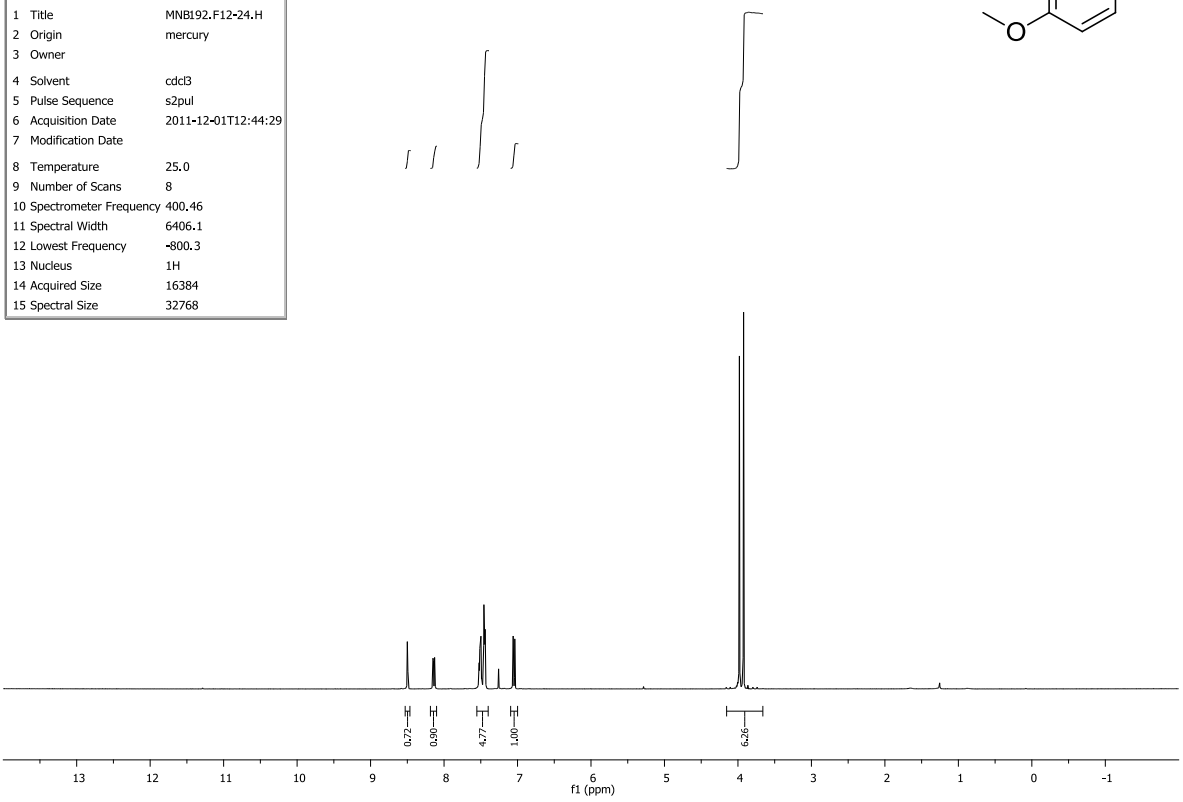
	Parameter	Value
1	Title	MNB224.F5-11.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-09T17:10:37
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



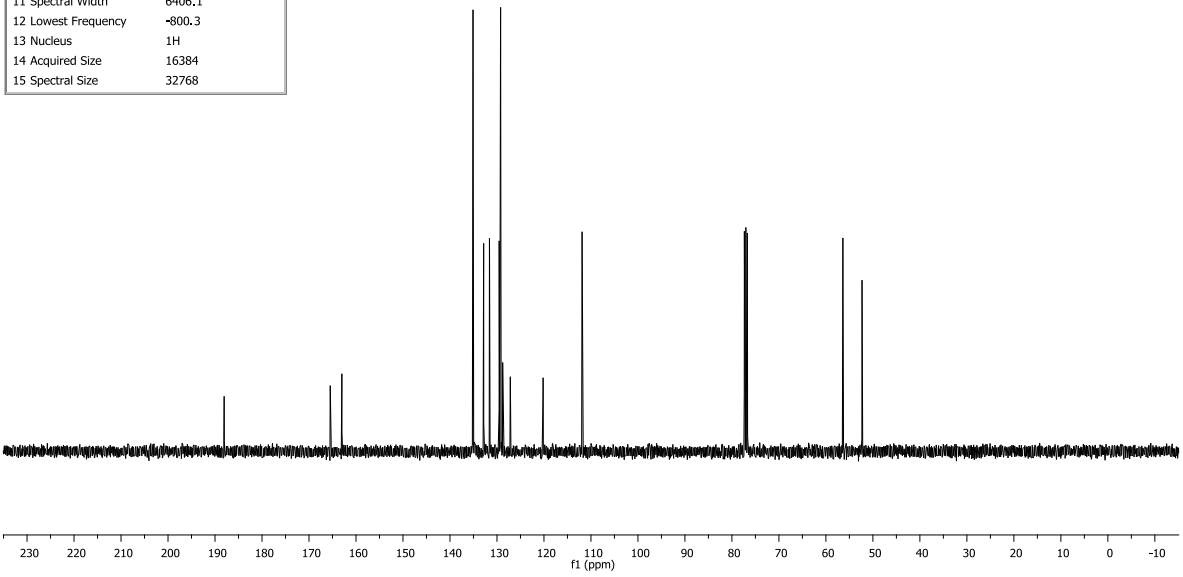
Methyl 2-methoxy-5-((phenylthio)carbonyl)benzoate (27)



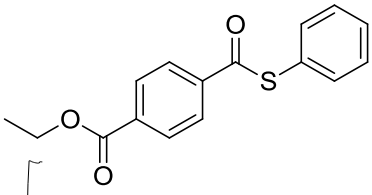
	Parameter	Value
1	Title	MNB192.F12-24.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-12-01T12:44:29
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



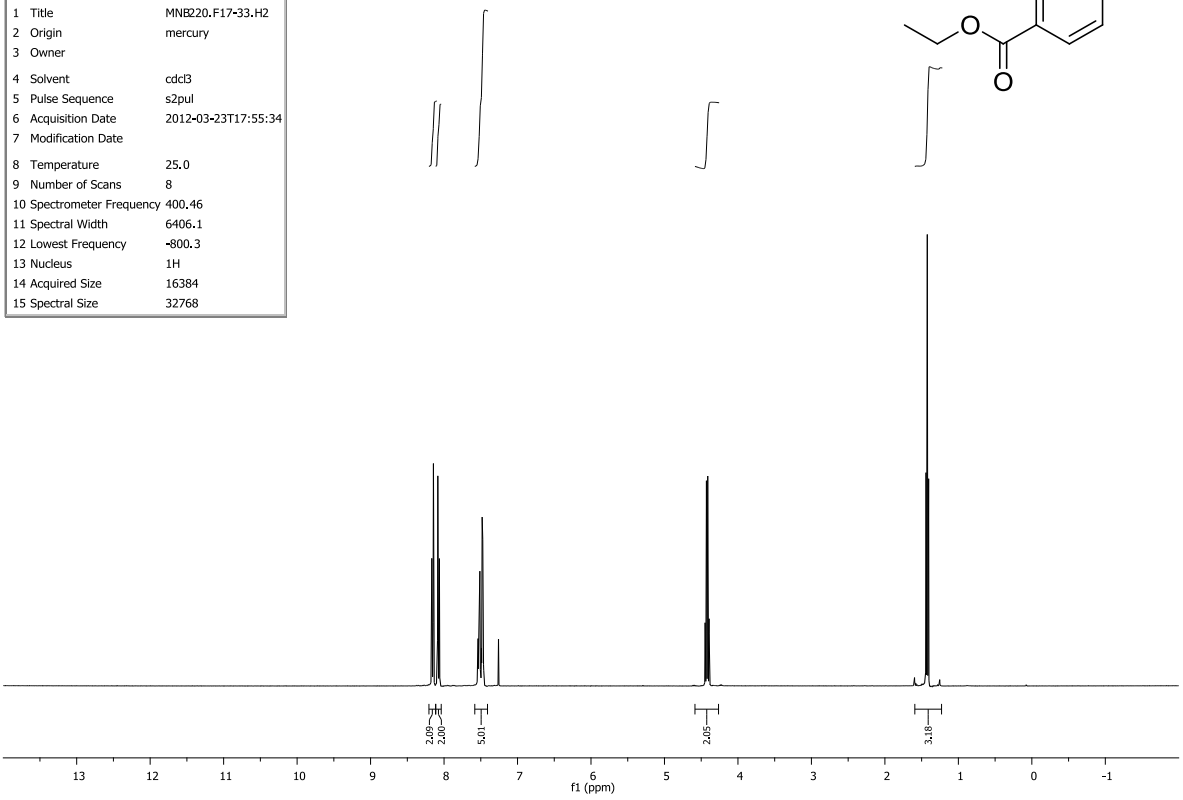
	Parameter	Value
1	Title	MNB192.F12-24.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-12-01T12:44:29
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



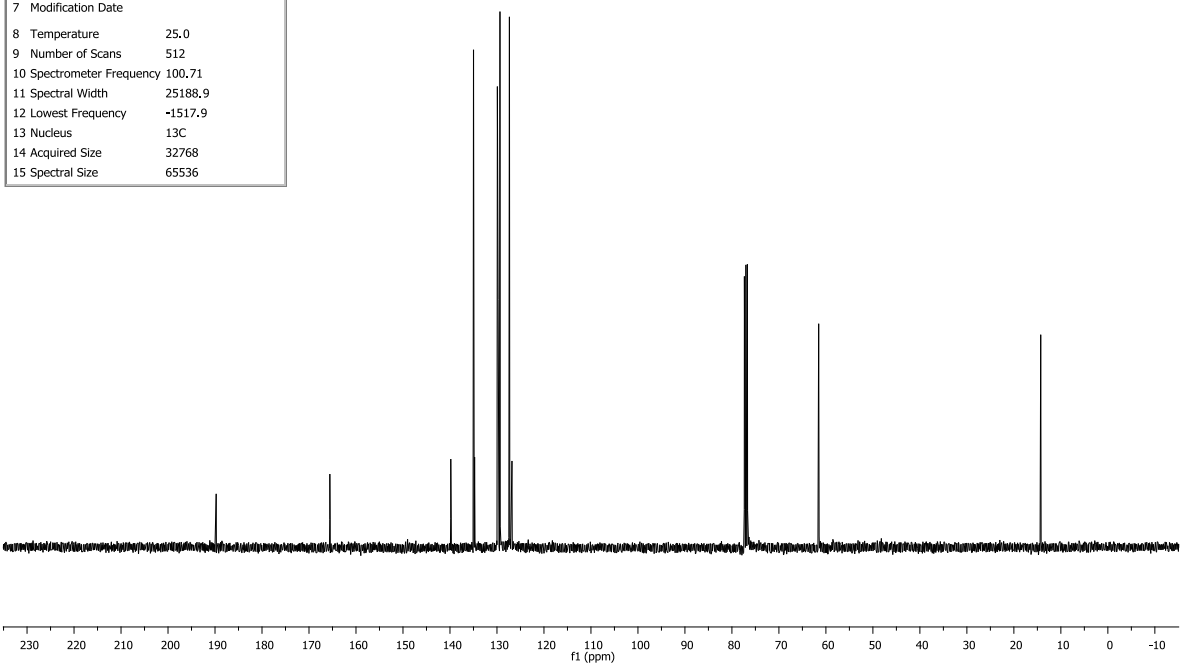
Ethyl 4-((phenylthio)carbonyl)benzoate (28)



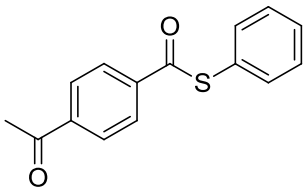
	Parameter	Value
1	Title	MNB220.F17-33.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-23T17:55:34
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



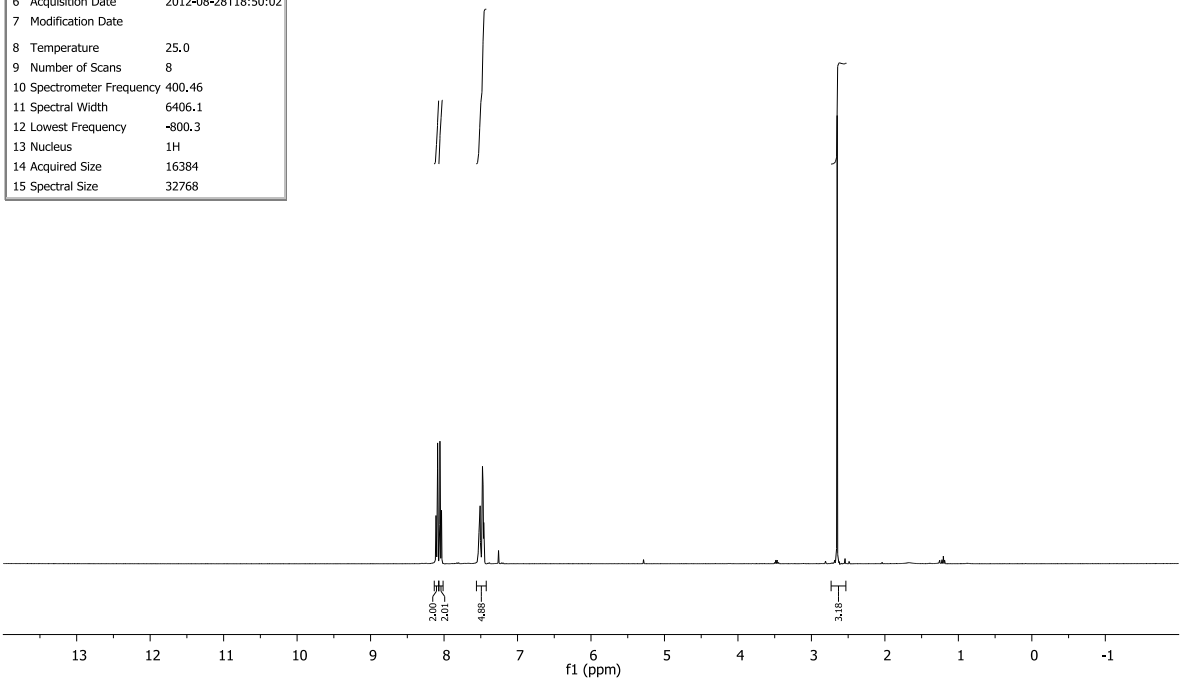
	Parameter	Value
1	Title	MNB220.F17-33.C2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-23T18:16:30
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	512
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



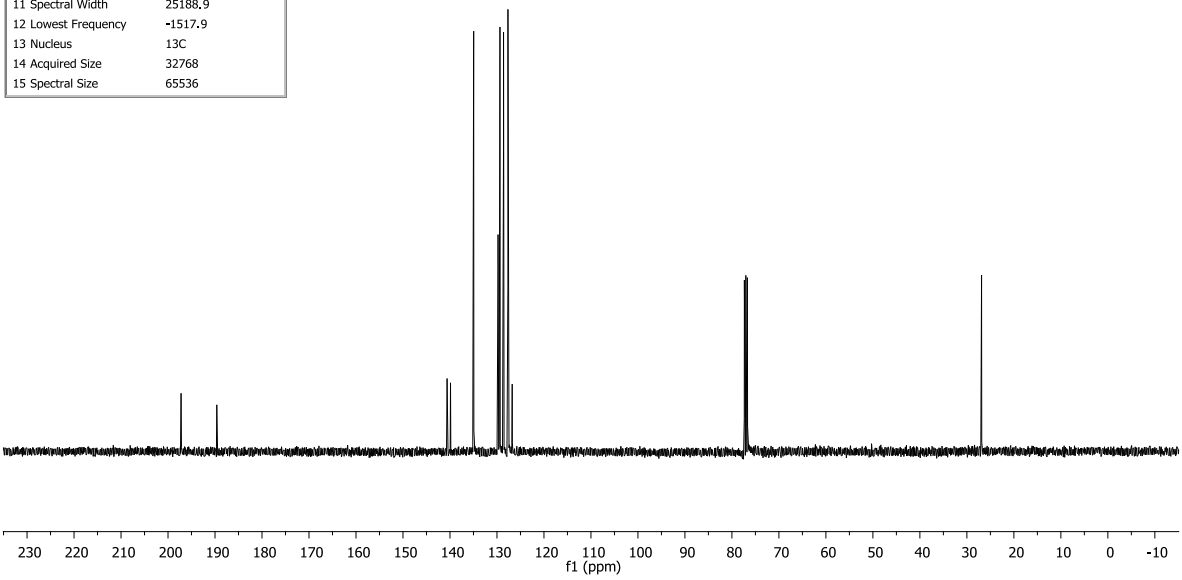
S-phenyl 4-acetylbenzothioate (29)



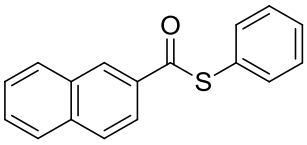
	Parameter	Value
1	Title	MNB291.F23-36.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-08-28T18:50:02
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



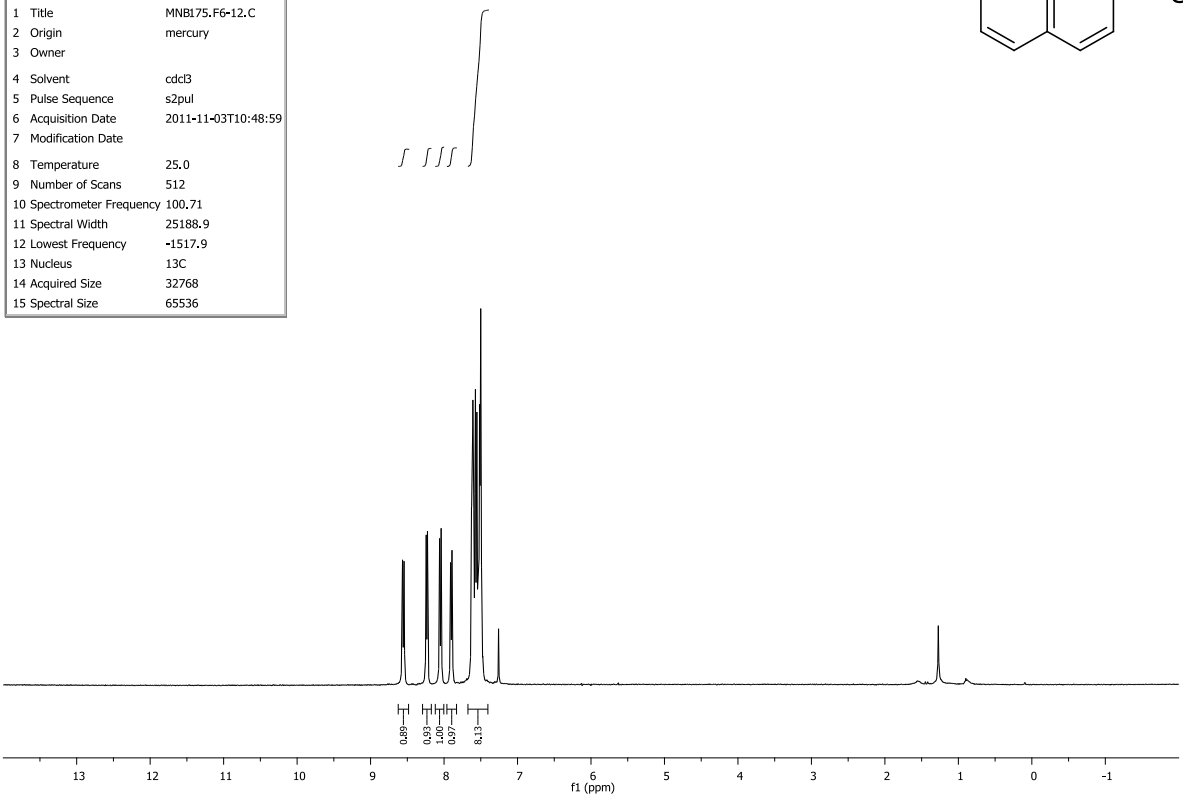
	Parameter	Value
1	Title	MNB291.F23-36.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-08-28T19:01:15
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



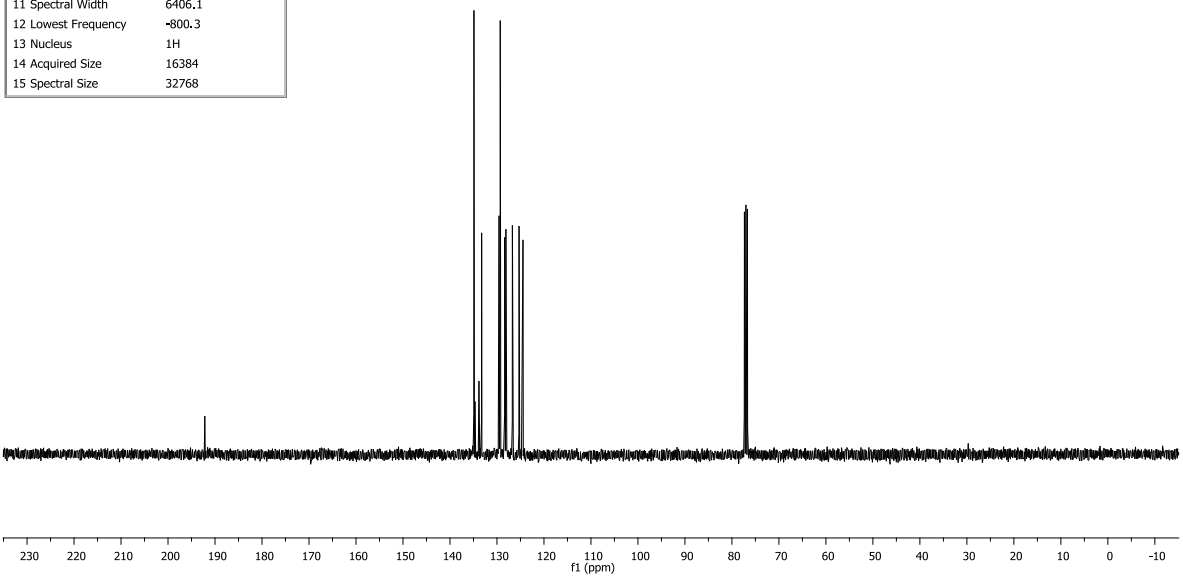
S-Phenyl naphthalene-2-carbothioate (30)



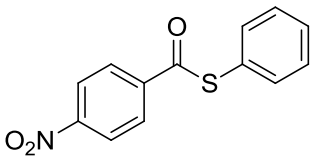
	Parameter	Value
1	Title	MNB175.F6-12.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-03T10:48:59
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	512
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



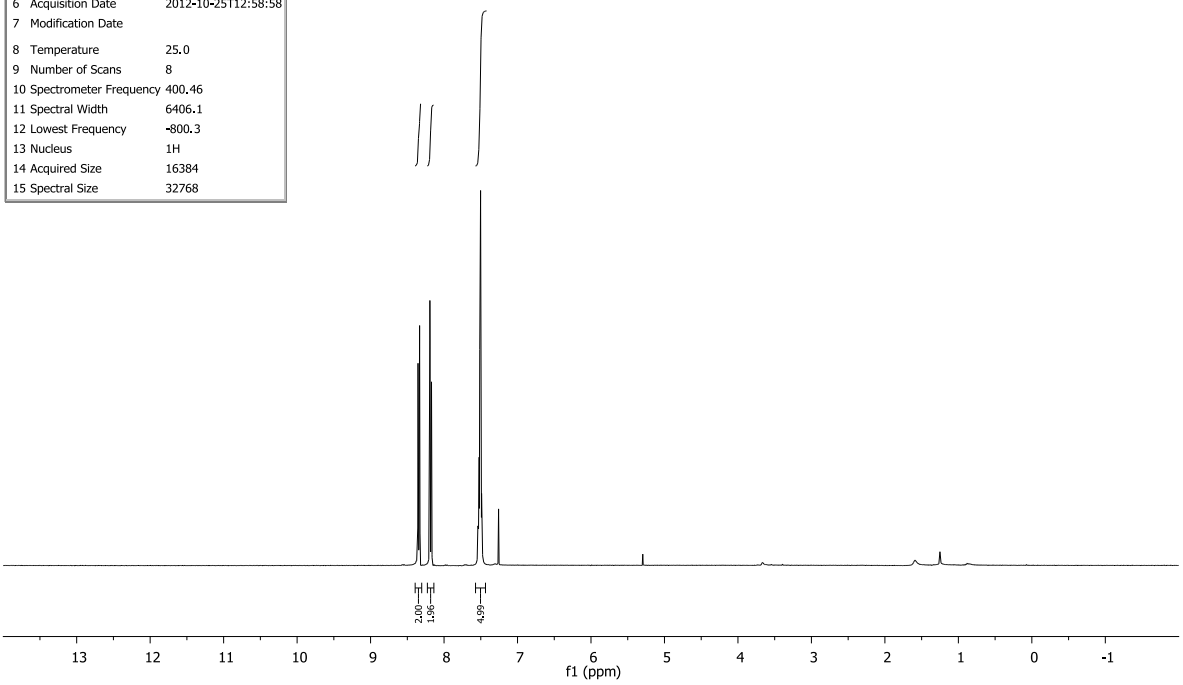
	Parameter	Value
1	Title	MNB175.F6-12.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-03-09T17:05:30
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



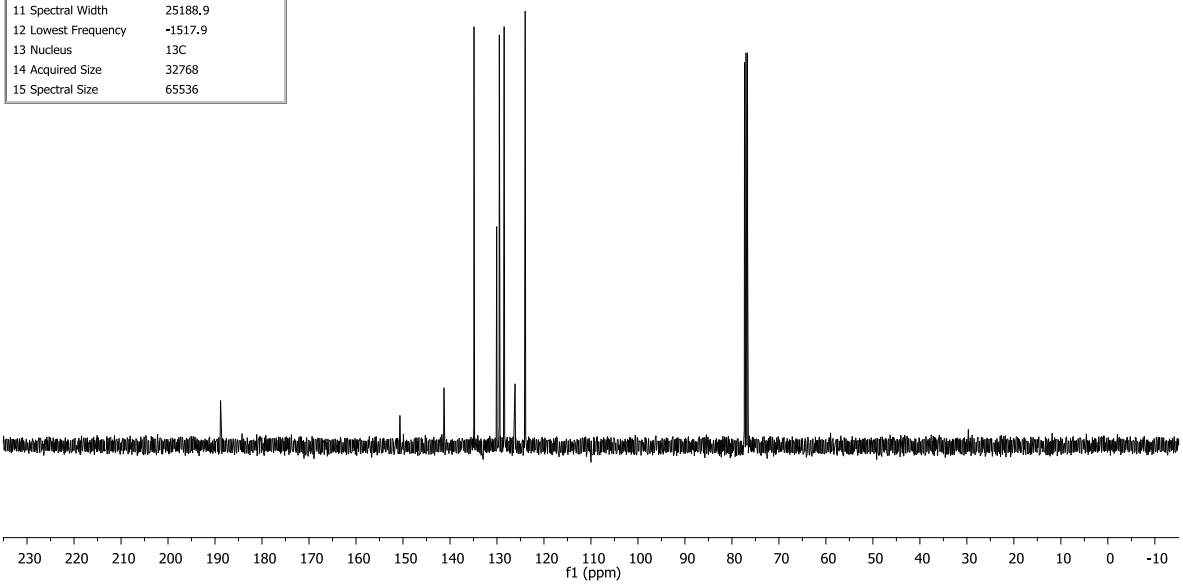
S-phenyl 4-nitrobenzothioate (31)



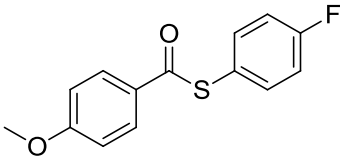
	Parameter	Value
1	Title	MNB317.F17-28.F
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-10-25T12:58:58
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



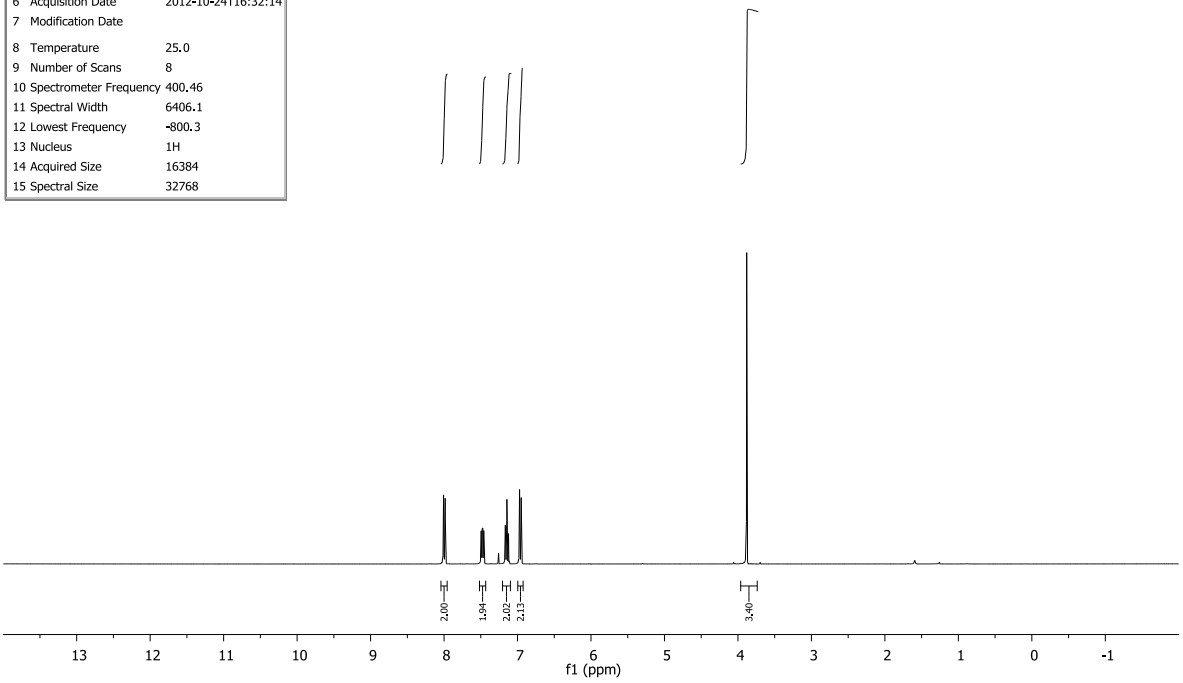
	Parameter	Value
1	Title	MNB290.F13-21.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-08-28T11:07:54
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	444
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



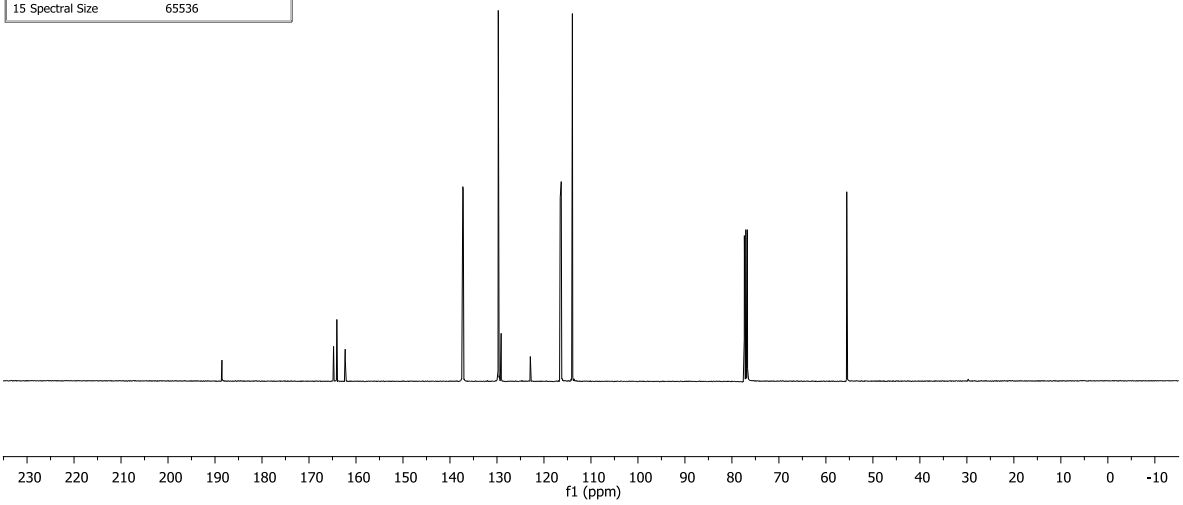
S-(4-fluorophenyl) 4-methoxybenzothioate (32)



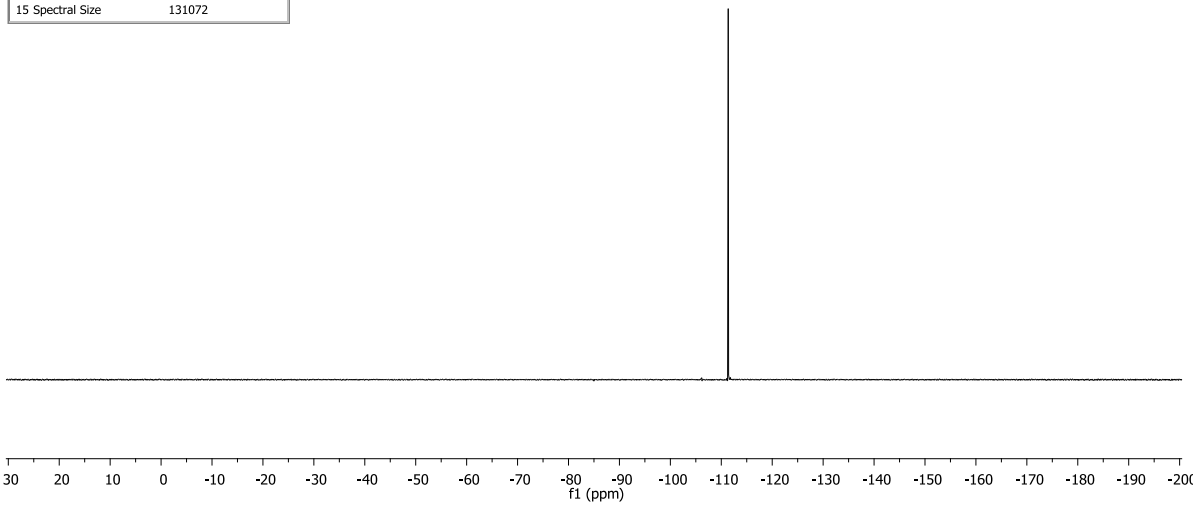
	Parameter	Value
1	Title	MNB313.F15-23.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-10-24T16:32:14
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



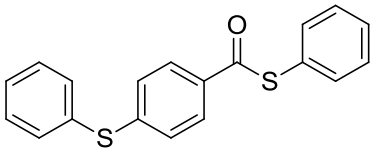
	Parameter	Value
1	Title	MNB313.F15-23.o/ n.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-10-24T16:40:55
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	23980
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



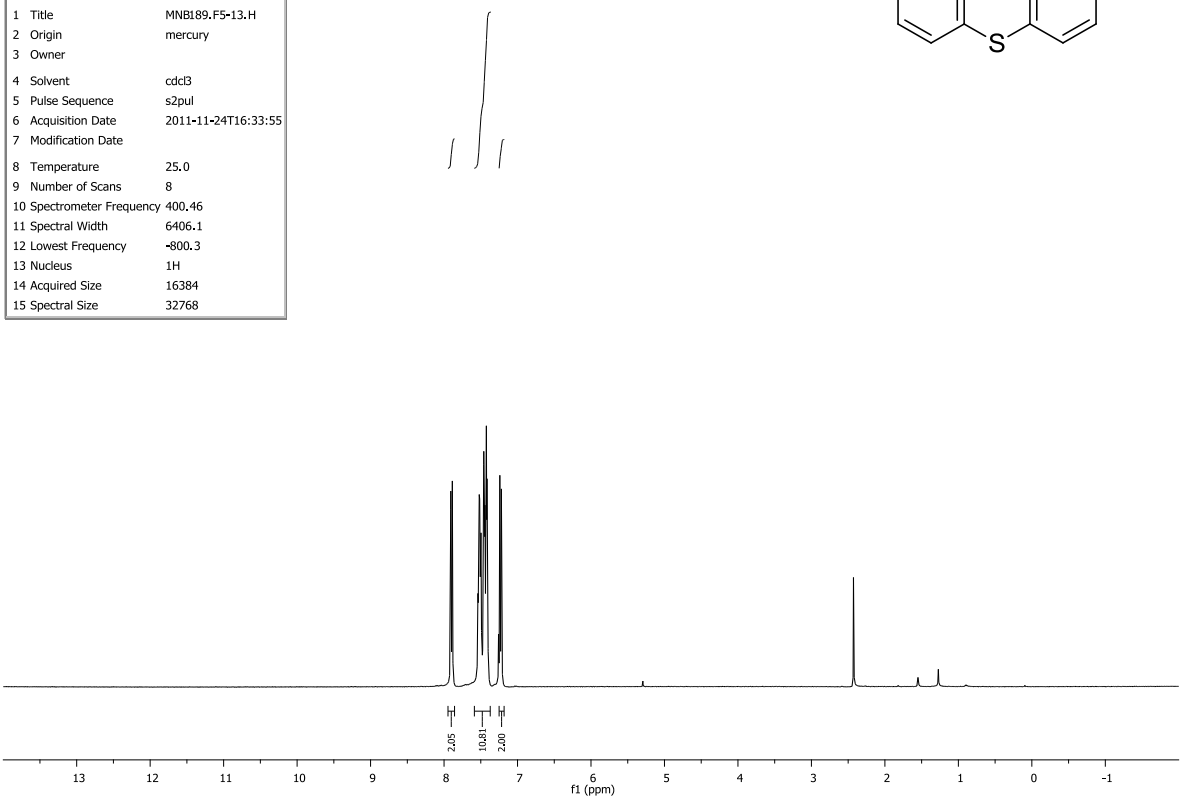
	Parameter	Value
1	Title	MNB313.F15-23.F
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-10-24T16:34:41
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	16
10	Spectrometer Frequency	376.78
11	Spectral Width	86956.5
12	Lowest Frequency	-75507.1
13	Nucleus	19F
14	Acquired Size	64000
15	Spectral Size	131072



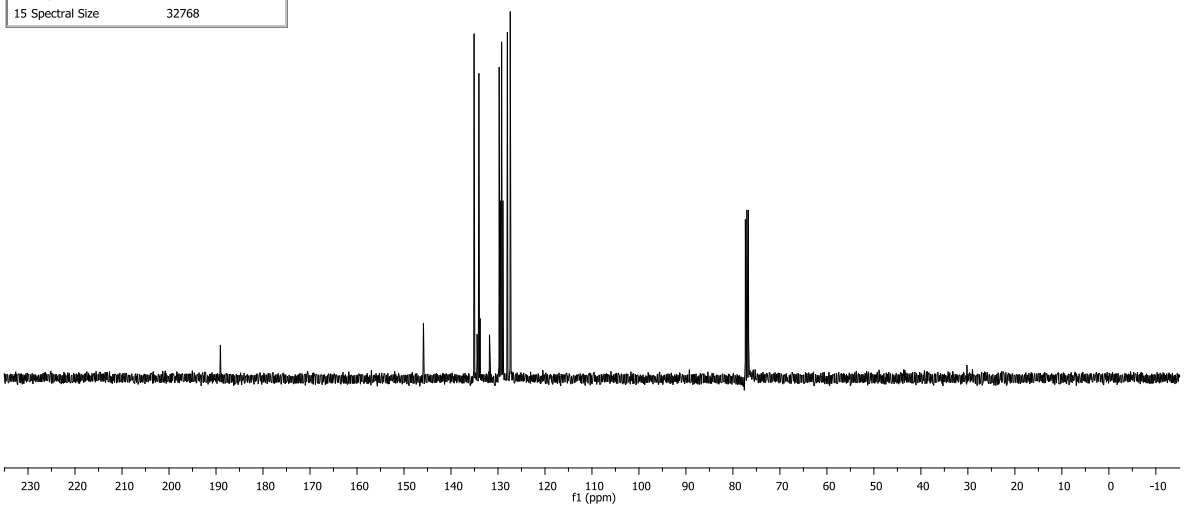
S-Phenyl 4-(phenylthio)benzothioate (33)



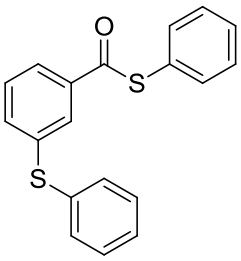
	Parameter	Value
1	Title	MNB189.F5-13.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-24T16:33:55
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



	Parameter	Value
1	Title	MNB189.F5-13.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2011-11-24T16:33:55
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

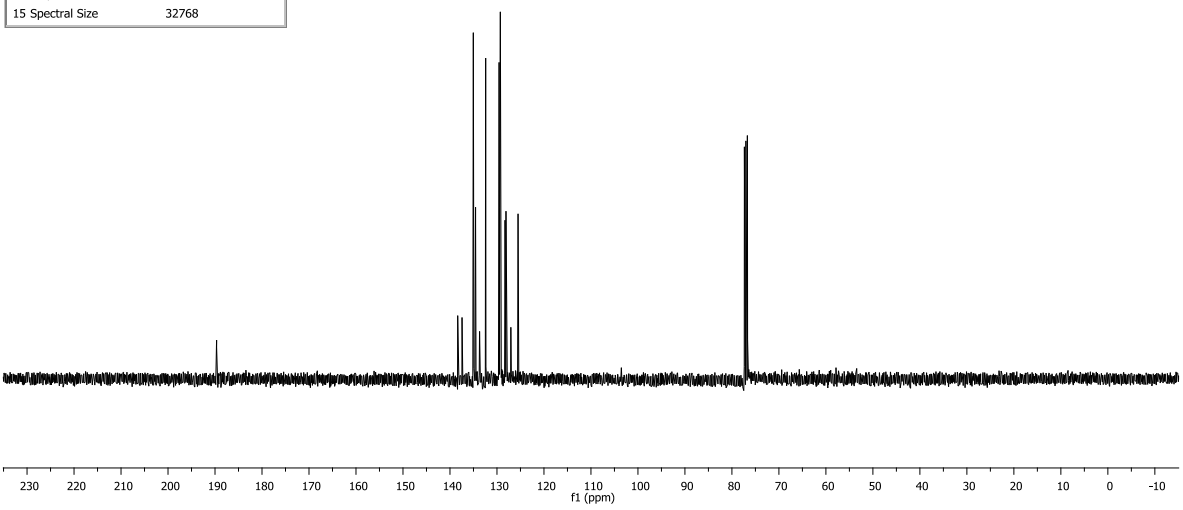


S-Phenyl 3-(phenylthio)benzothioate (34)

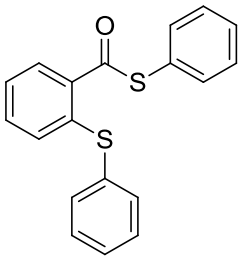


	Parameter	Value
1	Title	MNB255.F7-12.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-07T10:00:21
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

	Parameter	Value
1	Title	MNB255.F6-14.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-04-19T09:03:57
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

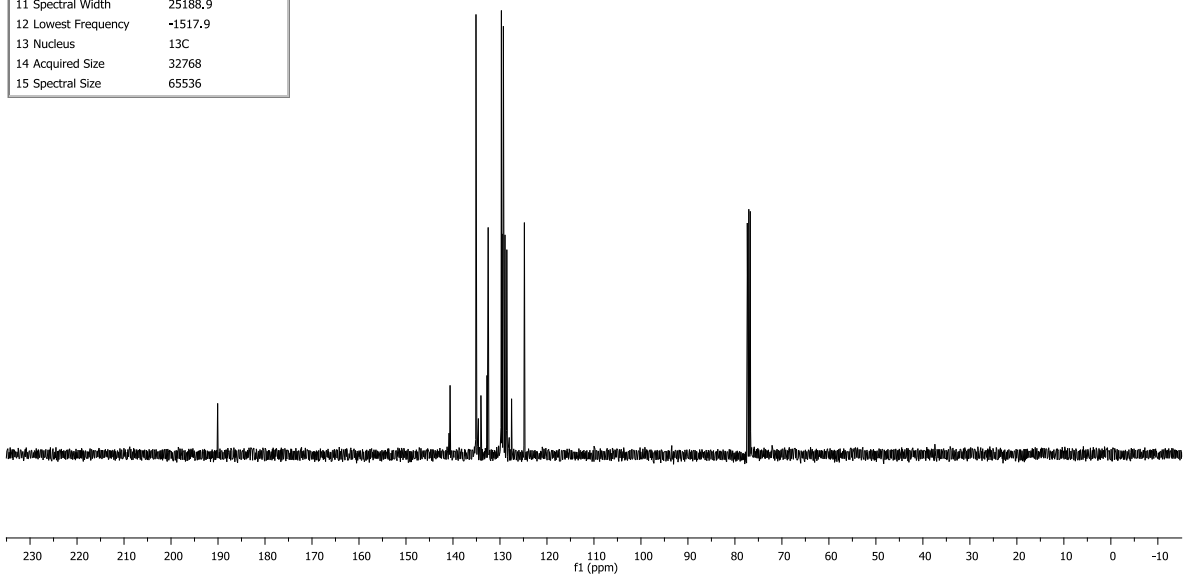


S-Phenyl 2-(phenylthio)benzothioate (35)

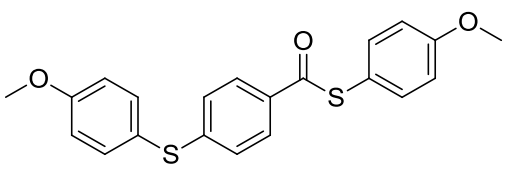


	Parameter	Value
1	Title	MNB256.F6-14.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-04-19T09:14:53
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536

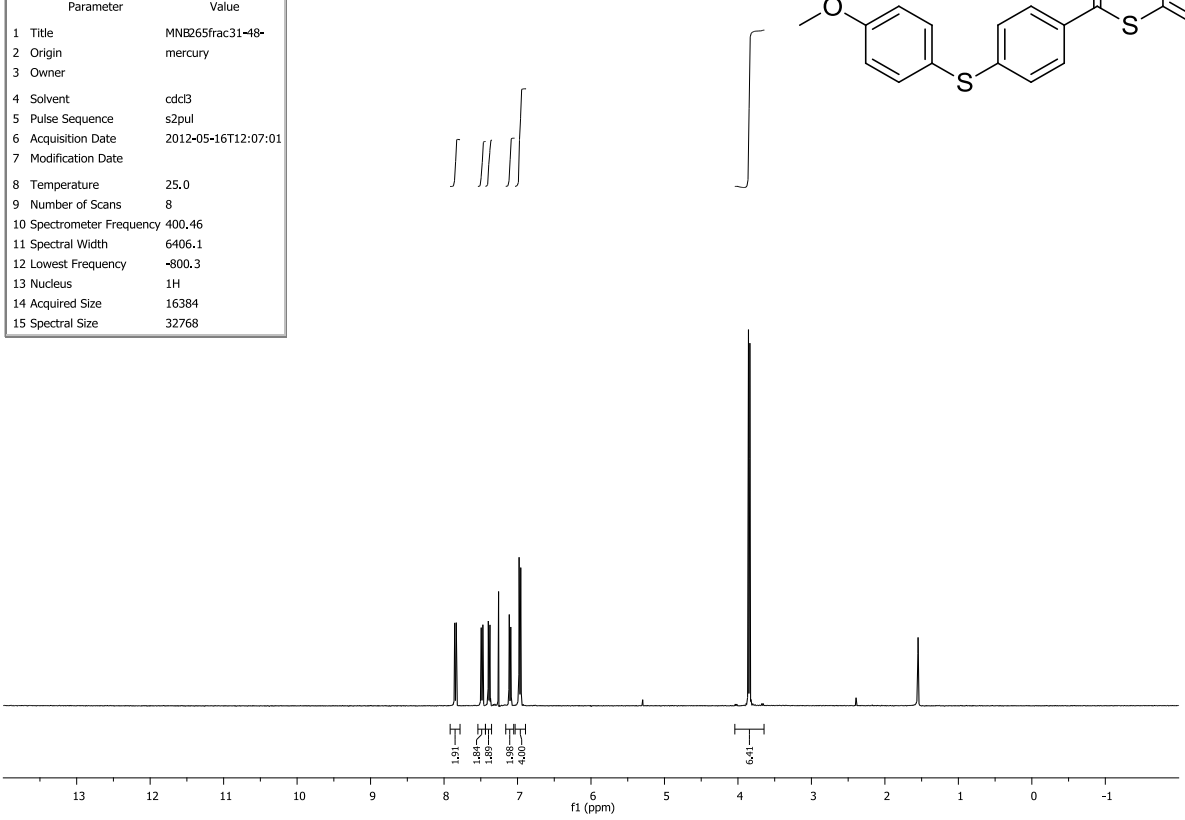
	Parameter	Value
1	Title	MNB256.F6-14.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-04-19T09:14:53
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



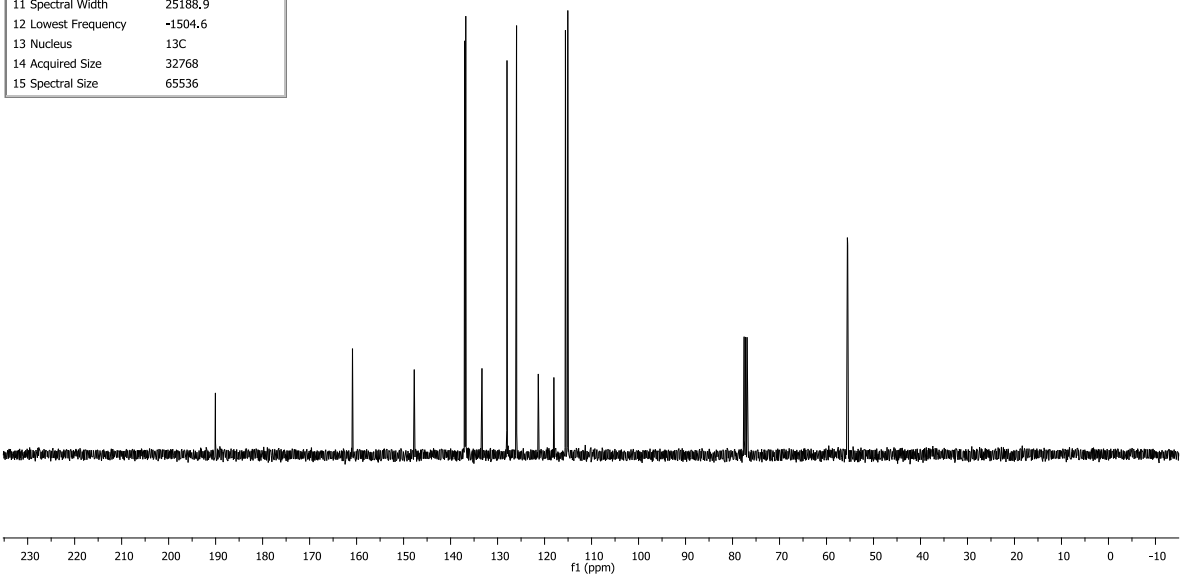
S-(4-Methoxyphenyl) 4-((4-methoxyphenyl)thio)benzothioate (36)



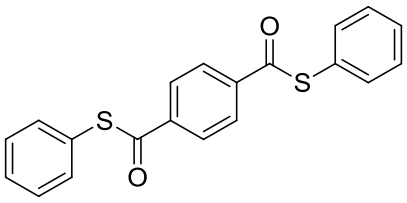
	Parameter	Value
1	Title	MNB265frac31-48-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-16T12:07:01
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



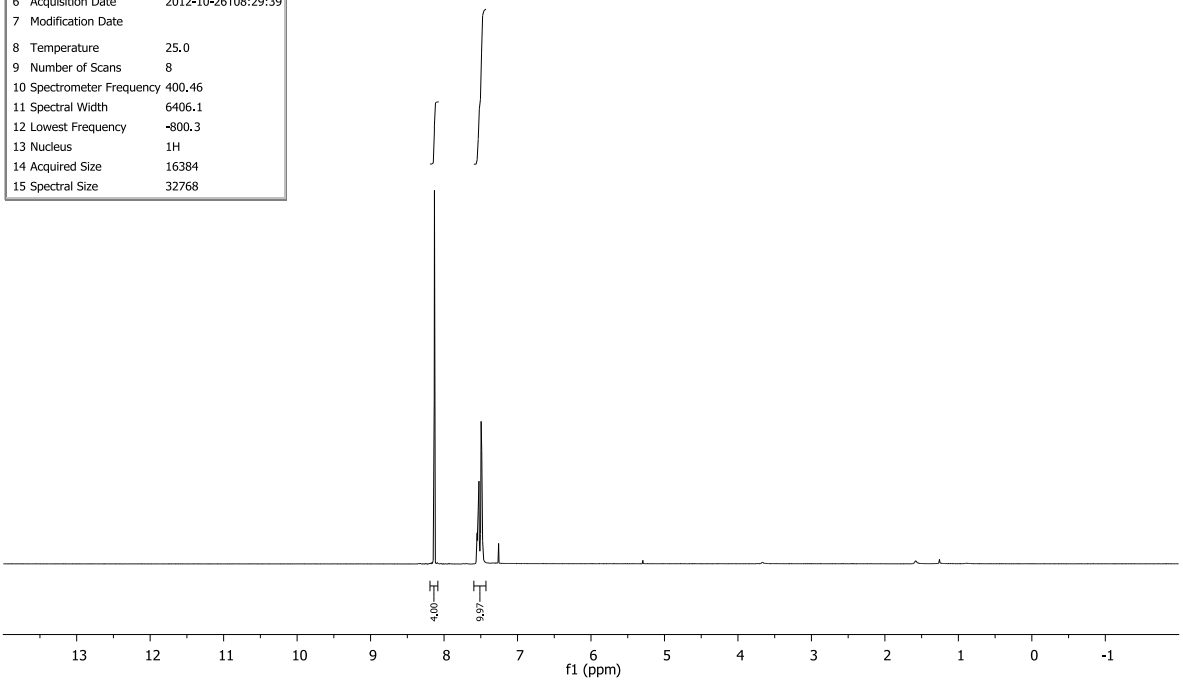
	Parameter	Value
1	Title	MNB265frac31-48_C-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-16T14:26:09
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	104
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1504.6
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



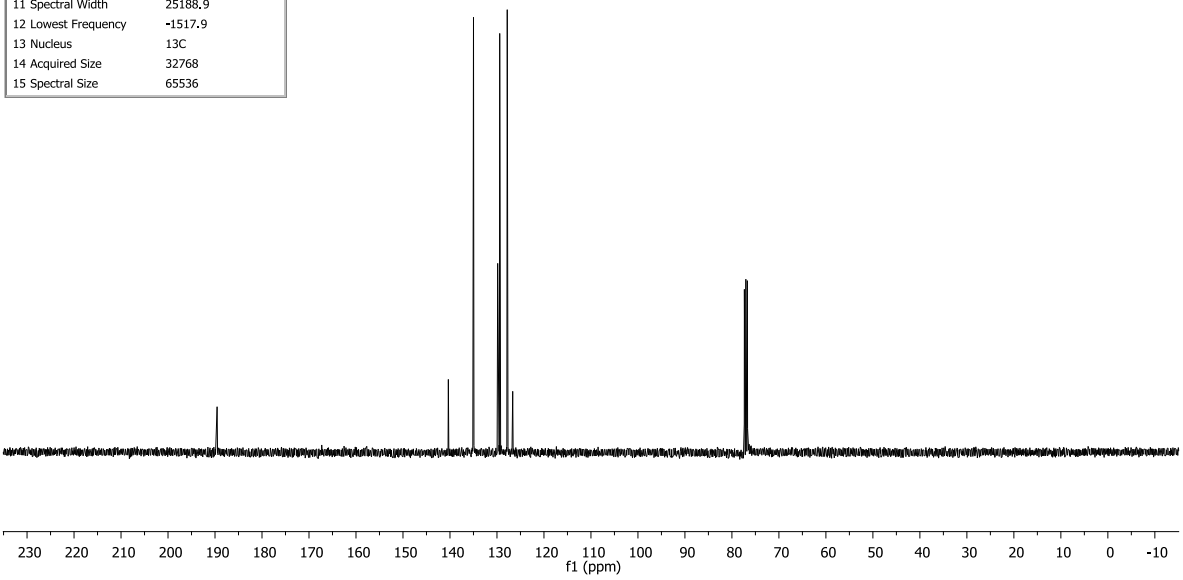
S,S-diphenyl benzene-1,4-bis(carbothioate) (37)



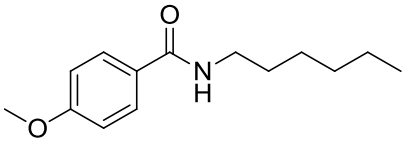
	Parameter	Value
1	Title	MNB316.F13-28.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-10-26T08:29:39
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



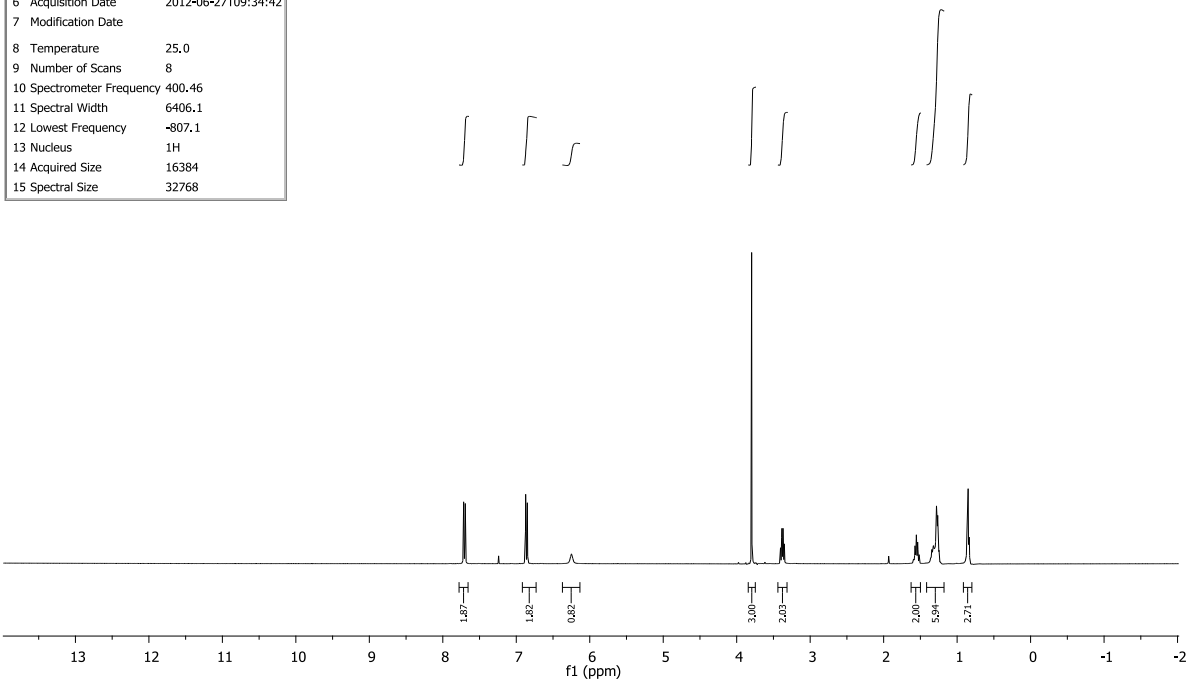
	Parameter	Value
1	Title	MNB316.F13-28.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-10-26T08:30:23
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	236
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



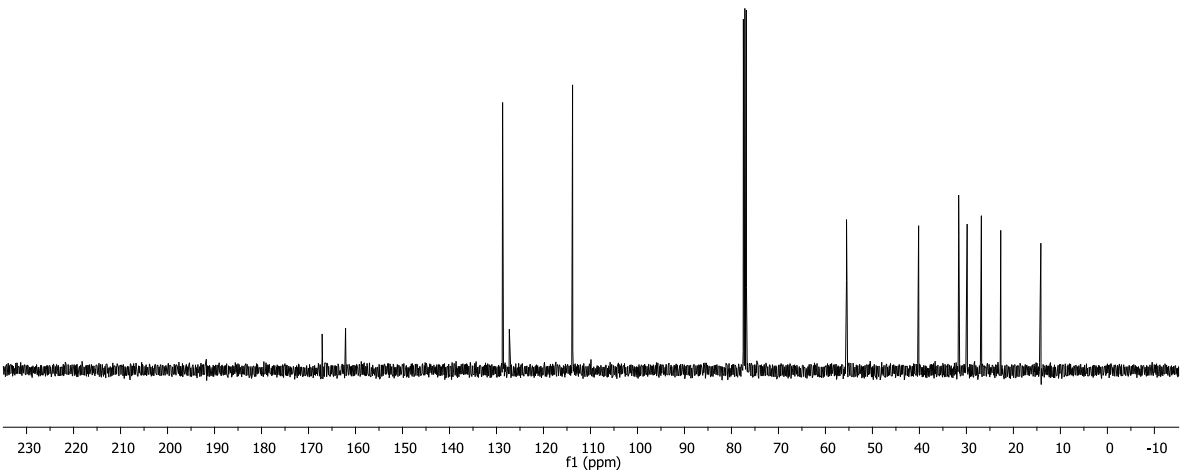
N-hexyl-4-methoxybenzamide (38)



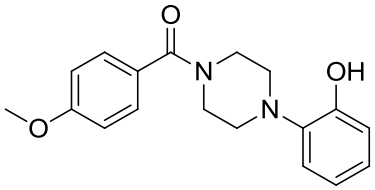
	Parameter	Value
1	Title	RH915a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-06-27T09:34:42
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.1
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



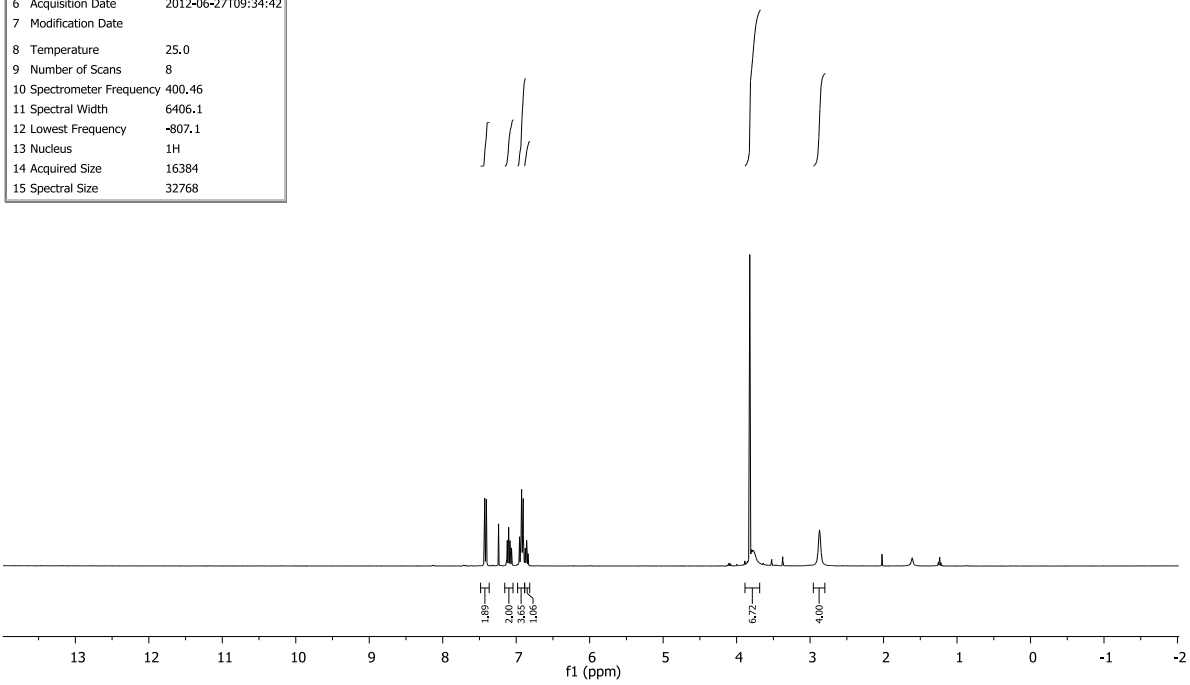
	Parameter	Value
1	Title	carbon571a
2	Origin	mercury
3	Owner	
4	Solvent	CDCl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2010-08-05T07:54:21
7	Modification Date	
8	Temperature	26.0
9	Number of Scans	456
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1527.6
13	Nucleus	13C
14	Acquired Size	30211
15	Spectral Size	65536



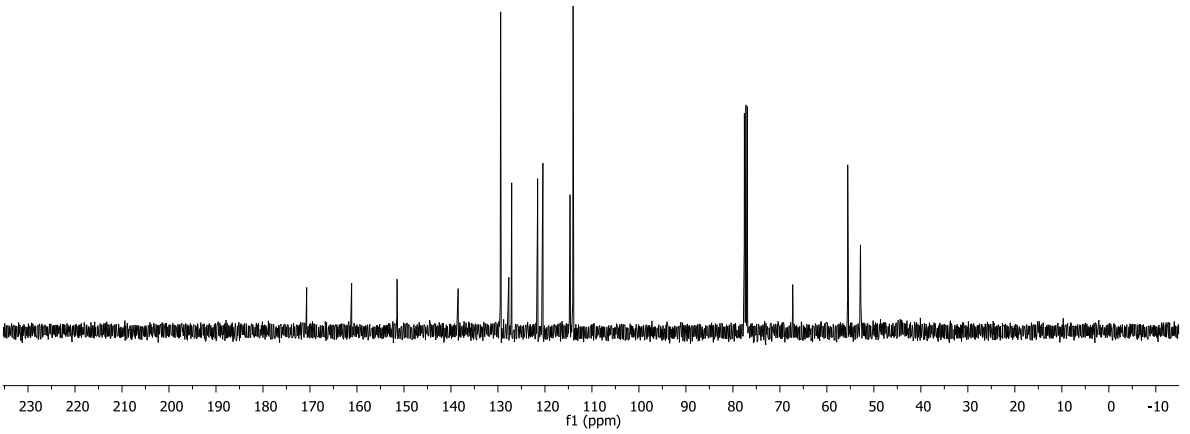
(4-(2-hydroxyphenyl)piperazin-1-yl)(4-methoxyphenyl)methanone (39)



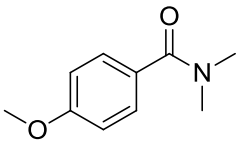
	Parameter	Value
1	Title	RH915a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-06-27T09:34:42
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.1
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



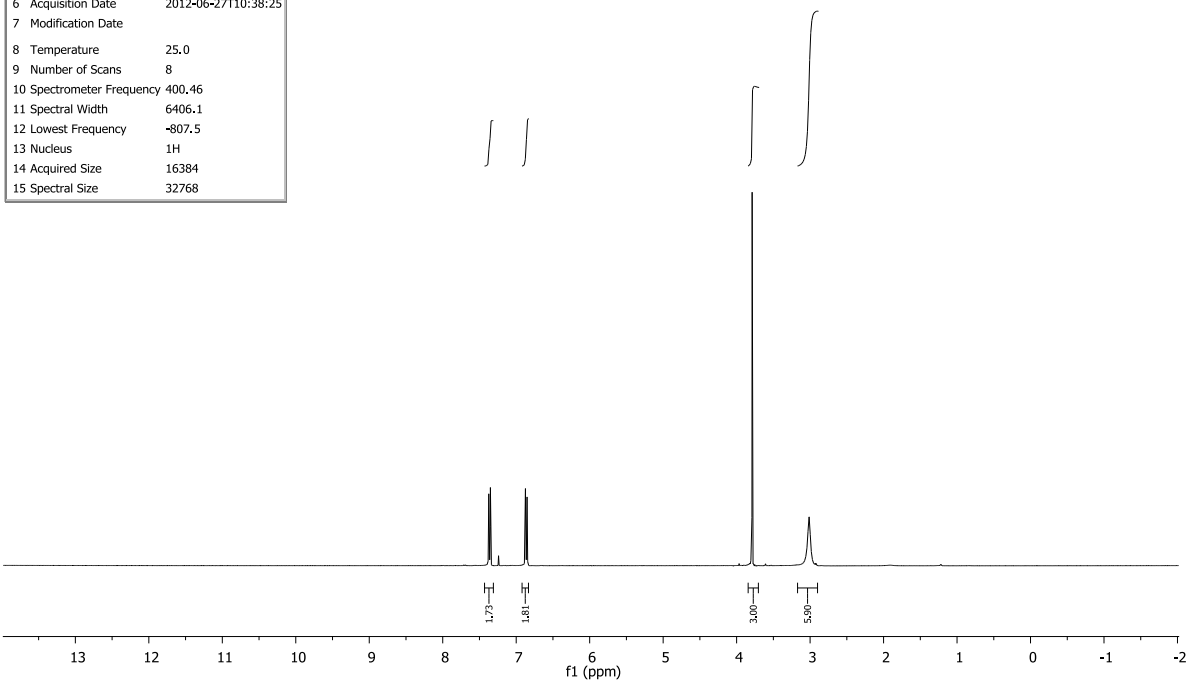
	Parameter	Value
1	Title	carbon928a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-10-10T08:06:37
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	328
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1497.1
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



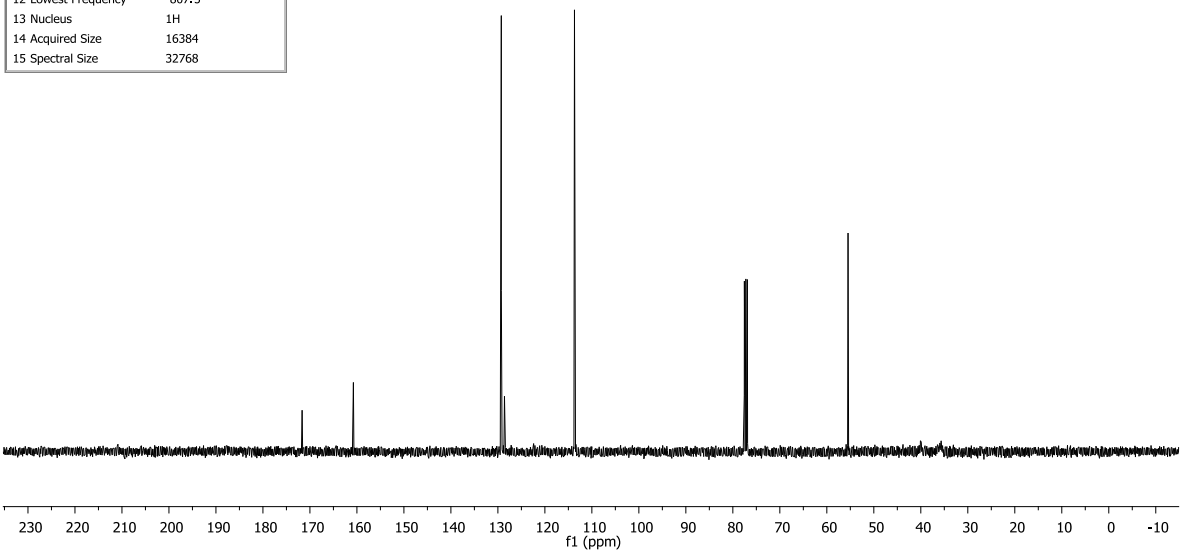
4-methoxy-*N*,*N*-dimethylbenzamide (40)



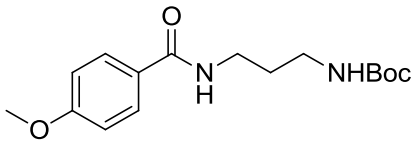
	Parameter	Value
1	Title	RH930a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-06-27T10:38:25
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.5
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



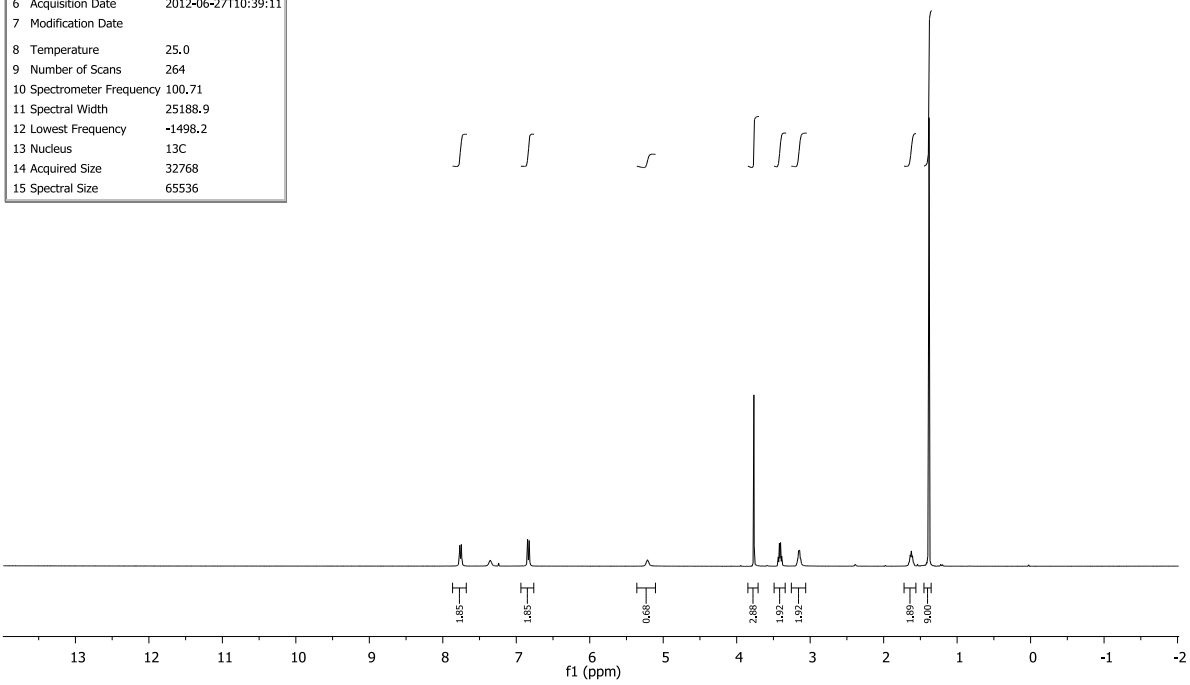
	Parameter	Value
1	Title	RH930a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-06-27T10:38:25
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.5
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



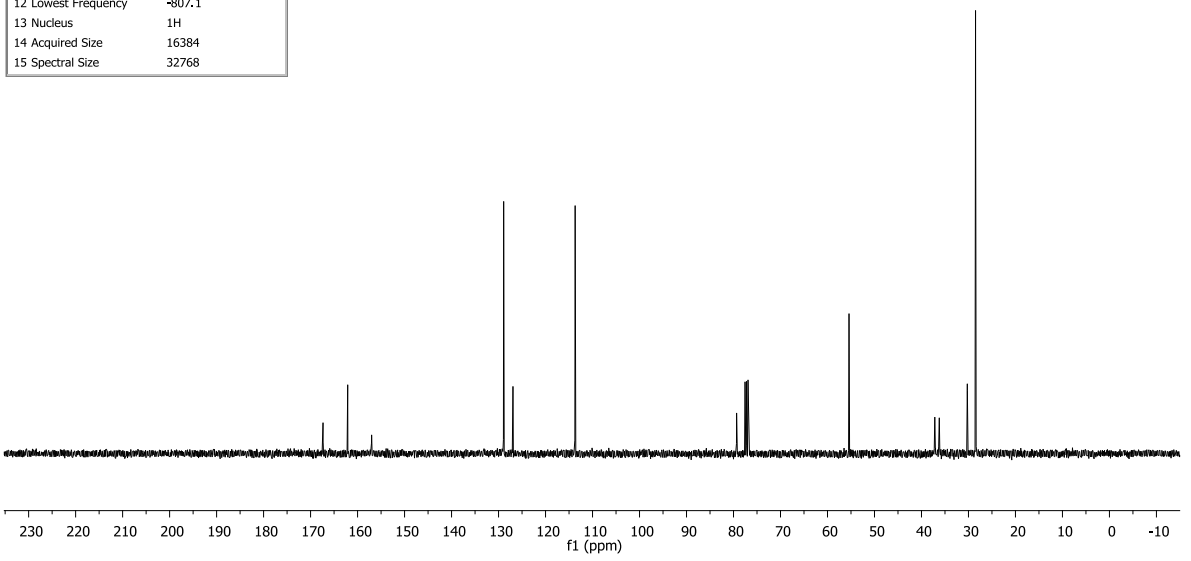
tert-butyl (3-(4-methoxybenzamido)propyl)carbamate (41)



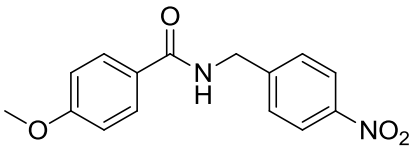
	Parameter	Value
1	Title	carbon930a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-06-27T10:39:11
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	264
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1498.2
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



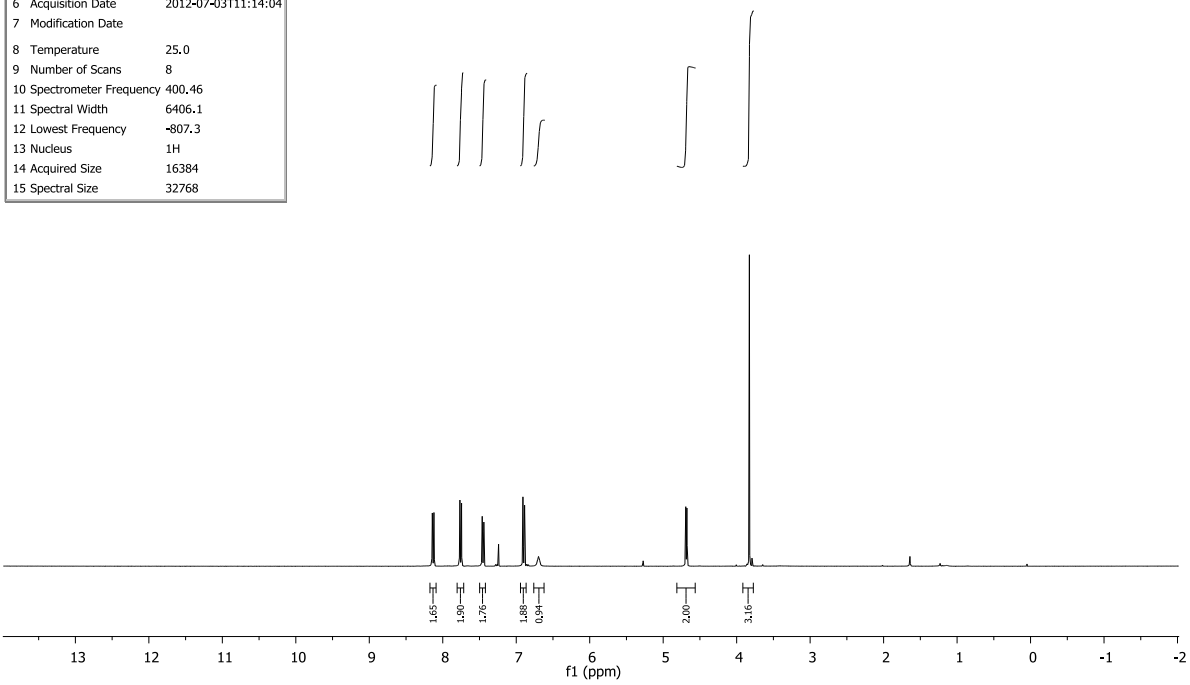
	Parameter	Value
1	Title	RH938a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-07-03T11:35:01
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.1
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



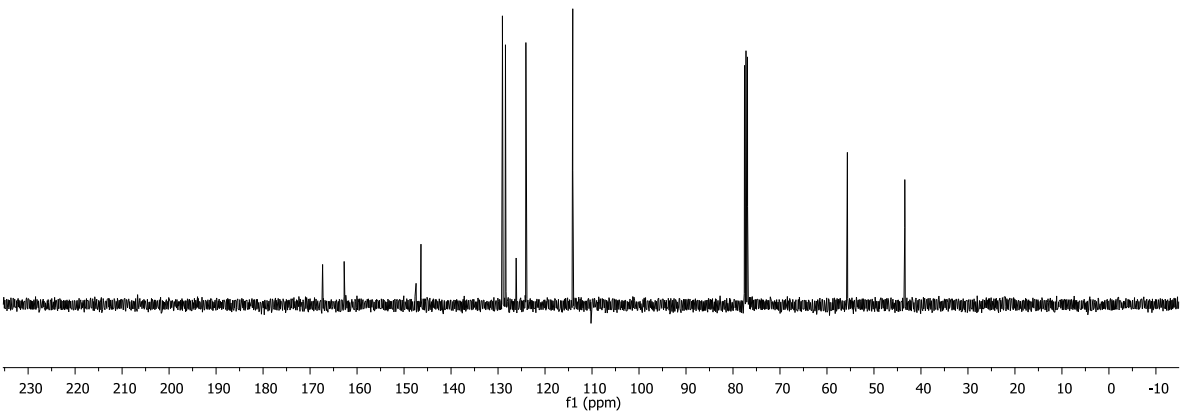
4-methoxy-*N*-(4-nitrobenzyl)benzamide (42)



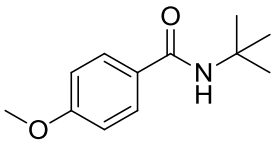
	Parameter	Value
1	Title	RH937a
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-07-03T11:14:04
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



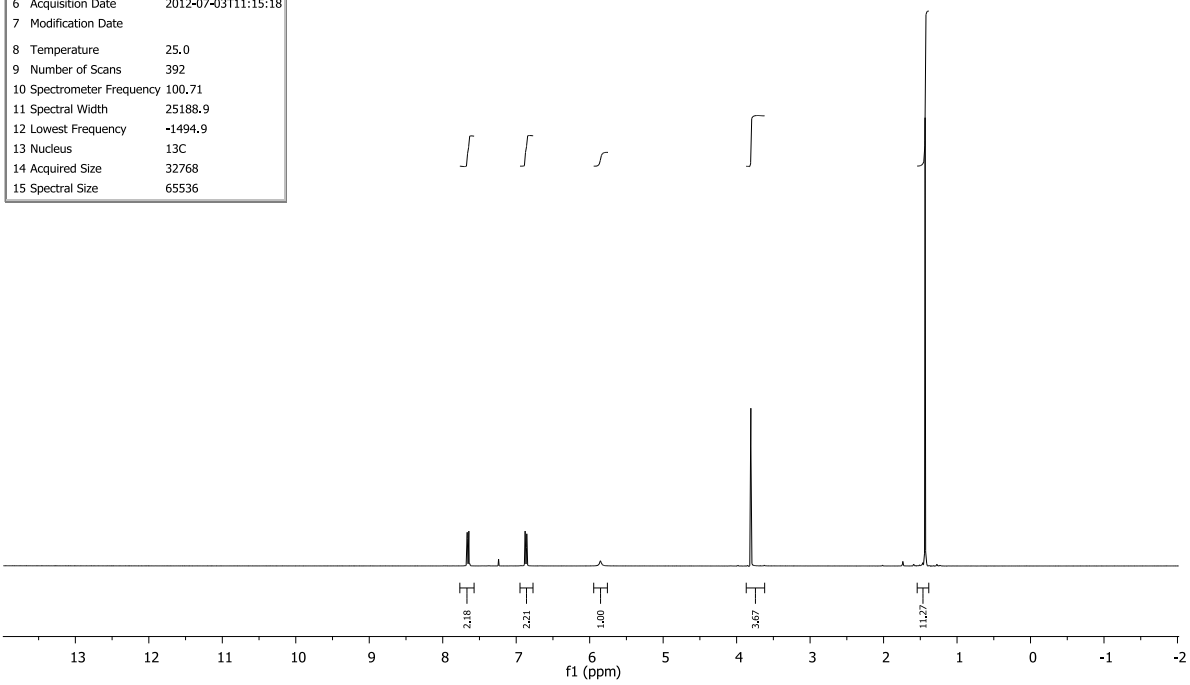
	Parameter	Value
1	Title	carbon937a
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-07-03T11:15:18
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	392
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1494.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



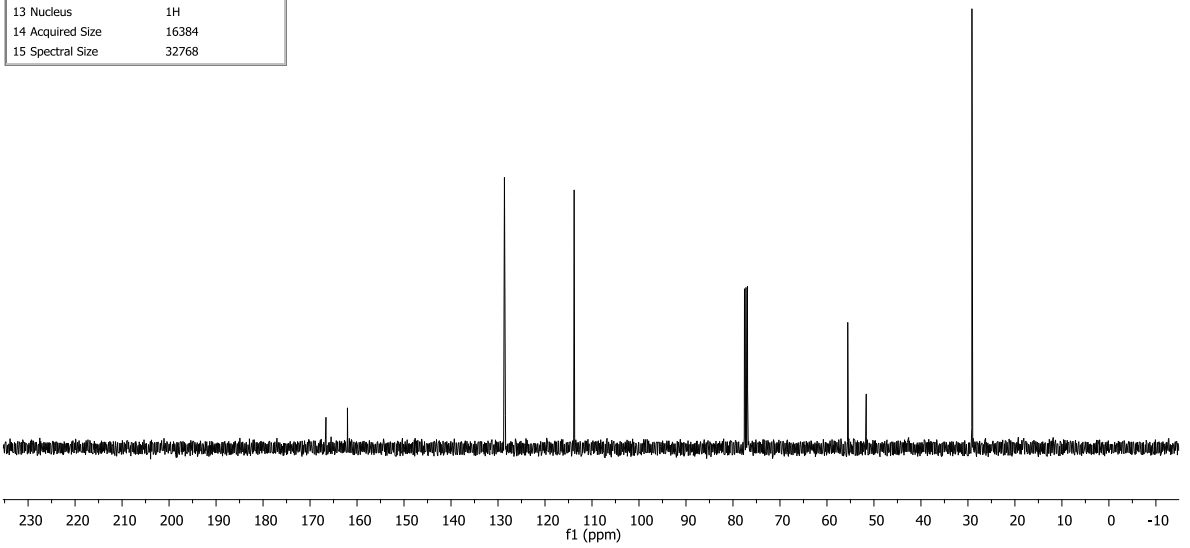
N-(tert-butyl)-4-methoxybenzamide (43)



	Parameter	Value
1	Title	carbon937a
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-07-03T11:15:18
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	392
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1494.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536

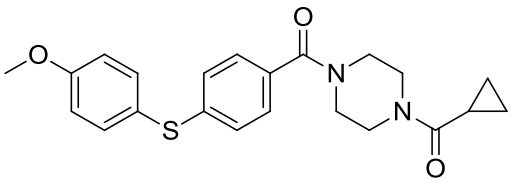


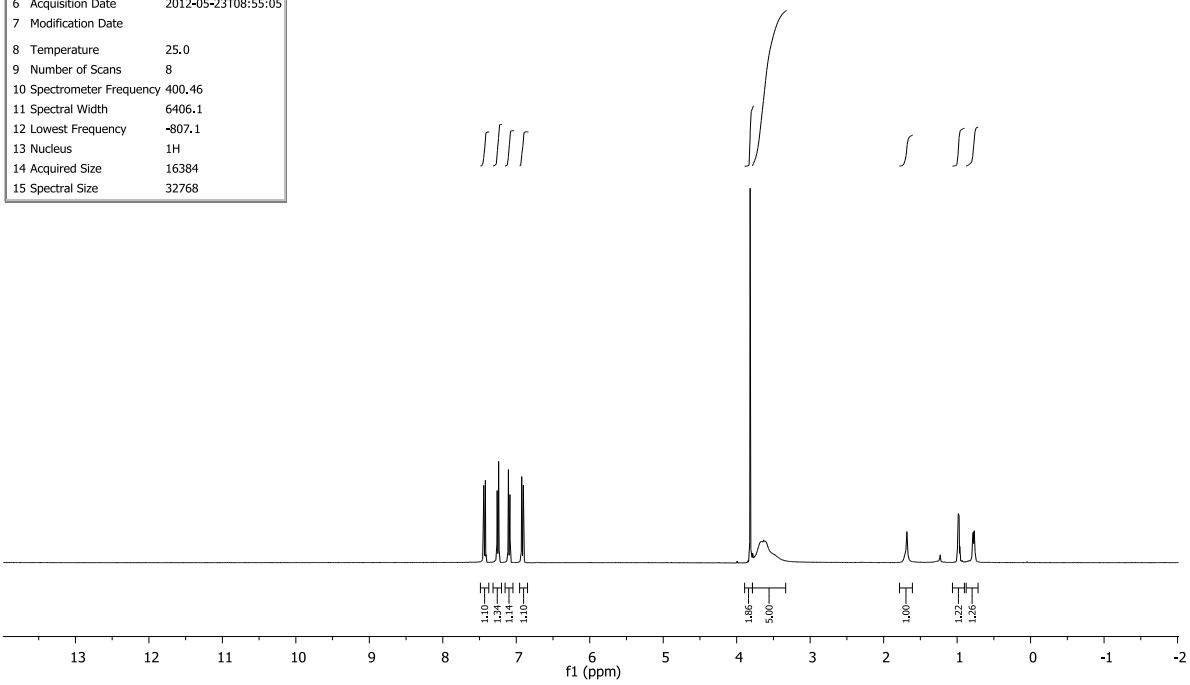
	Parameter	Value
1	Title	RH931a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-06-27T10:51:24
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.5
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



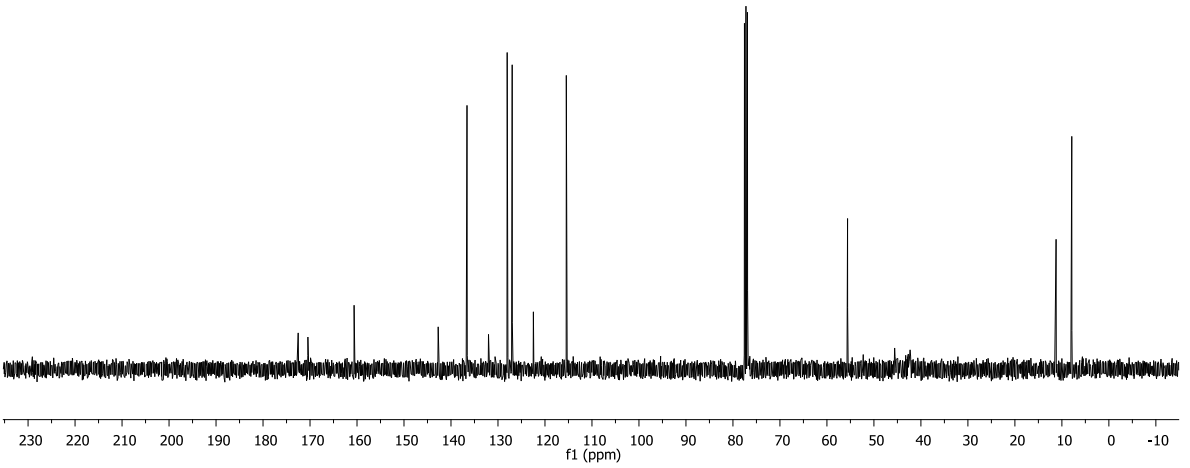
(4-(cyclopropanecarbonyl)piperazin-1-yl)(4-((4-methoxyphenyl)thio)phenyl)methanone (44)

	Parameter	Value
1	Title	RH906a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-23T08:55:05
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.1
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



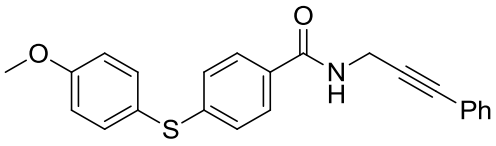


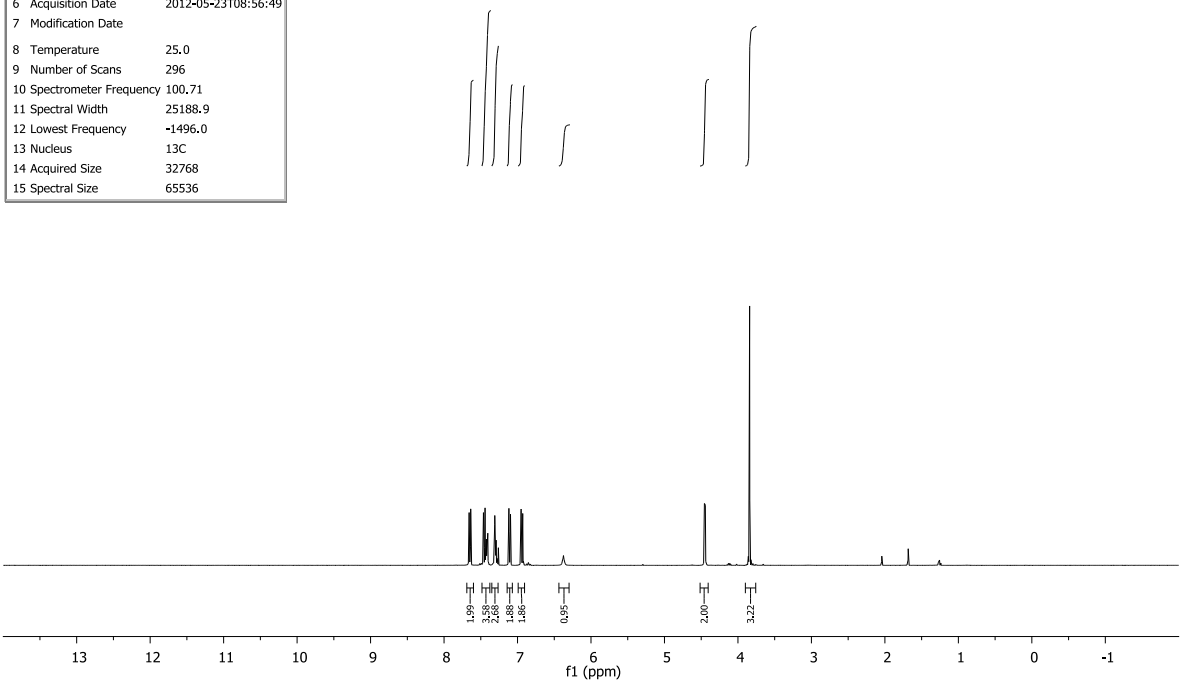
	Parameter	Value
1	Title	RH906a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-23T08:55:05
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-807.1
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



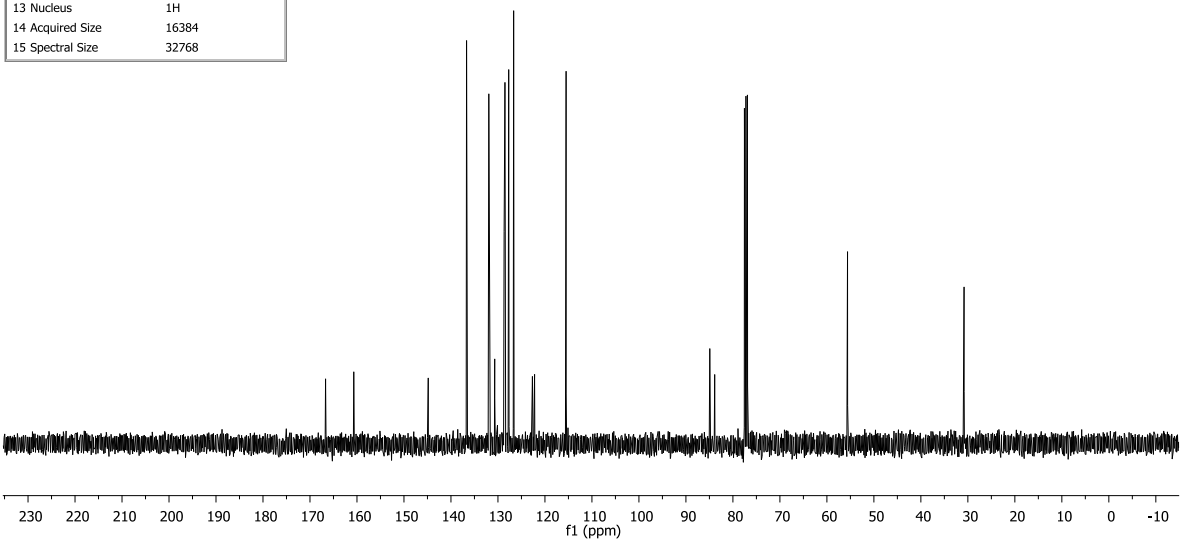
4-((4-methoxyphenyl)thio)-*N*-(3-phenylprop-2-yn-1-yl)benzamide (45)

	Parameter	Value
1	Title	carbon906a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-23T08:56:49
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	296
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1496.0
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



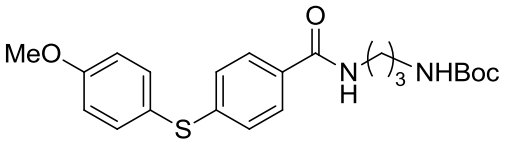


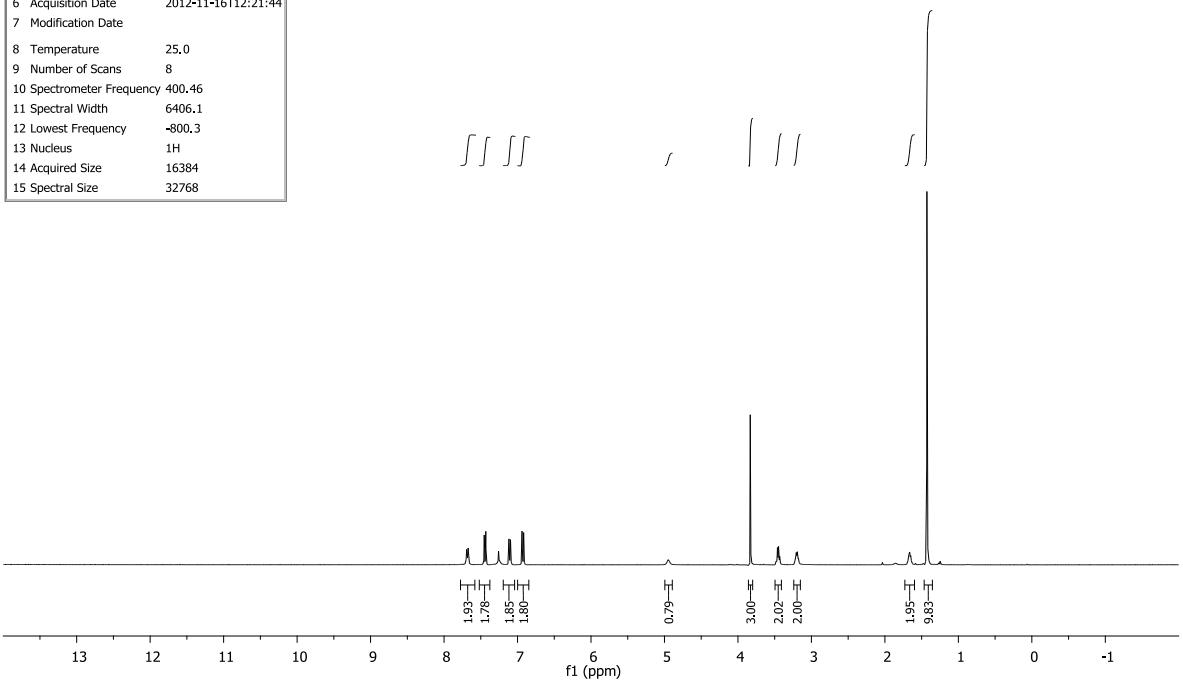
	Parameter	Value
1	Title	RH907a-
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-05-23T11:35:05
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



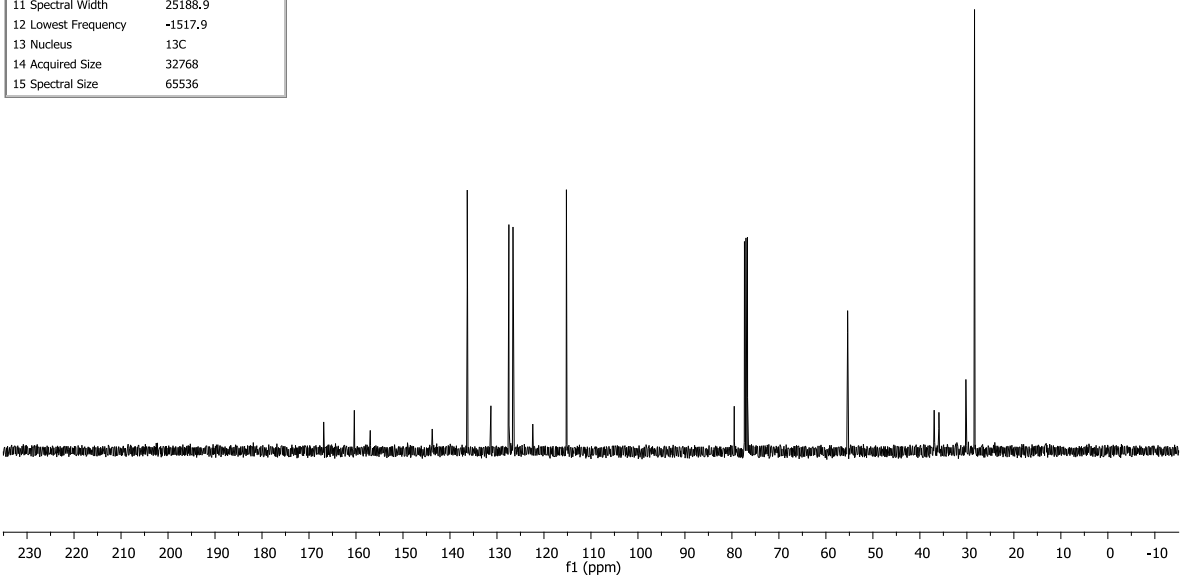
tert-butyl (3-(4-((4-methoxyphenyl)thio)benzamido)propyl)carbamate (46)

	Parameter	Value
1	Title	MNB320.F43-51.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-16T12:21:44
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

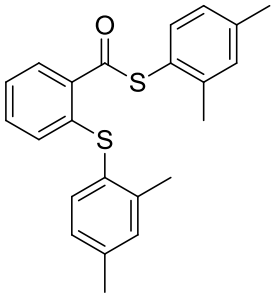




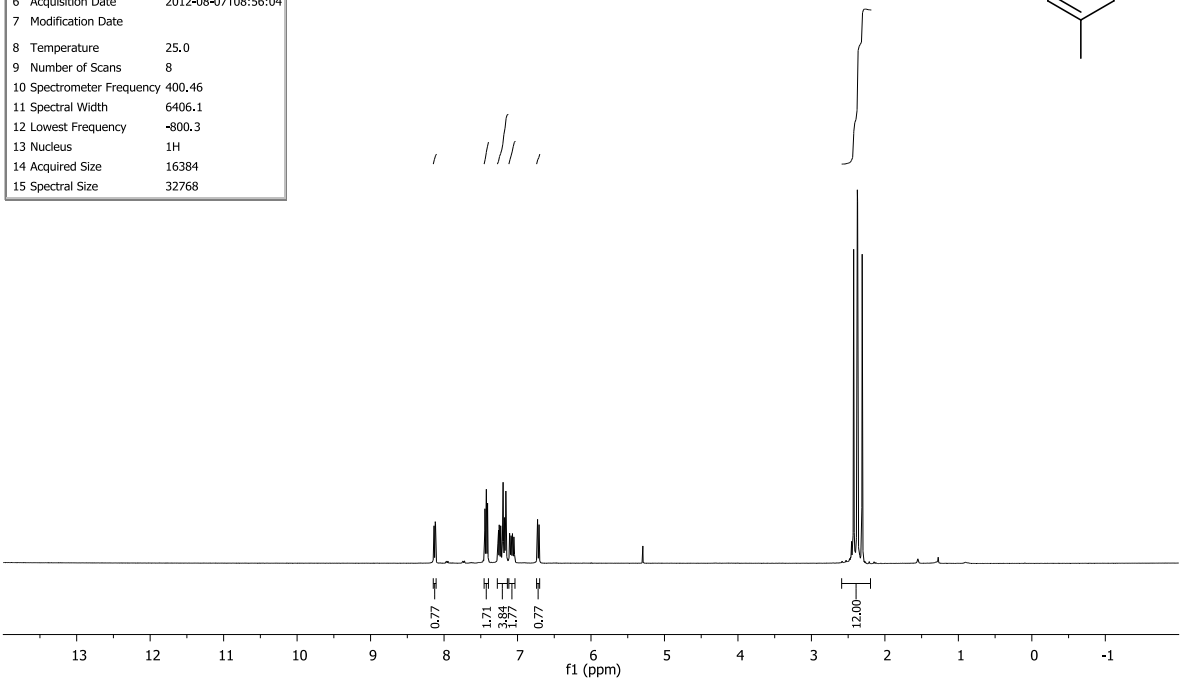
	Parameter	Value
1	Title	MNB320.F43-51.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-16T12:32:21
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



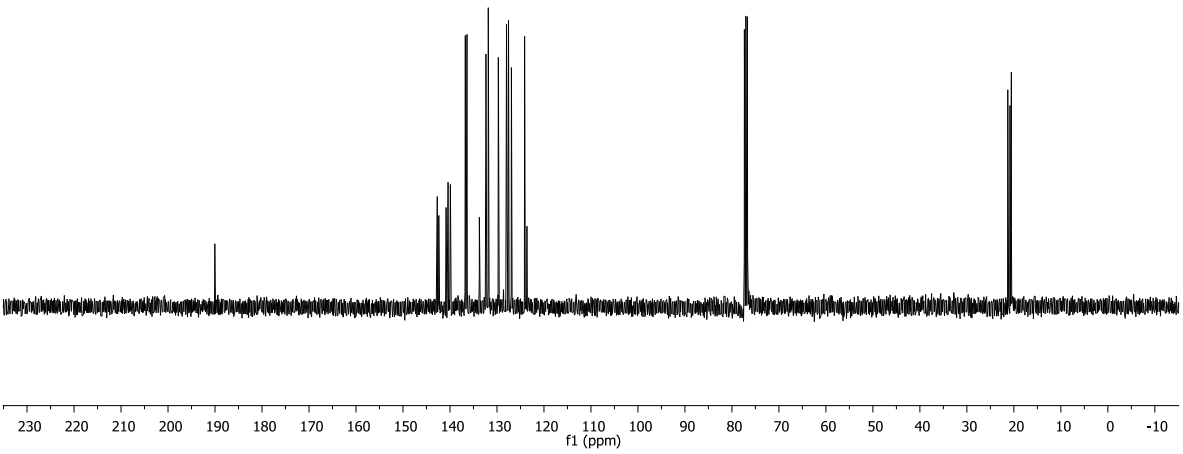
S-(2,4-dimethylphenyl) 2-((2,4-dimethylphenyl)thio)benzothioate (47)



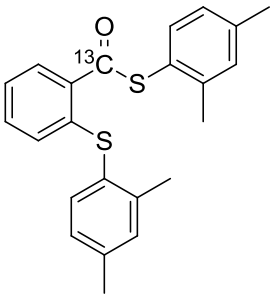
	Parameter	Value
1	Title	MNB270-2.F9-17.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-08-07T08:56:04
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



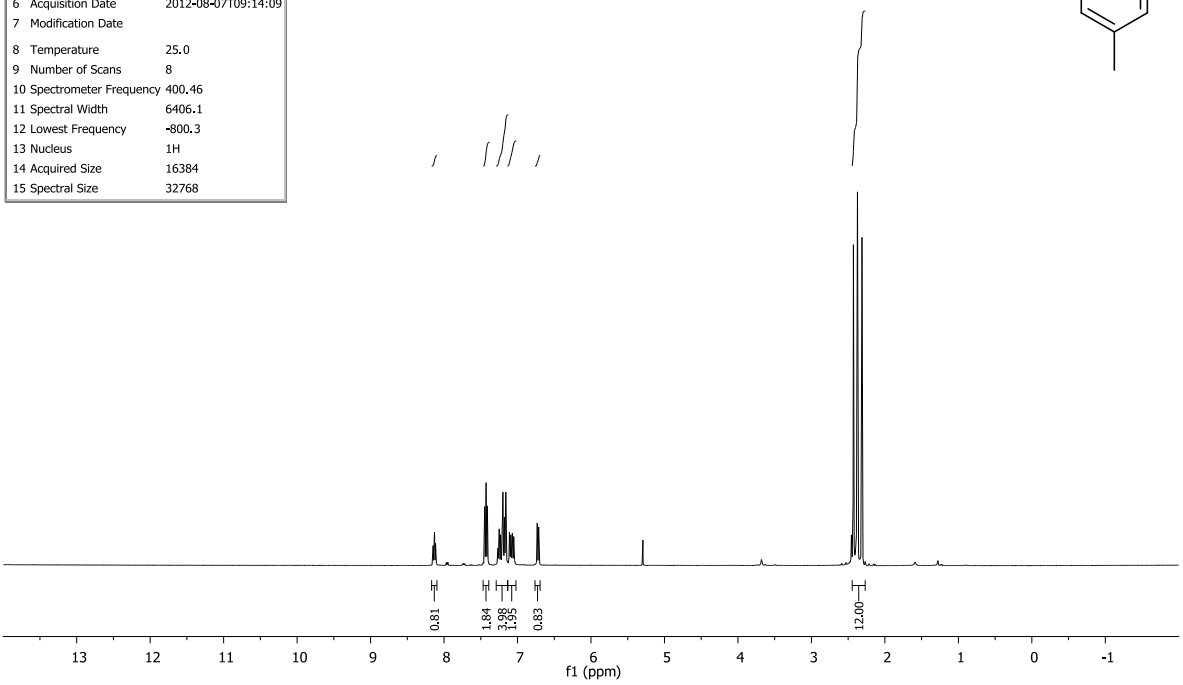
	Parameter	Value
1	Title	MNB270-2.F9-17.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-08-07T09:07:00
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



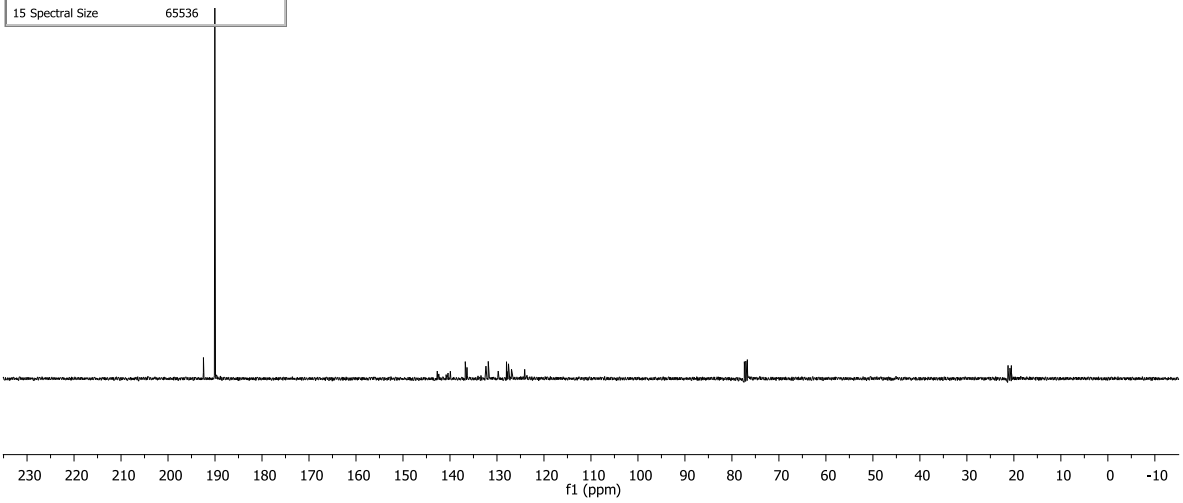
S-(2,4-dimethylphenyl) 2-((2,4-dimethylphenyl)thio)[^{13}C]benzothioate (^{13}C-47)



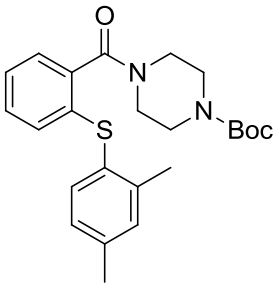
	Parameter	Value
1	Title	MNB271.F9-19.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-08-07T09:14:09
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



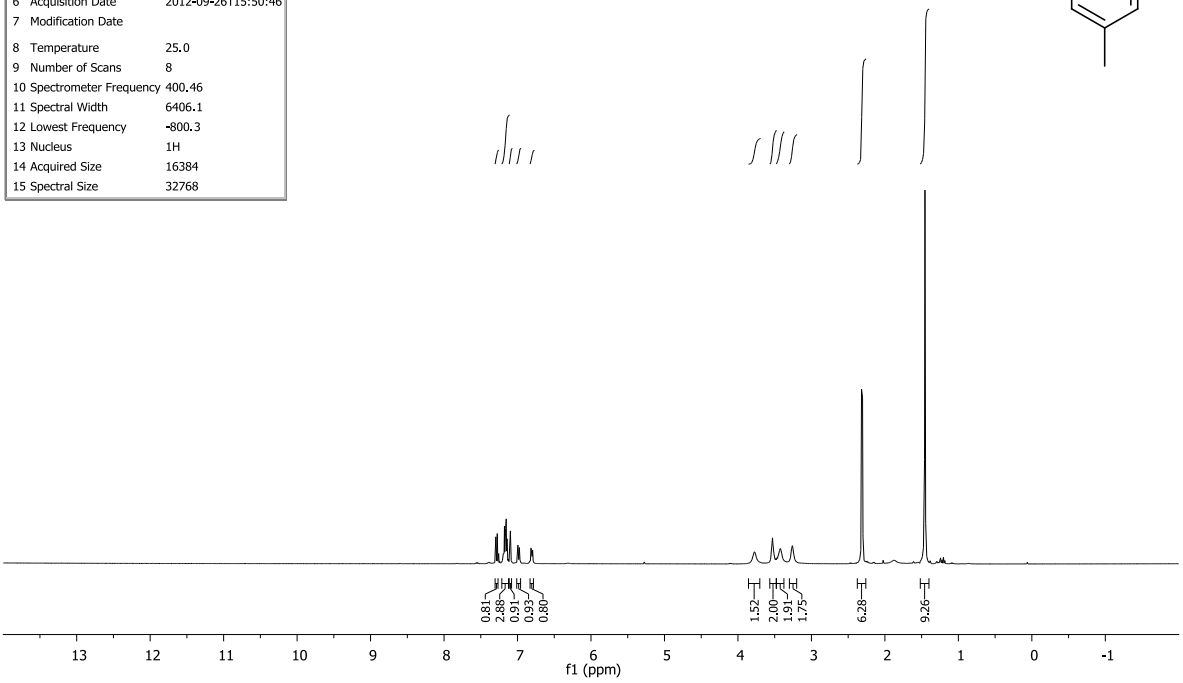
	Parameter	Value
1	Title	MNB271.F9-19.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-08-07T09:14:58
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	24
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



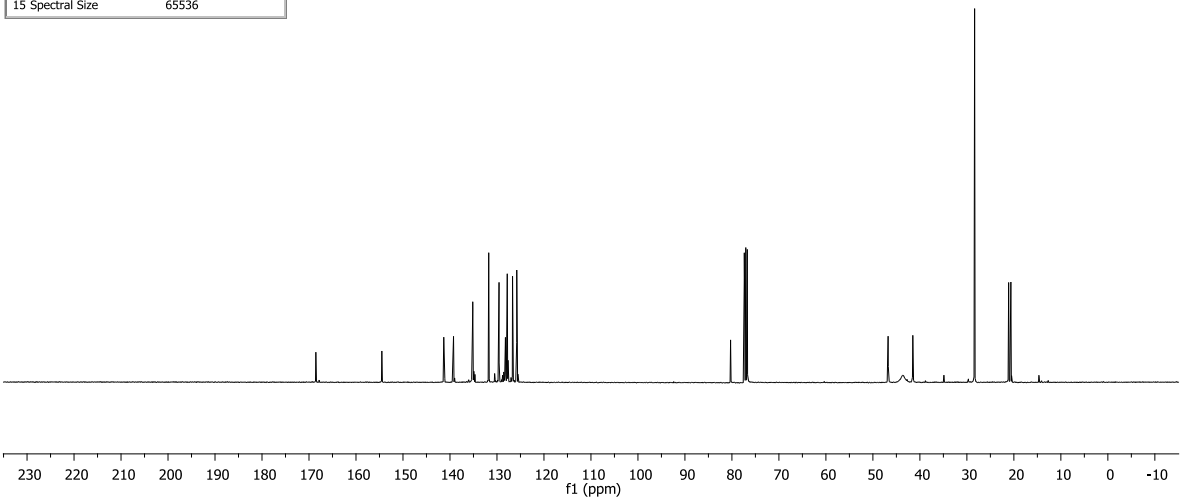
tert-butyl 4-(2-((2,4-dimethylphenyl)thio)benzoyl)piperazine-1-carboxylate (48)



	Parameter	Value
1	Title	MNB294.F7-16.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-09-26T15:50:46
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

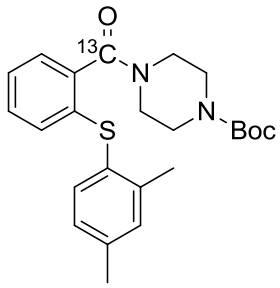


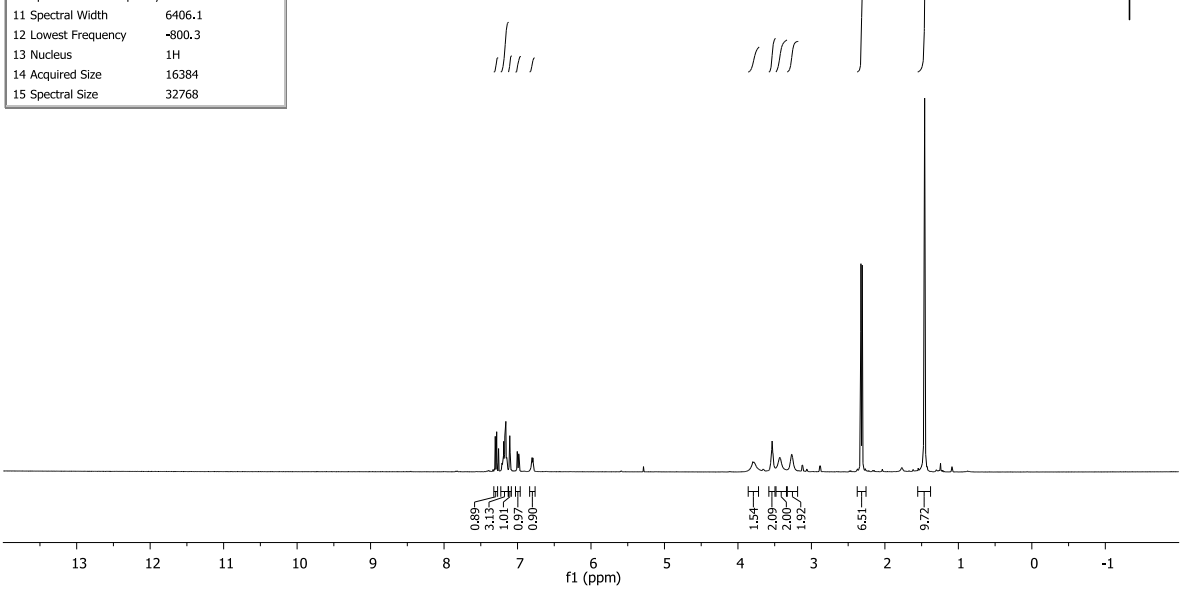
	Parameter	Value
1	Title	MNB294.F7-16.o/ n.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-09-26T16:15:17
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	23892
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



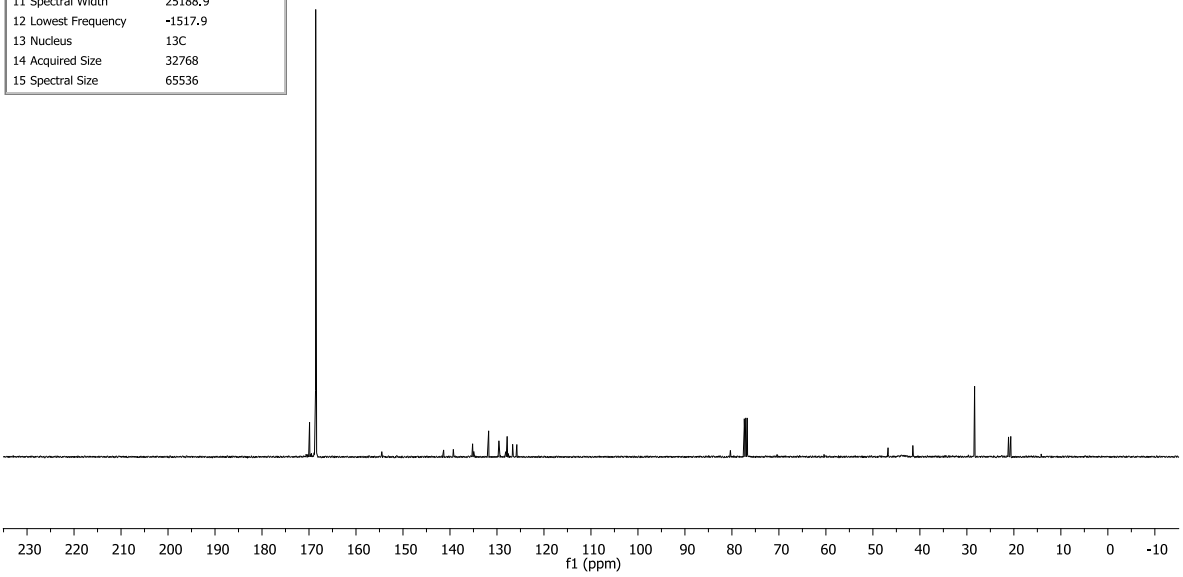
tert-butyl 4-(2-((2,4-dimethylphenyl)thio)[^{13}C]benzoyl)piperazine-1-carboxylate (^{13}C-48)

	Parameter	Value
1	Title	MNB310.F9-24.H2
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-10-23T09:23:29
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768

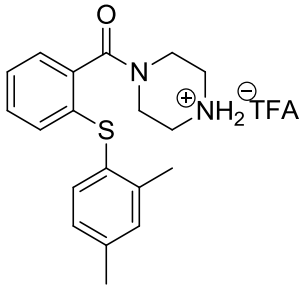




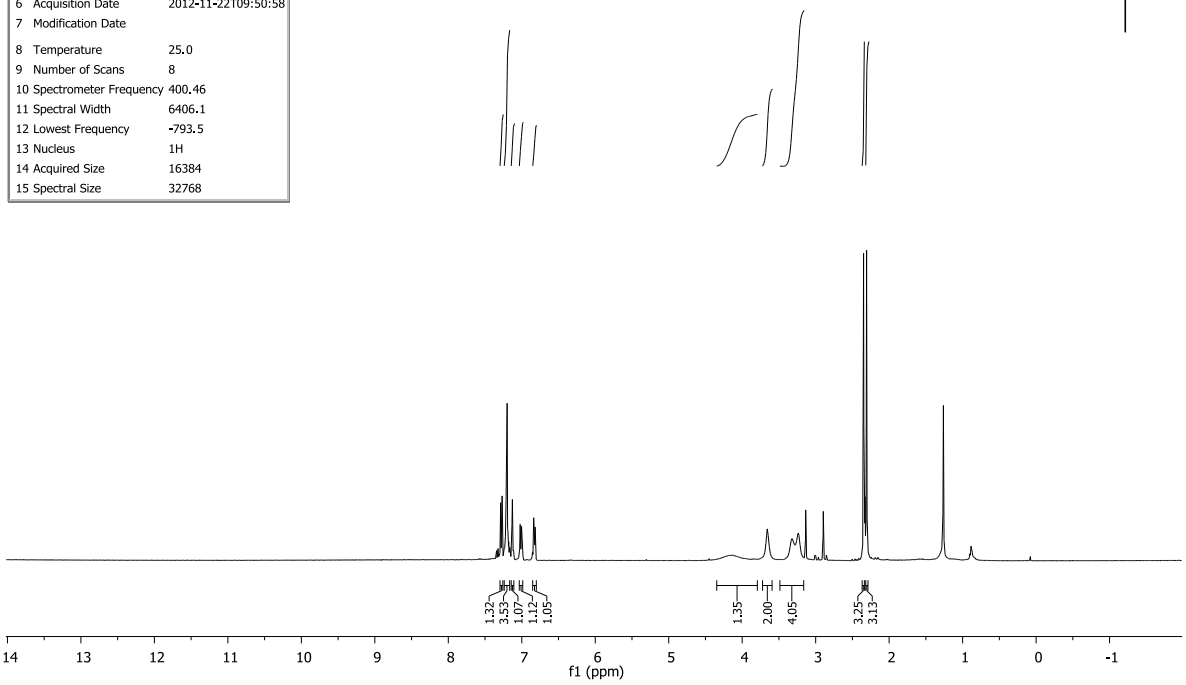
	Parameter	Value
1	Title	MNB326.F11-28.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-06T12:42:33
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	256
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



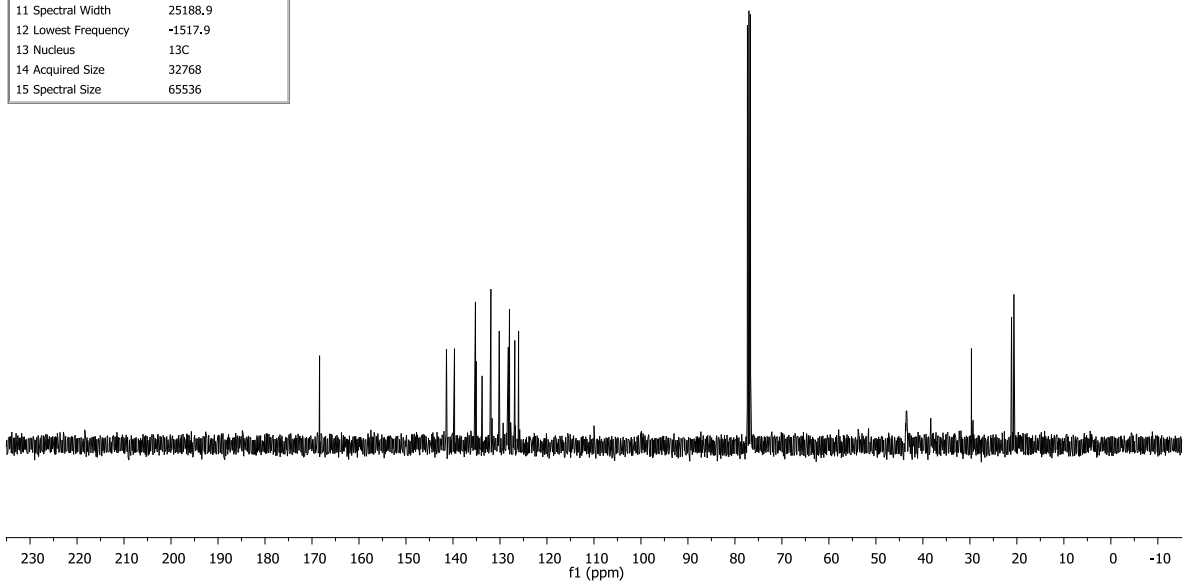
4-(2-((2,4-dimethylphenyl)thio)benzoyl)piperazin-1-ium trifluoroacetate (49)



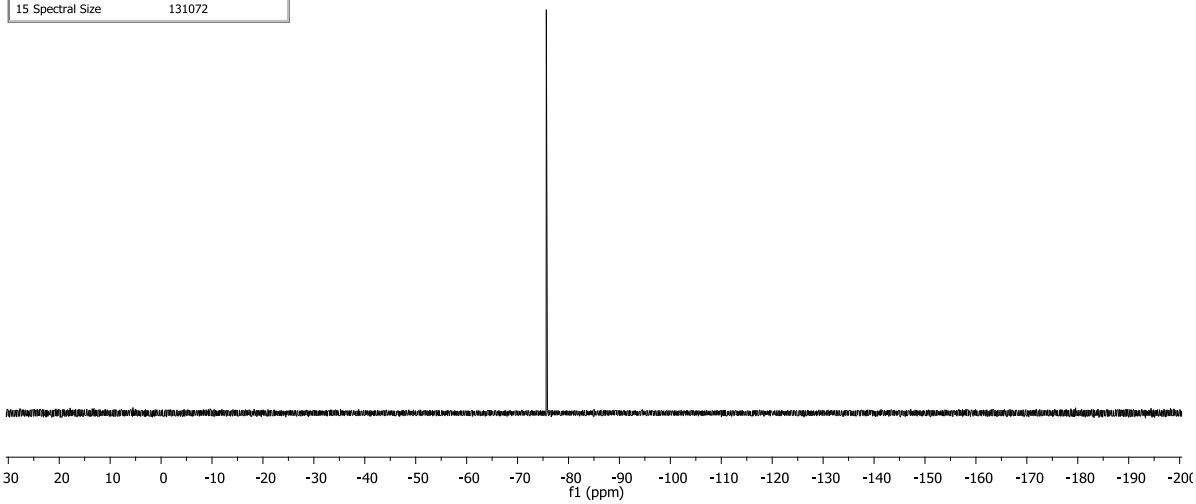
	Parameter	Value
1	Title	MNB328.vac.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-22T09:50:58
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-793.5
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768



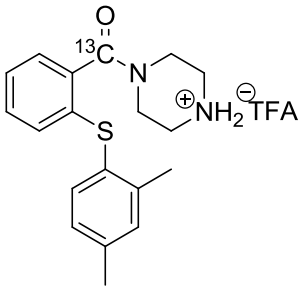
	Parameter	Value
1	Title	MNB328.vac.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-22T10:03:35
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	300
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



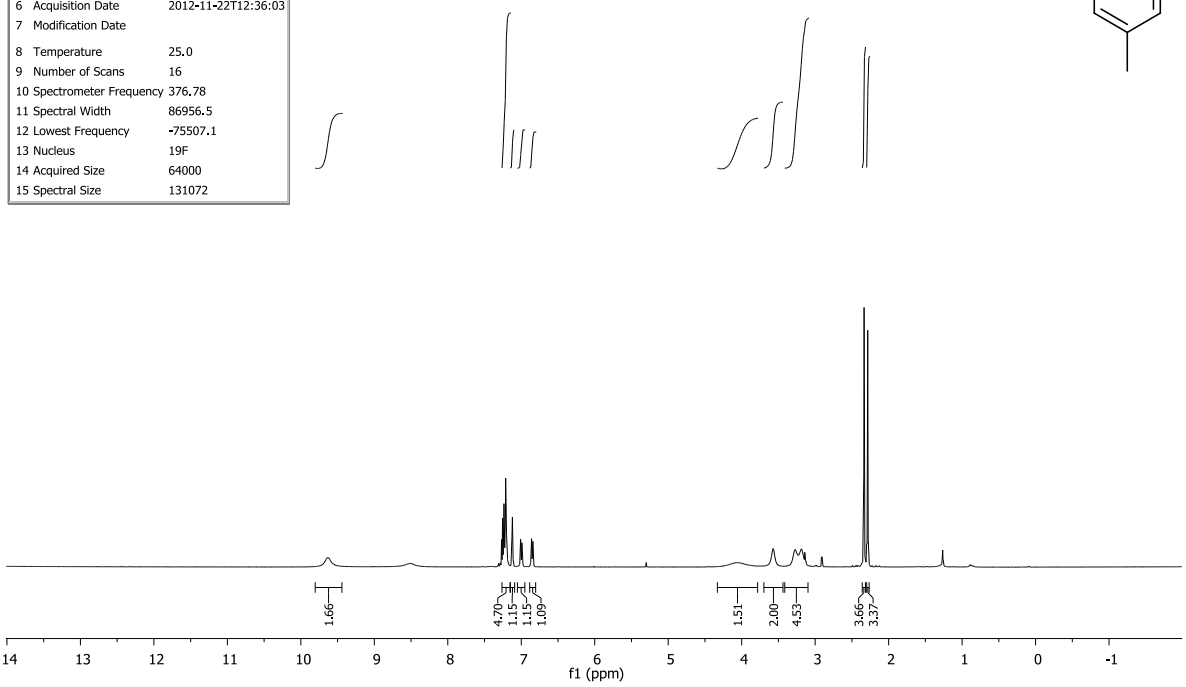
	Parameter	Value
1	Title	MNB328.vac.F
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-22T12:33:28
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	16
10	Spectrometer Frequency	376.78
11	Spectral Width	86956.5
12	Lowest Frequency	-75507.1
13	Nucleus	19F
14	Acquired Size	64000
15	Spectral Size	131072



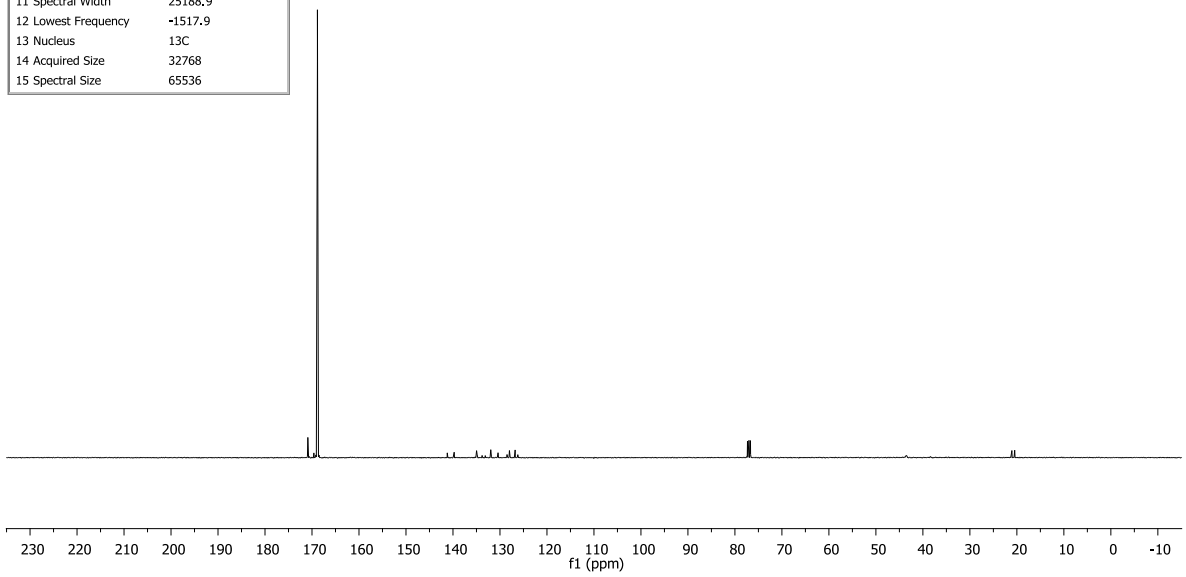
4-(2-((2,4-dimethylphenyl)thio)[^{13}C]benzoyl)piperazin-1-ium trifluoroacetate (^{13}C-49)



	Parameter	Value
1	Title	MNB329.vac.F
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-22T12:36:03
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	16
10	Spectrometer Frequency	376.78
11	Spectral Width	86956.5
12	Lowest Frequency	-75507.1
13	Nucleus	19F
14	Acquired Size	64000
15	Spectral Size	131072



	Parameter	Value
1	Title	MNB329.vac.C
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-22T10:50:31
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	350
10	Spectrometer Frequency	100.71
11	Spectral Width	25188.9
12	Lowest Frequency	-1517.9
13	Nucleus	13C
14	Acquired Size	32768
15	Spectral Size	65536



	Parameter	Value
1	Title	MNB382.wu.H
2	Origin	mercury
3	Owner	
4	Solvent	cdcl3
5	Pulse Sequence	s2pul
6	Acquisition Date	2012-11-05T12:32:11
7	Modification Date	
8	Temperature	25.0
9	Number of Scans	8
10	Spectrometer Frequency	400.46
11	Spectral Width	6406.1
12	Lowest Frequency	-800.3
13	Nucleus	1H
14	Acquired Size	16384
15	Spectral Size	32768