Electronic Supplementary Material (ESI) for Chemical Communications

Facile carbon-sulfur bond cleavage in diarylsulfonium ylides: a catalytic sulfur-to-silicon group transfer

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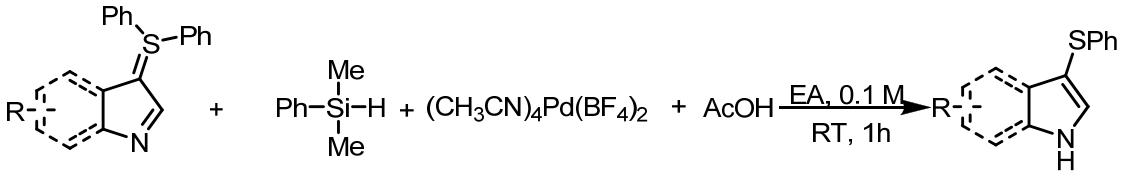
Part I Experimental part

General information

Unless otherwise indicated, all glassware was oven dried by a heat gun before use and all reactions were performed under an atmosphere of Argon. All solvents were distilled from appropriate drying agents prior to use. All reagents were used as received from commercial suppliers unless otherwise stated. All the ylides were prepared according to the procedures reported by our group.[1] Reaction progress was monitored by thin layer chromatography (TLC) performed on plastic plates coated with kieselgel F_{254} with 0.2 mm thickness or GC-MS. Visualization was achieved by ultraviolet light (254 nm). Flash column chromatography was performed using silica gel 60 (230-400 mesh, Merck and co.). Mass spectra were obtained using a Finnigan MAT 8200 or (70 eV) or an Agilent 5973 (70 eV) spectrometer, using electrospray ionization (ESI). All ^{1}H NMR, ^{13}C NMR spectra were recorded on Bruker AV-500, AV-400 or AV-300 in $CDCl_3$. Chemical shifts were given in parts per million (ppm, δ), referenced to the peak of tetramethylsilane, defined at δ = 0.00 (^{1}H NMR), or the solvent peak of $CDCl_3$, defined at δ = 77.0 (^{13}C NMR). Coupling constants were quoted in Hz (*J*). ^{1}H NMR Spectroscopy splitting patterns were designated as singlet (s), doublet (d), triplet (t), quartet (q), pentet (p), sextet (se), septet (sep), octet (o). Splitting patterns that could not be interpreted or easily visualized were designated as multiplet (m) or broad (br).

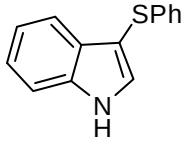
[1] X. Huang, R. Goddard, N. Maulide, *Angew. Chem. Int. Ed.* **2010**, *49*, 8979.

1.1 Palladium-catalysed dearylation of diphenyl sulfonium ylides



Typical procedure for the dephenylation of sulfonium ylides: Under an argon atmosphere, $(CH_3CN)_4Pd(BF_4)_2$ (0.005 mmol, 2.2 mg) and sulfonium ylide (0.1 mmol, 37.3 mg) were added into a dried Schlenk tube. The tube was stopped, evacuated and back filled with argon three times. Ethyl acetate (1 mL, 0.1 M), AcOH (57μL, 1.0 mmol) were added by syringe, followed by dimethylphenylsilane (30 μL, 0.2 mmol). The mixture was stirred under argon atmosphere at room temperature for 1h. The resultant mixture was filtered through a short plug of silica gel, and eluted with ethyl acetate. The filtrate was concentrated on a rotatory evaporator to afford a crude mixture, which was purified by flash column chromatography on silica gel to afford the title compound.

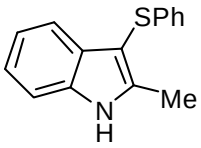
3-(Phenylthio)-1H-indole (**3b**)[2]



Compound **3b** was obtained in 67% yield as white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (br, 1H), 7.61 (d, J = 7.9 Hz, 1H), 7.48-7.42 (m, 2H), 7.28-7.24 (m, 1H), 7.18-7.14 (m, 3H), 7.11-7.09 (m, 2H) 7.06-7.03 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 139.2, 136.4, 130.7, 129.1, 128.7, 125.8, 124.7, 123.0, 123.9, 119.6, 111.5, 102.8.

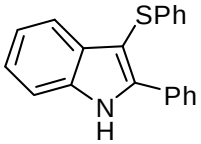
[2] Fang, X.-L.; Tang, R.-Y.; Zhong, P.; Li, J.-H. *Synthesis* **2009**, 4183.

2-Methyl-3-(phenylthio)-1H-indole (**3c**)[1]



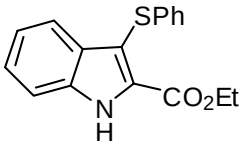
Compound **3c** was obtained in 92% yield as pale yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (br, 1H), 7.47 (d, *J* = 7.8 Hz, 1H), 7.28-7.26 (m, 1H), 7.14-7.03 (m, 4H), 6.98-6.94 (m, 3H), 2.45 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.1, 139.3, 135.4, 130.3,128.4, 124.5, 122.2, 119.0, 110.6, 99.4, 12.1.

2-Phenyl-3-(phenylthio)-1H-indole (**3d**)[3]



Compound **3d** was obtained in 89% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (br, 1H), 7.67-7.66 (m, 2H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.37-7.33 (m, 3H), 7.31-7.28 (m, 1H), 7.19 (t, *J* = 7.3 Hz, 1H), 7.10-7.06 (m, 3H), 7.02-7.01 (m, 2H), 6.98-6.95 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 142.0, 139.2, 135.8, 131.4, 131.1, 128.8, 128.74, 128.67, 128.1, 125.5, 124.6, 123.3, 121.1, 119.9, 111.1.

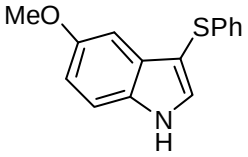
Ethyl 3-(phenylthio)-1H-indole-2-carboxylate (**3a**)[4]



Compound **3a** was obtained in 81% yield as white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.26 (br, 1H), 7.54 (dd, *J* = 8.1 Hz, *J* = 0.9 Hz, 1H), 7.39-7.36 (m, 1H), 7.31-7.25 (m, 1H), 7.10-6.98 (m, 6H), 4.32 (q, *J* = 7.1 Hz, 2H), 1.23 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 161.3, 137.9, 135.7, 130.1, 128.8, 128.7, 127.4,. 126.1, 125.3, 121,7, 121.5, 112.1, 110.5, 61.5, 14.2.

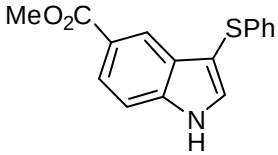
[3] Gou, Y.-J.; Tang, R.-Y.; Li, J.-H.; Zhong, P.; Zhang, X.-G. *Adv. Synth. Catal.* **2009**, *351*, 2615.
[4] Tudge, M.; Tamiya, M.; Savarin,C.; Humphrey, G. R. *Org. Lett.* **2006**, *8*, 565.

5-Methoxy-3-(phenylthio)-1H-indole (3e)[3]



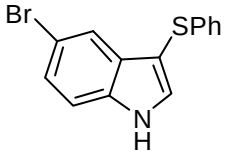
Compound **3e** obtained in 86% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (br, 1H), 7.42 (d, *J* = 2.7 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 1H), 7.18-7.15 (m, 2H), 7.10-7.04 (m, 4H), 6.91 (dd, *J* = 8.8 Hz, *J* = 2.4 Hz, 1H), 3.78 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.1, 139.3, 131.3, 129.9, 128.7, 125.6, 124.7, 113.6, 112.4, 102.1, 100.7, 55.7.

Methyl 3-(phenylthio)-1H-indole-5-carboxylate (3f)[3]



Compound **3f** was obtained in 88% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.81 (br, 1H), 8.38 (s, 1H), 7.97 (dd, *J* = 8.6 Hz, *J* = 1.5 Hz, 1H), 7.54 (d, *J* = 2.5 Hz, 1H), 7.45 (d, *J* = 8.6 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 2H), 7.09-7.05 (m, 3H), 3.89 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.9, 139.1, 138.8, 132.2, 128.9, 128.8, 125.9, 125.0, 124.4, 123.1, 122.4, 111.5, 104.6, 52.0.

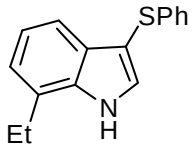
5-Bromo-3-(phenylthio)-1H-indole (3g)[1,5]



Compound **3g** was obtained in 66% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (br, 1H), 7.68 (d, *J* = 1.6 Hz, 1H), 7.40 (d, *J* = 2.5 Hz, 1H), 7.28-7.22 (m, 2H), 7.12-7.09 (m, 2H), 7.01-6.99 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 138.7, 135.1, 131.8, 130.9, 128.8, 126.1, 125.8, 125.0, 122.2, 114.5, 113.0, 102.7.

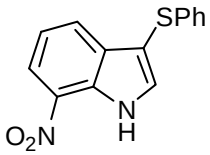
[5] Yadav, J. S.; Reddy, B. V. S.; Reddy, Y. J.; Praneeth, K. *Synthesis* **2009**, 1520.

7-Ethyl-3-(phenylthio)-1H-indole (**3h**)[1,4]



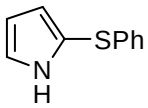
Compound **3h** was obtained in 95% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.27 (br, 1H), 7.40-7.37 (m, 2H), 7.09-7.02 (m, 6H), 6.98-6.95 (m, 1H), 2.81 (q, *J* = 7.6 Hz, 2H), 1.31 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 139.3, 135.3, 130.3, 128.8, 128.6, 126.9, 125.8, 124.7, 121.5, 121.1, 117.3, 103.1, 23.8, 13.8.

7-Nitro-3-(phenylthio)-1H-indole (**3i**)



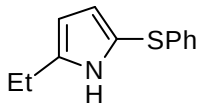
Compound **3i** was obtained in 74% yield as yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.1 (br, 1H), 8.15-8.13 (m, 1H), 7.87 (d, *J* = 7.8 Hz, 1H), 7.62 (d, *J* = 2.5 Hz, 1H), 7.19-7.17 (m, 1H), 7.13-7.10 (m, 2H), 7.03-7.01 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 137.9, 133.4, 132.7, 132.5, 129.9, 128.9, 127.8, 126.3, 125.4, 120.3, 105.6; EIMS *m/z* (%):270 (100), 253 (19), 223 (41); HRMS-(EI) (*m/z*): $[M]^+$ calcd for $C_{14}H_{10}N_2O_2S$, 270.0463; found 270.0461.

2-(Phenylthio)-1H-pyrrole (**3j**)[6]



Compound **3j** was obtained in 88% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (br, 1H), 7.15-7.12 (m, 2H), 7.04-7.00 (m, 1H), 6.95-6.94 (m, 2H), 6.87 (se, *J* = 1.4 Hz, 1H), 6.50 (Hep, *J* = 1.2 Hz, 1H), 6.25 (q, *J* = 3.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 139.1, 128.9, 125.6, 125.3, 121.8, 118.7, 115.5, 110.4.

2-Ethyl-5-(phenylthio)-1H-pyrrole (**3k**)

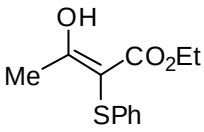


Compound **3k** was obtained in 88% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.91 (br, 1H), 7.16-7.13 (m, 2H), 7.04-7.00 (m,

[6] (a) Gillis, H. M.; Greene, L.; Thompson, A. *Synlett* **2009**, 112. (b) Thamyongkit, P.; Bhise, A. D.; Taniguchi, M.; Lindsey, J. S.; *J. Org. Chem.* **2006**, *71*, 903.

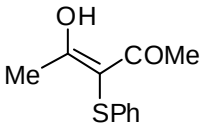
1H), 6.97-6.96 (m, 2H), 6.41 (t, J = 3.0 Hz, 1H), 5.95-5.94 (m, 1H), 2.56 (q, J = 7.6 Hz, 2H), 1.18 (t, J = 7.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 139.7, 138.6, 128.9, 125.5, 125.2, 119.3, 112.9, 106.7, 21.1, 13.3; EIMS *m/z* (%):203 (78), 188 (100); HRMS-(EI) (*m/z*): $[M]^+$ calcd for $C_{12}H_{13}NS$, 203.0769; found 203.0770.

(*E*)-Ethyl 3-hydroxy-2-(phenylthio)but-2-enoate (6a)[7]



$Pd(OAc)_2$ (10 mol%) was employed as the catalyst. The mixture was stirred in 1,2-dichloroethane at room temperature for 2h. Compound **6a** was obtained in 76% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.78 (d, J = 0.5 Hz, 1H), 7.19-7.16 (m, 2H), 7.07-7.03 (m, 3H), 4.14 (q, J = 7.1 Hz, 2H), 2.26 (d, J = 0.5 Hz, 3H), 1.11 (t, J = 7.1 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 184.3, 172.6, 137.8, 128.5, 125.3, 124.8, 61.3, 20.6, 13.7.

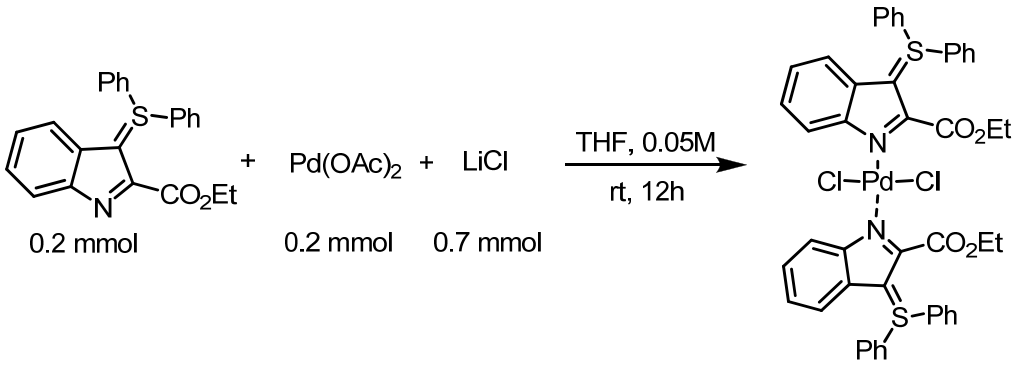
(*E*)-4-hydroxy-3-(phenylthio)pent-3-en-2-one (6b)[8]



$Pd(OAc)_2$ (10 mol%) was employed as the catalyst. The mixture was stirred in 1,2-dichloroethane at room temperature for 2h. The reaction was carried out in 0.2 mmol scale. Compound **6b** was obtained in 83% yield as colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33-7.30 (m, 2H), 7.18-7.12 (m, 3H), 2.37 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 198.3, 137.7, 129.2, 125.2, 124.6, 101.5, 24.4.

[7] Brownbridge, P.; Hunt, P. G.; Warren, S. *J. Chem. Soc. Perkin Trans. I* **1986**, 1695.
[8] Rashid, M. A.; Rasool, N.; Adeel, M.; Reinke, H.; Fischer, C.; Langer, P. *Tetrahedron* **2008**, *64*, 3782.

1.2 Preparation of palladium complex 7



To a solution of ylide (74.6 mg, 0.2 mmol) and $Pd(OAc)_2$ (44.8 mg, 0.2 mmol) in dry THF (2 mL, 0.1M), was added LiCl (30 mg, 0.7 mmol). The mixture was stirred at room temperature for 36h and the solvent was removed under vacuum. The resulting solid was washed carefully with THF, then diethyl ether. The crude yellow solid (89 mg) was re-dissolved by large amount of dichloromethane, filtered, and a portion of the filtrate was used for the preparation of the crystal. NMR of the crude solid: ^{1}H NMR (500 MHz, CD_2Cl_2) δ 9.30 (d, *J* = 8.4 Hz, 2H), 7.72-7.69 (m, 4H), 7.65-7.59 (m, 16H), 7.39 (t, *J* = 7.6 Hz, 2H), 6.98 (t, *J* = 7.6 Hz, 2H), 6.57 (d, *J* = 8.2 Hz, 2H), 4.79 (q, *J* = 7.0 Hz, 4H), 1.63 (t, *J* = 7.10 Hz, 6H); ^{13}C NMR (125 MHz, CD_2Cl_2) δ 163.4, 147.6, 144.9, 133.2, 131.3, 131.1, 129.8, 129.7, 128.8, 128.0, 123.3, 122.8, 122.6, 117.4, 84.6, 62.6, 15.0. EIMS *m/z* (%): 889 (100), 701 (15).

1.3 Crystal structure of the palladium complex 7

Crystals were prepared by slow diffusion of pentane into a solution of **7** in dichloromethane. Several crystals were investigated, all of which contained solute dichloromethane. The results described here stem from the crystal of best quality.

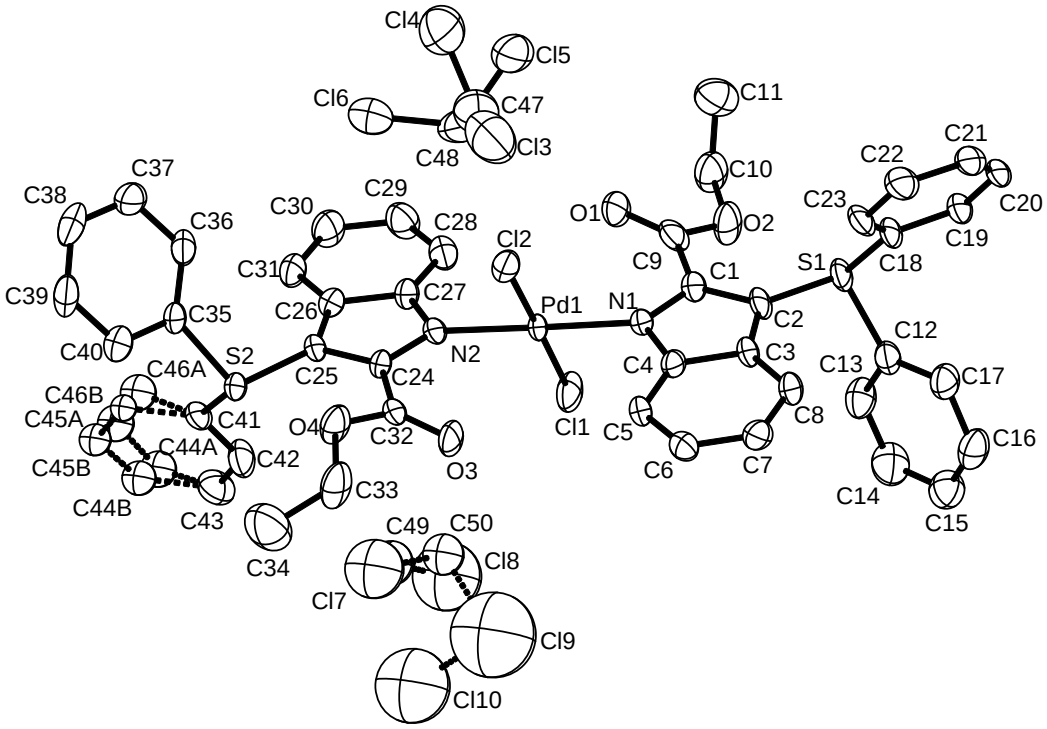


Figure S-1. The molecular structure of **7**. Atomic displacement ellipsoids are shown at the 50% probability level. H atoms omitted for clarity.

Crystal Data for 7: $[C_{46}\,H_{38}\,Cl_2\,N_2\,O_4\,Pd\,S_2] \cdot 3(C\,H_2\,Cl_2)$, M_r = 1178.98 g · mol^{-1}, yellow-orange plate, crystal size 0.06 x 0.14 x 0.23 mm^3, monoclinic, space group *C*2/c, a = 28.301(2) Å, b = 20.495(2) Å, c = 18.092(1) Å, β = 105.211(7)°, V = 10126.3(15) Å^3, T = 100 K, Z = 8, D_{calc} = 1.547 g·cm^3, Mo-K_α radiation, λ = 0.71073 Å, μ = 0.917 mm^{-1},

Gaussian absorption correction (T_{min} = 0.88566, T_{max} = 0.95945), minimum and maximum estimated transmissions from the multi-scan scaling: 0.5513 and 1.0 (SADABS), Bruker AXS Enraf-Nonius KappaCCD diffractometer, 2.81 < θ < 27.10°, 100126 measured reflections, 11175 independent reflections (R_{int} = 0.104), 7729 reflections with $I > 2\sigma(I)$. Structure solved by direct methods and refined by full-matrix least-squares against F^2 to R_1 = 0.0799 [$I > 2\sigma(I)$], wR_2 = 0.2300, 590 parameters (G. M. Sheldrick, *Acta Cryst.* **2008**, *A64*, 112-122). S = 1.530, indicating that on average the standard uncertainties of the intensities are systematically underestimated, residual electron density +1.78 / -1.52 e Å^{-3}. CCDC 894535.

Data were collected to a resolution of 0.78 Å with an average redundancy of almost 9 (see statistics, below). A minimum theta value of 2.81° was chosen in order to avoid possible loss of intensity resulting from the shadow cast by the beamstop. 13 reflections diffract at angles less than this minimum theta value, owing to the large unit cell parameters, and were not included in the data set. Although the face-indexed absorption correction was undertaken with as much care as possible, the observed residual electron density of 1.78 eÅ^{-3}, 0.92 Å from Pd1, may be due to the difficulty of accurately correcting for the effects of X-ray absorption for a thin plate composed of a substance with a relatively high linear absorption coefficient (μ = 0.917 mm^{-1}).

INTENSITY STATISTICS FOR DATASET

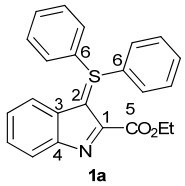
Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	R(int)	Rsigma
Inf - 2.14	576	593	97.1	11.08	22.8	30.75	0.0664	0.0255
2.14 - 1.70	585	585	100.0	11.77	12.1	28.33	0.0628	0.0256
1.70 - 1.48	576	576	100.0	11.69	7.9	24.70	0.0686	0.0278
1.48 - 1.34	615	615	100.0	11.34	6.1	22.32	0.0729	0.0308
1.34 - 1.24	613	613	100.0	10.75	4.8	18.91	0.0843	0.0362
1.24 - 1.16	659	659	100.0	10.24	3.9	15.86	0.0983	0.0433

1.16 - 1.10	612	612	100.0	9.78	3.6	14.23	0.1072	0.0481
1.10 - 1.05	650	650	100.0	9.52	2.8	12.18	0.1254	0.0580
1.05 - 1.01	606	606	100.0	9.10	2.4	10.67	0.1428	0.0681
1.01 - 0.97	709	709	100.0	8.90	2.2	9.21	0.1598	0.0782
0.97 - 0.94	604	604	100.0	8.38	2.0	8.39	0.1749	0.0893
0.94 - 0.91	705	705	100.0	8.26	1.7	7.01	0.1940	0.1066
0.91 - 0.88	781	781	100.0	7.99	1.4	5.61	0.2343	0.1417
0.88 - 0.86	599	599	100.0	7.60	1.2	4.84	0.2737	0.1691
0.86 - 0.84	632	632	100.0	6.71	1.0	3.54	0.3388	0.2363
0.84 - 0.82	759	759	100.0	6.05	1.0	3.35	0.3233	0.2489
0.82 - 0.80	767	767	100.0	5.52	0.9	2.84	0.3444	0.2992
0.80 - 0.78	444	444	100.0	5.20	0.7	2.09	0.4334	0.4348
0.88 - 0.78	3454	3454	100.0	6.35	1.0	3.53	0.3159	0.2446
Inf - 0.78	11492	11509	99.9	8.82	4.1	12.10	0.0981	0.0544

Merged [A], lowest resolution = 7.25 Angstroms, 3194 outliers downweighted

The crystal contains three solute dichloromethane molecules per Pd complex. One of the dichloromethane molecules is badly disordered about a two-fold axis of symmetry. Allocation of atoms was based on chemical intuition. The deepest hole in the residual electron density map is -1.51 $eÅ^{-3}$ at x = 0.0789, y = 0.3393 and z = 0.3834, 0.62 Å from Cl7 in the disordered dichloromethane molecule. One of the phenyl groups on one of the diphenylsulphonium ylide groups in close vicinity to the disordered dichloromethane is also slightly disordered. Disordered atoms were refined with isotropic atomic displacement parameters. H atom positions were calculated and refined using a riding model. Intensities at high 2θ angles are disproportionately weak, presumably owing to loss of solute from the crystal during transfer from solution to the diffractometer at 100 K. The suggested second term for weighting scheme proposed by SHELXL was not adopted, since it would have given too little weight to these weak reflections, which also contain important structural information.

Table S-1. Comparison of selected distances (Å) and angles (°) for the free ligand **1a** and the Pd complex **7**.



1a

bond	isolated ligand (CSD refcode LAFTAP)[1]	Pd complex **7**
N=C1	1.336(1)	1.342(6)[a]
C1-C2	1.424(1)	1.414(4)[a]
C2=S	1.710(1)	1.721(11)[a]
S-C6 (Ph)	1.790(4)[a]	1.799(5)[a]
C1-C5 (O_2Et)	1.482(2)	1.481(23)[a]
C2-C3	1.434(1)	1.419(24)[a]
C3-C4	1.426(1)	1.415(4)[a]
N-C4	1.378(1)	1.395(8)[a]
C4-N-C1	105.43(8)	107.8(2)
N-C1-C2	112.62(9)	110.0(2)
C1-C2-C3	105.68(8)	107.3(2)[a]

[a] Average value. [1] Reference 1.

Table S-2. Atomic coordinates and equivalent isotropic displacement parameters (Å²).

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
C(1)	0.1068(2)	0.8882(2)	0.2069(3)	0.032(1)
C(2)	0.1079(2)	0.9564(2)	0.1968(3)	0.031(1)
C(3)	0.1295(2)	0.9679(2)	0.1367(3)	0.030(1)
C(4)	0.1402(2)	0.9056(2)	0.1119(3)	0.029(1)
C(5)	0.1606(2)	0.8969(3)	0.0507(3)	0.034(1)
C(6)	0.1713(2)	0.9524(3)	0.0151(3)	0.038(1)
C(7)	0.1627(2)	1.0151(3)	0.0388(3)	0.037(1)
C(8)	0.1412(2)	1.0238(3)	0.0991(3)	0.035(1)
C(9)	0.0904(2)	0.8480(3)	0.2647(3)	0.038(1)
C(10)	0.0410(3)	0.8415(3)	0.3503(4)	0.053(2)
C(11)	0.0765(3)	0.8467(4)	0.4264(4)	0.061(2)
C(12)	0.0392(2)	1.0544(3)	0.1671(3)	0.035(1)
C(13)	-0.0004(2)	1.0179(3)	0.1273(4)	0.046(2)
C(14)	-0.0332(3)	1.0451(4)	0.0647(4)	0.059(2)
C(15)	-0.0262(2)	1.1086(3)	0.0421(4)	0.051(2)
C(16)	0.0117(2)	1.1440(3)	0.0827(4)	0.049(2)
C(17)	0.0460(2)	1.1181(3)	0.1468(4)	0.041(1)
C(18)	0.1249(2)	1.0716(2)	0.2883(3)	0.034(1)
C(19)	0.1077(3)	1.1218(3)	0.3277(3)	0.040(1)
C(20)	0.1413(3)	1.1675(3)	0.3650(3)	0.045(2)
C(21)	0.1906(3)	1.1637(3)	0.3648(3)	0.045(2)
C(22)	0.2069(3)	1.1128(3)	0.3273(4)	0.045(2)
C(23)	0.1732(2)	1.0661(3)	0.2881(3)	0.041(2)
C(24)	0.1484(2)	0.6318(2)	0.0722(3)	0.029(1)
C(25)	0.1444(2)	0.5637(2)	0.0823(3)	0.027(1)
C(26)	0.1187(2)	0.5544(3)	0.1402(3)	0.033(1)
C(27)	0.1088(2)	0.6185(2)	0.1616(3)	0.032(1)
C(28)	0.0840(2)	0.6298(3)	0.2169(3)	0.041(1)
C(29)	0.0688(2)	0.5754(3)	0.2506(4)	0.046(2)

C(30)	0.0783(2)	0.5116(3)	0.2302(4)	0.046(2)
C(31)	0.1021(2)	0.5010(3)	0.1743(3)	0.038(1)
C(32)	0.1680(2)	0.6674(2)	0.0166(3)	0.033(1)
C(33)	0.2097(3)	0.6520(3)	-0.0811(4)	0.057(2)
C(34)	0.2043(4)	0.5951(5)	-0.1352(5)	0.095(3)
C(35)	0.2104(2)	0.4578(2)	0.0837(3)	0.032(1)
C(36)	0.2196(2)	0.4533(3)	0.1610(4)	0.040(1)
C(37)	0.2575(2)	0.4109(3)	0.2003(4)	0.047(2)
C(38)	0.2826(2)	0.3750(3)	0.1592(4)	0.046(2)
C(39)	0.2743(3)	0.3827(3)	0.0811(4)	0.049(2)
C(40)	0.2375(2)	0.4247(3)	0.0421(4)	0.045(2)
C(41)	0.1106(2)	0.4520(3)	-0.0010(3)	0.035(1)
C(42)	0.0658(2)	0.4798(3)	-0.0334(4)	0.043(2)
C(43)	0.0253(2)	0.4415(3)	-0.0603(4)	0.050(2)
C(44B)	0.0349(6)	0.3710(8)	-0.0620(10)	0.043(4)
C(44A)	0.0235(7)	0.3811(8)	-0.0471(10)	0.048(4)
C(45A)	0.0661(6)	0.3518(7)	-0.0106(10)	0.049(4)
C(45B)	0.0811(5)	0.3442(6)	-0.0347(8)	0.037(4)
C(46A)	0.1097(6)	0.3885(7)	0.0172(11)	0.047(4)
C(46B)	0.1214(5)	0.3845(5)	-0.0042(8)	0.025(3)
C(47)	0.3203(4)	0.7505(5)	0.3286(6)	0.089(3)
C(48)	0.1871(4)	0.6711(4)	0.3397(5)	0.082(3)
C(49)	0.0354(6)	0.6315(9)	-0.1239(11)	0.073(5)
C(50)	0.0390(5)	0.6811(8)	-0.1084(9)	0.062(4)
Cl(1)	0.0445(1)	0.7635(1)	0.0872(1)	0.047(1)
Cl(2)	0.2124(1)	0.7602(1)	0.1834(1)	0.038(1)
Cl(3)	0.3643(2)	0.7937(2)	0.2929(2)	0.141(1)
Cl(4)	0.3465(1)	0.7117(1)	0.4091(2)	0.096(1)
Cl(5)	0.2099(1)	0.7125(1)	0.4209(1)	0.089(1)
Cl(6)	0.2215(1)	0.5996(1)	0.3305(1)	0.089(1)
Cl(7)	0.0784(2)	0.6399(3)	-0.1416(3)	0.128(2)
Cl(8)	-0.0142(3)	0.6619(5)	-0.1211(6)	0.176(3)
Cl(9)	0.0263(5)	0.7416(6)	-0.1886(8)	0.271(6)
Cl(10)	0.0000	0.6639(10)	-0.2500	0.206(7)
N(1)	0.1266(2)	0.8579(2)	0.1568(2)	0.028(1)
N(2)	0.1275(2)	0.6642(2)	0.1201(2)	0.030(1)

O(1)	0.1054(2)	0.7945(2)	0.2834(2)	0.046(1)
O(2)	0.0581(2)	0.8788(2)	0.2919(3)	0.049(1)
O(3)	0.1580(2)	0.7222(2)	-0.0035(3)	0.055(1)
O(4)	0.1975(2)	0.6296(2)	-0.0111(3)	0.045(1)
Pd(1)	0.1281(1)	0.7614(1)	0.1372(1)	0.028(1)
S(1)	0.0803(1)	1.0115(1)	0.2445(1)	0.033(1)
S(2)	0.1621(1)	0.5070(1)	0.0254(1)	0.030(1)

Table S-3. Selected bond lengths [Å] and angles [°].

C(1)-N(1)	1.337(7)	C(1)-C(2)	1.410(7)
C(1)-C(9)	1.497(8)	C(2)-C(3)	1.402(7)
C(2)-S(1)	1.728(5)	C(3)-C(4)	1.411(7)
C(3)-C(8)	1.415(7)	C(4)-C(5)	1.388(8)
C(4)-N(1)	1.388(7)	C(5)-C(6)	1.381(8)
C(5)-H(5)	0.9500	C(6)-C(7)	1.395(8)
C(6)-H(6)	0.9500	C(7)-C(8)	1.394(8)
C(7)-H(7)	0.9500	C(8)-H(8)	0.9500
C(9)-O(1)	1.193(7)	C(9)-O(2)	1.308(7)
C(10)-C(11)	1.480(10)	C(10)-O(2)	1.484(7)
C(10)-H(10A)	0.9900	C(10)-H(10B)	0.9900
C(11)-H(11B)	0.9800	C(11)-H(11C)	0.9800
C(11)-H(11A)	0.9800	C(12)-C(13)	1.381(8)
C(12)-C(17)	1.382(8)	C(12)-S(1)	1.798(6)
C(13)-C(14)	1.380(9)	C(13)-H(13)	0.9500
C(14)-C(15)	1.395(10)	C(14)-H(14)	0.9500
C(15)-C(16)	1.341(9)	C(15)-H(15)	0.9500
C(16)-C(17)	1.408(9)	C(16)-H(16)	0.9500
C(17)-H(17)	0.9500	C(18)-C(23)	1.375(9)
C(18)-C(19)	1.407(7)	C(18)-S(1)	1.792(5)
C(19)-C(20)	1.379(8)	C(19)-H(19)	0.9500
C(20)-C(21)	1.399(10)	C(20)-H(20)	0.9500
C(21)-C(22)	1.389(9)	C(21)-H(21)	0.9500
C(22)-C(23)	1.404(8)	C(22)-H(22)	0.9500
C(23)-H(23)	0.9500	C(24)-N(2)	1.346(7)
C(24)-C(25)	1.416(7)	C(24)-C(32)	1.465(7)
C(25)-C(26)	1.438(7)	C(25)-S(2)	1.713(5)
C(26)-C(31)	1.397(8)	C(26)-C(27)	1.418(7)
C(27)-C(28)	1.383(8)	C(27)-N(2)	1.389(7)
C(28)-C(29)	1.392(8)	C(28)-H(28)	0.9500
C(29)-C(30)	1.404(9)	C(29)-H(29)	0.9500
C(30)-C(31)	1.371(8)	C(30)-H(30)	0.9500
C(31)-H(31)	0.9500	C(32)-O(3)	1.191(6)
C(32)-O(4)	1.329(7)	C(33)-O(4)	1.471(7)

C(33)-C(34)	1.504(11)	C(33)-H(33B)	0.9900
C(33)-H(33A)	0.9900	C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800	C(34)-H(34A)	0.9800
C(35)-C(36)	1.356(8)	C(35)-C(40)	1.386(8)
C(35)-S(2)	1.799(6)	C(36)-C(37)	1.418(8)
C(36)-H(36)	0.9500	C(37)-C(38)	1.371(9)
C(37)-H(37)	0.9500	C(38)-C(39)	1.379(10)
C(38)-H(38)	0.9500	C(39)-C(40)	1.392(9)
C(39)-H(39)	0.9500	C(40)-H(40)	0.9500
C(41)-C(46A)	1.343(15)	C(41)-C(42)	1.373(8)
C(41)-C(46B)	1.421(12)	C(41)-S(2)	1.806(6)
C(42)-C(43)	1.368(8)	C(42)-H(42)	0.9500
C(43)-C(44A)	1.265(17)	C(43)-C(44B)	1.474(17)
C(43)-H(43)	0.9500	C(44B)-C(45B)	1.38(2)
C(44B)-H(44)	0.9500	C(44A)-C(45A)	1.35(2)
C(44A)-H(44A)	0.9500	C(45A)-C(46A)	1.42(2)
C(45A)-H(45)	0.9500	C(45B)-C(46B)	1.399(16)
C(45B)-H(45A)	0.9500	C(46A)-H(46)	0.9500
C(46B)-H(46A)	0.9500	C(47)-Cl(4)	1.655(10)
C(47)-Cl(3)	1.779(11)	C(47)-H(47B)	0.9900
C(47)-H(47A)	0.9900	C(48)-Cl(5)	1.672(9)
C(48)-Cl(6)	1.793(10)	C(48)-H(48B)	0.9900
C(48)-H(48A)	0.9900	C(49)-Cl(7)	1.348(17)
C(49)-Cl(8)	1.549(18)	C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900	C(50)-Cl(8)	1.516(17)
C(50)-Cl(7)	1.633(16)	C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900	Cl(1)-Pd(1)	2.3010(16)
Cl(2)-Pd(1)	2.3131(15)	Cl(8)-Cl(10)	2.470(10)
Cl(9)-Cl(9)#1	2.33(3)	Cl(10)-Cl(8)#1	2.470(10)
N(1)-Pd(1)	2.013(4)	N(2)-Pd(1)	2.015(4)

N(1)-C(1)-C(2)	110.2(5)	N(1)-C(1)-C(9)	118.7(5)
C(2)-C(1)-C(9)	131.0(5)	C(3)-C(2)-C(1)	107.2(5)
C(3)-C(2)-S(1)	128.7(4)	C(1)-C(2)-S(1)	123.7(4)
C(2)-C(3)-C(4)	105.5(5)	C(2)-C(3)-C(8)	135.5(5)
C(4)-C(3)-C(8)	119.0(5)	C(5)-C(4)-N(1)	127.8(5)

C(5)-C(4)-C(3)	122.6(5)	N(1)-C(4)-C(3)	109.7(5)
C(6)-C(5)-C(4)	117.0(5)	C(6)-C(5)-H(5)	121.5
C(4)-C(5)-H(5)	121.5	C(5)-C(6)-C(7)	122.6(5)
C(5)-C(6)-H(6)	118.7	C(7)-C(6)-H(6)	118.7
C(8)-C(7)-C(6)	120.4(5)	C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8	C(7)-C(8)-C(3)	118.5(5)
C(7)-C(8)-H(8)	120.8	C(3)-C(8)-H(8)	120.8
O(1)-C(9)-O(2)	124.6(6)	O(1)-C(9)-C(1)	123.5(5)
O(2)-C(9)-C(1)	111.9(5)	C(11)-C(10)-O(2)	110.9(6)
C(11)-C(10)-H(10A)	109.5	O(2)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10B)	109.5	O(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1	C(10)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5	H(11B)-C(11)-H(11C)	109.5
C(10)-C(11)-H(11A)	109.5	H(11B)-C(11)-H(11A)	109.5
H(11C)-C(11)-H(11A)	109.5	C(13)-C(12)-C(17)	121.5(6)
C(13)-C(12)-S(1)	114.3(4)	C(17)-C(12)-S(1)	124.1(5)
C(14)-C(13)-C(12)	119.3(6)	C(14)-C(13)-H(13)	120.3
C(12)-C(13)-H(13)	120.3	C(13)-C(14)-C(15)	120.0(6)
C(13)-C(14)-H(14)	120.0	C(15)-C(14)-H(14)	120.0
C(16)-C(15)-C(14)	119.9(7)	C(16)-C(15)-H(15)	120.0
C(14)-C(15)-H(15)	120.0	C(15)-C(16)-C(17)	121.8(6)
C(15)-C(16)-H(16)	119.1	C(17)-C(16)-H(16)	119.1
C(12)-C(17)-C(16)	117.4(6)	C(12)-C(17)-H(17)	121.3
C(16)-C(17)-H(17)	121.3	C(23)-C(18)-C(19)	122.5(5)
C(23)-C(18)-S(1)	121.9(4)	C(19)-C(18)-S(1)	115.4(5)
C(20)-C(19)-C(18)	117.4(6)	C(20)-C(19)-H(19)	121.3
C(18)-C(19)-H(19)	121.3	C(19)-C(20)-C(21)	121.4(6)
C(19)-C(20)-H(20)	119.3	C(21)-C(20)-H(20)	119.3
C(22)-C(21)-C(20)	120.2(6)	C(22)-C(21)-H(21)	119.9
C(20)-C(21)-H(21)	119.9	C(21)-C(22)-C(23)	119.4(6)
C(21)-C(22)-H(22)	120.3	C(23)-C(22)-H(22)	120.3
C(18)-C(23)-C(22)	119.1(5)	C(18)-C(23)-H(23)	120.4
C(22)-C(23)-H(23)	120.4	N(2)-C(24)-C(25)	109.9(5)
N(2)-C(24)-C(32)	120.5(4)	C(25)-C(24)-C(32)	129.5(5)
C(24)-C(25)-C(26)	107.3(4)	C(24)-C(25)-S(2)	123.1(4)
C(26)-C(25)-S(2)	129.2(4)	C(31)-C(26)-C(27)	119.5(5)

C(31)-C(26)-C(25)	135.9(5)	C(27)-C(26)-C(25)	104.5(5)
C(28)-C(27)-N(2)	128.0(5)	C(28)-C(27)-C(26)	121.7(5)
N(2)-C(27)-C(26)	110.3(5)	C(27)-C(28)-C(29)	117.2(5)
C(27)-C(28)-H(28)	121.4	C(29)-C(28)-H(28)	121.4
C(28)-C(29)-C(30)	121.8(6)	C(28)-C(29)-H(29)	119.1
C(30)-C(29)-H(29)	119.1	C(31)-C(30)-C(29)	120.5(6)
C(31)-C(30)-H(30)	119.8	C(29)-C(30)-H(30)	119.8
C(30)-C(31)-C(26)	119.2(5)	C(30)-C(31)-H(31)	120.4
C(26)-C(31)-H(31)	120.4	O(3)-C(32)-O(4)	123.9(5)
O(3)-C(32)-C(24)	125.1(5)	O(4)-C(32)-C(24)	111.0(4)
O(4)-C(33)-C(34)	108.2(5)	O(4)-C(33)-H(33B)	110.1
C(34)-C(33)-H(33B)	110.1	O(4)-C(33)-H(33A)	110.1
C(34)-C(33)-H(33A)	110.1	H(33B)-C(33)-H(33A)	108.4
C(33)-C(34)-H(34B)	109.5	C(33)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5	C(33)-C(34)-H(34A)	109.5
H(34B)-C(34)-H(34A)	109.5	H(34C)-C(34)-H(34A)	109.5
C(36)-C(35)-C(40)	122.8(5)	C(36)-C(35)-S(2)	123.7(4)
C(40)-C(35)-S(2)	113.5(4)	C(35)-C(36)-C(37)	118.4(5)
C(35)-C(36)-H(36)	120.8	C(37)-C(36)-H(36)	120.8
C(38)-C(37)-C(36)	119.2(6)	C(38)-C(37)-H(37)	120.4
C(36)-C(37)-H(37)	120.4	C(37)-C(38)-C(39)	121.4(6)
C(37)-C(38)-H(38)	119.3	C(39)-C(38)-H(38)	119.3
C(38)-C(39)-C(40)	119.6(6)	C(38)-C(39)-H(39)	120.2
C(40)-C(39)-H(39)	120.2	C(35)-C(40)-C(39)	118.4(6)
C(35)-C(40)-H(40)	120.8	C(39)-C(40)-H(40)	120.8
C(46A)-C(41)-C(42)	115.7(9)	C(42)-C(41)-C(46B)	124.9(7)
C(46A)-C(41)-S(2)	127.2(8)	C(42)-C(41)-S(2)	116.4(4)
C(46B)-C(41)-S(2)	116.7(6)	C(43)-C(42)-C(41)	120.4(6)
C(43)-C(42)-H(42)	119.8	C(41)-C(42)-H(42)	119.8
C(44A)-C(43)-C(42)	124.5(10)	C(42)-C(43)-C(44B)	115.4(8)
C(44A)-C(43)-H(43)	117.8	C(42)-C(43)-H(43)	117.8
C(44B)-C(43)-H(43)	123.3	C(45B)-C(44B)-C(43)	122.9(12)
C(45B)-C(44B)-H(44)	118.5	C(43)-C(44B)-H(44)	118.5
C(43)-C(44A)-C(45A)	116.7(14)	C(43)-C(44A)-H(44A)	121.6
C(45A)-C(44A)-H(44A)	121.6	C(44A)-C(45A)-C(46A)	121.2(14)
C(44A)-C(45A)-H(45)	119.4	C(46A)-C(45A)-H(45)	119.4

C(44B)-C(45B)-C(46B)	120.3(12)	C(44B)-C(45B)-H(45A)	119.9
C(46B)-C(45B)-H(45A)	119.9	C(41)-C(46A)-C(45A)	119.7(13)
C(41)-C(46A)-H(46)	120.1	C(45A)-C(46A)-H(46)	120.1
C(45B)-C(46B)-C(41)	115.3(10)	C(45B)-C(46B)-H(46A)	122.4
C(41)-C(46B)-H(46A)	122.4	Cl(4)-C(47)-Cl(3)	111.4(6)
Cl(4)-C(47)-H(47B)	109.4	Cl(3)-C(47)-H(47B)	109.4
Cl(4)-C(47)-H(47A)	109.4	Cl(3)-C(47)-H(47A)	109.4
H(47B)-C(47)-H(47A)	108.0	Cl(5)-C(48)-Cl(6)	113.7(5)
Cl(5)-C(48)-H(48B)	108.8	Cl(6)-C(48)-H(48B)	108.8
Cl(5)-C(48)-H(48A)	108.8	Cl(6)-C(48)-H(48A)	108.8
H(48B)-C(48)-H(48A)	107.7	Cl(7)-C(49)-Cl(8)	147.1(15)
Cl(7)-C(49)-H(49A)	100.0	Cl(8)-C(49)-H(49A)	100.0
Cl(7)-C(49)-H(49B)	100.0	Cl(8)-C(49)-H(49B)	100.0
H(49A)-C(49)-H(49B)	104.2	Cl(8)-C(50)-Cl(7)	123.9(12)
Cl(8)-C(50)-H(50A)	106.4	Cl(7)-C(50)-H(50A)	106.4
Cl(8)-C(50)-H(50B)	106.4	Cl(7)-C(50)-H(50B)	106.4
H(50A)-C(50)-H(50B)	106.4	C(50)-Cl(8)-Cl(10)	74.7(7)
C(49)-Cl(8)-Cl(10)	66.5(8)	Cl(8)-Cl(10)-Cl(8)#1	178.1(11)
C(1)-N(1)-C(4)	107.4(4)	C(1)-N(1)-Pd(1)	127.4(4)
C(4)-N(1)-Pd(1)	124.6(3)	C(24)-N(2)-C(27)	108.1(4)
C(24)-N(2)-Pd(1)	126.8(3)	C(27)-N(2)-Pd(1)	124.9(3)
C(9)-O(2)-C(10)	114.2(5)	C(32)-O(4)-C(33)	117.0(4)
N(1)-Pd(1)-N(2)	177.66(18)	N(1)-Pd(1)-Cl(1)	89.07(13)
N(2)-Pd(1)-Cl(1)	89.58(13)	N(1)-Pd(1)-Cl(2)	90.75(13)
N(2)-Pd(1)-Cl(2)	90.66(13)	Cl(1)-Pd(1)-Cl(2)	178.05(6)
C(2)-S(1)-C(18)	108.2(3)	C(2)-S(1)-C(12)	102.4(3)
C(18)-S(1)-C(12)	104.2(3)	C(25)-S(2)-C(35)	108.9(3)
C(25)-S(2)-C(41)	103.9(3)	C(35)-S(2)-C(41)	104.0(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z-1/2

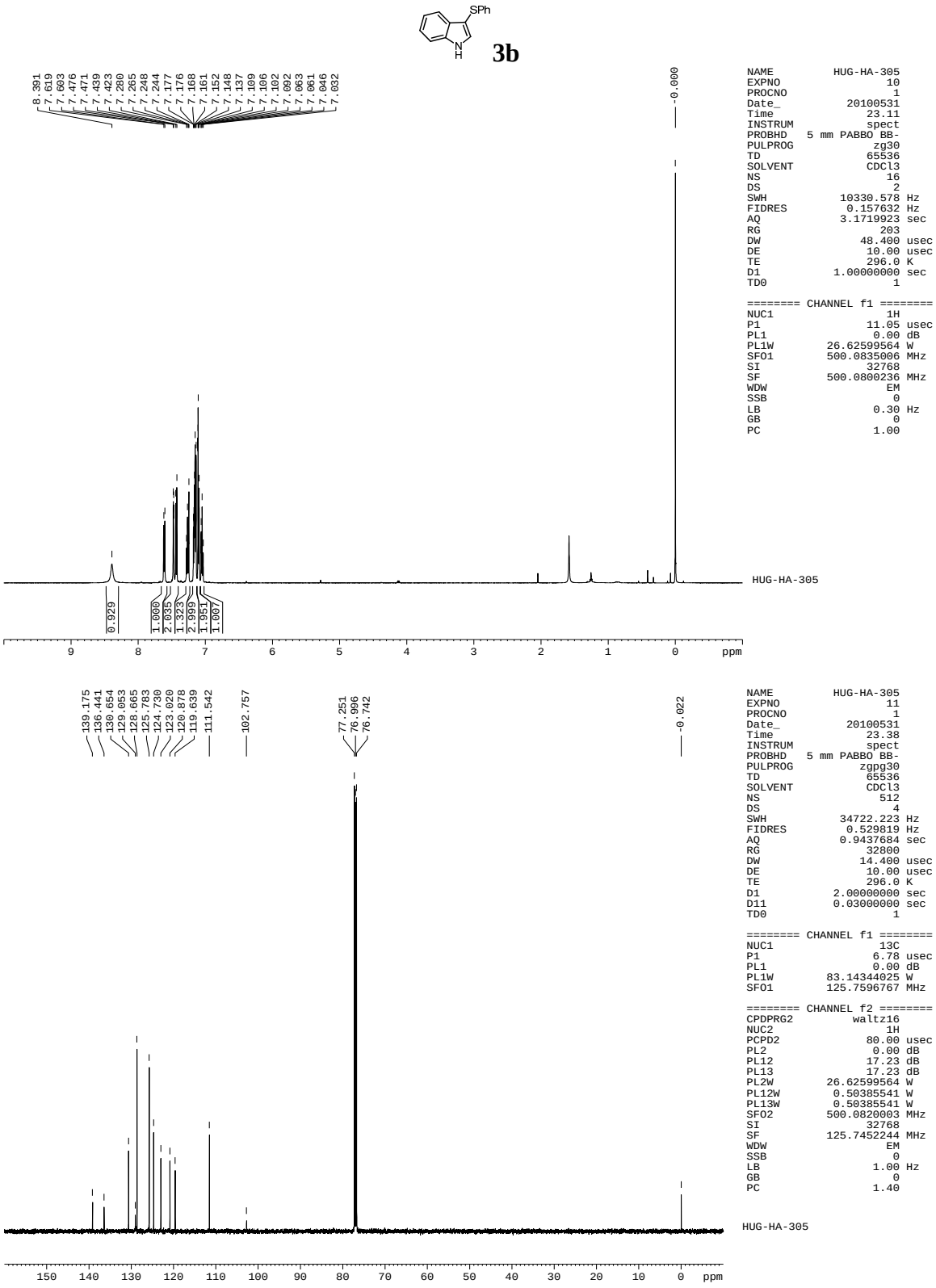
Table S-4. Anisotropic displacement parameters (Å^2).

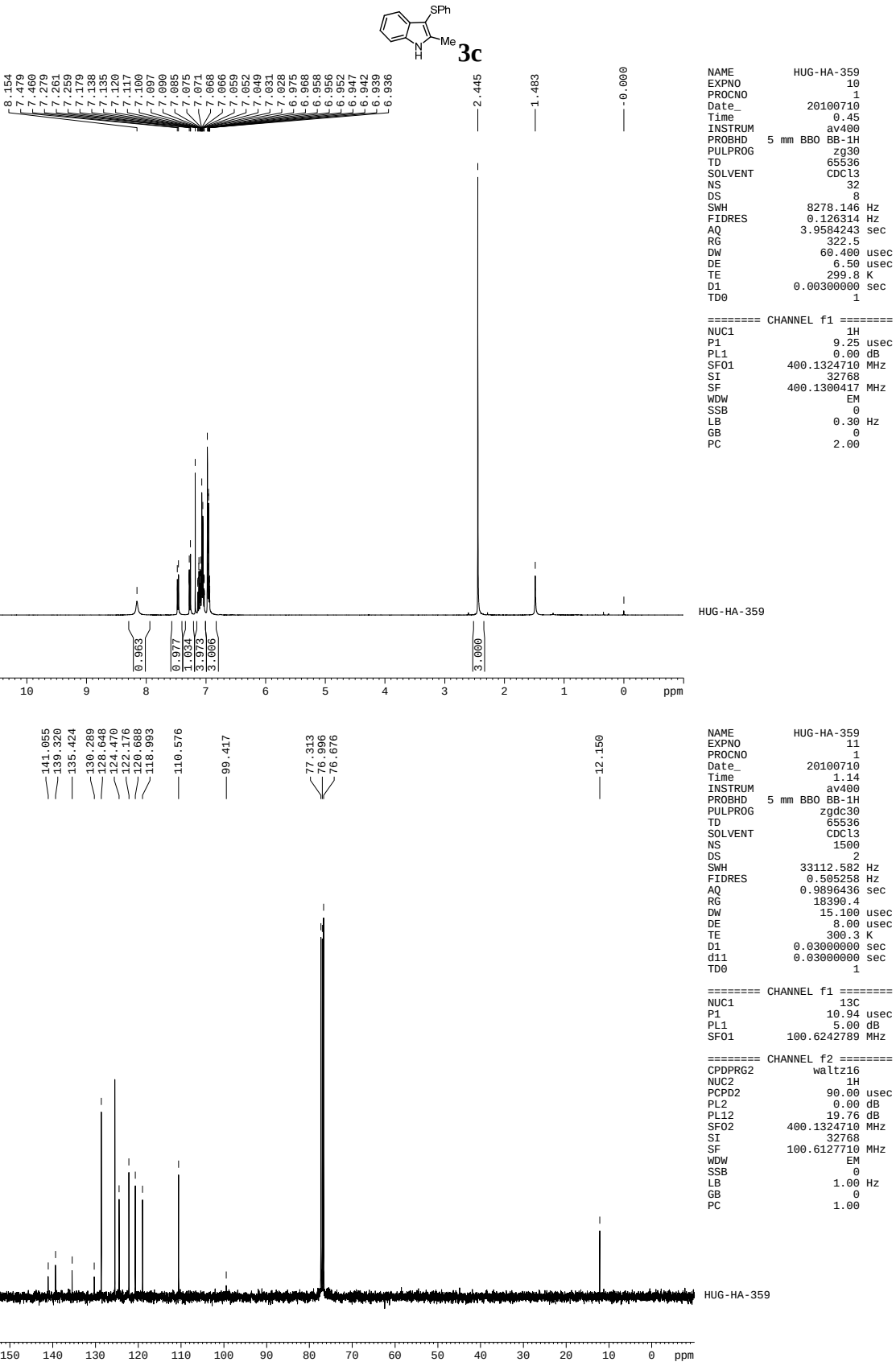
The anisotropic displacement factor exponent takes the form:
$-2\pi^2[\ h^2a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	0.044(3)	0.020(3)	0.032(3)	-0.003(2)	0.007(3)	-0.001(2)
C(2)	0.044(3)	0.016(2)	0.034(3)	-0.010(2)	0.009(3)	-0.006(2)
C(3)	0.040(3)	0.017(2)	0.031(3)	-0.007(2)	0.007(2)	-0.002(2)
C(4)	0.034(3)	0.018(2)	0.030(3)	-0.001(2)	0.001(2)	-0.002(2)
C(5)	0.048(4)	0.020(3)	0.031(3)	-0.006(2)	0.006(3)	0.004(2)
C(6)	0.052(4)	0.033(3)	0.029(3)	-0.002(2)	0.014(3)	0.003(3)
C(7)	0.051(4)	0.026(3)	0.033(3)	0.004(2)	0.008(3)	-0.004(2)
C(8)	0.047(3)	0.018(3)	0.039(3)	-0.006(2)	0.007(3)	-0.003(2)
C(9)	0.049(4)	0.032(3)	0.032(3)	-0.012(2)	0.009(3)	-0.008(3)
C(10)	0.072(5)	0.036(3)	0.058(5)	0.006(3)	0.029(4)	0.002(3)
C(11)	0.077(5)	0.059(5)	0.049(4)	0.002(3)	0.019(4)	-0.017(4)
C(12)	0.042(3)	0.025(3)	0.039(3)	-0.005(2)	0.013(3)	0.001(2)
C(13)	0.042(4)	0.031(3)	0.064(4)	-0.002(3)	0.012(3)	-0.002(3)
C(14)	0.043(4)	0.053(4)	0.072(5)	-0.012(4)	0.001(4)	-0.003(3)
C(15)	0.046(4)	0.049(4)	0.056(4)	-0.001(3)	0.011(3)	0.004(3)
C(16)	0.059(4)	0.031(3)	0.061(4)	0.010(3)	0.023(4)	0.004(3)
C(17)	0.046(4)	0.027(3)	0.048(4)	-0.001(3)	0.009(3)	-0.002(3)
C(18)	0.056(4)	0.014(2)	0.031(3)	-0.006(2)	0.011(3)	-0.005(2)
C(19)	0.064(4)	0.021(3)	0.031(3)	-0.005(2)	0.009(3)	0.000(3)
C(20)	0.085(5)	0.018(3)	0.026(3)	-0.006(2)	0.002(3)	0.001(3)
C(21)	0.073(5)	0.021(3)	0.032(3)	-0.003(2)	-0.003(3)	-0.012(3)
C(22)	0.057(4)	0.036(3)	0.038(4)	-0.003(3)	0.006(3)	-0.008(3)
C(23)	0.069(5)	0.024(3)	0.029(3)	-0.010(2)	0.014(3)	-0.006(3)
C(24)	0.042(3)	0.015(2)	0.029(3)	0.001(2)	0.005(2)	0.003(2)
C(25)	0.039(3)	0.017(2)	0.025(3)	-0.004(2)	0.007(2)	0.001(2)
C(26)	0.044(3)	0.023(3)	0.031(3)	0.003(2)	0.007(3)	0.004(2)
C(27)	0.041(3)	0.018(2)	0.034(3)	-0.001(2)	0.007(3)	-0.001(2)
C(28)	0.053(4)	0.032(3)	0.040(4)	-0.004(3)	0.015(3)	0.004(3)
C(29)	0.059(4)	0.043(4)	0.043(4)	-0.005(3)	0.023(3)	-0.002(3)
C(30)	0.061(4)	0.033(3)	0.049(4)	0.007(3)	0.023(3)	-0.002(3)

C(31)	0.051(4)	0.023(3)	0.041(3)	0.003(2)	0.014(3)	0.003(2)
C(32)	0.052(4)	0.019(3)	0.024(3)	-0.005(2)	0.003(3)	0.001(2)
C(33)	0.081(5)	0.031(3)	0.075(5)	0.019(3)	0.051(4)	0.008(3)
C(34)	0.153(10)	0.074(6)	0.068(6)	-0.005(5)	0.047(6)	-0.009(6)
C(35)	0.042(3)	0.016(2)	0.036(3)	-0.002(2)	0.007(3)	0.001(2)
C(36)	0.050(4)	0.024(3)	0.046(4)	-0.003(3)	0.015(3)	0.007(3)
C(37)	0.061(4)	0.031(3)	0.041(4)	0.002(3)	0.001(3)	-0.002(3)
C(38)	0.032(3)	0.025(3)	0.076(5)	0.007(3)	0.005(3)	0.004(2)
C(39)	0.060(4)	0.026(3)	0.065(5)	-0.001(3)	0.023(4)	0.011(3)
C(40)	0.057(4)	0.028(3)	0.048(4)	0.003(3)	0.012(3)	0.004(3)
C(41)	0.053(4)	0.021(3)	0.027(3)	-0.005(2)	0.005(3)	-0.006(2)
C(42)	0.041(4)	0.029(3)	0.055(4)	-0.014(3)	0.004(3)	0.001(3)
C(43)	0.047(4)	0.052(4)	0.045(4)	-0.012(3)	0.002(3)	-0.006(3)
C(47)	0.085(7)	0.086(7)	0.077(7)	-0.016(5)	-0.012(5)	0.014(5)
C(48)	0.101(7)	0.073(6)	0.053(5)	0.015(4)	-0.014(5)	-0.008(5)
Cl(1)	0.043(1)	0.021(1)	0.067(1)	-0.007(1)	-0.002(1)	0.000(1)
Cl(2)	0.043(1)	0.027(1)	0.040(1)	0.002(1)	0.005(1)	0.005(1)
Cl(3)	0.246(4)	0.095(2)	0.086(2)	-0.014(2)	0.049(3)	0.010(2)
Cl(4)	0.106(2)	0.072(2)	0.094(2)	-0.012(1)	-0.001(2)	0.000(1)
Cl(5)	0.150(2)	0.043(1)	0.057(1)	0.007(1)	-0.001(1)	-0.007(1)
Cl(6)	0.138(2)	0.079(2)	0.045(1)	-0.002(1)	0.014(1)	0.017(1)
N(1)	0.037(3)	0.019(2)	0.025(2)	-0.003(2)	0.002(2)	0.002(2)
N(2)	0.046(3)	0.017(2)	0.024(2)	-0.004(2)	0.003(2)	-0.002(2)
O(1)	0.074(3)	0.021(2)	0.043(3)	0.001(2)	0.016(2)	-0.004(2)
O(2)	0.071(3)	0.024(2)	0.064(3)	0.005(2)	0.037(3)	0.000(2)
O(3)	0.109(4)	0.021(2)	0.042(3)	0.011(2)	0.032(3)	0.017(2)
O(4)	0.060(3)	0.029(2)	0.054(3)	0.013(2)	0.028(2)	0.005(2)
Pd(1)	0.043(1)	0.012(1)	0.025(1)	-0.003(1)	0.004(1)	0.002(1)
S(1)	0.049(1)	0.016(1)	0.036(1)	-0.008(1)	0.015(1)	-0.003(1)
S(2)	0.045(1)	0.015(1)	0.028(1)	-0.001(1)	0.007(1)	0.000(1)

Part II NMR spectra

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7.117
7.100
7.097
7.090
7.085
7.075
7.071
7.068
7.066
7.059
7.052
7.049
7.031
7.028
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6.952
6.947
6.942
6.939
6.936
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PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 8
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.50 usec
TE 299.8 K
D1 0.00300000 sec
TD0 1
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NUC1 1H
P1 9.25 usec
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SFO1 400.1324710 MHz
SI 32768
SF 400.1300417 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 2.00
141.055
139.320
135.424
130.289
128.648
124.470
122.176
120.688
118.993
110.576
99.417
77.313
76.996
76.676
12.150
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PULPROG zgdc30
TD 65536
SOLVENT CDCl3
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FIDRES 0.505258 Hz
AQ 0.9896436 sec
RG 18390.4
DW 15.100 usec
DE 8.00 usec
TE 300.3 K
D1 0.03000000 sec
d11 0.03000000 sec
TD0 1
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NUC1 13C
P1 10.94 usec
PL1 5.00 dB
SFO1 100.6242789 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 19.76 dB
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SI 32768
SF 100.6127710 MHz
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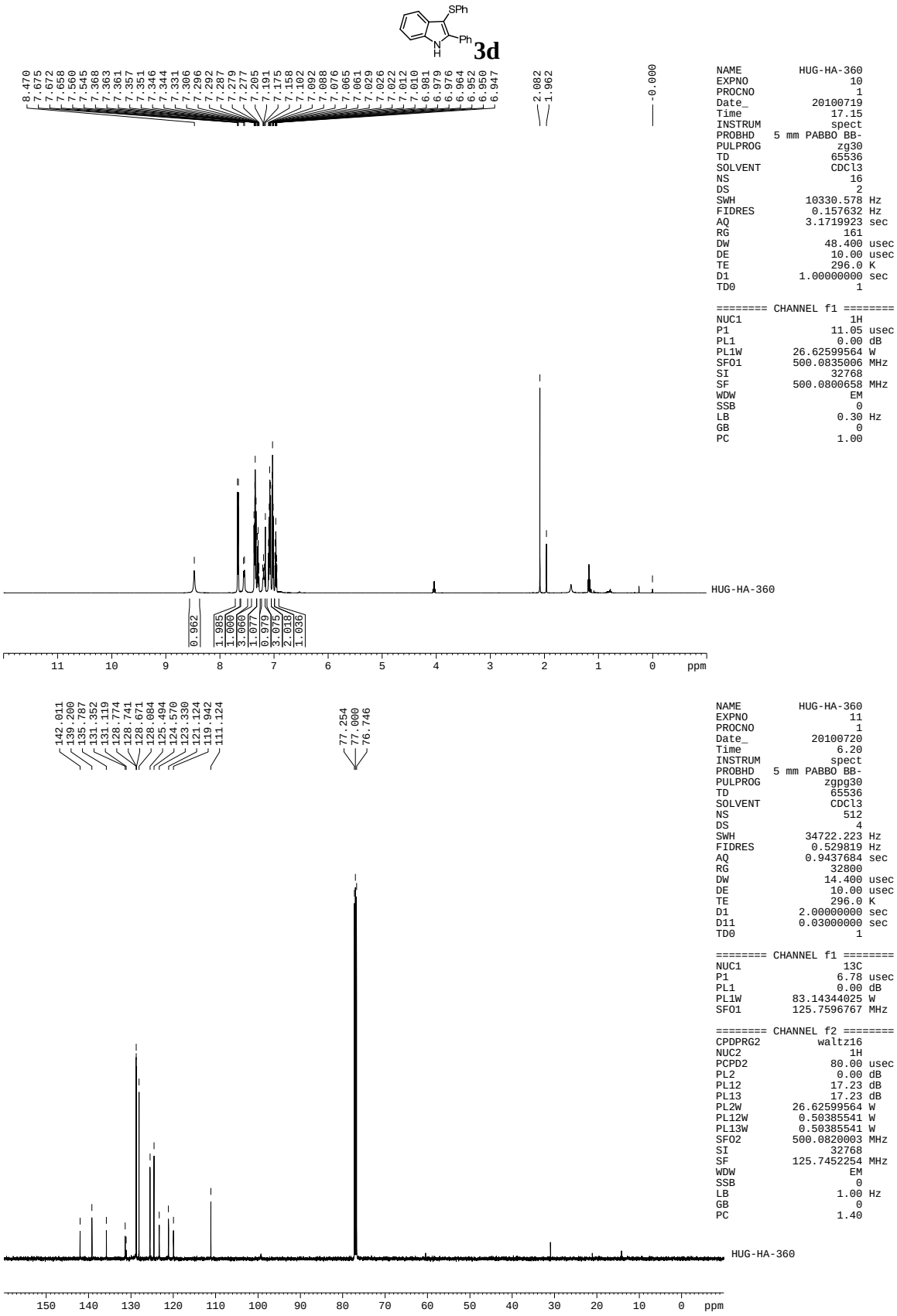
SSB 0
LB 1.00 Hz
GB 0
PC 1.00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7.351
7.346
7.344
7.331
7.306
7.296
7.292
7.287
7.279
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7.175
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7.102
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7.076
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7.061
7.029
7.026
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7.012
7.010
6.981
6.979
6.976
6.964
6.952
6.950
6.947
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PROCNO 1
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Time 17.15
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PULPROG zg30
TD 65536
SOLVENT CDCl3
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DE 10.00 usec
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SI 32768
SF 500.0800658 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HA-360
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1.000
3.060
1.077
0.979
3.075
2.018
1.036
11
10
9
8
7
6
5
4
3
2
1
0
ppm
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139.200
135.787
131.352
131.119
128.774
128.741
128.671
128.084
125.494
124.570
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121.124
119.942
111.124
77.254
77.000
76.746
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EXPNO 11
PROCNO 1
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Time 6.20
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.7596767 MHz
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CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.0820003 MHz
SI 32768
SF 125.7452254 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HA-360
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110
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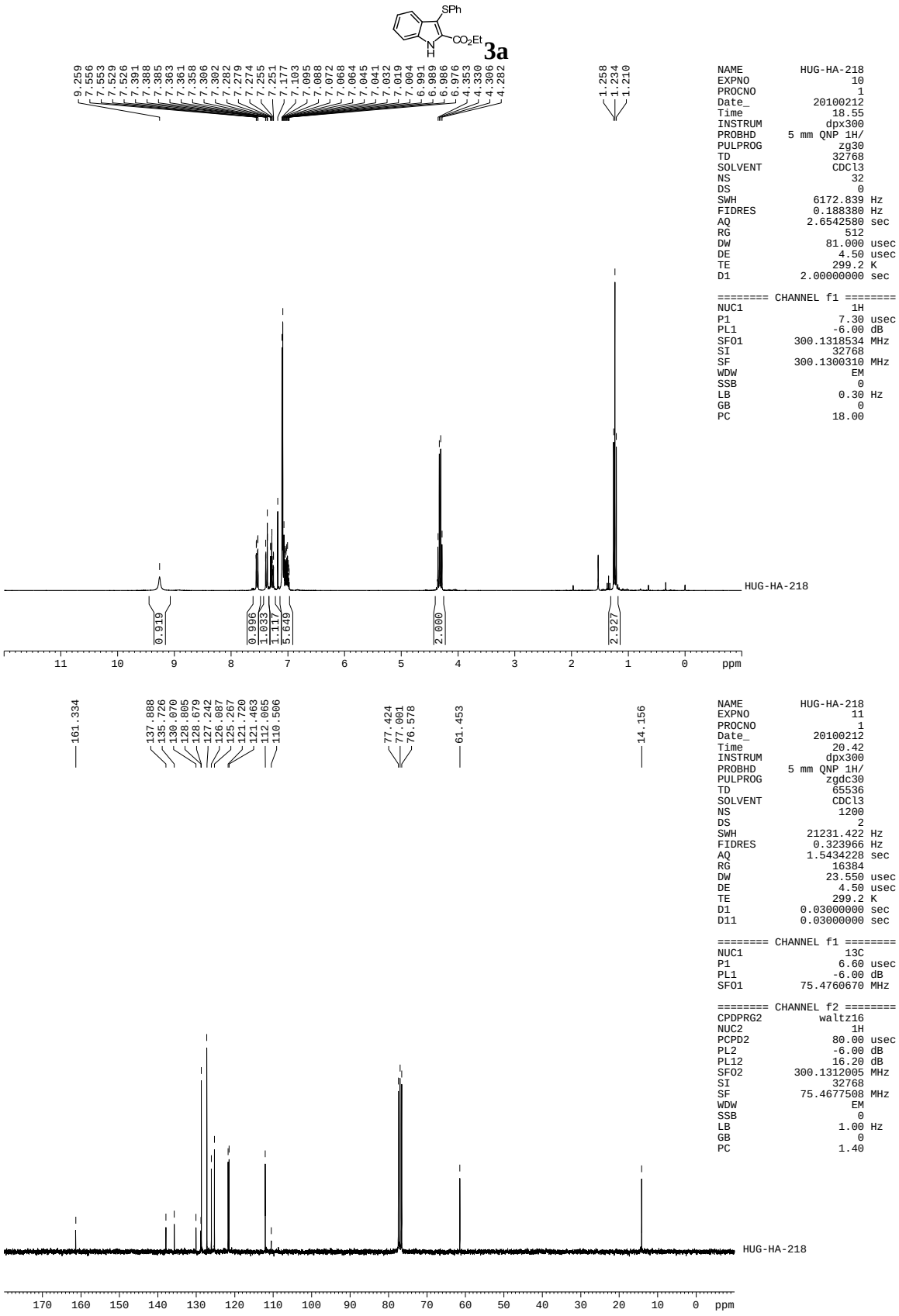
30
20
10
0
ppm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7.306
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7.041
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4.282
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1.234
1.210
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PROCNO 1
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Time 18.55
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PULPROG zg30
TD 32768
SOLVENT CDCl3
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FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 512
DW 81.000 usec
DE 4.50 usec
TE 299.2 K
D1 2.00000000 sec
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NUC1 1H
P1 7.30 usec
PL1 -6.00 dB
SFO1 300.1318534 MHz
SI 32768
SF 300.1300310 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 18.00
HUG-HA-218
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0.906
1.033
1.117
5.649
2.000
2.927
11 10 9 8 7 6 5 4 3 2 1 0 ppm
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137.888
135.726
130.070
128.805
128.679
127.242
126.087
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121.720
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76.578
61.453
14.156
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EXPNO 11
PROCNO 1
Date_ 20100212
Time 20.42
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PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1200
DS 2
SWH 21231.422 Hz
FIDRES 0.323966 Hz
AQ 1.5434228 sec
RG 16384
DW 23.550 usec
DE 4.50 usec
TE 299.2 K
D1 0.03000000 sec
D11 0.03000000 sec
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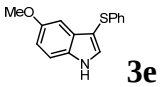
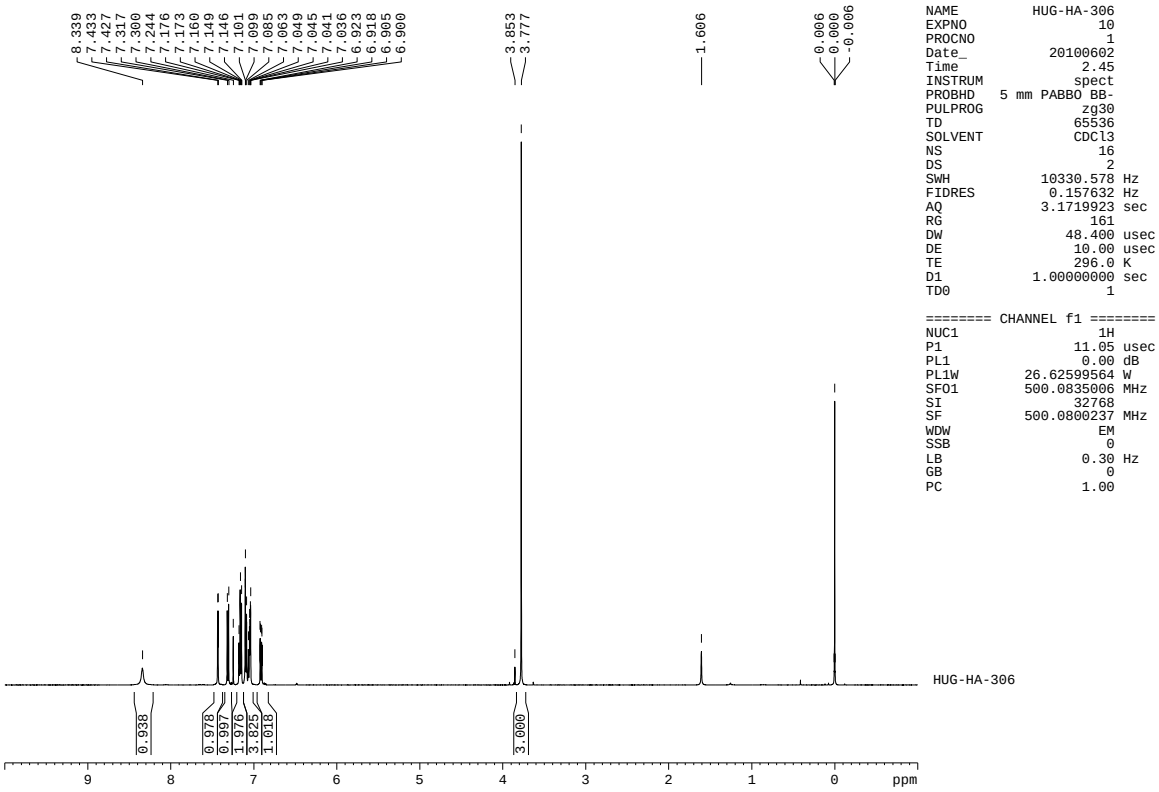
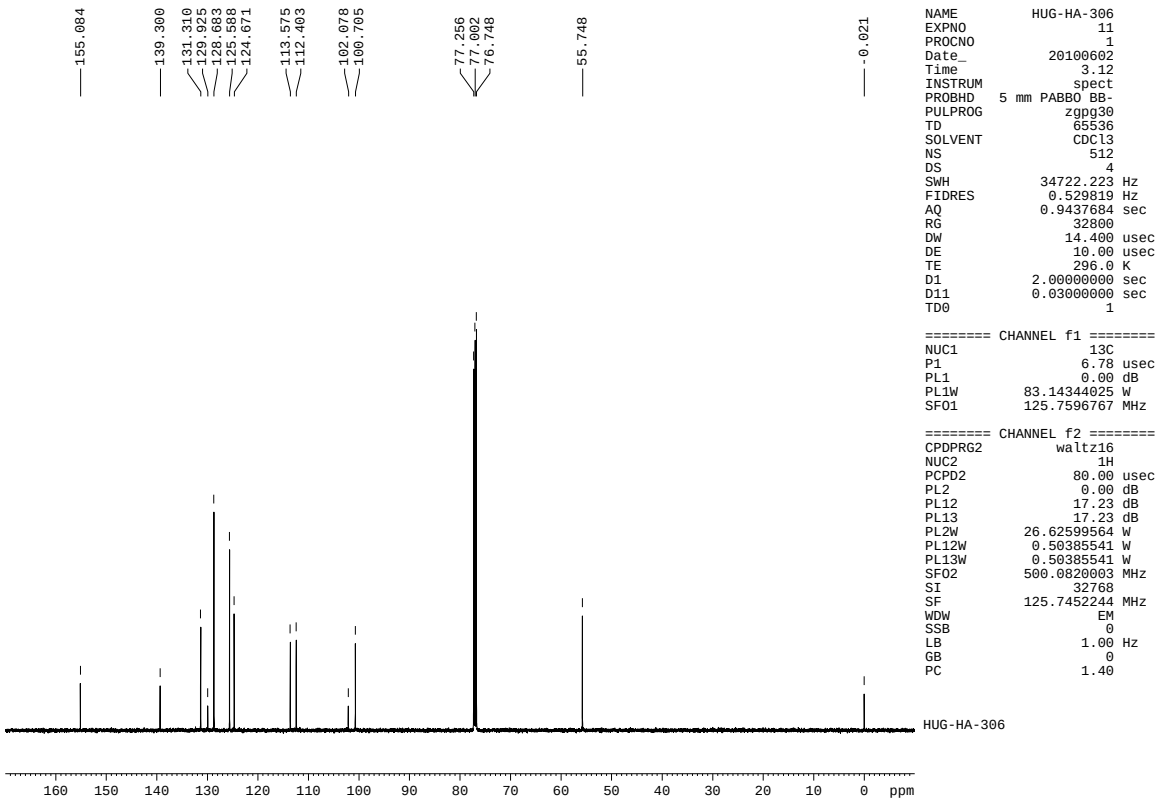
NUC1 13C
P1 6.60 usec
PL1 -6.00 dB
SFO1 75.4760670 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 16.20 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677508 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HA-218
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



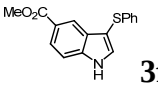
3e



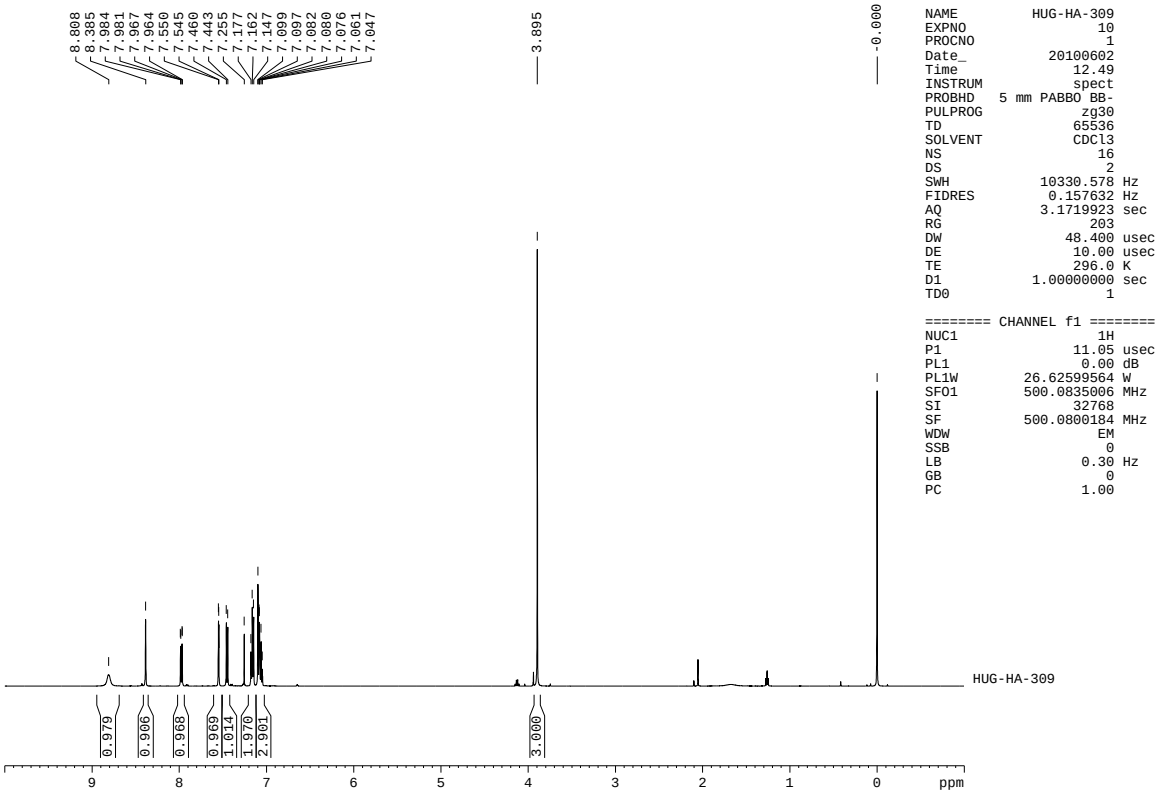

```
NAME          HUG-HA-306
EXPNO                 10
PROCNO                 1
Date_           20100602
Time                2.45
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   161
DW                48.400 usec
DE                10.00 usec
TE                296.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1         500.0835006 MHz
SI                 32768
SF           500.0800237 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

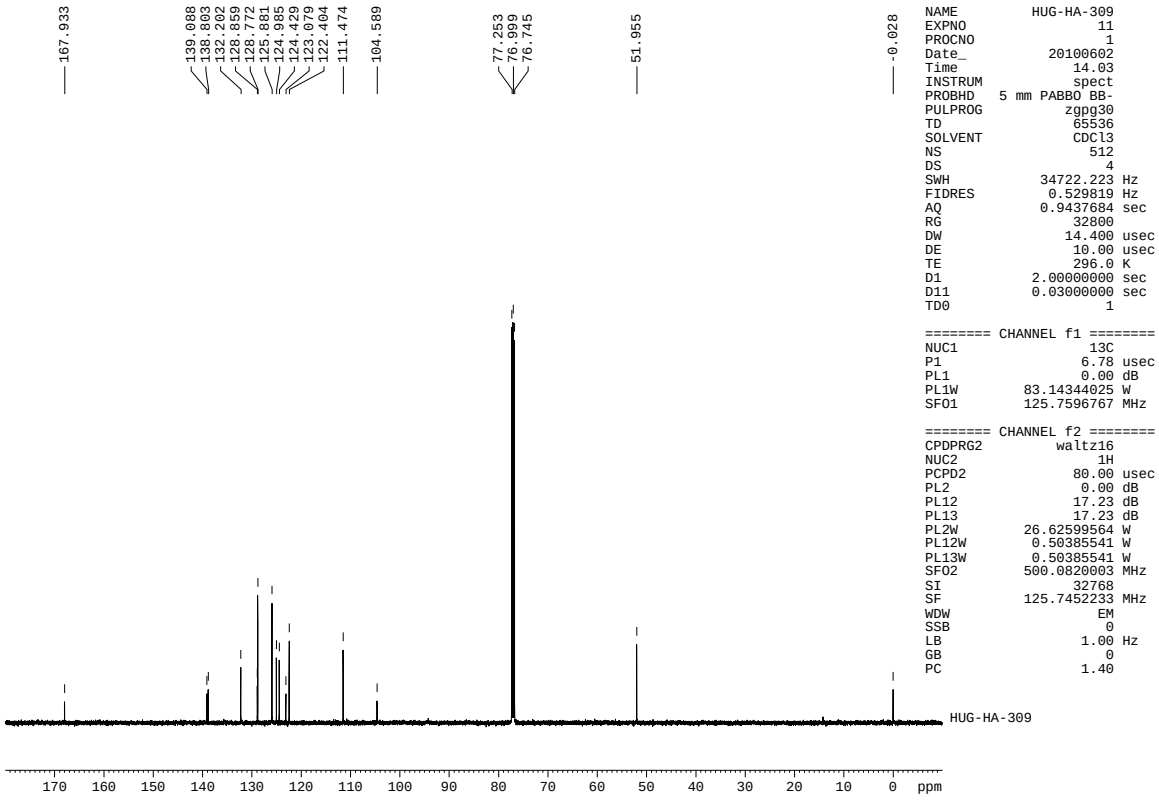


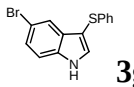

```
NAME          HUG-HA-306
EXPNO                 11
PROCNO                 1
Date_           20100602
Time                3.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1         125.7596767 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12              17.23 dB
PL13              17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.0820003 MHz
SI                 32768
SF           125.7452244 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```


MeO2C
SPh
N
H

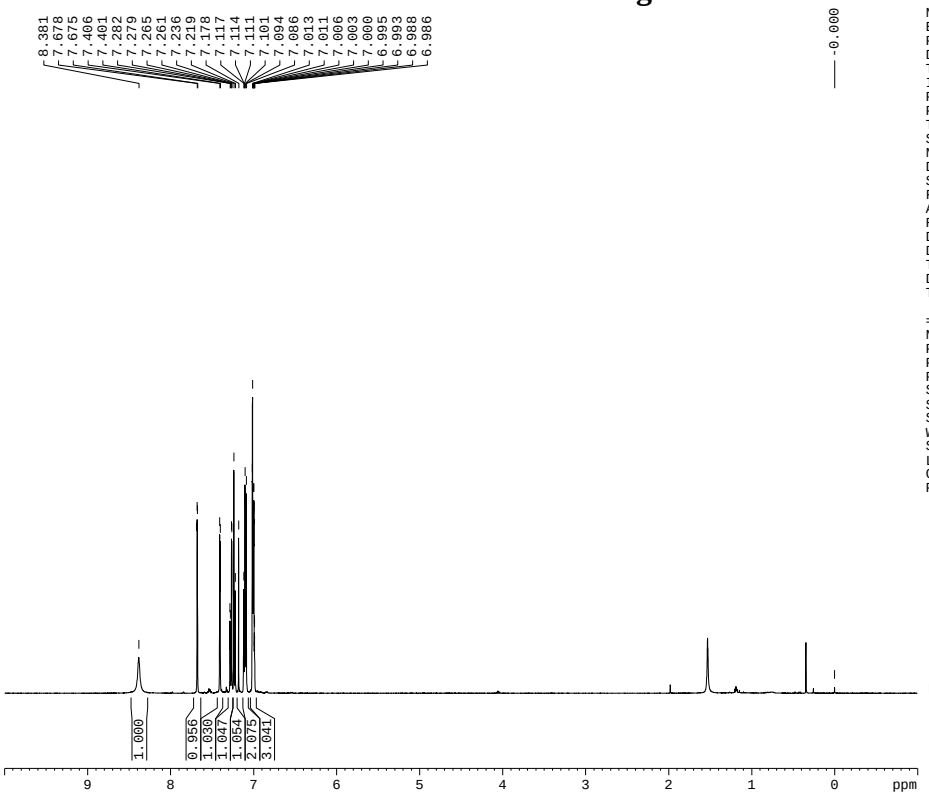
3f


8.808
8.385
7.984
7.981
7.967
7.964
7.550
7.545
7.460
7.443
7.255
7.177
7.162
7.147
7.099
7.097
7.082
7.080
7.076
7.061
7.047
3.895
-0.000
NAME HUG-HA-309
EXPNO 10
PROCNO 1
Date_ 20100602
Time 12.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 203
DW 48.400 usec
DE 10.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.0835006 MHz
SI 32768
SF 500.0800184 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HA-309
0.979
0.906
0.968
0.969
1.014
1.970
2.901
3.000
9
8
7
6
5
4
3
2
1
0
ppm

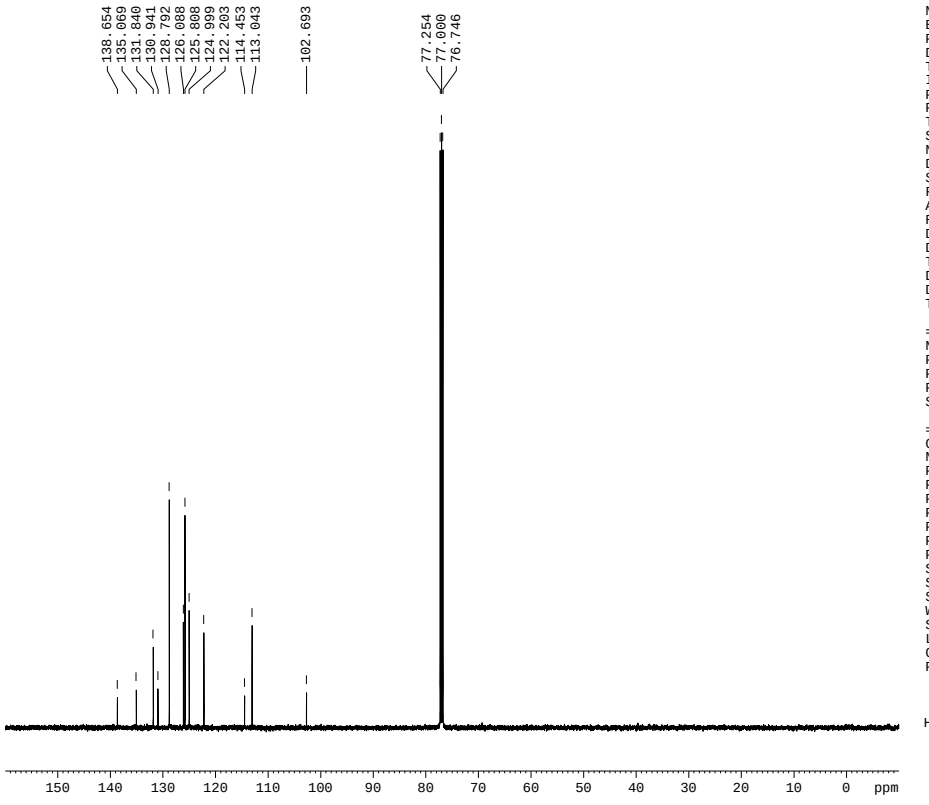

167.933
139.088
138.803
132.202
128.859
128.772
125.881
124.985
124.429
123.079
122.404
111.474
104.589
77.253
76.999
76.745
51.955
-0.028
NAME HUG-HA-309
EXPNO 11
PROCNO 1
Date_ 20100602
Time 14.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.7596767 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.0820003 MHz
SI 32768
SF 125.7452233 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HA-309
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



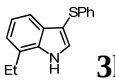
3g



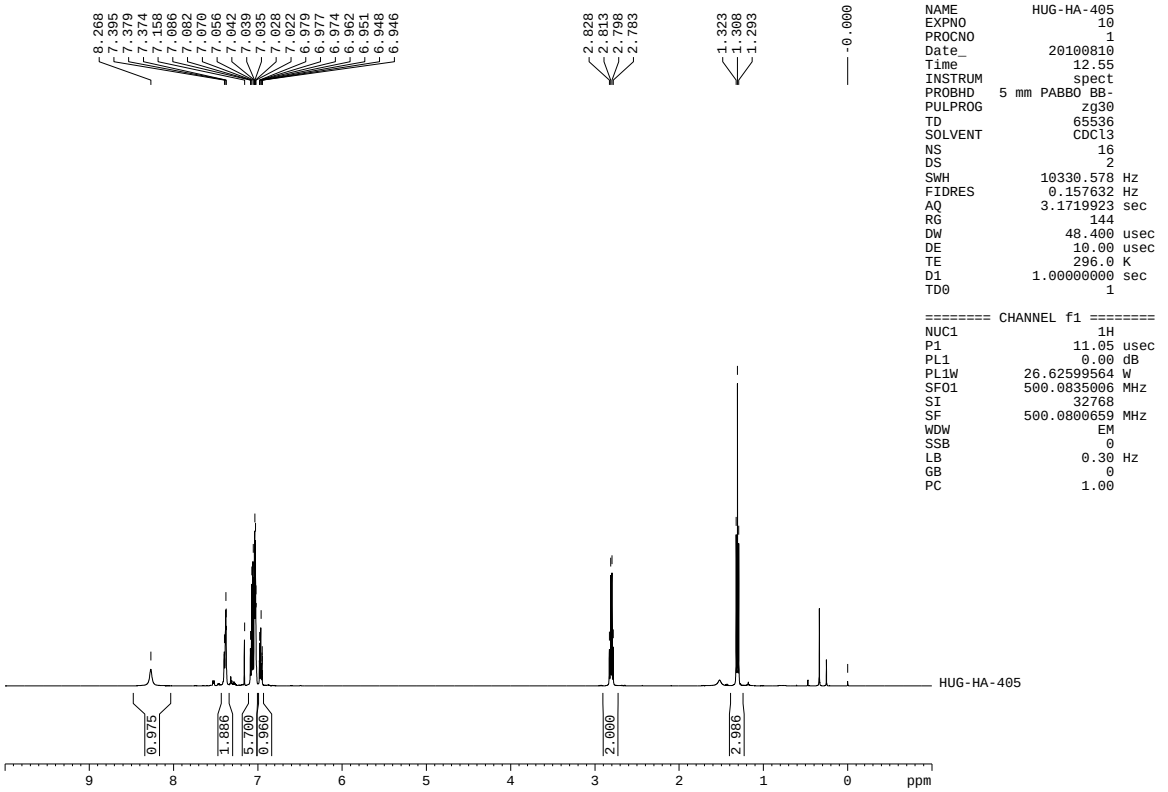

```
NAME          HUG-HA-352
EXPNO                 10
PROCNO                 1
Date_           20100705
Time               18.22
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   228
DW                48.400 usec
DE                10.00 usec
TE                296.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W         26.62599564 W
SFO1         500.0835006 MHz
SI                 32768
SF           500.0800558 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



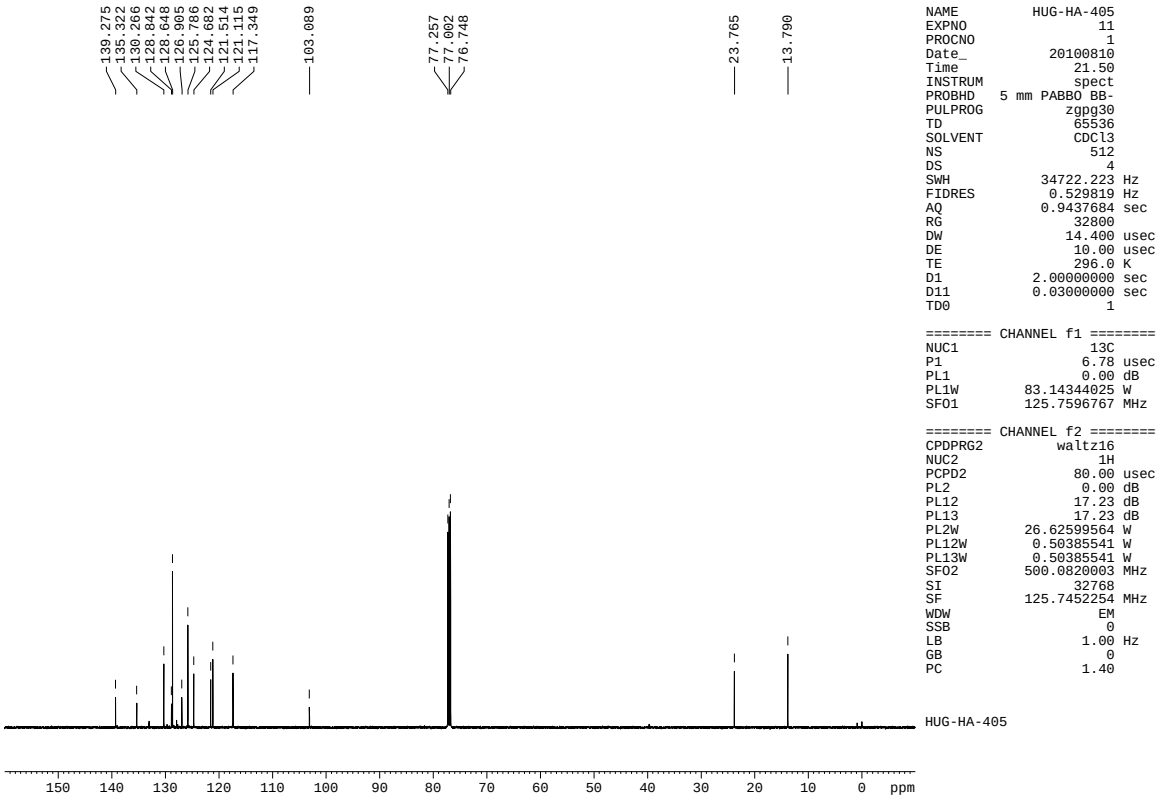

```
NAME          HUG-HA-352
EXPNO                 11
PROCNO                 1
Date_           20100706
Time               14.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W         83.14344025 W
SFO1         125.7596767 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.0820003 MHz
SI                 32768
SF           125.7452233 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



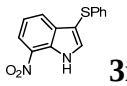
3h



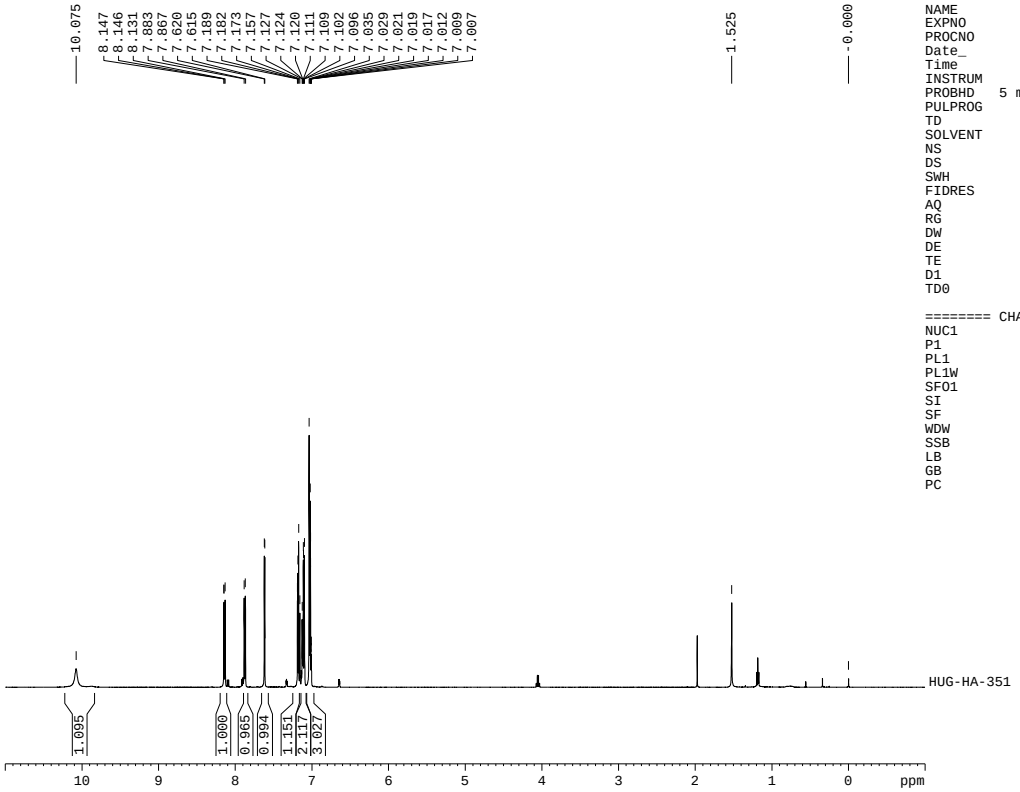

```
NAME          HUG-HA-405
EXPNO                 10
PROCNO                 1
Date_           20100810
Time               12.55
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   144
DW                48.400 usec
DE                10.00 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1         500.0835006 MHz
SI                 32768
SF           500.0800659 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



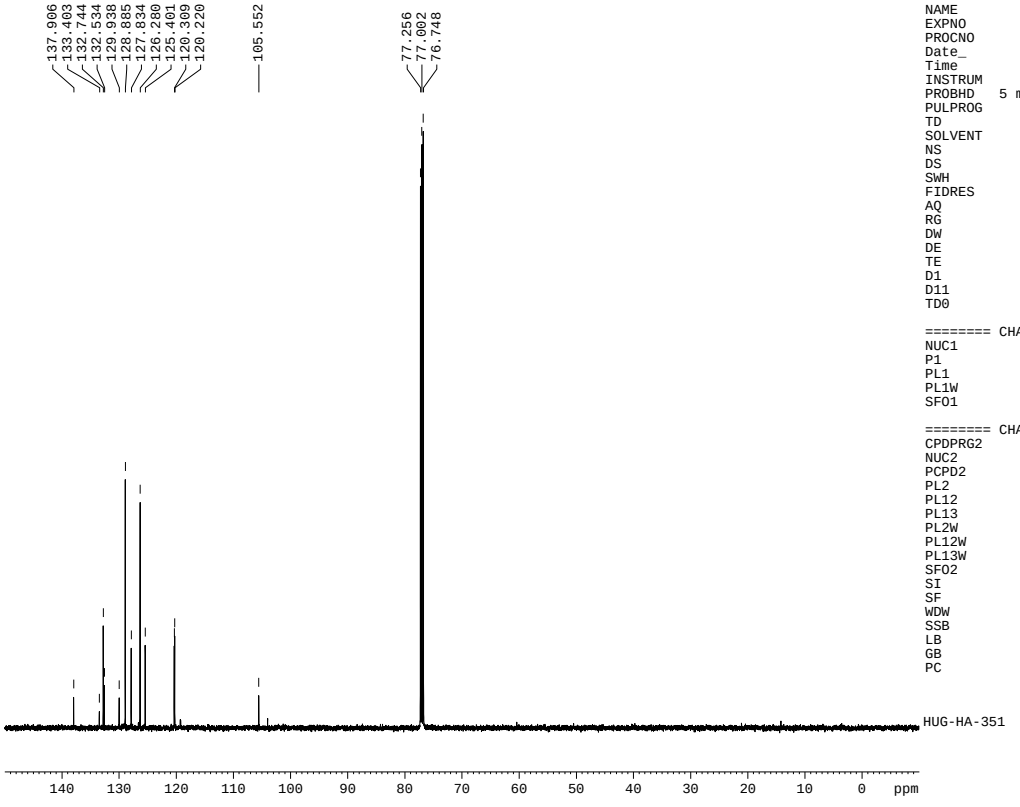

```
NAME          HUG-HA-405
EXPNO                 11
PROCNO                 1
Date_           20100810
Time               21.50
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1         125.7596767 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.0820003 MHz
SI                 32768
SF           125.7452254 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```



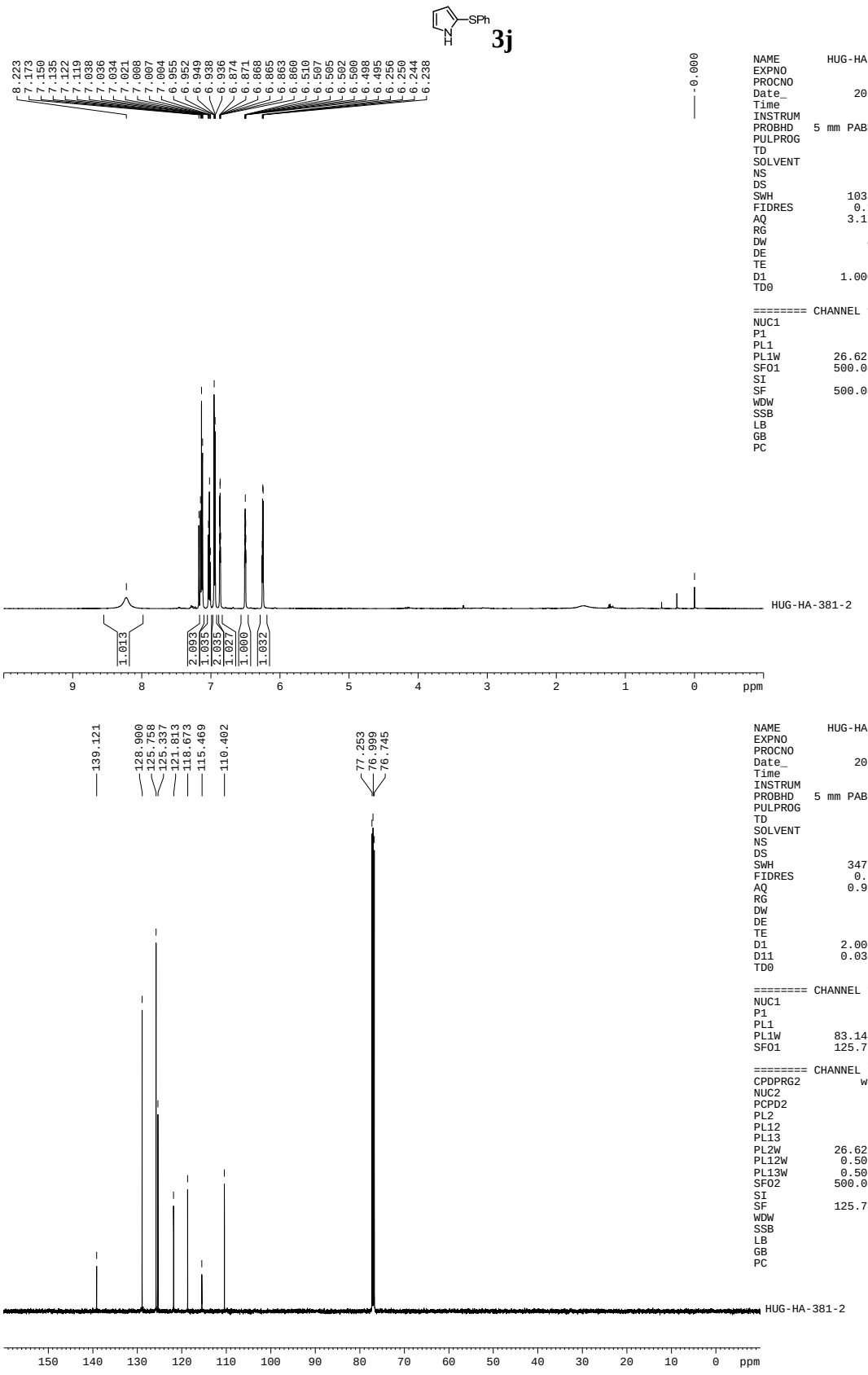
3i

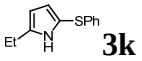



```
NAME          HUG-HA-351
EXPNO                 10
PROCNO                 1
Date_           20100705
Time               18.17
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   228
DW                48.400 usec
DE                10.00 usec
TE                296.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                 0.00 dB
PL1W         26.62599564 W
SFO1         500.0835006 MHz
SI                 32768
SF           500.0800537 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

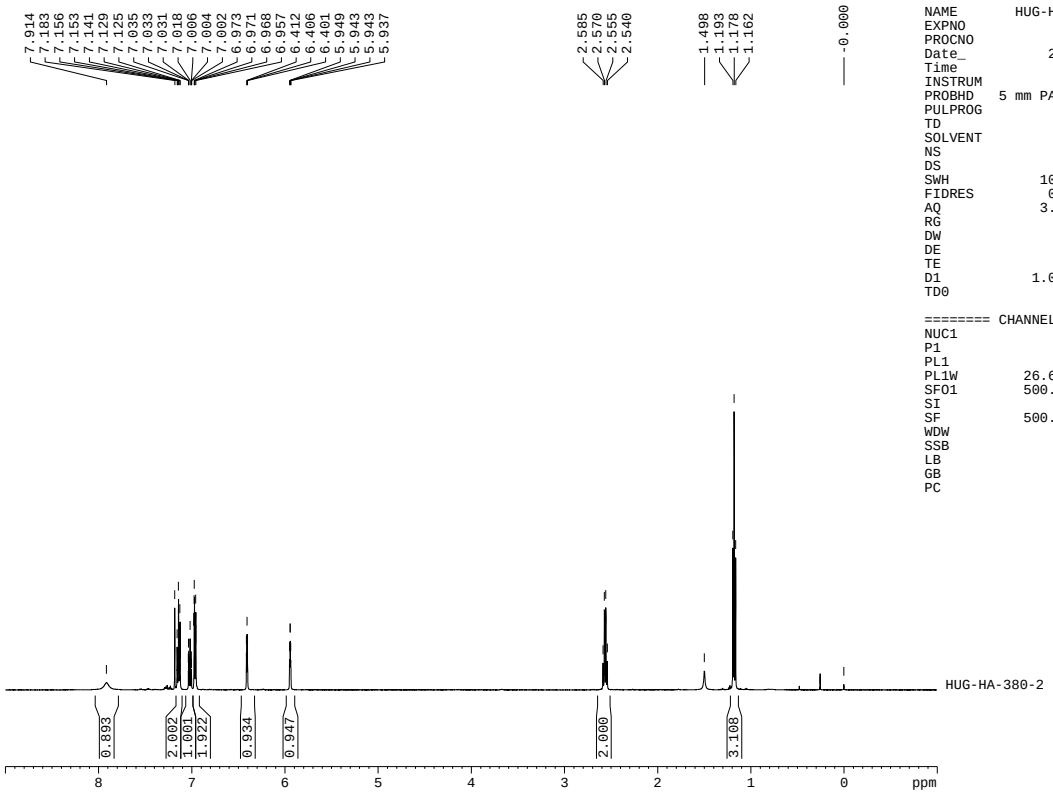



```
NAME          HUG-HA-351
EXPNO                 11
PROCNO                 1
Date_           20100706
Time               10.28
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  6.78 usec
PL1                 0.00 dB
PL1W         83.14344025 W
SFO1         125.7596767 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               17.23 dB
PL13               17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.0820003 MHz
SI                 32768
SF           125.7452222 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

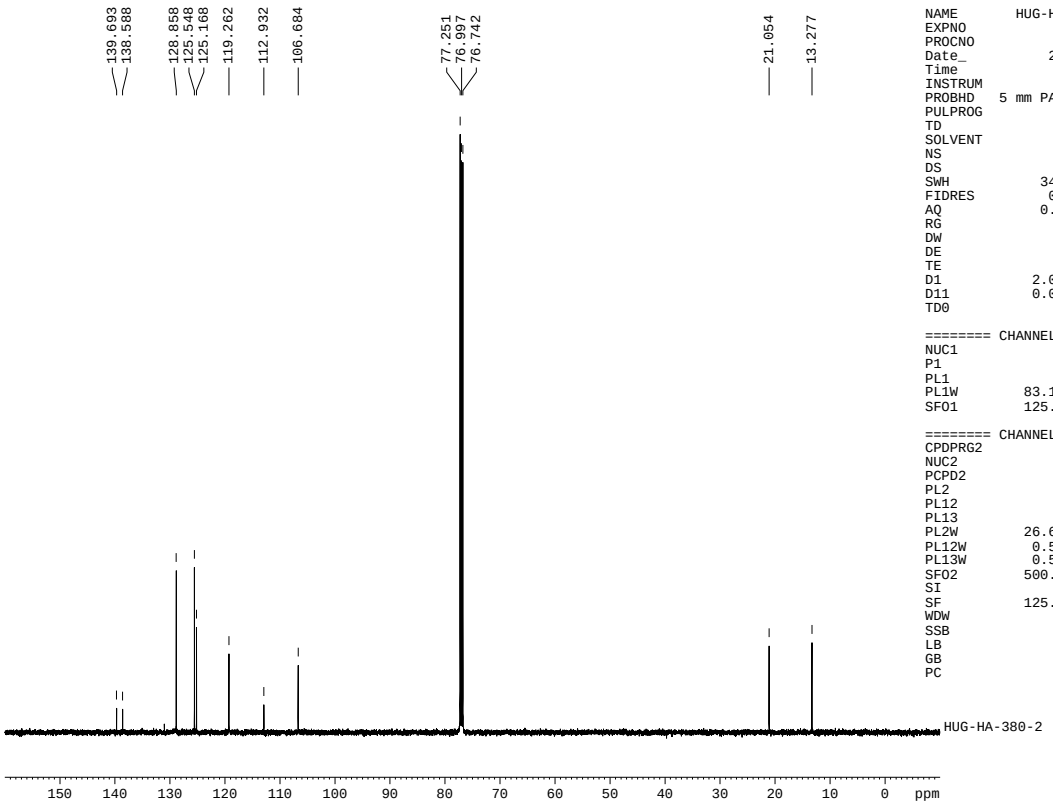

SPh
N
H
3j
8.223
7.173
7.150
7.135
7.122
7.119
7.038
7.036
7.034
7.021
7.008
7.007
7.004
6.955
6.952
6.949
6.938
6.936
6.874
6.871
6.868
6.865
6.863
6.860
6.510
6.507
6.505
6.502
6.500
6.498
6.495
6.256
6.250
6.244
6.238
-0.000
NAME HUG-HA-381-2
EXPNO 10
PROCNO 1
Date_ 20100726
Time 12.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 181
DW 48.400 usec
DE 10.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.0835006 MHz
SI 32768
SF 500.0800583 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HA-381-2
1.013
2.093
1.035
2.035
1.027
1.000
1.032
9
8
7
6
5
4
3
2
1
0
ppm
139.121
128.900
125.758
125.337
121.813
118.673
115.469
110.402
77.253
76.999
76.745
NAME HUG-HA-381-2
EXPNO 11
PROCNO 1
Date_ 20100726
Time 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 34722.223 Hz
FIDRES 0.529819 Hz
AQ 0.9437684 sec
RG 32800
DW 14.400 usec
DE 10.00 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.78 usec
PL1 0.00 dB
PL1W 83.14344025 W
SFO1 125.7596767 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 17.23 dB
PL13 17.23 dB
PL2W 26.62599564 W
PL12W 0.50385541 W
PL13W 0.50385541 W
SFO2 500.0820003 MHz
SI 32768
SF 125.7452244 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
HUG-HA-381-2
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



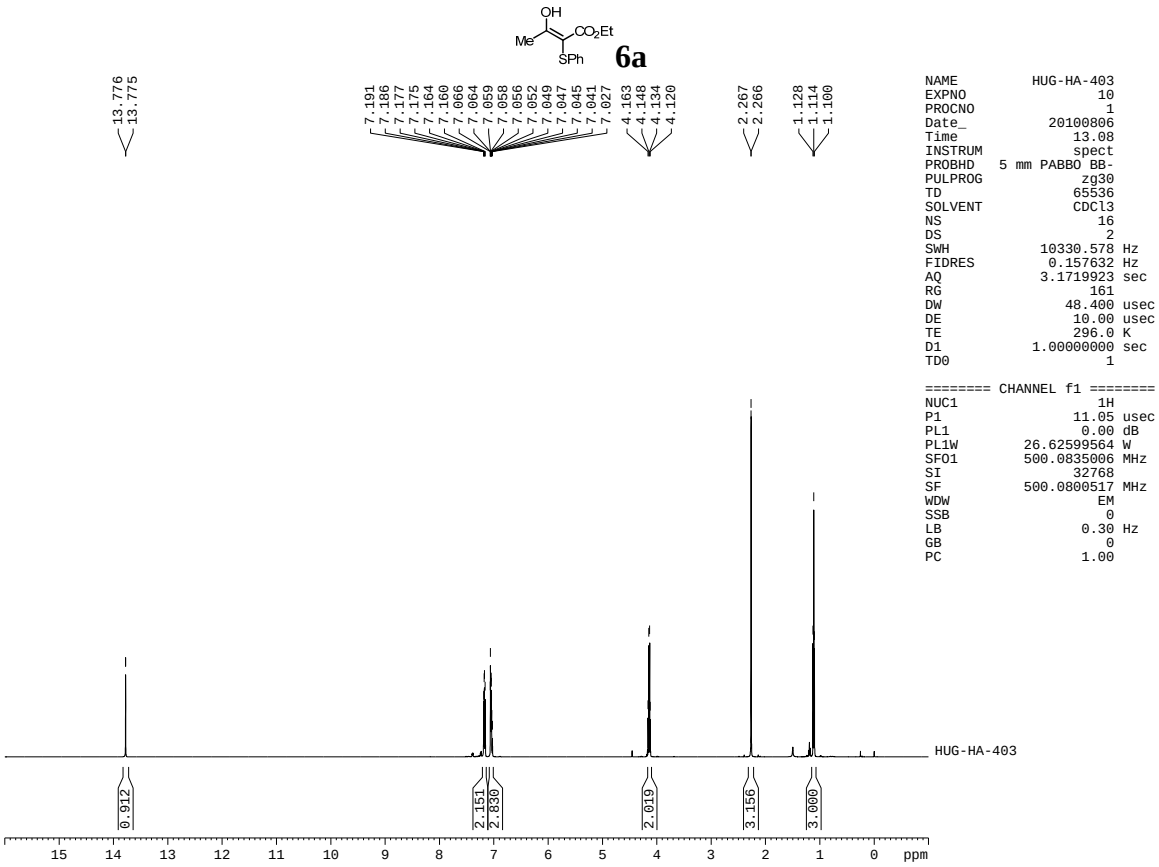
3k

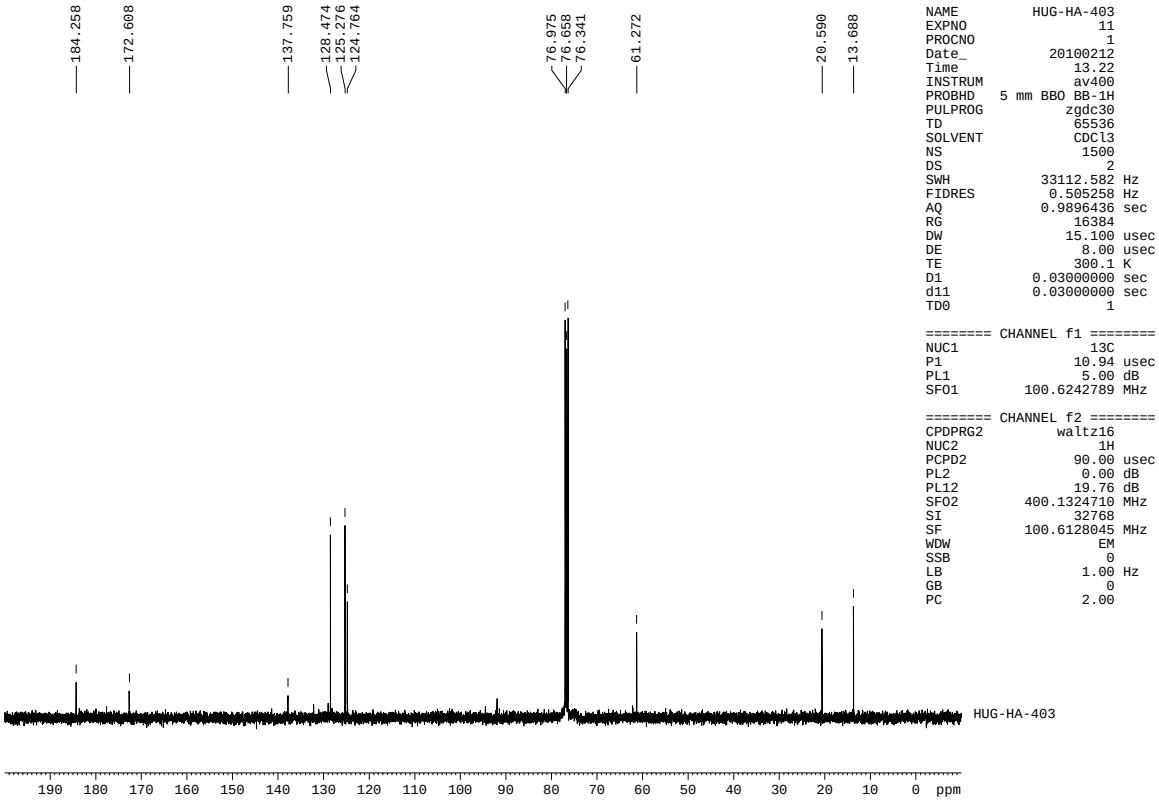


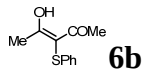

```
NAME       HUG-HA-380-2
EXPNO                10
PROCNO                1
Date_          20100723
Time              14.35
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ            3.1719923 sec
RG                  228
DW               48.400 usec
DE               10.00 usec
TE                296.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1         500.0835006 MHz
SI                 32768
SF           500.0800536 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



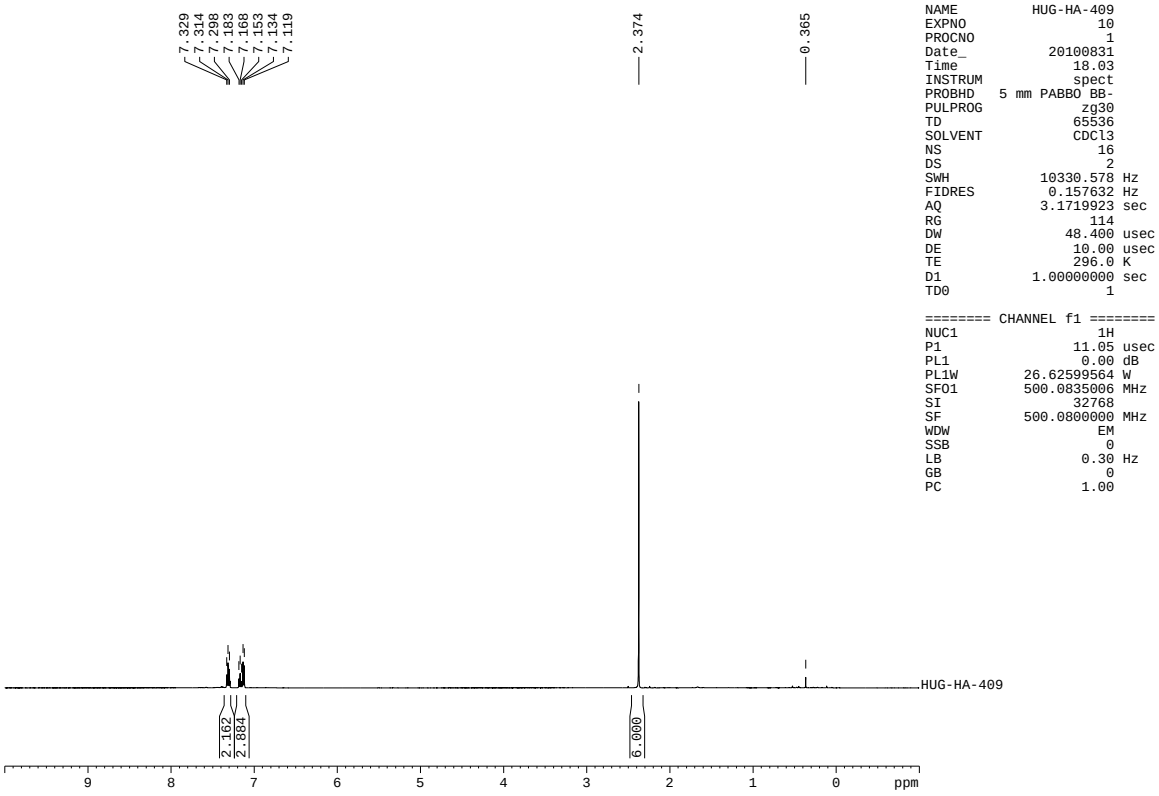

```
NAME       HUG-HA-380-2
EXPNO                11
PROCNO                1
Date_          20100723
Time              17.21
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ            0.9437684 sec
RG                32800
DW               14.400 usec
DE               10.00 usec
TE                295.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1         125.7596767 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              17.23 dB
PL13              17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.0820003 MHz
SI                 32768
SF           125.7452222 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```


OH
Me
CO2Et
SPh
6a
13.776
13.775
7.191
7.186
7.177
7.175
7.164
7.160
7.066
7.064
7.059
7.058
7.056
7.052
7.049
7.047
7.045
7.041
7.027
4.163
4.148
4.134
4.120
2.267
2.266
1.128
1.114
1.100
NAME HUG-HA-403
EXPNO 10
PROCNO 1
Date_ 20100806
Time 13.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 161
DW 48.400 usec
DE 10.00 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 11.05 usec
PL1 0.00 dB
PL1W 26.62599564 W
SFO1 500.0835006 MHz
SI 32768
SF 500.0800517 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
HUG-HA-403
0.912
2.151
2.830
2.019
3.156
3.000
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

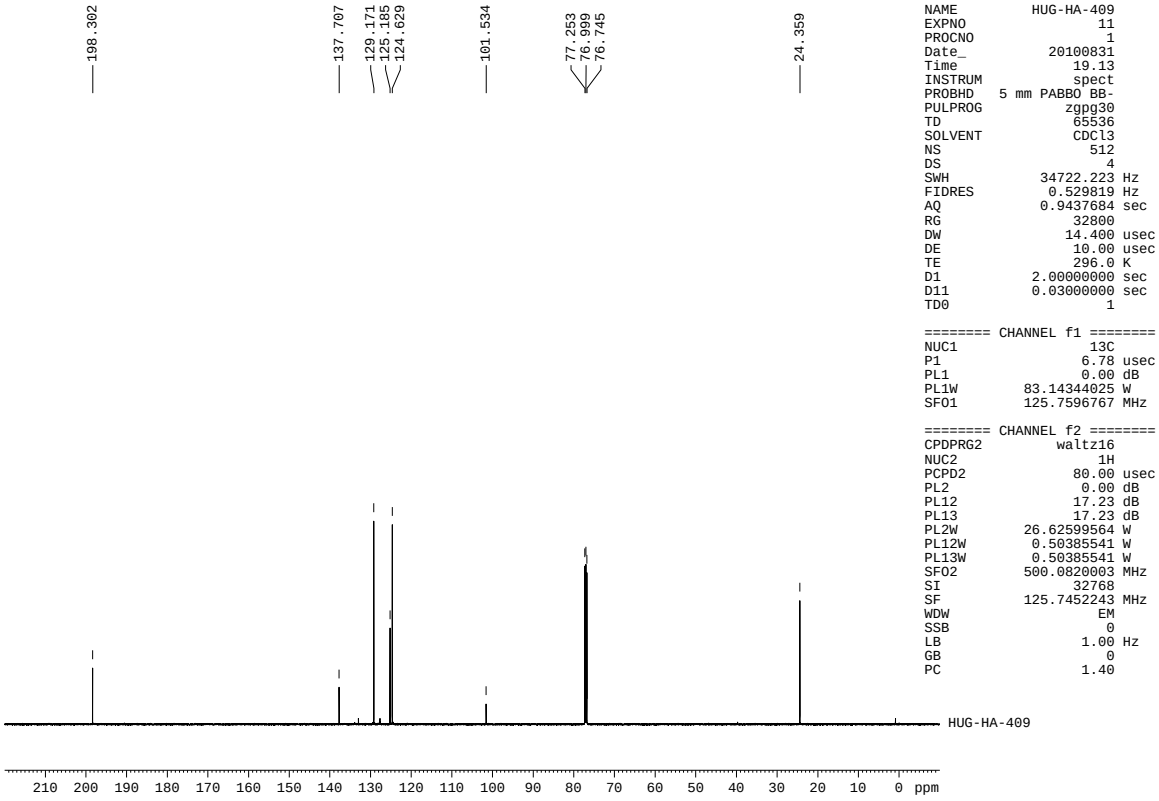

184.258
172.608
137.759
128.474
125.276
124.764
76.975
76.658
76.341
61.272
20.590
13.688
NAME HUG-HA-403
EXPNO 11
PROCNO 1
Date_ 20100212
Time 13.22
INSTRUM av400
PROBHD 5 mm BBO BB-1H
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1500
DS 2
SWH 33112.582 Hz
FIDRES 0.505258 Hz
AQ 0.9896436 sec
RG 16384
DW 15.100 usec
DE 8.00 usec
TE 300.1 K
D1 0.03000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.94 usec
PL1 5.00 dB
SFO1 100.6242789 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 19.76 dB
SFO2 400.1324710 MHz
SI 32768
SF 100.6128045 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
HUG-HA-403
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



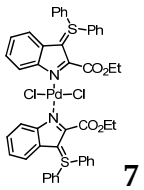
6b



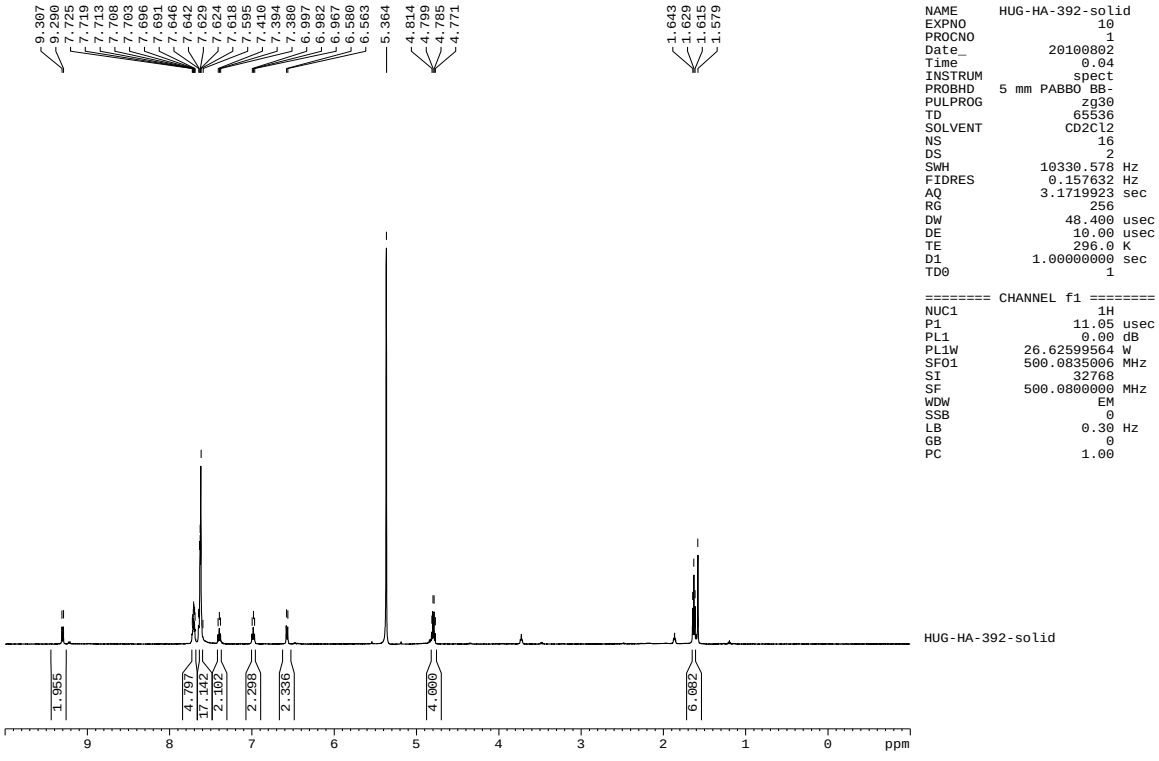

```
NAME          HUG-HA-409
EXPNO                 10
PROCNO                 1
Date_           20100831
Time               18.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                   114
DW                48.400 usec
DE                10.00 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1         500.0835006 MHz
SI                 32768
SF           500.0800000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```



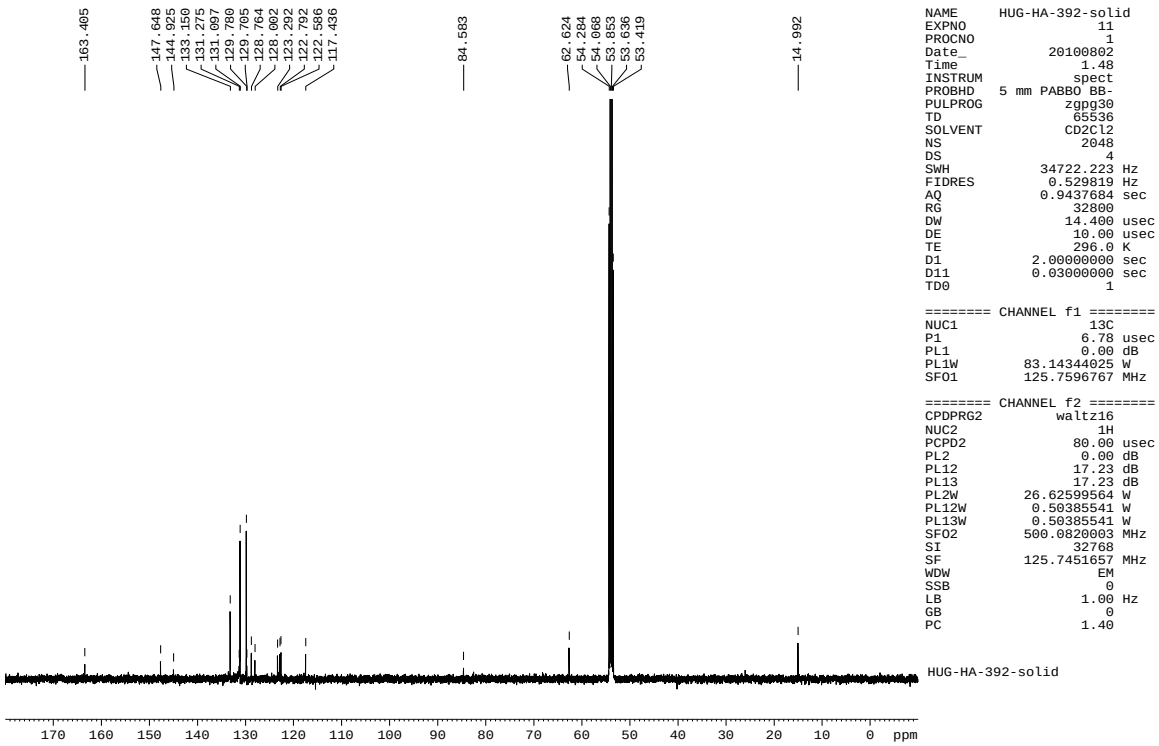

```
NAME          HUG-HA-409
EXPNO                 11
PROCNO                 1
Date_           20100831
Time               19.13
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                 32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1         125.7596767 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              17.23 dB
PL13              17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.0820003 MHz
SI                 32768
SF           125.7452243 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```



7




```
NAME      HUG-HA-392-solid
EXPNO               10
PROCNO               1
Date_          20100802
Time               0.04
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CD2Cl2
NS                   16
DS                    2
SWH           10330.578 Hz
FIDRES         0.157632 Hz
AQ             3.1719923 sec
RG                  256
DW                48.400 usec
DE                10.00 usec
TE                296.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                11.05 usec
PL1                0.00 dB
PL1W         26.62599564 W
SFO1         500.0835006 MHz
SI                32768
SF           500.0800000 MHz
WDW                EM
SSB                 0
LB                0.30 Hz
GB                  0
PC                1.00
```




```
NAME      HUG-HA-392-solid
EXPNO               11
PROCNO               1
Date_          20100802
Time               1.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CD2Cl2
NS                 2048
DS                    4
SWH           34722.223 Hz
FIDRES         0.529819 Hz
AQ             0.9437684 sec
RG                32800
DW                14.400 usec
DE                10.00 usec
TE                296.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               13C
P1                 6.78 usec
PL1                0.00 dB
PL1W         83.14344025 W
SFO1         125.7596767 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              17.23 dB
PL13              17.23 dB
PL2W         26.62599564 W
PL12W         0.50385541 W
PL13W         0.50385541 W
SFO2         500.0820003 MHz
SI                32768
SF           125.7451657 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```