An Experimental and Theoretical Study on the Interaction of *N*-Heterocyclic Carbene-derived 1,3-Dipoles with Methoxycarbonylallenes: Highly Regio- and Stereoselective [3+2]-Cycloadditions Controlled by the Structures of *N*-Heterocycles of 1,3-Dipoles

Ying Cheng*, Bo Wang, Xiao-Rong Wang, Jian-Hong Zhang and De-Cai Fang*

College of Chemistry, Beijing Normal University, Beijing, 100875, China

E-mail: ycheng2@bnu.edu.cn; dcfang@bnu.edu.cn

Table of contents:

Melting points are uncorrected. ^{1}H NMR (500, 400 or 300 MHz) and ^{13}C NMR (125, 100 or 75 MHz) were recorded in the indicated solvents. Column chromatography was performed using 200-300 mesh silica gel or neutral Al_2O_3. The solvents benzene and toluene were distilled from sodium benzophenone ketyl. The 2-arylthiocarbamoyl benzimidazolium, -imidazolinium and -triazolium inner salts **5**, **10** and **14** were prepared, respectively, from the reactions of benzimidazolium, imidazolinium, and triazolium salts with aryl isothiocyanates in the presence of NaH as described in our previous publications.[1] [1. (a) Cheng, Y.; Liu, M.-F.; Fang, D.-C.; Lei, X.-M. *Chem. Eur. J*. **2007**, 4282. (b) Liu, M.-F.; Wang, B.; Cheng, Y.; *Chem. Commun.*, **2006**, 1215.]

General procedure for the reaction of 2-arylthiocarbamoyl benzimidazolium salts 5 with methoxycarbonylallenes 6. 2-Arylthiocarbamoyl benzimidazolium salts **5** (1 mmol) were mixed with methoxycarbonylallenes **6** (1.5 mmol) in dry benzene (40 mL) under nitrogen atmosphere. The reaction mixture was stirred at room temperature (20-30 ^{o}C) for 24-48 h or at the refluxing temperature of benzene for 2-4 h. After removal of the solvent under vacuum, the residue was chromatographied on a silica gel column eluting with a mixture of petroleum ether (30-60 ^{o}C) and ethyl acetate (8:1) to afford benzimidazole-spiro-thiophenes **7** in 56-90% yields from the reaction at room temperature (or 69-82 % from the reaction in refluxing benzene). In some cases, a tiny amount of by-products were also detected, but only benzimidazole-spiro-pyrrole **9d** (9%) has been fully characterized. (Note: yields in parentheses correspond to the reaction in refluxing benzene.)

(*Z, Z*)-Methyl

2-[1,3,4'-tribenzyl-1,3-dihydro-2'-(phenylimino)spiro[2*H*-benzo[*d*]imidazole-2,3'(2'*H*)-thiophen]-5'-ylidene] acetate (7a): 559mg, 90% (509mg, 82%), mp 140-141 ^{o}C.[2] (2. Wang, B.; Li, J.-Q.; Cheng, Y. *Tetrahedron Lett.*, **2008**, *49*, 485.)

(*Z, Z*)-Methyl

2-[4'-benzyl-1,3,4',5'-tetrahydro-1,3-bis(4-methoxybenzyl)-2'-(phenylimino)spiro[2*H*-benzo[*d*]imidazole-2,3' (2'*H*)-thiophen]-5'-ylidene]acetate (7b): 510mg, 75% (470mg, 69%), yellow crystals (dichloromethane and petroleum ether), mp 168-170 ^{o}C; IR *v* (cm^{-1}) 1708, 1610, 1512, 1494; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.33-7.37 (m, 6H), 7.16-7.17 (m, 4H), 6.89 (d, *J* = 8.7 Hz, 2H), 6.88 (d, *J* = 8.2 Hz, 2H), 6.82 (d, *J* = 8.6 Hz, 2H), 6.77 (t, *J* = 3.4 Hz, 2H), 6.61 (t, *J* = 7.5 Hz, 1H), 6.55 (t, *J* = 7.0 Hz, 1H), 6.32 (d, *J* = 7.3 Hz, 1H), 6.15 (d, *J* = 7.4 Hz, 1H), 5.87 (d, *J* = 2.2 Hz, 1H), 4.82 (d, *J* = 16.8 Hz, 1H), 4.54 (d, *J* = 16.3 Hz, 1H), 4.46 (d, *J* = 16.9 Hz, 1H), 4.42 (d, *J* = 16.3 Hz, 1H), 3.84 (s, 3H), 3.80 (s, 3H), 3.74 (d, *J* = 15.6 Hz, 1H), 3.64 (s, 3H), 3.53 (d, *J* = 10.0 Hz, 1H), 2.88 (dd, *J* = 15.9, 10.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 166.4, 164.8, 159.0, 158.9, 157.8, 150.2, 141.2, 139.8, 138.8, 130.7, 129.5, 129.2, 128.9, 128.8, 128.7, 128.4, 128.3, 128.0, 126.4, 125.4, 119.9, 118.9, 118.4, 114.3, 114.0, 113.8, 111.6, 105.3, 104.1, 98.4, 55.4, 55.3, 51.5, 50.9, 49.1, 48.8, 33.3; MS (ESI): 682 (M+1). Anal. Calcd for $C_{42}H_{39}N_3O_4S$: C 73.98, H 5.77, N 6.16; Found: C 73.98, H 5.95, N 6.05.

(*Z, Z*)-Methyl

2-[4'-benzyl-1,3-bis(4-chlorobenzyl)-1,3,4',5'-tetrahydro-2'-(phenylimino)spiro[2*H*-benzo[*d*]imidazole-2,3'(2 '*H*)-thiophen]-5'-ylidene]acetate (7c): 573mg, 83% (552mg, 80%), yellow crystals (dichloromethane and petroleum ether), mp 171-172 ^{o}C; IR *v* (cm^{-1}) 1701, 1611, 1596, 1499; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.31-7.38 (m, 8H), 7.25 (d, *J* = 8.3 Hz, 2H), 7.16-7.21 (m, 4H), 6.84 (d, *J* = 7.6 Hz, 2H), 6.79 (t, *J* = 4.1 Hz, 2H), 6.62 (t, *J* = 7.5 Hz, 1H), 6.57 (t, *J* = 7.6 Hz, 1H), 6.25 (d, *J* = 7.2 Hz, 1H), 6.11 (d, *J* = 7.2 Hz, 1H), 5.90 (d, *J* = 2.2 Hz, 1H), 4.81 (d, *J* = 17.1 Hz, 1H), 4.56 (d, *J* = 16.7 Hz, 1H), 4.45 (d, *J* = 17.1 Hz, 1H), 4.43 (d, *J* = 16.7 Hz, 1H), 3.72 (d, *J* = 15.5 Hz, 1H), 3.65 (s, 3H), 3.47 (d, *J* = 9.8 Hz, 1H), 2.88 (dd, *J* = 15.9, 9.9 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 166.3, 164.4, 157.3, 149.8, 140.8, 139.4, 138.3, 137.0, 135.9, 133.2, 133.1, 129.3, 129.1, 128.84, 128.81, 128.52, 128.47, 127.8, 126.7, 125.6, 119.9, 119.3, 118.8, 111.9, 105.3, 104.4, 98.3, 51.6, 50.9, 49.1, 48.7, 33.2; MS (ESI): 690 (M+1). Anal. Calcd for $C_{40}H_{33}Cl_2N_3O_2S$: C 69.56, H 4.82, N 6.08; Found: C 69.61, H 5.03, N 5.95.

(*Z, Z*)-Methyl

2-[1,3-dibenzyl-1,3,4',5'-tetrahydro-4'-methyl-2'-(phenylimino)spiro[2*H*-benzo[*d*]imidazole-2,3'(2'*H*)-thioph en]-5'-ylidene]acetate (7d): 305mg, 56% (382mg, 70%), yellow crystals (dichloromethane and petroleum ether), mp 148-149 ^{o}C; IR *v* (cm^{-1}) 1705, 1645, 1602, 1495; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.47 (d, *J* = 7.5 Hz, 2H), 7.28-7.41 (m, 10H), 7.15 (t, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 7.9 Hz, 2H), 6.56 (t, *J* = 7.5 Hz, 1H), 6.50 (t, *J* = 7.5 Hz, 1H), 6.21(d, *J* = 7.3 Hz, 1H), 6.04 (d, *J* = 7.3 Hz, 1H), 6.00 (d, *J* = 2.0 Hz, 1H), 4.78 (d, *J* = 17.0 Hz, 1H), 4.51 (d, *J* = 16.5 Hz, 1H), 4.45 (d, *J* = 17.0 Hz, 1H), 4.37 (d, *J* = 16.5 Hz, 1H), 3.73 (s, 3H), 3.15-3.17 (m, 1H), 1.51 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 166.5, 165.0, 159.1, 150.2, 141.0, 139.7, 138.6, 137.3, 129.3, 128.8, 128.6, 127.3, 127.13, 127.07, 126.8, 125.4, 119.9, 118.8, 118.5, 110.1, 105.4, 104.3, 98.2, 51.7, 49.7, 49.1, 45.9, 11.9; MS (MALDI-TOF): 546 (M+1). Anal. Calcd for $C_{34}H_{31}N_3O_2S$: C 74.83, H 5.73, N 7.70; Found: C 74.81, H 5.74, N 7.68.

(*Z*)-Methyl

2-[1,3-dibenzyl-1,3-dihydro-4'-methyl-1'-phenyl-2'-thioxospiro[2*H*-benzo[*d*]imidazole-2,3'-pyrrolidine]-5'-yl idene]acetate (9d): 49mg, 9% from the reaction in refluxing benzene, red crystals (dichloromethane and petroleum ether), mp 125-126 ^{o}C; IR *v* (cm^{-1}) 1702, 1662, 1600, 1495; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.17-7.36 (m, 13H), 6.99 (d, *J* = 6.5 Hz, 2H), 6.49 (t, *J* = 8.2 Hz, 1H), 6.42 (t, *J* = 7.5 Hz, 1H), 6.07 (d, *J* = 7.3 Hz, 1H), 6.00 (d, *J* = 7.3 Hz, 1H), 5.03 (d, *J* = 2.2 Hz, 1H), 4.58 (d, *J* = 17.5 Hz, 1H), 4.32 (s, 2H), 4.17 (d, *J* = 17.5 Hz, 1H), 3.12 (dq, *J* = 6.6, 2.1 Hz, 1H), 3.00 (s, 3H), 1.31 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz,$CDCl_3$) δ (ppm) 199.0, 164.6, 153.5, 141.0, 140.0, 138.5, 138.4, 137.0, 128.8, 128.5, 127.3, 127.25, 127.2, 126.5, 119.3, 118.4,

105.5, 103.9, 99.4, 97.2, 51.3, 49.5, 48.8, 43.0, 10.7; HRMS (TOF-EI): 545.2139; $C_{34}H_{31}N_3O_2S$ required 545.2137.

(*Z, Z*)-Methyl 2-[1,3-dibenzyl-4'-ethyl-1,3,4',5'-tetrahydro-2'-(phenylimino)spiro[2*H*-benzo[*d*]imidazole-2,3'(2'*H*)-thiophen]-5'-ylidene]acetate (7e): 352mg, 63% (458mg, 82%), yellow crystals (dichloromethane and petroleum ether), mp 144-145 ^oC; IR ν (cm^{-1}) 1699, 1663, 1600, 1509; ^1H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.46 (d, J = 7.3 Hz, 2H), 7.29-7.40 (m, 10H), 7.15 (t, J = 7.3 Hz, 1H), 6.86 (d, J = 7.5 Hz, 2H), 6.58 (t, J = 7.4 Hz, 1H), 6.50 (t, J = 7.4 Hz, 1H), 6.26 (d, J = 7.2 Hz, 1H), 6.05 (s, 1H), 6.04 (d, J = 10.6 Hz, 1H), 4.81 (d, J = 17.1 Hz, 1H), 4.47 (d, J = 16.6 Hz, 1H), 4.42 (d, J = 17.2 Hz, 1H), 4.35 (d, J = 16.5 Hz, 1H), 3.73 (s, 3H), 2.84 (d, J = 7.9 Hz, 1H), 2.32-2.36 (m, 1H), 1.72-1.75 (m, 1H), 0.91 (t, J = 7.4 Hz, 3H); ^{13}C NMR (125 MHz) δ (ppm) 166.4, 165.1, 158.8, 150.2, 141.1, 139.8, 138.7, 137.6, 129.4, 129.2, 128.8, 128.6, 128.4, 127.3, 127.1, 127.0, 126.9, 125.3, 119.9, 118.9, 118.4, 110.2, 109.9, 105.2, 104.0, 98.1, 53.1, 51.6, 49.5, 49.3, 20.4, 13.8; MS (ESI): 560 (M+1). Anal. Calcd for $C_{35}H_{33}N_3O_2S$: C 75.10, H 5.94, N 7.51; Found: C 74.98, H 5.89, N 7.29.

(*Z, Z*)-Methyl 2-[4'-benzyl-1,3-diethyl-1,3,4',5'-tetrahydro-2'-(phenylimino)spiro[benzo[*d*]imidazole-2,3'(2'*H*)-thiophen]-5'-ylidene]acetate (7f): 407mg, 82%, mp 162-163 ^oC.[2] (2. Wang, B.; Li, J.-Q.; Cheng, Y. *Tetrahedron Lett.*, **2008**, 49, 485.)

(*Z, Z*)-Methyl 2-[4'-benzyl-1,3-dibutyl-1,3,4',5'-tetrahydro-2'-(phenylimino)spiro[benzo[*d*]imidazole-2,3'(2'*H*)-thiophen]-5'-ylidene]acetate (7g): 481mg, 87%, mp 121-122 ^oC.[2] (2. Wang, B.; Li, J.-Q.; Cheng, Y. *Tetrahedron Lett.*, **2008**, 49, 485.)

General procedure for the reaction of 2-arylthiocarbamoyl imidazolinium salts 10 with methoxycarbonylallenes 6. Under nitrogen atmosphere, 2-arylthiocarbamoyl imidazolinium salts **10** (1 mmol) were mixed with methoxycarbonylallenes **6** (1.5 mmol) in dry benzene (40 mL). The reaction mixture was stirred at ambient temperature (20-30 ^oC) for 24h or in refluxing benzene for 2-13 h. For the reaction at ambient temperature, solvent benzene was evaporated under vacuum at 30-35 ^oC, and the products **11** (58-83%) and **12** (7-17%) were isolated by chromatography on a neutral Al_2O_3 column eluting with a mixture of petroleum ether (30-60 ^oC) and ethyl acetate (30:1) followed by evaporating solvents at room temperature. For the reaction in refluxing benzene, products **13** (63-74%) and **12** (11-14%) were isolated by chromatography on a silica gel column eluting with a mixture of petroleum ether (30-60 ^oC) and ethyl acetate (30:1).

(*2'Z*, *5'E*)-Methyl 1,3-dibenzyl-4',5'-dihydro-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[imidazolidine-2,3'(2'*H*)-thiophene]-4'-carboxylate (11a): 430mg, 75%, white crystals (ethyl acetate and petroleum ether), mp 136-137 ^oC; IR ν (cm^{-1}) 1738, 1643, 1619, 1591; ^1H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.49 (d, J = 7.4 Hz, 2H), 7.45 (t, J = 7.7 Hz, 2H), 7.41 (d, J = 7.6 Hz, 2H), 7.38 (t, J = 7.4 Hz, 2H), 7.33 (t, J = 7.8 Hz, 2H), 7.18-7.30 (m, 6H), 7.14 (d, J = 10.1 Hz, 2H), 7.12 (d, J = 8.3 Hz, 2H), 5.71 (t, J = 6.4 Hz, 1H), 4.52 (d, J = 13.6 Hz, 1H), 4.40 (s, 1H), 4.16 (d, J = 13.7 Hz, 1H), 3.86 (d, J = 13.8 Hz, 1H), 3.80 (d, J = 13.6 Hz, 1H), 3.72 (s, 3H), 3.40-3.47 (m, 2H), 3.21-3.25 (m, 1H), 3.08-3.13 (m, 2H), 2.90-2.93 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 169.5, 168.1, 151.8, 139.4, 139.3, 139.0, 131.0, 129.4, 128.6, 128.5, 128.4, 128.35, 128.25, 128.2, 127.2, 126.8, 126.4, 125.0, 124.8, 120.0, 95.7, 55.4, 55.1, 53.2, 52.6, 50.6, 49.0, 35.9; MS (MALDI-TOF): 573 (M^+). Anal. Calcd for $C_{36}H_{35}N_3O_2S$: C 75.36, H 6.15, N 7.32; Found: C 75.27, H 6.42, N 7.23.

(*E*)-Methyl 1,3-dibenzyl-1'-phenyl-5'-(2-phenylethylidene)-2'-thioxospiro[imidazolidine-2,3'-pyrrolidine]-4'-carboxylate (12a): 92mg, 16%, yellow crystals (ethyl acetate and petroleum ether), mp 165-166 ^oC; IR ν (cm^{-1}) 1744, 1681, 1602, 1494; ^1H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.58 (t, J = 7.4 Hz, 2H), 7.53 (d, J = 7.5 Hz, 2H), 7.49 (t, J = 7.5 Hz, 1H), 7.38-7.43 (m, 4H), 7.30-7.35 (m, 4H), 7.22-7.29 (m, 4H), 7.18 (t,

J = 6.9 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 2H), 4.86 (t, *J* = 7.8 Hz, 1H), 4.42 (s, 1H), 4.32 (d, *J* = 13.1 Hz, 1H), 4.10 (d, *J* = 13.9 Hz, 1H), 3.98 (d, *J* = 13.9 Hz, 1H), 3.87 (d, *J* = 13.1 Hz, 1H), 3.77 (s, 3H), 3.29-3.35 (m, 2H), 3.14-3.24 (m, 3H), 3.07-3.10 (m, 1H); ^{13}C NMR (125 MHz) δ (ppm) 197.8, 169.0, 141.6, 139.5, 138.9, 138.8, 137.4, 130.1, 129.3, 128.9, 128.55, 128.48, 128.44, 128.3, 128.2, 127.2, 126.9, 126.4, 109.1, 94.8, 54.3, 52.7, 51.7, 50.2, 48.9, 33.9; MS (MALDI-TOF): 573 (M^+). Anal. Calcd for $C_{36}H_{35}N_3O_2S$: C 75.36, H 6.15, N 7.32; Found: C 75.07, H 6.58, N 7.24.

(*Z, Z*)-Methyl 2-[1,3,4'-tribenzyl-4',5'-dihydro-2'-(phenylimino)spiro[imidazolidine-2,3'(2'*H*)-thiophen]-5'-ylidene]acetate (13a): 424mg, 74%, white crystals (ethyl acetate and petroleum ether), mp 101-102 ^{o}C; IR *v* (cm^{-1}) 1711, 1638, 1593; ^{1}H NMR (400 MHz, CD_3COCD_3) 7.39 (d, *J* = 7.4 Hz, 2H), 7.31-7.36 (m, 4H), 7.27 (d, *J* = 7.6 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.14-7.22 (m, 5H), 7.07-7.12 (m, 3H), 7.03 (dd, *J* = 8.2, 1.2 Hz, 2H), 5.95 (d, *J* = 2.3 Hz,1H), 4.36 (d, *J* = 14.4 Hz, 1H), 3.99 (d, *J* = 12.8 Hz, 1H), 3.90 (d, *J* = 14.4 Hz, 1H), 3.78 (d, *J* = 9.4 Hz, 1H), 3.73 (d, *J* = 15.8 Hz, 1H), 3.43 (d, *J* = 13.0 Hz, 1H), 3.41 (s, 3H), 3.08-3.14 (m, 2H), 2.91-2.96 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 168.0, 166.6, 161.2, 150.9, 140.8, 139.4, 138.4, 129.5, 128.9, 128.6, 128.5, 128.4, 128.2, 128.1, 127.3, 127.0, 126.3, 125.1, 120.0, 110.3, 90.9, 54.1, 53.9, 51.4, 50.1, 49.8, 48.1, 33.2; MS (ESI): 574 (M+1). Anal. Calcd for $C_{36}H_{35}N_3O_2S$: C 75.36, H 6.15, N 7.32; Found: C 75.23, H 6.31, N 7.14.

(*2' Z, 5'E*)-Methyl 4',5'-dihydro-1,3-bis(4-methoxybenzyl)-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[imidazolidine-2,3'(2'*H*)-thiophene]-4'-carboxylate (11b): 411mg, 65%, yellow solid (without recrystallization), mp 68-70 ^{o}C; IR *v* (cm^{-1}) 1736, 1612, 1590, 1512; ^{1}H NMR (400 MHz, CD_3COCD_3) δ (ppm) 7.40-7.46 (m, 4H), 7.36 (d, *J* = 8.6 Hz, 2H), 7.17-7.27 (m, 6H), 7.13 (dd, *J* = 8.4, 1.0 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H), 6.90 (d, *J* = 8.8 Hz, 2H), 5.72 (dt, *J* = 7.7, 2.4 Hz, 1H), 4.52 (d, *J* = 1.0 Hz, 1H), 4.44 (d, *J* = 12.9 Hz, 1H), 4.16 (d, *J* = 13.4 Hz, 1H), 3.80 (d, *J* = 13.5 Hz, 1H), 3.80 (s, 3H), 3.79 (s, 3H), 3.78 (s, 3H), 3.69 (d, *J* = 12.9 Hz, 1H), 3.44 (d, *J* = 6.8 Hz, 2H), 3.02-3.07 (m, 2H), 2.97-3.00 (m, 1H), 2.82-2.88 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 169.2, 167.9, 159.0, 158.8, 152.1, 139.6, 131.2, 131.1, 130.8, 129.46, 129.45, 129.3, 128.43, 128.35, 126.2, 124.74, 124.71, 119.9, 113.6, 113.4, 95.3, 54.61, 54.55, 54.5, 54.4, 52.1, 51.9, 49.9, 48.5, 35.6; MS (ESI): 634 (M+1). Anal. Calcd for $C_{38}H_{39}N_3O_4S$: C 72.01, H 6.20, N 6.63; Found: C 72.35, H 6.40, N 6.28.

(*E*)-Methyl 1,3-bis(4-methoxybenzyl)-1'-phenyl-5'-(2-phenylethylidene)-2'-thioxospiro[imidazolidine-2,3'-pyrrolidine]-4'-carboxylate (12b): 76mg, 12%, yellow crystals (ethyl acetate and petroleum ether), mp: 152-153 ^{o}C; IR *v* (cm^{-1}) 1744, 1678, 1610, 1511; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.47 (t, *J* = 7.4 Hz, 2H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 2H), 7.23 (d, *J* = 8.5 Hz, 2H), 7.15 (t, *J* = 7.2 Hz, 3H), 7.08 (t, *J* = 7.2 Hz, 2H), 6.98 (d, *J* = 7.3 Hz, 2H), 6.82 (d, *J* = 8.5 Hz, 2H), 6.78 (d, *J* = 8.5 Hz, 2H), 4.75 (dt, *J* = 7.3, 2.0 Hz, 1H), 4.30 (s, 1H), 4.11 (d, *J* = 12.6 Hz, 1H), 3.93 (d, *J* = 13.7 Hz, 1H), 3.81 (d, *J* = 13.5 Hz, 1H), 3.75 (s, 3H), 3.73 (s, 3H), 3.69 (s, 3H), 3.69 (d, *J* = 12.6 Hz, 1H), 2.93-3.26 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.9, 169.0, 158.8, 158.5, 141.6, 139.5, 137.4, 131.0, 130.8, 130.0, 129.6, 129.56, 129.2, 128.5, 128.2, 128.1, 126.3, 113.8, 113.5, 109.0, 94.5, 55.3, 55.2, 53.5, 52.6, 52.0, 51.5, 49.9, 48.8, 33.9; MS (ESI): 634(M+1). Anal. Calcd for $C_{38}H_{39}N_3O_4S$: C 72.01, H 6.20, N 6.63; Found: C 72.11, H 6.34, N 6.50.

(*Z, Z*)-Methyl 2-[4'-benzyl-4',5'-dihydro-1,3-bis(4-methoxybenzyl)-2'-(phenylimino)spiro[imidazolidine-2,3'(2'*H*)-thiophen]-5'-ylidene]acetate (13b): 443mg, 70%, white crystals (ethyl acetate and petroleum ether), mp 163-164 ^{o}C; IR *v* (cm^{-1}) 1706, 1650, 1612, 1511; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.44 (t, *J* = 7.1 Hz, 2H), 7.34-7.37 (m, 6H), 7.28-7.29 (m, 3H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.11 (d, *J* = 7.2 Hz, 2H), 6.92 (d, *J* = 7.8 Hz, 2H), 6.85 (d, *J* = 7.8 Hz, 2H), 6.09 (s, 1H), 4.21 (d, *J* = 13.9 Hz, 1H), 4.04 (d, *J* = 12.8 Hz, 1H), 3.97 (d, *J* = 13.8 Hz, 1H), 3.88 (d, *J* = 12.9 Hz, 1H), 3.84 (s, 3H), 3.82 (s, 3H), 3.68 (d, *J* = 8.6 Hz, 1H), 3.63 (s, 3H), 3.44 (d, *J* = 12.7 Hz, 1H), 3.22-3.23 (m, 1H), 3.09 (brs, 3H), 3.01-3.02 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) 168.2, 166.7, 161.4, 159.0, 158.8, 151.1, 141.0, 131.5, 130.6, 129.6, 129.4, 129.3, 129.0, 128.5, 126.4, 125.2, 120.2, 114.1, 114.0,

110.3, 90.9, 55.44, 55.39, 53.6, 53.3, 51.5, 50.1, 49.8, 48.1, 33.3; MS (ESI): 634 (M+1). Anal. Calcd for $C_{38}H_{39}N_3O_4S$: C 72.01, H 6.20, N 6.63; Found: C 72.12, H 6.48, N 6.50.

(*2' Z*, *5'E*)-Methyl 1,3-bis(4-chlorobenzyl)-4',5'-dihydro-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[imidazolidine-2,3'(2'*H*)-thiophene]-4'-carboxylate (11c): 404mg, 63%, white crystals (ethyl acetate and petroleum ether), mp 128-129 ^oC; IR ν (cm^{-1}) 1742, 1618, 1590, 1488; ^1H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.45 (t, *J* = 7.5 Hz, 2H), 7.41 (d, *J* = 8.1 Hz, 2H), 7.35 (d, *J* = 8.1 Hz, 4H), 7.31 (d, *J* = 8.3 Hz, 2H), 7.19-7.27 (m, 4H), 7.13 (d, *J* = 7.3 Hz, 2H), 7.09 (d, *J* = 7.7 Hz, 2H), 5.72 (t, *J* = 6.9 Hz, 1H), 4.45 (d, *J* = 13.7 Hz, 1H), 4.33 (s, 1H), 4.09 (d, *J* = 14.0 Hz, 1H), 3.82 (d, *J* = 14.0 Hz, 1H), 3.73 (d, *J* = 13.7 Hz, 1H), 3.72 (s, 3H), 3.36-3.48 (m, 2H), 3.16-3.20 (m, 1H), 3.05-3.10 (m, 2H), 2.87-2.89 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$)) δ (ppm) 169.4, 167.7, 151.5, 139.2, 137.7, 137.5, 132.9, 132.5, 130.7, 129.7, 129.6, 129.4, 128.65, 128.59, 128.35, 128.30, 126.5, 125.2, 125.1, 120.0, 95.6, 54.9, 54.8, 52.6, 52.5, 50.4, 48.9, 35.8; MS (ESI): 642 (M+1). Anal. Calcd for $C_{36}H_{33}Cl_2N_3O_2S$: C 67.28, H 5.18, N 6.54; Found: C 67.45, H 5.09, N 6.55.

(*E*)-Methyl 1,3-bis(4-chlorobenzyl)-1'-phenyl-5'-(2-phenylethylidene)-2'-thioxospiro[imidazolidine-2,3'-pyrrolidine]-4'-carboxylate (12c): 109mg, 17%, yellow crystals (ethyl acetate and petroleum ether), mp 172-173 ^oC; IR ν (cm^{-1}) 1749, 1492; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.56 (t, *J* = 7.7 Hz, 2H), 7.47 (t, *J* = 7.4 Hz, 1H), 7.42 (d, *J* = 8.3 Hz, 2H), 7.28-7.34 (m, 6H), 7.14-7.24 (m, 5H), 7.05 (d, *J* = 7.4 Hz, 2H), 4.86 (dt, *J* = 7.7, 1.6 Hz, 1H), 4.32 (s, 1H), 4.23 (d, *J* = 13.2 Hz, 1H), 4.00 (d, *J* = 14.1 Hz, 1H), 3.91 (d, *J* = 14.0 Hz, 1H), 3.79 (d, *J* = 13.3 Hz, 1H), 3.75 (s, 3H), 3.00-3.34 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$)) δ (ppm) 197.4, 168.9, 141.3, 139.3, 137.3, 137.22, 137.16, 132.9, 132.6, 130.1, 129.8, 129.7, 129.3, 128.6, 128.5, 128.3, 128.2, 128.0, 126.4, 109.3, 94.5, 53.6, 52.7, 52.0, 51.5, 50.0, 48.7, 33.8; MS (ESI): 642 (M+1). Anal. Calcd for $C_{36}H_{33}Cl_2\ N_3O_2S$: C 67.28, H 5.18, N 6.54; Found: C 67.28, H 5.29, N 6.28.

(*Z, Z*)-Methyl 2-[4'-benzyl-1,3-bis(4-chlorobenzyl)-4',5'-dihydro-2'-(phenylimino)spiro[imidazolidine-2,3'(2'*H*)-thiophen]-5'-ylidene]acetate (13c): 455mg, 71%, white crystals (ethyl acetate and petroleum ether), mp 171-172 ^oC; IR ν (cm^{-1}) 1708, 1641, 1607, 1488; ^1H NMR (500 MHz, CD_3COCD_3) δ (ppm) 7.59 (d, *J* = 8.1 Hz, 2H), 7.41-7.50 (m, 8H), 7.33-7.37 (m, 4H), 7.27 (t, *J* = 7.5 Hz, 1H), 7.24 (t, *J* = 7.5 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 6.10 (s, 1H), 4.51 (d, *J* = 14.7 Hz, 1H), 4.10 (d, *J* = 13.1 Hz, 1H), 4.06 (d, *J* = 14.8 Hz, 1H), 3.92 (d, *J* = 9.1 Hz, 1H), 3.84 (d, *J* = 15.6 Hz, 1H), 3.60 (d, *J* = 13.1 Hz, 1H), 3.56 (s, 3H), 3.23-3.28 (m, 2H), 3.08-3.10 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.8, 166.6, 160.8, 150.7, 140.5, 137.8, 136.8, 133.0, 132.7, 129.55, 129.51, 129.3, 129.0, 128.7, 128.6, 128.4, 128.3, 126.5, 125.3, 120.0, 110.5, 90.9, 53.5, 53.2, 51.5, 49.9, 49.7, 48.1, 33.1; MS (ESI): 642 (M+1). Anal. Calcd for $C_{36}H_{33}Cl_2N_3O_2S$: C 67.28, H 5.18, N 6.54; Found: C 67.32, H 5.20, N 6.51.

(*2' Z*, *5'E*)-Methyl 2'-(4-bromophenylimino)-1,3-bis(4-chlorobenzyl)-4',5'-dihydro-5'-(2-phenylethylidene)spiro[imidazolidine-2,3'(2'*H*)-thiophene]-4'-carboxylate (11d): 597mg, 83%, white crystals (ethyl acetate and petroleum ether), mp 109-110 ^oC; IR ν (cm^{-1}) 1747, 1614, 1579, 1490, 1480; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 7.60 (d, *J* = 7.7 Hz, 2H), 7.53 (d, *J* = 7.7 Hz, 2H), 7.46 (d, *J* = 7.9 Hz, 2H), 7.38 (t, *J* = 8.1 Hz, 4H), 7.24 (t, *J* = 7.7 Hz, 2H), 7.17-7.20 (m, 3H), 7.12 (d, *J* = 7.5 Hz, 2H), 5.77 (t, *J* = 7.2 Hz, 1H), 4.55 (s, 1H), 4.47 (d, *J* = 13.5 Hz, 1H), 4.24 (d, *J* = 14.1 Hz, 1H), 3.87 (d, *J* = 14.1Hz, 1H), 3.78 (s, 3H), 3.73 (d, *J* = 13.5 Hz, 1H), 3.37-3.48 (m, 2H), 3.00-3.11 (m, 3H), 2.86-2.89 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 169.97, 169.94, 151.9, 140.4, 139.2, 139.0, 133.2, 133.0, 132.9, 131.0, 130.9, 129.3, 129.24, 129.17, 129.0, 127.1, 126.4, 123.0, 118.2, 96.4, 55.2, 55.1, 52.9, 52.8, 50.7, 49.5, 36.5; MS (ESI): 720 (M+1). Anal. Calcd for $C_{36}H_{32}BrCl_2N_3O_2S$: C 59.93, H 4.47, N 5.82; Found: C 59.61, H 4.73, N 5.73.

(*E*)-Methyl 1'-(4-bromophenyl)-1,3-bis(4-chlorobenzyl)-5'-(2-phenylethylidene)-2'-thioxospiro[imidazolidine-2,3'-pyrrolidine]-4'-carboxylate (12d): 79mg, 11%, yellow crystals (ethyl acetate and petroleum ether), mp 207-208 ^oC; IR ν

(cm^{-1}) 1739, 1672, 1489; ^1H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.67 (d, *J* = 8.8 Hz, 2H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.29-7.34 (m, 6H), 7.16-7.25 (m, 3H), 7.09 (brs, 2H), 7.05 (d, *J* = 6.9 Hz, 2H), 4.85 (dt, *J* = 7.9, 2.2 Hz, 1H), 4.32 (t, *J* = 1.0 Hz, 1H), 4.18 (d, *J* = 13.2 Hz, 1H), 3.98 (d, *J* = 14.0 Hz, 1H), 3.88 (d, *J* = 14.0 Hz, 1H), 3.76 (s, 3H), 3.74 (d, *J* = 13.2 Hz, 1H), 2.98-3.33 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.5, 168.8, 141.0, 139.1, 137.1, 137.0, 136.1, 133.5, 133.0, 132.6, 129.83, 129.76, 129.69, 128.6, 128.3, 128.2, 126.5, 123.4, 109.5, 94.5, 53.6, 52.8, 52.0, 51.4, 49.9, 48.7, 33.8; MS (ESI): 720 (M+1). Anal. Calcd for $C_{36}H_{32}BrCl_2N_3O_2S$: C 59.93, H 4.47, N 5.82; Found: C 59.88, H 4.78, N 5.71.

(*2' Z*, *5'E*)-Methyl

1,3-bis(4-chlorobenzyl)-2'-(3,4-dichlorophenylimino)-4',5'-dihydro-5'-(2-phenylethylidene)spiro[imidazolidine-2,3'(2'*H*)-thiophene]-4'-carboxylate (11e): 426mg, 60%, white crystals (ethyl acetate and petroleum ether), mp 113-114°C; IR *v* (cm^{-1}) 1747, 1609, 1582, 1490; ^1H NMR (400 MHz, CD_3COCD_3) δ (ppm) 7.63 (d, *J* = 8.5 Hz, 1H), 7.54 (d, *J* = 8.3 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.36-7.40 (m, 5H), 7.15-7.26 (m, 6H), 5.80 (dt, *J* = 7.9, 2.4 Hz, 1H), 4.56 (d, *J* = 1.0 Hz, 1H), 4.47 (d, *J* = 13.4 Hz, 1H), 4.26 (d, *J* = 14.1 Hz, 1H), 3.88 (d, *J* = 14.2 Hz, 1H), 3.78 (s, 3H), 3.74 (d, *J* = 13.5 Hz, 1H), 3.38-3.49 (m, 2H), 3.03-3.12 (m, 3H), 2.87-2.90 (m, 1H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 170.8, 169.0, 151.5, 139.4, 138.2, 138.0, 132.4, 132.2, 132.0, 131.3, 130.01, 129.98, 129.8, 128.5, 128.4, 128.3, 128.1, 127.6, 126.2, 125.9, 122.0, 120.3, 95.6, 54.3, 54.1, 52.1, 51.9, 49.8, 48.6, 35.7; MS (ESI): 710 (M+1). Anal. Calcd for $C_{36}H_{31}Cl_4N_3O_2S$: C 60.77, H 4.39, N 5.91; Found: C 60.85, H 4.48, N 5.81.

(*E*)-Methyl

1,3-bis(4-chlorobenzyl)-1'-(3,4-dichlorophenyl)-5'-(2-phenylethylidene)-2'-thioxospiro[imidazolidine-2,3'-pyrrolidine]-4'-carboxylate (12e): 50mg, 7%, yellow crystals (ethyl acetate and petroleum ether), mp 173-174 °C; IR *v* (cm^{-1}) 1737, 1674, 1490, 1471; ^1H NMR (400 MHz) δ (ppm) 7.62 (d, *J* = 8.5 Hz, 1H), 7.40 (d, *J* = 8.4 Hz, 2H), 7.28-7.34 (m, 7H), 7.22-7.25 (m, 2H), 7.16-7.20 (m, 1H), 7.07 (brs, 1H), 7.06 (dd, *J* = 6.9, 1.2 Hz, 2H), 4.86 (dt, *J* = 7.9, 2.2 Hz, 1H), 4.31 (t, *J* = 1.0 Hz, 1H), 4.16 (d, *J* = 13.2 Hz, 1H), 3.96 (d, *J* = 14.0 Hz, 1H), 3.86 (d, *J* = 14.0 Hz, 1H), 3.76 (s, 3H), 3.72 (d, *J* = 13.5 Hz, 1H), 3.32 (dd, *J* = 16.2, 7.2 Hz, 1H), 3.19-3.24 (m, 1H), 3.06-3.17 (m, 2H), 2.97-3.02 (m, 1H); ^{13}C NMR (100 MHz) δ (ppm) 197.7, 168.7, 140.8, 139.0, 137.0, 136.9, 136.2, 134.1, 133.9, 133.0, 132.7, 131.9, 130.3, 129.8, 129.7, 128.64, 128.61, 128.3, 128.2, 127.7, 126.6, 109.5, 94.4, 53.6, 52.8, 52.0, 51.4, 49.9, 48.7, 33.8; MS (ESI): 710 (M+1). Anal. Calcd for $C_{36}H_{31}Cl_4N_3O_2S$: C 60.77, H 4.39, N 5.91; Found: C 60.56, H 4.47, N 5.73.

(*Z, Z*)-Methyl

2-[4'-benzyl-1,3-bis(4-chlorobenzyl)-2'-(3,4-dichlorophenylimino)-4',5'-dihydrospiro[imidazolidine-2,3'(2'*H*)-thiophen]-5'-ylidene]acetate (13e): 448mg, 63%, white crystals (ethyl acetate and petroleum ether), mp 162-163 °C; IR *v* (cm^{-1}) 1703, 1601, 1490, 1464; ^1H NMR (500 MHz, CD_3COCD_3) δ (ppm) 7.68 (d, *J* = 8.5 Hz, 1H), 7.58 (d, *J* = 8.2 Hz, 2H), 7.40-7.46 (m, 7H), 7.33-7.37 (m, 4H), 7.27 (t, *J* = 7.3 Hz, 1H), 7.20 (dd, *J* = 8.5, 2.2 Hz, 1H), 6.13 (d, *J* = 2.1 Hz, 1H), 4.53 (d, *J* = 14.8 Hz, 1H), 4.09 (d, *J* = 13.0 Hz, 1H), 4.04 (d, *J* = 14.8 Hz, 1H), 3.94 (d, *J* = 9.2 Hz, 1H), 3.83 (d, *J* = 15.4 Hz, 1H), 3.61 (d, *J* = 13.0 Hz, 1H), 3.58 (s, 3H), 3.24-3.29 (m, 2H), 3.05-3.10 (m, 3H); ^{13}C NMR (100 MHz, CD_3COCD_3) δ (ppm) 172.7, 166.7, 160.5, 152.0, 141.6, 139.6, 138.2, 133.3, 132.8, 132.3, 131.1, 130.6, 129.7, 129.33, 129.30, 129.2, 128.5, 127.2, 122.8, 121.2, 111.6, 91.9, 53.8, 53.7, 51.7, 50.4, 50.2, 48.6, 33.6; MS (ESI): 710 (M+1). Anal. Calcd for $C_{36}H_{31}Cl_4N_3O_2S$: C 60.77, H 4.39, N 5.91; Found: C 60.86, H 4.72, N 5.85.

(*2' Z*, *5'E*)-Methyl

1,3-dibenzyl-4',5'-dihydro-2'-(phenylimino)-5'-propylidenespiro[imidazolidine-2,3'(2'*H*)-thiophene]-4'-carboxylate (11f): 297mg, 58%, white crystals (ethyl acetate and petroleum ether), mp 140-141 °C; IR *v* (cm^{-1}) 1743, 1731, 1619, 1592; ^1H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.52 (d, *J* = 7.4 Hz, 2H), 7.45 (t, *J* = 7.7 Hz, 2H), 7.37-7.41 (m, 4H), 7.30-7.34 (m, 3H), 7.20-7.26 (m, 2H), 7.12 (d, *J* = 7.4 Hz, 2H), 5.47 (dt, *J* = 7.9, 2.1 Hz, 1H), 4.50 (d, *J* = 13.5 Hz, 1H), 4.30 (s, 1H), 4.18 (d, *J* = 13.9 Hz, 1H), 3.86 (d, *J* = 13.8 Hz, 1H), 3.77 (s, 3H), 3.74 (d, *J* = 13.5 Hz, 1H), 3.19-3.23 (m, 1H), 3.07-3.14 (m, 2H), 2.88-2.92 (m, 1H), 2.04-2.11 (m, 2H), 0.98 (t, *J* = 7.5 Hz,

3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 169.6, 168.4, 151.9, 139.3, 139.2, 129.3, 128.9, 128.4, 128.35, 128.3, 128.2, 128.1, 127.1, 126.7, 124.9, 120.0, 95.7, 55.3, 54.7, 53.1, 52.5, 50.4, 49.0, 23.5, 13.5; MS (ESI): 512(M+1). Anal. Calcd for $C_{31}H_{33}N_3O_2S$: C 72.77, H 6.50, N 8.21; Found: C 72.73, H 6.53, N 8.08.

(*E*)-Methyl

1,3-dibenzyl-1'-phenyl-5'-propylidene-2'-thioxospiro[imidazolidine-2,3'-pyrrolidine]-4'-carboxylate (12f): 87mg, 17%, yellow crystals (ethyl acetate and petroleum ether), mp 144-145 ^{o}C; IR *v* (cm^{-1}) 1740, 1675, 1496, 1412, 1362; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.50 (t, *J* = 8.2 Hz, 2H), 7.39-7.45 (m, 3H), 7.27-7.31 (m, 4H), 7.20-7.24 (m, 3H), 7.14 (t, *J* = 7.2 Hz, 2H), 7.12 (bs, 1H), 4.50 (td, *J* = 7.7, 2.3 Hz, 1H), 4.24 (t, *J* = 1.0 Hz, 1H), 4.19 (d, *J* = 13.1 Hz, 1H), 4.00 (d, *J* = 14.0 Hz, 1H), 3.88 (d, *J* = 14.0 Hz, 1H), 3.72 (d, *J* = 13.0 Hz, 1H), 3.72 (s, 3H), 3.18-3.22 (m, 1H), 3.04-3.11 (m, 2H), 2.96-3.01 (m, 1H), 1.72-1.88 (m, 2H), 0.80 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 197.4, 169.0, 140.1, 139.0, 138.9, 137.5, 130.0, 129.0, 128.4, 128.2, 128.19, 128.1, 128.06, 127.1, 126.8, 112.2, 94.8, 77.3, 77.0, 76.7, 54.1, 52.6, 52.57, 51.4, 50.0, 48.9, 21.5, 13.6; MS (ESI): 512 (M+1).Anal. Calcd for $C_{31}H_{33}N_3O_2S$: C 72.77, H 6.50, N 8.21; Found: C 72.69, H 6.14, N 8.13.

(*2' Z*, *5'E*)-Methyl

1,3-dibenzyl-5'-(*iso*-butylidene)-4',5'-dihydro-2'-(phenylimino)spiro[imidazolidine-2,3'(2'*H*)-thiophene]-4'-carboxylate (11g): 331mg, 63%, white crystals (ethyl acetate and petroleum ether), mp 132-133 ^{o}C; IR *v* (cm^{-1}) 1742, 1730, 1618, 1594; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.51 (d, *J* = 7.4 Hz, 2H), 7.45 (t, *J* = 7.9 Hz, 2H), 7.37-7.41 (m, 4H), 7.30-7.35 (m, 3H), 7.20-7.26 (m, 2H), 7.11 (d, *J* = 7.5 Hz, 2H), 5.31 (dd, *J* = 10.4, 1.9 Hz, 1H), 4.50 (d, *J* = 13.7 Hz, 1H), 4.33 (d, *J* = 1.9 Hz, 1H), 4.16 (d, *J* = 13.7 Hz, 1H), 3.85 (d, *J* = 13.7 Hz, 1H), 3.79 (d, *J* = 13.7 Hz, 1H), 3.74 (s, 3H), 3.20-3.23 (m, 1H), 3.06-3.12 (m, 2H), 2.87-2.90 (m, 1H), 2.46-2.50 (m, 1H), 0.96 (d, *J* = 6.5 Hz, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 169.9, 168.5, 151.9, 139.5, 139.1, 133.6, 129.3, 128.4, 128.2, 128.1, 127.5, 127.1, 126.7, 124.9, 120.0, 95.5, 55.4, 55.0, 53.2, 52.5, 50.6, 48.9, 29.8, 22.7, 21.9; MS (ESI): 526 (M+1). Anal. Calcd for $C_{32}H_{35}N_3O_2S$: C 73.11, H 6.71, N 7.99; Found: C 73.17, H 6.77, N 7.77.

(*E*)-Methyl

1,3-dibenzyl-5'-(*iso*-butylidene)-1'-phenyl-2'-thioxospiro[imidazolidine-2,3'-pyrrolidine]-4'-carboxylate (12g): 89mg, 17%, yellow crystals (ethyl acetate and petroleum ether), mp 166-167 ^{o}C; IR *v* (cm^{-1}) 1742, 1674, 1597, 1496; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.58 (t, *J* = 8.2 Hz, 2H), 7.47-7.52 (m, 3H), 7.35-7.40 (m, 4H), 7.28-7.32 (m, 3H), 7.22 (t, *J* = 7.2 Hz, 2H), 7.20 (brs, 1H), 4.43 (dd, *J* = 10.6, 2.2 Hz, 1H), 4.33 (d, *J* = 2.2 Hz, 1H), 4.27 (d, *J* = 13.3 Hz, 1H), 4.06 (d, *J* = 13.9 Hz, 1H), 3.94 (d, *J* = 13.9 Hz, 1H), 3.84 (d, *J* = 13.3 Hz, 1H), 3.77 (s, 3H), 3.26-3.31 (m, 1H), 3.18-3.22 (m, 1H), 3.11-3.15 (m, 1H), 3.02-3.07 (m, 1H), 2.13-2.22 (m, 1H), 0.88 (d, *J* = 6.4 Hz, 3H), 0.86 (d, *J* = 6.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 197.4, 169.3, 139.0, 138.9, 138.87, 137.6, 129.9, 129.0, 128.4, 128.39, 128.3, 128.2, 128.1, 127.2, 126.7, 117.7, 94.7, 54.3, 52.7, 52.5, 51.6, 50.2, 48.9, 28.1, 23.0, 22.0; MS (ESI): 526 (M+1). Anal. Calcd for $C_{32}H_{35}N_3O_2S$: C 73.11, H 6.71, N 7.99; Found: C 73.09, H 6.32, N 8.00.

General procedure for the reaction of 2-arylthiocarbamoyl triazolium salts 14 with methoxycarbonylallenes 6. 2-Arylthiocarbamoyl triazolium salts **14** (2 mmol) were mixed with methoxycarbonylallenes **6** (3 mmol) in dry benzene or toluene (60 mL) under nitrogen atmosphere. The reaction mixture in benzene was stirred at ambient temperature (20-30 ^{o}C) for 15-24 h or in refluxing toluene for 2-12 h. For the reaction at ambient temperature, solvent benzene was evaporated under vacuum at 30-35 ^{o}C, and the products **15-I** (52-65%), **15-II** (10-13%) and **16-I** (14-24%), **16-II** (4-6%) were isolated by chromatography on a silica gel column eluting with a mixture of petroleum ether (30-60 ^{o}C) and ethyl acetate (15:1) followed by evaporating solvents at room temperature. For the reaction in refluxing toluene, products **17** (52-63%) and **18** (19-22%) were isolated by chromatography on a silica gel column eluting with a mixture of petroleum ether (30-60 ^{o}C) and ethyl acetate (15:1).

(*5S, 4'R, 2' Z*, *5'E*) or (*5R, 4'S*, *2' Z*, *5'E*)-Methyl

1,4,4',5'-tetrahydro-1,3,4-triphenyl-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15a-I): 806mg, 65%, yellow solid (without recrystallization), mp 96-97 ^{o}C; IR *v* (cm^{-1}) 1744, 1626, 1593, 1492; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.59 (dd, *J* = 7.3, 1.5 Hz, 2H), 7.37 (t, *J* = 8.0 Hz, 2H), 7.26-7.32 (m, 9H), 7.23-7.24 (m, 5H), 7.14-7.18 (m, 4H), 7.07 (t, *J* = 7.5 Hz, 1H), 6.97 (t, *J* = 7.0 Hz, 1H), 6.08 (d, *J* = 7.5 Hz, 2H), 5.88 (dt, *J* = 6.1, 2.6 Hz, 1H), 4.91 (t, *J* = 1.1 Hz, 1H), 3.67 (s, 3H), 3.48 (dd, *J* = 16.1, 6.2 Hz, 1H), 3.30 (dd, *J* = 16.2, 8.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 169.8, 165.0, 151.5, 147.5, 140.8, 139.4, 139.0, 129.24, 129.20, 129.0, 128.7, 128.6, 128.44, 128.38, 127.8, 127.7, 127.4, 127.2, 126.60, 126.56, 125.0, 119.9, 118.5, 114.7, 98.1, 53.4, 52.9, 36.6; HRMS (TOF-EI): 620.2252; $C_{39}H_{32}N_4O_2S$ required 620.2246.

(*5R, 4'R, 2' Z, 5'E*) or (*5S, 4'S, 2' Z, 5'E*)-Methyl 1,4,4',5'-tetrahydro-1,3,4-triphenyl-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15a-II): 160mg, 13%, yellow crystals, mp 153-154 ^{o}C; IR *v* (cm^{-1}) 1750, 1633, 1592, 1487; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.55 (d, *J* = 7.2 Hz, 2H), 7.44 (d, *J* = 7.8 Hz, 2H), 7.23-7.35 (m, 10H), 7.13-7.21 (m, 7H), 7.00-7.06 (m, 2H), 6.20 (d, *J* = 7.7 Hz, 2H), 5.86 (t, *J* = 6.8 Hz, 1H), 4.58 (s, 1H), 3.64 (s, 3H), 3.49 (dd, *J* = 16.2, 6.6 Hz, 1H), 3.35 (dd, *J* = 16.1, 8.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 168.7, 166.1, 151.6, 149.5, 143.7, 139.0, 138.5, 129.4, 129.2, 129.1, 128.7, 128.44, 128.39, 128.3, 128.22, 127.8, 127.1, 127.0, 126.5, 124.9, 122.0, 119.5, 118.5, 99.8, 57.0, 52.9, 36.2; MS (-c ESI): 619 (M-1). Anal. Calcd for $C_{39}H_{32}N_4O_2S$: C 75.46, H 5.20, N 9.03; Found: C 75.62, H 5.38, N 8.74.

(*5S, 4'R, E*) or (*5R, 4'S, E*)-Methyl 1,4-dihydro-1,1',3,4-tetraphenyl-5'-(2-phenylethylidene)-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'-pyrrolidine]-4'-carboxylate (16a-I): 186mg, 15%, yellow crystals, mp 177-178 ^{o}C; IR *v* (cm^{-1}) 1746, 1594, 1492; ^{1}H NMR (500 MHz) δ (ppm) 7.56 (d, *J* = 7.3 Hz, 2H), 7.53 (brs, 1H), 7.41 (brs, 2H), 7.37 (t, *J* = 7.7 Hz, 2H), 7.20-7.32 (m, 14H), 7.17 (d, *J* = 7.7 Hz, 2H), 6.99 (t, *J* = 7.2 Hz, 1H), 6.66 (brs, 1H), 5.19 (t, *J* = 7.0 Hz, 1H), 5.03 (s, 1H), 3.57 (s, 3H), 3.48 (dd, *J* = 16.5, 7.0 Hz, 1H), 3.24 (dd, *J* = 16.4, 8.1Hz, 1H); ^{13}C NMR (125 MHz) δ (ppm) 190.4, 169.2, 147.5, 141.3, 139.3, 139.1, 138.9, 137.3, 130.2, 129.4, 129.3, 129.2, 128.6, 128.4, 128.0, 127.7, 127.0, 126.5, 126.4, 120.6, 115.6, 112.2, 97.2, 52.8, 49.4, 34.3; MS (-c ESI): 619 (M-1). Anal. Calcd for $C_{39}H_{32}N_4O_2S$: C 75.46, H 5.20, N 9.03; Found: C 75.29, H 5.40, N 8.92.

(*5R, 4'R, E*) or (*5S, 4'S, E*)-Methyl 1,4-dihydro-1,1',3,4-tetraphenyl-5'-(2-phenylethylidene)-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'-pyrrolidine]-4'-carboxylate (16a-II): 62mg, 5%, yellow crystals, mp 164-165 ^{o}C; IR *v* (cm^{-1}) 1748, 1593, 1493; ^{1}H NMR (500 MHz) δ (ppm) 7.49 (t, *J* = 7.3 Hz, 4H), 7.43 (d, *J* = 7.1 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.26-7.36 (m, 10H), 7.22 (t, *J* = 6.9 Hz, 2H), 7.18 (t, *J* = 7.0 Hz, 1H), 6.99-7.03 (m, 5H), 5.10 (t, *J* = 7.6 Hz, 1H), 4.43 (s, 1H), 3.77 (s, 3H), 3.40 (dd, *J* = 16.7, 6.9 Hz, 1H), 3.16 (dd, *J* = 16.4, 8.2 Hz, 1H); ^{13}C NMR (125 MHz) δ (ppm) 193.1, 168.1, 149.9, 143.6, 139.4, 139.3, 137.9, 137.3, 130.2, 129.5, 129.3, 128.5, 128.3, 128.2, 127.7, 127.2, 126.3, 122.4, 119.3, 111.6, 99.0, 52.9, 51.3, 33.9; MS (-c ESI): 619 (M-1). Anal. Calcd for $C_{39}H_{32}N_4O_2S$: C 75.46, H 5.20, N 9.03; Found: C 75.16, H 5.42, N 8.78.

(*Z*) Methyl 1,4-dihydro-5'-phenethyl-1,3,4-triphenyl-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (17a): 768mg, 62%, red crystals, mp 110-111 ^{o}C; IR *v* (cm^{-1}) 1699, 1641, 1593, 1493; ^{1}H NMR (500 MHz) δ (ppm) 7.54 (d, *J* = 6.7 Hz, 2H), 7.22-7.32 (m, 15H), 7.11-7.13 (m, 3H), 7.04 (d, *J* = 6.5 Hz, 2H), 6.88 (t, *J* = 6.7 Hz, 1H), 6.50 (d, *J* = 7.3 Hz, 2H), 3.72 (s, 3H), 3.21-3.27 (m, 2H), 2.82 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR (125 MHz) δ (ppm) 166.6, 162.4, 159.8, 151.2, 147.3, 143.0, 140.0, 138.6, 129.6, 129.2, 129.1, 128.7, 128.6, 128.3, 128.2, 128.0, 127.5, 126.6, 126.5, 125.6, 120.1, 119.9, 118.8, 114.7, 98.0, 51.8, 34.3, 34.1; MS (-c ESI): 619 (M-1). Anal. Calcd for $C_{39}H_{32}N_4O_2S$: C 75.46, H 5.20, N 9.03; Found: C 75.57, H 5.32, N 8.98.

Methyl 1,4-dihydro-5'-phenethyl-1,1',3,4-tetraphenyl-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-pyrrole]-4'-carboxylate (18a): 273mg, 22%, green crystals, mp 167-168 ^{o}C; IR *v* (cm^{-1}) 1705, 1629, 1594, 1492; ^{1}H NMR (500 MHz)

δ (ppm) 7.57-7.61 (m, 3H), 7.54 (d, *J* = 7.3 Hz, 2H), 7.23-7.34 (m, 8H), 7.15-7.21 (m, 4H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 7.5 Hz, 2H), 6.88 (t, *J* = 6.8 Hz, 2H), 6.84 (d, *J* = 7.0 Hz, 2H), 3.74 (s, 3H), 2.91-2.97 (m, 1H), 2.82-2.87 (m, 1H), 2.53 (t, *J* = 8.4 Hz, 2H); ^{13}C NMR (125 MHz) δ (ppm) 207.4, 162.5, 160.4, 147.4, 143.2, 139.9, 138.1, 135.9, 130.2, 130.1, 129.9, 129.1, 128.8, 128.7, 128.6, 128.4, 128.2, 128.1, 127.8, 127.5, 126.9, 126.5, 120.1, 114.8, 111.2, 95.2, 51.4, 33.4, 29.2; MS (-c ESI): 619 (M-1). Anal. Calcd for $C_{39}H_{32}N_4O_2S$: C 75.46, H 5.20, N 9.03; Found: C 75.16, H 5.42, N 8.79.

(*5S, 4'R, 2' Z*, *5'E*) or (*5R, 4'S*, *2' Z*, *5'E*)-Methyl 1,4,4',5'-tetrahydro-4-(4-methoxyphenyl)-1,3-diphenyl-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[3*H*-1, 2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15b-I): 793mg, 61%, yellow crystals, mp 179-180 °C; IR *ν* (cm^{-1}) 1740, 1629, 1594, 1507, 1495, 1486; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.58 (dd, *J* = 7.7, 2.2 Hz, 2H), 7.37 (d, *J* = 7.7 Hz, 2H), 7.24-7.32 (m, 7H), 7.17-7.22 (m, 7H), 7.06 (t, *J* = 7.4 Hz, 1H), 6.96 (t, *J* = 7.3 Hz, 1H), 6.78 (d, *J* = 7.3 Hz, 1H), 6.21 (d, *J* = 7.5 Hz, 2H), 5.86 (dt, *J* = 8.7, 2.5 Hz, 1H), 4.90 (s, 1H), 3.79 (s, 3H), 3.67 (s, 3H), 3.48 (dd, *J* = 16.3, 6.2 Hz, 1H), 3.48 (dd, *J* = 16.2, 8.5 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 169.8, 164.7, 158.2, 151.4, 147.9, 140.9, 139.0, 132.0, 130.6, 129.2, 129.1, 129.0, 128.7, 128.4, 128.3, 127.7, 127.4, 127.1, 126.5, 125.1, 119.7, 118.7, 114.6, 113.7, 98.2, 55.5, 52.9, 52.8, 36.6; MS (+c ESI): 651 (M+1). Anal. Calcd for $C_{40}H_{34}N_4O_3S$: C 73.82, H 5.27, N 8.61; Found: C 73.85, H 5.74, N 8.26.

(*5R, 4'R, 2' Z*, *5'E*) or (*5S, 4'S*, *2' Z*, *5'E*)-Methyl 1,4,4',5'-tetrahydro-4-(4-methoxyphenyl)-1,3-diphenyl-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[3*H*-1, 2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15b-II): 143mg, 11%, yellow solid (without recrystallization), mp 88-90 °C; IR *ν* (cm^{-1}) 1749, 1625, 1593, 1510, 1493; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.53 (d, *J* = 7.1 Hz, 2H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.26-7.33 (m, 8H), 7.22 (t, *J* = 7.7 Hz, 2H), 7.16 (d, *J* = 8.8 Hz, 2H), 7.13 (d, *J* = 7.3 Hz, 2H), 7.06 (t, *J* = 7.4 Hz, 1H), 7.00 (t, *J* = 7.3 Hz, 1H), 6.82 (d, *J* = 8.9 Hz, 2H), 6.30 (d, *J* = 7.8 Hz, 2H), 5.83 (dt, *J* = 8.5, 2.1 Hz, 1H), 4.55 (d, *J* = 0.8 Hz, 1H), 3.82 (s, 3H), 3.64 (s, 3H), 3.49 (dd, *J* = 16.2, 6.8 Hz, 1H), 3.35 (dd, *J* = 16.2, 8.3 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 168.8, 166.5, 158.7, 151.7, 149.8, 143.8, 139.0, 130.8, 130.5, 129.3, 129.1, 128.6, 128.4, 128.3, 128.2, 128.1, 127.7, 126.8, 126.5, 124.9, 121.8, 119.3, 118.6, 114.4, 99.9, 56.3, 55.4, 52.9, 36.2; MS (+c ESI): 651 (M+1). Anal. Calcd for $C_{40}H_{34}N_4O_3S$: C 73.82, H 5.27, N 8.61; Found: C 73.87, H 5.06, N 8.53.

(*5S, 4'R, E*) or (*5R, 4'S*, *E*)-Methyl 1,4-dihydro-4-(4-methoxyphenyl)-1,1',3-triphenyl-5'-(2-phenylethylidene)-2'-thioxospiro[3*H*-1,2,4-triazole-5 ,3'-pyrrolidine]-4'-carboxylate (16b-I): 221mg, 17%, yellow crystals, mp 218-219 °C; IR *ν* (cm^{-1}) 1744, 1597, 1510, 1493; ^{1}H NMR (500 MHz) δ (ppm) 7.56 (d, *J* = 6.6 Hz, 2H), 7.52 (brs, 1H), 7.41 (brs, 2H), 7.36 (t, *J* = 7.8 Hz, 2H), 7.28-7.30 (m, 7H), 7.21-7.25 (m, 3H), 7.16 (d, *J* = 7.5 Hz, 2H), 6.97 (t, *J* = 7.3 Hz, 1H), 6.77 (d, *J* = 8.5 Hz, 2H), 6.61 (brs, 1H), 5.15 (dt, *J* = 8.1, 2.2 Hz, 1H), 5.02 (s, 1H), 3.77 (s, 3H), 3.66 (s, 3H), 3.47 (dd, *J* = 16.5, 7.1 Hz, 1H), 3.23 (dd, *J* = 16.4, 8.1Hz, 1H); ^{13}C NMR (75 MHz) δ (ppm) 190.6, 169.2, 158.0, 147.8, 141.3, 139.4, 139.1, 137.3, 131.5, 130.1, 129.6, 129.4, 129.20, 129.16, 128.6, 128.3, 127.8, 127.7, 127.1, 126.5, 120.4, 115.5, 113.5, 112.1, 97.1, 55.4, 52.8, 49.2, 34.2; HRMS (TOF-ESI) 651.2420 (M+1), $C_{40}H_{35}N_4O_3S$ required 651.2430.

(*5R, 4'R, E*) or (*5S, 4'S*, *E*)-Methyl 1,4-dihydro-4-(4-methoxyphenyl)-1,1',3-triphenyl-5'-(2-phenylethylidene)-2'-thioxospiro[3*H*-1,2,4-triazole-5 ,3'-pyrrolidine]-4'-carboxylate (16b-II): 78mg, 6%, yellow crystals, mp 199-200 °C; IR *ν* (cm^{-1}) 1743, 1597, 1510, 1493; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.49 (t, *J* = 7.6 Hz, 4H), 7.42 (t, *J* = 7.2 Hz, 1H), 7.38 (d, *J* = 7.8 Hz, 2H), 7.19-7.36 (m, 10H), 6.98-7.02 (m, 5H), 6.85 (d, *J* = 8.7 Hz, 2H), 5.09 (dt, *J* = 9.1, 1.7 Hz, 1H), 4.45 (s, 1H), 3.85 (s, 3H), 3.77 (s, 3H), 3.41 (dd, *J* = 16.5, 7.0 Hz, 1H), 3.17 (dd, *J* = 16.5, 8.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 193.4, 168.2, 158.7, 150.2, 143.7, 139.5, 139.3, 137.3, 130.2, 129.34, 129.30, 128.5, 128.3, 128.1, 127.7, 127.3, 126.3, 122.1, 119.1, 114.6, 111.4, 99.0, 55.4, 52.9, 51.0, 33.9; HRMS (TOF-EI): 650.2356; $C_{40}H_{34}N_4O_3S$ required 650.2352.

(*Z*) Methyl 1,4-dihydro-4-(4-methoxyphenyl)-5'-phenethyl-1,3-diphenyl-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'

***H*)-thiophene]-4'-carboxylate (17b)**: 819mg, 63%, red solid (without recrystallization), mp 75-77 ^{o}C; IR *v* (cm^{-1}) 1708, 1648, 1593, 1507, 1493; ^{1}H NMR (500 MHz) δ (ppm) 7.54 (d, *J* = 7.0 Hz, 2H), 7.21-7.32 (m, 11H), 7.14 (t, *J* = 7.1 Hz, 1H), 7.10 (d, *J* = 7.8 Hz, 2H), 7.01 (d, *J* = 8.4 Hz, 2H), 6.88 (t, *J* = 6.9 Hz, 1H), 6.76 (d, *J* = 8.4 Hz, 2H), 6.57 (d, *J* = 7.5 Hz, 2H), 3.79 (s, 3H), 3.75 (s, 3H), 3.23 (t, *J* = 8.8 Hz, 2H), 2.82 (t, *J* = 7.9 Hz, 2H); ^{13}C NMR (125 MHz) δ (ppm) 166.8, 162.5, 159.4, 158.4, 151.2, 147.4, 143.1, 140.1, 131.0, 129.5, 129.2, 128.95, 128.86, 128.6, 128.3, 128.1, 128.0, 126.5, 125.6, 120.2, 119.6, 119.0, 114.5, 114.1, 98.2, 55.4, 51.7, 34.3, 34.1; MS (+c ESI): 651 (M+1). Anal. Calcd for $C_{40}H_{34}N_4O_3S$: C 73.82, H 5.27, N 8.61; Found: C 73.76, H 5.27, N 8.45.

Methyl

1,4-dihydro-4-(4-methoxyphenyl)-5'-phenethyl-1,1',3-triphenyl-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-pyrrole]-4'-carboxylate (18b): 260mg, 20%, green solid (without recrystallization), mp 89-90 ^{o}C; IR *v* (cm^{-1}) 1704, 1636, 1596, 1508, 1494; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.52-7.60 (m, 5H), 7.23-7.37 (m, 12H), 7.18 (d, *J* = 7.3 Hz, 2H), 7.10 (d, *J* = 7.9 Hz, 2H), 7.02 (d, *J* = 8.5 Hz, 2H), 6.77-7.86 (m, 5H), 3.78 (s, 3H), 3.75 (s, 3H), 2.87-2.89 (m, 2H), 2.53-2.56 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 208.0, 162.6, 160.2, 158.5, 147.6, 143.3, 139.9, 136.0, 130.6, 130.1, 129.9, 129.4, 129.0, 128.7, 128.6, 128.5, 128.12, 128.07, 128.0, 127.9, 126.5, 119.9, 118.9, 114.6, 114.0, 111.4, 95.4, 55.4, 51.4, 33.4, 29.2; MS (+c ESI): 651 (M+1). Anal. Calcd for $C_{40}H_{34}N_4O_3S$: C 73.82, H 5.27, N 8.61; Found: C 73.70, H 5.64, N 8.35.

(*5S, 4'R, 2' Z, 5'E*) or (*5R, 4'S, 2' Z, 5'E*)-Methyl

1,4,4',5'-tetrahydro-3-(4-methylphenyl)-1,4-diphenyl-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15c-I): 684mg, 54%, yellow crystals, mp 155-156 ^{o}C; IR *v* (cm^{-1}) 1742, 1625, 1593, 1497; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.37 (d, *J* = 8.2 Hz, 2H), 7.23-7.27 (m, 4H), 7.09-7.21 (m, 8H), 7.03-7.07 (m, 4H), 6.97 (d, *J* = 8.0 Hz, 2H), 6.91 (tt, *J* = 7.4, 1.1 Hz, 1H), 6.85 (tt, *J* = 7.3, 1.0 Hz, 1H), 5.98 (dd, *J* = 8.5, 1.2 Hz, 2H), 5.77 (dt, *J* = 8.6, 2.5 Hz, 1H), 4.79 (s, 1H), 3.56 (s, 3H), 3.37 (dd, *J* = 16.3, 6.5 Hz, 1H), 3.19 (dd, *J* = 16.2, 8.5 Hz, 1H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 169.8, 165.0, 151.5, 147.6, 140.9, 139.5, 139.3, 139.0, 129.2, 129.1, 128.9, 128.6, 128.5, 128.4, 127.6, 127.3, 127.2, 126.50, 126.48, 125.0, 124.9, 119.8, 118.5, 114.7, 96.1, 53.4, 52.8, 36.6, 21.4; HRMS (TOF-EI): 634.2407; $C_{40}H_{34}N_4O_2S$ required 634.2402

(*5R, 4'R, 2' Z, 5'E*) or (*5S, 4'S, 2' Z, 5'E*)-Methyl

1,4,4',5'-tetrahydro-3-(4-methylphenyl)-1,4-diphenyl-5'-(2-phenylethylidene)-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15c-II): 152mg, 12%, yellow crystals, mp 122-123 ^{o}C; IR *v* (cm^{-1}) 1745, 1627, 1593, 1492; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.41 (dd, *J* = 8.1, 2.0 Hz, 4H), 7.24-7.29 (m, 6H), 7.11-7.23 (m, 8H), 6.07 (d, *J* = 8.3 Hz, 2H), 6.97-7.03 (m, 2H), 6.17 (d, *J* = 7.5 Hz, 2H), 5.84 (dt, *J* = 8.4, 2.1 Hz, 1H), 4.56 (s, 1H), 3.62 (s, 3H), 3.47 (dd, *J* = 16.1, 7.0 Hz, 1H), 3.34 (dd, *J* = 16.1, 8.2 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 168.8, 166.1, 151.6, 149.5, 143.8, 139.5, 139.0, 138.6, 129.1, 129.0, 128.9, 128.6, 128.5, 128.4, 128.3, 128.2, 128.1, 126.94, 126.91, 126.4, 124.94, 124.86, 121.9, 119.4, 118.4, 99.7, 57.1, 52.9, 36.2, 21.4; MS (-c ESI): 633(M-1). Anal. Calcd for $C_{40}H_{34}N_4O_2S$: C 75.68, H 5.40, N 8.83; Found: C 75.52, H 5.65, N 8.70.

(*5S, 4'R, E*) or (*5R, 4'S, E*)-Methyl

1,4-dihydro-3-(4-methylphenyl)-1,1',4-triphenyl-5'-(2-phenylethylidene)-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'-pyrrolidine]-4'-carboxylate (16c-I): 177mg, 14%, yellow crystals, mp 179-180 ^{o}C; IR *v* (cm^{-1}) 1744, 1594, 1491; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.42 (d, *J* = 8.2 Hz, 2H), 7.35-7.47 (m, 3H), 7.35 (d, *J* = 7.3 Hz, 2H), 7.33 (d, *J* = 7.3 Hz, 2H), 7.13-7.18 (m, 4H), 7.20-7.30 (m, 7H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.95 (tt, *J* = 7.3, 1.0 Hz, 1H), 6.63 (brs, 1H), 5.15 (dt, *J* = 8.1, 2.5 Hz, 1H), 4.99 (s, 1H), 3.64 (s, 3H), 3.45 (dd, *J* = 16.4, 6.8 Hz, 1H), 3.21 (dd, *J* = 16.3, 8.1 Hz, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.5, 169.2, 147.5, 141.4, 139.4, 139.3, 139.2, 139.0, 137.3, 130.1, 129.3, 129.2, 129.1, 128.6, 128.33, 128.27, 128.0, 127.6, 127.0, 126.4, 126.3, 124.8, 120.4, 115.6, 112.0, 97.1, 52.7, 49.4, 34.2, 21.4; MS (TOF-EI): 529 (100), 634 (M^+, 10%); Anal. Calcd for $C_{40}H_{34}N_4O_2S$: C 75.68, H 5.40, N 8.83; Found: C 75.42, H 5.85, N 8.66.

(*5R, 4'R, E*) or (*5S, 4'S, E*)-Methyl

1,4-dihydro-3-(4-methylphenyl)-1,1',4-triphenyl-5'-(2-phenylethylidene)-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'-pyrrolidine]-4'-carboxylate (16c-II): 50mg, 4%, yellow crystals, mp 136-137 °C; IR *v* (cm^{-1}) 1756, 1742, 1595, 1491; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.46 (dt, *J* = 7.8, 1.2 Hz, 2H), 7.34-7.42 (m, 5H), 7.24-7.32 (m, 7H), 7.16-7.23 (m, 3H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.96-7.00 (m, 5H), 5.05-5.09 (dt, *J* = 7.2, 2.4 Hz, 1H), 4.41 (t, *J* = 1.1 Hz, 1H), 3.74 (s, 3H), 3.38 (dd, *J* = 16.4, 7.2 Hz, 1H), 3.14 (dd, *J* = 16.6, 8.1 Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 193.2, 168.1, 150.0, 143.7, 139.5, 139.4, 139.3, 138.0, 137.3, 130.0, 129.4, 129.3, 128.8, 128.5, 128.3, 128.2, 128.1, 127.3, 127.1, 126.3, 124.7, 122.2, 119.3, 111.5, 98.9, 52.9, 51.3, 33.9, 21.4; HRMS (TOF-EI): 634.2407; $C_{40}H_{34}N_4O_2S$ required 634.2402.

(*Z*) Methyl

1,4-dihydro-3-(4-methylphenyl)-5'-phenethyl-1,4-diphenyl-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (17c): 760mg, 60%, red solid (without recrystallization), mp 88-89 °C; IR *v* (cm^{-1}) 1709, 1650, 1594, 1494; ^{1}H NMR (300 MHz, $CDCl_3$) δ (ppm) 7.44 (d, *J* = 7.6 Hz, 2H), 7.22-7.35 (m, 12H), 7.05-7.14 (m, 7H), 6.88 (t, *J* = 7.0 Hz, 1H), 6.51 (d, *J* = 7.8 Hz, 2H), 3.72 (s, 3H), 3.22-3.26 (m, 2H), 2.83 (t, *J* = 8.1Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 166.7, 162.4, 159.6, 151.2, 147.3, 143.1, 140.1, 139.1, 138.7, 129.2, 128.9, 128.84, 128.80, 128.6, 128.3, 127.9, 127.5, 126.5, 125.5, 125.1, 120.2, 119.7, 118.8, 114.7, 97.9, 51.7, 34.3, 34.1, 21.4; HRMS (TOF-ESI): 635.2471 (M+1); $C_{40}H_{35}N_4O_2S$ required 635.2481.

Methyl

1,4-dihydro-3-(4-methylphenyl)-5'-phenethyl-1,1'4-triphenyl-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-pyrrole]-4'-carboxylate (18c): 252mg, 20%, green crystals, mp 182-183 °C; IR *v* (cm^{-1}) 1692, 1628, 1596, 1497; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.54-7.60 (m, 3H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.23-7.26 (m, 5H), 7.14-7.21 (m, 4H), 7.09 (t, *J* = 7.3 Hz, 4H), 7.06 (d, *J* = 7.5 Hz, 2H), 6.87 (t, *J* = 7.5 Hz, 2H), 6.83 (d, *J* = 7.5 Hz, 2H), 3.73 (s, 3H), 2.90-2.96 (m, 1H), 2.81-2.86 (m, 1H), 2.52 (t, *J* = 8.2 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 207.0, 162.0, 159.8, 146.9, 142.7, 139.4, 138.6, 137.7, 135.4, 129.6, 129.4, 128.3, 128.2, 128.1, 128.0, 127.9, 127.5, 127.4, 127.3, 127.1, 126.3, 125.9, 124.5, 119.4, 114.2, 110.8, 94.7, 50.9, 32.8, 28.6, 20.9; MS (TOF-EI): 529 (100), 634 (M^+, 5%); Anal. Calcd for $C_{40}H_{34}N_4O_2S$: C 75.68, H 5.40, N 8.83; Found: C 75.72, H 4.84, N 8.64.

(*5S, 4'R, 2' Z, 5'E*) or (*5R, 4'S, 2' Z, 5'E*)-Methyl

1,4,4',5'-tetrahydro-1,3,4-triphenyl-2'-(phenylimino)-5'-propylidenespiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15d-I): 580mg, 52%, yellow crystals, mp 165-166 °C; IR *v* (cm^{-1}) 1736, 1626, 1593, 1492; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.57 (dd, *J* = 7.3, 1.5 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.31 (br, 2H), 7.21-7.28 (m, 8H), 7.15 (t, *J* = 7.9 Hz, 2H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.94 (t, *J* = 7.0 Hz, 1H), 6.07 (d, *J* = 7.4 Hz, 2H), 5.67 (dt, *J* = 6.8, 2.6 Hz, 1H), 4.80 (t, *J* = 1.2 Hz, 1H), 3.65 (s, 3H), 2.09-2.15 (m, 1H), 1.93-1.99 (m, 1H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 169.7, 165.2, 151.6, 147.4, 140.9, 139.4, 130.6, 129.2, 128.9, 128.5, 128.4, 127.9, 127.7, 126.5, 125.4, 124.9, 119.8, 118.5, 114.7, 98.1, 53.2, 52.7, 24.2, 13.4; MS (+c ESI): 559 (M+1). Anal. Calcd for $C_{34}H_{30}N_4O_2S$: C 73.09, H 5.41, N 10.03; Found: C 72.99, H 5.12, N 10.02.

(*5R, 4'R, 2' Z, 5'E*) or (*5S, 4'S, 2' Z, 5'E*)-Methyl

1,4,4',5'-tetrahydro-1,3,4-triphenyl-2'-(phenylimino)-5'-propylidenespiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15d-II): 112mg, 10%, yellow crystals, mp 148-149 °C IR *v* (cm^{-1}) 1746, 1625, 1591, 1494; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.57 (d, *J* = 7.2 Hz, 2H), 7.41 (d, *J* = 8.0 Hz,), 7.25-7.32 (m, 8H), 7.18 (t, *J* = 7.5 Hz, 4H), 6.98-7.04 (m, 2H), 6.16 (d, *J* = 7.7 Hz, 2H), 5.62 (t, *J* = 6.5 Hz, 1H), 4.50 (s, 1H), 3.66 (s, 3H), 2.08-2.14 (m, 1H), 1.97-2.03 (m, 1H), 1.00 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 169.3, 167.1, 152.7, 149.8, 145.0, 139.4, 131.1, 130.2, 129.97, 129.96, 129.7, 129.14, 129.09, 128.9, 128.7, 128.0, 127.2, 125.6, 122.0, 119.7, 119.1, 100.5, 57.9, 53.0, 24.4, 13.6; HRMS (TOF-EI): 558.2092; $C_{34}H_{30}N_4O_2S$ required 558.2089. Anal. Calcd for $C_{34}H_{30}N_4O_2S$: C 73.09, H 5.41, N 10.03; Found: C 72.53, H 5.47, N 9.72.

(*5S, 4'R, E*) or (*5R, 4'S, E*)-Methyl

1,4-dihydro-1,1',3,4-tetraphenyl-5'-propylidene-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'-pyrrolidine]-4'-carboxylate (16d-I): 268mg, 24%, yellow crystals, mp 187-188 °C; IR *v* (cm^{-1}) 1745, 1593, 1491; ^{1}H NMR (400 MHz,

$CDCl_3$) δ (ppm) 7.45 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.34-7.36 (m, 2H), 7.25 (t, *J* = 7.5 Hz, 3H), 7.12-7.21 (m, 10H), 7.06 (t, *J* = 7.0 Hz, 1H), 6.86 (t, *J* = 7.2 Hz, 1H), 6.54 (brs, 1H), 4.82-4.86 (m, 2H), 3.56 (s, 3H), 1.94-2.01 (m, 1H), 1.75-1.82 (m, 1H), 0.91 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 190.0, 169.1, 147.4, 141.3, 138.9, 137.9, 137.4, 130.0, 129.3, 129.2, 129.1, 128.31, 128.25, 128.0, 127.8, 127.7, 127.1, 126.3, 120.4, 115.6, 115.3, 97.2, 52.6, 49.2, 21.9, 13.7; MS (-c ESI): 557 (M-1). Anal. Calcd for $C_{34}H_{30}N_4O_2S$: C 73.09, H 5.41, N 10.03; Found: C 72.93, H 5.65, N 9.86.

(*5R, 4'R, E*) or (*5S, 4'S, E*)-Methyl 1,4-dihydro-1,1',3,4-tetraphenyl-5'-propylidene-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'-pyrrolidine]-4'-carboxylate (16d-II): 70mg, 6%, yellow crystals, mp 150-151 °C; IR *v* (cm^{-1}) 1755, 1623, 1595, 1493; ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) 7.38-7.42 (m, 4H), 7.34 (tt, *J* = 7.4, 1.7 Hz, 1H), 7.28 (dd, *J* = 8.8, 1.2 Hz, 2H), 7.16-7.24 (m, 10H), 6.90 (tt, *J* = 7.3, 1.2 Hz, 3H), 4.74 (dt, *J* = 8.0, 2.4 Hz, 1H), 4.32-4.33 (m, 1H), 3.70 (s, 3H), 1.88-1.97 (m, 1H), 1.64-1.75 (m, 1H), 0.82 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ (ppm) 192.6, 168.0, 150.0, 143.7, 137.9, 137.8, 137.4, 129.9, 129.3, 129.2, 128.3, 128.21, 128.15, 128.1, 127.8, 127.3, 127.1, 122.4, 119.6, 114.9, 99.1, 52.8, 51.1, 21.8, 13.6; HRMS (TOF-EI): 558.2093; $C_{34}H_{30}N_4O_2S$ required 558.2089.

(*Z*) Methyl 1,4-dihydro-1,3,4-triphenyl-2'-(phenylimino)-5'-propylspiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (17d): 603mg, 54%, red crystals, mp 133-134 °C; IR *v* (cm^{-1}) 1709, 1655, 1593, 1493; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.54 (d, *J* = 6.9 Hz, 2H), 7.21-7.29 (m, 10H), 7.13 (d, *J* = 8.2 Hz, 2H), 7.12 (t, *J* = 7.8 Hz, 1H), 7.06 (d, *J* = 7.1 Hz, 2H), 6.88 (t, *J* = 7.2 Hz, 1H), 6.51 (d, *J* = 7.6 Hz, 2H), 3.69 (s, 3H), 2.99 (quintet, *J* = 7.4 Hz, 1H), 2.89 (quintet, *J* = 6.4 Hz, 1H), 1.57 (sextet, *J* = 7.5 Hz, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.0, 162.5, 161.0, 151.3, 147.2, 143.1, 138.6, 129.2, 129.0, 128.9, 128.6, 128.2, 128.1, 128.0, 127.6, 127.3, 126.6, 125.5, 119.8, 118.9, 114.7, 98.2, 51.6, 33.9, 21.9, 14.0; MS (+c ESI): 559 (M+1). Anal. Calcd for $C_{34}H_{30}N_4O_2S$: C 73.09, H 5.41, N 10.03; Found: C 72.84, H 4.91, N 9.87.

Methyl 1,4-dihydro-1,1',3,4-tetraphenyl-5'-propyl-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-pyrrole]-4'-carboxylate (18d): 245mg, 22%, green crystals, mp 172-173 °C; IR *v* (cm^{-1}) 1698, 1638, 1595, 1493; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.56-7.59 (m, 1H), 7.51 (d, *J* = 6.7 Hz, 4H), 7.18-7.32 (m, 9H), 7.09 (d, *J* = 8.0 Hz, 2H), 7.03 (d, *J* = 7.2 Hz, 2H), 6.84-6.87 (m, 2H), 3.69 (s, 3H), 2.63-2.67 (m, 1H), 2.53-2.58 (m, 1H), 1.26-1.31 (m, 2H), 0.72 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 207.7, 162.6, 161.5, 147.4, 143.2, 138.1, 136.1, 130.0, 129.8, 129.4, 129.0, 128.8, 128.6, 128.3, 128.14, 128.06, 127.8, 127.5, 126.8, 120.0, 114.8, 111.0, 95.2, 51.3, 28.3, 21.0, 14.1; MS (+c ESI): 559 (M+1). Anal. Calcd for $C_{34}H_{30}N_4O_2S$: C 73.09, H 5.41, N 10.03; Found: C 73.15, H 5.34, N 9.93.

(*5S, 4'R, 2' Z, 5'E*) or (*5R, 4'S, 2' Z, 5'E*)-Methyl 1,4,4',5'-tetrahydro-5'-(*iso*-butylidene)-1,3,4-triphenyl-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15e-I): 664mg, 58%, yellow crystals, mp 148-149 °C; IR *v* (cm^{-1}) 1737, 1627, 1594, 1493; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.58 (dd, *J* = 7.9, 2.0 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 2H), 7.32 (br, 2H), 7.25-7.29 (m, 4H), 7.21 (d, *J* = 8.4 Hz, 4H), 7.16 (t, *J* = 7.8 Hz, 2H), 7.03 (t, *J* = 7.4 Hz, 1H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.08 (d, *J* = 7.5 Hz, 2H), 5.50 (dd, *J* = 10.6, 2.5 Hz, 1H), 4.83 (d, *J* = 2.5 Hz, 1H), 3.66 (s, 3H), 2.27-2.32 (m, 1H)， 1.09 (d, *J* = 6.5 Hz, 3H), 0.92 (d, *J* =6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 170.2, 165.3, 151.5, 147.5, 140.9, 139.4, 135.9, 129.1, 128.9, 128.5, 128.3, 127.9, 127.7, 126.5, 124.9, 123.9, 119.8, 118.5, 114.7, 98.0, 53.2, 52.7, 30.5, 22.7, 21.6; MS (+c ESI): 573 (M+1). Anal. Calcd for $C_{35}H_{32}N_4O_2S$: C 73.40, H 5.63, N 9.78; Found: C 73.41, H 5.40, N 9.64.

(*5R, 4'R, 2' Z, 5'E*) or (*5S, 4'S, 2' Z, 5'E*)-Methyl 5'-(*iso*-butylidene)-1,4,4',5'-tetrahydro-1,3,4-triphenyl-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (15e-II): 137mg, 12%, yellow crystals, mp 158-159 °C; IR *v* (cm^{-1}) 1743, 1626, 1592, 1492; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.55 (dd, *J* = 7.2, 1.1 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.31 (t, *J* = 7.2 Hz, 1H), 7.22-7.28 (m, 7H), 7.15-7.18 (m, 4H), 7.01 (t, *J* = 7.3 Hz, 1H), 6.95 (t, *J* = 7.3 Hz, 1H), 6.17 (d, *J* =

7.9 Hz, 2H), 5.45 (dd, *J* = 10.4, 1.9 Hz, 1H), 4.54 (d, *J* = 1.9 Hz, 1H), 3.57 (s, 3H), 2.37 (m, 1H)，1.01 (d, *J* = 6.5 Hz, 3H), 0.95 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 169.1, 166.2, 151.7, 149.0, 143.4, 138.6, 135.8, 129.3, 129.05, 129.01, 128.5, 128.22, 128.18, 127.9, 127.0, 124.9, 124.8, 121.5, 118.7, 118.4, 99.2, 57.4, 52.8, 30.2, 22.6, 21.8; MS (+c ESI): 573 (M+1). Anal. Calcd for $C_{35}H_{32}N_4O_2S$: C 73.40, H 5.63, N 9.78; Found: C 73.29, H 5.33, N 9.76.

(*5S, 4'R, E*) or (*5R, 4'S*, *E*)-Methyl 5'-(*iso*-butylidene)-1,4-dihydro-1,1',3,4-tetraphenyl-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'-pyrrolidine]-4'-carboxylate (16e-I): 229mg, 20%, yellow crystals, mp 187-188 °C; IR *v* (cm^{-1}) 1748, 1595, 1492; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) 7.52 (dd, *J* = 6.8, 1.5 Hz, 2H), 7.49 (br, 1H), 7.42 (t, *J* = 7.0 Hz, 1H), 7.32 (t, *J* = 7.9 Hz, 2H), 7.23-7.29 (m, 7H), 7.20-7.22 (m, 4H), 7.13 (t, *J* = 7.5 Hz, 1H), 6.93 (t, *J* = 7.2 Hz, 1H), 6.60 (bs, 1H), 4.95 (d, *J* = 2.5 Hz, 1H), 4.76 (dd, *J* = 10.7, 2.3 Hz, 1H), 3.63 (s, 3H), 2.19 (m, 1H), 1.07 (d, *J* = 6.5 Hz, 3H), 0.88 (d, *J* =6.6 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ (ppm) 190.1, 169.4, 147.4, 141.3, 138.9, 137.5, 136.6, 130.0, 129.2, 129.1, 128.3, 128.2, 128.0, 127.8, 127.7, 127.1, 126.3, 120.7, 120.4, 115.6, 97.2, 52.6, 49.1, 28.4, 23.2, 22.2; MS (+c ESI): 573 (M+1). Anal. Calcd for $C_{35}H_{32}N_4O_2S$: C 73.40, H 5.63, N 9.78; Found: C 73.39, H 5.37, N 9.70.

(*5R, 4'R, E*) or (*5S, 4'S*, *E*)-Methyl 5'-(*iso*-butylidene)-1,4-dihydro-1,1',3,4-tetraphenyl-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'-pyrrolidine]-4'-carboxylate (16e-II): 57mg, 5%, yellow crystals, mp 210-212 °C; IR *v* (cm^{-1}) 1745, 1592, 1493; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.44-7.53 (m, 5H), 7.28-7.38 (m, 12H), 6.98 (t, *J* = 7.0 Hz, 1H), 6.96 (br, 2H), 4.67 (d, *J* = 10.7 Hz, 1H), 4.45 (d, *J* = 1.5 Hz, 1H), 3.74 (s, 3H), 2.11-2.18 (m, 1H), 1.01 (d, *J* = 6.4 Hz, 3H), 0.79 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 192.6, 168.4, 149.5, 143.4, 137.9, 137.4, 136.6, 130.0, 129.4, 129.3, 129.2, 128.3, 128.22, 128.17, 128.1, 127.7, 127.3, 127.2, 122.1, 120.2, 119.1, 98.8, 52.8, 51.3, 28.3, 22.9, 22.3; MS (-c ESI): 571 (M-1). Anal. Calcd for $C_{35}H_{32}N_4O_2S$: C 73.40, H 5.63, N 9.78; Found: C 73.33, H 5.87, N 9.73.

(*Z*) Methyl 5'-(*iso*-butyl)-1,4-dihydro-1,3,4-triphenyl-2'-(phenylimino)spiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-thiophene]-4'-carboxylate (17e): 595mg, 52%, red crystals, mp 154-155 °C; IR *v* (cm^{-1}) 1701, 1654, 1593, 1493; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.53 (d, *J* = 6.4 Hz, 2H), 7.20-7.29 (m, 11H), 7.12 (t, *J* = 7.4 Hz, 2H), 7.07 (d, *J* = 7.2 Hz, 2H), 6.89 (br, 1H), 6.54 (d, *J* = 7.5 Hz, 2H), 3.70 (s, 3H), 2.91 (dd, *J* = 13.9, 7.2 Hz, 2H), 2.84 (dd, *J* = 13.9, 7.2 Hz, 2H), 1.88 (m, 1H), 0.94 (d, *J* = 6.6 Hz, 3H), 0.88 (d, *J* =6.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 167.0, 162.6, 160.3, 151.3, 147.2, 143.0, 138.5, 129.2, 129.0, 128.9, 128.2, 128.0, 127.7, 126.7, 125.5, 119.8, 118.9, 114.8, 98.3, 51.6, 40.7, 28.9, 22.7, 22.5; MS (+c ESI): 573 (M+1). Anal. Calcd for $C_{35}H_{32}N_4O_2S$: C 73.40, H 5.63, N 9.78; Found: C 73.39, H 5.37, N 9.70.

Methyl 5'-(*iso*-butyl)-1,4-dihydro-1,1',3,4-tetraphenyl-2'-thioxospiro[3*H*-1,2,4-triazole-5,3'(2'*H*)-pyrrole]-4'-carboxylate (18e): 217mg, 19%, green crystals, mp 132-133 °C; IR *v* (cm^{-1}) 1694, 1633, 1595, 1493; ^{1}H NMR (500 MHz, $CDCl_3$) δ (ppm) 7.56-7.58 (m, 1H), 7.50-7.54 (m, 4H), 7.20-7.30 (m, 9H), 7.10 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 7.3 Hz, 2H), 6.90 (d, *J* = 6.4 Hz, 1H), 6.86 (t, *J* = 7.2 Hz, 1H), 3.69 (s, 3H), 2.66 (dd, *J* = 12.9, 7.1 Hz, 1H), 2.57 (dd, *J* = 13.0, 6.9 Hz, 1H), 1.50-1.55 (m, 1H), 0.68 (d, *J* = 6.6 Hz, 3H), 0.56 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm) 208.1, 162.6, 160.6, 147.4, 143.2, 138.1, 136.3, 129.8, 129.6, 129.0, 128.9, 128.6, 128.1, 127.7, 127.0, 120.0, 114.9, 111.9, 95.4, 51.2, 34.6, 28.1, 22.6, 22.2; MS (+c ESI): 573 (M+1). Anal. Calcd for $C_{35}H_{32}N_4O_2S$: C 73.40, H 5.63, N 9.78; Found: C 73.16, H 5.60, N 9.70.

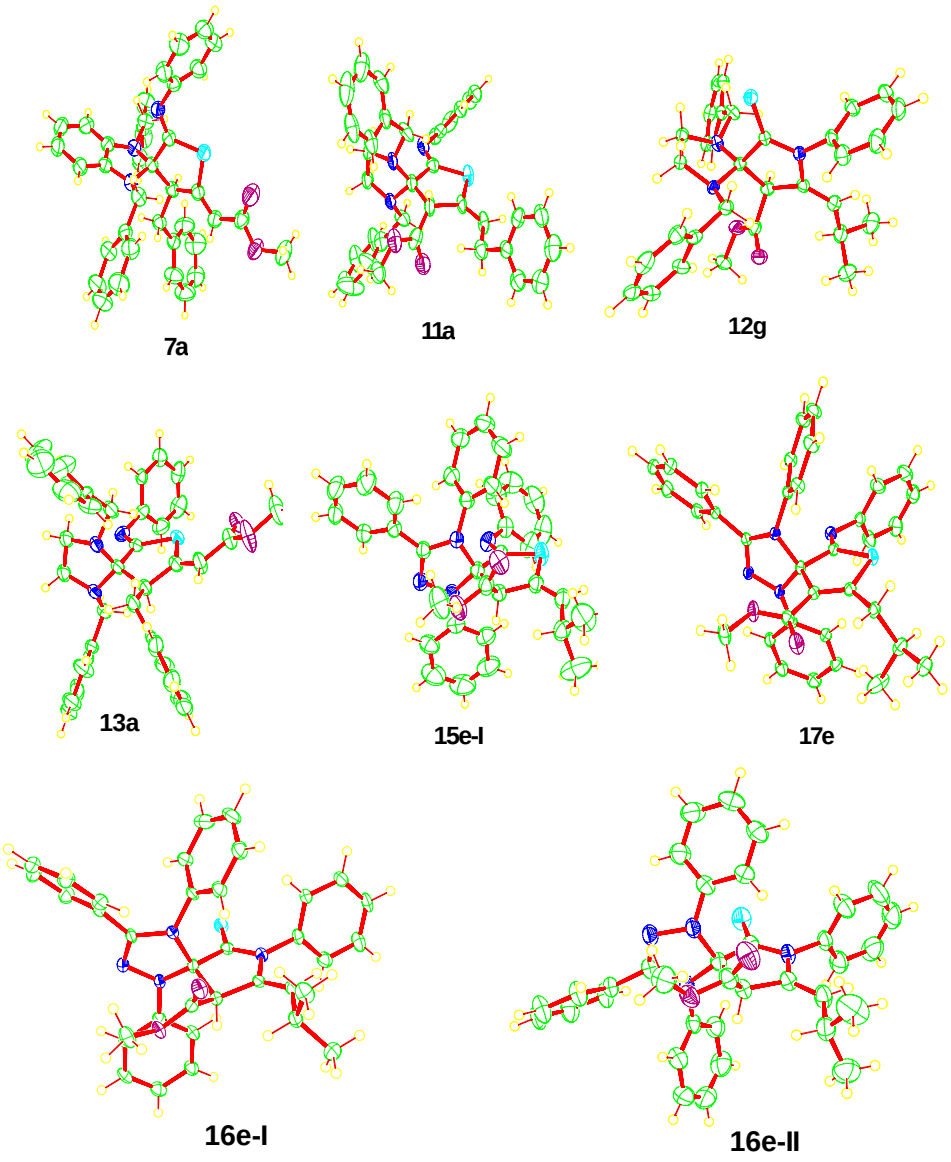


Figure S1.Ortep drawing of X-ray structures of **7a**, **11a, 12g, 13a, 15e-I, 16e-I, 16e-II** and **17e**.

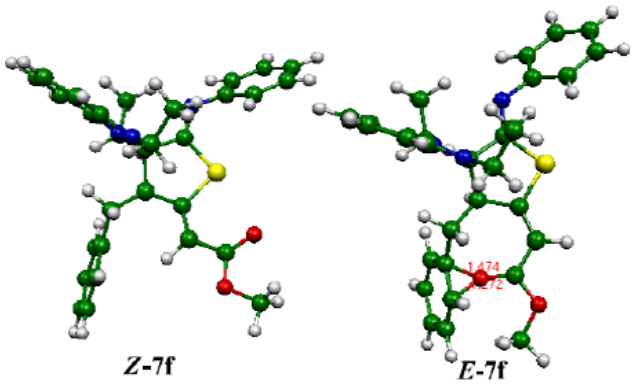


Figure S2. The Molekel drawing of structures for experimental product ***Z*-7f** and the fancy isomer of ***E*-7f**.

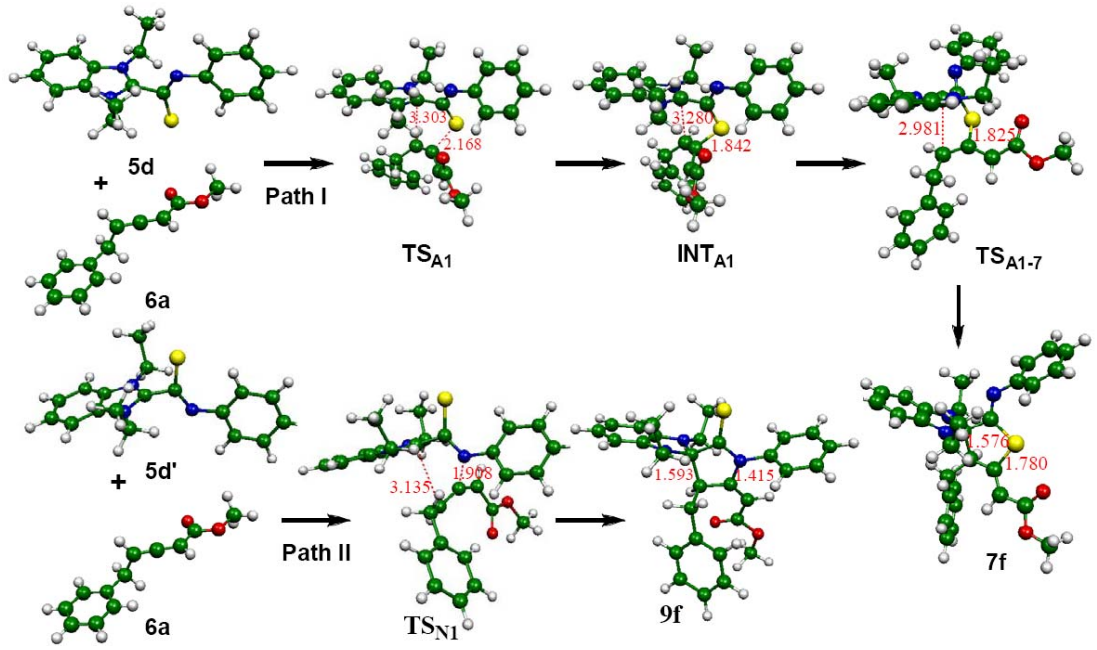


Figure S3. The obtained reaction pathways for **5d**+**6a**→**7f** and **5d'**+**6a**→**9f**, along with the bond lengths (Å) for the main reaction coordinates.

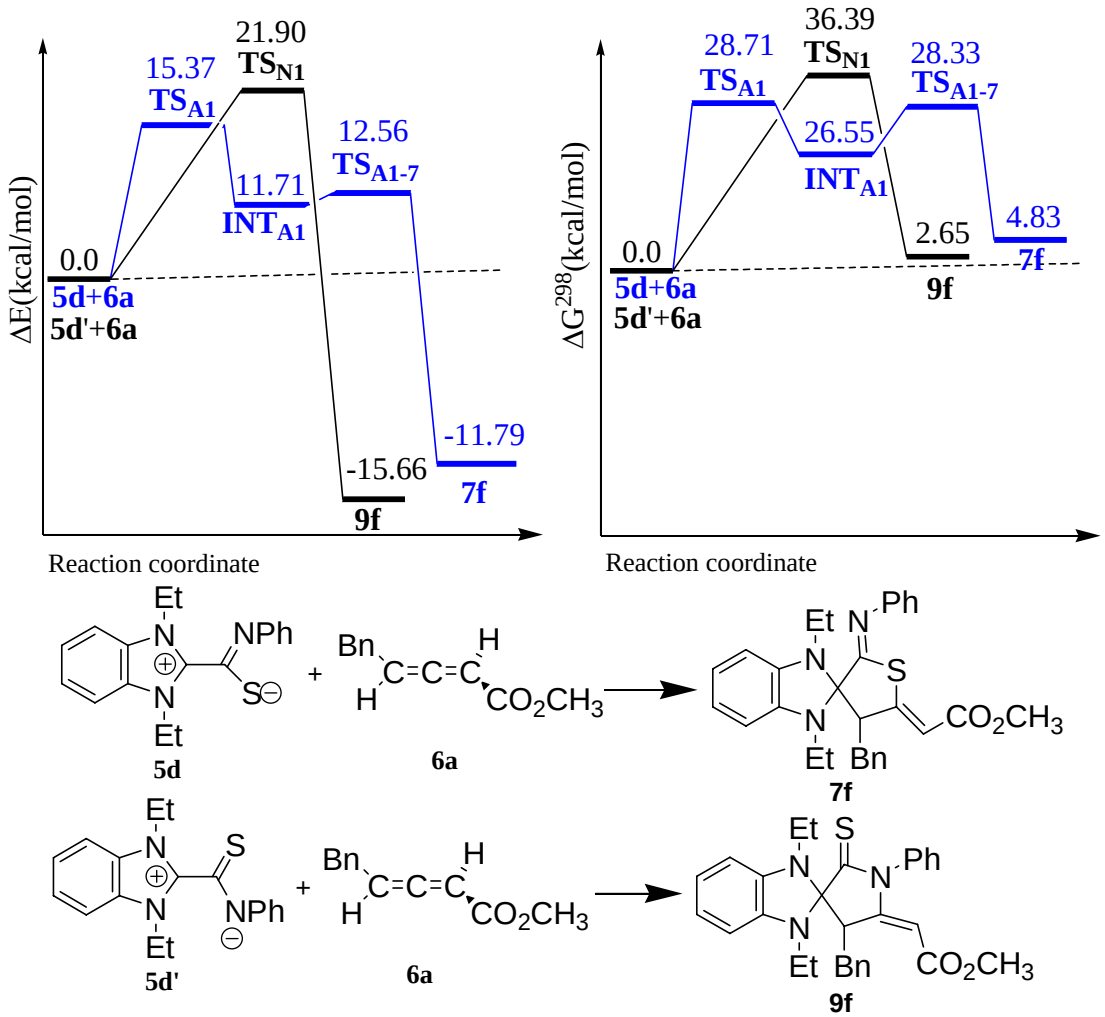


Figure S4. The energy profiles (ΔE and ΔG^{298}) for the reactions of **5d**+**6a**→**7f** and **5d'**+**6a**→**9f**.

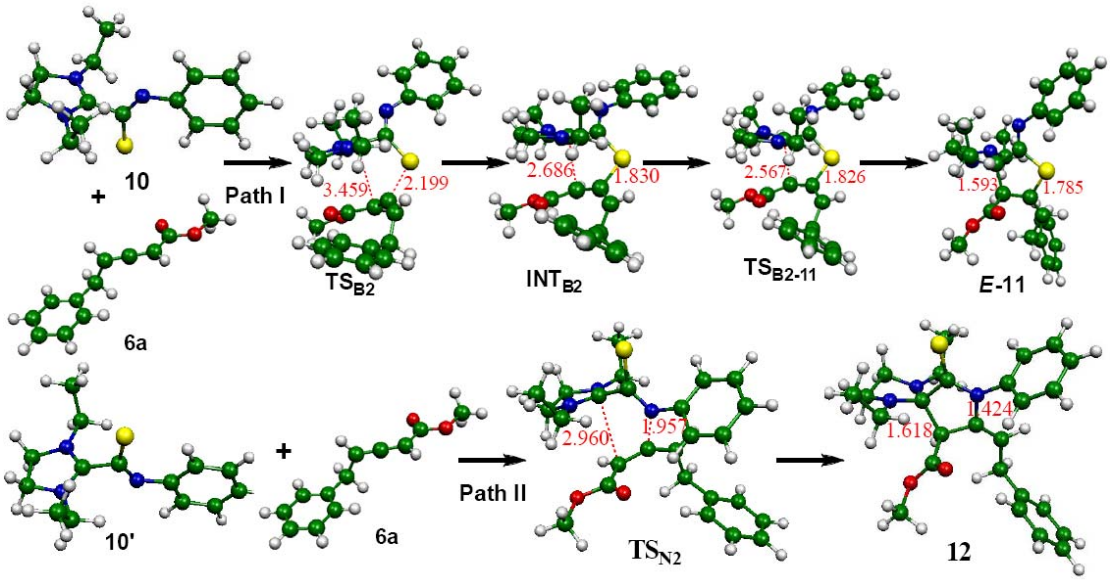


Figure S5.

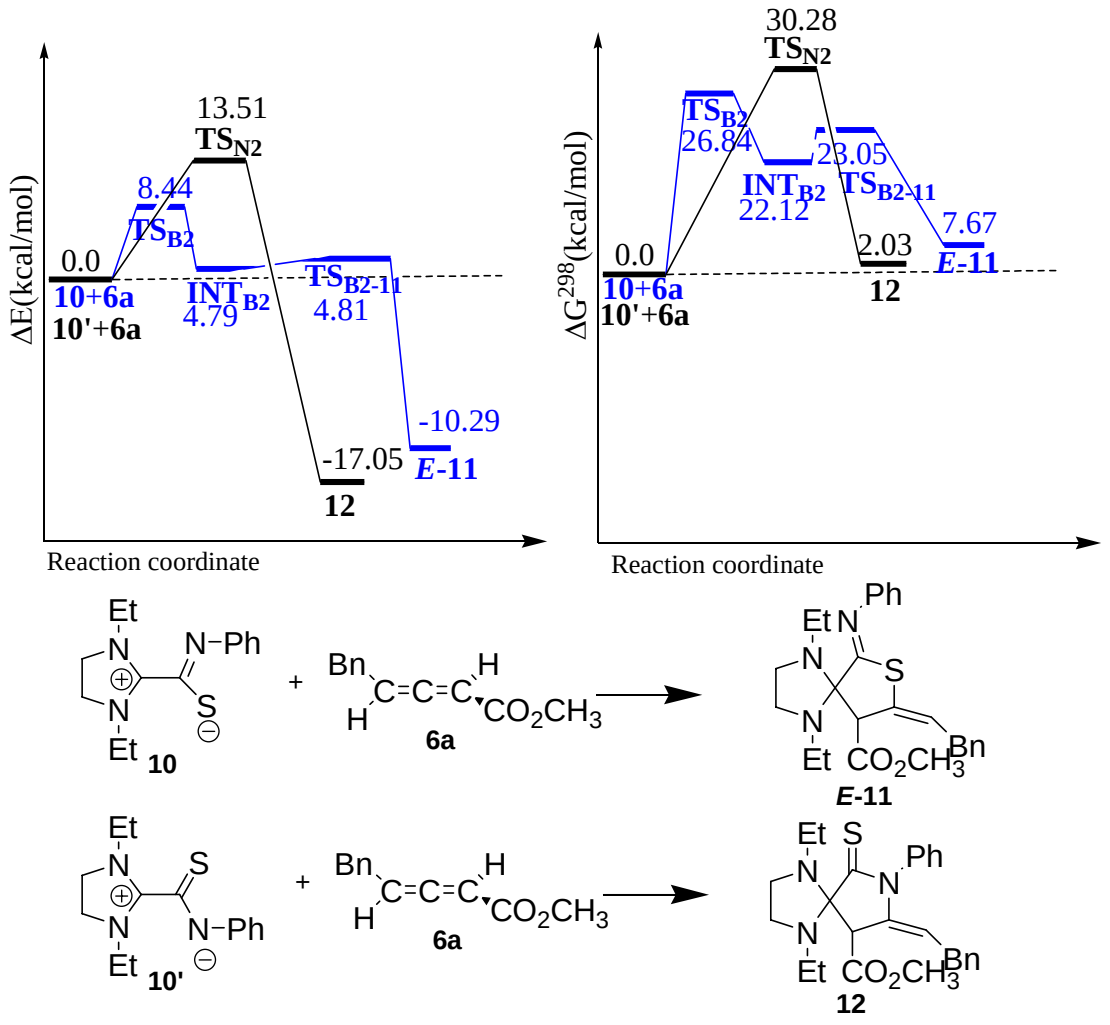


Figure S6. The energy profiles (ΔE and ΔG^{298}) for the reactions of **10+6a**→*E*-**11** and **10'+6a**→**12**.

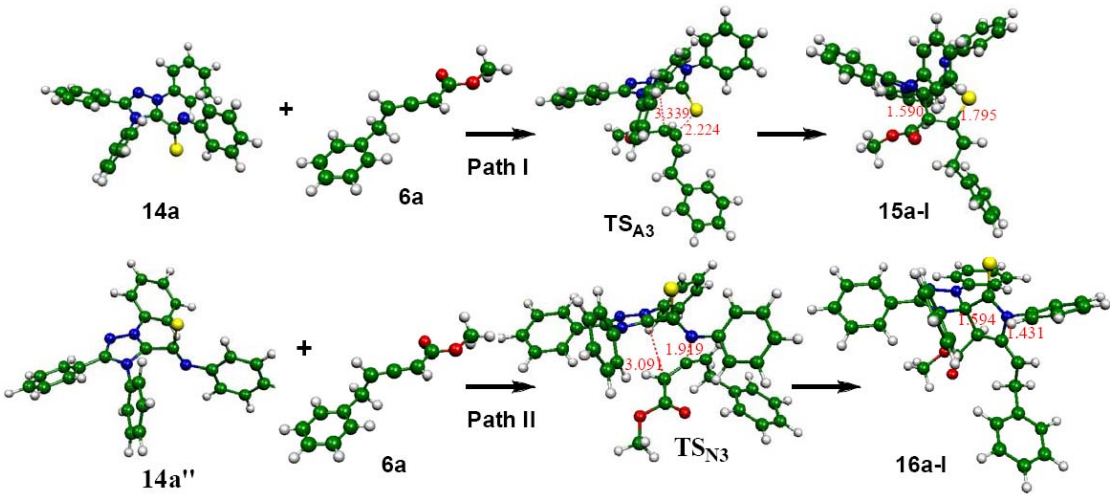


Figure S7. The reaction pathways for **14a**+**6a**→**15a-I** and **14a”**+**6a**→**16a-I**, along with the bond lengths (Å) for the main reaction coordinates.

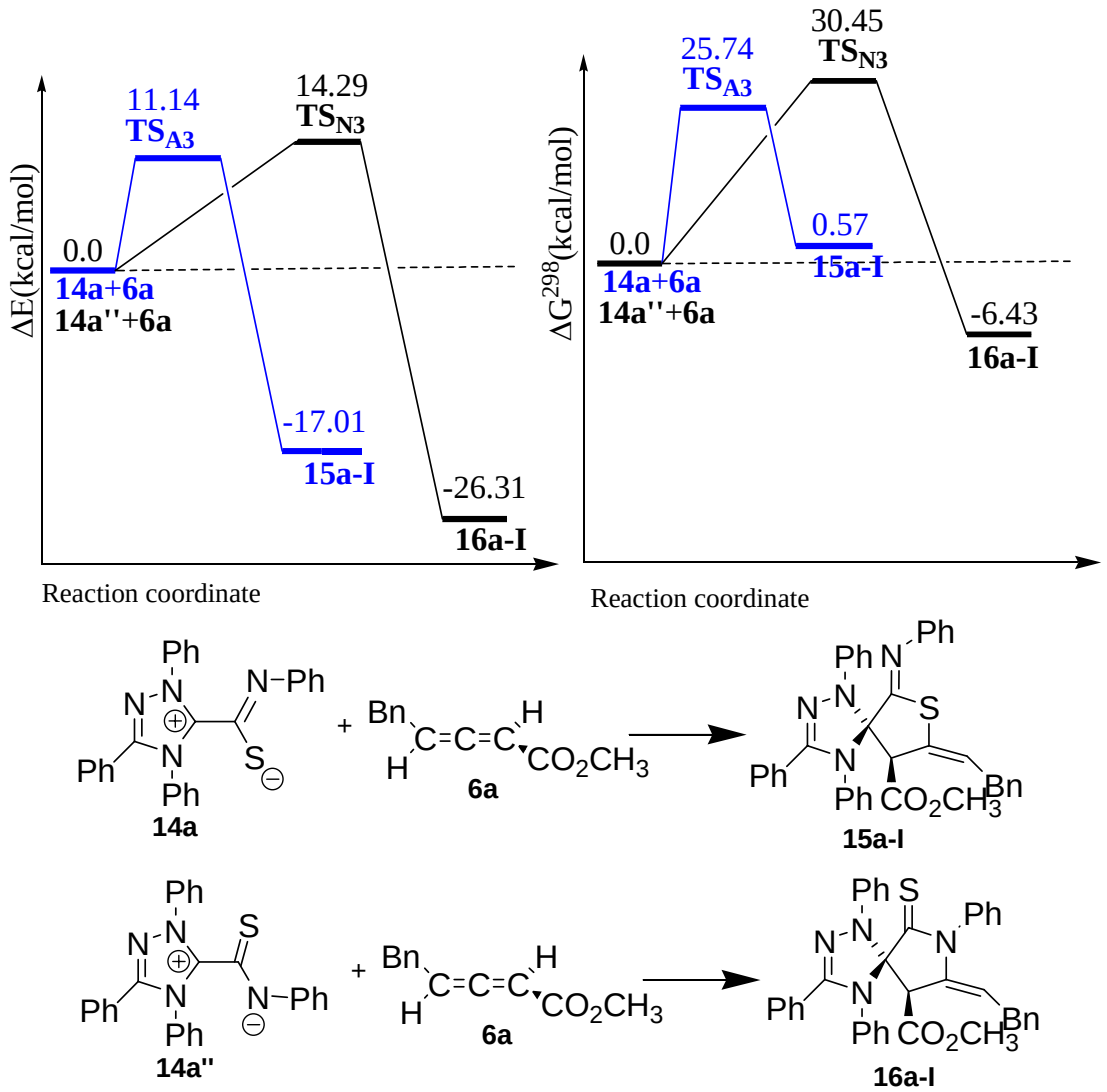


Figure S8. The energy profiles (ΔE and ΔG^{298}) for the reactions of **14a**+**6a**→**15a-I** and **14a”**+**6a**→**16a-I**.

Table S1. The Cartesian coordinates for the stationary points of the reactions **5d**+**6a**→**7f**, **5d**+**6a**→**27**, and **5d'**+**6a**→**9f.**

5d:

C	2.775378	-0.687827	-0.072459
C	2.758123	0.717473	-0.021448
N	1.476176	-1.110792	0.206015
N	1.448974	1.086816	0.285230
C	0.697536	-0.027734	0.420772
C	-0.754523	-0.054409	0.765427
N	-1.506270	0.019595	-0.294347
S	-0.927225	-0.167530	2.474657
C	0.934001	2.456484	0.414472
C	0.994124	-2.498298	0.233641
C	0.492556	-2.963279	-1.133502
C	0.125150	2.416904	1.147457
C	0.203136	-2.536687	0.986351
C	1.822946	-3.114949	0.593847
C	1.290334	-2.932603	-1.883609
C	-0.330365	-2.324864	-1.467406
C	0.128903	-3.993723	-1.060786
H	0.451648	3.021161	-0.921703
H	0.067176	4.036021	-0.774917
H	1.264695	3.064660	-1.654569
H	-0.351893	2.396055	-1.321084
H	1.739152	3.059572	0.844742
H	3.910088	1.468025	-0.252693
H	5.079776	0.764274	-0.536944
H	5.096901	-0.639927	-0.588542
H	3.945110	-1.390965	-0.357465
H	3.900524	2.552320	-0.216786
H	5.996643	1.314816	-0.723974
C	6.026778	-1.152702	-0.814545
H	3.961891	-2.474876	-0.401014
H	-2.906347	0.021549	-0.329406
H	-3.463666	0.092323	-1.624198
H	-3.787726	-0.036955	0.772205
C	-4.839780	0.104232	-1.820644
C	-2.778380	0.136708	-2.466144
C	-5.167440	-0.023822	0.564591
C	-3.385637	-0.091538	1.775244
H	-5.703237	0.046159	-0.722367
H	-5.241287	0.158925	-2.829710
H	-5.831224	-0.069133	1.424942
H	-6.780234	0.055451	-0.869261

TS_{A1}:

6a:

C	-1.165678	0.410112	0.458191
C	-0.102767	-0.314655	0.678216
C	-2.230355	1.146826	0.228506
H	0.159216	-0.562392	1.707873
H	-2.169069	2.232306	0.192817
C	0.818000	-0.850224	-0.404730
H	0.433148	-0.543782	-1.384142
H	0.784297	-1.947274	-0.380761
C	2.257057	-0.390814	-0.232849
C	3.285636	-1.315341	-0.021451
C	2.580618	0.972337	-0.285830
C	4.608697	-0.892938	0.128013
H	3.050486	-2.376642	0.022712
C	3.899752	1.397971	-0.138241
H	1.789839	1.702622	-0.440637
C	4.919452	0.465386	0.069545
H	5.394193	-1.626508	0.290050
H	4.133151	2.458537	-0.184934
H	5.947836	0.796990	0.185211
C	-3.596107	0.611477	0.002365
O	-4.564077	1.316216	-0.203159
O	-3.646543	-0.739340	0.047594
C	-4.948132	-1.303797	-0.166610
H	-5.334653	-1.022033	-1.149974
H	-4.811373	-2.383960	-0.103948
H	-5.649153	-0.960918	0.599487

INT_{A1}:

C	-0.716868	2.594592	1.377098	C	0.018874	2.931897	1.193262
N	-0.177645	2.303732	-0.778522	N	0.243959	2.225443	-0.920347
N	0.243987	1.591866	1.260691	N	0.709712	1.721910	1.171277
C	0.550566	1.439059	-0.038331	C	0.817468	1.317604	-0.103553
C	1.565857	0.488690	-0.587602	C	1.558156	0.102684	-0.571256
N	2.773934	0.904260	-0.400996	N	2.823769	0.279627	-0.656244
S	0.916235	-0.894827	-1.440092	S	0.584711	-1.290530	-1.072273
C	3.922924	0.180461	-0.779147	C	3.737424	-0.735619	-1.025011
C	4.942533	0.878241	-1.445153	C	4.724087	-0.413445	-1.967627
C	4.124486	-1.162961	-0.417760	C	3.749459	-1.993590	-0.397495
C	6.127855	0.232417	-1.791130	C	5.688464	-1.355582	-2.321284
H	4.787841	1.925788	-1.688877	H	4.720463	0.575683	-2.417063
C	5.326159	-1.788994	-0.744302	C	4.737286	-2.914752	-0.741494
H	3.356813	-1.686768	0.142628	H	3.005483	-2.224279	0.360543
C	6.325482	-1.105022	-1.441556	C	5.699722	-2.609795	-1.707958
H	6.903182	0.779290	-2.321876	H	6.439723	-1.103017	-3.065099
H	5.479916	-2.825334	-0.453868	H	4.750587	-3.883885	-0.249534
H	7.254119	-1.606679	-1.700496	H	6.458943	-3.340613	-1.973270
C	0.839729	0.838858	2.384214	C	1.298595	1.049567	2.348378
H	1.128276	-0.149633	2.012075	H	1.401654	-0.015905	2.110855
H	0.034365	0.689709	3.109774	H	0.561837	1.136947	3.152251
C	-0.049087	2.499613	-2.231424	C	0.218412	2.163467	-2.389204
H	0.201524	1.526100	-2.658137	H	0.261922	1.107924	-2.663596
H	-1.040251	2.778542	-2.600450	H	-0.757366	2.543383	-2.705389
C	-0.697969	-1.623808	-0.189974	C	-0.936395	-1.104847	-0.050501
C	-1.788616	-0.868324	-0.371376	C	-1.932302	-0.383847	-0.651756
C	-0.380708	-2.811996	0.450696	C	-0.985054	-1.837928	1.169039
H	-1.833541	-0.143655	-1.180191	H	-1.817571	-0.080292	-1.689202
C	-0.983454	3.052993	0.076493	C	-0.278085	3.253911	-0.140899
C	-1.909318	4.069402	-0.164910	C	-0.979935	4.414156	-0.474649
H	-2.115862	4.428459	-1.167513	H	-1.212561	4.665811	-1.503866
C	-2.560214	4.604850	0.943006	C	-1.373014	5.235196	0.577713
C	-2.296347	4.143215	2.246469	C	-1.076349	4.911984	1.916059
H	-2.825206	4.587630	3.083893	H	-1.403384	5.579251	2.707347
C	-1.371632	3.131017	2.487202	C	-0.376320	3.756493	2.248247
H	-1.168098	2.778857	3.492523	H	-0.151882	3.507254	3.279450
H	-3.288334	5.396819	0.797509	H	-1.923361	6.145656	0.361692
C	-3.033440	-0.996857	0.482664	C	-3.267446	-0.099187	-0.011625
H	-3.254307	-0.032054	0.963965	H	-3.529920	0.960028	-0.156516
H	-2.830725	-1.714091	1.287081	H	-3.179402	-0.245071	1.073696
C	-4.266722	-1.429305	-0.298208	C	-4.426356	-0.940531	-0.538656
C	-4.228984	-2.550822	-1.139351	C	-4.288344	-2.322815	-0.733325
C	-5.472178	-0.726419	-0.183149	C	-5.663781	-0.350867	-0.825726
C	-5.365454	-2.961799	-1.834759	C	-5.360154	-3.090250	-1.188765
H	-3.296843	-3.098533	-1.251154	H	-3.330731	-2.793867	-0.529231
C	-6.613166	-1.133688	-0.878326	C	-6.738675	-1.115091	-1.285477
H	-5.518794	0.149081	0.461822	H	-5.787415	0.721766	-0.686240

C	-6.563745	-2.254567	-1.707078	C	-6.590768	-2.490100	-1.467738
H	-5.315501	-3.835697	-2.479603	H	-5.233010	-4.160938	-1.329437
H	-7.538789	-0.572921	-0.772912	H	-7.689362	-0.634282	-1.504031
H	-7.449063	-2.574023	-2.250727	H	-7.424107	-3.088768	-1.826618
H	-0.941922	-3.705030	0.188503	H	-1.965408	-2.147741	1.516256
C	0.756339	-2.983800	1.291947	C	0.106783	-2.271903	1.947257
O	0.903960	-4.290434	1.693167	O	-0.299557	-3.121029	2.965784
O	1.566787	-2.120454	1.663321	O	1.321059	-1.980865	1.850802
C	2.009468	-4.543842	2.554940	C	0.736064	-3.580888	3.822611
H	1.943062	-5.601881	2.818171	H	0.244060	-4.201649	4.575965
H	2.961714	-4.343347	2.052159	H	1.477599	-4.175968	3.277992
H	1.961966	-3.926724	3.458290	H	1.260607	-2.750239	4.309077
C	2.024857	1.580990	2.999556	C	2.640714	1.670185	2.734468
H	1.738132	2.565077	3.387850	H	2.551632	2.733332	2.985210
H	2.424223	0.987474	3.828240	H	3.035992	1.143905	3.609259
H	2.814682	1.710786	2.254508	H	3.357854	1.560651	1.915578
C	1.001896	3.553846	-2.579180	C	1.366170	2.953671	-3.017827
H	1.068689	3.658278	-3.667051	H	1.306383	2.879488	-4.108548
H	0.747067	4.530876	-2.155013	H	1.323516	4.012888	-2.743470
H	1.982488	3.252695	-2.199189	H	2.329548	2.548686	-2.694439
TS_{A1-7}:				**7f:**			
C	-0.109942	2.664239	1.504415	C	0.759271	2.616202	1.473324
N	0.312436	2.244998	-0.655625	N	0.679748	2.001488	-0.705358
N	0.527485	1.431069	1.382399	N	0.469152	1.255800	1.428517
C	0.734181	1.186350	0.074578	C	0.384674	0.785083	0.041628
C	1.561488	0.063260	-0.476068	C	1.391056	-0.377153	-0.235232
N	2.758098	0.429578	-0.776202	N	2.607505	-0.154285	-0.513112
S	0.818275	-1.519487	-0.707428	S	0.598410	-1.990258	-0.081175
C	3.756863	-0.459340	-1.227904	C	3.574631	-1.164133	-0.698545
C	4.566839	-0.046330	-2.297464	C	4.387149	-1.104698	-1.842342
C	4.037135	-1.677330	-0.582110	C	3.813081	-2.166740	0.256023
C	5.607291	-0.856384	-2.746810	C	5.384474	-2.054592	-2.046745
H	4.364158	0.910287	-2.770398	H	4.218167	-0.314357	-2.567086
C	5.096803	-2.467443	-1.024061	C	4.828787	-3.101141	0.053575
H	3.439102	-1.991654	0.267767	H	3.217801	-2.201754	1.163002
C	5.878410	-2.070113	-2.111347	C	5.612388	-3.056625	-1.099795
H	6.215847	-0.531881	-3.586863	H	5.994549	-2.004782	-2.944803
H	5.308562	-3.403532	-0.514333	H	5.004592	-3.867564	0.803696
H	6.697187	-2.696380	-2.454543	H	6.399051	-3.789270	-1.256244
C	1.025675	0.617700	2.509001	C	0.338927	0.431956	2.619270
H	1.097355	-0.428049	2.190451	H	-0.196959	-0.483217	2.355584
H	0.255306	0.658257	3.284080	H	-0.304047	0.971139	3.329310
C	0.389404	2.363680	-2.116245	C	0.806078	2.070892	-2.151983
H	0.511345	1.354815	-2.513922	H	0.516435	1.097331	-2.559588
H	-0.580576	2.736140	-2.460992	H	0.079492	2.801530	-2.540719
C	-0.841495	-1.285344	0.015535	C	-1.032053	-1.283918	0.024242
C	-1.655034	-0.426445	-0.684278	C	-1.024759	0.186328	-0.331611

C	-1.150850	-2.076770	1.147105	C	-2.125125	-2.005182	0.347969
H	-1.366892	-0.127171	-1.688955	C	1.672862	0.085718	3.294737
C	-0.249585	3.181612	0.205696	H	2.220754	0.993497	3.565899
C	-0.869039	4.410446	-0.029146	H	1.494641	-0.494771	4.207442
H	-0.984299	4.809967	-1.031094	H	2.311042	-0.503486	2.630005
C	-1.336376	5.103753	1.084873	C	2.212449	2.422631	-2.655126
C	-1.190117	4.589625	2.386289	H	2.221639	2.430818	-3.751537
H	-1.567837	5.161160	3.228373	H	2.530112	3.409213	-2.306965
C	-0.574914	3.362051	2.619859	H	2.934636	1.689705	-2.290584
H	-0.468353	2.965657	3.623662	H	-3.097235	-1.528105	0.370432
H	-1.825420	6.062798	0.944609	H	-1.054716	0.218137	-1.430202
C	-3.036860	-0.026215	-0.233199	C	-2.187293	1.044225	0.210344
H	-3.164064	1.061743	-0.343844	C	-2.086333	-3.440471	0.647620
H	-3.133595	-0.234300	0.841304	C	0.869997	3.084549	0.148970
C	-4.182506	-0.703442	-0.980051	C	1.088475	4.428828	-0.113496
C	-4.153859	-2.077579	-1.259051	H	1.152346	4.803152	-1.129915
C	-5.300433	0.033631	-1.390763	C	1.220434	5.308182	0.980773
C	-5.217657	-2.695011	-1.916685	C	1.128206	4.842240	2.286227
H	-3.286904	-2.660908	-0.961451	H	1.238041	5.531080	3.118959
C	-6.366432	-0.579925	-2.052250	C	0.892057	3.477974	2.551497
H	-5.337117	1.102682	-1.188016	H	0.813338	3.119994	3.573290
C	-6.329340	-1.949176	-2.316729	H	1.399520	6.362680	0.791101
H	-5.177059	-3.762312	-2.120297	H	-2.351172	0.813159	1.267792
H	-7.223162	0.013354	-2.363288	H	-1.849668	2.087522	0.174571
H	-7.156200	-2.430817	-2.832417	C	-3.501228	0.937517	-0.544688
H	-2.197632	-2.301601	1.322370	C	-3.574650	1.220258	-1.916684
C	-0.234285	-2.635936	2.076858	C	-4.686471	0.605019	0.124468
O	-0.876124	-3.492664	2.954467	C	-4.788767	1.156784	-2.599520
O	0.988014	-2.435786	2.201348	H	-2.674685	1.504455	-2.458090
C	-0.041493	-4.080141	3.944867	C	-5.905369	0.541104	-0.554238
H	-0.698958	-4.705888	4.553587	H	-4.655459	0.397040	1.191975
H	0.746423	-4.693343	3.494293	C	-5.960290	0.813918	-1.920690
H	0.437522	-3.319963	4.572474	H	-4.821023	1.380360	-3.662727
C	2.370686	1.134269	3.020536	H	-6.810155	0.278412	-0.012448
H	2.307906	2.167274	3.380662	H	-6.906487	0.764248	-2.452522
H	2.702242	0.499415	3.848393	O	-3.316440	-3.899464	0.985827
H	3.126704	1.087040	2.230518	O	-1.097263	-4.154339	0.606606
C	1.535609	3.271472	-2.561796	C	-3.383657	-5.300476	1.286647
H	1.557038	3.325010	-3.655344	H	-3.065536	-5.895748	0.426203
H	1.418160	4.288027	-2.172418	H	-2.743413	-5.543728	2.139269
H	2.488544	2.869060	-2.208003	H	-4.429378	-5.498835	1.524192

TS_{B1}:

C	-1.824754	-2.296407	1.046690
N	-2.448415	-0.906199	-0.593157
N	-1.241292	-1.046478	1.239993
C	-1.630127	-0.227930	0.242377
C	-1.348175	1.241511	0.116812

27:

C	-2.153191	-2.242187	0.813968
N	-1.793403	-1.104889	-1.107273
N	-1.371011	-1.131360	1.114658
C	-0.964592	-0.456093	-0.112299
C	-1.212494	1.083180	-0.018169

N	-2.456873	1.914300	0.109877	N	-2.358125	1.570732	-0.254799
S	0.306364	1.767613	-0.057319	S	0.276347	1.965666	0.435487
C	-2.565582	3.312702	0.067196	C	-2.679994	2.933702	-0.110003
C	-3.700667	3.829854	-0.586213	C	-3.359124	3.570185	-1.161737
C	-1.685678	4.212471	0.698342	C	-2.425843	3.650187	1.071537
C	-3.924223	5.201567	-0.652237	C	-3.733694	4.906354	-1.049943
H	-4.395060	3.133516	-1.046930	H	-3.577143	3.005144	-2.062821
C	-1.932686	5.583615	0.653144	C	-2.825545	4.982006	1.183466
H	-0.823047	3.836058	1.234253	H	-1.939146	3.156374	1.907006
C	-3.040917	6.087647	-0.030037	C	-3.471198	5.619106	0.123304
H	-4.797389	5.579610	-1.177713	H	-4.244648	5.390166	-1.878222
H	-1.246416	6.263207	1.151801	H	-2.630101	5.521575	2.106444
H	-3.219360	7.158674	-0.070509	H	-3.776588	6.657781	0.212833
C	-0.331367	-0.731514	2.355915	C	-0.893280	-0.828516	2.457511
H	0.208771	0.172492	2.079373	H	0.001678	-0.208752	2.379950
H	0.397367	-1.545692	2.382327	H	-0.565153	-1.767742	2.918984
C	-3.050555	-0.403058	-1.836626	C	-1.785514	-0.771513	-2.521234
H	-2.518436	0.508247	-2.106168	H	-1.082023	0.053818	-2.666700
H	-2.844755	-1.152938	-2.607410	H	-1.394759	-1.625141	-3.096031
C	1.543600	-0.032059	-0.515696	C	1.354658	0.541892	0.214544
C	0.975081	-0.977111	-1.341892	C	0.609007	-0.592954	-0.441992
C	2.666933	0.171345	0.173238	C	2.645623	0.638615	0.556962
C	-1.078596	-0.547584	3.676468	C	-1.948381	-0.141749	3.332830
H	-1.636276	-1.444239	3.965530	H	-2.851545	-0.755251	3.414781
H	-0.356678	-0.327589	4.469849	H	-1.553321	0.022533	4.342379
H	-1.782391	0.288769	3.614337	H	-2.240921	0.826291	2.913985
C	-4.547483	-0.133556	-1.689981	C	-3.159844	-0.349737	-3.054500
H	-4.943417	0.245312	-2.638278	H	-3.086430	-0.092458	-4.117717
H	-5.102108	-1.040810	-1.429672	H	-3.895744	-1.152086	-2.949936
H	-4.712505	0.615427	-0.911852	H	-3.524488	0.515653	-2.496115
H	2.723938	0.929067	0.950795	H	2.975237	1.562449	1.031650
H	0.608509	-0.716408	-2.330993	H	0.686739	-0.482044	-1.529371
C	0.889320	-2.350356	-0.929358	C	1.067189	-1.989771	-0.071567
C	-2.593976	-2.207396	-0.120863	C	-2.401010	-2.237533	-0.573644
C	-3.311454	-3.301731	-0.609903	C	-3.127120	-3.256973	-1.171606
H	-3.897491	-3.240319	-1.520151	H	-3.306979	-3.270562	-2.241573
C	-3.237984	-4.480686	0.124751	C	-3.626632	-4.286826	-0.349126
C	-2.463433	-4.569734	1.298151	C	-3.393676	-4.283227	1.021426
H	-2.422791	-5.511504	1.836696	H	-3.788981	-5.082639	1.641769
C	-1.738042	-3.483642	1.775380	C	-2.645568	-3.253247	1.625953
H	-1.117204	-3.563967	2.659935	H	-2.459328	-3.258802	2.695190
H	-3.784977	-5.353649	-0.218091	H	-4.202169	-5.090223	-0.800233
C	3.918029	-0.645914	-0.069769	C	3.732720	-0.390842	0.344816
H	3.797848	-1.190721	-1.014307	H	3.453046	-1.073286	-0.467265
H	4.003454	-1.416888	0.709290	H	3.823879	-1.018348	1.241132
O	1.187841	-2.844597	0.160365	O	1.428379	-2.354580	1.026639
O	0.399220	-3.140876	-1.954144	O	0.956362	-2.812439	-1.136605

C	0.407359	-4.541964	-1.690839	C	1.198723	-4.205815	-0.866306
H	-0.242872	-4.797665	-0.848733	H	0.473832	-4.577272	-0.137853
H	0.041586	-5.017197	-2.604478	H	1.075673	-4.712681	-1.823386
H	1.418569	-4.896316	-1.464808	H	2.210238	-4.350254	-0.478648
C	5.190285	0.183341	-0.098422	C	5.078356	0.239202	0.026988
C	5.282909	1.324121	-0.909122	C	5.224181	1.102147	-1.068792
C	6.305596	-0.179361	0.666180	C	6.202688	-0.034455	0.814115
C	6.457111	2.074793	-0.957769	C	6.460432	1.672368	-1.370392
H	4.421436	1.623248	-1.501441	H	4.358990	1.329041	-1.687900
C	7.484297	0.568520	0.620625	C	7.443140	0.533532	0.515367
H	6.250172	-1.059868	1.303146	H	6.105957	-0.699690	1.669358
C	7.564097	1.699243	-0.192564	C	7.575820	1.389120	-0.578262
H	6.508520	2.955378	-1.593563	H	6.553806	2.338229	-2.224531
H	8.338006	0.268297	1.223405	H	8.304001	0.308052	1.139570
H	8.479240	2.284723	-0.229147	H	8.539658	1.833322	-0.812180
5d'				**TS_{N1}**			
C	-2.670773	-0.320488	-0.704376	N	-2.510543	0.604295	-0.837888
C	-2.677672	-0.333655	0.701160	N	-2.498560	-0.847052	0.818752
N	-1.332953	-0.263743	-1.094066	C	-0.894791	-1.320533	1.089728
N	-1.343545	-0.285975	1.104896	N	0.370284	-1.063866	-0.826560
C	-0.552393	-0.262776	0.009209	S	-1.681870	2.380180	2.168072
C	0.941569	-0.248284	0.013904	C	1.469102	-1.716174	-1.447933
N	1.407453	0.965665	-0.000484	C	2.613938	-0.937778	-1.680793
S	1.536123	-1.865724	0.029528	C	1.492652	-3.082925	-1.763453
C	-0.861652	-0.299107	2.493066	C	3.745315	-1.505414	-2.260084
C	-0.837699	-0.248602	-2.477408	H	2.614239	0.109024	-1.394450
C	-0.830259	-1.638839	-3.113299	C	2.635217	-3.645379	-2.331995
C	0.150874	0.106934	2.473469	H	0.625455	-3.699048	-1.566782
C	0.166598	0.176395	-2.442200	C	3.760208	-2.861946	-2.591733
C	-1.473336	0.447624	-3.034585	H	4.620660	-0.887454	-2.439919
C	-1.834897	-2.074285	-3.140026	H	2.641724	-4.705281	-2.572327
C	-0.169791	-2.305149	-2.551827	H	4.645385	-3.306527	-3.038584
C	-0.462047	-1.565301	-4.142120	C	-2.197459	-2.041247	1.621669
H	-0.883882	-1.698187	3.108442	H	-1.215779	-2.394936	1.312270
H	-0.521113	-1.645797	4.140445	H	-2.106025	-1.715655	2.662229
H	-1.896143	-2.116178	3.122848	C	-2.269289	1.208592	-2.157767
H	-0.230977	-2.366754	2.540780	H	-1.312268	0.826954	-2.513828
H	-1.489434	0.400625	3.054904	H	-2.158421	2.286222	-2.003030
H	-3.870434	-0.361168	1.422632	C	0.796064	-0.288783	0.864376
H	-5.055843	-0.377975	0.688458	C	0.526096	1.021518	0.887397
H	-5.048885	-0.366219	-0.716614	C	1.340558	-1.272378	1.637979
H	-3.856094	-0.336376	-1.438425	C	-1.913955	-0.508453	0.350297
H	-3.880019	-0.369263	2.507334	C	-3.383075	0.890405	-3.155806
H	-6.004739	-0.401432	1.215462	H	-4.353434	1.265222	-2.815067
C	-5.992355	-0.381011	-1.253624	H	-3.151321	1.365933	-4.114574
H	-3.854649	-0.326466	-2.523253	H	-3.453268	-0.189447	-3.309390
H	2.754631	1.346622	-0.003888	C	-3.254872	-3.132452	1.450790

H	2.971891	2.740804	-0.035701	H	-2.986593	-3.994099	2.070916
H	3.882780	0.497587	0.021942	H	-4.247947	-2.788279	1.757267
C	4.255847	3.273479	-0.042775	H	-3.302220	-3.454640	0.406665
C	2.097746	3.385402	-0.054734	H	0.970932	-2.292440	1.628153
C	5.167499	1.041869	0.015632	C	2.536321	-1.029331	2.417801
C	3.742951	-0.575106	0.046023	H	0.406400	1.438185	1.887527
H	5.365680	2.423235	-0.016918	C	0.553915	2.009622	-0.245937
H	4.393749	4.351802	-0.068009	C	-3.489074	0.087547	1.114302
H	6.024776	0.372786	0.035909	C	-3.499070	1.011256	0.057629
H	6.372297	2.833606	-0.021916	C	-4.369988	2.101158	0.050805
				C	-4.347712	0.218087	2.205906
				H	-4.336657	-0.489704	3.027539
				C	-5.218941	1.305436	2.198411
				C	-5.229804	2.230488	1.139707
				H	-5.921100	3.066855	1.171626
				H	-5.901664	1.442370	3.031205
				H	-4.377766	2.821210	-0.760246
				H	0.571436	1.460666	-1.195874
				H	-0.370985	2.606790	-0.246124
				C	1.729284	2.987710	-0.223414
				C	1.626942	4.195037	-0.930434
				C	2.919234	2.707071	0.460578
				C	2.688271	5.097905	-0.969261
				H	0.703032	4.430317	-1.457404
				C	3.982044	3.615053	0.423156
				H	3.010961	1.791027	1.039856
				C	3.874580	4.808616	-0.290277
				H	2.588009	6.028093	-1.523602
				H	4.896543	3.383833	0.963676
				H	4.703303	5.511855	-0.313605
				O	3.178482	0.008974	2.531117
				O	2.904648	-2.170826	3.092256
				C	4.076954	-2.040759	3.894975
				H	4.948081	-1.782876	3.284164
				H	3.950856	-1.266341	4.658503
				H	4.223044	-3.015454	4.365834

9f:

N	2.381840	-0.349163	-1.031791
N	2.09100	0.177926	1.15896
C	0.836680	1.597574	-0.466670
N	-0.514720	1.595759	-0.212574
S	1.722532	2.894970	-0.953330
C	-1.335006	2.776277	-0.287119
C	-2.192319	2.942373	-1.375366
C	-1.285970	3.725574	0.735263
C	-3.007068	4.072912	-1.441255
H	-2.214050	2.193684	-2.161462

C	-2.102701	4.853202	0.662023
H	-0.608885	3.582225	1.571185
C	-2.962988	5.027905	-0.424162
H	-3.673570	4.206468	-2.288399
H	-2.065237	5.595554	1.453958
H	-3.597606	5.907908	-0.477965
C	1.494260	0.517755	2.44231
H	0.42218	0.682206	2.30499
H	1.583113	-0.346812	3.116016
C	2.403508	-0.198108	-2.483372
H	1.49218	0.328197	-2.775613
H	2.35520	-1.191768	-2.955043
C	-1.010213	0.365367	0.278861
C	0.025002	-0.681435	-0.026936
C	-2.205682	0.258015	0.897694
C	1.369055	0.168171	-0.121305
C	3.616789	0.567885	-3.024490
H	4.557811	0.088448	-2.742264
H	3.56709	0.598237	-4.119505
H	3.62489	1.589889	-2.639923
C	2.131210	1.753948	3.08952
H	1.68143	1.943270	4.07174
H	3.20770	1.612905	3.22838
H	1.99186	2.639029	2.46075
H	-2.860654	1.118214	0.972774
C	-2.666703	-0.970348	1.562503
H	0.09024	-1.411930	0.779581
C	-0.301120	-1.430686	-1.354885
C	3.234066	-0.611016	1.054048
C	3.418889	-0.935004	-0.303719
C	4.476700	-1.736720	-0.705664
C	4.108678	-1.071932	2.026683
H	3.97294	-0.820334	3.073937
C	5.189428	-1.878947	1.618284
C	5.369902	-2.204507	0.279306
H	6.20594	-2.830145	-0.020296
H	5.88533	-2.248196	2.366361
H	4.61418	-2.008704	-1.747264
H	-0.449146	-0.696332	-2.155782
H	0.59579	-2.002770	-1.610360
C	-1.490018	-2.366534	-1.314034
C	-2.746026	-1.964740	-1.785411
C	-1.348268	-3.673089	-0.826559
C	-3.836775	-2.836873	-1.756262
H	-2.872766	-0.960489	-2.183510
C	-2.432236	-4.547535	-0.795454
H	-0.378878	-4.004156	-0.460931

C	-3.683170	-4.131322	-1.258916
H	-4.802620	-2.505563	-2.129049
H	-2.300804	-5.556010	-0.412318
H	-4.528042	-4.814950	-1.242087
O	-1.998283	-1.948922	1.844812
O	-3.980582	-0.858391	1.884543
C	-4.543173	-2.002336	2.542547
H	-4.474664	-2.883453	1.898836
H	-4.019859	-2.206448	3.480837
H	-5.585970	-1.745803	2.733832

Table S2. The Cartesian coordinates for the stationary points of the reactions **10**+**6a**→*E*-**11, 10**+**6a**→*Z*-**11, 10**+**6a**→**13** and **10'**+**6a**→**12**.

10:

C	-3.403458	0.784923	-0.517421
C	-3.480569	-0.759819	-0.426283
N	-1.960228	1.110859	0.007284
N	-2.106965	-1.093940	-0.078542
C	-1.290856	0.005237	0.202833
C	0.190326	-0.003397	0.682657
N	0.499399	0.018097	-0.313060
S	0.967734	-0.046415	2.402432
C	-1.692170	-2.467729	0.058846
C	-1.806142	-3.027588	-1.251682
C	-1.381015	2.478784	0.120192
C	-1.433547	3.020160	-1.197493
C	-3.926739	1.141591	-1.549466
C	-3.809600	1.259825	0.088949
C	-4.190732	-1.230626	-1.370688
C	-3.750168	-1.115871	0.359637
C	-0.663490	-2.466283	0.842220
C	-2.317643	-3.070084	0.423355
H	-2.837141	-3.041090	-2.040920
H	-1.485865	-4.055157	-1.100584
H	-1.165006	-2.417629	-1.586843
H	-0.350707	2.471284	0.899394
H	-1.925592	3.097358	0.483776
H	-2.463831	3.046235	-1.983494
H	-0.874743	2.393638	-1.533064
H	-0.982346	4.042028	-1.053046
H	1.786876	0.011270	-0.229790
H	1.833582	0.025589	-1.473534
H	3.007002	-0.007576	0.944654
H	3.040885	0.020478	-1.551065
H	0.890468	0.040343	-2.372559
H	4.213559	-0.012118	0.856370
H	2.997968	-0.018664	1.910527
H	4.243139	0.001517	-0.381423
H	3.046640	0.031461	-2.523334
H	5.143387	-0.026739	1.771921
H	5.190286	-0.002468	-0.435630

TS_{A2}:

N	-0.025441	-2.819708	0.065805
N	-0.327185	-1.525559	1.830938
C	-0.595149	-1.710653	0.548104
C	-1.457763	-0.798058	-0.273395
N	-2.712497	-0.987920	-0.043363
S	-0.603273	0.214648	-1.413971
C	-3.743849	-0.236953	-0.644455
C	-4.846159	-0.936129	-1.159783
C	-3.753570	1.168698	-0.643086
C	-5.923488	-0.244960	-1.710931
H	-4.841020	-2.022190	-1.125661
C	-4.849730	1.847957	-1.171877
H	-2.923036	1.709883	-0.200686
C	-5.930529	1.151340	-1.718933
H	-6.764028	-0.798511	-2.122031
H	-4.855418	2.935091	-1.159967
H	-6.775018	1.691879	-2.138194
C	-0.752256	-0.395844	2.670592
H	-0.957631	0.463919	2.025334
H	0.111427	-0.130127	3.291314
C	-0.280234	-3.409000	-1.251068
H	-0.435298	-2.580828	-1.946444
H	0.640133	-3.920994	-1.553326
C	1.087279	1.023073	-0.320499
C	2.050491	0.097572	-0.217209
C	0.947290	2.375916	-0.053925
H	1.997405	-0.824228	-0.790888
C	3.279587	0.283644	0.649063
H	3.339484	-0.524616	1.396179
H	3.170059	1.220264	1.208945
C	4.588344	0.294803	-0.129171
C	4.737986	1.087781	-1.275867
C	5.680310	-0.472731	0.294202
C	5.946874	1.119141	-1.970190
H	3.895131	1.677830	-1.625842
C	6.892925	-0.445186	-0.398114
H	5.581758	-1.096393	1.181055
C	7.030452	0.352431	-1.534187
H	6.042928	1.742475	-2.855698
H	7.727614	-1.048955	-0.050234
H	7.971781	0.375568	-2.077007
H	1.652748	3.065970	-0.509299
C	-0.168618	2.944393	0.628513
O	-0.111767	4.318062	0.641957

O	-1.114274	2.351721	1.169040
C	-1.181609	4.966776	1.323139
H	-0.946077	6.033068	1.296556
H	-2.140310	4.784124	0.825706
H	-1.261936	4.623291	2.359672
C	-1.965284	-0.748522	3.532017
H	-1.768976	-1.597142	4.198751
H	-2.230321	0.113640	4.152637
H	-2.820061	-0.991631	2.894317
C	-1.474004	-4.367461	-1.258778
H	-1.617017	-4.769243	-2.267459
H	-1.323464	-5.214592	-0.579925
H	-2.385305	-3.839084	-0.963244
C	0.585528	-2.568280	2.325278
C	0.645225	-3.562090	1.144343
H	0.196301	-3.018527	3.242547
H	1.561049	-2.118508	2.543195
H	0.104393	-4.492210	1.355549
H	1.668961	-3.815506	0.853334

INT_{A2}:

N	-0.891822	-0.986668	2.403345
N	-0.621827	1.209909	2.142578
C	-0.903450	0.046252	1.524454
C	-1.524123	-0.054584	0.166183
N	-2.622375	-0.728407	0.131790
S	-0.695775	0.774754	-1.171641
C	-3.409579	-0.934649	-1.007292
C	-4.046566	-2.185749	-1.120126
C	-3.662479	0.043085	-1.987638
C	-4.861099	-2.471684	-2.209972
H	-3.875256	-2.925124	-0.343309
C	-4.499723	-0.244553	-3.065925
H	-3.239729	1.037073	-1.888121
C	-5.091958	-1.501301	-3.190499
H	-5.328132	-3.449800	-2.290333
H	-4.687957	0.522980	-3.811805
H	-5.737979	-1.720533	-4.035999
C	-1.025372	2.563326	1.722516
H	-0.758546	2.727176	0.677169
H	-0.405627	3.250511	2.307725
C	-0.902862	-2.405486	2.052647
H	-1.010479	-2.485170	0.972389
H	0.072599	-2.833633	2.323404
C	0.984519	0.663315	-0.500403
C	1.275498	-0.599159	0.007909
C	1.812400	1.788946	-0.520906
H	0.701398	-1.445607	-0.357029

$TS_{A2\text{-}13}$:

N	-0.026291	-2.113258	1.415606
N	-0.166852	-0.046880	2.203645
C	-0.378784	-0.845885	1.164603
C	-1.505128	-0.512298	0.183390
N	-2.698960	-0.990236	0.198704
S	-0.719530	0.446593	-1.068539
C	-3.673833	-0.705855	-0.778965
C	-4.477776	-1.768688	-1.221586
C	-3.938067	0.595444	-1.242855
C	-5.494429	-1.545663	-2.146930
H	-4.286312	-2.764674	-0.832832
C	-4.974677	0.811140	-2.149580
H	-3.347516	1.431206	-0.880857
C	-5.748959	-0.254142	-2.614366
H	-6.097886	-2.380543	-2.493574
H	-5.174107	1.821419	-2.496711
H	-6.549757	-0.078237	-3.327210
C	-0.707580	1.306641	2.398377
H	-0.752747	1.819392	1.431553
H	0.030307	1.848906	2.998785
C	0.022000	-3.200813	0.440921
H	-0.256626	-2.789550	-0.530253
H	1.063200	-3.540622	0.363565
C	0.955679	0.689590	-0.385344
C	1.361079	-0.524511	-0.056910
C	1.338975	2.023039	-0.114426
H	1.019452	-1.416822	-0.574282

C	2.560810	-0.933578	0.724012	C	2.761764	-0.568700	0.503769
H	2.347959	-1.603453	1.571268	H	2.875219	-1.441209	1.167242
H	2.980089	-0.018189	1.164089	H	2.922413	0.314951	1.136632
C	3.624493	-1.614617	-0.134732	C	3.870546	-0.646935	-0.542057
C	3.913881	-1.162363	-1.430389	C	3.866024	0.193646	-1.665170
C	4.346896	-2.705902	0.364242	C	4.924978	-1.557198	-0.399153
C	4.904811	-1.777664	-2.195413	C	4.892549	0.131102	-2.607010
H	3.354384	-0.326358	-1.839959	H	3.047330	0.895027	-1.800300
C	5.337909	-3.326034	-0.399458	C	5.953041	-1.625899	-1.342224
H	4.130986	-3.075791	1.365230	H	4.942001	-2.222079	0.462929
C	5.621655	-2.862131	-1.684105	C	5.940967	-0.779462	-2.450707
H	5.115478	-1.410140	-3.196700	H	4.871973	0.793742	-3.468794
H	5.883923	-4.173242	0.008640	H	6.759981	-2.343072	-1.211185
H	6.390821	-3.342577	-2.283271	H	6.737967	-0.829892	-3.188144
H	2.866605	1.633573	-0.319030	H	2.402647	2.236612	-0.101642
C	1.436293	3.140829	-0.804622	C	0.488209	3.138917	0.113228
O	2.544968	3.962788	-0.800646	O	1.224023	4.310692	0.188148
O	0.313700	3.609537	-1.019638	O	-0.745188	3.181968	0.263216
C	2.279104	5.334167	-1.080783	C	0.462141	5.486263	0.432571
H	3.250458	5.833649	-1.062654	H	1.184351	6.305792	0.468516
H	1.810273	5.456759	-2.062567	H	-0.267524	5.665578	-0.364472
H	1.616294	5.775544	-0.328366	H	-0.081488	5.425402	1.382386
C	-2.512843	2.844961	1.958013	C	-2.076750	1.296231	3.083889
H	-2.799470	2.726972	3.009791	H	-2.044565	0.843206	4.081957
H	-2.734851	3.875974	1.663074	H	-2.426412	2.327685	3.195984
H	-3.139255	2.178910	1.356146	H	-2.808050	0.751674	2.478059
C	-2.038455	-3.155542	2.748976	C	-0.908999	-4.353414	0.817437
H	-2.012125	-4.214514	2.469584	H	-0.840135	-5.146004	0.064872
H	-1.958176	-3.098457	3.840541	H	-0.646454	-4.791611	1.786878
H	-3.001543	-2.734346	2.447331	H	-1.943626	-4.001098	0.862598
C	-0.357650	0.972044	3.568229	C	0.407496	-0.810953	3.321916
C	-0.260795	-0.557263	3.654747	C	0.715458	-2.179664	2.682170
H	-1.189357	1.364925	4.167053	H	-0.326925	-0.886987	4.132114
H	0.561568	1.476280	3.880222	H	1.300107	-0.309183	3.705445
H	-0.780915	-0.972183	4.522593	H	0.379163	-3.022408	3.291702
H	0.783908	-0.897704	3.679450	H	1.784997	-2.302351	2.469148
13:				**TS_{B2}:**			
C	0.641142	-2.583817	2.385678	C	-0.190373	2.104807	2.077596
C	0.044036	-3.426935	1.266423	C	-0.906548	0.773321	2.383145
H	0.256453	-2.849258	3.378073	H	-0.877785	2.824857	1.630231
H	1.737972	-2.687754	2.395763	H	0.299173	2.538262	2.956924
H	-1.007624	-3.692954	1.485063	H	-1.910112	0.753119	1.950243
H	0.601044	-4.356493	1.108859	H	-0.952653	0.550365	3.452557
N	0.187147	-1.250668	2.015567	N	0.824657	1.707807	1.084168
N	0.189387	-2.531745	0.131606	N	-0.065435	-0.218947	1.687604
C	0.174943	-1.140231	0.553637	C	0.840082	0.390224	0.928457
C	1.423278	-0.402720	-0.029507	C	1.811902	-0.316704	0.025107

N	2.536716	-0.988826	-0.174627	N	3.006104	-0.287066	0.515896
S	1.087265	1.350189	-0.325965	S	1.141956	-0.974145	-1.454383
C	3.699173	-0.372879	-0.675797	C	4.164748	-0.863915	-0.021482
C	4.871519	-0.435111	0.094823	C	5.375884	-0.352728	0.486810
C	3.749199	0.212281	-1.951996	C	4.221646	-1.914770	-0.958835
C	6.057064	0.117164	-0.384294	C	6.601735	-0.841102	0.048568
H	4.832807	-0.917358	1.066957	H	5.322941	0.438036	1.229240
C	4.945818	0.744911	-2.430866	C	5.454925	-2.412830	-1.378054
H	2.855178	0.231247	-2.567670	H	3.307527	-2.346728	-1.345591
C	6.101795	0.708703	-1.649301	C	6.647267	-1.876863	-0.888948
H	6.953308	0.074900	0.229265	H	7.522772	-0.422143	0.445433
H	4.971601	1.191195	-3.421619	H	5.480696	-3.225941	-2.098970
H	7.030537	1.128421	-2.025415	H	7.602847	-2.266682	-1.229120
C	-0.294717	-2.925009	-1.177259	C	-0.346126	-1.651936	1.759455
H	-0.004790	-2.143961	-1.889703	H	0.161852	-2.129889	0.920405
H	-1.399128	-2.997377	-1.215313	H	-1.423460	-1.778248	1.601369
C	0.516457	-0.142641	2.908060	C	1.640837	2.686578	0.364847
H	0.071984	0.769803	2.500180	H	2.117360	2.166258	-0.466338
H	-0.012500	-0.340641	3.851705	H	0.956769	3.425336	-0.066886
C	-0.638263	1.165532	0.045408	C	-0.840594	-0.057366	-1.709456
C	-1.471476	2.209090	0.247542	C	-0.822364	1.307444	-1.963094
C	-1.049961	-0.293516	0.047983	C	-1.704348	-1.072739	-1.643290
C	0.315977	-4.245480	-1.654329	C	0.095299	-2.272728	3.086782
H	0.002327	-5.090897	-1.032578	H	-0.411745	-1.813264	3.942332
H	-0.005775	-4.455779	-2.680214	H	-0.149241	-3.340214	3.090724
H	1.408960	-4.187445	-1.632478	H	1.175934	-2.165915	3.225135
C	2.000559	0.103735	3.229784	C	2.692439	3.344862	1.259040
H	2.081751	0.911611	3.966521	H	3.273562	4.064045	0.672168
H	2.469923	-0.786491	3.663036	H	2.238642	3.888985	2.094947
H	2.574766	0.395660	2.347104	H	3.374491	2.589271	1.659934
H	-1.153103	-0.554469	-1.014395	H	-1.391117	-2.046372	-1.277375
H	-2.519039	2.028787	0.460551	H	-0.222544	1.694410	-2.781583
C	-1.047896	3.611072	0.179080	C	-1.519184	2.258269	-1.167809
C	-2.373800	-0.637916	0.757265	C	-3.154997	-0.968368	-2.073611
H	-2.240265	-1.602780	1.255101	O	-1.320230	3.546061	-1.647968
O	-2.075368	4.443820	0.482837	O	-2.232318	2.082503	-0.165546
O	0.067467	4.009626	-0.113683	H	-3.356573	0.050675	-2.415785
C	-1.761436	5.842339	0.433456	C	-2.133106	4.553159	-1.054093
H	-0.975589	6.087805	1.153402	H	-3.195013	4.293204	-1.109280
H	-1.423522	6.127636	-0.566773	H	-1.877075	4.718670	-0.000828
H	-2.687610	6.359369	0.687109	H	-1.939483	5.464526	-1.624737
H	-2.543895	0.074174	1.575484	H	-3.320508	-1.641187	-2.927836
C	-3.614561	-0.713327	-0.120283	C	-4.109622	-1.354528	-0.954781
C	-4.653226	-1.581271	0.250910	C	-4.744250	-2.602319	-0.947419
C	-3.786581	0.058356	-1.277977	C	-4.351093	-0.469921	0.108750
C	-5.824879	-1.671379	-0.499236	C	-5.602918	-2.965632	0.093544
H	-4.537855	-2.196166	1.141203	H	-4.569371	-3.295676	-1.767880

C	-4.957130	-0.031809	-2.035373	C	-5.212220	-0.830599	1.145903
H	-3.005740	0.743637	-1.595263	H	-3.858458	0.499959	0.107135
C	-5.981846	-0.894914	-1.649170	C	-5.839839	-2.079874	1.144599
H	-6.612452	-2.353595	-0.189422	H	-6.089246	-3.938026	0.078349
H	-5.064709	0.577154	-2.929322	H	-5.401233	-0.130141	1.956494
H	-6.891931	-0.965268	-2.238783	H	-6.512246	-2.356756	1.952767
INT_{B2}:				**TS_{B2}-11:**			
C	0.360211	2.894538	1.597098	C	0.475299	2.963865	1.532933
C	-0.570366	1.831246	2.212730	C	-0.439730	1.935311	2.223663
H	-0.182297	3.568074	0.926268	H	-0.087871	3.625704	0.866097
H	0.879365	3.491403	2.352742	H	1.032585	3.577166	2.246970
H	-1.621590	2.017013	1.985034	H	-1.499466	2.156203	2.081224
H	-0.435439	1.742792	3.296303	H	-0.224508	1.850895	3.295192
N	1.321430	2.097992	0.817494	N	1.390253	2.127523	0.742873
N	-0.135148	0.588403	1.554747	N	-0.094622	0.676906	1.547093
C	0.878658	0.827128	0.717385	C	0.886698	0.870913	0.651925
C	1.712221	-0.257988	0.079571	C	1.705454	-0.256294	0.061397
N	2.926762	-0.267872	0.489584	N	2.923492	-0.268665	0.457105
S	0.963949	-1.335107	-1.129047	S	0.935056	-1.372720	-1.095579
C	3.909072	-1.192439	0.096832	C	3.884481	-1.226751	0.091607
C	5.204317	-0.688171	-0.116163	C	5.180177	-0.755151	-0.183406
C	3.691756	-2.577334	-0.004598	C	3.646035	-2.611633	0.076609
C	6.242433	-1.540004	-0.480059	C	6.196950	-1.642364	-0.522508
H	5.370933	0.378468	0.000386	H	5.364413	0.313824	-0.133908
C	4.744639	-3.427611	-0.342175	C	4.678115	-3.495981	-0.237156
H	2.710482	-2.988102	0.207073	H	2.664740	-2.994255	0.336240
C	6.017936	-2.915187	-0.593476	C	5.951385	-3.018302	-0.549547
H	7.233483	-1.132601	-0.661208	H	7.188341	-1.260934	-0.752055
H	4.564264	-4.497035	-0.411035	H	4.481490	-4.564785	-0.238813
H	6.832047	-3.581799	-0.863743	H	6.749273	-3.711572	-0.800437
C	-0.668758	-0.705796	1.984635	C	-0.654231	-0.591930	2.013691
H	-0.411584	-1.444383	1.227118	H	-0.456229	-1.347681	1.255546
H	-1.760164	-0.622402	1.983051	H	-1.741630	-0.471789	2.056834
C	2.158553	2.763020	-0.182927	C	2.210282	2.753384	-0.294755
H	2.644885	1.986956	-0.773068	H	2.659732	1.954646	-0.884410
H	1.500966	3.330305	-0.853882	H	1.550660	3.327577	-0.958648
C	-0.603465	-0.439116	-1.428770	C	-0.621534	-0.464979	-1.392372
C	-0.404369	0.971855	-1.637379	C	-0.398670	0.950509	-1.568324
C	-1.694349	-1.241012	-1.415340	C	-1.722527	-1.250197	-1.400963
C	-0.145480	-1.141821	3.357822	C	-0.091243	-1.035386	3.369136
H	-0.419515	-0.436611	4.149904	H	-0.309525	-0.315467	4.165329
H	-0.578758	-2.113540	3.617964	H	-0.545223	-1.990255	3.655427
H	0.944908	-1.243325	3.347997	H	0.994029	-1.172538	3.316760
C	3.214373	3.658763	0.462987	C	3.308977	3.632680	0.300812
H	3.829503	4.121490	-0.316042	H	3.913557	4.062776	-0.504840
H	2.766552	4.468149	1.050492	H	2.900942	4.465633	0.884413
H	3.865703	3.073440	1.119912	H	3.962392	3.042239	0.950961

H	-1.572483	-2.274379	-1.093909	H	-1.613652	-2.291966	-1.101983
H	0.422444	1.275636	-2.271305	H	0.404974	1.248518	-2.234783
C	-1.311968	1.981424	-1.240321	C	-1.314415	1.964387	-1.183520
C	-3.094802	-0.864288	-1.837506	C	-3.117802	-0.850446	-1.818455
O	-0.916307	3.236939	-1.720982	O	-0.936474	3.208558	-1.695006
O	-2.309593	1.904286	-0.505974	O	-2.297835	1.889114	-0.434489
H	-3.164112	0.213705	-1.990177	H	-3.175131	0.230050	-1.957698
C	-1.821335	4.299209	-1.443273	C	-1.834398	4.275622	-1.407753
H	-2.834378	4.058784	-1.780049	H	-2.855578	4.029465	-1.713867
H	-1.870769	4.530204	-0.371143	H	-1.853628	4.519816	-0.337840
H	-1.439223	5.166717	-1.987203	H	-1.466787	5.134808	-1.973907
H	-3.317912	-1.351453	-2.799604	H	-3.343812	-1.321575	-2.787676
C	-4.129269	-1.309667	-0.815486	C	-4.159938	-1.298685	-0.805223
C	-4.818927	-2.518724	-0.965267	C	-4.869646	-2.492643	-0.980263
C	-4.388280	-0.526532	0.320449	C	-4.406621	-0.534339	0.345901
C	-5.741668	-2.944365	-0.006134	C	-5.801023	-2.921525	-0.031120
H	-4.635625	-3.132397	-1.845395	H	-4.695314	-3.091759	-1.872161
C	-5.312412	-0.948010	1.277228	C	-5.339432	-0.959017	1.292687
H	-3.861450	0.417764	0.425459	H	-3.863380	0.397871	0.472376
C	-5.991092	-2.160003	1.120084	C	-6.038749	-2.155482	1.110169
H	-6.268869	-3.885524	-0.143445	H	-6.343844	-3.850667	-0.187786
H	-5.511773	-0.324314	2.146083	H	-5.528428	-0.350134	2.174188
H	-6.712668	-2.485455	1.865359	H	-6.766793	-2.483420	1.847997
***E*-11:**				**TS_{B2-A2}:**			
C	-0.501146	1.866045	2.779001	N	-0.536144	-2.318188	1.383925
C	-1.592923	2.664591	2.081971	N	-0.692503	-0.335371	2.360211
H	0.483679	2.363469	2.68409	C	-0.839037	-1.022786	1.234320
H	-0.705687	1.712110	3.842251	C	-1.507010	-0.483491	-0.001793
H	-1.450327	3.749544	2.173158	N	-2.717145	-0.902198	-0.116563
H	-2.574067	2.407813	2.507315	S	-0.583603	0.530932	-1.107080
N	-0.569528	0.606574	2.048598	C	-3.600129	-0.486052	-1.133984
N	-1.446907	2.238013	0.695695	C	-4.409258	-1.465393	-1.731935
C	-0.767916	0.943669	0.634113	C	-3.774149	0.863016	-1.492013
C	-1.579270	-0.213425	-0.028432	C	-5.340980	-1.111750	-2.704909
N	-2.762148	-0.469586	0.344390	H	-4.289245	-2.500307	-1.424766
S	-0.624034	-1.114023	-1.251682	C	-4.727463	1.208401	-2.448581
C	-3.558180	-1.494806	-0.198856	H	-3.179740	1.633491	-1.010754
C	-4.148821	-2.413217	0.683877	C	-5.505716	0.227261	-3.066912
C	-3.849112	-1.576582	-1.570677	H	-5.949071	-1.882296	-3.171641
C	-4.977941	-3.420159	0.196606	H	-4.858253	2.254201	-2.713396
H	-3.939009	-2.324089	1.745513	H	-6.240838	0.504562	-3.817305
C	-4.697370	-2.576937	-2.046482	C	-1.214190	1.009798	2.643835
H	-3.427238	-0.845223	-2.253592	H	-1.174437	1.610867	1.728860
C	-5.258049	-3.506915	-1.169938	H	-0.511136	1.470711	3.345491
H	-5.416864	-4.134253	0.888610	C	-0.436042	-3.306663	0.312348
H	-4.919681	-2.626359	-3.109292	H	-0.624215	-2.793991	-0.632069
H	-5.914973	-4.286420	-1.545583	H	0.599260	-3.670945	0.283479

C	-2.466545	2.653477	-0.273320	C	1.027420	0.676367	-0.259951
H	-2.333325	2.054575	-1.175826	C	1.752908	-0.491726	-0.212459
H	-2.246051	3.689630	-0.571131	C	1.402087	1.973497	0.160493
C	0.396316	-0.425074	2.403943	H	1.446785	-1.327501	-0.835883
H	0.322714	-1.227747	1.663171	C	3.098692	-0.614168	0.459770
H	1.438148	-0.050827	2.367479	H	3.143305	-1.544461	1.048773
C	0.884262	-0.222586	-0.911113	H	3.213599	0.206363	1.181481
C	2.073285	-0.682711	-1.322802	C	4.293624	-0.619939	-0.489622
C	0.601480	1.066584	-0.171134	C	4.396023	0.316661	-1.528949
C	-3.927038	2.578911	0.194984	C	5.321775	-1.558552	-0.338967
H	-4.128262	3.274369	1.017837	C	5.500161	0.318958	-2.380789
H	-4.585418	2.861078	-0.635371	H	3.599458	1.041863	-1.670253
H	-4.186389	1.569323	0.521872	C	6.427530	-1.562261	-1.192361
C	0.121756	-1.012755	3.790522	H	5.256397	-2.297544	0.458002
H	0.818581	-1.833206	3.994930	C	6.521290	-0.620903	-2.217242
H	0.247921	-0.269017	4.584610	H	5.561878	1.055548	-3.178170
H	-0.900766	-1.399676	3.842905	H	7.212245	-2.302984	-1.057387
H	1.393610	1.269167	0.55282	H	7.379047	-0.620447	-2.884939
C	0.580153	2.238985	-1.143470	H	2.463236	2.165235	0.280773
O	1.413534	3.219347	-0.725850	C	0.547499	3.080366	0.414301
O	-0.058729	2.299368	-2.171523	O	1.286669	4.228274	0.651270
H	2.112136	-1.644872	-1.832515	O	-0.693941	3.132238	0.466882
C	3.396720	0.027725	-1.178820	C	0.519681	5.391731	0.934370
H	3.273830	0.944771	-0.588685	H	1.245114	6.192270	1.099931
H	3.729041	0.359973	-2.173307	H	-0.139921	5.651687	0.099397
C	4.490699	-0.837154	-0.569576	H	-0.100936	5.259415	1.828107
C	4.263747	-1.558276	0.610788	C	-2.631132	0.977471	3.223144
C	5.755146	-0.915355	-1.165258	H	-2.685424	0.433330	4.173592
C	5.274718	-2.330074	1.182895	H	-2.964033	2.004273	3.406351
H	3.283415	-1.517602	1.079556	H	-3.326739	0.513868	2.516393
C	6.770547	-1.686574	-0.596095	C	-1.422666	-4.459535	0.498445
H	5.947130	-0.366161	-2.084698	H	-1.312261	-5.177454	-0.321123
C	6.533385	-2.396702	0.581297	H	-1.250675	-4.997622	1.437391
H	5.079235	-2.882212	2.098660	H	-2.448683	-4.080098	0.496786
H	7.744730	-1.734915	-1.076003	C	-0.226426	-1.221634	3.438173
H	7.321091	-2.999609	1.025207	C	0.100968	-2.530125	2.690921
C	1.462505	4.382105	-1.569573	H	-1.024456	-1.354398	4.177820
H	0.478897	4.855984	-1.623243	H	0.643735	-0.786476	3.937177
H	2.185781	5.051644	-1.102939	H	-0.301422	-3.417812	3.185727
H	1.781856	4.111642	-2.579410	H	1.181019	-2.663345	2.549302
TS'$_{B2}$:				***Z*-11:**			
C	-2.038059	-2.882724	1.312549	C	2.447959	-2.939204	1.45397
C	-0.949538	-2.438372	2.310205	C	2.953507	-2.927885	0.01903
H	-1.713920	-3.757237	0.745977	H	1.651653	-3.696162	1.59277
H	-3.005557	-3.078063	1.788871	H	3.241865	-3.141552	2.17830
H	-0.006512	-2.956378	2.112557	H	2.981212	-3.930134	-0.429138
H	-1.248035	-2.566472	3.354093	H	3.968323	-2.505009	-0.018241

N	-2.148944	-1.719396	0.412065	N	1.956350	-1.573049	1.58909
N	-0.782978	-1.007585	1.990784	N	1.964436	-2.089912	-0.645703
C	-1.423612	-0.705781	0.864882	C	1.285221	-1.236562	0.32692
C	-1.362724	0.634702	0.188121	C	1.436822	0.29903	0.09115
N	-2.485474	1.264107	0.296587	N	2.574653	0.81637	-0.10753
S	0.148464	1.029665	-0.607932	S	-0.125031	1.181550	0.217372
C	-2.789097	2.548806	-0.174458	C	2.794273	2.18893	-0.32682
C	-4.161774	2.814609	-0.349671	C	3.738837	2.84637	0.47737
C	-1.867605	3.585928	-0.419876	C	2.170808	2.89340	-1.36988
C	-4.600218	4.056481	-0.795988	C	4.019498	4.19438	0.26922
H	-4.867610	2.018950	-0.130451	H	4.235208	2.28507	1.26323
C	-2.317218	4.835729	-0.844406	C	2.473579	4.23853	-1.58264
H	-0.809158	3.418496	-0.265495	H	1.468838	2.38013	-2.02020
C	-3.677460	5.076242	-1.045446	C	3.390039	4.89734	-0.76187
H	-5.662991	4.234419	-0.937960	H	4.741583	4.69594	0.90838
H	-1.593468	5.626368	-1.024791	H	1.988775	4.77174	-2.39630
H	-4.016477	6.050832	-1.386024	H	3.619810	5.94591	-0.92927
C	0.006653	-0.107549	2.827136	C	2.201520	-1.695092	-2.037113
H	0.307634	0.741356	2.211228	H	1.506693	-0.889295	-2.280366
H	0.919935	-0.643750	3.108436	H	1.915080	-2.540049	-2.682289
C	-2.925732	-1.763540	-0.828397	C	1.311154	-1.224010	2.849109
H	-2.662184	-0.879069	-1.408149	H	0.860689	-0.232986	2.73692
H	-2.584502	-2.636309	-1.394982	H	0.488466	-1.920105	3.10265
C	1.205397	-0.874190	-0.902309	C	-1.037946	-0.273940	0.699287
C	0.482007	-1.793330	-1.646498	C	-2.255959	-0.244985	1.253405
C	2.430229	-0.811379	-0.368884	C	-0.276628	-1.535513	0.354472
C	-0.757319	0.365756	4.066811	C	3.634472	-1.274293	-2.393704
H	-1.062910	-0.472489	4.702704	H	4.342734	-2.103068	-2.281170
H	-0.117981	1.023422	4.665420	H	3.666412	-0.961320	-3.444211
H	-1.652239	0.925259	3.776696	H	3.970053	-0.443391	-1.768937
C	-4.432537	-1.805800	-0.570632	C	2.309016	-1.180539	4.00893
H	-4.965140	-1.835984	-1.527012	H	1.806887	-0.843868	4.92270
H	-4.727761	-2.693254	0.000390	H	2.742417	-2.164976	4.21596
H	-4.749836	-0.913513	-0.022672	H	3.126015	-0.488025	3.78264
H	3.107529	-1.579760	-0.744608	H	-0.464999	-2.306806	1.104703
H	0.047060	-1.507619	-2.599601	C	-0.770952	-2.082444	-0.978871
C	0.276050	-3.133344	-1.205627	O	-1.041681	-3.401406	-0.884197
C	3.033577	0.118162	0.649907	O	-0.933621	-1.437157	-1.993599
O	-0.406836	-3.868354	-2.173875	H	-2.721751	-1.204677	1.479445
O	0.594247	-3.672091	-0.137946	C	-3.085737	0.975038	1.551139
H	2.312380	0.903940	0.902376	H	-2.488516	1.881815	1.38610
C	-0.503543	-5.265771	-1.919325	H	-3.357132	0.979172	2.61589
H	0.479155	-5.703111	-1.717545	C	-4.364335	1.050470	0.72394
H	-1.154300	-5.484966	-1.063779	C	-4.347525	0.790809	-0.653887
H	-0.932079	-5.703783	-2.824091	C	-5.578223	1.405187	1.32425
H	3.226635	-0.437631	1.580378	C	-5.515409	0.893385	-1.409997
C	4.339959	0.754183	0.196704	H	-3.416991	0.497479	-1.133703

C	5.454936	0.784853	1.042707	C	-6.748187	1.508966	0.56948
C	4.447846	1.346425	-1.069332	H	-5.607590	1.604327	2.39362
C	6.645227	1.395563	0.642681	C	-6.720031	1.253823	-0.801907
H	5.391011	0.323391	2.026334	H	-5.483777	0.689440	-2.477287
C	5.634442	1.958207	-1.473151	H	-7.680857	1.785356	1.05479
H	3.594837	1.317234	-1.742577	H	-7.629417	1.331846	-1.391974
C	6.738640	1.985839	-0.618027	C	-1.509497	-4.020541	-2.094323
H	7.499853	1.404987	1.314729	H	-0.755061	-3.940808	-2.881352
H	5.698094	2.411881	-2.459131	H	-1.687212	-5.065315	-1.837679
H	7.664433	2.459655	-0.933948	H	-2.432231	-3.544908	-2.436732
10':				**TS_{N2}:**			
C	-3.352001	0.894569	-1.104786	C	-4.242890	0.794604	0.908619
C	-3.451065	-0.647914	-1.048208	C	-3.908816	-0.047519	2.156417
N	-2.038658	1.156330	-0.503736	H	-5.295115	0.722033	0.621138
N	-2.094800	-1.044496	-0.648186	H	-3.976075	1.851981	1.029370
C	-1.378076	0.019417	-0.274264	H	-4.682939	-0.794553	2.370215
C	-0.010630	-0.049895	0.334978	H	-3.753104	0.560732	3.052404
N	0.917079	0.027597	-0.571795	N	-3.372288	0.203972	-0.115365
S	-0.153804	-0.195948	2.04522	N	-2.657977	-0.712516	1.763824
C	-1.696878	-2.441777	-0.483364	C	-1.391018	-1.292511	-0.334945
C	-2.370009	-3.130292	0.706316	N	-0.193364	-0.759760	-0.353015
C	-1.526921	2.506395	-0.274569	S	-2.067470	-2.671879	-1.070855
C	-2.120576	3.165011	0.972239	C	0.868025	-1.236608	-1.165082
H	-3.373062	1.280014	-2.132124	C	1.595333	-0.274180	-1.882281
H	-4.149237	1.384416	-0.537632	C	1.244762	-2.587462	-1.230779
H	-3.710762	-1.093458	-2.013928	C	2.674372	-0.667581	-2.671939
H	-4.182907	-0.984869	-0.304651	H	1.28272	0.764239	-1.821505
H	-1.932470	-2.960259	-1.421539	C	2.334681	-2.964954	-2.014313
H	-0.611550	-2.448181	-0.368918	H	0.68399	-3.332120	-0.679089
H	-2.114892	-2.610909	1.634311	C	3.051105	-2.010750	-2.739671
H	-2.015308	-4.164212	0.775954	H	3.22459	0.082391	-3.234264
H	-3.460523	-3.160998	0.599185	H	2.61927	-4.013048	-2.061441
H	-1.745808	3.095613	-1.174605	H	3.89659	-2.312442	-3.352441
H	-0.441518	2.427029	-0.192906	C	-1.920012	-1.594907	2.664934
H	-1.860896	2.584512	1.862011	H	-0.962087	-1.809903	2.191223
H	-3.211779	3.248966	0.908136	H	-1.702064	-1.028274	3.577718
H	-1.714226	4.176204	1.082787	C	-3.396137	0.665769	-1.505241
C	2.300666	0.000365	-0.358615	H	-2.435280	0.416542	-1.957512
C	3.079681	0.070837	-1.533284	H	-3.462851	1.758357	-1.475495
C	2.971981	-0.082874	0.880887	C	0.214151	0.766947	0.85968
C	4.468899	0.057905	-1.482875	C	-0.697339	1.786919	0.757513
H	2.554121	0.135640	-2.481814	C	1.273024	0.406617	1.57473
C	4.366679	-0.093369	0.921219	C	-2.444405	-0.564602	0.453735
H	2.397158	-0.137670	1.796055	C	-4.550756	0.056289	-2.301082
C	5.123145	-0.024184	-0.249825	H	-5.524075	0.308144	-1.863848
H	5.043865	0.112802	-2.404279	H	-4.534442	0.447567	-3.323952
H	4.866745	-0.157077	1.885021	H	-4.451449	-1.031794	-2.340593

H	6.209195	-0.033570	-0.203668	C	-2.666497	-2.891547	2.988215
				H	-2.048138	-3.508313	3.648850
				H	-3.614308	-2.701483	3.504304
				H	-2.869972	-3.454564	2.072432
				H	1.33529	-0.662354	1.782527
				C	2.414354	1.233651	2.11775
				H	2.21773	2.296704	1.97310
				H	2.46958	1.075396	3.20555
				C	3.762383	0.880934	1.50108
				C	4.266499	-0.427183	1.536032
				C	4.544113	1.874937	0.89858
				C	5.507503	-0.732753	0.977985
				H	3.68526	-1.216544	2.006781
				C	5.788887	1.574651	0.33999
				H	4.17822	2.899351	0.87704
				C	6.273958	0.267364	0.37491
				H	5.87862	-1.753792	1.016910
				H	6.37942	2.364607	-0.117481
				H	7.24184	0.029294	-0.058217
				H	-1.323157	2.019557	1.614738
				C	-0.883000	2.563553	-0.434669
				O	-0.276803	2.481561	-1.498911
				O	-1.903491	3.491313	-0.270941
				C	-2.055698	4.407421	-1.356417
				H	-1.126913	4.955669	-1.541540
				H	-2.336902	3.891217	-2.280404
				H	-2.846540	5.098001	-1.054805

12:

C	3.818313	-2.075056	0.58416
C	3.898636	-1.096790	1.75011
H	4.79458	-2.253092	0.12377
H	3.40366	-3.049385	0.90354
H	4.67631	-0.339607	1.56243
H	4.112424	-1.585609	2.70958
N	2.94515	-1.351239	-0.32108
N	2.54938	-0.554417	1.75815
C	1.758336	0.836600	-0.22571
N	0.45540	1.181626	-0.02239
S	2.912861	1.756350	-0.97008
C	-0.123709	2.419167	-0.46746
C	-0.924729	2.406133	-1.611278
C	0.097166	3.600841	0.23999
C	-1.507764	3.593941	-2.05095
H	-1.078253	1.469610	-2.13861
C	-0.489376	4.784851	-0.20765
H	0.72868	3.590079	1.12243
C	-1.291102	4.782875	-1.35080

H	-2.129366	3.589983	-2.94185
H	-0.317325	5.708929	0.33699
H	-1.745630	5.707302	-1.69633
C	2.171812	0.404180	2.78736
H	1.114104	0.652926	2.65305
H	2.23560	-0.120241	3.75278
C	2.765205	-1.786598	-1.69368
H	2.01998	-1.135730	-2.15667
H	2.36648	-2.816082	-1.74125
C	-0.343889	0.167177	0.57674
C	0.458069	-1.109165	0.53871
C	-1.573303	0.370381	1.06879
C	1.980980	-0.578885	0.40834
C	4.056436	-1.706850	-2.51475
H	4.82951	-2.383973	-2.13449
H	3.85387	-1.992611	-3.55347
H	4.44851	-0.686064	-2.49733
C	3.002887	1.695165	2.88268
H	2.63329	2.309430	3.71311
H	4.05803	1.476363	3.08058
H	2.95292	2.283359	1.96269
H	-1.998687	1.369399	1.01841
C	-2.456749	-0.696616	1.66393
H	-1.952211	-1.670680	1.62813
H	-2.622956	-0.480074	2.72892
C	-3.813516	-0.800616	0.97759
C	-4.997416	-0.702358	1.71708
C	-3.901641	-1.005675	-0.407394
C	-6.243263	-0.811789	1.09517
H	-4.944810	-0.539094	2.79159
C	-5.144542	-1.116254	-1.030387
H	-2.991463	-1.075380	-0.998004
C	-6.320368	-1.019704	-0.281848
H	-7.151244	-0.731658	1.68752
H	-5.195199	-1.276163	-2.104537
H	-7.288067	-1.103977	-0.769424
H	0.40000	-1.681775	1.46283
C	-0.029570	-1.984416	-0.600929
O	-0.494912	-1.590196	-1.652689
O	0.09884	-3.291999	-0.28950
C	-0.340956	-4.214461	-1.302021
H	-1.394449	-4.046451	-1.539244
H	0.25423	-4.095285	-2.21128
H	-0.195112	-5.206750	-0.874711

Table S3. The Cartesian coordinates for the stationary points of the reactions **14a**+**6a**→**15a-I**, **14a'+6a**→**15a-II**, **14a**+**6a**→**19** and **14a"+6a**→**16a-I**

14 a:				**14 a':**			
C	2.121131	0.699162	-0.114182	C	-2.159467	0.606743	-0.086968
N	0.249030	1.695243	0.138627	N	-0.353428	1.739031	-0.002664
N	1.145362	-0.261817	0.129339	N	-1.103318	-0.272216	0.141352
C	-0.038798	0.392536	0.296289	C	0.034326	0.474581	0.229326
C	-1.351671	-0.253117	0.594639	C	1.393047	-0.038904	0.579872
N	-2.051584	-0.424830	-0.486157	N	2.034960	-0.480518	-0.460160
S	-1.461832	-0.557109	2.284682	S	1.610666	0.121528	2.277594
C	-3.321597	-1.004597	-0.577115	C	3.314520	-1.047069	-0.471024
C	-3.852068	-1.059870	-1.883822	C	3.760139	-1.473522	-1.740602
C	-4.099680	-1.525278	0.480209	C	4.179005	-1.223954	0.631590
C	-5.103587	-1.610828	-2.134080	C	5.011137	-2.055483	-1.910754
H	-3.247984	-0.652574	-2.689592	H	3.088586	-1.333409	-2.582917
C	-5.354319	-2.076546	0.218718	C	5.433295	-1.807295	0.450126
H	-3.715909	-1.493380	1.491439	H	3.862784	-0.902327	1.615125
C	-5.864672	-2.124872	-1.079688	C	5.858434	-2.226384	-0.811653
H	-5.488347	-1.639388	-3.150749	H	5.328067	-2.376081	-2.900357
H	-5.939772	-2.473184	1.045073	H	6.086050	-1.934679	1.310734
H	-6.844236	-2.556565	-1.268961	H	6.838098	-2.680110	-0.938616
N	1.586075	1.894416	-0.109165	N	-1.711835	1.834742	-0.175194
C	1.305475	-1.688225	0.256965	C	-1.140312	-1.715129	0.173074
C	0.668369	-2.525651	-0.658980	C	-0.851293	-2.386203	1.361316
C	2.083006	-2.198128	1.296531	C	-1.469696	-2.404801	-0.994461
C	0.827884	-3.905893	-0.532260	C	-0.899608	-3.781104	1.372602
H	0.039546	-2.098634	-1.433025	H	-0.565214	-1.822595	2.242907
C	2.241226	-3.578573	1.405603	C	-1.523262	-3.797303	-0.965797
H	2.544655	-1.524336	2.010522	H	-1.674527	-1.857142	-1.908814
C	1.616502	-4.431463	0.492801	C	-1.238997	-4.485283	0.216125
H	0.329529	-4.567926	-1.233952	H	-0.666181	-4.314524	2.289163
H	2.842193	-3.986543	2.212759	H	-1.776943	-4.343016	-1.869756
H	1.736804	-5.506919	0.586901	H	-1.274790	-5.570862	0.232739
C	-0.631245	2.828535	0.139382	C	0.446571	2.925990	-0.044222
C	-0.359826	3.869456	-0.752492	C	-0.071362	4.098677	0.508502
C	-1.709442	2.888638	1.023425	C	1.701766	2.896897	-0.653968
C	-1.193430	4.985167	-0.763723	C	0.691693	5.263007	0.454661
H	0.491121	3.797895	-1.419976	H	-1.052452	4.088828	0.969242
C	-2.538856	4.009989	0.990277	C	2.456422	4.069008	-0.688262
H	-1.889603	2.081853	1.725793	H	2.073924	1.976396	-1.089757
C	-2.286504	5.056630	0.102976	C	1.956211	5.250267	-0.138452
H	-0.989917	5.796437	-1.456721	H	0.298606	6.179518	0.884928
H	-3.382391	4.062190	1.672220	H	3.436718	4.054886	-1.155216
H	-2.937233	5.926362	0.087148	H	2.549368	6.159689	-0.172458
C	3.553653	0.469249	-0.354696	C	-3.582897	0.266466	-0.225119
C	4.027436	-0.652354	-1.053411	C	-4.173832	-0.798020	0.473768
C	4.463499	1.444547	0.086365	C	-4.380194	1.078674	-1.049450
C	5.392442	-0.795211	-1.296269	C	-5.538758	-1.046486	0.339602
H	3.335101	-1.402713	-1.417931	H	-3.576918	-1.420902	1.129953

C	5.825373	1.293685	-0.160172	C	-5.742622	0.823845	-1.177085
H	4.090965	2.312182	0.620765	H	-3.919956	1.903763	-1.582884
C	6.293660	0.172474	-0.849055	C	-6.325098	-0.241229	-0.485836
H	5.750247	-1.663785	-1.841527	H	-5.988145	-1.869327	0.887987
H	6.521674	2.050509	0.189426	H	-6.349321	1.455239	-1.819873
H	7.356926	0.054421	-1.038440	H	-7.388068	-0.440998	-0.588456

TS_{A3}: **15a-I:**

C	-1.008186	1.694287	-1.670050	C	2.370620	-1.247330	0.604304
N	-0.400607	-0.285212	-2.169892	N	1.001741	-0.065431	1.766015
N	0.145390	1.398815	-0.949273	N	1.453972	-0.743650	-0.337153
C	0.501724	0.128928	-1.270530	C	0.432550	0.018698	0.423334
C	1.644126	-0.652195	-0.708060	C	0.331999	1.477131	-0.099158
N	2.783573	-0.248702	-1.168508	N	1.247573	2.302528	0.186207
S	1.185074	-1.974007	0.327189	S	-1.142217	1.743937	-1.065604
C	4.025474	-0.769793	-0.755367	C	1.281534	3.630346	-0.279554
C	4.975622	-1.049624	-1.750593	C	1.451607	4.654290	0.665616
C	4.378758	-0.908222	0.598828	C	1.229997	3.950936	-1.645923
C	6.244344	-1.510738	-1.404459	C	1.520639	5.981832	0.251363
H	4.701542	-0.903613	-2.792092	H	1.515480	4.388525	1.716312
C	5.660304	-1.343199	0.931446	C	1.323293	5.282913	-2.050770
H	3.661872	-0.640483	1.368931	H	1.149836	3.156756	-2.381771
C	6.592707	-1.659892	-0.060490	C	1.458327	6.302756	-1.107735
H	6.965225	-1.740238	-2.185297	H	1.635033	6.768827	0.992141
H	5.930989	-1.439953	1.980046	H	1.290237	5.521587	-3.110645
H	7.585196	-2.009236	0.211897	H	1.525307	7.338618	-1.428493
C	-0.383709	-1.200008	1.615022	C	-1.863999	0.150912	-0.661897
C	-1.548510	-1.174053	0.950298	C	-1.021823	-0.617627	0.332937
C	0.045128	-1.021378	2.917709	C	-3.053478	-0.187235	-1.174623
H	-1.654293	-1.693035	0.001182	H	-3.524911	0.501433	-1.874886
N	-1.345156	0.672035	-2.420435	H	-1.459833	-0.507496	1.331128
C	-1.777237	2.947599	-1.648437	C	-0.901626	-2.110517	0.051501
C	-3.168556	2.868230	-1.827424	C	-3.846867	-1.439098	-0.875849
C	-1.167424	4.205210	-1.517165	H	-3.498268	-1.893643	0.059521
C	-3.937384	4.028280	-1.862142	H	-3.660162	-2.185231	-1.659759
H	-3.634654	1.894586	-1.936900	O	-0.958326	-2.648786	-1.033769
C	-1.944673	5.361201	-1.555553	O	-0.687260	-2.771276	1.203847
H	-0.093143	4.284048	-1.397401	C	-0.436816	-4.183540	1.079490
C	-3.327973	5.277196	-1.723685	H	0.472256	-4.355509	0.497890
H	-5.013026	3.956278	-1.994226	H	-0.312676	-4.545359	2.099850
H	-1.464685	6.330444	-1.456952	H	-1.279425	-4.678866	0.590756
H	-3.928817	6.181946	-1.748343	C	-5.338930	-1.169526	-0.777178
C	0.800151	2.249146	0.022035	C	-5.847258	-0.329596	0.224100
C	0.116533	2.584545	1.188377	C	-6.236412	-1.750537	-1.679938
C	2.078683	2.734615	-0.249668	C	-7.215818	-0.081854	0.322261
C	0.726272	3.445197	2.098154	H	-5.162122	0.133770	0.930690
H	-0.863272	2.164688	1.386720	C	-7.608210	-1.504688	-1.585978
C	2.678599	3.588999	0.674949	H	-5.857825	-2.403897	-2.463046

H	2.594679	2.425753	-1.151405	C	-8.102151	-0.669623	-0.583900
C	2.001949	3.949312	1.841378	H	-7.591499	0.569822	1.106960
H	0.207829	3.707629	3.015244	H	-8.288926	-1.966700	-2.296422
H	3.678108	3.966929	0.482258	H	-9.169037	-0.477278	-0.508033
H	2.475380	4.614587	2.557863	N	2.102890	-0.898248	1.817438
C	-0.459801	-1.528718	-2.883597	C	3.454983	-2.182956	0.276190
C	0.709409	-2.098825	-3.387707	C	4.574838	-2.258819	1.122009
C	-1.708345	-2.119743	-3.081493	C	3.376217	-3.041018	-0.833117
C	0.619766	-3.301272	-4.087450	C	5.590717	-3.174204	0.863038
H	1.665587	-1.611043	-3.235818	H	4.632243	-1.594013	1.977706
C	-1.780658	-3.317499	-3.789555	C	4.398815	-3.954144	-1.087350
H	-2.599642	-1.645462	-2.686884	H	2.511834	-2.999902	-1.487302
C	-0.619518	-3.911017	-4.289391	C	5.508827	-4.023773	-0.243938
H	1.524212	-3.756901	-4.478839	H	6.452506	-3.221072	1.523422
H	-2.746560	-3.788866	-3.944030	H	4.324794	-4.614200	-1.947402
H	-0.681070	-4.847269	-4.836456	H	6.306047	-4.733485	-0.447822
C	-2.791112	-0.498972	1.493495	C	1.849102	-0.371066	-1.668849
H	-3.152786	0.257811	0.779063	C	1.036667	-0.711332	-2.756310
H	-2.519529	0.036368	2.412238	C	3.045352	0.327098	-1.879441
C	-3.942857	-1.453625	1.781184	C	1.422735	-0.346555	-4.047404
C	-3.731592	-2.651389	2.478834	H	0.121528	-1.267953	-2.584034
C	-5.246368	-1.144455	1.373176	C	3.432372	0.669421	-3.174246
C	-4.794277	-3.506635	2.768811	H	3.658940	0.604073	-1.028383
H	-2.723313	-2.913979	2.787602	C	2.619987	0.338099	-4.261411
C	-6.313719	-1.997974	1.660614	H	0.787838	-0.611050	-4.888645
H	-5.428424	-0.220802	0.826517	H	4.363545	1.206964	-3.330843
C	-6.090981	-3.183499	2.361281	H	2.920416	0.611330	-5.269338
H	-4.609134	-4.429628	3.312694	C	0.450246	0.423541	2.953192
H	-7.317498	-1.737037	1.333889	C	-0.614870	1.344343	2.953679
H	-6.918471	-3.851687	2.585318	C	0.973660	-0.004949	4.189594
H	-0.445340	-1.593780	3.700904	C	-1.141588	1.808226	4.159665
C	1.217346	-0.287796	3.285075	H	-1.024752	1.724769	2.025730
O	1.466573	-0.384857	4.639072	C	0.438042	0.474015	5.379814
O	1.961492	0.367485	2.551602	H	1.795426	-0.709193	4.193767
C	2.622847	0.312298	5.089292	C	-0.625614	1.380914	5.381499
H	2.576641	1.374840	4.828124	H	-1.962420	2.520358	4.131501
H	2.640524	0.190657	6.174955	H	0.858878	0.128101	6.320744
H	3.536580	-0.106143	4.652705	H	-1.039354	1.748119	6.316070
TS_{B3}:				**19:**			
C	1.871789	-1.881250	-0.464884	C	1.413717	-2.183985	-0.220864
N	2.144168	-0.342357	0.984591	N	0.535678	-1.225016	1.495295
N	1.238782	-0.730206	-0.923657	N	0.861122	-0.993839	-0.733762
C	1.428071	0.228780	0.014829	C	0.199056	-0.298933	0.408777
C	0.990720	1.659975	-0.075756	C	0.773522	1.122400	0.610724
N	1.895025	2.356484	-0.687586	N	1.886840	1.287672	1.188795
S	-0.549918	2.044646	0.635521	S	-0.321192	2.380384	-0.068269
C	1.890703	3.724907	-0.987816	C	2.498478	2.542133	1.383588

C	3.054101	4.178128	-1.645245	C	2.905971	2.878538	2.684037
C	0.871585	4.660698	-0.712436	C	2.785340	3.413761	0.320780
C	3.202006	5.509962	-2.014781	C	3.548114	4.091046	2.921973
H	3.832785	3.450222	-1.854006	H	2.701364	2.182213	3.491534
C	1.027386	5.994516	-1.089617	C	3.450045	4.615179	0.567839
H	-0.033772	4.345391	-0.211452	H	2.512266	3.134926	-0.692109
C	2.184846	6.428000	-1.737927	C	3.825042	4.963939	1.866053
H	4.108850	5.833554	-2.519133	H	3.844531	4.350198	3.934986
H	0.231578	6.701893	-0.870519	H	3.672638	5.281174	-0.261645
H	2.294292	7.470615	-2.024227	H	4.337428	5.903431	2.053447
C	-1.631817	0.157302	1.096627	C	-1.595691	1.198573	-0.448609
C	-1.061685	-0.655938	2.056222	C	-1.345876	-0.129856	0.233777
C	-2.725823	0.213624	0.334631	C	-2.666854	1.492658	-1.213583
H	-2.793719	0.898424	-0.505389	H	-1.727620	-0.006669	1.255898
H	-0.785869	-0.257597	3.027677	N	1.201945	-2.346945	1.041799
C	-0.837443	-2.048260	1.821276	C	2.075855	-3.211217	-1.037857
C	-3.921629	-0.682511	0.583226	C	2.975155	-4.097434	-0.419207
H	-3.794641	-1.167561	1.558808	C	1.803240	-3.363219	-2.406771
H	-3.928783	-1.495847	-0.156731	C	3.583576	-5.110525	-1.153931
O	-1.002071	-2.705749	0.787561	H	3.185173	-3.977209	0.638446
O	-0.377169	-2.672817	2.974770	C	2.418021	-4.378672	-3.137665
C	-0.328584	-4.095751	2.916810	H	1.104612	-2.694534	-2.897191
H	0.318042	-4.447912	2.108176	C	3.310226	-5.254249	-2.517186
H	0.064835	-4.419675	3.883146	H	4.278370	-5.786625	-0.662919
H	-1.327668	-4.517351	2.760996	H	2.195069	-4.486438	-4.195743
C	-5.250458	0.052071	0.527695	H	3.790473	-6.042330	-3.090833
C	-5.460763	1.207436	1.294333	C	1.506363	-0.263748	-1.789506
C	-6.300296	-0.412796	-0.273272	C	0.745118	0.250738	-2.844734
C	-6.685591	1.873289	1.265238	C	2.894480	-0.073827	-1.780479
H	-4.650887	1.585135	1.913718	C	1.365731	0.953809	-3.877960
C	-7.529273	0.250132	-0.306032	H	-0.330082	0.103513	-2.850708
H	-6.154036	-1.306625	-0.876555	C	3.511971	0.612840	-2.825069
C	-7.726243	1.396485	0.464103	H	3.479620	-0.459701	-0.952136
H	-6.828417	2.766691	1.868257	C	2.749992	1.131725	-3.874504
H	-8.330749	-0.128733	-0.935636	H	0.765006	1.355541	-4.689121
H	-8.680882	1.915737	0.439740	H	4.589474	0.751489	-2.811605
N	2.430280	-1.650437	0.700130	H	3.232678	1.671944	-4.684178
C	1.989128	-3.168566	-1.163174	C	0.159927	-1.147639	2.839703
C	2.109106	-4.331591	-0.385896	C	-0.364282	0.031230	3.406340
C	2.060166	-3.262917	-2.561486	C	0.307336	-2.282598	3.663943
C	2.281738	-5.568870	-0.998418	C	-0.742520	0.057953	4.749473
H	2.064073	-4.250526	0.693799	H	-0.453129	0.939596	2.823217
C	2.232097	-4.506256	-3.167557	C	-0.066531	-2.231307	5.002177
H	1.995493	-2.373234	-3.176817	H	0.717294	-3.188887	3.237258
C	2.339062	-5.660686	-2.391003	C	-0.600292	-1.066329	5.560395
H	2.365634	-6.463285	-0.387907	H	-1.142930	0.981425	5.159990
H	2.287414	-4.569213	-4.250510	H	0.058084	-3.120515	5.615245

H	2.469311	-6.627870	-2.868530	H	-0.893223	-1.035987	6.605679
C	0.417517	-0.588031	-2.106064	C	-2.020512	-1.380368	-0.370254
C	-0.765967	-1.322862	-2.182587	H	-1.882560	-1.388387	-1.455969
C	0.835256	0.264288	-3.128601	H	-1.472766	-2.250447	0.013340
C	-1.539877	-1.205710	-3.337779	C	-3.491748	-1.558187	-0.035080
H	-1.065484	-1.944878	-1.342447	C	-4.442424	-1.723802	-1.050528
C	0.041383	0.374882	-4.270609	C	-3.926870	-1.615139	1.297744
H	1.750143	0.836598	-3.018746	C	-5.791352	-1.924933	-0.749498
C	-1.139626	-0.363162	-4.377461	H	-4.122623	-1.698776	-2.090395
H	-2.464855	-1.769149	-3.418047	C	-5.273027	-1.814700	1.602217
H	0.347590	1.038863	-5.073511	H	-3.207085	-1.514891	2.107269
H	-1.752578	-0.275124	-5.270186	C	-6.211884	-1.967973	0.579354
C	2.611240	0.229336	2.218116	H	-6.510443	-2.048533	-1.555047
C	3.354560	1.408868	2.196895	H	-5.588087	-1.855902	2.641604
C	2.325190	-0.446420	3.405120	H	-7.260573	-2.123461	0.817710
C	3.812231	1.930565	3.407092	H	-3.425173	0.739727	-1.390601
H	3.564497	1.902607	1.254806	C	-2.896617	2.816179	-1.802887
C	2.799157	0.085772	4.602903	O	-4.011761	2.818011	-2.573988
H	1.725045	-1.350008	3.383077	O	-2.197936	3.803266	-1.639333
C	3.539036	1.271007	4.606389	C	-4.331153	4.076795	-3.183323
H	4.389120	2.850582	3.406870	H	-5.237942	3.899601	-3.762725
H	2.579562	-0.423916	5.536370	H	-4.506415	4.840897	-2.420772
H	3.900920	1.681302	5.544965	H	-3.517719	4.409015	-3.834329
TS'$_{A3}$:				**15a-II:**			
N	-2.039826	-0.204893	0.048179	N	1.392706	-1.090495	0.131296
N	-0.561546	-0.321844	1.600442	N	0.954809	0.116429	-1.733947
C	-0.930872	0.400279	0.541898	C	0.403788	-0.125431	-0.364460
C	-0.368145	1.710604	0.076042	C	0.359426	1.193261	0.456280
N	-1.167170	2.662583	0.442242	N	1.428527	1.710589	0.899248
S	1.155493	1.690521	-0.761125	S	-1.289761	1.849399	0.591353
C	-1.018298	4.037120	0.212736	C	1.442948	2.968270	1.543183
C	-1.769380	4.867979	1.068463	C	1.782145	3.042448	2.902247
C	-0.248165	4.640156	-0.801895	C	1.201838	4.149145	0.823308
C	-1.730770	6.252286	0.942173	C	1.850606	4.281236	3.536956
H	-2.376541	4.392949	1.833732	H	1.975569	2.124490	3.448986
C	-0.232548	6.028441	-0.935236	C	1.287230	5.383949	1.466615
H	0.320803	4.025611	-1.487330	H	0.971886	4.090387	-0.236138
C	-0.960303	6.841228	-0.064545	C	1.605978	5.457164	2.823610
H	-2.308694	6.872945	1.622185	H	2.101637	4.327264	4.593565
H	0.362483	6.477426	-1.726508	H	1.103321	6.293114	0.900034
H	-0.931752	7.922277	-0.171651	H	1.669077	6.421401	3.320190
C	1.822785	-0.436745	-0.984074	C	-2.068412	0.401512	-0.122555
C	0.951580	-1.253826	-1.673444	C	-1.062593	-0.706962	-0.353146
C	3.016505	-0.476450	-0.393760	C	-3.397828	0.376257	-0.279719
H	3.343367	0.316240	0.272499	H	-3.952387	1.281333	-0.033693
H	0.610622	-0.981160	-2.667730	H	-1.100793	-1.371990	0.515789
C	0.465119	-2.476915	-1.108587	C	-1.289845	-1.557750	-1.597934

C	3.967946	-1.637227	-0.594146	C	-4.251587	-0.784218	-0.736480
H	3.597121	-2.252220	-1.423528	H	-3.703448	-1.727573	-0.625080
H	3.938518	-2.284944	0.293692	H	-4.460061	-0.688385	-1.810133
O	0.713745	-2.981440	-0.012317	O	-1.853097	-1.216284	-2.613341
O	-0.400499	-3.115580	-1.991453	O	-0.745870	-2.779781	-1.421920
C	-0.809976	-4.421672	-1.587274	C	-0.781941	-3.642537	-2.575335
H	-1.367805	-4.396152	-0.646210	H	-0.253629	-3.176306	-3.409927
H	-1.447330	-4.795382	-2.392458	H	-0.281912	-4.560408	-2.266390
H	0.053478	-5.082060	-1.457011	H	-1.815358	-3.844176	-2.868379
C	5.404105	-1.213854	-0.852740	C	-5.562608	-0.876281	0.027506
C	5.702422	-0.227802	-1.804058	C	-5.570489	-0.973414	1.426533
C	6.465619	-1.814333	-0.164715	C	-6.788540	-0.877082	-0.647472
C	7.022080	0.142180	-2.062676	C	-6.770388	-1.072750	2.129880
H	4.887684	0.253494	-2.339485	H	-4.626436	-0.966394	1.966963
C	7.788787	-1.448763	-0.420820	C	-7.992920	-0.976884	0.052707
H	6.252298	-2.579340	0.579255	H	-6.800233	-0.799491	-1.732462
C	8.071825	-0.467925	-1.371837	C	-7.987542	-1.075346	1.444137
H	7.231749	0.909172	-2.804313	H	-6.755882	-1.147312	3.214283
H	8.597196	-1.928356	0.125817	H	-8.934345	-0.975268	-0.490695
H	9.100479	-0.178988	-1.571817	H	-8.923403	-1.151693	1.991295
C	0.548309	-0.120441	2.492565	C	0.783215	1.362702	-2.416393
C	1.427553	-1.184701	2.690764	C	-0.479041	1.729198	-2.901482
C	0.688332	1.100262	3.150274	C	1.882450	2.203549	-2.642135
C	2.477394	-1.010567	3.591238	C	-0.637767	2.938434	-3.578711
H	1.296170	-2.094877	2.114071	H	-1.320607	1.058319	-2.774807
C	1.753718	1.258712	4.036695	C	1.716153	3.398916	-3.340056
H	-0.018412	1.903255	2.969536	H	2.856535	1.906780	-2.272214
C	2.641789	0.204944	4.261116	C	0.454409	3.777751	-3.804310
H	3.176928	-1.824219	3.759149	H	-1.621875	3.213063	-3.949360
H	1.882474	2.204122	4.555117	H	2.576980	4.039889	-3.513021
H	3.466946	0.332697	4.956243	H	0.326403	4.711849	-4.344647
C	-2.811939	0.282535	-1.075216	N	2.240333	-0.432121	-1.840771
C	-3.842945	1.190960	-0.840411	C	2.457459	-1.126869	-0.777135
C	-2.499906	-0.161155	-2.360021	C	3.682013	-1.934231	-0.624054
C	-4.587575	1.657585	-1.923165	C	4.866409	-1.466402	-1.219508
H	-4.038084	1.537891	0.168068	C	3.700885	-3.168095	0.044958
C	-3.252255	0.316698	-3.434074	C	6.039471	-2.211149	-1.141072
H	-1.695769	-0.875348	-2.503438	H	4.848777	-0.516369	-1.742658
C	-4.293049	1.221843	-3.216981	C	4.879752	-3.909627	0.121477
H	-5.390969	2.368380	-1.754727	H	2.795081	-3.557302	0.494973
H	-3.019969	-0.019540	-4.440148	C	6.052515	-3.434773	-0.466358
H	-4.873221	1.592089	-4.057485	H	6.947373	-1.833295	-1.603500
N	-1.400861	-1.378878	1.812496	H	4.877621	-4.864553	0.640271
C	-2.301953	-1.303981	0.863464	H	6.970002	-4.013451	-0.400828
C	-3.442509	-2.229306	0.779239	C	1.460591	-1.505639	1.500074
C	-3.995740	-2.655093	-0.437953	C	2.356637	-0.901663	2.391956
C	-3.961888	-2.729453	1.986007	C	0.647986	-2.558828	1.942505

C	-5.060970	-3.554650	-0.441236	C	2.425672	-1.341003	3.713868
H	-3.585647	-2.307719	-1.377723	H	2.983037	-0.091885	2.037060
C	-5.023636	-3.629075	1.973121	C	0.707755	-2.980430	3.272174
H	-3.525043	-2.405296	2.924585	H	0.002544	-3.065163	1.231256
C	-5.579416	-4.040711	0.759556	C	1.595558	-2.372102	4.160223
H	-5.479540	-3.881678	-1.388685	H	3.128571	-0.873368	4.398109
H	-5.419155	-4.006429	2.911728	H	0.072744	-3.796250	3.606637
H	-6.410191	-4.740797	0.750299	H	1.648177	-2.705888	5.192893

14a": **TS_{N3}:**

C	-2.159313	0.607621	-0.086623	N	-2.429972	0.091540	0.375278
N	-0.352447	1.738623	-0.002695	N	-1.265183	1.901546	0.281986
N	-1.103802	-0.272073	0.141651	C	-0.256808	0.062277	1.720587
C	0.034439	0.473928	0.22937	N	0.913117	-0.253790	1.224118
C	1.392872	-0.040299	0.57986	S	-0.898618	0.005290	3.296647
N	2.03577	-0.479861	-0.460385	C	1.975820	-0.769729	2.012103
S	1.609138	0.117415	2.27805	C	2.621716	-1.932119	1.564740
C	3.315153	-1.046892	-0.471002	C	2.436005	-0.110644	3.161583
C	3.760796	-1.473705	-1.740469	C	3.698721	-2.441917	2.287478
C	4.179589	-1.223492	0.63168	H	2.27742	-2.413023	0.653075
C	5.011686	-2.055984	-1.910382	C	3.524419	-0.623242	3.865697
H	3.08933	-1.333608	-2.582871	H	1.93972	0.791040	3.50012
C	5.433795	-1.807096	0.45043	C	4.154781	-1.793008	3.437221
H	3.86335	-0.901583	1.61512	H	4.19089	-3.346654	1.940764
C	5.858896	-2.226694	-0.811183	H	3.87624	-0.107350	4.755405
H	5.32860	-2.376897	-2.899885	H	5.00032	-2.191632	3.991593
H	6.08650	-1.934274	1.311104	C	1.282195	0.015941	-0.639526
H	6.83850	-2.680595	-0.937952	C	0.407645	-0.607721	-1.510460
N	-1.710824	1.835303	-0.174925	C	2.377989	0.760829	-0.626417
C	-1.141790	-1.714972	0.172985	C	-1.252679	0.651714	0.773066
C	-0.855294	-2.386632	1.361507	H	2.81293	1.109014	0.30602
C	-1.469623	-2.404064	-0.995335	C	3.122685	1.121088	-1.893856
C	-0.904580	-3.781477	1.372264	H	2.52273	0.806697	-2.754853
H	-0.570269	-1.823502	2.243718	H	3.22815	2.213125	-1.951013
C	-1.524176	-3.796559	-0.967213	C	4.503096	0.482958	-1.958795
H	-1.672575	-1.855976	-1.909868	C	5.655362	1.268988	-2.069564
C	-1.242412	-4.485084	0.214984	C	4.638699	-0.913181	-1.920056
H	-0.673063	-4.315334	2.289046	C	6.919970	0.680743	-2.148313
H	-1.776711	-4.341812	-1.871780	H	5.56276	2.353087	-2.098205
H	-1.278925	-5.570647	0.231170	C	5.900772	-1.500990	-2.000446
C	0.448231	2.925179	-0.04399	H	3.75304	-1.537235	-1.820579
C	-0.068672	4.097767	0.50996	C	7.045739	-0.707844	-2.114818
C	1.703006	2.895847	-0.65459	H	7.80377	1.308239	-2.234619
C	0.694933	5.261758	0.45640	H	5.99031	-2.584104	-1.971870
H	-1.049446	4.088092	0.97138	H	8.02796	-1.169729	-2.175739
C	2.458213	4.067606	-0.68858	H	-0.407132	-0.061367	-1.978028
H	2.07435	1.975430	-1.09123	C	0.573862	-1.990373	-1.835463
C	1.959023	5.248756	-0.13761	O	1.46192	-2.761088	-1.466099

H	0.30263	6.178147	0.88763	O	-0.433855	-2.440145	-2.678724
H	3.43817	4.053313	-1.15623	C	-0.267216	-3.777545	-3.149159
H	2.55268	6.157853	-0.17141	H	0.65758	-3.880417	-3.725971
C	-3.582930	0.268269	-0.225098	H	-0.233448	-4.492097	-2.320536
C	-4.174947	-0.795161	0.474491	H	-1.130637	-3.977344	-3.788087
C	-4.379255	1.080193	-1.050657	C	-3.108180	1.048705	-0.370372
C	-5.539980	-1.042800	0.339886	C	-0.293795	2.948488	0.420855
H	-3.578775	-1.417878	1.131511	C	0.026043	3.705101	-0.707934
C	-5.741795	0.826200	-1.178704	C	0.270246	3.219783	1.66756
H	-3.918175	1.904443	-1.584669	C	0.946627	4.743254	-0.584511
C	-6.325358	-0.237785	-0.486705	H	-0.440995	3.476457	-1.659133
H	-5.990210	-1.864814	0.888821	C	1.199317	4.255719	1.77088
H	-6.347733	1.457391	-1.822406	H	-0.020939	2.640807	2.537723
H	-7.388414	-0.436913	-0.589651	C	1.539332	5.015958	0.65109
				H	1.20388	5.335922	-1.457440
				H	1.64663	4.473538	2.73613
				H	2.26017	5.823518	0.74095
				C	-2.917099	-1.213870	0.768065
				C	-3.852515	-1.289495	1.800029
				C	-2.458620	-2.349905	0.104896
				C	-4.343000	-2.539199	2.173026
				H	-4.169470	-0.386930	2.310462
				C	-2.954753	-3.595795	0.494942
				H	-1.751586	-2.259925	-0.712095
				C	-3.892535	-3.691350	1.523866
				H	-5.067251	-2.612098	2.978737
				H	-2.603716	-4.490053	-0.011150
				H	-4.272268	-4.664281	1.822866
				N	-2.406483	2.154329	-0.436067
				C	-4.433931	0.916489	-0.993631
				C	-4.899385	-0.288879	-1.541418
				C	-5.233372	2.069496	-1.078734
				C	-6.150600	-0.336432	-2.153870
				H	-4.285936	-1.180940	-1.506154
				C	-6.481283	2.012509	-1.692346
				H	-4.866966	3.000324	-0.658836
				C	-6.944685	0.808762	-2.228413
				H	-6.500778	-1.272417	-2.579150
				H	-7.093884	2.907705	-1.748229
				H	-7.920147	0.764592	-2.704724

16a-I:

N	-1.561944	-0.488477	0.403853
N	-2.032057	1.536112	-0.471241
C	-0.082672	1.394377	1.154653
N	1.23915	1.198690	0.89309
S	-0.759018	2.124129	2.465502
C	2.274083	1.579702	1.81743

C	2.638535	0.701918	2.83899
C	2.907931	2.814856	1.67322
C	3.649643	1.070203	3.72651
H	2.12564	-0.249619	2.935001
C	3.918016	3.174965	2.56488
H	2.607011	3.484434	0.87330
C	4.289666	2.303681	3.59083
H	3.93515	0.392170	4.52570
H	4.411023	4.137136	2.45921
H	5.07614	2.586816	4.28485
C	1.540074	0.642340	-0.390376
C	0.229284	0.539259	-1.133163
C	2.792893	0.393663	-0.795959
C	-0.883756	0.761700	-0.013625
H	3.59857	0.578380	-0.090328
C	3.233142	-0.077548	-2.159733
H	2.37334	-0.355308	-2.775857
H	3.72370	0.762926	-2.672828
C	4.216693	-1.237196	-2.088813
C	5.577406	-1.036883	-2.347034
C	3.778472	-2.524196	-1.744971
C	6.485743	-2.094887	-2.265249
H	5.93056	-0.044041	-2.618827
C	4.683387	-3.582535	-1.666391
H	2.72288	-2.688543	-1.548731
C	6.040471	-3.371941	-1.924186
H	7.53869	-1.919963	-2.471218
H	4.32785	-4.576143	-1.404772
H	6.74397	-4.198156	-1.862352
H	0.13779	1.378570	-1.830412
C	-0.044311	-0.732403	-1.912105
O	0.44476	-1.827233	-1.719668
O	-0.971002	-0.487638	-2.854582
C	-1.430586	-1.631521	-3.598451
H	-0.593067	-2.122199	-4.100220
H	-1.921591	-2.343061	-2.929979
H	-2.140775	-1.236337	-4.324209
C	-2.904057	-0.375131	-0.003155
C	-1.999099	2.760316	-1.150974
C	-3.103292	3.155898	-1.930857
C	-0.891316	3.623579	-1.062142
C	-3.085870	4.374655	-2.600475
H	-3.959580	2.497648	-1.997588
C	-0.889676	4.838521	-1.747616
H	-0.043588	3.372445	-0.436250
C	-1.980856	5.226631	-2.522721
H	-3.949880	4.658307	-3.196342

H	-0.023296	5.489102	-1.659044
H	-1.974630	6.175499	-3.051008
C	-1.158961	-1.256146	1.548460
C	-1.942931	-1.257158	2.709905
C	0.012079	-2.021776	1.499983
C	-1.564519	-2.028937	3.806647
H	-2.837820	-0.645654	2.751570
C	0.395924	-2.773769	2.612982
H	0.59967	-2.046088	0.588892
C	-0.391063	-2.784901	3.765743
H	-2.180750	-2.024028	4.701412
H	1.30410	-3.369054	2.565564
H	-0.094667	-3.380328	4.624976
N	-3.177404	0.761537	-0.547647
C	-3.881076	-1.471496	0.055243
C	-3.482283	-2.817958	0.020731
C	-5.252071	-1.164520	0.091811
C	-4.438533	-3.832784	0.022784
H	-2.427350	-3.068401	-0.016769
C	-6.200839	-2.182853	0.092095
H	-5.555662	-0.123144	0.119170
C	-5.798639	-3.521105	0.060472
H	-4.117270	-4.870477	-0.006346
H	-7.257715	-1.931940	0.123442
H	-6.540822	-4.314771	0.067071

Table S4. The total energy (TE, in au), relative energy (RE, in kcal/mol), zero-point energy (ZPE, in kcal/mol), total free energy (TFE, in au) and relative free energy (RFE, in kcal/mol).

	TE	ZPE	RE	FE	RFE
5d+6a	-1874.71620	344.08	0.0	-1874.26017	0.0
5d'+6a	-1874.71619	344.10		-1874.26012	
TS_{A1}	-1874.69171	344.18	15.37	-1874.21442	28.71
TS_{B1}	-1874.69051	344.31	16.13	-1874.21306	29.56
TS_{N1}	-1874.68131	344.49	21.90	-1874.20218	36.39
INT_{A1}	-1874.69755	345.11	11.71	-1874.21786	26.55
TS_{A1-7}	-1874.69620	344.90	11.56	-1874.21502	28.33
7f	-1874.73500	345.77	-11.79	-1874.25231	4.83
27	-1874.72593	345.45	-6.10	-1874.24524	9.37
9f	-1874.74116	346.79	-15.66	-1874.25579	2.65
10+6a	-1722.27306	328.80	0.0	-1721.83486	0.0
10'+6a	-1722.27311	328.76		-1721.83492	
TS_{A2}	-1722.24352	329.35	14.89	-1721.78738	29.80
TS_{B2}	-1722.25379	330.19	8.44	-1721.79209	26.84
TS_{N2}	-1722.24730	329.86	13.51	-1721.78962	30.28
INT_{B2}	-1722.25961	330.62	4.79	-1721.79962	22.12
TS_{B2-11}	-1722.25958	330.43	4.81	-1721.79813	23.05

***E*-11**	-1722.28364	331.19	-10.29	-1721.82267	7.67
INT_{A2}	-1722.25058	330.27	10.46	-1722.79212	26.83
TS'_{B2}	-1722.24546	329.47	13.68	-1722.78919	28.66
***Z*-11**	-1722.28510	331.19	-11.20	-1722.82423	6.68
TS_{A2-13}	-1722.25049	330.09	10.52	-1722.79076	27.68
13	-1722.29067	331.50	-14.70	-1722.82796	4.34
12	-1722.29708	332.12	-17.05	-1722.83320	2.03
TS_{B2-A2}	-1722.24845	330.23	10.80	-1722.78822	29.27
14a+6a	-2272.98530	387.49	0.0	-2272.47092	0.0
14a'+6a	-2272.98577	387.54	-0.29	-2272.47159	-0.42
14a"+6a	-2272.98526	387.44		-2272.47088	
TS_{A3}	-2272.96755	387.87	11.14	-2272.42990	25.74
TS_{B3}	-2272.95528	387.40	18.84	-2272.41795	33.24
TS_{N3}	-2272.96251	388.13	14.29	-2272.42239	30.45
15a-I	-2273.01241	389.44	-17.01	-2272.47001	0.57
16a-I	-2273.02726	390.55	-26.31	-2272.48117	-6.43
19	-2273.02096	389.74	-22.34	-2272.47722	-3.95
$TS_{A3'}$	-2272.96295	387.59	14.02	-2272.42714	27.47
15a-II	-2273.00636	389.41	-13.22	-2272.46401	4.34

Table S5. The vibrational frequencies (cm^{-1}) obtained for the stationary points.

5d:

16. 28. 38. 55. 70. 73. 80. 111. 138. 146. 183. 199. 210. 229. 234. 284. 288. 312. 314. 335. 407. 424. 449. 451. 515. 527. 569. 573. 581. 596. 625. 636. 668. 688. 706. 721. 758. 760. 776. 784. 787. 805. 841. 856. 859. 873. 927. 928. 952. 969. 971. 977. 992. 1007. 1015. 1047. 1055. 1055. 1110. 1120. 1121. 1153. 1172. 1176. 1188. 1194. 1202. 1224. 1244. 1265. 1325. 1325. 1335. 1363. 1378. 1385. 1401. 1404. 1422. 1441. 1444. 1487. 1494. 1508. 1517. 1520. 1525. 1530. 1531. 1536. 1538. 1542. 1545. 1582. 1624. 1657. 1659. 1669. 3061. 3061. 3090. 3091. 3126. 3127. 3142. 3144. 3156. 3158. 3174. 3183. 3197. 3201. 3206. 3212. 3222. 3227. 3248.

5d':

11. 31. 39. 62. 74. 86. 91. 112. 140. 147. 185. 194. 201. 221. 235. 280. 291. 309. 315. 330. 409. 424. 445. 455. 516. 533. 562. 570. 573. 596. 625. 647. 669. 686. 706. 717. 758. 760. 776. 785. 787. 804. 838. 856. 859. 874. 927. 929. 950. 969. 970. 977. 993. 1007. 1015. 1047. 1055. 1056. 1110. 1120. 1121. 1153. 1172. 1175. 1187. 1194. 1201. 1223. 1244. 1266. 1324. 1326. 1335. 1363. 1377. 1380. 1400. 1406. 1422. 1442. 1443. 1488. 1494. 1506. 1518. 1518. 1524. 1530. 1531. 1536. 1537. 1541. 1544. 1584. 1624. 1657. 1660. 1669. 3062. 3062. 3082. 3083. 3128. 3128. 3149. 3151. 3163. 3163. 3173. 3182. 3198. 3201. 3208. 3212. 3223. 3227. 3248.

6a:

18. 27. 44. 60. 81. 130. 155. 183. 237. 270. 314. 354. 397. 417. 467. 517. 556. 615. 637. 680. 715. 718. 764. 804. 837. 861. 862. 907. 923. 928. 967. 996. 1018. 1035. 1059. 1074. 1113. 1146. 1186. 1193. 1208. 1214. 1220. 1224. 1295. 1302. 1337. 1363. 1372. 1455. 1494. 1499. 1509. 1513. 1526. 1546. 1645. 1665. 1803. 2059. 3046. 3073. 3091. 3146. 3148. 3175. 3178. 3180. 3186. 3190. 3198. 3210.

TS_{A1}:

-178i 14. 16. 18. 28. 31. 35. 42. 50. 53. 61. 68. 71. 86. 95. 98. 105. 112. 128. 137. 150. 152. 160. 178. 201. 212. 222. 237. 247. 264. 270. 291. 294. 309. 322. 328. 380. 397. 417. 417. 421. 451. 454. 457. 475. 487. 501. 528. 550. 564. 569. 583. 598. 600. 623. 634. 636. 641. 647. 675. 708. 714. 723. 733. 760. 762. 764. 768. 778. 783. 788. 809. 812. 842. 857. 859. 862. 863. 870. 915. 926. 931. 936. 953. 956. 965. 969. 974. 983. 992. 997. 1003. 1017. 1018. 1026. 1046. 1049. 1056. 1058. 1081. 1111. 1111. 1118. 1118. 1154. 1155. 1171. 1177. 1184. 1189.

1191. 1195. 1198. 1207. 1213. 1217. 1219. 1219. 1224. 1244. 1267. 1309. 1325. 1332. 1336. 1362. 1365. 1369. 1373. 1374. 1383. 1404. 1415. 1433. 1442. 1442. 1452. 1493. 1496. 1498. 1499. 1505. 1508. 1511. 1518. 1520. 1529. 1530. 1533. 1536. 1538. 1543. 1545. 1548. 1558. 1594. 1633. 1643. 1655. 1660. 1663. 1670. 1678. 1765. 3010. 3054. 3058. 3063. 3073. 3078. 3093. 3117. 3119. 3129. 3133. 3143. 3153. 3154. 3156. 3167.
3177. 3179. 3179. 3182. 3186. 3188. 3198. 3198. 3203. 3207. 3207. 3215. 3220. 3225. 3230.

TS_{B1}:

-151i 12. 16. 22. 23. 27. 32. 38. 48. 60. 65. 72. 79. 91. 94. 109. 111. 116. 124. 137. 153. 153. 177. 184. 199. 208. 221. 241. 241. 248. 268. 271.287. 309. 320. 323. 370. 381. 401. 418. 420. 427. 446. 449. 474. 511. 520. 533. 557. 566. 572. 588. 599. 615. 623. 635. 637. 655. 668. 702. 705. 715. 718. 724. 758. 761. 766. 767. 778. 782. 785. 801. 811. 827. 844. 846. 860. 863. 871. 915. 922. 932. 936. 951. 954. 963. 967. 973. 980. 989. 992. 1005. 1016. 1018. 1026. 1048. 1054. 1056. 1059. 1080. 1110. 1113. 1117. 1120. 1135. 1154. 1170. 1177. 1183. 1187. 1191. 1191. 1196. 1205. 1212. 1213. 1215. 1225. 1229. 1243. 1266. 1306. 1320. 1327. 1336. 1359. 1365. 1366. 1372. 1376. 1379. 1403. 1412. 1423. 1438. 1444. 1445. 1493. 1494. 1495. 1496. 1502. 1503. 1511. 1516. 1521. 1522. 1528. 1532. 1534. 1537. 1540. 1542. 1546. 1550. 1580. 1630. 1643. 1655. 1664. 1665. 1671. 1706. 1795. 3031. 3057. 3063. 3067. 3074. 3089. 3115. 3125. 3131. 3132. 3139. 3148. 3158. 3170. 3177. 3178. 3180. 3181. 3182. 3183. 3186. 3191. 3194. 3202. 3204. 3205. 3212. 3215. 3228. 3238. 3238.

TS_{N1}:

-319i 13. 17. 23. 30. 36. 42. 46. 51. 54. 68. 79. 84. 93. 102. 109. 112. 119. 126. 135. 144. 169. 171. 186. 196. 203. 218. 230. 234. 236. 268. 279. 288. 296. 311. 331. 351. 392. 418. 418. 421. 428. 449. 460. 479. 503. 517. 545. 566. 568. 570. 579. 595. 607. 629. 635. 651. 667. 690. 694. 697. 706. 717. 735. 754. 759. 762. 768. 771. 780. 784. 792. 806. 825. 836. 846. 862. 870. 889. 904. 928. 933. 934. 950. 957. 965. 974. 977. 982. 992. 1014. 1017. 1024. 1032. 1049. 1049. 1052. 1059. 1060. 1077. 1116. 1117. 1118. 1120. 1153. 1164. 1171. 1174. 1185. 1191. 1193. 1195. 1198. 1206. 1211. 1214. 1217. 1222. 1223. 1235. 1267. 1297. 1324. 1327. 1344. 1347. 1366. 1368. 1373. 1375. 1382. 1398. 1408. 1421. 1441. 1442. 1445. 1483. 1487. 1496. 1497. 1501. 1506. 1510. 1516. 1517. 1519. 1523. 1526. 1530. 1538. 1538. 1540. 1542. 1547. 1550. 1638. 1642. 1655. 1662. 1662. 1669. 1736. 1819. 3001. 3058. 3062. 3065. 3067. 3092. 3098. 3125. 3133. 3134. 3150. 3153. 3155. 3156. 3156. 3171. 3177. 3184. 3186. 3190. 3194. 3195. 3195. 3203. 3204. 3207. 3215. 3220. 3226. 3230. 3251.

INT_{A1}

12. 17. 26. 29. 33. 38. 43. 53. 57. 61. 71. 78. 92. 94. 104. 109. 113. 134. 150. 152. 166. 174. 181. 195. 207. 216. 219. 235. 263. 265. 292. 297. 315. 326. 340. 371. 398. 415. 418. 421. 445. 453. 454. 476. 493. 508. 527. 551. 567. 570. 587. 598. 602. 616. 629. 635. 636. 643. 672. 707.710. 714. 725. 726. 740. 753. 758. 761.766. 779. 785. 791. 817. 822. 843. 861. 862. 862. 865. 909. 933. 933. 937. 953. 966. 971. 976. 984. 985. 991. 1007. 1016. 1017. 1022. 1028. 1046. 1049. 1056. 1059. 1099. 1112. 1113. 1116. 1118. 1156. 1170. 1173. 1178. 1185. 1190. 1190. 1197. 1201. 1209. 1213. 1214. 1217. 1224. 1238. 1243. 1268. 1313. 1323. 1332. 1337. 1362. 1367. 1372. 1373. 1379. 1382. 1404. 1417. 1435. 1442. 1458. 1464. 1495. 1497. 1502. 1505. 1508. 1509. 1512. 1519. 1519. 1529. 1532. 1534. 1537. 1540. 1544. 1546. 1553. 1563. 1616. 1631. 1635. 1642. 1655. 1660. 1662. 1666. 1672. 3003. 3044. 3046. 3054. 3061. 3064. 3096. 3104. 3115. 3131. 3132. 3141. 3144. 3149. 3159. 3163. 3176. 3177. 3181. 3186. 3190. 3197. 3198. 3200. 3204. 3204. 3208. 3210. 3215. 3225. 3232.

7f:

16. 23. 27. 28. 37. 42. 49. 53. 60. 62. 83. 96. 99. 106. 108. 121. 132. 135. 151. 161. 175. 182. 194. 199. 214. 218. 232. 237. 265. 280. 284. 302. 324. 345. 361. 370. 397. 405. 419. 419. 430. 448. 467. 501. 526. 536. 541. 563. 569. 573. 584. 592. 612. 635. 637. 646. 661. 688. 706. 713. 725. 731. 738. 747. 749. 761. 768. 779. 788. 801. 823. 833. 837. 845. 858. 862. 875. 887. 898. 915. 927. 933. 936. 938. 956. 962. 968. 987. 989. 996. 998. 1016. 1018. 1038. 1039. 1056. 1056. 1060. 1074. 1097. 1105. 1112. 1113. 1115. 1131. 1152. 1154. 1180. 1185. 1192. 1193. 1194. 1206. 1216. 1217. 1219. 1222. 1233. 1236. 1245. 1249. 1271. 1325. 1334. 1341. 1345. 1349. 1363. 1364. 1367. 1373. 1376. 1379. 1398. 1412. 1416. 1433. 1440. 1466. 1492. 1496. 1499. 1505. 1508. 1511. 1515. 1516. 1519. 1521. 1525. 1535. 1537. 1543. 1547. 1556. 1634. 1643. 1652. 1653. 1660. 1665. 1667. 1724. 1777. 3002. 3030.

3031. 3056. 3061. 3064. 3072. 3096. 3104. 3120. 3132. 3136. 3145. 3147. 3169. 3173. 3175. 3179. 3185. 3186. 3189. 3193. 3198. 3199. 3206. 3210. 3211. 3213. 3217. 3217. 3241.

9f:

19. 26. 28. 34. 38. 43. 48. 55. 65. 73. 80. 82. 89. 106. 121. 132. 147. 149. 155. 173. 175. 190. 197. 207. 215. 228. 237. 243. 258. 270. 282. 309. 314. 330. 354. 361. 384. 416. 419. 424. 444. 453. 461. 494. 514. 535. 548. 560. 569. 578. 621. 626. 636. 637. 656. 670. 677. 701. 709. 714. 734. 736. 741. 753. 770. 778. 779. 786. 807. 825. 842. 850. 855. 856. 859. 870. 882. 886. 920. 933. 934. 938. 958. 961. 963. 968. 972. 992. 1000. 1012. 1018. 1019. 1022. 1051. 1053. 1055. 1059. 1074. 1087. 1104. 1110. 1114. 1115. 1121. 1147. 1154. 1161. 1178. 1187. 1192. 1192. 1195. 1207. 1208. 1215. 1216. 1223. 1237. 1239. 1256. 1271. 1324. 1327. 1331. 1341. 1343. 1352. 1355. 1358. 1363. 1367. 1374. 1376. 1386. 1415. 1419. 1432. 1438. 1441. 1462. 1494. 1500. 1503. 1504. 1512. 1513. 1517. 1518. 1520. 1525. 1525. 1537. 1542. 1545. 1547. 1553. 1644. 1649. 1652. 1657. 1665. 1667. 1691. 1787. 3003. 3025. 3054. 3054. 3064. 3073. 3112. 3113. 3121. 3125. 3138. 3141. 3148. 3151. 3166. 3175. 3177. 3178. 3185. 3187. 3192. 3198. 3198. 3201. 3208. 3209. 3209. 3215. 3217. 3223. 3229.

$TS_{A1\text{-}7}$:

-25i 15. 18. 27. 31. 32. 36. 51. 61. 65. 78. 80. 83. 92. 100. 105. 113. 135. 139. 158. 169. 174. 178. 200. 205. 213. 221. 238. 251. 269. 289. 298. 317. 321. 341. 371. 398. 408. 418. 420. 448. 451. 453. 476. 497. 513. 529. 558. 564. 570. 586. 596. 609. 617. 633. 635. 639. 656. 665.690. 708. 713. 726. 730. 742. 756. 759. 761. 765. 779. 785. 791. 815. 821. 838. 856. 861. 861. 865. 909. 928. 933. 933. 953. 966. 970. 973. 982. 985. 992. 997. 1012. 1017. 1020. 1034. 1047. 1051. 1056. 1059. 1098. 1111. 1114. 1114. 1121. 1154. 1166. 1174. 1177. 1185. 1190. 1191. 1195. 1201. 1207. 1213. 1214. 1217. 1225. 1239. 1243. 1268. 1312. 1325. 1330. 1335. 1362. 1366. 1368. 1370. 1380. 1381. 1400. 1417. 1434. 1441. 1449. 1465. 1493. 1496. 1497. 1503. 1503. 1506. 1510. 1518. 1519. 1526. 1531. 1532. 1534. 1538. 1541. 1543. 1545. 1553. 1602. 1618. 1633. 1642. 1657. 1659. 1662. 1666. 1675. 3001. 3048. 3052. 3056. 3066. 3066. 3088. 3109. 3118. 3131. 3134. 3145. 3145. 3150. 3162. 3163. 3174. 3177. 3183. 3187. 3192. 3199. 3203. 3203. 3203. 3208. 3210. 3215. 3217. 3225. 3231.

27:

12. 19. 21. 26. 28. 36. 43. 46. 59. 68. 74. 80. 93. 106. 114. 120. 126. 146. 155. 166. 182. 196. 201. 208. 217. 229. 234. 244. 267. 269. 284. 303. 318. 323. 360. 365. 390. 416. 417. 420. 424. 438. 448. 457. 497. 522. 539. 557. 560. 567. 575. 596. 614. 631. 636. 641. 651. 671. 707. 716. 723. 732. 739. 755. 763. 771. 779. 786. 794. 810. 821. 828. 838. 848. 857. 863. 878. 890. 916. 919. 922. 937. 937. 941. 960. 963. 968. 975. 984. 990. 996. 999. 1016. 1019. 1037. 1051. 1056. 1057. 1060. 1097. 1108. 1111. 1112. 1116. 1125. 1135. 1155. 1179. 1186. 1192. 1193. 1193. 1198. 1205. 1215. 1216. 1221. 1228. 1232. 1240. 1250. 1270.

1322. 1325. 1333. 1342. 1358. 1362. 1364. 1369. 1372. 1373. 1382. 1402. 1410. 1416. 1435. 1439. 1466. 1492. 1492. 1495. 1502. 1505. 1513. 1515. 1516. 1520. 1521. 1522. 1535. 1537. 1541. 1547. 1555. 1633. 1644. 1653. 1654. 1665. 1666. 1706. 1724. 1813. 3012. 3043. 3056. 3062. 3063. 3073. 3076. 3080. 3100. 3122. 3129. 3135. 3149. 3156. 3159. 3160. 3175. 3178. 3184. 3185. 3188. 3189. 3192. 3197. 3199. 3205. 3209. 3211. 3211. 3216. 3217.

10:

24. 33. 55. 58. 65. 71. 79. 94. 124. 159. 161. 193. 225. 240. 243. 314. 316. 363. 387. 401. 424. 451. 541. 560. 604. 605. 626. 674. 679. 702. 706. 785. 804. 808. 809. 855. 860. 923. 927. 930. 968. 971. 992. 999. 1014. 1017. 1055. 1072. 1101. 1110. 1117. 1133. 1146. 1187. 1192. 1204. 1224. 1237. 1240. 1263. 1305. 1328. 1336. 1343. 1363. 1363. 1391. 1405. 1413. 1442. 1442. 1494. 1514. 1515. 1523. 1524. 1532. 1535. 1538. 1539. 1547. 1575. 1590. 1617. 1624. 1657. 3050. 3053. 3055. 3058. 3066. 3070. 3096. 3112. 3117. 3117. 3137. 3139. 3151. 3151. 3173. 3182. 3196. 3205. 3248.

10':

9. 29. 51. 54. 63. 68. 80. 84. 128. 155. 164. 188. 228. 237. 243. 310. 314. 352. 386. 391. 424. 456. 542. 551. 603. 614. 625. 672. 675. 697. 706. 785. 797. 802. 808. 856. 858. 921. 928. 930. 969. 973. 992. 1000. 1014. 1014. 1055. 1067. 1096. 1109. 1115. 1130. 1151. 1186. 1189. 1201. 1222. 1237. 1239. 1261. 1307. 1324. 1333. 1339.

1360. 1363. 1390. 1404. 1410. 1439. 1441. 1494. 1509. 1513. 1522. 1523. 1532. 1533. 1536. 1536. 1545. 1576. 1592. 1616. 1625. 1657. 3050. 3053. 3054. 3055. 3056. 3061. 3097. 3112. 3119. 3119. 3145. 3146. 3155. 3156. 3173. 3182. 3197. 3207. 3247.

TS_{A2}:

-178i 17. 19. 22. 30. 37. 41. 51. 54. 56. 63. 68. 80. 86. 94. 100. 103. 112. 132. 136. 142. 156. 169. 175. 198. 214. 224. 244. 251. 267. 281. 303. 321. 351. 380. 393. 403. 410. 418. 421. 452. 457. 474. 491. 526. 551. 556. 586. 597. 608. 625. 636. 642. 646. 676. 708. 714. 714. 723. 759. 768. 780. 804. 808. 812. 816. 851. 855. 858. 861. 912. 916. 923. 929. 936. 958. 966. 969. 974. 992. 1001. 1003. 1015. 1016. 1017. 1025. 1057. 1059. 1068. 1081. 1094. 1111. 1112. 1114. 1129. 1141. 1153. 1183. 1189. 1191. 1191. 1197. 1211. 1214. 1217. 1219. 1221. 1222. 1234. 1237. 1264. 1302. 1308. 1331. 1337. 1348. 1361. 1365. 1365. 1371. 1375. 1395. 1410. 1432. 1441. 1443. 1454. 1495. 1496. 1498. 1504. 1512. 1516. 1519. 1526. 1527. 1530. 1533. 1537. 1538. 1542. 1545. 1548. 1586. 1602. 1633. 1640. 1643. 1656. 1663. 1682. 1764. 2986. 3051. 3054. 3057. 3061. 3062. 3068. 3075. 3076. 3108. 3111. 3118. 3121. 3125. 3127. 3139. 3149. 3150. 3153. 3165. 3177. 3178. 3180. 3181. 3186. 3189. 3197. 3199. 3207. 3208. 3218.

TS_{B2}:

-147i 15. 18. 24. 31. 39. 47. 50. 57. 61. 63. 72. 82. 85. 97. 112. 126. 137. 153. 157. 164. 173. 180. 185. 198. 211. 233. 245. 256. 265. 301. 315. 319. 346. 357. 368. 384. 390. 420. 420. 422. 464. 486. 522. 537. 558. 571. 595. 599. 610. 620. 636. 652. 670. 702. 707. 716. 719. 722. 767. 770. 785. 796. 806. 812. 820. 849. 859. 862. 872. 914. 922. 925. 931. 937.

950. 967. 977. 978. 993. 1005. 1012. 1014. 1016. 1016. 1017. 1056. 1060. 1063. 1078. 1092. 1113. 1114. 1115. 1131. 1143. 1149. 1180. 1185. 1190. 1191. 1193. 1203. 1205. 1213. 1218. 1225. 1227. 1237. 1254. 1279. 1312. 1318. 1336. 1338. 1345. 1359. 1364. 1364. 1372. 1379. 1402. 1411. 1417. 1440. 1442. 1450. 1495. 1497. 1500. 1508. 1509. 1514. 1515. 1518. 1523. 1525. 1529. 1533. 1534. 1535. 1539. 1548. 1598. 1603. 1629. 1642. 1646. 1659. 1662. 1677. 1781. 3023. 3047. 3059. 3059. 3068. 3075. 3084. 3089. 3111. 3115. 3123. 3123. 3137. 3139. 3144. 3150. 3152. 3155. 3165. 3169. 3174. 3182. 3186. 3190. 3191. 3191. 3194. 3202. 3204. 3212. 3242.

TS_{N2}:

-239i 14. 19. 25. 33. 38. 51. 51. 57. 60. 68. 70. 73. 75. 83. 96. 124. 126. 129. 139. 160. 162. 176. 186. 191. 218. 231. 240. 243. 267. 289. 311. 312. 343. 370. 384. 398. 418. 419. 423. 435. 465. 483. 495. 529. 551. 577. 586. 598. 618. 631. 635. 640. 663. 674. 693. 714. 718. 721. 765. 769. 791. 793. 797. 810. 815. 848. 856. 867. 883. 928. 929. 932. 934. 951. 962. 971. 975. 978. 1000. 1004. 1008. 1017. 1017. 1021. 1024. 1057. 1059. 1075. 1080. 1093. 1112. 1115. 1116. 1129. 1136. 1149. 1173. 1185. 1188. 1192. 1192. 1208. 1214. 1216. 1217. 1218. 1223. 1234. 1241. 1258. 1313. 1319. 1327. 1336. 1341. 1358. 1363. 1367. 1371. 1377. 1392. 1406. 1411. 1434. 1440. 1443. 1493. 1496. 1500. 1508. 1509. 1510. 1513. 1522. 1523. 1529. 1531. 1532. 1536. 1537. 1542. 1547. 1556. 1588. 1622. 1638. 1644. 1653. 1663. 1721. 1838. 3037. 3054. 3056. 3058. 3059. 3060. 3068. 3082. 3092. 3112. 3119. 3122. 3126. 3129. 3145. 3148. 3154. 3157. 3160. 3169. 3176. 3179. 3181. 3188. 3192. 3194. 3196. 3204. 3206. 3213. 3221.

INT_{A2}:

12. 20. 24. 32. 37. 40. 49. 55. 60. 69. 84. 88. 91. 104. 106. 110. 118. 131. 142. 172. 183. 190. 201. 208. 213. 224. 229. 246. 253. 298. 315. 331. 362. 375. 378. 388. 417. 418. 423. 456. 470. 485. 517. 521. 542. 574. 584. 608. 615. 622. 632. 635. 656. 660. 675. 706. 714. 729. 732. 740. 759. 771. 781. 802. 806. 819. 820. 848. 853. 862. 907. 913. 925. 931. 932. 966. 967. 976. 990. 991. 994. 1011. 1015. 1017. 1025. 1036. 1056. 1060. 1077. 1091. 1097. 1111. 1113. 1114. 1127. 1142. 1179. 1184. 1185. 1191. 1191. 1208. 1210. 1212. 1216. 1220. 1222. 1232. 1239. 1245. 1257. 1299. 1310. 1324. 1335. 1339. 1361. 1362. 1366. 1370. 1381. 1387. 1410. 1428. 1440. 1445. 1471. 1495. 1495. 1499. 1500. 1503. 1508. 1510. 1520. 1522. 1525. 1528. 1530. 1535. 1536. 1537. 1545. 1561. 1573. 1582. 1614. 1630. 1642. 1658. 1662. 1707. 2999. 3033. 3037. 3047. 3049. 3053. 3055. 3057. 3083. 3106. 3116. 3117. 3117. 3120. 3137. 3147. 3152. 3154. 3164. 3179. 3181. 3184. 3188. 3189. 3193. 3202. 3205. 3207. 3212. 3212. 3220.

TS_{A2-13}:

-32i 15. 21. 29. 33. 36. 40. 46. 54. 63. 81. 87. 90. 100. 104. 116. 126. 130. 140. 172. 184. 185. 199. 210. 216. 224. 234. 247. 252. 299. 309. 325. 360. 369. 375. 388. 413. 418. 423. 458. 469. 486. 518. 520. 538. 575. 585. 606. 614. 620. 633. 636. 651. 659. 675. 707. 714. 735. 737. 751. 761. 780. 782. 797. 802. 819. 822. 849. 854. 863. 908. 912. 925. 930. 932. 966. 968. 974. 990. 991. 995. 1010. 1015. 1017. 1024. 1038. 1055. 1060. 1075. 1090. 1097. 1109. 1114. 1114. 1127. 1143. 1179. 1183. 1185. 1191. 1192. 1207. 1212. 1213. 1217. 1220. 1222. 1232. 1241. 1244. 1256. 1297. 1309. 1320. 1334. 1337. 1360. 1362. 1366. 1369. 1380. 1385. 1410. 1424. 1438. 1441. 1468. 1492. 1495. 1496. 1497. 1503. 1505. 1510. 1518. 1521. 1524. 1527. 1530. 1534. 1536. 1538. 1545. 1562. 1567. 1581. 1620. 1631. 1642. 1659. 1662. 1715. 3000. 3027. 3034. 3044. 3048. 3055. 3056. 3057. 3080. 3101. 3112. 3118. 3120. 3120. 3136. 3145. 3155. 3157. 3163. 3177. 3179. 3184. 3186. 3189. 3192. 3202. 3204. 3207. 3212. 3212. 3219.

13:

16. 21. 27. 32. 39. 48. 49. 59. 64. 66. 95. 99. 108. 110. 116. 124. 137. 158. 171. 181. 197. 203. 218. 226. 232. 242. 267. 271. 274. 293. 304. 346. 361. 366. 387. 418. 419. 427. 448. 471. 496. 518. 537. 541. 580. 582. 604. 609. 619. 635. 637. 657. 692. 707. 712. 730. 738. 752. 762. 773. 793. 806. 818. 826. 846. 847. 859. 868. 884. 900. 914. 930. 943. 954. 961. 970. 978. 986. 988. 994. 1000. 1015. 1018. 1033. 1042. 1052. 1055. 1062. 1078. 1085. 1104. 1104. 1109. 1117. 1142. 1146. 1157. 1185. 1191. 1193. 1195. 1203. 1215. 1218. 1220. 1224. 1231. 1243. 1245. 1250. 1257. 1277. 1302. 1315. 1325. 1332. 1349. 1358. 1362. 1369. 1371. 1377. 1395. 1404. 1414. 1420. 1425. 1440. 1444. 1493. 1495. 1499. 1509. 1512. 1512. 1523. 1525. 1525. 1527. 1530. 1535. 1540. 1543. 1549. 1559. 1633. 1642. 1651. 1656. 1665. 1732. 1778. 2934. 2938. 2998. 3023. 3037. 3050. 3057. 3058. 3071. 3072. 3073. 3087. 3107. 3108. 3123. 3123. 3136. 3144. 3151. 3173. 3178. 3182. 3183. 3190. 3192. 3202. 3203. 3210. 3210. 3214. 3226**.**

12:

19. 22. 31. 33. 34. 43. 44. 53. 69. 79. 87. 96. 101. 106. 123. 136. 147. 153. 171. 185. 197. 202. 209. 225. 237. 247. 254. 259. 275. 295. 313. 324. 349. 369. 386. 396. 420. 421. 442. 454. 496. 503. 522. 532. 582. 591. 599. 609. 632. 635. 650. 662. 685. 711. 718. 745. 760. 765. 789. 790. 815. 817. 818. 855. 857. 865. 874. 920. 925. 931. 935. 945. 946. 956. 971. 972. 974. 980. 998. 1001. 1007. 1018. 1021. 1031. 1050. 1054. 1060. 1086. 1096. 1100. 1108. 1108. 1114. 1128. 1143. 1148. 1182. 1185. 1193. 1194. 1194. 1201. 1205. 1212. 1217. 1221. 1227. 1235. 1246. 1251. 1270. 1288. 1310. 1326. 1335. 1345. 1355. 1358. 1362. 1364. 1375. 1379. 1384. 1407. 1418. 1424. 1427. 1434. 1438. 1447. 1491. 1500. 1500. 1510. 1512. 1513. 1520. 1521. 1522. 1525. 1535. 1538. 1544. 1544. 1547. 1556. 1644. 1648. 1658. 1664. 1740. 1792. 2948. 2960. 3000. 3013. 3026. 3052. 3054. 3061. 3068. 3077. 3096. 3102. 3111. 3116. 3131. 3146. 3147. 3153. 3154. 3172. 3181. 3185. 3188. 3191. 3191. 3199. 3199. 3208. 3209. 3219. 3221.

INT_{B2}:

15. 20. 28. 36. 45. 46. 51. 60. 66. 72. 82. 89. 96. 101. 109. 113. 125. 134. 149. 169. 170. 181. 190. 203. 215. 227. 233. 238. 252. 301. 321. 330. 343. 358. 370. 382. 397. 416. 421. 421. 436. 476. 520. 522. 537. 565. 590. 602. 613. 617. 634. 636. 660. 666. 687. 706. 720. 724. 746. 765. 772. 781. 798. 802. 809. 820. 845. 850. 867. 869. 904. 918. 918. 929. 933. 966. 969. 976. 977. 992. 992. 1004. 1013. 1016. 1018. 1019. 1055. 1060. 1069. 1086. 1090. 1111. 1112. 1114. 1126. 1146. 1150. 1173. 1186. 1188. 1190. 1192. 1206. 1212. 1214. 1215. 1224. 1225. 1238. 1241. 1278. 1291. 1325. 1329. 1336. 1341. 1358. 1363. 1365. 1372. 1381. 1394. 1406. 1419. 1439. 1445. 1465. 1495. 1498. 1501. 1502. 1509. 1511. 1514. 1522. 1524. 1525. 1526. 1534. 1534. 1536. 1537. 1544. 1564. 1604. 1631. 1637. 1641. 1660. 1662. 1667. 1692. 3007. 3036. 3057. 3058. 3067. 3069. 3080. 3095. 3106. 3118. 3122. 3125. 3134. 3136. 3144. 3147. 3148. 3159. 3167. 3169. 3173. 3178. 3185. 3186. 3194. 3195. 3200. 3206. 3213. 3214. 3222.

TS_{B2-11}:

-38i 20. 27. 28. 38. 45. 46. 51. 63. 71. 84. 86. 97. 98. 103. 113. 129. 136. 147. 168. 169. 178. 188. 204. 214. 225. 230. 237. 255. 301. 320. 329. 341. 357. 370. 382. 396. 418. 421. 421. 436. 477. 516. 521. 535. 564. 589. 602. 613.

617. 634. 636. 654. 664. 691. 707. 720. 732. 757. 768. 775. 781. 795. 805. 808. 821. 848. 850. 865. 869. 905. 919. 920. 928. 934. 966. 970. 976. 977. 992. 992. 1004. 1012. 1016. 1018. 1022. 1055. 1060. 1068. 1085. 1090. 1111. 1112. 1114. 1126. 1146. 1151. 1172. 1186. 1186. 1190. 1192. 1205. 1213. 1214. 1215. 1224. 1225. 1234. 1241. 1271. 1293. 1322. 1327. 1334. 1338. 1358. 1360. 1365. 1371. 1377. 1394. 1407. 1417. 1438. 1445. 1463. 1495. 1496. 1500. 1502. 1508. 1510. 1511. 1521. 1524. 1525. 1526. 1533. 1534. 1536. 1537. 1545. 1562. 1587. 1632. 1640. 1642. 1662. 1664. 1673. 1699. 3009. 3040. 3056. 3057. 3060. 3063. 3076. 3091. 3109. 3113. 3121. 3124. 3133. 3136. 3140. 3143. 3151. 3158. 3164. 3167. 3174. 3179. 3185. 3186. 3190. 3194. 3200. 3206. 3214. 3214. 3221.

***E*-11:**

16. 23. 29. 35. 40. 45. 49. 55. 58. 71. 86. 103. 109. 119. 125. 132. 138. 142. 156. 168. 192. 204. 224. 231. 237. 254. 263. 287. 288. 312. 344. 356. 362. 364. 383. 403. 417. 418. 435. 486. 503. 520. 541. 572. 587. 595. 606. 610. 627. 636. 639. 654. 665. 702. 708. 716. 731. 738. 771. 775. 794. 817. 821. 840. 848. 859. 861. 868. 872. 890. 913. 918. 935. 945. 956. 962. 966. 986. 988. 995. 998. 1015. 1018. 1036. 1041. 1055. 1059. 1065. 1078. 1085. 1100. 1106. 1108. 1114. 1123. 1127. 1150. 1184. 1190. 1191. 1193. 1196. 1204. 1206. 1214. 1220. 1235. 1236. 1250. 1253. 1268. 1281. 1304. 1310. 1317. 1332. 1344. 1355. 1357. 1363. 1365. 1367. 1381. 1390. 1415. 1422. 1426. 1437. 1445. 1491. 1495. 1502. 1512. 1516. 1518. 1523. 1525. 1525. 1527. 1536. 1537. 1544. 1547. 1547. 1557. 1633. 1643. 1654. 1660. 1665. 1736. 1794. 2929. 2947. 2994. 3012. 3054. 3056. 3057. 3061. 3074. 3076. 3102. 3106. 3113. 3118. 3121. 3128. 3135. 3148. 3160. 3169. 3180. 3182. 3183. 3189. 3191. 3198. 3204. 3210. 3210. 3215. 3216.

TS'$_{B2}$:

-175. 14. 17. 21. 24. 28. 37. 43. 51. 57. 62. 68. 74. 77. 93. 103. 114. 130. 144. 147. 152. 160. 175. 184. 196. 221. 229. 238. 250. 260. 286. 298. 329. 349. 360. 368. 386. 395. 417. 421. 423. 460. 479. 525. 534. 556. 561. 593. 598. 609. 620. 636. 650. 668. 689. 702. 712. 714. 717. 757. 766. 785. 795. 804. 805. 815. 841. 848. 849. 861. 904. 915. 922. 925. 932. 944. 966. 967. 975. 992. 993. 1010. 1012. 1016. 1018. 1035. 1056. 1059. 1068. 1079. 1091. 1111. 1113. 1115. 1131. 1146.

1168. 1184. 1187. 1190. 1191. 1191. 1204. 1212. 1213. 1214. 1221. 1225. 1237. 1253. 1271. 1295. 1315. 1336. 1338. 1343. 1351. 1362. 1362. 1364. 1374. 1402. 1406. 1414. 1438. 1440. 1444. 1493. 1494. 1496. 1503. 1506. 1514. 1515. 1516. 1522. 1523. 1527. 1532. 1534. 1534. 1538. 1546. 1597. 1603. 1629. 1643. 1644. 1658. 1664. 1698. 1780. 3009. 3042. 3058. 3058. 3067. 3075. 3078. 3085. 3091. 3109. 3123. 3123. 3137. 3138. 3142. 3143. 3149. 3152. 3156. 3168. 3169. 3179. 3182. 3188. 3191. 3191. 3197. 3204. 3206. 3213. 3241.

***Z*-11:**

14. 17. 22. 27. 32. 38. 48. 50. 58. 61. 75. 93. 109. 121. 125. 138. 142. 146. 171. 179. 196. 202. 221. 227. 243. 245. 252. 266. 285. 306. 313. 341. 362. 372. 399. 416. 418. 422. 427. 478. 483. 517. 531. 538. 555. 582. 601. 611. 617. 634. 635. 645. 658. 703. 708. 715. 753. 758. 773. 781. 793. 807. 812. 830. 849. 859. 864. 871. 875. 916. 920. 929. 943. 945. 963. 967. 972. 984. 988. 998. 1003. 1015. 1018. 1027. 1033. 1054. 1057. 1059. 1082. 1090. 1102. 1109. 1110. 1113. 1126.

1141. 1151. 1183. 1188. 1191. 1192. 1201. 1204. 1204. 1216. 1218. 1225. 1234. 1245. 1248. 1251. 1261. 1280. 1306. 1315. 1332. 1341. 1355. 1363. 1363. 1368. 1372. 1383. 1390. 1416. 1419. 1424. 1438. 1444. 1490. 1495. 1500. 1508. 1512. 1516. 1518. 1523. 1523. 1524. 1535. 1537. 1542. 1544. 1547. 1556. 1633. 1644. 1654. 1664. 1713. 1736. 1808. 2934. 2940. 3003. 3014. 3030. 3054. 3056. 3057. 3065. 3076. 3099. 3107. 3110. 3111. 3125. 3136. 3139. 3151. 3152. 3158. 3172. 3181. 3182. 3182. 3190. 3191. 3198. 3204. 3208. 3211. 3215.

14a:

13. 18. 23. 36. 37. 42. 56. 57. 66. 83. 96. 117. 132. 166. 173. 184. 218. 247. 254. 269. 295. 310. 322. 382. 412. 416. 419. 420. 423. 457. 476. 491. 526. 531. 542. 583. 594. 625. 630. 630. 633. 679. 684. 691. 697. 702. 704. 706. 709. 718. 734. 760. 777. 785. 786. 794. 826. 850. 854. 859. 865. 927. 934. 942. 943. 946. 969. 970. 980. 981. 991. 1001. 1005. 1006. 1007. 1014. 1019. 1021. 1022. 1044. 1055. 1056. 1061. 1078. 1109. 1111. 1112. 1118. 1138. 1157. 1187. 1195. 1196. 1197. 1201. 1210. 1216. 1220. 1237. 1239. 1333. 1337. 1343. 1347. 1359. 1363. 1366.

1372. 1372. 1406. 1443. 1483. 1493. 1494. 1505. 1519. 1534. 1543. 1545. 1548. 1584. 1596. 1624. 1642. 1652. 1654. 1657. 1657. 1658. 1664. 3173. 3183. 3192. 3193. 3196. 3197. 3203. 3205. 3207. 3208. 3213. 3214. 3216. 3221. 3226. 3226. 3230. 3232. 3236. 3248.

14a':

18. 20. 22. 33. 42. 47. 50. 57. 66. 83. 96. 117. 135. 166. 176. 184. 218. 246. 254. 271. 295. 311. 317. 393. 410. 416. 421. 422. 424. 460. 471. 488. 522. 536. 544. 586. 594. 625. 629. 630. 633. 681. 685. 691. 698. 703. 705. 707. 707. 715. 732. 762. 778. 785. 787. 796. 824. 852. 854. 858. 864. 927. 935. 943. 945. 947. 969. 973. 979. 981. 991. 1001. 1005. 1006. 1006. 1014. 1019. 1021. 1022. 1045. 1055. 1056. 1061. 1078. 1108. 1111. 1112. 1118. 1138. 1159. 1187. 1196. 1196. 1197. 1201. 1210. 1214. 1221. 1238. 1241. 1333. 1337. 1344. 1346. 1359. 1363. 1366. 1371. 1373. 1405. 1440. 1485. 1494. 1495. 1503. 1520. 1534. 1543. 1545. 1550. 1585. 1594. 1624. 1642. 1651. 1655. 1656. 1657. 1659. 1664. 3173. 3182. 3192. 3193. 3195. 3197. 3203. 3206. 3206. 3207. 3213. 3214. 3215. 3222. 3226. 3227. 3231. 3233. 3237. 3248.

14a":

19. 20. 22. 33. 42. 47. 50. 57. 66. 83. 96. 117. 135. 166. 176. 184. 218. 246. 254. 271. 295. 311. 317. 393. 410. 416. 421. 422. 424. 460. 470. 488. 522. 536. 544. 586. 594. 625. 629. 630. 633. 681. 685. 691. 698. 703. 705. 707. 707. 715. 732. 762. 778. 785. 787. 796. 824. 852. 854. 859. 864. 927. 935. 943. 945. 947. 969. 973. 979. 981. 991. 1001. 1005. 1006. 1006. 1014. 1019. 1021. 1022. 1045. 1055. 1056. 1061. 1078. 1108. 1111. 1112. 1118. 1138. 1159. 1187. 1196. 1196. 1197. 1201. 1210. 1214. 1221. 1237. 1241. 1333. 1337. 1344. 1346. 1358. 1363. 1366. 1371. 1373. 1405. 1440. 1485. 1494. 1495. 1503. 1520. 1534. 1543. 1545. 1550. 1585. 1594. 1624. 1642. 1651. 1655. 1656. 1657. 1659. 1664. 3173. 3182. 3192. 3193. 3195. 3197. 3203. 3206. 3206. 3207. 3213. 3214. 3215. 3222. 3226. 3228. 3231. 3233. 3237. 3248.

TS_{A3}:

-179i 11. 14. 18. 21. 24. 31. 37. 39. 42. 44. 46. 49. 57. 59. 65. 74. 76. 90. 106. 108. 123. 130. 141. 144. 154. 163. 174. 196. 220. 244. 247. 248. 260. 263. 271. 300. 313. 317. 368. 377. 406. 414. 416. 418. 419. 420. 431. 448. 456. 460. 473. 492. 511. 513. 529. 541. 552. 582. 589. 600. 625. 629. 630. 632. 636. 648. 655. 682. 690. 698. 703. 706. 708. 711. 714. 716. 722. 744. 758. 760. 769. 776. 780. 787. 795. 808. 826. 839. 854. 859. 859. 862. 864. 912. 923. 927. 931. 941. 945. 946. 960. 963. 966. 970. 978. 979. 992. 996. 1002. 1004. 1005. 1007. 1016. 1017. 1019. 1022. 1023. 1027. 1046. 1056. 1056. 1059. 1061. 1078. 1082. 1111. 1111. 1113. 1114. 1118. 1139. 1155. 1163. 1183. 1187. 1189. 1191. 1197. 1197. 1198. 1209. 1210. 1213. 1213. 1216. 1218. 1221. 1223. 1233. 1244. 1307. 1333. 1336. 1343. 1350. 1360. 1361. 1363. 1367. 1370. 1370. 1371. 1375. 1397. 1441. 1453. 1493. 1494. 1495. 1496. 1496. 1504. 1505. 1511. 1525. 1531. 1537. 1542. 1543. 1545. 1551. 1582. 1590. 1632. 1641. 1643. 1654. 1654. 1656. 1657. 1658. 1663. 1664. 1705. 1763. 2994. 3051. 3066. 3113. 3149. 3165. 3176. 3177. 3179. 3183. 3185. 3188. 3194. 3195. 3195. 3198. 3199. 3204. 3205. 3207. 3209. 3209. 3214. 3216. 3217. 3218. 3225. 3233. 3234. 3234. 3236. 3238.

TS_{B3}:

-146i 8. 14. 17. 23. 26. 27. 29. 39. 39. 46. 49. 54. 60. 63. 70. 72. 80. 85. 98. 101. 111. 119. 137. 152. 163. 173. 176. 207. 225. 237. 245. 247. 250. 266. 273. 306. 309. 322. 325. 368. 402. 414. 418. 422. 424. 424. 426. 429. 445. 457. 472. 513. 517. 521. 539. 545. 557. 587. 594. 614. 622. 629. 631. 633. 637. 665. 682. 691. 697. 702. 703. 705. 711. 714. 715. 716. 718. 748. 759. 765. 765. 781. 787. 789. 799. 810. 831. 846. 852. 861. 863. 867. 871. 915. 929. 930. 944. 944. 951. 953. 955. 967. 970. 979. 988. 992. 993. 996. 1003. 1004. 1008. 1015. 1017. 1018. 1020. 1022. 1024. 1027. 1045. 1056. 1057. 1059. 1063. 1077. 1082. 1110. 1112. 1115. 1115. 1118. 1137. 1143. 1160. 1176. 1183. 1190. 1191. 1196. 1197. 1197. 1203. 1212. 1213. 1213. 1215. 1217. 1221. 1224. 1231. 1251. 1307. 1334. 1337. 1345. 1349. 1357. 1360. 1364. 1368. 1372. 1372. 1375. 1377. 1396. 1445. 1461. 1492. 1493. 1494. 1495. 1500. 1502. 1505. 1508. 1529. 1532. 1536. 1544. 1545. 1546. 1559. 1589. 1592. 1626. 1643. 1643. 1649. 1654. 1655. 1657. 1658. 1664. 1665. 1695. 1786. 3026. 3059. 3075. 3126. 3154. 3170. 3178. 3181. 3187. 3190. 3191. 3191. 3194. 3195. 3195. 3197. 3198. 3203. 3203. 3205. 3207. 3208. 3211. 3213. 3215. 3216. 3228. 3229. 3234. 3235. 3239. 3252.

TS_{N3}:

-242i 14. 17. 19. 25. 32. 33. 36. 42. 46. 47. 55. 59. 60. 65. 67. 70. 75. 86. 103. 104. 122. 137. 137. 147. 163. 177. 185. 192. 219. 223. 246. 255. 259. 271. 290. 305. 312. 318. 367. 369. 396. 414. 418. 419. 420. 421. 436. 448. 457. 470. 484. 487. 506. 527. 529. 542. 558. 581. 587. 609. 629. 630. 631. 634. 635. 641. 676. 686. 692. 697. 701. 705. 707. 713. 715. 719. 723. 735. 759. 765. 768. 779. 787. 790. 797. 815. 830. 854. 856. 860. 863. 868. 882. 929. 931. 935. 942. 944. 947. 952. 972. 975. 978. 979. 982. 983. 1002. 1004. 1007. 1007. 1009. 1011. 1017. 1018. 1019. 1021. 1024. 1024. 1046. 1056. 1059. 1060. 1062. 1078. 1080. 1112. 1114. 1115. 1117. 1119. 1133. 1142. 1159. 1174. 1186. 1192. 1192. 1196. 1196. 1198. 1211. 1212. 1214. 1214. 1217. 1218. 1222. 1224. 1230. 1239. 1317. 1333. 1342. 1344. 1349. 1357. 1362. 1366. 1371. 1372. 1372. 1375. 1378. 1401. 1431. 1446. 1483. 1493. 1494. 1497. 1499. 1502. 1508. 1510. 1515. 1532. 1538. 1542. 1544. 1546. 1548. 1557. 1591. 1637. 1642. 1644. 1652. 1653. 1654. 1655. 1657. 1663. 1664. 1713. 1829. 3037. 3057. 3093. 3124. 3152. 3167. 3173. 3178. 3181. 3186. 3192. 3193. 3194. 3195. 3195. 3196. 3202. 3204. 3204. 3206. 3209. 3209. 3214. 3215. 3217. 3222. 3226. 3233. 3234. 3236. 3240. 3242.

15a-I:

9. 17. 21. 22. 24. 29. 35. 40. 42. 46. 51. 60. 62. 66. 74. 78. 88. 105. 112. 121. 134. 138. 156. 175. 185. 192. 200. 221. 224. 230. 248. 255. 270. 273. 288. 302. 319. 352. 364. 386. 400. 416. 417. 418. 423. 424. 427. 434. 454. 475. 485. 506. 520. 525. 530. 541. 559. 580. 600. 615. 630. 632. 634. 635. 636. 657. 671. 675. 687. 695. 706. 708. 708. 715. 716. 723. 747. 760. 766. 776. 782. 783. 799. 810. 823. 836. 850. 851. 862. 862. 862. 879. 893. 894. 922. 924. 926. 936. 942. 958. 960. 965. 966. 967. 975. 980. 984. 990. 991. 995. 996. 998. 1006. 1009. 1015. 1017. 1019. 1021. 1035. 1048. 1055. 1055. 1057. 1059. 1066. 1083. 1104. 1107. 1110. 1112. 1116. 1119. 1134. 1156. 1184. 1188. 1191. 1193. 1193. 1194. 1194. 1205. 1208. 1214. 1215. 1216. 1220. 1221. 1231. 1234. 1252. 1278. 1308. 1327. 1334. 1336. 1341. 1349. 1358. 1359. 1363. 1365. 1369. 1371. 1371. 1378. 1397. 1436. 1491. 1494. 1496. 1496. 1499. 1503. 1506. 1514. 1521. 1537. 1544. 1546. 1547. 1553. 1628. 1634. 1634. 1641. 1645. 1653. 1656. 1660. 1663. 1665. 1674. 1707. 1731. 1811. 3041. 3076. 3077. 3080. 3158. 3160. 3175. 3178. 3182. 3183. 3185. 3186. 3189. 3189. 3191. 3192. 3195. 3197. 3197. 3205. 3207. 3208. 3209. 3209. 3214. 3217. 3221. 3222. 3224. 3227. 3228. 3252.

16a-I:

11. 18. 22. 28. 30. 30. 34. 44. 53. 53. 59. 63. 66. 70. 74. 79. 98. 112. 122. 129. 142. 148. 159. 178. 184. 197. 205. 219. 225. 237. 246. 250. 257. 277. 287. 308. 316. 331. 372. 389. 390. 418. 418. 419. 420. 424. 426. 436. 473. 484. 497. 509. 512. 526. 528. 545. 576. 592. 605. 631. 632. 634. 636. 636. 659. 669. 675. 686. 695. 700. 704. 710. 713. 715. 718. 743. 752. 760. 770. 782. 785. 795. 811. 821. 831. 849. 856. 860. 865. 866. 877. 892. 910. 926. 932. 937. 939. 940. 954. 956. 964. 971. 972. 974. 975. 978. 984. 986. 998. 998. 1000. 1000. 1011. 1017. 1018. 1020. 1021. 1044. 1054. 1056. 1058. 1060. 1063. 1070. 1095. 1104. 1109. 1111. 1113. 1116. 1118. 1145. 1159. 1172. 1187. 1192. 1192. 1194. 1194. 1194. 1198. 1207. 1213. 1216. 1216. 1218. 1219. 1224. 1232. 1243. 1262. 1310. 1311. 1335. 1341. 1343. 1345. 1350. 1356. 1362. 1362. 1365. 1370. 1371. 1374. 1376. 1401. 1431. 1440. 1493. 1494. 1498. 1499. 1500. 1505. 1506. 1515. 1522. 1544. 1545. 1546. 1547. 1553. 1628. 1635. 1641. 1644. 1648. 1656. 1658. 1660. 1663. 1664. 1677. 1737. 1805. 3022. 3081. 3084. 3110. 3159. 3171. 3181. 3182. 3185. 3185. 3189. 3190. 3192. 3192. 3192. 3195. 3196. 3200. 3205. 3208. 3208. 3209. 3209. 3215. 3217. 3222. 3224. 3224. 3226. 3230. 3232. 3253.

19:

14. 15. 17. 25. 27. 33. 34. 44. 47. 51. 53. 60. 64. 67. 70. 95. 99. 107. 111. 123. 130. 133. 146. 167. 175. 185. 203. 213. 220. 232. 248. 252. 272. 280. 285. 306. 342. 347. 362. 381. 404. 416. 418. 418. 423. 424. 429. 457. 475. 476. 505. 520. 528. 530. 540. 552. 580. 588. 606. 612. 630. 632. 634. 636. 640. 670. 672. 676. 694. 699. 707. 707. 708. 711. 715. 727. 745. 751. 760. 763. 776. 779. 782. 794. 826. 838. 850. 852. 854. 860. 863. 876. 880. 894. 901. 922. 926. 934. 935. 957. 960. 966. 968. 970. 972. 973. 985. 990. 991. 996. 998. 998. 1008. 1014. 1017. 1017. 1018. 1021. 1051. 1053. 1055. 1056. 1060. 1062. 1075. 1086. 1102. 1109. 1110. 1114. 1115. 1122. 1150. 1165. 1185. 1191. 1192. 1193. 1193. 1194. 1201. 1205. 1210. 1216. 1217. 1219. 1220. 1223. 1235. 1239. 1250. 1285. 1308.

1333. 1335. 1340. 1347. 1349. 1356. 1359. 1364. 1364. 1366. 1370. 1374. 1375. 1401. 1433. 1493. 1494. 1496. 1498. 1499. 1505. 1508. 1512. 1525. 1536. 1543. 1545. 1548. 1553. 1627. 1633. 1634. 1641. 1643. 1653. 1656. 1660. 1661. 1663. 1665. 1674. 1735. 1777. 3051. 3056. 3072. 3107. 3145. 3172. 3178. 3179. 3182. 3184. 3185. 3188. 3189. 3190. 3193. 3195. 3198. 3199. 3206. 3208. 3209. 3209. 3210. 3215. 3218. 3218. 3222. 3224. 3227. 3231. 3239. 3250.

TS'$_{A3}$:

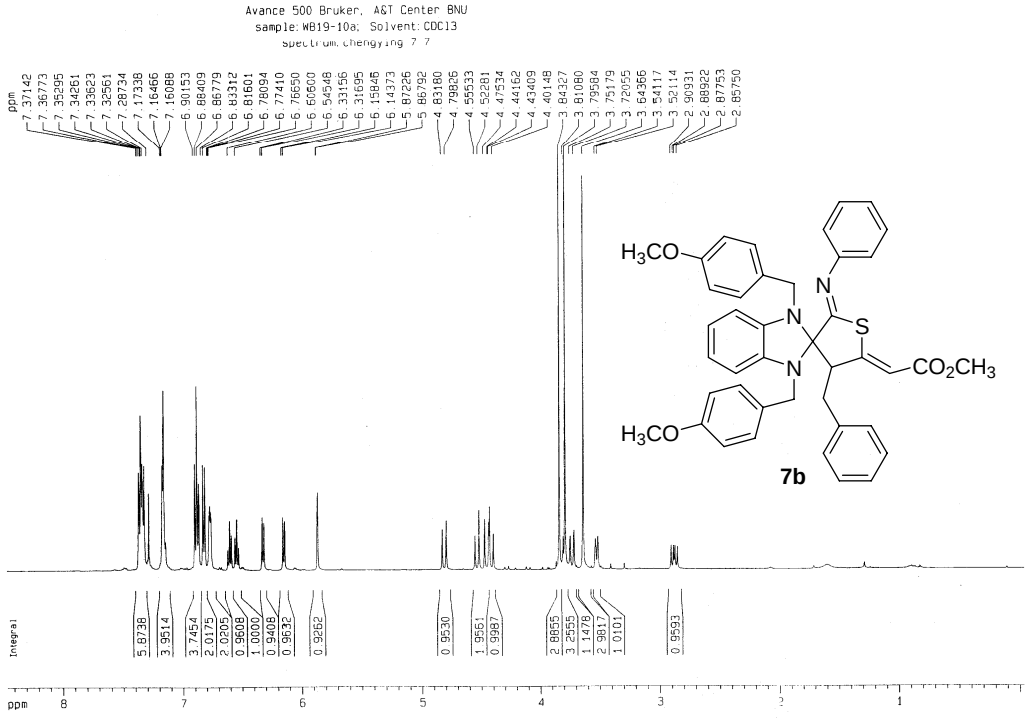
-155i 11. 12. 16. 18. 23. 24. 28. 31. 35. 37. 44. 54. 56. 57. 64. 66. 73. 84. 94. 111. 114. 123. 135. 154. 157. 165. 179. 201. 225. 235. 245. 246. 253. 264. 269. 287. 316. 324. 331. 373. 406. 413. 419. 419. 421. 421. 423. 426. 453. 463. 472. 490. 519. 526. 535. 546. 556. 591. 592. 612. 622. 629. 631. 634. 637. 660. 680. 691. 698. 699. 703. 705. 708. 711. 714. 716. 728. 749. 755. 758. 763. 780. 785. 789. 801. 811. 828. 847. 850. 855. 859. 863. 864. 914. 927. 930. 937. 942. 948. 950. 952. 967. 968. 976. 981. 984. 992. 992. 1003. 1005. 1006. 1008. 1015. 1017. 1019. 1022. 1022. 1024. 1045. 1055. 1056. 1059. 1062. 1077. 1082. 1111. 1112. 1113. 1114. 1118. 1134. 1140. 1161. 1173. 1186. 1190. 1191. 1196. 1197. 1198. 1203. 1211. 1212. 1213. 1214. 1215. 1222. 1224. 1233. 1250. 1304. 1334. 1337. 1344. 1348. 1356. 1358. 1364. 1366. 1367. 1372. 1372. 1377. 1393. 1444. 1458. 1491. 1493. 1494. 1495. 1502. 1502. 1503. 1509. 1530. 1532. 1535. 1542. 1545. 1546. 1557. 1586. 1590. 1628. 1642. 1643. 1651. 1653. 1655. 1656. 1657. 1665. 1665. 1712. 1799. 3029. 3058. 3073. 3127. 3149. 3170. 3177. 3180. 3187. 3188. 3189. 3192. 3193. 3195. 3196. 3199. 3202. 3203. 3205. 3206. 3208. 3210. 3214. 3214. 3217. 3227. 3227. 3228. 3231. 3234. 3247. 3249.

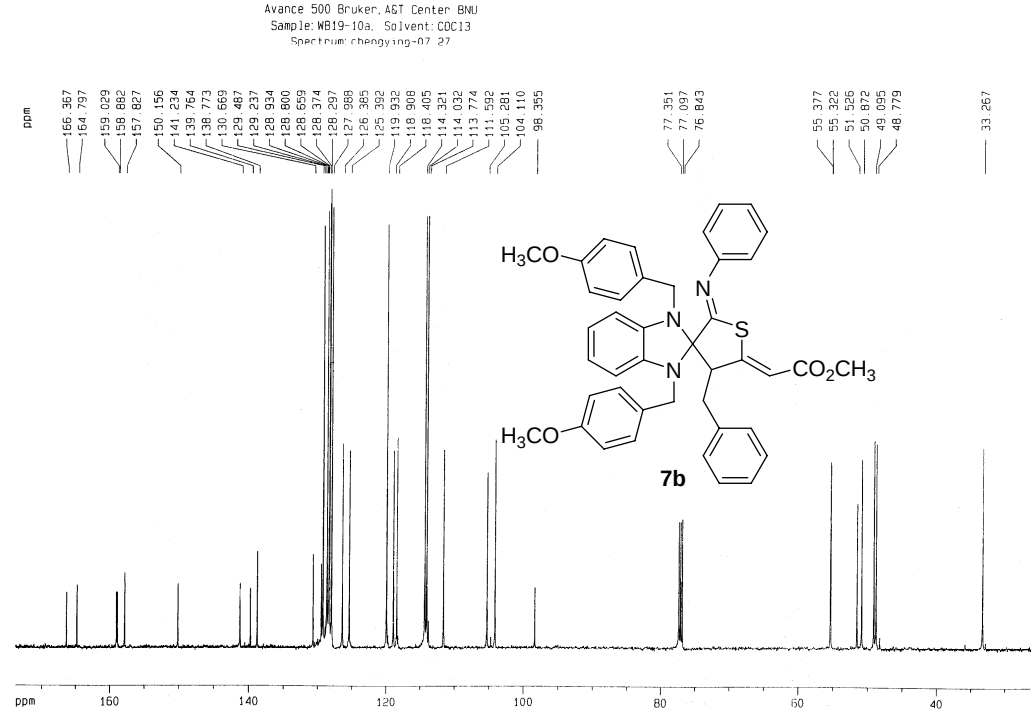
15a-II:

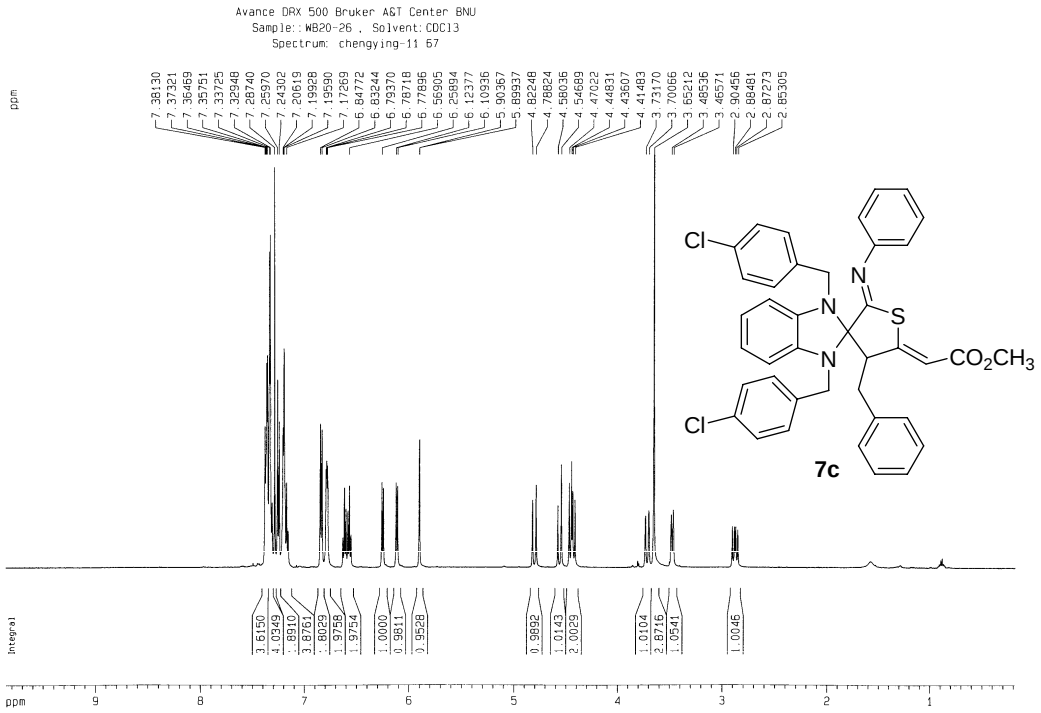
11. 16. 20. 22. 27. 32. 33. 35. 40. 44. 48. 56. 66. 69. 72. 76. 91. 104. 112. 114. 131. 144. 164. 171. 176. 194. 204. 218. 227. 230. 242. 261. 266. 268. 285. 311. 315. 357. 368. 396. 415. 416. 417. 421. 425. 429. 433. 446. 450. 478. 491. 509. 515. 525. 533. 547. 560. 589. 601. 617. 630. 631. 632. 635. 636. 649. 671. 676. 677. 696. 706. 708. 711. 715. 721. 722. 750. 763. 773. 779. 783. 784. 799. 814. 818. 826. 850. 857. 859. 862. 866. 880. 892. 919. 922. 927. 933. 934. 946. 953. 963. 964. 967. 970. 971. 986. 988. 990. 994. 996. 996. 998. 1004. 1015. 1018. 1019. 1019. 1021. 1038. 1041. 1055. 1057. 1058. 1059. 1065. 1071. 1079. 1109. 1109. 1112. 1113. 1117. 1127. 1147. 1180. 1185. 1191. 1191. 1193. 1194. 1194. 1205. 1205. 1209. 1215. 1216. 1218. 1221. 1229. 1232. 1249. 1271. 1300. 1324. 1329. 1333. 1335. 1343. 1349. 1357. 1361. 1363. 1365. 1369. 1371. 1372. 1401. 1416. 1491. 1491. 1492. 1495. 1496. 1500. 1502. 1512. 1522. 1536. 1543. 1545. 1547. 1550. 1630. 1634. 1638. 1640. 1644. 1654. 1655. 1658. 1664. 1665. 1677. 1708. 1728. 1822. 3043. 3077. 3081. 3084. 3157. 3161. 3175. 3178. 3181. 3182. 3184. 3187. 3189. 3189. 3191. 3192. 3195. 3196. 3197. 3205. 3206. 3207. 3208. 3209. 3212. 3216. 3216. 3227. 3232. 3238. 3238. 3241.

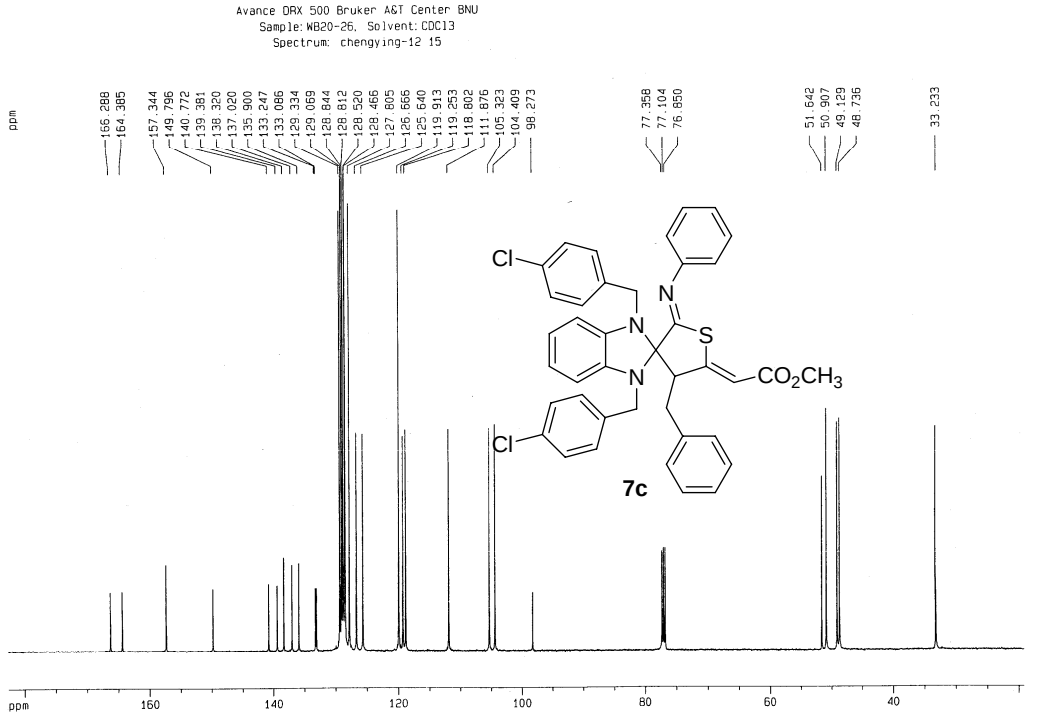
Gaussian 03 reference: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C. and Pople, J. A. *Gaussian 03, Revision C.02*, Gaussian, Inc., Wallingford CT, **2004**.

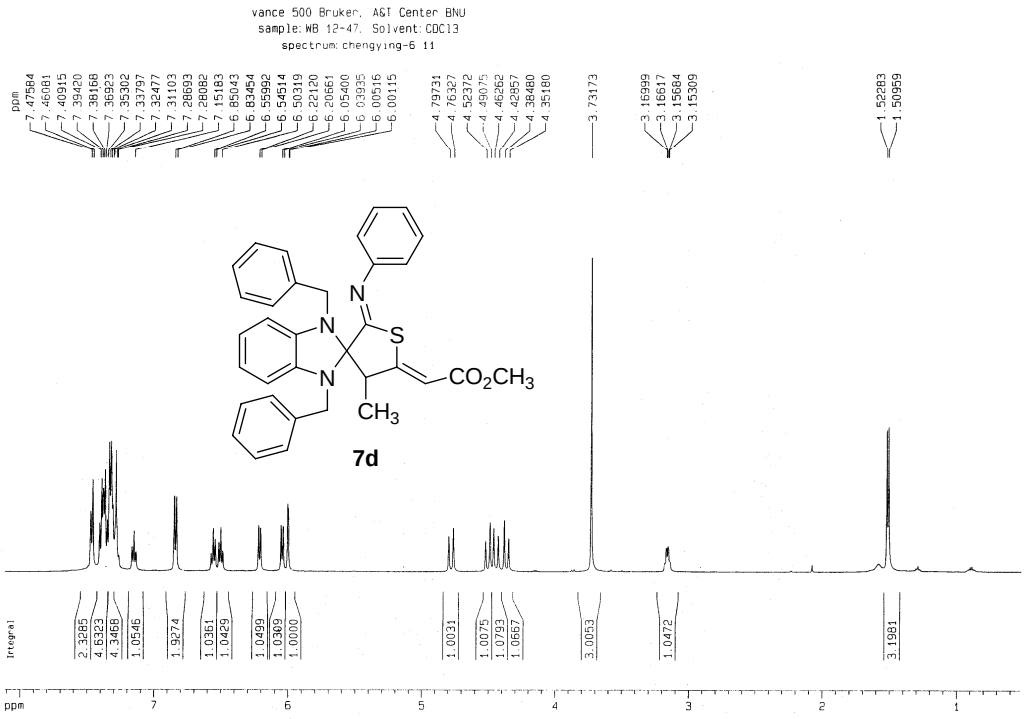
Copies of NMR spectra of products **7, 11, 12, 13, 15, 16, 17** and **18**.

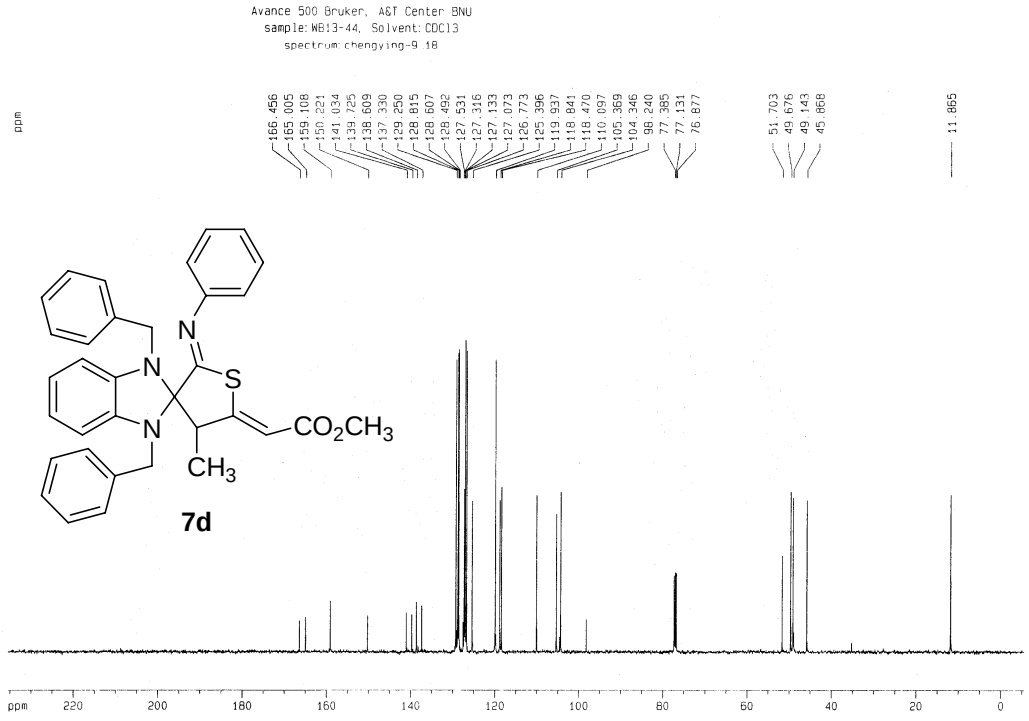

Avance 500 Bruker, A&T Center BNU
sample: WB19-10a; Solvent: CDCl3
Spectrum: chengying 7 7
ppm
Integral
7b

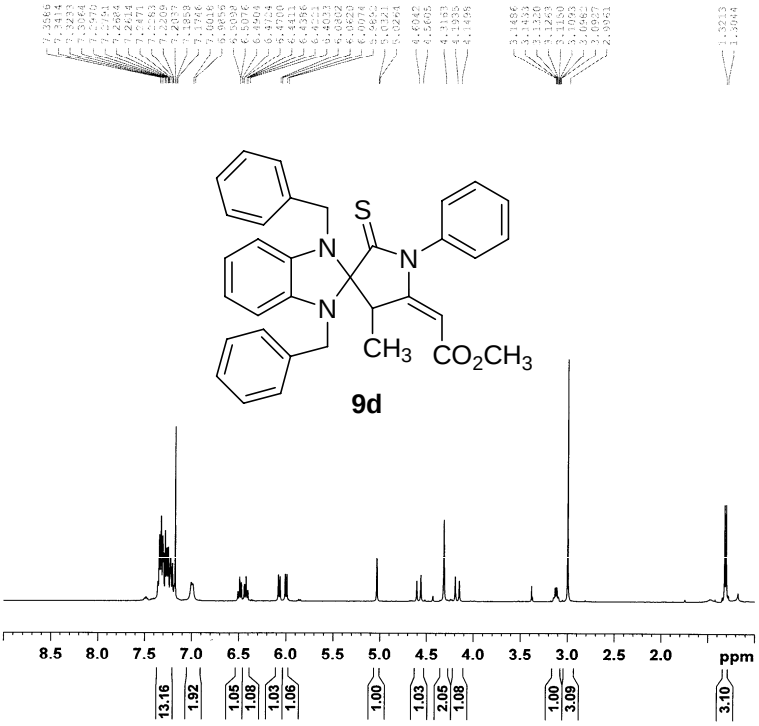

Avance 500 Bruker, A&T Center BNU
Sample: WB19-10a; Solvent: CDCl3
Spectrum: chengying-07 27
ppm
7b


Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-26 , Solvent: CDCl3
Spectrum: chengying-11 67
ppm
Integral
ppm
Cl
N
N
S
N
CO2CH3
Cl
7c


Avance DRX 500 Bruker A&T Center BNU
Sample: WB20-26, Solvent: CDCl3
Spectrum: chengying-12 15
ppm
Cl
N
N
S
N
CO2CH3
Cl
7c

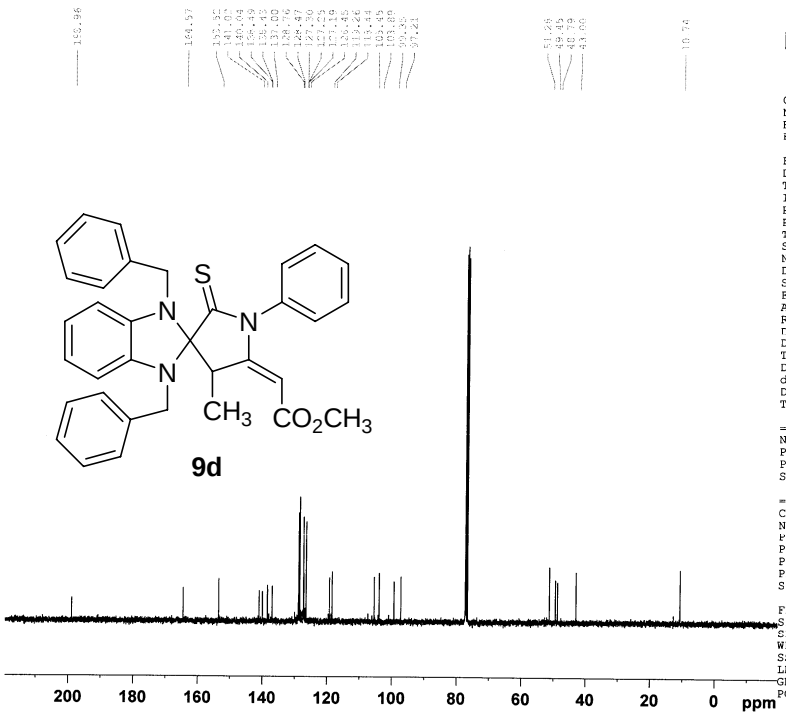

vance 500 Bruker, A&T Center BNU
sample: WB 12-47, Solvent: CDCl3
spectrum: chengying-6 11
ppm
7.47584
7.46081
7.40915
7.39420
7.38166
7.36923
7.35302
7.33797
7.32477
7.31103
7.28693
7.28082
7.15183
6.85043
6.83454
6.55992
6.54514
6.50319
6.22120
6.20661
6.05400
6.03935
6.00516
6.00115
4.79731
4.76327
4.52372
4.49075
4.46262
4.42857
4.38480
4.35180
3.73173
3.16999
3.16617
3.15684
3.15309
1.52283
1.50959
N
N
S
N
CO2CH3
CH3
7d
Integral
2.3285
4.6323
4.3468
1.0546
1.9274
1.0361
1.0429
1.0499
1.0389
1.0000
1.0031
1.0075
1.0793
1.0657
3.0053
1.0472
3.1981
ppm
7
6
5
4
3
2
1


Avance 500 Bruker, A&T Center BNU
sample: WB13-44, Solvent: CDCl3
spectrum: chengying-9 18
ppm
166.456
165.005
159.108
150.221
141.034
139.725
138.609
137.330
129.250
128.815
128.607
128.492
127.531
127.316
127.133
127.073
126.773
125.396
119.937
118.841
118.470
110.097
105.369
104.346
98.240
77.385
77.131
76.877
51.703
49.676
49.143
45.868
11.865
N
N
S
N
CO2CH3
CH3
7d
ppm
220
200
180
160
140
120
100
80
60
40
20
0



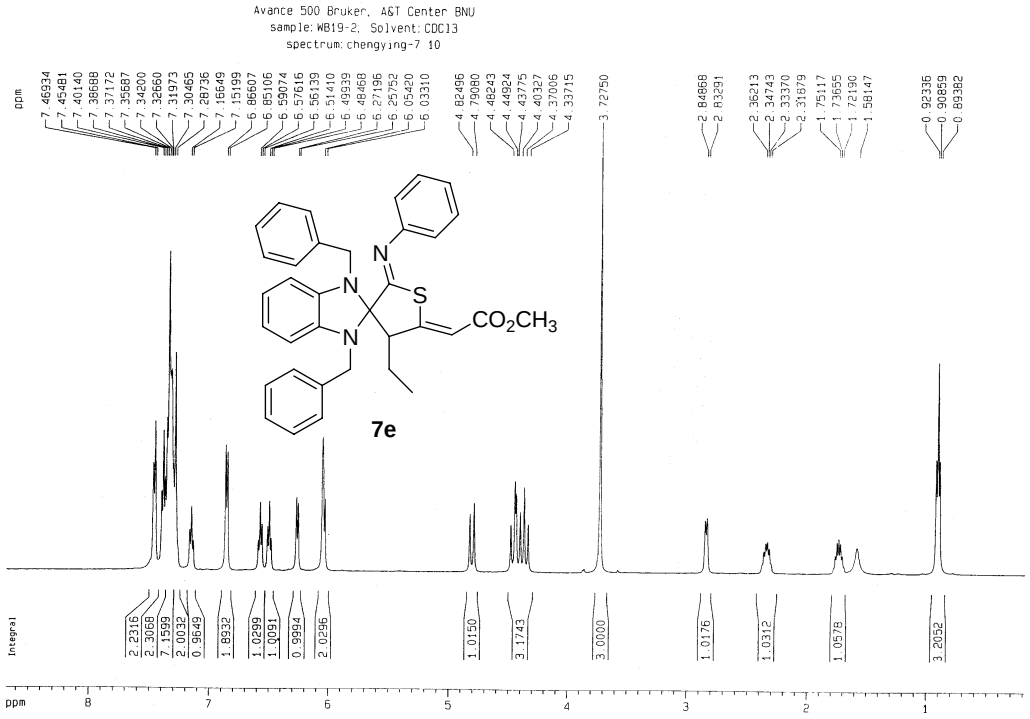
BRUKER

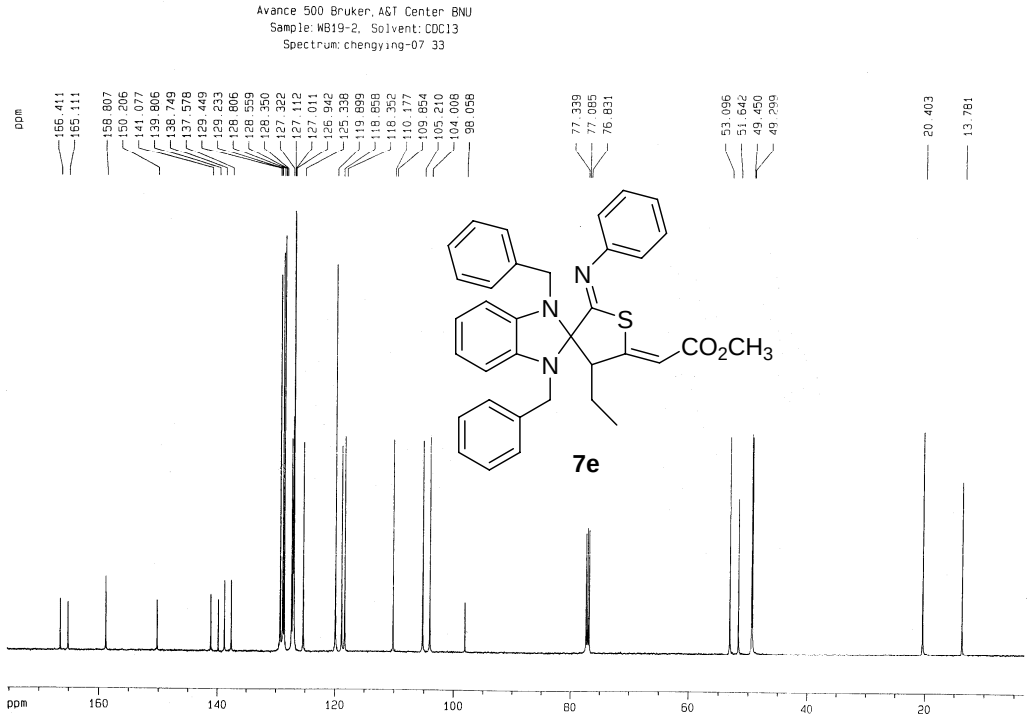
```
Current Data Parameters
NAME          WB21-23b-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080414
Time               15.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                299.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.50 usec
PL1                -1.00 dB
SFO1          400.1724712 MHz

F2 - Processing parameters
SI                 32768
SF            400.1700370 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

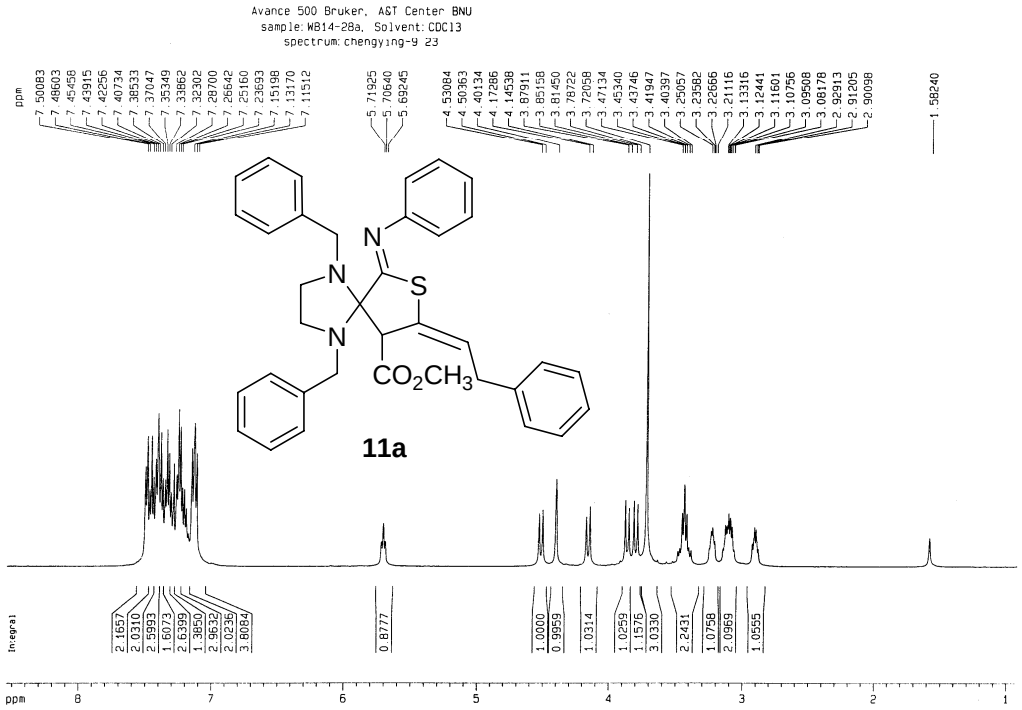


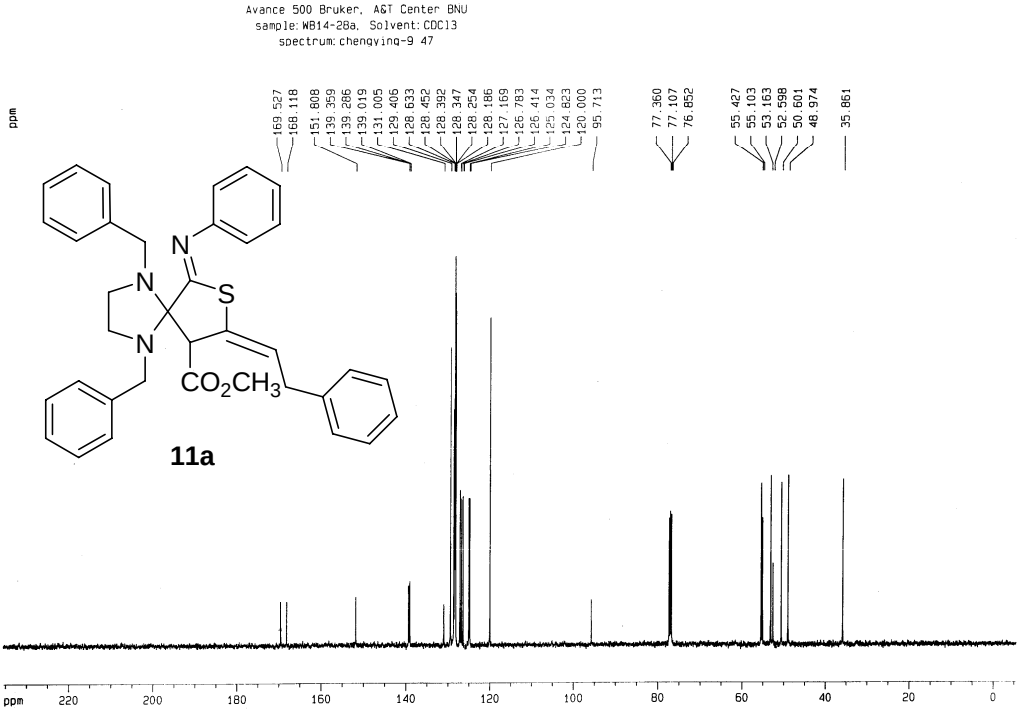
BRUKER

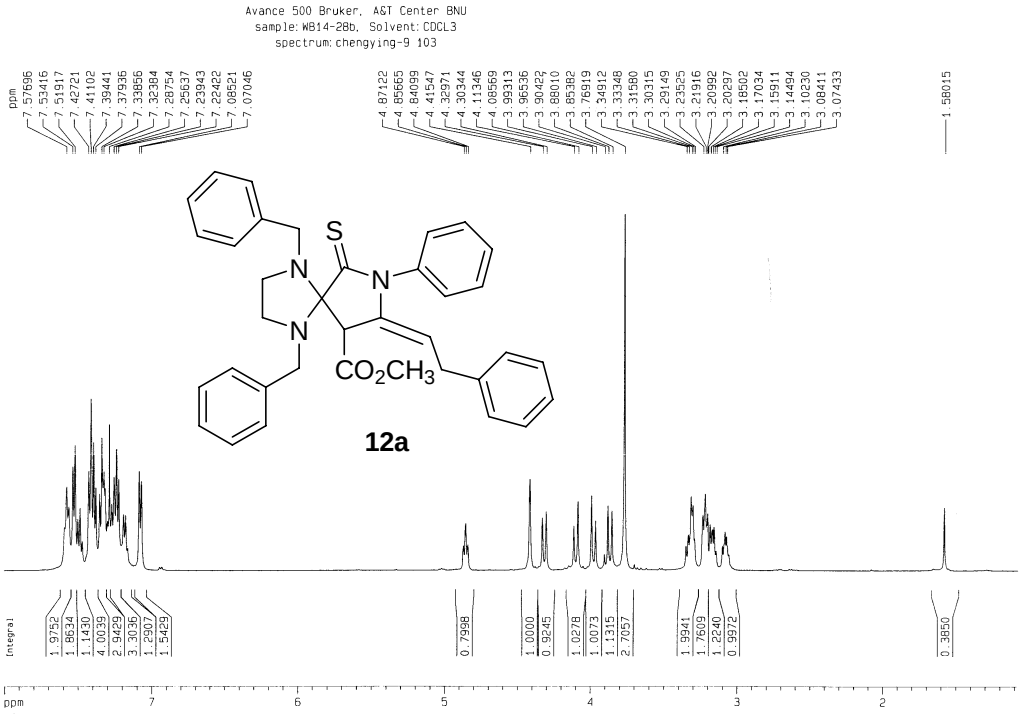
```
Current Data Parameters
NAME        WB21-23b-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080415
Time               15.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   509
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                301.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.40 usec
PL1                -2.00 dB
SFO1          100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL12               14.46 dB
PL13               14.46 dB
PL2                -1.00 dB
SFO2          400.1716007 MHz

F2 - Processing parameters
SI                 32768
SF            100.6228270 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

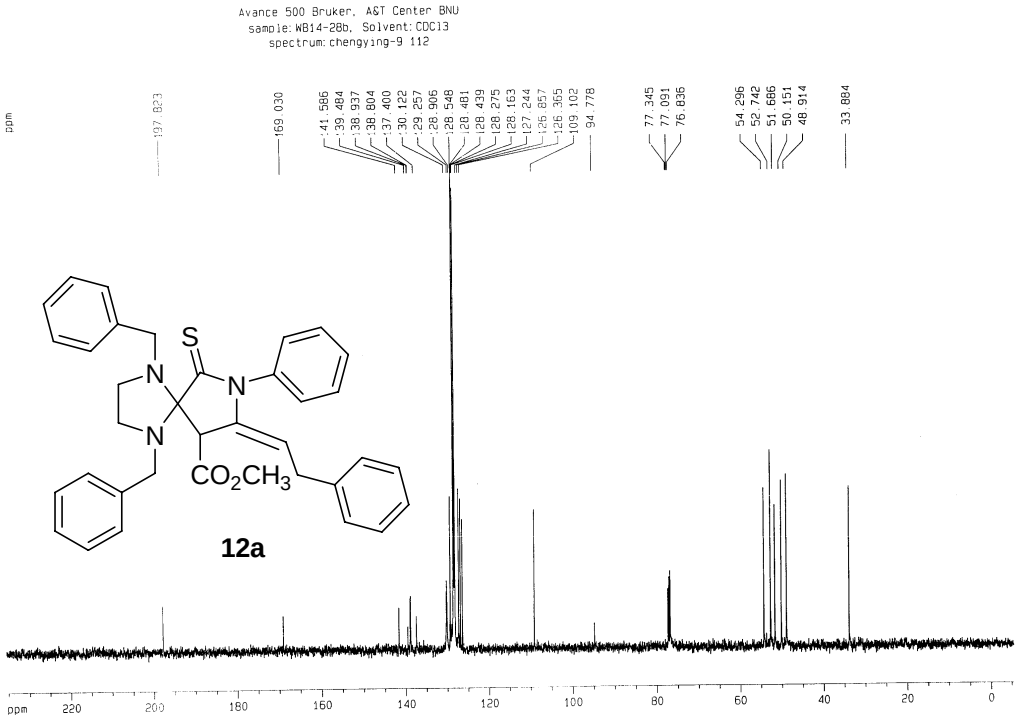

Avance 500 Bruker, A&T Center BNU
sample: WB19-2, Solvent: CDCl3
spectrum: chengying-7 10
ppm
7.46934
7.45481
7.40140
7.38688
7.37172
7.35687
7.34200
7.32660
7.31973
7.30465
7.28736
7.16649
7.15199
6.86607
6.85106
6.59074
6.57616
6.56139
6.51410
6.49939
6.48468
6.27196
6.25752
6.05420
6.03310
4.82496
4.79080
4.48243
4.44924
4.43775
4.40327
4.37006
4.33715
3.72750
2.84868
2.83291
2.36213
2.34743
2.33370
2.31879
1.75117
1.73655
1.72190
1.58147
0.92336
0.90859
0.89382
N
N
S
N
CO2CH3
7e
Integral
2.2316
2.3068
7.1599
2.0032
0.9649
1.8932
1.0299
1.0091
0.9994
2.0296
1.0150
3.1743
3.0000
1.0176
1.0312
1.0578
3.2052
ppm
8
7
6
5
4
3
2
1

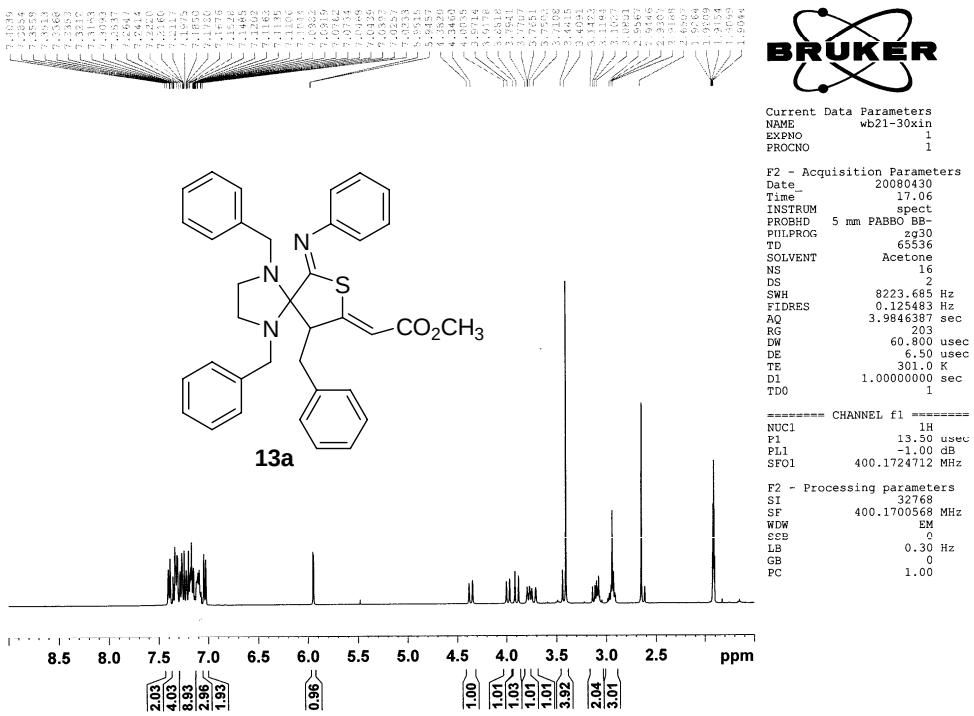

Avance 500 Bruker, A&T Center BNU
Sample: WB19-2, Solvent: CDCl3
Spectrum: chengying-07 33
ppm
166.411
165.111
158.807
150.206
141.077
139.806
138.749
137.578
129.449
129.233
128.806
128.559
128.350
127.322
127.112
127.011
126.942
125.338
119.899
118.858
118.352
110.177
109.854
105.210
104.006
98.058
77.339
77.085
76.831
53.096
51.642
49.450
49.299
20.403
13.781
N
N
S
N
CO2CH3
7e
ppm
160
140
120
100
80
60
40
20

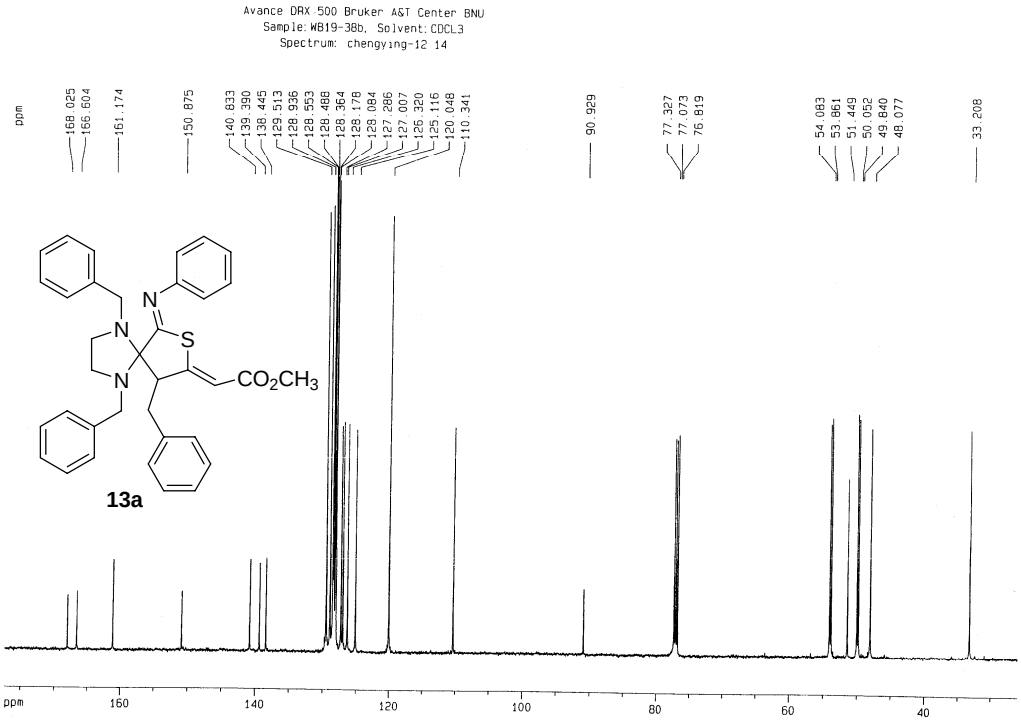

Avance 500 Bruker, A&T Center BNU
sample: WB14-28a, Solvent: CDCl3
spectrum: chengying-9 23
11a

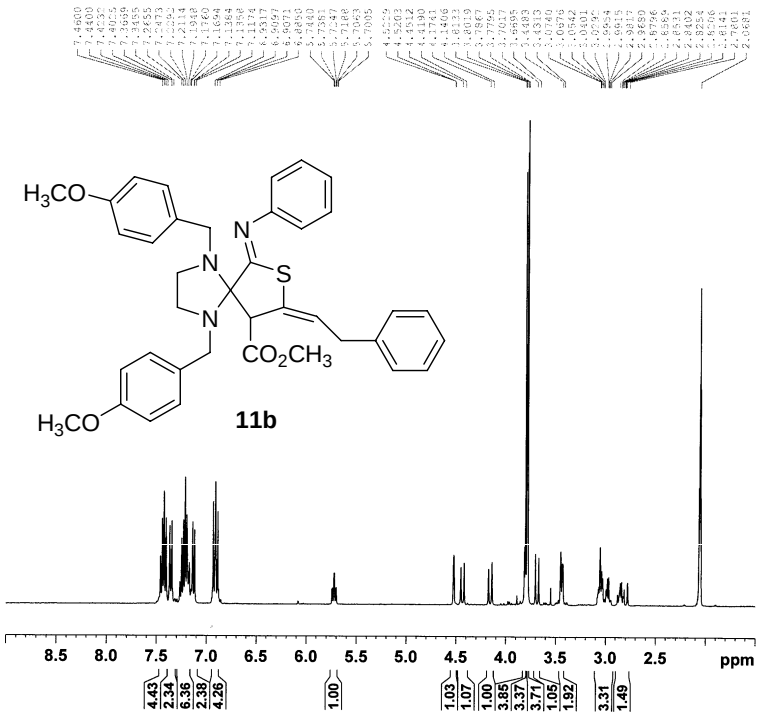

Avance 500 Bruker, A&T Center BNU
sample: WB14-28a, Solvent: CDCl3
spectrum: chengying-9 47
11a


Avance 500 Bruker, A&T Center BNU
sample: WB14-28b, Solvent: CDCL3
spectrum: chengying-9 103
12a

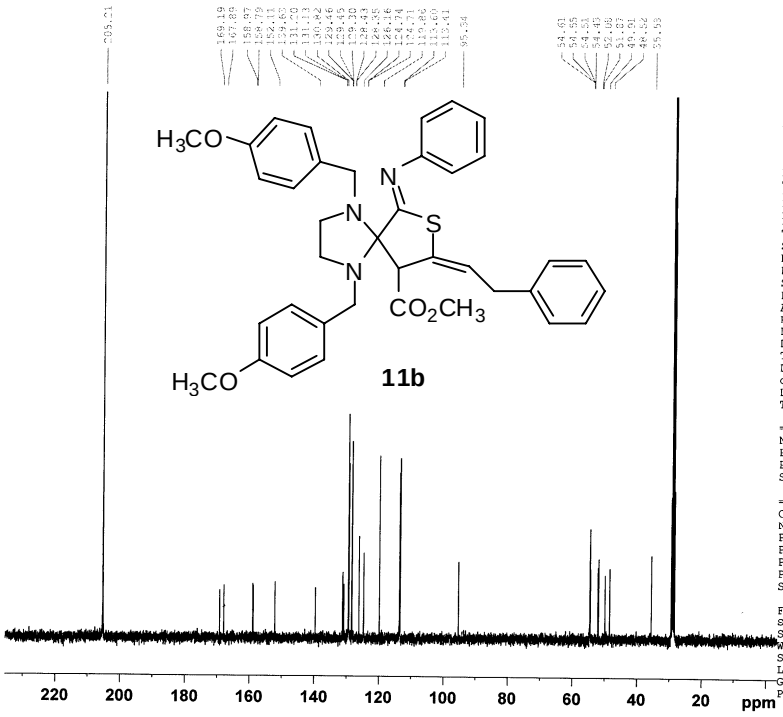

Avance 500 Bruker, A&T Center BNU
sample: WB14-28b, Solvent: CDCl3
spectrum: chengying-9 112
12a


BRUKER
Current Data Parameters
NAME wb21-30xin
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date 20080430
Time 17.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 301.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
SFO1 400.1724712 MHz
F2 - Processing parameters
SI 32768
SF 400.1700568 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
13a
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm
2.03 4.03 8.93 2.96 1.93 0.96 1.00 1.01 1.03 1.01 1.01 3.92 2.04 3.01

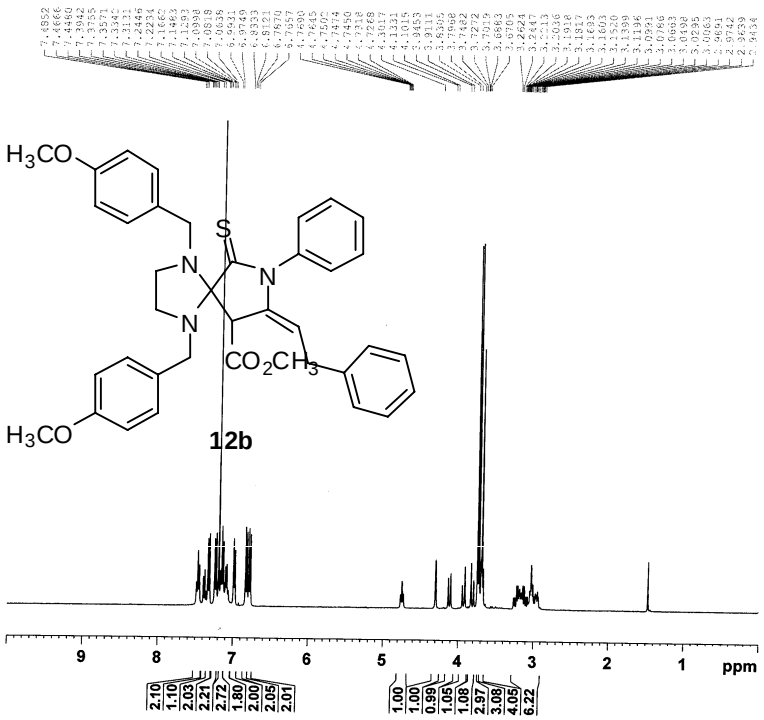

Avance DRX 500 Bruker A&T Center BNU
Sample: WB19-38b, Solvent: CDCL3
Spectrum: chengying-12 14
ppm
168.025
166.604
161.174
150.875
140.833
139.390
138.445
129.513
128.936
128.553
128.488
128.364
128.178
128.084
127.286
127.007
125.320
125.116
120.048
110.341
90.929
77.327
77.073
76.819
54.083
53.861
51.449
50.052
49.840
48.077
33.208
13a
ppm 160 140 120 100 80 60 40



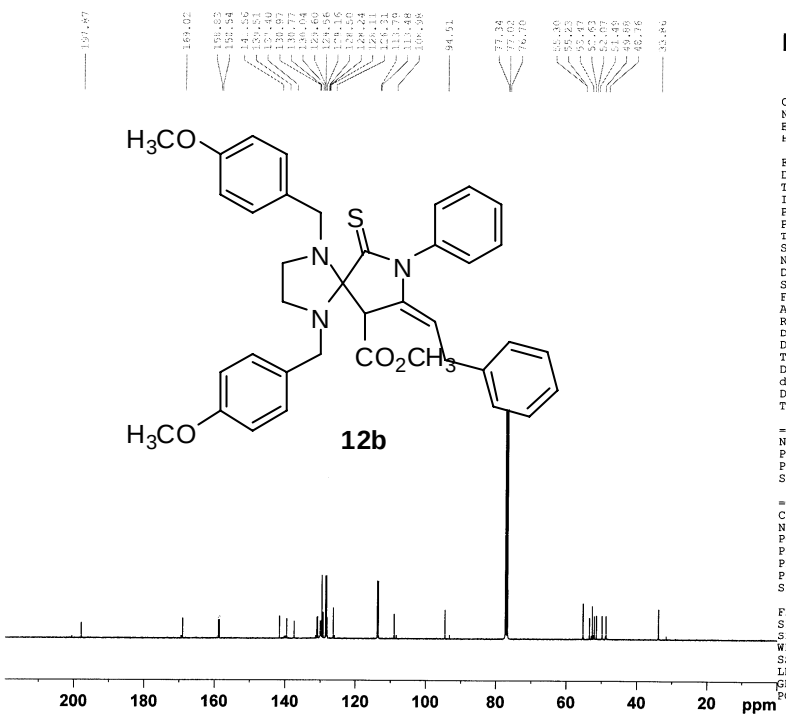

```
Current Data Parameters
NAME          WB21-18a-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080327
Time               14.40
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     0
SWH           4807.692 Hz
FIDRES        0.073360 Hz
AQ            6.8157940 sec
RG                     4
DW             104.000 usec
DE               6.50 usec
TE              297.5 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.50 usec
PL1               -1.00 dB
SFO1         400.1723210 MHz

F2 - Processing parameters
SI                 32768
SF          400.1700000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```



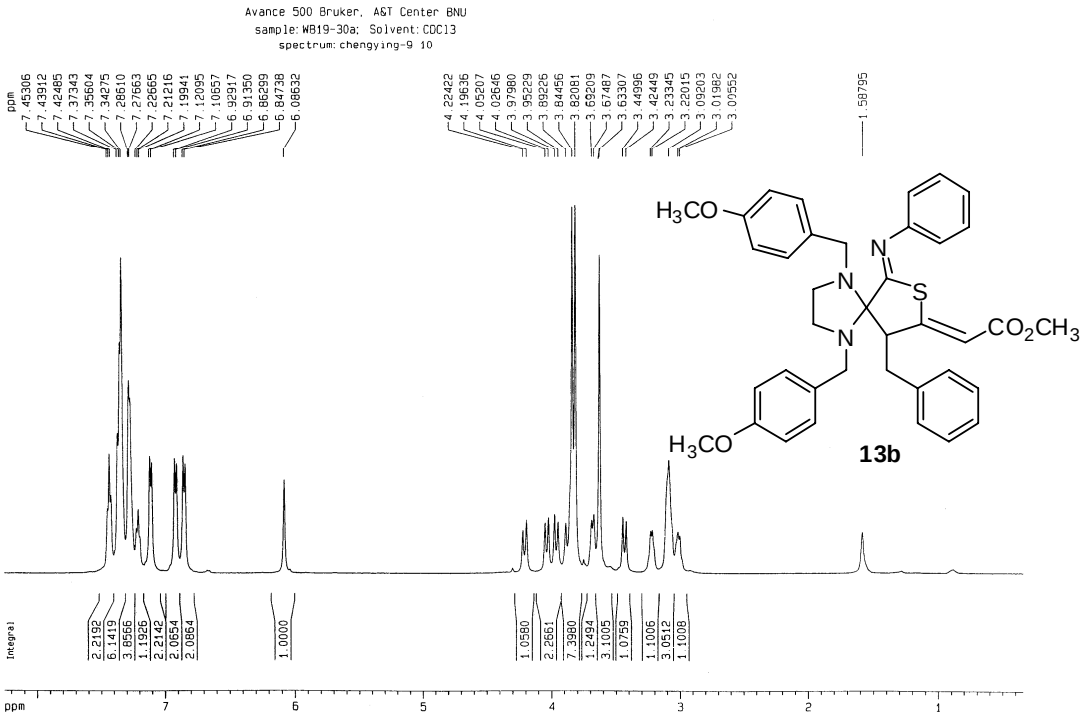

```
Current Data Parameters
NAME        WB21-18a-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080327
Time               15.39
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                    67
DS                     0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                   203
DW              20.800 usec
DE               6.50 usec
TE              298.1 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                8.40 usec
PL1              -2.00 dB
SFO1        100.6344992 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            80.00 usec
PL12             14.46 dB
PL13             14.46 dB
PL2              -1.00 dB
SFO2        400.1716007 MHz

F2 - Processing parameters
SI                 32768
SF          100.6228270 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

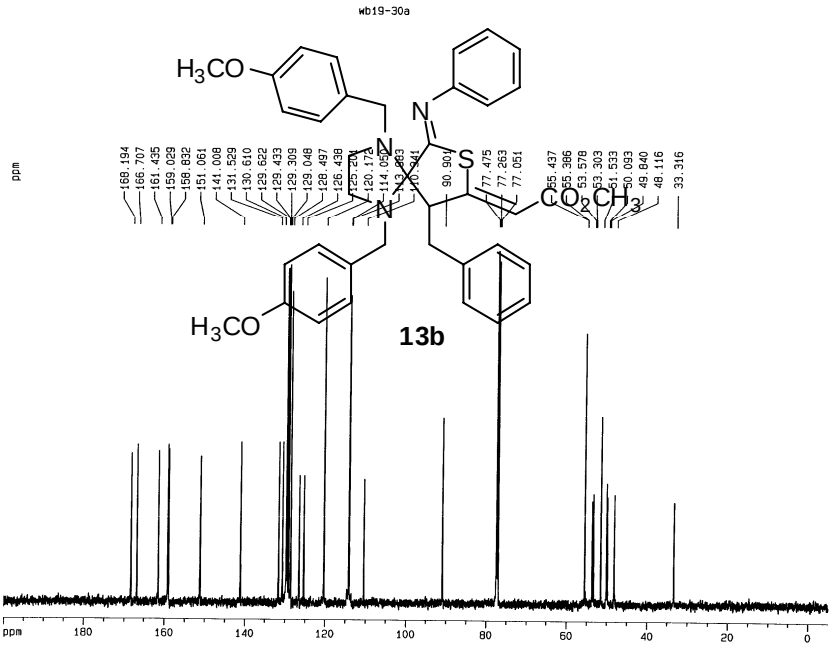



```
Current Data Parameters
NAME                  wb21-28b
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20080424
Time                      8.22
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                         203
DW                    60.800 usec
DE                     6.50 usec
TE                     296.3 K
D1                1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      13.50 usec
PL1                     -1.00 dB
SFO1             400.1724712 MHz

F2 - Processing parameters
SI                       32768
SF                400.1700311 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                        1.00
```

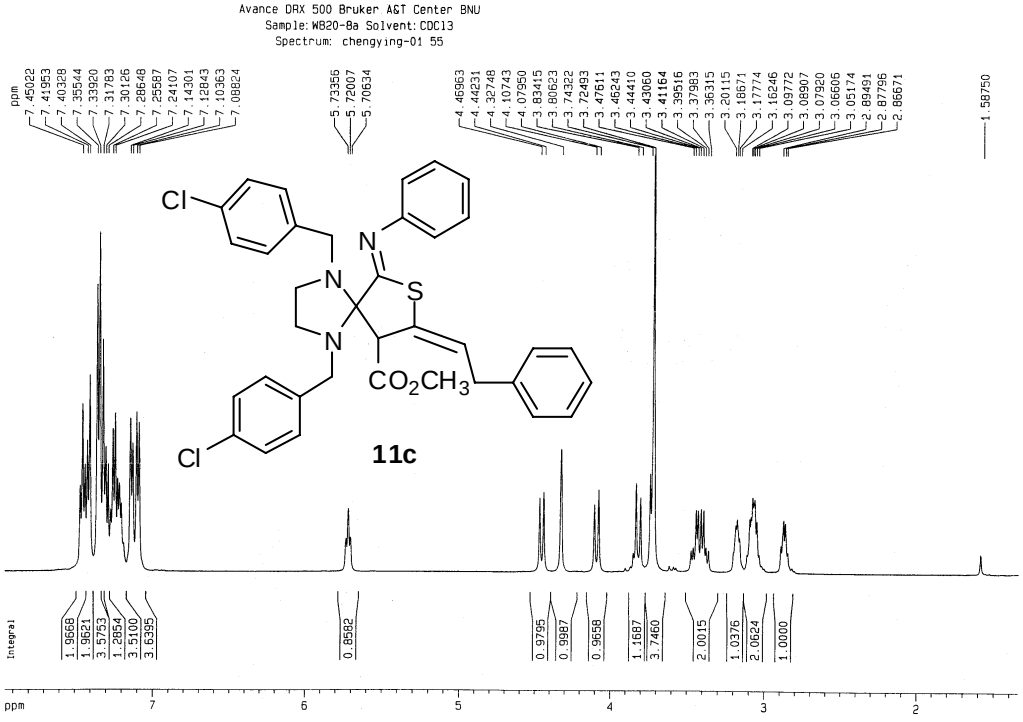


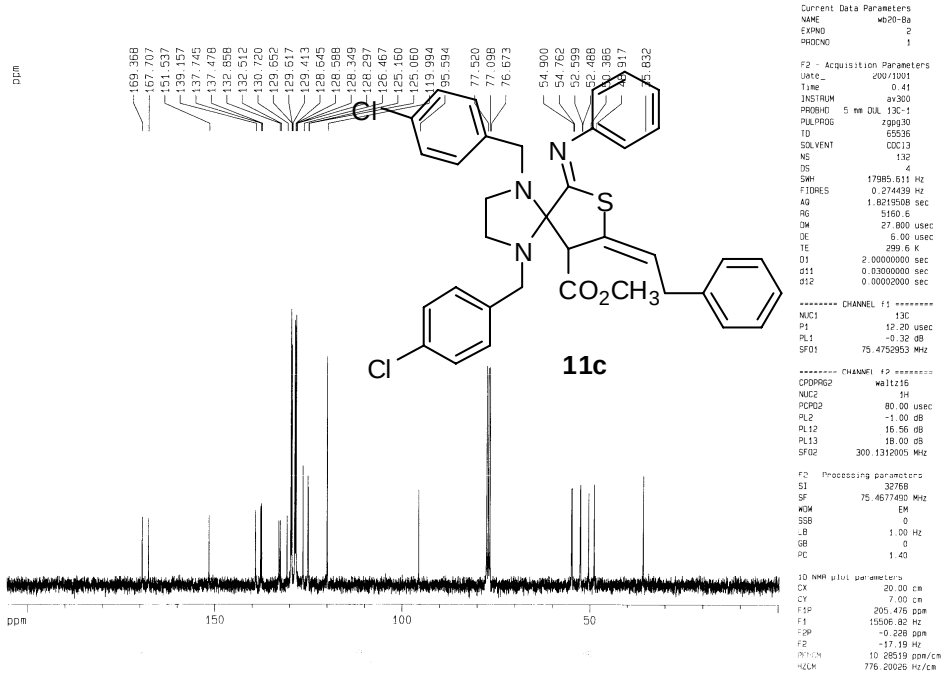

```
Current Data Parameters
NAME             WB21-28b-C13
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20080425
Time                      8.06
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        6000
DS                           4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                         203
DW                    20.800 usec
DE                     6.50 usec
TE                     297.5 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                      8.40 usec
PL1                    -2.00 dB
SFO1            100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                  80.00 usec
PL12                   14.46 dB
PL13                   14.46 dB
PL2                    -1.00 dB
SFO2            400.1716007 MHz

F2 - Processing parameters
SI                       32768
SF                100.6228270 MHz
WDW                         EM
SSB                          0
LB                      1.00 Hz
GB                           0
PC                        1.40
```

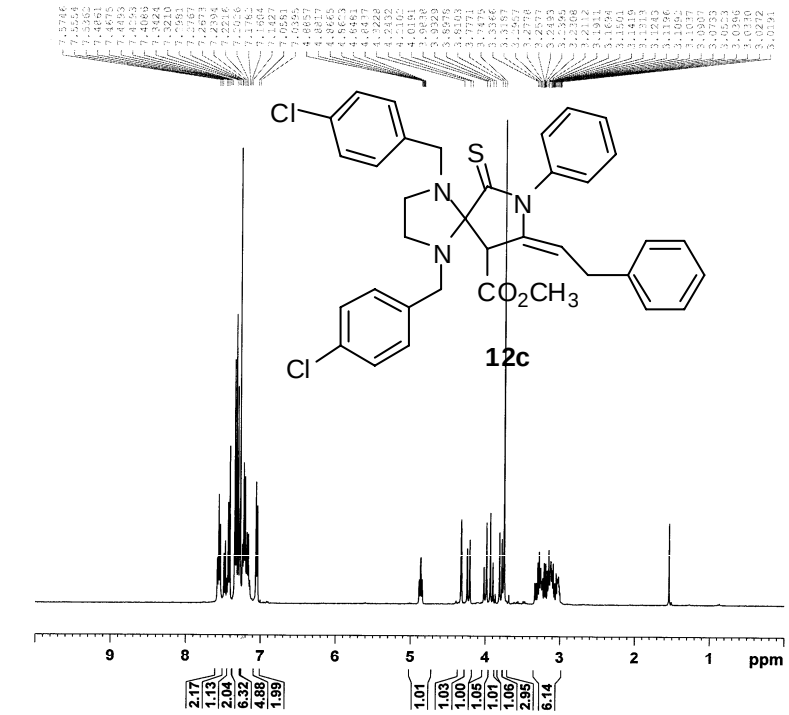





```
Current Data Parameters
NAME                  66
EXPNO                 66
PROCNO                 1

F2 - Acquisition Parameters
Date_           20070903
Time                9.32
INSTRUM           av600
PROBHD  5 mm BBI 1H-BB
PULPROG          zgig30
TD                65536
SOLVENT            DMSO
NS                   263
DS                     0
SWH           37593.984 Hz
FIDRES        0.573639 Hz
AQ            0.8716788 sec
RG                 812.7
DW                13.300 usec
DE                 6.00 usec
TE                297.7 K
D1             2.00000000 sec
D11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 14.50 usec
PL1                -2.00 dB
SFO1         150.9178993 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               19.40 dB
SF02         600.1342009 MHz

F2 - Processing parameters
SI                    32768
SF           150.9027956 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.10

1D NMR plot parameters
CX                 22.00 cm
CY                 10.00 cm
F1P              200.000 ppm
F1             30180.56 Hz
F2P               -5.000 ppm
F2              -754.51 Hz
PPMCM           9.31818 ppm/cm
HZCM         1406.13965 Hz/cm
```

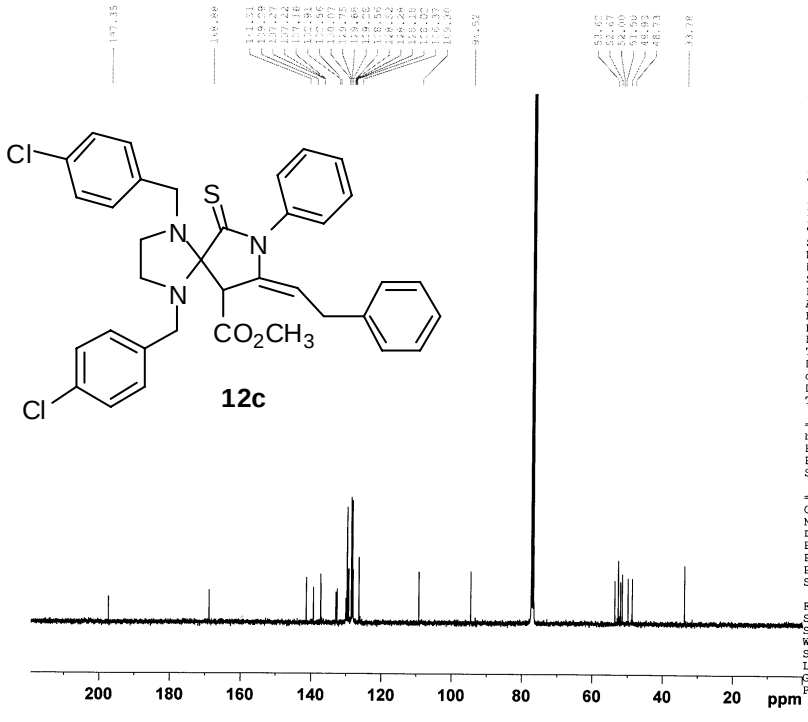

Avance DRX 500 Bruker A&T Center BNU
Sample: WB20-8a Solvent: CDCl3
Spectrum: chengying-01 55
11c


11c



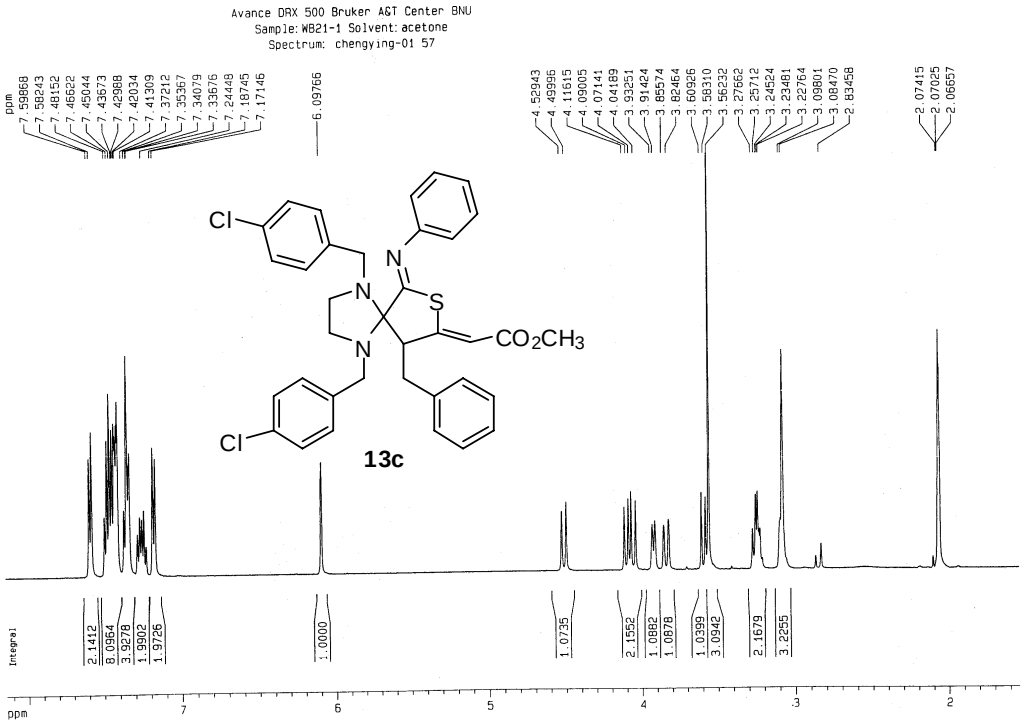
BRUKER

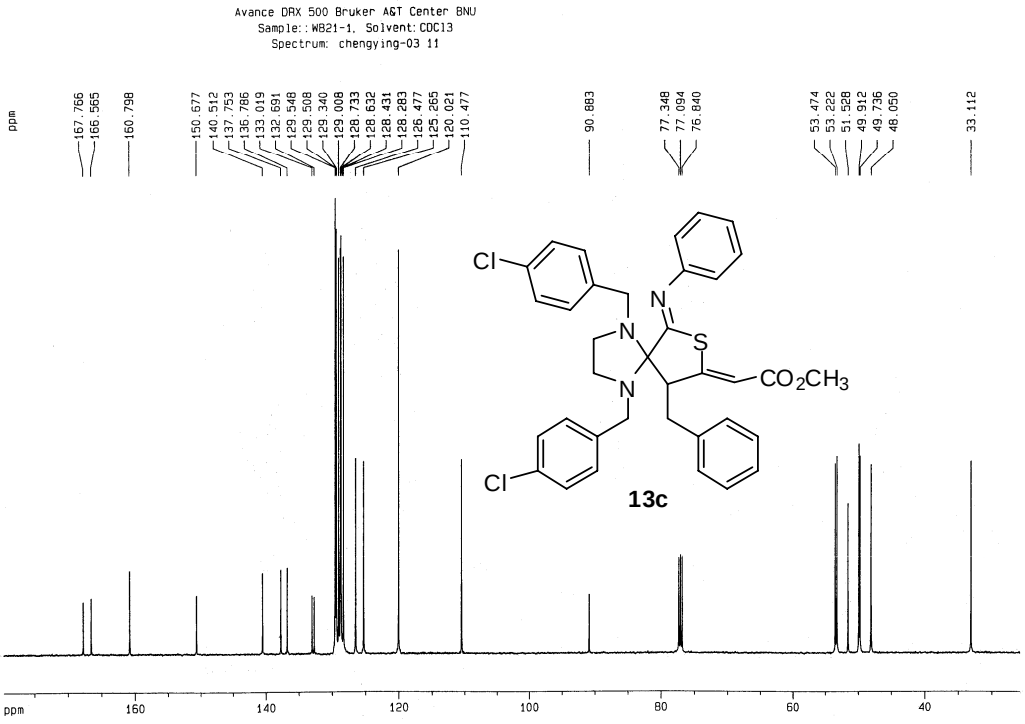
```
Current Data Parameters
NAME          WB21-24b-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080414
Time              14.58
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                  203
DW               60.800 usec
DE                6.50 usec
TE               299.3 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.50 usec
PL1               -1.00 dB
SFO1         400.1724712 MHz

F2 - Processing parameters
SI                 32768
SF          400.1700000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

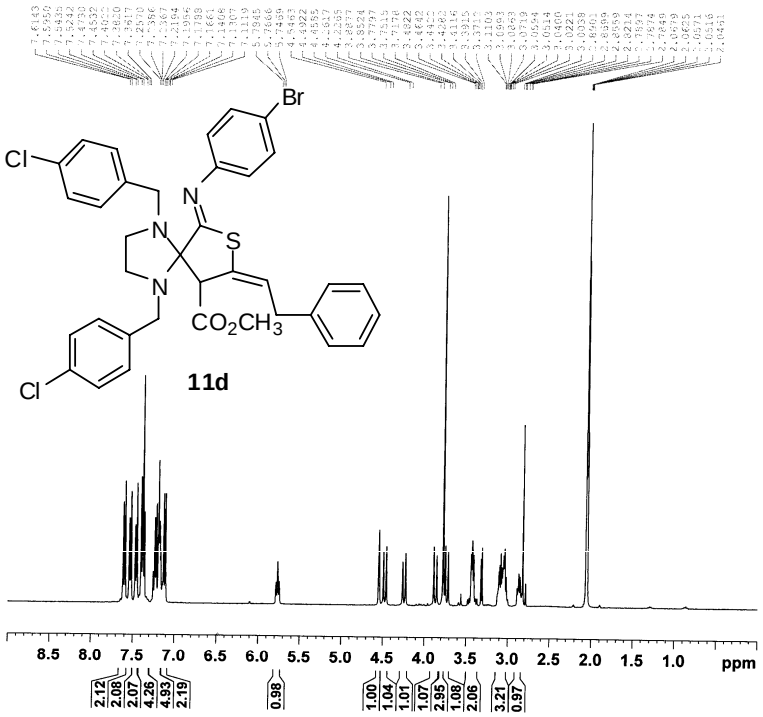


BRUKER

```
Current Data Parameters
NAME         WB21-24b-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080415
Time              23.12
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 6000
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               300.5 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                8.40 usec
PL1               -2.00 dB
SFO1         100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            80.00 usec
PL12              14.46 dB
PL13              14.46 dB
PL2               -1.00 dB
SFO2         400.1716007 MHz

F2 - Processing parameters
SI                 32768
SF          100.6228270 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

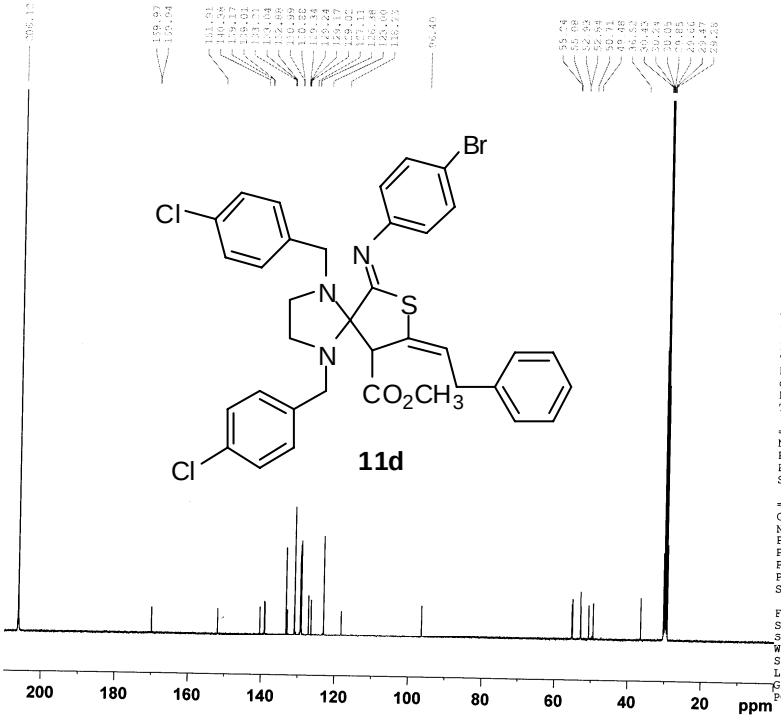

Avance DRX 500 Bruker A&T Center BNU
Sample: WB21-1 Solvent: acetone
Spectrum: chengying-01 57
13c


Avance DRX 500 Bruker A&T Center BNU
Sample: : WB21-1, Solvent: CDCl3
Spectrum: chengying-03 11
13c



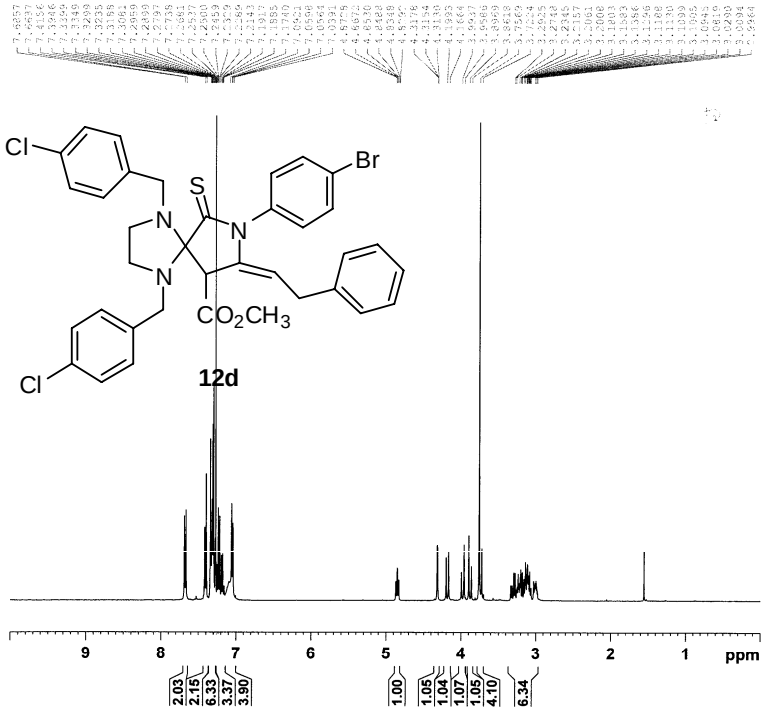
BRUKER

```
Current Data Parameters
NAME                  wb21-10ax
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20080410
Time                  10.47
INSTRUM               spect
PROBHD     5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT            Acetone
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      203
DW                 60.800 usec
DE                  6.50 usec
TE                  296.3 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                 13.50 usec
PL1                -1.00 dB
SFO1          400.1724712 MHz

F2 - Processing parameters
SI                    32768
SF              400.1700000 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00
```

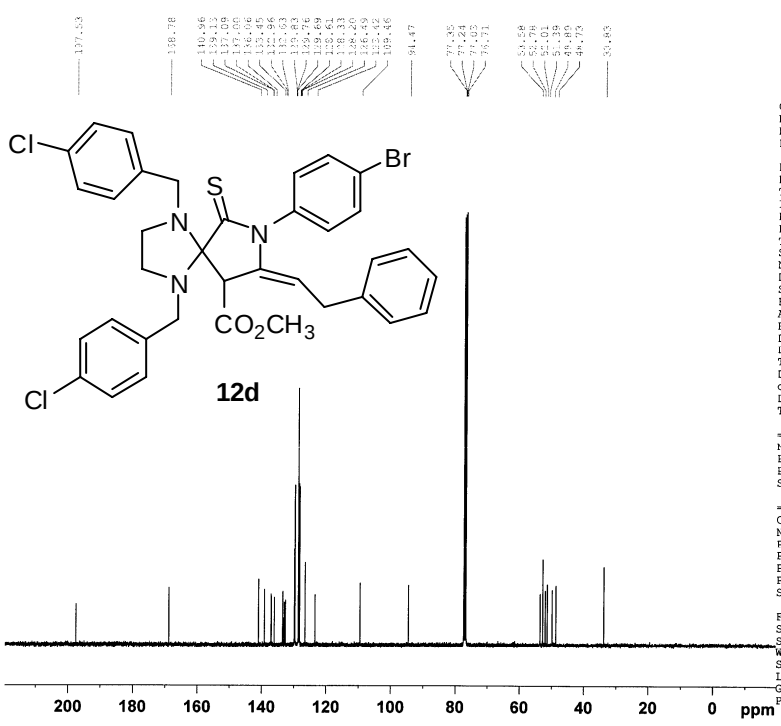


BRUKER

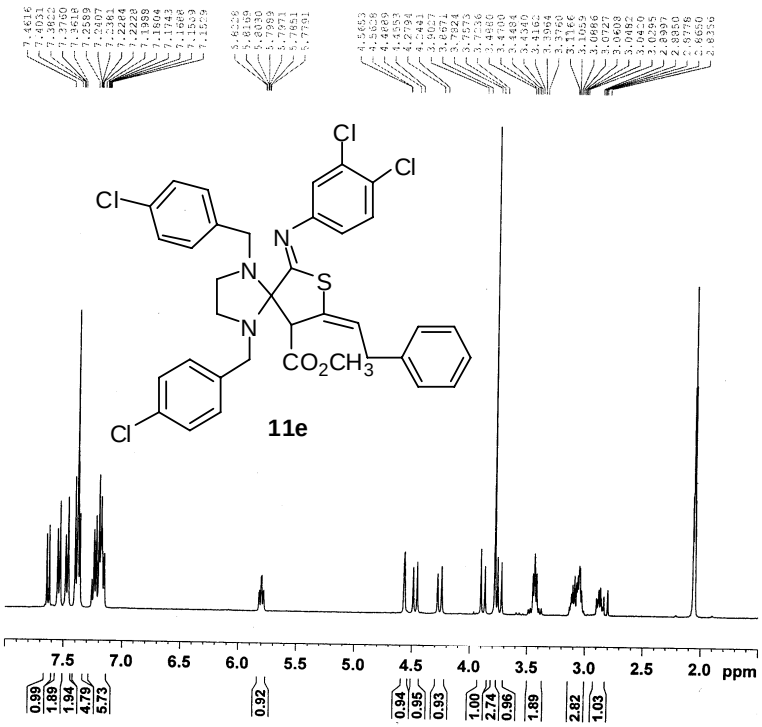
```
Current Data Parameters
NAME              WB21-10ax-C13
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20080410
Time                  11.24
INSTRUM               spect
PROBHD     5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    1200
DS                       4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      203
DW                 20.800 usec
DE                  6.50 usec
TE                  296.8 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                  8.40 usec
PL1                -2.00 dB
SFO1          100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2              80.00 usec
PL12               14.46 dB
PL13               14.46 dB
PL2                -1.00 dB
SFO2          400.1716007 MHz

F2 - Processing parameters
SI                    32768
SF              100.6227364 MHz
WDW                      EM
SSB                       0
LB                 1.00 Hz
GB                        0
PC                     1.40
```




```
Current Data Parameters
NAME          WB21-10b-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080402
Time               9.34
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT           CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                294.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.50 usec
PL1                -1.00 dB
SFO1         400.1724712 MHz

F2 - Processing parameters
SI                 32768
SF          400.1700000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

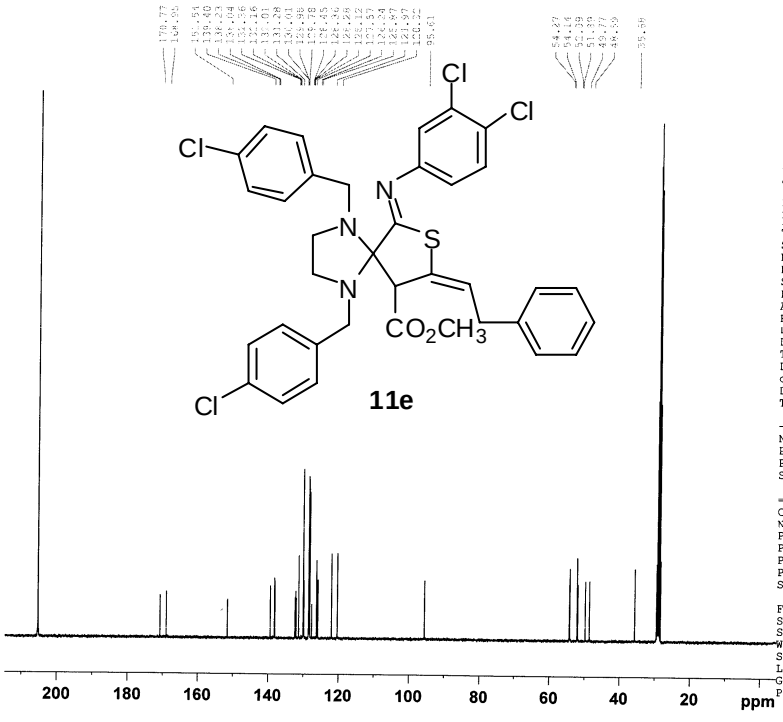



```
Current Data Parameters
NAME         WB21-10b-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080402
Time              15.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT           CDCl3
NS                   763
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                296.6 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.40 usec
PL1               -2.00 dB
SFO1         100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL12               14.46 dB
PL13               14.46 dB
PL2                -1.00 dB
SFO2         400.1716007 MHz

F2 - Processing parameters
SI                 32768
SF          100.6228270 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



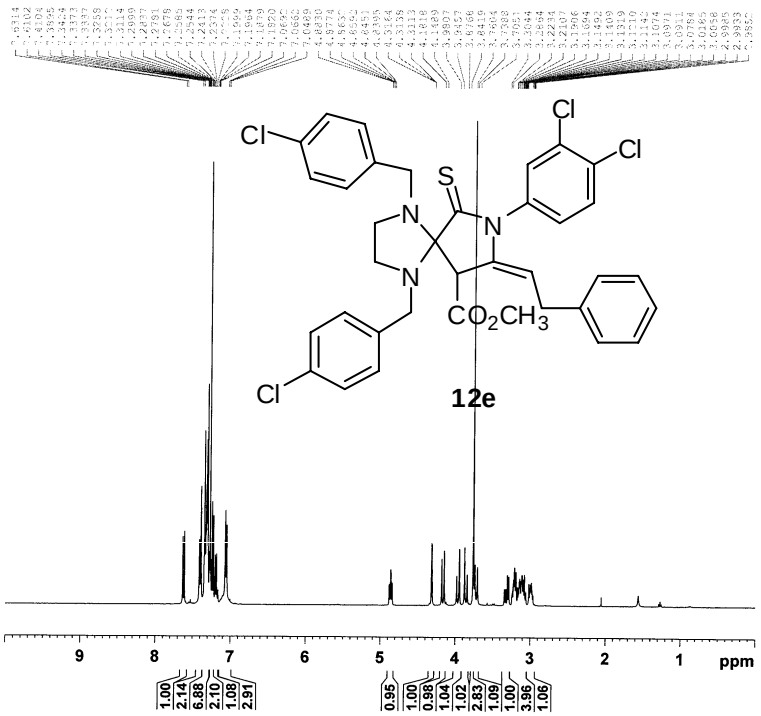
BRUKER

```
Current Data Parameters
NAME          WB-21-16a-H
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20080319
Time                  10.20
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT            Acetone
NS                        16
DS                         0
SWH                4401.409 Hz
FIDRES             0.067160 Hz
AQ                 7.4449396 sec
RG                         4
DW                   113.600 usec
DE                     6.50 usec
TE                    294.7 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.50 usec
PL1                    -1.00 dB
SFO1           400.1720009 MHz

F2 - Processing parameters
SI                        32768
SF                 400.1700000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



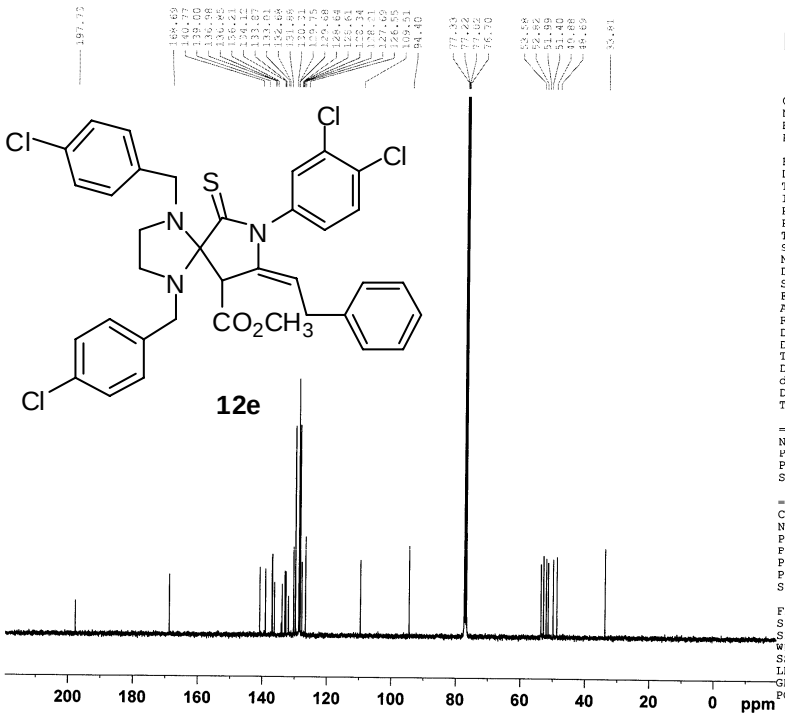
BRUKER

```
Current Data Parameters
NAME         WB-21-16a-C13
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20080319
Time                  11.07
INSTRUM               spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       331
DS                         0
SWH               22058.824 Hz
FIDRES             0.336591 Hz
AQ                 1.4855326 sec
RG                       203
DW                   22.667 usec
DE                     6.50 usec
TE                    295.4 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      8.40 usec
PL1                    -2.00 dB
SFO1           100.6333924 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL12                   14.46 dB
PL13                   17.46 dB
PL2                    -1.00 dB
SFO2           400.1716007 MHz

F2 - Processing parameters
SI                        32768
SF                 100.6228270 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```



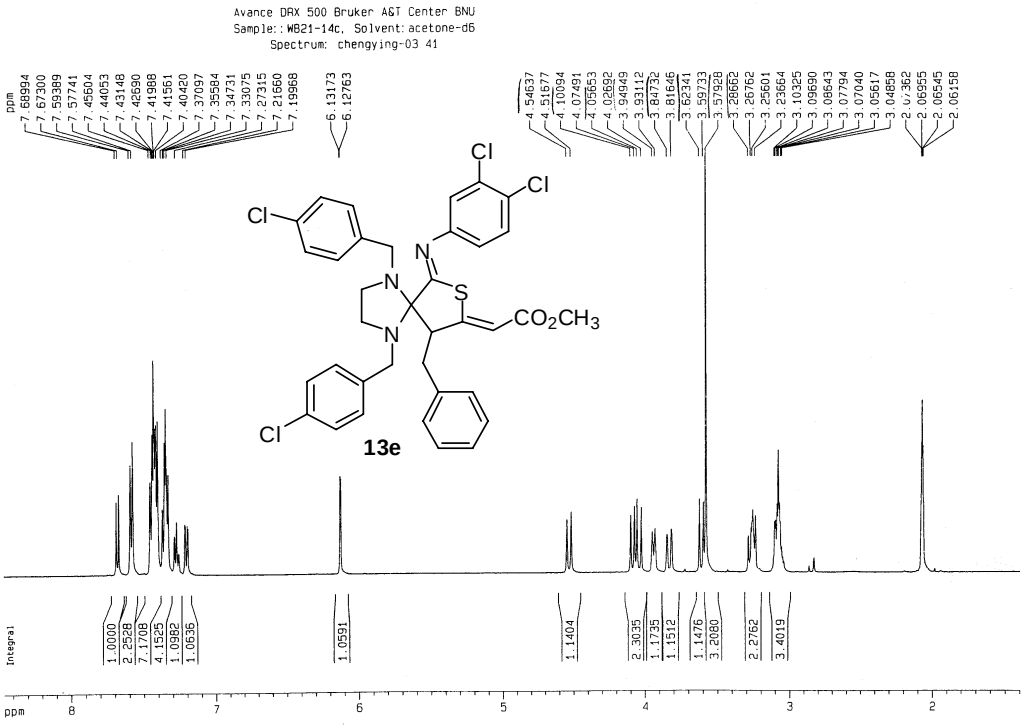
BRUKER

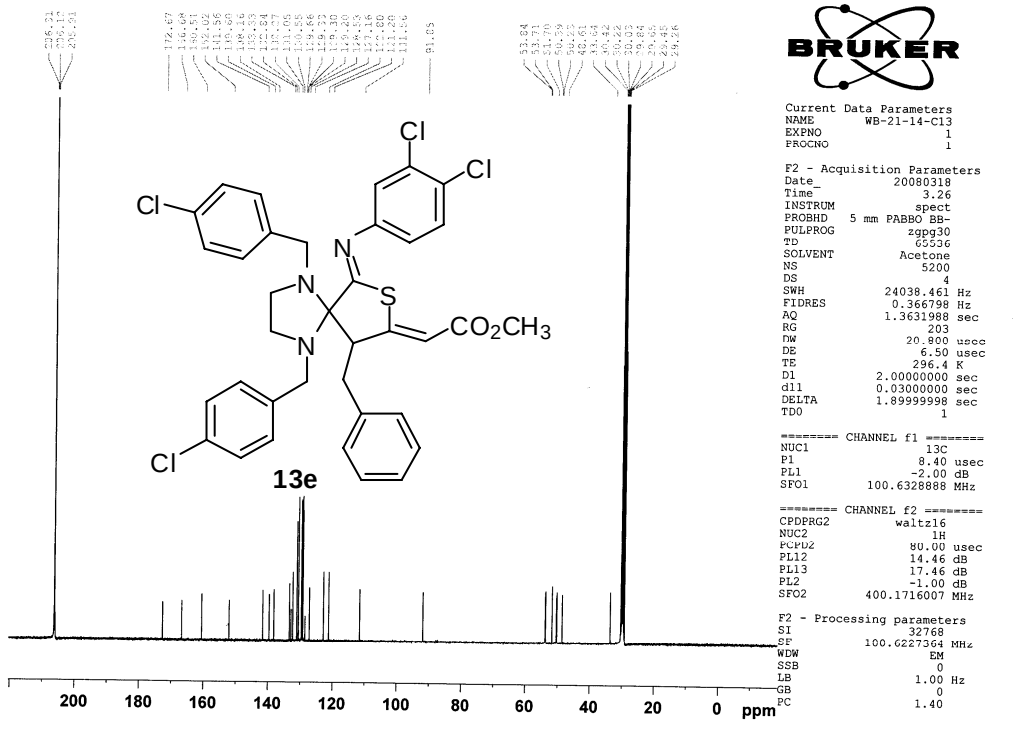
```
Current Data Parameters
NAME              WB21-15b
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20080403
Time                  9.55
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    203
DW                 60.800 usec
DE                  6.50 usec
TE                 293.8 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.50 usec
PL1                -1.00 dB
SFO1          400.1724712 MHz

F2 - Processing parameters
SI                  32768
SF            400.1700000 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

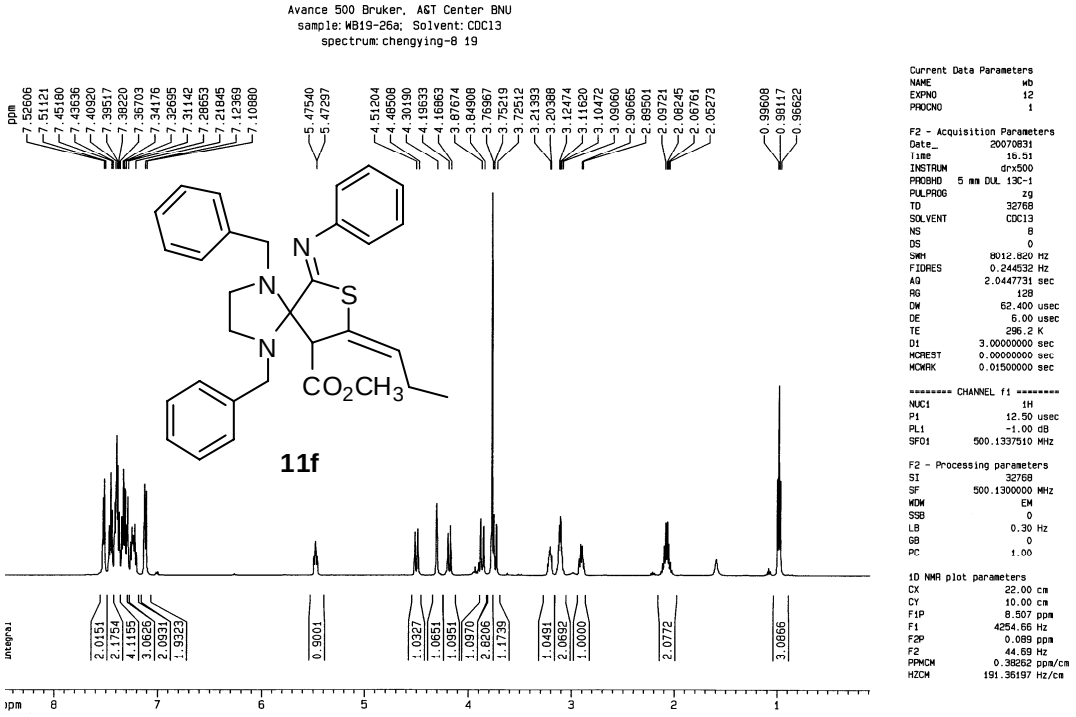


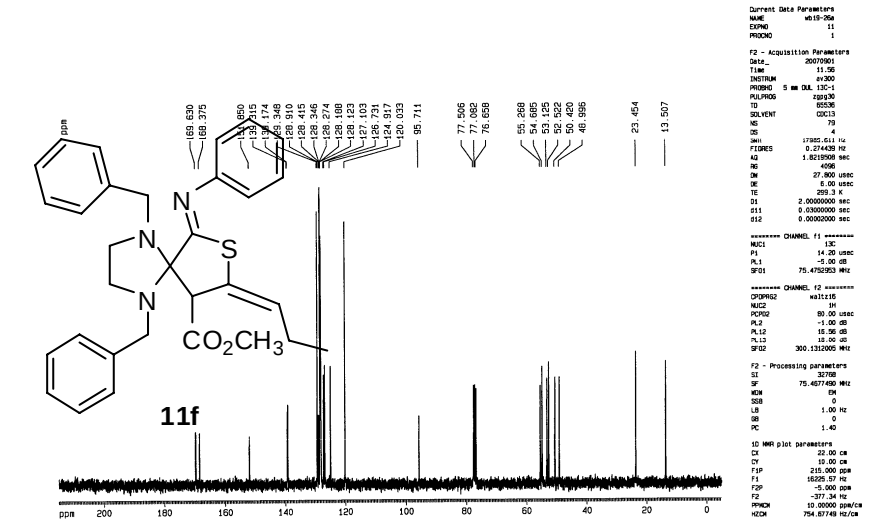
BRUKER

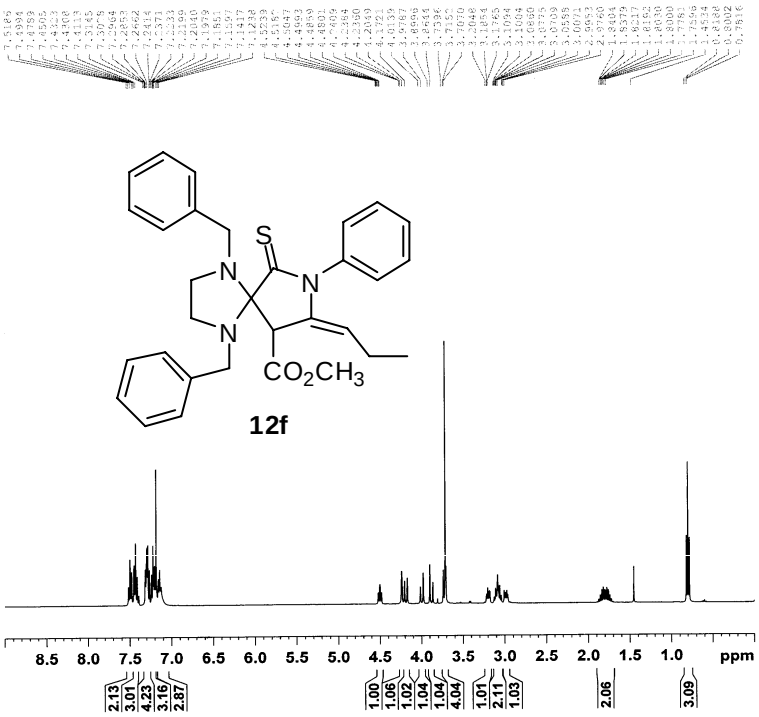
```
Current Data Parameters
NAME          WB21-15b-C13
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20080403
Time                 10.32
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   3690
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    203
DW                 20.800 usec
DE                  6.50 usec
TE                 295.3 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.40 usec
PL1                -2.00 dB
SFO1          100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL12               14.46 dB
PL13               14.46 dB
PL2                -1.00 dB
SFO2          400.1716007 MHz

F2 - Processing parameters
SI                  32768
SF            100.6228270 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```


Avance DRX 500 Bruker A&T Center BNU
Sample: : WB21-14c, Solvent: acetone-d6
Spectrum: chengying-03 41
13e


13e
Current Data Parameters
NAME WB-21-14-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080318
Time 3.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 5200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.40 usec
PL1 -2.00 dB
SFO1 100.6328888 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.46 dB
PL13 17.46 dB
PL2 -1.00 dB
SFO2 400.1716007 MHz
F2 - Processing parameters
SI 32768
SF 100.6227364 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


Avance 500 Bruker, A&T Center BNU
sample: WB19-26a; Solvent: CDCl3
spectrum: chengying-8 19
11f
Current Data Parameters
NAME wb
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070831
Time 16.51
INSTRUM drx500
PROBHD 5 mm DUL 13C-1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447731 sec
RG 128
DW 62.400 usec
DE 6.00 usec
TE 296.2 K
D1 3.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.50 usec
PL1 -1.00 dB
SFO1 500.1337510 MHz
F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 10.00 cm
F1P 8.507 ppm
F1 4254.66 Hz
F2P 0.089 ppm
F2 44.69 Hz
PPMCM 0.38262 ppm/cm
HZCM 191.36197 Hz/cm


11f
Current Data Parameters
NAME wb19-26a
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070901
Time 11.56
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 79
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 6.00 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 14.20 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.56 dB
PL13 16.56 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
CY 10.00 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.00000 ppm/cm
HZCM 754.67749 Hz/cm

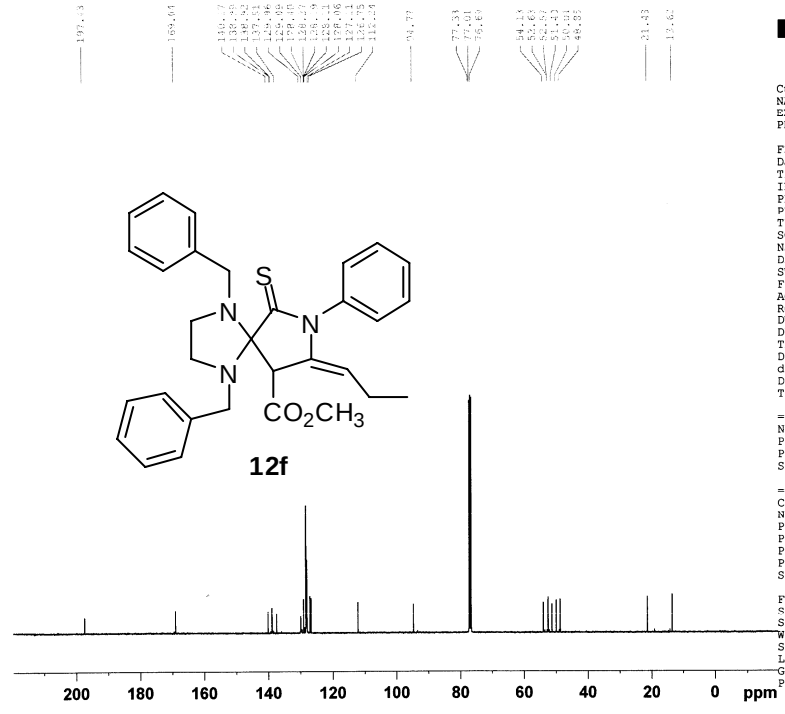


Current Data Parameters
NAME WB21-29b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080428
Time 17.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 301.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 13.50 usec
PL1 -1.00 dB
SFO1 400.1724712 MHz

F2 - Processing parameters
SI 32768
SF 400.1700329 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



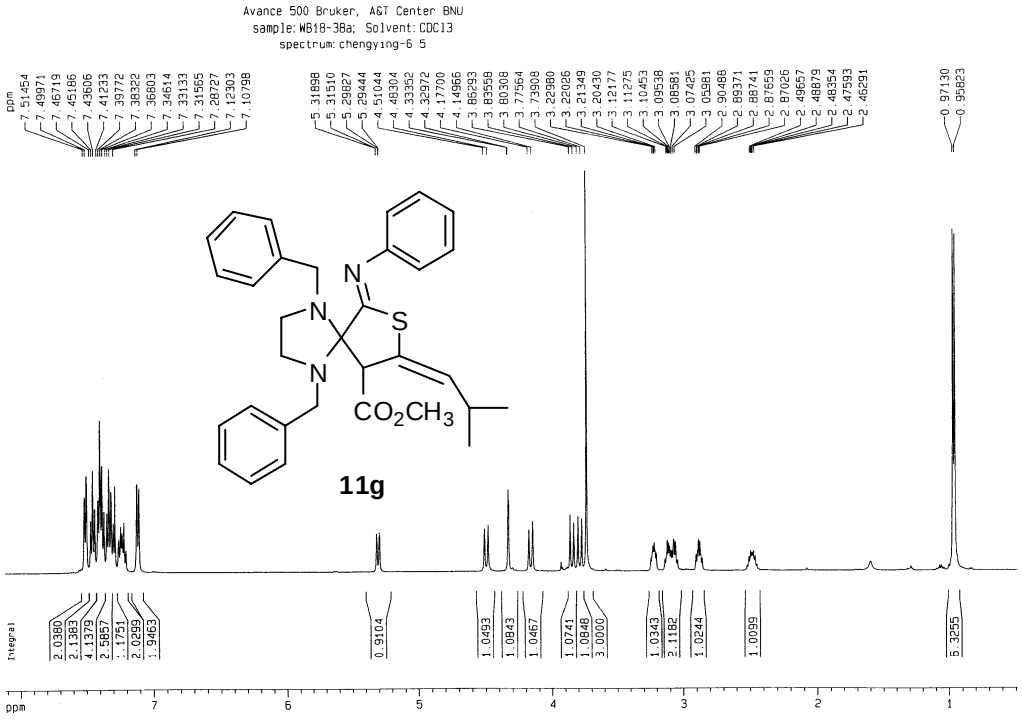
Current Data Parameters
NAME WB21-29b
EXPNO 1
PROCNO 1

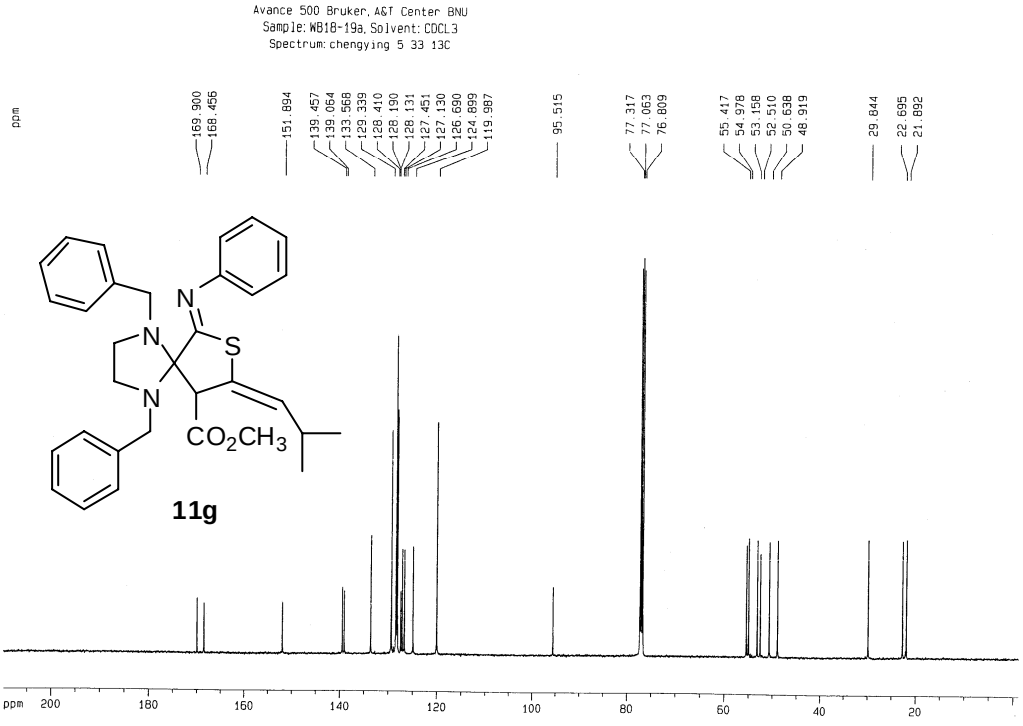
F2 - Acquisition Parameters
Date_ 20080429
Time 13.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2733
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

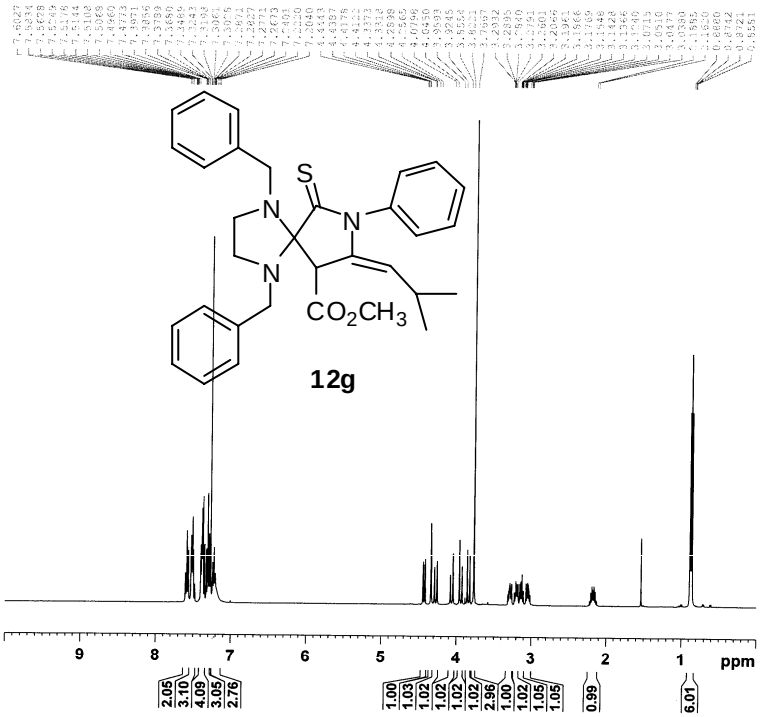
======== CHANNEL f1 ========
NUC1 13C
P1 8.40 usec
PL1 -2.00 dB
SFO1 100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.46 dB
PL13 14.46 dB
PL2 -1.00 dB
SFO2 400.1716007 MHz

F2 - Processing parameters
SI 32768
SF 100.6228270 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

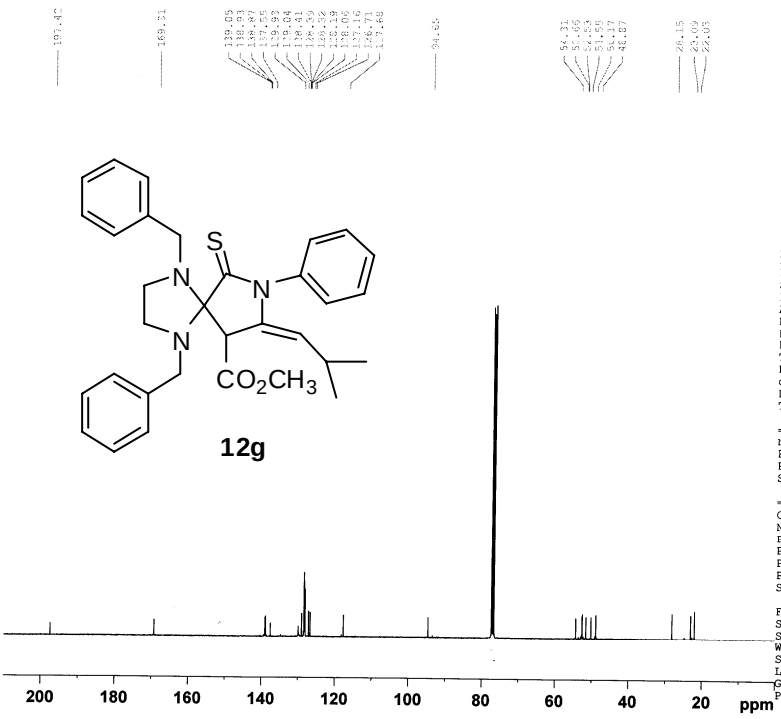

Avance 500 Bruker, A&T Center BNU
sample: WB18-38a; Solvent: CDCl3
spectrum: chengying-6 5
11g


Avance 500 Bruker, A&T Center BNU
Sample: WB18-19a, Solvent: CDCL3
Spectrum: chengying 5 33 13C
11g



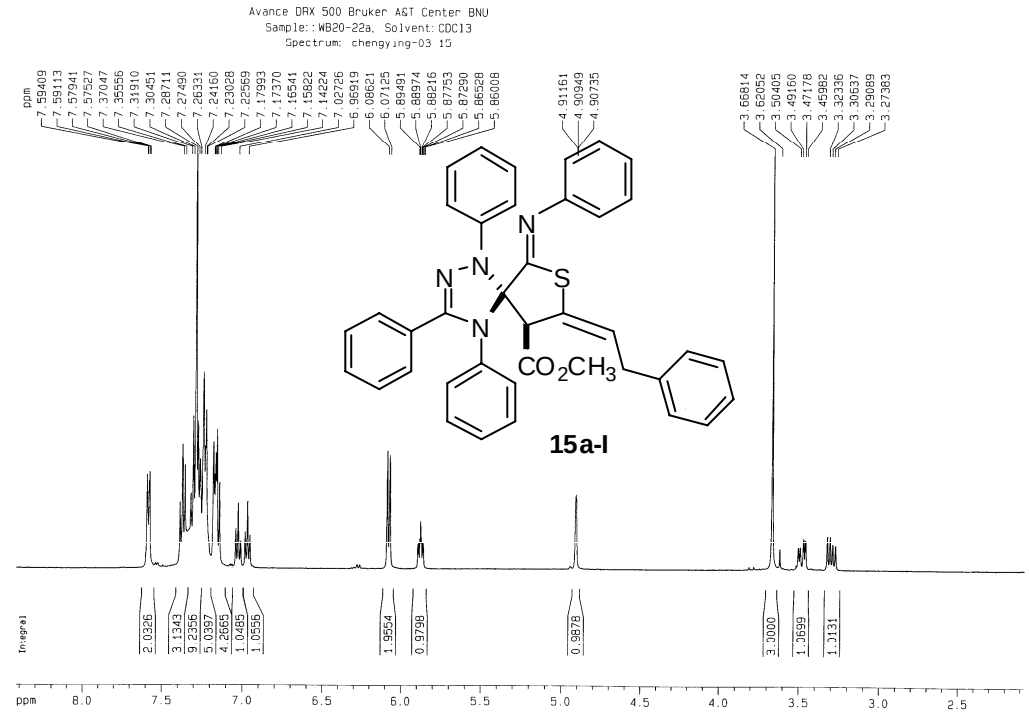
BRUKER

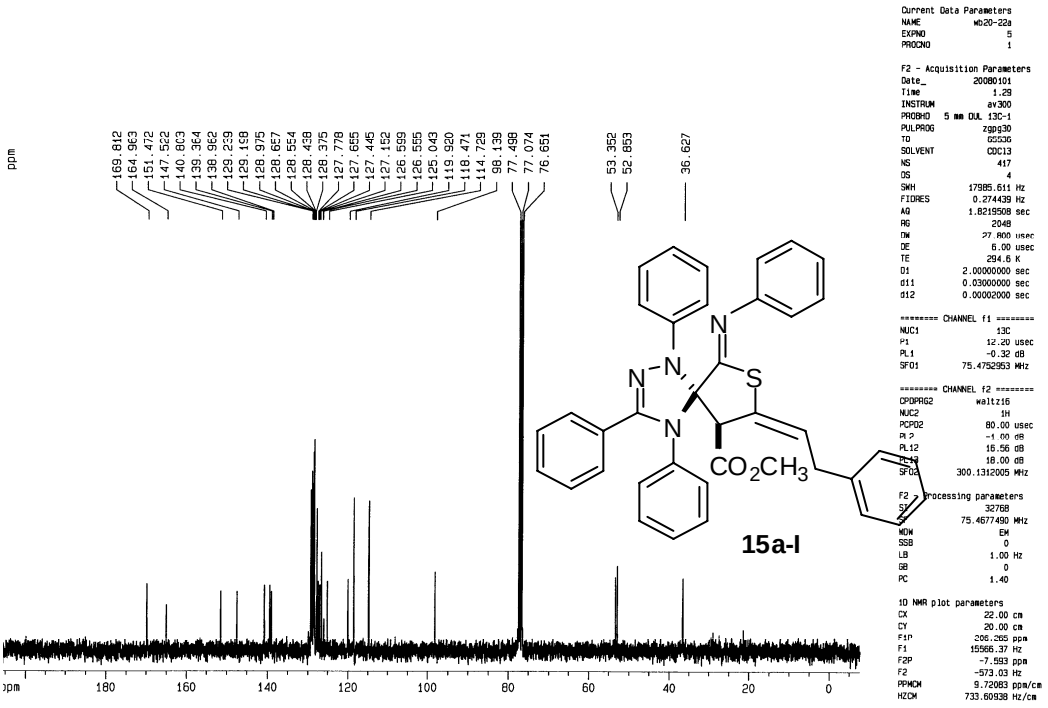
```
Current Data Parameters
NAME                  WB20-47b
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20080416
Time                     16.41
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                         203
DW                    60.800 usec
DE                     6.50 usec
TE                     300.8 K
D1                   1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       13.50 usec
PL1                      -1.00 dB
SFO1                400.1724712 MHz

F2 - Processing parameters
SI                       32768
SF                  400.1700000 MHz
WDW                         EM
SSB                          0
LB                        0.30 Hz
GB                           0
PC                        1.00
```

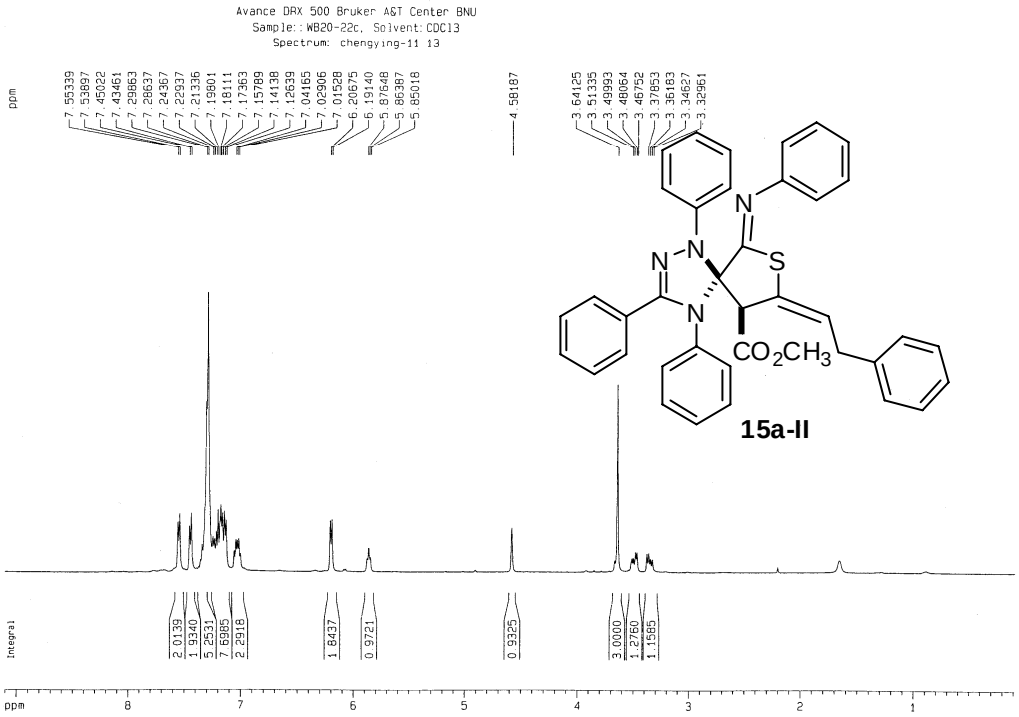


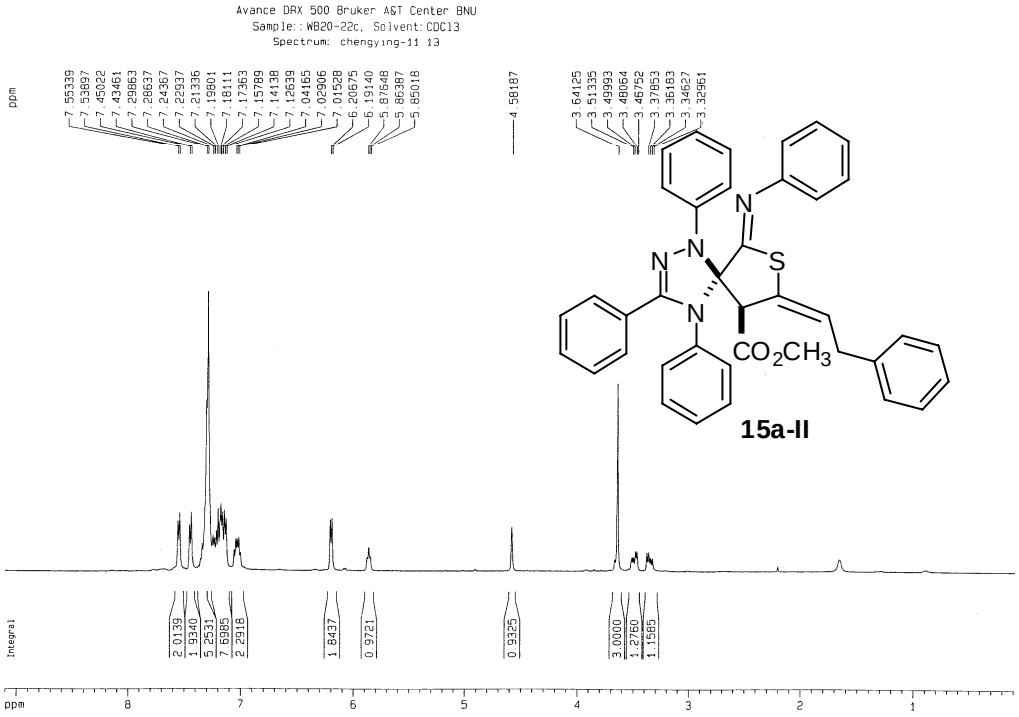
BRUKER

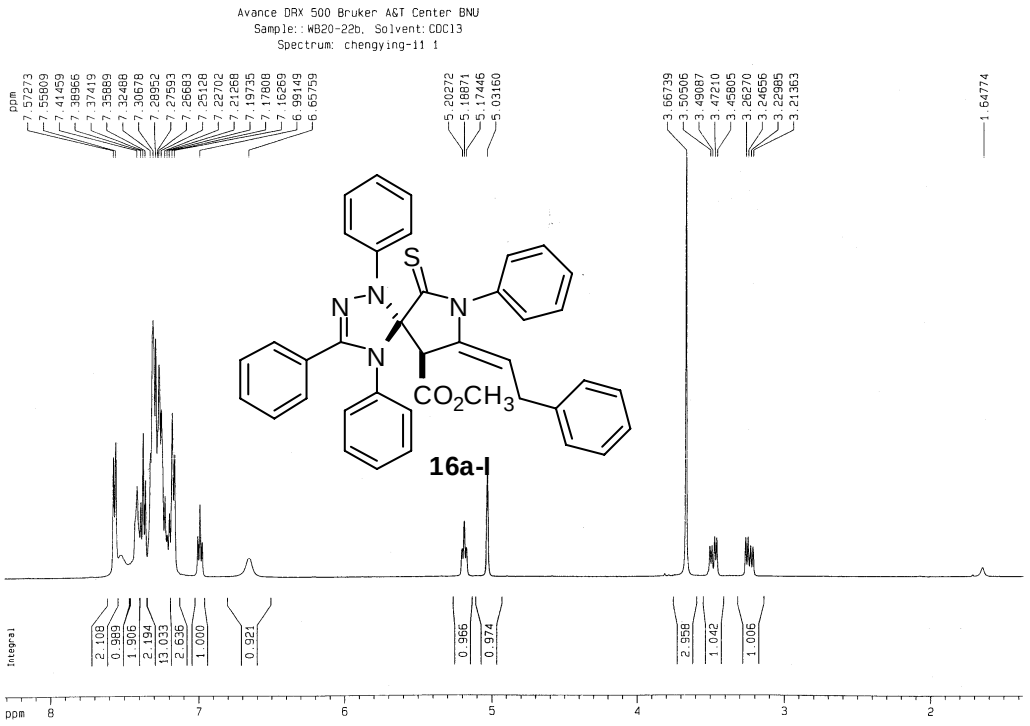
```
Current Data Parameters
NAME                  WB20-47b
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20080418
Time                     23.15
INSTRUM                  spect
PROBHD    5 mm PABBO BB-
PULPROG                 zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        6000
DS                           4
SWH                 24038.461 Hz
FIDRES               0.366798 Hz
AQ                   1.3631988 sec
RG                         203
DW                    20.800 usec
DE                     6.50 usec
TE                     301.4 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        13C
P1                        8.40 usec
PL1                      -2.00 dB
SFO1                100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                    80.00 usec
PL12                     14.46 dB
PL13                     14.46 dB
PL2                      -1.00 dB
SFO2                400.1716007 MHz

F2 - Processing parameters
SI                       32768
SF                  100.6228270 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

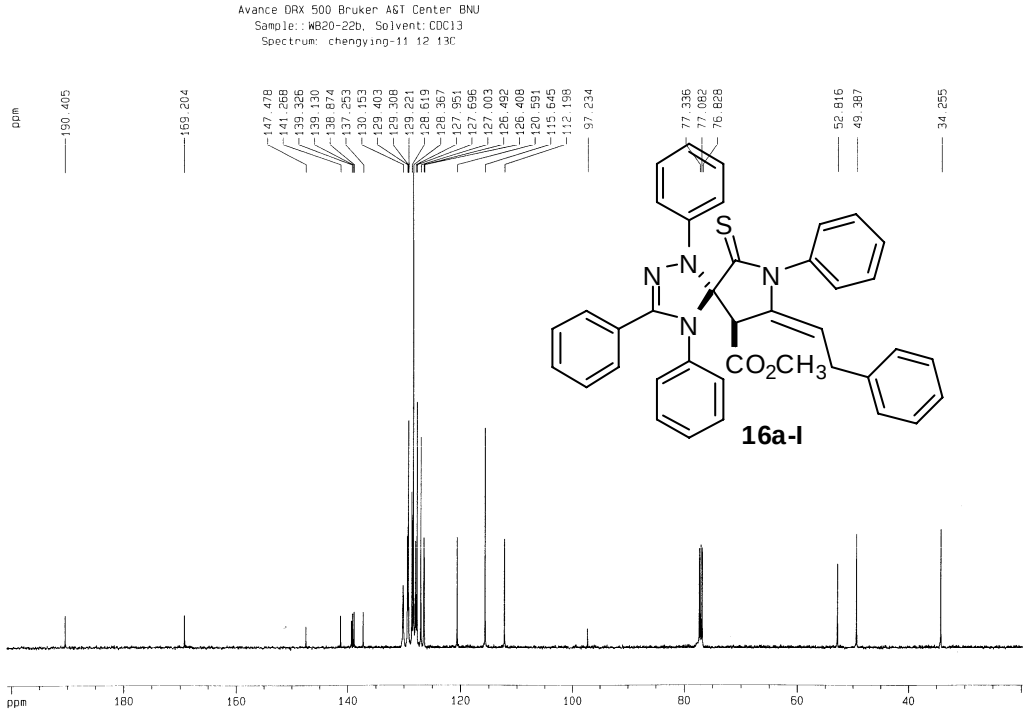

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-22a, Solvent: CDCl3
Spectrum: chengying-03 15
15a-l

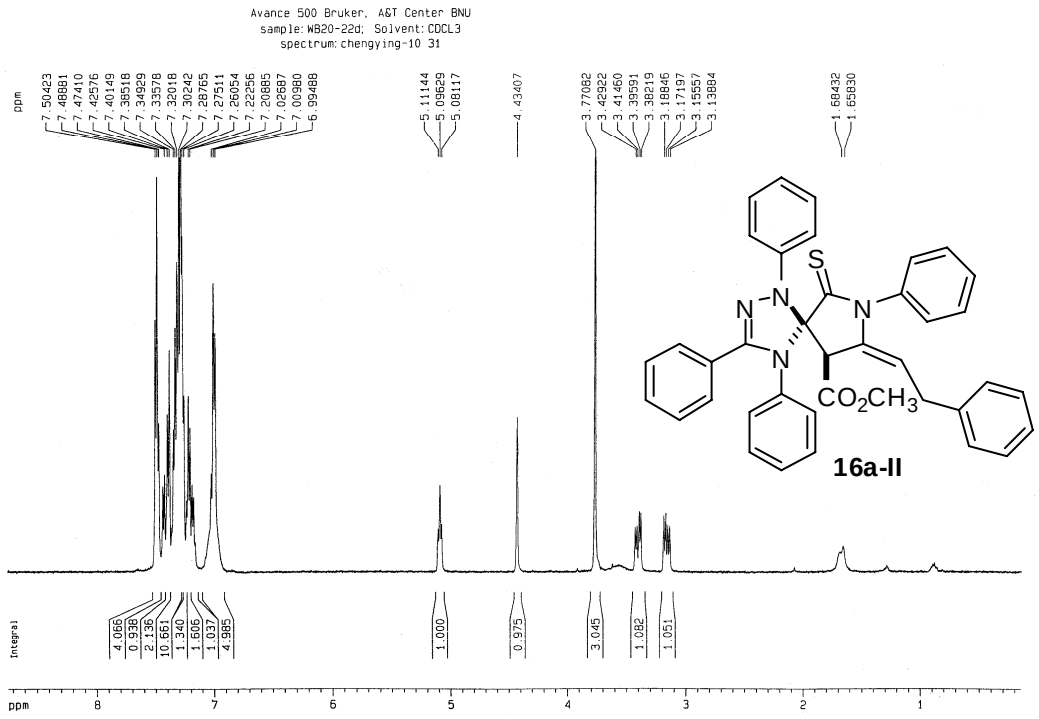

15a-l
Current Data Parameters
NAME wb20-22a
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20080101
Time 1.29
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 417
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 294.6 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 12.20 usec
PL1 -0.32 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.56 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 22.00 cm
CY 20.00 cm
F1P 206.265 ppm
F1 15566.37 Hz
F2P -7.593 ppm
F2 -573.03 Hz
PPMCM 9.72083 ppm/cm
HZCM 733.60938 Hz/cm

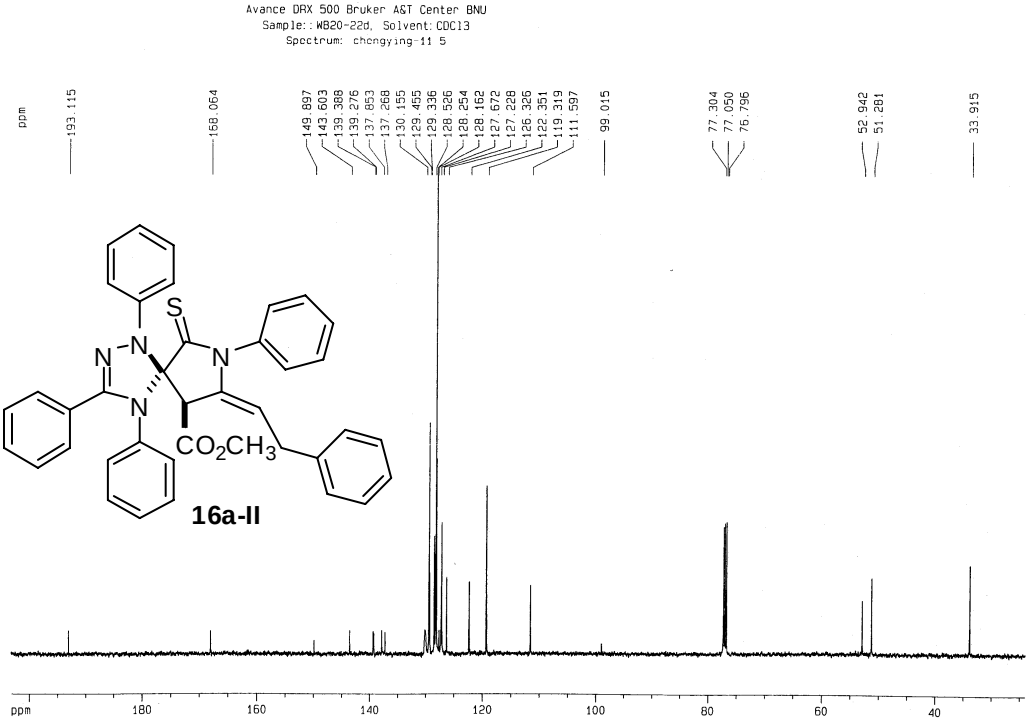

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-22c, Solvent: CDCl3
Spectrum: chengying-11 13
ppm
7.55339
7.53897
7.45022
7.43461
7.29863
7.28637
7.24367
7.22937
7.21336
7.19801
7.18111
7.17363
7.15789
7.14138
7.12639
7.04165
7.02906
7.01528
6.20675
6.19140
5.87648
5.86387
5.85018
4.58187
3.64125
3.51335
3.49993
3.49064
3.46752
3.37853
3.36183
3.34627
3.32961
Integral
2.0139
1.9340
5.2531
7.6985
2.2918
1.8437
0.9721
0.9325
3.0000
1.2760
1.1565
ppm
8
7
6
5
4
3
2
1
N
N
N
S
N
CO2CH3
15a-II

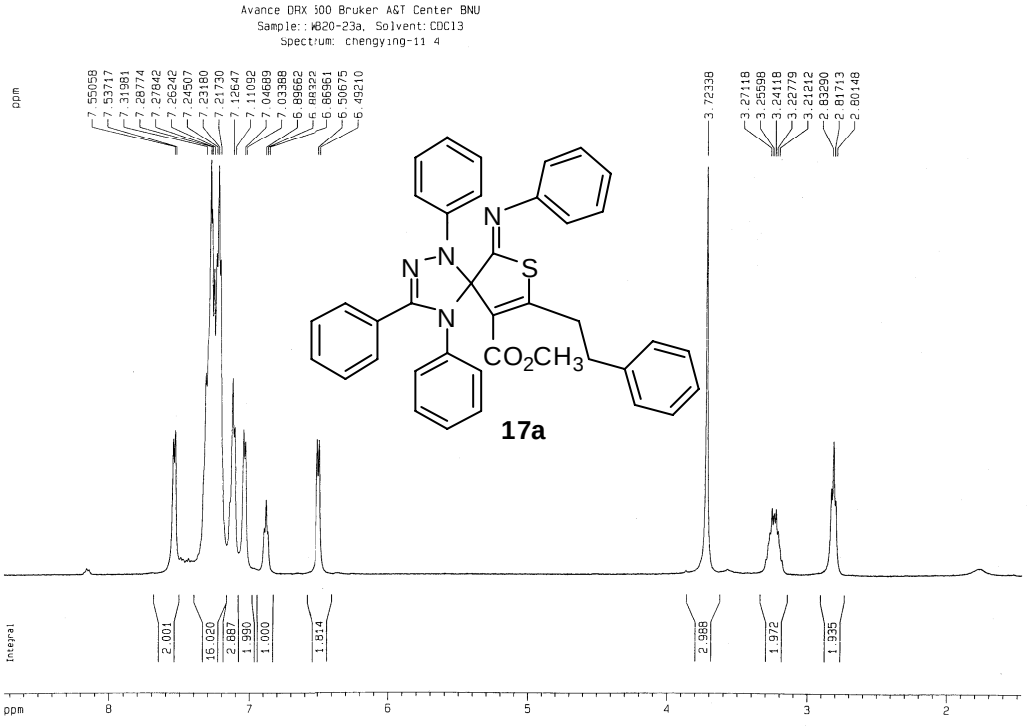

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-22c, Solvent: CDCl3
Spectrum: chengying-11 13
ppm
7.55339
7.53897
7.45022
7.43461
7.29863
7.28637
7.24367
7.22937
7.21336
7.19801
7.18111
7.17363
7.15789
7.14138
7.12639
7.04165
7.02906
7.01528
6.20675
6.19140
5.87648
5.86387
5.85018
4.58187
3.64125
3.51335
3.49993
3.49064
3.46752
3.37853
3.36183
3.34627
3.32961
Integral
2.0139
1.9340
5.2531
7.6985
2.2918
1.8437
0.9721
0.9325
3.0000
1.2760
1.1565
ppm
8
7
6
5
4
3
2
1
N
N
N
S
N
CO2CH3
15a-II

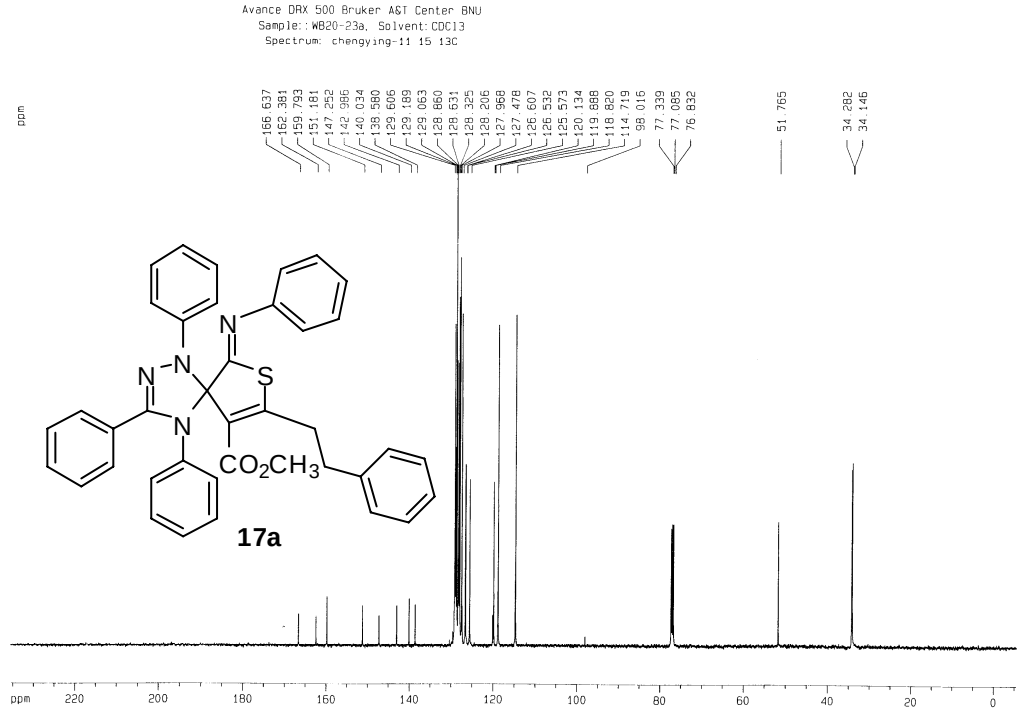

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-22b, Solvent: CDCl3
Spectrum: chengying-11 1
ppm
7.57273
7.55809
7.41459
7.38966
7.37419
7.35889
7.32488
7.30678
7.28952
7.27593
7.26683
7.25128
7.22702
7.21258
7.19735
7.17808
7.16269
6.99149
6.65759
5.20272
5.18871
5.17446
5.03160
3.66739
3.50506
3.49087
3.47210
3.45805
3.26270
3.24656
3.22985
3.21363
1.64774
S
N
N
N
N
CO2CH3
16a-l
Integral
2.108
0.989
1.906
2.194
13.033
2.636
1.000
0.921
0.966
0.974
2.958
1.042
1.006
ppm
8
7
6
5
4
3
2

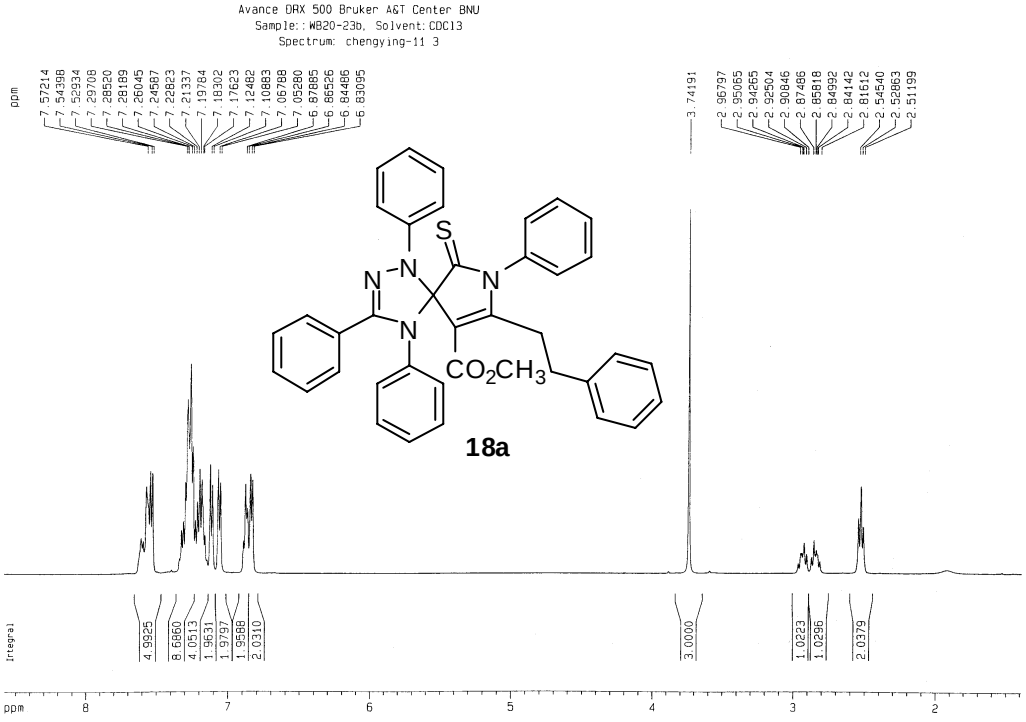

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-22b, Solvent: CDCl3
Spectrum: chengying-11 12 13C
ppm
190.405
169.204
147.478
141.268
139.326
139.130
138.874
137.253
130.153
129.403
129.308
129.221
128.619
128.367
127.951
127.696
127.003
126.492
126.408
120.591
115.645
112.198
97.234
77.336
77.082
76.828
52.816
49.387
34.255
S
N
N
N
N
CO2CH3
16a-l
ppm
180
160
140
120
100
80
60
40

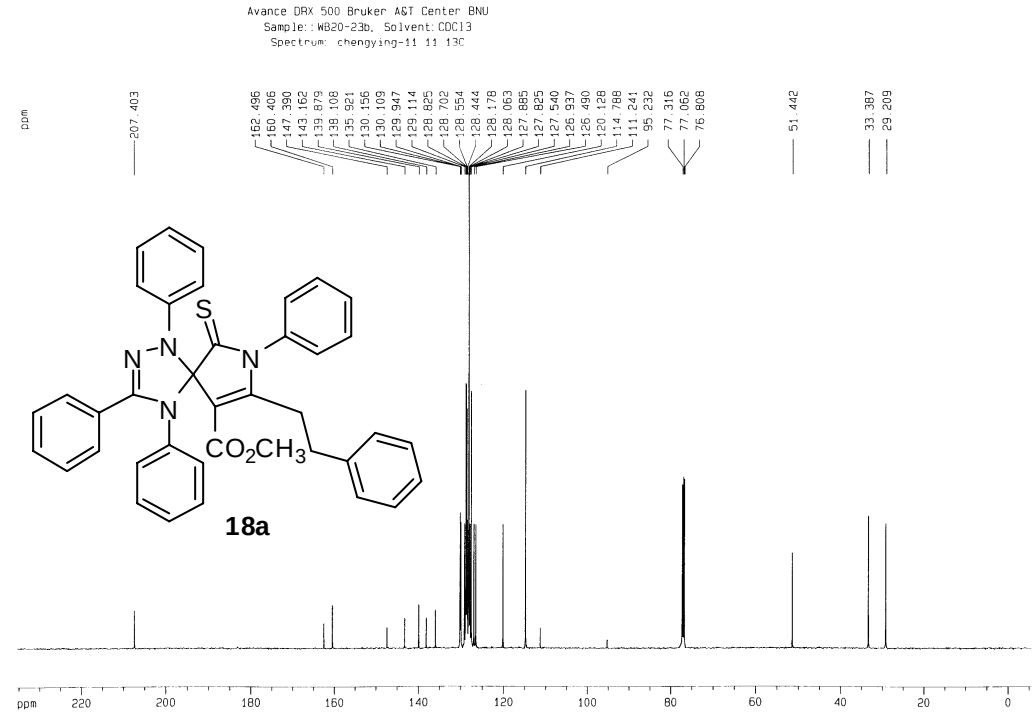

Avance 500 Bruker, A&T Center BNU
sample: WB20-22d; Solvent: CDCL3
spectrum: chengying-10 31
ppm
7.50423
7.48881
7.47410
7.42576
7.40149
7.38518
7.34929
7.33578
7.32018
7.30242
7.28765
7.27511
7.26054
7.22256
7.20885
7.02687
7.00980
6.99488
5.11144
5.09629
5.08117
4.43407
3.77082
3.42922
3.41460
3.39591
3.38219
3.18846
3.17197
3.15557
3.13884
1.68432
1.65830
Integral
4.066
0.938
2.136
10.661
1.340
1.606
1.037
4.985
1.000
0.975
3.045
1.082
1.051
ppm
8
7
6
5
4
3
2
1
S
N
N
N
N
CO2CH3
16a-II

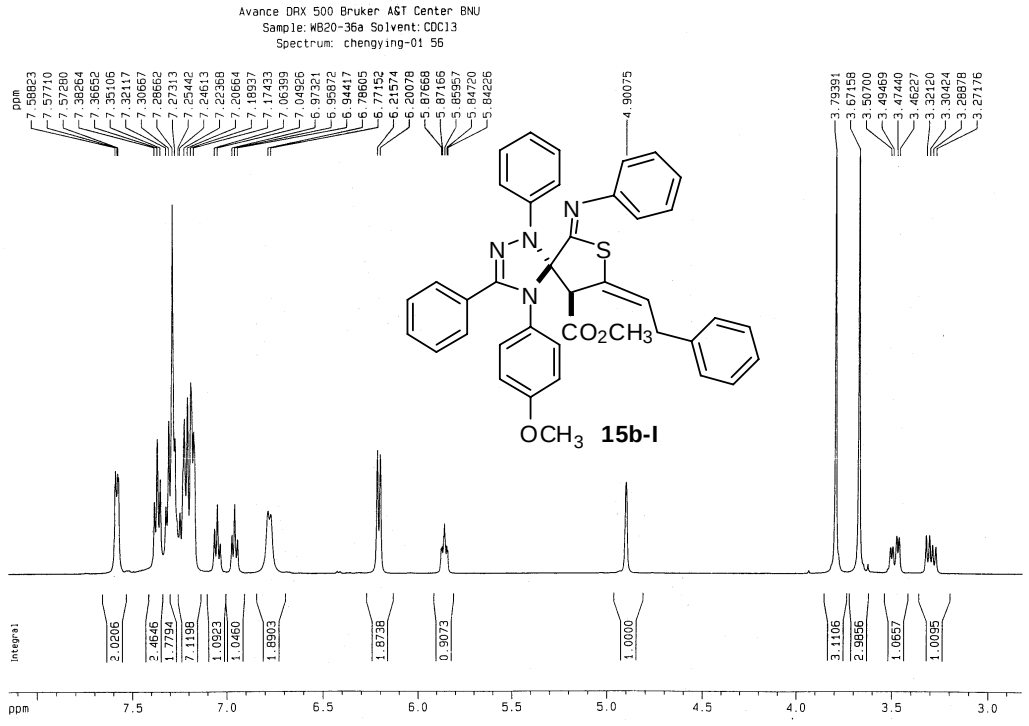

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-22d, Solvent: CDCl3
Spectrum: chengying-11 5
ppm
193.115
168.064
149.897
143.603
139.388
139.276
137.853
137.268
130.155
129.455
129.336
128.526
128.254
128.162
127.672
127.228
126.326
122.351
119.319
111.597
99.015
77.304
77.050
76.796
52.942
51.281
33.915
ppm
180
160
140
120
100
80
60
40
S
N
N
N
N
CO2CH3
16a-II

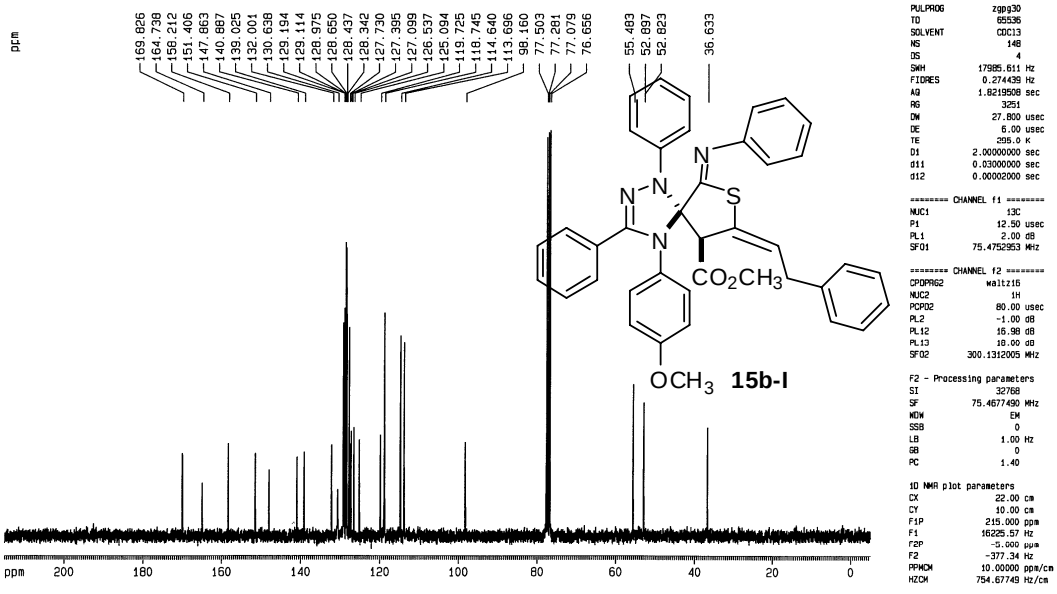

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-23a, Solvent: CDCl3
Spectrum: chengying-11 4
ppm
7.55058
7.53717
7.31981
7.28774
7.27842
7.26242
7.24507
7.23180
7.21730
7.12647
7.11092
7.04689
7.03388
6.89662
6.88322
6.86961
6.50675
6.49210
3.72338
3.27118
3.25598
3.24118
3.22779
3.21212
2.83290
2.81713
2.80148
Integral
2.001
16.020
2.887
1.980
1.000
1.814
2.988
1.972
1.935
ppm
8
7
6
5
4
3
2
N
N
N
S
CO2CH3
17a


Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-23a, Solvent: CDCl3
Spectrum: chengying-11 15 13C
ppm
166.637
162.381
159.793
151.181
147.252
142.986
140.034
138.580
129.606
129.189
129.063
128.860
128.631
128.325
128.206
127.988
127.478
126.607
126.532
125.573
120.134
119.888
118.820
114.719
98.016
77.339
77.085
76.832
51.765
34.282
34.146
ppm
220
200
180
160
140
120
100
80
60
40
20
0
N
N
N
S
CO2CH3
17a

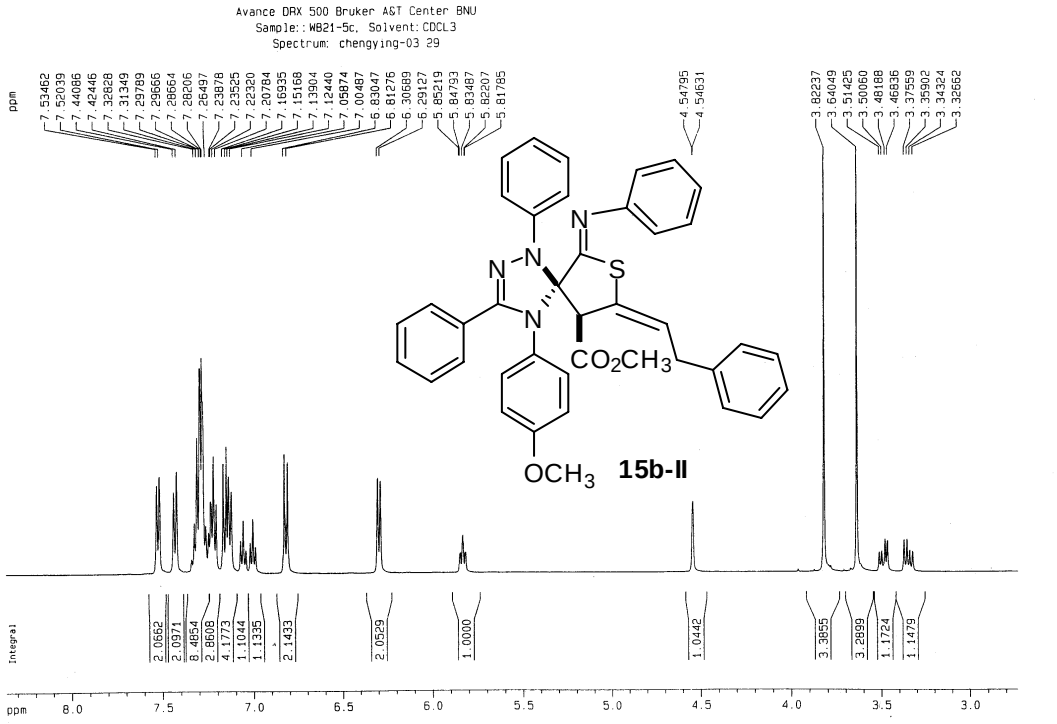

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-23b, Solvent: CDCl3
Spectrum: chengying-11 3
ppm
7.57214
7.54398
7.52934
7.29708
7.28520
7.28189
7.26045
7.24567
7.22823
7.21337
7.19784
7.18302
7.17623
7.12482
7.10883
7.06788
7.05280
6.87885
6.86526
6.84486
6.83095
3.74191
2.96797
2.95065
2.94265
2.92504
2.90846
2.87486
2.85818
2.84992
2.84142
2.81612
2.54540
2.52863
2.51199
S
N
N
N
N
CO2CH3
18a
Integral
4.0925
8.6860
4.0513
1.9631
1.9797
1.9588
2.0310
3.0000
1.0223
1.0296
2.0379
ppm
8
7
6
5
4
3
2

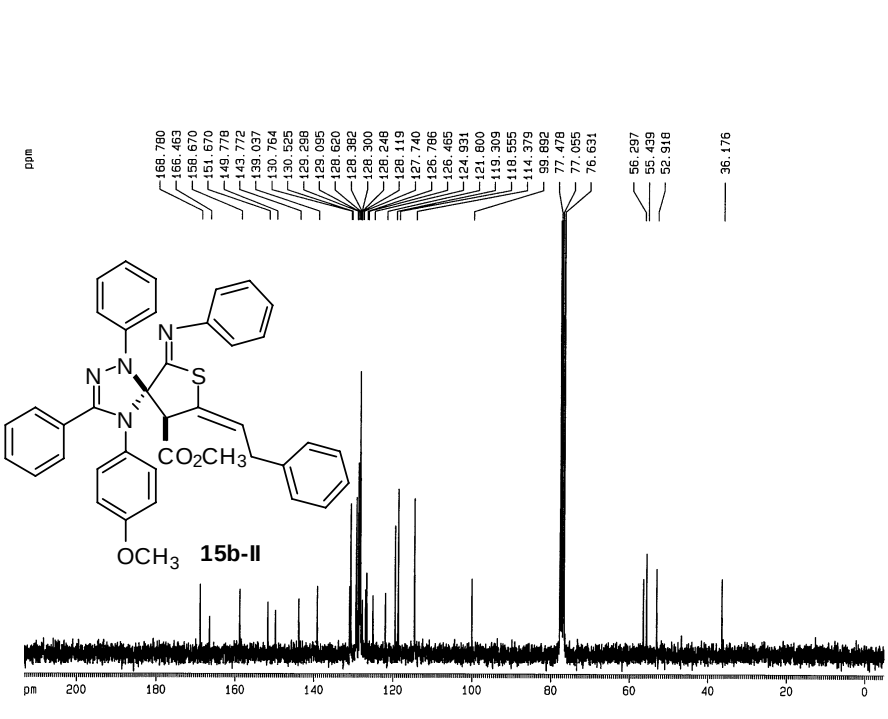

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-23b, Solvent: CDCl3
Spectrum: chengying-11 11 13C
ppm
207.403
162.496
160.406
147.390
143.162
139.879
138.108
135.921
130.156
130.109
129.947
129.114
128.825
128.702
128.554
128.444
128.178
128.063
127.885
127.825
127.540
126.937
126.490
120.128
114.788
111.241
95.232
77.316
77.062
76.808
51.442
33.387
29.209
S
N
N
N
N
CO2CH3
18a
ppm
220
200
180
160
140
120
100
80
60
40
20
0



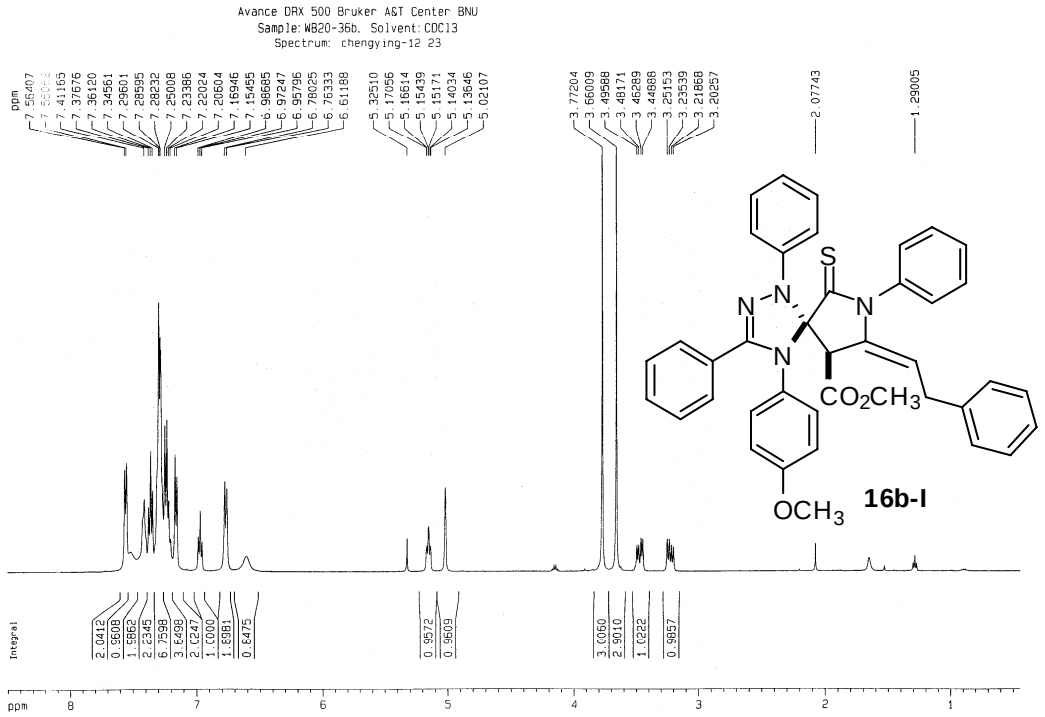


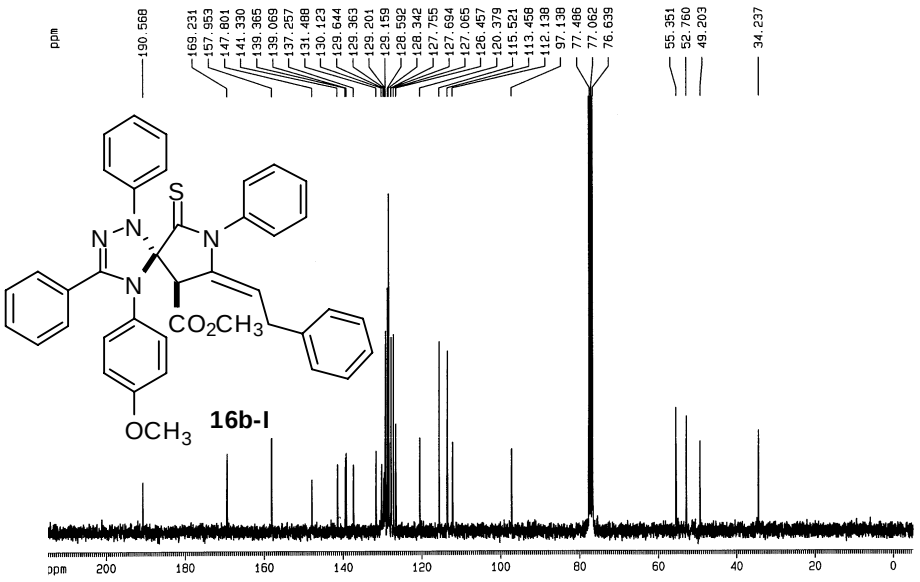

```
Current Data Parameters
NAME                  wb20-36a
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20080107
Time                    22.29
INSTRUM                 av300
PROBHD    5 mm DUL 13C-1
PULPROG                 zgpg30
TD                       65536
SOLVENT                 CDCl3
NS                         148
DS                           4
SWH                 17985.611 Hz
FIDRES                0.274439 Hz
AQ                    1.8219508 sec
RG                        3251
DW                      27.800 usec
DE                       6.00 usec
TE                      295.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
d12                0.00002000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                      12.50 usec
PL1                      2.00 dB
SF01               75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                     -1.00 dB
PL12                    16.98 dB
PL13                    18.00 dB
SF02              300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                 75.4677490 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40

1D NMR plot parameters
CX                         22.00 cm
CY                         10.00 cm
F1P                       215.000 ppm
F1                      16225.57 Hz
F2P                        -5.000 ppm
F2                       -377.34 Hz
PPMCM                  10.00000 ppm/cm
HZCM                  754.67749 Hz/cm
```



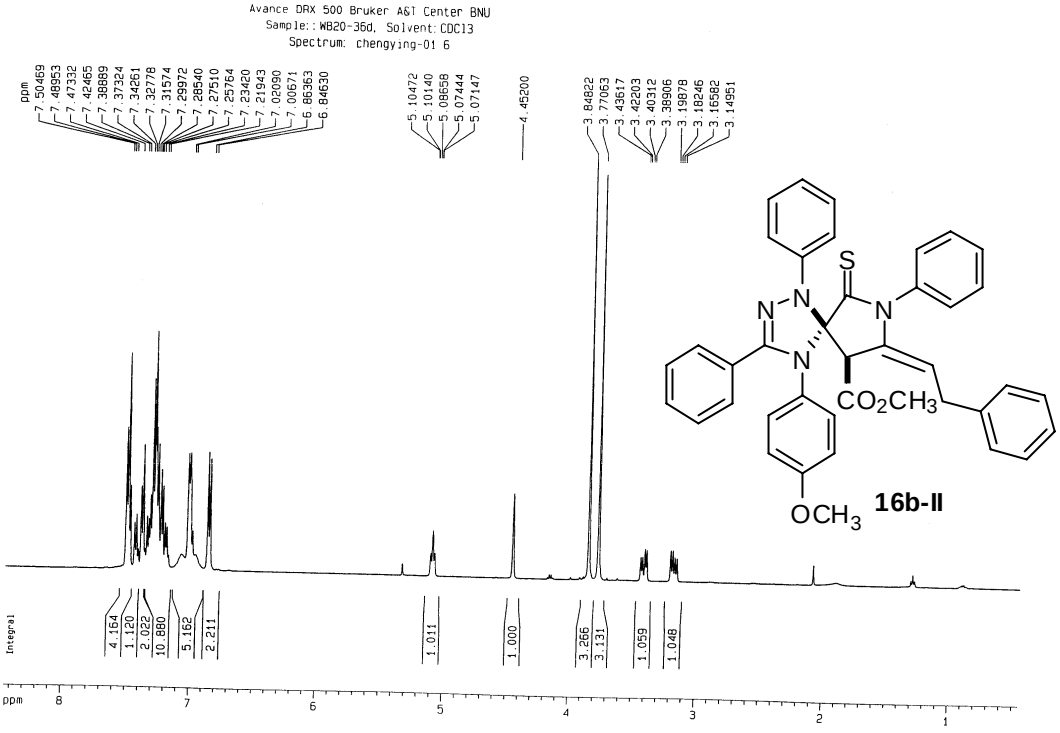


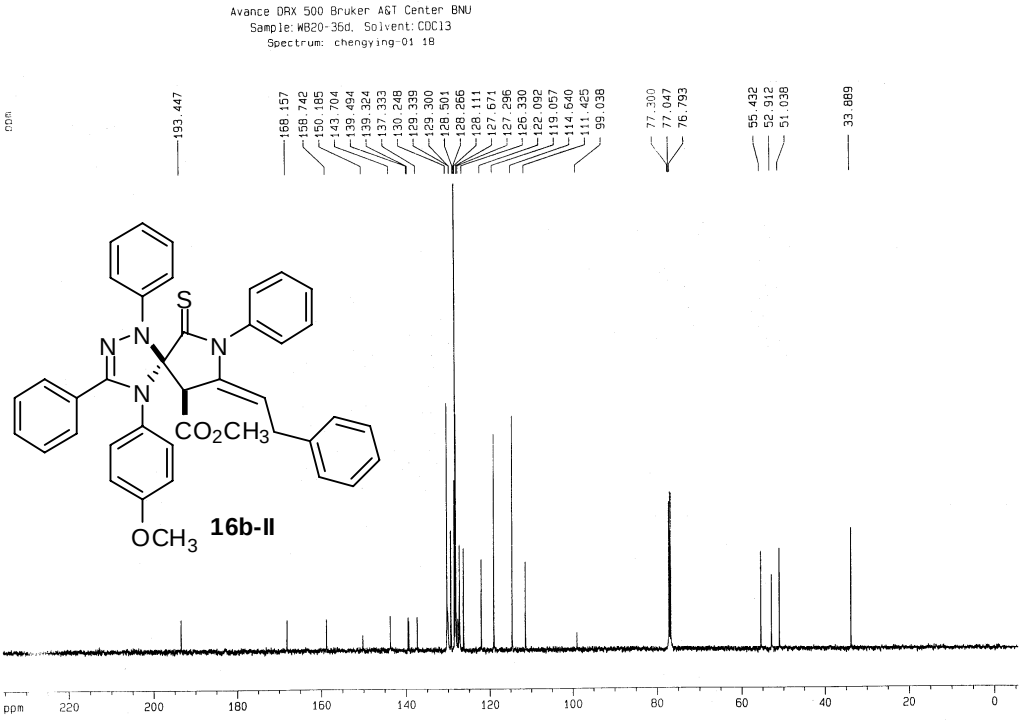

```
Current Data Parameters
NAME                 wb20-36c
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20080101
Time                    2.11
INSTRUM                av300
PROBHD  5 mm DUL 13C-1
PULPROG             zgpg30
TD                       65536
SOLVENT                 CDCl3
NS                        1024
DS                           4
SWH                 17985.611 Hz
FIDRES               0.274439 Hz
AQ                   1.8219508 sec
RG                       912.3
DW                      27.800 usec
DE                       6.00 usec
TE                      294.7 K
D1                   2.00000000 sec
d11                  0.03000000 sec
d12                  0.00002000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                       12.20 usec
PL1                      -0.32 dB
SF01                75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                        1H
PCPD2                   80.00 usec
PL2                      -1.00 dB
PL12                     16.56 dB
PL13                     16.00 dB
SF02               300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                  75.4677490 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                          1.40

1D NMR plot parameters
CX                        22.00 cm
CY                        30.00 cm
F1P                     215.000 ppm
F1                    16225.57 Hz
F2P                      -5.000 ppm
F2                     -377.34 Hz
PPMCM                 10.00000 ppm/cm
HZCM                  754.67749 Hz/cm
```

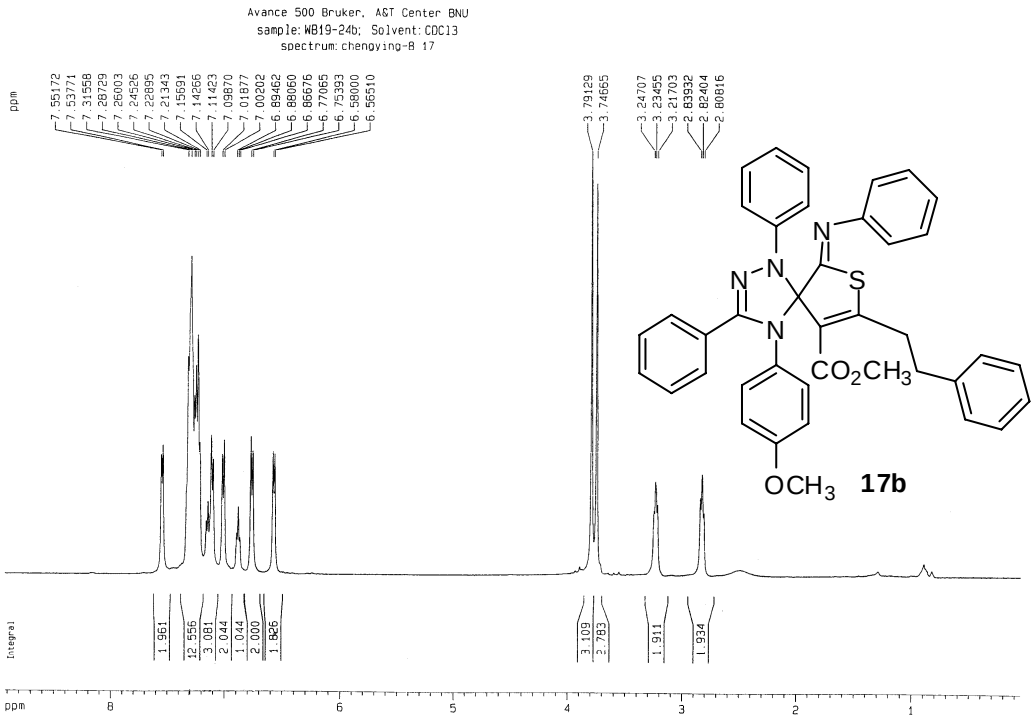


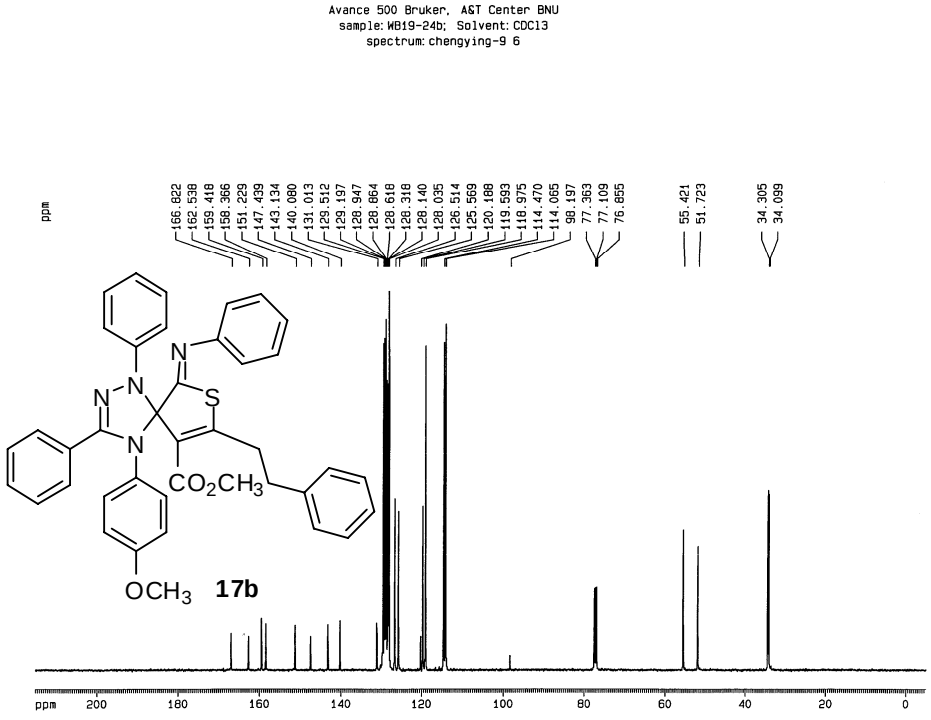


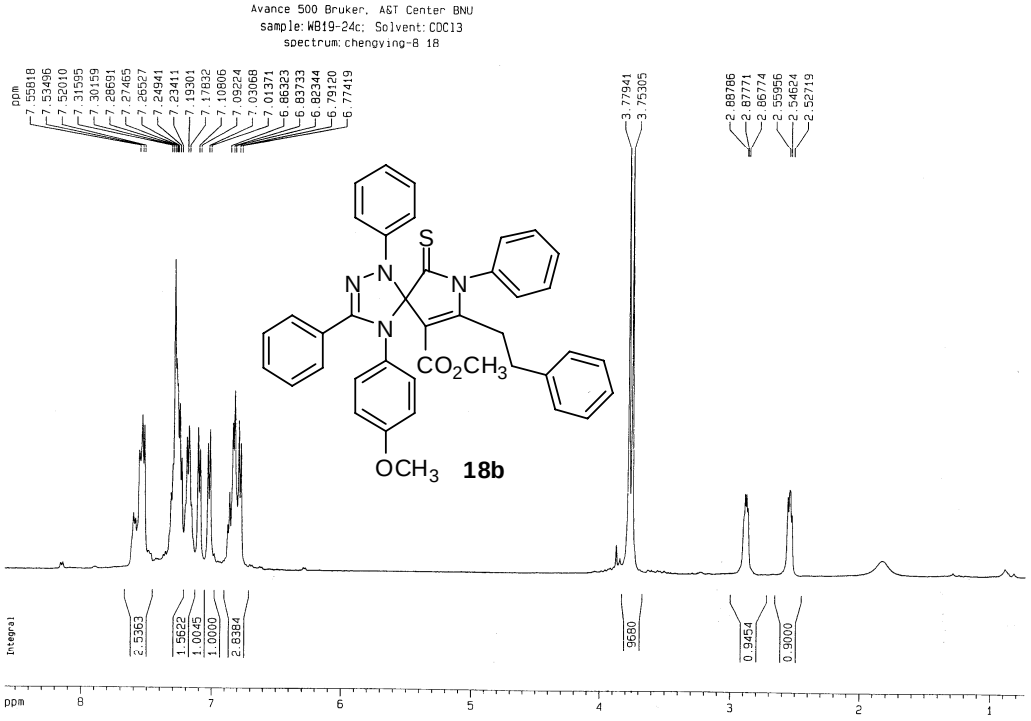

```
Current Data Parameters
NAME                  wb20-36b
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20080101
Time                     3.28
INSTRUM                  av300
PROBHD    5 mm DUL 13C-1
PULPROG                zgpg30
TD                       65536
SOLVENT                  CDCl3
NS                         797
DS                           4
SWH                17985.611 Hz
FIDRES                0.274439 Hz
AQ                    1.8219508 sec
RG                        1290.2
DW                       27.800 usec
DE                        6.00 usec
TE                       294.8 K
D1                 2.00000000 sec
d11                0.03000000 sec
d12                0.00002000 sec

======== CHANNEL f1 ========
NUC1                       13C
P1                       12.20 usec
PL1                      -0.32 dB
SF01               75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                    80.00 usec
PL2                      -1.00 dB
PL12                     16.56 dB
PL13                     18.00 dB
SF02              300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                 75.4677490 MHz
WDW                           EM
SSB                            0
LB                        1.00 Hz
GB                             0
PC                          1.40

1D NMR plot parameters
CX                        22.00 cm
CY                        20.00 cm
F1P                     215.000 ppm
F1                    16225.57 Hz
F2P                      -5.000 ppm
F2                     -377.34 Hz
PPMCM                 10.00000 ppm/cm
HZCM                754.67749 Hz/cm
```

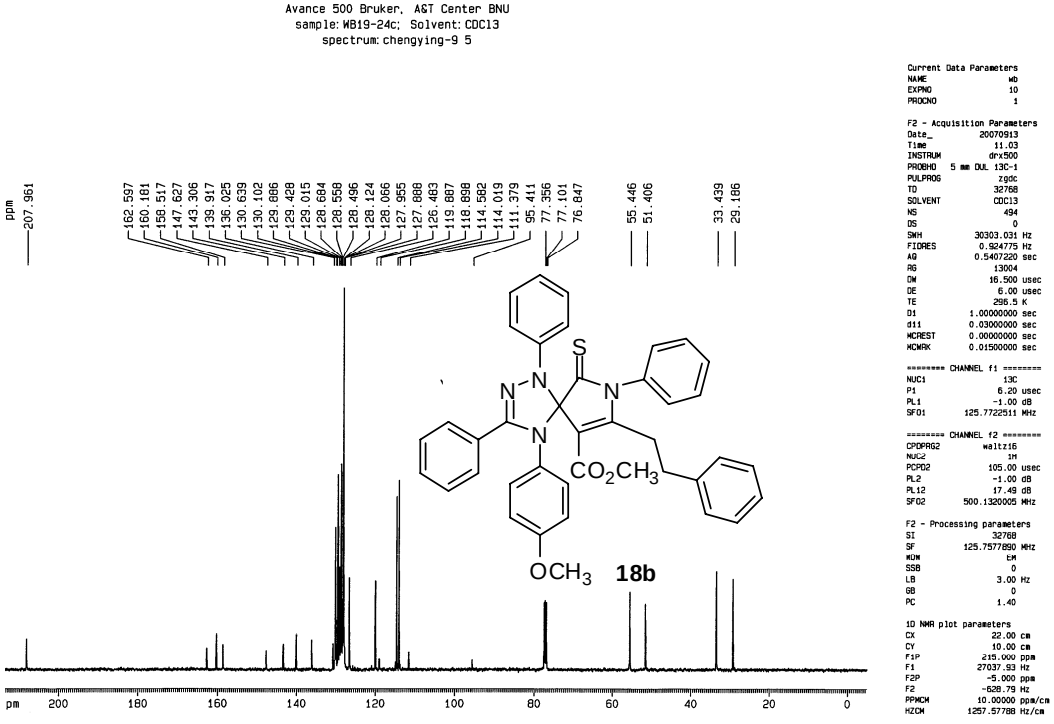

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-36d, Solvent: CDCl3
Spectrum: chengying-01 6
ppm
7.50469
7.48953
7.47332
7.42465
7.38889
7.37324
7.34261
7.32778
7.31574
7.29972
7.28540
7.27510
7.25764
7.23420
7.21943
7.02090
7.00671
6.86363
6.84630
5.10472
5.10140
5.08658
5.07444
5.07147
4.45200
3.84822
3.77063
3.43617
3.42203
3.40312
3.38906
3.19878
3.18246
3.16582
3.14951
Integral
4.164
1.120
2.022
10.880
5.162
2.211
1.011
1.000
3.266
3.131
1.059
1.048
ppm
8
7
6
5
4
3
2
1
S
N
N
N
N
CO2CH3
OCH3
16b-II


Avance DRX 500 Bruker A&T Center BNU
Sample: WB20-36d, Solvent: CDCl3
Spectrum: chengying-01 18
ppm
193.447
168.157
158.742
150.185
143.704
139.494
139.324
137.333
130.248
129.339
129.300
128.501
128.266
128.111
127.671
127.296
126.330
122.092
119.057
114.640
111.425
99.038
77.300
77.047
76.793
55.432
52.912
51.038
33.889
ppm
220
200
180
160
140
120
100
80
60
40
20
0
S
N
N
N
N
CO2CH3
OCH3
16b-II

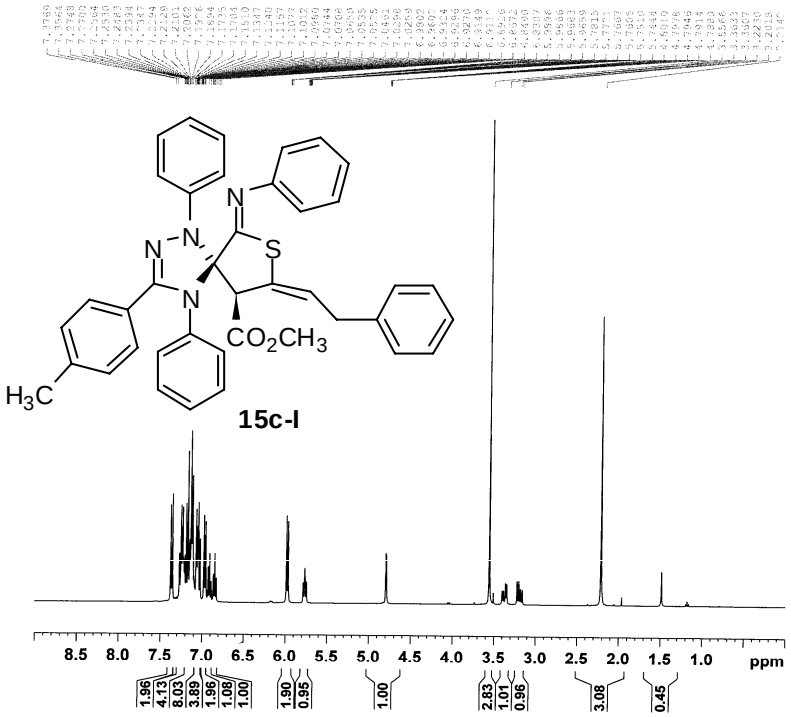

Avance 500 Bruker, A&T Center BNU
sample: WB19-24b; Solvent: CDCl3
spectrum: chengying-8 17
ppm
7.55172
7.53771
7.31558
7.28729
7.26003
7.24526
7.22895
7.21343
7.15591
7.14266
7.11423
7.09870
7.01877
7.00202
6.89462
6.88060
6.86676
6.77065
6.75393
6.58000
6.56510
3.79129
3.74665
3.24707
3.23455
3.21703
2.83932
2.82404
2.80816
Integral
1.961
12.556
3.081
2.044
1.044
2.000
1.826
3.109
2.783
1.911
1.934
ppm
8
6
5
4
3
2
1
N
N
N
S
CO2CH3
OCH3
17b


Avance 500 Bruker, A&T Center BNU
sample: WB19-24b; Solvent: CDCl3
spectrum: chengying-9 6
ppm
166.822
162.538
159.418
158.366
151.229
147.439
143.134
140.080
131.013
129.512
129.197
128.947
128.864
128.618
128.316
128.140
128.035
126.514
125.569
120.188
119.593
118.975
114.470
114.065
98.197
77.363
77.109
76.855
55.421
51.723
34.305
34.099
ppm
200
180
160
140
120
100
80
60
40
20
0
N
N
N
S
CO2CH3
OCH3
17b



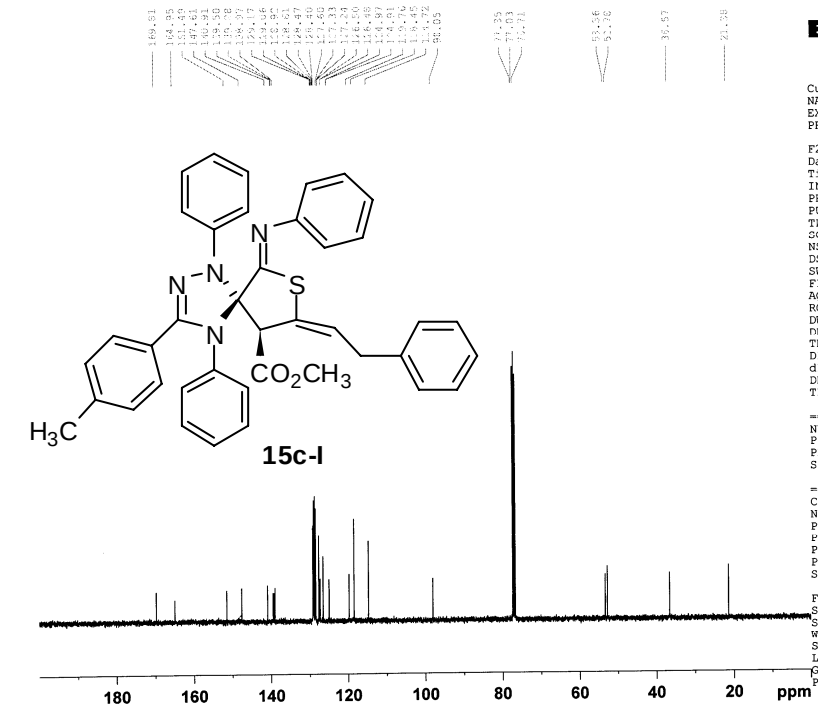



```
Current Data Parameters
NAME                  wb
EXPNO                 10
PROCNO                1

F2 - Acquisition Parameters
Date_           20070913
Time                11.03
INSTRUM           drx500
PROBHD   5 mm DUL 13C-1
PULPROG             zgdc
TD                 32768
SOLVENT             CDCl3
NS                    494
DS                      0
SWH           30303.031 Hz
FIDRES        0.924775 Hz
AQ            0.5407220 sec
RG                  13004
DW                16.500 usec
DE                 6.00 usec
TE                296.5 K
D1            1.00000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 6.20 usec
PL1               -1.00 dB
SFO1         125.7722511 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             105.00 usec
PL2               -1.00 dB
PL12              17.49 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF           125.7577890 MHz
WDW                   EM
SSB                    0
LB                3.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                22.00 cm
CY                10.00 cm
F1P              215.000 ppm
F1             27037.93 Hz
F2P               -5.000 ppm
F2              -628.79 Hz
PPMCM          10.00000 ppm/cm
HZCM         1257.57788 Hz/cm
```



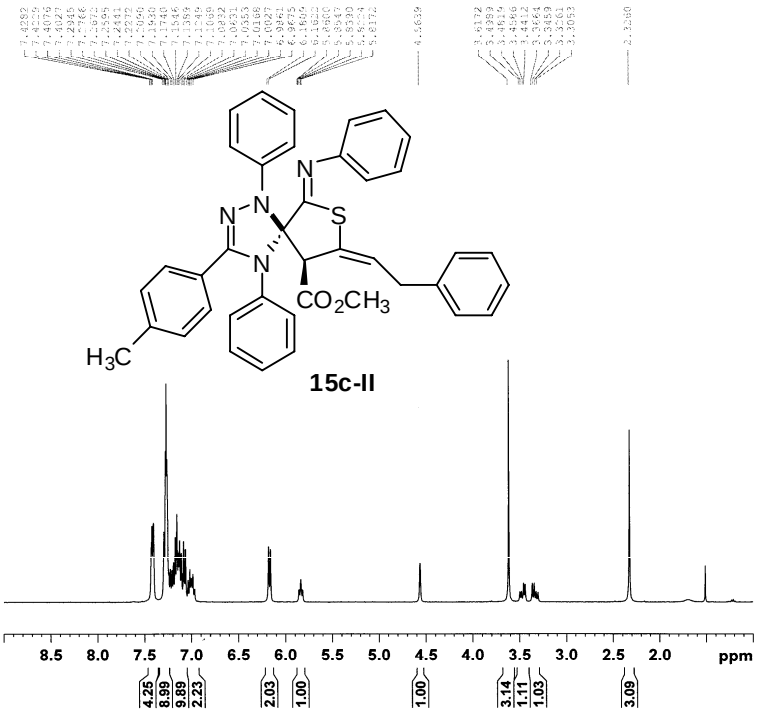
BRUKER

```
Current Data Parameters
NAME                 wb21-20a-x
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20080415
Time                   16.55
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      144
DW                   60.800 usec
DE                    6.50 usec
TE                   299.7 K
D1                1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                      1H
P1                     13.50 usec
PL1                    -1.00 dB
SFO1             400.1724712 MHz

F2 - Processing parameters
SI                        32768
SF               400.1700389 MHz
WDW                          EM
SSB                           0
LB                     0.30 Hz
GB                            0
PC                     1.00
```

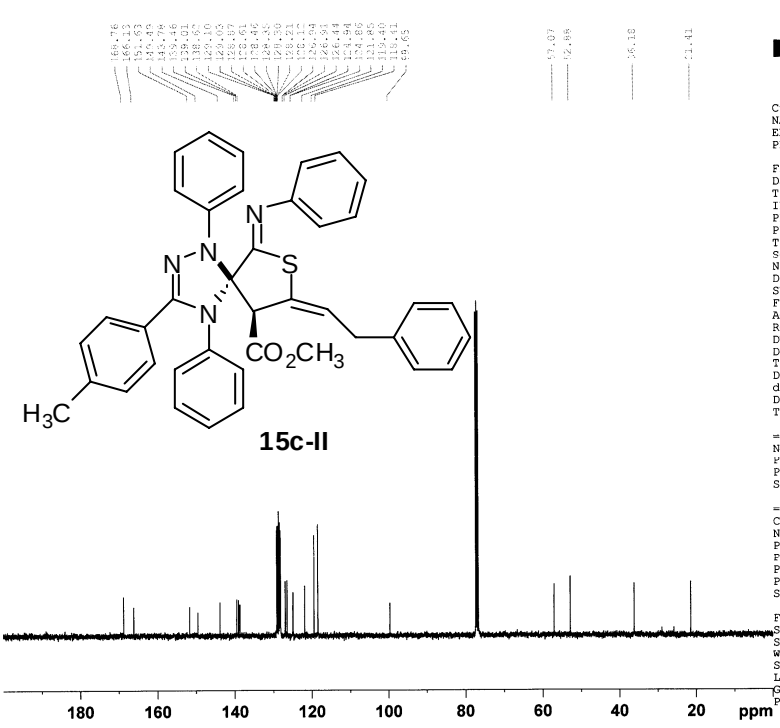


BRUKER

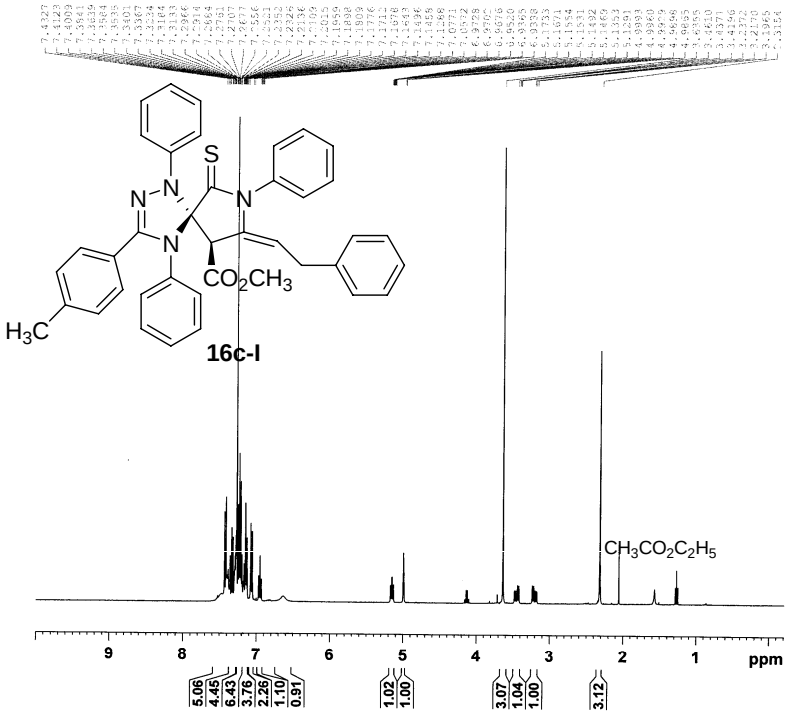
```
Current Data Parameters
NAME                 WB21-20a2
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20080415
Time                   11.40
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      177
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                      203
DW                   20.800 usec
DE                    6.50 usec
TE                   299.5 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                      13C
P1                     8.40 usec
PL1                   -2.00 dB
SFO1             100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL12                   14.46 dB
PL13                   14.46 dB
PL2                   -1.00 dB
SFO2             400.1716007 MHz

F2 - Processing parameters
SI                        32768
SF               100.6228270 MHz
WDW                          EM
SSB                           0
LB                     1.00 Hz
GB                            0
PC                     1.40
```




```
Current Data Parameters
NAME          WB21-20C-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080407
Time               9.21
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            4807.692 Hz
FIDRES        0.073360 Hz
AQ            6.8157940 sec
RG                    4
DW              104.000 usec
DE                6.50 usec
TE               295.8 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                13.50 usec
PL1               -1.00 dB
SFO1        400.1723210 MHz

F2 - Processing parameters
SI                32768
SF          400.1700000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

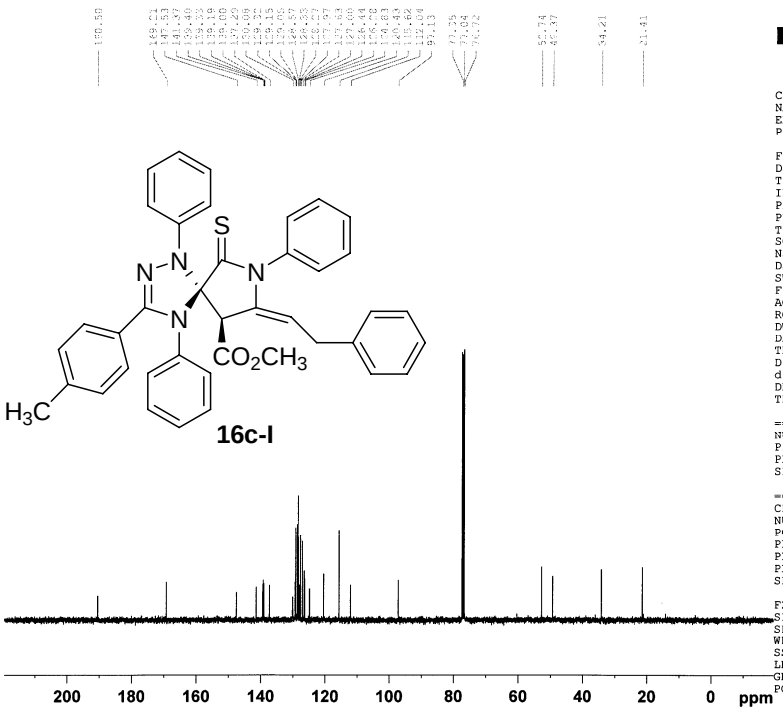



```
Current Data Parameters
NAME        WB21-20c-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080407
Time              15.20
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  501
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               298.5 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                8.40 usec
PL1              -2.00 dB
SFO1        100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            80.00 usec
PL12             14.46 dB
PL13             14.46 dB
PL2              -1.00 dB
SFO2        400.1716007 MHz

F2 - Processing parameters
SI                32768
SF          100.6228270 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



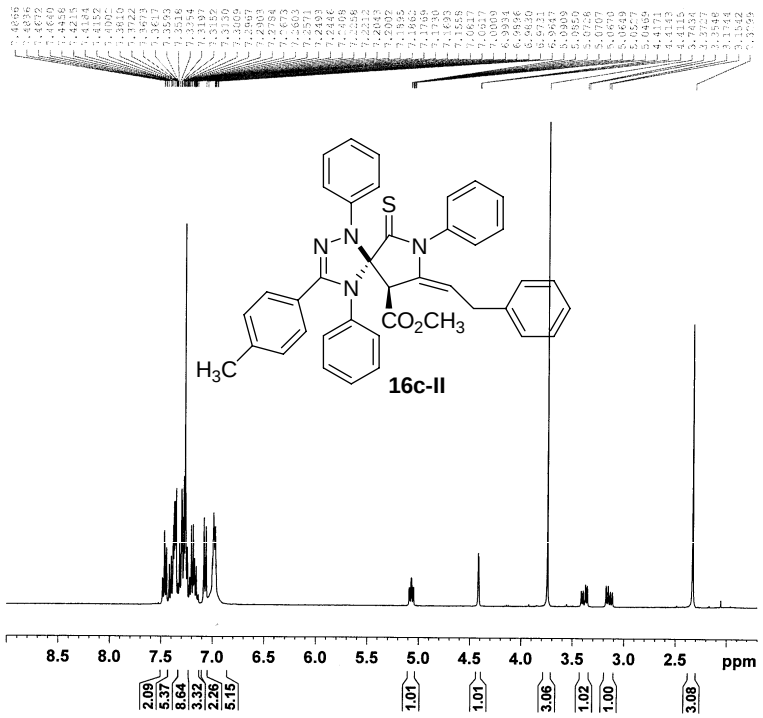
BRUKER

```
Current Data Parameters
NAME                  WB21-20b-H
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20080407
Time                        9.33
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                    zg30
TD                        65536
SOLVENT                   CDCl3
NS                           16
DS                            0
SWH                    4807.692 Hz
FIDRES                 0.073360 Hz
AQ                     6.8157940 sec
RG                            4
DW                       104.000 usec
DE                         6.50 usec
TE                        295.7 K
D1                     1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                         13.50 usec
PL1                        -1.00 dB
SFO1                400.1723210 MHz

F2 - Processing parameters
SI                            32768
SF                  400.1700000 MHz
WDW                            EM
SSB                             0
LB                           0.30 Hz
GB                              0
PC                           1.00
```

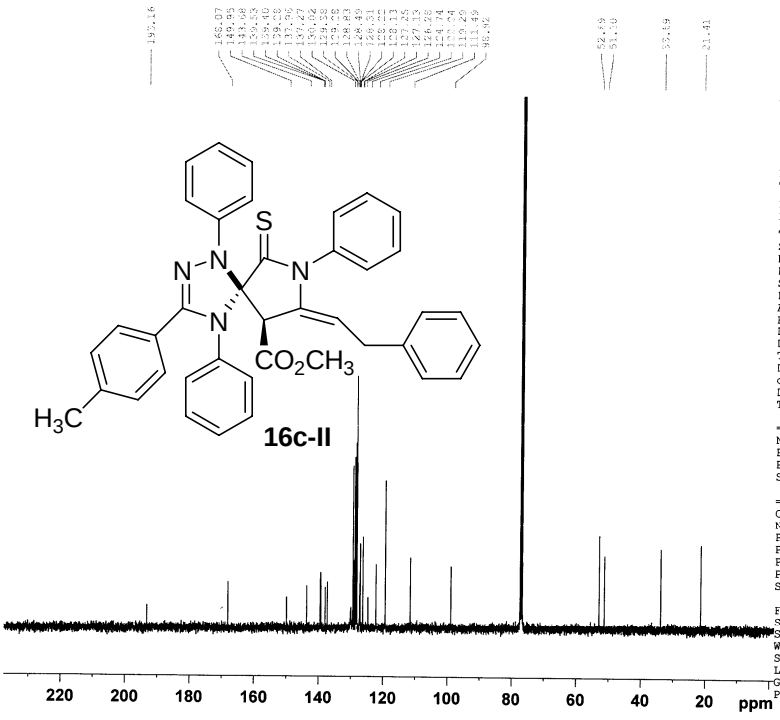


BRUKER

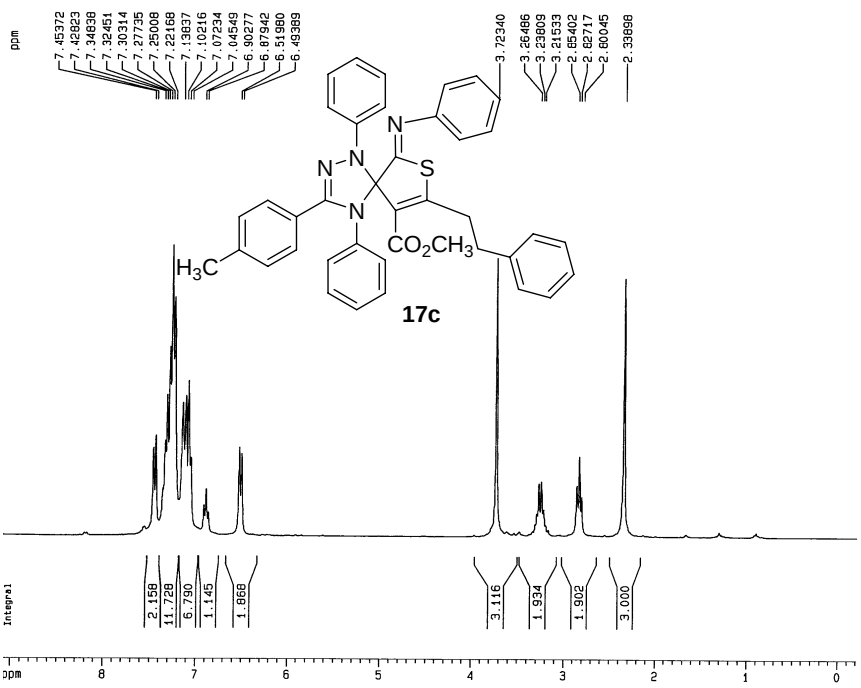
```
Current Data Parameters
NAME                  WB21-20b2-C13
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20080407
Time                       15.00
INSTRUM                    spect
PROBHD    5 mm PABBO BB-
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                          166
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                     1.3631988 sec
RG                          203
DW                        20.800 usec
DE                         6.50 usec
TE                        297.9 K
D1                     2.00000000 sec
d11                    0.03000000 sec
DELTA                  1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          13C
P1                          8.40 usec
PL1                        -2.00 dB
SFO1                100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2                   waltz16
NUC2                          1H
PCPD2                      80.00 usec
PL12                       14.46 dB
PL13                       14.46 dB
PL2                        -1.00 dB
SFO2                400.1716007 MHz

F2 - Processing parameters
SI                            32768
SF                  100.6228270 MHz
WDW                            EM
SSB                             0
LB                           1.00 Hz
GB                              0
PC                           1.40
```



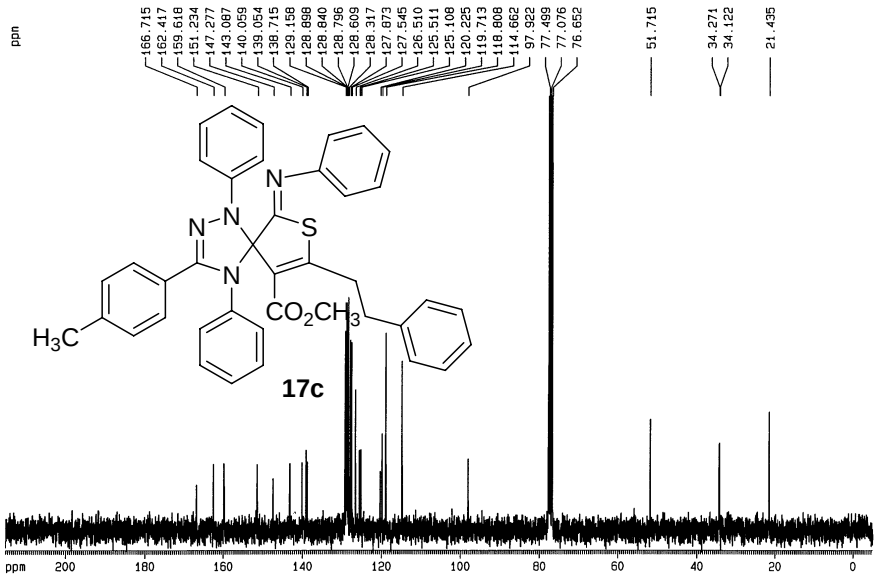

```
Current Data Parameters
NAME          WB21-20d-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080327
Time               16.16
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     0
SWH           4807.692 Hz
FIDRES        0.073360 Hz
AQ            6.8157940 sec
RG                     4
DW              104.000 usec
DE                6.50 usec
TE                297.1 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                13.50 usec
PL1               -1.00 dB
SFO1        400.1723210 MHz

F2 - Processing parameters
SI                 32768
SF          400.1700000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



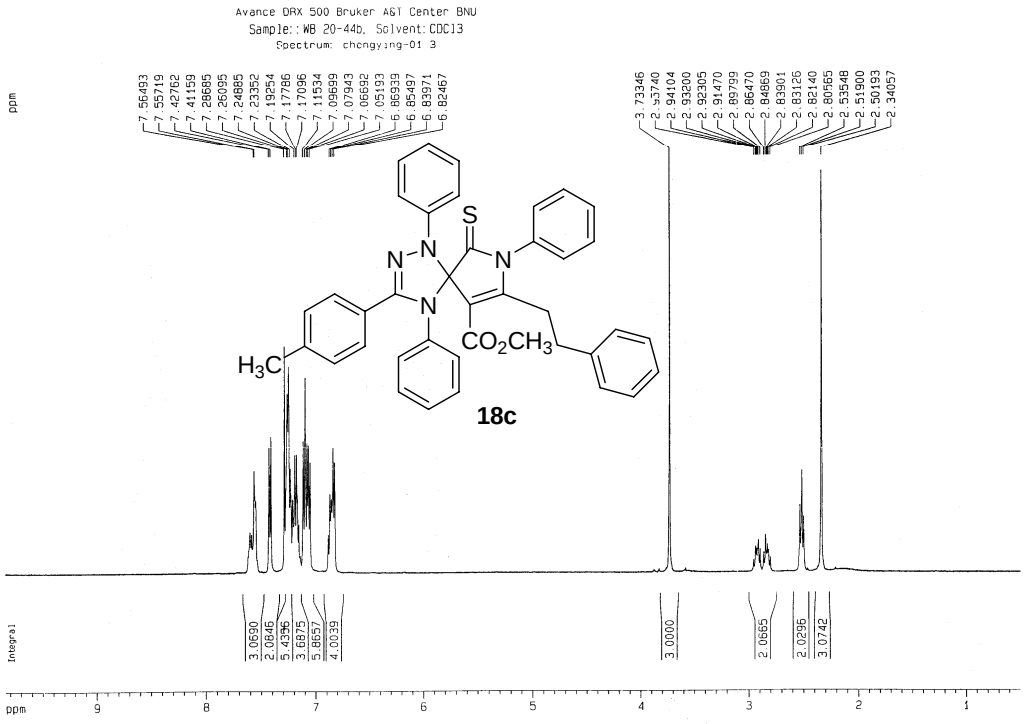

```
Current Data Parameters
NAME         WB21-20d-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080327
Time               16.48
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   829
DS                     0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                   203
DW              20.800 usec
DE                6.50 usec
TE                297.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                8.40 usec
PL1               -2.00 dB
SFO1        100.6347005 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            80.00 usec
PL12              14.46 dB
PL13              14.46 dB
PL2               -1.00 dB
SFO2        400.1716007 MHz

F2 - Processing parameters
SI                 32768
SF          100.6228270 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

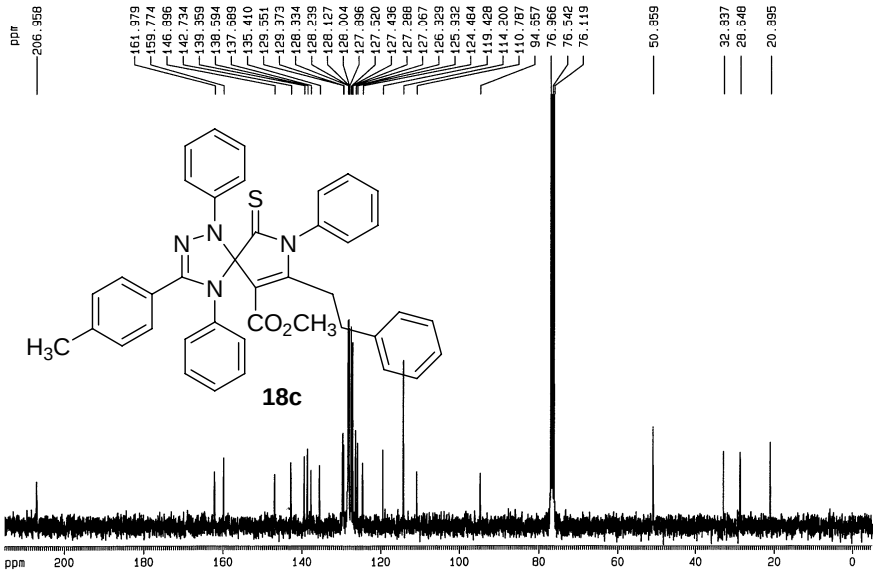



```
Current Data Parameters
NAME            wb20-44a
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_          20080101
Time               4.51
INSTRUM           av300
PROBHD   5 mm DUL 13C-1
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   0
SWH           8992.806 Hz
FIDRES        0.137219 Hz
AQ            3.6438515 sec
RG                 128
DW              55.600 usec
DE               6.00 usec
TE              294.4 K
D1           5.00000000 sec

======== CHANNEL f1 ========
NUC1                1H
P1               10.60 usec
PL1              -1.00 dB
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                 32768
SF          300.1300000 MHz
WDW                   EM
SSB                    0
LB                  0.35 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 22.00 cm
CY                  7.00 cm
F1P                9.086 ppm
F1               2726.90 Hz
F2P               -0.207 ppm
F2                -62.26 Hz
PPMCM          0.42242 ppm/cm
HZCM          126.77998 Hz/cm
```

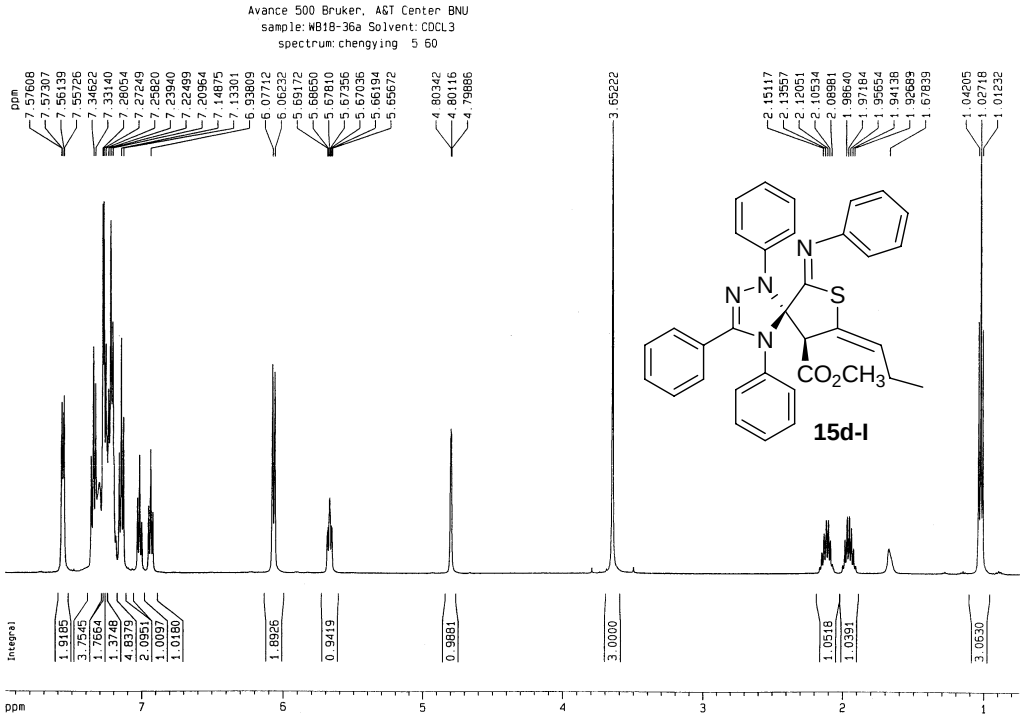


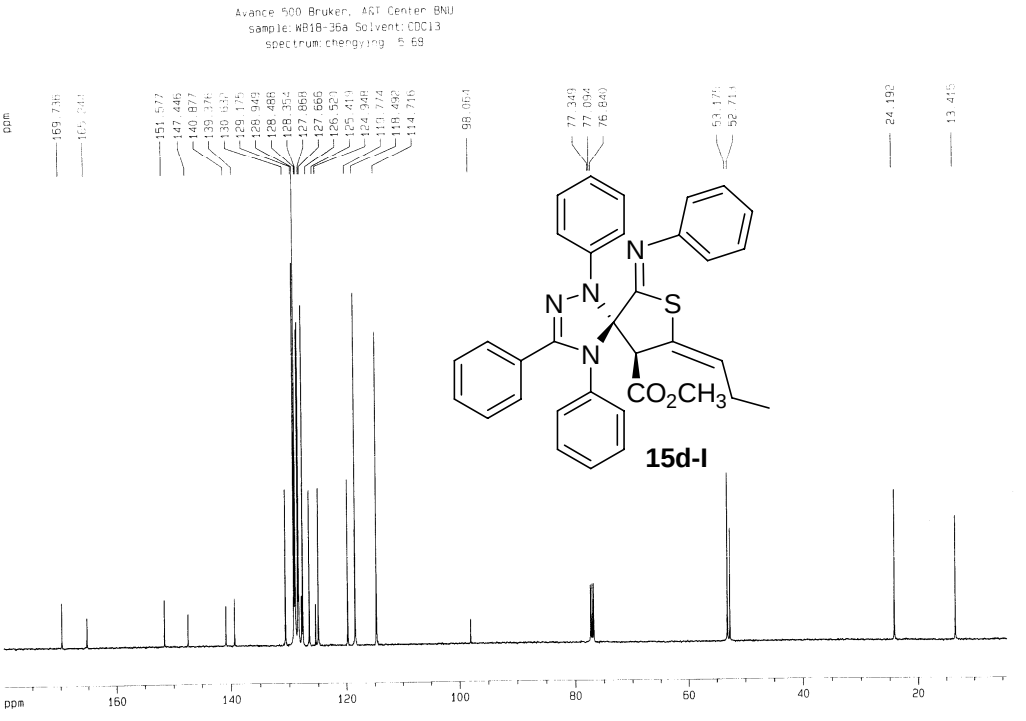

```
Current Data Parameters
NAME            wb20-44a
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_          20080101
Time               5.32
INSTRUM           av300
PROBHD   5 mm DUL 13C-1
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 237
DS                   4
SWH          17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG                 322.5
DW              27.800 usec
DE               6.00 usec
TE              294.7 K
D1           2.00000000 sec
d11          0.03000000 sec
d12          0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1               12.20 usec
PL1              -0.32 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -1.00 dB
PL12             16.96 dB
PL13             18.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                 22.00 cm
CY                 18.00 cm
F1P              215.000 ppm
F1             16225.57 Hz
F2P              -5.000 ppm
F2             -377.34 Hz
PPMCM         10.00000 ppm/cm
HZCM          754.67749 Hz/cm
```

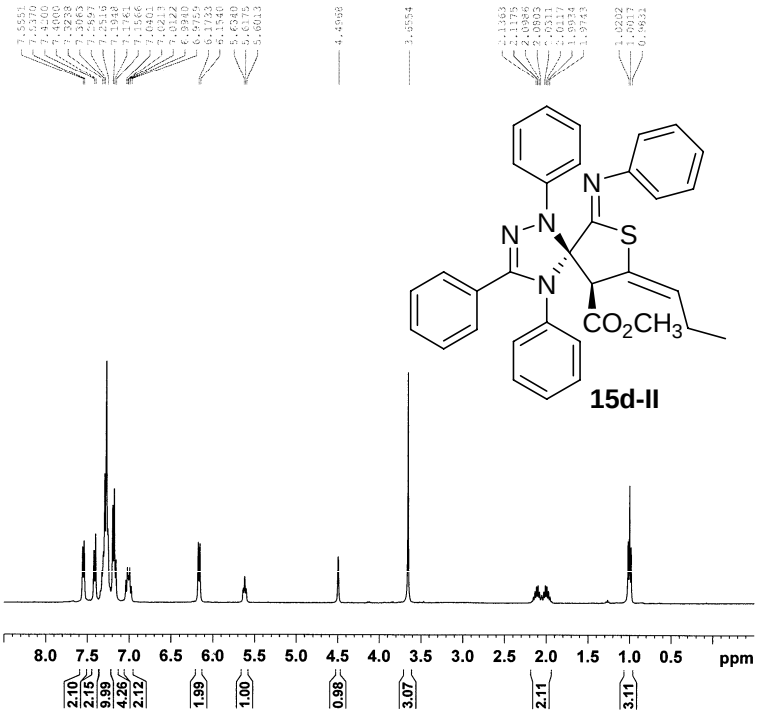





```
Current Data Parameters
NAME            wb20-44b
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20080101
Time               6.04
INSTRUM           av300
PROBHD  5 mm DUL 13C-1
PULPROG        zgpg30
TD              65536
SOLVENT         CDCl3
NS                 703
DS                   4
SWH          17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG               912.3
DW              27.800 usec
DE               6.00 usec
TE              294.8 K
D1           2.00000000 sec
d11          0.03000000 sec
d12          0.00002000 sec

======== CHANNEL f1 ========
NUC1              13C
P1              12.20 usec
PL1             -0.32 dB
SFO1       75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2        waltz16
NUC2              1H
PCPD2           80.00 usec
PL2             -1.00 dB
PL12            16.56 dB
PL13            18.00 dB
SFO2      300.1312005 MHz

F2 - Processing parameters
SI                32768
SF         75.4677904 MHz
WDW               EM
SSB                0
LB              1.00 Hz
GB                 0
PC              1.40

1D NMR plot parameters
CX              22.00 cm
CY              18.00 cm
F1P           215.000 ppm
F1          16225.58 Hz
F2P            -5.000 ppm
F2           -377.34 Hz
PPMCM       10.00000 ppm/cm
HZCM       754.67785 Hz/cm
```

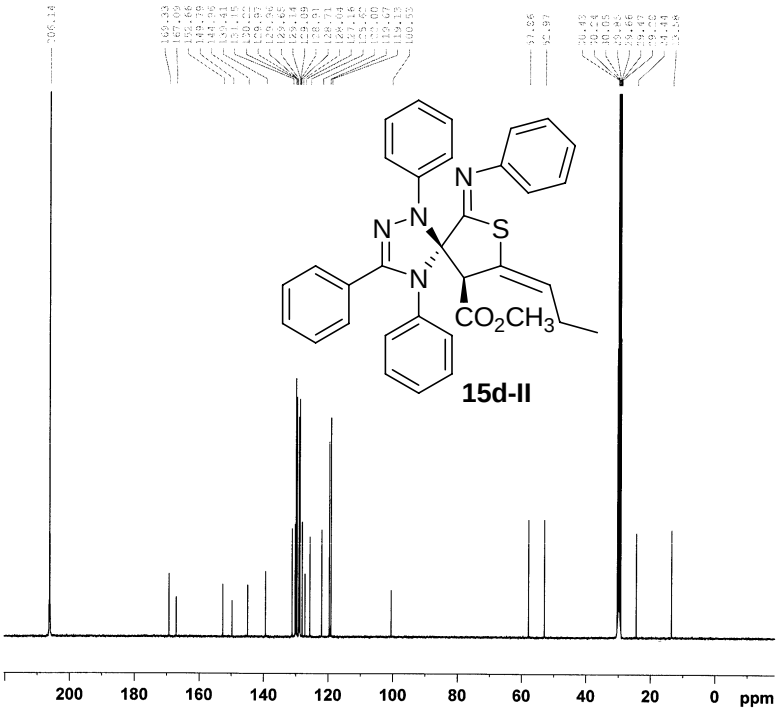

Avance 500 Bruker, A&T Center BNU
sample: WB18-36a Solvent: CDCL3
spectrum: chengying 5 60
ppm
7.57608
7.57307
7.56139
7.55726
7.34622
7.33140
7.28054
7.27249
7.25820
7.23940
7.22499
7.20964
7.14875
7.13301
6.93809
6.07712
6.06232
5.69172
5.68650
5.67810
5.67356
5.67036
5.66194
5.65672
4.80342
4.80116
4.79886
3.65222
2.15117
2.13557
2.12051
2.10534
2.08981
1.98640
1.97184
1.95554
1.94138
1.92689
1.67839
1.04205
1.02718
1.01232
Integral
1.9185
3.7545
1.7664
1.3748
4.8379
2.0951
1.0097
1.0180
1.8926
0.9419
0.9881
3.0000
1.0518
1.0391
3.0630
ppm
7
6
5
4
3
2
1
N
N
N
S
CO2CH3
15d-l


Avance 500 Bruker, A&T Center BNU
sample: WB18-36a Solvent: CDCl3
spectrum: chengying 5 69
ppm
169.738
165.341
151.577
147.446
140.877
139.317
130.653
129.175
128.949
128.488
128.354
127.868
127.666
126.523
125.411
124.949
111.774
119.492
114.716
98.0651
77.3493
77.0944
76.8400
53.1745
52.7114
24.1921
13.4155
ppm
160
140
120
100
80
60
40
20
N
N
N
S
CO2CH3
15d-l



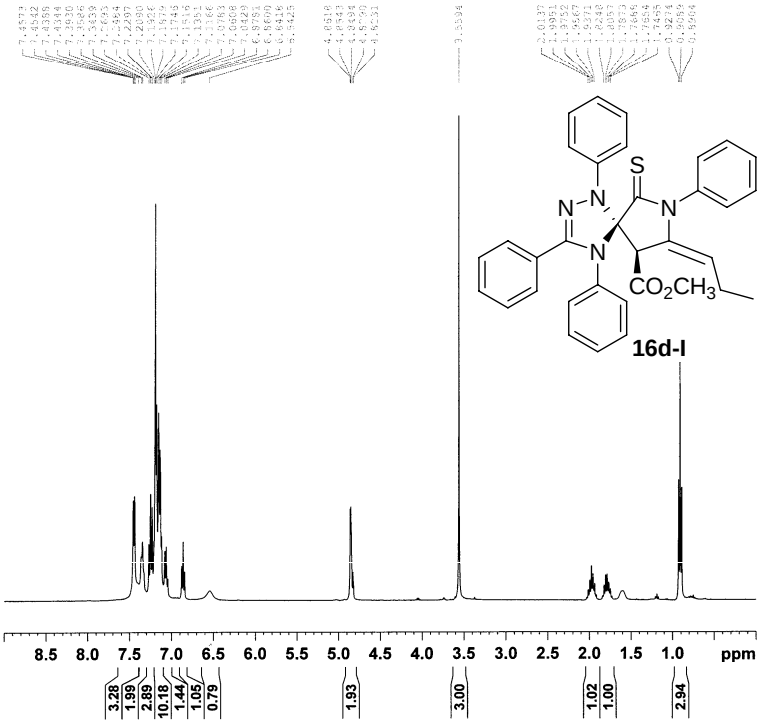
BRUKER

```
Current Data Parameters
NAME        WXR-1-17c2-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080320
Time              15.54
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           4401.409 Hz
FIDRES        0.067160 Hz
AQ            7.4449396 sec
RG                    4
DW              113.600 usec
DE                6.50 usec
TE               294.3 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                13.50 usec
PL1               -1.00 dB
SFO1        400.1720009 MHz

F2 - Processing parameters
SI                32768
SF          400.1700000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



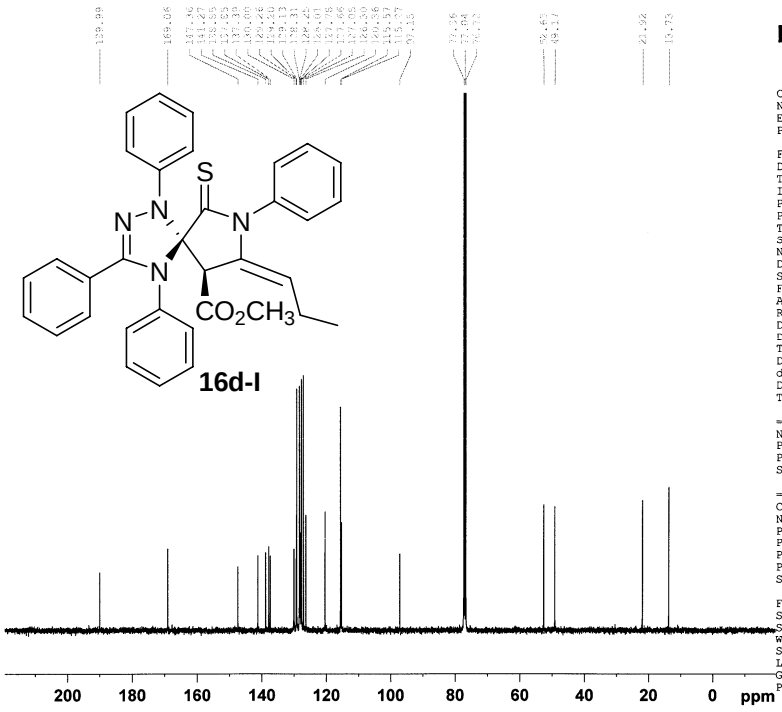
BRUKER

```
Current Data Parameters
NAME        WXR-1-17c-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080321
Time              0.10
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 7200
DS                    4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  203
DW              20.800 usec
DE                6.50 usec
TE               294.9 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                8.40 usec
PL1              -2.00 dB
SFO1        100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PL12              14.46 dB
PL13              14.46 dB
PL2               -1.00 dB
SFO2        400.1716007 MHz

F2 - Processing parameters
SI                32768
SF          100.6227364 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```



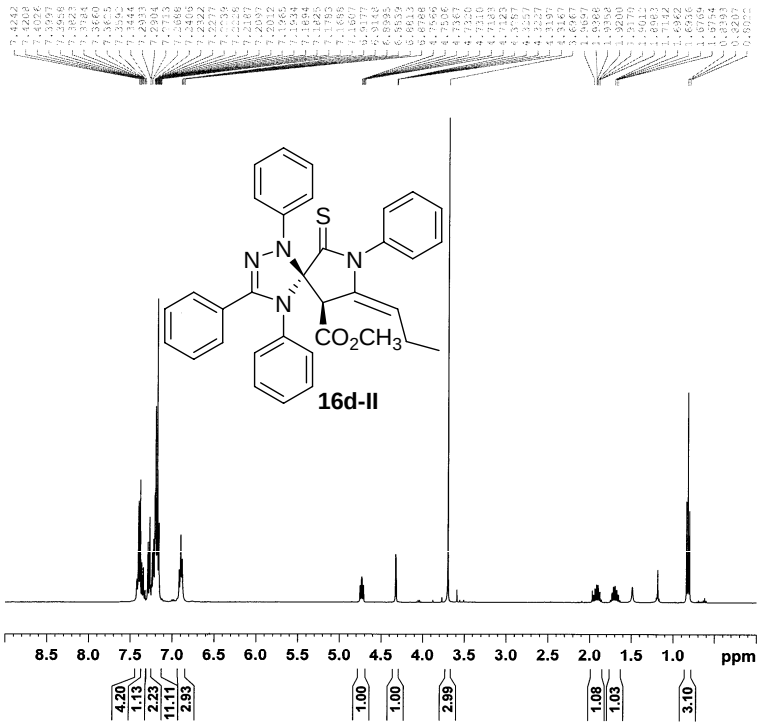
BRUKER

```
Current Data Parameters
NAME            WXR1-17b
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080409
Time_              10.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                296.7 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.50 usec
PL1                -1.00 dB
SFO1         400.1724712 MHz

F2 - Processing parameters
SI                 32768
SF           400.1700317 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

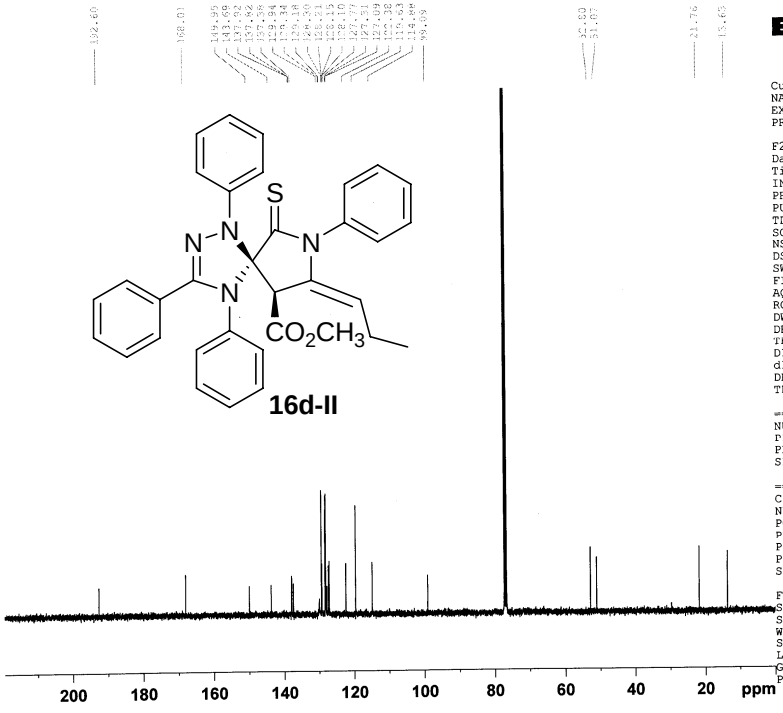


BRUKER

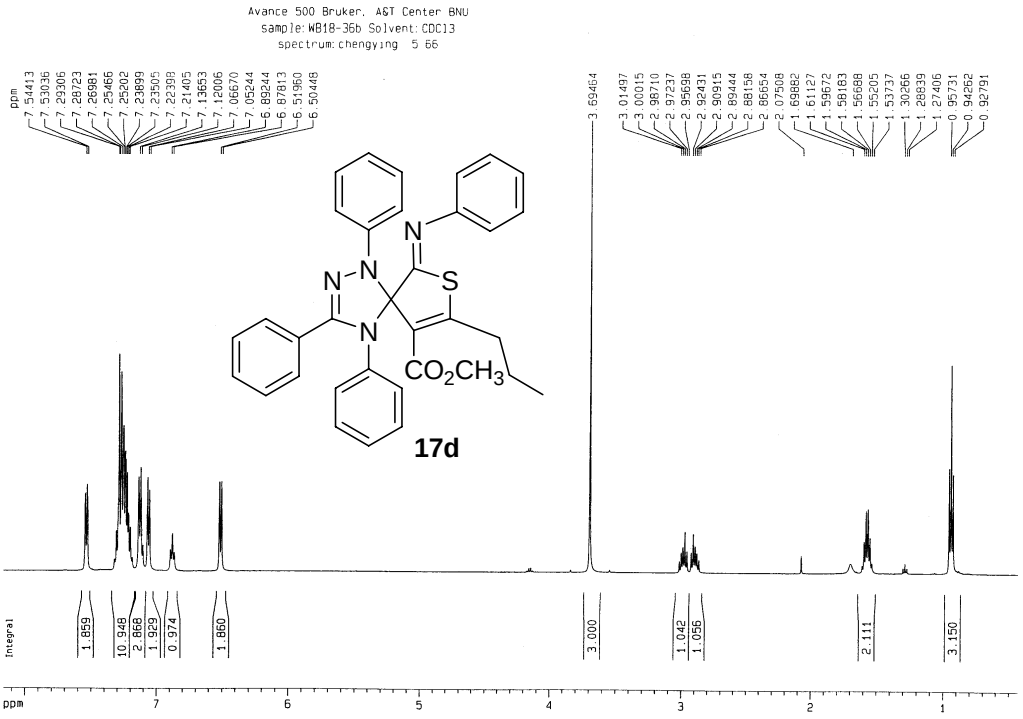
```
Current Data Parameters
NAME        WXR1-17b-C13
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080409
Time_              12.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1200
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.40 usec
PL1                -2.00 dB
SFO1         100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL12               14.46 dB
PL13               14.46 dB
PL2                -1.00 dB
SFO2         400.1716007 MHz

F2 - Processing parameters
SI                 32768
SF           100.6228270 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

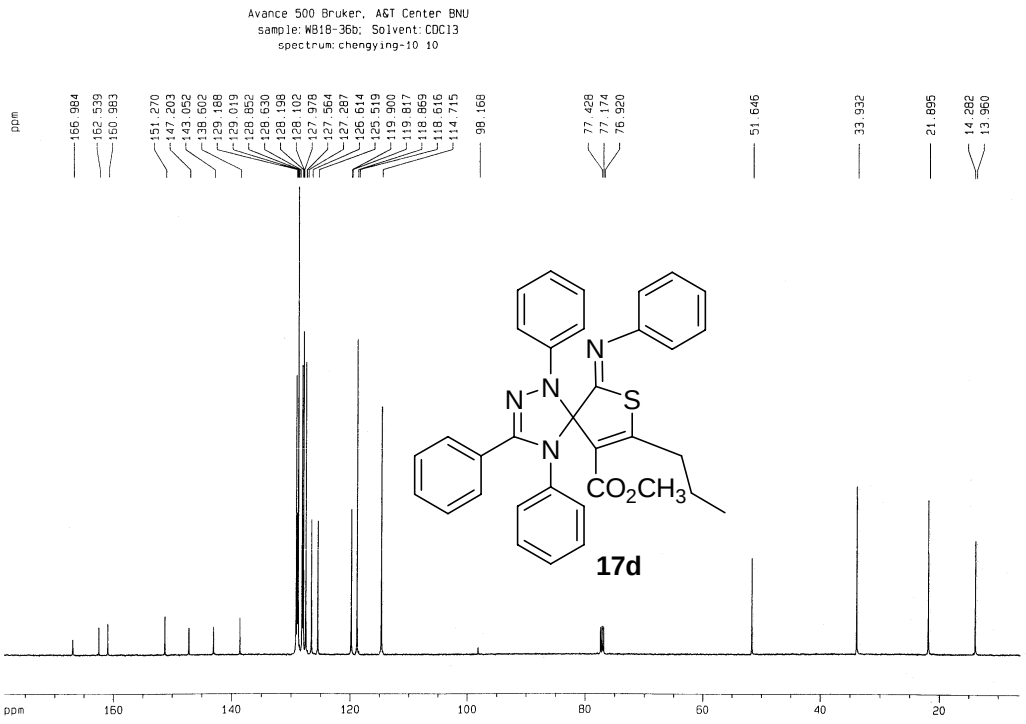


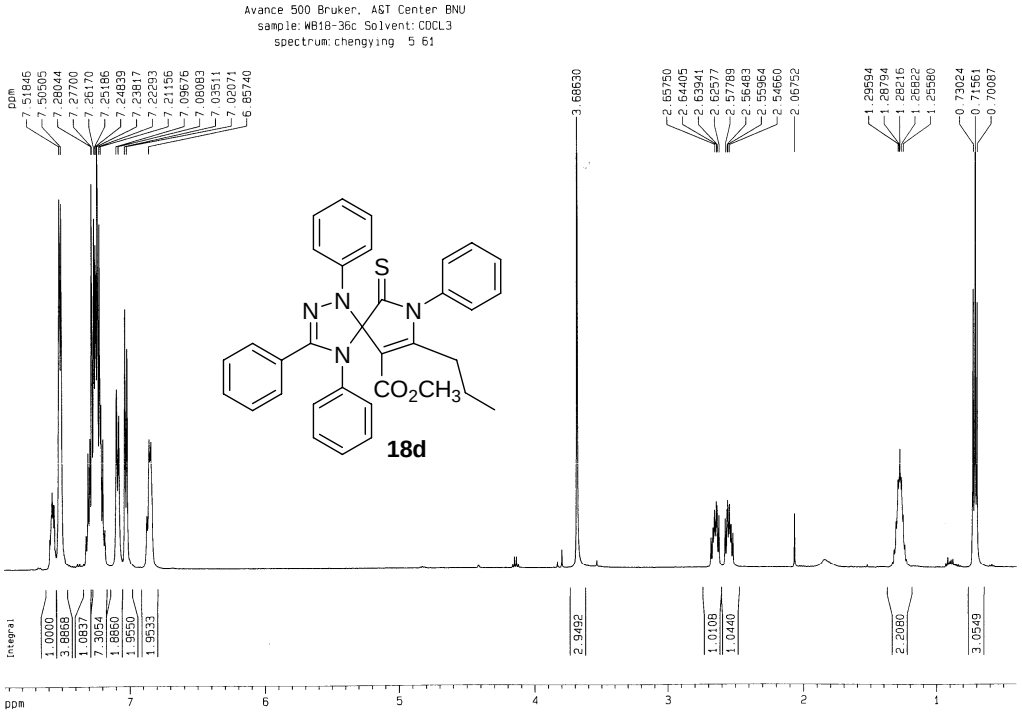

```
Current Data Parameters
NAME        wxr1-21d-xin
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080415
Time              16.49
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.50 usec
TE                299.8 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.50 usec
PL1                -1.00 dB
SFO1         400.1724712 MHz

F2 - Processing parameters
SI                 32768
SF           400.1700341 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

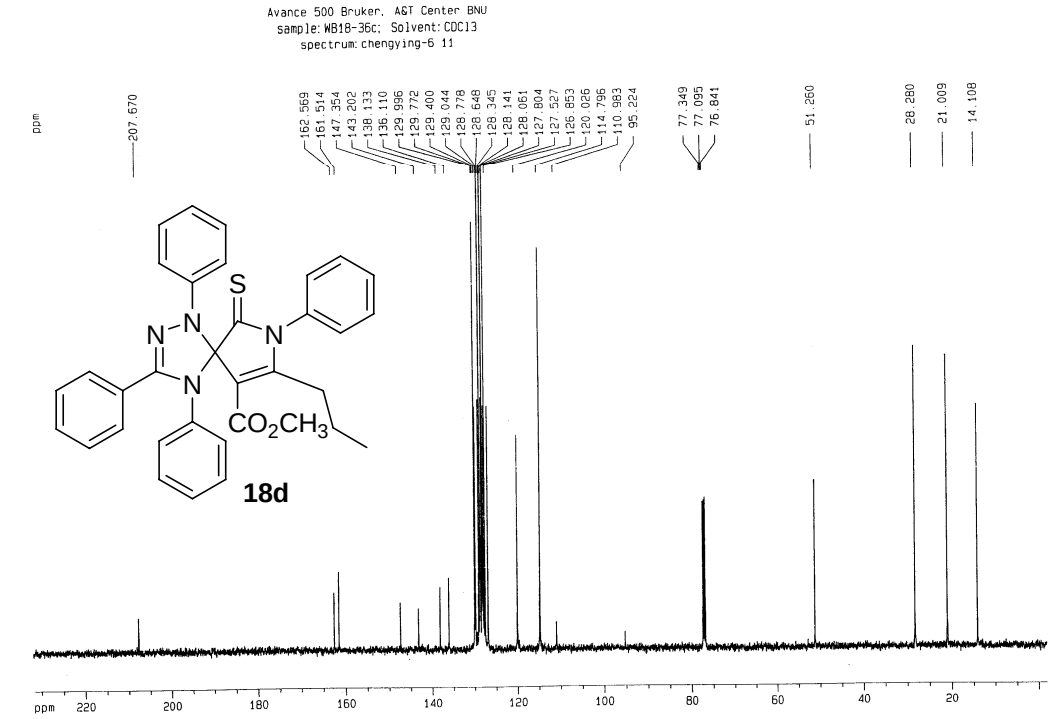


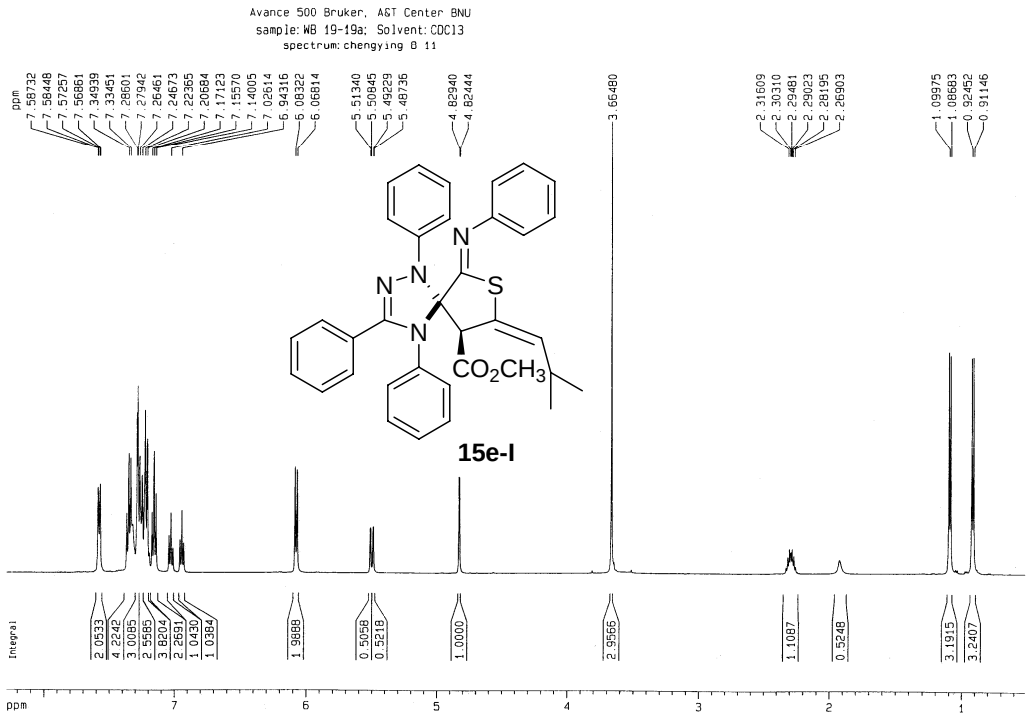

```
Current Data Parameters
NAME          WXR1-21D-X
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080416
Time              10.23
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   603
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                300.7 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.40 usec
PL1                -2.00 dB
SFO1         100.6328888 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL12               14.46 dB
PL13               14.46 dB
PL2                -1.00 dB
SFO2         400.1716007 MHz

F2 - Processing parameters
SI                 32768
SF           100.6228270 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

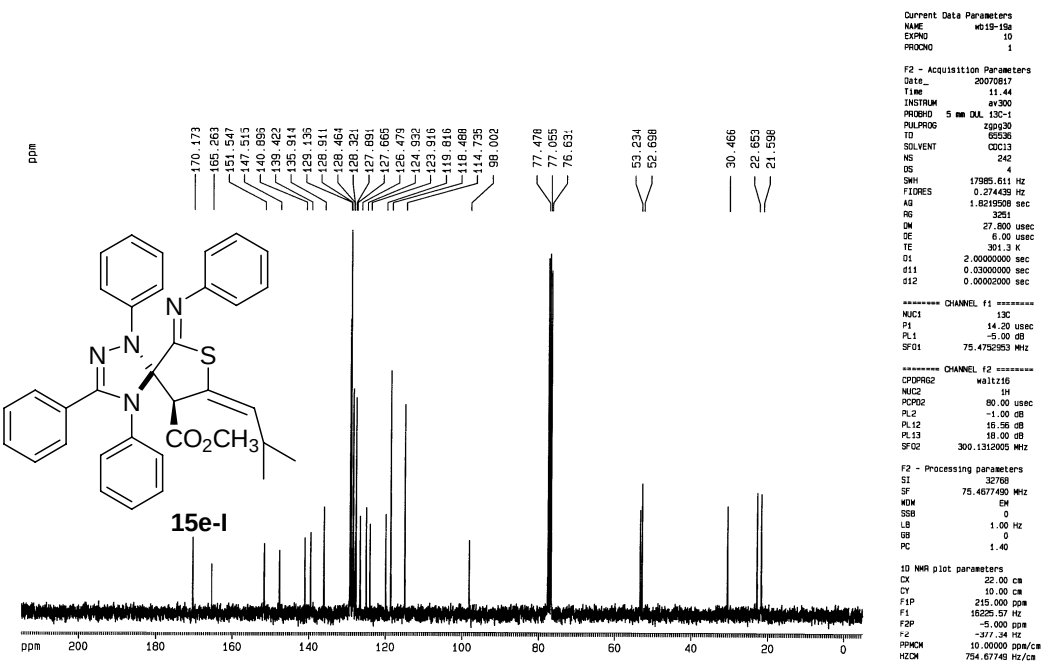

Avance 500 Bruker, A&T Center BNU
sample: WB18-36b Solvent: CDCl3
spectrum: chengying 5 66
17d


Avance 500 Bruker, A&T Center BNU
sample: WB18-36b; Solvent: CDCl3
spectrum: chengying-10 10
17d


Avance 500 Bruker, A&T Center BNU
sample: WB18-36c Solvent: CDCL3
spectrum: chengying 5 61
ppm
7.51845
7.50505
7.28044
7.27700
7.26170
7.25186
7.24839
7.23817
7.22293
7.21156
7.09676
7.08083
7.03511
7.02071
6.85740
3.68630
2.65750
2.64405
2.63941
2.62577
2.57789
2.56483
2.55964
2.54660
2.06752
1.29594
1.28794
1.28216
1.26822
1.25580
0.73024
0.71561
0.70087
Integral
1.0000
3.8858
1.0837
7.3054
1.8860
1.9550
1.9533
2.9492
1.0108
1.0440
2.2080
3.0549
S
N
N
N
N
CO2CH3
18d


Avance 500 Bruker, A&T Center BNU
sample: WB18-36c; Solvent: CDCl3
spectrum: chengying-6 11
ppm
207.670
162.569
161.514
147.354
143.202
138.133
136.110
129.996
129.772
129.400
129.044
128.778
128.648
128.345
128.141
128.061
127.804
127.527
126.853
120.026
114.796
110.983
95.224
77.349
77.095
76.841
51.260
28.280
21.009
14.108
S
N
N
N
N
CO2CH3
18d





Current Data Parameters
NAME wb19-19a
EXPNO 10
PROCNO 1

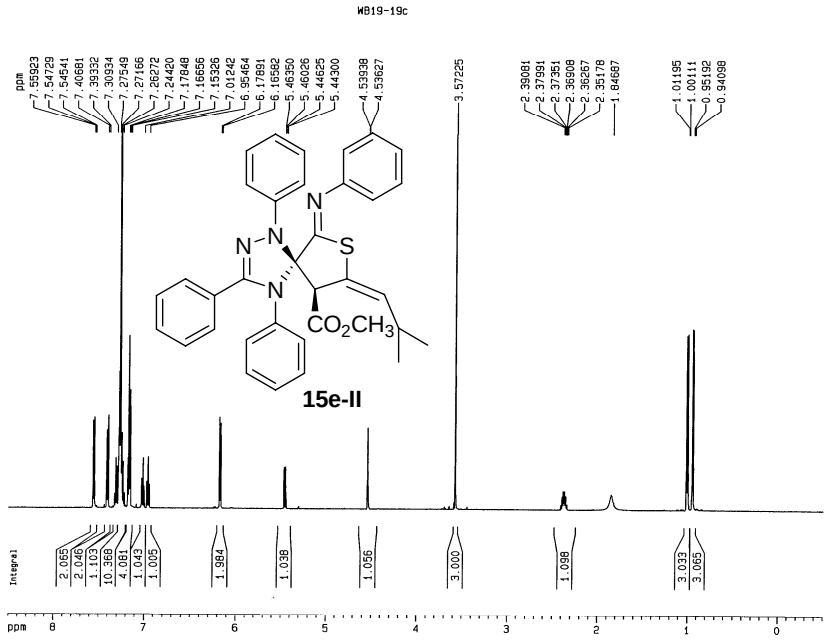
F2 - Acquisition Parameters
Date_ 20070817
Time 11.44
INSTRUM av300
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 242
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 3251
DW 27.800 usec
DE 6.00 usec
TE 301.3 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 14.20 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz

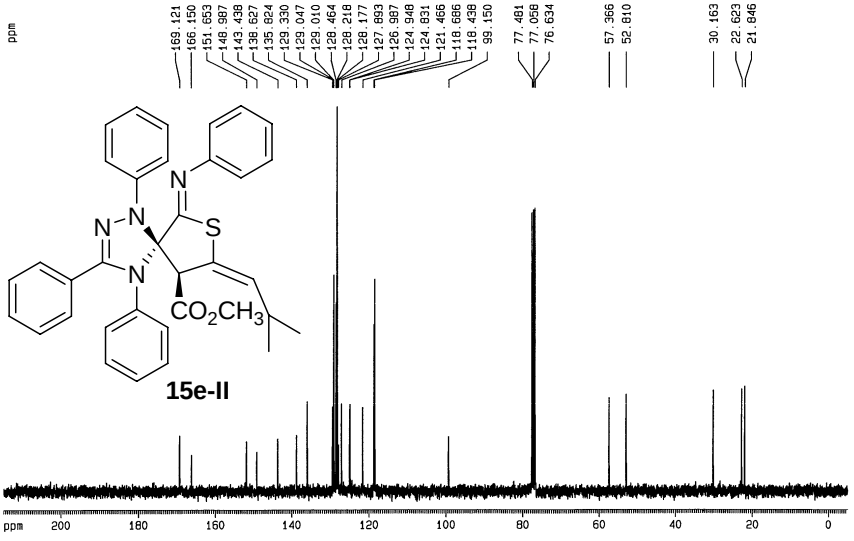
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 16.56 dB
PL13 18.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

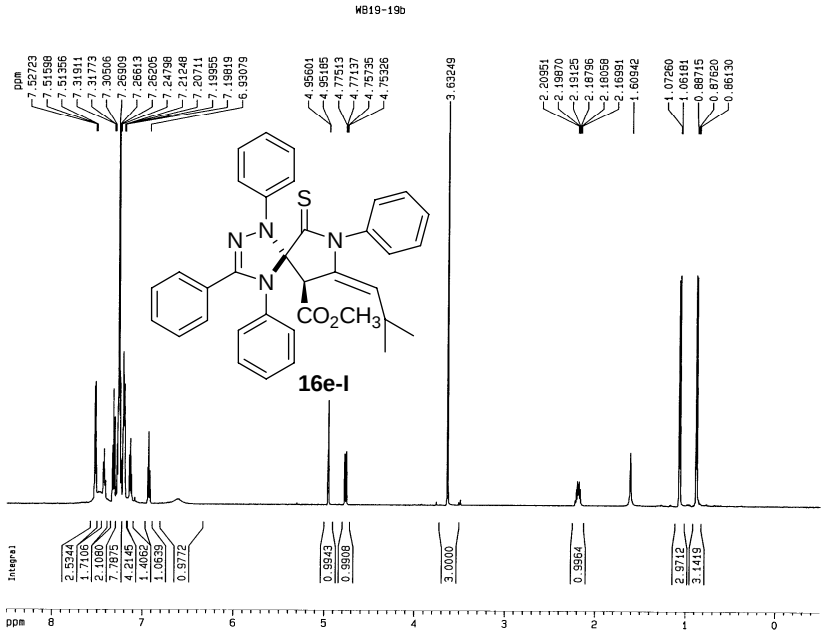
1D NMR plot parameters
CX 22.00 cm
CY 10.00 cm
F1P 215.000 ppm
F1 16225.57 Hz
F2P -5.000 ppm
F2 -377.34 Hz
PPMCM 10.00000 ppm/cm
HZCM 754.67749 Hz/cm



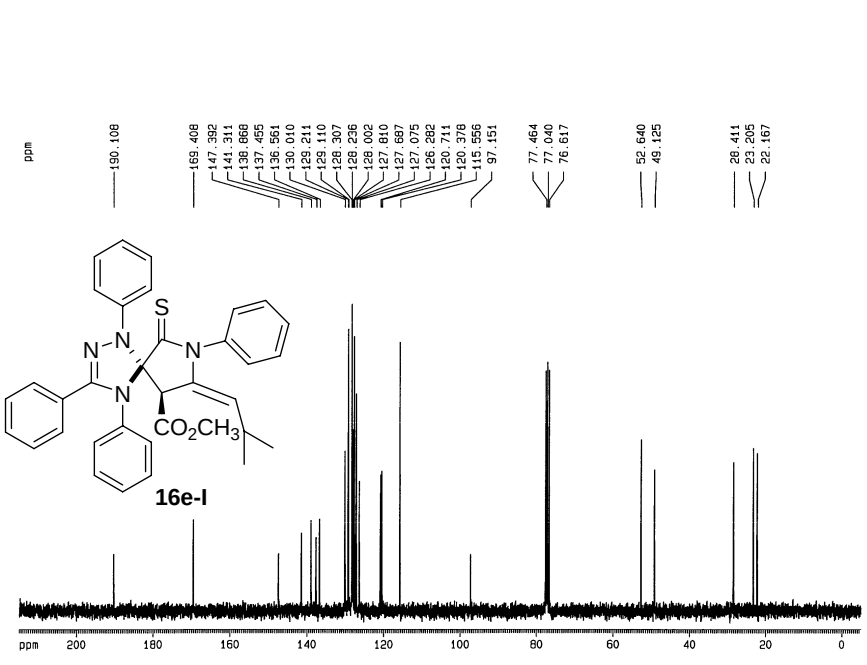

```
Current Data Parameters
NAME                  2
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20070816
Time              14.54
INSTRUM           av600
PROBHD   5 mm BBI 1H-BB
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                  362
DW                27.800 usec
DE                 6.00 usec
TE               298.4 K
D1            5.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1                8.60 usec
PL1              -1.00 dB
SFO1        600.1348010 MHz

F2 - Processing parameters
SI                32768
SF          600.1300088 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                22.00 cm
CY                20.00 cm
F1P               8.500 ppm
F1             5101.10 Hz
F2P              -0.500 ppm
F2             -300.07 Hz
PPMCM          0.40909 ppm/cm
HZCM          245.50774 Hz/cm
```



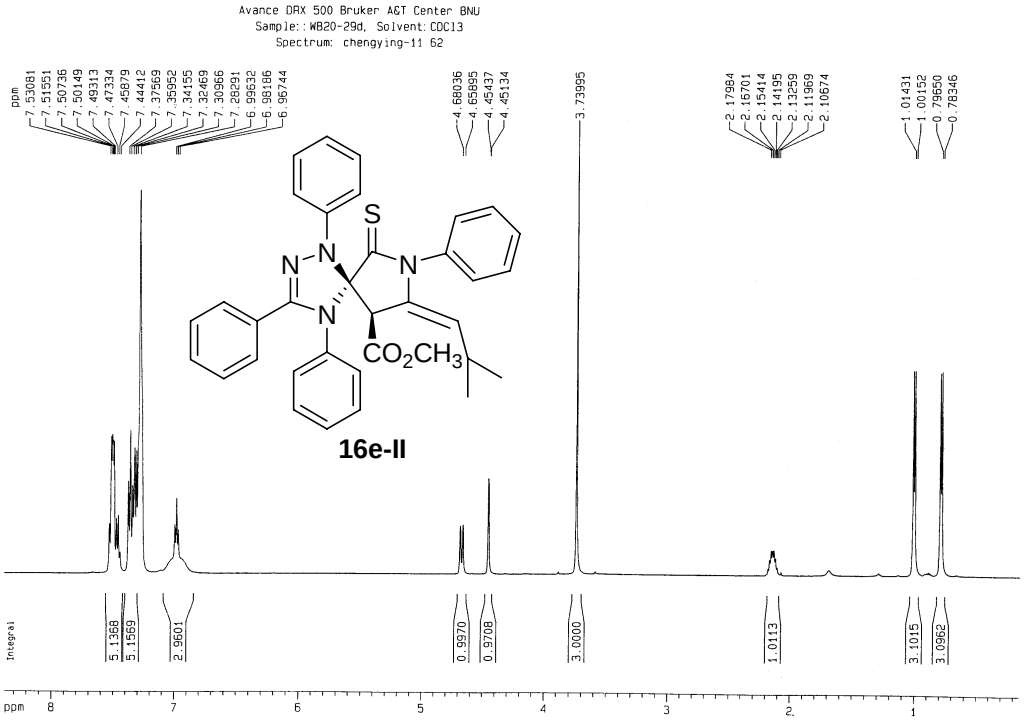

```
Current Data Parameters
NAME          wb19-19cxin
EXPNO                  20
PROCNO                  1

F2 - Acquisition Parameters
Date_          20070817
Time              11.22
INSTRUM           av300
PROBHD   5 mm DUL 13C-1
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                  272
DS                    4
SWH           17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                 2896.3
DW                27.800 usec
DE                 6.00 usec
TE               301.3 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                14.20 usec
PL1               -5.00 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              16.56 dB
PL13              18.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF          75.4677490 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                22.00 cm
CY                10.00 cm
F1P             215.000 ppm
F1             16225.57 Hz
F2P              -5.000 ppm
F2             -377.34 Hz
PPMCM         10.00000 ppm/cm
HZCM          754.67749 Hz/cm
```

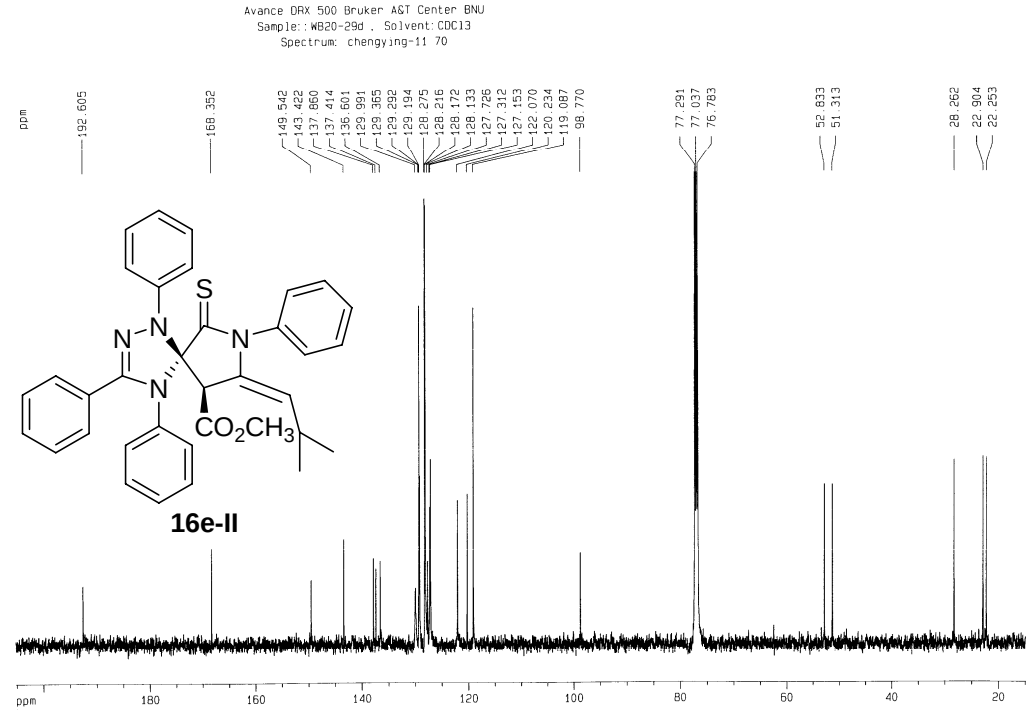


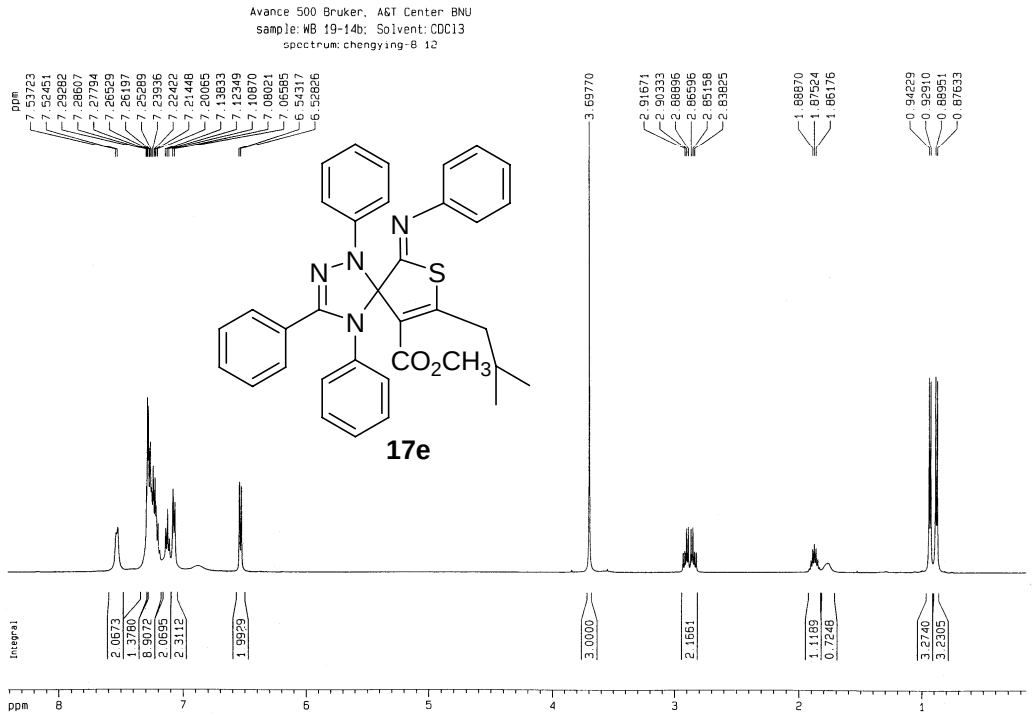

```
Current Data Parameters
NAME                  3
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20070816
Time               15.01
INSTRUM            av600
PROBHD   5 mm BBI 1H-BB
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG                  362
DW               27.800 usec
DE                6.00 usec
TE                298.5 K
D1            5.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                 8.50 usec
PL1               -1.00 dB
SFO1        600.1346010 MHz

F2 - Processing parameters
SI                32768
SF          600.1300088 MHz
WDW                  EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                22.00 cm
CY                20.00 cm
F1P               8.500 ppm
F1             5101.10 Hz
F2P              -0.500 ppm
F2             -300.07 Hz
PPMCM          0.40909 ppm/cm
HZCM           245.50774 Hz/cm
```

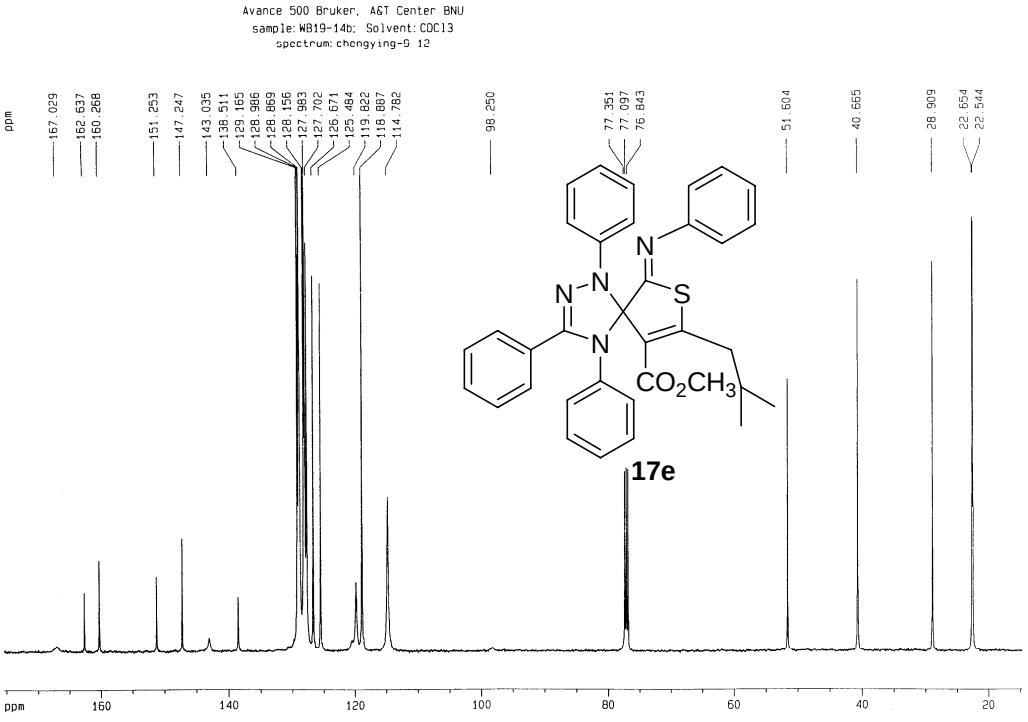


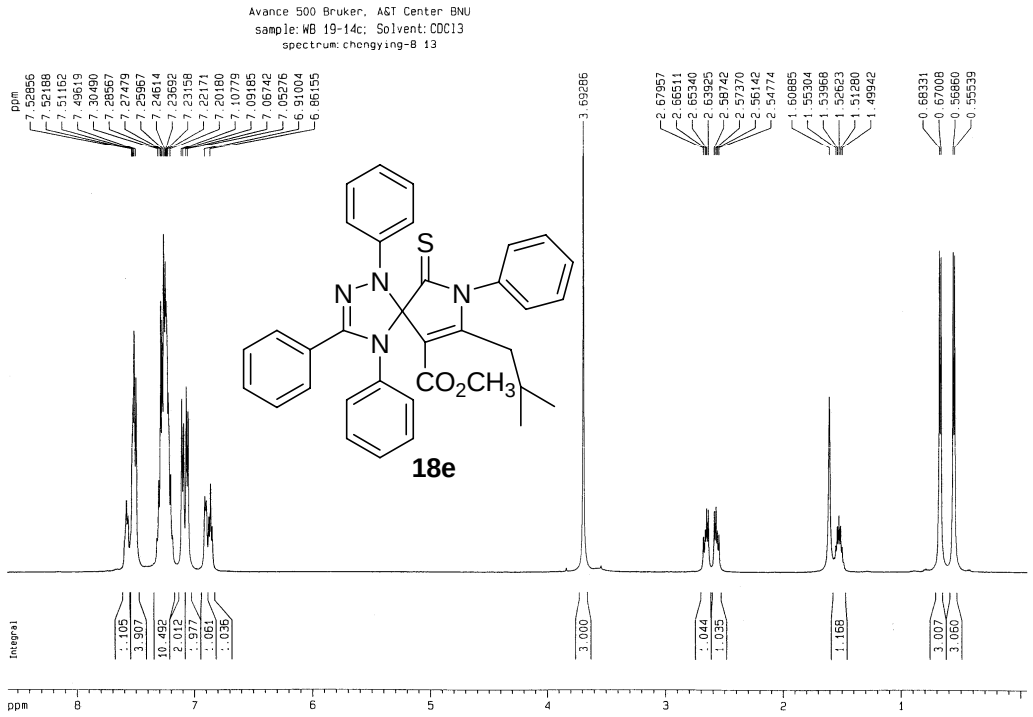

```
Current Data Parameters
NAME             wb19-19b
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_          20070817
Time               11.07
INSTRUM            av300
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  181
DS                    4
SWH           17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG                 2580.3
DW               27.800 usec
DE                6.00 usec
TE                301.3 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                14.20 usec
PL1               -5.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              16.56 dB
PL13              18.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677490 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                22.00 cm
CY                 8.00 cm
F1P             215.000 ppm
F1             16225.57 Hz
F2P              -5.000 ppm
F2             -377.34 Hz
PPMCM          10.00000 ppm/cm
HZCM           754.67749 Hz/cm
```

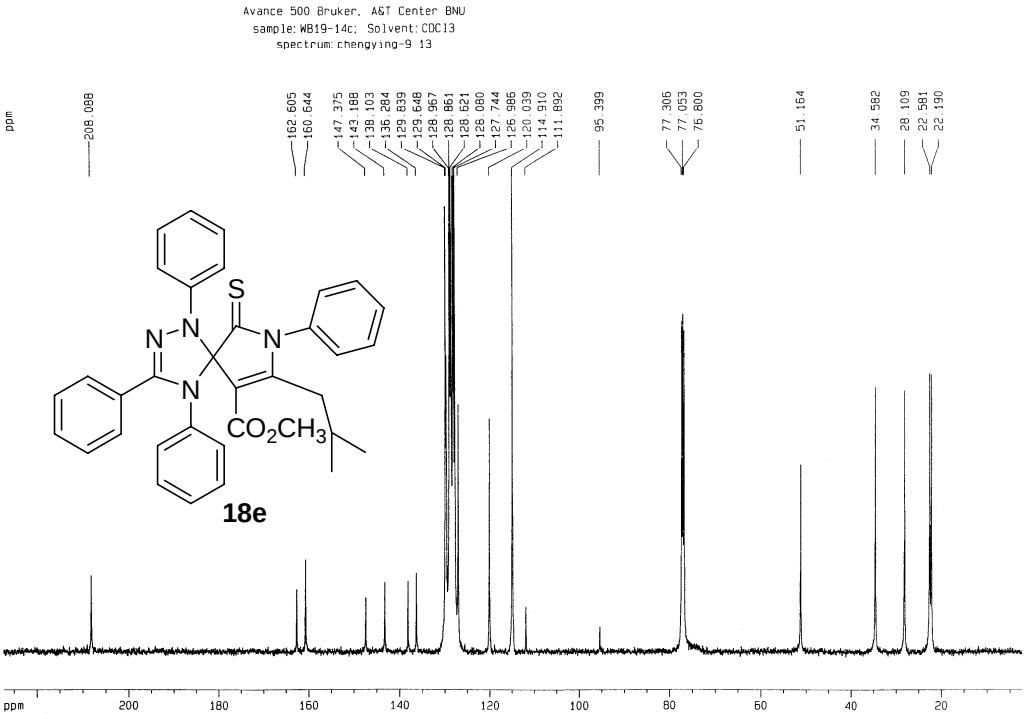

Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-29d, Solvent: CDCl3
Spectrum: chengying-11 62
16e-II


Avance DRX 500 Bruker A&T Center BNU
Sample: : WB20-29d , Solvent: CDCl3
Spectrum: chengying-11 70
16e-II


Avance 500 Bruker, A&T Center BNU
sample: WB 19-14b; Solvent: CDCl3
spectrum: chengying-8 12
ppm
7.53723
7.52451
7.29282
7.28607
7.27794
7.26529
7.26197
7.25289
7.23936
7.22422
7.21448
7.20065
7.13833
7.12349
7.10870
7.08021
7.06585
6.54317
6.52826
3.69770
2.91671
2.90333
2.88896
2.86596
2.85158
2.83825
1.88870
1.87524
1.86176
0.94229
0.92910
0.88951
0.87633
N
N-N
S
N
CO2CH3
17e
Integral
2.0673
1.3760
8.9072
2.0695
2.3112
1.9929
3.0000
2.1661
1.1189
0.7248
3.2740
3.2305
ppm
8
7
6
5
4
3
2
1


Avance 500 Bruker, A&T Center BNU
sample: WB19-14b; Solvent: CDCl3
spectrum: chengying-9 12
ppm
167.029
162.637
160.268
151.253
147.247
143.035
138.511
129.165
128.986
128.869
128.156
127.983
127.702
126.671
125.484
119.822
118.887
114.782
98.250
77.351
77.097
76.843
51.604
40.665
28.909
22.654
22.544
N
N-N
S
N
CO2CH3
17e
ppm
160
140
120
100
80
60
40
20


Avance 500 Bruker, A&T Center BNU
sample: WB 19-14c; Solvent: CDCl3
spectrum: chengying-B 13
ppm
7.52856
7.52188
7.51162
7.49619
7.30490
7.28567
7.27479
7.25967
7.24614
7.23692
7.23158
7.22171
7.20180
7.10779
7.09185
7.06742
7.05276
6.91004
6.86155
3.69286
2.67957
2.66511
2.65340
2.63925
2.58742
2.57370
2.56142
2.54774
1.60885
1.55304
1.53968
1.52623
1.51280
1.49942
0.68331
0.67008
0.56860
0.55539
S
N
N
N
N
CO2CH3
18e
Integral
1.105
3.907
10.492
2.012
.977
1.061
1.036
3.000
.044
1.035
1.168
3.007
3.050
ppm
8
7
6
5
4
3
2
1


Avance 500 Bruker, A&T Center BNU
sample: WB19-14c; Solvent: CDCl3
spectrum: chengying-9 13
ppm
208.088
162.605
160.644
147.375
143.188
138.103
136.284
129.839
129.648
128.967
128.861
128.621
126.080
127.744
126.985
120.039
114.910
111.892
95.399
77.306
77.053
76.800
51.164
34.582
28.109
22.581
22.190
S
N
N
N
N
CO2CH3
18e
ppm
200
180
160
140
120
100
80
60
40
20