Supporting Information

A combined experimental and theoretical study of the polar [3+2] cycloaddition of electrophilically activated carbonyl ylides with aldehydes and imines

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General Methods

Melting points were measured on a Kofler apparatus. ^{1}H and ^{13}C Nuclear Magnetic Resonance (NMR) spectra were recorded at 200 or 300 MHz, and at 50 or 75 MHz, respectively. ^{1}H chemical shifts (δ) are given in ppm relative to the solvent residual peak, and ^{13}C chemical shifts relative to the central peak of the solvent signal. Coupling constants (*J*) are given in Hz. Microwave reactions were performed in open glass containers (Prolabo Synthewave® 402) with accurate control of power (maximum power: 300 W) and temperature (by infrared detection).

Starting Materials

Oxiranes[1] and imines[2] were prepared according to described procedures. Toluene was distilled before use. Reactions were performed under dry argon. Petrol refers to petroleum ether (bp 40–60°C).

Compound Characterizations

Diastereoisomers of 2-phenyl-5-(3,4,5-trimethoxyphenyl)-1,3-dioxolane-4,4-dicarbonitrile (3a,b).[3] The general procedure 1 (reflux of 35 h), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and 3,4,5-trimethoxybenzaldehyde (**2a**, 0.39 g), gave a 77/23 mixture from which the preponderant diastereoisomer **3a** was isolated by recrystallization from petrol/Et_2O 85:15 in 40% yield as a beige powder: mp 122°C; ^{1}H NMR ($(CD_3)_2CO$) δ 3.83 (s, 3H), 3.93 (s, 6H), 6.04 (s, 1H), 6.59 (s, 1H), 7.03 (s, 2H), 7.6 (m, 3H), 7.8 (m, 2H); ^{13}C NMR ($(CD_3)_2CO$) δ 56.7 (2C), 60.7, 70.8, 87.9, 104.8 (2C), 108.5, 113.1, 113.4, 126.4, 128.4 (2C), 129.8 (2C), 132.0, 134.3, 141.0, 155.0 (2C); HRMS, *m*/*z*: 366.1189 found (calcd for $C_{20}H_{18}N_2O_5$, $M^{+\bullet}$ requires: 366.1216). The minor diastereoisomer **3b** was identified by the ^{1}H NMR spectra of an enriched fraction: ^{1}H NMR ($(CD_3)_2CO$) δ 3.83 (s, 3H), 3.93 (s, 6H), 5.94 (s, 1H), 6.98 (s, 1H), 7.03 (s, 2H), 7.6 (m, 3H), 7.8 (m, 2H). The general procedure 2 (60 W, 9 min to reach 100°C, 12 min to reach 120°C, and 45 min at 120°C), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and 3,4,5-trimethoxybenzaldehyde (**2a**, 0.39 g), gave a 68/32 mixture from

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[1] Baudy, M.; Robert, A.; Foucaud, A. *J. Org. Chem.* **1978**, *43*, 3732-3736.
[2] Chérouvrier, J.-R.; Carreaux, F.; Bazureau, J. P. *Tetrahedron Lett.* **2002**, *43*, 3581-3584.
[3] Bentabed, G.; Rahmouni, M.; Mongin, F.; Derdour, A.; Hamelin, J.; Bazureau, J. P. *Synth. Commun.* **2007**, *37*, 2935-2948.

which the preponderant diastereoisomer **3a** was isolated by recrystallization from petrol/Et_2O 85:15 in 49% yield.

Diastereoisomers of 2-(4-chlorophenyl)-5-(3,4,5-trimethoxyphenyl)-1,3-dioxolane-4,4-dicarbonitrile (4a,b).[3] The general procedure 1 (reflux of 68 h), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and 3,4,5-trimethoxybenzaldehyde (**2a**, 0.39 g), gave a 72/28 mixture from which the preponderant diastereoisomer **4a** was isolated by recrystallization from petrol/Et_2O 85:15 in 42% yield as a white powder: mp 123°C; ^{1}H NMR ($(CD_3)_2CO$) δ 3.80 (s, 3H), 3.89 (s, 6H), 6.00 (s, 1H), 6.57 (s, 1H), 6.99 (s, 2H), 7.60 (d, 2H, *J* = 8.4), 7.74 (d, 2H, *J* = 8.4); ^{13}C NMR ($(CD_3)_2CO$) δ 56.7 (2C), 60.7, 70.8, 87.9, 104.9 (2C), 107.6, 112.9, 113.3, 126.2, 130.0 (2C), 130.1 (2C), 133.1, 137.4, 141.0, 155.0 (2C); HRMS, *m*/*z*: 400.0830 found (calcd for $C_{20}H_{17}N_2O_5{}^{35}Cl$, $M^{+\bullet}$ requires: 400.0826). The minor diastereoisomer **4b** was identified by the ^{1}H NMR spectra of an enriched fraction: ^{1}H NMR ($(CD_3)_2CO$) δ 3.83 (s, 3H), 3.91 (s, 6H), 5.92 (s, 1H), 6.96 (s, 1H), 7.02 (s, 2H), 7.6 (m, 4H); ^{1}H NMR ($CDCl_3$) δ 4.03 (s, 3H), 4.07 (s, 6H), 5.43 (s, 1H), 6.84 (s, 1H), 6.89 (s, 2H), 7.5 (m, 4H). The general procedure 2 (60 W, 9 min to reach 100°C, 12 min to reach 120°C, and 40 min at 120°C), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and 3,4,5-trimethoxybenzaldehyde (**2a**, 0.39 g), gave a 71/29 mixture from which the preponderant diastereoisomer **4a** was isolated by recrystallization from petrol/Et_2O 85:15 in 45% yield.

Diastereoisomers of 2-(4-methoxyphenyl)-5-(3,4,5-trimethoxyphenyl)-1,3-dioxolane-4,4-dicarbonitrile (5a,b).[3] The general procedure 1 (reflux of 45 h), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and 3,4,5-trimethoxybenzaldehyde (**2a**, 0.39 g), gave a 68/32 mixture from which the preponderant diastereoisomer **5a** was isolated by recrystallization from petrol/Et_2O 85:15 in 52% yield as a white powder: mp 110°C; ^{1}H NMR ($(CD_3)_2CO$) δ 3.82 (s, 3H), 3.91 (s, 3H), 3.93 (s, 6H), 5.99 (s, 1H), 6.53 (s, 1H), 7.02 (s, 2H), 7.13 (d, 2H, *J* = 8.8), 7.68 (d, 2H, *J* = 8.8); ^{13}C NMR ($(CD_3)_2CO$) δ 55.8, 56.6 (2C), 60.7, 70.7, 87.7, 104.8 (2C), 108.7, 113.1, 113.5, 115.1 (2C), 126.1, 126.6, 130.1 (2C), 141.0, 155.0 (2C), 162.8; HRMS, *m*/*z*: 396.1356 found (calcd for $C_{21}H_{20}N_2O_6$, $M^{+\bullet}$ requires: 396.1321). The minor diastereoisomer **5b** was identified by the ^{1}H NMR spectra of an enriched fraction: ^{1}H NMR ($(CD_3)_2CO$) δ 3.86 (s, 3H), 3.89 (s, 3H), 3.95 (s, 6H), 5.96 (s, 1H), 6.89 (s, 1H), 7.02 (s, 2H), 7.13 (d, 2H, *J* = 8.8), 7.68 (d, 2H, *J* = 8.8). The general procedure 2 (60 W, 3 min to reach 60°C, 6 min to reach 80°C, and 35 min at 80°C), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and 3,4,5-trimethoxybenzaldehyde (**2a**, 0.39 g), gave a 70/30 mixture from which the preponderant diastereoisomer **5a** was isolated by recrystallization from petrol/Et_2O 85:15 in 55% yield.

Diastereoisomers of 5-(1,3-benzodioxol-5-yl)-2-phenyl-1,3-dioxolane-4,4-dicarbonitrile (6a,b).[3] The general procedure 1 (reflux of 96 h), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and piperonal (**2b**, 0.30 g), gave a 58/42 mixture from which the preponderant diastereoisomer **6a** was isolated by recrystallization from petrol/Et_2O 80:20 in 31% yield as a whitish powder: mp 126°C; ^{1}H NMR ($(CD_3)_2CO$) δ 6.04 (s, 1H), 6.17 (s, 2H), 6.58 (s, 1H), 7.08 (d, 1H, *J* = 7.7), 7.23 (s, 1H), 7.25 (d, 1H, *J* = 7.6), 7.6 (m, 3H), 7.8 (m, 2H); ^{13}C NMR ($(CD_3)_2CO$) δ 70.8, 87.7, 102.9, 107.3, 108.5, 109.6, 113.0, 113.4, 121.8, 124.7, 128.4 (2C), 129.8 (2C), 132.0, 134.3, 149.4, 150.6; HRMS, *m*/*z*: 320.0774 found (calcd for $C_{18}H_{12}N_2O_4$, $M^{+\bullet}$ requires: 320.0797). The minor diastereoisomer **6b** was identified by the ^{1}H NMR spectra of an enriched fraction: ^{1}H NMR ($(CD_3)_2CO$) δ 5.96 (s, 1H), 6.17 (s, 2H), 6.95 (s, 1H), 7.08 (d, 1H, *J* = 7.7), 7.23 (s, 1H), 7.25 (d, 1H, *J* = 7.6), 7.6 (m, 3H), 7.7 (m, 2H). The general procedure 2 (60 W, 6 min to reach 100°C, 9 min to reach 120°C, and 40 min at 120°C), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and piperonal (**2b**, 0.30 g), gave a 66/34 mixture from which the preponderant diastereoisomer **6a** was isolated by recristallization from petrol/Et_2O 80:20 in 25% yield.

Diastereoisomers of 5-(1,3-benzodioxol-5-yl)-2-(4-chlorophenyl)-1,3-dioxolane-4,4-dicarbonitrile (7a,b).[3] The general procedure 1 (reflux of 72 h), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and piperonal (**2b**, 0.30 g), gave a 60/40 mixture from which the preponderant diastereoisomer **7a** was isolated by recrystallization from petrol/Et_2O 80:20 in 28% yield as a white powder: mp 130°C; ^{1}H NMR ($(CD_3)_2CO$) δ 6.05 (s, 1H), 6.16 (s, 2H), 6.60 (s, 1H), 7.07 (d, 1H, *J* = 8.6), 7.23 (s, 1H), 7.24 (d, 1H, *J* = 7.1), 7.65 (d, 2H, *J* = 8.5), 7.79 (d, 2H, *J* = 8.5); ^{13}C NMR ($(CD_3)_2CO$) δ 70.8, 87.8, 102.9, 107.3, 107.5, 109.6, 112.9, 113.3, 121.8, 124.5, 130.0 (2C), 130.2 (2C), 133.2, 137.4, 149.4, 150.6; HRMS, *m*/*z*: 354.0406 found (calcd for $C_{18}H_{11}N_2O_4{}^{35}Cl$, $M^{+\bullet}$ requires: 354.0407). The minor diastereoisomer **7b** was identified by the ^{1}H NMR spectra of an enriched fraction: ^{1}H NMR ($(CD_3)_2CO$) δ 5.98 (s, 1H), 6.16 (s, 2H), 6.97 (s, 1H), 7.07 (d, 1H, *J* = 8.6), 7.23 (s, 1H), 7.24 (d, 1H, *J* = 7.1), 7.65 (d, 2H, *J* = 8.5), 7.79 (d, 2H, *J* = 8.5). The general procedure 2 (60 W, 6 min to reach 100°C, 9 min to reach 120°C, and 40 min at 120°C), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and piperonal (**2b**, 0.30 g), gave a 60/40 mixture from which the preponderant diastereoisomer **7a** was isolated by recristallization from petrol/Et_2O 80:20 in 39% yield.

Diastereoisomers of 5-(1,3-benzodioxol-5-yl)-2-(4-methoxyphenyl)-1,3-dioxolane-4,4-dicarbonitrile (8a,b).[3] The general procedure 1 (reflux of 48 h), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and piperonal (**2b**, 0.30 g), gave a 71/29 mixture from which the preponderant diastereoisomer **8a** was isolated by recrystallization from petrol/Et_2O 80:20 in 54%

yield as a beige powder: mp 137°C; ^{1}H NMR ($(CD_3)_2CO$) δ 3.91 (s, 3H), 5.98 (s, 1H), 6.16 (s, 2H), 6.51 (s, 1H), 7.1 (m, 5H), 7.67 (d, 2H, *J* = 6.7); ^{13}C NMR ($(CD_3)_2CO$) δ 55.8, 70.7, 87.5, 102.9, 107.3, 108.6, 109.6, 112.9, 113.3, 115.1 (2C), 121.7, 124.8, 126.1, 130.1 (2C), 149.4, 150.5, 162.8; HRMS, *m*/*z*: 350.0910 found (calcd for $C_{19}H_{14}N_2O_5$, $M^{+\bullet}$ requires: 350.0903). The minor diastereoisomer **8b** was identified by the ^{1}H NMR spectra of an enriched fraction: ^{1}H NMR ($(CD_3)_2CO$) δ 3.88 (s, 3H), 5.98 (s, 1H), 6.16 (s, 2H), 6.87 (s, 1H), 7.1 (m, 5H), 7.67 (d, 2H, *J* = 6.7). The general procedure 2 (60 W, 3 min to reach 60°C, 6 min to reach 80°C, and 30 min at 80°C), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and piperonal (**2b**, 0.30 g), gave a 67/33 mixture from which the preponderant diastereoisomer **8a** was isolated by recristallization from petrol/Et_2O 80:20 in 40% yield.

3-Methyl-2,4-diphenyloxazolidine-5,5-dicarbonitrile (26a).[3] The general procedure 3 (reflux of 24 h), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and *N*-(phenylmethylene)methanamine (**25a**, 0.24 g), gave 52% of **26a** as a brown powder: mp 128°C; ^{1}H NMR ($CDCl_3$) δ 2.17 (s, 3H), 4.27 (s, 1H), 5.12 (s, 1H), 7.6 (m, 10H); ^{13}C NMR ($CDCl_3$) δ 34.2, 71.3, 77.4, 100.8, 112.3, 112.8, 128.5 (2C), 128.7 (2C), 128.9 (2C), 129.4 (2C), 129.7, 130.7, 130.8, 134.7; HRMS, *m*/*z*: 288.1133 found (calcd for $C_{18}H_{14}N_3O$, $[M\text{-}H]^{+\bullet}$ requires: 288.1133). The general procedure 4 (120 W, 6 min to reach 100°C, 12 min to reach 125°C, and 55 min at 125°C), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and *N*-(phenylmethylene)methanamine (**25a**, 0.24 g), gave 35% of **26a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

2-(4-Chlorophenyl)-3-methyl-4-phenyloxazolidine-5,5-dicarbonitrile (27a).[3] The general procedure 3 (reflux of 20 h), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and *N*-(phenylmethylene)methanamine (**25a**, 0.24 g), gave 60% of **27a** as a brown glitter: mp 114°C; ^{1}H NMR ($CDCl_3$) δ 2.21 (s, 3H), 4.31 (s, 1H), 5.14 (s, 1H), 7.6 (m, 9H); ^{13}C NMR ($CDCl_3$) δ 30.9, 71.2, 77.3, 99.9, 112.2, 112.6, 128.5 (2C), 129.2 (2C), 129.4, 129.5 (2C), 130.0 (2C), 130.8, 133.3, 136.8; HRMS, *m*/*z*: 322.0739 found (calcd for $C_{18}H_{13}{}^{35}ClN_3O$, $[M\text{-}H]^{+\bullet}$ requires: 322.0747). The general procedure 4 (120 W, 6 min to reach 100°C, 12 min to reach 125°C, and 50 min at 125°C), using 3-phenyloxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and *N*-(phenylmethylene)methanamine (**25a**, 0.24 g), gave 48% of **27a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

2-(4-Methoxyphenyl)-3-methyl-4-phenyloxazolidine-5,5-dicarbonitrile (28a).[3] The general procedure 3 (reflux of 5 h), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and *N*-(phenylmethylene)methanamine (**25a**, 0.24 g), gave 78% of **28a** as a yellow glitter: mp 149°C; ^{1}H NMR ($CDCl_3$) δ 2.15 (s, 3H), 3.86 (s, 3H), 4.24 (s, 1H), 5.08 (s, 1H), 6.99 (d, 2H, *J* = 8.7), 7.6 (m, 7H); ^{13}C NMR ($CDCl_3$) δ 34.3, 55.4, 71.0, 77.3, 100.6, 112.4, 112.9, 114.3 (2C), 126.6, 128.5 (2C), 129.4

(2C), 129.8, 130.1 (2C), 130.6, 161.5; HRMS, *m*/*z*: 319.1330 found (calcd for $C_{19}H_{17}N_3O_2$, $M^{+\bullet}$ requires: 319.1321). The general procedure 4 (60 W, 3 min to reach 60°C, 6 min to reach 80°C, and 25 min at 80°C), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and *N*-(phenylmethylene)methanamine (**25a**, 0.24 g), gave 85% of **28a** after recrystallization from CH_2Cl_2.

3-Methyl-2-(4-nitrophenyl)-4-phenyloxazolidine-5,5-dicarbonitrile (29a).[3] The general procedure 3 (reflux of 35 h), using 3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (**1d**, 0.43 g) and *N*-(phenylmethylene)methanamine (**25a**, 0.24 g), gave 40% of **29a** as a beige powder: mp 164°C; ^{1}H NMR ($CDCl_3$) δ 2.22 (s, 3H), 4.38 (s, 1H), 5.22 (s, 1H), 7.6 (m, 5H), 7.82 (d, 2H, *J* = 8.7), 8.36 (d, 2H, *J* = 8.7); ^{13}C NMR ($CDCl_3$) δ 34.2, 71.4, 77.3, 99.0, 111.9, 112.3, 124.2 (2C), 128.4 (2C), 128.6, 128.9, 129.6 (2C), 129.7 (2C), 131.0, 141.5; HRMS, *m*/*z*: 333.0995 found (calcd for $C_{18}H_{13}N_4O_3$, $[M-H]^{+\bullet}$ requires: 333.0988). The general procedure 4 (150 W, 10 min to reach 100°C, 15 min to reach 125°C, and 60 min at 125°C), using 3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (**1d**, 0.43 g) and *N*-(phenylmethylene)methanamine (**25a**, 0.24 g), gave 33% of **29a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-2-phenyl-3-propyloxazolidine-5,5-dicarbonitrile (30a).[3] The general procedure 3 (reflux of 27 h), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and *N*-(1,3-benzodioxol-5-ylmethylene)propylamine (**25b**, 0.38 g), gave 48% of **30a** as a beige glitter: mp 101°C; ^{1}H NMR ($CDCl_3$) δ 0.66 (t, 3H, *J* = 7.3), 1.05 (n, 2H, *J* = 7.3), 2.6 (m, 2H), 4.41 (s, 1H), 5.33 (s, 1H), 6.05 (s, 2H), 6.91 (d, 1H, *J* = 8.0), 7.12 (dd, 1H, *J* = 8.0 and 1.5), 7.19 (d, 1H, *J* = 1.5), 7.4 (m, 3H), 7.6 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 11.6, 18.9, 49.9, 71.2, 75.5, 99.2, 101.7, 108.4, 108.9, 112.5, 112.9, 122.9, 123.7, 128.7 (2C), 128.8 (2C), 130.6, 135.9, 148.5, 149.5; HRMS, *m*/*z*: 361.1421 found (calcd for $C_{21}H_{19}N_3O_3$, $M^{+\bullet}$ requires: 361.1426). The general procedure 4 (120 W, 6 min to reach 100°C, 12 min to reach 125°C, and 55 min at 125°C), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and *N*-(1,3-benzodioxol-5-ylmethylene)propylamine (**25b**, 0.38 g), gave 32% of **30a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-2-(4-chlorophenyl)-3-propyloxazolidine-5,5-dicarbonitrile (31a).[3] The general procedure 3 (reflux of 25 h), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and *N*-(1,3-benzodioxol-5-ylmethylene)propylamine (**25b**, 0.38 g), gave 59% of **31a** as a beige powder: mp 140°C; ^{1}H NMR ($CDCl_3$) δ 0.64 (t, 3H, *J* = 7.3), 1.11 (n, 2H, *J* = 7.2), 2.5 (m, 2H), 4.41 (s, 1H), 5.31 (s, 1H), 6.06 (s, 2H), 6.91 (d, 1H, *J* = 8.0), 7.11 (dd, 1H, *J* = 8.0 and 1.7), 7.16 (d, 1H, *J* = 1.6), 7.44 (d, 2H, *J* = 8.5), 7.56 (d, 2H, *J* = 8.5); ^{13}C NMR ($CDCl_3$) δ 11.6, 19.1, 50.0, 71.1, 75.5, 98.4, 101.7, 108.3, 108.9, 112.4, 112.7, 122.9, 123.4, 129.2 (2C), 130.0 (2C), 134.6, 136.6, 148.6, 149.6; HRMS, *m*/*z*: 315.1013 found (calcd for $C_{18}H_{18}{}^{35}ClNO_2$, $[M-OC(CN)_2]^{+\bullet}$ requires: 315.1026). The

general procedure 4 (120 W, 6 min to reach 100°C, 12 min to reach 125°C, and 45 min at 125°C), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and *N*-(1,3-benzodioxol-5-ylmethylene)propylamine (**25b**, 0.38 g), gave 40% of **31a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-2-(4-methoxyphenyl)-3-propyloxazolidine-5,5-dicarbonitrile (32a).[3] The general procedure 3 (reflux of 9 h), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and *N*-(1,3-benzodioxol-5-ylmethylene)propylamine (**25b**, 0.38 g), gave 60% of **32a** as yellow needles: mp 138°C; ^{1}H NMR ($CDCl_3$) δ 0.65 (t, 3H, *J* = 7.3), 1.07 (n, 2H, *J* = 7.3), 2.5 (m, 2H), 3.85 (s, 3H), 4.41 (s, 1H), 5.31 (s, 1H), 6.05 (s, 2H), 7.0 (m, 3H), 7.11 (dd, 1H, *J* = 8.0 and 1.7), 7.18 (d, 1H, *J* = 1.6), 7.5 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 11.7, 18.9, 50.0, 55.4, 71.0, 75.5, 99.1, 101.7, 108.4, 108.9, 112.7, 113.0, 114.2 (2C), 122.9, 123.9, 127.9, 130.1 (2C), 148.5, 149.5, 161.4; HRMS, *m*/*z*: 311.1526 found (calcd for $C_{19}H_{21}NO_3$, $[M\text{-}OC(CN)_2]^{+\bullet}$ requires: 311.1521). The general procedure 4 (60 W, 3 min to reach 60°C, 6 min to reach 80°C, and 30 min at 80°C), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and *N*-(1,3-benzodioxol-5-ylmethylene)propylamine (**25b**, 0.38 g), gave 80% of **32a** after recrystallization from CH_2Cl_2.

4-(1,3-Benzodioxol-5-yl)-2-(4-nitrophenyl)-3-propyloxazolidine-5,5-dicarbonitrile (33a).[3] The general procedure 3 (reflux of 45 h), using 3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (**1d**, 0.43 g) and *N*-(1,3-benzodioxol-5-ylmethylene)propylamine (**25b**, 0.38 g), gave 35% of **33a** as a beige powder: mp 178°C; ^{1}H NMR ($CDCl_3$) δ 0.65 (t, 3H, *J* = 7.3), 1.11 (n, 2H, *J* = 7.6), 2.6 (m, 2H), 4.46 (s, 1H), 5.44 (s, 1H), 6.07 (s, 2H), 6.93 (d, 1H, *J* = 7.9), 7.12 (dd, 1H, *J* = 8.0 and 1.6), 7.16 (s, 1H), 7.82 (d, 2H, *J* = 8.7), 8.34 (d, 2H, *J* = 8.6); ^{13}C NMR ($CDCl_3$) δ 11.6, 19.4, 50.2, 71.3, 75.7, 97.6, 101.8, 108.2, 109.0, 112.2, 112.4, 122.9, 122.9, 124.1 (2C), 128.0, 129.7 (2C), 142.9, 148.7, 149.8; HRMS, *m*/*z*: 406.1260 found (calcd for $C_{21}H_{18}N_4O_5$, $M^{+\bullet}$ requires: 406.1277). The general procedure 4 (150 W, 10 min to reach 100°C, 15 min to reach 125°C, and 65 min at 125°C), using 3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (**1d**, 0.43 g) and *N*-(1,3-benzodioxol-5-ylmethylene)propylamine (**25b**, 0.38 g), gave 30% of **33a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-3-butyl-2-phenyloxazolidine-5,5-dicarbonitrile (34a).[3] The general procedure 3 (reflux of 32 h), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and *N*-(1,3-benzodioxol-5-ylmethylene)butylamine (**25c**, 0.41 g), gave 56% of **34a** as a beige glitter: mp 107°C; ^{1}H NMR ($CDCl_3$) δ 0.66 (t, 3H, *J* = 6.8), 1.1 (m, 4H), 2.6 (m, 2H), 4.41 (s, 1H), 5.33 (s, 1H), 6.05 (s, 2H), 6.91 (d, 1H, *J* = 8.0), 7.12 (d, 1H, *J* = 8.0), 7.18 (d, 1H, *J* = 1.5), 7.5 (m, 3H), 7.6 (m, 2H); ^{13}C NMR ($CDCl_3$) δ 13.6, 20.2, 27.3, 47.6, 71.2, 75.4, 99.1, 101.7, 108.4, 108.9, 112.5, 112.9, 122.9, 123.7, 128.7 (2C), 128.8 (2C), 130.6, 135.9, 148.5, 149.5; HRMS, *m*/*z*: 375.1573 found (calcd for

$C_{22}H_{21}N_3O_3$, $M^{+\bullet}$ requires: 375.1583). The general procedure 4 (120 W, 6 min to reach 100°C, 12 min to reach 125°C, and 60 min at 125°C), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and *N*-(1,3-benzodioxol-5-ylmethylene)butylamine (**25c**, 0.41 g), gave 40% of **34a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-3-butyl-2-(4-chlorophenyl)oxazolidine-5,5-dicarbonitrile (35a).[3] The general procedure 3 (reflux of 32 h), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and *N*-(1,3-benzodioxol-5-ylmethylene)butylamine (**25c**, 0.41 g), gave 59% of **35a** as a pale yellow powder: mp 138°C; ^{1}H NMR ($CDCl_3$) δ 0.67 (t, 3H, *J* = 6.8), 1.1 (m, 4H), 2.6 (m, 2H), 4.40 (s, 1H), 5.31 (s, 1H), 6.05 (s, 2H), 6.91 (d, 1H, *J* = 7.9), 7.11 (dd, 1H, *J* = 8.0 and 1.6), 7.15 (d, 1H, *J* = 1.4), 7.44 (d, 2H, *J* = 6.7), 7.56 (d, 2H, *J* = 6.5); ^{13}C NMR ($CDCl_3$) δ 13.5, 20.2, 27.4, 47.7, 71.1, 75.3, 98.2, 101.7, 108.3, 108.9, 112.5, 112.7, 122.9, 123.4, 129.1 (2C), 130.0 (2C), 134.6, 136.6, 148.6, 149.6; HRMS, *m*/*z*: 329.1197 found (calcd for $C_{19}H_{20}{}^{35}ClNO_2$, $[M\text{-}OC(CN)_2]^{+\bullet}$ requires: 329.1183). The general procedure 4 (120 W, 6 min to reach 100°C, 12 min to reach 125°C, and 60 min at 125°C), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and *N*-(1,3-benzodioxol-5-ylmethylene)butylamine (**25c**, 0.41 g), gave 49% of **35a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-3-butyl-2-(4-methoxyphenyl)oxazolidine-5,5-dicarbonitrile (36a).[3] The general procedure 3 (reflux of 9 h), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and *N*-(1,3-benzodioxol-5-ylmethylene)butylamine (**25c**, 0.41 g), gave 60% of **36a** as orange needles: mp 114°C; ^{1}H NMR ($CDCl_3$) δ 0.65 (t, 3H, *J* = 6.8), 1.1 (m, 4H), 2.6 (m, 2H), 3.86 (s, 3H), 4.38 (s, 1H), 5.29 (s, 1H), 6.05 (s, 2H), 6.91 (d, 1H, *J* = 8.0), 6.97 (d, 2H, *J* = 8.7), 7.11 (dd, 1H, *J* = 8.0 and 1.5), 7.17 (d, 1H, *J* = 1.5), 7.53 (d, 2H, *J* = 8.7); ^{13}C NMR ($CDCl_3$) δ 13.6, 20.3, 27.2, 47.6, 55.4, 71.0, 75.3, 98.9, 101.7, 108.4, 108.9, 112.6, 113.0, 114.2 (2C), 122.9, 123.8, 127.9, 130.1 (2C), 148.5, 149.5, 161.4; HRMS, *m*/*z*: 378.1597 found (calcd for $C_{22}H_{22}N_2O_4$, $[M\text{-}HCN]^{+\bullet}$ requires: 378.1580). The general procedure 4 (60 W, 3 min to reach 60°C, 6 min to reach 80°C, and 30 min at 80°C), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and *N*-(1,3-benzodioxol-5-ylmethylene)butylamine (**25c**, 0.41 g), gave 75% of **36a** after recrystallization from CH_2Cl_2.

4-(1,3-Benzodioxol-5-yl)-3-butyl-2-(4-nitrophenyl)oxazolidine-5,5-dicarbonitrile (37a).[3] The general procedure 3 (reflux of 65 h), using 3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (**1d,** 0.43 g) and *N*-(1,3-benzodioxol-5-ylmethylene)butylamine (**25c**, 0.41 g), gave 18% of **37a** as an orange powder: mp 126°C; ^{1}H NMR ($CDCl_3$) δ 0.66 (t, 3H, *J* = 6.8), 1.1 (m, 4H), 2.6 (m, 2H), 4.45 (s, 1H), 5.43 (s, 1H), 6.06 (s, 2H), 6.92 (d, 1H, *J* = 7.9), 7.10 (dd, 1H, *J* = 8.1 and 1.6), 7.14 (d, 1H, *J* = 1.6), 7.81 (d, 2H, *J* =8.8), 8.33 (d, 2H, *J* = 8.8); ^{13}C NMR ($CDCl_3$) δ 13.5, 20.2, 27.7, 47.9, 71.3, 75.5, 97.4, 101.8, 108.2,

109.0, 112.2, 112.4, 122.9, 122.9, 124.1 (2C), 128.0, 129.7 (2C), 142.9, 148.7, 149.8; HRMS, *m*/*z*: 420.1457 found (calcd for $C_{22}H_{20}N_4O_5$, $M^{+\bullet}$ requires: 420.1434). The general procedure 4 (150 W, 10 min to reach 100°C, 15 min to reach 125°C, and 75 min at 125°C), using 3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (**1d**, 0.43 g) and *N*-(1,3-benzodioxol-5-ylmethylene)butylamine (**25c**, 0.41 g), gave 22% of **37a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-3-benzyl-2-phenyloxazolidine-5,5-dicarbonitrile (38a).[3] The general procedure 3 (reflux of 40 h), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and *N*-(1,3-benzodioxol-5-ylmethylene)benzylamine (**25d**, 0.48 g), gave 60% of **38a** as a beige glitter: mp 132°C; ^{1}H NMR ($CDCl_3$) δ 3.64 (d, 1H, *J* = 15), 3.86 (d, 1H, *J* = 15), 4.28 (s, 1H), 5.25 (s, 1H), 6.08 (s, 2H), 6.7 (m, 2H), 6.97 (d, 1H, *J* = 7.8), 7.17 (d, 1H, *J* = 8.1), 7.3 (m, 4H), 7.6 (m, 5H); ^{13}C NMR ($CDCl_3$) δ 49.2, 70.8, 72.7, 96.4, 101.8, 108.6, 109.1, 112.7, 112.8, 122.8, 123.2, 128.3, 128.5 (2C), 128.9 (2C), 129.2 (2C), 130.1 (2C), 130.8, 131.4, 134.6, 148.7, 149.6; HRMS, *m*/*z*: 329.1426 found (calcd for $C_{22}H_{19}NO_2$, $[M\text{-}CO(CN)_2]^{+\bullet}$ requires: 329.1416). The general procedure 4 (120 W, 6 min to reach 100°C, 12 min to reach 125°C, and 70 min at 125°C), using 3-phenyloxirane-2,2-dicarbonitrile (**1a**, 0.34 g) and *N*-(1,3-benzodioxol-5-ylmethylene)benzylamine (**25d**, 0.48 g), gave 42% of **38a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-3-benzyl-2-(4-chlorophenyl)oxazolidine-5,5-dicarbonitrile (39a).[3] The general procedure 3 (reflux of 37 h), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and *N*-(1,3-benzodioxol-5-ylmethylene)benzylamine (**25d**, 0.48 g), gave 50% of **39a** as a white powder: mp 147°C; ^{1}H NMR ($CDCl_3$) δ 3.63 (d, 1H, *J* = 15), 3.85 (d, 1H, *J* = 15), 4.28 (s, 1H), 5.22 (s, 1H), 6.09 (s, 2H), 6.7 (m, 2H), 6.98 (d, 1H, *J* = 7.9), 7.3 (m, 5H), 7.46 (d, 2H, *J* = 8.4), 7.58 (d, 2H, *J* = 8.5); ^{13}C NMR ($CDCl_3$) δ 49.5, 70.8, 72.9, 95.7, 101.8, 108.6, 109.2, 112.6, 112.6, 122.6, 123.2, 128.4, 128.6 (2C), 129.3 (2C), 130.0 (2C), 130.5 (2C), 131.4, 133.2, 136.7, 148.8, 149.7; HRMS, *m*/*z*: 363.1040 found (calcd for $C_{22}H_{18}NO_2{}^{35}Cl$, $M^{+\bullet}$ requires: 363.1026). The general procedure 4 (120 W, 6 min to reach 100°C, 12 min to reach 125°C, and 60 min at 125°C), using 3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (**1b**, 0.41 g) and *N*-(1,3-benzodioxol-5-ylmethylene)benzylamine (**25d**, 0.48 g), gave 37% of **39a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

4-(1,3-Benzodioxol-5-yl)-3-benzyl-2-(4-methoxyphenyl)oxazolidine-5,5-dicarbonitrile (40a).[3] The general procedure 3 (reflux of 18 h), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and *N*-(1,3-benzodioxol-5-ylmethylene)benzylamine (**25d**, 0.48 g), gave 80% of **40a** as pale yellow needles: mp 116°C; ^{1}H NMR ($CDCl_3$) δ 3.63 (d, 1H, *J* = 15), 3.86 (d, 1H, *J* = 15), 3.88 (s, 3H), 4.24 (s, 1H), 5.21 (s, 1H), 6.08 (s, 2H), 6.9 (m, 2H), 7.0 (m, 3H), 7.2 (m, 5H), 7.59 (d, 2H, *J* = 8.0); ^{13}C NMR

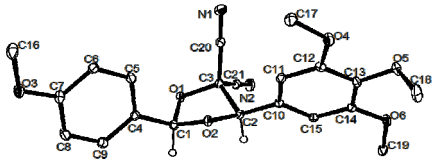
($CDCl_3$) δ 49.1, 55.4, 70.6, 72.5, 96.1, 101.7, 108.6, 109.1, 112.8, 112.9, 114.4 (2C), 122.9, 123.2, 126.4, 128.3, 128.5 (2C), 130.1 (2C), 130.6 (2C), 131.5, 148.7, 149.6, 161.5; HRMS, *m*/*z*: 412.1401 found (calcd for $C_{25}H_{20}N_2O_4$, $[M\text{-}HCN]^{+\bullet}$ requires: 412.1423). The general procedure 4 (60 W, 3 min to reach 60°C, 6 min to reach 80°C, and 35 min at 80°C), using 3-(4-methoxyphenyl)oxirane-2,2-dicarbonitrile (**1c**, 0.40 g) and *N*-(1,3-benzodioxol-5-ylmethylene)benzylamine (**25d**, 0.48 g), gave 70% of **40a** after recrystallization from CH_2Cl_2.

4-(1,3-Benzodioxol-5-yl)-3-benzyl-2-(4-nitrophenyl)oxazolidine-5,5-dicarbonitrile (41a).[3] The general procedure 3 (reflux of 72 h), using 3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (**1d,** 0.43 g) and *N*-(1,3-benzodioxol-5-ylmethylene)benzylamine (**25d**, 0.48 g), gave 27% of **41a** as a white powder: mp 187°C; ^{1}H NMR ($CDCl_3$) δ 3.70 (d, 1H, *J* = 15), 3.82 (d, 1H, *J* = 15), 4.36 (s, 1H), 5.34 (s, 1H), 6.11 (s, 2H), 6.9 (m, 2H), 7.00 (d, 1H, *J* = 8.0), 7.2 (m, 5H), 7.77 (d, 2H, *J* = 8.8), 8.29 (d, 2H, *J* = 8.8); ^{13}C NMR ($CDCl_3$) δ 50.3, 70.9, 73.6, 95.5, 101.9, 108.4, 109.3, 112.3, 112.4, 122.1, 123.2, 124.0 (2C), 128.0, 128.6, 128.7 (2C), 129.8 (2C), 130.1 (2C), 131.5, 141.7, 148.9, 149.9; HRMS, *m*/*z*: 374.1258 found (calcd for $C_{22}H_{18}N_2O_4$, $[M\text{-}CO(CN)_2]^{+\bullet}$ requires: 374.1267). The general procedure 4 (150 W, 10 min to reach 100°C, 15 min to reach 125°C, and 90 min at 125°C), using 3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (**1d**, 0.43 g) and *N*-(1,3-benzodioxol-5-ylmethylene)benzylamine (**25d**, 0.48 g), gave 18% of **41a** after isolation by column chromatography over silica gel (eluent: Et_2O/petrol 30:70).

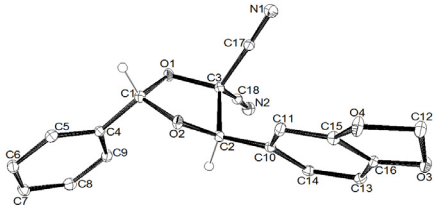
Crystallography

The samples were studied with graphite monochromatized $Mo_{K\alpha}$ radiation (λ = 0.71073 Å). X-ray diffraction data were collected at *T* = 100(2) K using APEXII Bruker-AXS diffractometer. The structure was solved by direct methods using the SIR97 program,[4] and then refined with full-matrix least-square methods based on F^2 (SHELX-97)[5] with the aid of the WINGX program.[6] All non-hydrogen atoms were refined with anisotropic thermal parameters. Except N-linked hydrogen that was introduced in the structural model through Fourier difference maps analysis, H atoms were finally included in their calculated positions. Molecular diagrams were generated by ORTEP-3 (version 1.08).[7]

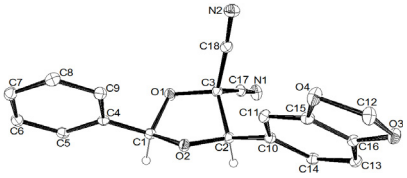
ORTEP Diagrams (30% Probability) - (Most of Hydrogens are Omitted for Clarity)



Racemic **5a**



Racemic **6b**



Racemic **6a**

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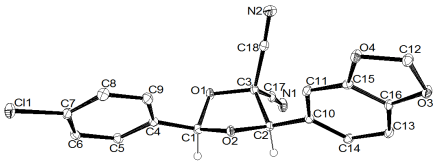
[4] Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G. G.; Polidori, G.; Spagna, R. *J. Appl. Cryst.* **1999**, *32*, 115-119.

[5] SHELX97 - Programs for Crystal Structure Analysis (Release 97-2). Sheldrick, G. M. Institüt für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Göttingen, Germany, 1998.

[6] Farrugia, L. J. *J. Appl. Cryst.* **1999**, *32*, 837-838.



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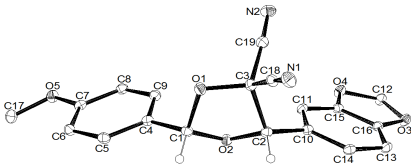

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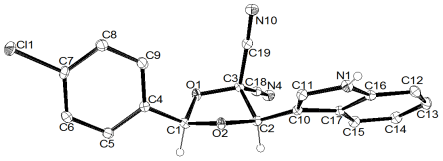

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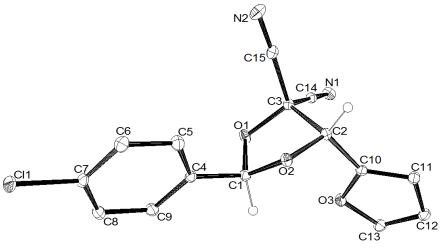
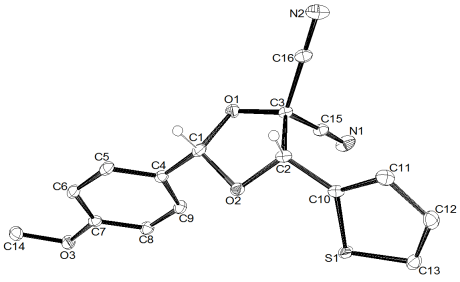


Racemic **20b**



Racemic **24a**

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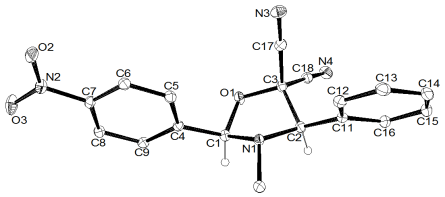
[7] Farrugia, L. J. *J. Appl. Crystallogr.* **1997**, *30*, 565.



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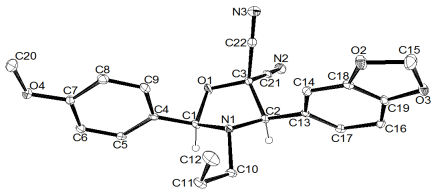

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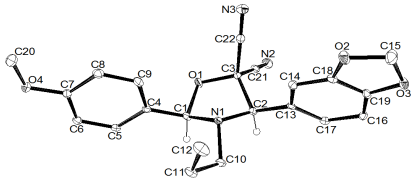

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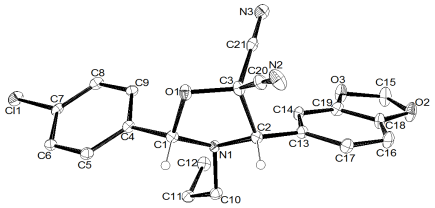
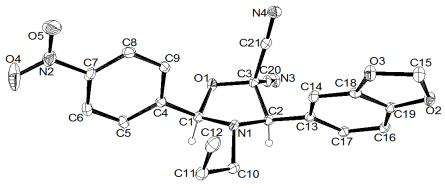
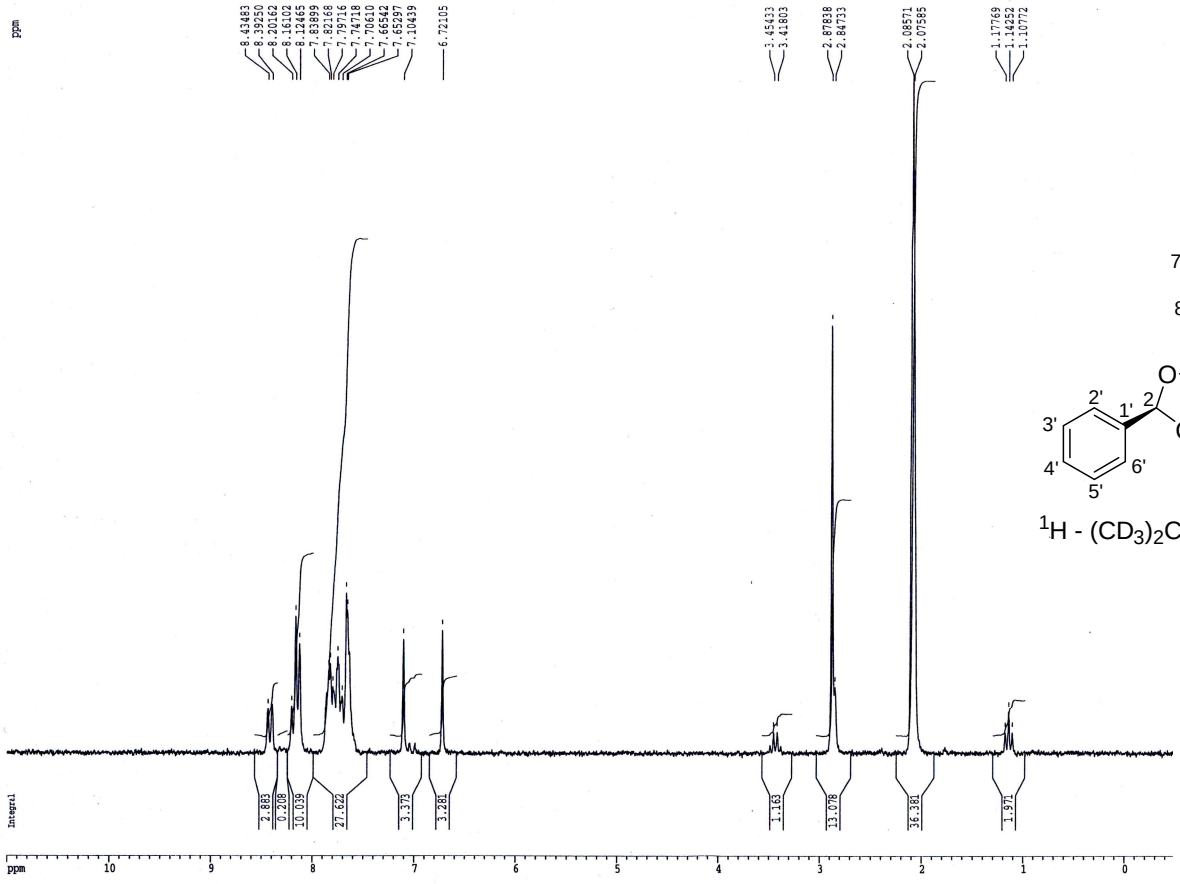
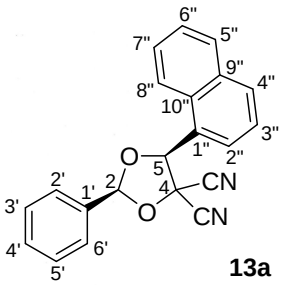


Racemic **33a**



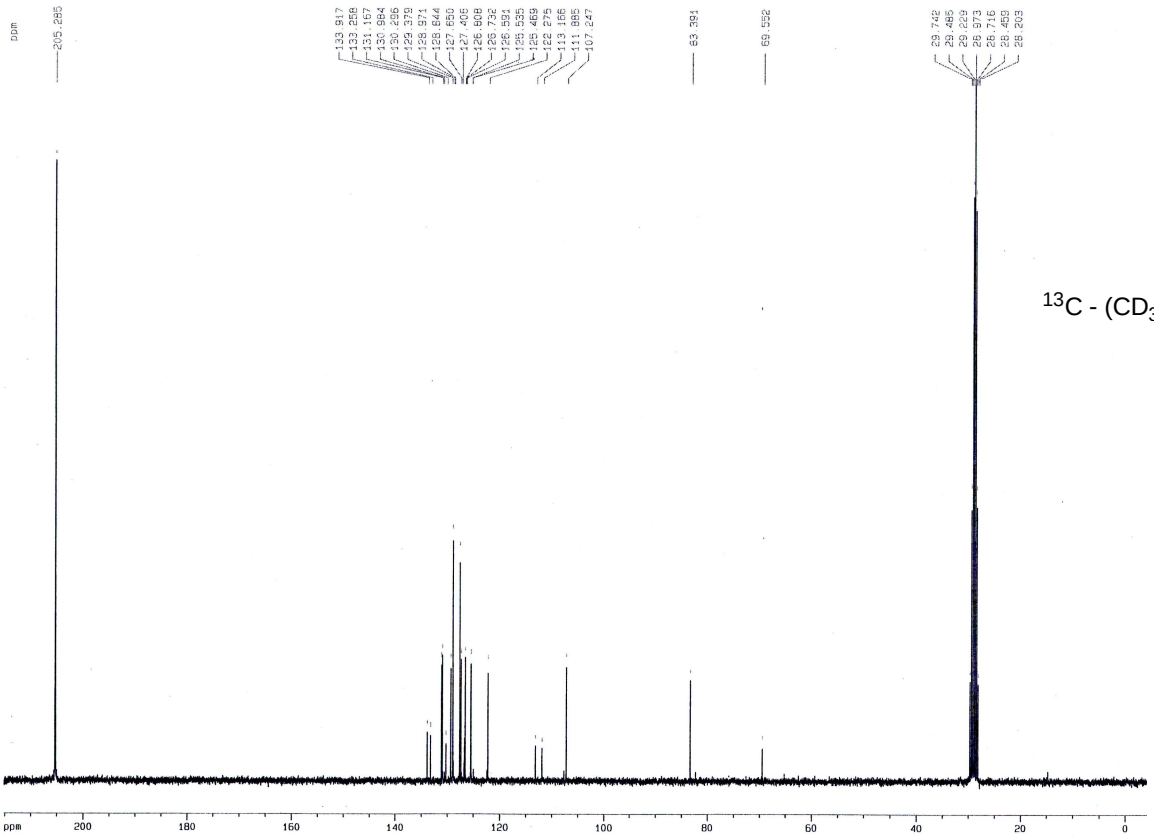
Racemic **39a**





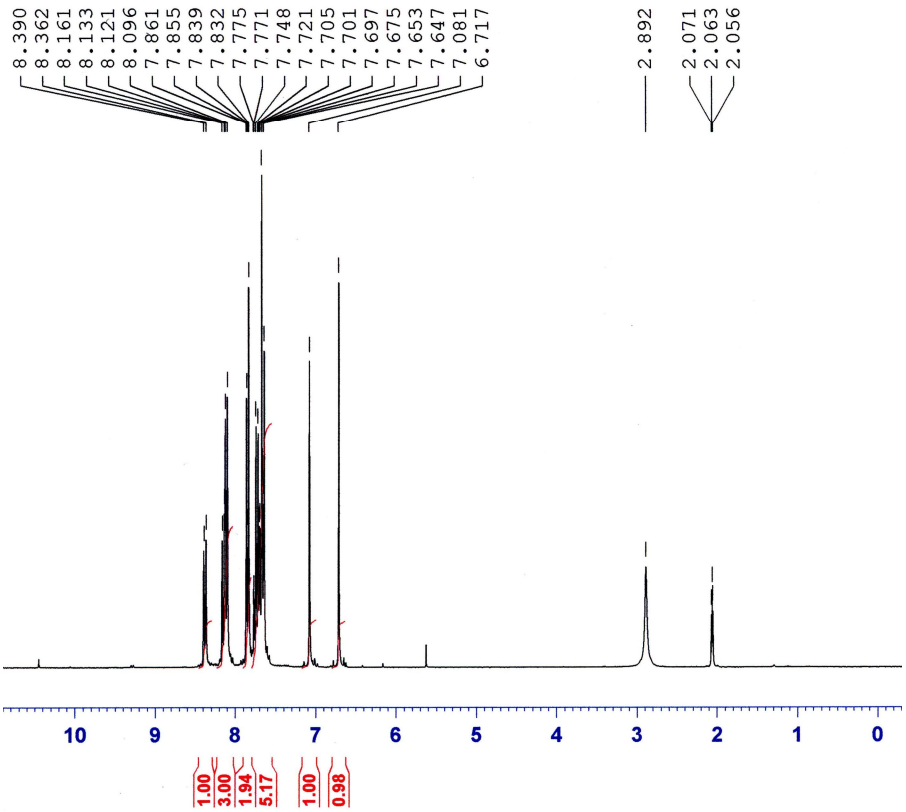
13a

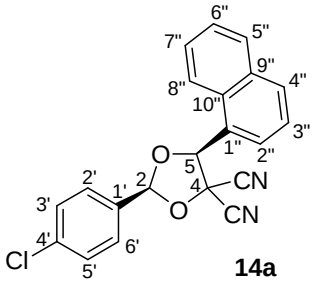
^{1}H - $(CD_3)_2CO$ - 200MHz



13a

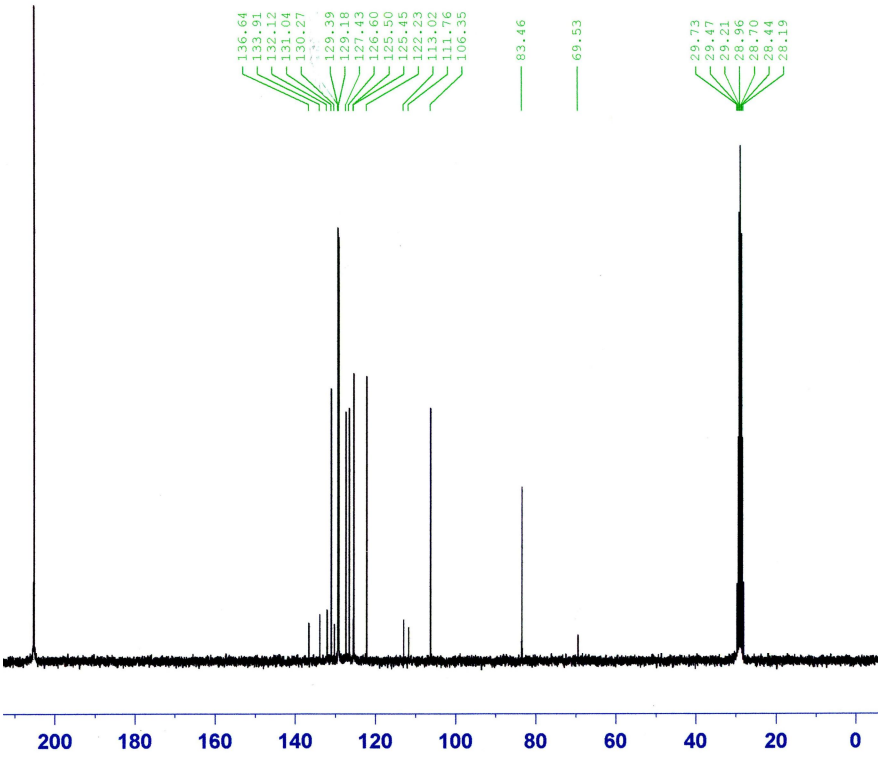
^{13}C - $(CD_3)_2CO$ - 75MHz





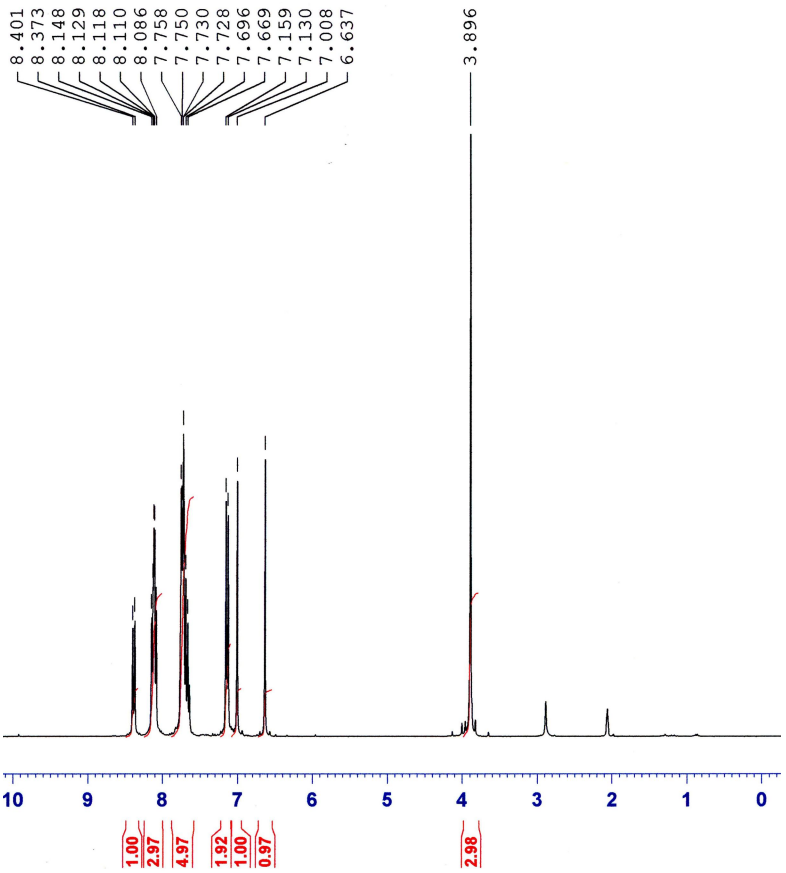
14a

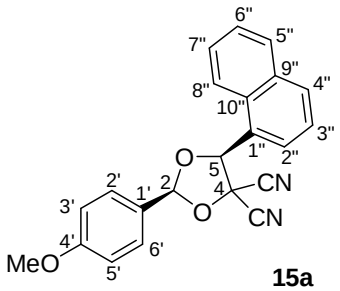
^{1}H - $(CD_3)_2CO$ - 300MHz



14a

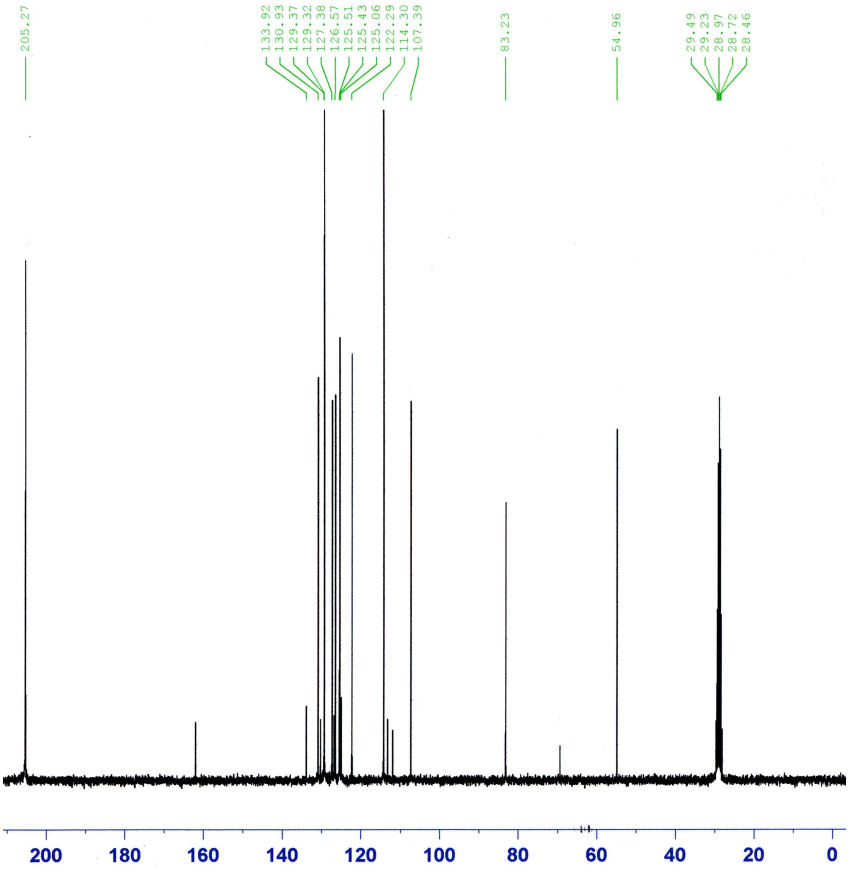
^{13}C - $(CD_3)_2CO$ - 75MHz





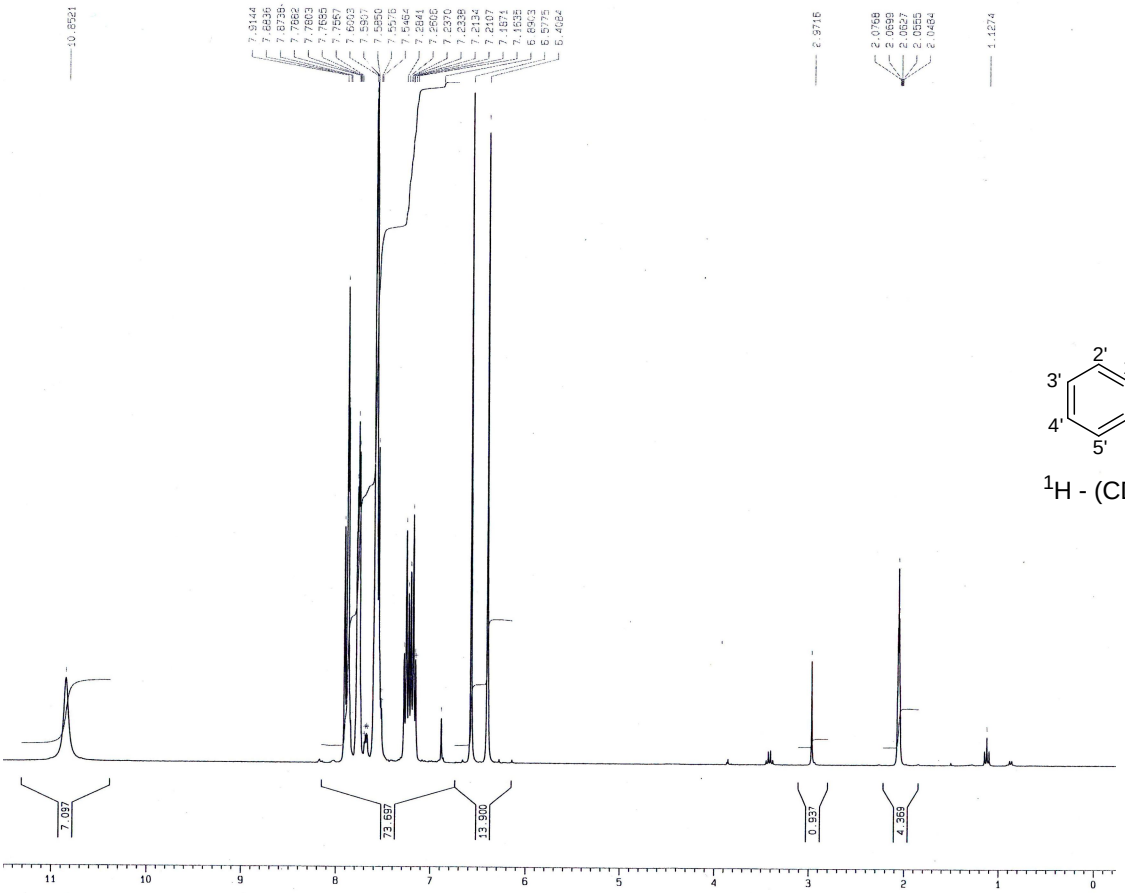
15a

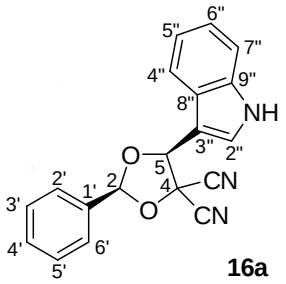
^{1}H - $(CD_3)_2CO$ - 300MHz



15a

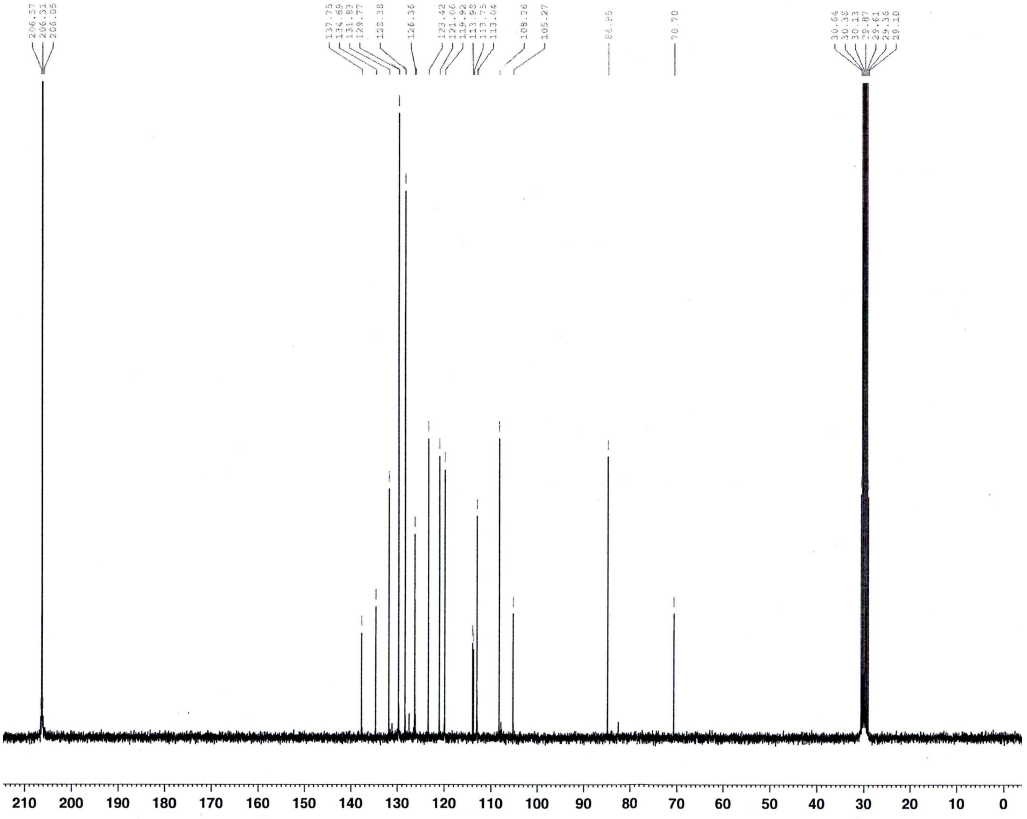
^{13}C - $(CD_3)_2CO$ - 75MHz





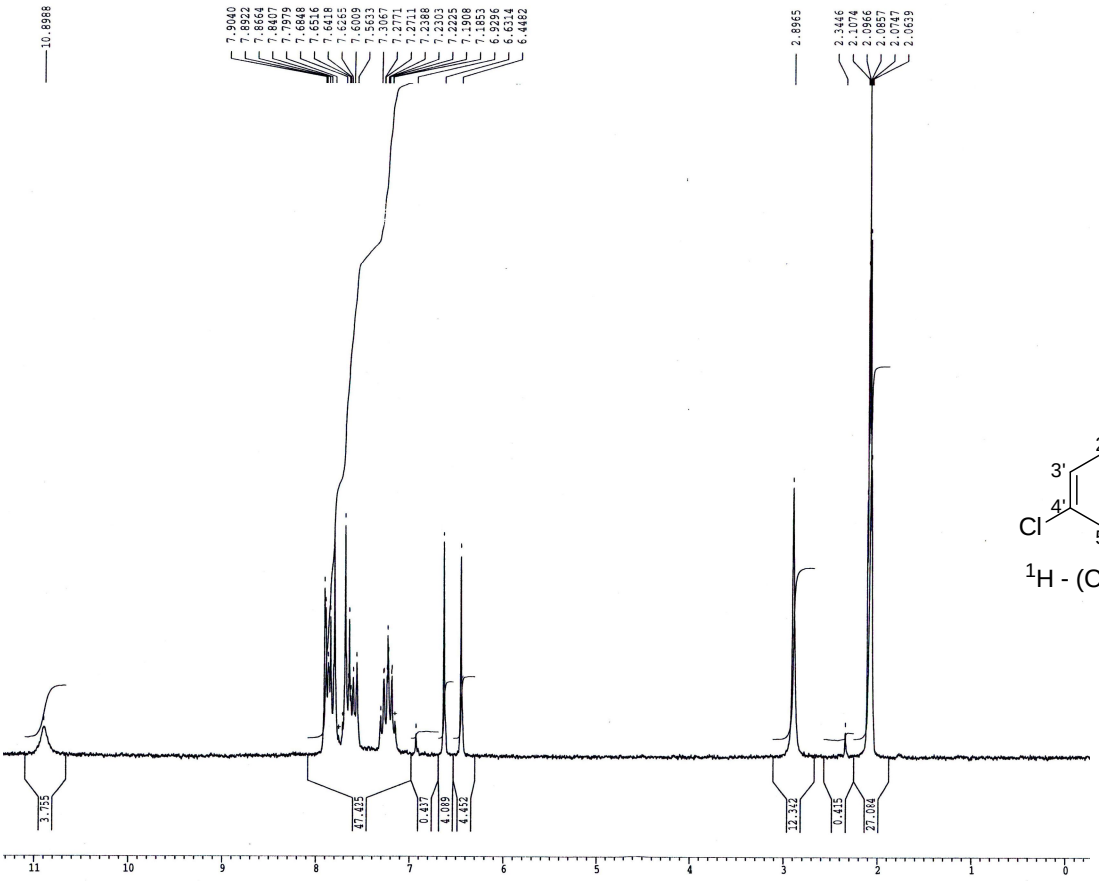
16a

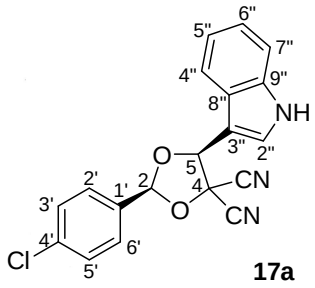
^{1}H - $(CD_3)_2CO$ - 300MHz



16a

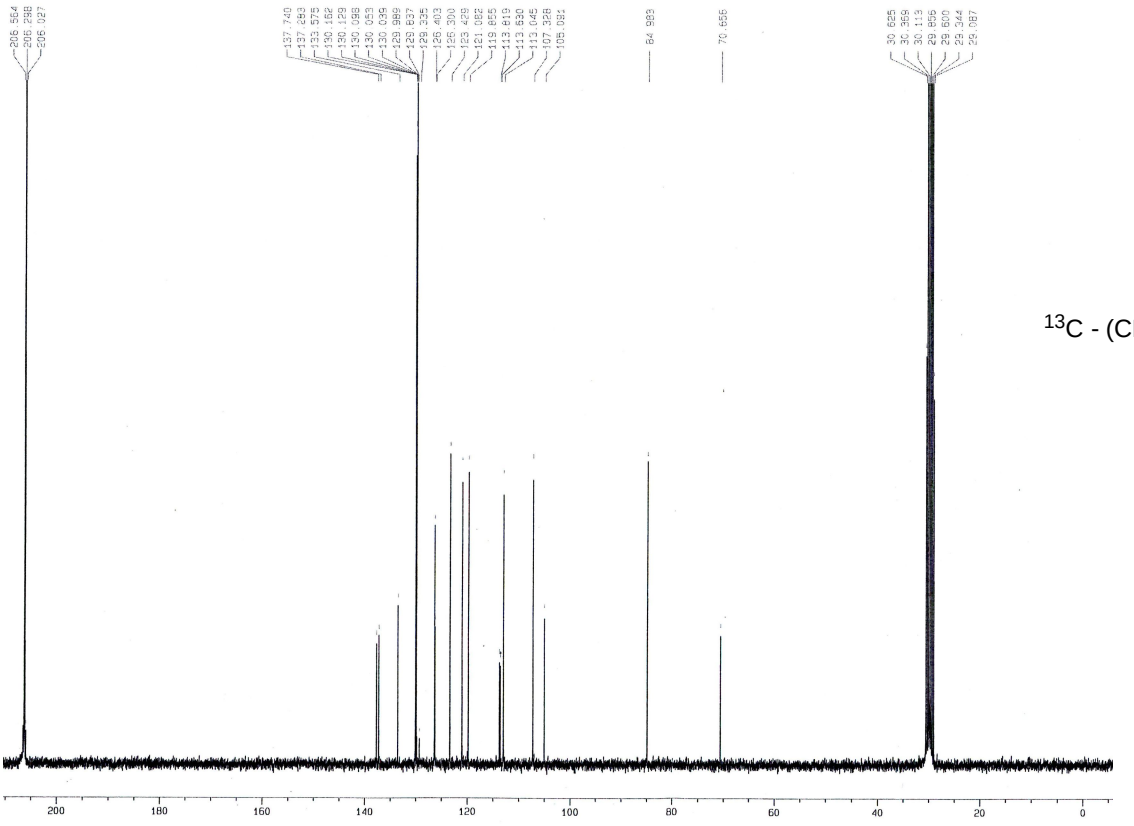
^{13}C - $(CD_3)_2CO$ - 75MHz





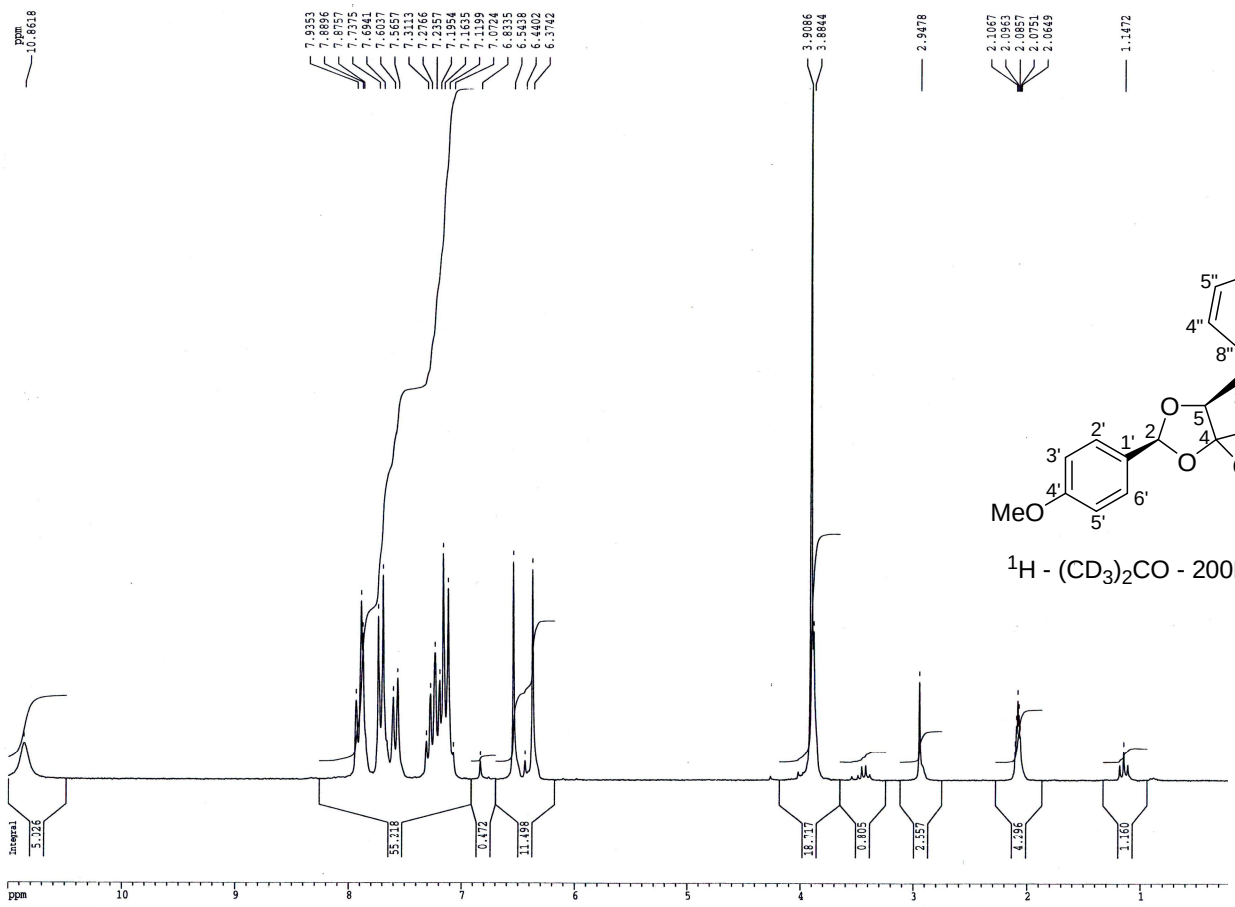
17a

^{1}H - $(CD_3)_2CO$ - 200MHz



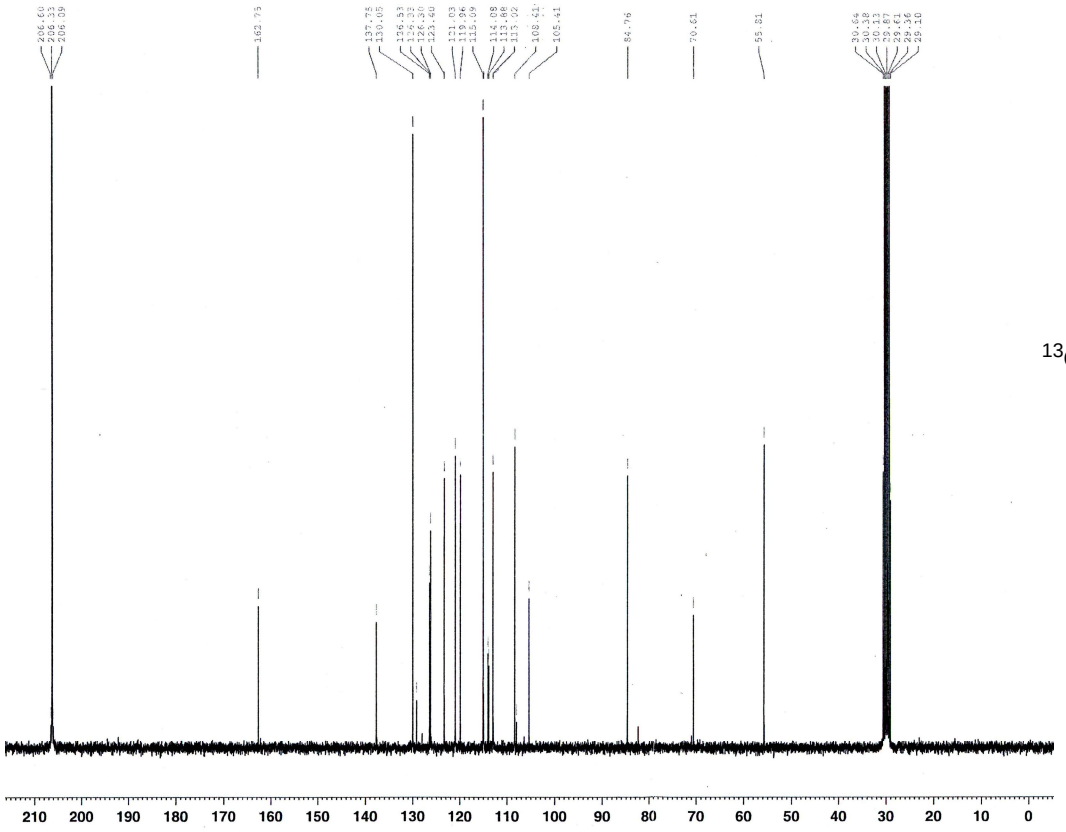
17a

^{13}C - $(CD_3)_2CO$ - 75MHz



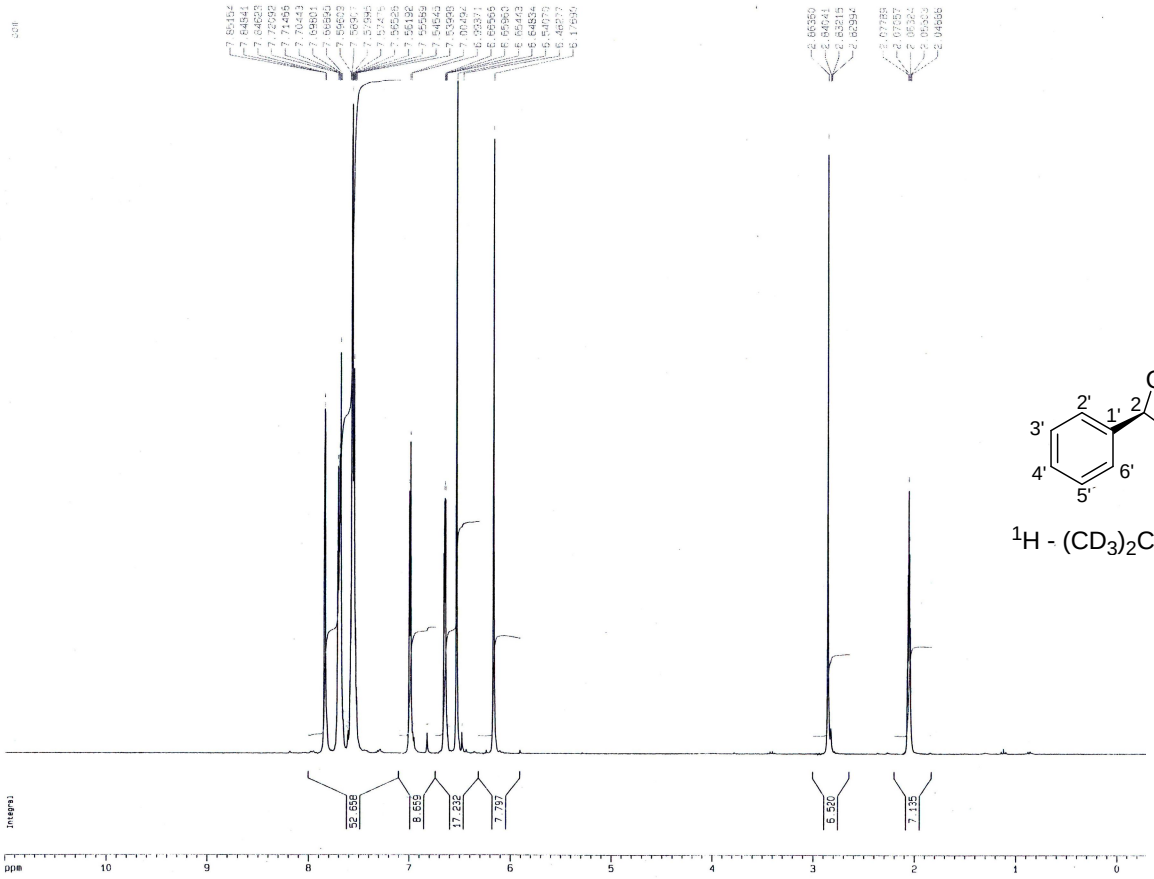
18a

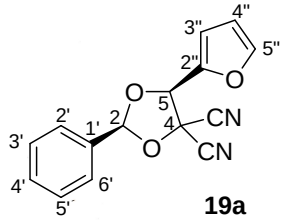
^{1}H - $(CD_3)_2CO$ - 200MHz



18a

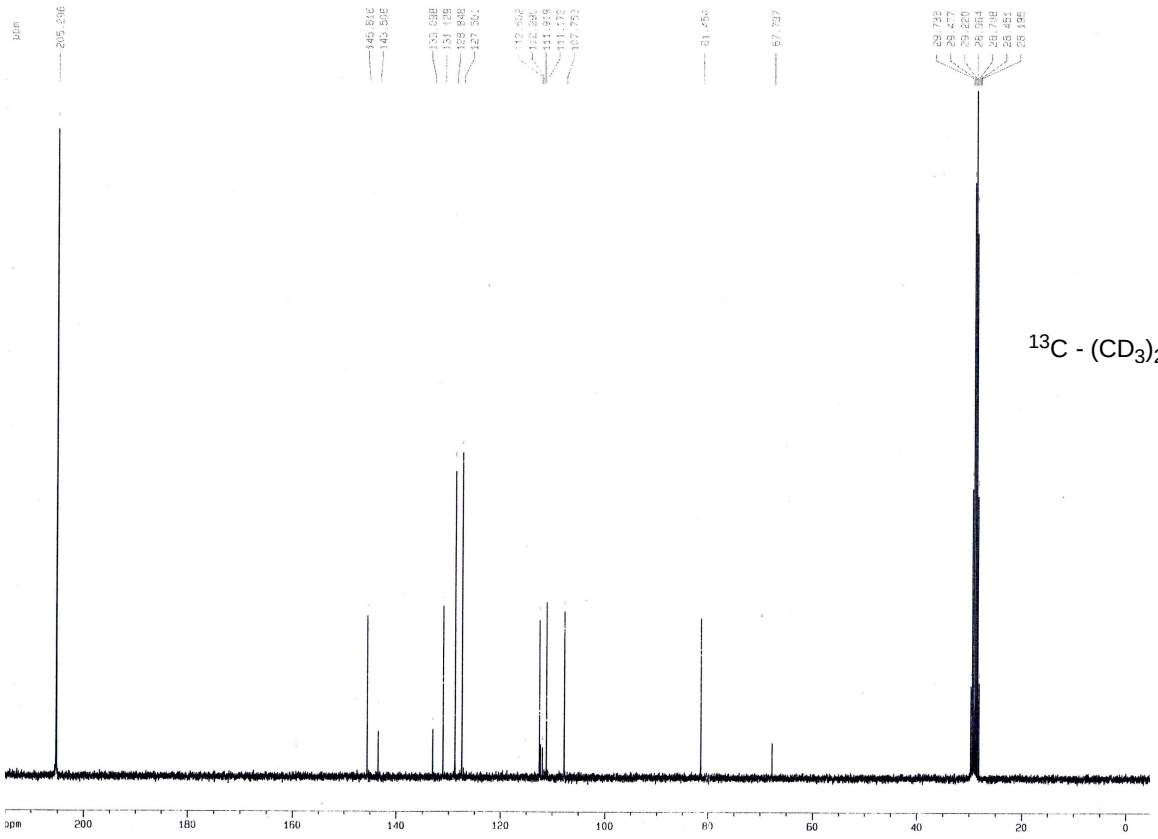
^{13}C - $(CD_3)_2CO$ - 75MHz





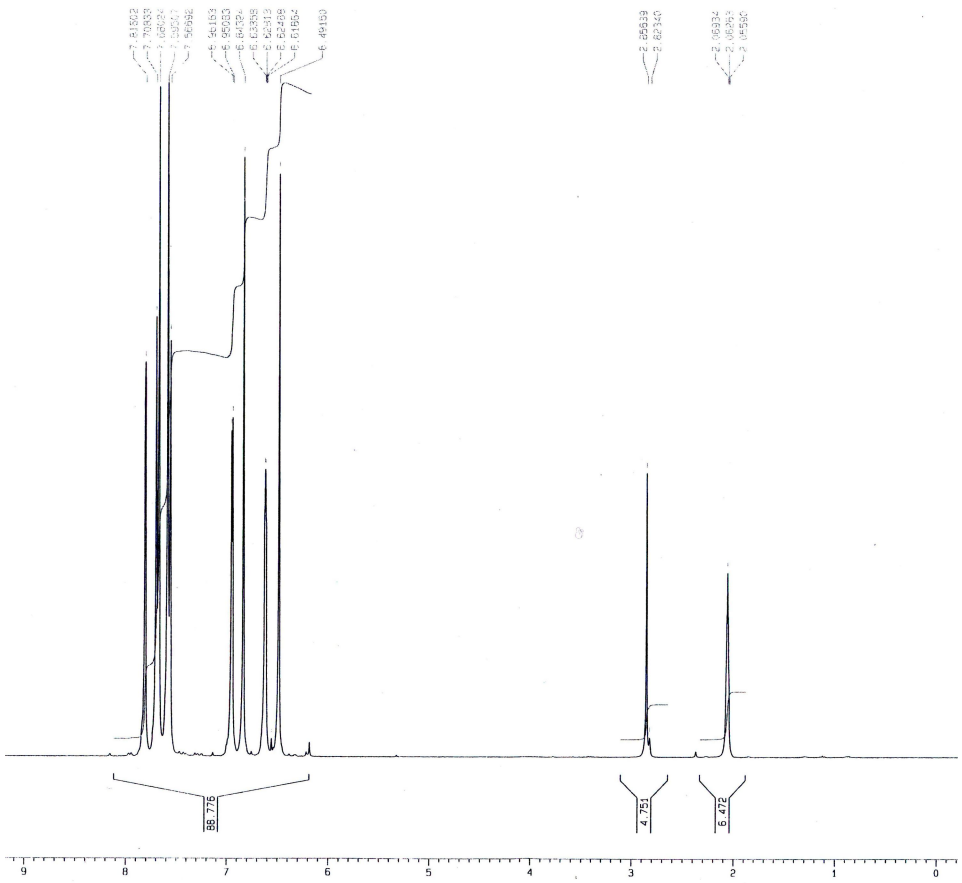
19a

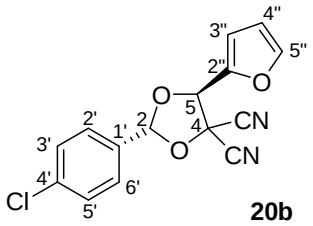
^{1}H - $(CD_3)_2CO$ - 300MHz



19a

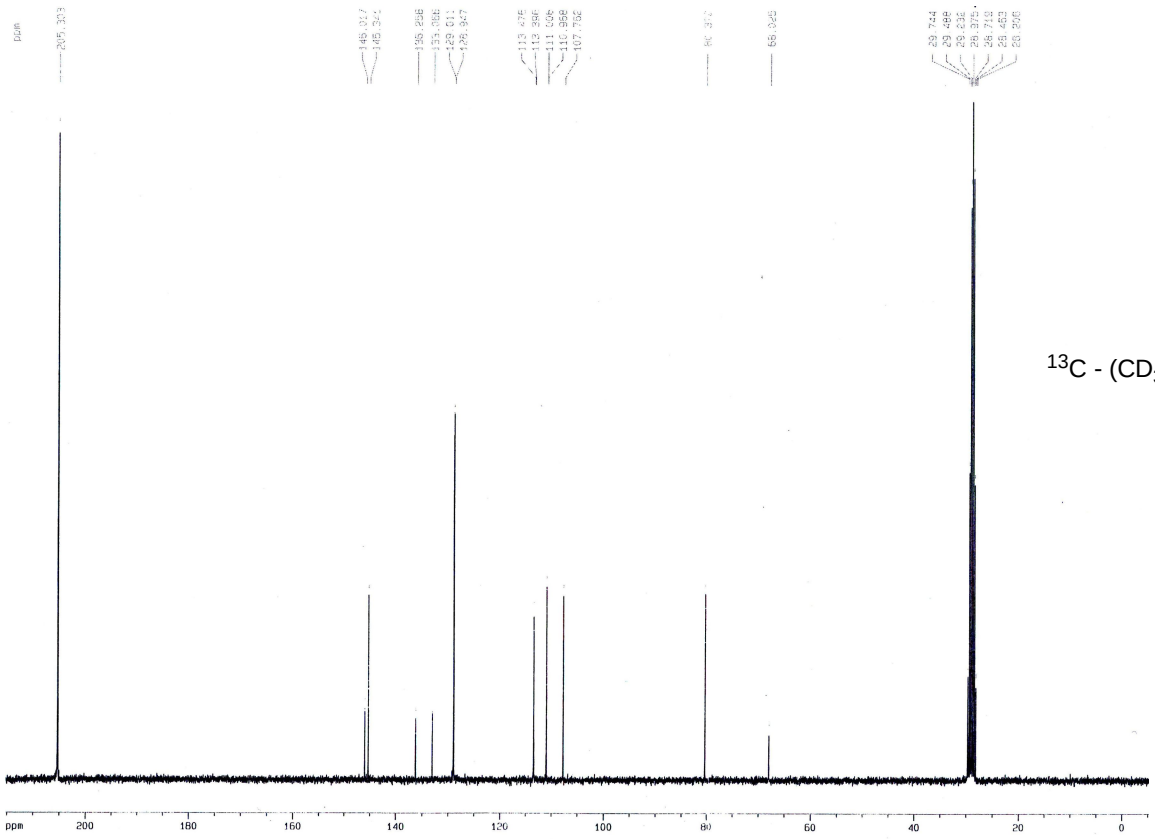
^{13}C - $(CD_3)_2CO$ - 75MHz





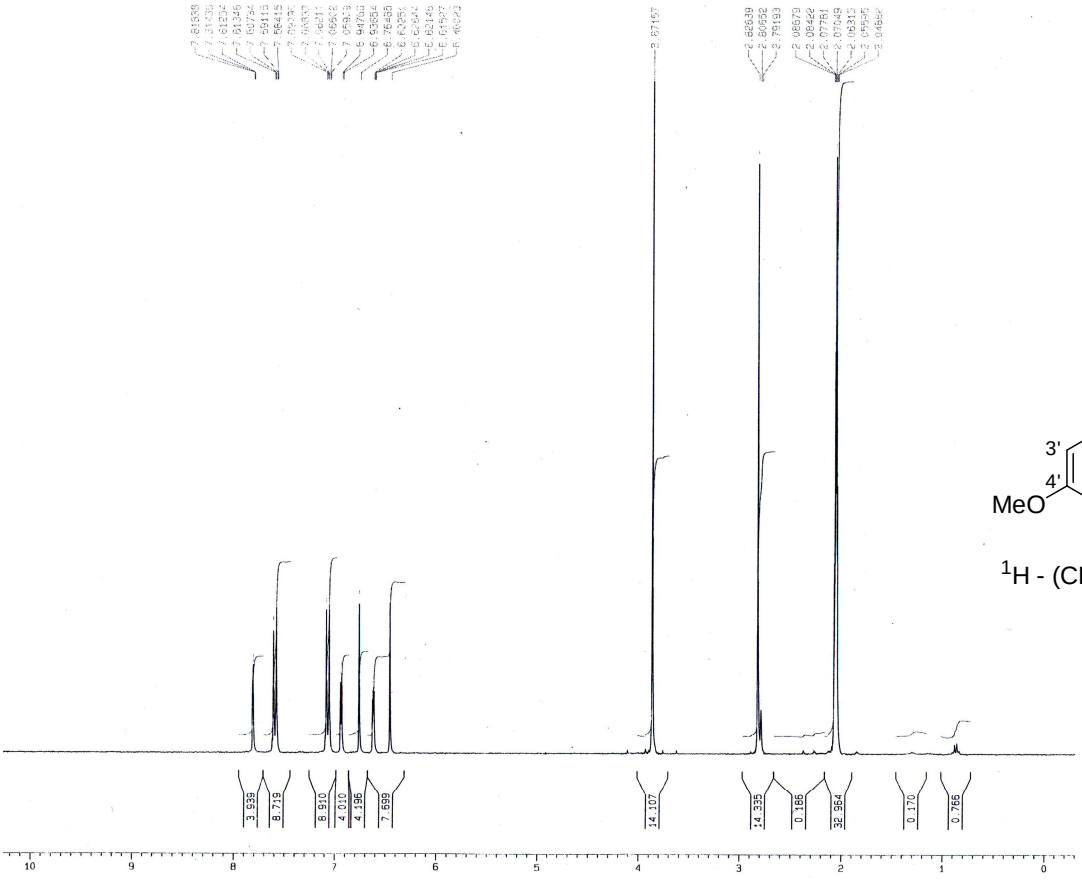
20b

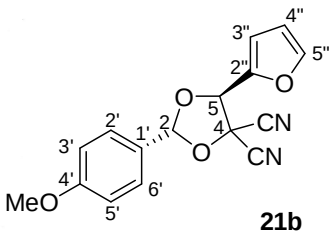
^{1}H - $(CD_3)_2CO$ - 300MHz



20b

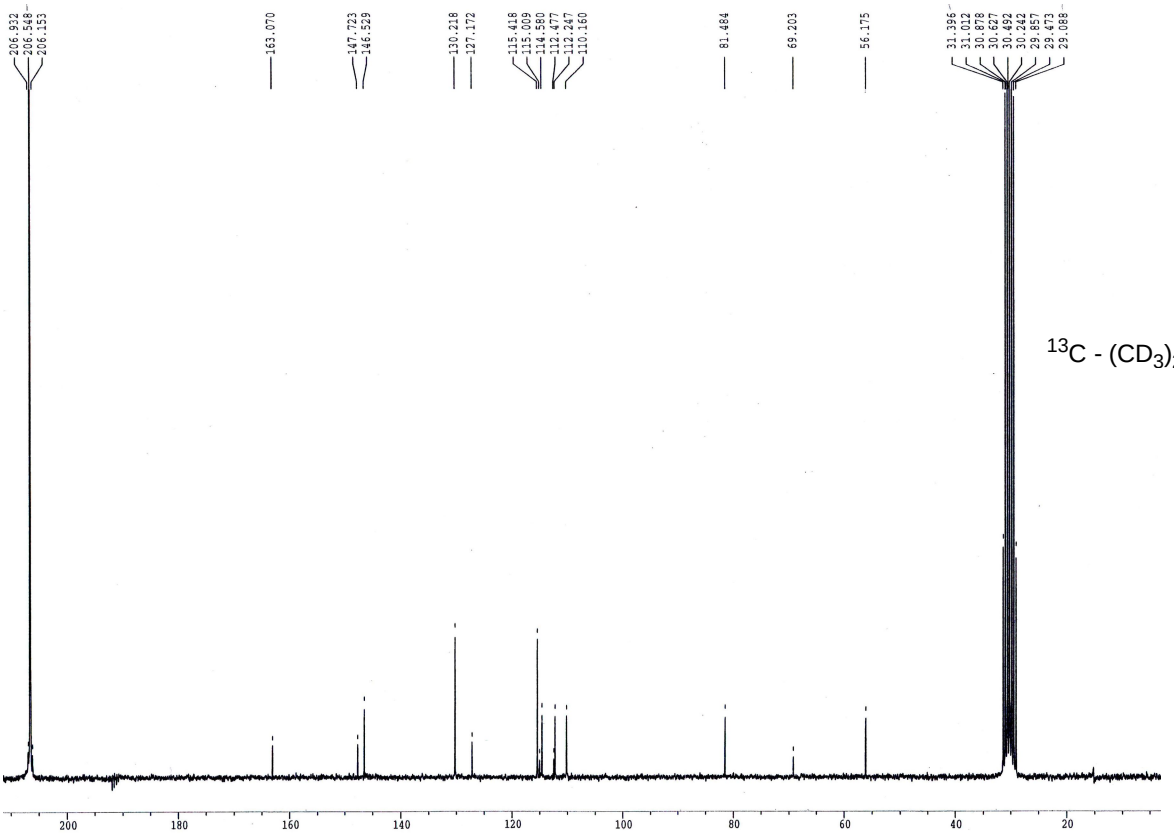
^{13}C - $(CD_3)_2CO$ - 75MHz





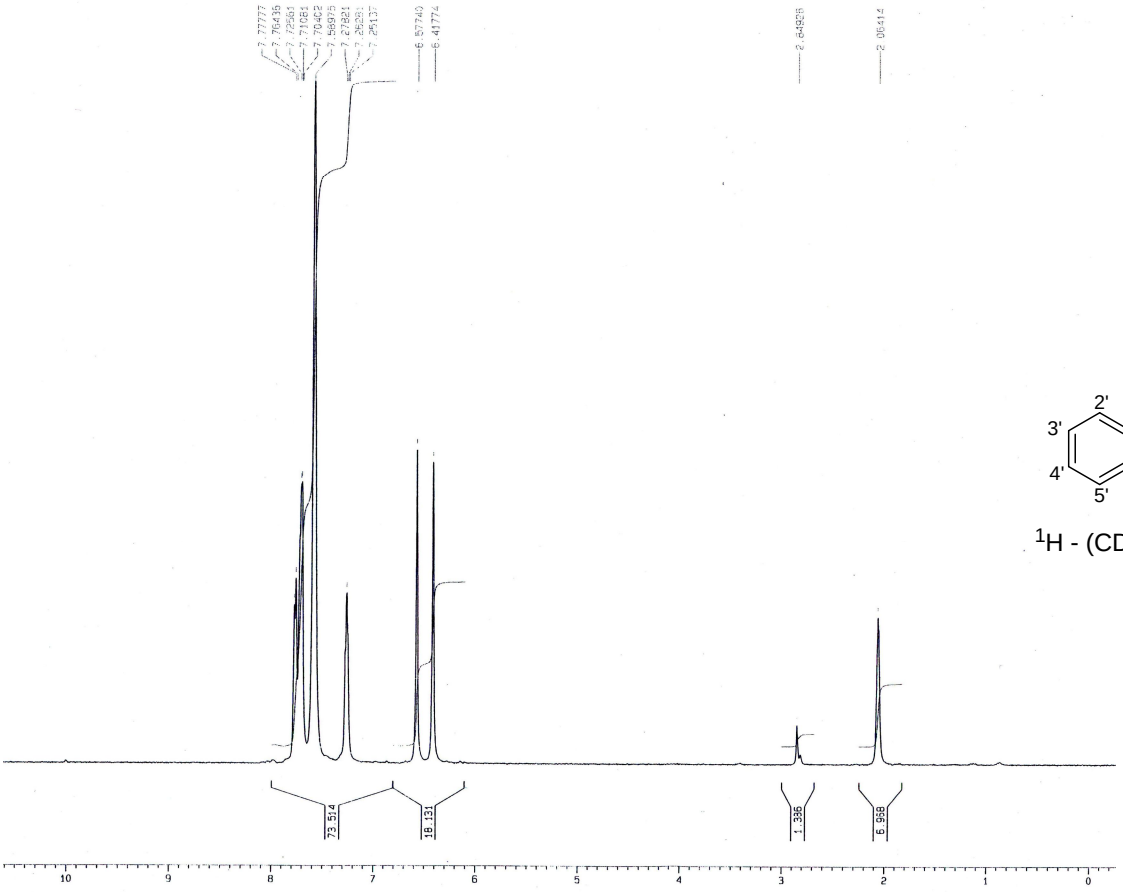
21b

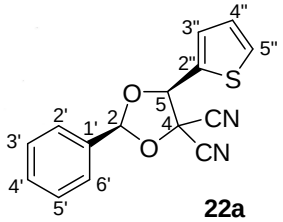
^{1}H - $(CD_3)_2CO$ - 300MHz



21b

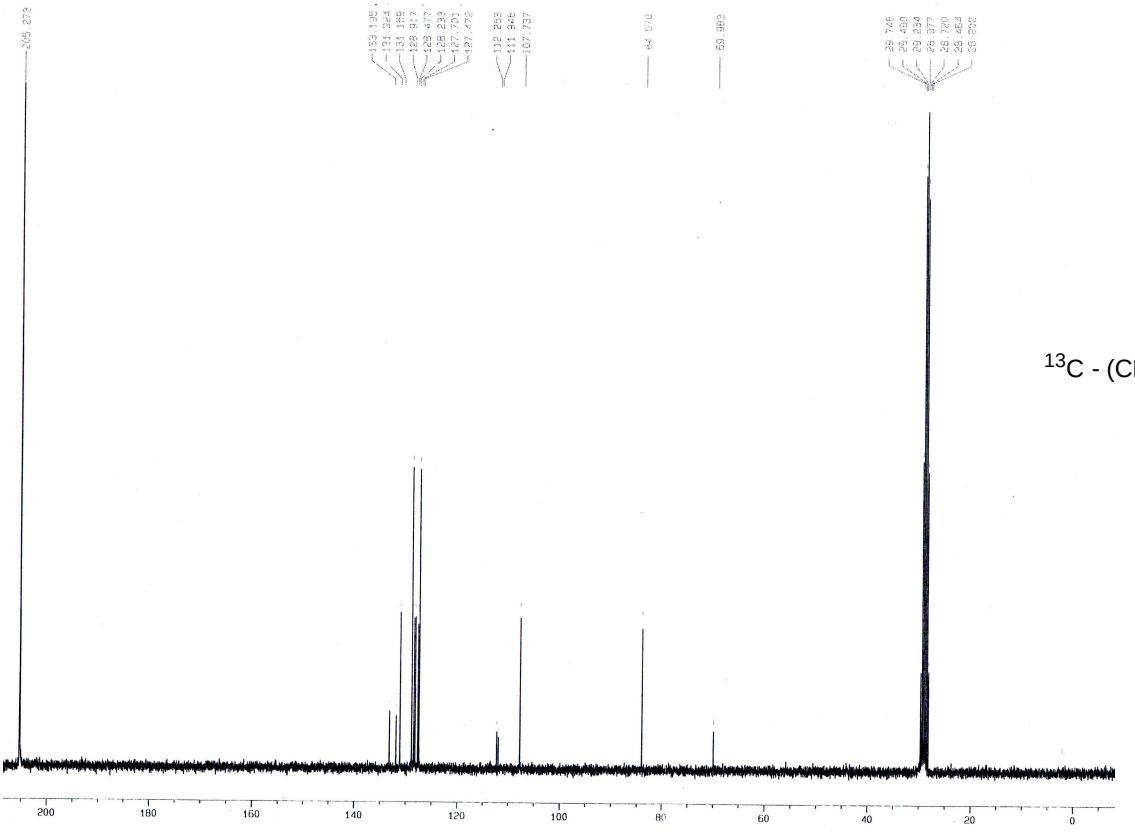
^{13}C - $(CD_3)_2CO$ - 50MHz





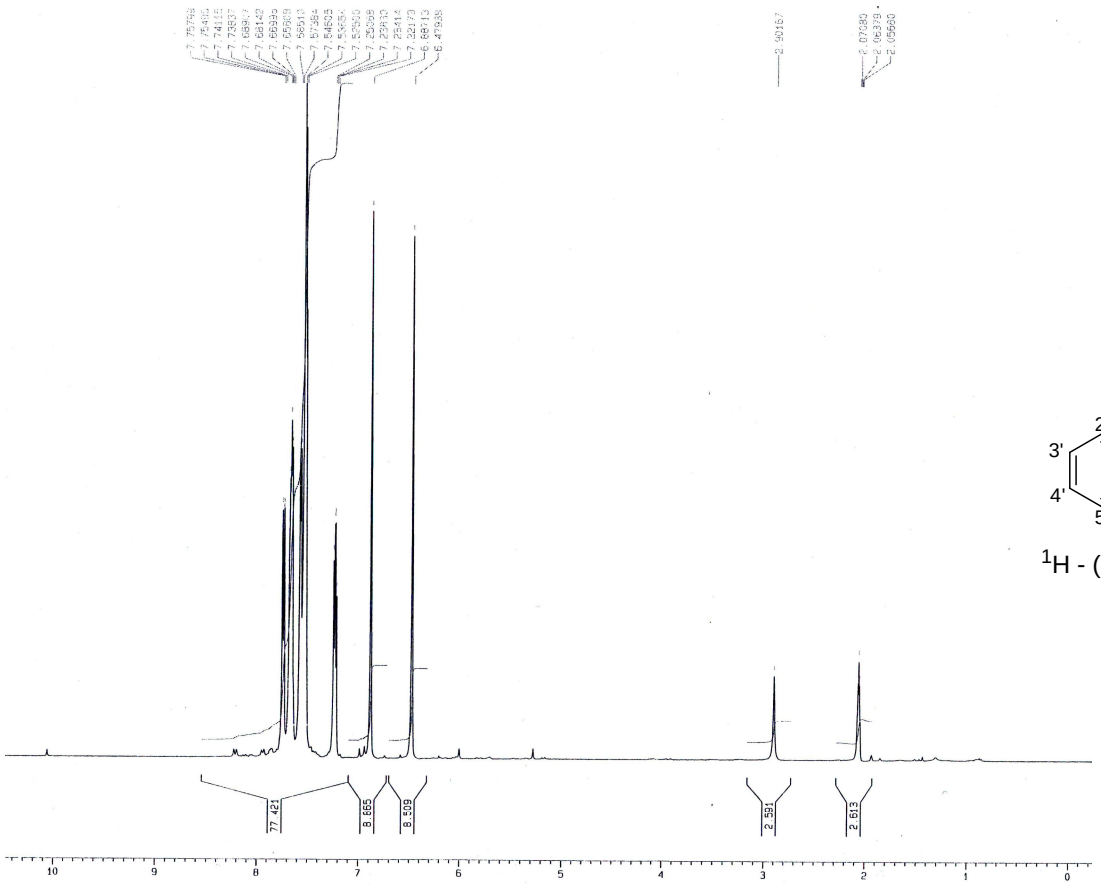
22a

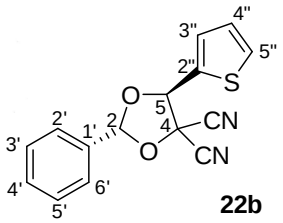
^{1}H - $(CD_3)_2CO$ - 300MHz



22a

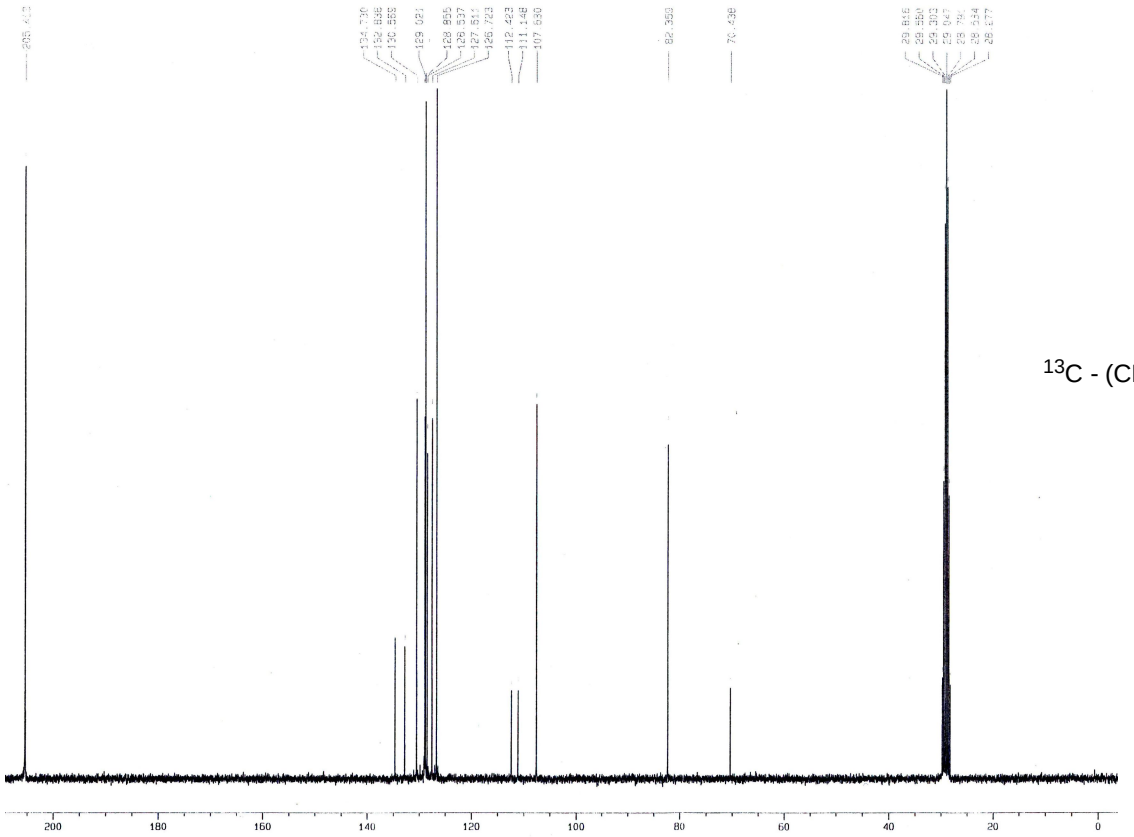
^{13}C - $(CD_3)_2CO$ - 75MHz





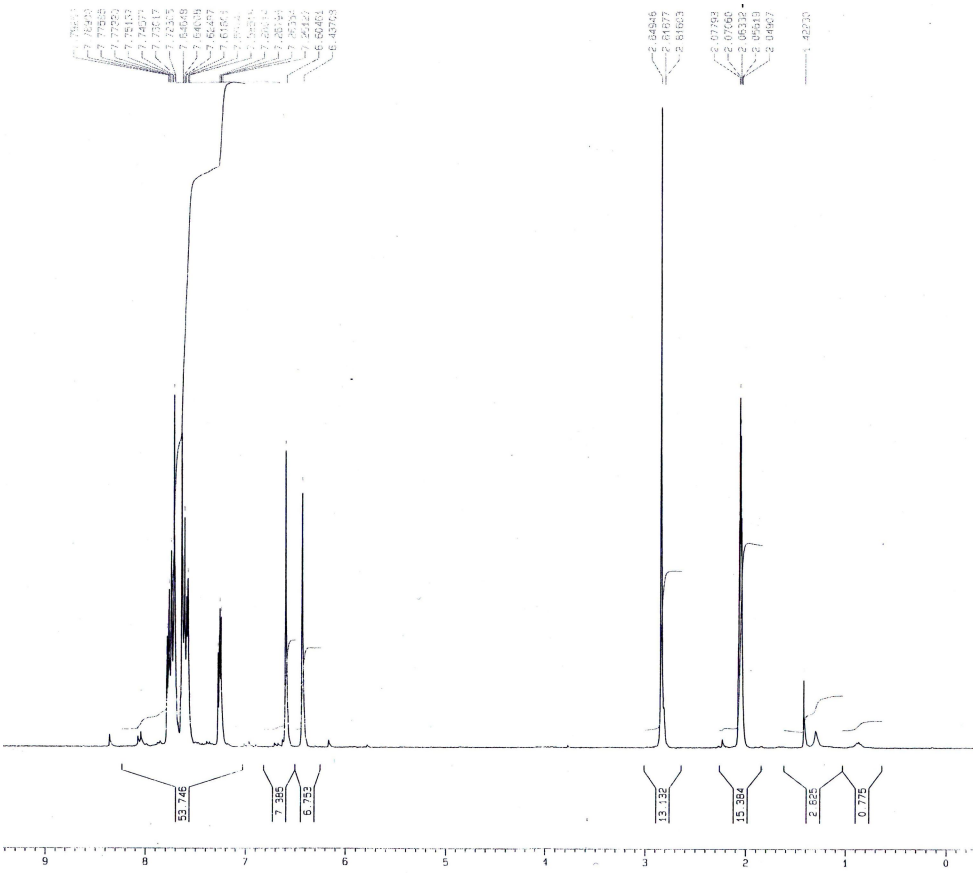
22b

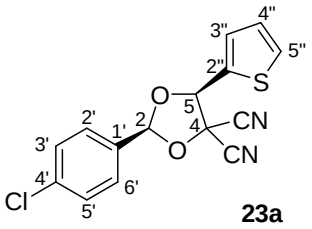
^{1}H - $(CD_3)_2CO$ - 300MHz



22b

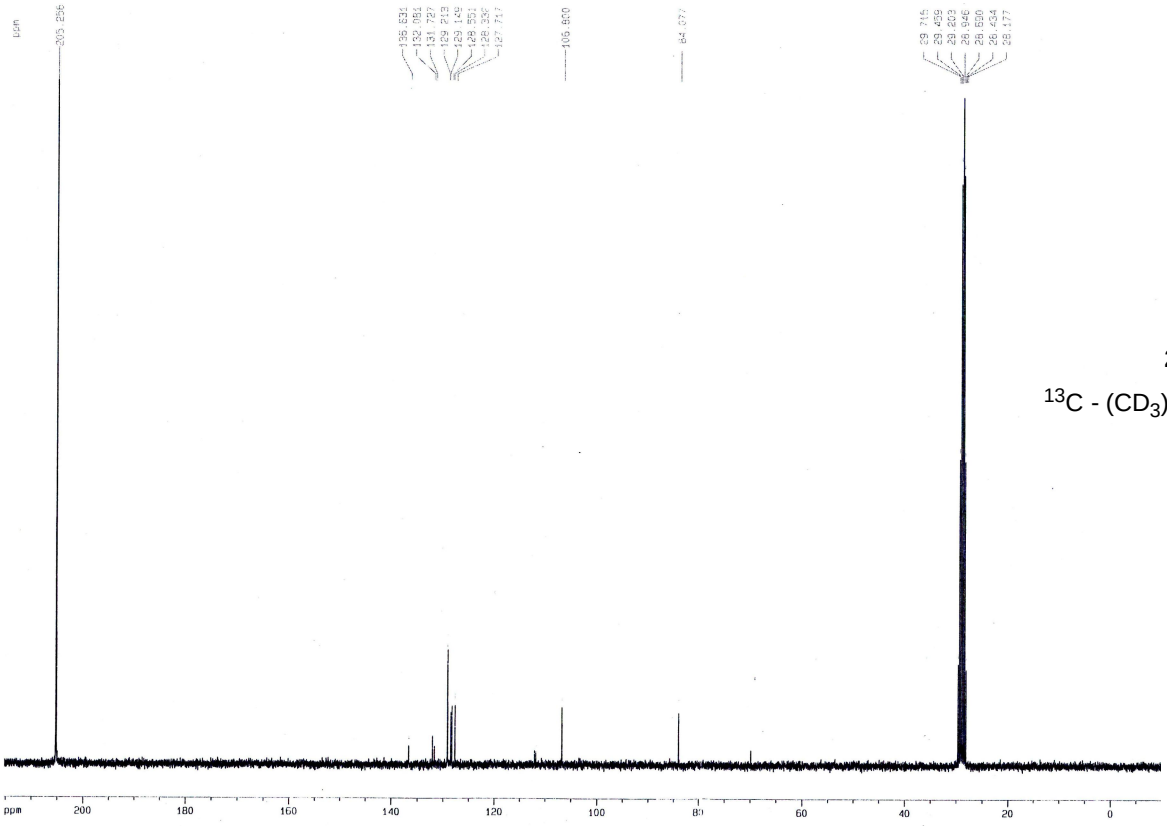
^{13}C - $(CD_3)_2CO$ - 75MHz





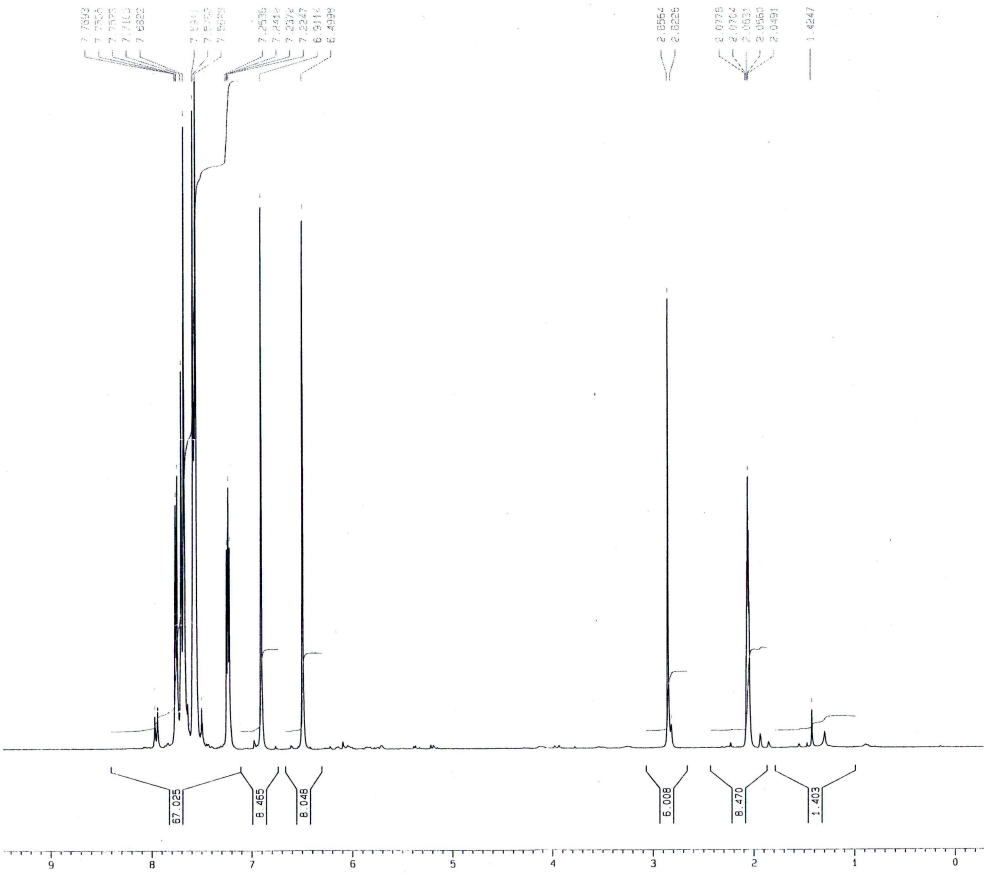
23a

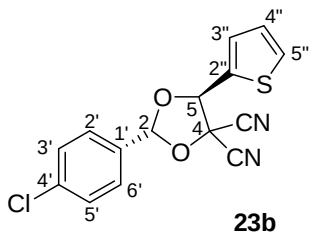
^{1}H - $(CD_3)_2CO$ - 300MHz



23a

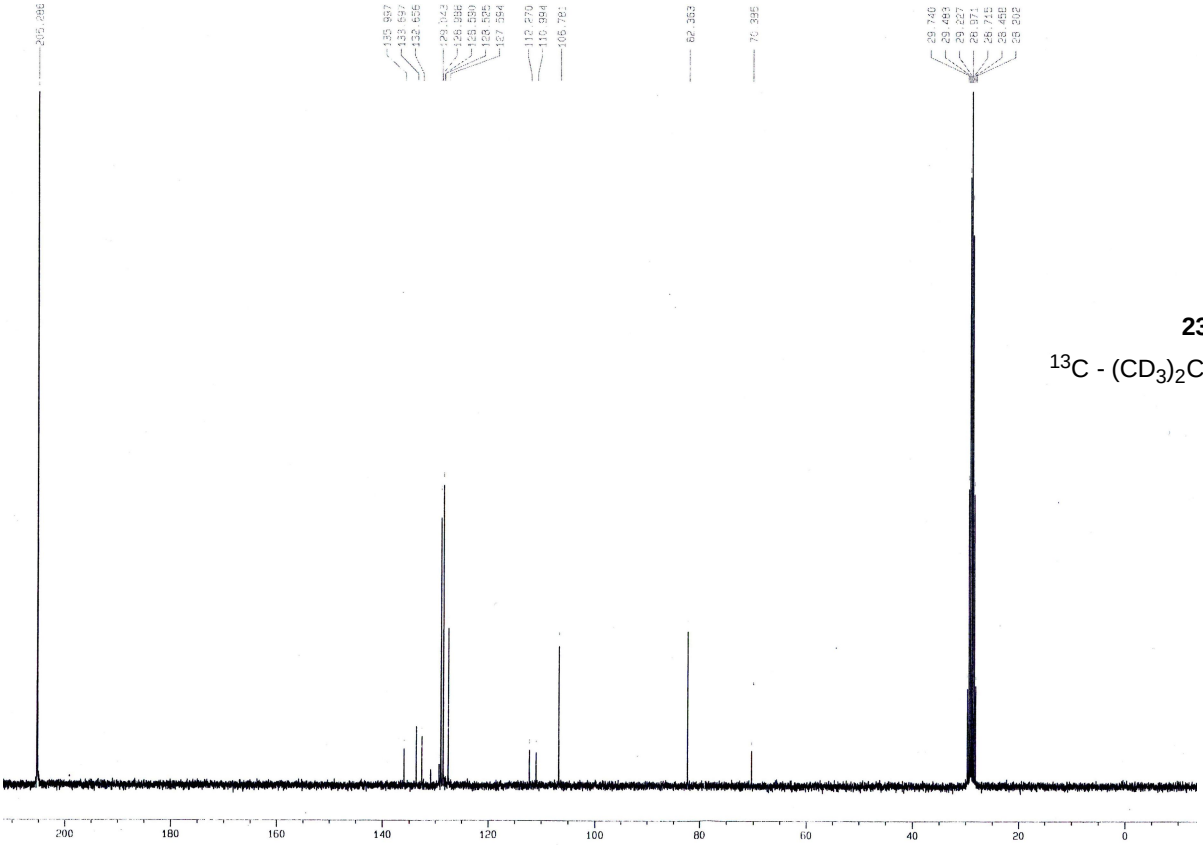
^{13}C - $(CD_3)_2CO$ - 75MHz





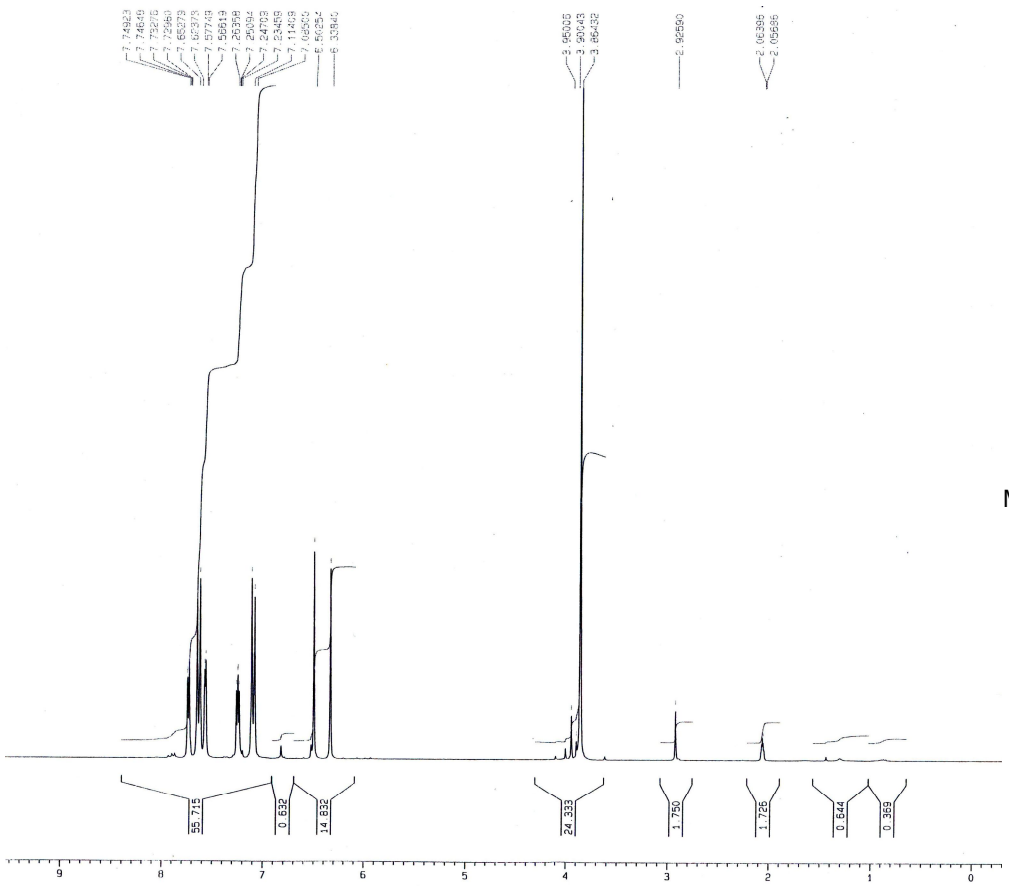
23b

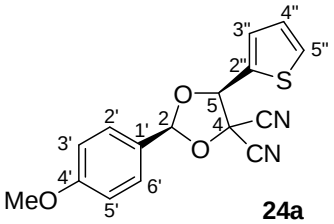
^{1}H - $(CD_3)_2CO$ - 300MHz



23b

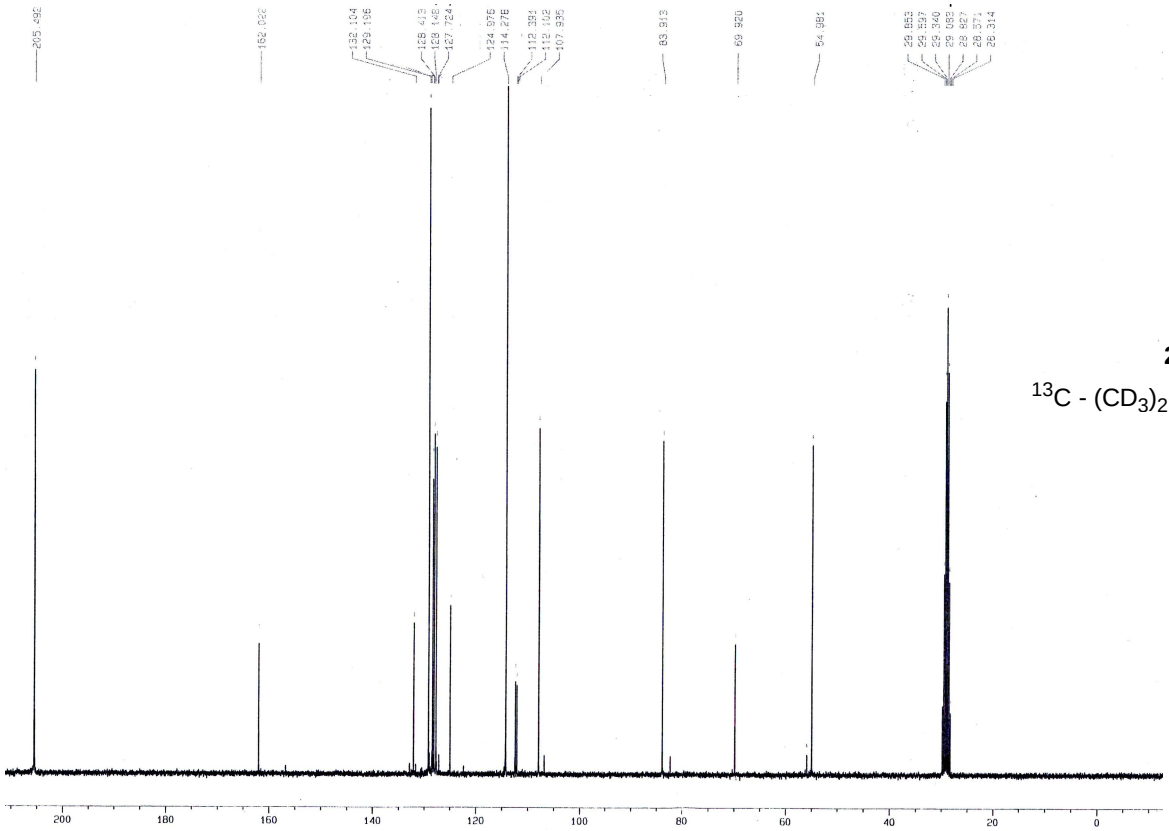
^{13}C - $(CD_3)_2CO$ - 75MHz





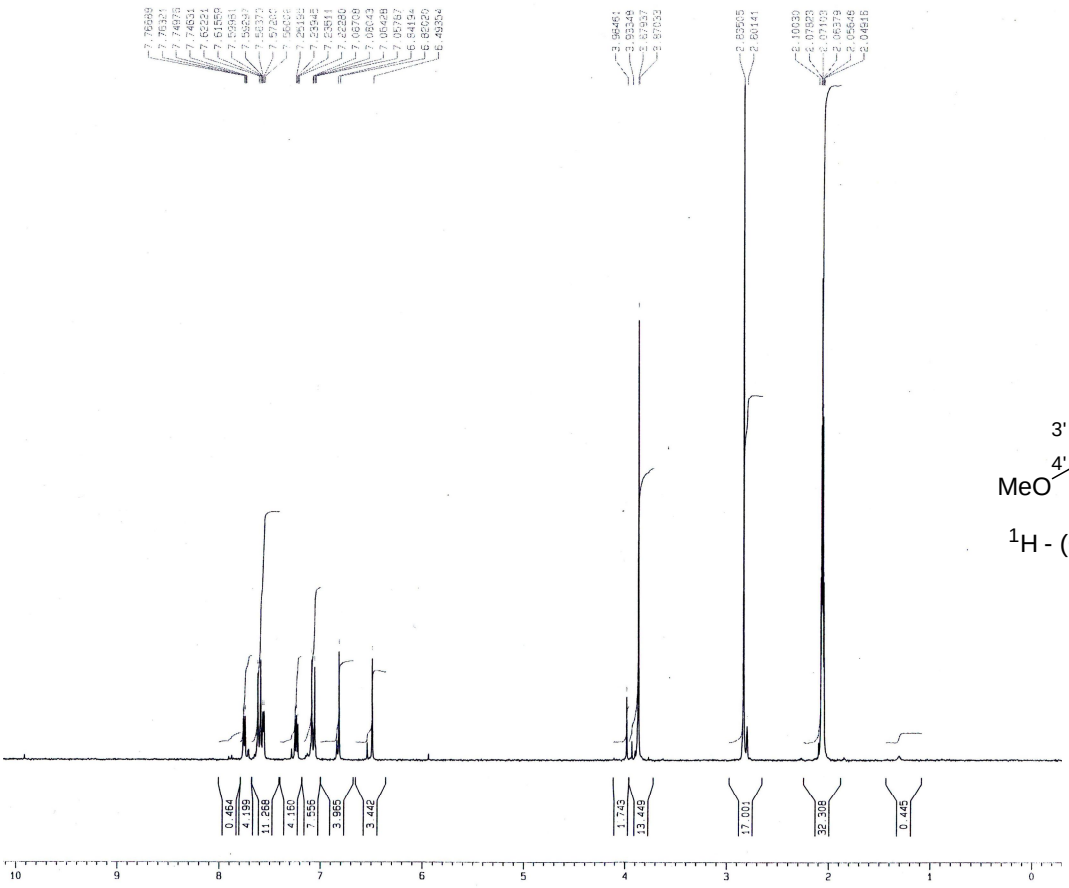
24a

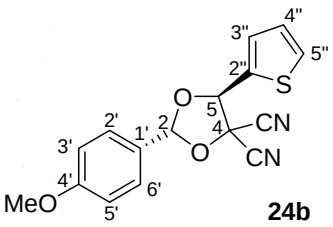
^{1}H - $(CD_3)_2CO$ - 300MHz



24a

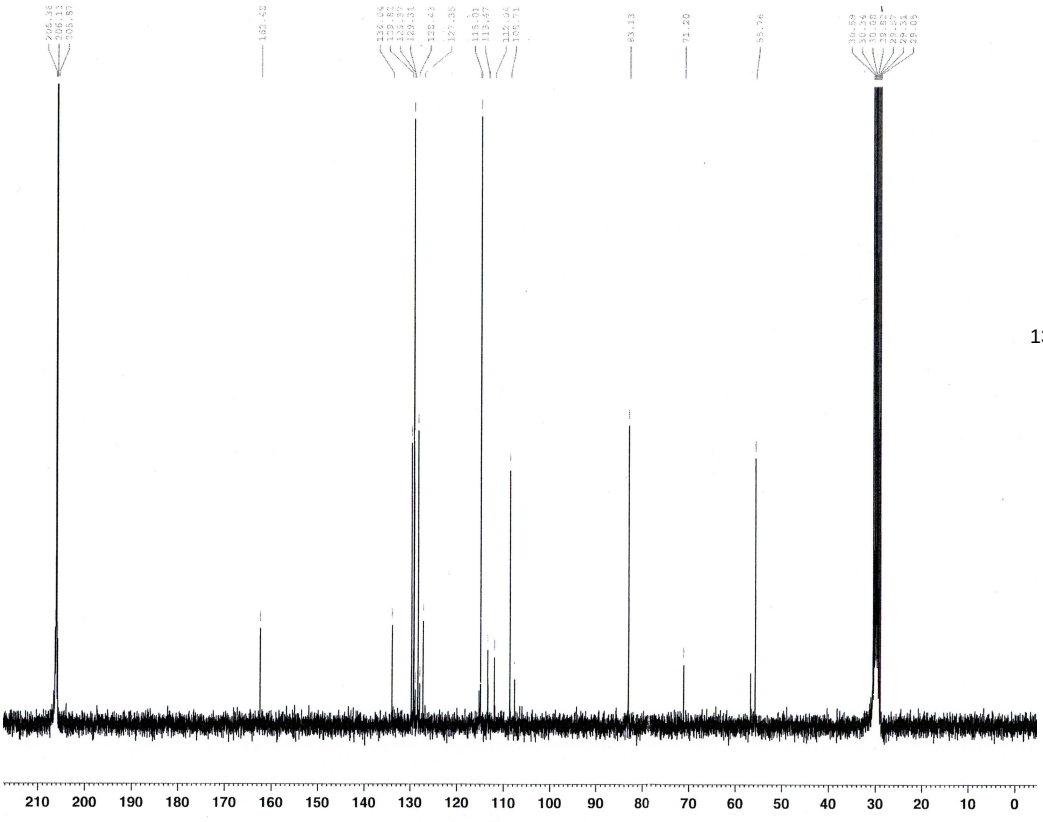
^{13}C - $(CD_3)_2CO$ - 75MHz





24b

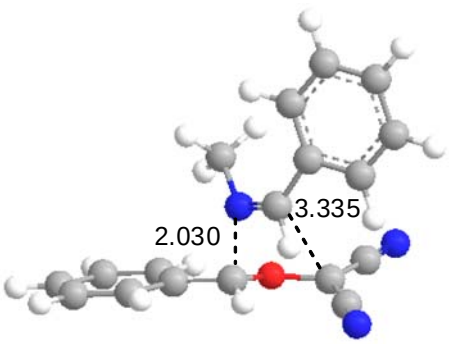
^{1}H - $(CD_3)_2CO$ - 300MHz



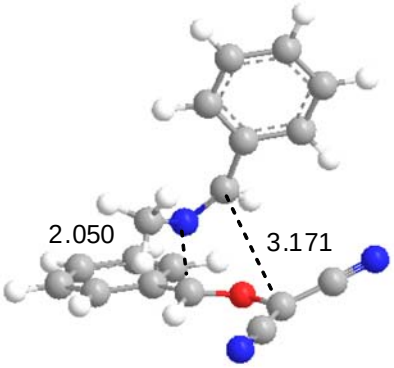
24b

^{13}C - $(CD_3)_2CO$ - 75MHz

Geometries of the TSs with the (*Z*)-Imine 25a



TSn1c-Z



TSn1t-Z

Transition Structures Involved in the Reaction of the Carbonyl Ylide **CYa** with the (*Z*)-Imine **25a**.

B3LYP/6-31G* Computed Total Energies, Unique Imaginary Frequencies, and Cartesian Coordinates of the TSs and Cycloadducts

TSo1c

E(RB+HF-LYP) = -914.858355204 A.U.
1 imaginary frequencies -301.9560 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.392105030000
C	1.213477481552	0.000000000000	2.098509710027
C	2.428577223912	-0.004206205066	1.393431284841
C	2.424420179628	-0.007014864818	0.002841374779
C	1.211992486576	-0.003798364884	-0.695424373851
C	1.196986614722	0.032676156289	3.565824033556
O	2.251393213145	0.192865208752	4.245745202653
H	1.212681736563	-0.006307604577	-1.782011787976
C	2.516568461683	-1.245693084766	5.577996178067
O	2.260168430149	-2.244475626851	4.773727102634
C	0.979488596054	-2.370019975155	4.219982993304
C	-0.127194033725	-2.175959753050	5.073081095187
N	-1.016807199364	-1.908092867741	5.783886169222
C	3.882011130952	-1.086188570495	6.042578717466
C	4.955030294852	-1.755914705483	5.427594116243
C	6.248504380608	-1.562651292895	5.898353072928
C	6.484457216749	-0.698687747675	6.973796226414
C	5.422628937780	-0.025143866525	7.582164411010
C	4.123962314313	-0.217684348390	7.119525660359
C	0.924767226920	-3.234718945995	3.107410301376
N	0.865429829942	-3.902081037049	2.151336985473
H	-0.939506095620	-0.001860011768	1.940109265911
H	0.214353036741	0.157330292672	4.044042004764
H	3.358004670118	0.002333784332	1.953645463881
H	3.364348267568	-0.010919383337	-0.542064272103
H	-0.940737248209	-0.002189181477	-0.542881452761
H	1.700595284007	-0.866755563444	6.187800534266
H	3.293237850122	0.305024693748	7.586271456679
H	5.606899408596	0.645976217641	8.415684182746
H	7.497890270971	-0.551051760889	7.336384021318
H	7.077197409049	-2.083558205785	5.427854556941
H	4.762396712579	-2.423246217938	4.594211757598

TSo1t

E(RB+HF-LYP) = -914.858332500 A.U.
1 imaginary frequencies -305.2925 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.406670070000
C	1.218877043889	0.000000000000	2.105445536100
C	2.423213653976	-0.000565088034	1.407786840692
C	2.417957194407	0.004341834521	0.010811247785
C	1.206679278496	0.006062517719	-0.689951415814
C	-1.232239646365	-0.015099620218	2.172647085062
O	-2.346819112545	0.236212805116	1.534057495906
C	-3.570113979689	0.016335292542	2.191297063466
C	-3.674223610452	0.451054664859	3.530894372911
N	-3.679698236189	0.744023243762	4.662198303101
C	-4.680682020241	0.003814557686	1.319797489753
N	-5.600053381229	-0.099584305619	0.607560943625
O	-1.610701865708	-1.890952576250	2.741881235331
C	-2.806844774042	-2.215237387622	2.478015043225
C	-3.708192261653	-2.787412052027	3.488821304699
C	-4.935474840837	-3.338225929709	3.084645473368
C	-3.351299835201	-2.801449486197	4.846812127820
C	-4.213488705831	-3.361054923558	5.784954458944
C	-5.433147697084	-3.909774539016	5.377492570183
C	-5.793940190613	-3.897318934126	4.026814900085
H	-2.399568095477	-2.374788879958	5.144209526930
H	-3.937940620273	-3.368732754635	6.835736843383
H	-6.103618209267	-4.346298192466	6.112883406232
H	-6.743708326988	-4.319886797037	3.711630275584
H	-1.200736238635	0.191927575483	3.238360776062
H	1.215233701985	-0.006436559867	3.192156777220
H	3.363664933382	-0.002283397573	1.950623431373
H	3.357850104308	0.007230469752	-0.534064530115
H	1.207009166065	0.010795879923	-1.775955250548
H	-0.943389839307	0.001165710828	-0.535775042558
H	-5.214356101235	-3.315048304674	2.033815903350
H	-3.114794778832	-2.346631994673	1.429544029652

TSo2c

E(RB+HF-LYP) = -914.841137978 A.U.

1 imaginary frequencies -453.8051 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.393997830000
C	1.208188271972	0.000000000000	2.104905010336
C	2.420439479256	-0.001160798975	1.399493813401
C	2.418962398583	0.005725379983	0.006016020926
C	1.210480266361	0.006199687243	-0.696752206754
C	1.199965356871	-0.025465979742	3.593235047233
O	2.262070082210	-0.292242698089	4.252739705883
C	0.942733090405	1.982238526365	4.200579732602
O	2.268496152719	2.247621570571	4.109233286053
C	3.121661949296	1.530581899637	4.841722250245

C	4.460763188897	1.522663401535	4.364643772883
N	5.555492310518	1.481969920619	3.969792405528
C	0.062004643053	2.796885870469	3.380762649913
C	-1.292505774096	2.900083307362	3.748717657149
C	-2.180410130734	3.634918722335	2.968247431920
C	-1.727386107454	4.280300743042	1.814829134497
C	-0.383373249646	4.180869994138	1.441349350667
C	0.507707311524	3.440045934219	2.210275315713
C	2.858990975953	1.294395490283	6.224404086990
N	2.631188005062	1.140492243035	7.356052575463
H	-0.942733632874	-0.005127605863	1.936755576570
H	0.232213083601	-0.278588373664	4.056545947411
H	3.354312818442	-0.029098056525	1.952128810069
H	3.361995191615	0.000397654553	-0.534001043568
H	1.212766096278	0.005077913134	-1.783514383863
H	-0.941982038481	-0.006691854201	-0.541697069278
H	0.602972868365	1.703048070470	5.196402795459
H	1.547989499894	3.355230785039	1.914730930752
H	-0.030591033406	4.680046507185	0.543481308049
H	-2.418617411201	4.859157341938	1.208814366236
H	-3.222651829614	3.712228206059	3.264170785502
H	-1.642807296088	2.407300973164	4.652672868936

TSo2t

E(RB+HF-LYP) = -914.841634504 A.U.

1 imaginary frequencies -455.8793 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.395363750000
C	1.209765813356	0.000000000000	2.103174395859
C	2.421674711607	0.003714563919	1.397642357570
C	2.418467754939	-0.000336640785	0.004604979775
C	1.209197951250	-0.003344460625	-0.697961325154
C	1.191042294726	0.020692377599	3.598009030025
O	2.228485907555	0.350543660636	4.265896653969
C	1.110002993825	-2.043655490132	4.015942321717
O	1.657827305937	-1.913743830359	5.245978295927
C	2.850542821738	-1.334418033281	5.379554052392
C	3.140337263567	-0.849061051303	6.683383576648
N	3.388945756745	-0.430907639194	7.741025565918
C	-0.227202822479	-2.616420260505	3.971987994687
C	-0.683187994759	-3.175984195619	2.764046440913
C	-1.974562960622	-3.689583102168	2.671034515194
C	-2.822663760519	-3.657720789868	3.779869484805
C	-2.376189609361	-3.103106404705	4.984511722644
C	-1.092175639062	-2.579032566248	5.083259125295
C	3.917962748798	-1.659373174711	4.492725403847
N	4.779337376698	-1.952787692110	3.764924093497
H	-0.941501259170	0.010525479735	1.939708360201

H	0.202862500309	0.217537391931	4.046840058312
H	3.355851886206	0.017137247783	1.950526042038
H	3.361189312539	0.004465957438	-0.535815133079
H	1.210633970867	-0.002753632251	-1.784626275691
H	-0.942687844580	0.007466415229	-0.540685396476
H	1.808463142818	-2.295245652390	3.220698068860
H	-0.747184355970	-2.147837644045	6.017690272238
H	-3.034304892898	-3.078390291436	5.848373657634
H	-3.827724487812	-4.063684908338	3.708316950712
H	-2.315774021822	-4.121677817595	1.734745702810
H	-0.022022822546	-3.204738299253	1.902666527211

TSn1c

E(RB+HF-LYP) = -934.290180643 A.U.

1 imaginary frequencies -281.5750 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	2.762036420000
C	2.090713320407	0.000000000000	1.676063120604
O	1.116733468900	-0.625822450491	2.459078539687
C	2.273147241800	1.388303948287	1.807456720575
N	2.348332552181	2.552380344883	1.912623503738
C	3.097527157470	-0.856318552758	1.202881576810
N	3.911291684347	-1.563003578018	0.749059432565
N	-0.779912011743	0.441895062355	0.955402281584
C	0.146628410671	-1.415657844238	-0.324851263164
C	-0.708013675849	-2.384491900318	0.234507339844
C	1.117139814133	-1.818476779697	-1.261008914426
C	-0.575846721282	-3.723484138462	-0.119560703405
H	-1.486665337683	-2.066925977354	0.919412440487
C	1.245067924567	-3.158601655577	-1.612274359287
H	1.781669943197	-1.077053400959	-1.695775477882
C	0.401491164509	-4.114216210878	-1.040346734734
H	-1.243994274319	-4.464296001615	0.311336192177
H	2.006921424291	-3.458843618071	-2.325321797458
H	0.500449063620	-5.160353310696	-1.316860024350
C	-1.094993649296	1.873558045442	0.919926761008
H	-1.938699615012	2.028619512462	0.238182706822
H	-1.414404628854	2.210955106252	1.910561553473
H	-0.252780505153	2.496893151286	0.595739025014
H	0.447988226588	0.712066737189	-0.702159285151
C	-0.961139494680	-0.750446038326	3.573784341747
C	-0.860515493200	-2.141655057601	3.746319798882
C	-2.004699420485	-0.051144951202	4.201113652948
C	-1.794583645206	-2.814081065292	4.528952951936
H	-0.048431992537	-2.681682215918	3.271728142712
C	-2.940255228231	-0.730278386140	4.977559673591
H	-2.079239232766	1.026858866600	4.083436142584
C	-2.837322752337	-2.113230317149	5.142654046572

H	-1.707843407985	-3.888374335272	4.664726495841
H	-3.743785567050	-0.180662972820	5.459190494669
H	-3.563337758090	-2.643298601000	5.752756878898
H	0.079438122493	1.071192347195	2.938090610329

TSn1t

E(RB+HF-LYP) = -934.293306790 A.U.

1 imaginary frequencies -261.9217 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	2.776406670000
C	2.194190877992	0.000000000000	1.897307476281
O	1.202588113443	-0.525535100541	2.726542030040
C	2.348065875693	1.390871305176	1.814381163382
N	2.435231077264	2.556253748607	1.733755654556
C	3.213615060459	-0.912867115411	1.575648112400
N	4.044798722782	-1.676888700860	1.269882024911
N	-0.644183275592	-0.666577102760	0.914004575202
C	-0.222366733239	1.420829952624	-0.257531675682
C	-1.347958255132	2.090788681946	0.260375805129
C	0.678906749950	2.130485864598	-1.069594894874
C	-1.553581454467	3.437787196276	-0.018188256498
H	-2.070430343839	1.528282071103	0.844164683676
C	0.469851344559	3.478727445466	-1.346162019252
H	1.551415440734	1.620933359666	-1.469753691513
C	-0.644198768053	4.135200027181	-0.819947949185
H	-2.429554401673	3.944803139153	0.377158163415
H	1.179405422875	4.019008971606	-1.965693825624
H	-0.807578097845	5.187088936906	-1.037215964906
C	-0.481908951834	-2.118176760231	0.899732876979
H	-0.595711712668	-2.517652009684	1.910802034229
H	-1.278016698325	-2.551581565823	0.283249914409
H	0.489630487064	-2.436800391981	0.497922044232
H	0.678750594418	-0.523979762271	-0.683274564470
C	-0.912672605198	-0.541916033544	3.775019920129
C	-0.591720110924	-1.679492108590	4.537855085292
C	-2.150783307144	0.094716356716	3.969837977299
C	-1.500238391234	-2.168417219929	5.472604829782
H	0.373377623430	-2.157506222321	4.405957545568
C	-3.053524284520	-0.399078077487	4.906031214592
H	-2.398124676217	0.975059858796	3.382985341486
C	-2.730931094175	-1.532406970216	5.658195196610
H	-1.245010206910	-3.043254945027	6.063578488356
H	-4.007253034509	0.099478537993	5.052595882853
H	-3.434973038893	-1.915579305218	6.391449012507
H	-0.107736244404	1.037119620159	2.469170367721

TSn2c

E(RB+HF-LYP) = -934.274359714 A.U.

1 imaginary frequencies -404.7659 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.394421620000
C	1.206406825291	0.000000000000	2.110809560075
C	2.418061123791	-0.004762569513	1.401071825815
C	2.415454621590	0.005218721651	0.007600990529
C	1.208767901710	0.007046376335	-0.697933886232
C	1.178909467651	-0.018899771698	3.593504934425
C	1.037244804322	2.077967799118	4.085894886513
O	2.335819171694	2.314501915438	3.828860617186
C	3.259130410981	1.685071469687	4.595520102172
C	4.543337814636	1.565447686828	4.000543963473
N	5.592351734414	1.425191473420	3.513444804720
C	0.067744836414	2.809293752140	3.290951950084
C	-1.249347736374	2.925902603691	3.774897545891
C	-2.217050315748	3.592676484552	3.029968631129
C	-1.882653878259	4.155897214592	1.795203891317
C	-0.577551866405	4.042591717959	1.306373498644
C	0.393385465563	3.369950328535	2.040878332325
C	3.145653238321	1.782377604216	6.008241676805
N	3.004500014596	1.851921073837	7.164769753758
H	-0.944072112516	-0.002453014884	1.934651957607
H	0.197280104004	-0.218141707171	4.044649039634
H	3.354082607414	-0.038276080813	1.948314834639
H	3.359985829010	0.000568440575	-0.529869852957
H	1.211667097910	0.007063276872	-1.784697508966
H	-0.943272186594	-0.006742726141	-0.539621254572
H	0.793819992109	1.879660693758	5.128467190496
H	1.403957884329	3.274851891821	1.658809636974
H	-0.317323595214	4.478041218240	0.345928734829
H	-2.636365343443	4.682173915082	1.216264514253
H	-3.228708583108	3.682090129050	3.415241800884
H	-1.506470453397	2.497447348324	4.740913614455
N	2.277624285232	-0.357182538285	4.268822716869
C	2.054109676119	-0.912175280454	5.595764370090
H	2.957820368201	-0.827723610113	6.202697745022
H	1.214971642026	-0.459322159316	6.149982410822
H	1.838021374612	-1.982270311285	5.474336446179

TSn2t

E(RB+HF-LYP) = -934.274440415 A.U.

1 imaginary frequencies -421.4817 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.395518640000
C	1.208070087603	0.000000000000	2.110553041628
C	2.418239042665	0.011944309850	1.399727805628
C	2.414336095009	0.007872273695	0.006507923190

C	1.207681284244	0.000000000000	-0.699157351551
C	1.164804218419	0.011887043490	3.598759648180
C	1.006209118873	-2.107572774465	3.989267503141
O	1.714279094197	-2.128304869932	5.127298771782
C	2.972225356323	-1.625585020505	5.131308904126
C	3.518057089068	-1.455358615153	6.431408411076
N	3.965601015158	-1.262349292207	7.490360423285
C	-0.371606555266	-2.570539686532	4.085075258289
C	-1.024459289840	-3.003647098122	2.916065488369
C	-2.352174082950	-3.422537823347	2.966467603907
C	-3.041468074158	-3.423385791604	4.180648894090
C	-2.397565920883	-2.998594734615	5.348307209015
C	-1.075934327808	-2.569426624533	5.305045981478
C	3.858790143613	-1.923351477616	4.056311413674
N	4.570302300823	-2.167782605254	3.166354027307
H	-0.943401590581	0.008173999687	1.936432065026
H	0.173391192708	0.216590356123	4.023194305747
H	3.354444248306	0.030077154730	1.946381276306
H	3.358797445690	0.015419225959	-0.530807597066
H	1.209822947921	0.000351412351	-1.785801794232
H	-0.943803150593	0.006764183444	-0.539044656210
H	1.563206214628	-2.325689038376	3.081320029367
H	-0.577145400008	-2.240738971734	6.211327211632
H	-2.930669506014	-3.002043259846	6.294842691438
H	-4.074983739304	-3.755661730081	4.219992226223
H	-2.845644367077	-3.757120233269	2.058457625531
H	-0.486704469779	-3.009068233346	1.972371543158
N	2.241882070545	0.364652320068	4.305440753971
C	1.939436288139	1.008859451658	5.581274531969
H	2.820693795385	1.017317985620	6.225158820969
H	1.670700805105	2.053057244616	5.370933302058
H	1.097731437384	0.552064925422	6.127025154713

TSn1c-Z

E(RB+HF-LYP) = -934.291743435 A.U.

1 imaginary frequencies -177.8591 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	2.818617250000
C	2.342962551780	0.000000000000	2.372816759573
O	1.192067431967	-0.486082143553	3.036709679142
C	2.303536647581	1.260016471465	1.791762922100
N	2.155701410129	2.311446818432	1.282148349024
C	3.458776189016	-0.834848331970	2.466402982997
N	4.389514959469	-1.543131466605	2.531696755498
N	-0.444398844085	-0.713596087166	0.970973043894
C	0.303982816711	-0.329099643907	-1.398820575019
C	-0.251897439086	-1.398896549539	-2.125710399714
C	1.210164884664	0.537495506560	-2.042293400653

C	0.108649382889	-1.602288612305	-3.455324363978
H	-0.987145673768	-2.051890254819	-1.671193174074
C	1.582042257081	0.316152850936	-3.364641472098
H	1.633106912218	1.368846017972	-1.483140569056
C	1.031055373215	-0.753957035933	-4.073438793758
H	-0.332882546977	-2.423941210473	-4.011903779286
H	2.295265392367	0.980413306256	-3.843594202858
H	1.313048438820	-0.922930086746	-5.108991536109
C	-0.673119011509	-2.146958406788	0.913781359268
H	0.063107216070	-2.657754685517	0.283308813293
H	-0.607745661606	-2.546753071681	1.929541154428
H	-1.681009406871	-2.358985875707	0.538659981986
H	0.225071714675	1.037890398958	0.257699577699
C	-1.067643828683	-0.493118995895	3.692273868312
C	-0.851499657896	-1.546361598745	4.597286808271
C	-2.337578128733	0.102107566067	3.612673514461
C	-1.893313179485	-1.991716140597	5.407239155020
H	0.134872167746	-1.992446166548	4.671032452030
C	-3.374674277262	-0.348333128700	4.424553986151
H	-2.505926269343	0.915506757783	2.911366471101
C	-3.155027004918	-1.396528669980	5.322767716174
H	-1.719046406501	-2.801069386083	6.110421912678
H	-4.352985045373	0.119379545093	4.360793755435
H	-3.963990945081	-1.744813077159	5.958806058519
H	-0.064759082522	1.021805373200	2.447795200942

TSn1t-Z

E(RB+HF-LYP) = -934.290881878 A.U.

1 imaginary frequencies -166.0848 cm**-1

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	2.801365520000
C	2.299075889219	0.000000000000	2.186583737547
O	1.091023191668	-0.669291663527	2.551481972426
C	2.402868308092	1.355138394801	2.479217468456
N	2.376807072321	2.494808100686	2.766560567584
C	3.108812994607	-0.745632470344	1.334777334982
N	3.744023969298	-1.391813207885	0.587773195025
N	-0.487680299395	0.713167603534	0.942803757649
C	0.127022284130	0.266762803274	-1.441468296747
C	-0.819873036659	0.986054322950	-2.191923739630
C	1.257006742620	-0.271697052063	-2.085573715623
C	-0.628189304309	1.176788195631	-3.558320151157
H	-1.721588362907	1.361116747281	-1.719006186774
C	1.453593114512	-0.054932533382	-3.447013914372
H	1.992046811570	-0.828524969808	-1.507598347236
C	0.511727019268	0.666267332735	-4.184724769851
H	-1.370096155428	1.721056558281	-4.135609761346
H	2.338564923475	-0.455447533393	-3.932525739139

H	0.660541464244	0.823614576728	-5.249436802073
C	-0.961490553373	2.079995289208	0.816742101600
H	-0.596452684666	2.567899172202	-0.092225115721
H	-2.057482715177	2.101180125665	0.824791432166
H	-0.597397708939	2.647556990668	1.679719204129
H	0.423079189530	-0.952937204938	0.327727163651
C	-1.157073132662	-0.774460177530	3.256290603777
C	-1.199331636825	-2.174017768460	3.140836960353
C	-2.251298119532	-0.091670670452	3.811232863321
C	-2.323336249596	-2.872359074180	3.571876992304
H	-0.345944928340	-2.702580997115	2.728978166909
C	-3.374492882287	-0.795649824577	4.238150213872
H	-2.215549889567	0.990313143575	3.913182627713
C	-3.412993978409	-2.186824602165	4.117902870659
H	-2.349463742135	-3.954901879163	3.486380985670
H	-4.215516688978	-0.261377389278	4.670653160364
H	-4.287221819780	-2.736884867684	4.454667664993
H	0.110018331959	1.025555852436	3.149875378348

CAo1c

E(RB+HF-LYP) = -914.913838580 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.400215600000
C	1.215691604341	0.000000000000	2.093904242108
C	2.418434453334	-0.000374090623	1.388499836550
C	2.416141947605	-0.010223851245	-0.007704468429
C	1.204931582539	-0.011727683563	-0.701656209662
C	-1.313645308525	-0.022761960704	2.130367395485
H	1.214012303165	0.012948595913	3.178340059019
H	3.359068874242	0.005084108242	1.931881598580
H	3.355620635477	-0.012648714985	-0.553461794101
H	1.196181882620	-0.014064288182	-1.787863296481
H	-2.089282361676	0.488826968183	1.540209971800
O	-1.229325304057	0.538884851278	3.424382663786
H	-0.942591566605	0.008716752820	-0.542488298573
C	-1.926965188005	-1.449129908679	2.486966325585
C	-2.421931374369	0.174949334646	4.084529784570
O	-2.703990112994	-1.183922571176	3.642542395462
H	-3.252008519632	0.807387041869	3.736904681735
C	-2.270557826847	0.239736628960	5.576009529067
C	-2.778110898543	-1.947523962459	1.389762314056
C	-0.887479857240	-2.450163251443	2.819278449490
C	-3.054462717384	1.129821779436	6.313322869180
C	-2.911060117842	1.210365846514	7.699743683642
C	-1.983892730673	0.396035970723	8.349766032496
C	-1.200805162414	-0.499039347018	7.614060657977
C	-1.342360685064	-0.579302331595	6.231108742032
H	-3.778112012777	1.761819050902	5.803780794813

H	-3.523579467313	1.904492718347	8.268130367133
H	-1.872214890403	0.454113532547	9.429088225235
H	-0.482085308249	-1.137026815857	8.120608164572
H	-0.741779498344	-1.280190866780	5.659198947002
N	-0.076065883842	-3.218978543587	3.129140936450
N	-3.444526664762	-2.291128234974	0.504701399959

CAo1t

E(RB+HF-LYP) = -914.910560931 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.399420760000
C	1.213173833674	0.000000000000	2.092179459359
C	2.421870344706	0.008804926717	1.393991512070
C	2.418218579578	0.011237931381	-0.000955636288
C	1.205711867640	0.004780362298	-0.697063376575
C	-1.290604803015	0.025010486742	2.170829084701
O	-1.844065611493	1.353791049270	2.145023134544
C	-3.247591962056	1.194067425024	2.254995903951
C	-3.645579919154	1.001322054587	3.671993105051
N	-3.891403897889	0.834027980234	4.793113310733
C	-3.919647662326	2.377282913152	1.696009891638
N	-4.475307588294	3.277212704318	1.221063681699
O	-2.295581263843	-0.828389090775	1.620895472248
C	-3.486033227302	-0.096329400000	1.372318303548
C	-4.731753733320	-0.893588756388	1.660417532879
C	-5.922019323746	-0.553840260913	1.005120277709
C	-4.726705148768	-1.945774413022	2.582573928631
C	-5.903494234570	-2.644949766341	2.849273490442
C	-7.091112245107	-2.296384815741	2.203510953947
C	-7.099109249078	-1.248611837162	1.280920586908
H	-3.800186532441	-2.220891805175	3.074545367036
H	-5.891453714246	-3.463687261524	3.563244005452
H	-8.006273082855	-2.842862881692	2.414126852658
H	-8.018168632391	-0.976242875427	0.769834122350
H	-1.128439574965	-0.271301420871	3.216066749454
H	1.213026879070	-0.006132424579	3.179723379862
H	3.361749007166	0.008944662179	1.938671921113
H	3.357539998896	0.013483744653	-0.547189266141
H	1.202014436157	0.001026957611	-1.783490071261
H	-0.942849864768	-0.017348241243	-0.538030636846
H	-5.929129211227	0.255166512342	0.278065142109
H	-3.500169862041	0.260539329967	0.333186280605

CAo2c

E(RB+HF-LYP) = -914.904879282 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.394088770000

C	1.205477289020	0.000000000000	2.106929851252
C	2.413905557449	-0.020482884183	1.401980956952
C	2.413640678175	-0.025994007863	0.006291922865
C	1.208990039938	-0.012036241354	-0.698041670252
C	1.158058368634	0.035605496248	3.617693848411
O	2.319767275727	-0.610353208610	4.196302522965
C	1.189112175092	1.442838410227	4.303384495497
O	2.605883882332	1.624417761788	4.530274993574
C	3.085468877156	0.359482105792	4.880399714291
C	4.511339897639	0.259371434920	4.476849782899
N	5.617683542593	0.167098052995	4.144187631100
C	0.617400173895	2.621251995955	3.564946266723
C	-0.685090562852	3.038791743873	3.861169129932
C	-1.258629914252	4.108594903257	3.173119702127
C	-0.524801076843	4.780287993696	2.194843050233
C	0.780683198898	4.376128400710	1.906144321213
C	1.349987039680	3.298454770026	2.582434941750
C	2.957737728648	0.130270135712	6.356655969919
N	2.819586062210	-0.031202085520	7.496901371896
H	-0.945142550718	0.003276548086	1.932493644967
H	0.278320011311	-0.511134567324	3.971473371777
H	3.356257919401	-0.052441015108	1.938732205900
H	3.358624192925	-0.047705909941	-0.529523840740
H	1.211560426489	-0.019809123064	-1.784561696998
H	-0.943140027190	0.000448991789	-0.539442295994
H	0.695139426821	1.347236628356	5.280238698081
H	2.364587962981	2.987527476460	2.359213781359
H	1.358647441705	4.901385511177	1.150893034392
H	-0.964943961658	5.620176018916	1.664309618518
H	-2.270652832780	4.423621675856	3.411616412441
H	-1.251979128387	2.530058318512	4.638038687053

CAo2t

E(RB+HF-LYP) = -914.909770388 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.398993590000
C	1.219963621952	0.000000000000	2.087750118911
C	2.422135312887	-0.000431331423	1.382036510563
C	2.417282664705	-0.009267131942	-0.015031251036
C	1.204490848261	-0.009937396385	-0.704903465730
C	-1.309170752282	-0.051648030825	2.140452003941
H	1.224286158773	0.023664539872	3.173287063918
H	3.363857565945	0.009832451338	1.923764564160
H	3.355624711364	-0.008548676200	-0.562813277355
H	1.193268505906	-0.009256676923	-1.791251358712
H	-2.129964989748	0.299563485413	1.502245351541
O	-1.245074072399	0.773588713096	3.328586324620
H	-0.944223499688	0.007318539840	-0.538834421326

C	-1.684664409849	-1.426200247954	2.739876439400
C	-2.167049733244	0.250333398534	4.253725900500
O	-2.542921601402	-1.044634218747	3.841829478037
C	-3.398756084409	1.091806685382	4.314173777343
C	-1.509592141156	0.211871969552	5.591026564446
H	-0.780444434689	-1.901816195276	3.139991028310
C	-2.409555854042	-2.361827289526	1.808435759345
N	-0.990108315203	0.151995840738	6.625731850105
N	-4.352024723343	1.751891248588	4.324574158332
C	-1.700048660278	-3.390969276749	1.179987573627
C	-2.336823627873	-4.229375460278	0.263993744028
C	-3.691089210135	-4.051360474181	-0.021117081338
C	-4.405876494316	-3.031294715529	0.611408541246
C	-3.769087775428	-2.186660185548	1.519633690560
H	-0.646725538361	-3.536333460006	1.406576425904
H	-1.776351219658	-5.025287215551	-0.218406780644
H	-4.190185586455	-4.708462076214	-0.727999757576
H	-5.462826240409	-2.894591524895	0.400170739824
H	-4.329023591552	-1.404176124328	2.022729330378

CAn1c

E(RB+HF-LYP) = -934.355788996 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	2.313214570000
C	1.491176283043	0.000000000000	0.510624807509
O	1.382026385529	0.172514008033	1.916577739994
C	2.255469739114	1.120691311456	-0.076126029832
N	2.821631438131	2.017189490295	-0.545984517347
C	2.195502635321	-1.276706907163	0.237082021657
N	2.748043626749	-2.282728455073	0.069590088045
N	-0.630635631758	-0.626589596251	1.155533113284
C	-0.252148120439	-0.676963998430	-1.327417078465
C	-0.412678734714	-2.065954983227	-1.420544621636
C	-0.305769535816	0.098713755971	-2.492122024931
C	-0.622325740922	-2.665410942618	-2.661994080560
H	-0.373245284301	-2.668036904285	-0.518738444051
C	-0.506634744536	-0.503557790249	-3.734147055386
H	-0.186108907700	1.177680887149	-2.426725031977
C	-0.666673007498	-1.887299000564	-3.820676579017
H	-0.746475275595	-3.742934456646	-2.723796394278
H	-0.542400926560	0.108626652323	-4.630886528902
H	-0.827533018981	-2.357502429872	-4.786929388033
C	-2.087920354795	-0.554577219826	1.175497483459
H	-2.489355942199	-1.074262173807	0.302847741647
H	-2.456223415260	-1.051194153498	2.076992464439
H	-2.461199646041	0.485682001115	1.168287025482
H	-0.278348420839	1.067701933635	-0.086307357190
C	-0.088914714726	-0.818832662428	3.576801493037

C	0.357598428539	-2.146839655412	3.593612835421
C	-0.613450427697	-0.252734635624	4.741480526486
C	0.275746137994	-2.895041102052	4.765287138716
H	0.768728199124	-2.583965460178	2.688869087992
C	-0.699063287791	-1.004019784510	5.915816842214
H	-0.954075529609	0.780353743557	4.731241728218
C	-0.254038814168	-2.325636747335	5.927813839025
H	0.626719794293	-3.923279551610	4.774500578014
H	-1.109182438930	-0.556145185037	6.816721804022
H	-0.316303177076	-2.912368017815	6.840398590137
H	-0.409702372314	1.011784967756	2.495923608182

CAn1t

E(RB+HF-LYP) = -934.348123887 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	2.301225620000
C	1.529504970588	0.000000000000	0.592424094606
O	1.382870702104	-0.312690374847	1.963624873048
C	2.227813653748	1.298185368601	0.449996102095
N	2.795586008333	2.308050620463	0.388949615968
C	2.333211093185	-1.055692553039	-0.054657408294
N	2.925277632081	-1.898959823051	-0.588443680586
N	-0.779443063654	-0.437484923030	1.153767084243
C	-0.438958926247	1.316177189576	-0.621089862039
C	-1.441147073060	2.103894269621	-0.047323771317
C	0.141747156634	1.727516210341	-1.829029977543
C	-1.838507091168	3.295197819749	-0.657357762196
H	-1.924972109030	1.764653213924	0.862292761344
C	-0.256052510548	2.915320003346	-2.438927864099
H	0.909759992795	1.116460520559	-2.298933100276
C	-1.246045974400	3.705886525336	-1.851293734851
H	-2.618034594975	3.898411690573	-0.199796208630
H	0.205102806567	3.221175625368	-3.373741281725
H	-1.557533505253	4.632166045781	-2.326076493651
C	-1.109560859838	-1.871739080465	1.121782813330
H	-1.736897133715	-2.114820612299	1.980897961416
H	-1.685368666468	-2.069190139350	0.213719685457
H	-0.227586026305	-2.529408246012	1.133256519607
H	-0.036296890490	-0.771897639307	-0.772899351965
C	-0.366544666066	-0.606870733582	3.632475002475
C	0.443849547728	-1.559438399852	4.257026123163
C	-1.552687632567	-0.194851805175	4.253454672161
C	0.066530808137	-2.097122547828	5.489351053833
H	1.369660472353	-1.866865260195	3.783745952595
C	-1.931013940441	-0.739219688664	5.479538614993
H	-2.181219968500	0.551197672698	3.773076170907
C	-1.120190809700	-1.692290831547	6.100900339929
H	0.704463440349	-2.833014750537	5.971044925361

H	-2.853797682707	-0.414893236449	5.952598931337
H	-1.410734567269	-2.112295062112	7.059968165533
H	-0.077557406081	1.094490850712	2.356899414821

CAn2c

E(RB+HF-LYP) = -934.350451877 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.395756840000
C	1.203798348310	0.000000000000	2.110229297747
C	2.413814630604	-0.016464528517	1.403161957239
C	2.414137094978	-0.028026381905	0.008927932734
C	1.208611757932	-0.015750072445	-0.696643802267
C	1.162925066487	0.027689738382	3.622023792065
C	1.435266966819	1.403381788467	4.318946781567
O	1.982033412645	1.022956996489	5.609680810456
C	2.205089538332	-0.367224391714	5.639860615959
C	3.523193020244	-0.649384208040	6.267896433983
N	4.558147008942	-0.875746692499	6.738910776372
C	2.363649070072	2.372428125180	3.621001995453
C	1.818975727679	3.335325661142	2.762747495794
C	2.644590011350	4.231691729442	2.085075867332
C	4.027310034901	4.183443982336	2.270165660355
C	4.576080176106	3.235939577221	3.136043853543
C	3.750082686902	2.334695066883	3.808911510734
C	1.123428028981	-1.010298718045	6.470915851741
N	0.249129073451	-1.524525926134	7.035388834070
H	-0.944704970579	-0.003830466982	1.935462996884
H	0.156870241064	-0.300158728755	3.940474660014
H	3.350365214120	-0.019704493807	1.950748113438
H	3.358879017906	-0.043705279870	-0.527640592772
H	1.212021627580	-0.023600251601	-1.783232295216
H	-0.943026076387	0.001663700234	-0.539785597248
H	0.477175440917	1.897188685676	4.509789008496
H	4.182642209129	1.612402781800	4.492981768523
H	5.650492324708	3.200154733105	3.294812744160
H	4.672400475528	4.886445711053	1.750099691882
H	2.207147689053	4.972775536154	1.421652611328
H	0.741575530968	3.382460246610	2.620636783177
N	2.194361431549	-0.805863950490	4.255900808845
C	2.114865580225	-2.248361978948	4.032379611960
H	2.948803525313	-2.737992271688	4.544047695687
H	1.169515076542	-2.686918138009	4.388827078317
H	2.211466994562	-2.436036736624	2.961474841838

CAn2t

E(RB+HF-LYP) = -934.355171113 A.U.

C	0.000000000000	0.000000000000	0.000000000000

C	0.000000000000	0.000000000000	1.396066610000
C	1.205328247744	0.000000000000	2.106596204713
C	2.415186137761	0.007300047214	1.398079732687
C	2.415124899145	0.013960516366	0.003759401996
C	1.207535254613	0.007785996447	-0.698909193081
C	1.189189718651	-0.054252287198	3.619242232257
C	1.589264054056	-1.432055471869	4.203218638567
O	2.114764554089	-1.105773390994	5.518384274558
C	2.368440942975	0.280148377225	5.589619932738
C	1.390421323043	0.875766210791	6.568681726279
N	0.580008373833	1.349008226101	7.252085413021
C	0.471720720287	-2.437745329011	4.313842421224
C	0.362417850206	-3.452187610834	3.356260493571
C	-0.693901348722	-4.362909571241	3.407325664403
C	-1.643950991870	-4.273054211229	4.425169013858
C	-1.534584259476	-3.268189898254	5.389592651957
C	-0.484504253138	-2.352826541916	5.334444316044
C	3.750884536523	0.528624207843	6.082229123530
N	4.830248093050	0.731245787383	6.454009521060
H	-0.942460985412	-0.003275730416	1.938240450314
H	0.178135460588	0.202975746264	3.980308974016
H	3.352889105588	0.022405968217	1.946538379062
H	3.358861093762	0.025106918376	-0.534865114181
H	1.208919947490	0.013144633282	-1.785491557433
H	-0.943415856634	-0.000955107500	-0.538988230721
H	2.411571297868	-1.842685162353	3.606770359254
H	-0.396145245006	-1.582119012186	6.094341643299
H	-2.266499276334	-3.198817996254	6.189682674212
H	-2.462559672910	-4.986148127198	4.471721371260
H	-0.767671051994	-5.146158112161	2.657882142041
H	1.106379237200	-3.529543754057	2.567108395841
N	2.213854387045	0.796116980754	4.239431771141
C	2.067924613139	2.242465565082	4.099535235258
H	2.925732334197	2.738401944383	4.563746984551
H	2.067668785952	2.485256592352	3.034905150475
H	1.142567047214	2.628209714900	4.555503534276