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Supporting Information

for

One-pot synthesis of oxazolidinones and five-membered cyclic carbonates from epoxides and chlorosulfonyl isocyanate: theoretical evidence for an asynchronous concerted pathway

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Experimental, analytical and calculated data

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EXPERIMENTAL

General remarks

The epoxides were synthesized from related alkenes with *m*-CPBA and purified in the filter column. All solvents and reagents were used as purchased from commercial suppliers without any purification. Melting points were determined on a melting-point apparatus (Gallenkamp; WA11373) and are uncorrected. IR spectra were obtained from solutions in 0.1mm cells and in CH_2Cl_2 with a Perkin–Elmer spectrophotometer. ^{1}H and ^{13}C NMR spectra were recorded on Varian and Bruker spectrometers at 400 and 100 MHz, respectively, and NMR shifts are presented as δ in ppm. Elemental analyses were performed on LECO CHNS-932 apparatus. MS spectra were carried out on an LC/MS High-Resolution Time of Flight (TOF) Agilent 1200/6530 instrument. All column chromatography was performed on silica gel (60-mesh, Merck).

General procedure for the synthesis of epoxides:

1 g of the alkene was dissolved in CH_2Cl_2 (40 mL) and cooled to 0 ºC. Then metachloroperbenzoic acid (1.2 equiv) was slowly added to the solution. The solution was left stirring for 12 h at ambient temperature. The solution was washed with 1 M Na_2SO_3 (3 × 30 mL, 1 M), a saturated solution of $NaHCO_3$ (3 × 30 mL) and brine. The organic phase was dried over sodium sulfate and the product obtained after removal of the solvent in vacuo (rotary evaporator), and purified by the column chromatography.

Hexahydro-4,7-methanobenzo[*d*][1,3]dioxol-2-one (8a): [48] [1] Colourless solid, (295 mg, yield 42%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 4.51 (d, J = 1.46 Hz, 2H), 2.51-2.53 (m, 2H), 1.10-1.75 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.9, 82.5, 40.4, 31.0, 23.0; IR ($CHCl_3$, cm^{-1}): 2969, 2879, 1802, 1784, 1372, 1164, 1068; Elemental Analysis Calcd for: C, 62.33; H, 6.54; found: 62.48; H, 6.42. HRMS (ESI) m/z calcd for $C_8H_{10}O_3$+: 154,0624; found [M+H]+ 154,0642.

Hexahydro-4,7-methanobenzo[*d*]oxazol-2(3*H*)-one (9a): [49] [2] Colourless solid, (263 mg, yield 38%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 4.80 (s, 1H), 3.92 (s, 2H), 2.68 (m, 2H). 1.93-0.83 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 157.2, 86.5, 57.6, 40.4, 31.3, 22.5; IR ($CHCl_3$, cm^{-1}): 3366, 2961, 2930, 2885, 1801, 1781, 1709, 1644, 1351, 1182, 1067, 1001; Elemental Analysis Calcd for: C, 62.73; H, 7.24; N, 9.14; found: 62.64; H, 7.49; N, 9.32; HRMS (ESI) m/z calcd for $C_8H_{11}NO_2$+: 153,0784; found [M+H]+ 153,0765.

Hexahydro-4*H*-cyclohepta[*d*][1,3]dioxol-2-one (8b): [50] [3]Colourless solid, (334 mg, yield 48%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 4.82 (m, 2H), 1.94 (m, 4H), 1.80 (m, 2H), 1.63 (m, 1H), 1.50 (m, 1H), 1.32 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.5, 79.6, 30.1, 29.7, 23.2; IR ($CHCl_3$, cm^{-1}): 2930, 2860, 1798, 1721, 1456, 1378, 1180, 1180, 1052; Elemental Analysis Calcd for: C, 61.52; H, 7.74; found: 61.58; H, 7.52; HRMS (ESI) m/z calcd for $C_8H_{12}O_3$+: 156,0781; found [M+H]+ 156,0769.

Octahydro-2*H*-cyclohepta[*d*]oxazol-2-one (9b): [51] [4] Colourless solid, (315 mg, yield 45%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 4.86-4.92 (m, 1H), 4.59-4.36 (m, 1H), 2.32-1.21 (m, 10H), ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 150.1, 79.2, 64.2, 30.3, 29.9, 28.5, 25.4, 22.7; IR ($CHCl_3$, cm^{-1}): 3250, 2931, 2859, 1803, 1748, 1414, 1369, 1176, 1087; Elemental Analysis Calcd for: C, 61.91; H, 8.44; N, 9.03; found: 61.73; H, 8.49; N, 9.34; HRMS (ESI) m/z calcd for $C_8H_{13}NO_2$+: 155,0941; found [M+H]+ 155,0964.

Octahydrocycloocta[*d*][1,3]dioxol-2-one (8c): [50] [3] Colourless solid, (342 mg, yield 51%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 4.72 (m, 2H), 1.99 (m, 4H), 1.73 (m, 2H), 1.48 (m, 4H), 1.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.4, 81.4, 26.5, 26.2, 26.1; IR ($CHCl_3$, cm^{-1}): 2924, 1801, 1472, 1359, 1203, 1174, 1054; Elemental Analysis Calcd for: C, 63.51; H, 8.29; found: 63.42; H, 8.39; HRMS (ESI) m/z calcd for $C_9H_{14}O_3$+: 170,0937; found [M+H]+ 170,0956.

***trans*-4,5-Diphenyl-1,3-dioxolan-2-one (8d):** [50] [3] Colourless solid, (263 mg, yield 43%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 5.42 (s, 2H), 7.31-7.33 (m, 3H), 7.43-7.45 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.3, 135.1, 130.0, 129.5, 126.3, 85.6; IR ($CHCl_3$, cm^{-1}): 3064, 2925, 1808, 1457, 1257, 1167, 1044; Elemental Analysis Calcd for: C, 74.99; H, 5.03; found: C, 75.32; H, 5.21; HRMS (ESI) m/z calcd for $C_{15}H_{12}O_3$+: 240,0781; found [M+H]+ 240,0796.

***trans*-4,5-Diphenyloxazolidin-2-one (9d):** [52] [5]Colourless solid, (208 mg, yield 34%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.39-7.42 (m, 6H) 7.25-7.32 (m, 4H), 5.48 (bs, 1H), 5.30 (m, 1H), 4.75 (d, *J* = 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 158.7, 138.5, 137.5, 129.5, 129.3, 129.2, 128.5, 126.7, 126.1, 86.4, 65.1; IR ($CHCl_3$, cm^{-1}): 3290, 2923, 2853, 1754, 1456, 1380, 1199, 1015; Elemental Analysis Calcd for: C, 75.30; H, 5.48; N, 5.85; found: C, 75.42; H, 5.36; N, 5.67; HRMS (ESI) m/z calcd for $C_{15}H_{13}NO_2$+; 239,0941; found [M+H]+ 239,0947.

***cis*-4,5-Diphenyl-1,3-dioxolan-2-one (8e):** [50] [3]Colourless solid, (269 mg, yield 44%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.42-7.45 (m, 6H). 7.30-7.33 (m, 4H). 5.44 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.3, 135.0, 130.0, 127.3, 126.3, 85.6; IR ($CHCl_3$, cm^{-1}): 2918, 1811, 1454, 1275,

1091; Elemental Analysis Calcd for: C, 74.99; H, 5.03; found: C, 75.12; H, 5.24; HRMS (ESI) m/z calcd for $C_{15}H_{12}O_3$+: 240,0781; found [M+H]+ 240,0794.

***cis*-4,5-Diphenyloxazolidin-2-one (9e):** [52] [5] Colourless solid, (250 mg, yield 41%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.12-7.09 (m, 6H), 6.98-6.94 (m, 4H), 5.95 (d, *J* = 8.1 Hz, 1H), 5.5 (bs, 1H), 5.2 (d, *J* = 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 160.1, 136.2, 128.6, 128.5, 128.3, 128.1, 127.2, 126.7, 126.3, 126.0, 82.6, 61.6; IR ($CHCl_3$, cm^{-1}): 3295, 2923, 1754, 1455, 1356, 1217, 1091, 1020; Elemental Analysis Calcd for: C, 75.30; H, 5.48; N, 5.85; found: C, 75.36; H, 5.57; N, 5.66; HRMS (ESI) m/z calcd for $C_{15}H_{13}NO_2$+: 239,0941; found [M+H]+ 239,0955.

4-Phenyl-1,3-dioxolan-2-one (8f): [16] [6] White solid, (355 mg, yield 49%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.27-7.46 (m, 5H), 5.68 (t, *J* = 8.6 Hz, 1H), 4.82 (t, *J* = 8.6 Hz, 1H), 4.36 (t, *J* = 8.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.0, 136.0, 129.5, 129.2, 126.0, 78.2, 71.4; IR ($CHCl_3$, cm^{-1}): 2932, 1809, 1795, 1457, 1358, 1270, 1168, 1067; Elemental Analysis Calcd for: C, 65.85; H, 4.91; found: C, 65.92; H, 4.85; HRMS (ESI) m/z calcd for $C_9H_8O_3$+: 164,0468; found [M+H]+ 164,0475.

4-Phenyloxazolidin-2-one (9f): [16] [6] White solid, (285 mg, yield 42%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.38-7.43 (m, 5H), 5.46 (s, 1H, NH), 4.98 (dd, *J* = 8.6, 7.0 Hz, 1H), 4.76 (dd, *J* = 8.6, 7.0 Hz, 1H), 4.21 (dd, *J* = 8.6, 7.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 56.6, 72.8, 126.3, 129.2, 129.5, 139.6. 158.2; IR ($CHCl_3$, cm^{-1}): 3284, 2922, 1744, 1457, 1404, 1238, 1040; Elemental Analysis Calcd for: C, 66.25; H, 5.56; N, 8.58; found: C, 66.48; H, 5.32; N, 8.45; HRMS (ESI) m/z calcd for $C_9H_9NO_2$+: 163,0628; found [M+H]+ 163,0643.

4-Benzyl-1,3-dioxolan-2-one (8g): [16] [6] Colourless oil, (270 mg, yield 41%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 2.99 (dd, *J* = 6.7, 14.2 Hz, 1H), 3.15 (dd, *J* = 6.4, 14.2 Hz, 1H), 4.17 (dd, *J* = 6.9, 8.6 Hz, 1H), 4.44 (t, *J* = 8.1 Hz, 1H), 4.93 (m, 1H), 7.18-7.25 (m, 2H), 7.28-7.36 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.1, 134.1, 129.6, 129.2, 127.8, 77.1, 68.7, 39.8; IR ($CHCl_3$, cm^{-1}): 2921, 1803, 1455, 1371, 1272, 1170, 1080; Elemental Analysis Calcd for: C, 67.41; H, 5.66; found: C, 67.49; H, 5.72; HRMS (ESI) m/z calcd for $C_{10}H_{10}O_3$+: 178,0624; found [M+H]+ 178,0643.

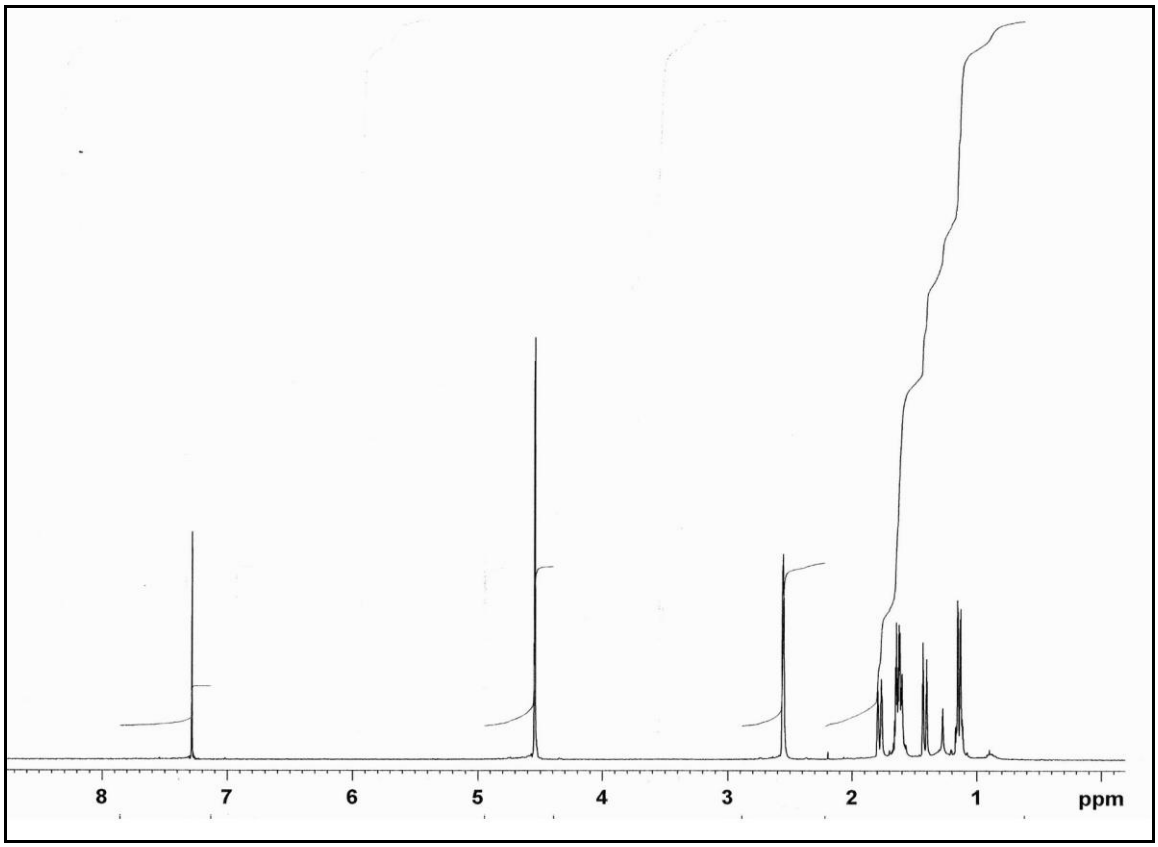
4-Benzyloxazolidin-2-one (9g): [53] [7]Colourless solid, (230 mg, yield 35%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.17-7.35 (m, 5H), 4.84 (bs, 1H), 4.47- 4.49 (m, 1H), 4.07-4.13 (m, 2H), 2.76-2.84 (m, 2H), ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 159.6, 135.8, 129.1, 128.9, 127.3, 69.6, 53.7, 41.4; IR ($CHCl_3$, cm^{-1}): 3282, 2925, 1744, 1456, 1410, 1223, 1030; Elemental Analysis Calcd for: C, 67.78; H,

6.26; N, 7.90 found: C, 67.71; H, 6.38; N, 7.75; HRMS (ESI) m/z calcd for $C_{10}H_{11}NO_2$+: 177,0784; found [M+H]+ 177,0789.

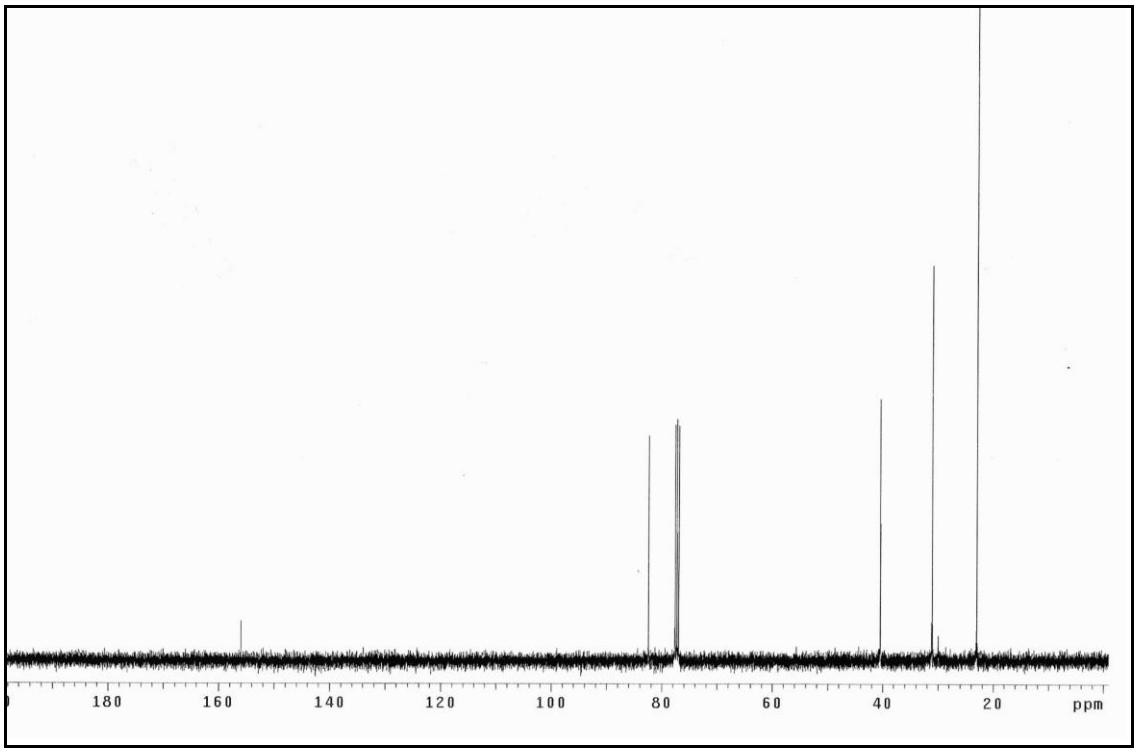
3a,8a-Dihydro-8*H*-indeno[1,2-*d*][1,3]dioxol-2-one (8h): [54] [8]White solid, (300 mg, yield 45%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.32-7.53 (m, 4H), 6.01 (d, J = 6.8 Hz, 1H), 5.44-5.46 (m, 1H), 3.40 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.9, 140.3, 136.7, 131.3, 128.5, 126.8, 125.6, 83.7, 79.7, 38.3; IR ($CHCl_3$, cm^{-1}): 2925, 1789, 1463, 1362, 1160, 1058, 1016; Elemental Analysis Calcd for: C, 68.18; H, 4.58; found: C, 68.34; H, 4.65; HRMS (ESI) m/z calcd for $C_{10}H_8O_3$+: 176,0468; found [M+H]+ 176,0478.

3,3a,8,8a-Tetrahydro-2*H*-indeno[1,2-*d*]oxazol-2-one (9h): [52] [5]White solid, (265 mg, yield 40%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.25 –7.36 (m, 4H), 7.10 (bs, 1H), 5.40–5.45 (m, 1H), 5.19 (d, *J* = 7.1 Hz, 1H), 3.42 (d, *J* = 18.5 Hz 1H), 3.34 (d, *J* = 16.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 159.7, 140.2, 139.6, 129.4, 127.7, 125.4, 124.9, 80.7, 61.3, 38.9; IR ($CHCl_3$, cm^{-1}): 3490, 2921, 1803, 1455, 1272, 1170, 1161; Elemental Analysis Calcd for: C, 68.56; H, 5.18; N, 8.00; found: C, 68.64; H, 5.34; N, 8.23; HRMS (ESI) m/z calcd for $C_{10}H_9NO_2$+: 175,0628; found [M+H]+ 175,0643.

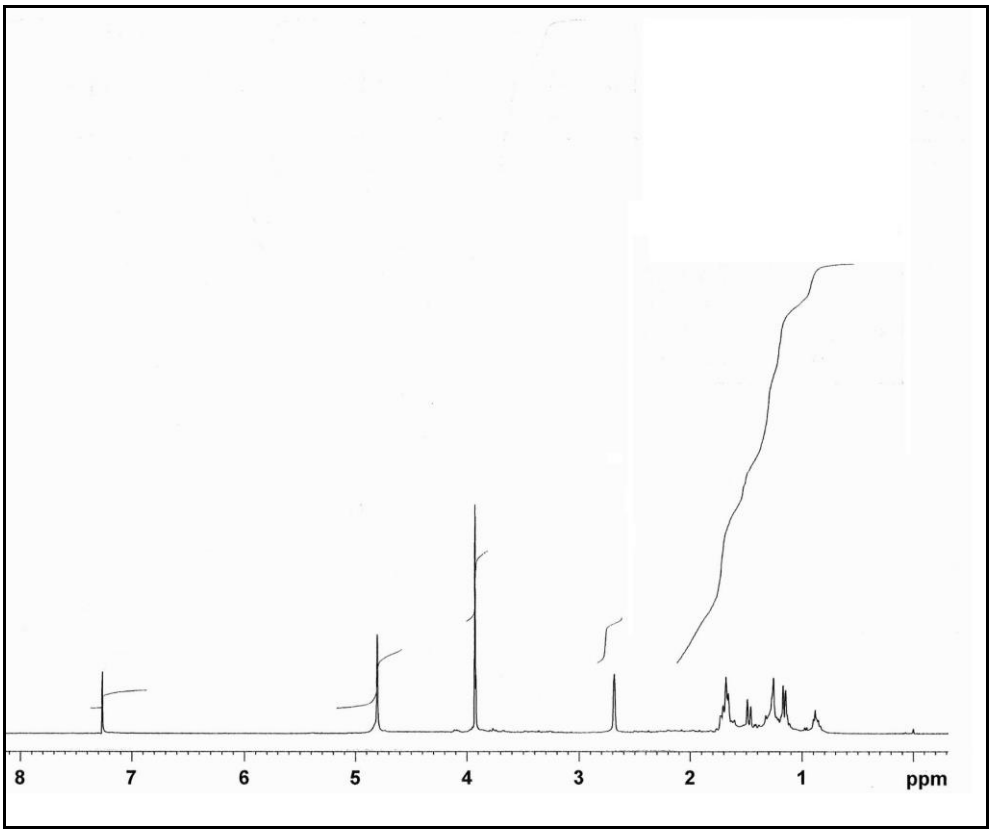
3a-Phenylhexahydrobenzo[*d*]oxazol-2(3*H*)-one (9j): [55] [9]Colourless oil, (265 mg, yield 42%). ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.42–7.38 (m, 2H), 7.36–7.33 (m, 2H), 7.30–7.26 (m, 1H), 4.66 (t, *J* = 4.2 Hz, 1H), 2.19–2.14 (m, 1H), 2.06–2.01 (m, 1H), 1.89–1.66 (m, 4H), 1.62–1.53 (m, 2H); ^{13}C-NMR (100 MHz, $CDCl_3$, ppm) δ 159.8, 143.3, 128.6, 127.8, 125.3, 82.0, 61.8, 34.8, 25.9, 19.5, 17.6; IR ($CHCl_3$, cm^{-1}): 3220, 2943, 1803, 1448, 1205, 1028, 1005; Elemental Analysis Calcd for: C, 71.87; H, 6.96; N, 6.45; found: C, 71.68; H, 6.91; N, 6.54; HRMS (ESI) m/z calcd for $C_{13}H_{15}NO_2$+: 217,1097; found [M+H]+ 217,1086.



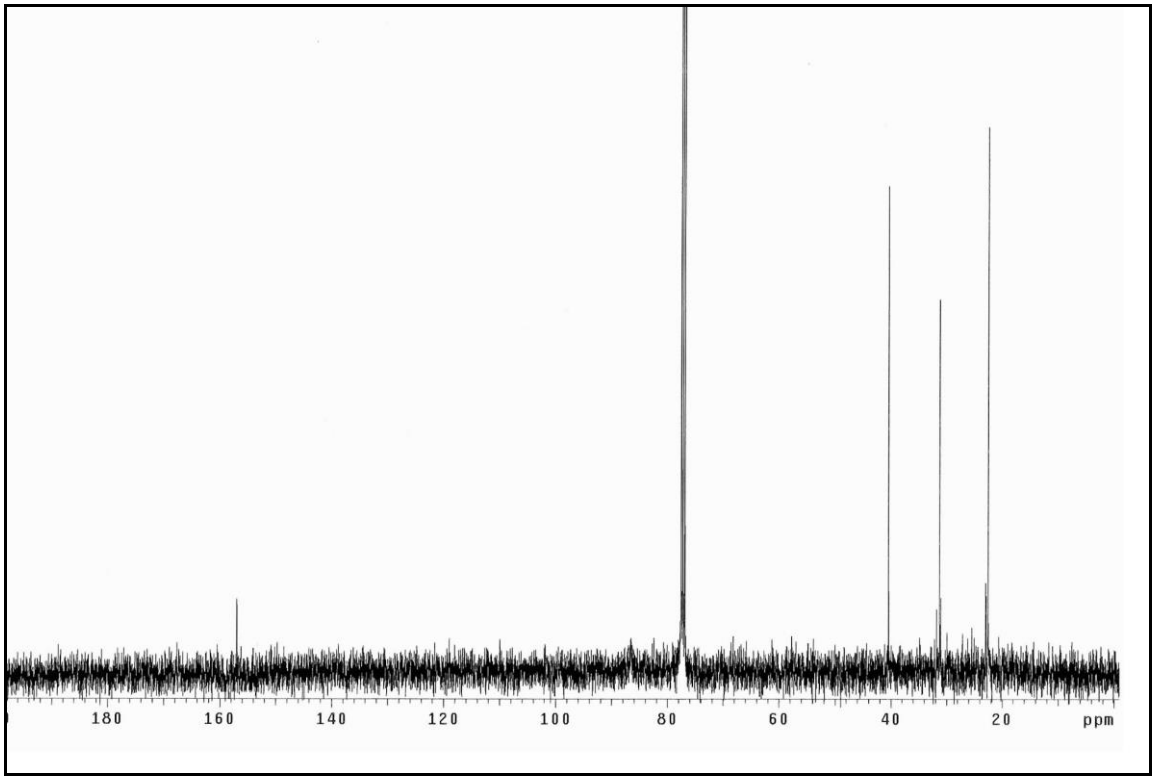
^{1}H NMR spectrum of hexahydro-4,7-methanobenzo[*d*][1,3]dioxol-2-one (**8a**)



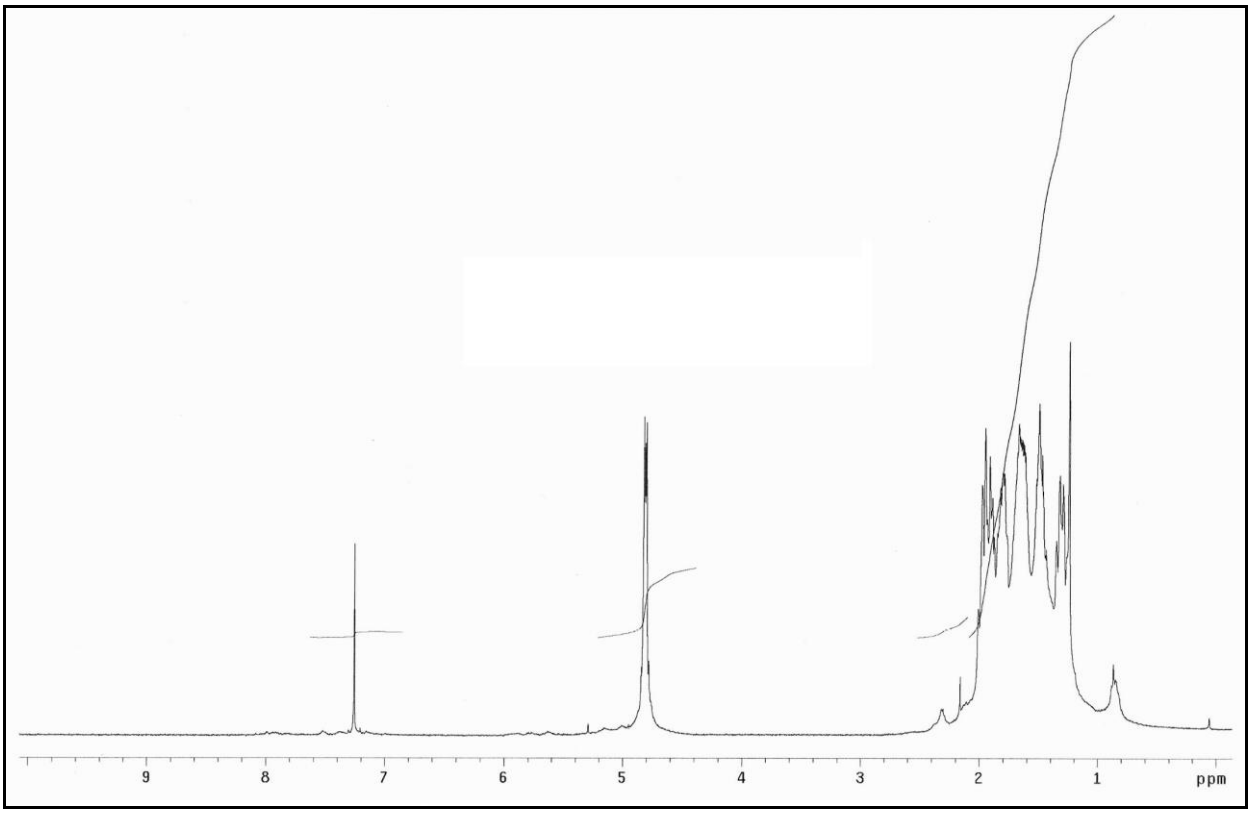
^{13}C NMR spectrum of hexahydro-4,7-methanobenzo[*d*][1,3]dioxol-2-one (**8a**)



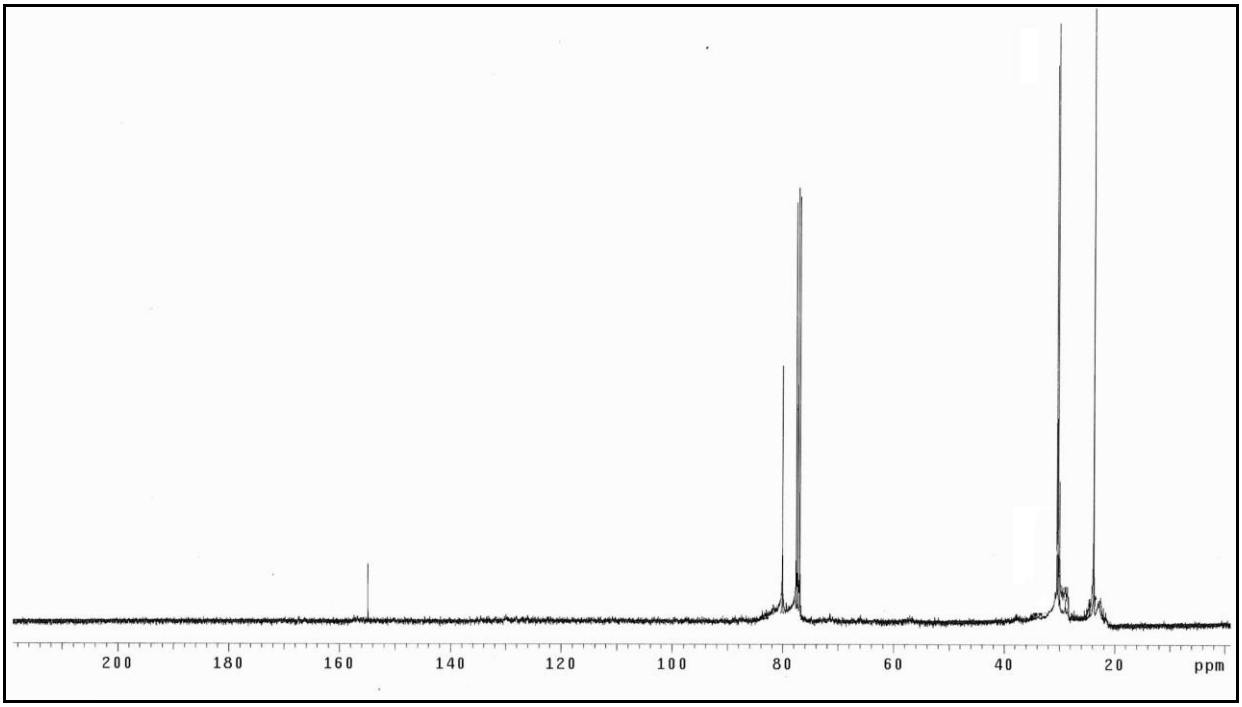
^{1}H NMR spectrum of hexahydro-4,7-methanobenzo[*d*]oxazol-2(3*H*)-one (**9a**)



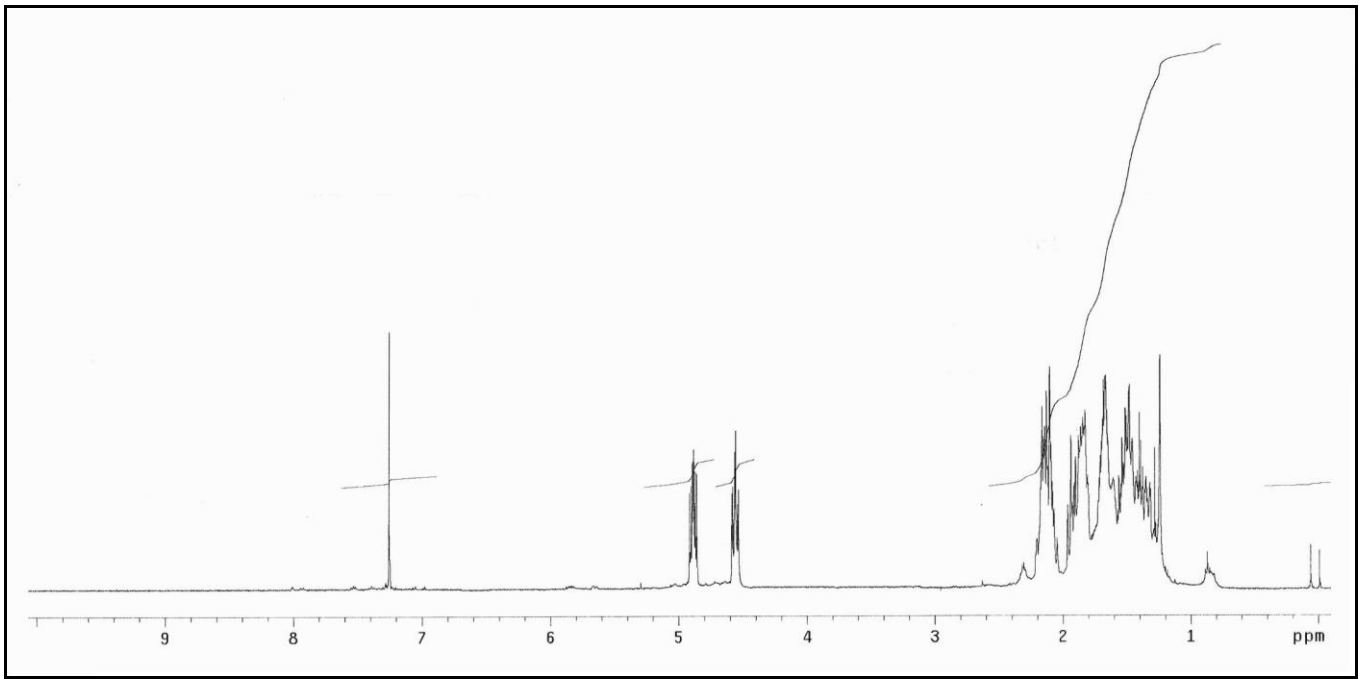
^{13}C NMR spectrum of hexahydro-4,7-methanobenzo[*d*]oxazol-2(3*H*)-one (**9a**)



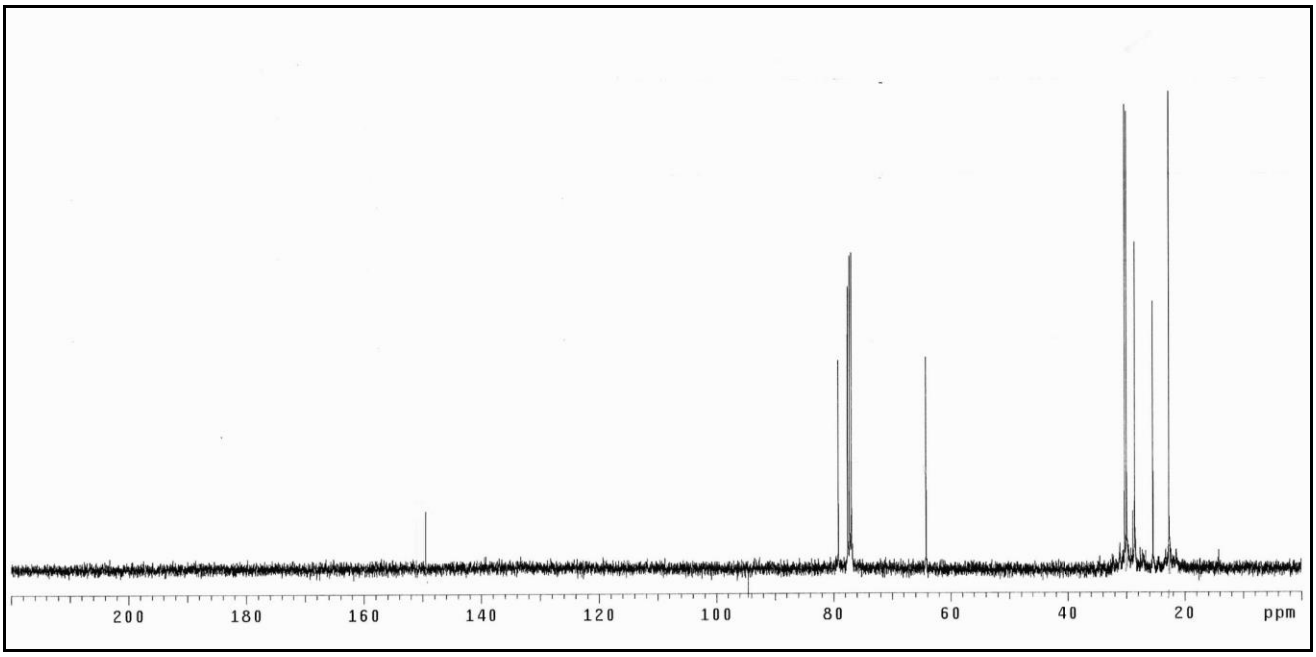
^{1}H NMR spectrum of hexahydro-4*H*-cyclohepta[*d*][1,3]dioxol-2-one (**8b**)



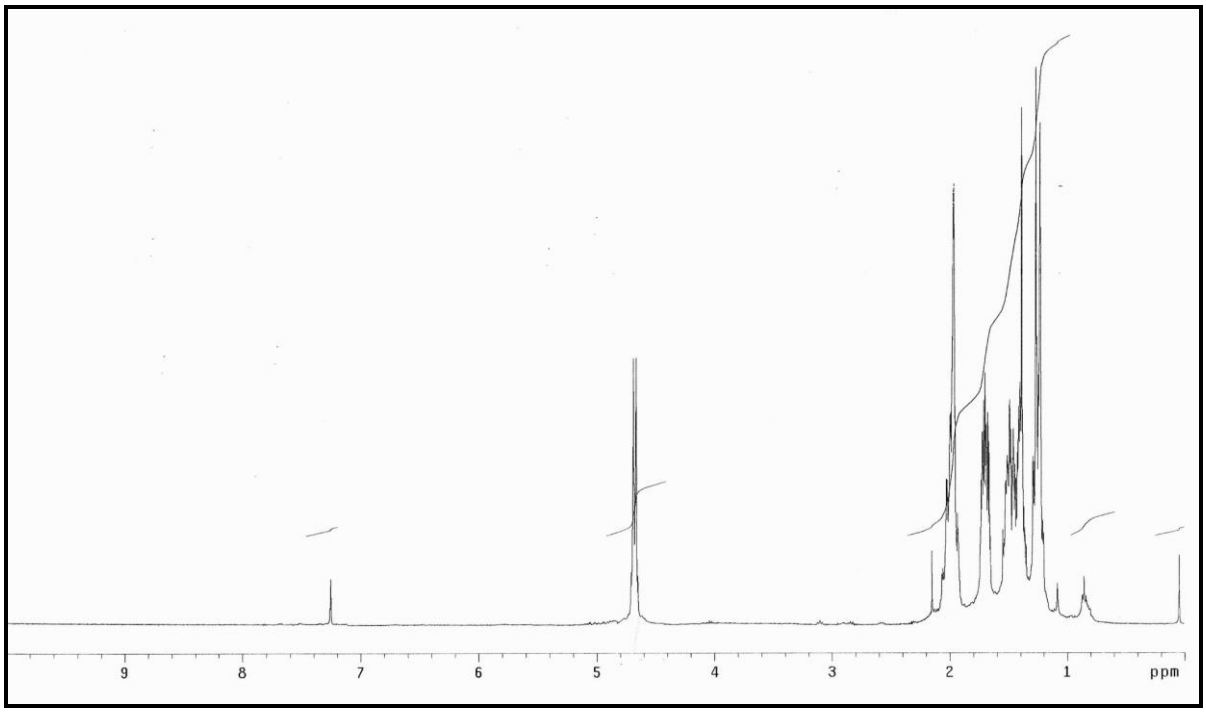
^{13}C NMR spectrum of hexahydro-4*H*-cyclohepta[*d*][1,3]dioxol-2-one (**8b**)



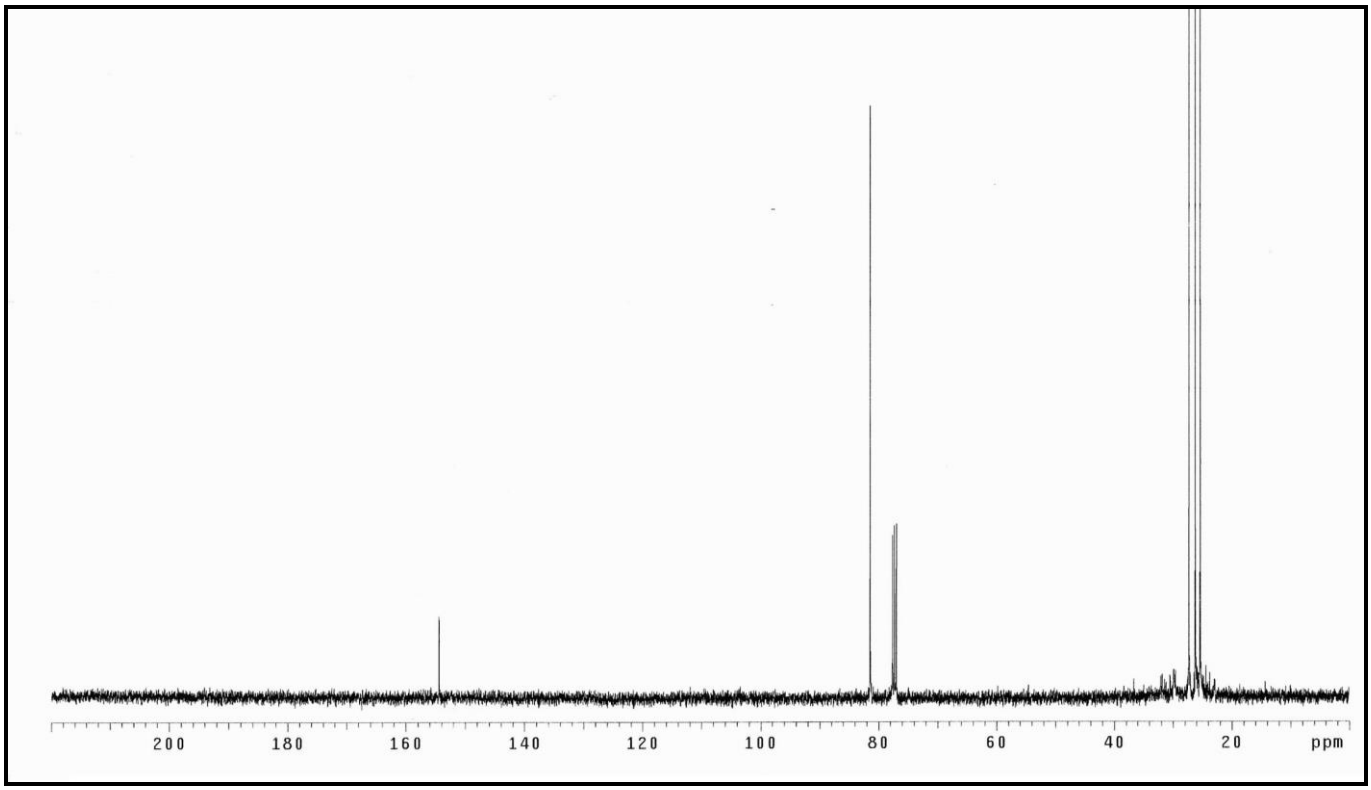
^{1}H NMR spectrum of octahydro-2*H*-cyclohepta[*d*]oxazol-2-one (**9b**)



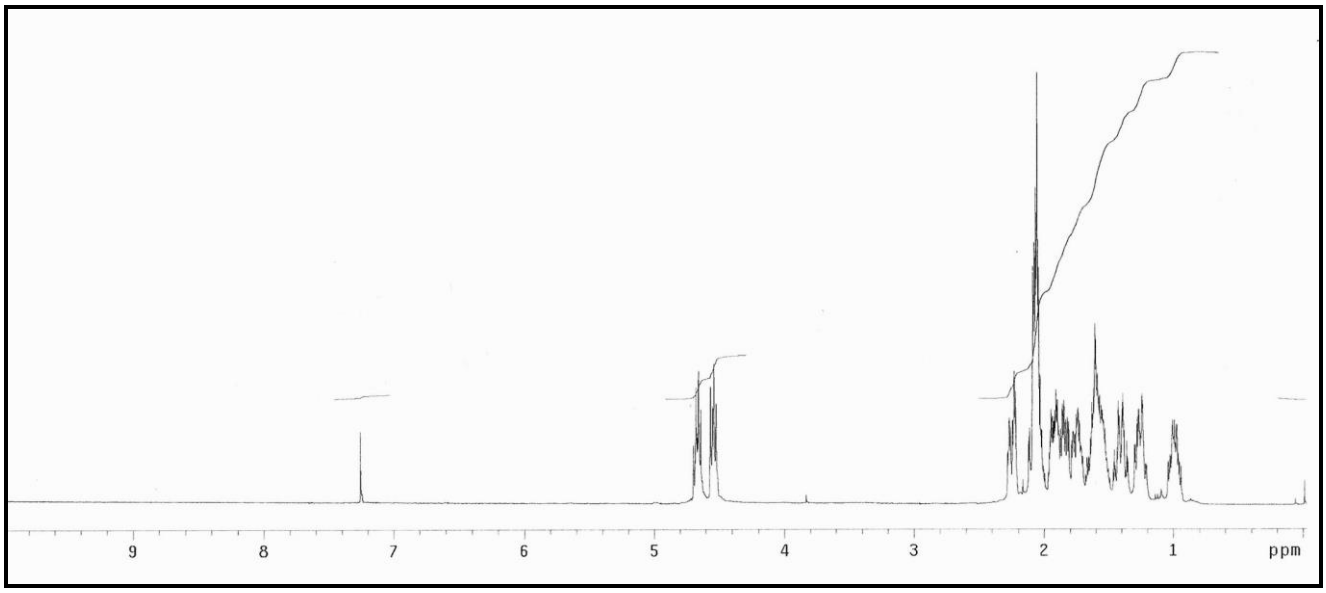
^{13}C NMR spectrum of octahydro-2*H*-cyclohepta[*d*]oxazol-2-one (**9b**)



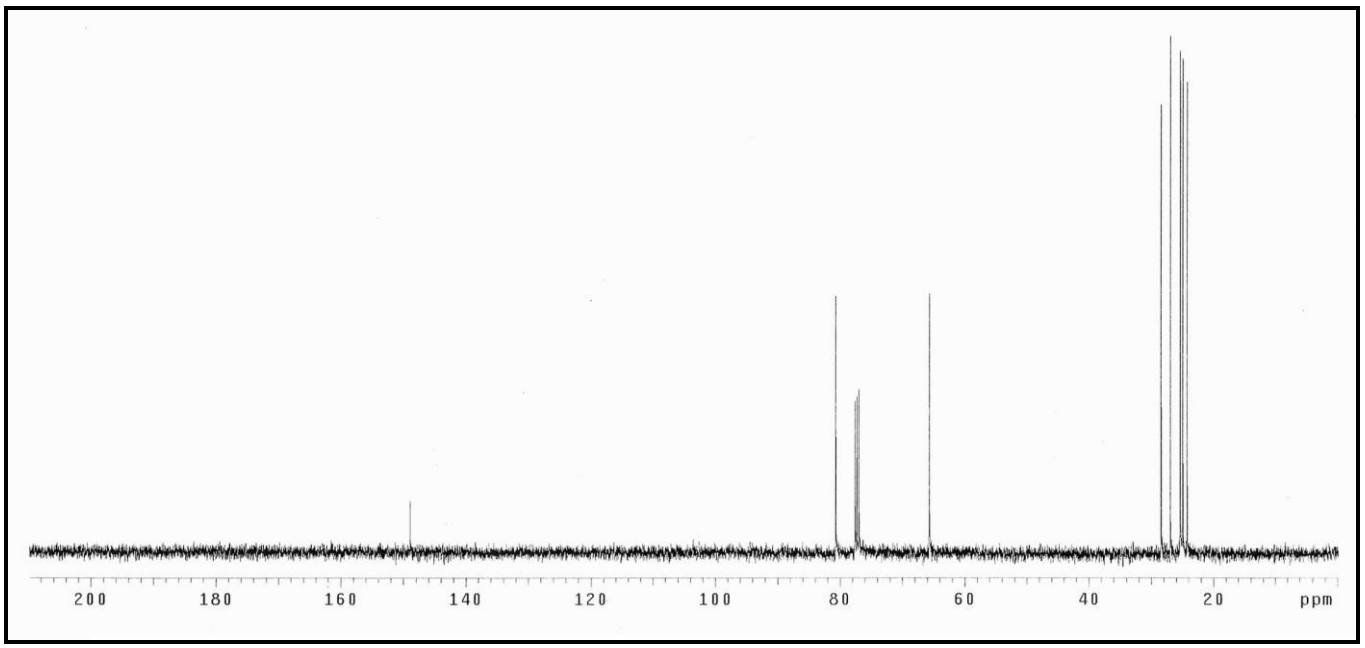
^{1}H NMR spectrum of octahydrocycloocta[*d*][1,3]dioxol-2-one (**8c**)



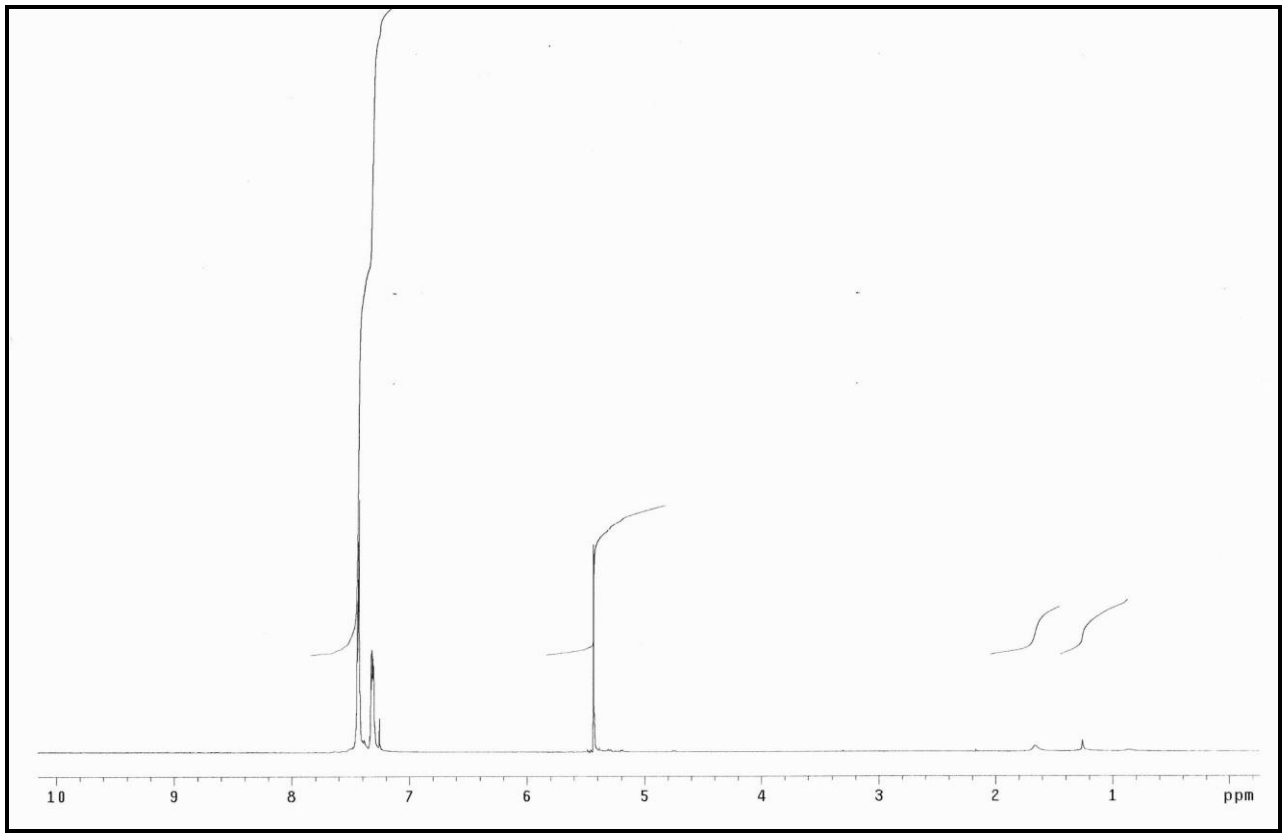
^{13}C NMR spectrum of octahydrocycloocta[*d*][1,3]dioxol-2-one (**8c**)



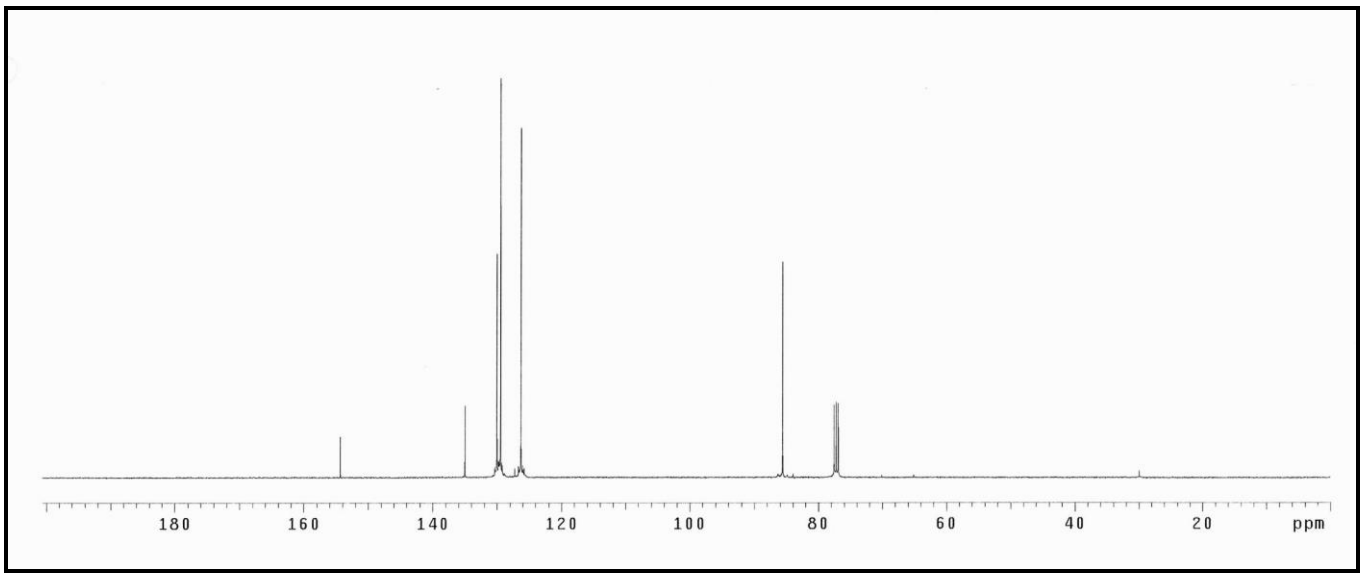
^{1}H NMR spectrum of octahydrocycloocta[*d*]oxazol-2(3*H*)-one (**9c**)



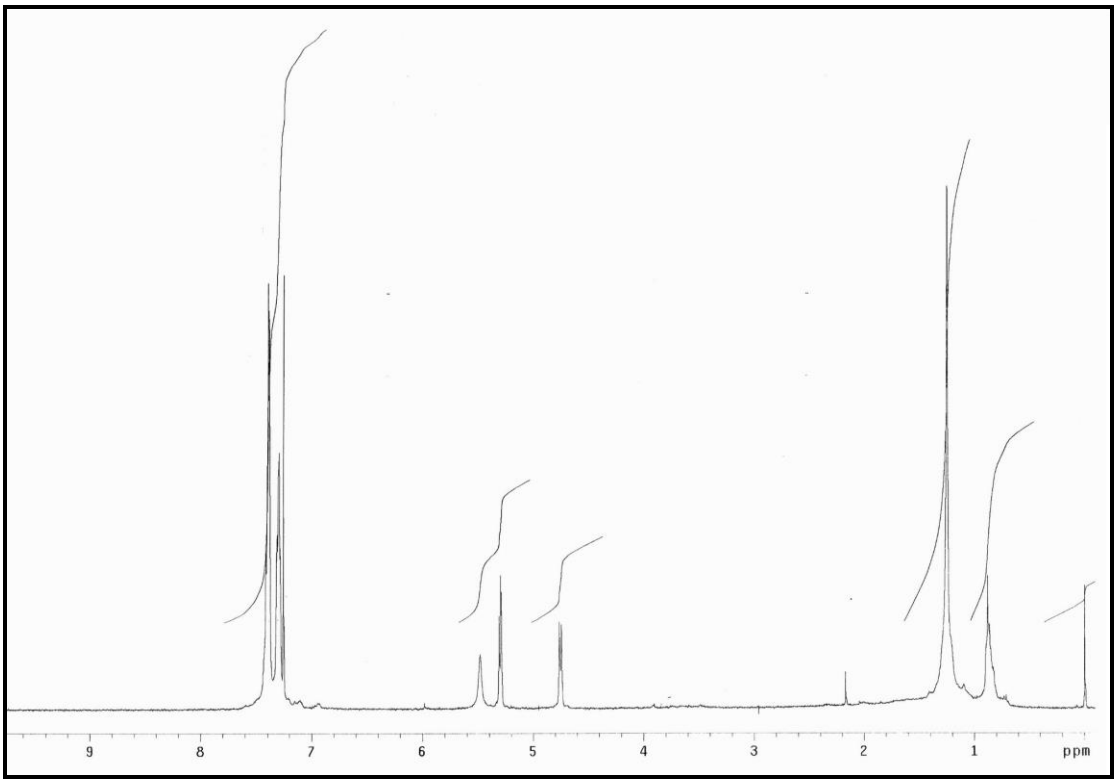
^{13}C NMR spectrum of octahydrocycloocta[*d*]oxazol-2(3*H*)-one (**9c**)



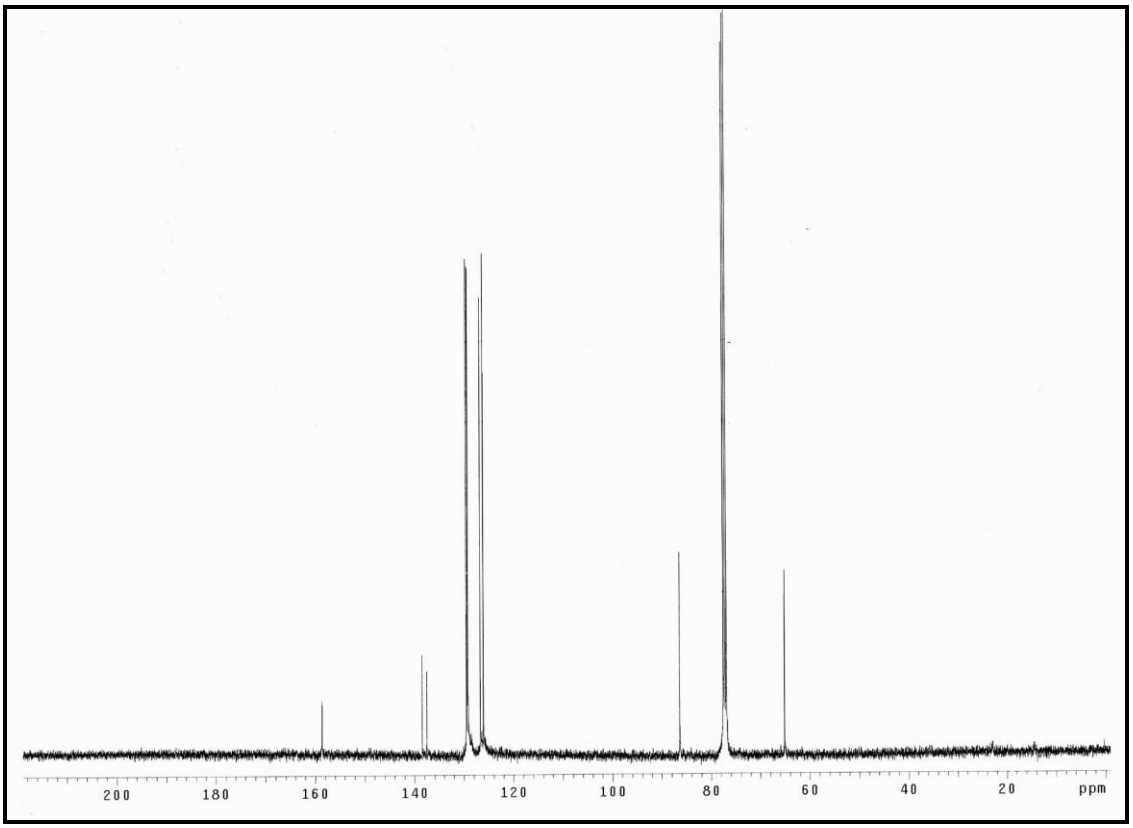
^{1}H NMR spectrum of *trans*-4,5-diphenyl-1,3-dioxolan-2-one (**8d**)



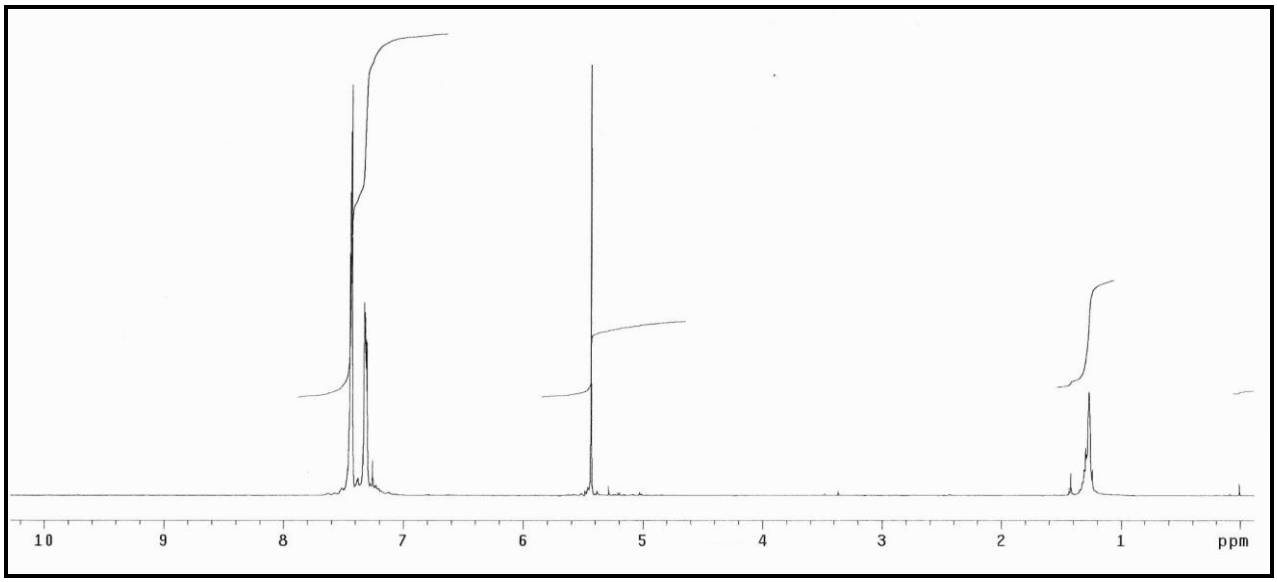
^{13}C NMR spectrum of *trans*-4,5-diphenyl-1,3-dioxolan-2-one (**8d**)



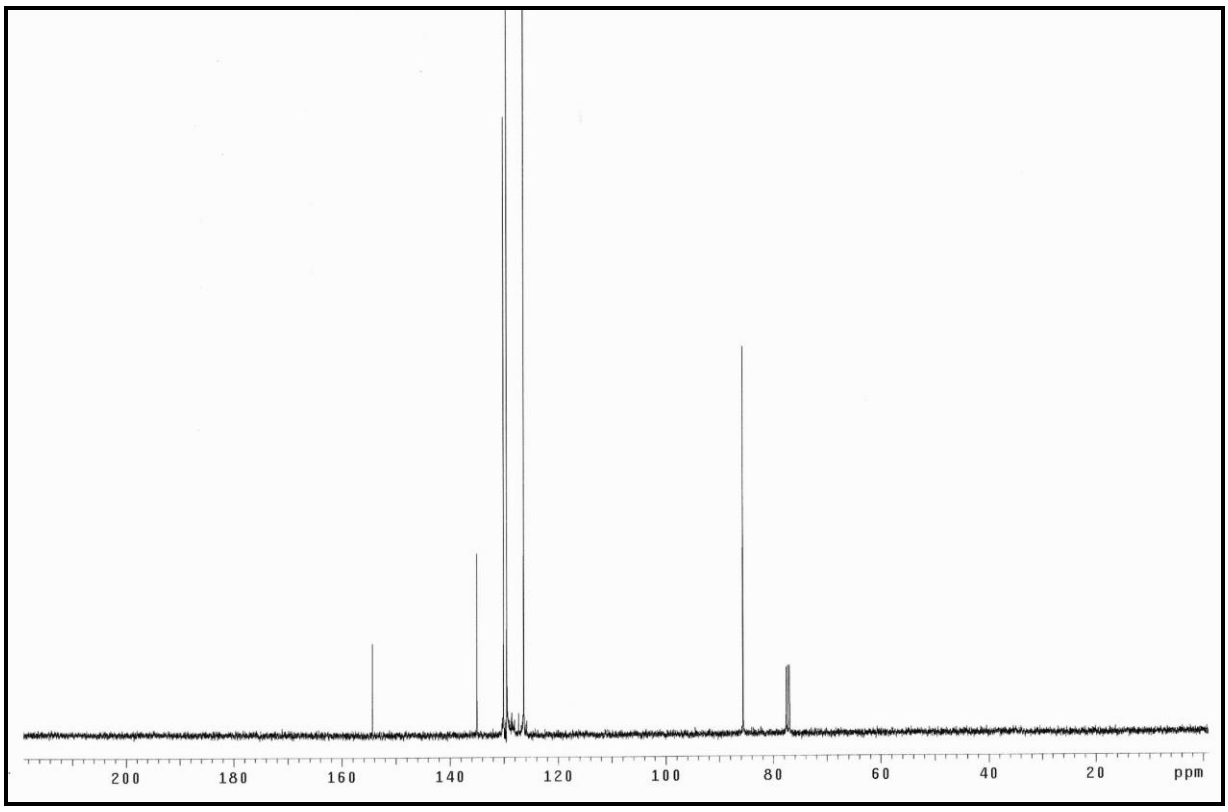
^{1}H NMR spectrum of *trans*-4,5-diphenyloxazolidin-2-one (**9d**)



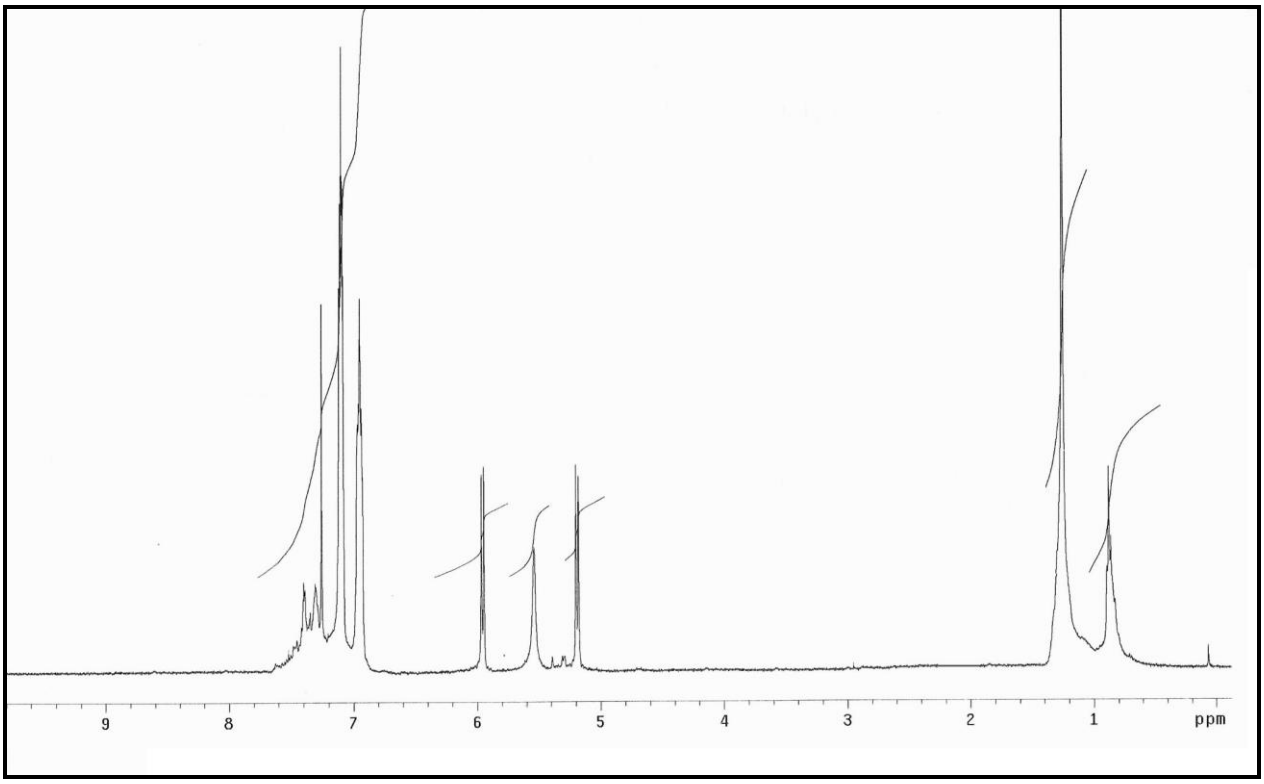
^{13}C NMR spectrum of *trans*-4,5-diphenyloxazolidin-2-one (**9d**)



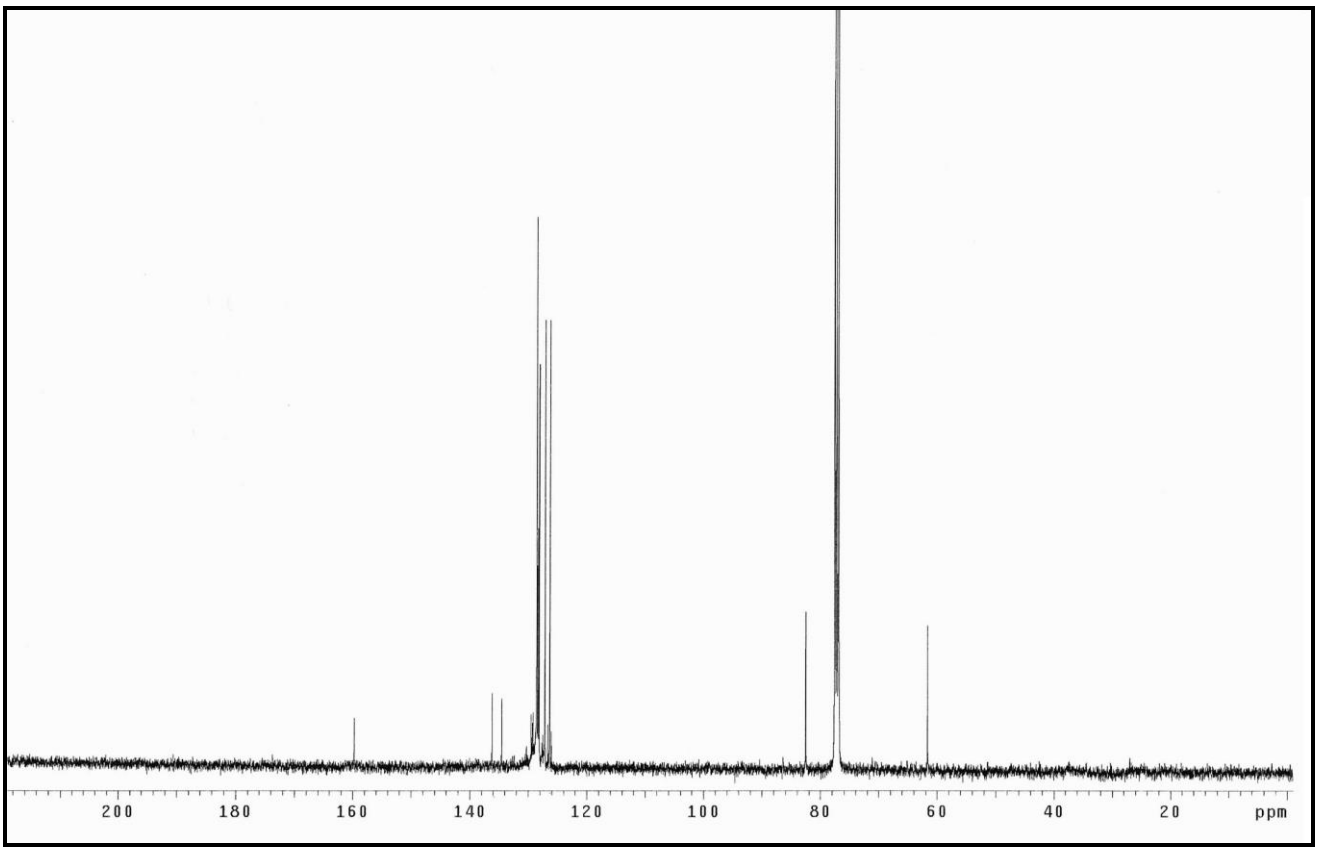
^{1}H NMR spectrum of *cis*-4,5-diphenyl-1,3-dioxolan-2-one (**8e**)



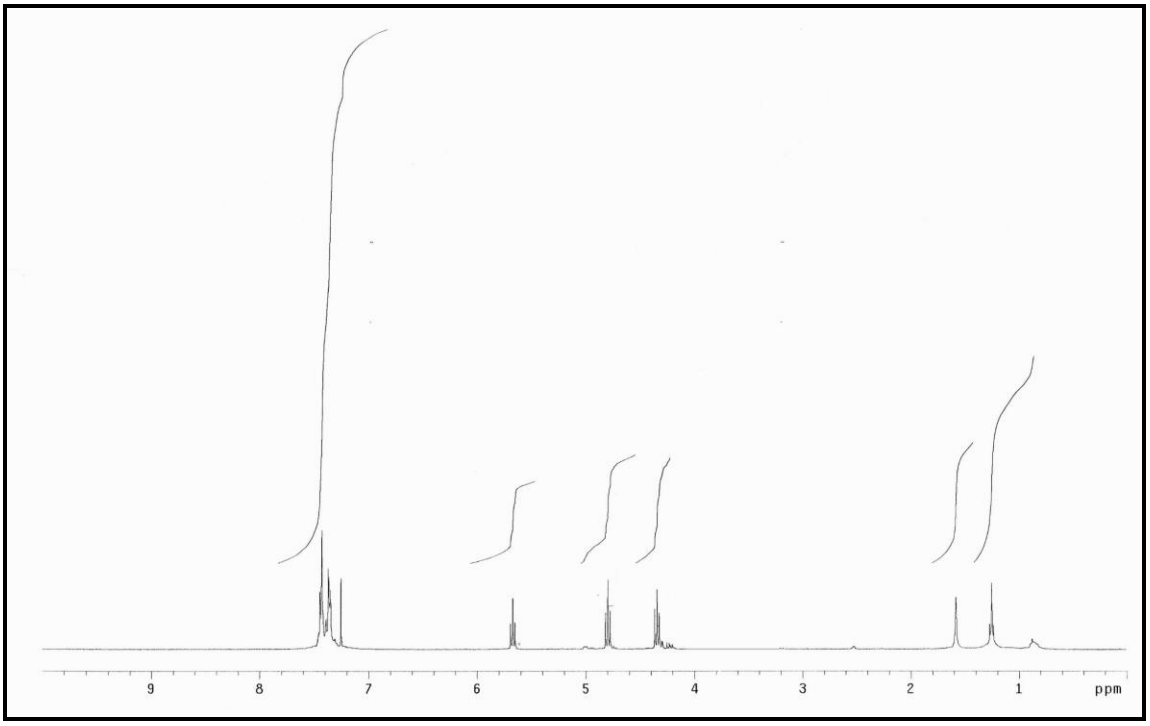
^{13}C NMR spectrum of *cis*-4,5-diphenyl-1,3-dioxolan-2-one (**8e**)



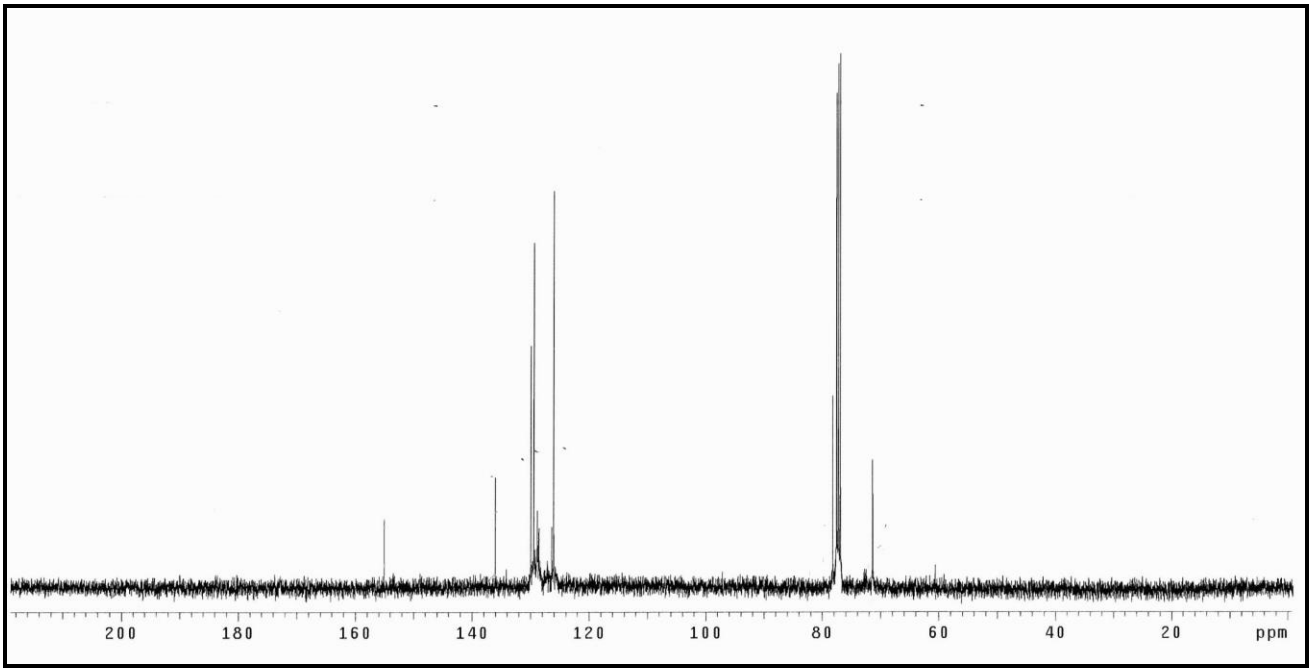
^{1}H NMR spectrum of *cis*-4,5-diphenyloxazolidin-2-one (**9e**)



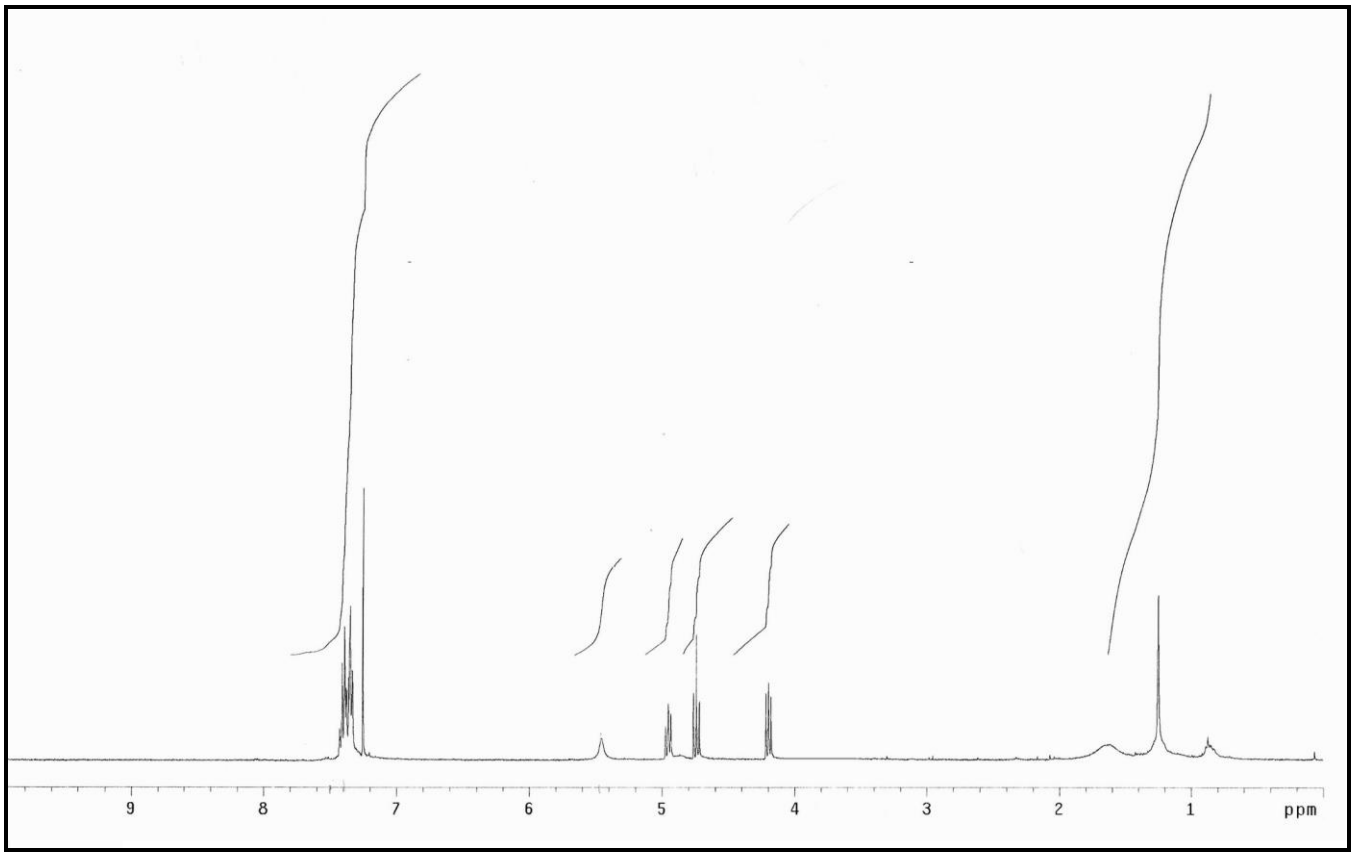
^{13}C NMR spectrum of *cis*-4,5-diphenyloxazolidin-2-one (**9e**)



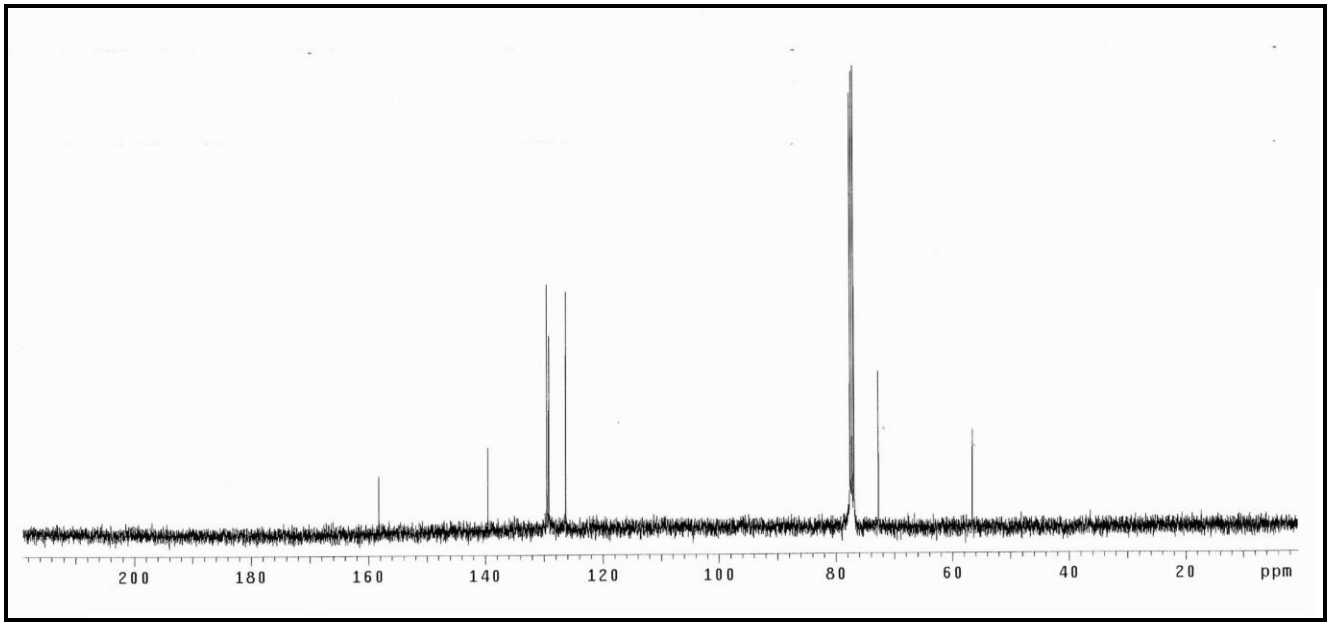
^{1}H NMR spectrum of 4-phenyl-1,3-dioxolan-2-one (**8f**)



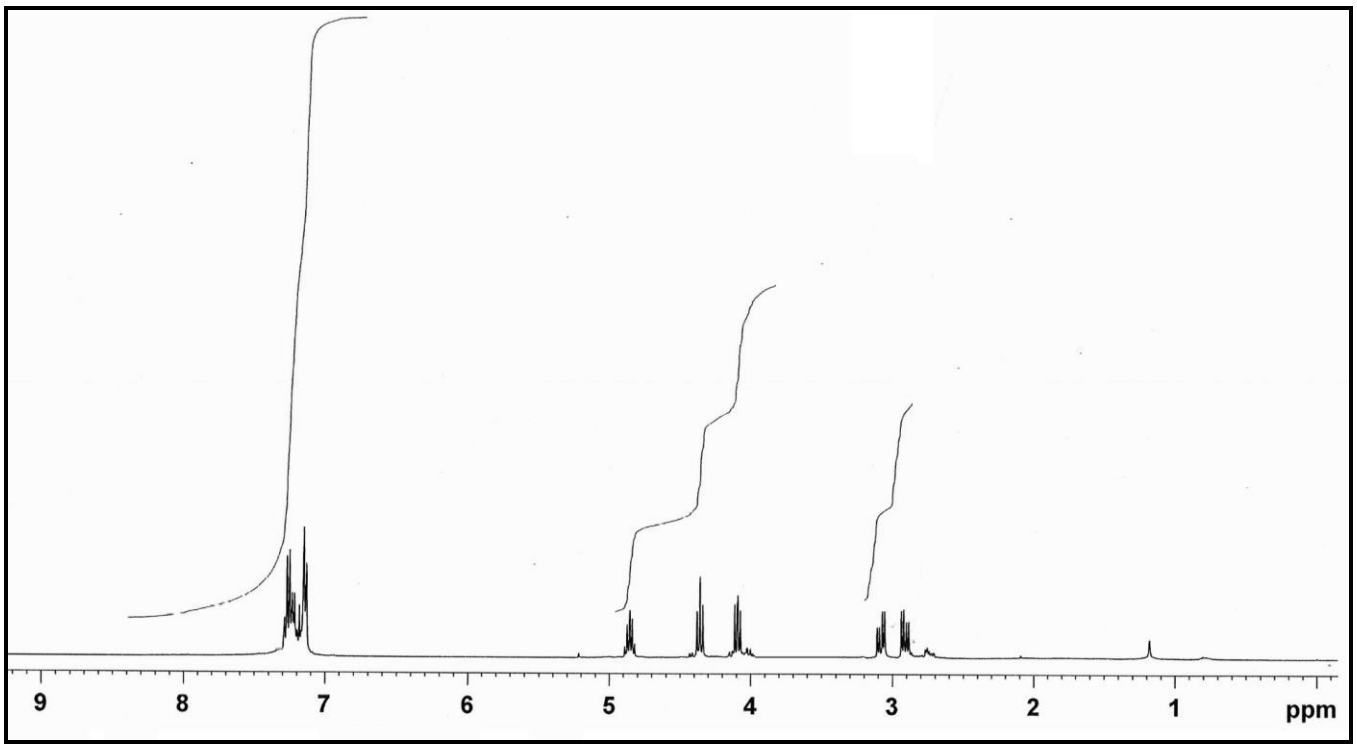
^{13}C NMR spectrum of 4-phenyl-1,3-dioxolan-2-one (**8f**)



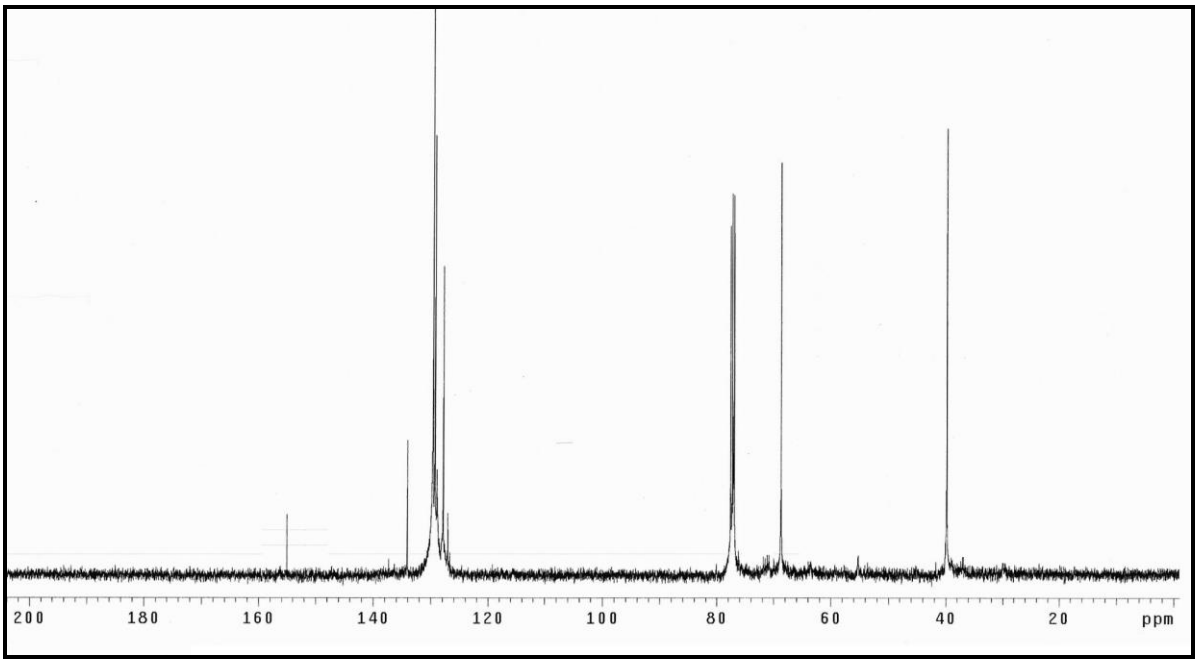
^{1}H NMR spectrum of 4-phenyloxazolidin-2-one (**9f**)



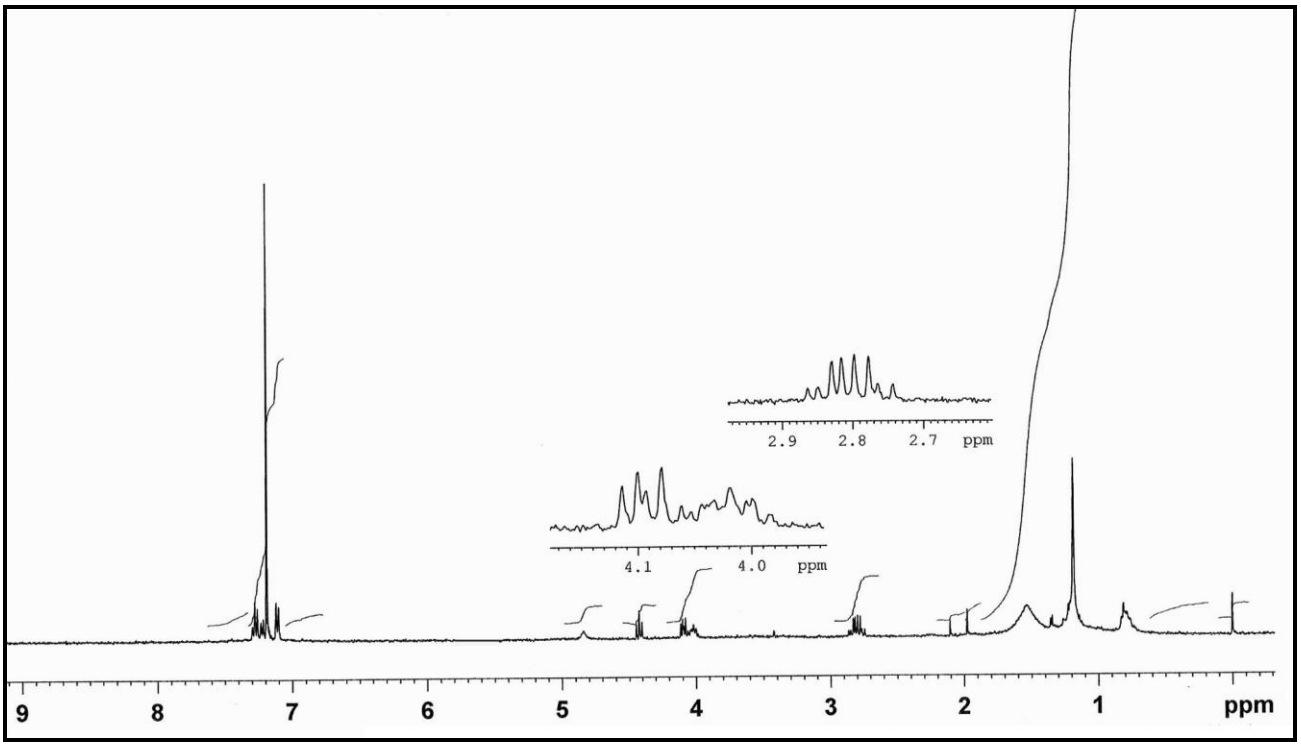
^{13}C NMR spectrum of 4-phenyloxazolidin-2-one (**9f**)



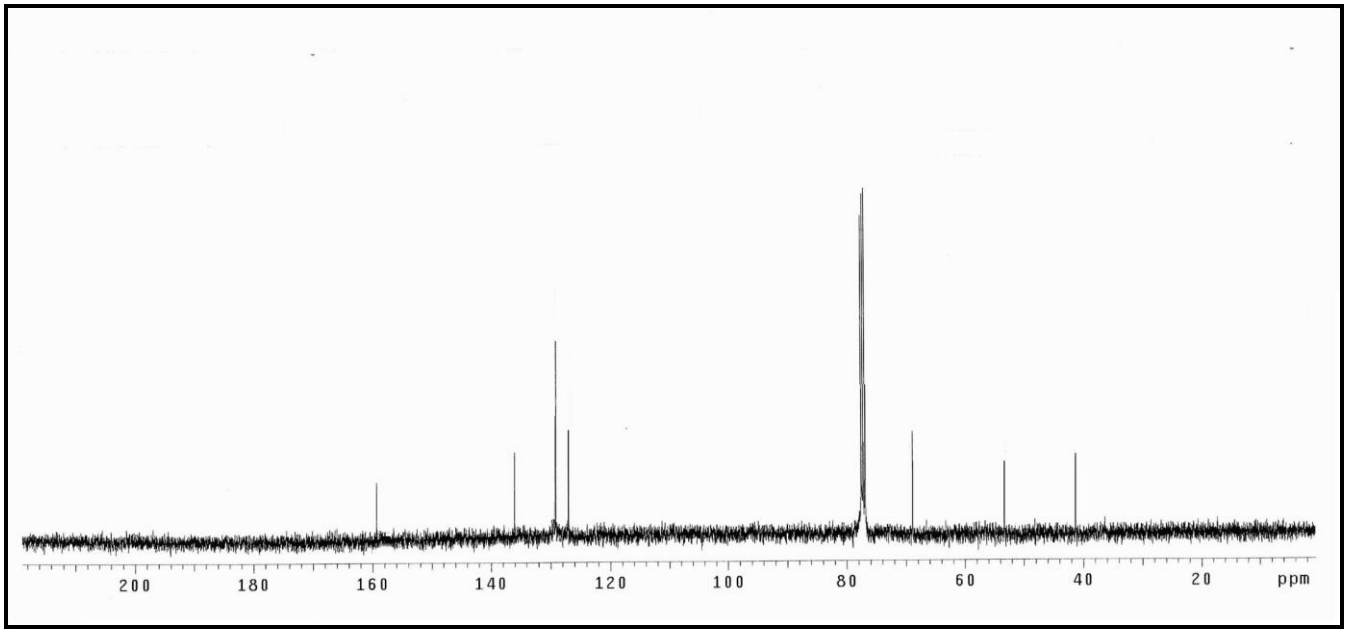
^{1}H NMR spectrum of 4-benzyl-1,3-dioxolan-2-one (**8g**)



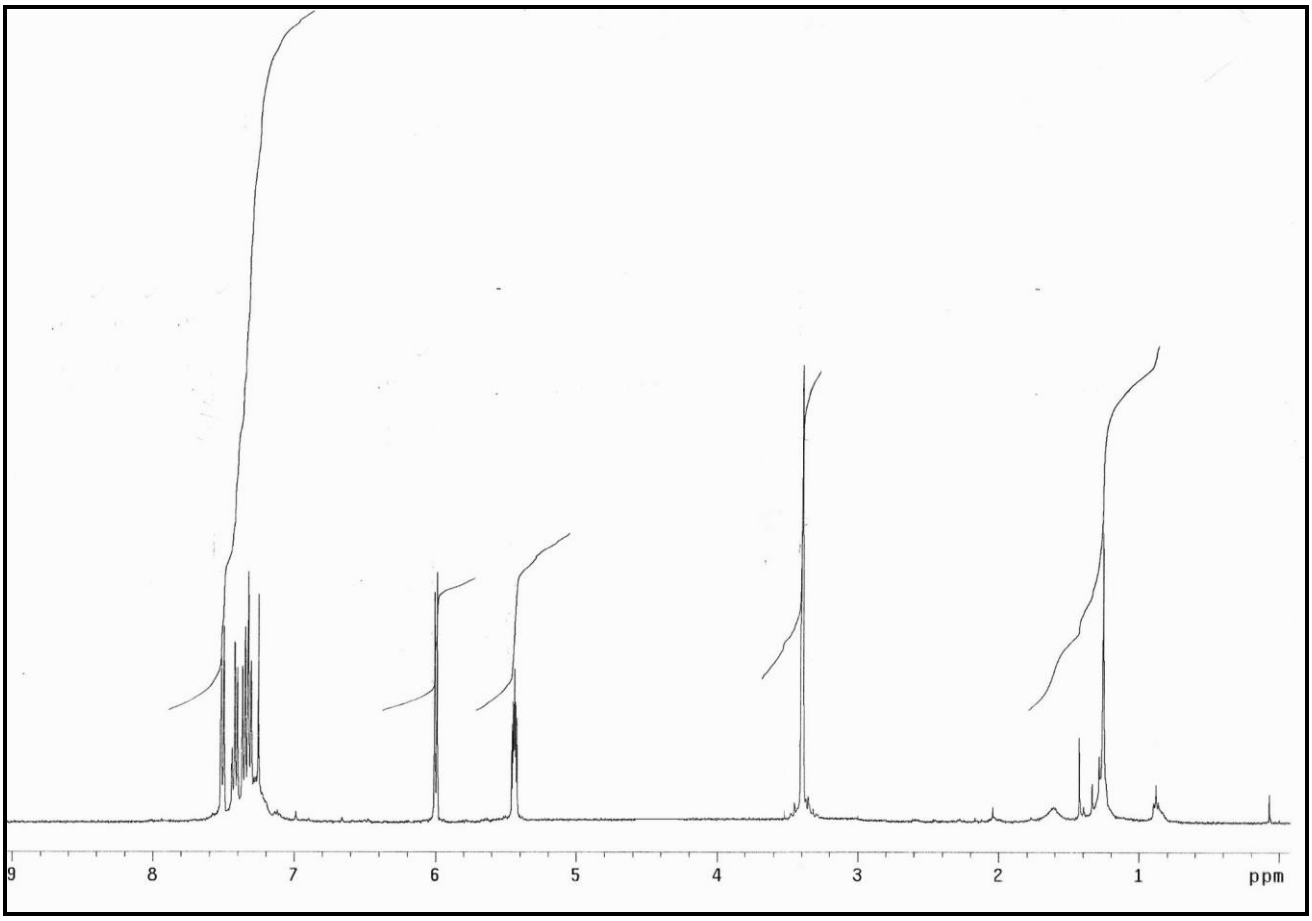
^{13}C NMR spectrum of 4-benzyl-1,3-dioxolan-2-one (**8g**)



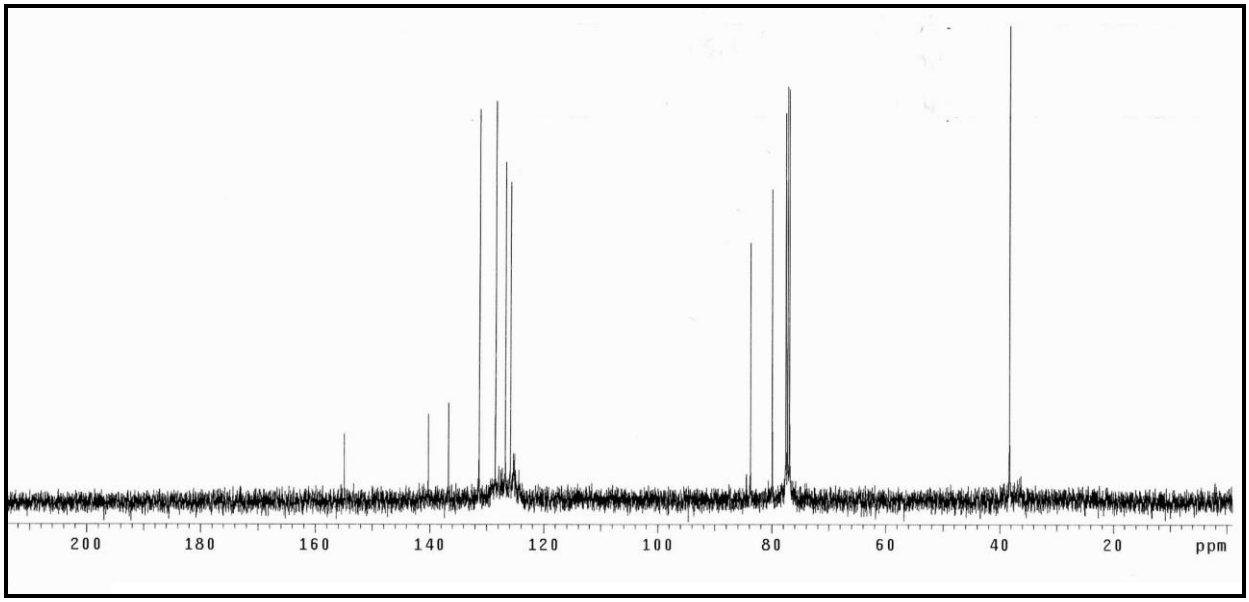
^{1}H NMR spectrum of 4-benzyloxazolidin-2-one (**9g**)



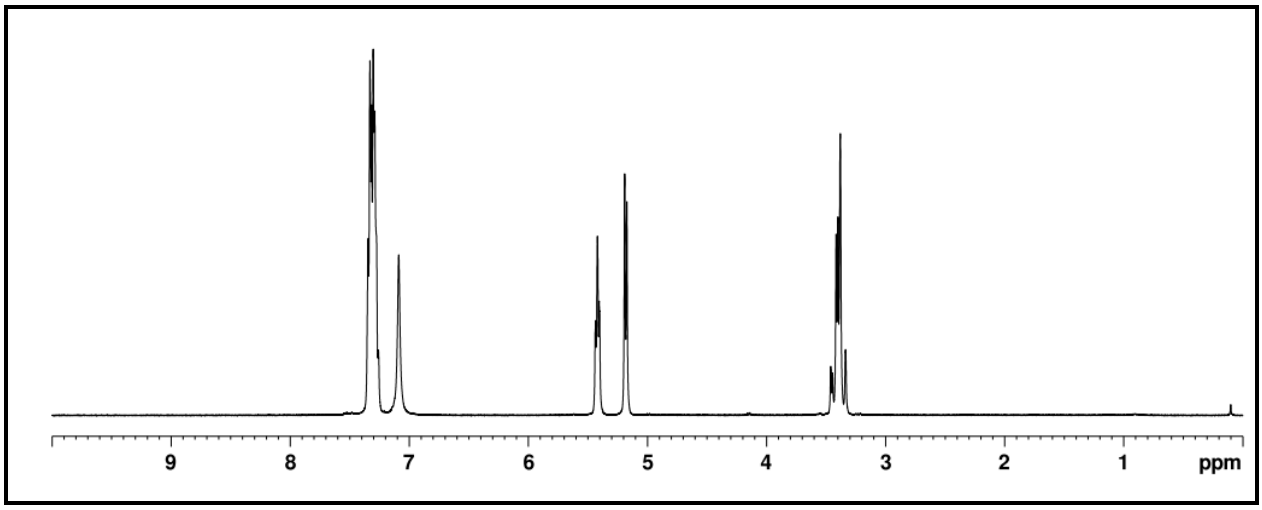
^{13}C NMR spectrum of 4-benzyloxazolidin-2-one (**9g**)



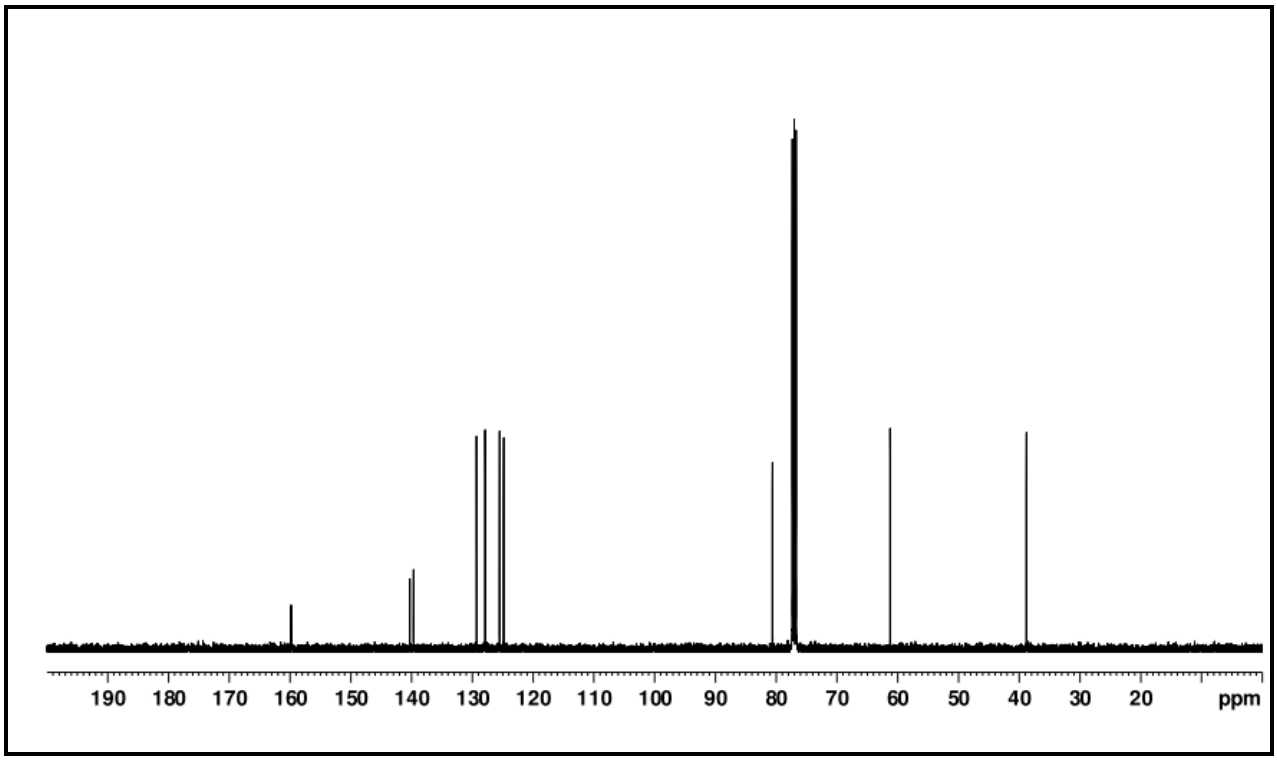
^{1}H NMR spectrum of 8,8a-dihydro-3a*H*-indeno[1,2-*d*][1,3]dioxol-2-one (**8h**)



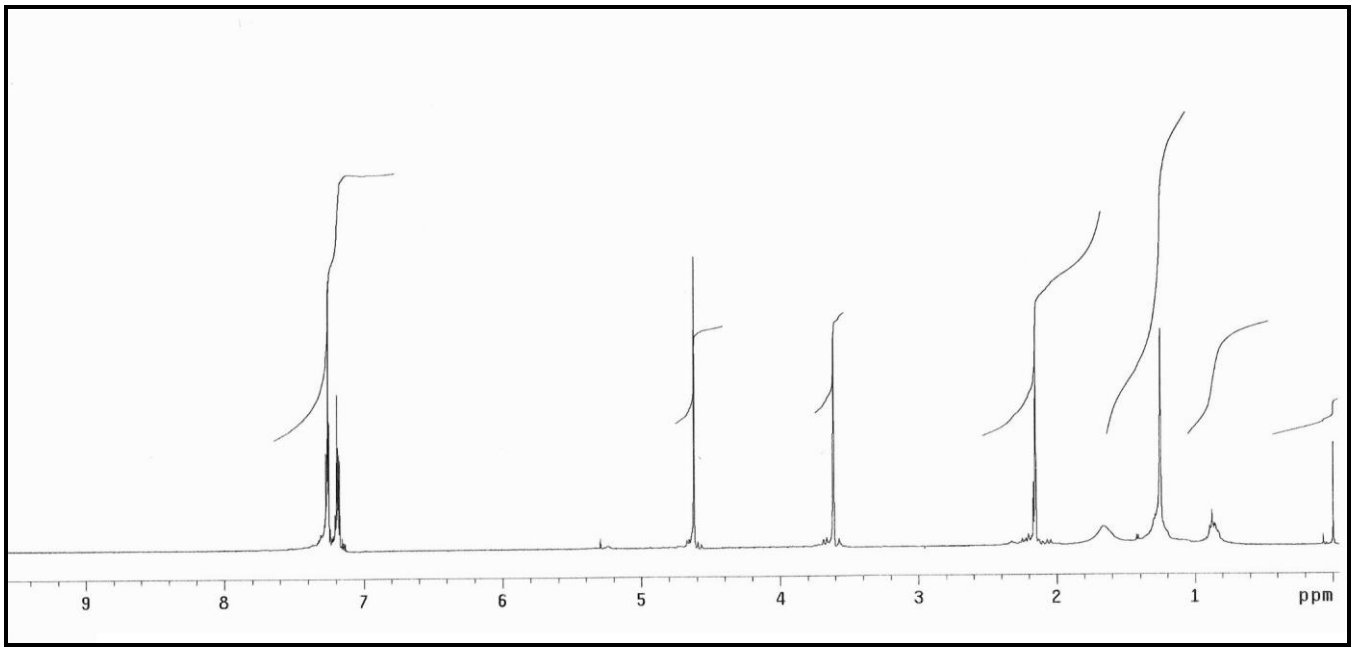
^{13}C NMR spectrum of 8,8a-dihydro-3a*H*-indeno[1,2-*d*][1,3]dioxol-2-one (**8h**)



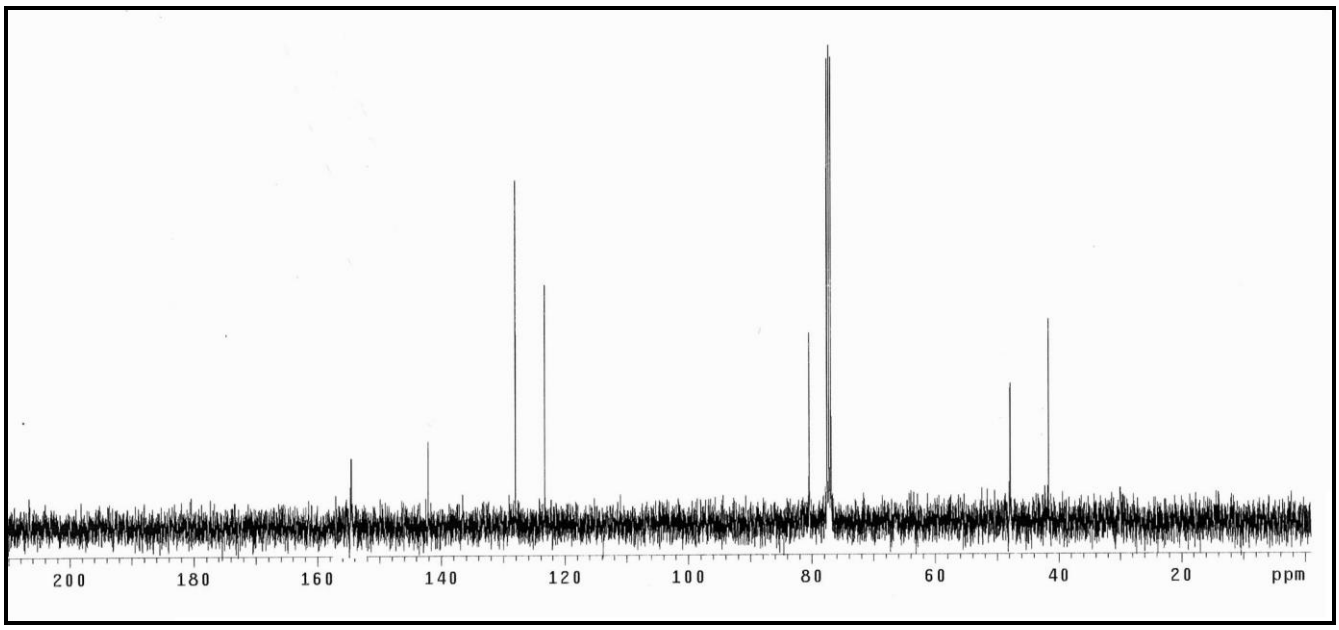
^{1}H NMR spectrum of 3,3a,8,8a-tetrahydro-2*H*-indeno[1,2-*d*]oxazol-2-one (**9h**)



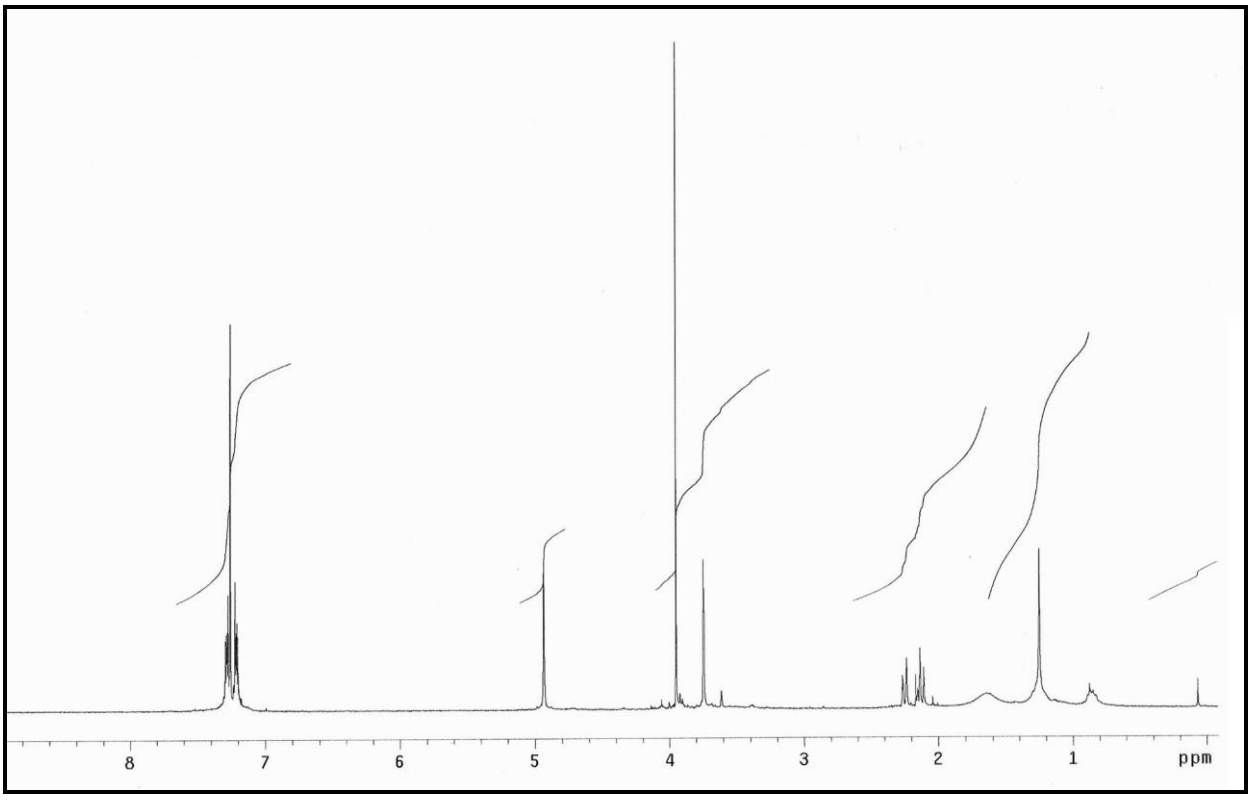
^{13}C NMR spectrum of 3,3a,8,8a-tetrahydro-2*H*-indeno[1,2-*d*]oxazol-2-one (**9h**)



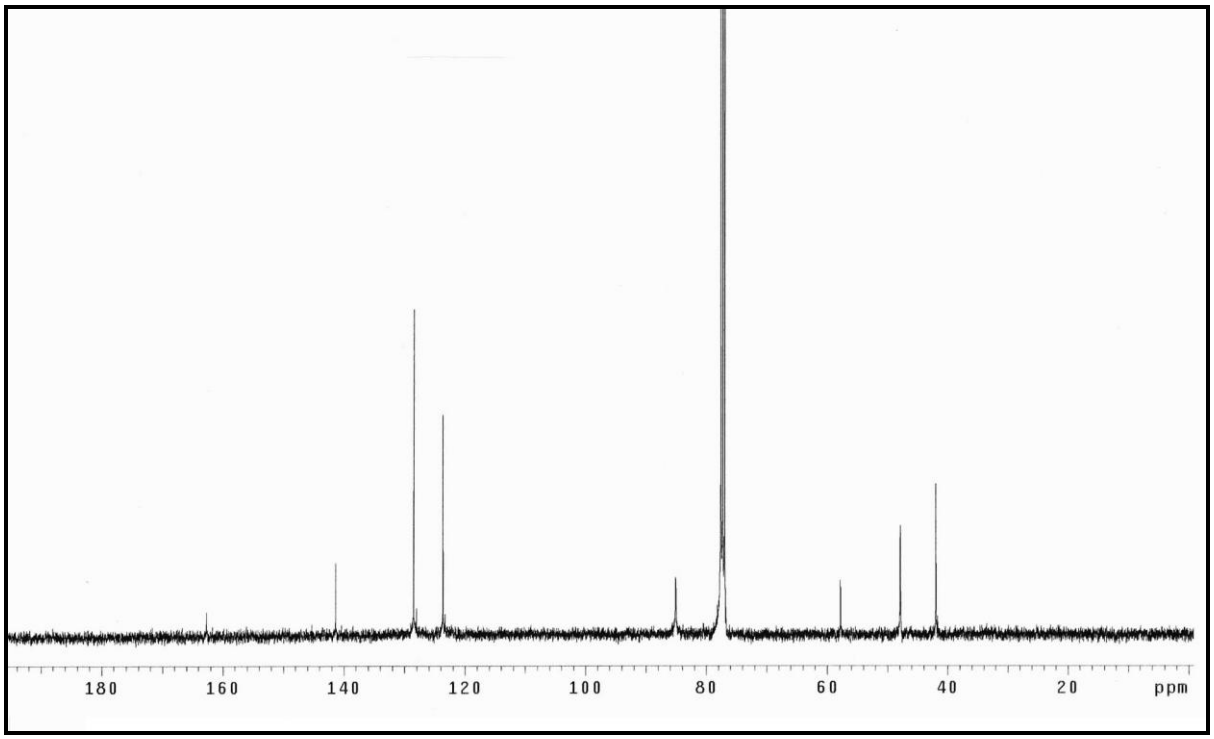
^{1}H NMR spectrum of 3a,4,9,9a-tetrahydro-4,9-methanonaphtho[2,3-*d*][1,3]dioxol-2-one (**8i**)



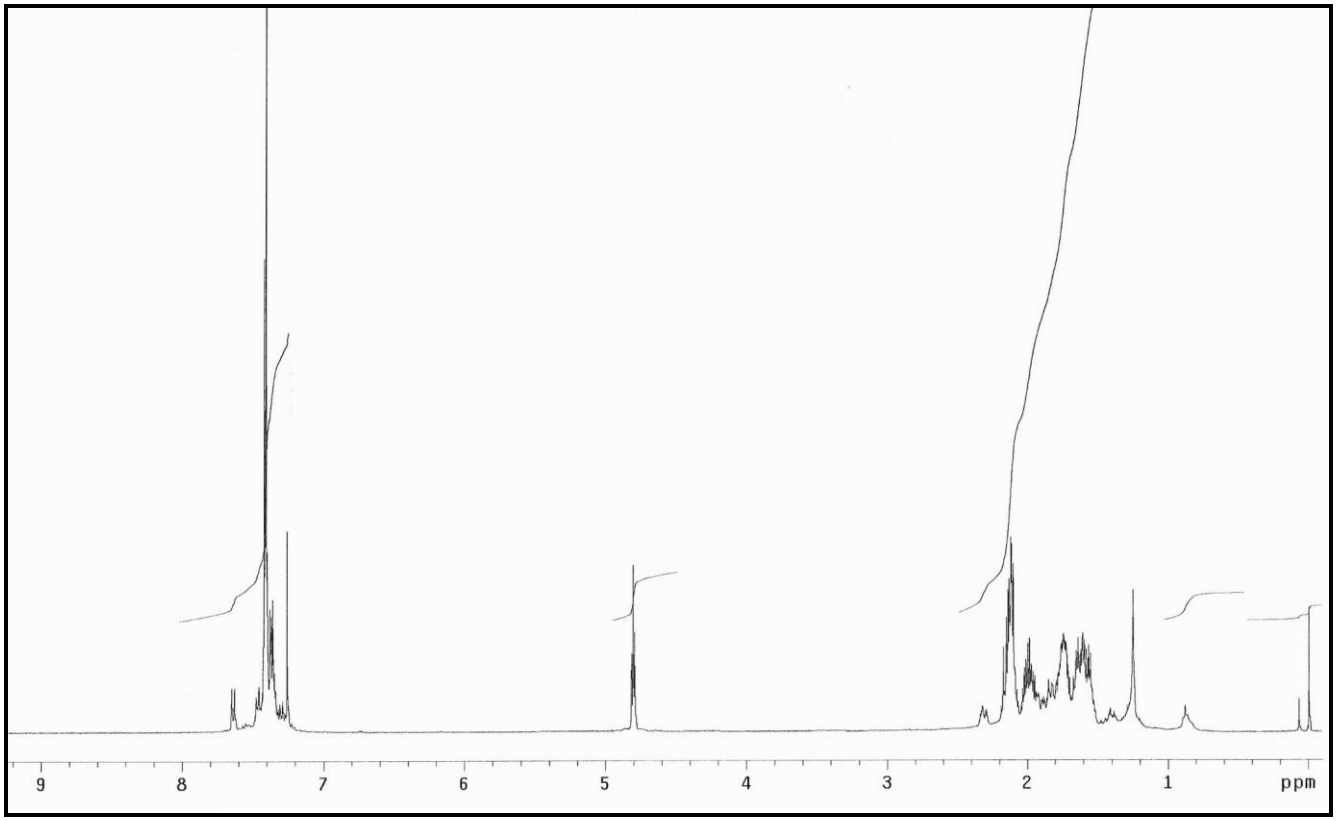
^{13}C NMR spectrum of 3a,4,9,9a-tetrahydro-4,9-methanonaphtho[2,3-*d*][1,3]dioxol-2-one (**8i**)



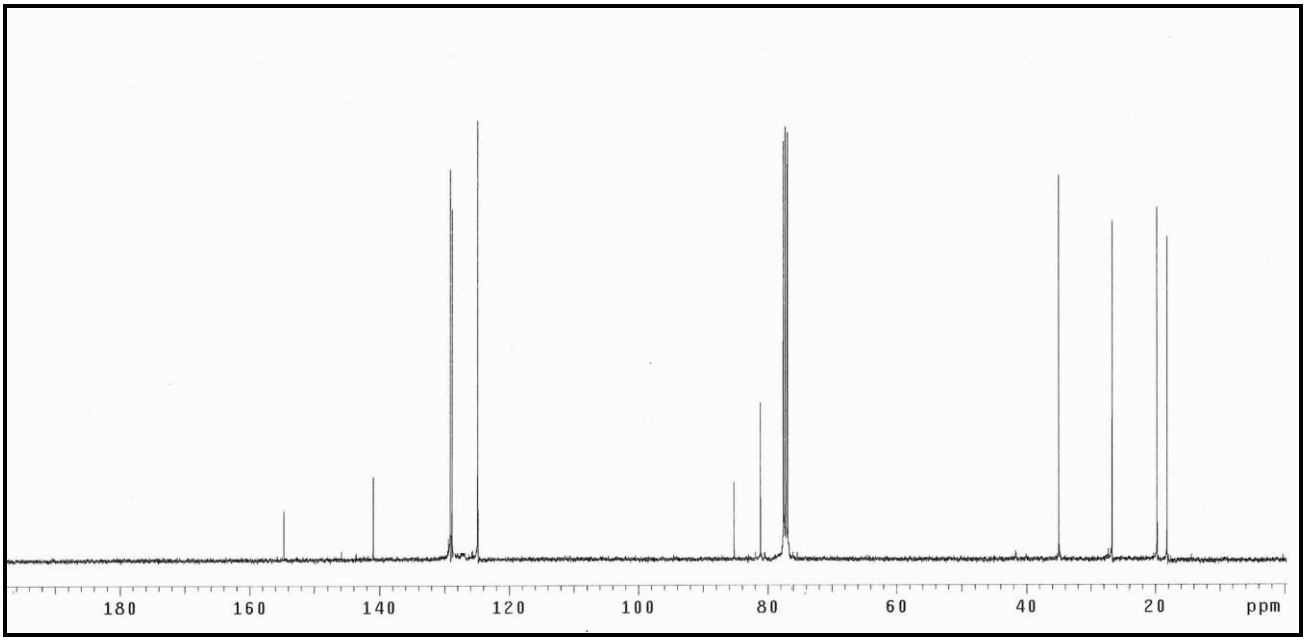
^{1}H NMR spectrum of 3a,4,9,9a-tetrahydro-4,9-methanonaphtho[2,3-*d*]oxazol-2(3*H*)-one (**9i**)



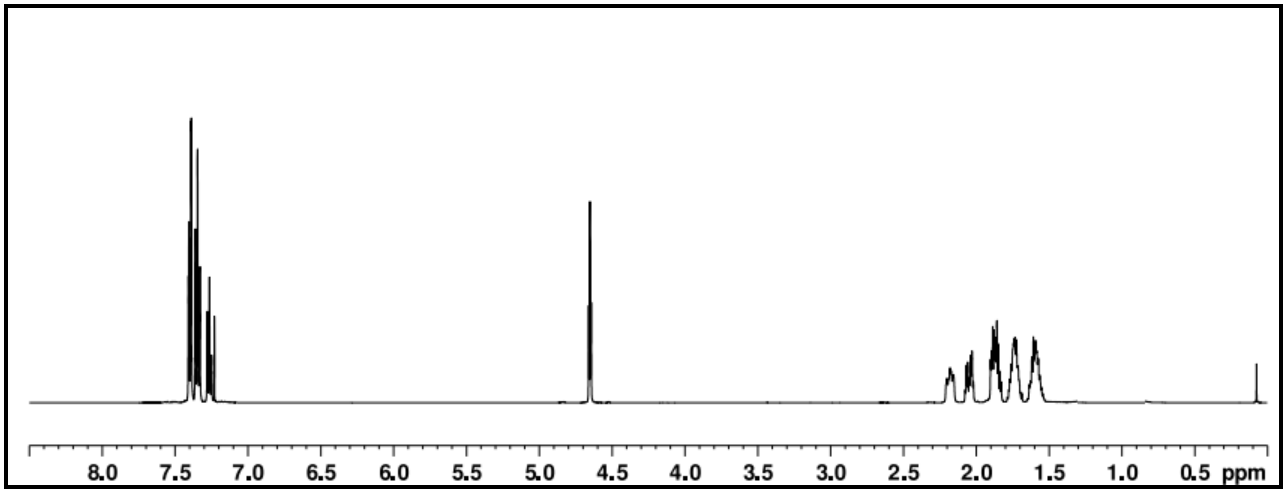
^{13}C NMR spectrum of 3a,4,9,9a-tetrahydro-4,9-methanonaphtho[2,3-*d*]oxazol-2(3*H*)-one (**9i**)



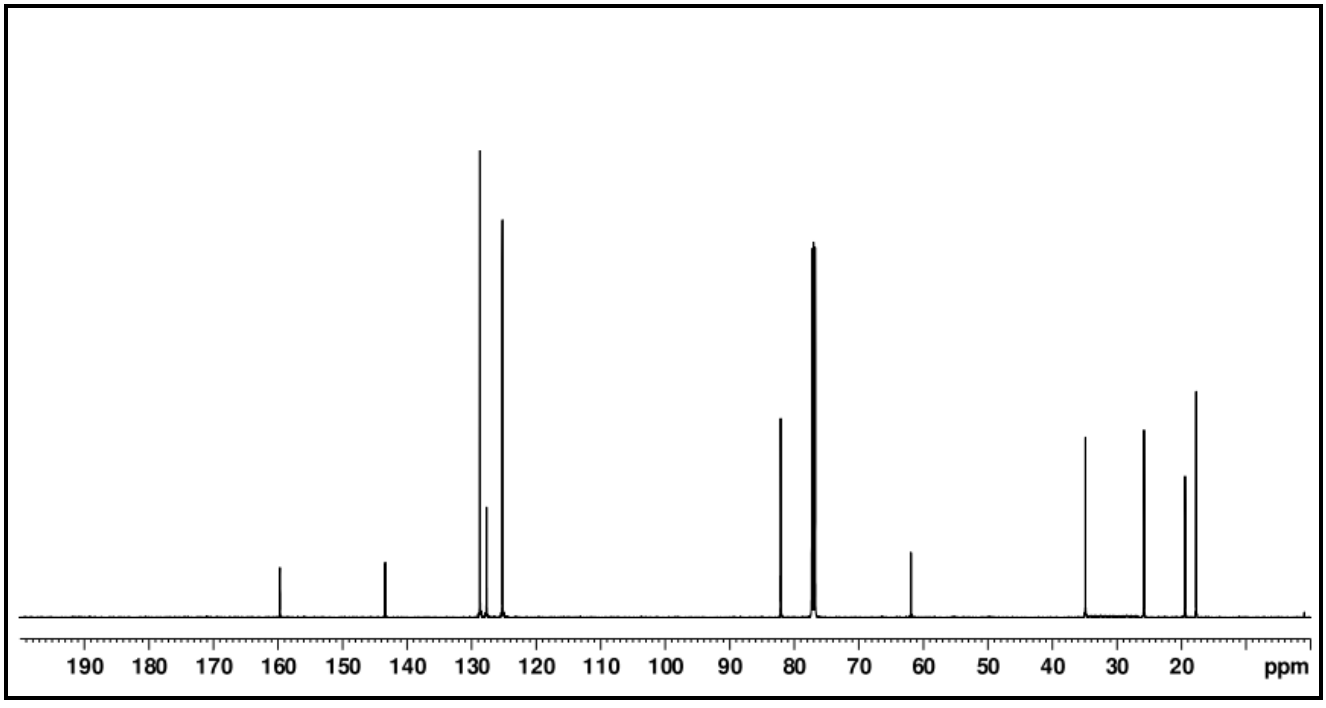
^{1}H NMR spectrum of 3a-phenylhexahydrobenzo[*d*][1,3]dioxol-2-one (**8j**)



^{13}C NMR spectrum of 3a-phenylhexahydrobenzo[*d*][1,3]dioxol-2-one (**8j**)



^{1}H NMR spectrum of 3a-phenylhexahydrobenzo[*d*]oxazol-2(3*H*)-one (**9j**)



^{13}C NMR spectrum of 3a-phenylhexahydrobenzo[*d*]oxazol-2(3*H*)-one (**9j**)

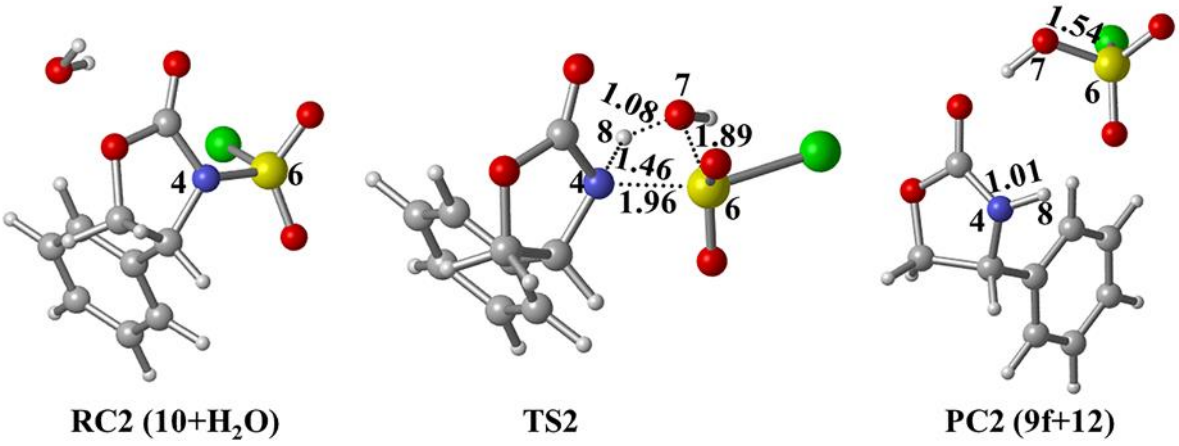


Figure S1. Optimized geometries for the stationary points of path 1a at PCM(DCM)/M06-2X/6-31+G(d,p)//M06-2X/6-31+G(d,p) level. Distances are given in Å.

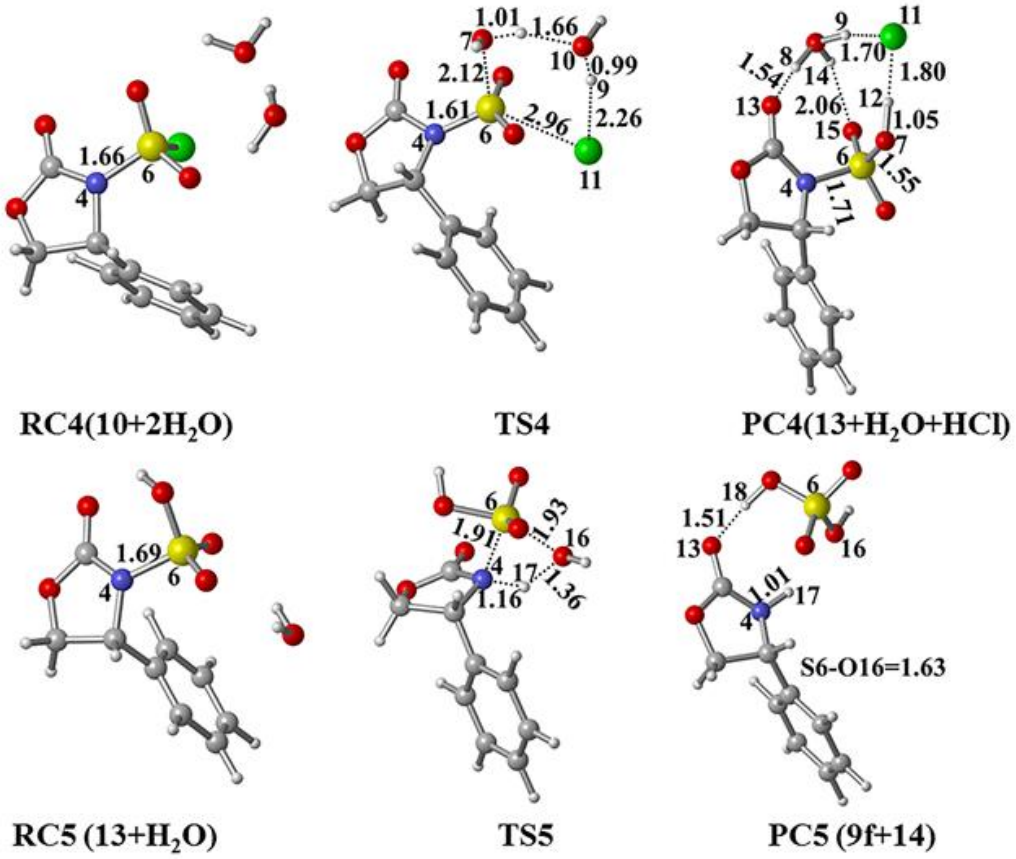


Figure S2. Optimized geometries for the stationary points of path 2 at PCM(DCM)/M06-2X/6-31+G(d,p)//M06-2X/6-31+G(d,p) level. Distances are given in Å.

Absolute energies of structures

Energies are given in terms of ZPE-corrected total energy (Eel+ZPE), enthalpy (Eel+H) and Gibbs free-energy (Eel+G) as extracted from Gaussian [10] output of each structure.

Table S1. Absolute energies of optimized structures for the formation of **10** and **11** in gas phase **(**M06-2X/6-31+G(d,p))

Compound No	***Eel***[a]***+ZPE***[b] ***(au)***	***Eel+H***[c] ***(au)***	***Eel+G***[d] ***(au)***	***Imaginary Frequency (i)***
RC1(7f+CSI)	-1561.194746	-1561.178848	-1561.241301	–
TS1	-1561.153888	-1561.138832	-1561.197491	-100.6
10	-1561.259136	-1561.244428	-1561.302205	–
RC(7f+CSI)	-1561.194356	-1561.177605	-1561.242869	–
TS1'	-1561.124586	-1561.109231	-1561.169734	-638.32
11	-1561.259812	-1561.244978	-1561.303961	–

[a] Eel = Total electronic energy. [b] ZPE = Zero point energy correction. [c] H = Enthalpy correction. [d] G = Gibbs free energy correction.

Table S2. Single point energies for the formation of **10** and **11** at PCM(DCM)/M06-2X/6-31+G(d,p)//M06-2X/6-31+G(d,p) level.

Compound No	***Eel***[a] ***(au)***	***Eel+G***[b] ***(au)***
RC1(7f+CSI)	-1561.369067	-1561.24944
TS1	-1561.361003	-1561.236926
10	-1561.443435	-1561.31507
RC(7f+CSI)	-1561.368896	-1561.250916
TS1'	-1561.315231	-1561.194255
11	-1561.444182	-1561.317096

Table S3. Absolute energies of optimized structures for path 1a, path 1b and path 2 in gas phase (M06-2X/6-31+G(d,p))

Compound No	***Eel***[a]***+ZPE***[b] ***(au)***	***Eel+H***[c] ***(au)***	***Eel+G***[d] ***(au)***	***Imaginary Frequency (i)***
RC2(10+H₂O)	-1637.645459	-1637.62761	-1637.691332	–
TS2	-1637.547131	-1637.530831	-1637.592093	-723.3
PC2(9f+12)	-1637.671332	-1637.655843	-1637.715451	–
RC3(10+2H₂O)	-1714.024727	-1714.003944	-1714.074618	–
TS3	-1713.958869	-1713.941923	-1714.004302	-527.9
PC3(9f+12+H₂O)	-1714.04547	-1714.025749	-1714.095205	–
RC4(10+2H₂O)	-1714.024112	-1714.002993	-1714.074864	–
TS4	-1713.935637	-1713.916326	-1713.983151	-230.1
13+H₂O+HCl	-1714.024503	-1714.003043	-1714.102387	–
RC5(13+H₂O)	-1253.279008	-1253.261331	-1253.323976	–
TS5	-1253.182873	-1253.166892	-1253.226232	-966.5
PC5(9f+14)	-1253.296965	-1253.28041	-1253.343945	–

Table S4. Single point energies for path 1a, path 1b and path 2 at PCM(DCM)/M06-2X/6-31+G(d,p)//M06-2X/6-31+G(d,p) level.

Compound No	*Eel*[a] *(au)*	*Eel+G*[b] *(au)*
RC2(10+H_2O)	-1637.855513	-1637.705082
TS2	-1637.758664	-1637.61003
PC2(9f+12)	-1637.881053	-1637.727922
RC3(10+2H_2O)	-1714.261539	-1714.089819
TS3	-1714.207323	-1714.032324
PC3(9f+12+H_2O)	-1714.286479	-1714.11308
RC4(10+2H_2O)	-1714.26671	-1714.096141
TS4	-1714.195502	-1714.021157
13+H_2O+HCl	-1714.262539	-1714.126365
RC5(13+H_2O)	-1253.504294	-1253.339321
TS5	-1253.407798	-1253.243687
PC5(9f+14)	-1253.523423	-1253.35909

Table S5. Absolute energies of optimized structures for the formation of **8f** in gas phase **(**M06-2X/6-31+G(d,p))

Compound No	*Eel*[a]*+ZPE*[b] *(au)*	*Eel+H*[c] *(au)*	*Eel+G*[d] *(au)*	*Imaginary Frequency (i)*
RC6(7f+CSI)	-1561.191475	-1561.174617	-1561.240605	–
TS6	-1561.150784	-1561.135859	-1561.194273	-118.2
16	-1561.239888	-1561.225413	-1561.282908	–
RC7(16+H_2O)	-1637.627309	-1637.609558	-1637.673558	–
TS7	-1637.566139	-1637.55039	-1637.60951	-1251.3
17	-1637.633906	-1637.617977	-1637.676911	–
RC8(17+H_2O)	-1637.632267	-1637.616177	-1637.676000	–
TS8	-1637.591580	-1637.575304	-1637.636346	-199.9
PC8(8f+18)	-1637.655022	-1637.639003	-1637.699032	–

Table S6. Single point energies for the formation of **8f** at PCM(DCM)/M06-2X/6-31+G(d,p)//M06-2X/6-31+G(d,p) level.

Compound No	*Eel*[a] *(au)*	*Eel+G*[b] *(au)*
RC6(7f+CSI)	-1561.366947	-1561.249535
TS6	-1561.362049	-1561.237508
16	-1561.426792	-1561.29803
RC7(16+H_2O)	-1637.839263	-1637.688891
TS7	-1637.777903	-1637.627503
17	-1637.845407	-1637.689378
RC8(17+H_2O)	-1637.843896	-1637.688757
TS8	-1637.809078	-1637.657218
PC8(8f+18)	-1637.866644	-1637.712687

Cartesian coordinates for the optimized structures given in paths

Structure No: ***RC1 (7f+CSI) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-0.798109	0.522489	1.479827
6	-1.373568	-0.051007	0.249713
6	1.574494	1.422758	-0.782489
1	0.196886	0.213123	1.796450
1	-0.756765	-0.766881	-0.294025
8	-0.839363	1.268893	0.268905
8	1.463753	2.534085	-1.056486
7	1.637964	0.216568	-0.502202
16	3.075441	-0.608660	-0.437455
8	4.067541	0.048924	-1.247780
8	2.757131	-2.000755	-0.563971
17	3.596030	-0.288139	1.523004
6	-2.845837	-0.178208	0.062732
6	-3.389973	-1.412364	-0.296976
6	-3.689281	0.917297	0.260336
6	-4.767974	-1.556567	-0.442116
1	-2.732476	-2.261921	-0.464759
6	-5.066157	0.772585	0.110871
1	-3.255753	1.881084	0.512137
6	-5.608852	-0.464159	-0.237018
1	-5.183425	-2.519758	-0.721611
1	-5.717461	1.628253	0.260341
1	-6.682326	-0.574233	-0.354675
1	-1.474970	0.875150	2.255146

Structure No: ***TS1 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-0.746216	-1.451023	-1.209600
6	-1.386374	-0.139017	-0.947315
6	0.950632	-1.049606	0.533417
1	0.077884	-1.374430	-1.918808
1	-0.704333	0.708499	-1.020047
8	-0.291363	-1.660322	0.126473
8	1.399860	-1.470137	1.563410
7	1.318437	-0.118350	-0.361517
16	2.575999	0.825516	-0.027956
8	2.550097	1.377228	1.310875
8	2.767044	1.703036	-1.164589
17	4.213499	-0.480106	-0.061291
6	-2.677897	0.075044	-0.442037
6	-3.038692	1.405546	-0.101599
6	-3.614286	-0.977427	-0.258861
6	-4.303987	1.679538	0.384917

1	-2.305498	2.197378	-0.226432
6	-4.871457	-0.694346	0.234825
1	-3.332656	-1.999469	-0.487731
6	-5.212226	0.629474	0.551292
1	-4.585905	2.693091	0.646088
1	-5.593109	-1.489060	0.385878
1	-6.203498	0.840681	0.941919
1	-1.429497	-2.262251	-1.460595

Structure No: ***10 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	0.375729	2.265702	-1.079604
6	0.420374	0.720367	-1.066649
6	-1.150129	1.614211	0.492966
1	-0.149068	2.645141	-1.960790
1	0.298508	0.316744	-2.074188
8	-0.372692	2.636244	0.085433
8	-1.979594	1.665385	1.348744
7	-0.803928	0.492707	-0.286480
16	-1.343430	-1.045719	0.061868
8	-1.254388	-1.319914	1.468490
8	-0.738958	-1.885540	-0.940627
17	-3.328576	-0.865909	-0.387980
6	1.666092	0.153059	-0.422441
6	2.690352	-0.327465	-1.238842
6	1.831520	0.153804	0.964804
6	3.876476	-0.794679	-0.677789
1	2.554219	-0.349979	-2.317404
6	3.016477	-0.317496	1.524972
1	1.034921	0.501092	1.618417
6	4.040857	-0.789153	0.705985
1	4.664663	-1.173962	-1.320174
1	3.134701	-0.322289	2.603573
1	4.960789	-1.161268	1.145366
1	1.368012	2.708037	-1.000391

Structure No: ***RC (7f+CSI) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.438491	0.000450	0.382318
6	0.971381	0.812900	1.520024
6	-1.523119	1.324335	-0.796683
1	0.771168	-0.789788	0.037167
1	1.714710	1.286689	2.157790
1	0.001298	0.596796	1.964320
8	0.924597	1.314257	0.188709
6	2.889546	-0.196491	0.107086
6	3.400190	-1.488341	-0.033865
6	3.748266	0.900254	0.004633
6	4.760934	-1.683995	-0.260227
1	2.731003	-2.342651	0.033231

6	5.107362	0.703181	-0.225529
1	3.338057	1.902460	0.089147
6	5.617357	-0.588480	-0.355534
1	5.151283	-2.691203	-0.367486
1	5.769562	1.559406	-0.308900
1	6.676732	-0.740633	-0.536403
8	-1.325215	2.225761	-1.482797
7	-1.677045	0.329367	-0.073218
16	-3.169430	-0.171235	0.450579
8	-4.108650	0.919234	0.394546
8	-2.945068	-0.947767	1.635540
17	-3.678317	-1.478920	-1.041584

Structure No: ***TS1' (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-1.181822	0.244875	0.215947
6	-0.636570	-0.066117	1.537576
6	0.849790	-0.956046	-0.534661
1	-0.703392	1.095990	-0.272530
1	-1.096992	-0.907508	2.048672
1	0.140326	0.495802	2.037599
8	-0.572733	-1.009155	-0.172141
6	-2.673399	0.210146	0.055054
6	-3.366718	1.415375	-0.068211
6	-3.362757	-1.003851	0.066238
6	-4.755242	1.407249	-0.172619
1	-2.823295	2.356489	-0.093887
6	-4.750758	-1.005492	-0.046705
1	-2.812895	-1.937675	0.132000
6	-5.446859	0.197090	-0.161226
1	-5.293476	2.343785	-0.274249
1	-5.288303	-1.947990	-0.051942
1	-6.528300	0.190510	-0.250887
8	1.158763	-1.456840	-1.572251
7	1.456667	-0.325998	0.476694
16	3.053492	-0.050553	0.449462
8	3.826110	-1.199915	0.049035
8	3.359366	0.679993	1.658176
17	3.242807	1.331140	-1.109056

Structure No: ***11 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	0.957091	-0.182730	-0.617830
6	0.034819	-0.567907	0.555749
6	-0.778568	1.330080	-0.634340
1	0.785012	-0.851093	-1.468993
1	0.495973	-0.373007	1.527090
1	-0.283050	-1.611428	0.508837
8	0.499544	1.126663	-1.008001
6	2.417226	-0.152884	-0.266534
6	3.259809	-1.165786	-0.721165

6	2.926747	0.860523	0.549212
6	4.605399	-1.175404	-0.355198
1	2.867098	-1.946267	-1.368138
6	4.271485	0.856451	0.905022
1	2.273801	1.661693	0.885496
6	5.111504	-0.164288	0.456861
1	5.256823	-1.966422	-0.712259
1	4.666317	1.650546	1.530552
1	6.160128	-0.165844	0.736775
8	-1.491302	2.190349	-1.042608
7	-1.090689	0.348948	0.348740
16	-2.639675	-0.126238	0.679388
8	-3.510374	1.008883	0.705277
8	-2.535671	-1.087584	1.746088
17	-3.110772	-1.209166	-1.022792

Structure No: ***RC2 (10+H_2O) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-0.229395	1.660957	-2.106377
6	0.110273	0.235196	-1.630581
6	-1.640787	1.232389	-0.358845
1	0.652158	2.296847	-2.178833
1	-0.778878	1.652040	-3.050852
1	0.102303	-0.471514	-2.462380
8	-1.088030	2.208731	-1.093262
16	-1.391469	-1.433851	-0.043277
8	-2.789532	-1.539772	0.254211
7	-1.102572	0.009477	-0.808709
8	-2.436838	1.398091	0.519222
1	-1.193022	2.786282	1.708530
8	-0.286914	2.648922	2.013925
1	-0.348960	1.914823	2.634664
8	-0.660140	-2.415890	-0.802365
17	-0.419815	-1.230558	1.757660
6	1.397372	0.112124	-0.846017
6	2.217887	-0.998913	-1.039568
6	1.746491	1.080334	0.100854
6	3.390634	-1.140768	-0.299411
1	1.926047	-1.764449	-1.753923
6	2.916431	0.934542	0.839941
1	1.097997	1.931047	0.301491
6	3.740633	-0.173558	0.639801
1	4.024070	-2.008522	-0.453251
1	3.178183	1.687332	1.577067
1	4.652871	-0.283584	1.218064

Structure No: ***TS2 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.007142	2.021434	-1.355524
6	0.816134	0.534068	-0.994339

6	-0.349353	1.958244	0.479078
1	2.056529	2.299083	-1.462170
1	0.452214	2.298097	-2.255828
1	0.446749	-0.031432	-1.850509
8	0.462721	2.748714	-0.250820
16	-1.927947	-0.316124	-0.280721
8	-2.716173	0.869457	-0.518394
7	-0.235815	0.610836	0.037414
8	-1.020582	2.332244	1.394777
1	-0.412789	-0.251756	1.207207
8	-1.369825	-0.674169	1.488510
1	-1.492090	-1.611493	1.725514
8	-1.339386	-1.251149	-1.220536
17	-3.590431	-1.606022	0.324688
6	2.046214	-0.148138	-0.436911
6	2.392553	-1.428308	-0.868898
6	2.818848	0.478042	0.547504
6	3.503781	-2.076867	-0.328477
1	1.787629	-1.919283	-1.627360
6	3.925407	-0.169092	1.088369
1	2.554862	1.476449	0.892677
6	4.270140	-1.448723	0.649719
1	3.768356	-3.071690	-0.672741
1	4.519713	0.323851	1.851200
1	5.134794	-1.952056	1.070537

Structure No: ***PC2 (9f+12) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	2.297702	2.413899	0.264136
6	1.943435	1.332819	-0.783303
6	0.078736	2.031120	0.381231
1	3.116527	2.123757	0.921535
1	2.498766	3.382245	-0.201759
1	2.353452	1.608586	-1.759300
8	1.107364	2.545705	1.059439
16	-2.821242	-0.431823	-0.510358
8	-4.016935	-1.002742	-1.056715
7	0.496353	1.484337	-0.778496
8	-1.067927	2.104186	0.824851
1	-0.127670	0.847324	-1.269455
8	-3.093328	0.991763	0.006697
1	-2.199495	1.485281	0.330043
8	-1.573290	-0.463655	-1.257602
17	-2.401704	-1.446860	1.237359
6	2.417094	-0.059267	-0.405316
6	3.765885	-0.376255	-0.595507
6	1.560514	-1.015077	0.139993
6	4.256085	-1.625747	-0.230818
1	4.437184	0.358646	-1.036242
6	2.052064	-2.269320	0.503038
1	0.503103	-0.804028	0.269770
6	3.397117	-2.576810	0.322006
1	5.304463	-1.860720	-0.385136

1	1.373373	-3.005652	0.921528
1	3.775806	-3.554250	0.603000

Structure No: ***RC3 (10+2H$_2$O) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-0.148129	2.358322	-1.045614
6	0.175299	0.865674	-1.150016
6	-0.876138	1.408377	0.900881
1	0.689124	3.004432	-1.305418
1	-1.032854	2.626347	-1.629085
1	-0.166064	0.430543	-2.091083
8	-0.448676	2.556301	0.348727
16	-1.730366	-0.891451	-0.194610
8	-1.955043	-1.505192	1.081461
7	-0.670138	0.369969	-0.037198
8	-1.315917	1.296280	2.007636
1	0.893516	-2.053940	1.256147
8	0.743045	-2.653174	0.503175
8	-1.368080	-1.592749	-1.394876
17	-3.490037	0.124960	-0.640004
6	1.613584	0.487281	-0.860468
6	2.070383	-0.767020	-1.264148
6	2.446486	1.314640	-0.096547
6	3.348671	-1.192667	-0.911099
1	1.407001	-1.433201	-1.808094
6	3.726531	0.887498	0.252495
1	2.104751	2.289941	0.241600
6	4.177784	-0.368112	-0.154131
1	3.683421	-2.180202	-1.209631
1	4.367449	1.533974	0.843767
1	5.170885	-0.704038	0.126449
1	0.107198	-3.304605	0.816831
8	1.031945	-0.653873	2.479928
1	1.596808	0.031109	2.100867
1	0.181195	-0.235944	2.675349

Structure No: ***TS3 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-0.060067	2.344481	-0.474309
6	0.291738	0.861801	-0.701873
6	-1.087629	1.206764	1.233614
1	0.818500	2.988192	-0.427253
1	-0.769084	2.692705	-1.224183
1	-0.115657	0.524686	-1.656615
8	-0.706004	2.403244	0.806987
16	-1.642104	-1.099734	-0.145645
8	-2.979679	-1.120476	0.400205
7	-0.465216	0.181453	0.397695
8	-1.732686	0.954358	2.201930
1	0.388400	-1.932951	1.632296
8	-0.996751	-2.180666	1.078624

8	-1.027994	-1.729141	-1.290719
17	-2.551665	0.770078	-1.608147
6	1.752656	0.483677	-0.583179
6	2.208830	-0.630394	-1.295937
6	2.613794	1.125982	0.312120
6	3.509220	-1.099459	-1.110758
1	1.529984	-1.138434	-1.976660
6	3.914721	0.658320	0.495981
1	2.268748	1.981651	0.888204
6	4.362476	-0.457815	-0.211530
1	3.854786	-1.963788	-1.668951
1	4.574963	1.161423	1.195123
1	5.374433	-0.822522	-0.067324
1	-1.722799	-2.312300	1.709439
8	1.098541	-1.207600	1.796703
1	1.933857	-1.398930	1.338129
1	0.494490	-0.463393	1.208151

Structure No: ***PC3 (9f+12+H_2O) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.628801	2.130400	-1.326401
6	1.018560	0.921455	-0.592372
6	0.319357	2.922963	0.358625
1	2.685129	2.255740	-1.062400
1	1.516036	2.080611	-2.409328
1	0.151805	0.538795	-1.149036
8	0.889240	3.249658	-0.835829
16	-2.587216	-1.146905	-0.254031
8	-3.804178	-1.577569	-0.873564
7	0.601518	1.598231	0.625887
8	-0.305751	3.695076	1.033690
1	0.394575	-1.459037	0.919188
8	-2.565683	-1.651126	1.226883
8	-1.288399	-1.383260	-0.852198
17	-2.709451	0.885391	0.007387
6	1.984765	-0.213361	-0.348817
6	1.874787	-1.397975	-1.082168
6	2.983787	-0.100363	0.625668
6	2.756797	-2.456388	-0.848616
1	1.086099	-1.497286	-1.823626
6	3.860947	-1.155673	0.857963
1	3.051301	0.813782	1.209521
6	3.748047	-2.337795	0.122057
1	2.660932	-3.373193	-1.421716
1	4.632395	-1.058762	1.615711
1	4.430366	-3.161252	0.307624
8	-0.084499	-1.215360	1.730305
1	0.490574	-1.419991	2.476943
1	-0.010650	1.126211	1.279641
1	-1.623993	-1.553311	1.585267

Structure No: ***RC4 (10+2H_2O) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-1.988521	1.943252	1.488851
6	-1.157976	0.659023	1.325844
6	-0.543547	2.345288	-0.240589
1	-3.060194	1.748589	1.520056
1	-1.675702	2.515717	2.365530
1	-0.745171	0.327538	2.280147
8	-1.711756	2.722557	0.314730
16	1.262385	0.364246	0.061204
8	2.328878	1.278856	-0.247622
8	1.378116	-0.674224	1.055897
17	0.701756	-0.524676	-1.685858
7	-0.067395	1.243233	0.512137
8	-0.031917	2.846649	-1.192408
8	4.160305	-1.716636	1.724697
1	3.220415	-1.575015	1.877188
8	4.116934	-0.755807	-1.015263
1	4.757088	-0.977079	-1.698313
1	4.028446	0.205827	-1.002914
1	4.281970	-1.478219	0.793901
6	-1.865985	-0.483781	0.631291
6	-1.612123	-1.793571	1.038005
6	-2.726443	-0.248829	-0.446714
6	-2.212814	-2.863397	0.376507
1	-0.924896	-1.976459	1.859521
6	-3.325431	-1.317517	-1.106346
1	-2.926182	0.766849	-0.781851
6	-3.067862	-2.626083	-0.696589
1	-2.006390	-3.879429	0.696828
1	-3.990966	-1.128823	-1.942559
1	-3.534941	-3.458039	-1.213967

Structure No: ***TS4 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-1.267644	2.751753	-0.339769
6	-0.950427	1.501327	0.497927
6	0.986114	2.456622	-0.591936
1	-1.744609	2.470070	-1.282461
1	-1.878529	3.474354	0.198923
1	-0.867522	1.756187	1.560664
8	0.000481	3.359062	-0.627003
16	1.250469	-0.112010	0.176955
8	2.318927	-0.161672	-0.754381
8	0.504414	-0.940673	1.067032
17	0.788094	-2.633546	-1.314520
7	0.412770	1.249503	-0.032137
8	2.115629	2.622572	-0.908298
8	2.702771	0.177739	1.696558
1	2.316023	0.157207	2.584570
8	3.041867	-2.324792	0.973058

1	2.321994	-2.601922	0.348683
1	3.855750	-2.624226	0.552144
1	3.048108	-0.761254	1.524921
6	-1.954081	0.394996	0.299043
6	-2.945123	0.221415	1.265751
6	-1.932032	-0.419094	-0.834488
6	-3.921359	-0.757221	1.094075
1	-2.949379	0.842282	2.158741
6	-2.888611	-1.417745	-0.986653
1	-1.144418	-0.332839	-1.579553
6	-3.889315	-1.580204	-0.030047
1	-4.690579	-0.889783	1.847804
1	-2.826259	-2.082086	-1.841506
1	-4.632922	-2.361044	-0.151551

Structure No: ***13 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-0.078237	2.401228	-0.191584
6	0.165129	0.949901	-0.660306
6	-1.966906	1.245022	0.315756
1	0.490986	2.614200	0.717374
1	0.141461	3.141378	-0.959870
1	0.040753	0.855000	-1.745768
8	-1.478851	2.478360	0.120802
16	-1.344714	-1.325735	-0.101434
8	-1.515428	-1.835442	1.232086
8	-0.399476	-1.869105	-1.035378
7	-0.968808	0.321596	0.027071
8	-3.096218	0.992672	0.654639
8	-2.755159	-1.281123	-0.836589
1	-3.396407	-0.825983	-0.250102
6	1.514093	0.414983	-0.248591
6	2.524963	0.300311	-1.200926
6	1.771689	0.074109	1.081428
6	3.793202	-0.141016	-0.827644
1	2.316391	0.540799	-2.240413
6	3.035621	-0.375736	1.451396
1	0.976857	0.137838	1.821077
6	4.049304	-0.479718	0.498708
1	4.574252	-0.233691	-1.575344
1	3.227609	-0.652477	2.483075
1	5.033079	-0.833885	0.789516

Structure No: ***RC5 (13+H_2O) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	0.678470	-2.522285	-0.870992
6	0.157845	-1.075253	-1.062515
6	2.013775	-1.199027	0.410163
1	-0.115571	-3.213796	-0.591940
1	1.212734	-2.880912	-1.754076
1	0.117255	-0.818041	-2.123554

8	1.617344	-2.460740	0.218203
16	1.262150	1.291765	-0.135101
8	0.693760	1.543020	1.167917
8	0.704645	1.899966	-1.314909
7	1.287355	-0.368866	-0.437395
8	2.873386	-0.844822	1.180584
8	2.815597	1.580694	-0.104651
1	3.210973	1.048539	0.623022
8	-1.972464	2.612927	0.119657
1	-1.428500	2.307087	0.855604
1	-1.362208	2.649136	-0.626540
6	-1.178803	-0.798197	-0.413885
6	-2.280851	-0.506671	-1.215882
6	-1.330252	-0.861993	0.974562
6	-3.530317	-0.286882	-0.639872
1	-2.157994	-0.432597	-2.293805
6	-2.577020	-0.638441	1.548885
1	-0.474701	-1.066847	1.614885
6	-3.678205	-0.351800	0.741628
1	-4.379581	-0.041054	-1.268504
1	-2.687573	-0.678589	2.627729
1	-4.646705	-0.164161	1.193608

Structure No: ***TS5 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	0.101777	1.708283	-1.433272
6	0.355352	0.289690	-0.895374
6	-0.931682	1.619273	0.609177
1	1.017611	2.208918	-1.747392
1	-0.640993	1.705157	-2.231843
1	0.029135	-0.465360	-1.614646
8	-0.438888	2.437540	-0.323249
16	-2.068304	-0.887280	-0.021255
8	-3.267586	-0.725536	0.778458
8	-1.647045	-1.998350	-0.865341
7	-0.563706	0.247820	0.275775
8	-1.547434	1.930458	1.575912
8	-2.444039	0.242583	-1.234162
1	-3.385487	0.446347	-1.135423
8	-1.084515	-1.572142	1.496047
1	-0.335016	-0.499704	1.127004
1	-0.823454	-2.484052	1.308137
6	1.766638	0.002218	-0.438440
6	2.311778	-1.264025	-0.655694
6	2.512417	0.968845	0.243255
6	3.596514	-1.560880	-0.203350
1	1.726711	-2.017094	-1.178335
6	3.794211	0.670793	0.696320
1	2.093060	1.956913	0.423756
6	4.338012	-0.594221	0.471955
1	4.016741	-2.545927	-0.379104
1	4.368000	1.425055	1.224945
1	5.338459	-0.824788	0.823792

Structure No: ***PC5 (9f+14) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.174365	2.052064	-0.936788
6	1.057776	0.554249	-0.599895
6	-0.693955	1.748379	0.292789
1	1.953784	2.531715	-0.336251
1	1.331499	2.252176	-1.995786
1	0.608586	0.009323	-1.441219
8	-0.098608	2.598415	-0.554233
16	-3.018254	-0.915701	-0.152190
8	-4.052538	-1.882973	-0.392920
8	-2.116313	-0.462204	-1.183892
7	0.088265	0.654779	0.486016
8	-1.781792	1.993953	0.800474
8	-3.647427	0.293253	0.606236
1	-2.936656	1.025398	0.732189
8	-2.006540	-1.522302	0.973600
1	-0.357652	-0.179497	0.853589
1	-2.516333	-2.004376	1.644624
6	2.367855	-0.085710	-0.214807
6	3.033727	-0.894402	-1.136134
6	2.945459	0.150418	1.035972
6	4.268600	-1.457150	-0.817991
1	2.579627	-1.091276	-2.104246
6	4.175986	-0.416201	1.356378
1	2.419778	0.768372	1.759230
6	4.841024	-1.219178	0.429392
1	4.777146	-2.087161	-1.540791
1	4.615989	-0.234602	2.331995
1	5.799170	-1.662254	0.681982

Structure No: ***RC6 (7f+CSI) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	-1.620993	1.963123	-1.090884
6	-1.966637	1.128917	0.075091
6	1.497227	1.116206	0.226556
1	-1.042956	2.873962	-0.944971
1	-1.618458	1.471838	1.050020
8	-0.921954	0.755165	-0.815713
16	3.166980	-0.815755	0.278629
8	3.093381	-2.098942	-0.352960
8	3.249576	-0.646451	1.706445
17	4.776242	0.165637	-0.531294
1	-2.268282	1.926543	-1.964518
6	-3.181237	0.266130	0.083645
6	-3.406850	-0.654132	-0.942328
6	-4.110579	0.389575	1.118089
6	-4.560017	-1.435039	-0.936341
1	-2.663936	-0.764583	-1.726975

6	-5.265673	-0.389282	1.120039
1	-3.929778	1.096544	1.924148
6	-5.492796	-1.302708	0.091943
1	-4.727059	-2.154713	-1.731663
1	-5.984729	-0.286980	1.926693
1	-6.389424	-1.914287	0.095662
8	1.075562	2.091751	0.678761
7	1.918519	0.097002	-0.323083

Structure No: ***TS6 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.045920	2.092945	0.117007
6	1.763376	1.101620	-0.726534
6	-0.888221	0.679200	0.094663
1	0.439793	2.775323	-0.479322
1	1.256343	0.843205	-1.656176
8	0.252416	1.153043	0.828300
16	-2.845938	-0.864243	0.274267
8	-3.582333	-1.500762	1.340604
8	-2.461383	-1.629104	-0.896363
17	-4.140614	0.634275	-0.444510
1	1.665494	2.623674	0.838659
6	2.888176	0.355554	-0.349992
6	3.564667	0.568255	0.881971
6	3.349882	-0.649188	-1.242203
6	4.674025	-0.190883	1.192022
1	3.190987	1.304737	1.584782
6	4.470162	-1.395759	-0.926988
1	2.809374	-0.820333	-2.168941
6	5.125155	-1.163775	0.287013
1	5.190938	-0.045871	2.133751
1	4.830439	-2.160958	-1.604891
1	5.998813	-1.756897	0.540624
8	-0.969444	1.001465	-1.079483
7	-1.618518	-0.043230	0.924813

Structure No: 16 (M06-2X/6-31+G(d,p))

	X	Y	Z
6	-1.104860	2.425217	-0.367748
6	-1.191637	1.304232	0.680614
6	0.665180	1.061799	-0.574577
1	-0.804399	3.384880	0.060397
1	-1.310422	1.698872	1.691952
8	-0.048302	1.966754	-1.227710
16	2.463768	-0.695221	-0.368665
8	3.633030	-1.019323	-1.137511
8	1.490162	-1.707893	-0.018969
17	3.161502	0.086304	1.427485
1	-2.007717	2.529602	-0.968148
6	-2.222702	0.239732	0.380464
6	-1.855055	-1.077295	0.106934

6	-3.573124	0.601833	0.394585
6	-2.844820	-2.023402	-0.164987
1	-0.808838	-1.369799	0.116214
6	-4.554081	-0.345943	0.123883
1	-3.862798	1.625885	0.624137
6	-4.188821	-1.662903	-0.159243
1	-2.556089	-3.047209	-0.379658
1	-5.600815	-0.059458	0.136709
1	-4.952888	-2.404529	-0.369071
8	0.140190	0.756593	0.606514
7	1.748145	0.598492	-1.082755

Structure No: ***RC7 (16+H_2O) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.191579	1.145638	-0.308652
6	1.060149	2.070167	0.921935
6	-0.686803	0.664031	0.852614
1	1.182411	1.726329	-1.234052
8	-0.046499	0.412524	-0.272422
8	-0.066629	1.524565	1.630141
7	-1.815029	0.152293	1.216518
16	-2.431518	-1.063090	0.324514
8	-1.436450	-2.053186	-0.021527
8	-3.697101	-1.435166	0.893956
17	-2.926233	-0.102576	-1.496486
8	-1.309446	2.822996	-0.746311
1	-1.997156	3.391822	-0.384123
1	-1.775371	2.162670	-1.277911
1	1.925269	2.024172	1.583251
1	0.815699	3.095526	0.645453
6	2.359996	0.191142	-0.262835
6	2.183322	-1.174512	-0.042156
6	3.646385	0.711257	-0.431998
6	3.298806	-2.011095	0.020868
1	1.183183	-1.586603	0.060368
6	4.754460	-0.126872	-0.365729
1	3.783841	1.774223	-0.621878
6	4.581102	-1.492361	-0.136053
1	3.158003	-3.073873	0.189584
1	5.750445	0.283220	-0.498970
1	5.444165	-2.148530	-0.087958

Structure No: ***TS7 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.142330	1.436558	-0.108117
6	0.549296	1.822607	1.246928
6	-1.127517	1.415452	-0.217610
1	1.441165	2.326826	-0.675330
8	-0.019984	0.864582	-0.747575
8	-0.812075	2.129489	0.906345
7	-2.311765	0.652458	-0.239680

16	-2.280046	-0.815990	0.394738
8	-1.253107	-0.878046	1.422695
8	-3.623678	-1.276614	0.632105
17	-1.551543	-2.048674	-1.128448
8	-1.757853	2.442311	-1.236418
1	-1.973234	3.264306	-0.762476
1	-2.591973	1.654151	-1.150693
1	0.554493	0.978264	1.942740
1	1.004086	2.706976	1.692230
6	2.256191	0.431508	-0.063223
6	2.003047	-0.870113	0.381707
6	3.545365	0.801958	-0.443146
6	3.044294	-1.791006	0.440273
1	0.993522	-1.157853	0.667048
6	4.588379	-0.120607	-0.371965
1	3.735215	1.810578	-0.802374
6	4.336622	-1.417748	0.067384
1	2.845891	-2.803702	0.776314
1	5.590554	0.171652	-0.668620
1	5.145126	-2.140527	0.116130

Structure No: ***17 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.067852	1.418514	-0.070462
6	0.437125	1.735436	1.288023
6	-1.180452	1.542099	-0.323577
1	1.374399	2.341600	-0.579227
8	-0.062184	0.866210	-0.764030
8	-0.911991	2.058938	0.940303
7	-2.335820	0.648335	-0.285724
16	-2.254807	-0.852508	0.362376
8	-1.311880	-0.821820	1.452726
8	-3.603752	-1.336619	0.493659
17	-1.397304	-2.033526	-1.101519
8	-1.524875	2.565063	-1.193024
1	-1.818580	3.313980	-0.657023
1	-2.953546	0.722399	-1.089292
1	0.439954	0.862344	1.946310
1	0.887238	2.596929	1.782798
6	2.201514	0.434080	-0.038741
6	1.983507	-0.873508	0.406979
6	3.480747	0.827732	-0.428849
6	3.041816	-1.775061	0.455535
1	0.984647	-1.179495	0.707431
6	4.542857	-0.074028	-0.370082
1	3.647060	1.840912	-0.786338
6	4.322947	-1.376510	0.070060
1	2.867803	-2.790825	0.796356
1	5.536132	0.239508	-0.675093
1	5.146696	-2.082330	0.111576

Structure No: ***RC8 (17+H_2O) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.304566	1.220124	0.112038
6	0.430818	1.035137	1.355965
6	-0.863980	1.365418	-0.511113
1	1.609155	2.270103	0.006957
8	0.364476	0.900027	-0.920018
8	-0.866780	1.420301	0.886000
7	-1.893367	0.475582	-1.035306
16	-2.245578	-0.960326	-0.350529
8	-3.120013	-1.664180	-1.251733
8	-1.031582	-1.520514	0.186543
17	-3.422218	-0.494405	1.289298
8	-1.137897	2.620989	-1.032448
1	-1.491445	3.159980	-0.312409
1	0.404094	-0.012089	1.671357
1	0.709365	1.685201	2.186126
6	2.499733	0.313829	0.037384
6	2.323920	-1.060809	-0.147013
6	3.783530	0.835632	0.189442
6	3.432459	-1.901319	-0.179771
1	1.320015	-1.457507	-0.272974
6	4.892276	-0.009815	0.166174
1	3.919746	1.906608	0.319256
6	4.717100	-1.378512	-0.020896
1	3.294078	-2.967349	-0.330410
1	5.889193	0.402766	0.284447
1	5.579132	-2.037712	-0.046375
1	-2.660972	0.919923	-1.528434

Structure No: ***TS8 (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.674487	1.465716	0.374970
6	0.573169	1.371293	1.444451
6	-0.305607	2.146621	-0.429245
1	2.339963	2.315146	0.550374
8	0.887905	1.845753	-0.817053
8	-0.510224	2.131762	0.847923
7	-1.516355	0.244095	-0.867694
16	-2.002300	-0.854464	0.149548
8	-1.483788	-2.189852	-0.121893
8	-1.916488	-0.337781	1.510213
17	-4.084852	-1.059589	-0.179686
8	-1.105760	2.751208	-1.244338
1	-1.980087	2.317973	-1.131406
1	0.197447	0.361210	1.616713
1	0.834647	1.858040	2.381883
6	2.465370	0.218713	0.122442

6	1.826745	-1.004153	-0.109029
6	3.859458	0.287863	0.124700
6	2.586620	-2.146764	-0.335969
1	0.743010	-1.079231	-0.127006
6	4.617763	-0.860009	-0.094477
1	4.354176	1.240328	0.297833
6	3.980195	-2.076759	-0.325980
1	2.082938	-3.090888	-0.515299
1	5.701207	-0.802065	-0.087627
1	4.568286	-2.972544	-0.499346
1	-1.390187	-0.196036	-1.780355

Structure No: ***PC8 (8f+18) (M06-2X/6-31+G(d,p))***

	X	Y	Z
6	1.635477	1.405601	0.272449
6	0.531303	1.122422	1.299755
6	-0.404986	1.887831	-0.601689
1	2.144214	2.350766	0.493291
8	0.860841	1.609937	-0.928065
8	-0.605421	1.773770	0.721775
7	-3.279486	0.198271	-1.178984
16	-2.539281	-0.942753	-0.311282
8	-3.231078	-2.192532	-0.482817
8	-1.114362	-0.798003	-0.514351
17	-2.846851	-0.434113	1.685085
8	-1.262623	2.208272	-1.382034
1	-2.787600	1.099460	-1.219681
1	0.314813	0.053035	1.382922
1	0.725128	1.558105	2.279153
6	2.639136	0.303613	0.091018
6	2.235099	-0.945930	-0.389600
6	3.975459	0.520044	0.424489
6	3.169870	-1.966226	-0.533389
1	1.194834	-1.112299	-0.656986
6	4.908564	-0.507308	0.289530
1	4.291291	1.495731	0.785532
6	4.506003	-1.750245	-0.191728
1	2.854507	-2.932612	-0.913524
1	5.947221	-0.332003	0.551008
1	5.231757	-2.549330	-0.305196
1	-4.289209	0.214851	-1.090636

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