Electronic Supplementary Information (ESI)

Electronic effects in tautomeric equilibria: The case of chiral imines from D-glucamine and 2-hydroxyacetophenones

Esther Matamoros, [a]* Pedro Cintas,[a] Mark E. Light,[b] and Juan C. Palacios[a]*

[a]Departamento de Química Orgánica e Inorgánica, Facultad de Ciencias, and IACYS-Unidad de Química Verde y Desarrollo Sostenible, Universidad de Extremadura, E-06006 Badajoz, Spain

[b]Department of Chemistry, Faculty of Natural and Environmental Sciences, The University of Southampton, Southampton SO17 1BJ, U.K.

E-mail: esthermc@unex.es; palacios@unex.es

ORCID
Esther Matamoros: 0000-0003-4460-2065
Pedro Cintas: 0000-0002-2608-3604
Mark E. Light: 0000-0002-0585-0843
Juan Carlos Palacios: 0000-0002-5004-4744

Summary

Experimental methods

General. Melting points have been determined in an Electrothermal IA 9000 Series apparatus and are uncorrected. Quantitative elemental analyses were performed on a Leco® CHNS-932 analyzer. Optical rotations were measured on a Perkin-Elmer 241 polarimeter, with sodium light (D line, λ = 589 nm) and mercury light (λ = 578, 546, 463 nm). Thin layer chromatography was used with qualitative analytical character, using chromatograms (7 x 3 cm) made of Polygram Silica G/UV254 supplied by Aldrich®. UV light of wavelengths 254 and 360 nm, and iodine vapors were used as developers. Infrared absorption spectra were performed on a Perkin-Elmer 399 spectrophotometer and a Fourier-transform Thermo IR-300 in the range of 4000-600 cm^{-1}. The spectra of solid products were recorded using dry potassium bromide pellets (Merck® for spectroscopy). Nuclear magnetic resonance spectra were recorded on Bruker Avance 400 and 500 spectrometers (400 MHz and 500 MHz for ^{1}H, and 100 MHz and 125 MHz for ^{13}C nuclei, respectively). Chloroform-d_1, DMSO-d_6 and benzene-d_6 were used as solvents. Chemical shifts (δ, ppm) refer to tetramethylsilane (Me_4Si, TMS) as internal reference (δ = 0.0 ppm). The coupling constants (*J*) are given in Hz and correspond to the values of the apparent coupling constants, measured directly on the recorded spectrum. Structural elucidation was facilitated through a) DEPT (Distortionless Enhancement by Polarization Transfer), b) 2D correlation spectroscopy (COSY), c) heteronuclear multiple-quantum correlation (HMQC), d) heteronuclear multiple bond correlation (HMBC), e) isotope exchange with deuterium oxide, f) nuclear Overhauser effect (NOE) and g) variable-temperature NMR experiments. High-resolution mass spectra (HRMS) were carried out using ESI ionization techniques with a 6520 Accurate-Mass Q-TOF LC/MS equipment from Agilent Technologies at the *Servicio de Apoyo a la Investigación* (SAIUEX) in the University of Extremadura.

1-Deoxy-1-(2-hydroxy-α-methylbenzylidene)amino-D-glucitol (8). Following the general procedure and from 2-hydroxyacetophenone, the title compound was obtained. Yield: 58%; m.p. 156-159 ºC; $[\alpha]_D^{19}$ -22.1°; $[\alpha]_{578}^{19}$ -23.3°; $[\alpha]_{546}^{19}$ -27.8° (*c* 0.5, pyridine) IR (KBr) $\bar{\nu}_{max}/cm^{-1}$ 3500-3000 (OH), 1617 (C=N), 1540 (arom), 1104, 1084, 1040 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6) δ 16.66 (s, 1H, OH-arom), 7.61 (dd, *J* = 1.2 Hz, *J* = 8.0 Hz, 1H, H-arom), 7.25 (dt, *J* = 1.6 Hz, *J* = 8.4 Hz, 1H, H-arom), 6.71 (m, 2H, H-arom), 4.89 (d, $J_{2,OH}$ = 4.8 Hz, 1H, C2-OH), 4.50 (d, $J_{3,OH}$ = 4.8 Hz, 1H, C3-OH), 4.47 (bs, 1H, OH), 4.42 (d, *J* = 6.4 Hz, 1H, OH), 4.37 (t, $J_{6,OH} \approx J_{6',OH}$ = 5.6 Hz, 1H, C6-OH), 3.86 (m, 1H, H-2), 3.73 (m, 1H, H-1), 3.70 (m, 1H, H-3), 3.59 (m, 2H, H-1', H-6), 3.49 (m, 2H, H-4, H-5), 3.41 (m, 1H, H-6'), 2.36 (s, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.7 (C=N), 164.8 (C-OH), 132.3, 128.7, 118.6, 118.5, 115.9, 115.9 (C-arom), 72.5 (C-2), 71.5, 71.5 (C-4, C-5), 70.0 (C-3), 63.3 (C-6), 51.3 (C-1), 14.4 (CH_3). Anal. Calculated for $C_{14}H_{21}NO_6$: C, 56.18, H, 7.07, N, 4.68. Found: C, 55.89, H, 6.91, N, 4.60.

1-(5-Bromo-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (9). Following the general procedure and from 5-bromo-2-hydroxyacetophenone, the title compound was obtained. Yield: 94%; m.p. 186-188 ºC; $[\alpha]_D^{19}$ -17.7°; $[\alpha]_{578}^{19}$ -15.7°; $[\alpha]_{546}^{19}$ -19.4° (*c* 0.5, pyridine). IR (KBr) $\bar{\nu}_{max}/cm^{-1}$ 3500-3300 (OH), 1617 (C=N), 1603, 1541 (arom), 1087, 1076, 1068 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6) δ 16.98 (s, 1H, OH-arom), 7.72 (d, *J* = 2.0 Hz, 1H, H-arom), 7.35 (dd, *J* = 2.4 Hz, *J* = 9.2 Hz, 1H, H-arom), 6.68 (d, *J* = 8.8 Hz, 1H, H-arom), 4.94 (d, $J_{2,OH}$ = 4.4 Hz, 1H, C2-OH), 4.50 (d, $J_{3,OH}$ = 4.8 Hz, 1H, C3-OH), 4.48 (bs, 1H, OH), 4.45 (d, *J* = 6.4 Hz, 1H, OH), 4.37 (t, $J_{6,OH} \approx J_{6',OH}$ = 5.2 Hz, 1H, C6-OH), 3.84 (m, 1H, H-2), 3.75 (d, *J* = 14.4 Hz, 1H, H-1), 3.69 (t, $J_{3,OH} \approx J_{2,3}$ = 5.2 Hz, 1H, H-3), 3.61 (m, 2H, H-1', H-6), 3.48 (m, 2H, H-4, H-5), 3.40 (m, 1H, H-6'), 2.38 (s, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.5 (C=N) 165.6 (C-OH), 135.1, 130.8,

121.6, 119.4, 105.8 (C-arom), 72.2 (C-2), 71.4, 71.3 (C-4, C-5), 70.1 (C-3), 63.3 (C-6), 50.8 (C-1), 14.5 (CH_3). Anal. Calculated for $C_{14}H_{20}BrNO_6$: C, 44.46, H, 5.33, N, 3.70. Found: C, 44.53, H, 5.06, N, 3.58.

1-Deoxy-1-(2-hydroxy-α-methyl-5-methoxybenzylidene)amino-D-glucitol (10). Following the general procedure and from 2-hydroxy-5-methoxyacetophenone, the title compound was obtained. Yield: 97%; m.p. 179-181 ºC; $[\alpha]_D^{19}$ -16.5°; $[\alpha]_{578}^{19}$ -16.5°; $[\alpha]_{546}^{19}$ -19.6° (*c* 0.5, pyridine) IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 3400-3200 (OH), 1617 (C=N), 1525 (arom), 1084, 1028 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6) δ 15.79 (s, 1H, OH-arom), 7.12 (d, J = 3.2 Hz, 1H, H-arom), 6.92 (dd, J = 2.8 Hz, J = 8.8 Hz, 1H, H-arom), 6.71 (d, J = 8.8 Hz, 1H, H-arom), 4.84 (d, $J_{2,OH}$ = 4.8 Hz, 1H, C2-OH), 4.50 (d, $J_{3,OH}$ = 4.8 Hz, 1H, C3-OH), 4.49 (m, 1H, OH), 4.40 (d, J = 6.4 Hz, 1H, OH), 4.37 (t, $J_{6,OH} \approx J_{6',OH}$ = 5.6 Hz, 1H, C6-OH), 3.86 (m, 1H, H-2), 3.72 (s, 3H, OCH_3), 3.70 (m, *2*H, H-1, H-3), 3.58 (m, 2H, H-1', H-6), 3.49 (m, 2H, H-4, H-5), 3.40 (m, 1H, H-6), 2.34 (s, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ 171.9 (C=N), 157.5 (C-OH), 150.0, 119.3, 118.7, 118.4, 112.3 (C-arom), 72.7 (C-2), 71.7, 71.5 (C-4, C-5), 70.0 (C-3), 63.3 (C-6), 55.6 (OCH_3), 52.0 (C-1), 14.7 (CH_3). Anal. Calculated for $C_{15}H_{23}NO_7$: C, 54.70, H, 7.04, N, 4.25. Found: C, 54.43, H, 6.91, N, 4.12.

1-(5-Chloro-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (11). Following the general procedure and from 5-chloro-2-hydroxyacetophenone, the title compound was obtained. Yield: 90%; m.p. 175-177 ºC; $[\alpha]_D^{19}$ -19.8°; $[\alpha]_{578}^{19}$ -21.0°; $[\alpha]_{546}^{19}$ -26.6° (*c* 0.5, pyridine) IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 3500-3300 (OH), 1608 (C=N), 1544, 1511 (arom), 1086, 1066, 1026 (C-O); ^{1}H NMR (400 MHz, DMSO-d_6) δ 16.93 (s, 1H, OH-arom), 7.63 (s, 1H, H-arom), 7.25 (dd, J = 2.4 Hz, J = 8.8 Hz, 1H, H-arom), 6.74 (d, J = 8.8 Hz, 1H, H-arom), 4.94 (d, $J_{2,OH}$ = 4.4 Hz, 1H, C2-OH), 4.51 (d, $J_{3,OH}$ = 4.4 Hz, 1H, C3-OH), 4.48 (bs, 1H, OH), 4.45 (d, J = 6.0 Hz, 1H, OH), 4.37 (t, $J_{6,OH} \approx J_{6',OH}$ = 4.8 Hz, 1H, C6-OH), 3.85 (m, 1H, H-2), 3.75 (d, J = 16.4 Hz, 1H, H-1), 3.69 (t, $J_{3,OH} \approx J_{2,3}$ = 5.2 Hz 1H, H-3), 3.60 (m, 2H, H-1', H-6), 3.49 (m, 2H, H-4, H-5), 3.40 (m, 1H, H-6'), 2.38 (s, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ 172.5 (C=N), 165.0 (C-OH), 132.4, 127.9, 121.0, 118.8, 118.6 (C-arom), 72.3 (C-2), 71.4, 71.3 (C-4, C-5), 70.1 (C-3), 63.3 (C-6), 50.9 (C-1), 14.5 (CH_3). Anal. Calculated for $C_{14}H_{20}ClNO_6$: C, 50.38, H, 6.04, N, 4.20. Found: C, 50.32, H, 5.82, N, 3.98.

1-Deoxy-1-(2-hydroxy-α-methyl-5-nitrobenzylidene)amino-D-glucitol (12). Following the general procedure and from 2-hydroxy-5-nitroacetophenone, the title compound was obtained. Yield: 40%; m.p. 183-185 ºC; $[\alpha]_D^{19}$ -10.3°; $[\alpha]_{578}^{19}$ -11.1°; $[\alpha]_{546}^{19}$ -12.2° (*c* 0.5, pyridine) IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 3500-3200 (OH), 1616 (C=N), 1559 (NO_2), 1447 (arom), 1317 (NO_2), 1080, 1034 (C-O); ^{1}H NMR (500 MHz, DMSO-d_6) δ 16.61 (s, 1H, OH-arom), 8.55 (d, J = 3.0 Hz, 1H, H-arom), 8.01 (dd, J = 3.0 Hz, J = 9.5 Hz, 1H, H-arom), 6.58 (d, J = 10.0 Hz, 1H, H-arom), 5.22 (d, $J_{2,OH}$ = 5 Hz, 1H, C2-OH), 4.58 (d, $J_{3,OH}$ = 6.5 Hz, 1H, C3-OH), 4.53 (d, J = 5.0 Hz, 1H, OH), 4.49 (d, J = 6.0 Hz, 1H, OH), 4.38 (t, $J_{6,OH} \approx J_{6',OH}$ = 5.5 Hz, 1H, C6-OH), 3.90 (m, 1H, H-1), 3.85 (m, 1H, H-2), 3.75 (m, 1H, H-1'), 3.70 (t, $J_{3,OH} \approx J_{2,3}$ = 5.5 Hz, 1H, H-3), 3.60 (m, 1H, H-6), 3.50 (m, 2H, H-4, H-5), 3.41 (m, 1H, H-6'), 2.61 (s, 3H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6) δ 178.4 (C-OH), 176.1 (C=N), 132.7, 128.6, 128.5, 123.4, 113.6 (C-arom), 71.4 (C-2), 71.2, 70.6 (C-4, C-5), 70.3 (C-3), 63.3 (C-6), 48.7 (C-1), 14.6 (CH_3). Anal. Calculated for $C_{14}H_{20}N_2O_8$: C, 48.84, H, 5.85, N, 8.14. Found: C, 48.63, H, 5.65, N, 8.04.

1-Deoxy-1-(5-fluoro-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (13). Following the general procedure and from 5-fluoro-2-hydroxyacetophenone, the title compound was obtained. Yield: 36%; m.p. 155-157 ºC; $[\alpha]_D^{20}$ -27.6°; $[\alpha]_{578}^{20}$ -27.8°; $[\alpha]_{546}^{20}$ -34.2° (*c* 0.5, pyridine) IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 3500-3100 (OH), 1624 (C=N), 1543 (arom), 1108, 1080, 1054, 1028 (C-O); ^{1}H NMR (500 MHz, DMSO-d_6) δ 16.35 (s, 1H, OH-arom), 7.46 (dd, J = 3.0 Hz, J = 10.5 Hz, 1H, H-arom), 7.13 (dt, J = 3.0 Hz, J = 9.0 Hz, 1H, H-arom), 6.76

(dd, J = 5.0 Hz, J = 9.0 Hz, 1H, H-arom), 4.87 (d, $J_{2,OH}$ = 5.0 Hz, 1H, C2-OH), 4.49 (d, $J_{3,OH}$ = 5.5 Hz, 1H, C3-OH), 4.46 (bs, 1H, OH), 4.41 (d, J = 6.5 Hz, 1H, OH), 4.35 (t, $J_{6,OH} \approx J_{6',OH}$ = 6.0 Hz, 1H, C6-OH), 3.86 (m, 1H, H-2), 3.73 (dd, $J_{1,2}$ = 4.0 Hz, $J_{1,1'}$ = 14.5 Hz, 1H, H-1), 3.69 (dt, $J_{3,4}$ = 1.5 Hz, $J_{3,OH} \approx J_{2,3}$ = 6.5 Hz 1H, H-3), 3.60 (m, 1H, H-1'), 3.58 (m, 1H, H-6), 3.50 (m, 2H, H-4, H-5), 3.41 (m, 1H, H-6'), 2.34 (s, 3H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6) δ 171.8 (C=N), 160.5 (C-OH), 153.1 (d, J = 229.5 Hz, 1C, C-arom), 119.3 (d, J = 23.1 Hz, 1C, C-arom), 119.1 (d, J = 7.1 Hz, 1C, C-arom), 118.3 (d, J = 7.1 Hz, 1C, C-arom), 113.8 (d, J = 23.5 Hz, 1C, C-arom), 72.4 (C-2), 71.5, 71.4 (C-4, C-5), 70.1 (C-3), 63.3 (C-6), 51.7 (C-1), 14.6 (CH_3). Anal. Calculated for $C_{14}H_{20}FNO_6$: C, 52.85, H, 6.35, N, 4.41. Found: C, 52.85, H, 6.24, N, 4.32.

1-(5-Bromo-2-hydroxy-α-methyl-3-nitrobenzylidene)amino-1-deoxy-D-glucitol (14). Following the general procedure and from 5-bromo-2-hydroxy-3-nitroacetophenone, the title compound was obtained. Yield: 58%; m.p. 159-156 ºC; $[\alpha]_D^{19}$ -44.5°; $[\alpha]_{578}^{19}$ -49.1°; $[\alpha]_{546}^{19}$ -64.5° (*c* 0.5, pyridine) IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 3500-3100 (OH), 1627 (C=N), 1518 (NO_2), 1415 (arom), 1251 (NO_2), 1083 (C-O); ^{1}H NMR (500 MHz, DMSO-d_6) δ 16.67 (s, 1H, OH-arom), 8.03 (m, 2H, H-arom), 5.28 (d, $J_{2,OH}$ = 5.0 Hz, 1H, C2-OH), 4.60 (d, $J_{3,OH}$ = 6.5 Hz, 1H, C3-OH), 4.53 (d, J = 5.0 Hz, 1H, OH), 4.48 (d, J = 6.0 Hz, 1H, OH), 4.38 (t, $J_{6,OH} \approx J_{6',OH}$ = 5.5 Hz, 1H, C6-OH), 3.87 (m, 1H, H-1), 3.84 (m, 1H, H-2), 3.74 (m, 1H, H-1'), 3.70 (t, $J_{3,OH} \approx J_{2,3}$ = 6.0 Hz, 1H, H-3), 3.60 (m, 1H, H-6), 3.43 (m, 2H, H-4, H-5), 3.39 (m, 1H, H-6'), 2.59 (s, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ 175.7 (C=N), 165.3 (C-OH), 142.8, 137.6, 132.7, 120.3, 98.4 (C-arom), 71.4 (C-2), 71.0, 70.5 (C-4, C-5), 70.3(C-3), 63.3 (C-6), 48.7 (C-1), 15.2 (CH_3). HRMS-ESI ($C_{14}H_{20}BrN_2O_8$ $[M+H]^+$): Calcd. 423.0405 and 425.0385; Found 423.0399 and 425.0381.

1-Deoxy-1-(4,5-dimethoxy-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (15). Following the general procedure and from 4,5-dimethoxy-2-hydroxyacetophenone, the title compound was obtained. Yield: 28%; m.p. 188-190 ºC; $[\alpha]_D^{20}$ -31.3°; $[\alpha]_{578}^{20}$ -35.9°; $[\alpha]_{546}^{20}$ -40.2° (*c* 0.5, DMSO) IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 3500-3000 (OH), 1614 (C=N), 1540 (arom), 1059, 1033 (C-O); ^{1}H NMR (500 MHz, DMSO-d_6) δ 16.50 (s, 1H, OH-arom), 6.94 (s, 1H, H-arom), 6.19 (s, 1H, H-arom), 4.90 (d, $J_{2,OH}$ = 4.5 Hz, 1H, C2-OH), 4.48 (d, $J_{3,OH}$ = 5.0 Hz, 1H, C3-OH), 4.42 (bs, 1H, OH), 4.41 (d, J = 6.5 Hz, 1H, OH), 4.35 (t, $J_{6,OH} \approx J_{6',OH}$ = 5.5 Hz, 1H, C6-OH), 3.82 (m, 1H, H-2), 3.73 (s, 3H, OCH_3), 3.70 (m, 2H, H-1, H-3), 3.69 (s, 3H, OCH_3), 3.60 (m, 1H, H-6), 3.52 (m, 1H, H-1'), 3.49 (m, 2H, H-4, H-5), 3.41 (m, 1H, H-6'), 2.35 (s, 3H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6) δ 171.1 (C=N), 166.9 (C-OH), 154.9, 139.2, 111.3, 108.8, 102.3 (C-arom), 72.3 (C-2), 71.5, 71.4 (C-4, C-5), 70.1 (C-3), 63.3 (C-6), 56.5, 55.1 (OCH_3), 49.3 (C-1), 14.3 (CH_3). Anal. Calculated for $C_{16}H_{25}NO_8$: C, 53.47, H, 7.01, N, 3.90. Found: C, 53.23, H, 6.71, N, 3.70.

2,3,4,5,6-Penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (28) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (29). Applying the general procedure a white solid (70%) was obtained; recrystallized from ethanol it afforded colorless crystals (42%) with m.p. 120-122 ºC; $[\alpha]_D^{22}$ -9.9°; $[\alpha]_{578}^{22}$ -10.9°; $[\alpha]_{546}^{22}$ -12.6°; $[\alpha]_{436}^{22}$ -25.8° (*c* 0.5, $CHCl_3$); IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 1748 (C=O), 1652 (amide), 1543 (arom), 1086, 1062, 1040, 1020 (C-O); ^{1}H NMR (500 MHz, C_6D_6) δ 7.87 (bs, 1H, H-arom), 7.51 (d,1H, H-arom), 7.06 (dd, 2H, H-arom), 6.60 (d, 1H, H-arom), 6.49 (d, 1H, H-arom), 5.74 (dd, $J_{3,4}$ = 4.5 Hz, $J_{4,5}$ = 7.0 Hz 1H, H-4 (**28**)), 5.72 (ddd, $J_{1,2}$ = 3.5 Hz, $J_{2,3}$ = 6.0 Hz, $J_{1',2}$ = 8.5 Hz, 1H, H-2 (**28**)), 5.58 (dd, $J_{3,4}$ = 5.0 Hz, $J_{2,3}$ = 5.5 Hz 1H, H-3 (**28**)), 5.51 (dd, $J_{1',2'}$ = 2 Hz, $J_{2',3'}$ = 9.0 Hz, 1H, H-2' (**29**)), 5.44 (bs, 1H, H-1 (**29**)), 5.36 (dt, $J_{5,6}$ = 3.5 Hz, $J_{5,4}$ = $J_{5,6'}$ = 8.0 Hz, 1H, H-5 (**28**)), 5.30 (ddd, $J_{3',4'}$ = 2.0 Hz, $J_{3',4''}$ = 4.0 Hz, $J_{3',2'}$ = 9.0 Hz, 1H, H-3' (**29**)), 5.09 (s, 1H, CH_2 (**28**)), 4.93 (s, 1H, CH_2 (**28**)), 4.41 (dd, $J_{5,6}$ = 3.5 Hz, $J_{6,6'}$ = 12.0 Hz, 1H, H-6 (**28**)), 4.29 (dd, $J_{3',4'}$ = 2.5 Hz, $J_{4',4''}$ = 13.0 Hz, 1H, H-4' (**29**)), 4.22 (dd, $J_{3',4''}$ = 4.0 Hz, $J_{4',4''}$ = 12.5 Hz, 1H, H-4'' (**29**)), 4.17 (dt, J = 6.0

Hz, *J* = 9.5 Hz, 1H, H-5 (**29**)), 4.13 (dd, $J_{5,6'}$ = 8.0 Hz, $J_{6,6'}$ = 12.5 Hz, 1H, H-6' (**28**)), 3.86 (dd, $J_{1,2}$ = 2.0 Hz, $J_{1,1'}$ = 14.5 Hz, 1H, H-1 (**28**)), 3.45 (dd, $J_{1',2}$ = 8.0 Hz, $J_{1,1'}$ = 14.0 Hz, 1H, H-1' (**28**)), 3.28 (bs, 1H, H-4a (**29**)), 3.15 (bs, 1H, H-4b (**29**)), 1.96, 1.95, 1.87,1.86,1.80, 1.78, 1.77, 1.74, 1.73, 1.65, 1.49 (s, 39H, CH_3); ^{13}C NMR (125 MHz, C_6D_6) δ 170.0, 169.7, 169.7, 169.6, 169.6, 169.4, 169.4, 169.3, 169.2, 168.0, 167.7, 165.8 (C=O), 148.0, 147.4, 143.7, 135.4, 133.0, 132.9, 132.0, 131.6, 130.8, 126.3, 125.5, 119.2, 118.3 (C-arom, C-2 (**29**), $C=CH_2$ (**28**)), 117.0 (CH_2 (**28**), 74.6 (C-5 (**29**)), 70.0 (C-2 (**28**)), 69.6 (C-3 (**28**)), 69.2, 69.0, 69.0 (C-4 (**28**)), C-2' (**29**), C-5 (**28**)), 68.8 (C-1' (**29**)), 68.3 (C-3' (**29**)), 61.6 (C-6 (**28**)), 61.4 (C-4' (**29**)), 48.2 (C-4 (**29**)), 45.6 (C-1 (**28**)), 23.8, 22.9, 21.9, 20.8, 20.3, 20.2, 20.1, 20.0, 20.0, 19.9, 19.9, 18.2 (CH_3).

^1H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, *J* = 2.0 Hz, 1H, H-arom), 7.53 (dd, *J* = 2.0 Hz, *J* = 8.5 Hz, 1H, H-arom), 7.45 (d, *J* = 2.0 Hz, 1H, H-arom), 7.44 (bs, 1H, H-arom), 6.99 (d, *J* = 9.0 Hz, 1H, H-arom), 6.94 (d, *J* = 8.0 Hz, 1H, H-arom), 5.52 (s, 1H, CH_2 (**28**)), 5.42 (dd, $J_{3,4}$ = 4.5 Hz, $J_{4,5}$ = 6.5 Hz 1H, H-4 (**28**)), 5.39 (m, 1H, H-2' (**29**)), 5.38 (s, 1H, CH_2 (**28**)), 5,37 (m, 2H, H-1' (**29**),H-2 (**28**)), 5.27 (dd, $J_{3,4}$ = 5.0 Hz, $J_{2,3}$ = 5.5 Hz 1H, H-3 (**28**)), 5.09 (bs, 1H, H-3' (**29**)), 5.06 (dt, $J_{5,6}$ = 3.5 Hz, $J_{5,4}$ = $J_{5,6'}$ = 6.5 Hz, 1H, H-5 (**28**)), 4.43 (bs, 1H, H-5 (**29**)), 4.26 (dd, $J_{5,6}$ = 3.5 Hz, $J_{6,6'}$ = 12.5 Hz, 2H, H-6 (**28**), H-4' (**29**)) 4.20 (dd, $J_{3',4''}$ = 4.5 Hz, $J_{4',4''}$ = 12.5 Hz, 1H, H-4'' (**29**)), 4.13 (dd, $J_{5,6'}$ = 6.0 Hz, $J_{6,6'}$ = 12.5 Hz, 1H, H-6' (**28**)), 3.87 (bs, 1H, H-4a (**29**)), 3.49 (m, 2H, H-1 (**28**), H-4b (**29**)), 3.40 (dd, $J_{1',2}$ = 8.0 Hz, $J_{1,1'}$ = 14.0 Hz, 1H, H-1' (**28**)), 2.33, 2.26, 2.20, 2.15, 2.12, 2.10, 2.09, 2.08, 2.08, 2.07, 2.05, 2.04, 1.96 (s, 39H, CH_3); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.9, 170.5, 170.2, 169.9, 169.8, 169.8, 168.8, 168.6 (C=O), 147.7, 147.4, 143.1, 133.3, 132.6,131.6, 130.4, 128.3, 125.4, 122.4, 119.6 (C-arom, C-2 (**29**), $C=CH_2$ (**28**)), 117.8 (CH_2 (**28**)), 74.5 (C-5 (**29**)), 69.8, 69.4, 69.2, 68.8, 68.8, 68.2 (C-2 (**28**), C-3 (**28**), C-4 (**28**), C-5 (**29**), C-1' (**29**), C-2' (**29**), C-3' (**29**)), 61.6, 61.5 (C-6 (**28**), C-4' (**28**)), 48.6 (C-4 (**29**)), 45.5 (C-1 (**28**)), 22.3, 21.4, 20.9, 20.8, 20.8, 20.7, 20.6, 20.5 (CH_3).

^1H NMR (500 MHz, DMSO-d_6) δ 7.67 (d, *J* = 2.0 Hz, *J* = 8.5 Hz, 1H, H-arom), 7.54 (m, 3H, H-arom), 7.19 (d, *J* = 9.0 Hz, 1H, H-arom), 7.05 (d, *J* = 8.0 Hz, 1H, H-arom), 5.56 (s, 1H, CH_2 (**28**)), 5.27 (s, 1H, CH_2 (**28**)), 5,26 (m, 3H, H-1' (**29**), H-2' (**29**), H-4 (**28**)), 5,22 (m, 1H, H-2 (**28**)), 5.17 (dd, $J_{3,4}$ = 4.0 Hz, $J_{2,3}$ = 6.0 Hz 1H, H-3 (**28**)), 5.01 (m, 1H, H-3' (**29**)), 4.96 (dt, $J_{5,6}$ = 3.0 Hz, $J_{5,4}$ = $J_{5,6'}$ = 6.5 Hz, 1H, H-5 (**28**)), 4.49 (m, 1H, H-5 (**29**)), 4.22 (dd, $J_{5,6}$ = 3.0 Hz, $J_{6,6'}$ = 12.5 Hz, 1H, H-6 (**28**)), 4.18 (dd, $J_{3',4'}$ = 3.0 Hz, $J_{4',4''}$ = 12.0 Hz, 1H, H-4' (**29**)) 4.10 (dd, $J_{3',4''}$ = 5.5 Hz, $J_{4',4''}$ = 12.5 Hz, 1H, H-4'' (**29**)), 4.01 (dd, $J_{5,6'}$ = 6.5 Hz, $J_{6,6'}$ = 12.5 Hz, 1H, H-6' (**28**)), 3.82 (dd, $J_{4a,5}$ = 6.5 Hz, $J_{4a,4b}$ = 9.5 Hz, 1H, H-4a (**29**)), 3.51 (m, 1H, H-4b (**29**)), 3.51 (m, 1H, H-4b (**29**)), 3.39 (m, 1H, H-1 (**28**)), 3.13 (m, 1H, H-1' (**28**)), 2.29, 2.17, 2.08, 2.05, 2.04, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.84 (s, 39H, CH_3); ^{13}C NMR (125 MHz, DMSO-d_6) δ 170.6, 170.5, 170.5, 170.1, 169.9, 169.9, 169.8, 169.2, 168.8, 168.8 (C=O), 147.6, 142.9, 135.5, 133.5, 133.0, 132.4, 131.8, 130.9, 127.0, 126.7, 119.1 (C-arom, C-2 (**28**), $C=CH_2$ (**28**)), 118.3 (CH_2 (**28**)), 74.8 (C-5 (**28**)), 69.9, 69.6, 69.3, 68.8, 68.7, 68.5 (C-2 (**28**), C-3 (**28**), C-4 (**28**), C-5 (**28**), C-1' (**29**), C-2' (**29**), C-3' (**29**)), 61.9, 61.8 (C-6 (**28**), C-4' (**28**)), 48.3 (C-4 (**29**)), 45.3 (C-1 (**28**)), 23.1, 23.0, 22.5, 21.6, 21.1, 21.0, 21.0, 20.8(CH_3). HRMS-ESI of **28** ($C_{28}H_{34}BrNO_{13}$ $[M+H]^+$): calculated 672.1292 and 674.1271; found 672.1306 and 674.1295. HRMS-ESI of **29** ($C_{26}H_{33}BrNO_{12}$ $[M+H]^+$): calculated 630.1136 and 632.1166; found 630.1185 and 632.1171.

2,3,4,5,6-Penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-chlorophenyl)vinyl]amino-D-glucitol (30) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-chlorophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (31). Applying the general procedure an oil was obtained. Yield: 38%; m.p. 80-82 ºC; IR (KBr) $\bar{\nu}_{max}$/cm^{-1} 1746 (C=O), 1665 (amide), 1078, 1042 (C-O); ^1H NMR (500 MHz, C_6D_6) δ 7.42 (bs, 1H, H-arom), 7.18 (m,1H, H-arom), 7.00 (dd, 1H, H-arom), 6.67(m, 1H, H-arom), 6.59 (m, 2H, H-arom), 5.76 (dd, $J_{3,4}$ = 5.0 Hz, $J_{4,5}$ = 6.5 Hz, 1H, H-4 (**30**)), 5.73 (m, 1H, H-2 (**30**)), 5.60(t, $J_{3,4}$ = $J_{2,3}$ = 5.5 Hz 1H, H-3 (**30**)),

5.50 (dd, $J_{1',2'}$ = 2.0 Hz, $J_{2',3'}$ = 9.0 Hz, 1H, H-2' (**31**)), 5.41 (bs, 1H, H-1' (**31**)), 5.36 (dt, $J_{5,6}$ = 3.5 Hz, $J_{5,4}$ = $J_{5,6'}$ = 6 Hz, 1H, H-5 (**30**)), 5.29 (m, 1H, H-3' (**31**)), 5.13 (s, 1H, CH_2 (**30**)), 5.01 (s, 1H, CH_2 (**30**)), 4.42 (dd, $J_{5,6}$ = 3.5 Hz, $J_{6,6'}$ = 12.5 Hz, 1H, H-6 (**30**)), 4.29 (dd, $J_{3',4'}$ = 2.5 Hz, $J_{4',4''}$ = 13.0 Hz, 1H, H-4' (**31**)), 4.23 (dd, $J_{3',4''}$ = 4.5 Hz, $J_{4',4''}$ = 12.5 Hz, 1H, H-4'' (**31**)), 4.12 (m, 1H, H-5 (**31**)), 4.10 (m, 1H, H-6' (**30**)), 3.87 (dd, $J_{1,2}$ = 2.5 Hz, $J_{1,1'}$ = 14.5 Hz, 1H, H-1 (**30**)), 3.49 (dd, $J_{1',2}$ = 8.5 Hz, $J_{1,1'}$ =14.0 Hz, 1H, H-1' (**30**)), 3.35 (bs, 1H, H-4a (**31**)), 3.15 (bs, 1H, H-4b (**31**)), 1.98, 1.97, 1.96, 1.86, 1.85, 1.80, 1.79, 1.77, 1.76, 1.74, 1.65, 1.52 (s, 39H, CH_3); ^{13}C NMR (125 MHz, C_6D_6) δ 169.7, 169.7, 169.6, 169.5, 169.5, 169.5, 169.3, 169.3, 169.2, 168.1, 165.9 (C=O), 160.6, 158.7, 144.8, 144.3, 116.7, 116.5 (C-arom, C-2 (**31**), C=CH_2 (**30**)), 115.5 (CH_2 (**30**), 74.7 (C-5 (**31**)), 70.0 (C-2 (**30**)), 70.0 (C-3 (**30**)), 69.6, 69.1, 69.0 (C-4 (**30**), C-2' (**31**), C-5 (**30**)), 68.8 (C-1' (**31**)), 68.3 (C-3' (**31**)), 61,5 (C-6 (**30**)), 61.3 (C-4' (**31**)), 48.3 (C-4 (**31**)), 45.6 (C-1 (**30**)), 23.7, 21.8, 20.3, 20.2, 20.2, 20.1, 20.0, 19.9, 19.9, 19.8, 19.5 (CH_3).

(2*S*, 3*E*, 5*S*)-3-Acetyl-2-(2-acetoxy-5-methoxyphenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (33). Applying the general procedure an oil was obtained. Yield: 32%; ^{1}H NMR (500 MHz, C_6D_6) δ 7.26 (bs, 1H, H-arom), 6.83 (d, 1H, H-arom), 6.48 (d, 2H, H-arom), 5.53 (d, $J_{2',3'}$ = 9.0 Hz, 1H, H-2'), 5.49 (bs, 1H, H-1'), 5.31 (m, 1H, H-3'), 4.30 (dd, $J_{3',4'}$ = 2.5 Hz, $J_{4',4''}$ = 12.5 Hz, 1H, H-4'), 4.25 (m, 2H, H-4'', H-5), 3.41 (m, 1H, H-4a), 3.26 (m, 4H, H-4b, OCH_3), 2.09, 1.87, 1.73, 1.67, 1.60 (s, 21H, CH_3); ^{13}C NMR (125 MHz, C_6D_6) δ 167.7, 169.7, 169.6, 169.5, 169.3, 168.7 (C=O), 156.8, 142.5, 114.9, 113.3 (C-arom, C-2), 74.1 (C-5), 69.1, 69.0 (C-2', C-1'), 68.3 (C-3'), 61.4 (C-4'), 54.8 (OCH_3), 48.3 (C-4), 23.9, 20.6, 20.0, 20.0, 19.9(CH_3).

Crystallographic Data

Acquisition data. A clear colourless prism-shaped crystal with dimensions 0.25×0.05×0.04 was mounted on a MITIGEN holder in perfluoroether oil. Data were collected using a Rigaku AFC12 FRE-HF diffractometer equipped with an Oxford Cryosystems low-temperature apparatus operating at T = 100(2) K. Data were measured using profile data from ω-scans of 1.0° per frame for 8.0 s using MoKα radiation (Rotating-anode X-ray tube, 45.0 kV, 55.0 mA). The total number of runs and images was based on the strategy calculation from the program CrysAlisPro (Rigaku). The maximum resolution achieved was Θ = 30.872°. Cell parameters were retrieved using the CrysAlisPro (Rigaku) software[1] and refined using CrysAlisPro (Rigaku) on 35897 reflections, 60 % of the observed reflections. Data reduction was performed using the CrysAlisPro (Rigaku) software that corrects for Lorentz polarisation. The final completeness is 99.90 % out to 30.872° in Θ. A multi-scan absorption correction was performed using CrysAlisPro (Rigaku)[1] using spherical harmonics as implemented in SCALE3 ABSPACK. The absorption coefficient μ of this material is 1.462 mm^{-1} at this wavelength (λ = 0.711Å) and the minimum and maximum transmissions are 0.939 and 1.000. The structure was solved in the space group $P2_1$ (# 4) by direct using the ShelXT structure solution program and refined by full matrix least squares on F^2 using version 2016/6 of ShelXL.[2,3] All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. There is a single molecule in the asymmetric unit, which is represented by the reported sum formula. In other words: Z is 2 and Z' is 1.

The Flack parameter was refined to –0.0045(16). Determination of absolute structure using Bayesian statistics on Bijvoet differences using the Olex2 results in None.[4] **Note:** The Flack parameter is used to determine chirality of the crystal studied, the value should be near 0, a value of 1 means that the stereochemistry is wrong and the model should be inverted. A value of 0.5 means that the crystal consists of a racemic mixture of the two enantiomers.

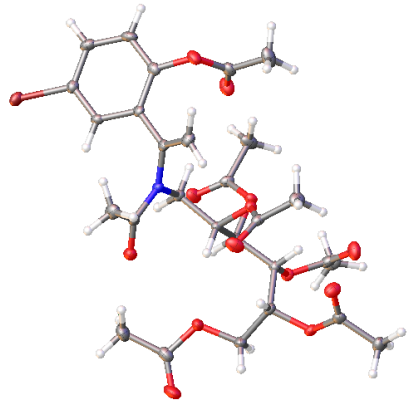
References

1. *CrysAlisPro Software System*, Agilent Technologies UK Ltd, Yarnton, Oxford, UK (2014).

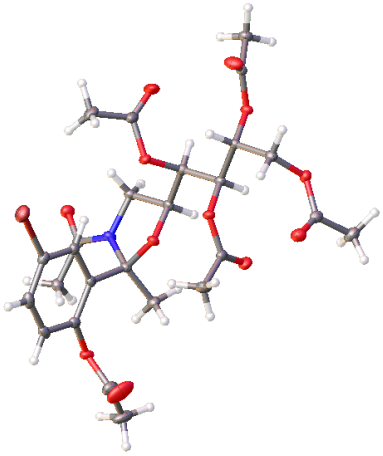
2. G. M. Sheldrick, *Acta Cryst.*, 2015, **C27**, 3-8.

3. G. M. Sheldrick, *Acta Cryst.*, 2015, **A71**, 3-8.

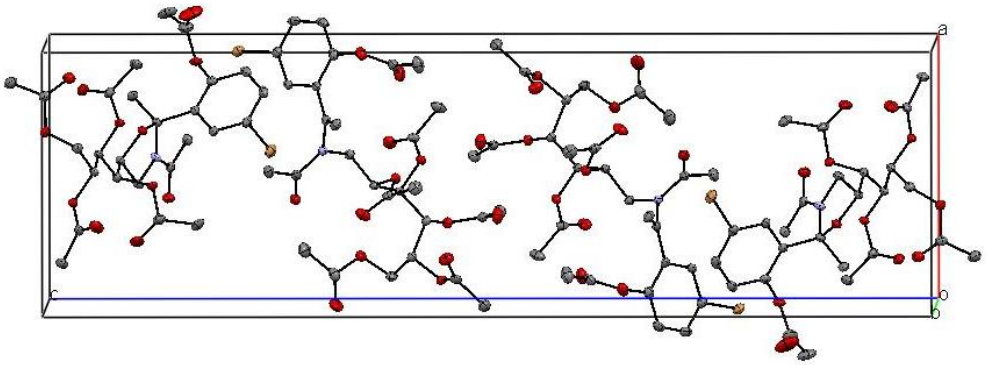
4. O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339-341.



28



29



Representation of the unit cell composed of two molecules of compounds **28** and **29**

Table S1. Summary of crystal parameters

Compounds	**28** and **29**
Formulas	$C_{28}H_{34}BrNO_{13}$ (**28**) and $C_{26}H_{32}BrNO_{12}$ (**29**)
Formula (full unit cell)	$C_{54}H_{66}Br_2N_2O_{25}$
$D_{calc.}$/ g cm^{-3}	1.470
μ/mm^{-1}	1.462
Formula Weight	1302.90
Colour	clear colourless
Shape	prism
Size/mm^3	0.25×0.05×0.04
T/K	100(2)
Crystal System	monoclinic
Flack Parameter	-0.0045(16)
Space Group	$P2_1$
a/Å	10.06056(13)
b/Å	8.66685(10)
c/Å	33.7640(4)
α/°	90
β/°	90.1091(12)
γ/°	90
V/Å^3	2943.99(6)
Z	2
Z'	1
Wavelength/Å	0.71073
Radiation type	MoKα
Θ_{min}/°	2.113
Θ_{max}/°	30.872
Measured Reflections	60113
Independent Reflections	16894
Reflections with I > 2(I)	15295
R_{int}	0.0338
Parameters	762
Restraints	4
Largest Peak	0.292
Deepest Hole	-0.326
GooF	1.025
wR_2 (all data)	0.0662
wR_2	0.0636
R_1 (all data)	0.0379
R_1	0.0310

Calculation of the HOMA index.

Geometrical parameters of the rings and quasi-rings (C-C, C-N, and C-O bond lengths) were used to calculate the aromaticity index HOMA (harmonic oscillator model of aromaticity)[5] as a geometry-based indicator of local aromaticity. According to its definition, HOMA can be expressed by the following equation:

$$HOMA = 1 - \frac{1}{n}\sum_{j=1}^{n} \alpha_i \, (R_{\mathrm{opt,i}} - R_j)^2$$

$$HOMA = 1 - \frac{1}{n}\sum_{j=1}^{n} \alpha \, (R_{opt} - R_j)^2$$

Where R_{opt} and α_i are obtained as follows:

$$R_{opt} = (R_s + 2R_d)/3$$

$$\alpha = 2/[(R_{opt} - R_s)^2 + (R_{opt} - R_d)^2]$$

where n represents the total number of bonds taken into the summation and α_i is a normalization constant fixed to give HOMA = 0 for a model nonaromatic system, e.g., the Kekulé structure of benzene and HOMA = 1 for the system with all bonds equal to the optimal value $R_{opt,i}$ assumed to be realized for fully aromatic systems. The higher the HOMA value, the more "aromatic" is the ring in question and hence the more delocalized are the π-electrons of the system. HOMA may be estimated for the set of bonds forming the ring but also for any part of that ring or other sequence of bonds for which delocalization can be considered. In the case of quasi-rings the HOMA was estimated for the sequence of (H)O-C=C-C=N bonds.

Constants R_s and R_d denote specific bonds and can be obtained from model compounds; herein ethane and ethene (for C-C and C=C bonds), methylamine and methylenimine (for C-N and C=N bonds), and formic acid (for C-O and C=O bonds). Table S1 shows the R_{opt} and α values used for the calculation of the HOMA index.

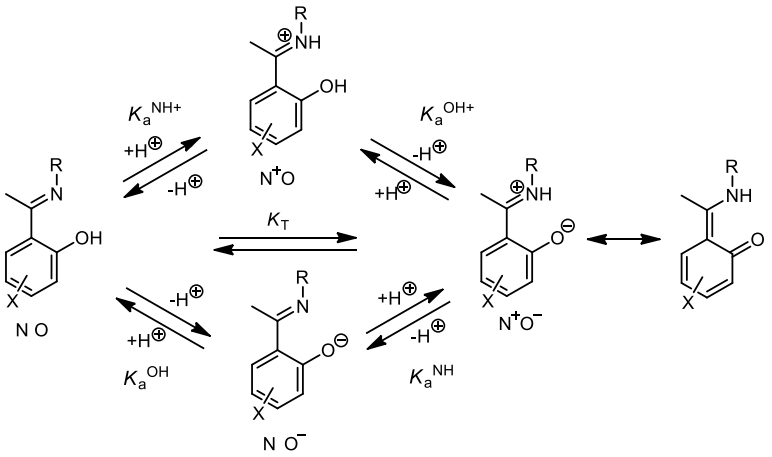
Table S2. R_{opt} and α parameters used for the calculation of HOMA indices

	Gas phase			**DMSO**		
Parameter	-C	-N	-O	-C	-N	-O
R_{opt}	1.395	1.333	1.247	1.395	1.335	1.248
A	86.89	89.10	164.420	88.80	89.29	186.00

5. a) T. M. Krygowski and M. K. Cyrański*, Chem. Rev.,* 2001, **101**, 1385-419; b) J. Kruszewski and T. M. Krygowski, *Tetrahedron Lett.,* 1972, **13**, 3839-3842; c) T. M. Krygowski, *J. Chem. Inf. Comput. Sci.,* 1993, **33**, 70-78; d) T. M. Krygowskiand and M. Cyrański, *Tetrahedron,* 1996, **52**, 1713-1722; e) P. V. R. Schleyer, *Chem. Rev*., 2001, **101**, 1115-1118; f) E. Matito, M. Duran and M. Solà, *J. Chem. Phys*., 2005, **122**, 014109 (1-8).

Deduction of equation [5]

In scheme 4 (main text) the multiple equilibria associated to the phenolimine-ketoenamine tautomerism in 2-hydroxyacetophenones are represented as follows:[6]



Scheme 4 Proton transfer equilibria for phenol-imine and keto-enamine tautomers.

The acid dissociation constants are defined by the following expressions:

$$K_a^{OH} = \frac{[NO^-][H^+]}{[NO]} \quad , \quad K_a^{NH} = \frac{[NO^-][H^+]}{[N^+O^-]} \quad ,$$
$$K_a^{NH+} = \frac{[NO][H^+]}{[N^+O]} \quad , \quad K_a^{OH+} = \frac{[N^+O^-][H^+]}{[N^+O]} \qquad [1S]$$

Then, the tautomeric equilibrium constant K_T can be expressed as:

$$K_T = \frac{[N^+O^-]}{[NO]} = \frac{K_a^{OH}}{K_a^{NH}} = \frac{K_a^{OH+}}{K_a^{NH+}} \qquad [2S]$$

We should consider the electronic effects exerted by the substituents on both the phenolic hydroxyl and the iminic nitrogen. Assuming independent behavior of the phenolic and iminic groups, the effect of substituents on the first group are modeled by the Hammett equation [3S],

$$\log K_a^{OH} = \rho^{OH} \sigma_x^{OH} + a \qquad [3S]$$

Similarly, the effect caused by substituents on the imine group are described by equation [4S],

$$\log K_a^{NH} = \rho^{NH} \sigma_x^{NH} + b \qquad [4S]$$

where $\sigma_x^{OH} = \sigma_{para}^{x}$ if the substituent is in position C-5 and $\sigma_x^{OH} = \sigma_{meta}^{x}$ if it is in position C-4. Analogously, $\sigma_x^{NH} = \sigma_{para}^{x}$ if the substituent is in position C-4 and $\sigma_x^{NH} = \sigma_{meta}^{x}$ when it is in position C-5.

By substituting both equations into the logarithmic form of equation [2S] gives rise to equation [5S], where c = a-b.

$$\log K_T = \log K_a^{OH} - \log K_a^{NH} = \rho^{OH} \sigma_x^{OH} - \rho^{NH} \sigma_x^{NH} + c \qquad [5S]$$

Since the effect of two different substituents (X and Y) on a chemical function attached to an aromatic ring can be represented by the same value of ρ, which make them additive, equation [6S] is obtained:

$$\log K_{xy} = \rho_x\sigma_x+\rho_y\sigma_y = \rho(\sigma_x+\sigma_y) = \rho\Sigma\sigma_{xy} \quad [6S]$$

where $\rho_x = \rho_y = \rho$; $\Sigma\sigma_{xy} = \sigma_x+\sigma_y$. Similarly, in the case of acetophenone imines, one can accept the hypothesis that $\rho^{OH} = \rho^{NH} = \rho$, thereby simplifying equation [5S] to equation [7S]:

$$\log K_T = \rho\,(\sigma_x^{OH} - \sigma_x^{NH}) + c = \rho\,\sigma_{ef} + c \quad [7S]$$

The difference $\sigma_{ef} = \sigma_x^{OH} - \sigma_x^{NH}$, represents the net or effective effect of a given substituent on the delocalized cyclic tautomeric system, whereas c is a constant different from zero, since the tautomeric termini are distinct each other.

The above treatment may be extended to polysubstituted acetophenones. For several substituents X, Y, ... one can write,

$$\log K_T = \rho\,(\sigma_x^{OH} - \sigma_x^{NH}) + \rho\,(\sigma_y^{OH} - \sigma_y^{NH}) + \ldots\ldots + c = \rho\,\Sigma(\sigma_i^{OH} - \sigma_i^{NH}) + c$$

$$\log K_T = \rho\,\sigma_{ef}^{x} + \rho\,\sigma_{ef}^{y} + \ldots\ldots + c = \rho\,\Sigma\sigma_{ef}^{i} + c = \rho\,\sigma_{ef}^{T} + c$$

$$\log K_T = \rho\,\Sigma(\sigma_i^{OH} - \sigma_i^{NH}) + c = \rho\,(\Sigma\sigma_i^{OH} - \Sigma\sigma_i^{NH}) + c$$

and such equations can then be transformed into equation [8S]:

$$\log K_T = \rho\,(\Sigma\sigma_i^{OH} - \Sigma\sigma_i^{NH}) + c = \rho\,\sigma_{ef}^{T} + c \quad [8S]$$

where now $\sigma_{ef}^{T} = \Sigma\sigma_{ef}^{i} = \Sigma\sigma_i^{OH} - \Sigma\sigma_i^{NH}$ and c is a constant.

6. R. F. Martínez, *PhD Dissertation*, Universidad de Extremadura, Badajoz, Spain, 2010.

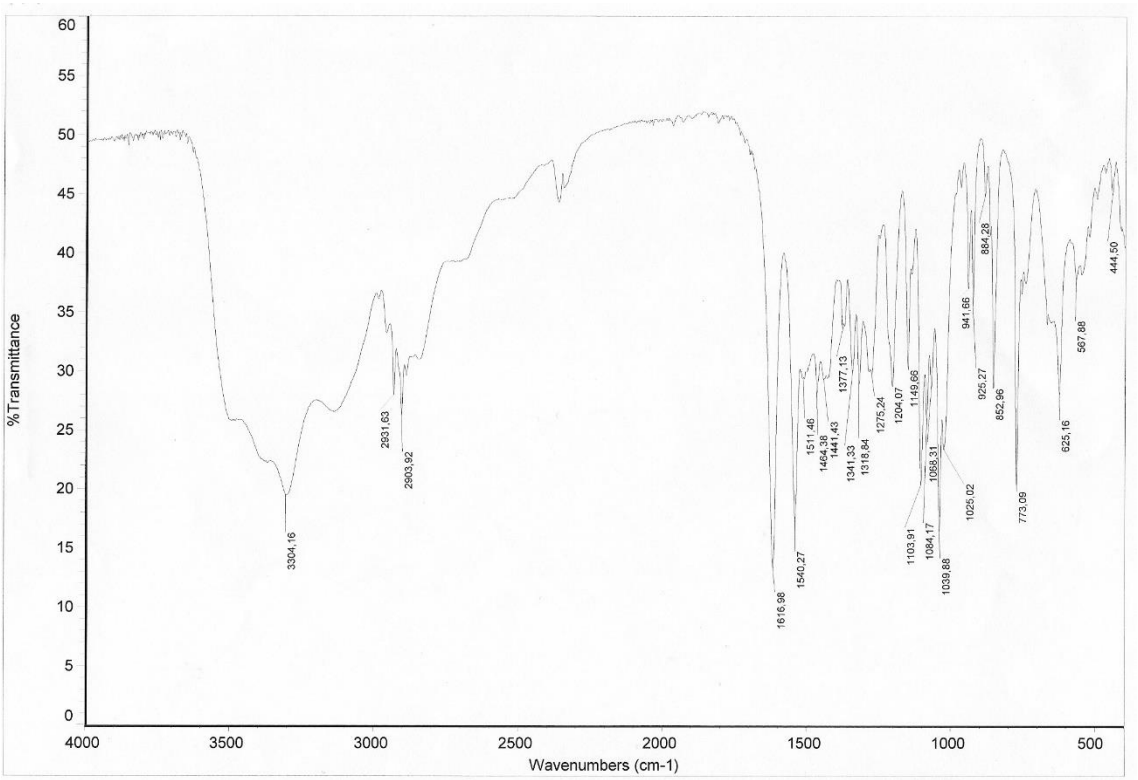


Figure S1. IR spectrum of 1-deoxy-1-(2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**8**).

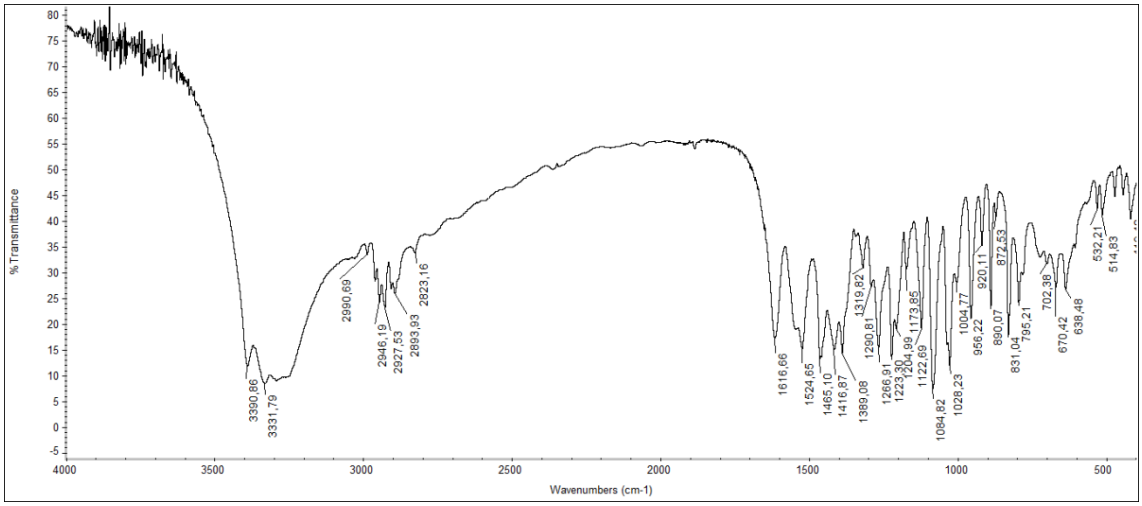


Figure S2. IR spectrum of 1-(5-bromo-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (**9**).

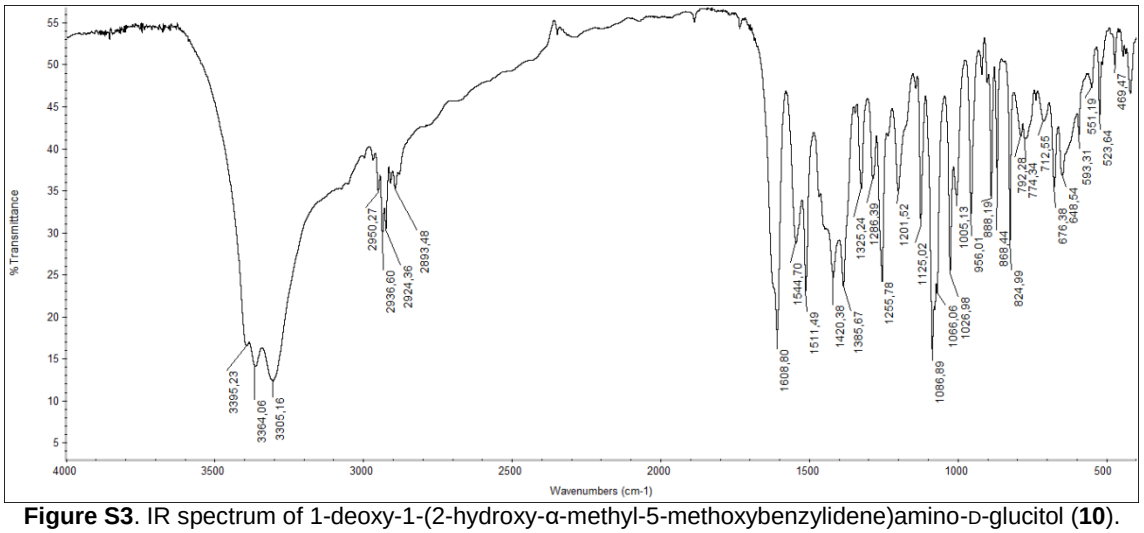


Figure S3. IR spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-methoxybenzylidene)amino-D-glucitol (**10**).

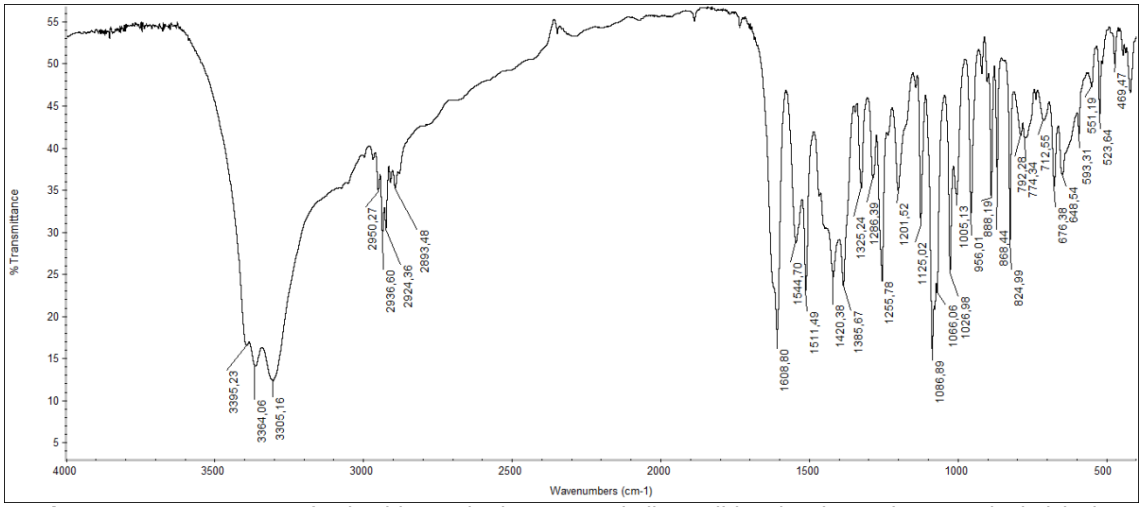


Figure S4. IR spectrum of 1-(5-chloro-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (**11**).

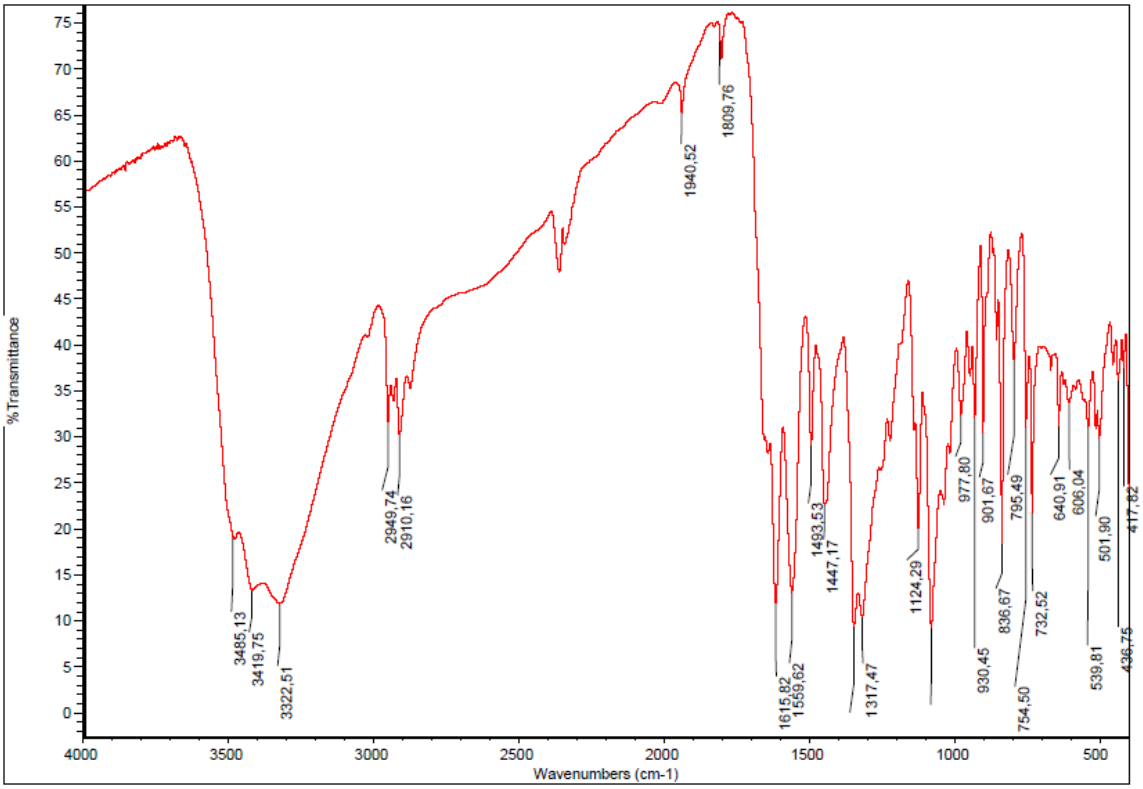


Figure S5. IR spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-nitrobenzylidene)amino-D-glucitol (**12**).

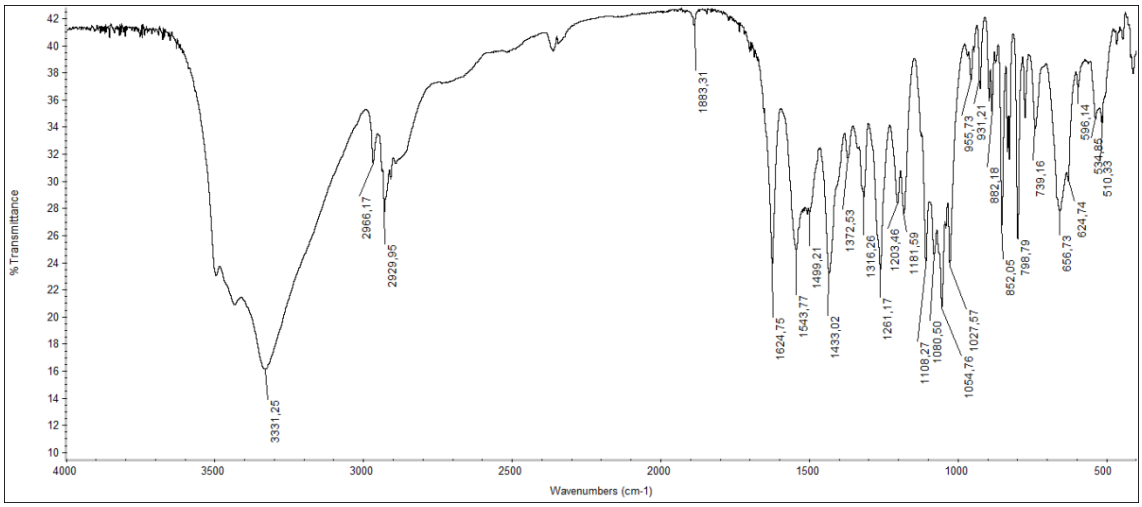


Figure S6. IR spectrum of 1-deoxy-1-(5-fluoro-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**13**).

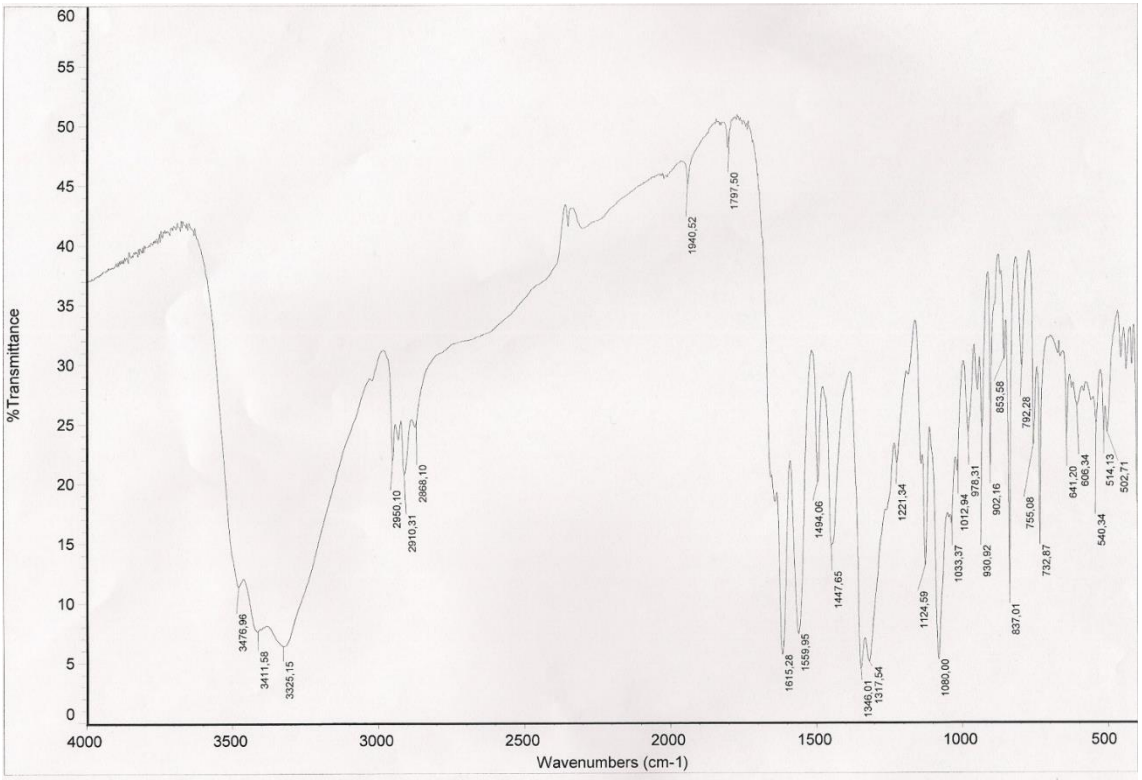


Figure S7. IR spectrum of 1-(5-bromo-2-hydroxy-α-methyl-3-nitrobenzylidene)amino-1-deoxy-D-glucitol (**14**).

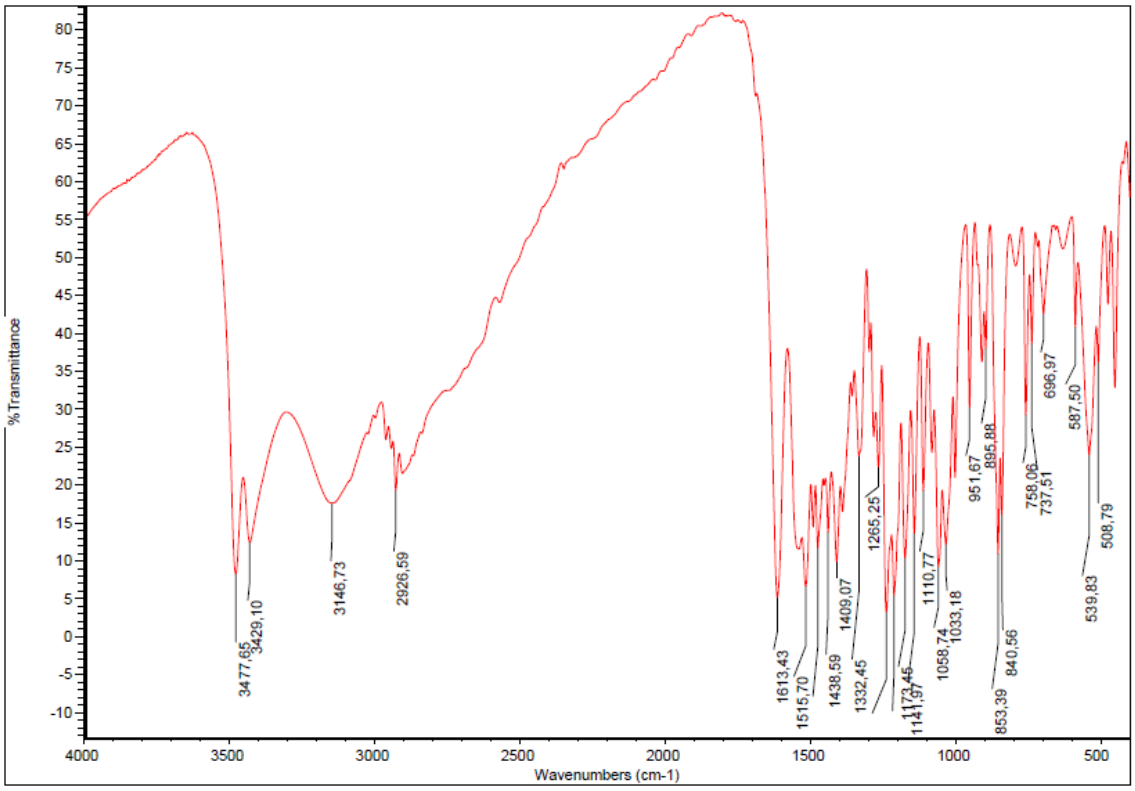


Figure S8. IR spectrum of 1-deoxy-1-(4,5-dimethoxy-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**15**).

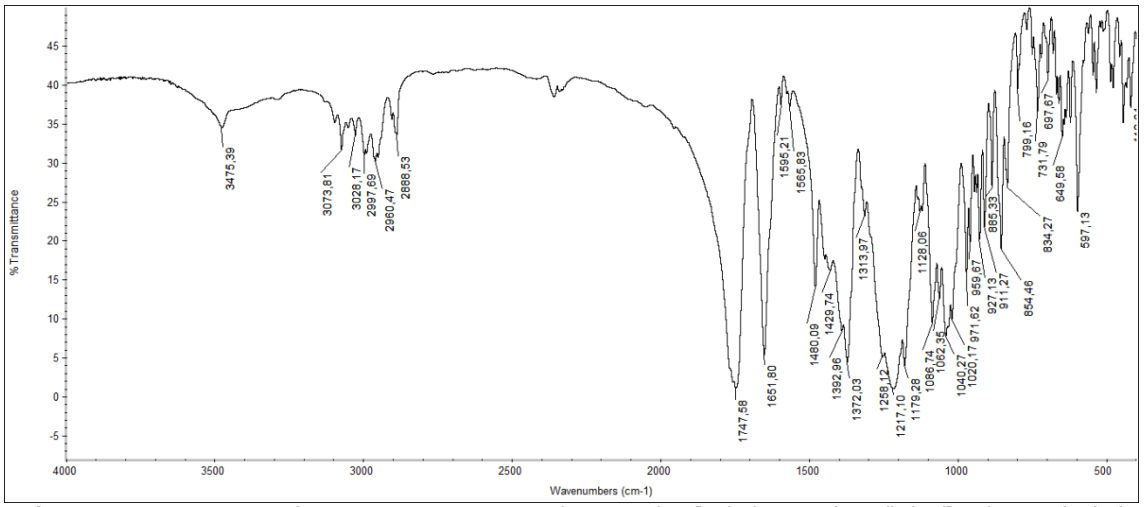


Figura S9. IR spectrum of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**).

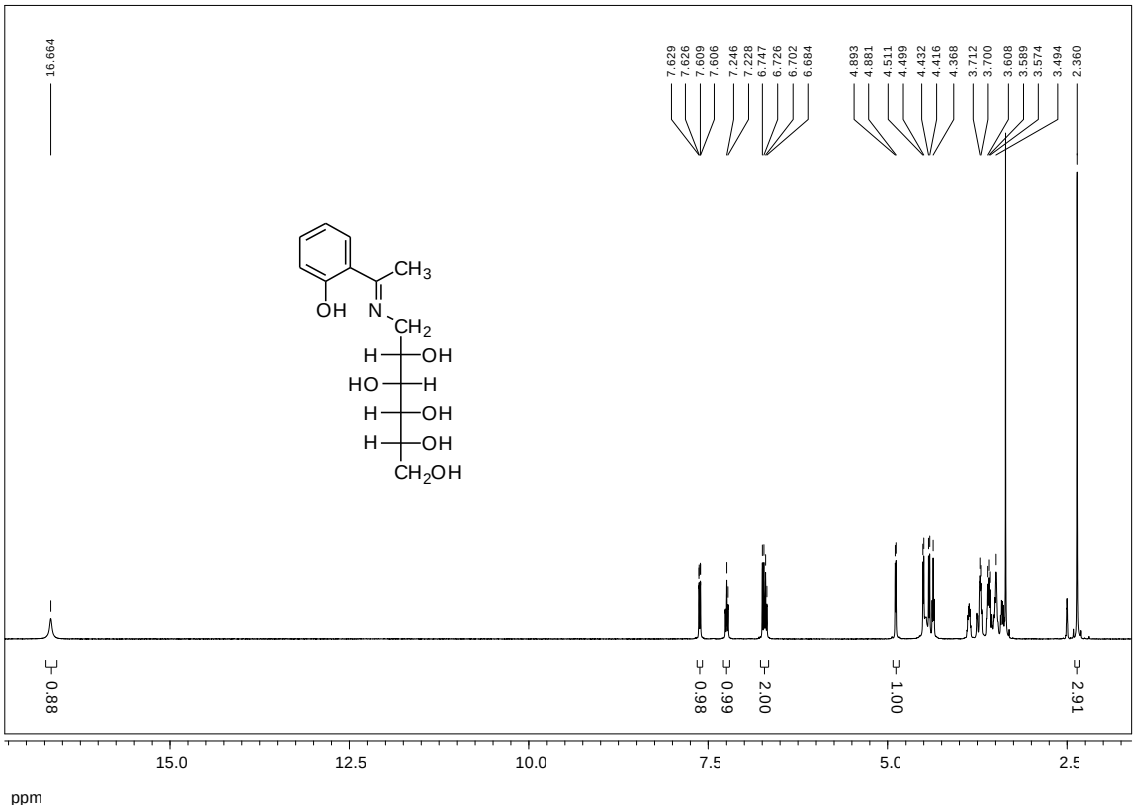


Figure S10. ^{1}H NMR spectrum of 1-deoxy-1-(2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**8**), recorded in DMSO-d_6.

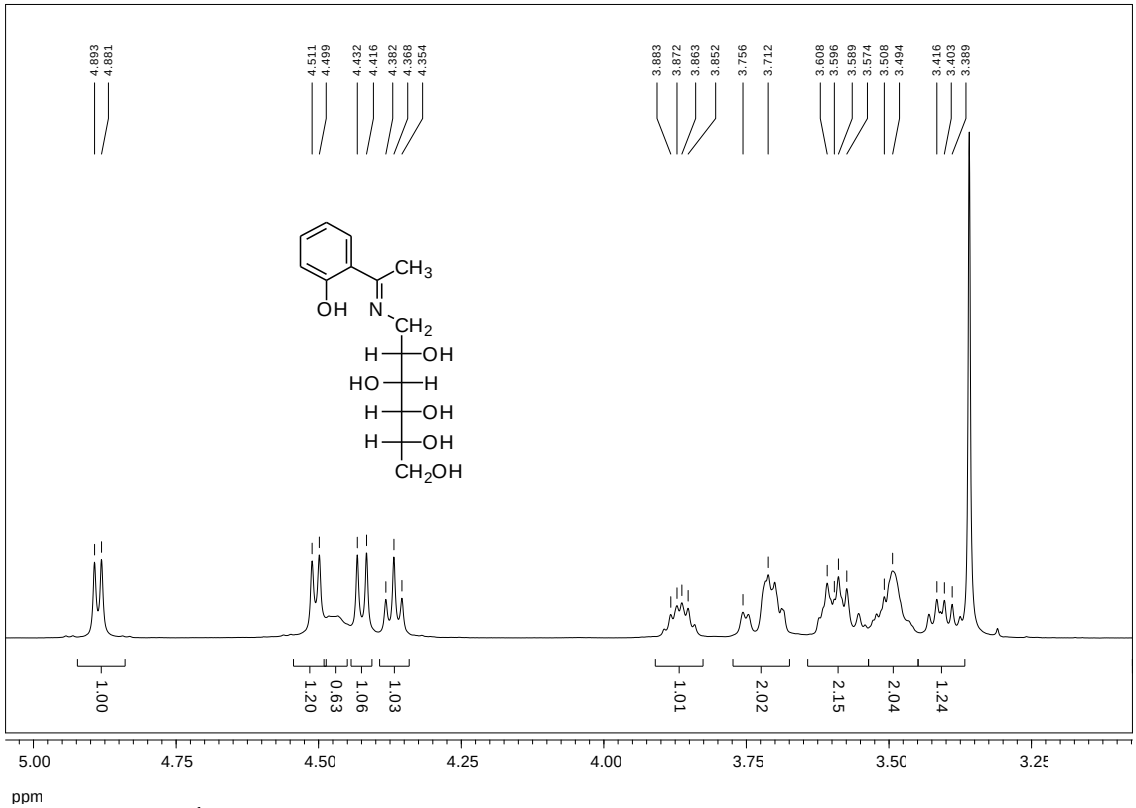


Figure S10a. ^{1}H NMR spectrum of 1-deoxy-1-(2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**8**), recorded in DMSO-d_6 (magnified zone between 3.0 and 5.0 ppm).

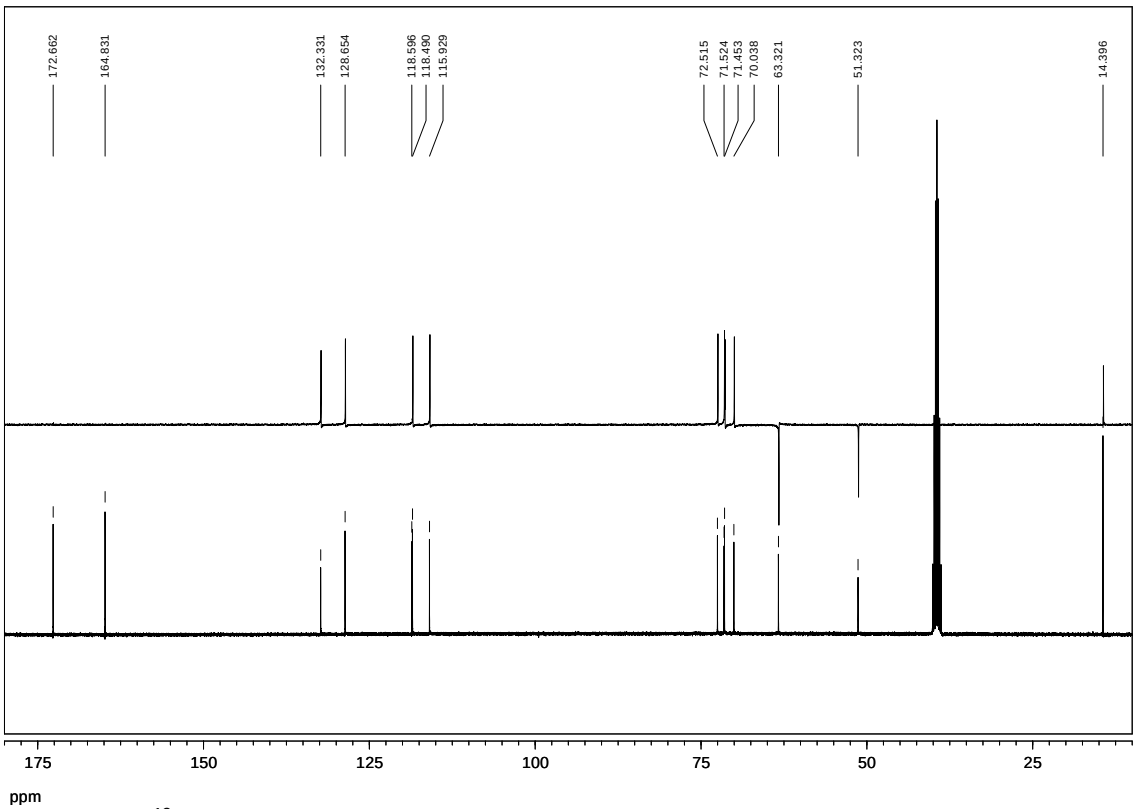


Figure S11. ^{13}C NMR and DEPT spectra of 1-deoxy-1-(2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**8**), recorded in DMSO-d_6.

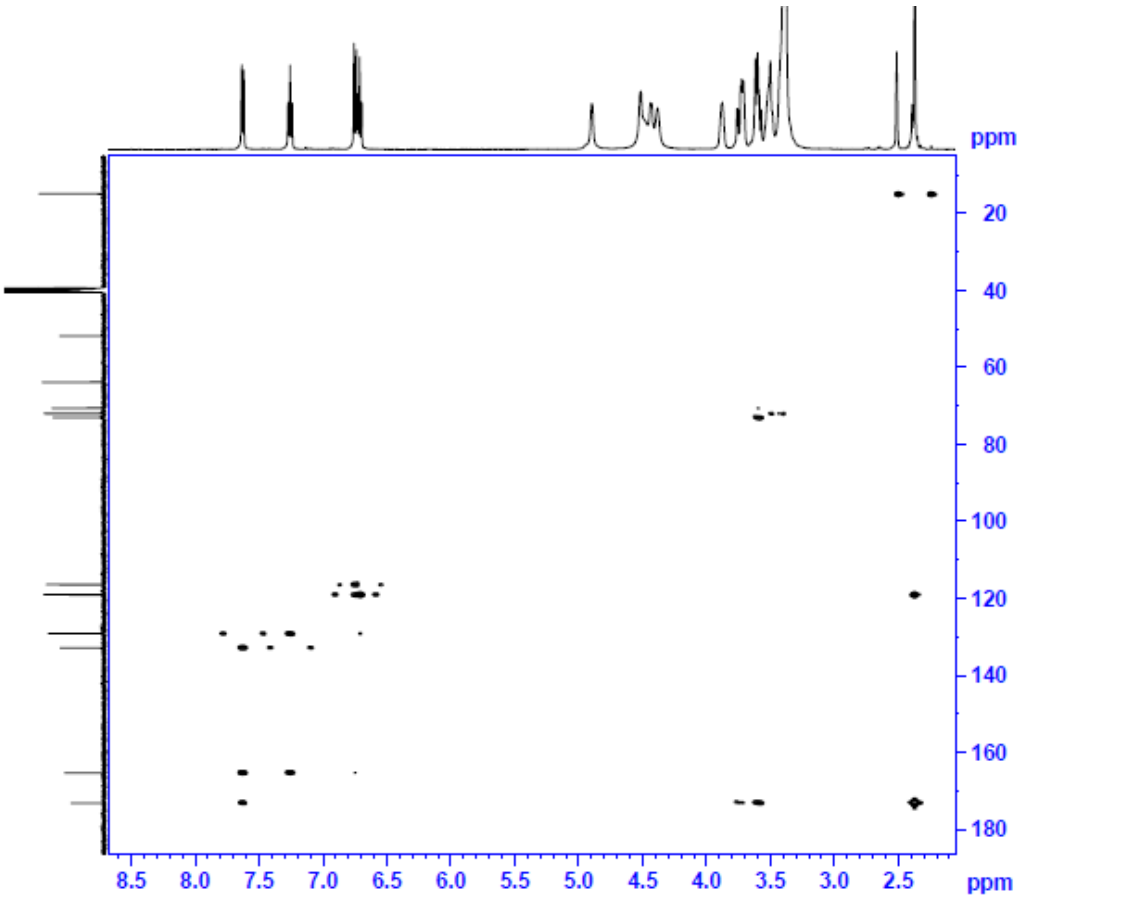


Figure S12. HMBC spectrum of 1-deoxy-1-(2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**8**), recorded in DMSO-d_6.

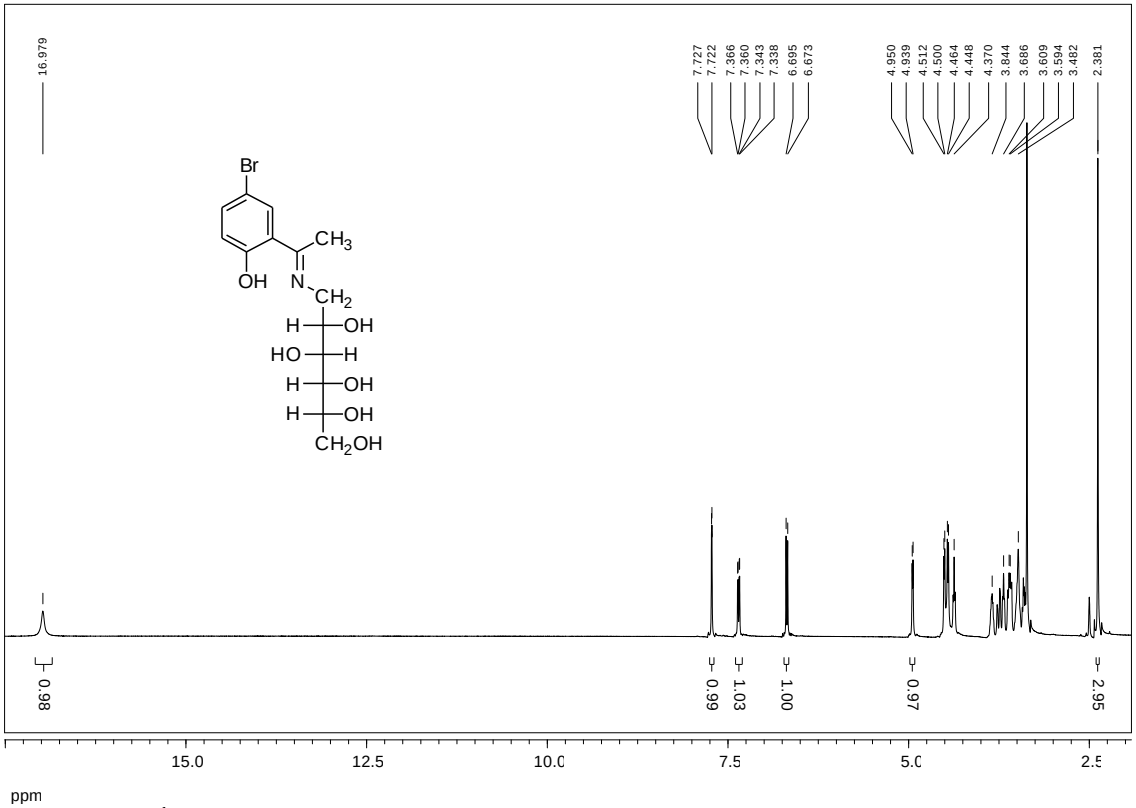


Figure S13. ^{1}H NMR spectrum of 1-(5-bromo-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (**9**), recorded in DMSO-d_6.

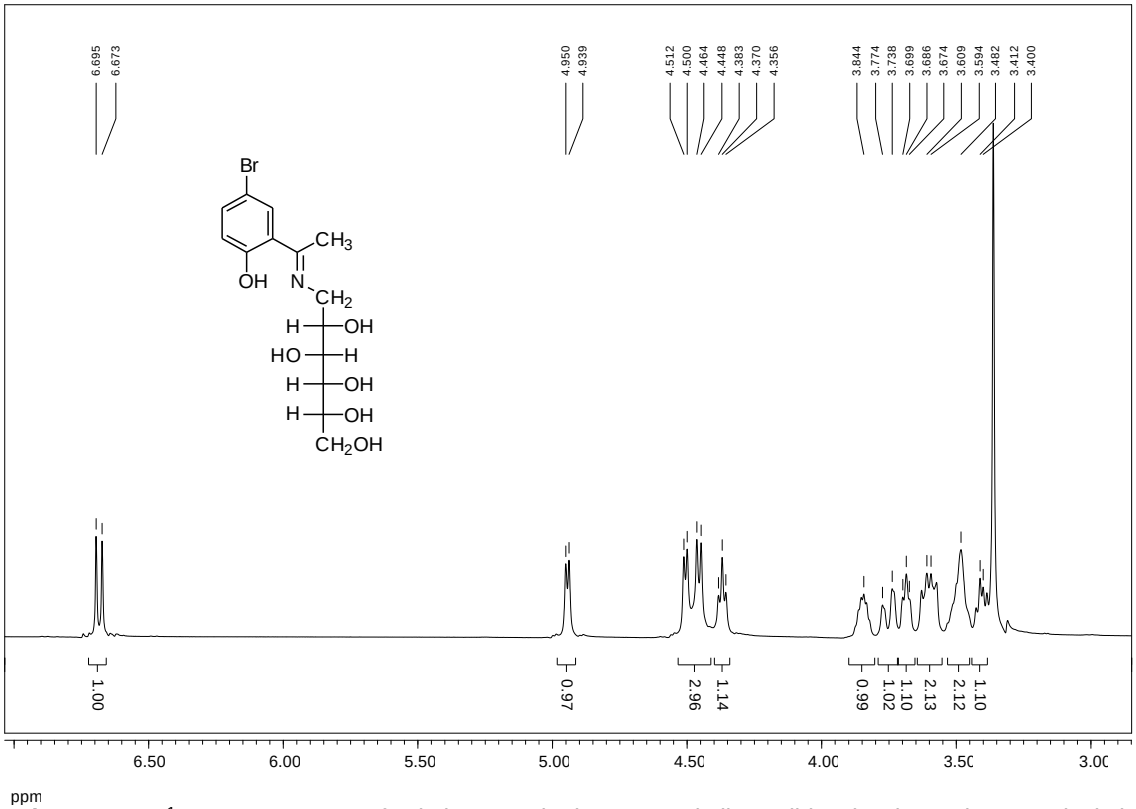


Figure S13a. ^{1}H NMR spectrum of 1-(5-bromo-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (**9**), recorded in DMSO-d_6 (magnified zone between 3.0 and 7.0 ppm).

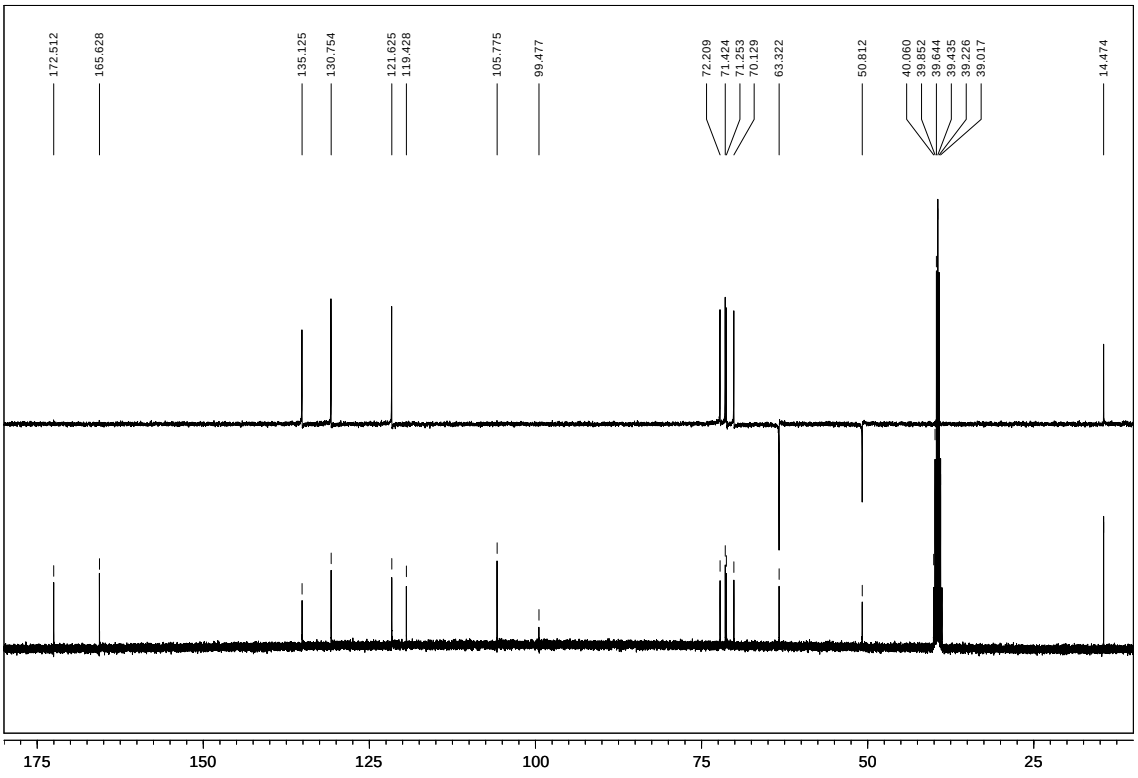


Figure S14. ^{13}C NMR and DEPT spectra of 1-(5-bromo-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (**9**), recorded in DMSO-*d*$_6$.

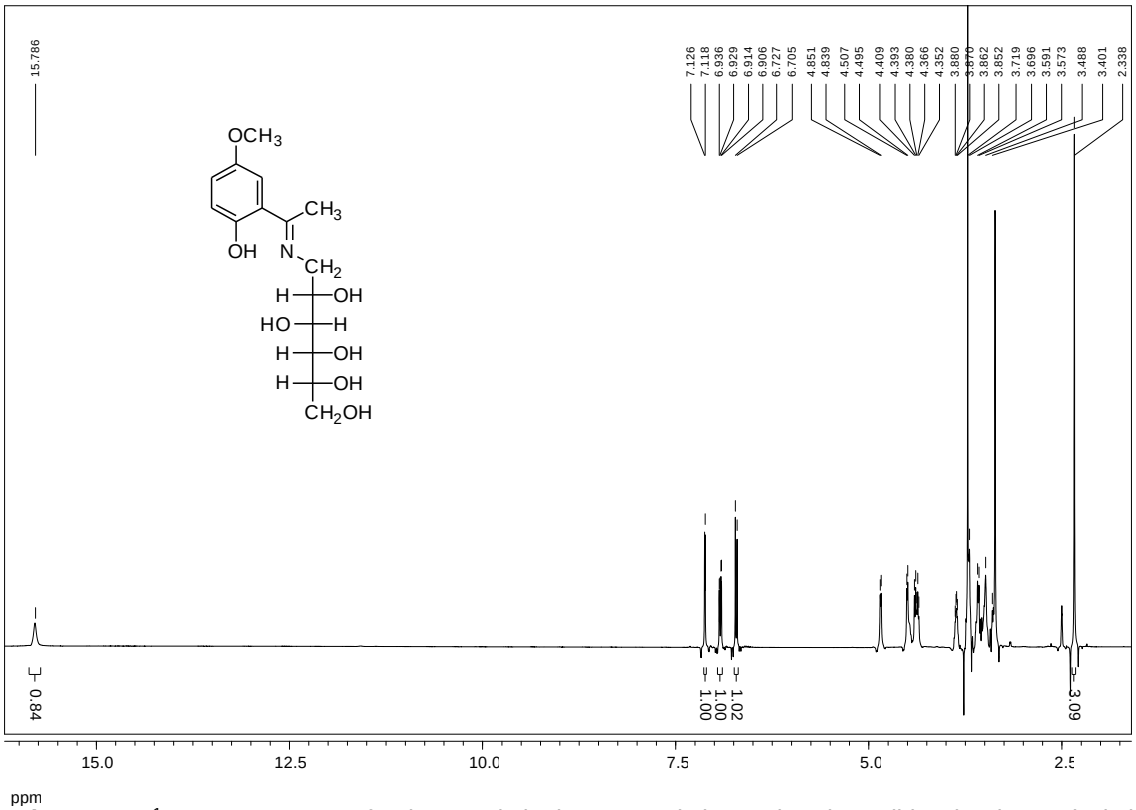


Figure S15. ^{1}H NMR spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-methoxybenzylidene)amino-D-glucitol (**10**), recorded in DMSO-*d*$_6$.

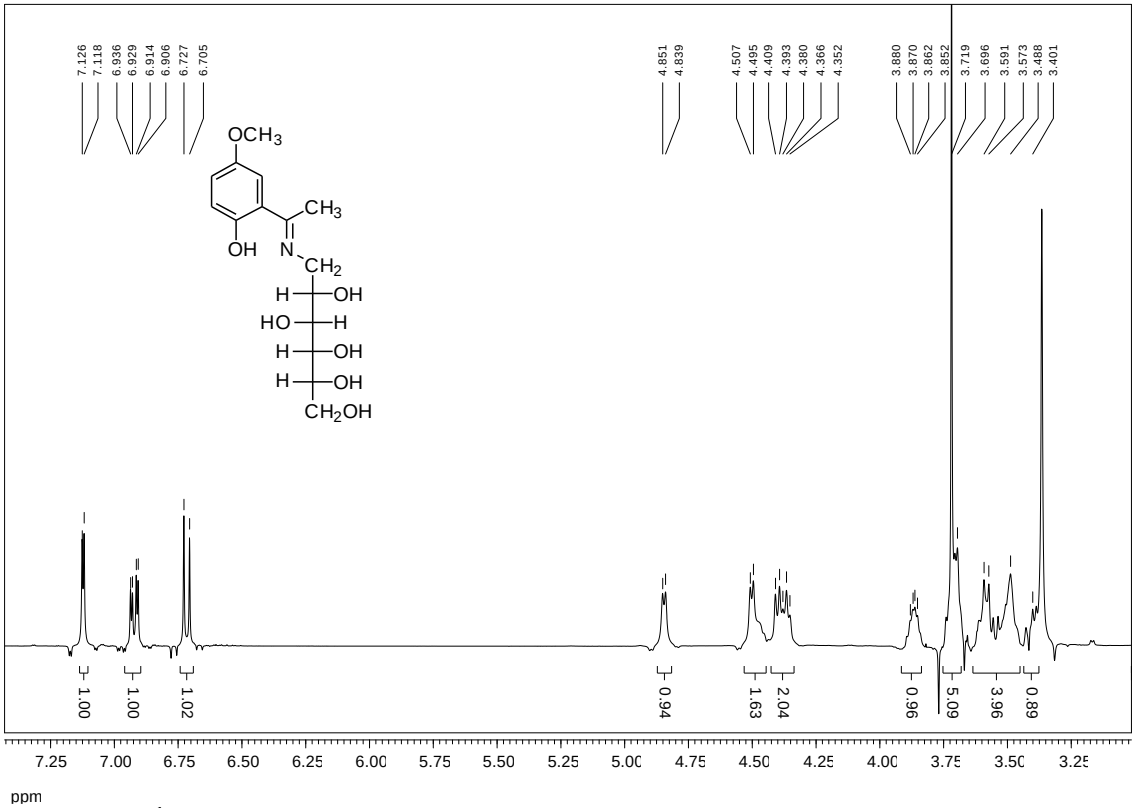


Figure S15a. ^{1}H NMR spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-methoxybenzylidene)amino-D-glucitol (**10**), recorded in DMSO-*d*$_6$ (magnified zone between 3.0 and 7.25 ppm).

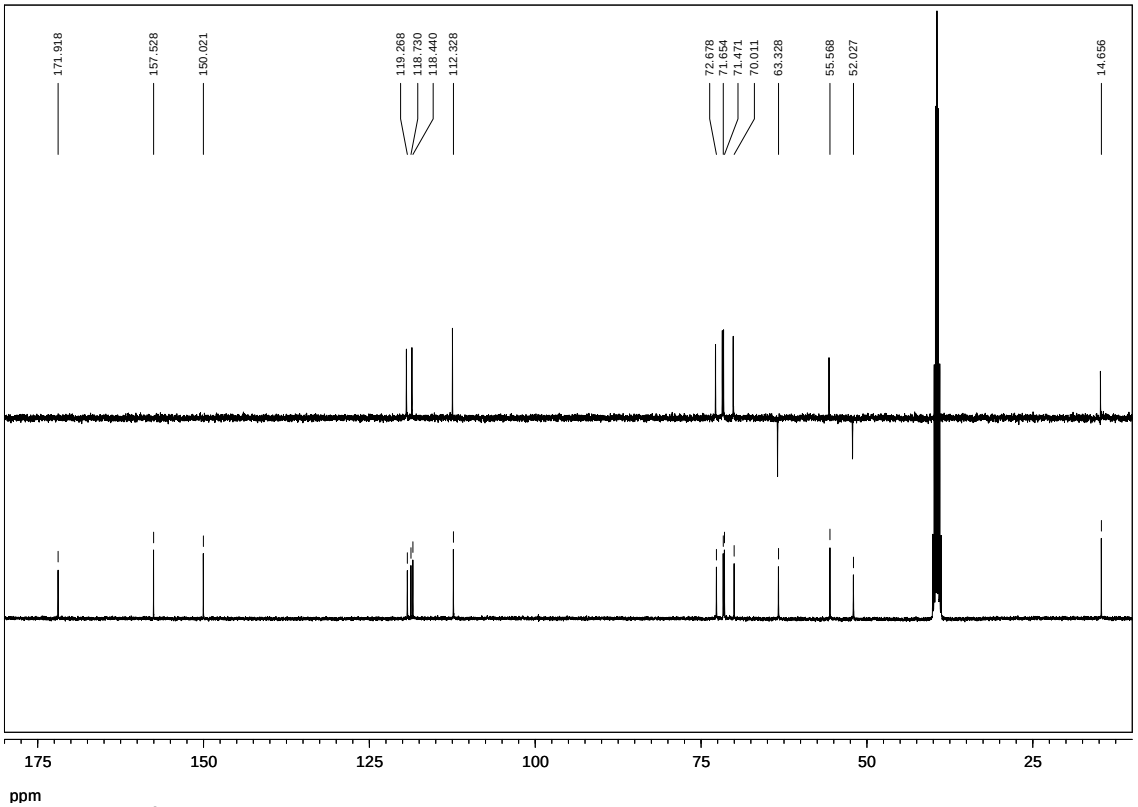


Figure S16. ^{13}C NMR and DEPT spectra of 1-deoxy-1-(2-hydroxy-α-methyl-5-methoxybenzylidene)amino-D-glucitol (**10**), recorded in DMSO-*d*$_6$.

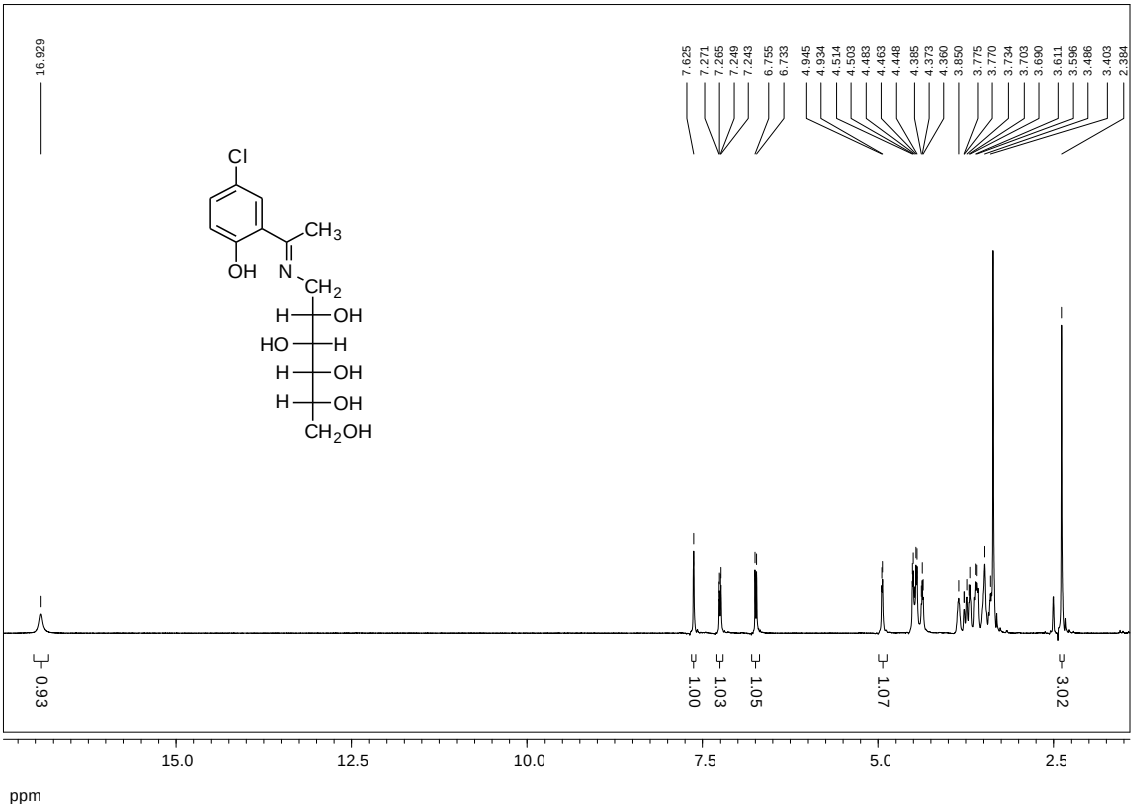


Figure S17. ^{1}H NMR spectrum of 1-(5-chloro-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (**11**), recorded in DMSO-d_6.

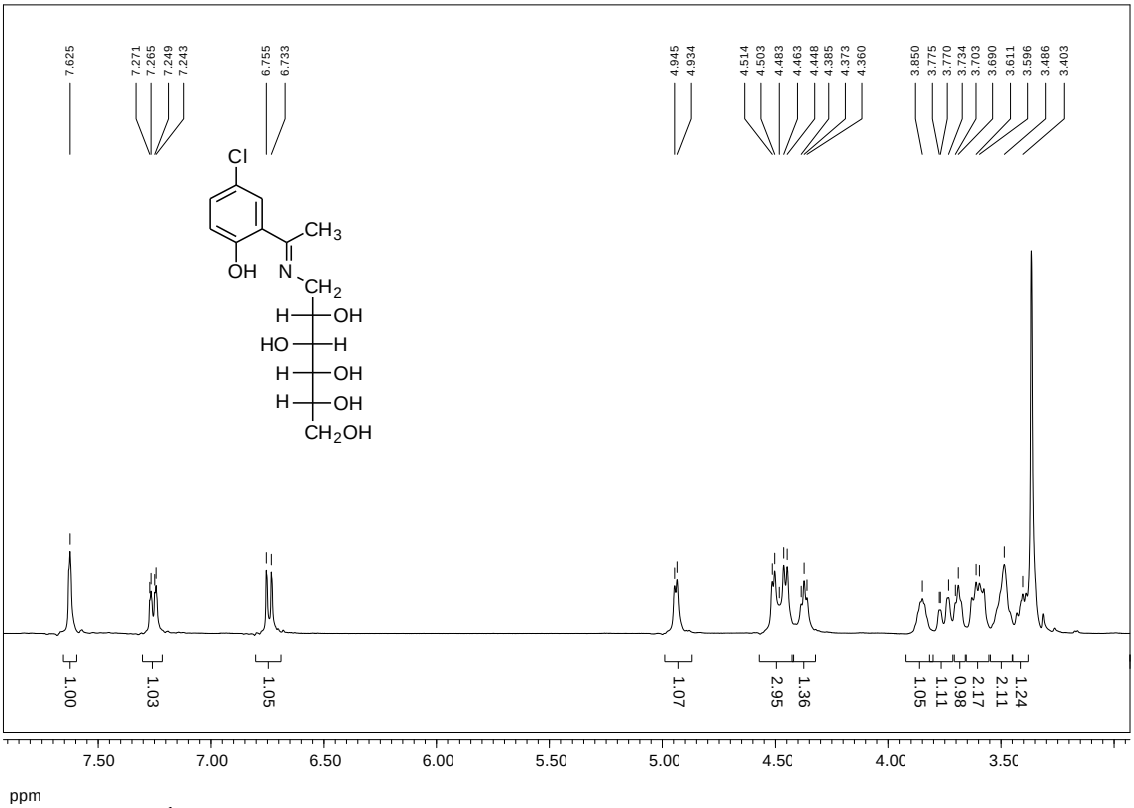


Figure S17a. ^{1}H NMR spectrum of 1-(5-chloro-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (**11**), recorded in DMSO-d_6 (magnified zone between 3.0 and 8.0 ppm).

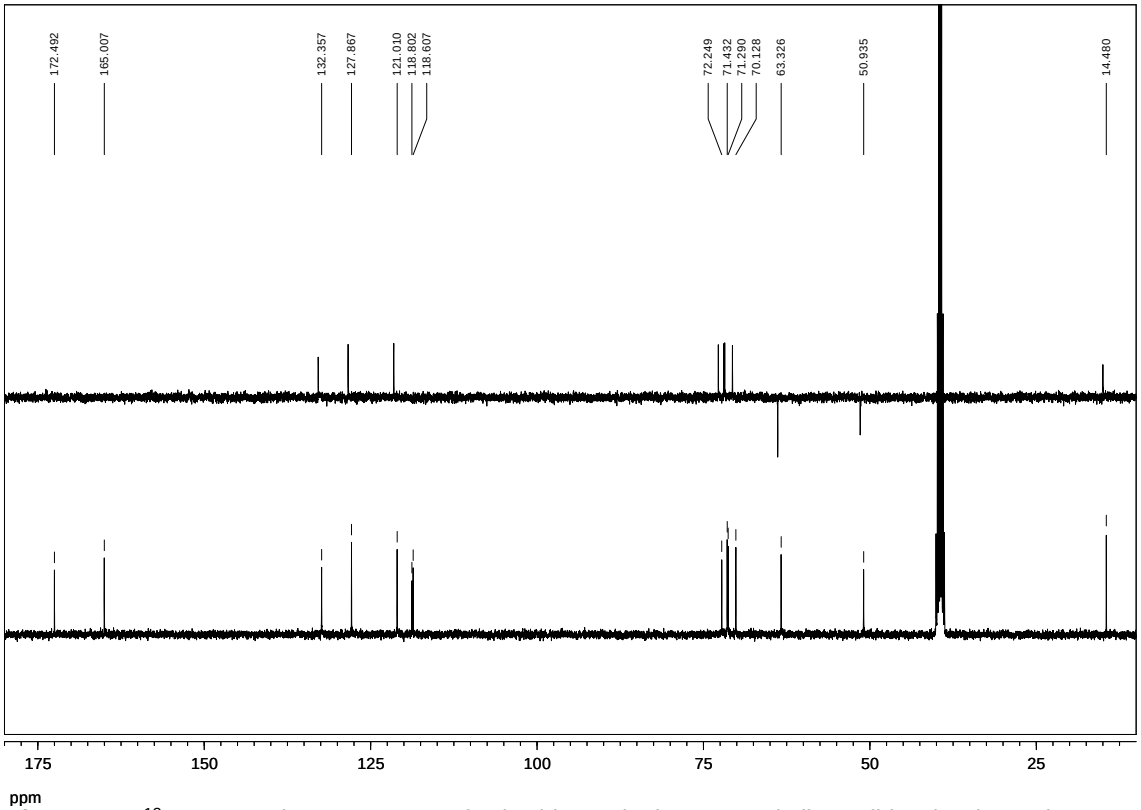


Figure S18. ^{13}C NMR and DEPT spectra of 1-(5-chloro-2-hydroxy-α-methylbenzylidene)amino-1-deoxy-D-glucitol (**11**), recorded in DMSO-*d*$_6$.

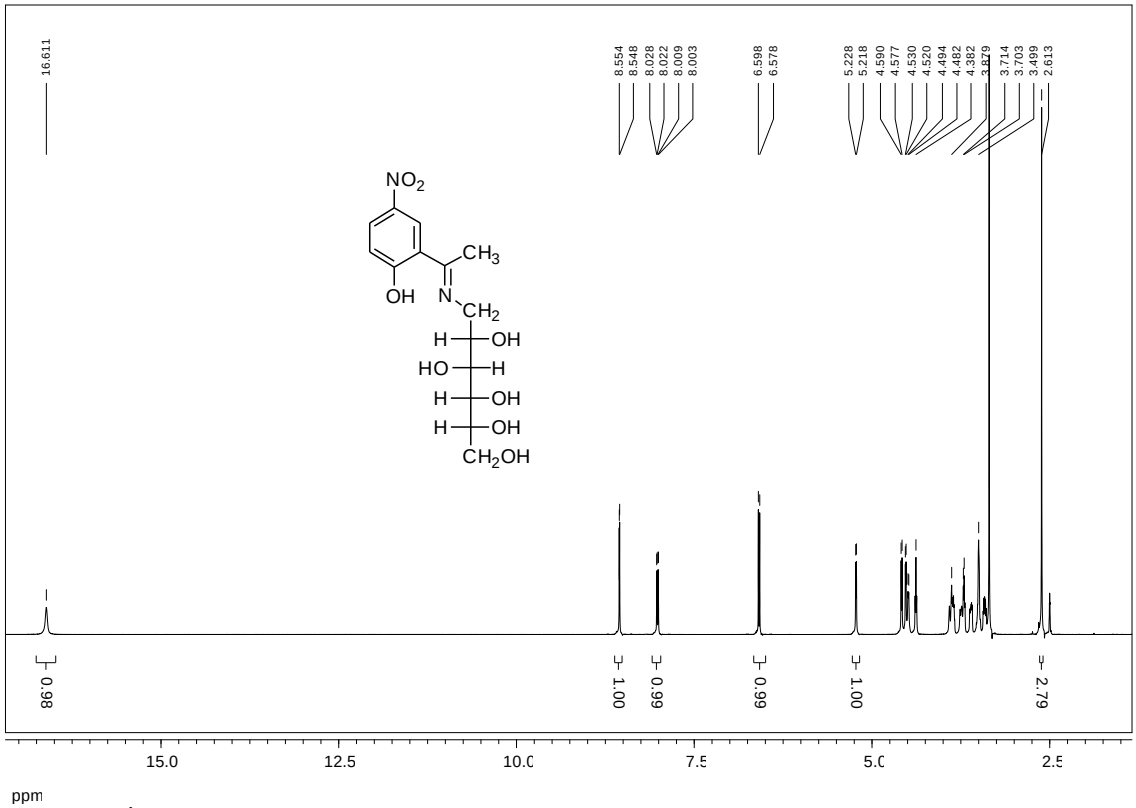


Figure S19. ^{1}H NMR spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-nitrobenzylidene)amino-D-glucitol (**12**), recorded in DMSO-*d*$_6$.

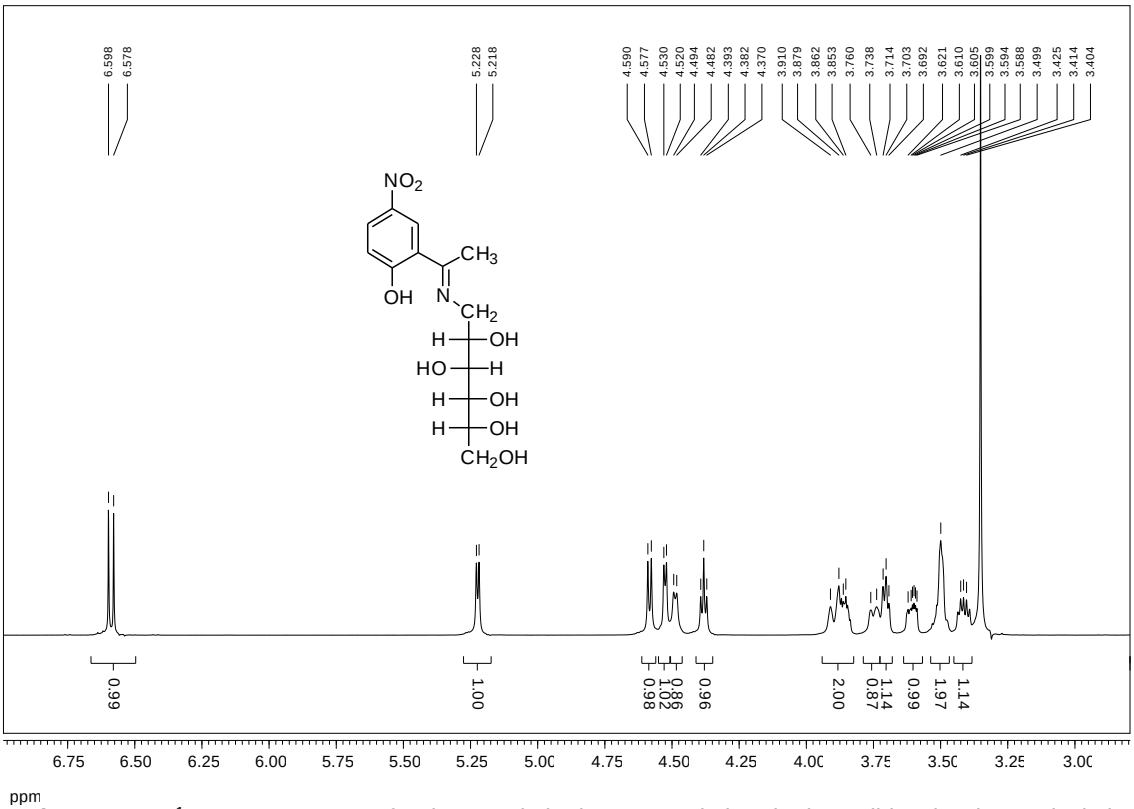


Figure S19a. ^{1}H NMR spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-nitrobenzylidene)amino-D-glucitol (**12**), recorded in DMSO-*d*$_6$ (magnified zone between 3.0 and 7.0 ppm).

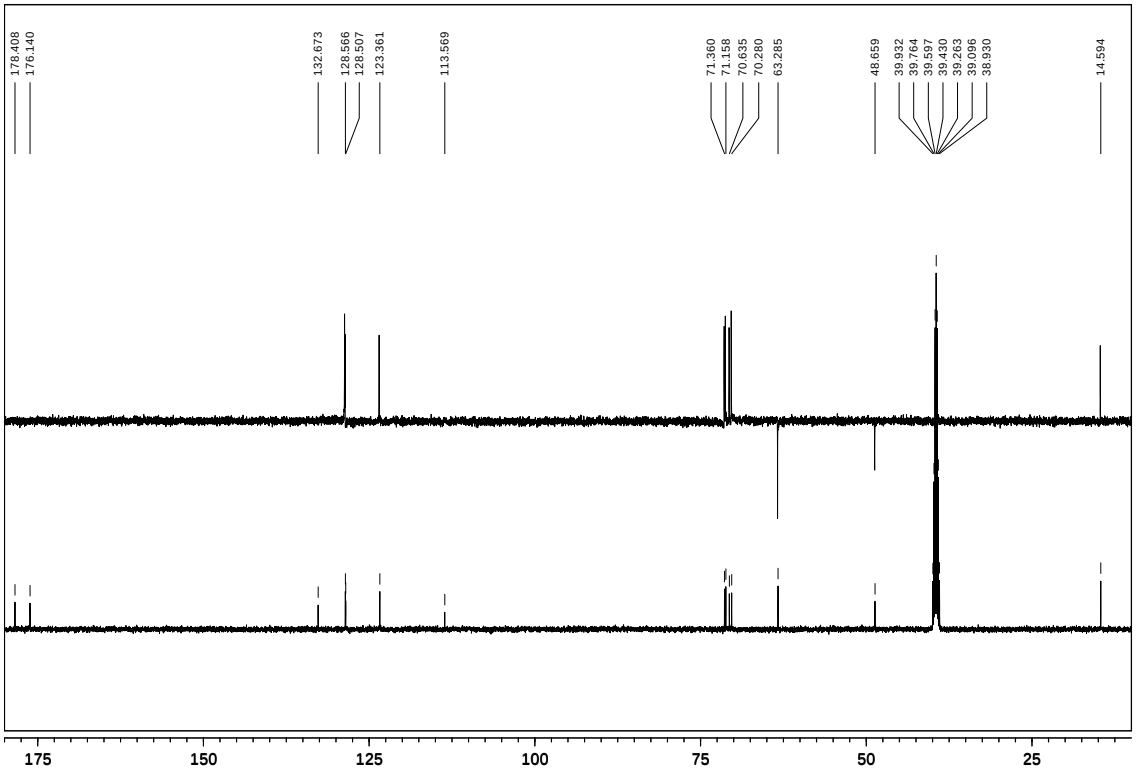


Figure S20. ^{13}C NMR and DEPT spectra of 1-deoxy-1-(2-hydroxy-α-methyl-5-nitrobenzylidene)amino-D-glucitol (**12**), recorded in DMSO-*d*$_6$.

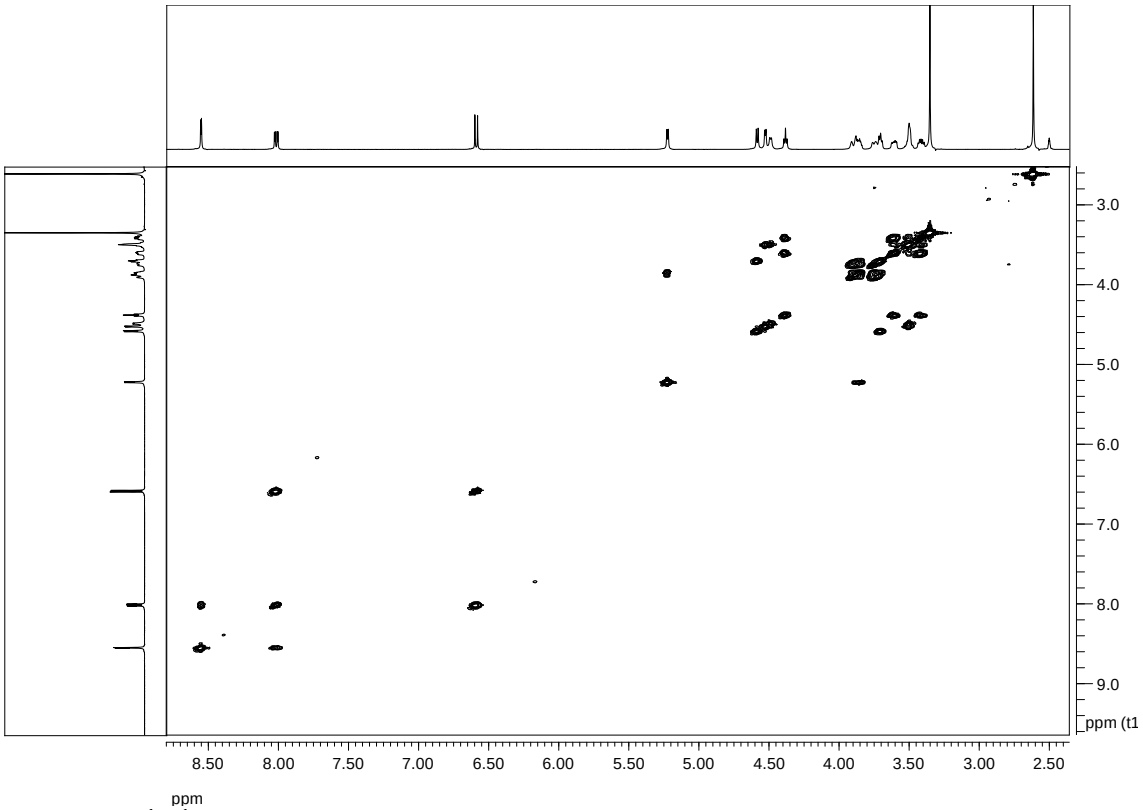


Figure S21. ^{1}H-^{1}H COSY spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-nitrobenzylidene)amino-D-glucitol (**12**), recorded in DMSO-d_6.

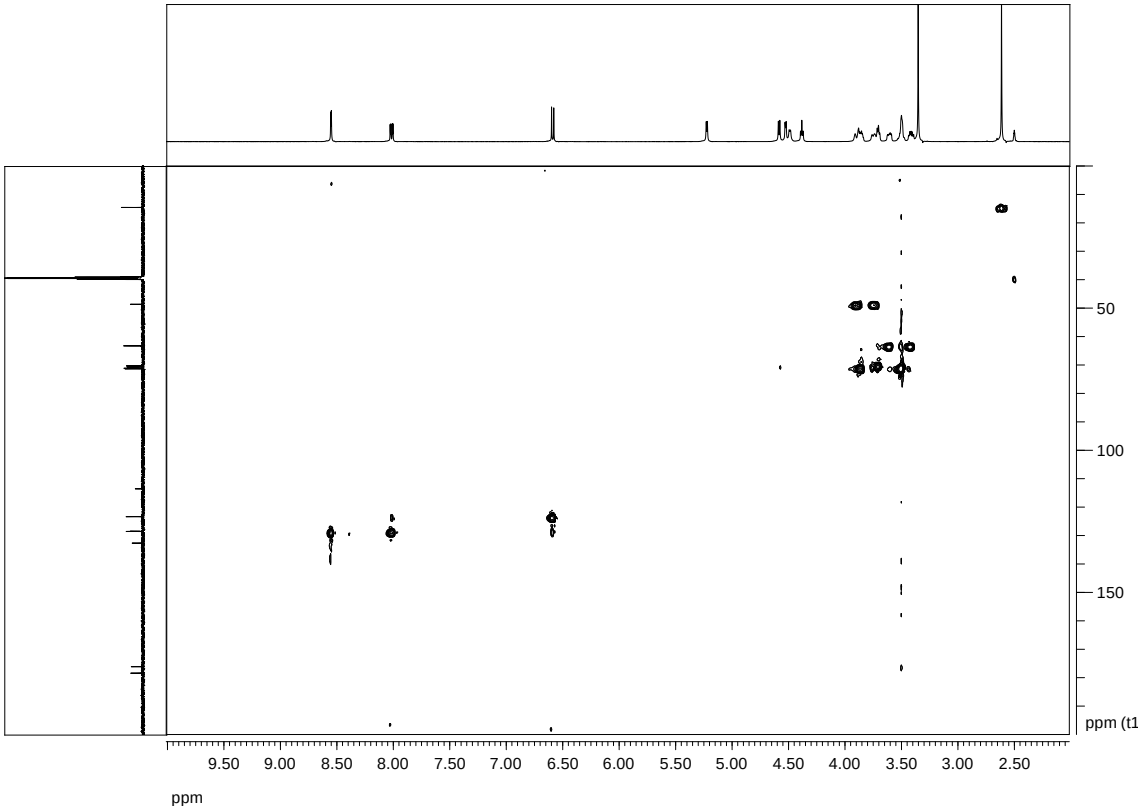


Figure S22. HMQC spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-nitrobenzylidene)amino-D-glucitol (**12**), recorded in DMSO-d_6.

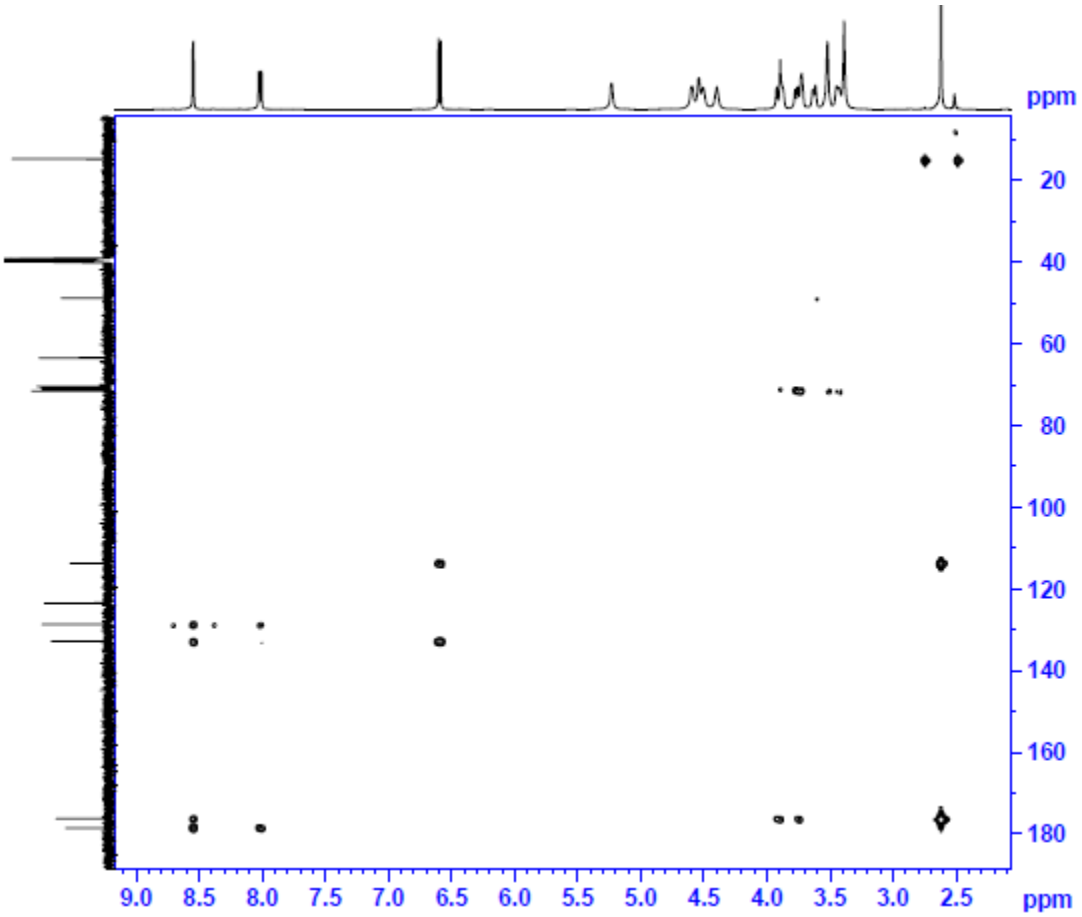


Figure S23. HMBC spectrum of 1-deoxy-1-(2-hydroxy-α-methyl-5-nitrobenzylidene)amino-D-glucitol (**12**), recorded in DMSO-d_6.

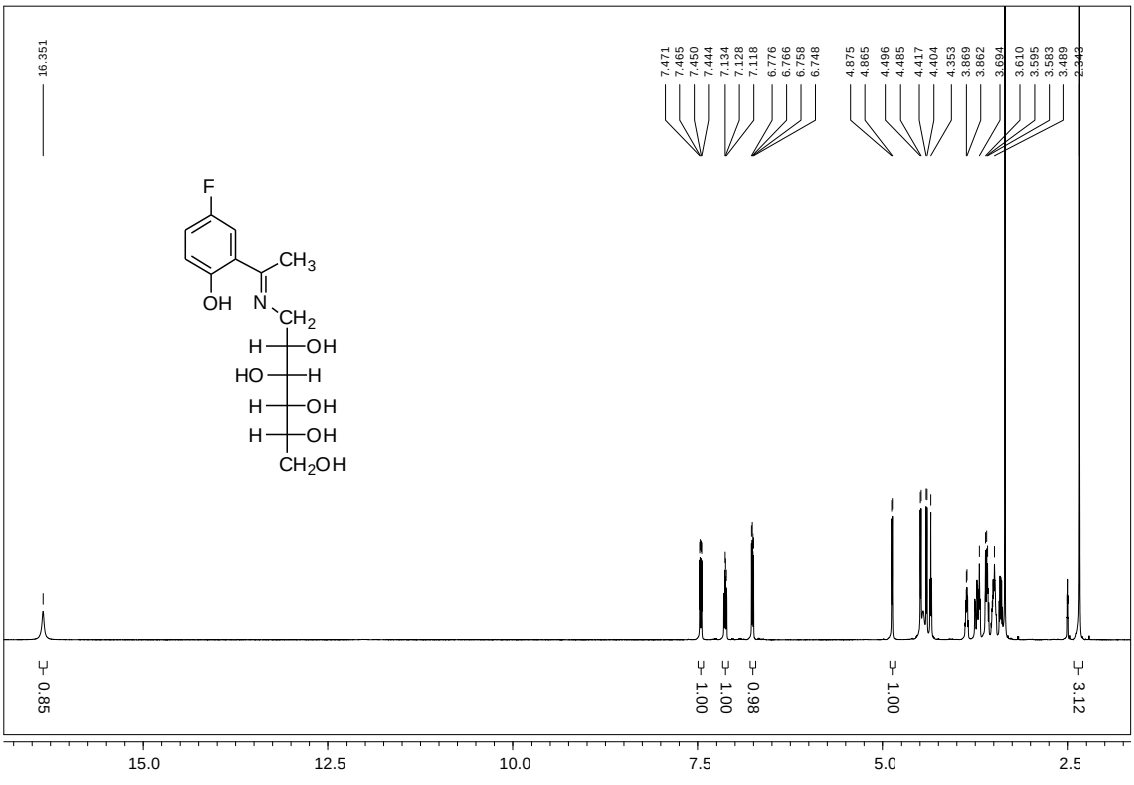


Figure S24. ^{1}H NMR spectrum of 1-deoxy-1-(5-fluoro-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**13**), recorded in DMSO-d_6.

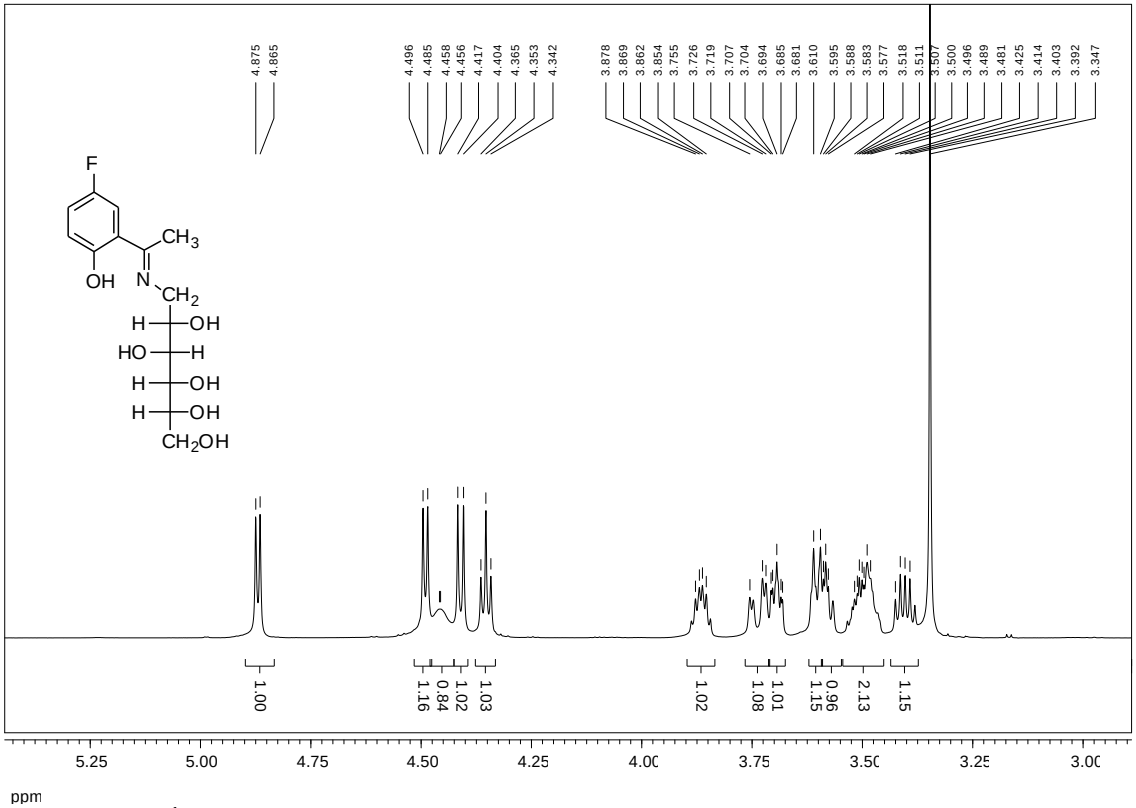


Figure S24a. ^{1}H NMR spectrum of 1-deoxy-1-(5-fluoro-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**13**), recorded in DMSO-d_6 (magnified zone between 3.0 and 5.5 ppm).

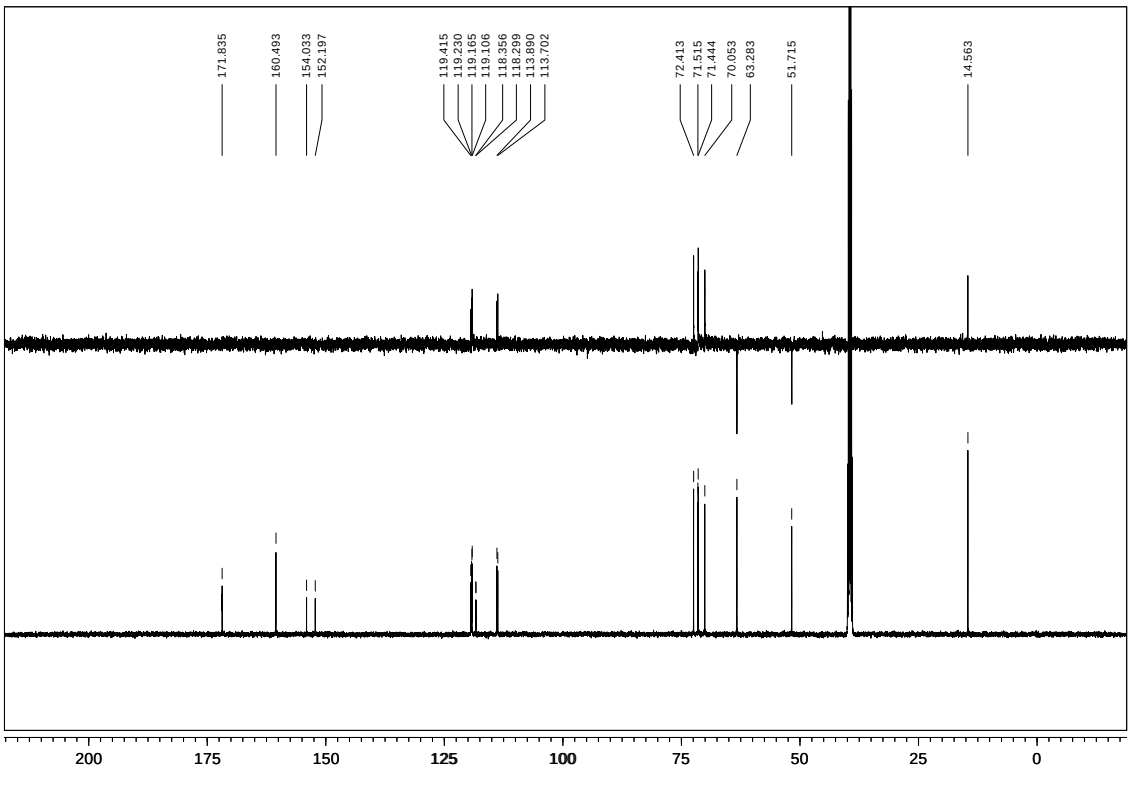


Figure S25. ^{13}C NMR and DEPT spectra of 1-deoxy-1-(5-fluoro-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**13**), recorded in DMSO-*d*$_6$.

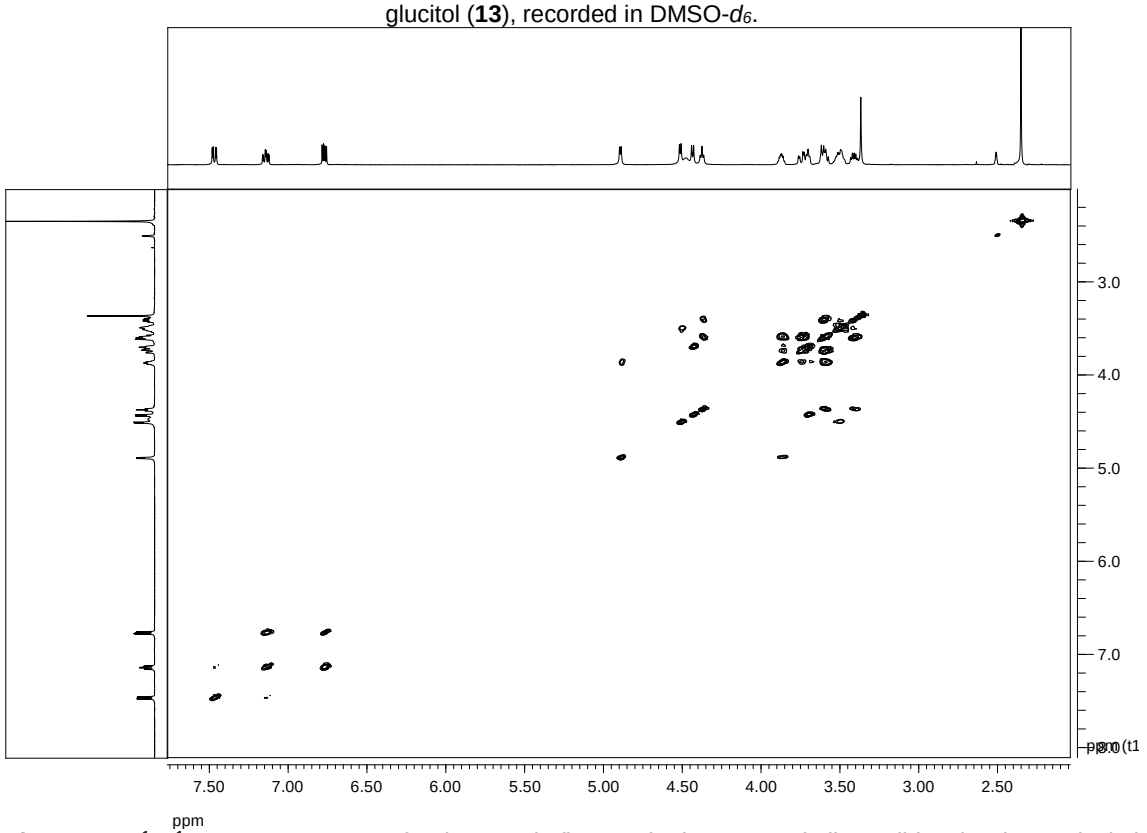


Figure S26. ^{1}H-^{1}H COSY spectrum of 1-deoxy-1-(5-fluoro-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**13**), recorded in DMSO-*d*$_6$.

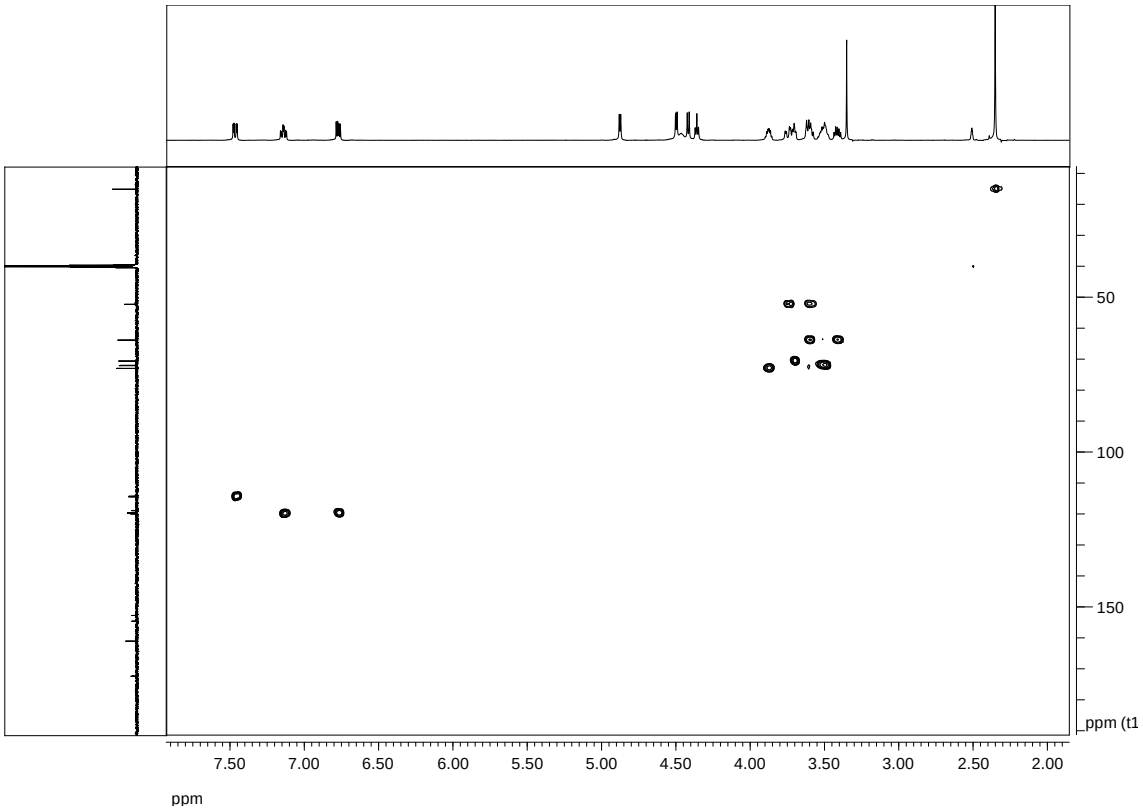


Figure S27. HMQC spectrum of 1-deoxy-1-(5-fluoro-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**13**), recorded in DMSO-d_6.

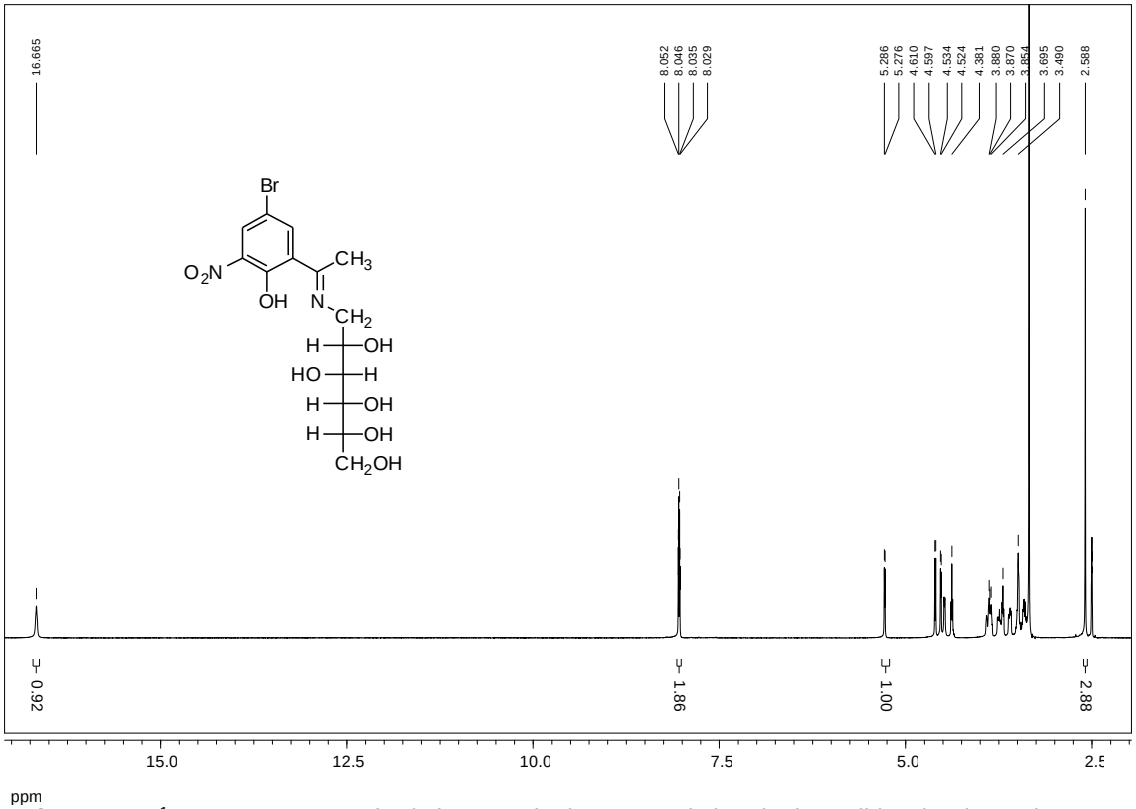


Figure S28. ^{1}H NMR spectrum of 1-(5-bromo-2-hydroxy-α-methyl-3-nitrobenzylidene)amino-1-deoxy-D-glucitol (**14**), recorded in DMSO-d_6.

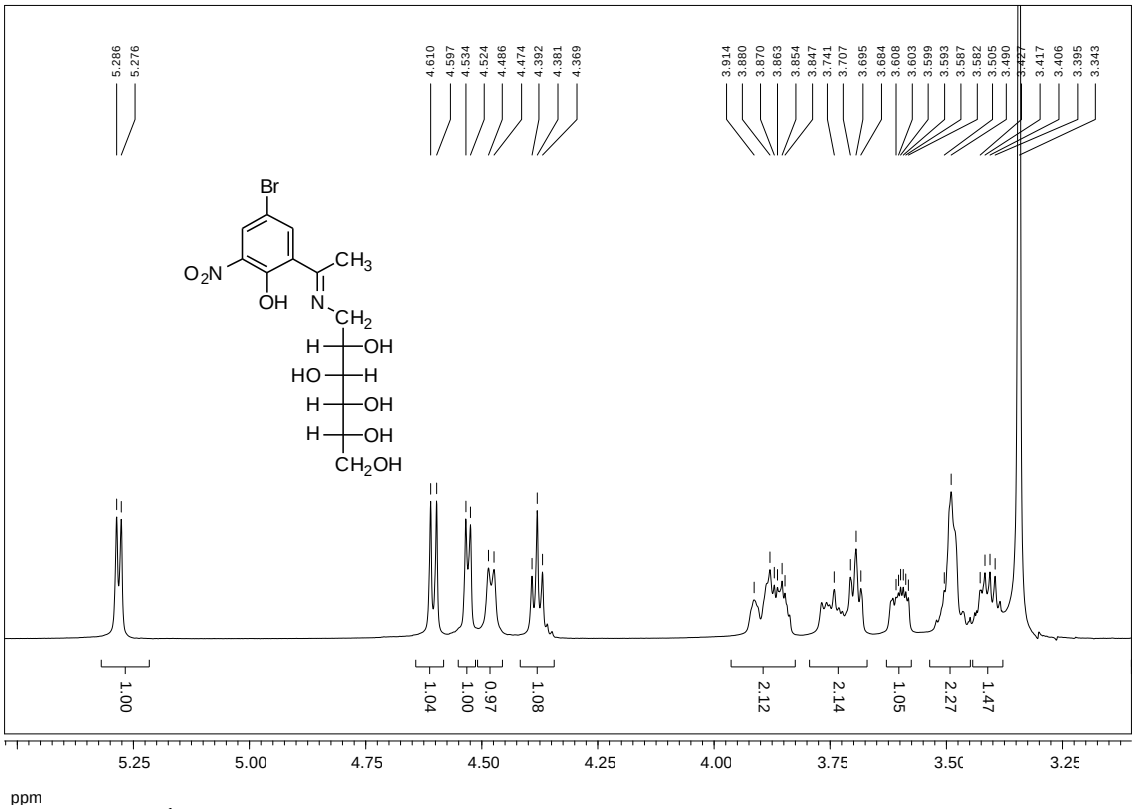


Figure S28a. ^{1}H NMR spectrum of 1-(5-bromo-2-hydroxy-α-methyl-3-nitrobenzylidene)amino-1-deoxy-D-glucitol (**14**), recorded in DMSO-*d*$_6$ (magnified zone between 3.0 and 5.5 ppm).

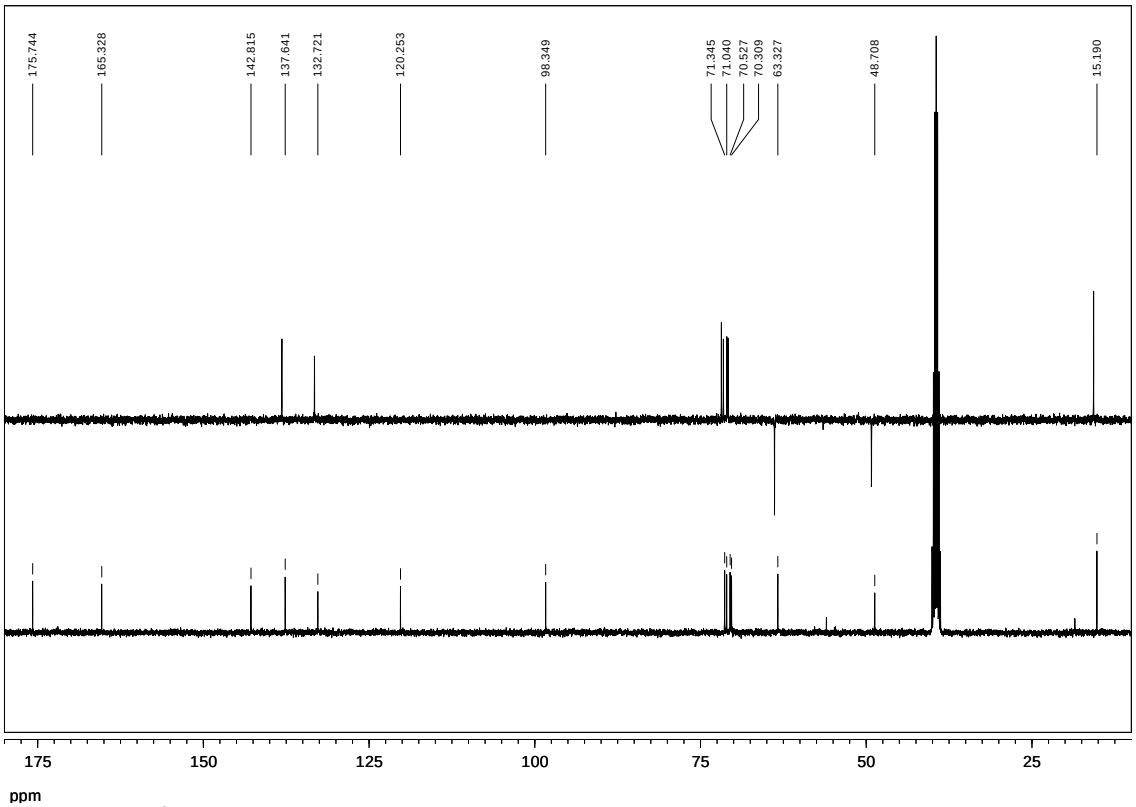


Figure S29. ^{13}C NMR and DEPT spectra of 1-(5-bromo-2-hydroxy-α-methyl-3-nitrobenzylidene)amino-1-deoxy-D-glucitol (**14**), recorded in DMSO-*d*$_6$.

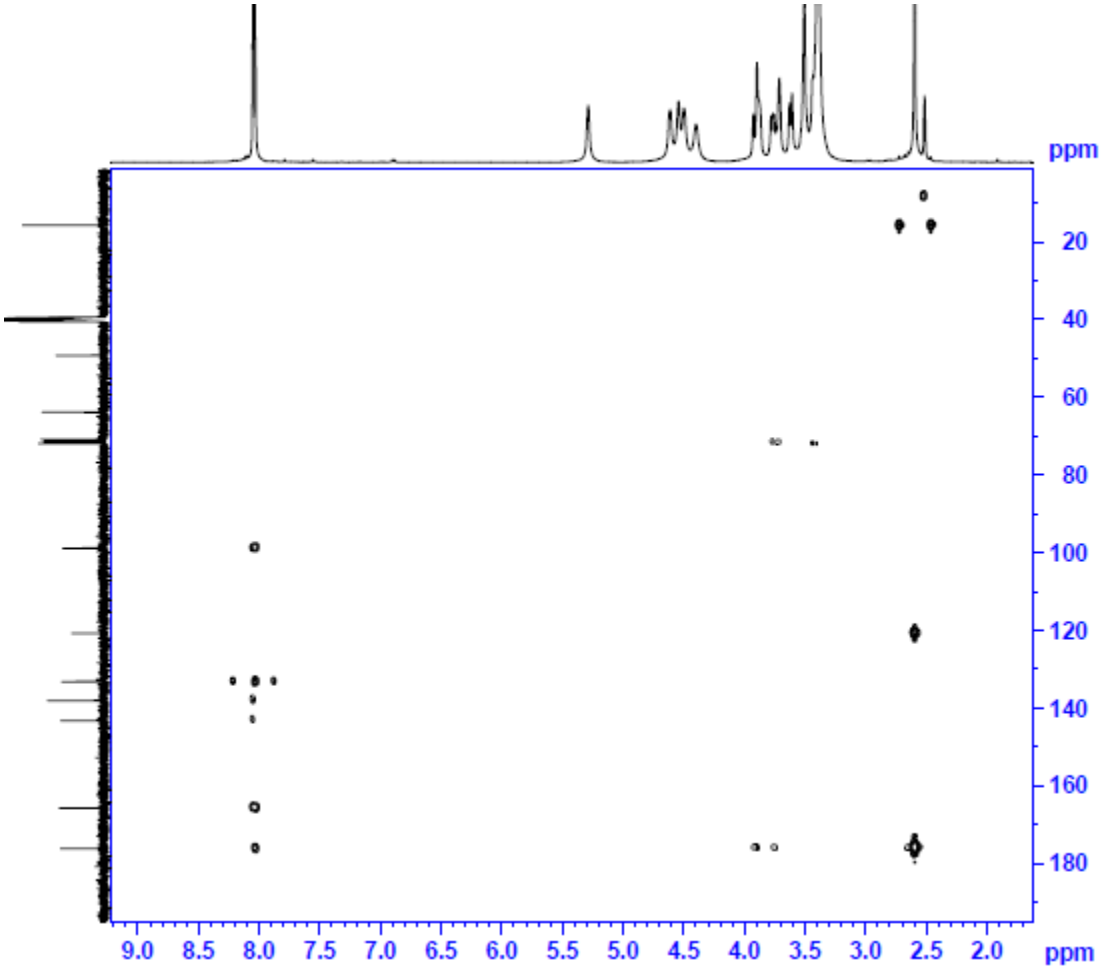


Figure S30. HMBC spectrum of 1-(5-bromo-2-hydroxy-α-methyl-3-nitrobenzylidene)amino-1-deoxy-D-glucitol (**14**), recorded in DMSO-d_6.

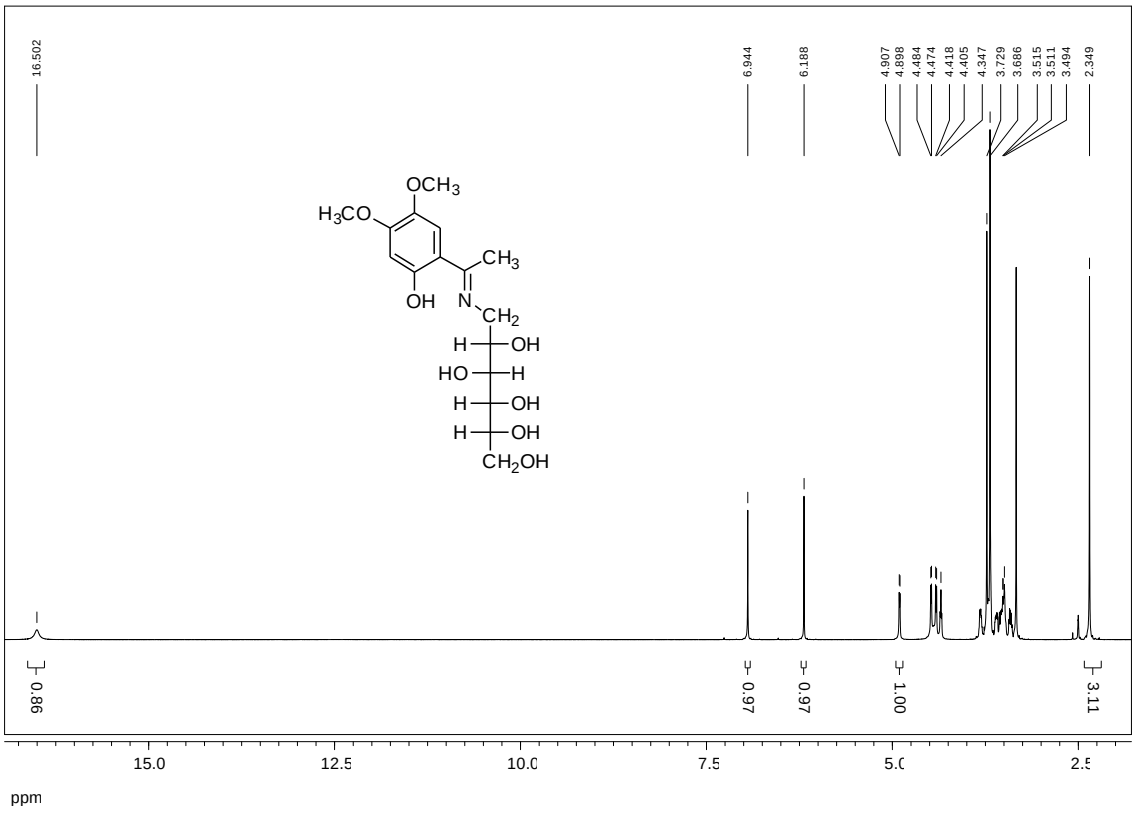


Figure S31. ^{1}H NMR spectrum of 1-deoxy-1-(4,5-dimethoxy-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**15**), recorded in DMSO-*d*$_6$.

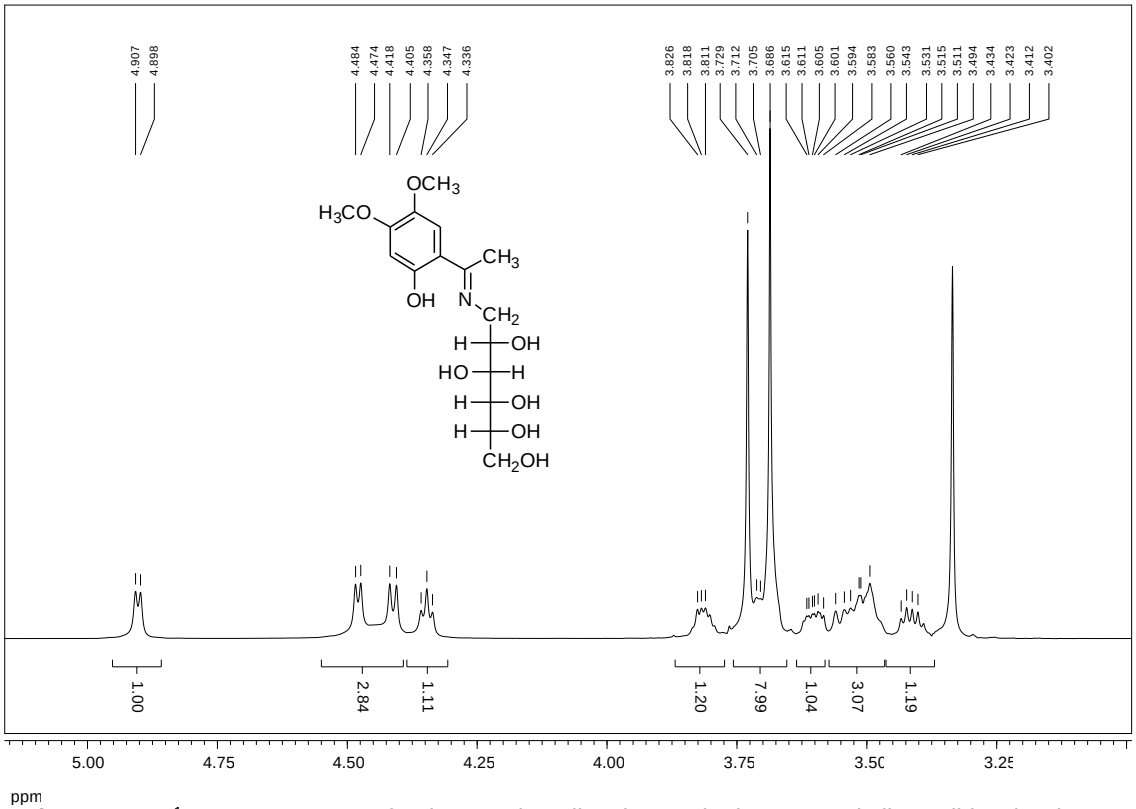


Figure S31a. ^{1}H NMR spectrum of 1-deoxy-1-(4,5-dimethoxy-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**15**), recorded in DMSO-*d*$_6$ (magnified zone between 3.0 and 5.0 ppm).

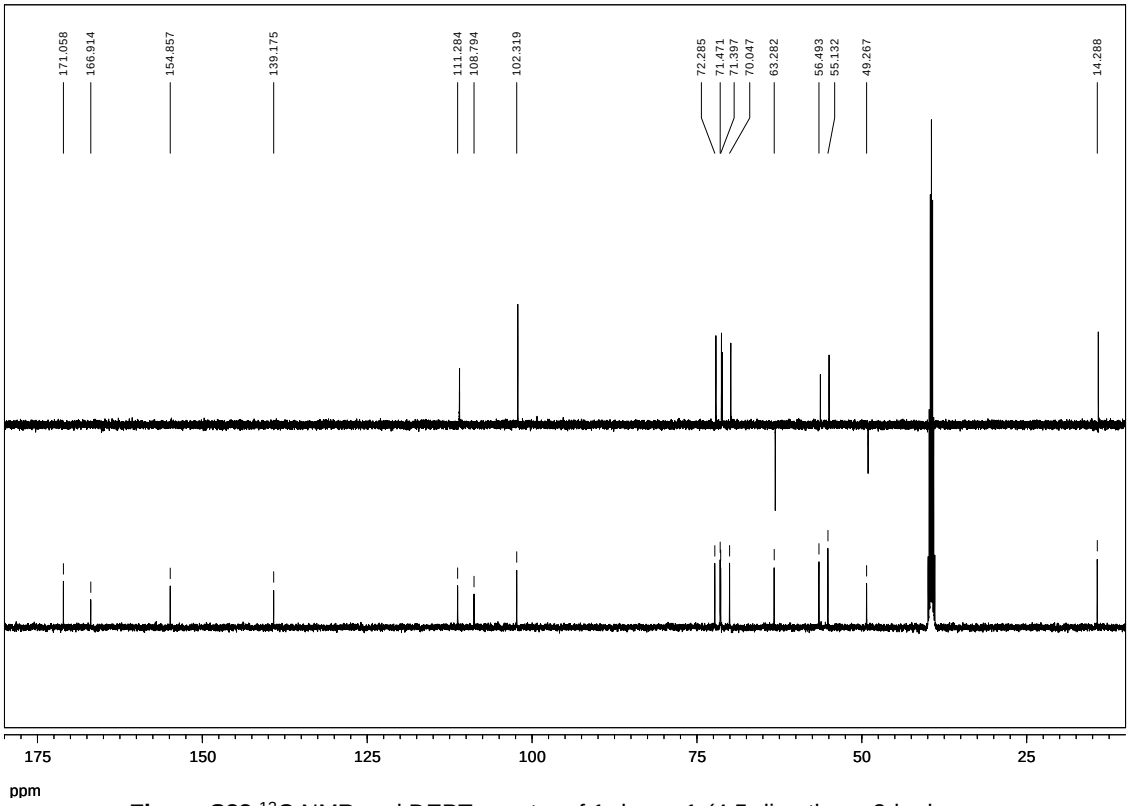


Figure S32 ^{13}C NMR and DEPT spectra of 1-deoxy-1-(4,5-dimethoxy-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**15**), recorded in DMSO-*d*$_6$.

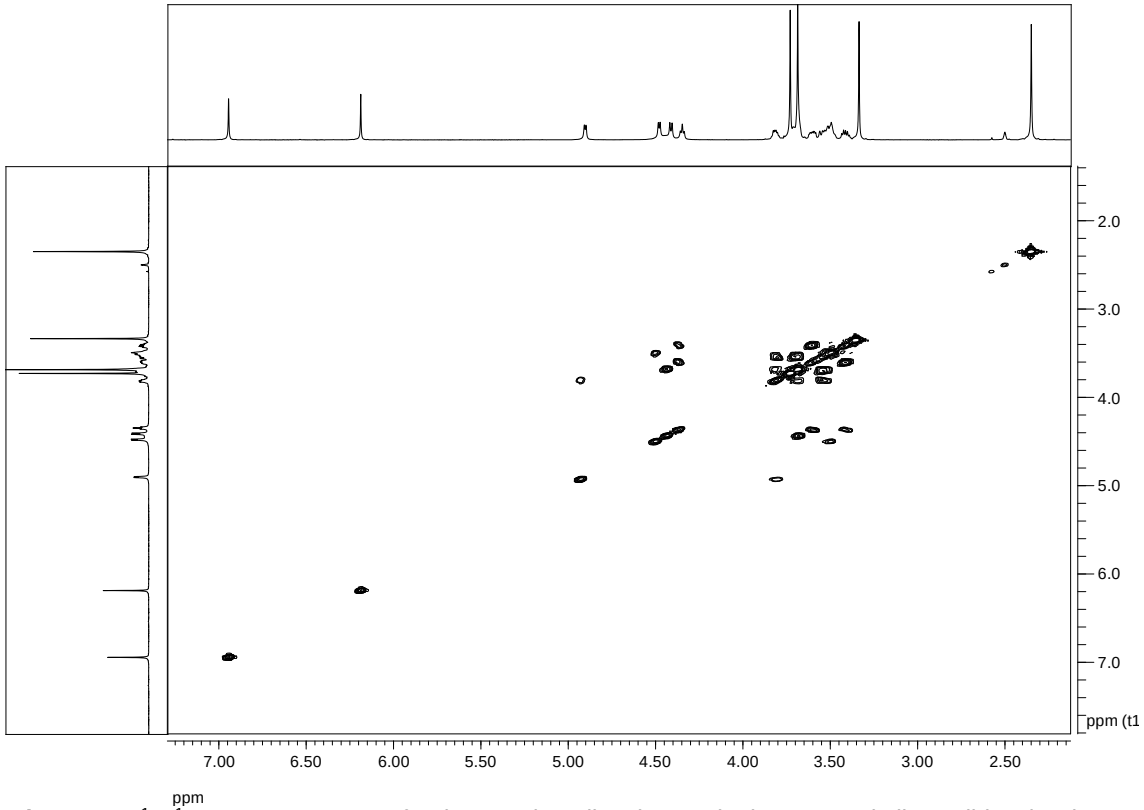


Figure S33 ^{1}H-^{1}H COSY spectrum of 1-deoxy-1-(4,5-dimethoxy-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**15**), recorded in DMSO-*d*$_6$.

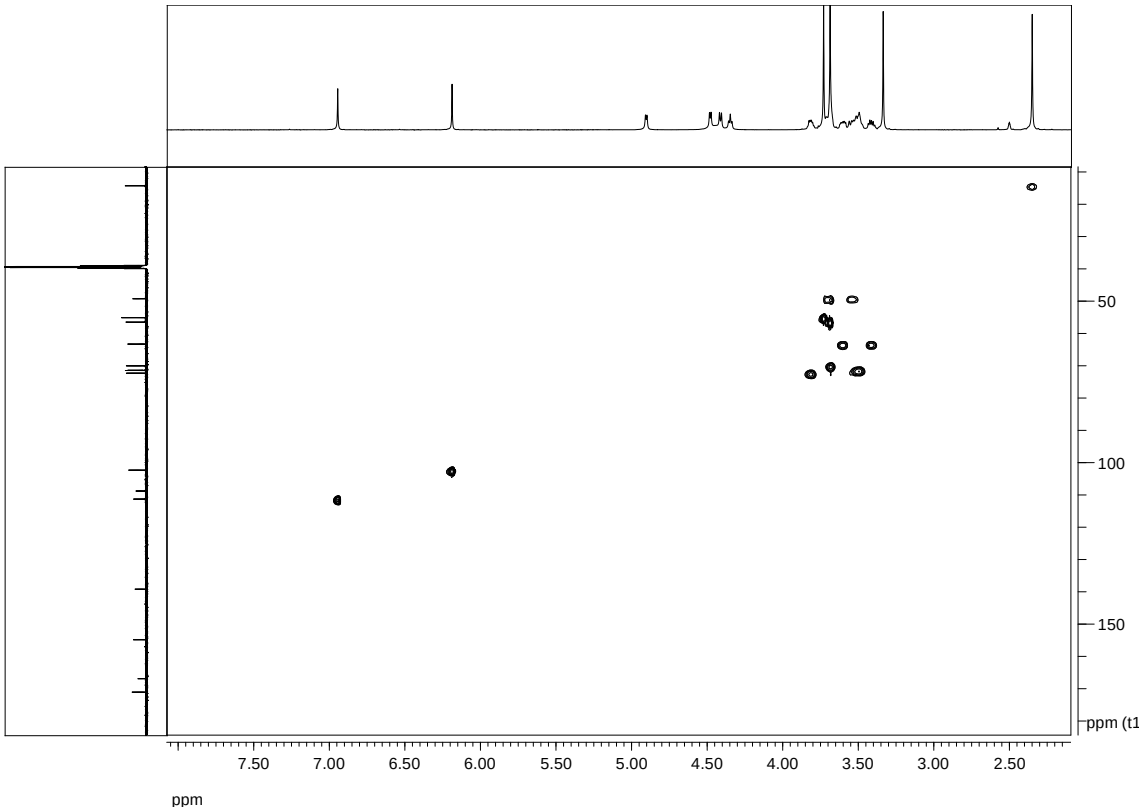


Figure S34. HMQC spectrum of 1-deoxy-1-(4,5-dimethoxy-2-hydroxy-α-methylbenzylidene)amino-D-glucitol (**15**), recorded in DMSO-d_6.

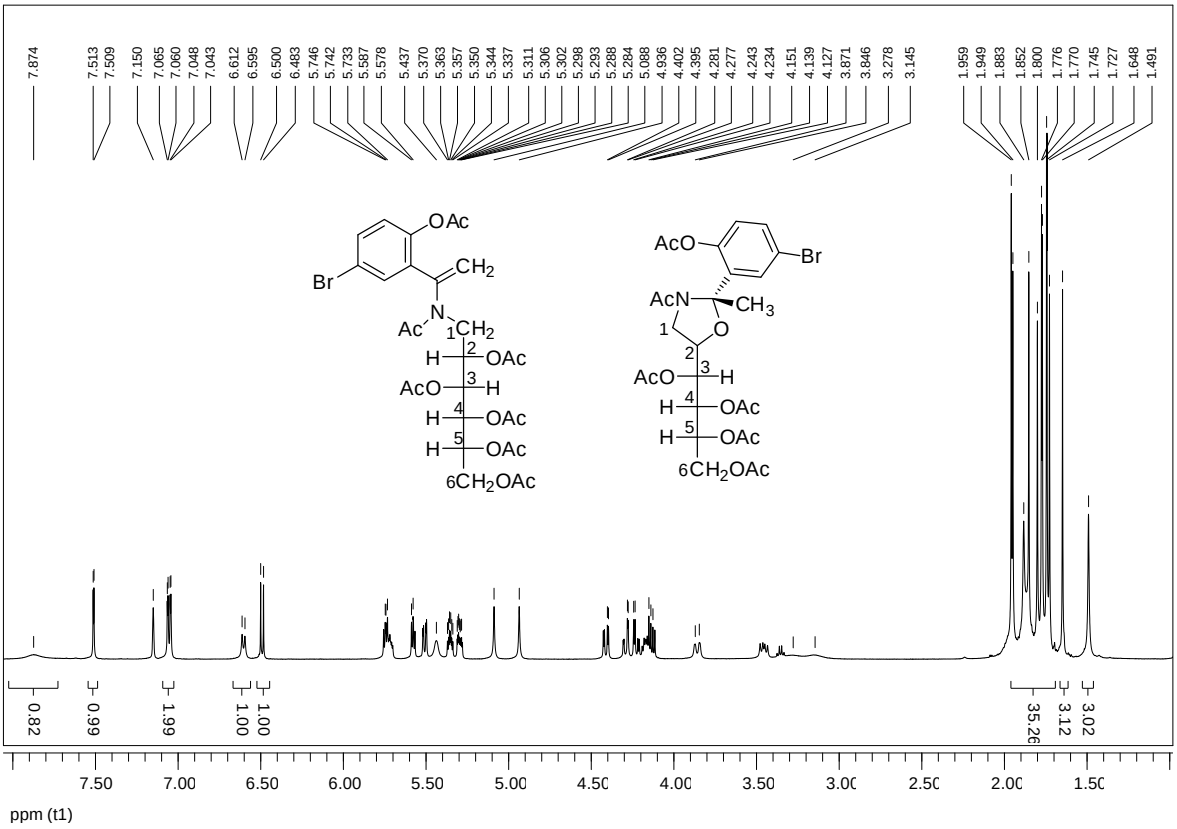


Figure S35. ^{1}H NMR spectrum of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**), recorded in benzene-d_6.

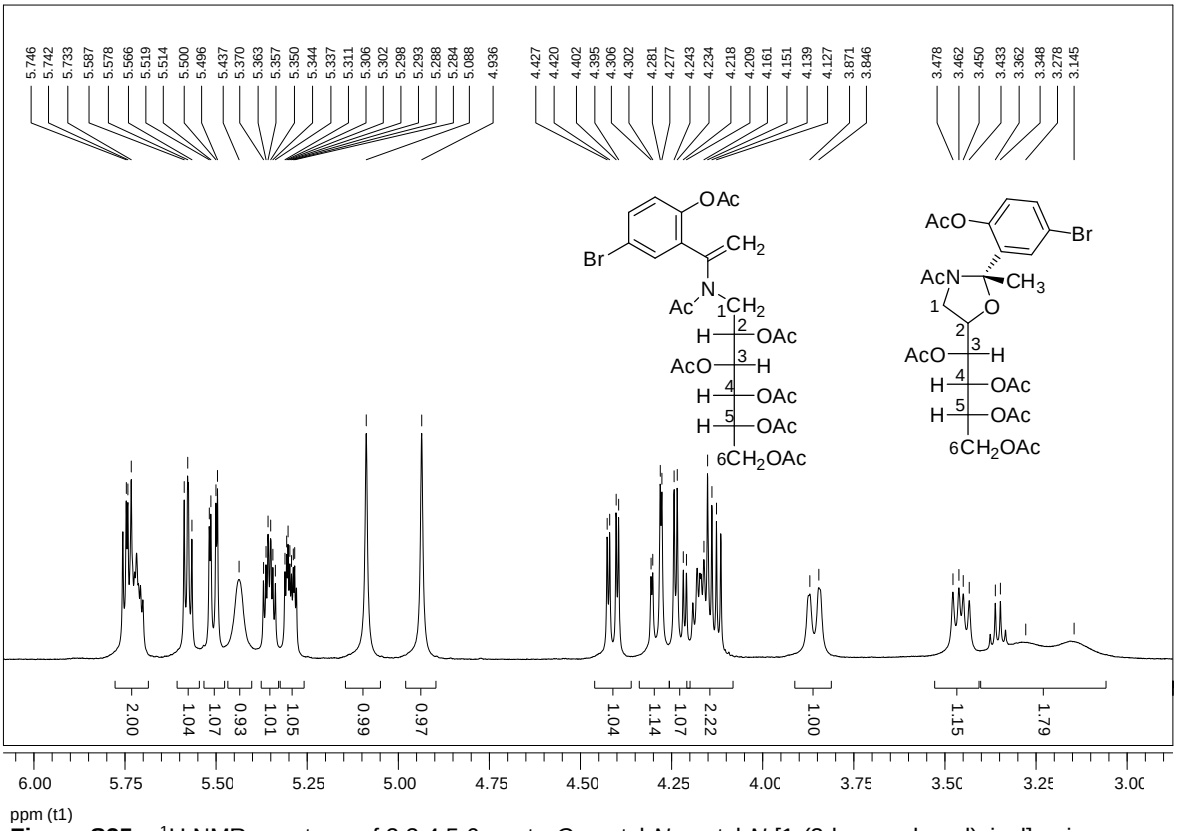


Figure S35a. ^{1}H NMR spectrum of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**), recorded in benzene-d_6 (magnified zone between 3.0 and 6.0 ppm).

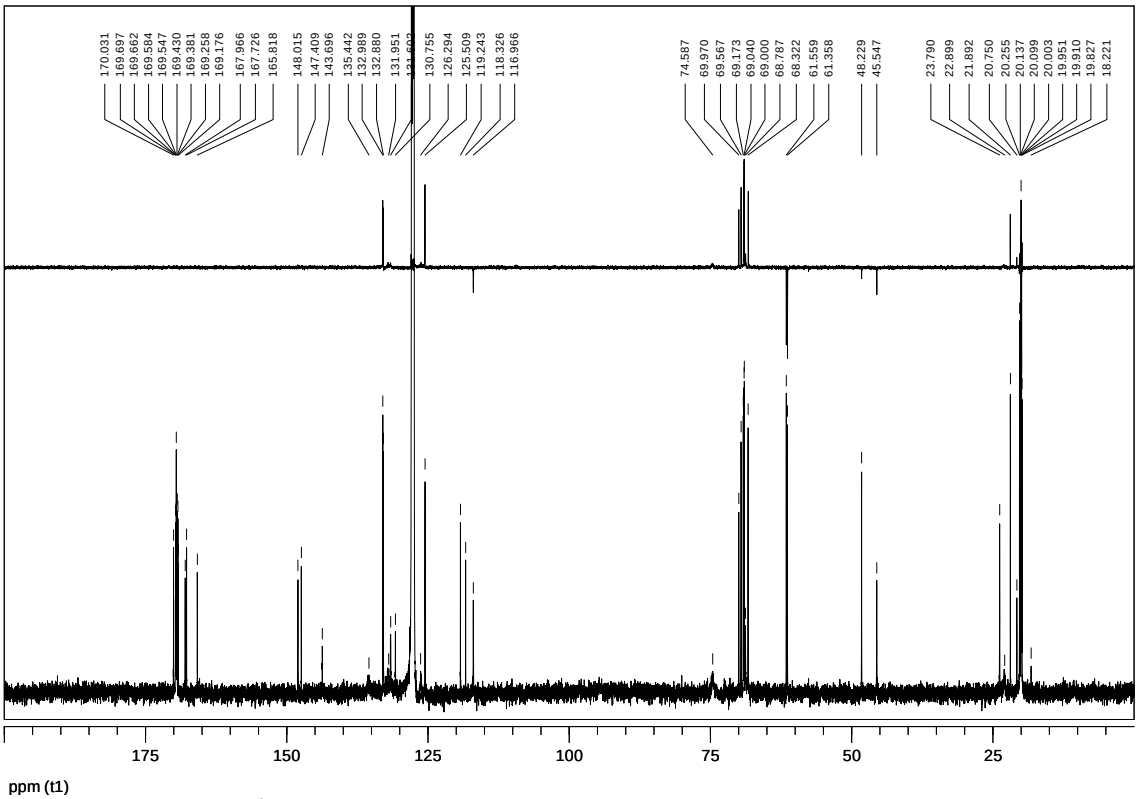


Figure S36. ^{13}C NMR and DEPT spectra of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**), recorded in benzene-d_6.

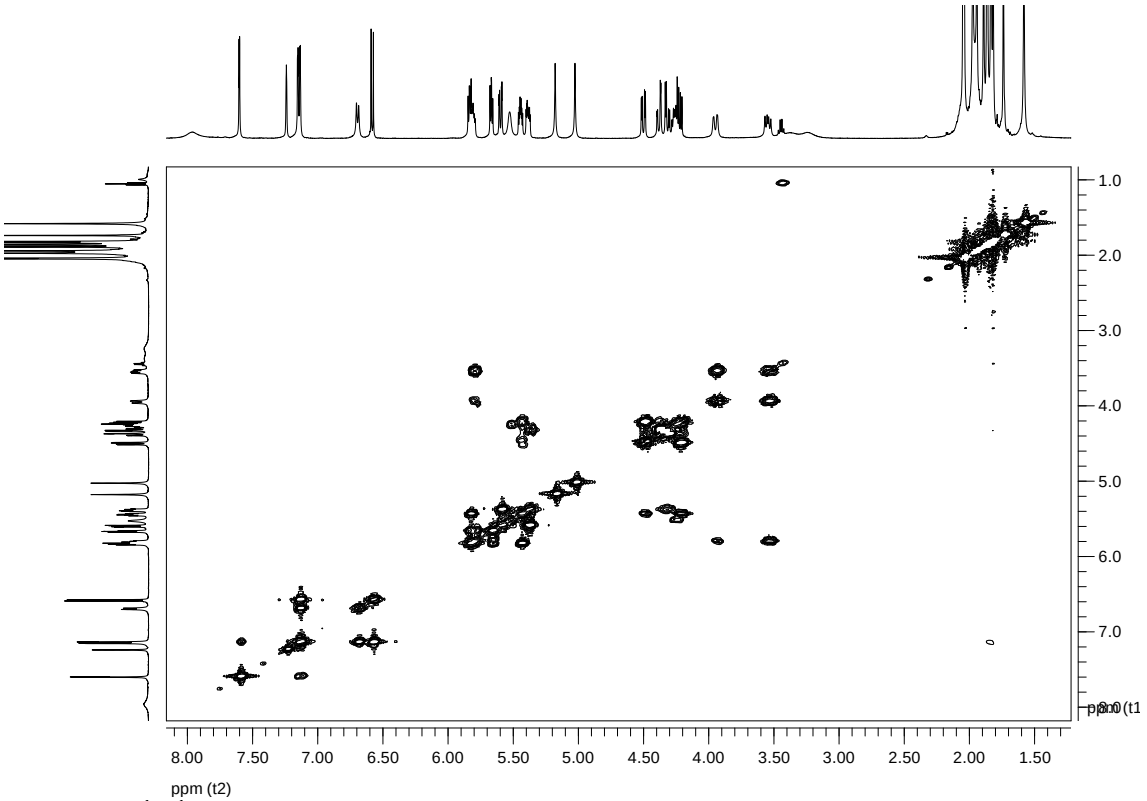


Figure S37. ^{1}H-^{1}H COSY spectrum of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**), recorded in benzene-d_6.

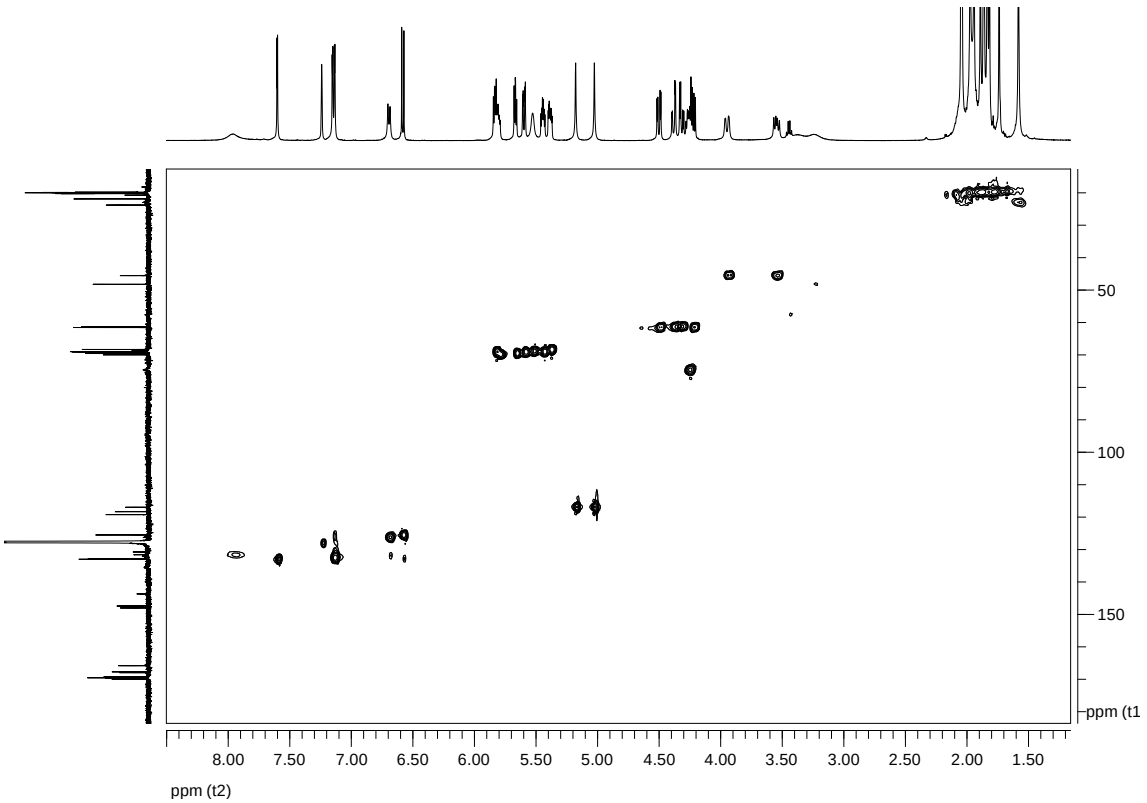


Figure S38. HMQC spectrum of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**), recorded in benzene-d_6.

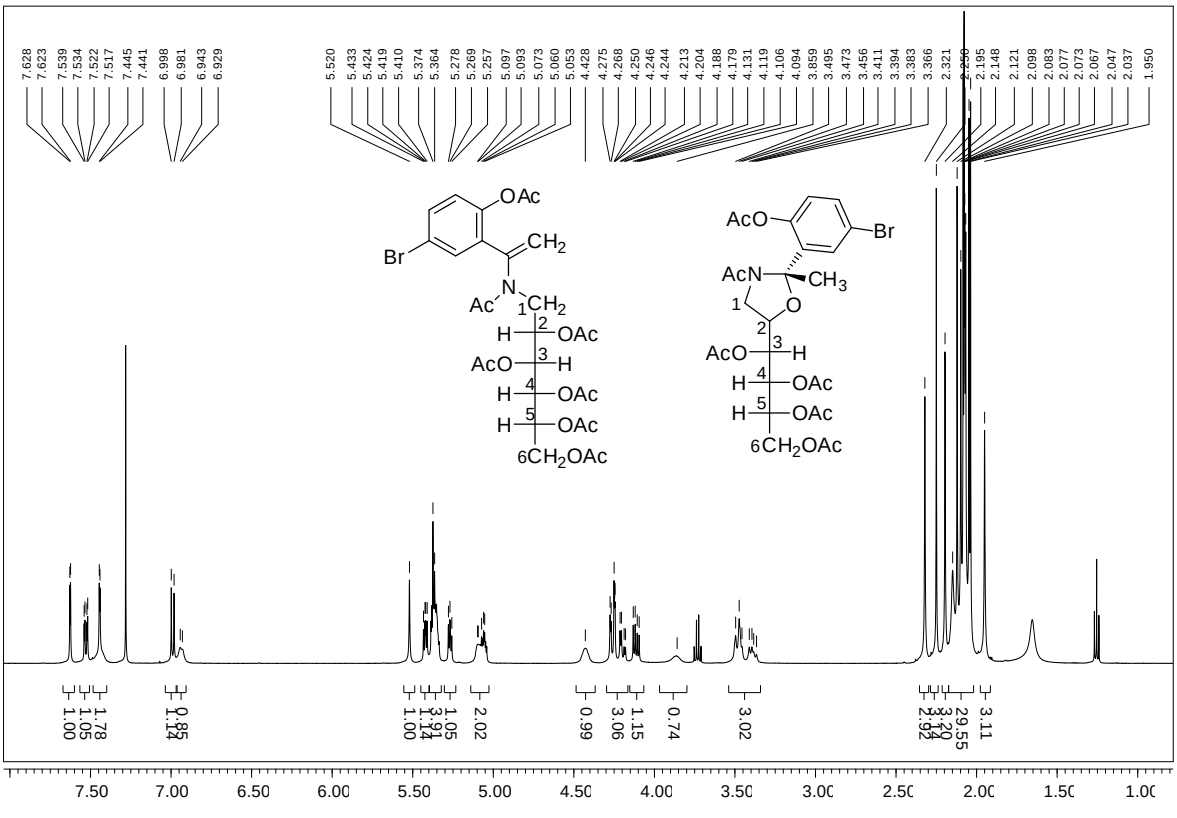


Figure S39. ^{1}H NMR spectrum of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**), recorded in $CDCl_3$.

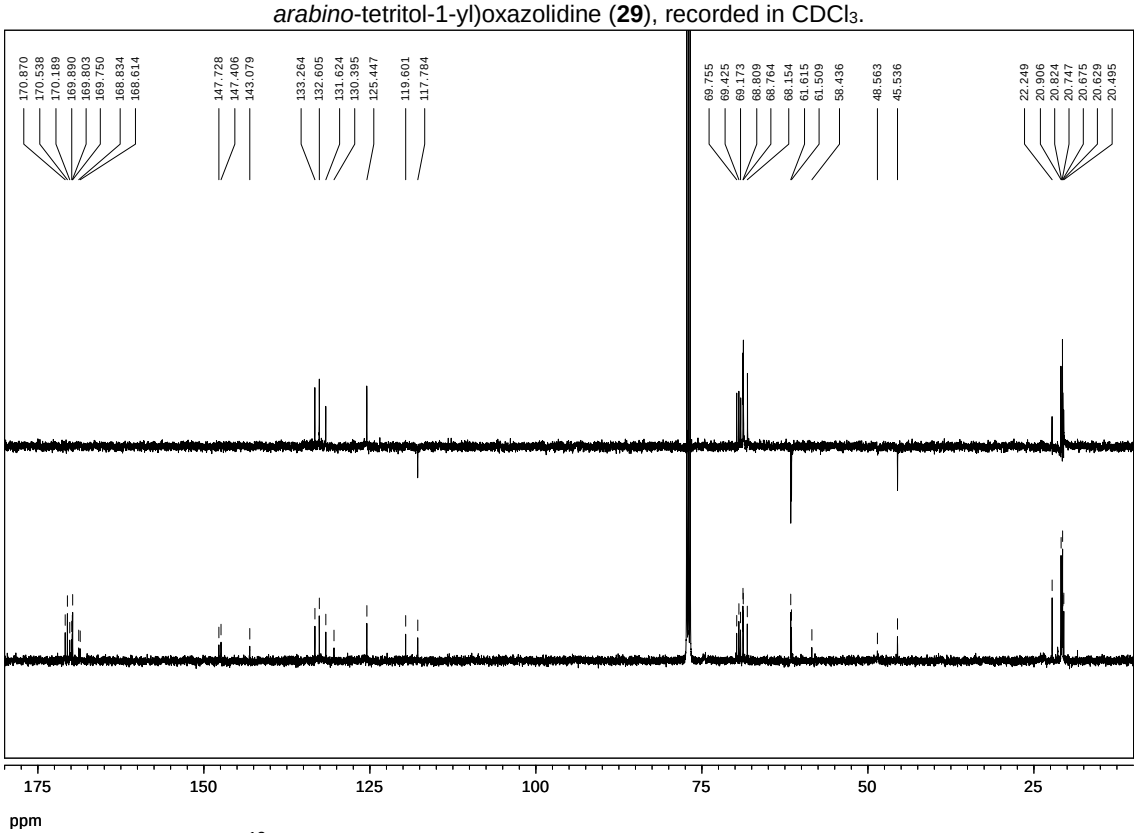


Figure S40. ^{13}C NMR and DEPT spectra of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**), recorded in $CDCl_3$.

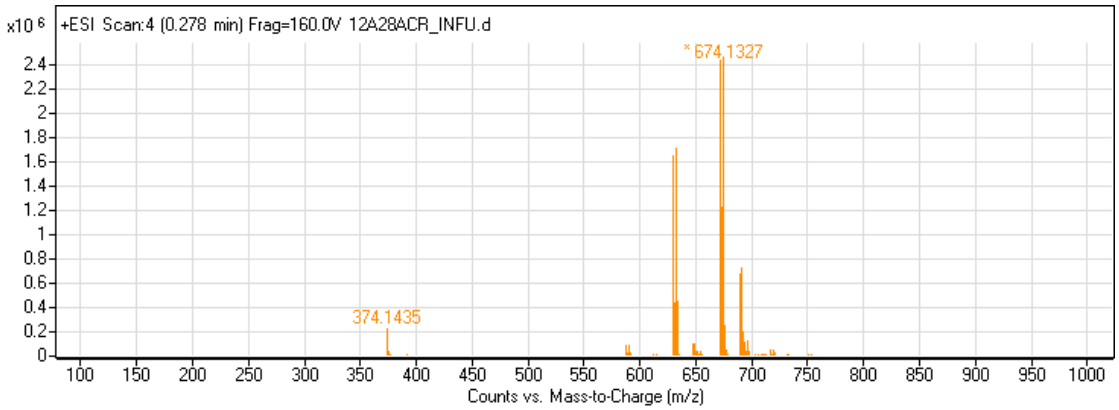


Figure S41. Mass spectrum of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**) and (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**).

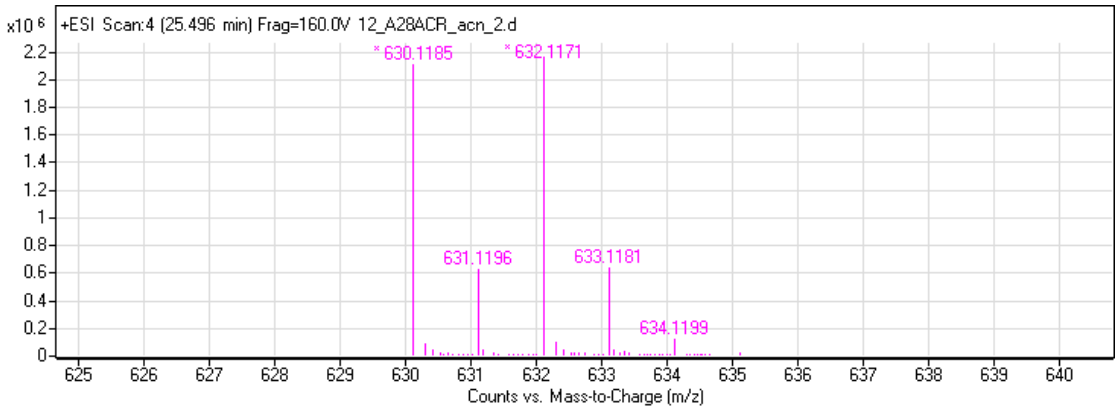
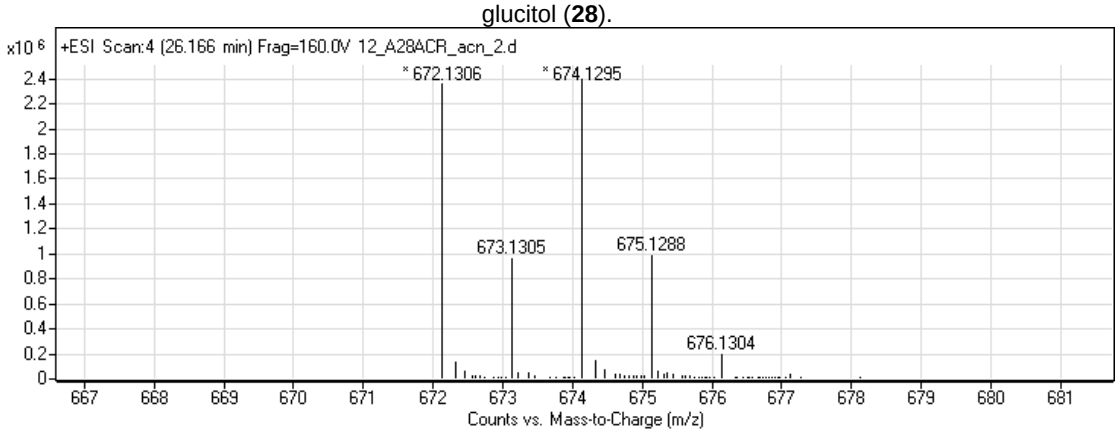


Figure S42. Mass spectrum of 2,3,4,5,6-penta-*O*-acetyl-*N*-acetyl-*N*-[1-(3-bromophenyl)vinyl]amino-D-glucitol (**28**).



FigureS43. Mass spectrum of (2*S*, 3*E*, 5*S*)-3-acetyl-2-(2-acetoxy-5-bromophenyl)-2-methyl-5-(1,2,3,4-tetra-*O*-acetyl-D-*arabino*-tetritol-1-yl)oxazolidine (**29**).

Additional information on NMR data

Coupled ^{13}C NMR spectra were recorded in order to assess the coupling pattern involving carbon atoms with the protons located in neighboring atoms. Thus, the phenolic carbon will have as neighbors one or two protons, depending on either enamine (C3-H) or imine structure (C3-H and phenolic OH). On the other hand, the iminic carbon will have as neighbors at least the three hydrogens of the methyl group and, in the enamine structure, that of the NH. Accordingly, the multiplicity of the C=N signal must be greater than that of aromatic C-OH, which could be used to distinguish the chemical environments of both carbon atoms. The coupled spectra of **10**, **13** and **14** show well-differentiated signals, whose identification, on the basis of previous work by Hansen and Filarowski[7] shows no ambiguity, and the coupling patterns allow the assignment of the homonymous signals of **12** (Table S4). As explicitly displayed in Figure S44, the aromatic C-OH signal resonates as triplet in **10** and **13**, whilst for **14** it is a double doublet; the latter exhibiting the same multiplicity as the signal recorded for **12** at ~178 ppm. Moreover, the C=N signal appears in all cases as broad multiplet. In addition, the HMBC spectra of **8** and **14** (Figures S12 and S30) show the C2 signal at ~165 ppm, while in the case of **12** it is observed at ~178 ppm (Figure S23). In summary, this analysis shows that the C2 signal at ~178 ppm for **12** is very close to that of a carbonyl carbon.

7. P. E. Hansen and A. Filarowski, *J. Mol. Struct.*, 2004, **707**, 69-81.

Table S3. IR data[a] and proton chemical shifts ((δ, ppm)[b] for compounds **8**-**15**

Compound	$\bar{\nu}_{max}$ (C=N)	OH (arom)	H-1	H-1'	H-2	H-3	H-4	H-5	H-6	H-6'
8[c]	1617	16.66	3.73	3.59	3.86	3.70	3.49	3.49	3.59	3.41
9[c]	1617	16.98	3.75	3.61	3.84	3.69	3.48	3.48	3.61	3.40
10[c]	1617	15.79	3.70	3.58	3.86	3.70	3.49	3.49	3.58	3.40
11[c]	1608	16.93	3.75	3.60	3.85	3.69	3.49	3.49	3.60	3.40
12[d]	1616	16.61	3.90	3.75	3.85	3.70	3.50	3.50	3.60	3.41
13[d]	1624	16.35	3.73	3.60	3.86	3.69	3.50	3.50	3.58	3.41
14[d]	1627	16.67	3.87	3.74	3.84	3.70	3.43	3.43	3.60	3.39
15[d]	1614	16.50	3.70	3.52	3.82	3.70	3.49	3.49	3.60	3.41

[a] In cm^{-1}; [b]In DMSO-d_6; [c]At 400 MHz; [d] At 500 MHz

Table S4. Carbon chemical shifts (δ, ppm) for compounds **8**-**15**[a]

Compound	C-OH	C=N	C-1	C-2	C-3	C-4, C-5[d]	C-6	CH_3
8[b]	164.8	172.7	51.3	72.5	70.0	71.5, 71.5	63.3	14.4
9[b]	165.6	172.5	50.8	72.2	70.1	71.4, 71.3	63.3	14.5
10[b]	157.5	171.9	52.0	72.7	70.0	71.7, 71.5	63.3	14.7
11[b]	165.0	172.5	50.9	72.2	70.1	71.4, 71.3	63.3	14.5
12[c]	178.4	176.1	48.7	71.4	70.3	71.2, 70.6	63.3	14.6
13[c]	160.5	171.8	51.7	72.4	70.1	71.5, 71.4	63.3	14.6
14[c]	165.3	175.7	48.7	71.4	70.3	71.0, 70.5	63.3	15.2
15[b]	166.9	171.1	49.3	72.3	70.1	71.5, 71.4	63.3	14.3

[a]In DMSO-d_6; [b]At 100 MHz; [c]At 125 MHz; [d]These two carbons could be interchanged

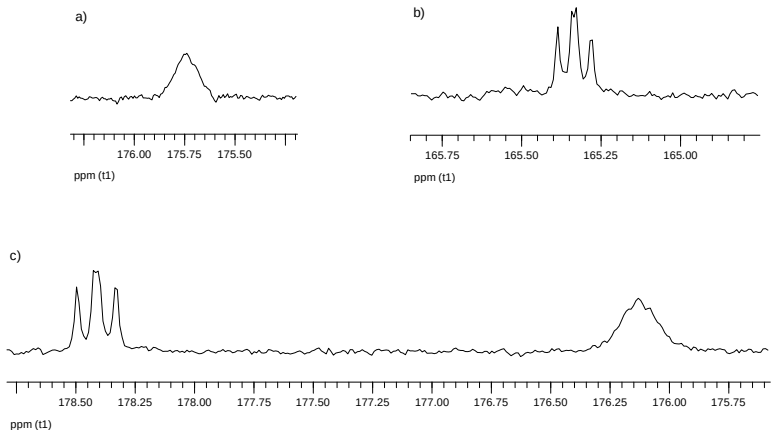


Fig. S44 Zoomed regions of proton-coupled ^{13}C NMR spectra for **14** (a and b) and **12** (c).

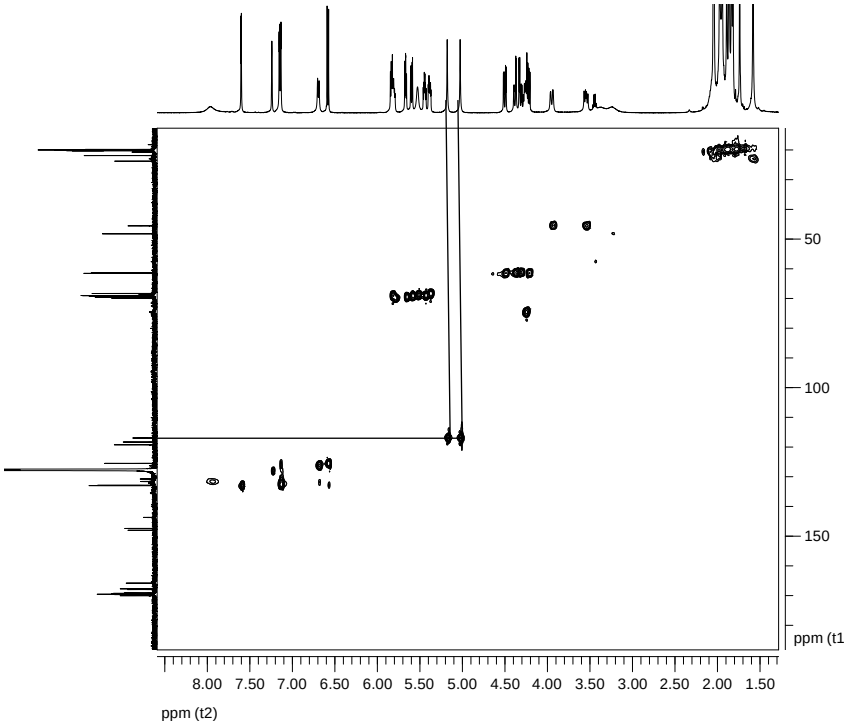


Fig. S45 2D-HMQC spectrum of compound **24**.

Table S5. Geometric and energy data for intramolecular hydrogen bonds in compounds **8-10**, **12**, **16**-**18** and **20**[a]

		D-H···*A*	*d*(*D*-H)[b]	*d*(H···*A*)[b]	*d*(*D*···*A*)[b]	<(*DHA*)[c]	E_{HB}[d,e]
8	G.phase	O-H···N	1.002	1.644	2.560	149.676	-14.6
	DMSO[f]	O-H···N	1.011	1.612	2.542	150.646	-15.7
9	G.phase	O-H···N	1.003	1.642	2.558	149.580	-14.7
	DMSO[f]	O-H···N	1.013	1.607	2.539	150.565	-15.9
10	G.phase	O-H···N	1.000	1.651	2.563	149.280	-14.4
	DMSO[f]	O-H···N	1.008	1.626	2.549	150.136	-15.3
12	G.phase	O-H···N	1.010	1.619	2.545	150.112	-15.5
	DMSO[f]	O-H···N	1.024	1.576	2.522	151.180	-17.1
16	G.phase	N-H···O	1.069	1.525	2.498	148.336	-18.8
	DMSO[f]	N-H···O	1.051	1.608	2.544	145.350	-15.6
17	G.phase	N-H···O	1.065	1.538	2.505	147.881	-18.3
	DMSO[f]	N-H···O	1.051	1.612	2.550	145.803	-15.2
18	G.phase	N-H···O	1.061	1.549	2.508	147.308	-18.1
	DMSO[f]	N-H···O	1.055	1.593	2.539	146.225	-15.9
20	G.phase	N-H···O	1.062	1.559	2.518	147.295	-17.3
	DMSO[f]	N-H···O	1.046	1.648	2.573	144.579	-13.8

[a]At the B3LYP/6-311G(d,p). [b]In degrees. [c]In Å. [d]In kcal/mol. [e]Estimated as described in Ref.29. [f]SMD method.

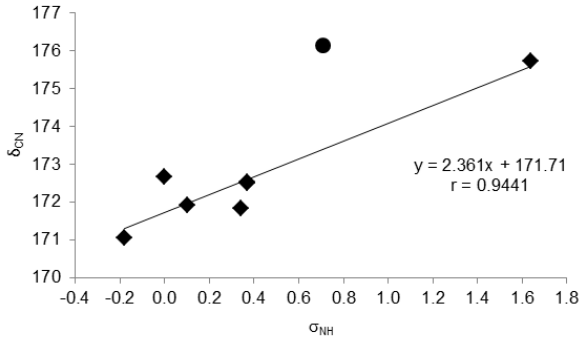


Fig. S46 Linear correlation between chemical shifts ($\delta_{C=N}$) and electronic effects of substituents (plotted against σ_{NH} omitted compound **12**).

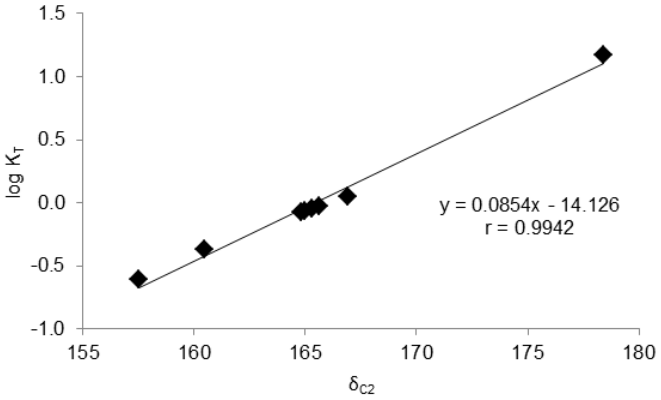


Fig.S47 Linear correlation between tautomeric equilibrium constants and chemical shifts ($\delta_{C\text{-}2}$) for compounds **8**-**15**

Cartesian Coordinates and Calculated Energies at the B3LYP/6-311G(d,p) and M06-2x/6-311G(d,p) level in Gas Phase, $CHCl_3$ and DMSO (SMD Model)

Structure 8 (B3LYP, Gas Phase)

Energy (Hartrees): = - 1052.5031436
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.824636	-0.689756	0.353588
2	1	0	-4.439821	0.158793	0.678521
3	6	0	-4.733027	-1.725584	-0.281518
4	1	0	-4.126340	-2.560393	-0.656221
5	1	0	-5.280699	-1.270750	-1.112813
6	6	0	-2.774064	-0.148562	-0.626890
7	1	0	-2.320487	-0.991581	-1.164393
8	6	0	-1.621143	0.567141	0.125181
9	1	0	-0.875278	-0.190071	0.383784
10	6	0	-0.960487	1.663159	-0.720941
11	1	0	-0.817073	1.307982	-1.743421
12	6	0	0.384996	2.123427	-0.150872
13	8	0	-5.610922	-2.168083	0.762027
14	1	0	-6.096001	-2.937444	0.452263
15	8	0	-3.155719	-1.262791	1.486887
16	1	0	-3.825242	-1.785916	1.947393
17	8	0	-3.448199	0.643784	-1.599875
18	1	0	-3.230450	1.574870	-1.438472
19	8	0	-2.059452	1.238448	1.313925
20	1	0	-2.388120	0.546006	1.905761
21	8	0	-1.857942	2.780489	-0.806768
22	1	0	-2.162425	2.931668	0.100212
23	1	0	0.700442	3.003881	-0.722421
24	1	0	0.228770	2.434122	0.888661
25	7	0	1.363121	1.050525	-0.252157
26	6	0	2.546379	1.128586	0.254587
27	6	0	3.060448	2.345910	0.993890
28	1	0	3.344531	2.084370	2.016502
29	1	0	3.950902	2.743498	0.500126
30	1	0	2.316846	3.137617	1.038502
31	6	0	3.448143	-0.031708	0.103370
32	6	0	4.755802	-0.015331	0.625907
33	6	0	3.015763	-1.211684	-0.567527
34	6	0	5.609808	-1.098480	0.502661
35	1	0	5.110830	0.868427	1.140523
36	6	0	3.887841	-2.304040	-0.686548
37	6	0	5.165636	-2.248588	-0.158350
38	1	0	6.610238	-1.053231	0.915430
39	1	0	3.523811	-3.183814	-1.203231
40	1	0	5.824355	-3.103993	-0.261380
41	8	0	1.794422	-1.325314	-1.102252
42	1	0	1.343099	-0.446930	-0.931015

Structure 8 (B3LYP, DMSO)

Energy (Hartrees): = - 1052.5290417
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.801364	-0.721454	0.359337
2	1	0	-4.446074	0.094838	0.709191
3	6	0	-4.671553	-1.786515	-0.278573
4	1	0	-4.039973	-2.601460	-0.652056
5	1	0	-5.232970	-1.356931	-1.115187
6	6	0	-2.787580	-0.116081	-0.623437
7	1	0	-2.328991	-0.922078	-1.210060
8	6	0	-1.635229	0.597229	0.125195
9	1	0	-0.893410	-0.164403	0.382057
10	6	0	-0.960289	1.682228	-0.723422
11	1	0	-0.814247	1.316637	-1.741691
12	6	0	0.386115	2.138776	-0.154715
13	8	0	-5.548825	-2.258695	0.754203
14	1	0	-5.918881	-3.101779	0.469208
15	8	0	-3.093148	-1.283689	1.477294
16	1	0	-3.741199	-1.829417	1.944666
17	8	0	-3.508761	0.714090	-1.538888
18	1	0	-3.235139	1.631197	-1.379466
19	8	0	-2.075601	1.267257	1.315290

20	1	0	-2.400528	0.569993	1.903823
21	8	0	-1.849513	2.811097	-0.828214
22	1	0	-2.126244	3.007342	0.079581
23	1	0	0.717191	3.008159	-0.733042
24	1	0	0.241367	2.462943	0.881231
25	7	0	1.359215	1.058902	-0.249435
26	6	0	2.535514	1.131253	0.274974
27	6	0	3.049357	2.329453	1.032752
28	1	0	3.316189	2.051791	2.056294
29	1	0	3.953156	2.719835	0.556974
30	1	0	2.314850	3.130041	1.074759
31	6	0	3.431283	-0.037660	0.110935
32	6	0	4.730122	-0.042579	0.653354
33	6	0	3.000448	-1.196845	-0.596507
34	6	0	5.579613	-1.130708	0.513533
35	1	0	5.081643	0.825716	1.195823
36	6	0	3.866112	-2.292522	-0.732369
37	6	0	5.138966	-2.260257	-0.183670
38	1	0	6.574470	-1.102826	0.942055
39	1	0	3.510535	-3.160951	-1.275387
40	1	0	5.792984	-3.117804	-0.300046
41	8	0	1.782493	-1.280504	-1.150014
42	1	0	1.338520	-0.395510	-0.944375

Structure 8 (M06-2X, Gas Phase)

Energy (Hartrees): = - 1052.0721773
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.855835	-0.801392	0.342334
2	1	0	-4.439321	0.004090	0.805896
3	6	0	-4.811969	-1.768242	-0.318218
4	1	0	-4.235480	-2.551754	-0.825960
5	1	0	-5.424461	-1.229723	-1.046925
6	6	0	-2.903724	-0.160934	-0.663194
7	1	0	-2.472817	-0.945399	-1.299380
8	6	0	-1.727731	0.516788	0.064065
9	1	0	-0.957236	-0.238724	0.240462
10	6	0	-1.124531	1.659973	-0.750222
11	1	0	-1.035072	1.360799	-1.796793
12	6	0	0.245757	2.063033	-0.222276
13	8	0	-5.590282	-2.322030	0.737373
14	1	0	-6.136956	-3.026722	0.386343
15	8	0	-3.089155	-1.479214	1.331352
16	1	0	-3.707003	-2.056168	1.794771
17	8	0	-3.665512	0.689272	-1.500245
18	1	0	-3.426625	1.606075	-1.308592
19	8	0	-2.120405	1.113609	1.297174
20	1	0	-2.351305	0.388426	1.889537
21	8	0	-2.014832	2.772646	-0.713574
22	1	0	-2.240286	2.891863	0.218212
23	1	0	0.560863	2.968629	-0.754926
24	1	0	0.150506	2.315447	0.842140
25	7	0	1.182206	0.976499	-0.443177
26	6	0	2.337106	1.035870	0.084873
27	6	0	2.827931	2.190304	0.928833
28	1	0	2.431656	2.107720	1.944647
29	1	0	3.912721	2.200214	0.998881
30	1	0	2.482386	3.134648	0.504592
31	6	0	3.269858	-0.092444	-0.210948
32	6	0	3.226553	-0.701854	-1.464982
33	6	0	4.174535	-0.589382	0.735808
34	6	0	4.069315	-1.753880	-1.793245
35	1	0	2.505525	-0.321402	-2.177890
36	6	0	5.021150	-1.647923	0.414749
37	6	0	4.972204	-2.224810	-0.846520
38	1	0	4.022633	-2.202036	-2.777489
39	1	0	5.712203	-2.023704	1.163362
40	1	0	5.638070	-3.045763	-1.083892
41	8	0	4.178963	-0.028845	1.979195
42	1	0	4.820624	-0.486152	2.528695

Structure 8 (M06-2X, DMSO)

Energy (Hartrees): = - 1052.1009678
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-3.840567	-0.848573	0.320050
2	1	0	-4.443868	-0.103338	0.854399
3	6	0	-4.768841	-1.814289	-0.379774
4	1	0	-4.173554	-2.542743	-0.942703
5	1	0	-5.419652	-1.268558	-1.070188
6	6	0	-2.944381	-0.097024	-0.660803
7	1	0	-2.522623	-0.808423	-1.382907
8	6	0	-1.758337	0.544018	0.075800
9	1	0	-0.999772	-0.229716	0.221086
10	6	0	-1.136399	1.697297	-0.709966
11	1	0	-1.058709	1.422607	-1.764795
12	6	0	0.243762	2.067191	-0.183251
13	8	0	-5.514684	-2.458355	0.648557
14	1	0	-5.948498	-3.229745	0.271966
15	8	0	-3.015577	-1.555150	1.241897
16	1	0	-3.596749	-2.187690	1.682319
17	8	0	-3.759494	0.820437	-1.376722
18	1	0	-3.454003	1.713810	-1.170626
19	8	0	-2.136611	1.103831	1.330733
20	1	0	-2.363026	0.360244	1.902638
21	8	0	-2.004602	2.830457	-0.644847
22	1	0	-2.190934	2.964336	0.294647
23	1	0	0.581562	2.970835	-0.704593
24	1	0	0.165197	2.311046	0.884236
25	7	0	1.164332	0.966346	-0.415414
26	6	0	2.333538	1.036405	0.084418
27	6	0	2.834163	2.205459	0.895203
28	1	0	2.333051	2.239016	1.867169
29	1	0	3.906698	2.152999	1.063890
30	1	0	2.599164	3.136225	0.371888
31	6	0	3.269892	-0.085874	-0.221772
32	6	0	3.293045	-0.635972	-1.504757
33	6	0	4.121230	-0.627262	0.752237
34	6	0	4.151785	-1.676949	-1.833048
35	1	0	2.623923	-0.219012	-2.248627
36	6	0	4.983594	-1.674814	0.430742
37	6	0	5.000427	-2.193273	-0.857633
38	1	0	4.162129	-2.078602	-2.838824
39	1	0	5.631576	-2.085160	1.199486
40	1	0	5.677088	-3.006109	-1.094880
41	8	0	4.050575	-0.124896	2.012037
42	1	0	4.686349	-0.585078	2.574388

Structure 9 (B3LYP, Gas Phase)

Energy (Hartrees): = - 3626.0448746
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.051679	-0.893776	0.479526
2	1	0	-5.696306	-0.105533	0.888769
3	6	0	-5.934619	-1.957046	-0.146523
4	1	0	-5.303967	-2.730219	-0.604821
5	1	0	-6.567923	-1.500906	-0.913735
6	6	0	-4.107992	-0.238057	-0.538823
7	1	0	-3.637179	-1.023138	-1.144507
8	6	0	-2.956192	0.523646	0.169927
9	1	0	-2.140390	-0.187436	0.331501
10	6	0	-2.442904	1.710070	-0.656114
11	1	0	-2.351937	1.421963	-1.705382
12	6	0	-1.095279	2.240937	-0.156563
13	8	0	-6.705420	-2.506543	0.929946
14	1	0	-7.163074	-3.290245	0.614360
15	8	0	-4.270198	-1.473754	1.534601
16	1	0	-4.871560	-2.061696	2.010908
17	8	0	-4.895442	0.545878	-1.429947
18	1	0	-4.750469	1.481891	-1.222766
19	8	0	-3.349469	1.097343	1.423181
20	1	0	-3.590913	0.353175	1.994224
21	8	0	-3.422154	2.757919	-0.611219
22	1	0	-3.671362	2.833357	0.321853
23	1	0	-0.887600	3.173527	-0.693392
24	1	0	-1.192437	2.478386	0.908993
25	7	0	-0.050681	1.254960	-0.393937
26	6	0	1.157440	1.396260	0.030938
27	6	0	1.640392	2.601363	0.807943
28	1	0	2.032097	2.300034	1.782940
29	1	0	2.450916	3.101759	0.271305
30	1	0	0.845045	3.324647	0.968833
31	6	0	2.123831	0.314978	-0.261792

32	6	0	3.461247	0.406225	0.167734
33	6	0	1.724565	-0.851203	-0.973683
34	6	0	4.363523	-0.607632	-0.093301
35	1	0	3.797344	1.277946	0.710591
36	6	0	2.661969	-1.864451	-1.224003
37	6	0	3.970764	-1.751712	-0.790116
38	1	0	2.327952	-2.739544	-1.767762
39	1	0	4.683028	-2.541798	-0.990376
40	8	0	0.478706	-1.025860	-1.423695
41	1	0	-0.020322	-0.195559	-1.162044
42	35	0	6.179579	-0.442652	0.510978

Structure 9 (B3LYP, DMSO)

Energy (Hartrees): = - 3626.0725497
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.987265	-0.966598	0.475440
2	1	0	-5.680539	-0.255540	0.942166
3	6	0	-5.790639	-2.075872	-0.175760
4	1	0	-5.109518	-2.777334	-0.672342
5	1	0	-6.476843	-1.655848	-0.919234
6	6	0	-4.135902	-0.178493	-0.532165
7	1	0	-3.661334	-0.879793	-1.231049
8	6	0	-2.987585	0.575817	0.177013
9	1	0	-2.178348	-0.143431	0.332276
10	6	0	-2.454483	1.755721	-0.644456
11	1	0	-2.353227	1.461076	-1.691090
12	6	0	-1.106753	2.278618	-0.139113
13	8	0	-6.503446	-2.728982	0.885027
14	1	0	-6.803214	-3.585843	0.561159
15	8	0	-4.126088	-1.525651	1.481546
16	1	0	-4.667539	-2.176765	1.949544
17	8	0	-5.020026	0.652963	-1.289987
18	1	0	-4.767942	1.575300	-1.125885
19	8	0	-3.385150	1.137871	1.435898
20	1	0	-3.595394	0.382860	2.004361
21	8	0	-3.426691	2.818724	-0.620663
22	1	0	-3.652752	2.943384	0.313442
23	1	0	-0.880040	3.204111	-0.679057
24	1	0	-1.195311	2.524468	0.924551
25	7	0	-0.067976	1.283537	-0.370531
26	6	0	1.139679	1.424291	0.056560
27	6	0	1.631163	2.616624	0.835521
28	1	0	2.046069	2.301839	1.796899
29	1	0	2.430274	3.125357	0.288545
30	1	0	0.837309	3.335102	1.024030
31	6	0	2.097501	0.333023	-0.249750
32	6	0	3.437248	0.413058	0.170716
33	6	0	1.684946	-0.823895	-0.969482
34	6	0	4.327174	-0.609446	-0.106571
35	1	0	3.775944	1.282937	0.715418
36	6	0	2.610513	-1.844322	-1.233288
37	6	0	3.924887	-1.746824	-0.806678
38	1	0	2.273771	-2.717142	-1.780296
39	1	0	4.622972	-2.546553	-1.020073
40	8	0	0.432519	-0.976551	-1.413356
41	1	0	-0.052696	-0.134971	-1.126591
42	35	0	6.155781	-0.462434	0.486037

Structure 9 (M06-2X, Gas Phase)

Energy (Hartrees): = - 3625.6590079
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.925476	-0.942451	0.498449
2	1	0	-5.579881	-0.188263	0.954308
3	6	0	-5.789312	-2.009627	-0.135015
4	1	0	-5.142598	-2.741977	-0.634525
5	1	0	-6.459245	-1.549360	-0.866780
6	6	0	-4.044807	-0.235259	-0.527802
7	1	0	-3.558664	-0.988349	-1.161374
8	6	0	-2.918177	0.547794	0.175269
9	1	0	-2.079412	-0.138763	0.326786
10	6	0	-2.454685	1.752911	-0.644343

11	1	0	-2.373671	1.479007	-1.699145
12	6	0	-1.114552	2.284768	-0.148597
13	8	0	-6.498728	-2.614972	0.939720
14	1	0	-6.968448	-3.383588	0.611798
15	8	0	-4.089649	-1.526693	1.491307
16	1	0	-4.642200	-2.159051	1.965387
17	8	0	-4.878397	0.535852	-1.371222
18	1	0	-4.776177	1.468491	-1.142052
19	8	0	-3.322790	1.098987	1.423941
20	1	0	-3.497036	0.351236	2.009069
21	8	0	-3.440582	2.774028	-0.559911
22	1	0	-3.656546	2.849048	0.379159
23	1	0	-0.904201	3.224603	-0.669585
24	1	0	-1.205557	2.494751	0.923651
25	7	0	-0.083035	1.297115	-0.412918
26	6	0	1.114969	1.420534	0.020157
27	6	0	1.604394	2.599157	0.824472
28	1	0	1.959537	2.267029	1.802532
29	1	0	2.442085	3.078577	0.313480
30	1	0	0.823773	3.340316	0.971382
31	6	0	2.078716	0.337384	-0.287450
32	6	0	3.403949	0.413824	0.164996
33	6	0	1.680460	-0.803283	-1.025693
34	6	0	4.303331	-0.597065	-0.104988
35	1	0	3.736426	1.270056	0.736165
36	6	0	2.613915	-1.813262	-1.288926
37	6	0	3.914018	-1.718486	-0.834906
38	1	0	2.280253	-2.671450	-1.858455
39	1	0	4.627605	-2.505622	-1.042016
40	8	0	0.442701	-0.965113	-1.491944
41	1	0	-0.059655	-0.147194	-1.225145
42	35	0	6.088970	-0.464790	0.532198

Structure 9 (M06-2X, DMSO)

Energy (Hartrees): = - 3625.6876563
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.872054	-1.002261	-0.489754
2	1	0	5.546824	-0.309967	-1.009573
3	6	0	5.696254	-2.086632	0.165260
4	1	0	5.029734	-2.766912	0.708787
5	1	0	6.408509	-1.641248	0.866913
6	6	0	4.070923	-0.189466	0.524726
7	1	0	3.588390	-0.871658	1.236790
8	6	0	2.946670	0.585535	-0.181070
9	1	0	2.114862	-0.109362	-0.329761
10	6	0	2.462161	1.785721	0.632449
11	1	0	2.373053	1.507363	1.685716
12	6	0	1.121196	2.309332	0.131892
13	8	0	6.357439	-2.768187	-0.896018
14	1	0	6.732469	-3.582815	-0.548016
15	8	0	3.965787	-1.585498	-1.422286
16	1	0	4.471162	-2.258664	-1.895108
17	8	0	4.981379	0.622024	1.252795
18	1	0	4.789901	1.546415	1.046465
19	8	0	3.359466	1.126492	-1.432570
20	1	0	3.508168	0.373087	-2.017479
21	8	0	3.440473	2.822128	0.563073
22	1	0	3.630252	2.942254	-0.377832
23	1	0	0.890066	3.239404	0.660521
24	1	0	1.204367	2.533802	-0.937586
25	7	0	0.095930	1.309775	0.381669
26	6	0	-1.106067	1.445933	-0.038481
27	6	0	-1.607233	2.630601	-0.814898
28	1	0	-1.983990	2.308711	-1.788964
29	1	0	-2.435404	3.104027	-0.281804
30	1	0	-0.828571	3.372690	-0.969960
31	6	0	-2.060865	0.349740	0.269979
32	6	0	-3.391583	0.424389	-0.162997
33	6	0	-1.644789	-0.794880	0.993474
34	6	0	-4.277825	-0.599016	0.113016
35	1	0	-3.729022	1.289359	-0.719140
36	6	0	-2.565746	-1.814915	1.260993
37	6	0	-3.874591	-1.725757	0.825230
38	1	0	-2.227258	-2.681049	1.817120
39	1	0	-4.573662	-2.524904	1.038930
40	8	0	-0.396826	-0.942038	1.440291
41	1	0	0.089902	-0.108516	1.153171
42	35	0	-6.079325	-0.475421	-0.498059

Structure 10 (B3LYP, Gas Phase)

Energy (Hartrees): = - 1167.053118
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.467317	-0.732823	0.453863
2	1	0	-5.084556	0.098362	0.817423
3	6	0	-5.381582	-1.776337	-0.159926
4	1	0	-4.775168	-2.593276	-0.572517
5	1	0	-5.971270	-1.319365	-0.960754
6	6	0	-3.469845	-0.156496	-0.561592
7	1	0	-3.026294	-0.981943	-1.133694
8	6	0	-2.296901	0.566171	0.150625
9	1	0	-1.530409	-0.183255	0.368341
10	6	0	-1.688649	1.681918	-0.708983
11	1	0	-1.588798	1.342007	-1.741830
12	6	0	-0.322637	2.150410	-0.197839
13	8	0	-6.207378	-2.251945	0.911217
14	1	0	-6.689294	-3.026392	0.609286
15	8	0	-3.740846	-1.309572	1.549046
16	1	0	-4.380291	-1.853237	2.028103
17	8	0	-4.200260	0.640603	-1.489327
18	1	0	-3.987585	1.572161	-1.324085
19	8	0	-2.694354	1.215846	1.365532
20	1	0	-2.985260	0.510857	1.962167
21	8	0	-2.602612	2.788790	-0.737821
22	1	0	-2.868824	2.922009	0.183884
23	1	0	-0.048431	3.045631	-0.767872
24	1	0	-0.429804	2.440598	0.854236
25	7	0	0.660344	1.090466	-0.362967
26	6	0	1.882962	1.199805	0.033996
27	6	0	2.435412	2.443675	0.698323
28	1	0	2.826153	2.208619	1.691893
29	1	0	3.260913	2.854904	0.111050
30	1	0	1.678664	3.216892	0.804841
31	6	0	2.788953	0.051872	-0.170060
32	6	0	4.144171	0.119741	0.232479
33	6	0	2.318421	-1.147389	-0.761189
34	6	0	5.003236	-0.953552	0.059884
35	1	0	4.511596	1.029777	0.681981
36	6	0	3.203572	-2.225763	-0.925666
37	6	0	4.518966	-2.135183	-0.523840
38	1	0	2.817593	-3.130578	-1.379117
39	1	0	5.202775	-2.965947	-0.650804
40	8	0	1.053970	-1.305982	-1.181454
41	1	0	0.602199	-0.432285	-0.999239
42	8	0	6.325875	-0.970261	0.418712
43	6	0	6.874119	0.194699	1.009144
44	1	0	6.817402	1.056490	0.332783
45	1	0	6.373893	0.444138	1.953019
46	1	0	7.919949	-0.033757	1.209122

Structure 10 (B3LYP, DMSO)

Energy (Hartrees): = - 1167.080843
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.476439	-0.743484	0.447247
2	1	0	-5.114244	0.070684	0.814240
3	6	0	-5.359535	-1.807347	-0.174503
4	1	0	-4.735519	-2.623200	-0.558535
5	1	0	-5.934221	-1.376533	-1.001404
6	6	0	-3.486970	-0.134667	-0.557726
7	1	0	-3.040922	-0.939135	-1.155777
8	6	0	-2.318042	0.582417	0.162087
9	1	0	-1.562290	-0.174306	0.391627
10	6	0	-1.680032	1.679205	-0.700172
11	1	0	-1.568952	1.322910	-1.726155
12	6	0	-0.315466	2.140021	-0.181648
13	8	0	-6.219777	-2.277756	0.873122
14	1	0	-6.596402	-3.120038	0.594406
15	8	0	-3.741541	-1.307698	1.547049
16	1	0	-4.377940	-1.853283	2.030214
17	8	0	-4.231041	0.693307	-1.456799

18	1	0	-3.970591	1.613040	-1.290385
19	8	0	-2.726962	1.240545	1.369980
20	1	0	-3.035207	0.537293	1.960502
21	8	0	-2.580918	2.802107	-0.763175
22	1	0	-2.829918	2.985014	0.155329
23	1	0	-0.024481	3.028495	-0.752191
24	1	0	-0.412625	2.436249	0.868801
25	7	0	0.664073	1.073542	-0.340356
26	6	0	1.890299	1.198578	0.041148
27	6	0	2.448256	2.446076	0.679589
28	1	0	2.832018	2.226328	1.679896
29	1	0	3.283473	2.834718	0.090495
30	1	0	1.699171	3.229410	0.765721
31	6	0	2.794697	0.042901	-0.165160
32	6	0	4.149754	0.112800	0.230108
33	6	0	2.318447	-1.158156	-0.749262
34	6	0	5.010011	-0.963951	0.058892
35	1	0	4.518702	1.024717	0.674392
36	6	0	3.201075	-2.237011	-0.915161
37	6	0	4.521892	-2.146485	-0.519195
38	1	0	2.820708	-3.148189	-1.362729
39	1	0	5.197430	-2.984158	-0.650568
40	8	0	1.046452	-1.309638	-1.161108
41	1	0	0.601418	-0.428501	-0.959259
42	8	0	6.329662	-0.974042	0.416757
43	6	0	6.879652	0.214881	0.980979
44	1	0	6.826989	1.053708	0.278152
45	1	0	6.377450	0.490500	1.914635
46	1	0	7.924868	-0.009783	1.191139

Structure 10 (M06-2X, Gas Phase)

Energy (Hartrees): = - 1166.5940703
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.374837	-0.757574	0.446953
2	1	0	-4.999617	0.048826	0.852107
3	6	0	-5.276387	-1.790995	-0.189963
4	1	0	-4.656425	-2.575358	-0.642104
5	1	0	-5.887233	-1.313260	-0.961208
6	6	0	-3.414132	-0.138339	-0.564594
7	1	0	-2.951787	-0.939292	-1.156100
8	6	0	-2.268183	0.595926	0.157622
9	1	0	-1.485892	-0.137860	0.374270
10	6	0	-1.689391	1.730503	-0.689393
11	1	0	-1.591953	1.405693	-1.728252
12	6	0	-0.331008	2.188370	-0.170858
13	8	0	-6.063072	-2.320962	0.870898
14	1	0	-6.564080	-3.070197	0.544454
15	8	0	-3.615681	-1.356897	1.490638
16	1	0	-4.223089	-1.941348	1.958939
17	8	0	-4.168511	0.656172	-1.460030
18	1	0	-4.000449	1.587411	-1.265858
19	8	0	-2.688974	1.224390	1.364022
20	1	0	-2.929389	0.514609	1.972156
21	8	0	-2.603390	2.820757	-0.684188
22	1	0	-2.848292	2.948368	0.241900
23	1	0	-0.039630	3.085148	-0.727658
24	1	0	-0.440394	2.458050	0.886951
25	7	0	0.629393	1.114103	-0.345300
26	6	0	1.848565	1.211567	0.035680
27	6	0	2.425561	2.447307	0.683813
28	1	0	2.840778	2.200486	1.663225
29	1	0	3.236637	2.846101	0.070181
30	1	0	1.677018	3.224541	0.810933
31	6	0	2.740691	0.047944	-0.165823
32	6	0	4.100670	0.119917	0.203365
33	6	0	2.245158	-1.152778	-0.710338
34	6	0	4.944113	-0.962745	0.040306
35	1	0	4.483824	1.040843	0.617922
36	6	0	3.114897	-2.242545	-0.865144
37	6	0	4.436721	-2.153143	-0.497594
38	1	0	2.707249	-3.154264	-1.283564
39	1	0	5.113480	-2.990597	-0.615021
40	8	0	0.973820	-1.314715	-1.097465
41	1	0	0.532194	-0.437950	-0.947877
42	8	0	6.267998	-0.978554	0.368249
43	6	0	6.812461	0.200328	0.913303
44	1	0	6.737725	1.036661	0.209136
45	1	0	6.315578	0.471947	1.851524
46	1	0	7.861095	-0.011274	1.110048

Structure 10 (M06-2X, DMSO)

Energy (Hartrees): = - 1166.623141
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.380299	-0.771871	0.438723
2	1	0	-5.013309	0.014909	0.869349
3	6	0	-5.268316	-1.806780	-0.212640
4	1	0	-4.642175	-2.588217	-0.659322
5	1	0	-5.872626	-1.335508	-0.993927
6	6	0	-3.437113	-0.111263	-0.563406
7	1	0	-2.977627	-0.885230	-1.191263
8	6	0	-2.290333	0.610709	0.165615
9	1	0	-1.519987	-0.133692	0.388281
10	6	0	-1.680745	1.729769	-0.680377
11	1	0	-1.574254	1.393083	-1.714621
12	6	0	-0.322570	2.176349	-0.153990
13	8	0	-6.077320	-2.342775	0.829416
14	1	0	-6.501949	-3.141616	0.502760
15	8	0	-3.600926	-1.380716	1.465171
16	1	0	-4.201526	-1.970095	1.938301
17	8	0	-4.211992	0.721367	-1.414241
18	1	0	-3.989374	1.640511	-1.215104
19	8	0	-2.717854	1.242995	1.368230
20	1	0	-2.967590	0.533953	1.973894
21	8	0	-2.579462	2.838359	-0.702003
22	1	0	-2.794808	3.020386	0.223198
23	1	0	-0.011693	3.064701	-0.712502
24	1	0	-0.422657	2.454957	0.901719
25	7	0	0.632924	1.093894	-0.318860
26	6	0	1.855938	1.207944	0.047543
27	6	0	2.437465	2.447277	0.670532
28	1	0	2.867563	2.211556	1.646893
29	1	0	3.242580	2.838048	0.043168
30	1	0	1.690257	3.226061	0.798687
31	6	0	2.746822	0.037656	-0.156625
32	6	0	4.109625	0.116614	0.191978
33	6	0	2.243033	-1.169302	-0.682600
34	6	0	4.954459	-0.969543	0.029820
35	1	0	4.496025	1.044017	0.589901
36	6	0	3.110188	-2.259446	-0.838451
37	6	0	4.440349	-2.165584	-0.488260
38	1	0	2.707019	-3.181612	-1.240855
39	1	0	5.108576	-3.010573	-0.608856
40	8	0	0.961323	-1.325947	-1.048885
41	1	0	0.529282	-0.437917	-0.883596
42	8	0	6.278669	-0.974298	0.343522
43	6	0	6.823197	0.224022	0.869737
44	1	0	6.746005	1.044662	0.149067
45	1	0	6.328753	0.511078	1.803299
46	1	0	7.873336	0.018103	1.068264

Structure 12 (B3LYP, Gas Phase)

Energy (Hartrees): = - 1257.0631392
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.643019	-0.858069	0.486371
2	1	0	-5.282637	-0.047323	0.857712
3	6	0	-5.532037	-1.936399	-0.104505
4	1	0	-4.906153	-2.733171	-0.527542
5	1	0	-6.155366	-1.504764	-0.893726
6	6	0	-3.681749	-0.254832	-0.547867
7	1	0	-3.213569	-1.069604	-1.114989
8	6	0	-2.528914	0.524126	0.141808
9	1	0	-1.719446	-0.186971	0.334114
10	6	0	-2.001922	1.677365	-0.721752
11	1	0	-1.902880	1.351802	-1.759287
12	6	0	-0.657324	2.220272	-0.226302
13	8	0	-6.315213	-2.434935	0.987276
14	1	0	-6.782505	-3.223563	0.699213
15	8	0	-3.877156	-1.403374	1.571058
16	1	0	-4.488659	-1.966062	2.064863

17	8	0	-4.448807	0.498621	-1.481270
18	1	0	-4.311204	1.440993	-1.300342
19	8	0	-2.924653	1.145057	1.370968
20	1	0	-3.182944	0.424560	1.964984
21	8	0	-2.973851	2.731718	-0.723243
22	1	0	-3.230744	2.843541	0.204106
23	1	0	-0.437538	3.131276	-0.794033
24	1	0	-0.764821	2.495502	0.828571
25	7	0	0.389580	1.225766	-0.418257
26	6	0	1.580552	1.359553	0.052586
27	6	0	2.050546	2.559268	0.842821
28	1	0	2.383580	2.258148	1.839580
29	1	0	2.900761	3.033780	0.345989
30	1	0	1.265938	3.303053	0.954698
31	6	0	2.545670	0.266153	-0.203268
32	6	0	3.856274	0.332728	0.278679
33	6	0	2.160169	-0.895079	-0.941878
34	6	0	4.751077	-0.698261	0.043063
35	1	0	4.207359	1.182525	0.845030
36	6	0	3.091992	-1.925620	-1.166209
37	6	0	4.378487	-1.835103	-0.679877
38	1	0	2.762543	-2.788478	-1.730990
39	1	0	5.104102	-2.619400	-0.844650
40	8	0	0.937216	-1.041934	-1.436260
41	1	0	0.437363	-0.202201	-1.179940
42	7	0	6.116194	-0.589325	0.566846
43	8	0	6.887467	-1.515192	0.342542
44	8	0	6.409695	0.420620	1.199488

Structure 12 (B3LYP, DMSO)

Energy (Hartrees): = - 1257.0922579
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.675686	-0.857879	0.466036
2	1	0	-5.335072	-0.060484	0.832010
3	6	0	-5.531554	-1.951896	-0.141111
4	1	0	-4.887153	-2.752487	-0.523739
5	1	0	-6.124902	-1.544750	-0.966684
6	6	0	-3.711330	-0.227780	-0.550174
7	1	0	-3.240758	-1.023618	-1.140421
8	6	0	-2.564262	0.538211	0.156953
9	1	0	-1.775525	-0.187444	0.377415
10	6	0	-1.983960	1.663148	-0.709776
11	1	0	-1.859638	1.312798	-1.736237
12	6	0	-0.644364	2.193851	-0.192862
13	8	0	-6.369753	-2.438383	0.917004
14	1	0	-6.723309	-3.293893	0.648500
15	8	0	-3.916834	-1.392467	1.564558
16	1	0	-4.533712	-1.952908	2.056095
17	8	0	-4.485328	0.561843	-1.458022
18	1	0	-4.276239	1.493649	-1.286828
19	8	0	-2.984917	1.178675	1.369902
20	1	0	-3.265515	0.464261	1.961142
21	8	0	-2.936180	2.742465	-0.767092
22	1	0	-3.188497	2.913804	0.152867
23	1	0	-0.398780	3.096844	-0.761266
24	1	0	-0.753591	2.479058	0.858657
25	7	0	0.397801	1.188789	-0.360555
26	6	0	1.599190	1.355647	0.072623
27	6	0	2.083769	2.584399	0.793898
28	1	0	2.477818	2.319422	1.778870
29	1	0	2.897504	3.054734	0.234404
30	1	0	1.292178	3.317470	0.926705
31	6	0	2.561394	0.253087	-0.174109
32	6	0	3.882460	0.338116	0.265768
33	6	0	2.156588	-0.930316	-0.867238
34	6	0	4.773866	-0.702188	0.035165
35	1	0	4.235121	1.211696	0.793433
36	6	0	3.082447	-1.968509	-1.087273
37	6	0	4.381479	-1.863039	-0.640866
38	1	0	2.746307	-2.852585	-1.614967
39	1	0	5.093760	-2.659199	-0.807231
40	8	0	0.920072	-1.083753	-1.320101
41	1	0	0.429477	-0.224835	-1.055926
42	7	0	6.144633	-0.578452	0.510491
43	8	0	6.911367	-1.523424	0.325896
44	8	0	6.478231	0.463417	1.075535

Structure 12 (M06-2X, Gas Phase)

Energy (Hartrees): = - 1256.5746501
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.603473	-0.850200	0.426665
2	1	0	-5.255831	-0.058944	0.818209
3	6	0	-5.467578	-1.910657	-0.218172
4	1	0	-4.820308	-2.678935	-0.659733
5	1	0	-6.082004	-1.453240	-0.998771
6	6	0	-3.641449	-0.212315	-0.571554
7	1	0	-3.145534	-1.005556	-1.145634
8	6	0	-2.530887	0.561368	0.166927
9	1	0	-1.727689	-0.146118	0.396229
10	6	0	-1.981795	1.716095	-0.672883
11	1	0	-1.858282	1.396547	-1.710654
12	6	0	-0.649851	2.225897	-0.134069
13	8	0	-6.251297	-2.457403	0.835567
14	1	0	-6.731628	-3.219130	0.506811
15	8	0	-3.844477	-1.423812	1.484969
16	1	0	-4.442863	-2.022227	1.947616
17	8	0	-4.395059	0.551325	-1.492855
18	1	0	-4.287606	1.487779	-1.282784
19	8	0	-2.986237	1.176456	1.366522
20	1	0	-3.221301	0.460657	1.970059
21	8	0	-2.931983	2.772845	-0.679452
22	1	0	-3.194391	2.892621	0.243011
23	1	0	-0.387395	3.137461	-0.679939
24	1	0	-0.779603	2.479631	0.924975
25	7	0	0.362355	1.196912	-0.302306
26	6	0	1.576688	1.360797	0.065768
27	6	0	2.109150	2.619793	0.700565
28	1	0	2.548892	2.394949	1.674518
29	1	0	2.894858	3.050570	0.075634
30	1	0	1.329480	3.364222	0.836101
31	6	0	2.517145	0.234437	-0.144830
32	6	0	3.862405	0.353269	0.201343
33	6	0	2.066050	-0.997820	-0.691761
34	6	0	4.725906	-0.707724	0.014780
35	1	0	4.262955	1.267246	0.617499
36	6	0	2.969869	-2.058904	-0.863969
37	6	0	4.293851	-1.922136	-0.514057
38	1	0	2.586443	-2.981338	-1.280275
39	1	0	5.003634	-2.728074	-0.641445
40	8	0	0.808506	-1.191721	-1.056595
41	1	0	0.333836	-0.324412	-0.884864
42	7	0	6.135386	-0.546522	0.385444
43	8	0	6.869908	-1.496731	0.221223
44	8	0	6.482384	0.526810	0.833490

Structure 12 (M06-2X, DMSO)

Energy (Hartrees): = - 1256.6042617
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.615189	-0.860711	0.406169
2	1	0	-5.288117	-0.085413	0.795390
3	6	0	-5.444811	-1.936506	-0.255790
4	1	0	-4.777843	-2.703867	-0.666377
5	1	0	-6.036604	-1.499562	-1.066049
6	6	0	-3.654145	-0.192665	-0.574008
7	1	0	-3.147308	-0.965056	-1.165710
8	6	0	-2.559355	0.582586	0.180499
9	1	0	-1.769862	-0.128865	0.441534
10	6	0	-1.967219	1.712353	-0.664178
11	1	0	-1.822055	1.368388	-1.691216
12	6	0	-0.640387	2.214268	-0.108536
13	8	0	-6.271332	-2.480334	0.768025
14	1	0	-6.665663	-3.294043	0.439845
15	8	0	-3.858052	-1.423875	1.474352
16	1	0	-4.457795	-2.023067	1.936307
17	8	0	-4.417114	0.595112	-1.476189
18	1	0	-4.266305	1.524923	-1.261136
19	8	0	-3.047932	1.216633	1.358335
20	1	0	-3.295797	0.508234	1.965627

21	8	0	-2.901590	2.788440	-0.721094
22	1	0	-3.148855	2.971425	0.195927
23	1	0	-0.353001	3.114539	-0.659421
24	1	0	-0.770354	2.483998	0.945986
25	7	0	0.366908	1.175555	-0.253840
26	6	0	1.584429	1.358140	0.097264
27	6	0	2.120070	2.626150	0.696315
28	1	0	2.594471	2.415909	1.657739
29	1	0	2.881409	3.054980	0.039339
30	1	0	1.337108	3.364313	0.848232
31	6	0	2.523026	0.225995	-0.110254
32	6	0	3.874838	0.356155	0.194993
33	6	0	2.058689	-1.017949	-0.620227
34	6	0	4.735149	-0.711503	0.007352
35	1	0	4.271703	1.287020	0.576363
36	6	0	2.956668	-2.085393	-0.789352
37	6	0	4.289559	-1.940409	-0.478496
38	1	0	2.572454	-3.022400	-1.172949
39	1	0	4.985902	-2.757688	-0.609841
40	8	0	0.792052	-1.208422	-0.950778
41	1	0	0.329008	-0.320915	-0.775881
42	7	0	6.149124	-0.541674	0.326207
43	8	0	6.886721	-1.496869	0.176179
44	8	0	6.523166	0.545179	0.724821

Structure 16 (B3LYP, Gas Phase)

Energy (Hartrees): = - 1052.4967813
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.752112	-0.693986	0.343160
2	1	0	-4.389318	0.141282	0.661056
3	6	0	-4.630690	-1.750460	-0.300323
4	1	0	-4.001336	-2.571200	-0.668150
5	1	0	-5.180488	-1.309092	-1.137487
6	6	0	-2.701859	-0.133226	-0.627335
7	1	0	-2.232101	-0.964716	-1.166638
8	6	0	-1.562464	0.593215	0.136804
9	1	0	-0.805044	-0.157522	0.379228
10	6	0	-0.933992	1.721450	-0.694479
11	1	0	-0.798485	1.390823	-1.726574
12	6	0	0.406965	2.207467	-0.130219
13	8	0	-5.508418	-2.211272	0.735150
14	1	0	-5.963237	-2.999486	0.426770
15	8	0	-3.084633	-1.251677	1.484800
16	1	0	-3.746317	-1.793317	1.935432
17	8	0	-3.375405	0.653405	-1.605961
18	1	0	-3.222518	1.588811	-1.405773
19	8	0	-2.006163	1.237928	1.337681
20	1	0	-2.336425	0.531665	1.913370
21	8	0	-1.846831	2.823654	-0.741279
22	1	0	-2.158932	2.931808	0.169893
23	1	0	0.705795	3.093895	-0.698382
24	1	0	0.259427	2.499590	0.913937
25	7	0	1.404126	1.151739	-0.236767
26	6	0	2.632361	1.138477	0.251887
27	6	0	3.171225	2.349263	0.967642
28	1	0	3.380529	2.111950	2.013824
29	1	0	4.109083	2.673293	0.512253
30	1	0	2.474289	3.184006	0.939274
31	6	0	3.410629	-0.045676	0.083540
32	6	0	4.745980	-0.123696	0.567481
33	6	0	2.815687	-1.208651	-0.572918
34	6	0	5.495603	-1.263463	0.434581
35	1	0	5.185906	0.739187	1.054036
36	6	0	3.644950	-2.377002	-0.680044
37	6	0	4.925931	-2.397968	-0.197999
38	1	0	3.203193	-3.239121	-1.165666
39	1	0	5.521106	-3.299997	-0.302008
40	8	0	1.628448	-1.205307	-1.032682
41	1	0	1.189278	0.218921	-0.711737
42	1	0	6.511445	-1.301262	0.808367

Structure 16 (B3LYP, DMSO)

Energy (Hartrees): = - 1052.5273783
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.774075	-0.736730	0.378880
2	1	0	-4.423040	0.087014	0.702856
3	6	0	-4.638892	-1.823759	-0.228597
4	1	0	-4.003636	-2.646591	-0.577509
5	1	0	-5.201694	-1.421704	-1.077706
6	6	0	-2.757964	-0.160147	-0.618619
7	1	0	-2.290302	-0.983478	-1.171897
8	6	0	-1.614953	0.587814	0.113353
9	1	0	-0.862637	-0.158475	0.385201
10	6	0	-0.964140	1.667476	-0.762051
11	1	0	-0.816654	1.284320	-1.773924
12	6	0	0.372098	2.173761	-0.208561
13	8	0	-5.514219	-2.268356	0.817830
14	1	0	-5.879883	-3.121811	0.559254
15	8	0	-3.066208	-1.263003	1.514511
16	1	0	-3.712937	-1.798127	1.996026
17	8	0	-3.473516	0.628429	-1.573875
18	1	0	-3.251224	1.558474	-1.413976
19	8	0	-2.059500	1.278702	1.288492
20	1	0	-2.382107	0.592399	1.891651
21	8	0	-1.866822	2.779162	-0.881807
22	1	0	-2.149726	2.982810	0.022923
23	1	0	0.674564	3.045008	-0.796681
24	1	0	0.237585	2.488048	0.827968
25	7	0	1.391002	1.131452	-0.292625
26	6	0	2.556577	1.110987	0.322768
27	6	0	2.938888	2.258620	1.210665
28	1	0	2.705703	2.017515	2.253342
29	1	0	4.005474	2.467253	1.149471
30	1	0	2.400351	3.166496	0.944751
31	6	0	3.411734	-0.028903	0.129255
32	6	0	4.658340	-0.121000	0.804628
33	6	0	2.989239	-1.120843	-0.745613
34	6	0	5.490195	-1.206075	0.655712
35	1	0	4.965313	0.681439	1.464174
36	6	0	3.902152	-2.225074	-0.871115
37	6	0	5.097588	-2.264097	-0.198087
38	1	0	3.597918	-3.036622	-1.523792
39	1	0	5.753832	-3.120517	-0.321982
40	8	0	1.881170	-1.118401	-1.374342
41	1	0	1.253665	0.283832	-0.899020
42	1	0	6.434464	-1.251900	1.185077

Structure 17 (B3LYP, Gas Phase)

Energy (Hartrees): = - 3626.0392324
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.958925	-0.953973	0.460824
2	1	0	-5.632144	-0.186013	0.863488
3	6	0	-5.801522	-2.044214	-0.174811
4	1	0	-5.141896	-2.796235	-0.627176
5	1	0	-6.441721	-1.608423	-0.948077
6	6	0	-4.022571	-0.271783	-0.547112
7	1	0	-3.522684	-1.040816	-1.147869
8	6	0	-2.898858	0.523206	0.174465
9	1	0	-2.055396	-0.159323	0.314184
10	6	0	-2.448899	1.751076	-0.629922
11	1	0	-2.358299	1.490939	-1.686758
12	6	0	-1.125632	2.343078	-0.127532
13	8	0	-6.564417	-2.617614	0.894429
14	1	0	-6.990723	-3.417910	0.576485
15	8	0	-4.173131	-1.510462	1.525213
16	1	0	-4.760126	-2.120418	1.991963
17	8	0	-4.816892	0.487935	-1.453482
18	1	0	-4.760215	1.421974	-1.203190
19	8	0	-3.303042	1.056914	1.441270
20	1	0	-3.533844	0.293619	1.992637
21	8	0	-3.466110	2.754719	-0.547580
22	1	0	-3.720686	2.780709	0.387363
23	1	0	-0.958259	3.286426	-0.656415
24	1	0	-1.224292	2.556604	0.940596
25	7	0	-0.034573	1.407210	-0.366950
26	6	0	1.211482	1.482518	0.064753
27	6	0	1.663880	2.674596	0.864871
28	1	0	1.973880	2.365804	1.866329
29	1	0	2.524507	3.148099	0.387542
30	1	0	0.879330	3.421140	0.964561

31	6	0	2.096445	0.404848	-0.247036
32	6	0	3.454066	0.436170	0.175385
33	6	0	1.593140	-0.750938	-0.984473
34	6	0	4.295047	-0.605624	-0.102158
35	1	0	3.832148	1.289455	0.722129
36	6	0	2.535883	-1.808078	-1.234438
37	6	0	3.835277	-1.740896	-0.812721
38	1	0	2.166735	-2.668103	-1.780117
39	1	0	4.521320	-2.553429	-1.019832
40	8	0	0.392976	-0.838262	-1.392001
41	1	0	-0.181784	0.507052	-0.917194
42	35	0	6.128521	-0.547640	0.472133

Structure 17 (B3LYP, DMSO)

Energy (Hartrees): = - 3626.0716479
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.834950	-1.102677	0.496812
2	1	0	-5.549090	-0.427030	0.984503
3	6	0	-5.604059	-2.233263	-0.159038
4	1	0	-4.903640	-2.902977	-0.672243
5	1	0	-6.314871	-1.830637	-0.888699
6	6	0	-4.026413	-0.268551	-0.509545
7	1	0	-3.526187	-0.940868	-1.217126
8	6	0	-2.908214	0.536280	0.199965
9	1	0	-2.042962	-0.127081	0.289761
10	6	0	-2.500797	1.793197	-0.579122
11	1	0	-2.423703	1.561024	-1.643448
12	6	0	-1.180112	2.402510	-0.091194
13	8	0	-6.278435	-2.923460	0.903319
14	1	0	-6.552575	-3.786474	0.573048
15	8	0	-3.938855	-1.643787	1.482885
16	1	0	-4.449074	-2.319633	1.951209
17	8	0	-4.945937	0.523127	-1.267687
18	1	0	-4.820474	1.449629	-1.011622
19	8	0	-3.293660	1.011231	1.496596
20	1	0	-3.461068	0.217978	2.027546
21	8	0	-3.539320	2.777935	-0.457042
22	1	0	-3.746141	2.821324	0.489227
23	1	0	-1.044855	3.368202	-0.586489
24	1	0	-1.236608	2.568439	0.984799
25	7	0	-0.064123	1.516658	-0.411354
26	6	0	1.123870	1.470306	0.152249
27	6	0	1.482140	2.417447	1.257964
28	1	0	1.663257	1.866208	2.184704
29	1	0	2.401629	2.952110	1.009939
30	1	0	0.703064	3.152866	1.440385
31	6	0	2.061985	0.487585	-0.328652
32	6	0	3.346021	0.388742	0.267053
33	6	0	1.693769	-0.416563	-1.412585
34	6	0	4.248711	-0.548631	-0.165229
35	1	0	3.613677	1.058334	1.073033
36	6	0	2.696957	-1.367141	-1.812967
37	6	0	3.928808	-1.436739	-1.214633
38	1	0	2.438278	-2.043290	-2.620386
39	1	0	4.653507	-2.170964	-1.547201
40	8	0	0.560511	-0.387517	-1.989537
41	1	0	-0.153147	0.817630	-1.191154
42	35	0	5.986261	-0.671333	0.665570

Structure 18 (B3LYP, Gas Phase)

Energy (Hartrees): = - 1167.0470817
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.384225	-0.782489	0.436256
2	1	0	-5.030234	0.025899	0.802276
3	6	0	-5.260840	-1.849222	-0.192857
4	1	0	-4.625842	-2.642680	-0.607926
5	1	0	-5.859751	-1.404816	-0.993904
6	6	0	-3.395906	-0.169233	-0.566934
7	1	0	-2.926584	-0.974319	-1.145256
8	6	0	-2.245012	0.576388	0.160495

9	1	0	-1.454249	-0.154818	0.351526
10	6	0	-1.691542	1.741768	-0.672884
11	1	0	-1.596275	1.438017	-1.717670
12	6	0	-0.339802	2.256776	-0.163152
13	8	0	-6.077810	-2.359051	0.869072
14	1	0	-6.525514	-3.151578	0.561350
15	8	0	-3.650191	-1.345995	1.533207
16	1	0	-4.275302	-1.916604	1.999958
17	8	0	-4.136957	0.616140	-1.496879
18	1	0	-4.004426	1.551448	-1.282031
19	8	0	-2.652406	1.180465	1.394912
20	1	0	-2.932730	0.451824	1.969015
21	8	0	-2.639958	2.814666	-0.650564
22	1	0	-2.911506	2.891953	0.276616
23	1	0	-0.098248	3.165696	-0.723312
24	1	0	-0.445355	2.521313	0.893953
25	7	0	0.681072	1.235738	-0.343584
26	6	0	1.945913	1.264992	0.056790
27	6	0	2.489455	2.498368	0.728841
28	1	0	2.850413	2.260310	1.732522
29	1	0	3.335316	2.896687	0.162945
30	1	0	1.740467	3.282735	0.813064
31	6	0	2.754663	0.116628	-0.165460
32	6	0	4.133173	0.106240	0.223071
33	6	0	2.161706	-1.066703	-0.774512
34	6	0	4.910845	-1.005521	0.032219
35	1	0	4.558785	0.992931	0.670518
36	6	0	3.033748	-2.202424	-0.937778
37	6	0	4.341373	-2.170447	-0.555087
38	1	0	2.597272	-3.086554	-1.386803
39	1	0	4.987583	-3.031314	-0.688029
40	8	0	0.948102	-1.123743	-1.151244
41	1	0	0.460680	0.304502	-0.800818
42	8	0	6.237560	-1.125312	0.360749
43	6	0	6.876283	-0.007221	0.947300
44	1	0	7.908878	-0.305739	1.122929
45	1	0	6.860875	0.863035	0.279021
46	1	0	6.412540	0.267132	1.903270

Structure 18 (B3LYP, DMSO)

Energy (Hartrees): = - 1167.0765229
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.387828	-0.959993	0.423840
2	1	0	-5.088289	-0.200775	0.795306
3	6	0	-5.182493	-2.085795	-0.208741
4	1	0	-4.494722	-2.840531	-0.608674
5	1	0	-5.798648	-1.694939	-1.025347
6	6	0	-3.443143	-0.269927	-0.571908
7	1	0	-2.929932	-1.032977	-1.168976
8	6	0	-2.338672	0.534404	0.161417
9	1	0	-1.518799	-0.159486	0.370019
10	6	0	-1.811293	1.705707	-0.678294
11	1	0	-1.670090	1.385703	-1.712756
12	6	0	-0.501594	2.294823	-0.143533
13	8	0	-5.991414	-2.641617	0.838145
14	1	0	-6.294643	-3.510670	0.552072
15	8	0	-3.615182	-1.475645	1.521793
16	1	0	-4.207253	-2.079067	1.992754
17	8	0	-4.238843	0.497186	-1.480053
18	1	0	-4.104715	1.434188	-1.270288
19	8	0	-2.793464	1.128080	1.384479
20	1	0	-3.047660	0.388857	1.957343
21	8	0	-2.806572	2.741641	-0.710585
22	1	0	-3.075591	2.871987	0.211819
23	1	0	-0.291826	3.214798	-0.696191
24	1	0	-0.626435	2.547383	0.911397
25	7	0	0.594294	1.344364	-0.312293
26	6	0	1.803588	1.418994	0.207177
27	6	0	2.182633	2.577377	1.081995
28	1	0	2.390736	2.231113	2.098261
29	1	0	3.092203	3.051515	0.707256
30	1	0	1.400635	3.331165	1.128459
31	6	0	2.735897	0.364385	-0.088700
32	6	0	4.047810	0.402830	0.451067
33	6	0	2.332024	-0.750246	-0.934277
34	6	0	4.968935	-0.590850	0.200781
35	1	0	4.356279	1.227845	1.080734
36	6	0	3.330337	-1.753546	-1.158629

37	6	0	4.594262	-1.683625	-0.617800
38	1	0	3.050171	-2.593501	-1.785342
39	1	0	5.300598	-2.477665	-0.828142
40	8	0	1.168338	-0.848370	-1.456855
41	1	0	0.487254	0.488128	-0.919998
42	8	0	6.209613	-0.445346	0.773199
43	6	0	7.183791	-1.457464	0.536836
44	1	0	8.079200	-1.139155	1.070575
45	1	0	6.864731	-2.430898	0.926060
46	1	0	7.421409	-1.553445	-0.528653

Structure 20 (B3LYP, Gas Phase)

Energy (Hartrees): = - 1257.060052
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.532630	-0.921201	0.488872
2	1	0	-5.198842	-0.134358	0.865953
3	6	0	-5.386066	-2.028615	-0.101457
4	1	0	-4.734382	-2.800749	-0.530856
5	1	0	-6.029502	-1.617734	-0.885620
6	6	0	-3.594163	-0.285014	-0.546773
7	1	0	-3.103215	-1.080905	-1.119025
8	6	0	-2.460730	0.527642	0.141399
9	1	0	-1.618698	-0.154460	0.294260
10	6	0	-2.012881	1.728498	-0.703243
11	1	0	-1.927212	1.435917	-1.752031
12	6	0	-0.687475	2.334475	-0.220977
13	8	0	-6.143619	-2.557125	0.993796
14	1	0	-6.581885	-3.363215	0.708278
15	8	0	-3.745494	-1.443517	1.569612
16	1	0	-4.333942	-2.032432	2.061220
17	8	0	-4.381596	0.445442	-1.481663
18	1	0	-4.335747	1.385891	-1.255166
19	8	0	-2.849065	1.102318	1.394302
20	1	0	-3.089521	0.358800	1.968836
21	8	0	-3.024848	2.737447	-0.647332
22	1	0	-3.276645	2.793443	0.287131
23	1	0	-0.514928	3.258970	-0.780227
24	1	0	-0.783314	2.579761	0.839291
25	7	0	0.405821	1.391046	-0.430505
26	6	0	1.619425	1.427149	0.078615
27	6	0	2.041106	2.573395	0.956461
28	1	0	2.183919	2.229362	1.984477
29	1	0	2.992071	2.984906	0.615338
30	1	0	1.306376	3.375054	0.961310
31	6	0	2.507735	0.341185	-0.222102
32	6	0	3.818125	0.327062	0.291546
33	6	0	2.039327	-0.779793	-1.045480
34	6	0	4.663579	-0.723913	0.027201
35	1	0	4.195794	1.132075	0.906036
36	6	0	2.983005	-1.844305	-1.280539
37	6	0	4.246112	-1.820860	-0.766903
38	1	0	2.636103	-2.669161	-1.890533
39	1	0	4.948553	-2.622964	-0.949392
40	8	0	0.872781	-0.825169	-1.530594
41	1	0	0.274930	0.523498	-1.028011
42	7	0	6.013908	-0.705191	0.577334
43	8	0	6.747385	-1.656327	0.321606
44	8	0	6.347603	0.257314	1.266674

Structure 20 (B3LYP, DMSO)

Energy (Hartrees): = - 1257.0954108
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.471229	-1.016099	0.513699
2	1	0	-5.192207	-0.315052	0.952817
3	6	0	-5.229447	-2.181580	-0.092353
4	1	0	-4.520979	-2.872292	-0.565071
5	1	0	-5.934427	-1.819174	-0.848509
6	6	0	-3.648807	-0.237349	-0.525403
7	1	0	-3.154715	-0.946698	-1.201151
8	6	0	-2.520931	0.577075	0.153079
9	1	0	-1.684341	-0.109804	0.311686

10	6	0	-2.050690	1.759555	-0.702698
11	1	0	-1.956584	1.448580	-1.745421
12	6	0	-0.721256	2.359094	-0.227008
13	8	0	-5.911858	-2.822757	0.995046
14	1	0	-6.180492	-3.701179	0.702999
15	8	0	-3.589643	-1.501378	1.540283
16	1	0	-4.103479	-2.157518	2.032140
17	8	0	-4.556857	0.536382	-1.314785
18	1	0	-4.376582	1.473006	-1.142612
19	8	0	-2.918799	1.154691	1.403002
20	1	0	-3.107206	0.406660	1.989277
21	8	0	-3.053490	2.786940	-0.678368
22	1	0	-3.277779	2.911534	0.256844
23	1	0	-0.530384	3.273079	-0.795437
24	1	0	-0.796830	2.613185	0.830399
25	7	0	0.371263	1.410135	-0.439668
26	6	0	1.552949	1.400198	0.126943
27	6	0	1.934435	2.452870	1.121246
28	1	0	2.138515	1.994945	2.092647
29	1	0	2.848245	2.955907	0.796948
30	1	0	1.158846	3.203228	1.247020
31	6	0	2.476536	0.346365	-0.241344
32	6	0	3.744515	0.299172	0.350544
33	6	0	2.094983	-0.677352	-1.220389
34	6	0	4.645266	-0.699568	0.026558
35	1	0	4.046074	1.042074	1.074452
36	6	0	3.085407	-1.687096	-1.511953
37	6	0	4.311794	-1.703228	-0.915398
38	1	0	2.808548	-2.445091	-2.235428
39	1	0	5.037564	-2.470691	-1.149070
40	8	0	0.969643	-0.694571	-1.792479
41	1	0	0.254520	0.634722	-1.132071
42	7	0	5.942450	-0.716008	0.658340
43	8	0	6.729798	-1.617771	0.353229
44	8	0	6.219526	0.167133	1.477035

Structure $TS_{8/16}$ (B3LYP, Gas Phase)

Energy (Hartrees): = - 1052.4960206
Imaginary frequency -874.45

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.758577	-0.681586	0.339123
2	1	0	-4.391197	0.160627	0.647463
3	6	0	-4.640996	-1.734800	-0.304228
4	1	0	-4.015709	-2.562939	-0.662405
5	1	0	-5.180984	-1.294019	-1.148059
6	6	0	-2.697788	-0.134141	-0.627255
7	1	0	-2.228601	-0.972516	-1.156781
8	6	0	-1.560595	0.591460	0.140339
9	1	0	-0.810754	-0.161459	0.398610
10	6	0	-0.912988	1.704637	-0.695648
11	1	0	-0.766295	1.360807	-1.721663
12	6	0	0.425254	2.183240	-0.120136
13	8	0	-5.530240	-2.182473	0.727362
14	1	0	-5.991361	-2.966922	0.418780
15	8	0	-3.103195	-1.237593	1.488646
16	1	0	-3.772745	-1.769915	1.938652
17	8	0	-3.360952	0.649886	-1.615082
18	1	0	-3.188833	1.585265	-1.429667
19	8	0	-2.013100	1.251716	1.329806
20	1	0	-2.350152	0.553336	1.910750
21	8	0	-1.818292	2.813171	-0.767621
22	1	0	-2.137332	2.938057	0.138826
23	1	0	0.738148	3.062608	-0.692393
24	1	0	0.266990	2.488852	0.919470
25	7	0	1.414197	1.119172	-0.206763
26	6	0	2.635143	1.144780	0.265781
27	6	0	3.195500	2.360720	0.956548
28	1	0	3.479275	2.118054	1.983598
29	1	0	4.095748	2.706003	0.442778
30	1	0	2.481284	3.180852	0.982128
31	6	0	3.424275	-0.051435	0.096677
32	6	0	4.761178	-0.140149	0.551069
33	6	0	2.812811	-1.197909	-0.541007
34	6	0	5.496449	-1.293746	0.399081
35	1	0	5.220181	0.718144	1.028247
36	6	0	3.604408	-2.373034	-0.676224
37	6	0	4.901145	-2.413731	-0.220138
38	1	0	6.519427	-1.344119	0.751267
39	1	0	3.140879	-3.228043	-1.153738
40	1	0	5.479298	-3.324466	-0.339968

41	8	0	1.594920	-1.160230	-0.976718
42	1	0	1.248904	0.055943	-0.683574

Structure $TS_{8/16}$ (B3LYP, DMSO)

Energy (Hartrees): = - 1052.5245738
Imaginary frequency -1095.73

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.753107	-0.719872	0.369331
2	1	0	-4.402702	0.101203	0.698597
3	6	0	-4.616642	-1.802661	-0.247403
4	1	0	-3.980542	-2.622603	-0.601600
5	1	0	-5.178406	-1.394478	-1.094343
6	6	0	-2.736661	-0.133939	-0.622427
7	1	0	-2.269738	-0.951937	-1.184724
8	6	0	-1.593163	0.604474	0.116833
9	1	0	-0.846706	-0.147079	0.389767
10	6	0	-0.928430	1.681879	-0.750390
11	1	0	-0.776105	1.300227	-1.761924
12	6	0	0.408587	2.170052	-0.184194
13	8	0	-5.493526	-2.255812	0.794140
14	1	0	-5.858061	-3.107532	0.528333
15	8	0	-3.046688	-1.254407	1.501995
16	1	0	-3.693996	-1.793402	1.978321
17	8	0	-3.453566	0.667148	-1.566375
18	1	0	-3.207924	1.592633	-1.412646
19	8	0	-2.040827	1.293099	1.292548
20	1	0	-2.364850	0.605302	1.892953
21	8	0	-1.824722	2.799958	-0.875753
22	1	0	-2.108427	3.007790	0.027570
23	1	0	0.739508	3.024054	-0.783040
24	1	0	0.257807	2.513527	0.842831
25	7	0	1.400452	1.103840	-0.237562
26	6	0	2.568103	1.126713	0.340035
27	6	0	3.055586	2.292241	1.149482
28	1	0	3.882739	2.784932	0.629227
29	1	0	2.273894	3.029491	1.318729
30	1	0	3.433970	1.957666	2.117516
31	6	0	3.407734	-0.049844	0.142426
32	6	0	4.700214	-0.144366	0.698537
33	6	0	2.896801	-1.142775	-0.644686
34	6	0	5.488339	-1.264686	0.507789
35	1	0	5.087092	0.679189	1.286875
36	6	0	3.727371	-2.279036	-0.818575
37	6	0	4.987552	-2.334731	-0.255375
38	1	0	6.479329	-1.318322	0.942679
39	1	0	3.338881	-3.101822	-1.408781
40	1	0	5.599792	-3.218255	-0.406656
41	8	0	1.709375	-1.090463	-1.186000
42	1	0	1.317209	0.035653	-0.829484

Structure $TS_{10/18}$ (B3LYP, Gas Phase)

Energy (Hartrees): = - 1167.0459085
Imaginary frequency -964.22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.388097	-0.779329	0.427927
2	1	0	-5.035058	0.032277	0.784737
3	6	0	-5.261935	-1.846802	-0.203528
4	1	0	-4.625467	-2.643729	-0.609728
5	1	0	-5.852955	-1.404446	-1.011559
6	6	0	-3.390951	-0.171772	-0.569847
7	1	0	-2.917586	-0.980078	-1.140894
8	6	0	-2.245890	0.575121	0.163993
9	1	0	-1.461342	-0.157215	0.373815
10	6	0	-1.671888	1.726372	-0.673951
11	1	0	-1.560690	1.409260	-1.712954
12	6	0	-0.324725	2.235936	-0.148612
13	8	0	-6.089339	-2.350244	0.853532
14	1	0	-6.537679	-3.141882	0.544494
15	8	0	-3.664111	-1.339268	1.533447
16	1	0	-4.294782	-1.905237	1.998264
17	8	0	-4.125453	0.611586	-1.506656

18	1	0	-3.972974	1.547774	-1.308370
19	8	0	-2.668070	1.194362	1.386386
20	1	0	-2.953283	0.472538	1.966208
21	8	0	-2.615499	2.805407	-0.680956
22	1	0	-2.896996	2.900708	0.241356
23	1	0	-0.069660	3.139638	-0.712049
24	1	0	-0.445123	2.512342	0.904697
25	7	0	0.692752	1.208826	-0.306364
26	6	0	1.942731	1.283744	0.083585
27	6	0	2.499078	2.520995	0.739099
28	1	0	2.884136	2.284816	1.734400
29	1	0	3.331858	2.917698	0.152606
30	1	0	1.749557	3.303176	0.838461
31	6	0	2.767525	0.123838	-0.141695
32	6	0	4.142241	0.101218	0.225699
33	6	0	2.162090	-1.038314	-0.738214
34	6	0	4.906774	-1.024265	0.016497
35	1	0	4.582573	0.981934	0.671173
36	6	0	2.993256	-2.180375	-0.929469
37	6	0	4.314159	-2.170802	-0.565697
38	1	0	2.538378	-3.056032	-1.376525
39	1	0	4.942428	-3.041650	-0.715742
40	8	0	0.915223	-1.056286	-1.094206
41	1	0	0.541016	0.133389	-0.777218
42	8	0	6.236852	-1.156070	0.327084
43	6	0	6.894559	-0.046103	0.908537
44	1	0	6.878768	0.826971	0.244037
45	1	0	6.448641	0.228887	1.872726
46	1	0	7.926600	-0.355590	1.067609

Structure $TS_{10/18}$ (B3LYP, DMSO)

Energy (Hartrees): = - 1167.0757861
Imaginary frequency -1105.60

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.423881	-0.774946	0.445082
2	1	0	-5.076973	0.033667	0.797501
3	6	0	-5.285991	-1.859509	-0.170273
4	1	0	-4.647125	-2.669881	-0.541237
5	1	0	-5.862266	-1.447503	-1.005527
6	6	0	-3.434777	-0.164083	-0.559054
7	1	0	-2.970028	-0.968906	-1.141453
8	6	0	-2.284468	0.581547	0.163428
9	1	0	-1.516348	-0.159977	0.401755
10	6	0	-1.667373	1.688641	-0.702397
11	1	0	-1.543937	1.330787	-1.726513
12	6	0	-0.319616	2.189431	-0.175814
13	8	0	-6.145091	-2.330926	0.877755
14	1	0	-6.505006	-3.183397	0.608037
15	8	0	-3.689453	-1.315293	1.557183
16	1	0	-4.321160	-1.866113	2.040769
17	8	0	-4.180614	0.638089	-1.479392
18	1	0	-3.961195	1.566428	-1.304358
19	8	0	-2.710922	1.239029	1.364615
20	1	0	-3.013282	0.534504	1.957073
21	8	0	-2.588100	2.791841	-0.772803
22	1	0	-2.847840	2.971111	0.143700
23	1	0	-0.038293	3.073824	-0.755040
24	1	0	-0.431340	2.491458	0.870062
25	7	0	0.694228	1.150570	-0.306859
26	6	0	1.929629	1.250591	0.101826
27	6	0	2.466501	2.485167	0.765493
28	1	0	2.970882	2.230973	1.700308
29	1	0	3.206387	2.963963	0.116581
30	1	0	1.682730	3.207941	0.981264
31	6	0	2.784114	0.095731	-0.135309
32	6	0	4.148941	0.097206	0.249587
33	6	0	2.217666	-1.058338	-0.770533
34	6	0	4.950050	-1.006157	0.021106
35	1	0	4.559848	0.976462	0.724474
36	6	0	3.072796	-2.171329	-0.984453
37	6	0	4.394708	-2.145071	-0.600818
38	1	0	2.652674	-3.049360	-1.462430
39	1	0	5.035934	-3.003429	-0.771120
40	8	0	0.964863	-1.090936	-1.147508
41	1	0	0.574225	0.048157	-0.810547
42	8	0	6.275711	-1.103352	0.353194
43	6	0	6.884061	0.016311	0.990381
44	1	0	6.865047	0.905815	0.350377
45	1	0	6.402134	0.248341	1.946765

46	1	0	7.920001	-0.267618	1.173703

Structure $TS_{12/20}$ (B3LYP, Gas Phase)

Energy (Hartrees): = - 1257.0583144
Imaginary frequency -1014.76

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.554805	-0.907244	0.470961
2	1	0	-5.222948	-0.114308	0.831059
3	6	0	-5.404077	-2.014702	-0.124862
4	1	0	-4.749521	-2.793518	-0.537667
5	1	0	-6.031996	-1.606021	-0.922656
6	6	0	-3.598112	-0.281825	-0.554450
7	1	0	-3.101365	-1.083696	-1.114035
8	6	0	-2.473131	0.529872	0.146051
9	1	0	-1.642770	-0.157928	0.332560
10	6	0	-1.988152	1.709372	-0.707520
11	1	0	-1.879201	1.397009	-1.748145
12	6	0	-0.666117	2.302454	-0.204071
13	8	0	-6.183079	-2.531661	0.961062
14	1	0	-6.620564	-3.337380	0.673388
15	8	0	-3.787290	-1.424754	1.568080
16	1	0	-4.386997	-2.005724	2.055352
17	8	0	-4.371133	0.446989	-1.502641
18	1	0	-4.296091	1.391270	-1.299722
19	8	0	-2.887935	1.129211	1.379297
20	1	0	-3.138553	0.397002	1.963190
21	8	0	-2.991150	2.730976	-0.696060
22	1	0	-3.260392	2.813096	0.231327
23	1	0	-0.469468	3.216868	-0.772745
24	1	0	-0.785206	2.570288	0.849990
25	7	0	0.417839	1.344033	-0.378686
26	6	0	1.620755	1.443889	0.110336
27	6	0	2.074732	2.623633	0.926451
28	1	0	2.380014	2.300232	1.924747
29	1	0	2.942558	3.094378	0.458326
30	1	0	1.293807	3.373272	1.029799
31	6	0	2.525510	0.340998	-0.172786
32	6	0	3.846272	0.333543	0.291479
33	6	0	2.032594	-0.783539	-0.941451
34	6	0	4.674366	-0.736555	0.016222
35	1	0	4.250557	1.152155	0.870164
36	6	0	2.928897	-1.861062	-1.196421
37	6	0	4.218453	-1.840361	-0.730227
38	1	0	2.550301	-2.695714	-1.772941
39	1	0	4.902722	-2.655609	-0.922190
40	8	0	0.820641	-0.808382	-1.384349
41	1	0	0.367967	0.293336	-0.979498
42	7	0	6.048022	-0.719328	0.512863
43	8	0	6.762501	-1.681861	0.250136
44	8	0	6.414071	0.255384	1.165997

Structure $TS_{12/20}$ (B3LYP, DMSO)

Energy (Hartrees): = - 1257.0902598
Imaginary frequency -1076.95

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.443113	-1.034445	0.502992
2	1	0	-5.164553	-0.341208	0.953398
3	6	0	-5.200147	-2.195822	-0.112108
4	1	0	-4.491461	-2.880025	-0.593952
5	1	0	-5.908454	-1.827644	-0.862413
6	6	0	-3.630060	-0.239372	-0.530947
7	1	0	-3.134837	-0.938239	-1.217313
8	6	0	-2.504531	0.574047	0.151045
9	1	0	-1.665971	-0.110746	0.307151
10	6	0	-2.031891	1.760301	-0.697666
11	1	0	-1.931280	1.453026	-1.740649
12	6	0	-0.704873	2.355267	-0.211753
13	8	0	-5.877680	-2.849645	0.970919
14	1	0	-6.146672	-3.725049	0.670319
15	8	0	-3.554441	-1.527405	1.519686
16	1	0	-4.064254	-2.188882	2.008434
17	8	0	-4.548900	0.539128	-1.303202

18	1	0	-4.348773	1.474707	-1.145145
19	8	0	-2.906411	1.143139	1.404326
20	1	0	-3.087581	0.390843	1.986952
21	8	0	-3.042490	2.783642	-0.677948
22	1	0	-3.266088	2.911685	0.256638
23	1	0	-0.509856	3.266836	-0.784944
24	1	0	-0.798213	2.626568	0.842266
25	7	0	0.382686	1.406588	-0.416964
26	6	0	1.535903	1.448003	0.173215
27	6	0	1.938670	2.496878	1.165872
28	1	0	2.195609	2.032532	2.121847
29	1	0	2.829807	3.020775	0.809655
30	1	0	1.153776	3.229912	1.334488
31	6	0	2.479470	0.383224	-0.196077
32	6	0	3.750039	0.303647	0.371547
33	6	0	2.077172	-0.604580	-1.166933
34	6	0	4.618216	-0.716253	0.004653
35	1	0	4.077777	1.029748	1.101440
36	6	0	2.997972	-1.627752	-1.515436
37	6	0	4.244363	-1.686765	-0.941402
38	1	0	2.686460	-2.363242	-2.247310
39	1	0	4.942503	-2.468581	-1.207481
40	8	0	0.899945	-0.559956	-1.715993
41	1	0	0.413473	0.404783	-1.205783
42	7	0	5.934216	-0.779989	0.611037
43	8	0	6.686431	-1.698227	0.278364
44	8	0	6.248188	0.084041	1.432834

Structure 28 (M06-2X, Gas Phase)

Energy (Hartrees): = - 4693.8030792
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-6.179241	2.081228	0.941884
2	8	0	-3.541642	-3.109587	-0.618450
3	8	0	-1.942244	-2.949583	0.965295
4	8	0	-0.542950	2.500881	-1.702281
5	8	0	1.062117	-1.161223	-0.989193
6	8	0	1.303670	-0.280165	-3.045716
7	8	0	1.287984	-0.888432	1.750688
8	8	0	0.169465	0.553835	3.083969
9	8	0	3.836737	-0.016611	1.903130
10	8	0	4.695353	-2.090547	1.684729
11	8	0	5.278434	0.289830	-0.501153
12	8	0	4.604825	-1.319751	-1.941623
13	8	0	2.811548	2.829698	0.100749
14	8	0	3.765898	4.837132	-0.225541
15	7	0	-1.419158	0.471238	-1.288455
16	6	0	-5.324406	0.457537	0.463332
17	6	0	-5.896559	-0.742132	0.857536
18	1	0	-6.706938	-0.758293	1.353844
19	6	0	-5.255437	-1.918351	0.506944
20	1	0	-5.616244	-2.753608	0.780190
21	6	0	-4.091906	-1.883664	-0.237423
22	6	0	-3.517474	-0.681480	-0.670927
23	6	0	-4.148698	0.504311	-0.276603
24	1	0	-3.772926	1.342290	-0.515576
25	6	0	-2.427844	-3.531164	0.034309
26	6	0	-1.941770	-4.790034	-0.592499
27	1	0	-2.577945	-5.512284	-0.412158
28	1	0	-1.066333	-5.024571	-0.218688
29	1	0	-1.860611	-4.661879	-1.560866
30	6	0	-2.320017	-0.627240	-1.561846
31	6	0	-2.061096	-1.473904	-2.548823
32	1	0	-1.281286	-1.360699	-3.080487
33	1	0	-2.655365	-2.195270	-2.724572
34	6	0	-1.301931	1.601224	-2.047137
35	6	0	-2.131524	1.702863	-3.314791
36	1	0	-2.257345	2.645178	-3.546803
37	1	0	-3.005590	1.282658	-3.167584
38	1	0	-1.668426	1.244110	-4.045809
39	6	0	-0.612470	0.369113	-0.071626
40	1	0	-0.943810	-0.384166	0.479265
41	1	0	-0.712313	1.199608	0.457787
42	6	0	0.865785	0.148959	-0.389324
43	1	0	1.180040	0.855782	-1.023365
44	6	0	1.331642	-1.232826	-2.312607
45	6	0	1.646061	-2.634583	-2.716631
46	1	0	2.528067	-2.885848	-2.368955
47	1	0	1.648049	-2.699431	-3.694971
48	1	0	0.966147	-3.239501	-2.351365

49	6	0	1.715082	0.183783	0.868106
50	1	0	1.616829	1.069087	1.325801
51	6	0	0.523053	-0.563023	2.823152
52	6	0	0.196900	-1.800625	3.603900
53	1	0	-0.287681	-2.431200	3.031212
54	1	0	-0.362549	-1.563455	4.372705
55	1	0	1.025343	-2.216760	3.917713
56	6	0	3.190601	-0.118061	0.613061
57	1	0	3.265816	-1.064585	0.299221
58	6	0	4.466315	-1.129574	2.364928
59	6	0	4.795264	-0.984992	3.812752
60	1	0	4.998042	-0.048049	4.011206
61	1	0	5.573447	-1.540632	4.028206
62	1	0	4.029137	-1.274807	4.352530
63	6	0	3.919066	0.776126	-0.387770
64	1	0	3.466206	0.718329	-1.278900
65	6	0	5.487529	-0.756979	-1.342406
66	6	0	6.940282	-1.084490	-1.423365
67	1	0	7.408990	-0.376625	-1.914643
68	1	0	7.056753	-1.936681	-1.890097
69	1	0	7.310641	-1.153208	-0.518755
70	6	0	4.112842	2.232464	-0.015113
71	1	0	4.599201	2.302332	0.845144
72	1	0	4.640569	2.694826	-0.713190
73	6	0	2.787682	4.191262	-0.010472
74	6	0	1.398309	4.710435	0.200172
75	1	0	0.764011	4.166078	-0.313388
76	1	0	1.347740	5.641995	-0.103230
77	1	0	1.172639	4.664101	1.152013

Structure 29 (M06-2X, Gas Phase)

Energy (Hartrees): = - 4541.2005979
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-2.242222	-3.195547	-2.413058
2	8	0	-4.451167	1.709778	0.319761
3	8	0	-4.141965	3.105085	-1.419855
4	8	0	-2.512540	-1.615352	4.058137
5	8	0	-0.485165	0.534032	0.722238
6	8	0	1.218776	-1.568936	0.281841
7	8	0	2.716398	-2.949712	1.237894
8	8	0	1.693991	0.957764	-0.877136
9	8	0	1.257368	2.941946	0.109660
10	8	0	4.537566	-0.494903	0.809678
11	8	0	5.551848	-1.986231	-0.538142
12	8	0	4.703410	2.150945	-0.551544
13	8	0	3.595519	3.190515	-2.226580
14	7	0	-1.749721	-0.313330	2.409248
15	6	0	-2.925438	-1.620097	-1.587572
16	6	0	-4.081755	-1.027813	-2.079761
17	1	0	-4.531008	-1.389664	-2.832854
18	6	0	-4.559367	0.097605	-1.447693
19	1	0	-5.361099	0.507561	-1.751482
20	6	0	-3.873873	0.639933	-0.365034
21	6	0	-2.696129	0.078209	0.108800
22	6	0	-2.228751	-1.087748	-0.525677
23	1	0	-1.432914	-1.508199	-0.221564
24	6	0	-4.522713	2.933960	-0.308241
25	6	0	-5.067254	3.949699	0.636541
26	1	0	-5.698217	3.519179	1.250180
27	1	0	-5.530917	4.649268	0.130770
28	1	0	-4.332841	4.347795	1.147777
29	6	0	-1.810233	0.622065	1.251742
30	6	0	-2.044904	2.059761	1.700375
31	1	0	-1.332631	2.329935	2.316437
32	1	0	-2.911194	2.123698	2.152596
33	1	0	-2.040650	2.651046	0.917862
34	6	0	-2.754221	-0.779251	3.190119
35	6	0	-4.148011	-0.237691	3.029856
36	1	0	-4.797858	-0.952004	3.203532
37	1	0	-4.266851	0.095563	2.115820
38	1	0	-4.288842	0.494137	3.665043
39	6	0	-0.380973	-0.810268	2.617789
40	1	0	-0.284463	-1.745576	2.310390
41	1	0	-0.114786	-0.748834	3.568178
42	6	0	0.429364	0.150074	1.747408
43	1	0	0.689944	0.951863	2.283323
44	6	0	1.666441	-0.459640	1.098888
45	1	0	2.258384	-0.818068	1.821941
46	6	0	1.796396	-2.782583	0.497169

47	6	0	1.113139	-3.839689	-0.311479
48	1	0	0.167774	-3.882438	-0.059238
49	1	0	1.536612	-4.706556	-0.140918
50	1	0	1.186933	-3.621678	-1.264717
51	6	0	2.471047	0.525978	0.260851
52	1	0	2.709585	1.319426	0.819909
53	6	0	1.083050	2.173298	-0.792132
54	6	0	0.196229	2.387937	-1.976436
55	1	0	0.744066	2.445601	-2.787620
56	1	0	-0.306090	3.221665	-1.862078
57	1	0	-0.429116	1.639039	-2.054183
58	6	0	3.743642	-0.079653	-0.328298
59	1	0	3.498136	-0.889018	-0.863043
60	6	0	5.352283	-1.564455	0.571725
61	6	0	5.926047	-2.107179	1.833753
62	1	0	6.279918	-1.372788	2.374902
63	1	0	6.647982	-2.735762	1.619754
64	1	0	5.225110	-2.575605	2.335232
65	6	0	4.505631	0.879922	-1.217438
66	1	0	5.384104	0.488041	-1.450019
67	1	0	4.001075	1.022876	-2.057993
68	6	0	4.189174	3.247068	-1.179206
69	6	0	4.459429	4.495941	-0.396565
70	1	0	3.870575	4.526175	0.385715
71	1	0	4.290569	5.278817	-0.963003
72	1	0	5.392687	4.500228	-0.102859

Structure 28 + 29 (M06-2X, Gas Phase)

Energy (Hartrees): = - 9235.003811
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-13.976681	-2.643762	2.289737
2	8	0	-9.181588	-4.546519	-0.828393
3	8	0	-7.710442	-3.395187	0.437342
4	8	0	-11.021437	1.629678	-1.165654
5	8	0	-7.306623	0.041124	-1.580860
6	8	0	-8.290003	0.927335	-3.400610
7	8	0	-6.550978	0.287368	1.065032
8	8	0	-7.901182	0.516460	2.863177
9	8	0	-5.277426	2.662919	0.945548
10	8	0	-3.384887	1.753018	0.123050
11	8	0	-5.138963	3.968132	-1.550492
12	8	0	-4.974083	2.392611	-3.166042
13	8	0	-8.360397	4.098762	0.031923
14	8	0	-9.084959	6.224890	-0.008466
15	7	0	-10.202604	-0.462417	-1.060329
16	6	0	-12.453073	-3.218886	1.318152
17	6	0	-11.965092	-4.498510	1.533559
18	1	0	-12.385925	-5.085366	2.151455
19	6	0	-10.847059	-4.899985	0.822036
20	1	0	-10.481171	-5.765112	0.964093
21	6	0	-10.259274	-4.047799	-0.093047
22	6	0	-10.758382	-2.763252	-0.345977
23	6	0	-11.863308	-2.349739	0.407799
24	1	0	-12.210735	-1.473709	0.296504
25	6	0	-7.937609	-4.114547	-0.496304
26	6	0	-6.953177	-4.671641	-1.462973
27	1	0	-6.881212	-5.639857	-1.335440
28	1	0	-6.077706	-4.256316	-1.314011
29	1	0	-7.252753	-4.485061	-2.377405
30	6	0	-10.200774	-1.867872	-1.403309
31	6	0	-9.746309	-2.267118	-2.583169
32	1	0	-9.420128	-1.629319	-3.207991
33	1	0	-9.745928	-3.192059	-2.804291
34	6	0	-11.069027	0.468804	-1.558675
35	6	0	-12.078167	0.023210	-2.602027
36	1	0	-12.845216	0.630811	-2.593353
37	1	0	-12.379749	-0.887343	-2.396658
38	1	0	-11.659689	0.035916	-3.487474
39	6	0	-9.223653	-0.030901	-0.061681
40	1	0	-8.811886	-0.827075	0.359331
41	1	0	-9.684634	0.483540	0.647414
42	6	0	-8.127698	0.835261	-0.680778
43	1	0	-8.544785	1.589201	-1.188691
44	6	0	-7.443721	0.225559	-2.913670
45	6	0	-6.424508	-0.561790	-3.667530
46	1	0	-5.540908	-0.153098	-3.548500
47	1	0	-6.657222	-0.569383	-4.619971
48	1	0	-6.407466	-1.481945	-3.328928
49	6	0	-7.196291	1.393942	0.379414

50	1	0	-7.712047	1.952105	1.031605
51	6	0	-6.999176	-0.042562	2.302551
52	6	0	-6.203879	-1.196133	2.835824
53	1	0	-6.297281	-1.964381	2.234586
54	1	0	-6.535538	-1.437427	3.725808
55	1	0	-5.260399	-0.942673	2.895562
56	6	0	-6.031448	2.196416	-0.197206
57	1	0	-5.451502	1.572349	-0.720908
58	6	0	-3.979247	2.267801	1.028771
59	6	0	-3.432414	2.541974	2.389326
60	1	0	-3.842666	3.354223	2.750309
61	1	0	-2.461435	2.663419	2.332971
62	1	0	-3.631803	1.784890	2.980401
63	6	0	-6.381849	3.384893	-1.089749
64	1	0	-6.915293	3.067095	-1.875229
65	6	0	-4.548328	3.383574	-2.625982
66	6	0	-3.333686	4.144989	-3.037323
67	1	0	-3.602209	5.000037	-3.435949
68	1	0	-2.829168	3.623737	-3.694129
69	1	0	-2.772345	4.313738	-2.252068
70	6	0	-7.087022	4.561647	-0.445289
71	1	0	-6.546522	4.912395	0.307243
72	1	0	-7.212671	5.286816	-1.107049
73	6	0	-9.294073	5.076261	0.230768
74	6	0	-10.552034	4.492544	0.797405
75	1	0	-10.790391	3.681975	0.298843
76	1	0	-11.279179	5.146721	0.721738
77	1	0	-10.412247	4.266971	1.740088
78	35	0	4.645306	-0.592580	-0.770046
79	8	0	7.569208	4.261331	1.303671
80	8	0	8.136508	5.073305	-0.718114
81	8	0	7.779303	0.405394	5.028968
82	8	0	9.415145	0.561031	0.886731
83	8	0	8.892947	-2.100588	0.483075
84	8	0	9.216710	-4.177464	1.286328
85	8	0	10.547179	-0.656408	-1.286425
86	8	0	11.979849	0.981102	-0.680288
87	8	0	11.926898	-3.790236	-0.138820
88	8	0	11.079133	-5.491551	-1.345578
89	8	0	13.397705	-2.031033	-2.042203
90	8	0	12.839849	-0.439607	-3.548867
91	7	0	8.601518	0.820504	2.992394
92	6	0	5.583208	0.949642	-0.160011
93	6	0	5.089481	2.216547	-0.445154
94	1	0	4.295956	2.326388	-0.953254
95	6	0	5.780599	3.308798	0.027637
96	1	0	5.450598	4.185074	-0.134740
97	6	0	6.961901	3.137377	0.742700
98	6	0	7.484122	1.876769	0.998206
99	6	0	6.757622	0.764161	0.534782
100	1	0	7.076725	-0.115073	0.701335
101	6	0	8.156054	5.182653	0.464087
102	6	0	8.835639	6.234228	1.272305
103	1	0	8.346339	6.368419	2.110513
104	1	0	8.851943	7.073561	0.766895
105	1	0	9.752879	5.953302	1.469680
106	6	0	8.814521	1.558522	1.716304
107	6	0	9.813478	2.697539	1.883752
108	1	0	10.663966	2.340075	2.213525
109	1	0	9.461483	3.349395	2.524246
110	1	0	9.957773	3.135490	1.018109
111	6	0	7.907377	1.193685	4.094558
112	6	0	7.341035	2.583199	4.195205
113	1	0	6.492938	2.555263	4.687810
114	1	0	7.183550	2.938694	3.295503
115	1	0	7.975031	3.160590	4.668003
116	6	0	9.199318	-0.522300	2.933907
117	1	0	8.508415	-1.221920	2.825301
118	1	0	9.736023	-0.714749	3.741854
119	6	0	10.081498	-0.410833	1.690606
120	1	0	10.985208	-0.071857	1.948243
121	6	0	10.224511	-1.698081	0.887343
122	1	0	10.600113	-2.405332	1.487669
123	6	0	8.494096	-3.363254	0.798577
124	6	0	7.051709	-3.559512	0.453283
125	1	0	6.507239	-2.914924	0.950502
126	1	0	6.779484	-4.470028	0.691473
127	1	0	6.923571	-3.421142	-0.509043
128	6	0	11.131596	-1.566501	-0.329630
129	1	0	12.023430	-1.218305	-0.042582
130	6	0	11.028831	0.618495	-1.311568
131	6	0	10.208530	1.460839	-2.234965
132	1	0	10.319441	1.139168	-3.154582
133	1	0	10.505102	2.393173	-2.177477
134	1	0	9.266121	1.402420	-1.977278
135	6	0	11.320317	-2.879291	-1.087490
136	1	0	10.421351	-3.234453	-1.346367
137	6	0	11.623539	-5.105693	-0.343450

138	6	0	12.044335	-5.950212	0.808151
139	1	0	12.962520	-5.725420	1.060743
140	1	0	11.995290	-6.896236	0.553720
141	1	0	11.445965	-5.786449	1.567987
142	6	0	12.164811	-2.732490	-2.335393
143	1	0	12.372732	-3.628359	-2.700862
144	1	0	11.655508	-2.231577	-3.021864
145	6	0	13.614565	-0.876984	-2.735766
146	6	0	14.918133	-0.248414	-2.347363
147	1	0	14.832079	0.164699	-1.463305
148	1	0	15.158794	0.437241	-3.006317
149	1	0	15.614950	-0.934689	-2.320428

Structure 29E (M06-2X, Gas Phase)

Energy (Hartrees): = - 4541.5099467
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-2.494013	-3.429431	-2.050886
2	8	0	-4.273929	1.951211	0.031052
3	8	0	-3.226020	3.060671	-1.625427
4	8	0	-2.422970	-1.219142	4.170547
5	8	0	-0.426003	0.577088	0.614591
6	8	0	1.326101	-1.534658	0.235049
7	8	0	2.323765	-2.939424	1.680720
8	8	0	1.725993	1.163208	-0.859536
9	8	0	1.387226	2.965769	0.437701
10	8	0	4.469137	-0.755636	0.411053
11	8	0	4.468719	-2.696268	-0.725655
12	8	0	4.775755	2.000515	-0.666372
13	8	0	3.541802	3.297464	-2.035850
14	7	0	-1.670201	-0.144460	2.353485
15	6	0	-3.028827	-1.727486	-1.399248
16	6	0	-4.165653	-1.125403	-1.929193
17	1	0	-4.740877	-1.617140	-2.702075
18	6	0	-4.537398	0.115003	-1.446475
19	1	0	-5.415782	0.620124	-1.828348
20	6	0	-3.790552	0.738793	-0.452204
21	6	0	-2.653107	0.145227	0.081438
22	6	0	-2.280792	-1.108981	-0.417723
23	1	0	-1.376068	-1.572215	-0.043886
24	6	0	-3.932245	3.079524	-0.664502
25	6	0	-4.539518	4.288352	-0.018305
26	1	0	-5.595740	4.116376	0.185790
27	1	0	-4.402471	5.149001	-0.667041
28	1	0	-4.037140	4.462452	0.936008
29	6	0	-1.724511	0.725182	1.158891
30	6	0	-1.907765	2.190961	1.541662
31	1	0	-1.105155	2.455721	2.231255
32	1	0	-2.866003	2.378982	2.022115
33	1	0	-1.800826	2.814884	0.651999
34	6	0	-2.657427	-0.469851	3.244623
35	6	0	-4.025898	0.154300	3.075367
36	1	0	-4.761174	-0.598594	3.353378
37	1	0	-4.241743	0.530864	2.078843
38	1	0	-4.107666	0.978575	3.788020
39	6	0	-0.326373	-0.673192	2.558835
40	1	0	-0.267149	-1.725693	2.263208
41	1	0	-0.044254	-0.598258	3.608583
42	6	0	0.489983	0.233129	1.645109
43	1	0	0.812343	1.138365	2.174725
44	6	0	1.718110	-0.406901	1.022261
45	1	0	2.370923	-0.747269	1.828900
46	6	0	1.736983	-2.759587	0.648434
47	6	0	1.394748	-3.811328	-0.360089
48	1	0	0.445314	-3.595435	-0.847734
49	1	0	1.379345	-4.783095	0.126970
50	1	0	2.189283	-3.799675	-1.110831
51	6	0	2.520579	0.559431	0.154145
52	1	0	2.933075	1.330151	0.808531
53	6	0	1.165478	2.363198	-0.580349
54	6	0	0.258552	2.794499	-1.686145
55	1	0	0.796874	2.742293	-2.632460
56	1	0	-0.088874	3.807300	-1.499671
57	1	0	-0.592099	2.109418	-1.725691
58	6	0	3.649931	-0.140447	-0.589767
59	1	0	3.242124	-0.909531	-1.246498
60	6	0	4.789266	-2.061146	0.240981
61	6	0	5.541693	-2.589096	1.423755
62	1	0	6.201615	-1.828023	1.835682
63	1	0	6.094989	-3.477475	1.129949

64	1	0	4.798445	-2.861028	2.177219
65	6	0	4.461952	0.832395	-1.428766
66	1	0	5.403872	0.365833	-1.717622
67	1	0	3.896468	1.117037	-2.314428
68	6	0	4.204314	3.168638	-1.044273
69	6	0	4.469528	4.246361	-0.035297
70	1	0	3.665411	4.192252	0.703647
71	1	0	4.427406	5.215375	-0.526862
72	1	0	5.424463	4.093909	0.462957

Structure 29E (M06-2X, $CHCl_3$)

Energy (Hartrees): = - 4541.5492769
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-2.659194	-3.079548	-2.475211
2	8	0	-4.293215	1.910164	0.504853
3	8	0	-3.588166	3.269680	-1.143125
4	8	0	-2.313926	-1.872047	3.880749
5	8	0	-0.399051	0.479974	0.652331
6	8	0	1.470161	-1.595937	0.235553
7	8	0	2.523805	-2.934280	1.703832
8	8	0	1.724601	1.092470	-0.892357
9	8	0	1.364476	2.951697	0.316150
10	8	0	4.578283	-0.624305	0.434011
11	8	0	4.693117	-2.606089	-0.621687
12	8	0	4.737033	2.102112	-0.720461
13	8	0	3.468925	3.311079	-2.134755
14	7	0	-1.592941	-0.419214	2.338966
15	6	0	-3.150115	-1.498400	-1.537675
16	6	0	-4.328232	-0.845155	-1.885345
17	1	0	-4.967383	-1.226358	-2.670906
18	6	0	-4.665240	0.308777	-1.202340
19	1	0	-5.577019	0.844506	-1.438048
20	6	0	-3.842950	0.797041	-0.192314
21	6	0	-2.662869	0.150340	0.159368
22	6	0	-2.327643	-1.017223	-0.536916
23	1	0	-1.401278	-1.521851	-0.291753
24	6	0	-4.130152	3.133966	-0.086257
25	6	0	-4.698598	4.210267	0.780837
26	1	0	-5.733355	3.974529	1.033109
27	1	0	-4.638071	5.163468	0.261957
28	1	0	-4.127643	4.255778	1.711193
29	6	0	-1.680005	0.583176	1.252598
30	6	0	-1.836869	1.991684	1.816467
31	1	0	-0.998358	2.183423	2.487565
32	1	0	-2.758618	2.108079	2.382652
33	1	0	-1.799241	2.723521	1.006319
34	6	0	-2.587704	-1.019949	3.049686
35	6	0	-4.019906	-0.631103	2.769942
36	1	0	-4.391572	-1.222012	1.928307
37	1	0	-4.154774	0.423699	2.533426
38	1	0	-4.603836	-0.884675	3.653030
39	6	0	-0.209554	-0.829965	2.559650
40	1	0	-0.073837	-1.874595	2.263925
41	1	0	0.071294	-0.728093	3.608402
42	6	0	0.550627	0.136796	1.653961
43	1	0	0.852470	1.033591	2.207003
44	6	0	1.799408	-0.441287	1.014141
45	1	0	2.470977	-0.736545	1.822865
46	6	0	1.935925	-2.793633	0.664256
47	6	0	1.626409	-3.874744	-0.320772
48	1	0	0.554443	-3.901023	-0.521491
49	1	0	1.964156	-4.830066	0.073006
50	1	0	2.142866	-3.652959	-1.256709
51	6	0	2.551214	0.554378	0.136053
52	1	0	2.912173	1.358814	0.779293
53	6	0	1.136500	2.287846	-0.662015
54	6	0	0.193592	2.635798	-1.766321
55	1	0	0.700366	2.536196	-2.726875
56	1	0	-0.175680	3.649734	-1.632285
57	1	0	-0.637566	1.926280	-1.743278
58	6	0	3.725463	-0.092908	-0.588250
59	1	0	3.373705	-0.904016	-1.226545
60	6	0	4.979663	-1.911397	0.316533
61	6	0	5.775384	-2.334997	1.509937
62	1	0	6.460304	-1.544842	1.815885
63	1	0	6.313528	-3.252282	1.283049
64	1	0	5.071756	-2.520290	2.325718
65	6	0	4.482298	0.897852	-1.452939
66	1	0	5.447307	0.474737	-1.734636

67	1	0	3.903719	1.125713	-2.346208
68	6	0	4.137847	3.238545	-1.138369
69	6	0	4.401513	4.361914	-0.184456
70	1	0	3.790860	4.196432	0.706836
71	1	0	4.116496	5.304305	-0.645905
72	1	0	5.449800	4.373607	0.113183

Structure 29Z (M06-2X, Gas Phase)

Energy (Hartrees): = - 4541.5123568
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-2.389244	-3.393185	-2.103951
2	8	0	-4.419698	1.823502	0.160050
3	8	0	-3.635663	2.977465	-1.609727
4	8	0	-3.850237	0.293869	2.750203
5	8	0	-0.395025	0.640865	0.534672
6	8	0	1.346102	-1.496430	0.226861
7	8	0	2.169720	-2.892196	1.784756
8	8	0	1.816314	1.179662	-0.898153
9	8	0	1.493884	3.006403	0.368179
10	8	0	4.488138	-0.775992	0.467157
11	8	0	4.408635	-2.759204	-0.592115
12	8	0	4.859597	1.963825	-0.652459
13	8	0	3.703107	3.246818	-2.100375
14	7	0	-1.660251	0.014856	2.300088
15	6	0	-3.011216	-1.742602	-1.392226
16	6	0	-4.256994	-1.263985	-1.775536
17	1	0	-4.871892	-1.817275	-2.472575
18	6	0	-4.685699	-0.058917	-1.247699
19	1	0	-5.649671	0.353203	-1.518660
20	6	0	-3.894143	0.645549	-0.348154
21	6	0	-2.646907	0.169026	0.040117
22	6	0	-2.214174	-1.044357	-0.505388
23	1	0	-1.229391	-1.413396	-0.246750
24	6	0	-4.242331	2.953350	-0.581105
25	6	0	-4.877741	4.123826	0.109437
26	1	0	-5.885813	3.867851	0.433300
27	1	0	-4.885804	4.977876	-0.562257
28	1	0	-4.292452	4.360196	1.001119
29	6	0	-1.701727	0.817753	1.056965
30	6	0	-1.910928	2.293240	1.366559
31	1	0	-1.075751	2.629173	1.983642
32	1	0	-2.847916	2.445308	1.897791
33	1	0	-1.895132	2.867016	0.437650
34	6	0	-2.787964	-0.219125	3.035551
35	6	0	-2.616767	-1.146201	4.219381
36	1	0	-3.595962	-1.306807	4.662819
37	1	0	-1.950745	-0.702475	4.962956
38	1	0	-2.187697	-2.101985	3.910558
39	6	0	-0.344125	-0.569047	2.505573
40	1	0	-0.308620	-1.620320	2.197541
41	1	0	-0.020264	-0.493391	3.544576
42	6	0	0.498254	0.311465	1.583048
43	1	0	0.817624	1.221620	2.107099
44	6	0	1.732049	-0.359766	1.004569
45	1	0	2.357521	-0.694757	1.835094
46	6	0	1.670915	-2.723554	0.704300
47	6	0	1.345248	-3.789726	-0.293417
48	1	0	0.362428	-3.620274	-0.733730
49	1	0	1.398576	-4.761439	0.190364
50	1	0	2.095953	-3.734084	-1.085084
51	6	0	2.574306	0.574921	0.140967
52	1	0	2.990342	1.345638	0.793371
53	6	0	1.274365	2.395386	-0.644619
54	6	0	0.400165	2.830667	-1.774499
55	1	0	0.978784	2.807893	-2.698510
56	1	0	0.029100	3.833747	-1.581734
57	1	0	-0.431669	2.127672	-1.860457
58	6	0	3.705495	-0.161212	-0.564117
59	1	0	3.297133	-0.933699	-1.216530
60	6	0	4.744668	-2.101104	0.353537
61	6	0	5.448334	-2.619447	1.570425
62	1	0	6.137981	-1.876876	1.967373
63	1	0	5.961983	-3.544564	1.321415
64	1	0	4.679384	-2.826342	2.319205
65	6	0	4.555196	0.782832	-1.398115
66	1	0	5.499233	0.298863	-1.649608
67	1	0	4.017767	1.054568	-2.305240
68	6	0	4.326295	3.133023	-1.082263
69	6	0	4.583746	4.231158	-0.093626

70	1	0	3.793752	4.174017	0.659928
71	1	0	4.518653	5.191319	-0.599448
72	1	0	5.548950	4.101597	0.392047

Structure 29Z (M06-2X, $CHCl_3$)

Energy (Hartrees): = - 4541.5504651
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	-2.507278	-3.385775	-2.095037
2	8	0	-4.422449	1.854566	0.215261
3	8	0	-3.790312	2.986138	-1.624217
4	8	0	-3.833014	0.296739	2.790478
5	8	0	-0.407902	0.634565	0.511910
6	8	0	1.352025	-1.506814	0.211241
7	8	0	2.223444	-2.896690	1.748462
8	8	0	1.830491	1.152390	-0.933471
9	8	0	1.528155	3.016014	0.282883
10	8	0	4.494880	-0.785220	0.479348
11	8	0	4.488601	-2.766546	-0.582555
12	8	0	4.918538	1.912332	-0.654845
13	8	0	3.789162	3.234129	-2.085170
14	7	0	-1.652776	0.015713	2.297654
15	6	0	-3.093902	-1.723079	-1.372046
16	6	0	-4.337974	-1.225938	-1.738404
17	1	0	-4.976051	-1.764364	-2.427112
18	6	0	-4.741328	-0.015684	-1.201189
19	1	0	-5.704910	0.409158	-1.456501
20	6	0	-3.923462	0.674119	-0.313115
21	6	0	-2.676058	0.180732	0.055536
22	6	0	-2.271714	-1.040565	-0.494954
23	1	0	-1.293242	-1.429602	-0.239619
24	6	0	-4.311652	2.978757	-0.546583
25	6	0	-4.893682	4.153043	0.174030
26	1	0	-5.882115	3.903660	0.560448
27	1	0	-4.944701	5.005016	-0.499350
28	1	0	-4.252098	4.393624	1.025698
29	6	0	-1.705908	0.820649	1.055910
30	6	0	-1.900757	2.297017	1.369998
31	1	0	-1.057764	2.624097	1.982112
32	1	0	-2.828319	2.462192	1.913323
33	1	0	-1.894827	2.877128	0.444225
34	6	0	-2.757043	-0.211048	3.060028
35	6	0	-2.557424	-1.120394	4.248398
36	1	0	-3.520993	-1.270241	4.730163
37	1	0	-1.860549	-0.674126	4.962273
38	1	0	-2.148155	-2.084266	3.936428
39	6	0	-0.332371	-0.569389	2.487640
40	1	0	-0.311093	-1.619561	2.175463
41	1	0	0.002216	-0.493736	3.522163
42	6	0	0.498107	0.309310	1.556704
43	1	0	0.817788	1.220509	2.076163
44	6	0	1.732607	-0.363737	0.984982
45	1	0	2.349890	-0.689255	1.824655
46	6	0	1.700879	-2.728967	0.677666
47	6	0	1.369094	-3.796782	-0.313659
48	1	0	0.356684	-3.661446	-0.695129
49	1	0	1.481985	-4.773453	0.150741
50	1	0	2.065089	-3.705796	-1.151050
51	6	0	2.583903	0.559898	0.120410
52	1	0	2.991443	1.337902	0.768836
53	6	0	1.312128	2.382240	-0.717738
54	6	0	0.469876	2.813663	-1.872899
55	1	0	1.061589	2.763060	-2.788256
56	1	0	0.113065	3.827730	-1.709253
57	1	0	-0.372605	2.125100	-1.970076
58	6	0	3.720855	-0.185596	-0.568433
59	1	0	3.319073	-0.964539	-1.217078
60	6	0	4.798782	-2.098606	0.367891
61	6	0	5.519835	-2.590891	1.582045
62	1	0	6.228302	-1.845924	1.942013
63	1	0	6.021284	-3.528193	1.352473
64	1	0	4.771398	-2.764073	2.359943
65	6	0	4.584596	0.739509	-1.405862
66	1	0	5.517307	0.237133	-1.664001
67	1	0	4.053040	1.020609	-2.313093
68	6	0	4.417169	3.096156	-1.069420
69	6	0	4.718302	4.180627	-0.082112
70	1	0	3.984883	4.101239	0.725332
71	1	0	4.611390	5.150535	-0.562573

72	1	0	5.715043	4.058909	0.339821

Structure 34 (B3LYP, Gas Phase)

Energy (Hartrees): = -1052.4806857
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.724596	-0.747290	0.178820
2	1	0	-4.346641	0.003640	0.681226
3	6	0	-4.633343	-1.684819	-0.593171
4	1	0	-4.021591	-2.412087	-1.143694
5	1	0	-5.238619	-1.108417	-1.299850
6	6	0	-2.746654	0.006872	-0.731926
7	1	0	-2.284489	-0.705006	-1.430195
8	6	0	-1.590321	0.631737	0.085097
9	1	0	-0.819508	-0.131628	0.217298
10	6	0	-0.965995	1.844383	-0.613217
11	1	0	-0.840109	1.631412	-1.676229
12	6	0	0.395485	2.216766	-0.019828
13	8	0	-5.441656	-2.347126	0.389444
14	1	0	-5.937668	-3.048342	-0.041092
15	8	0	-2.979769	-1.490049	1.155556
16	1	0	-3.613905	-2.102623	1.550690
17	8	0	-3.508871	0.927156	-1.509195
18	1	0	-3.245270	1.826613	-1.258460
19	8	0	-2.020188	1.119545	1.366251
20	1	0	-2.272345	0.338170	1.876447
21	8	0	-1.876934	2.953472	-0.527555
22	1	0	-2.156339	2.982056	0.398906
23	1	0	0.730550	3.148439	-0.493852
24	1	0	0.270337	2.420805	1.052356
25	7	0	1.332175	1.135025	-0.269163
26	6	0	2.467993	1.121949	0.304663
27	6	0	2.964684	2.202585	1.250069
28	1	0	3.976214	2.008897	1.603328
29	1	0	2.938307	3.187488	0.773799
30	1	0	2.307260	2.254936	2.124346
31	6	0	3.377208	-0.033218	0.029724
32	6	0	4.712650	0.193588	-0.320495
33	6	0	2.929625	-1.367863	0.098205
34	6	0	5.584848	-0.846197	-0.627148
35	1	0	5.068826	1.216788	-0.373426
36	6	0	3.807970	-2.414457	-0.196659
37	6	0	5.124378	-2.157935	-0.563319
38	1	0	6.608442	-0.634227	-0.911381
39	1	0	3.450371	-3.438784	-0.134668
40	1	0	5.786695	-2.984906	-0.792826
41	8	0	1.648612	-1.616252	0.491605
42	1	0	1.521118	-2.568980	0.547689

Structure 34 (B3LYP, DMSO)

Energy (Hartrees): = -1052.5090447
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.882955	-0.839865	0.205077
2	1	0	-4.523575	-0.106630	0.710863
3	6	0	-4.761090	-1.782352	-0.594615
4	1	0	-4.132033	-2.498707	-1.136630
5	1	0	-5.361139	-1.216635	-1.315551
6	6	0	-2.895749	-0.055484	-0.671899
7	1	0	-2.441796	-0.737988	-1.402704
8	6	0	-1.735289	0.519616	0.173173
9	1	0	-0.999962	-0.278995	0.302767
10	6	0	-1.039726	1.710393	-0.493281
11	1	0	-0.879399	1.494827	-1.551505
12	6	0	0.304618	2.049921	0.155754
13	8	0	-5.592033	-2.460382	0.359756
14	1	0	-5.974909	-3.232381	-0.071970
15	8	0	-3.144415	-1.587756	1.185241
16	1	0	-3.775604	-2.223045	1.551460
17	8	0	-3.646241	0.921544	-1.400184
18	1	0	-3.312743	1.795775	-1.142227
19	8	0	-2.169195	0.997575	1.455484
20	1	0	-2.476311	0.215675	1.935913

21	8	0	-1.916050	2.855619	-0.446410
22	1	0	-2.191682	2.934118	0.478966
23	1	0	0.671768	2.984195	-0.287317
24	1	0	0.146339	2.239181	1.225159
25	7	0	1.251392	0.964908	-0.066012
26	6	0	2.405647	1.022792	0.475293
27	6	0	2.879807	2.155743	1.359778
28	1	0	2.190035	2.321395	2.193411
29	1	0	3.877183	1.977197	1.758579
30	1	0	2.906082	3.085581	0.780338
31	6	0	3.357309	-0.108254	0.231415
32	6	0	3.925861	-0.774382	1.324741
33	6	0	3.707849	-0.536292	-1.064148
34	6	0	4.785405	-1.856913	1.160609
35	1	0	3.670991	-0.442449	2.325842
36	6	0	4.583296	-1.615329	-1.231363
37	6	0	5.112982	-2.275820	-0.127830
38	1	0	5.195991	-2.363096	2.026449
39	1	0	4.849892	-1.929067	-2.236652
40	1	0	5.786124	-3.112405	-0.279076
41	8	0	3.210204	0.136048	-2.138588
42	1	0	3.589070	-0.244721	-2.942660

Structure 34 (M06-2X, Gas Phase)

Energy (Hartrees): = -1052.0658053
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.828473	-0.806603	-0.291373
2	1	0	4.435915	-0.011345	-0.741659
3	6	0	4.746222	-1.753240	0.448019
4	1	0	4.141361	-2.522940	0.944061
5	1	0	5.317382	-1.194672	1.195099
6	6	0	2.819687	-0.143396	0.641135
7	1	0	2.353832	-0.912315	1.271757
8	6	0	1.685956	0.511255	-0.169757
9	1	0	0.928593	-0.250976	-0.370996
10	6	0	1.032512	1.670315	0.579378
11	1	0	0.875704	1.395035	1.624429
12	6	0	-0.303072	2.055653	-0.042446
13	8	0	5.582255	-2.335500	-0.546385
14	1	0	6.114991	-3.023221	-0.143901
15	8	0	3.120328	-1.512218	-1.304143
16	1	0	3.764586	-2.098266	-1.717683
17	8	0	3.532462	0.730669	1.496728
18	1	0	3.294248	1.641132	1.276041
19	8	0	2.148126	1.079392	-1.392860
20	1	0	2.418981	0.340331	-1.950295
21	8	0	1.921125	2.785328	0.572224
22	1	0	2.203515	2.884548	-0.346257
23	1	0	-0.655097	2.973183	0.444741
24	1	0	-0.140820	2.282805	-1.105251
25	7	0	-1.246002	0.968177	0.138107
26	6	0	-2.400223	1.067512	-0.378606
27	6	0	-2.863657	2.254387	-1.198530
28	1	0	-2.317298	2.303386	-2.145643
29	1	0	-3.930139	2.210515	-1.409407
30	1	0	-2.653992	3.181439	-0.660056
31	6	0	-3.359472	-0.061834	-0.202188
32	6	0	-4.105799	-0.507765	-1.292837
33	6	0	-3.533127	-0.708289	1.032114
34	6	0	-4.984004	-1.579173	-1.195922
35	1	0	-3.977593	-0.008814	-2.247755
36	6	0	-4.424512	-1.776090	1.135282
37	6	0	-5.140512	-2.213540	0.029810
38	1	0	-5.538678	-1.911176	-2.064079
39	1	0	-4.555192	-2.263503	2.096956
40	1	0	-5.824927	-3.046998	0.132520
41	8	0	-2.852765	-0.254186	2.112006
42	1	0	-3.136433	-0.748425	2.885596

Structure 34 (M06-2X, DMSO)

Energy (Hartrees): = -1052.096362
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.790572	-0.878062	0.213711
2	1	0	-4.421964	-0.177574	0.775419
3	6	0	-4.681334	-1.797909	-0.588997
4	1	0	-4.058533	-2.477037	-1.182997
5	1	0	-5.315074	-1.208671	-1.259345
6	6	0	-2.861708	-0.052230	-0.673267
7	1	0	-2.406405	-0.706666	-1.428465
8	6	0	-1.711533	0.536476	0.158228
9	1	0	-0.955457	-0.244080	0.277636
10	6	0	-1.060283	1.746915	-0.507479
11	1	0	-0.922462	1.551036	-1.573465
12	6	0	0.285091	2.079376	0.124624
13	8	0	-5.454296	-2.523214	0.362580
14	1	0	-5.880157	-3.258362	-0.088603
15	8	0	-2.996532	-1.643190	1.115663
16	1	0	-3.588112	-2.310429	1.485719
17	8	0	-3.653959	0.912545	-1.351109
18	1	0	-3.358087	1.789568	-1.072643
19	8	0	-2.147296	0.997546	1.434510
20	1	0	-2.394334	0.210901	1.936039
21	8	0	-1.939617	2.868822	-0.405511
22	1	0	-2.166545	2.940380	0.531851
23	1	0	0.649023	3.021003	-0.303418
24	1	0	0.138033	2.240140	1.200678
25	7	0	1.227715	1.004086	-0.141522
26	6	0	2.340896	1.015834	0.472667
27	6	0	2.745829	2.067046	1.478474
28	1	0	2.123060	1.998183	2.376298
29	1	0	3.789538	1.966122	1.770351
30	1	0	2.594167	3.063781	1.055424
31	6	0	3.302726	-0.100504	0.223117
32	6	0	3.853271	-0.776637	1.313999
33	6	0	3.674850	-0.499757	-1.069884
34	6	0	4.720845	-1.848983	1.146944
35	1	0	3.578376	-0.458735	2.314897
36	6	0	4.557301	-1.568107	-1.240912
37	6	0	5.070820	-2.242311	-0.141031
38	1	0	5.121849	-2.366137	2.009912
39	1	0	4.843020	-1.861688	-2.246741
40	1	0	5.752787	-3.070527	-0.295308
41	8	0	3.193627	0.188864	-2.133163
42	1	0	3.590672	-0.167673	-2.937506

Structure 35 (B3LYP, Gas Phase)

Energy (Hartrees): = -1167.0311421
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.392326	-0.726255	0.066843
2	1	0	-5.034033	0.029723	0.535886
3	6	0	-5.265627	-1.656656	-0.753267
4	1	0	-4.630498	-2.388481	-1.270122
5	1	0	-5.827389	-1.075566	-1.491344
6	6	0	-3.361819	0.020212	-0.791077
7	1	0	-2.869882	-0.694726	-1.465139
8	6	0	-2.244739	0.636492	0.085321
9	1	0	-1.484392	-0.130591	0.252311
10	6	0	-1.582031	1.849834	-0.575339
11	1	0	-1.406872	1.642186	-1.632350
12	6	0	-0.247917	2.210316	0.083891
13	8	0	-6.130971	-2.313017	0.183799
14	1	0	-6.606422	-3.011917	-0.272916
15	8	0	-3.706190	-1.474888	1.081268
16	1	0	-4.365061	-2.082806	1.441599
17	8	0	-4.074459	0.946854	-1.607317
18	1	0	-3.826604	1.844146	-1.334002
19	8	0	-2.736133	1.120581	1.345872
20	1	0	-3.019285	0.338077	1.837936
21	8	0	-2.490420	2.963141	-0.526260
22	1	0	-2.815478	2.985802	0.385368
23	1	0	0.112417	3.145321	-0.364454
24	1	0	-0.421081	2.403279	1.151422
25	7	0	0.693534	1.126178	-0.135049
26	6	0	1.800290	1.096277	0.491796
27	6	0	2.260828	2.160686	1.473619
28	1	0	3.256064	1.956796	1.865640
29	1	0	2.257023	3.153342	1.012859
30	1	0	1.568205	2.201504	2.320977
31	6	0	2.707613	-0.068143	0.249698

32	6	0	4.058852	0.162428	-0.054332
33	6	0	2.243954	-1.390926	0.310325
34	6	0	4.934967	-0.886718	-0.323341
35	1	0	4.404839	1.186562	-0.099054
36	6	0	3.132632	-2.440673	0.053275
37	6	0	4.459007	-2.199245	-0.265113
38	1	0	2.774155	-3.465101	0.105352
39	1	0	5.143794	-3.013171	-0.468611
40	8	0	0.942948	-1.632840	0.656702
41	1	0	0.815555	-2.584108	0.727923
42	8	0	6.256652	-0.741745	-0.647146
43	6	0	6.791964	0.569771	-0.714904
44	1	0	6.290617	1.171821	-1.481867
45	1	0	6.723538	1.084737	0.250811
46	1	0	7.840744	0.450834	-0.982603

Structure 35 (B3LYP, DMSO)

Energy (Hartrees): = -1167.0613413
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.333871	-1.091474	0.175850
2	1	0	-4.965812	-0.567865	0.904253
3	6	0	-5.227575	-1.869816	-0.770324
4	1	0	-4.611731	-2.376123	-1.523357
5	1	0	-5.920934	-1.188186	-1.274569
6	6	0	-3.489143	-0.028911	-0.542407
7	1	0	-3.064292	-0.463616	-1.456803
8	6	0	-2.292515	0.419970	0.328758
9	1	0	-1.490905	-0.309413	0.184583
10	6	0	-1.761315	1.804113	-0.057766
11	1	0	-1.706958	1.882874	-1.145426
12	6	0	-0.381159	2.104458	0.531184
13	8	0	-5.928366	-2.827065	0.037810
14	1	0	-6.291567	-3.502721	-0.545714
15	8	0	-3.457564	-1.997213	0.866886
16	1	0	-4.010682	-2.752427	1.111273
17	8	0	-4.370072	1.027877	-0.937319
18	1	0	-4.084845	1.832779	-0.475972
19	8	0	-2.625457	0.510698	1.722516
20	1	0	-2.832661	-0.392821	2.001036
21	8	0	-2.708179	2.806401	0.368097
22	1	0	-2.888247	2.612988	1.300144
23	1	0	-0.148091	3.156928	0.326745
24	1	0	-0.424289	1.989375	1.622009
25	7	0	0.615651	1.218145	-0.053840
26	6	0	1.837419	1.339810	0.295756
27	6	0	2.333116	2.351288	1.307531
28	1	0	1.871702	2.181555	2.286419
29	1	0	3.415527	2.325500	1.422841
30	1	0	2.045460	3.360474	0.994123
31	6	0	2.844529	0.414382	-0.312683
32	6	0	3.723932	-0.275407	0.540660
33	6	0	2.943983	0.212449	-1.698443
34	6	0	4.665680	-1.174141	0.042035
35	1	0	3.642699	-0.105843	1.606228
36	6	0	3.903006	-0.679834	-2.194054
37	6	0	4.750058	-1.369993	-1.341358
38	1	0	3.984338	-0.827240	-3.267280
39	1	0	5.486533	-2.061182	-1.734469
40	8	0	2.133195	0.914712	-2.544463
41	1	0	2.393087	0.711778	-3.452916
42	8	0	5.535104	-1.897078	0.807425
43	6	0	5.504031	-1.708757	2.221888
44	1	0	5.741999	-0.675158	2.495097
45	1	0	4.531344	-1.983614	2.643438
46	1	0	6.268435	-2.370534	2.627808

Structure 35 (M06-2X, Gas Phase)

Energy (Hartrees): = -1166.5729898
No imaginary frequencies
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.292098	-1.070159	-0.200793
2	1	0	4.903680	-0.495868	-0.908241
3	6	0	5.213993	-1.838698	0.718698

4	1	0	4.611548	-2.374748	1.462857
5	1	0	5.888228	-1.140537	1.222910
6	6	0	3.417791	-0.079231	0.561535
7	1	0	2.966011	-0.587439	1.423653
8	6	0	2.256626	0.408385	-0.324896
9	1	0	1.434291	-0.306052	-0.231968
10	6	0	1.756283	1.791894	0.084018
11	1	0	1.686681	1.854248	1.171978
12	6	0	0.392461	2.094162	-0.521738
13	8	0	5.913612	-2.755879	-0.115962
14	1	0	6.419016	-3.356514	0.434159
15	8	0	3.450337	-1.975089	-0.906561
16	1	0	4.015504	-2.710747	-1.169571
17	8	0	4.259516	0.940592	1.066876
18	1	0	4.069636	1.761408	0.593248
19	8	0	2.635613	0.544518	-1.692763
20	1	0	2.805992	-0.347736	-2.017032
21	8	0	2.709107	2.769060	-0.328020
22	1	0	2.905369	2.563555	-1.251484
23	1	0	0.156357	3.147261	-0.325983
24	1	0	0.457590	1.963394	-1.610989
25	7	0	-0.596742	1.209091	0.063215
26	6	0	-1.803306	1.308399	-0.314525
27	6	0	-2.283782	2.288485	-1.365261
28	1	0	-3.365385	2.264047	-1.481321
29	1	0	-1.990519	3.302672	-1.081776
30	1	0	-1.815143	2.079851	-2.331794
31	6	0	-2.817438	0.399682	0.296508
32	6	0	-3.726996	-0.259405	-0.539562
33	6	0	-2.882728	0.190391	1.675751
34	6	0	-4.675741	-1.134846	-0.025443
35	1	0	-3.659007	-0.083942	-1.605802
36	6	0	-3.849474	-0.679250	2.186695
37	6	0	-4.732573	-1.338473	1.352854
38	1	0	-3.905987	-0.837965	3.259417
39	1	0	-5.478652	-2.017305	1.746281
40	8	0	-2.030925	0.863748	2.494512
41	1	0	-2.264232	0.669262	3.405596
42	8	0	-5.580114	-1.828301	-0.771511
43	6	0	-5.538979	-1.651827	-2.169569
44	1	0	-5.738228	-0.610649	-2.446081
45	1	0	-4.571089	-1.958082	-2.580975
46	1	0	-6.321049	-2.287990	-2.577780

Structure 35 (M06-2X, DMSO)

Energy (Hartrees): = -1166.6059177
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.252459	-0.785607	0.151359
2	1	0	-4.895007	-0.093637	0.711044
3	6	0	-5.128688	-1.735272	-0.632245
4	1	0	-4.495333	-2.409336	-1.220941
5	1	0	-5.777857	-1.168208	-1.306936
6	6	0	-3.353663	0.051331	-0.755850
7	1	0	-2.889409	-0.601709	-1.506850
8	6	0	-2.210362	0.683028	0.052490
9	1	0	-1.427644	-0.071334	0.173513
10	6	0	-1.608597	1.904410	-0.641264
11	1	0	-1.489015	1.698043	-1.707520
12	6	0	-0.256147	2.274000	-0.044370
13	8	0	-5.881223	-2.463608	0.333105
14	1	0	-6.291693	-3.214957	-0.105303
15	8	0	-3.431628	-1.520462	1.054438
16	1	0	-4.003355	-2.196842	1.438564
17	8	0	-4.178233	0.984582	-1.440297
18	1	0	-3.911025	1.872654	-1.168201
19	8	0	-2.644430	1.150540	1.328275
20	1	0	-2.856784	0.364033	1.845364
21	8	0	-2.514303	3.004072	-0.534259
22	1	0	-2.729383	3.075660	0.405850
23	1	0	0.100792	3.192912	-0.523815
24	1	0	-0.387560	2.482928	1.025016
25	7	0	0.672319	1.183015	-0.287712
26	6	0	1.727498	1.102830	0.415123
27	6	0	2.124261	2.095455	1.481828
28	1	0	3.131641	1.913738	1.851905
29	1	0	2.059017	3.119898	1.107324
30	1	0	1.433528	2.010320	2.327190
31	6	0	2.634345	-0.061006	0.172693

32	6	0	4.003415	0.168462	-0.021367
33	6	0	2.145154	-1.370254	0.135879
34	6	0	4.876822	-0.883124	-0.278116
35	1	0	4.364573	1.188958	0.017335
36	6	0	3.030443	-2.423299	-0.109829
37	6	0	4.377019	-2.186748	-0.319215
38	1	0	2.652805	-3.441195	-0.131458
39	1	0	5.060691	-3.005406	-0.510877
40	8	0	0.824931	-1.602868	0.374716
41	1	0	0.682265	-2.556419	0.409963
42	8	0	6.211087	-0.743819	-0.494228
43	6	0	6.749204	0.566041	-0.419887
44	1	0	6.306964	1.222517	-1.175758
45	1	0	6.600798	1.001327	0.573377
46	1	0	7.815678	0.465972	-0.612180

Structure 36 (B3LYP, Gas Phase)

Energy (Hartrees): =-1257.0389688
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.645824	-0.805552	0.045962
2	1	0	-5.314176	-0.048596	0.474401
3	6	0	-5.480284	-1.781955	-0.761118
4	1	0	-4.818580	-2.515156	-1.241566
5	1	0	-6.039810	-1.238160	-1.528671
6	6	0	-3.609451	-0.066580	-0.811260
7	1	0	-3.085431	-0.793980	-1.446926
8	6	0	-2.528862	0.601744	0.073424
9	1	0	-1.759295	-0.144884	0.285476
10	6	0	-1.871027	1.805134	-0.609619
11	1	0	-1.659219	1.565517	-1.653174
12	6	0	-0.567825	2.221027	0.077981
13	8	0	-6.348434	-2.426779	0.180428
14	1	0	-6.807585	-3.144751	-0.263287
15	8	0	-3.967753	-1.504340	1.101167
16	1	0	-4.621769	-2.114604	1.466733
17	8	0	-4.317064	0.816040	-1.677389
18	1	0	-4.098018	1.727672	-1.428556
19	8	0	-3.060743	1.117216	1.303378
20	1	0	-3.350311	0.347174	1.811481
21	8	0	-2.800827	2.899999	-0.626905
22	1	0	-3.151818	2.952221	0.273870
23	1	0	-0.218960	3.153379	-0.384003
24	1	0	-0.778444	2.437293	1.134092
25	7	0	0.413340	1.159559	-0.068310
26	6	0	1.534072	1.235006	0.527852
27	6	0	1.971923	2.394137	1.403939
28	1	0	2.954389	2.235050	1.845522
29	1	0	1.990545	3.329150	0.835147
30	1	0	1.252885	2.532708	2.217480
31	6	0	2.495883	0.103866	0.332071
32	6	0	3.826792	0.373693	0.024927
33	6	0	2.097857	-1.249789	0.428411
34	6	0	4.728132	-0.657903	-0.212668
35	1	0	4.180597	1.392816	-0.051011
36	6	0	3.024170	-2.275537	0.194098
37	6	0	4.338713	-1.989933	-0.133274
38	1	0	2.702343	-3.309391	0.274570
39	1	0	5.061191	-2.771783	-0.319844
40	8	0	0.824480	-1.531691	0.785114
41	1	0	0.717041	-2.486506	0.858492
42	7	0	6.121130	-0.332192	-0.548704
43	8	0	6.888053	-1.264699	-0.758157
44	8	0	6.434478	0.851642	-0.598321

Structure 36 (B3LYP, DMSO)

Energy (Hartrees): = -1257.0711744
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.474237	-1.226417	0.182564
2	1	0	-5.173697	-0.718673	0.858454
3	6	0	-5.266257	-2.103147	-0.767858

4	1	0	-4.579786	-2.599575	-1.464446
5	1	0	-5.975037	-1.492976	-1.338313
6	6	0	-3.669906	-0.138061	-0.544458
7	1	0	-3.194157	-0.573681	-1.432758
8	6	0	-2.526940	0.407022	0.343267
9	1	0	-1.680922	-0.278776	0.244744
10	6	0	-2.067574	1.808228	-0.073783
11	1	0	-1.998682	1.862115	-1.161978
12	6	0	-0.713208	2.193538	0.525779
13	8	0	-5.944834	-3.069008	0.048540
14	1	0	-6.246705	-3.783994	-0.523043
15	8	0	-3.573560	-2.042414	0.950101
16	1	0	-4.086586	-2.822128	1.204806
17	8	0	-4.595382	0.854788	-0.998983
18	1	0	-4.382266	1.683506	-0.541348
19	8	0	-2.903641	0.523380	1.723721
20	1	0	-3.073461	-0.380761	2.025296
21	8	0	-3.074191	2.765832	0.311722
22	1	0	-3.265393	2.579245	1.243036
23	1	0	-0.533529	3.254517	0.312457
24	1	0	-0.755433	2.085383	1.617151
25	7	0	0.334288	1.359705	-0.047313
26	6	0	1.542897	1.537213	0.317533
27	6	0	1.989735	2.562093	1.336065
28	1	0	1.530983	2.364243	2.310696
29	1	0	3.071672	2.583905	1.457278
30	1	0	1.658946	3.558867	1.026273
31	6	0	2.589263	0.651299	-0.287596
32	6	0	3.503123	0.010865	0.543972
33	6	0	2.689149	0.432603	-1.682091
34	6	0	4.462779	-0.849148	0.016948
35	1	0	3.467694	0.167434	1.613390
36	6	0	3.671390	-0.428696	-2.195454
37	6	0	4.556029	-1.077360	-1.354751
38	1	0	3.735017	-0.579157	-3.268285
39	1	0	5.310492	-1.743499	-1.748793
40	8	0	1.850710	1.090523	-2.506508
41	1	0	2.076342	0.878912	-3.424442
42	7	0	5.392504	-1.519275	0.920620
43	8	0	6.224910	-2.283355	0.435004
44	8	0	5.302176	-1.290760	2.125884

Structure 36 (M06-2X, Gas Phase)

Energy (Hartrees): = -1256.5516258
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.360307	1.244157	-0.203626
2	1	0	-4.996625	0.750759	-0.949142
3	6	0	-5.238591	2.071984	0.707137
4	1	0	-4.615140	2.526871	1.487444
5	1	0	-5.993030	1.427069	1.167081
6	6	0	-3.612581	0.154637	0.558792
7	1	0	-3.151744	0.594932	1.453265
8	6	0	-2.464981	-0.408752	-0.299458
9	1	0	-1.593945	0.238274	-0.164626
10	6	0	-2.090966	-1.835837	0.094363
11	1	0	-2.060939	-1.925055	1.182309
12	6	0	-0.739983	-2.237605	-0.482554
13	8	0	-5.817519	3.073600	-0.121384
14	1	0	-6.299743	3.694431	0.427072
15	8	0	-3.408806	2.080745	-0.851279
16	1	0	-3.888099	2.875270	-1.113612
17	8	0	-4.562246	-0.798230	0.997550
18	1	0	-4.418689	-1.624384	0.517535
19	8	0	-2.805533	-0.488980	-1.680776
20	1	0	-2.886434	0.419457	-1.994957
21	8	0	-3.103251	-2.724756	-0.369016
22	1	0	-3.255455	-2.483369	-1.292334
23	1	0	-0.581338	-3.302758	-0.275875
24	1	0	-0.773557	-2.108565	-1.572798
25	7	0	0.303825	-1.431146	0.123161
26	6	0	1.486415	-1.527665	-0.321925
27	6	0	1.904057	-2.427650	-1.465330
28	1	0	2.985765	-2.531862	-1.527530
29	1	0	1.465635	-3.419335	-1.338740
30	1	0	1.536182	-2.031188	-2.417077
31	6	0	2.539039	-0.660413	0.288187
32	6	0	3.458550	-0.027231	-0.537849
33	6	0	2.626248	-0.442016	1.677149

34	6	0	4.416929	0.819271	-0.003471
35	1	0	3.432902	-0.173423	-1.610286
36	6	0	3.608081	0.409879	2.193422
37	6	0	4.505598	1.050919	1.359420
38	1	0	3.663676	0.565098	3.265826
39	1	0	5.266836	1.715618	1.743595
40	8	0	1.774643	-1.093089	2.489151
41	1	0	1.985300	-0.885705	3.404161
42	7	0	5.365554	1.484464	-0.906380
43	8	0	6.186928	2.223844	-0.408665
44	8	0	5.269253	1.252186	-2.092370

Structure 36 (M06-2X, DMSO)

Energy (Hartrees): = -1256.5853776
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.526610	-0.847790	0.153011
2	1	0	-5.190846	-0.140242	0.665736
3	6	0	-5.371250	-1.842034	-0.609329
4	1	0	-4.714461	-2.534381	-1.149270
5	1	0	-6.007989	-1.314185	-1.326200
6	6	0	-3.616034	-0.038600	-0.767628
7	1	0	-3.124217	-0.716413	-1.477824
8	6	0	-2.502812	0.644088	0.041718
9	1	0	-1.713032	-0.092965	0.213383
10	6	0	-1.899993	1.844627	-0.686401
11	1	0	-1.745587	1.597090	-1.739202
12	6	0	-0.573224	2.263312	-0.066138
13	8	0	-6.140476	-2.535173	0.368492
14	1	0	-6.537706	-3.306118	-0.047416
15	8	0	-3.719382	-1.531254	1.107893
16	1	0	-4.292552	-2.196753	1.508602
17	8	0	-4.435345	0.852432	-1.511824
18	1	0	-4.187578	1.755337	-1.271881
19	8	0	-2.974969	1.157862	1.284885
20	1	0	-3.194999	0.391347	1.828414
21	8	0	-2.825902	2.931894	-0.650969
22	1	0	-3.070839	3.037698	0.278534
23	1	0	-0.228425	3.179844	-0.558646
24	1	0	-0.734834	2.493340	0.994600
25	7	0	0.396342	1.197837	-0.258934
26	6	0	1.450860	1.198897	0.447824
27	6	0	1.794523	2.247346	1.476999
28	1	0	2.793960	2.111058	1.885648
29	1	0	1.714955	3.250279	1.050217
30	1	0	1.079805	2.185563	2.303811
31	6	0	2.428141	0.087130	0.232195
32	6	0	3.775343	0.385837	0.076525
33	6	0	2.027519	-1.262661	0.170415
34	6	0	4.690692	-0.627656	-0.165887
35	1	0	4.117173	1.411898	0.129127
36	6	0	2.971957	-2.269785	-0.061052
37	6	0	4.306481	-1.959709	-0.236607
38	1	0	2.646402	-3.304174	-0.096568
39	1	0	5.039140	-2.734609	-0.416421
40	8	0	0.733856	-1.565062	0.370902
41	1	0	0.624587	-2.525642	0.360771
42	7	0	6.100206	-0.282660	-0.346396
43	8	0	6.880375	-1.182663	-0.588241
44	8	0	6.421548	0.885438	-0.247637

Structure 37 (B3LYP, Gas Phase)

Energy (Hartrees): = -1052.4801179
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.693823	-0.080790	-0.079374
2	1	0	-4.661504	-0.353793	-1.140684
3	6	0	-5.848745	-0.817077	0.573061
4	1	0	-5.858262	-0.597872	1.649260
5	1	0	-5.728261	-1.894199	0.420684
6	6	0	-3.336434	-0.471794	0.517565

7	1	0	-3.406845	-0.446424	1.618606
8	6	0	-2.258446	0.571630	0.133671
9	1	0	-2.447515	1.439750	0.779996
10	6	0	-0.836398	0.104962	0.440781
11	1	0	-0.784180	-0.121624	1.517041
12	6	0	0.223045	1.165074	0.112301
13	8	0	-7.039546	-0.317599	-0.052500
14	1	0	-7.801957	-0.649517	0.428615
15	8	0	-4.880071	1.334459	0.054841
16	1	0	-5.814753	1.488132	-0.133857
17	8	0	-3.091511	-1.802438	0.090795
18	1	0	-2.153177	-1.873609	-0.147580
19	8	0	-2.332278	0.967536	-1.232214
20	1	0	-3.145066	1.483706	-1.303781
21	8	0	-0.541566	-1.073350	-0.308557
22	1	0	0.423087	-1.184689	-0.248685
23	1	0	0.035804	1.530732	-0.903699
24	1	0	0.138910	2.016050	0.801668
25	7	0	1.513648	0.504337	0.206191
26	6	0	2.606889	1.109275	-0.038003
27	6	0	2.693505	2.580029	-0.404670
28	1	0	2.576686	3.211537	0.483075
29	1	0	3.640741	2.831149	-0.880137
30	1	0	1.883255	2.839503	-1.089709
31	6	0	3.876141	0.330990	0.056697
32	6	0	5.039019	0.950310	0.534923
33	6	0	3.962795	-1.031646	-0.307272
34	6	0	6.242758	0.269360	0.675958
35	1	0	4.990855	1.994567	0.821169
36	6	0	5.177232	-1.711753	-0.179753
37	6	0	6.308772	-1.072031	0.311748
38	1	0	7.116217	0.779942	1.062788
39	1	0	5.228046	-2.757542	-0.470574
40	1	0	7.237321	-1.623392	0.405458
41	8	0	2.867691	-1.668424	-0.812926
42	1	0	3.135448	-2.543498	-1.114312

Structure 37 (B3LYP, DMSO)

Energy (Hartrees): = -1052.5097167
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.698416	-0.097138	0.070472
2	1	0	4.721994	-0.336730	1.140923
3	6	0	5.825373	-0.842736	-0.618598
4	1	0	5.797009	-0.636065	-1.695355
5	1	0	5.714242	-1.920762	-0.458330
6	6	0	3.313441	-0.507303	-0.448002
7	1	0	3.345063	-0.581253	-1.546571
8	6	0	2.257552	0.572449	-0.119383
9	1	0	2.451870	1.401569	-0.810564
10	6	0	0.830990	0.113345	-0.407015
11	1	0	0.793841	-0.192648	-1.462285
12	6	0	-0.223269	1.201549	-0.182047
13	8	0	7.044979	-0.350632	-0.042660
14	1	0	7.771081	-0.593695	-0.627920
15	8	0	4.873700	1.315662	-0.109429
16	1	0	5.818024	1.473580	0.027546
17	8	0	3.049112	-1.794159	0.109672
18	1	0	2.094863	-1.837489	0.285937
19	8	0	2.350792	1.038066	1.228524
20	1	0	3.173706	1.543693	1.260813
21	8	0	0.501099	-1.013547	0.422362
22	1	0	-0.460011	-1.129541	0.317257
23	1	0	-0.073863	1.647465	0.807309
24	1	0	-0.113167	1.995681	-0.931047
25	7	0	-1.515316	0.539271	-0.286900
26	6	0	-2.604093	1.120517	0.035986
27	6	0	-2.699243	2.559089	0.494317
28	1	0	-2.638546	3.242419	-0.359892
29	1	0	-3.630104	2.760674	1.023685
30	1	0	-1.863686	2.799157	1.156383
31	6	0	-3.865992	0.328765	-0.067440
32	6	0	-5.036771	0.948650	-0.529085
33	6	0	-3.936164	-1.041015	0.273340
34	6	0	-6.232405	0.254401	-0.680788
35	1	0	-5.000422	2.000046	-0.790754
36	6	0	-5.142397	-1.735534	0.133975
37	6	0	-6.281152	-1.096931	-0.344234
38	1	0	-7.113771	0.762478	-1.054045

39	1	0	-5.179959	-2.785829	0.408923
40	1	0	-7.203708	-1.657223	-0.447450
41	8	0	-2.835709	-1.674393	0.773105
42	1	0	-3.094741	-2.567035	1.042154

Structure 37 (M06-2X, Gas Phase)

Energy (Hartrees): = -1052.0659394
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.644341	-0.067376	0.100674
2	1	0	4.573755	-0.329030	1.163367
3	6	0	5.808103	-0.817814	-0.505504
4	1	0	5.850267	-0.604200	-1.581279
5	1	0	5.667874	-1.890847	-0.346628
6	6	0	3.318155	-0.456494	-0.543554
7	1	0	3.424336	-0.414253	-1.639293
8	6	0	2.237454	0.573098	-0.167943
9	1	0	2.423649	1.449012	-0.803821
10	6	0	0.827526	0.090763	-0.475137
11	1	0	0.784728	-0.195259	-1.536462
12	6	0	-0.218006	1.170996	-0.206528
13	8	0	6.971422	-0.322852	0.149844
14	1	0	7.748625	-0.699774	-0.265547
15	8	0	4.838965	1.333965	-0.049040
16	1	0	5.765116	1.493567	0.165091
17	8	0	3.060814	-1.787904	-0.154528
18	1	0	2.154757	-1.841534	0.180062
19	8	0	2.293982	0.947185	1.195146
20	1	0	3.098851	1.468528	1.288344
21	8	0	0.528893	-1.030896	0.338388
22	1	0	-0.429766	-1.166670	0.271133
23	1	0	-0.035951	1.572569	0.796587
24	1	0	-0.128502	1.988093	-0.933278
25	7	0	-1.507130	0.512137	-0.287523
26	6	0	-2.583086	1.110738	0.010549
27	6	0	-2.666678	2.570053	0.400245
28	1	0	-2.671893	3.201265	-0.494095
29	1	0	-3.565190	2.783792	0.977041
30	1	0	-1.793944	2.850079	0.991240
31	6	0	-3.850017	0.328650	-0.051334
32	6	0	-5.033137	0.953280	-0.449488
33	6	0	-3.900269	-1.039687	0.273055
34	6	0	-6.234670	0.265935	-0.551063
35	1	0	-5.003515	2.007808	-0.700622
36	6	0	-5.109705	-1.727536	0.184864
37	6	0	-6.267796	-1.084208	-0.227916
38	1	0	-7.131521	0.778079	-0.874672
39	1	0	-5.135942	-2.782002	0.443388
40	1	0	-7.194193	-1.642111	-0.291671
41	8	0	-2.777244	-1.674445	0.702137
42	1	0	-3.019576	-2.554893	1.002678

Structure 37 (M06-2X, DMSO)

Energy (Hartrees): = -1052.0969557
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.651159	-0.074664	0.085786
2	1	0	4.640712	-0.296601	1.160373
3	6	0	5.790967	-0.832996	-0.554945
4	1	0	5.795708	-0.632416	-1.632962
5	1	0	5.663814	-1.907177	-0.386594
6	6	0	3.294641	-0.493436	-0.473733
7	1	0	3.354395	-0.545588	-1.571621
8	6	0	2.233534	0.565732	-0.140347
9	1	0	2.431092	1.416242	-0.803635
10	6	0	0.819731	0.100201	-0.449755
11	1	0	0.795814	-0.225517	-1.499032
12	6	0	-0.217727	1.201254	-0.252483
13	8	0	6.981279	-0.341080	0.053797
14	1	0	7.734174	-0.641018	-0.464168

15	8	0	4.826639	1.322990	-0.118708
16	1	0	5.761588	1.495221	0.047823
17	8	0	3.030664	-1.783193	0.052269
18	1	0	2.088481	-1.824405	0.268560
19	8	0	2.298670	0.979829	1.215107
20	1	0	3.108348	1.498697	1.286926
21	8	0	0.481170	-0.995412	0.398075
22	1	0	-0.475763	-1.125496	0.293333
23	1	0	-0.069282	1.653390	0.733914
24	1	0	-0.098691	1.980934	-1.013799
25	7	0	-1.510042	0.547305	-0.356503
26	6	0	-2.578734	1.123323	0.015244
27	6	0	-2.662313	2.549010	0.499318
28	1	0	-2.635613	3.236838	-0.351912
29	1	0	-3.577092	2.733662	1.060512
30	1	0	-1.806134	2.784142	1.134252
31	6	0	-3.839901	0.330828	-0.061526
32	6	0	-5.025715	0.952555	-0.461726
33	6	0	-3.878386	-1.040552	0.252221
34	6	0	-6.217959	0.250687	-0.582272
35	1	0	-5.004054	2.011426	-0.697411
36	6	0	-5.079027	-1.743557	0.145151
37	6	0	-6.238671	-1.105683	-0.274511
38	1	0	-7.118584	0.756660	-0.907524
39	1	0	-5.095835	-2.799692	0.397767
40	1	0	-7.159021	-1.672779	-0.353212
41	8	0	-2.753768	-1.665956	0.692939
42	1	0	-2.990575	-2.561294	0.967569

Structure 38 (B3LYP, Gas Phase)

Energy (Hartrees): = -1167.030707
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.374281	-0.080516	0.019108
2	1	0	5.406557	0.275313	-1.017407
3	6	0	6.538459	0.531605	0.775090
4	1	0	6.486111	0.230207	1.829950
5	1	0	6.487470	1.622568	0.703924
6	6	0	4.015408	0.345511	0.587821
7	1	0	4.032514	0.231034	1.685595
8	6	0	2.898910	-0.597226	0.076924
9	1	0	3.019910	-1.529561	0.645218
10	6	0	1.492721	-0.084746	0.383406
11	1	0	1.410983	0.031384	1.475263
12	6	0	0.391884	-1.043128	-0.089709
13	8	0	7.725973	0.009762	0.161443
14	1	0	8.483307	0.256548	0.698551
15	8	0	5.471934	-1.510319	0.047271
16	1	0	6.404276	-1.705911	-0.111924
17	8	0	3.868906	1.716178	0.254126
18	1	0	2.939859	1.868651	0.017336
19	8	0	3.001834	-0.870975	-1.317129
20	1	0	3.785026	-1.427420	-1.410772
21	8	0	1.289072	1.180049	-0.245707
22	1	0	0.331916	1.347502	-0.196234
23	1	0	0.596352	-1.308933	-1.132942
24	1	0	0.405448	-1.966000	0.506097
25	7	0	-0.863920	-0.325144	0.041954
26	6	0	-1.974979	-0.815540	-0.338973
27	6	0	-2.130281	-2.210705	-0.917901
28	1	0	-2.117195	-2.966948	-0.124968
29	1	0	-3.056680	-2.321236	-1.480476
30	1	0	-1.293041	-2.432653	-1.583211
31	6	0	-3.195796	0.030261	-0.197087
32	6	0	-4.417337	-0.580040	0.141047
33	6	0	-3.172106	1.424499	-0.382941
34	6	0	-5.584921	0.158397	0.311397
35	1	0	-4.430026	-1.650999	0.288210
36	6	0	-4.354218	2.156547	-0.225950
37	6	0	-5.545761	1.541944	0.119012
38	1	0	-4.333530	3.232362	-0.376502
39	1	0	-6.456531	2.114272	0.243934
40	8	0	-2.010953	2.053117	-0.745444
41	1	0	-2.218645	2.965484	-0.973285
42	8	0	-6.800230	-0.364023	0.657882
43	6	0	-6.898118	-1.763998	0.864155
44	1	0	-7.936343	-1.954183	1.131504
45	1	0	-6.652647	-2.324905	-0.045462
46	1	0	-6.248822	-2.098071	1.681993

Structure 38 (B3LYP, DMSO)

Energy (Hartrees): = -1167.0620398
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.384916	-0.073419	-0.032783
2	1	0	-5.462909	0.290821	0.999110
3	6	0	-6.527100	0.511409	-0.841921
4	1	0	-6.446122	0.176956	-1.883269
5	1	0	-6.486070	1.605716	-0.813974
6	6	0	-4.007436	0.355097	-0.554321
7	1	0	-3.993604	0.268445	-1.652371
8	6	0	-2.902112	-0.590784	-0.033128
9	1	0	-3.016504	-1.524967	-0.596064
10	6	0	-1.495703	-0.084071	-0.338429
11	1	0	-1.433300	0.070947	-1.425115
12	6	0	-0.388575	-1.058518	0.075473
13	8	0	-7.737401	0.018208	-0.247131
14	1	0	-8.453495	0.145586	-0.879448
15	8	0	-5.467256	-1.505799	-0.044608
16	1	0	-6.404098	-1.707298	0.085353
17	8	0	-3.849731	1.723405	-0.180846
18	1	0	-2.909154	1.856770	0.021157
19	8	0	-3.022181	-0.855587	1.366860
20	1	0	-3.805983	-1.414157	1.450151
21	8	0	-1.270618	1.167727	0.330612
22	1	0	-0.312093	1.323325	0.254039
23	1	0	-0.557471	-1.374357	1.110847
24	1	0	-0.415012	-1.953311	-0.558852
25	7	0	0.864414	-0.331797	-0.064239
26	6	0	1.975154	-0.814041	0.337720
27	6	0	2.132248	-2.196587	0.931682
28	1	0	2.132430	-2.956960	0.142678
29	1	0	3.055153	-2.298158	1.501692
30	1	0	1.289972	-2.419784	1.591038
31	6	0	3.193805	0.036184	0.187379
32	6	0	4.411997	-0.581452	-0.154287
33	6	0	3.172593	1.432563	0.367080
34	6	0	5.579653	0.155554	-0.339024
35	1	0	4.422537	-1.653810	-0.291803
36	6	0	4.354203	2.163578	0.194923
37	6	0	5.541475	1.542575	-0.157342
38	1	0	4.337392	3.239249	0.344926
39	1	0	6.448585	2.120230	-0.291011
40	8	0	2.018545	2.068192	0.741326
41	1	0	2.232300	2.991760	0.932451
42	8	0	6.787879	-0.373239	-0.690082
43	6	0	6.885938	-1.789712	-0.836683
44	1	0	7.923763	-1.990871	-1.099866
45	1	0	6.646230	-2.308473	0.097638
46	1	0	6.235312	-2.158591	-1.636720

Structure 38 (M06-2X, Gas Phase)

Energy (Hartrees): = -1166.5734535
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.311510	-0.071651	0.030292
2	1	0	-5.275895	0.262577	1.074134
3	6	0	-6.492161	0.585999	-0.646992
4	1	0	-6.500157	0.303114	-1.707468
5	1	0	-6.401670	1.672082	-0.554814
6	6	0	-3.989149	0.331185	-0.612928
7	1	0	-4.068276	0.207438	-1.704881
8	6	0	-2.873222	-0.619885	-0.143639
9	1	0	-3.005092	-1.545323	-0.720151
10	6	0	-1.479287	-0.095133	-0.453507
11	1	0	-1.422699	0.119905	-1.530775
12	6	0	-0.390839	-1.102880	-0.089324
13	8	0	-7.648109	0.082606	0.015084
14	1	0	-8.430747	0.403565	-0.435434
15	8	0	-5.442729	-1.486879	-0.029152

16	1	0	-6.366364	-1.672678	0.174686
17	8	0	-3.799897	1.696689	-0.313700
18	1	0	-2.902812	1.814537	0.029173
19	8	0	-2.946104	-0.901887	1.240938
20	1	0	-3.729005	-1.452144	1.353304
21	8	0	-1.254009	1.092465	0.287474
22	1	0	-0.305248	1.285534	0.218081
23	1	0	-0.577436	-1.445014	0.934589
24	1	0	-0.422392	-1.969862	-0.760869
25	7	0	0.864462	-0.386007	-0.198276
26	6	0	1.954623	-0.860039	0.237678
27	6	0	2.119801	-2.244559	0.824660
28	1	0	2.256839	-2.981320	0.026750
29	1	0	2.979554	-2.295781	1.491477
30	1	0	1.225477	-2.529015	1.379691
31	6	0	3.160534	0.012018	0.151564
32	6	0	4.406897	-0.564227	-0.128038
33	6	0	3.080040	1.395142	0.349053
34	6	0	5.555428	0.210132	-0.231060
35	1	0	4.451740	-1.635000	-0.278773
36	6	0	4.242127	2.163860	0.257304
37	6	0	5.464015	1.587121	-0.030643
38	1	0	4.181170	3.236364	0.415112
39	1	0	6.365037	2.182904	-0.103370
40	8	0	1.885836	1.979824	0.661097
41	1	0	2.054786	2.881374	0.947632
42	8	0	6.795925	-0.272741	-0.513735
43	6	0	6.919517	-1.661099	-0.728183
44	1	0	7.970653	-1.841932	-0.940695
45	1	0	6.627337	-2.229573	0.161325
46	1	0	6.315781	-1.986207	-1.582264

Structure 38 (M06-2X, DMSO)

Energy (Hartrees): = -1166.6061779
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.335363	-0.080844	-0.006026
2	1	0	-5.369886	0.276123	1.030881
3	6	0	-6.495234	0.519472	-0.767035
4	1	0	-6.452534	0.184927	-1.810416
5	1	0	-6.437267	1.611943	-0.734265
6	6	0	-3.986521	0.340665	-0.581121
7	1	0	-4.008234	0.230828	-1.675944
8	6	0	-2.879170	-0.591090	-0.065220
9	1	0	-2.993622	-1.535537	-0.610467
10	6	0	-1.483843	-0.076400	-0.380052
11	1	0	-1.433345	0.120293	-1.460265
12	6	0	-0.390442	-1.073130	-0.009415
13	8	0	-7.675482	0.036429	-0.131725
14	1	0	-8.426736	0.227279	-0.701195
15	8	0	-5.423601	-1.501525	-0.032883
16	1	0	-6.352303	-1.708331	0.128638
17	8	0	-3.817071	1.707530	-0.244126
18	1	0	-2.895425	1.832765	0.022151
19	8	0	-2.981084	-0.821758	1.331582
20	1	0	-3.755012	-1.385953	1.443440
21	8	0	-1.251151	1.133610	0.337597
22	1	0	-0.298476	1.307129	0.258925
23	1	0	-0.553379	-1.408522	1.020616
24	1	0	-0.425720	-1.948292	-0.668609
25	7	0	0.861582	-0.350155	-0.141348
26	6	0	1.956504	-0.832794	0.282408
27	6	0	2.112661	-2.214740	0.865398
28	1	0	2.174640	-2.955122	0.061074
29	1	0	3.009424	-2.297263	1.478048
30	1	0	1.243599	-2.468377	1.474846
31	6	0	3.170460	0.026081	0.163281
32	6	0	4.398111	-0.578090	-0.145930
33	6	0	3.118564	1.413942	0.348810
34	6	0	5.556777	0.175774	-0.291663
35	1	0	4.420126	-1.651533	-0.284893
36	6	0	4.291101	2.162175	0.214050
37	6	0	5.493401	1.558408	-0.104954
38	1	0	4.255115	3.236489	0.368005
39	1	0	6.398518	2.145180	-0.208437
40	8	0	1.946773	2.025127	0.691308
41	1	0	2.141299	2.942780	0.920018
42	8	0	6.776103	-0.334923	-0.604090
43	6	0	6.870464	-1.741752	-0.760564

44	1	0	7.914171	-1.951353	-0.986660
45	1	0	6.587997	-2.264323	0.158696
46	1	0	6.245257	-2.092033	-1.587849

Structure 39 (B3LYP, Gas Phase)

Energy (Hartrees): = -1257.0376977
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.646518	-0.061573	0.072245
2	1	0	5.708621	0.327075	-0.951014
3	6	0	6.796160	0.514897	0.877088
4	1	0	6.714350	0.180402	1.919998
5	1	0	6.756729	1.608120	0.840053
6	6	0	4.276321	0.358242	0.618761
7	1	0	4.265861	0.218225	1.713486
8	6	0	3.169618	-0.567732	0.058572
9	1	0	3.275233	-1.514138	0.606157
10	6	0	1.756732	-0.060383	0.343098
11	1	0	1.646709	0.028657	1.434802
12	6	0	0.673036	-1.008721	-0.185895
13	8	0	7.993170	0.001288	0.276407
14	1	0	8.739936	0.223663	0.838464
15	8	0	5.730722	-1.492250	0.056462
16	1	0	6.665325	-1.692401	-0.083181
17	8	0	4.143949	1.737337	0.314568
18	1	0	3.223715	1.901501	0.056007
19	8	0	3.302343	-0.806511	-1.338824
20	1	0	4.086800	-1.362090	-1.429634
21	8	0	1.568945	1.219558	-0.260127
22	1	0	0.610816	1.378540	-0.239903
23	1	0	0.908267	-1.242261	-1.230124
24	1	0	0.673383	-1.947575	0.383099
25	7	0	-0.594222	-0.303167	-0.083546
26	6	0	-1.695753	-0.837459	-0.428185
27	6	0	-1.834424	-2.256131	-0.946726
28	1	0	-1.844482	-2.974871	-0.119867
29	1	0	-2.747434	-2.394858	-1.525104
30	1	0	-0.981857	-2.507038	-1.580516
31	6	0	-2.939454	-0.020460	-0.286422
32	6	0	-4.130907	-0.645642	0.080272
33	6	0	-2.968777	1.381108	-0.494570
34	6	0	-5.300260	0.082789	0.257205
35	1	0	-4.165811	-1.713012	0.247151
36	6	0	-4.163229	2.094365	-0.322656
37	6	0	-5.331902	1.457711	0.057576
38	1	0	-4.166524	3.166868	-0.491789
39	1	0	-6.256243	2.000187	0.196748
40	8	0	-1.843396	2.019963	-0.891182
41	1	0	-2.053517	2.942191	-1.078494
42	7	0	-6.529388	-0.617460	0.658304
43	8	0	-7.542274	0.055180	0.806848
44	8	0	-6.468042	-1.830671	0.819372

Structure 39 (B3LYP, DMSO)

Energy (Hartrees): = -1257.0712458
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.657883	-0.061862	-0.128104
2	1	0	-5.805514	0.367233	0.870818
3	6	0	-6.752959	0.451265	-1.044150
4	1	0	-6.599338	0.055965	-2.055477
5	1	0	-6.729667	1.545886	-1.080585
6	6	0	-4.255879	0.354970	-0.591091
7	1	0	-4.176865	0.210091	-1.680250
8	6	0	-3.174587	-0.548304	0.041435
9	1	0	-3.264096	-1.518989	-0.460690
10	6	0	-1.756073	-0.060510	-0.237965
11	1	0	-1.642535	0.001311	-1.329669
12	6	0	-0.671205	-0.991593	0.310632
13	8	0	-7.991716	-0.027443	-0.498803
14	1	0	-8.668478	0.052369	-1.180313

15	8	0	-5.722845	-1.492608	-0.051554
16	1	0	-6.664251	-1.699910	0.026862
17	8	0	-4.133773	1.741896	-0.279093
18	1	0	-3.199833	1.904800	-0.070491
19	8	0	-3.356219	-0.715776	1.449350
20	1	0	-4.137237	-1.277380	1.537629
21	8	0	-1.562569	1.244400	0.331033
22	1	0	-0.601709	1.390262	0.288994
23	1	0	-0.879529	-1.198189	1.366009
24	1	0	-0.679540	-1.945353	-0.230172
25	7	0	0.594513	-0.286233	0.161208
26	6	0	1.699037	-0.812667	0.516662
27	6	0	1.838852	-2.204572	1.089456
28	1	0	1.835750	-2.952368	0.288576
29	1	0	2.761104	-2.322215	1.658233
30	1	0	0.995085	-2.428970	1.745431
31	6	0	2.944907	-0.008840	0.316888
32	6	0	4.111044	-0.656143	-0.087386
33	6	0	3.000582	1.394601	0.511142
34	6	0	5.282793	0.057365	-0.316716
35	1	0	4.113105	-1.726189	-0.240130
36	6	0	4.197536	2.092956	0.289709
37	6	0	5.339395	1.436737	-0.128681
38	1	0	4.220886	3.165418	0.454217
39	1	0	6.258981	1.977509	-0.302625
40	8	0	1.902795	2.051346	0.941213
41	1	0	2.130860	2.981135	1.091694
42	7	0	6.477844	-0.657156	-0.756803
43	8	0	7.506821	-0.008952	-0.937752
44	8	0	6.401627	-1.872753	-0.926880

Structure 39 (M06-2X, Gas Phase)

Energy (Hartrees): = -1256.5508808
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.603597	-0.071970	-0.053249
2	1	0	-5.634521	0.319891	0.970531
3	6	0	-6.763508	0.510711	-0.827791
4	1	0	-6.707239	0.168926	-1.869298
5	1	0	-6.707857	1.602496	-0.793366
6	6	0	-4.258900	0.336514	-0.645619
7	1	0	-4.275832	0.163360	-1.733636
8	6	0	-3.150388	-0.565709	-0.076211
9	1	0	-3.247572	-1.526049	-0.599624
10	6	0	-1.750211	-0.043397	-0.361672
11	1	0	-1.646218	0.091483	-1.448344
12	6	0	-0.674383	-1.009299	0.129193
13	8	0	-7.938022	0.010020	-0.198303
14	1	0	-8.705558	0.288470	-0.700527
15	8	0	-5.690468	-1.491399	-0.039358
16	1	0	-6.618409	-1.696485	0.122076
17	8	0	-4.118638	1.717490	-0.394988
18	1	0	-3.234619	1.879356	-0.039047
19	8	0	-3.274417	-0.762872	1.318897
20	1	0	-4.048800	-1.324281	1.435464
21	8	0	-1.568389	1.198178	0.297640
22	1	0	-0.616239	1.376773	0.277588
23	1	0	-0.902243	-1.260627	1.171101
24	1	0	-0.676784	-1.931695	-0.464266
25	7	0	0.589427	-0.302354	0.032431
26	6	0	1.677346	-0.842371	0.388810
27	6	0	1.810545	-2.260934	0.893647
28	1	0	1.885384	-2.958965	0.053807
29	1	0	2.693153	-2.384709	1.519850
30	1	0	0.928324	-2.537124	1.471640
31	6	0	2.921684	-0.027164	0.267166
32	6	0	4.114790	-0.650785	-0.078938
33	6	0	2.935495	1.368133	0.476794
34	6	0	5.276178	0.087143	-0.234426
35	1	0	4.153390	-1.719763	-0.243782
36	6	0	4.124456	2.087860	0.326369
37	6	0	5.300958	1.457391	-0.034826
38	1	0	4.118707	3.159466	0.495966
39	1	0	6.226148	2.002616	-0.159466
40	8	0	1.801175	1.993780	0.853290
41	1	0	2.000673	2.912048	1.060191
42	7	0	6.516443	-0.603787	-0.615276
43	8	0	7.512308	0.072583	-0.752686
44	8	0	6.465478	-1.805147	-0.767295

Structure 39 (M06-2X, DMSO)

Energy (Hartrees): = -1256.585091
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.619793	-0.075872	-0.098944
2	1	0	-5.736741	0.345663	0.907236
3	6	0	-6.736101	0.441633	-0.976965
4	1	0	-6.609398	0.043571	-1.990630
5	1	0	-6.706300	1.535319	-1.010861
6	6	0	-4.244772	0.349509	-0.606765
7	1	0	-4.195437	0.196436	-1.695672
8	6	0	-3.155770	-0.538973	0.010867
9	1	0	-3.240135	-1.513630	-0.484191
10	6	0	-1.750939	-0.033766	-0.274438
11	1	0	-1.649803	0.077652	-1.363138
12	6	0	-0.672772	-0.989006	0.224764
13	8	0	-7.947194	-0.033944	-0.397581
14	1	0	-8.660245	0.104331	-1.028240
15	8	0	-5.672187	-1.496965	-0.039034
16	1	0	-6.604639	-1.719844	0.070961
17	8	0	-4.122879	1.730564	-0.310537
18	1	0	-3.208091	1.893595	-0.042618
19	8	0	-3.319367	-0.689095	1.412232
20	1	0	-4.091160	-1.256729	1.522113
21	8	0	-1.558312	1.230705	0.355255
22	1	0	-0.602923	1.394320	0.315699
23	1	0	-0.873838	-1.227978	1.274697
24	1	0	-0.683879	-1.920617	-0.352250
25	7	0	0.589115	-0.280720	0.090210
26	6	0	1.678796	-0.817069	0.455734
27	6	0	1.805618	-2.216212	1.000629
28	1	0	1.822753	-2.938954	0.178273
29	1	0	2.715597	-2.341436	1.586072
30	1	0	0.946270	-2.454565	1.629450
31	6	0	2.927099	-0.014608	0.289670
32	6	0	4.100534	-0.661597	-0.080083
33	6	0	2.965007	1.383597	0.481591
34	6	0	5.265683	0.061780	-0.279767
35	1	0	4.108356	-1.734164	-0.227213
36	6	0	4.159614	2.087883	0.292088
37	6	0	5.314023	1.436899	-0.095956
38	1	0	4.172846	3.160395	0.455298
39	1	0	6.236136	1.980933	-0.248684
40	8	0	1.852615	2.029453	0.877386
41	1	0	2.069689	2.957594	1.042308
42	7	0	6.478626	-0.646071	-0.688908
43	8	0	7.482258	0.010501	-0.884077
44	8	0	6.422492	-1.853662	-0.813927

Structure 40 (B3LYP, Gas Phase)

Energy (Hartrees): = =-1052.4855591
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.720250	0.790330	-0.205607
2	1	0	3.196015	1.537454	0.402288
3	6	0	5.206457	0.854834	0.113180
4	1	0	5.731645	0.057750	-0.430205
5	1	0	5.365941	0.728233	1.186977
6	6	0	3.124350	-0.584095	0.095072
7	1	0	3.567343	-1.293514	-0.624188
8	6	0	1.608526	-0.608801	-0.143439
9	1	0	1.448039	-0.331639	-1.191932
10	6	0	1.014741	-2.013418	0.127665
11	1	0	1.685103	-2.782121	-0.269577
12	6	0	-0.365373	-2.220517	-0.505817
13	8	0	5.645523	2.145958	-0.339879
14	1	0	6.605476	2.166200	-0.314215
15	8	0	3.514230	1.044704	-1.594827
16	1	0	4.082980	1.796595	-1.800921

17	8	0	3.490604	-0.930582	1.424350
18	1	0	2.830466	-1.555611	1.757507
19	8	0	0.987191	0.332188	0.729770
20	1	0	0.053158	0.383013	0.460266
21	8	0	0.966901	-2.223700	1.544549
22	1	0	0.638035	-1.382237	1.899875
23	1	0	-0.245880	-2.294826	-1.597267
24	1	0	-0.758735	-3.183133	-0.153995
25	7	0	-1.261162	-1.125787	-0.159433
26	6	0	-2.467931	-1.104128	-0.571408
27	6	0	-3.083256	-2.200243	-1.423695
28	1	0	-3.269683	-3.099355	-0.826201
29	1	0	-4.020507	-1.890778	-1.882548
30	1	0	-2.392474	-2.486719	-2.220241
31	6	0	-3.334494	0.045521	-0.178337
32	6	0	-4.698640	-0.163568	0.069528
33	6	0	-2.836959	1.357611	-0.018145
34	6	0	-5.547356	0.859970	0.474535
35	1	0	-5.099941	-1.164257	-0.038374
36	6	0	-3.692376	2.390518	0.372068
37	6	0	-5.037470	2.146397	0.621848
38	1	0	-6.592662	0.655219	0.670829
39	1	0	-3.291644	3.394233	0.481920
40	1	0	-5.681395	2.962126	0.929697
41	8	0	-1.521459	1.607656	-0.276650
42	1	0	-1.349873	2.551625	-0.186860

Structure 40 (B3LYP, DMSO)

Energy (Hartrees): = -1052.5152604
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.793842	-0.766537	0.185620
2	1	0	3.273391	-1.553278	-0.375181
3	6	0	5.270742	-0.798262	-0.180623
4	1	0	5.791332	0.035710	0.306552
5	1	0	5.397880	-0.716439	-1.263541
6	6	0	3.143318	0.577046	-0.142704
7	1	0	3.609660	1.335117	0.506051
8	6	0	1.642740	0.594576	0.176627
9	1	0	1.542358	0.391578	1.249456
10	6	0	1.012175	1.972794	-0.131325
11	1	0	1.677285	2.765675	0.219657
12	6	0	-0.353610	2.173915	0.525877
13	8	0	5.772274	-2.055149	0.305900
14	1	0	6.732722	-1.994568	0.353171
15	8	0	3.649458	-0.988679	1.590750
16	1	0	4.291172	-1.681856	1.796737
17	8	0	3.419908	0.866505	-1.513730
18	1	0	2.703078	1.440805	-1.825571
19	8	0	0.989333	-0.414656	-0.595372
20	1	0	0.049967	-0.395090	-0.332082
21	8	0	0.924130	2.137066	-1.562234
22	1	0	0.492961	1.326741	-1.874709
23	1	0	-0.215939	2.228920	1.614580
24	1	0	-0.755772	3.141987	0.202270
25	7	0	-1.256609	1.083031	0.172957
26	6	0	-2.467815	1.090885	0.581881
27	6	0	-3.053241	2.200665	1.428027
28	1	0	-3.139345	3.125835	0.847531
29	1	0	-4.034944	1.948677	1.824714
30	1	0	-2.387944	2.414037	2.269469
31	6	0	-3.361185	-0.036066	0.180743
32	6	0	-4.704436	0.227864	-0.129566
33	6	0	-2.914103	-1.371457	0.071978
34	6	0	-5.577231	-0.769141	-0.551325
35	1	0	-5.066277	1.246598	-0.055477
36	6	0	-3.795421	-2.377994	-0.334839
37	6	0	-5.116499	-2.080578	-0.649711
38	1	0	-6.604132	-0.525222	-0.796564
39	1	0	-3.433969	-3.400135	-0.402561
40	1	0	-5.781315	-2.875644	-0.968336
41	8	0	-1.624750	-1.674387	0.396462
42	1	0	-1.504381	-2.632524	0.334978

Structure 40 (M06-2X, Gas Phase)

Energy (Hartrees): = -1052.0727314

No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.684901	-0.781923	0.208045
2	1	0	3.167476	-1.531956	-0.401558
3	6	0	5.167934	-0.829462	-0.102982
4	1	0	5.674176	-0.018284	0.436513
5	1	0	5.326045	-0.709500	-1.177162
6	6	0	3.096313	0.584613	-0.100057
7	1	0	3.547292	1.301804	0.604899
8	6	0	1.589759	0.604561	0.143797
9	1	0	1.428429	0.352266	1.199022
10	6	0	1.002237	2.001758	-0.158315
11	1	0	1.693204	2.774250	0.193374
12	6	0	-0.353026	2.221565	0.504975
13	8	0	5.616473	-2.099809	0.363610
14	1	0	6.571123	-2.136823	0.288672
15	8	0	3.476171	-1.023937	1.588335
16	1	0	4.041631	-1.771812	1.808137
17	8	0	3.445605	0.907284	-1.430414
18	1	0	2.763768	1.487574	-1.790565
19	8	0	0.989015	-0.355329	-0.705349
20	1	0	0.064673	-0.445218	-0.425697
21	8	0	0.900523	2.163236	-1.565805
22	1	0	0.521634	1.329907	-1.880961
23	1	0	-0.216522	2.277536	1.593744
24	1	0	-0.759002	3.181761	0.163819
25	7	0	-1.239666	1.123190	0.157542
26	6	0	-2.439293	1.105302	0.570724
27	6	0	-3.061207	2.203003	1.406765
28	1	0	-3.339207	3.051146	0.772818
29	1	0	-3.949609	1.857161	1.931661
30	1	0	-2.344183	2.570696	2.141746
31	6	0	-3.303956	-0.045510	0.182179
32	6	0	-4.666380	0.158101	-0.047864
33	6	0	-2.795002	-1.345136	0.012405
34	6	0	-5.509769	-0.869260	-0.446924
35	1	0	-5.070527	1.156905	0.072348
36	6	0	-3.642210	-2.381939	-0.372614
37	6	0	-4.989862	-2.147411	-0.605208
38	1	0	-6.558417	-0.674071	-0.630116
39	1	0	-3.233203	-3.380506	-0.492098
40	1	0	-5.629195	-2.967250	-0.909239
41	8	0	-1.478582	-1.580847	0.256032
42	1	0	-1.298189	-2.522267	0.177026

Structure 40 (M06-2X, DMSO)

Energy (Hartrees): = -1052.103762
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.752507	-0.756475	0.212995
2	1	0	3.243814	-1.549770	-0.348302
3	6	0	5.230402	-0.780417	-0.125075
4	1	0	5.729543	0.063484	0.367203
5	1	0	5.373159	-0.704742	-1.205919
6	6	0	3.116791	0.576871	-0.145434
7	1	0	3.583647	1.348815	0.485313
8	6	0	1.621841	0.594264	0.161610
9	1	0	1.508320	0.424933	1.239105
10	6	0	1.001331	1.960389	-0.199686
11	1	0	1.685200	2.759707	0.097828
12	6	0	-0.342644	2.189752	0.476132
13	8	0	5.724818	-2.019353	0.379808
14	1	0	6.685758	-1.984291	0.380969
15	8	0	3.582778	-0.949817	1.608656
16	1	0	4.205437	-1.646811	1.846132
17	8	0	3.393400	0.825923	-1.514620
18	1	0	2.659053	1.346959	-1.865355
19	8	0	1.002030	-0.438648	-0.586256
20	1	0	0.067791	-0.468712	-0.320620
21	8	0	0.868867	2.050981	-1.619248
22	1	0	0.394319	1.247206	-1.874778
23	1	0	-0.192736	2.251198	1.561385
24	1	0	-0.752387	3.149977	0.140616
25	7	0	-1.239626	1.094380	0.135868

26	6	0	-2.431001	1.092567	0.581603
27	6	0	-3.006491	2.189911	1.442588
28	1	0	-3.246679	3.064325	0.828647
29	1	0	-3.911041	1.870859	1.957051
30	1	0	-2.274212	2.506878	2.187258
31	6	0	-3.328482	-0.034363	0.194413
32	6	0	-4.686199	0.218302	-0.027680
33	6	0	-2.863919	-1.349561	0.016036
34	6	0	-5.563565	-0.779200	-0.431007
35	1	0	-5.057436	1.228614	0.103822
36	6	0	-3.746474	-2.357920	-0.371609
37	6	0	-5.086449	-2.074814	-0.598771
38	1	0	-6.606727	-0.548608	-0.608549
39	1	0	-3.370714	-3.369649	-0.492717
40	1	0	-5.754187	-2.871758	-0.904760
41	8	0	-1.556446	-1.634961	0.255006
42	1	0	-1.421998	-2.588115	0.171130

Structure 41 (B3LYP, Gas Phase)

Energy (Hartrees): = -1167.0362201
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.380905	0.776923	-0.155303
2	1	0	3.849054	1.527049	0.442134
3	6	0	5.861279	0.834817	0.190371
4	1	0	6.392647	0.035100	-0.343082
5	1	0	6.000548	0.707890	1.266958
6	6	0	3.773053	-0.594311	0.135505
7	1	0	4.225163	-1.306235	-0.575545
8	6	0	2.261479	-0.611866	-0.128763
9	1	0	2.119377	-0.334001	-1.179607
10	6	0	1.658621	-2.015001	0.133164
11	1	0	2.337673	-2.785989	-0.244476
12	6	0	0.294600	-2.221998	-0.534147
13	8	0	6.314611	2.123685	-0.254992
14	1	0	7.274001	2.139466	-0.211533
15	8	0	4.201374	1.030664	-1.548432
16	1	0	4.776126	1.780552	-1.744833
17	8	0	4.113433	-0.943184	1.471134
18	1	0	3.437121	-1.554834	1.796780
19	8	0	1.631612	0.332222	0.734477
20	1	0	0.707682	0.410814	0.439220
21	8	0	1.575762	-2.218809	1.548881
22	1	0	1.236492	-1.375856	1.890921
23	1	0	0.440886	-2.297209	-1.622370
24	1	0	-0.107795	-3.184667	-0.192212
25	7	0	-0.610028	-1.130501	-0.204183
26	6	0	-1.791376	-1.084482	-0.681797
27	6	0	-2.367320	-2.148667	-1.599775
28	1	0	-2.551283	-3.079243	-1.051780
29	1	0	-3.296741	-1.832359	-2.069689
30	1	0	-1.650652	-2.384436	-2.390586
31	6	0	-2.662181	0.068223	-0.306902
32	6	0	-4.039321	-0.146245	-0.113384
33	6	0	-2.156246	1.366149	-0.119250
34	6	0	-4.894973	0.882665	0.269972
35	1	0	-4.425565	-1.147107	-0.245834
36	6	0	-3.024388	2.399109	0.247372
37	6	0	-4.374965	2.168292	0.444440
38	1	0	-2.628140	3.401338	0.382755
39	1	0	-5.044167	2.968702	0.734380
40	8	0	-0.825102	1.612264	-0.325448
41	1	0	-0.658731	2.557507	-0.244600
42	8	0	-6.235607	0.744651	0.495464
43	6	0	-6.818955	-0.539188	0.337798
44	1	0	-7.875607	-0.416674	0.569787
45	1	0	-6.716901	-0.905675	-0.690508
46	1	0	-6.380937	-1.269097	1.028529

Structure 41 (B3LYP, DMSO)

Energy (Hartrees): = -1167.0675932
No imaginary frequencies

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	4.451714	-0.742606	0.108279
2	1	0	3.927238	-1.520072	-0.461452
3	6	0	5.921812	-0.753642	-0.284580
4	1	0	6.444890	0.071081	0.215714
5	1	0	6.028818	-0.641176	-1.366977
6	6	0	3.785071	0.602876	-0.176719
7	1	0	4.257957	1.349716	0.480132
8	6	0	2.290576	0.601026	0.170599
9	1	0	2.210669	0.376910	1.240752
10	6	0	1.642868	1.979364	-0.101988
11	1	0	2.311594	2.772392	0.241863
12	6	0	0.293690	2.162202	0.594026
13	8	0	6.441244	-2.019078	0.158324
14	1	0	7.402493	-1.955530	0.178197
15	8	0	4.333642	-0.998388	1.510235
16	1	0	4.981060	-1.693727	1.689036
17	8	0	4.032824	0.926744	-1.545858
18	1	0	3.301112	1.495006	-1.833406
19	8	0	1.632623	-0.399763	-0.608705
20	1	0	0.704094	-0.416415	-0.310225
21	8	0	1.517160	2.159379	-1.527929
22	1	0	1.097026	1.342444	-1.838884
23	1	0	0.461298	2.209700	1.678954
24	1	0	-0.126088	3.129382	0.290571
25	7	0	-0.609201	1.067364	0.255774
26	6	0	-1.800815	1.046924	0.717552
27	6	0	-2.366214	2.128201	1.613029
28	1	0	-2.478580	3.068548	1.062353
29	1	0	-3.331664	1.856835	2.035932
30	1	0	-1.674150	2.323388	2.437398
31	6	0	-2.686837	-0.093688	0.336611
32	6	0	-4.048766	0.161052	0.086060
33	6	0	-2.214143	-1.411170	0.199152
34	6	0	-4.921670	-0.850887	-0.307341
35	1	0	-4.408891	1.175218	0.186955
36	6	0	-3.100214	-2.427334	-0.175296
37	6	0	-4.434911	-2.157362	-0.430444
38	1	0	-2.731883	-3.445156	-0.266311
39	1	0	-5.112006	-2.950806	-0.724273
40	8	0	-0.900916	-1.696814	0.461529
41	1	0	-0.774949	-2.653901	0.403881
42	8	0	-6.245149	-0.672317	-0.587039
43	6	0	-6.789349	0.641894	-0.464842
44	1	0	-7.842770	0.553873	-0.727755
45	1	0	-6.706038	1.018080	0.560356
46	1	0	-6.305126	1.343459	-1.152275

Structure 41 (M06-2X, Gas Phase)

Energy (Hartrees): = -1166.5802547
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.336953	-0.775232	0.144523
2	1	0	3.806654	-1.517308	-0.463635
3	6	0	5.812439	-0.816719	-0.200704
4	1	0	6.330691	-0.013358	0.339135
5	1	0	5.945292	-0.680287	-1.276352
6	6	0	3.740414	0.594723	-0.131510
7	1	0	4.204240	1.302383	0.574750
8	6	0	2.238635	0.608984	0.141097
9	1	0	2.097077	0.345388	1.196367
10	6	0	1.643825	2.008710	-0.136886
11	1	0	2.342371	2.779053	0.204541
12	6	0	0.303740	2.222479	0.558274
13	8	0	6.272456	-2.093556	0.235891
14	1	0	7.223157	-2.134161	0.122843
15	8	0	4.159353	-1.036676	1.525794
16	1	0	4.728486	-1.788173	1.722268
17	8	0	4.063032	0.938246	-1.463609
18	1	0	3.368700	1.514812	-1.805335
19	8	0	1.624404	-0.342977	-0.706845
20	1	0	0.710647	-0.454095	-0.401173
21	8	0	1.509642	2.179497	-1.540402
22	1	0	1.127557	1.345999	-1.851761
23	1	0	0.464255	2.271361	1.644136
24	1	0	-0.111092	3.184509	0.232963
25	7	0	-0.588906	1.125888	0.222312
26	6	0	-1.773648	1.094782	0.674935

27	6	0	-2.374603	2.178054	1.544788
28	1	0	-2.656933	3.042061	0.934447
29	1	0	-3.255107	1.826037	2.078938
30	1	0	-1.641990	2.525446	2.274500
31	6	0	-2.637269	-0.063198	0.305647
32	6	0	-4.009352	0.145263	0.104951
33	6	0	-2.118920	-1.351440	0.137423
34	6	0	-4.852665	-0.893767	-0.266666
35	1	0	-4.399005	1.147426	0.225930
36	6	0	-2.974705	-2.394313	-0.219617
37	6	0	-4.323237	-2.174952	-0.422516
38	1	0	-2.569052	-3.393806	-0.342241
39	1	0	-4.988619	-2.980799	-0.704747
40	8	0	-0.790577	-1.580616	0.349945
41	1	0	-0.615957	-2.524900	0.304330
42	8	0	-6.187250	-0.767244	-0.494472
43	6	0	-6.752451	0.518788	-0.367045
44	1	0	-7.809948	0.407300	-0.594714
45	1	0	-6.641010	0.904323	0.652124
46	1	0	-6.301482	1.223205	-1.074087

Structure 41 (M06-2X, DMSO)

Energy (Hartrees): = -1166.6130318
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.413231	-0.732704	0.138985
2	1	0	3.897938	-1.518837	-0.426178
3	6	0	5.881543	-0.733761	-0.238087
4	1	0	6.385839	0.101288	0.264029
5	1	0	5.993912	-0.625947	-1.319857
6	6	0	3.756028	0.601527	-0.175244
7	1	0	4.231986	1.365407	0.458427
8	6	0	2.268877	0.599002	0.169344
9	1	0	2.183610	0.413154	1.246704
10	6	0	1.627262	1.964756	-0.157670
11	1	0	2.313026	2.765955	0.130086
12	6	0	0.299567	2.175313	0.555388
13	8	0	6.401610	-1.981024	0.217498
14	1	0	7.361722	-1.937946	0.184909
15	8	0	4.281108	-0.957607	1.534140
16	1	0	4.909637	-1.659437	1.740020
17	8	0	3.994759	0.881872	-1.545859
18	1	0	3.239096	1.388766	-1.871475
19	8	0	1.642148	-0.429977	-0.577907
20	1	0	0.719914	-0.489365	-0.277990
21	8	0	1.454627	2.070394	-1.571949
22	1	0	0.976568	1.266932	-1.822209
23	1	0	0.474863	2.221388	1.637656
24	1	0	-0.125516	3.137163	0.244552
25	7	0	-0.595422	1.076818	0.221917
26	6	0	-1.778016	1.059829	0.688990
27	6	0	-2.351678	2.145416	1.565691
28	1	0	-2.609443	3.021500	0.961269
29	1	0	-3.245440	1.814003	2.091366
30	1	0	-1.611072	2.464758	2.301196
31	6	0	-2.661393	-0.083868	0.316850
32	6	0	-4.027192	0.161204	0.106103
33	6	0	-2.172960	-1.385392	0.154369
34	6	0	-4.892870	-0.857999	-0.273180
35	1	0	-4.394615	1.171867	0.229363
36	6	0	-3.051551	-2.409235	-0.206382
37	6	0	-4.393170	-2.153869	-0.421441
38	1	0	-2.670645	-3.420124	-0.317450
39	1	0	-5.069873	-2.951113	-0.705098
40	8	0	-0.853107	-1.652215	0.378332
41	1	0	-0.716107	-2.607077	0.333642
42	8	0	-6.219226	-0.693686	-0.513122
43	6	0	-6.747865	0.616110	-0.381499
44	1	0	-7.807436	0.539357	-0.617399
45	1	0	-6.632983	0.991246	0.640195
46	1	0	-6.271249	1.309321	-1.081525

Structure 42 (B3LYP, Gas Phase)

Energy (Hartrees): =-1257.0423839
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.608369	0.854569	0.131138
2	1	0	-4.038803	1.612007	-0.420822
3	6	0	-6.076557	0.971182	-0.251068
4	1	0	-6.644715	0.163464	0.229681
5	1	0	-6.189483	0.898483	-1.335759
6	6	0	-4.033044	-0.521688	-0.199637
7	1	0	-4.532992	-1.249534	0.461410
8	6	0	-2.534618	-0.599251	0.121299
9	1	0	-2.427637	-0.366380	1.187322
10	6	0	-1.959960	-2.006518	-0.171100
11	1	0	-2.664766	-2.772308	0.167573
12	6	0	-0.618104	-2.269669	0.522550
13	8	0	-6.504265	2.250563	0.242742
14	1	0	-7.461133	2.299026	0.173992
15	8	0	-4.459598	1.046173	1.537333
16	1	0	-5.026562	1.797368	1.751447
17	8	0	-4.333481	-0.795596	-1.561326
18	1	0	-3.693408	-1.448325	-1.879005
19	8	0	-1.837790	0.356469	-0.677893
20	1	0	-0.915444	0.344334	-0.369469
21	8	0	-1.845664	-2.171130	-1.589415
22	1	0	-1.495330	-1.322150	-1.903481
23	1	0	-0.791951	-2.373674	1.603732
24	1	0	-0.229764	-3.229200	0.158718
25	7	0	0.324461	-1.188189	0.262125
26	6	0	1.516404	-1.232495	0.709984
27	6	0	2.075313	-2.385237	1.522879
28	1	0	2.280226	-3.248852	0.880875
29	1	0	2.994374	-2.119749	2.042520
30	1	0	1.344340	-2.707971	2.267307
31	6	0	2.434240	-0.097380	0.387063
32	6	0	3.789747	-0.351812	0.176830
33	6	0	1.990936	1.241931	0.257275
34	6	0	4.666949	0.668626	-0.165490
35	1	0	4.184948	-1.354237	0.260176
36	6	0	2.894858	2.258784	-0.076357
37	6	0	4.233662	1.982669	-0.294549
38	1	0	2.533872	3.278600	-0.165060
39	1	0	4.939134	2.758242	-0.557003
40	8	0	0.688370	1.527512	0.487055
41	1	0	0.538083	2.476917	0.409094
42	7	0	6.085755	0.349804	-0.389398
43	8	0	6.832200	1.272059	-0.692106
44	8	0	6.434823	-0.817253	-0.258542

Structure 42 (B3LYP, DMSO)

Energy (Hartrees): = -1257.0764998
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.650059	-0.837015	0.068665
2	1	0	4.090898	-1.599306	-0.488593
3	6	0	6.115215	-0.909890	-0.335932
4	1	0	6.674493	-0.103752	0.155162
5	1	0	6.218465	-0.809482	-1.419849
6	6	0	4.033487	0.530333	-0.226603
7	1	0	4.548655	1.268602	0.407629
8	6	0	2.548380	0.595302	0.150891
9	1	0	2.482727	0.390798	1.225790
10	6	0	1.945468	1.991226	-0.130321
11	1	0	2.644442	2.765882	0.194565
12	6	0	0.614404	2.228358	0.584765
13	8	0	6.585531	-2.192639	0.112577
14	1	0	7.548461	-2.166602	0.133893
15	8	0	4.534711	-1.073614	1.473987
16	1	0	5.157017	-1.791145	1.654385
17	8	0	4.268381	0.818121	-1.605822
18	1	0	3.566373	1.425300	-1.886701
19	8	0	1.829061	-0.388415	-0.597335
20	1	0	0.904621	-0.328388	-0.291545
21	8	0	1.804764	2.159112	-1.556315
22	1	0	1.367833	1.347137	-1.856858
23	1	0	0.802690	2.297460	1.664740

24	1	0	0.213332	3.197152	0.263574
25	7	0	-0.327430	1.148658	0.301399
26	6	0	-1.518057	1.200523	0.759046
27	6	0	-2.049106	2.344204	1.593195
28	1	0	-2.132282	3.255068	0.990422
29	1	0	-3.022540	2.127878	2.029584
30	1	0	-1.350388	2.561605	2.405887
31	6	0	-2.448807	0.077778	0.427058
32	6	0	-3.785489	0.361995	0.152976
33	6	0	-2.035052	-1.275620	0.359856
34	6	0	-4.673310	-0.649704	-0.196756
35	1	0	-4.145413	1.380058	0.195751
36	6	0	-2.949642	-2.284145	0.022595
37	6	0	-4.267584	-1.980898	-0.262161
38	1	0	-2.612348	-3.315059	-0.012499
39	1	0	-4.971785	-2.757012	-0.526536
40	8	0	-0.754313	-1.585921	0.652866
41	1	0	-0.639053	-2.547468	0.616288
42	7	0	-6.062371	-0.306774	-0.492402
43	8	0	-6.835486	-1.218305	-0.779573
44	8	0	-6.394822	0.875837	-0.440600

Structure 42 (M06-2X, Gas Phase)

Energy (Hartrees): = -1256.5568156
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.569891	-0.850241	0.144724
2	1	0	4.009659	-1.609949	-0.413003
3	6	0	6.037643	-0.949777	-0.222563
4	1	0	6.584479	-0.128728	0.259341
5	1	0	6.154992	-0.882130	-1.306478
6	6	0	4.004215	0.518373	-0.194722
7	1	0	4.509343	1.251824	0.454743
8	6	0	2.513628	0.593124	0.124159
9	1	0	2.401767	0.383841	1.195080
10	6	0	1.947966	1.993020	-0.199502
11	1	0	2.669692	2.759174	0.100690
12	6	0	0.628236	2.270891	0.512678
13	8	0	6.472355	-2.208926	0.284185
14	1	0	7.419865	-2.281947	0.160670
15	8	0	4.410929	-1.031342	1.540628
16	1	0	4.973980	-1.778075	1.770885
17	8	0	4.295010	0.768685	-1.553856
18	1	0	3.645424	1.396317	-1.893097
19	8	0	1.839052	-0.377797	-0.656251
20	1	0	0.922124	-0.399470	-0.342454
21	8	0	1.791636	2.113902	-1.605667
22	1	0	1.412904	1.268303	-1.886185
23	1	0	0.812893	2.363359	1.591407
24	1	0	0.229671	3.226208	0.151541
25	7	0	-0.303571	1.183159	0.254071
26	6	0	-1.493277	1.237253	0.688713
27	6	0	-2.067859	2.399625	1.467201
28	1	0	-2.401204	3.185570	0.781862
29	1	0	-2.916539	2.096609	2.078314
30	1	0	-1.309885	2.834369	2.118372
31	6	0	-2.410174	0.102218	0.370425
32	6	0	-3.765094	0.356293	0.185198
33	6	0	-1.960398	-1.226288	0.221853
34	6	0	-4.634785	-0.666945	-0.150577
35	1	0	-4.162113	1.357704	0.286233
36	6	0	-2.859490	-2.244368	-0.105401
37	6	0	-4.201948	-1.973925	-0.298790
38	1	0	-2.492628	-3.259869	-0.209390
39	1	0	-4.908969	-2.750319	-0.556286
40	8	0	-0.655904	-1.502295	0.427213
41	1	0	-0.498436	-2.448808	0.351245
42	7	0	-6.058783	-0.356388	-0.348837
43	8	0	-6.791977	-1.272509	-0.649036
44	8	0	-6.407584	0.794421	-0.198526

Structure 42 (M06-2X, DMSO)

Energy (Hartrees): = -1256.5915771
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.628148	-0.817635	-0.131638
2	1	0	-4.090383	-1.603714	0.412584
3	6	0	-6.097044	-0.873709	0.240754
4	1	0	-6.623474	-0.037204	-0.235363
5	1	0	-6.216376	-0.807161	1.325025
6	6	0	-4.012230	0.526243	0.222537
7	1	0	-4.520429	1.295887	-0.378234
8	6	0	-2.531210	0.586783	-0.139669
9	1	0	-2.454611	0.438179	-1.223315
10	6	0	-1.930042	1.961000	0.222073
11	1	0	-2.642248	2.748483	-0.038044
12	6	0	-0.618317	2.234469	-0.498790
13	8	0	-6.577632	-2.119470	-0.260582
14	1	0	-7.538899	-2.102781	-0.243811
15	8	0	-4.487871	-0.998911	-1.531944
16	1	0	-5.103677	-1.705314	-1.759491
17	8	0	-4.245334	0.746039	1.604800
18	1	0	-3.521397	1.293849	1.935372
19	8	0	-1.854976	-0.442138	0.565085
20	1	0	-0.930889	-0.430613	0.267133
21	8	0	-1.749158	2.033656	1.637325
22	1	0	-1.262205	1.230037	1.868697
23	1	0	-0.809969	2.315821	-1.575956
24	1	0	-0.214407	3.194675	-0.157162
25	7	0	0.316805	1.152035	-0.223280
26	6	0	1.490017	1.199055	-0.708546
27	6	0	2.013102	2.332953	-1.552922
28	1	0	2.244143	3.197094	-0.921350
29	1	0	2.911453	2.054213	-2.100817
30	1	0	1.252575	2.647193	-2.269847
31	6	0	2.426480	0.082503	-0.381884
32	6	0	3.774157	0.367932	-0.191641
33	6	0	2.002785	-1.254380	-0.235630
34	6	0	4.660601	-0.639697	0.153283
35	1	0	4.138481	1.381455	-0.299071
36	6	0	2.919400	-2.258129	0.093673
37	6	0	4.252537	-1.958459	0.295832
38	1	0	2.573002	-3.282008	0.188898
39	1	0	4.963502	-2.731173	0.554519
40	8	0	0.707118	-1.557899	-0.446033
41	1	0	0.583907	-2.515561	-0.382530
42	7	0	6.069076	-0.302561	0.364854
43	8	0	6.830867	-1.201941	0.659444
44	8	0	6.405511	0.858008	0.236550

Structure 43 (B3LYP, Gas Phase)

Energy (Hartrees): = -1052.4857266
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.642456	1.158026	0.153109
2	1	0	2.705938	0.969105	1.229094
3	6	0	3.869970	1.935809	-0.293999
4	1	0	3.871402	2.024956	-1.388263
5	1	0	4.772683	1.411284	0.028329
6	6	0	2.527555	-0.192625	-0.559402
7	1	0	2.481206	-0.005618	-1.645776
8	6	0	1.224196	-0.898333	-0.177077
9	1	0	0.418191	-0.277891	-0.563835
10	6	0	1.046885	-2.287840	-0.792771
11	1	0	1.226640	-2.237238	-1.869355
12	6	0	-0.382767	-2.837667	-0.524430
13	8	0	3.755780	3.231168	0.314930
14	1	0	4.417014	3.812996	-0.069018
15	8	0	1.467459	1.949932	-0.128142
16	1	0	1.749314	2.863272	0.028281
17	8	0	3.706680	-0.915632	-0.229917
18	1	0	3.502999	-1.856329	-0.336117
19	8	0	1.103683	-1.042961	1.244022
20	1	0	0.360094	-0.484966	1.511576
21	8	0	2.027098	-3.198376	-0.272055
22	1	0	1.941007	-3.143319	0.690324
23	1	0	-0.593055	-3.631169	-1.247050
24	1	0	-0.382433	-3.283835	0.476731
25	7	0	-1.327062	-1.750783	-0.703124
26	6	0	-2.107351	-1.357313	0.220774

27	6	0	-2.395505	-2.000406	1.559954
28	1	0	-3.476454	-2.137793	1.662390
29	1	0	-1.908578	-2.964452	1.695824
30	1	0	-2.088496	-1.329709	2.368077
31	6	0	-2.787122	-0.033662	-0.008009
32	6	0	-4.035820	0.078763	-0.618364
33	6	0	-2.110363	1.135191	0.374667
34	6	0	-4.599031	1.327730	-0.871716
35	1	0	-4.556493	-0.822943	-0.922422
36	6	0	-2.671922	2.386652	0.125364
37	6	0	-3.910611	2.480942	-0.503820
38	1	0	-5.564869	1.399081	-1.357973
39	1	0	-2.137751	3.277864	0.436286
40	1	0	-4.339275	3.457685	-0.697788
41	8	0	-0.907384	1.012070	1.040419
42	1	0	-0.199596	1.553275	0.632829

Structure 43 (B3LYP, DMSO)

Energy (Hartrees): = -1052.5100581
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.653196	-1.162990	0.162793
2	1	0	-2.720073	-0.998712	1.243206
3	6	0	-3.862680	-1.957258	-0.302993
4	1	0	-3.854441	-2.039953	-1.396408
5	1	0	-4.782525	-1.456896	0.011867
6	6	0	-2.552277	0.202379	-0.524960
7	1	0	-2.539390	0.040915	-1.614328
8	6	0	-1.240018	0.900169	-0.164672
9	1	0	-0.448379	0.265723	-0.557739
10	6	0	-1.049458	2.274212	-0.809885
11	1	0	-1.221580	2.190247	-1.885384
12	6	0	0.378845	2.823617	-0.545382
13	8	0	-3.741244	-3.256269	0.299463
14	1	0	-4.309078	-3.866178	-0.185123
15	8	0	-1.463167	-1.930716	-0.129206
16	1	0	-1.732588	-2.853087	0.002674
17	8	0	-3.716610	0.938316	-0.148101
18	1	0	-3.496302	1.873347	-0.274545
19	8	0	-1.095612	1.046304	1.255510
20	1	0	-0.325822	0.513099	1.499125
21	8	0	-2.031005	3.212605	-0.330269
22	1	0	-1.909185	3.253503	0.629741
23	1	0	0.593293	3.605681	-1.279442
24	1	0	0.388453	3.281900	0.449173
25	7	0	1.323446	1.729126	-0.708209
26	6	0	2.113285	1.358900	0.220878
27	6	0	2.412835	2.032660	1.536252
28	1	0	3.491462	2.212859	1.598836
29	1	0	1.896726	2.981657	1.670548
30	1	0	2.161029	1.368045	2.368716
31	6	0	2.792715	0.031949	0.003731
32	6	0	4.048523	-0.083878	-0.594298
33	6	0	2.104447	-1.136071	0.373999
34	6	0	4.603314	-1.336626	-0.854331
35	1	0	4.583427	0.816199	-0.878457
36	6	0	2.655443	-2.391048	0.113380
37	6	0	3.899688	-2.488577	-0.506857
38	1	0	5.574698	-1.411681	-1.329584
39	1	0	2.110158	-3.282594	0.404752
40	1	0	4.320499	-3.467410	-0.708668
41	8	0	0.904405	-1.008465	1.040832
42	1	0	0.192560	-1.549372	0.636740

Structure 43 (M06-2X, Gas Phase)

Energy (Hartrees): = -1052.0778263
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.537697	-1.180677	0.130683
2	1	0	-2.579443	-0.994561	1.208863
3	6	0	-3.771716	-1.952337	-0.293363

4	1	0	-3.795397	-2.024676	-1.388159
5	1	0	-4.663906	-1.430722	0.058511
6	6	0	-2.453055	0.162359	-0.582598
7	1	0	-2.415492	-0.025480	-1.668370
8	6	0	-1.162091	0.884419	-0.208663
9	1	0	-0.349460	0.274152	-0.605782
10	6	0	-1.028969	2.279475	-0.813879
11	1	0	-1.180486	2.227578	-1.894674
12	6	0	0.357724	2.887396	-0.497725
13	8	0	-3.636316	-3.244195	0.291675
14	1	0	-4.341479	-3.809510	-0.027701
15	8	0	-1.376885	-1.957823	-0.183449
16	1	0	-1.644301	-2.875724	-0.041697
17	8	0	-3.634323	0.851657	-0.231925
18	1	0	-3.478890	1.791862	-0.384763
19	8	0	-1.041748	1.035999	1.200022
20	1	0	-0.333227	0.446445	1.489101
21	8	0	-2.045054	3.138578	-0.303378
22	1	0	-1.968635	3.082410	0.658429
23	1	0	0.548531	3.705584	-1.194891
24	1	0	0.307443	3.303408	0.513183
25	7	0	1.349920	1.850516	-0.681972
26	6	0	1.979895	1.349629	0.297685
27	6	0	2.042797	1.800072	1.738170
28	1	0	3.075062	2.086509	1.960118
29	1	0	1.385185	2.631168	1.976526
30	1	0	1.803026	0.955808	2.389009
31	6	0	2.721974	0.076297	0.019809
32	6	0	3.944011	0.029740	-0.639859
33	6	0	2.100852	-1.118421	0.396619
34	6	0	4.546522	-1.190959	-0.925225
35	1	0	4.409197	0.959042	-0.948679
36	6	0	2.697099	-2.340991	0.111763
37	6	0	3.918512	-2.373592	-0.552062
38	1	0	5.496836	-1.219008	-1.443597
39	1	0	2.200549	-3.255016	0.416962
40	1	0	4.380428	-3.328117	-0.773964
41	8	0	0.903567	-1.044944	1.072486
42	1	0	0.205953	-1.563398	0.623790

Structure 43 (M06-2X, DMSO)

Energy (Hartrees): = -1052.1030683
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.541953	1.186480	0.141505
2	1	0	2.594266	1.021484	1.223130
3	6	0	3.749188	1.984942	-0.306833
4	1	0	3.748135	2.063815	-1.400445
5	1	0	4.665236	1.487491	0.020172
6	6	0	2.475219	-0.169766	-0.550377
7	1	0	2.465329	-0.004933	-1.638917
8	6	0	1.180490	-0.890156	-0.193089
9	1	0	0.376410	-0.266884	-0.585948
10	6	0	1.033121	-2.267207	-0.833445
11	1	0	1.180224	-2.180013	-1.912591
12	6	0	-0.355764	-2.871505	-0.528018
13	8	0	3.606989	3.271826	0.289498
14	1	0	4.216115	3.877905	-0.143104
15	8	0	1.358786	1.932665	-0.172892
16	1	0	1.606791	2.860414	-0.051766
17	8	0	3.644988	-0.867165	-0.159420
18	1	0	3.474305	-1.803987	-0.319374
19	8	0	1.050763	-1.054123	1.214762
20	1	0	0.308803	-0.501166	1.492001
21	8	0	2.045500	-3.156071	-0.359227
22	1	0	1.932341	-3.194240	0.600789
23	1	0	-0.550463	-3.677590	-1.238760
24	1	0	-0.319480	-3.299620	0.477663
25	7	0	-1.343679	-1.822519	-0.698491
26	6	0	-1.998031	-1.358310	0.286312
27	6	0	-2.095896	-1.861933	1.701601
28	1	0	-3.144679	-2.105318	1.899475
29	1	0	-1.488908	-2.738314	1.912707
30	1	0	-1.827440	-1.060335	2.395180
31	6	0	-2.727348	-0.071597	0.028523
32	6	0	-3.954427	-0.003869	-0.623168
33	6	0	-2.082770	1.113060	0.404159
34	6	0	-4.531823	1.229239	-0.913887

35	1	0	-4.448719	-0.923589	-0.917537
36	6	0	-2.651421	2.347612	0.108306
37	6	0	-3.874086	2.401533	-0.554413
38	1	0	-5.485773	1.274326	-1.425581
39	1	0	-2.133466	3.254844	0.400707
40	1	0	-4.314124	3.365101	-0.784154
41	8	0	-0.896093	1.017993	1.090755
42	1	0	-0.187054	1.536092	0.654919

Structure 44 (B3LYP, Gas Phase)

Energy (Hartrees): = -1167.0373946
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.137248	1.289230	0.004823
2	1	0	3.320633	1.093996	1.065976
3	6	0	4.258638	2.153728	-0.548989
4	1	0	4.143198	2.253960	-1.636214
5	1	0	5.222527	1.688845	-0.327828
6	6	0	3.042421	-0.058865	-0.714764
7	1	0	2.879053	0.134968	-1.788637
8	6	0	1.829961	-0.852726	-0.220756
9	1	0	0.952374	-0.282698	-0.520746
10	6	0	1.688762	-2.245624	-0.839253
11	1	0	1.764153	-2.172415	-1.926825
12	6	0	0.331374	-2.897968	-0.449381
13	8	0	4.120357	3.431716	0.090455
14	1	0	4.695880	4.062211	-0.350450
15	8	0	1.889218	1.999310	-0.146312
16	1	0	2.119746	2.928503	0.000155
17	8	0	4.292736	-0.704434	-0.511698
18	1	0	4.142938	-1.655657	-0.613607
19	8	0	1.854409	-1.019660	1.202363
20	1	0	1.115134	-0.501187	1.551680
21	8	0	2.772615	-3.091398	-0.425482
22	1	0	2.775416	-3.047541	0.541399
23	1	0	0.105514	-3.689696	-1.169084
24	1	0	0.459273	-3.363516	0.534397
25	7	0	-0.697429	-1.877291	-0.509674
26	6	0	-1.370122	-1.521436	0.509375
27	6	0	-1.435456	-2.161087	1.879730
28	1	0	-2.479826	-2.392562	2.112071
29	1	0	-0.849107	-3.074112	1.966712
30	1	0	-1.097936	-1.448641	2.637758
31	6	0	-2.159911	-0.247353	0.371581
32	6	0	-3.461271	-0.234813	-0.139266
33	6	0	-1.547113	0.952891	0.742489
34	6	0	-4.144875	0.971912	-0.298635
35	1	0	-3.910820	-1.173729	-0.433967
36	6	0	-2.238340	2.156530	0.591315
37	6	0	-3.522201	2.169880	0.068314
38	1	0	-1.761342	3.082493	0.893054
39	1	0	-4.067238	3.097123	-0.058654
40	8	0	-0.277043	0.921032	1.297856
41	1	0	0.351435	1.479560	0.795411
42	8	0	-5.410690	1.088080	-0.799830
43	6	0	-6.089351	-0.093288	-1.197388
44	1	0	-5.558740	-0.611089	-2.004615
45	1	0	-6.227564	-0.781499	-0.355371
46	1	0	-7.064103	0.230498	-1.558890

Structure 44 (B3LYP, DMSO)

Energy (Hartrees): = -1167.063439
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.159912	1.295197	0.023890
2	1	0	3.317982	1.132082	1.094987
3	6	0	4.276733	2.168950	-0.522317
4	1	0	4.181452	2.257119	-1.611209
5	1	0	5.247942	1.727558	-0.282311
6	6	0	3.094866	-0.071011	-0.665920

7	1	0	2.985031	0.094146	-1.749276
8	6	0	1.862847	-0.852743	-0.207810
9	1	0	1.003068	-0.267526	-0.529149
10	6	0	1.706730	-2.231627	-0.852052
11	1	0	1.783202	-2.128318	-1.936796
12	6	0	0.343677	-2.874599	-0.477300
13	8	0	4.117415	3.453261	0.101837
14	1	0	4.616692	4.099958	-0.409793
15	8	0	1.903100	1.982158	-0.172926
16	1	0	2.117937	2.920315	-0.052897
17	8	0	4.330132	-0.731921	-0.389717
18	1	0	4.160570	-1.678573	-0.507275
19	8	0	1.844877	-1.017354	1.217274
20	1	0	1.072837	-0.524386	1.531312
21	8	0	2.781769	-3.109133	-0.467801
22	1	0	2.740580	-3.169760	0.497994
23	1	0	0.114485	-3.656677	-1.206782
24	1	0	0.450738	-3.347883	0.503995
25	7	0	-0.678590	-1.840819	-0.533038
26	6	0	-1.389850	-1.527296	0.476633
27	6	0	-1.511154	-2.227170	1.807740
28	1	0	-2.568603	-2.439143	1.997136
29	1	0	-0.955421	-3.161896	1.865073
30	1	0	-1.178321	-1.566034	2.614257
31	6	0	-2.170728	-0.244606	0.352098
32	6	0	-3.484552	-0.227295	-0.129221
33	6	0	-1.539992	0.955214	0.701194
34	6	0	-4.160265	0.985515	-0.291927
35	1	0	-3.956555	-1.165057	-0.392012
36	6	0	-2.220825	2.164583	0.542595
37	6	0	-3.514845	2.183215	0.041848
38	1	0	-1.730234	3.091996	0.818505
39	1	0	-4.045494	3.119349	-0.087316
40	8	0	-0.270367	0.918493	1.253297
41	1	0	0.362852	1.475736	0.752951
42	8	0	-5.432773	1.102974	-0.765044
43	6	0	-6.141703	-0.090422	-1.101644
44	1	0	-5.645312	-0.639151	-1.908642
45	1	0	-6.259081	-0.745373	-0.232218
46	1	0	-7.124557	0.234001	-1.441474

Structure 44 (M06-2X, Gas Phase)

Energy (Hartrees): = -1166.5865779
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.041764	-1.278899	-0.022752
2	1	0	-3.225534	-1.083954	1.038963
3	6	0	-4.170170	-2.122464	-0.582441
4	1	0	-4.051529	-2.206974	-1.670267
5	1	0	-5.126376	-1.647284	-0.354263
6	6	0	-2.942483	0.058172	-0.743844
7	1	0	-2.766431	-0.140309	-1.814037
8	6	0	-1.742047	0.851779	-0.236012
9	1	0	-0.859655	0.278192	-0.523700
10	6	0	-1.614518	2.243479	-0.850652
11	1	0	-1.647433	2.168181	-1.940146
12	6	0	-0.302354	2.930180	-0.403474
13	8	0	-4.040874	-3.398749	0.036751
14	1	0	-4.656411	-4.009642	-0.371803
15	8	0	-1.810804	-1.991654	-0.181093
16	1	0	-2.039925	-2.921321	-0.050104
17	8	0	-4.190905	0.688073	-0.548328
18	1	0	-4.068327	1.633320	-0.699723
19	8	0	-1.792732	1.030651	1.173614
20	1	0	-1.098567	0.478166	1.556632
21	8	0	-2.721874	3.053826	-0.466395
22	1	0	-2.751754	3.004830	0.498478
23	1	0	-0.080946	3.745732	-1.094628
24	1	0	-0.479574	3.360715	0.586906
25	7	0	0.754727	1.944131	-0.458763
26	6	0	1.283061	1.478039	0.595410
27	6	0	1.152861	1.941772	2.027621
28	1	0	2.129230	2.310486	2.355754
29	1	0	0.410064	2.720116	2.179684
30	1	0	0.908507	1.086764	2.661756
31	6	0	2.107878	0.237489	0.424492
32	6	0	3.386591	0.259110	-0.129083
33	6	0	1.520335	-0.971385	0.787359
34	6	0	4.080811	-0.933522	-0.317866

35	1	0	3.802446	1.212527	-0.427092
36	6	0	2.220308	-2.161022	0.602011
37	6	0	3.488776	-2.143625	0.049823
38	1	0	1.758897	-3.097148	0.895010
39	1	0	4.047992	-3.057135	-0.107527
40	8	0	0.255880	-0.961263	1.344497
41	1	0	-0.365569	-1.491155	0.806913
42	8	0	5.328184	-1.021691	-0.851510
43	6	0	5.951812	0.179564	-1.250303
44	1	0	5.378381	0.683964	-2.034935
45	1	0	6.082726	0.859939	-0.402224
46	1	0	6.927117	-0.102467	-1.640321

Structure 44 (M06-2X, DMSO)

Energy (Hartrees): = -1166.6134029
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.048967	1.292590	-0.004052
2	1	0	3.210319	1.125920	1.066534
3	6	0	4.164904	2.157270	-0.553849
4	1	0	4.059656	2.238820	-1.642318
5	1	0	5.132759	1.709369	-0.316337
6	6	0	2.989659	-0.060717	-0.701132
7	1	0	2.863452	0.110918	-1.781362
8	6	0	1.776570	-0.853114	-0.228000
9	1	0	0.905507	-0.270850	-0.531915
10	6	0	1.640885	-2.230064	-0.870943
11	1	0	1.675113	-2.124076	-1.957688
12	6	0	0.323404	-2.912962	-0.440417
13	8	0	4.008897	3.432325	0.063366
14	1	0	4.547254	4.070941	-0.413937
15	8	0	1.803077	1.973482	-0.201112
16	1	0	2.008442	2.912985	-0.091546
17	8	0	4.228364	-0.695463	-0.435942
18	1	0	4.096245	-1.638052	-0.598178
19	8	0	1.793952	-1.036684	1.183233
20	1	0	1.055594	-0.525402	1.539891
21	8	0	2.741009	-3.066907	-0.512040
22	1	0	2.728862	-3.116496	0.454077
23	1	0	0.101316	-3.719305	-1.142729
24	1	0	0.481482	-3.352064	0.548569
25	7	0	-0.730459	-1.917411	-0.493132
26	6	0	-1.295067	-1.490482	0.561126
27	6	0	-1.210080	-2.001142	1.975486
28	1	0	-2.209530	-2.335112	2.272292
29	1	0	-0.510546	-2.820720	2.118696
30	1	0	-0.944540	-1.179410	2.645900
31	6	0	-2.114564	-0.243014	0.399647
32	6	0	-3.405002	-0.257393	-0.129537
33	6	0	-1.508782	0.963040	0.748584
34	6	0	-4.088883	0.943639	-0.320014
35	1	0	-3.848271	-1.208216	-0.397855
36	6	0	-2.193746	2.160505	0.552692
37	6	0	-3.471017	2.151690	0.016965
38	1	0	-1.717551	3.096996	0.822633
39	1	0	-4.013132	3.076219	-0.142504
40	8	0	-0.249492	0.939999	1.310935
41	1	0	0.382223	1.469563	0.781220
42	8	0	-5.343934	1.036402	-0.825724
43	6	0	-6.013502	-0.175875	-1.136265
44	1	0	-5.494963	-0.725054	-1.927862
45	1	0	-6.109844	-0.812290	-0.251407
46	1	0	-7.004079	0.108141	-1.485740

Structure 45 (B3LYP, Gas Phase)

Energy (Hartrees): = -1257.0432597
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.234667	1.437262	0.057539
2	1	0	3.468354	1.204529	1.100654
3	6	0	4.262152	2.419595	-0.483111

4	1	0	4.111018	2.555747	-1.561840
5	1	0	5.267849	2.032233	-0.303807
6	6	0	3.223959	0.123874	-0.731289
7	1	0	3.007666	0.357436	-1.787609
8	6	0	2.099594	-0.790593	-0.242247
9	1	0	1.170509	-0.276027	-0.476521
10	6	0	2.031906	-2.155706	-0.930684
11	1	0	2.048588	-2.021204	-2.014891
12	6	0	0.740450	-2.918049	-0.519157
13	8	0	4.028619	3.651333	0.216199
14	1	0	4.538652	4.349184	-0.203614
15	8	0	1.928714	2.057270	-0.014102
16	1	0	2.101610	2.996342	0.152914
17	8	0	4.528026	-0.424565	-0.598991
18	1	0	4.455984	-1.376069	-0.762443
19	8	0	2.197077	-1.029658	1.168646
20	1	0	1.423545	-0.614710	1.571383
21	8	0	3.189438	-2.939504	-0.611957
22	1	0	3.235257	-2.952220	0.354582
23	1	0	0.546564	-3.701277	-1.256981
24	1	0	0.930357	-3.400710	0.446172
25	7	0	-0.358614	-1.970512	-0.513564
26	6	0	-1.075544	-1.746377	0.511042
27	6	0	-1.126251	-2.489534	1.826132
28	1	0	-2.155681	-2.809706	2.015736
29	1	0	-0.481075	-3.365850	1.854101
30	1	0	-0.851584	-1.818875	2.645982
31	6	0	-1.945345	-0.517231	0.429266
32	6	0	-3.253792	-0.553744	-0.032940
33	6	0	-1.373646	0.723928	0.772109
34	6	0	-3.966100	0.634081	-0.174678
35	1	0	-3.722306	-1.486723	-0.315195
36	6	0	-2.102926	1.906459	0.618183
37	6	0	-3.403345	1.866943	0.136838
38	1	0	-1.647393	2.851378	0.890594
39	1	0	-3.989001	2.766357	0.009520
40	8	0	-0.110022	0.729497	1.291631
41	1	0	0.477216	1.403562	0.880205
42	7	0	-5.349466	0.583167	-0.677569
43	8	0	-5.942343	1.645647	-0.819900
44	8	0	-5.826289	-0.518446	-0.921903

Structure 45 (B3LYP, DMSO)

Energy (Hartrees): = -1257.0707889
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.259060	1.450058	0.075851
2	1	0	3.488984	1.246253	1.126372
3	6	0	4.263106	2.447767	-0.478642
4	1	0	4.096945	2.581757	-1.554087
5	1	0	5.281289	2.083887	-0.315474
6	6	0	3.274324	0.120384	-0.687330
7	1	0	3.099887	0.330922	-1.753994
8	6	0	2.136750	-0.786594	-0.221963
9	1	0	1.218028	-0.259167	-0.466823
10	6	0	2.053112	-2.138755	-0.933339
11	1	0	2.067792	-1.976255	-2.013523
12	6	0	0.757067	-2.894159	-0.533763
13	8	0	4.028814	3.679344	0.223409
14	1	0	4.430774	4.394817	-0.282402
15	8	0	1.939104	2.038887	-0.014731
16	1	0	2.087350	2.985406	0.138884
17	8	0	4.572040	-0.445477	-0.500495
18	1	0	4.478542	-1.394584	-0.669797
19	8	0	2.210101	-1.026801	1.191855
20	1	0	1.392848	-0.672805	1.565747
21	8	0	3.205582	-2.949606	-0.642591
22	1	0	3.220702	-3.050514	0.320659
23	1	0	0.562918	-3.672971	-1.276859
24	1	0	0.926410	-3.381105	0.432330
25	7	0	-0.338258	-1.936147	-0.529647
26	6	0	-1.103235	-1.766041	0.473312
27	6	0	-1.219112	-2.579410	1.735505
28	1	0	-2.269680	-2.848666	1.885496
29	1	0	-0.625627	-3.492421	1.719908
30	1	0	-0.926466	-1.977481	2.602488
31	6	0	-1.961652	-0.526985	0.408956
32	6	0	-3.278510	-0.553321	-0.026533
33	6	0	-1.371835	0.711668	0.739328

34	6	0	-3.979045	0.644148	-0.168946
35	1	0	-3.754676	-1.489954	-0.282882
36	6	0	-2.086208	1.903829	0.579161
37	6	0	-3.392634	1.874941	0.117809
38	1	0	-1.616062	2.847782	0.829853
39	1	0	-3.956643	2.788538	-0.006725
40	8	0	-0.112602	0.702876	1.255318
41	1	0	0.474057	1.395753	0.873173
42	7	0	-5.363641	0.605335	-0.641569
43	8	0	-5.963225	1.670246	-0.770696
44	8	0	-5.863714	-0.490556	-0.885853

Structure 45 (M06-2X, Gas Phase)

Energy (Hartrees): = -1256.5626636
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.114927	-1.430165	0.011383
2	1	0	-3.360132	-1.196459	1.052263
3	6	0	-4.142962	-2.397120	-0.543860
4	1	0	-3.978709	-2.521209	-1.621722
5	1	0	-5.144611	-1.999530	-0.369382
6	6	0	-3.097314	-0.128489	-0.779699
7	1	0	-2.862560	-0.365362	-1.830458
8	6	0	-1.990386	0.789712	-0.272171
9	1	0	-1.053102	0.279995	-0.498157
10	6	0	-1.945548	2.156167	-0.951755
11	1	0	-1.914481	2.027263	-2.036218
12	6	0	-0.713572	2.962671	-0.478024
13	8	0	-3.921392	-3.625285	0.142140
14	1	0	-4.469204	-4.309007	-0.247117
15	8	0	-1.822583	-2.048815	-0.054046
16	1	0	-1.990329	-2.989946	0.093634
17	8	0	-4.400166	0.400513	-0.661084
18	1	0	-4.353177	1.342181	-0.867094
19	8	0	-2.114266	1.032322	1.123977
20	1	0	-1.390380	0.568018	1.561409
21	8	0	-3.130432	2.890690	-0.664061
22	1	0	-3.205665	2.896751	0.299345
23	1	0	-0.527384	3.769242	-1.189281
24	1	0	-0.962602	3.407281	0.490198
25	7	0	0.418006	2.061030	-0.459271
26	6	0	0.961440	1.691971	0.623833
27	6	0	0.770527	2.205027	2.030371
28	1	0	1.708106	2.662977	2.359094
29	1	0	-0.031206	2.931324	2.130786
30	1	0	0.576339	1.364422	2.700633
31	6	0	1.877453	0.507885	0.507589
32	6	0	3.154827	0.583203	-0.021701
33	6	0	1.350396	-0.741873	0.864217
34	6	0	3.884997	-0.586096	-0.179968
35	1	0	3.575854	1.529346	-0.335083
36	6	0	2.098569	-1.903712	0.689842
37	6	0	3.377838	-1.830065	0.161146
38	1	0	1.671958	-2.857606	0.975648
39	1	0	3.984908	-2.712247	0.012693
40	8	0	0.093466	-0.779937	1.395910
41	1	0	-0.485557	-1.419255	0.925212
42	7	0	5.242141	-0.503076	-0.747188
43	8	0	5.854111	-1.539382	-0.888786
44	8	0	5.661621	0.596324	-1.035100

Structure 45 (M06-2X, DMSO)

Energy (Hartrees): = -1256.5904088
No imaginary frequencies

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.123686	1.447319	0.024600
2	1	0	3.363579	1.239822	1.072705
3	6	0	4.125600	2.434340	-0.540236
4	1	0	3.943288	2.562684	-1.613756
5	1	0	5.140693	2.060904	-0.386633
6	6	0	3.138165	0.130887	-0.744266

7	1	0	2.942570	0.345055	-1.806136
8	6	0	2.022370	-0.786343	-0.259405
9	1	0	1.092160	-0.268490	-0.493902
10	6	0	1.967914	-2.139988	-0.962241
11	1	0	1.939735	-1.984028	-2.043125
12	6	0	0.730367	-2.945209	-0.506353
13	8	0	3.902551	3.656873	0.157133
14	1	0	4.351841	4.364562	-0.315363
15	8	0	1.815407	2.032255	-0.058826
16	1	0	1.954702	2.980496	0.080357
17	8	0	4.437250	-0.408109	-0.572125
18	1	0	4.375879	-1.349125	-0.779121
19	8	0	2.127045	-1.033336	1.138721
20	1	0	1.357240	-0.626649	1.554482
21	8	0	3.147385	-2.897520	-0.693510
22	1	0	3.189622	-2.987940	0.268857
23	1	0	0.546253	-3.742736	-1.229175
24	1	0	0.960920	-3.401465	0.460439
25	7	0	-0.401489	-2.037854	-0.486328
26	6	0	-0.975440	-1.709743	0.596736
27	6	0	-0.821623	-2.268218	1.985248
28	1	0	-1.785506	-2.689076	2.288618
29	1	0	-0.060313	-3.038483	2.076459
30	1	0	-0.601236	-1.458653	2.686366
31	6	0	-1.887818	-0.519799	0.492944
32	6	0	-3.173900	-0.588486	-0.013478
33	6	0	-1.345449	0.728465	0.838751
34	6	0	-3.893337	0.589612	-0.173728
35	1	0	-3.605282	-1.538447	-0.301367
36	6	0	-2.080802	1.898654	0.658363
37	6	0	-3.366590	1.832907	0.146016
38	1	0	-1.641915	2.853607	0.923385
39	1	0	-3.953873	2.729242	-0.000050
40	8	0	-0.092151	0.751632	1.367437
41	1	0	0.490160	1.404784	0.915870
42	7	0	-5.252936	0.514750	-0.718812
43	8	0	-5.876947	1.549773	-0.839211
44	8	0	-5.685340	-0.579159	-1.022198