

Supplementary Materials for Intermolecular interactions of Edaravone in aqueous solutions of Ethaline and Glyceline inferred from experiments and quantum chemistry computations.

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Table S1. The solubility of edaravone dissolved in mixtures of water and DES comprising choline chloride and glycerol in 1:2 molar ratio (GLE) at various temperatures. Values expressed as mole fractions (x_E , $\cdot 10^4$) and concentrations (c_E , mg/ml). Standard deviation values are given in parentheses.

x_{GLE}^*	298.15 K		303.15 K		308.15 K		313.15 K	
	$x_E (\cdot 10^4)$	$c_E (mg/ml)$	$x_E (\cdot 10^4)$	$c_E (mg/ml)$	$x_E (\cdot 10^4)$	$c_E (mg/ml)$	$x_E (\cdot 10^4)$	$c_E (mg/ml)$
0.0	1.73(± 0.01)	1.72(± 0.01)	1.78(± 0.01)	1.79(± 0.02)	1.84(± 0.02)	1.87(± 0.01)	1.93(± 0.01)	1.96(± 0.01)
0.2	235.51(± 9.67)	115.11(± 4.41)	309.2(± 4.30)	148.29(± 1.98)	435.07(± 4.04)	201.28(± 1.21)	564.61(± 7.05)	251.54(± 2.67)
0.4	743.88(± 5.92)	233.13(± 1.43)	1116.64(± 2.70)	328.49(± 0.84)	1444.07(± 14.86)	402.14(± 2.73)	2014.09(± 17.34)	513.56(± 2.32)
0.5	1121.47(± 10.85)	298.98(± 3.19)	1673.69(± 20.61)	414.6(± 3.61)	2236.41(± 28.00)	517.95(± 3.12)	3065.17(± 55.82)	646.93(± 6.00)
0.6	1450.22(± 11.26)	344.22(± 2.54)	2089.77(± 58.10)	464.06(± 10.07)	2723.73(± 61.99)	567.03(± 8.81)	3567.08(± 42.51)	691.57(± 4.95)
0.8	1305.70(± 26.15)	265.81(± 4.17)	1852.98(± 39.43)	363.68(± 5.58)	2525.56(± 24.65)	471.98(± 3.89)	3420.95(± 31.16)	602.41(± 4.73)
1.0	1052.85(± 68.85)	191.06(± 11.91)	1606.43(± 50.52)	282.25(± 8.03)	2151.57(± 64.56)	369.09(± 11.3)	2991.42(± 64.10)	492.12(± 9.58)

Table S2. The solubility of edaravone dissolved in mixtures of water and DES comprising choline chloride and ethylene glycol in 1:2 molar ratio (ETA) at various temperatures. Values expressed as mole fractions (x_E , $\cdot 10^4$) and concentrations (c_E , mg/ml). Standard deviation values are given in parentheses.

x_{ETA}^*	298.15 K		303.15 K		308.15 K		313.15 K	
	$x_E (\cdot 10^4)$	$c_E (mg/ml)$	$x_E (\cdot 10^4)$	$c_E (mg/ml)$	$x_E (\cdot 10^4)$	$c_E (mg/ml)$	$x_E (\cdot 10^4)$	$c_E (mg/ml)$
0.0	1.73(± 0.01)	1.72(± 0.01)	1.78(± 0.01)	1.79(± 0.02)	1.84(± 0.02)	1.87(± 0.01)	1.93(± 0.01)	1.96(± 0.01)
0.2	454.10(± 5.48)	220.96(± 2.27)	574.18(± 8.89)	269.62(± 3.62)	742.26(± 18.45)	331.05(± 6.32)	890.33(± 10.84)	381.65(± 3.10)
0.4	1353.93(± 5.00)	406.66(± 1.15)	1819.02(± 41.45)	505.10(± 7.17)	2386.29(± 27.09)	602.61(± 3.89)	2954.32(± 49.04)	683.73(± 5.94)
0.5	1754.56(± 31.02)	456.55(± 6.04)	2316.25(± 38.27)	554.20(± 5.35)	3073.71(± 53.04)	663.59(± 6.82)	3822.75(± 61.93)	743.62(± 7.61)
0.6	1934.93(± 34.18)	459.69(± 5.59)	2552.36(± 52.56)	560.61(± 8.87)	3306.79(± 48.29)	670.27(± 6.19)	3982.72(± 70.26)	752.91(± 6.66)
0.8	1713.96(± 31.15)	363.37(± 5.15)	2241.64(± 42.78)	451.55(± 6.38)	2989.20(± 42.33)	561.30(± 6.00)	3720.80(± 28.54)	655.40(± 3.72)
1.0	1579.47(± 70.73)	302.96(± 11.01)	2135.68(± 42.46)	392.28(± 6.53)	2878.22(± 133.85)	499.02(± 18.34)	3602.21(± 117.41)	592.85(± 14.78)