

Supporting Information

Exploring the Role of Temperature on Hydrotrophy

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1. Figures

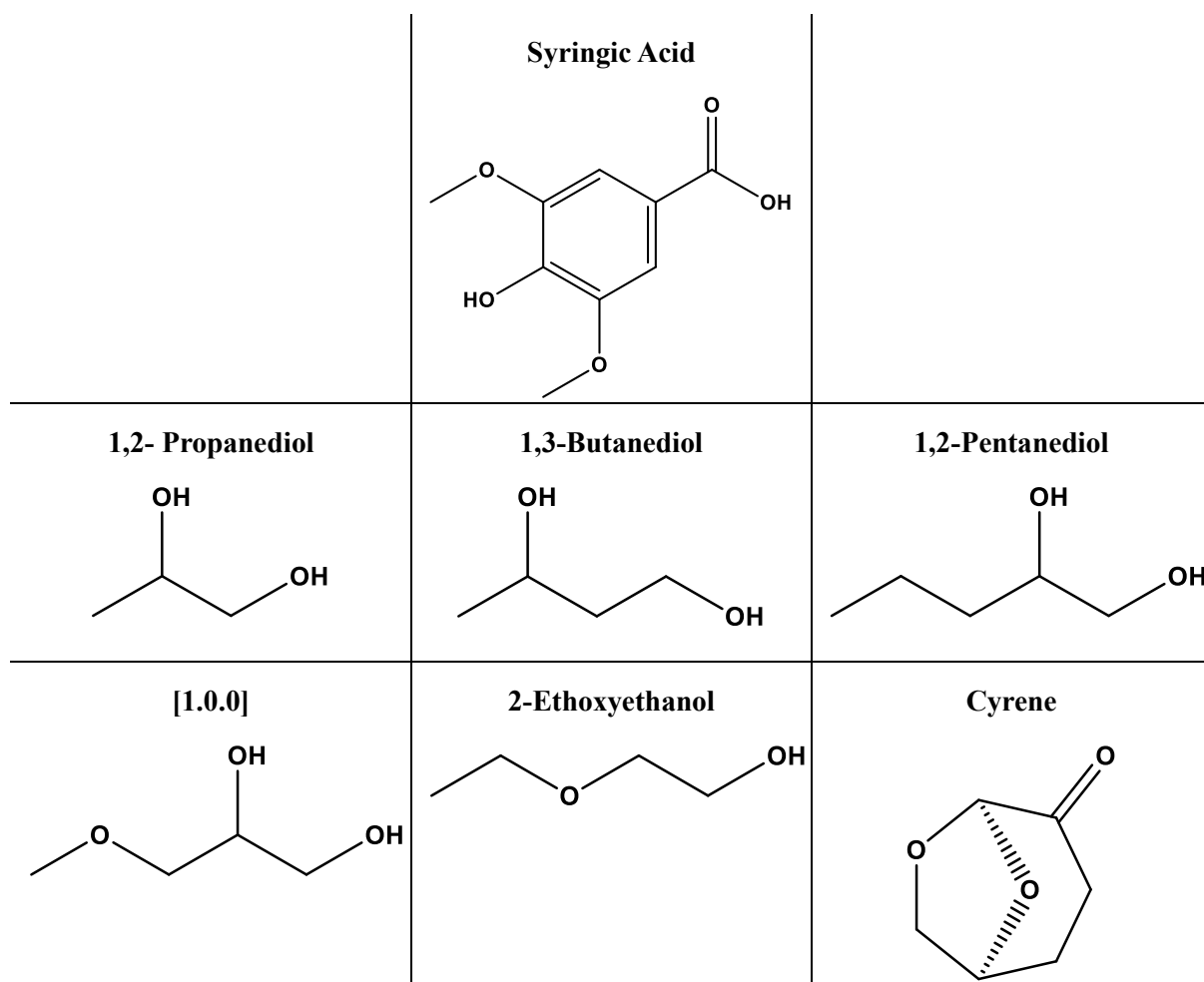


Figure S1. Chemical structures of the solute (syringic acid) and the hydrotropes studied in this work. See Table 1 of the main text for abbreviations.

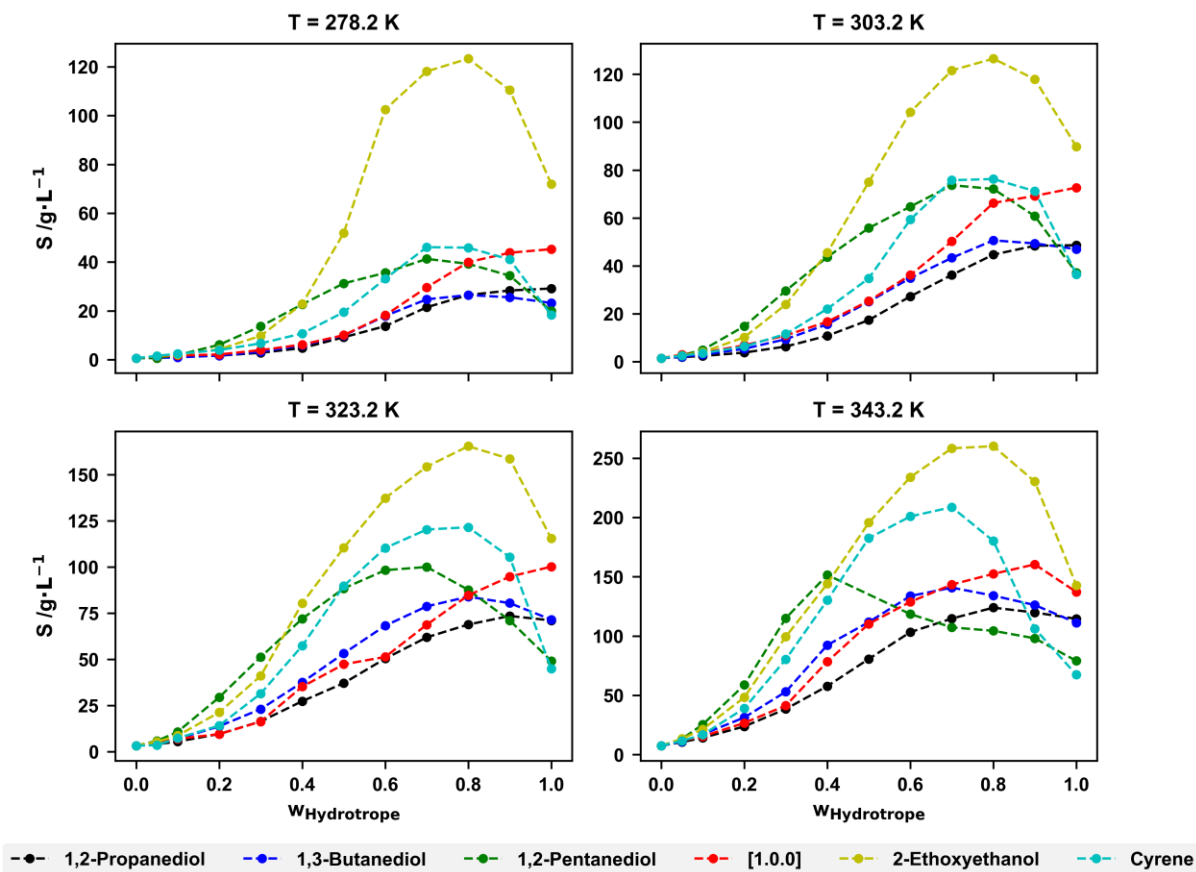


Figure S2. Solubility (mass of solute per volume of solution) of syringic acid in aqueous hydrotrope solutions as a function of the solute-free basis weight fraction of the hydrotrope. Each panel depicts different temperatures, circles represent experimental data measured in this work, and colors represent different hydrotropes. Lines are simple visual aids.

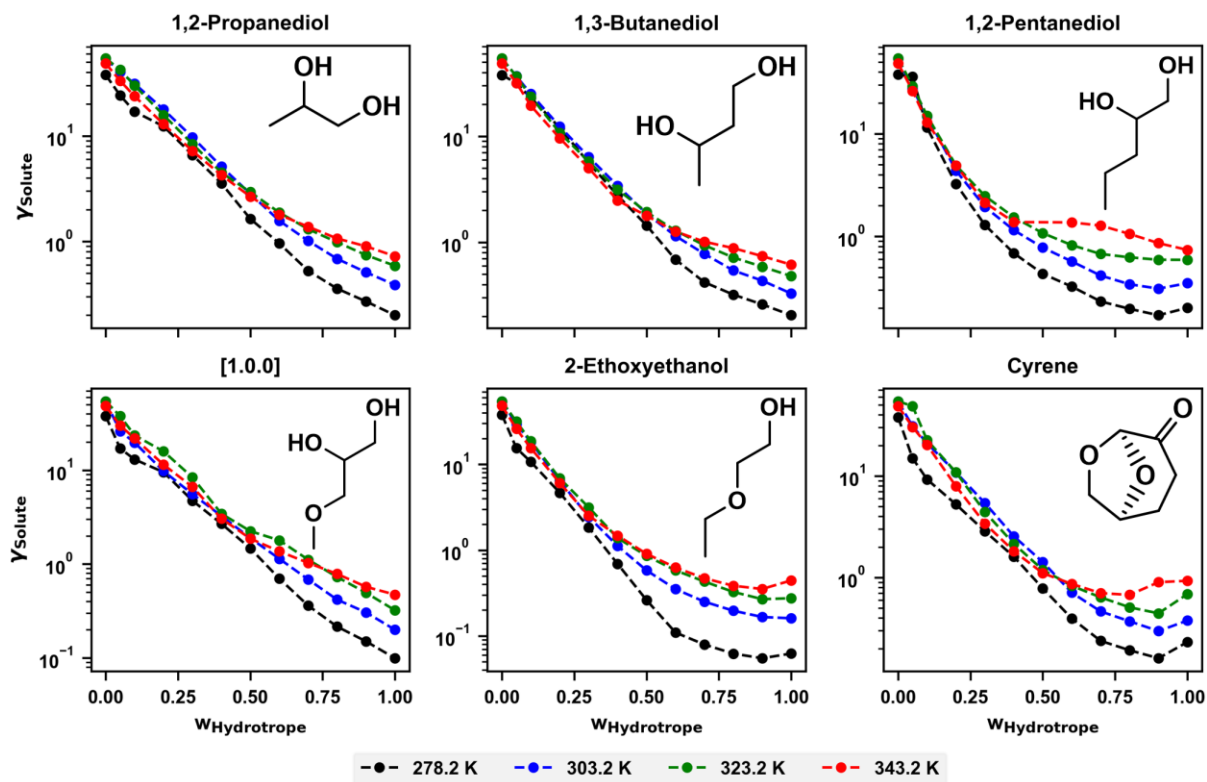


Figure S3. Activity coefficients of syringic acid in aqueous hydrotrope solutions as a function of the solute-free basis weight fraction of the hydrotrope. Each panel depicts different hydrotropes, circles represent experimental data measured in this work, and colors represent different temperatures. Lines are simple visual aids. The chemical structures of the hydrotropes are also shown.

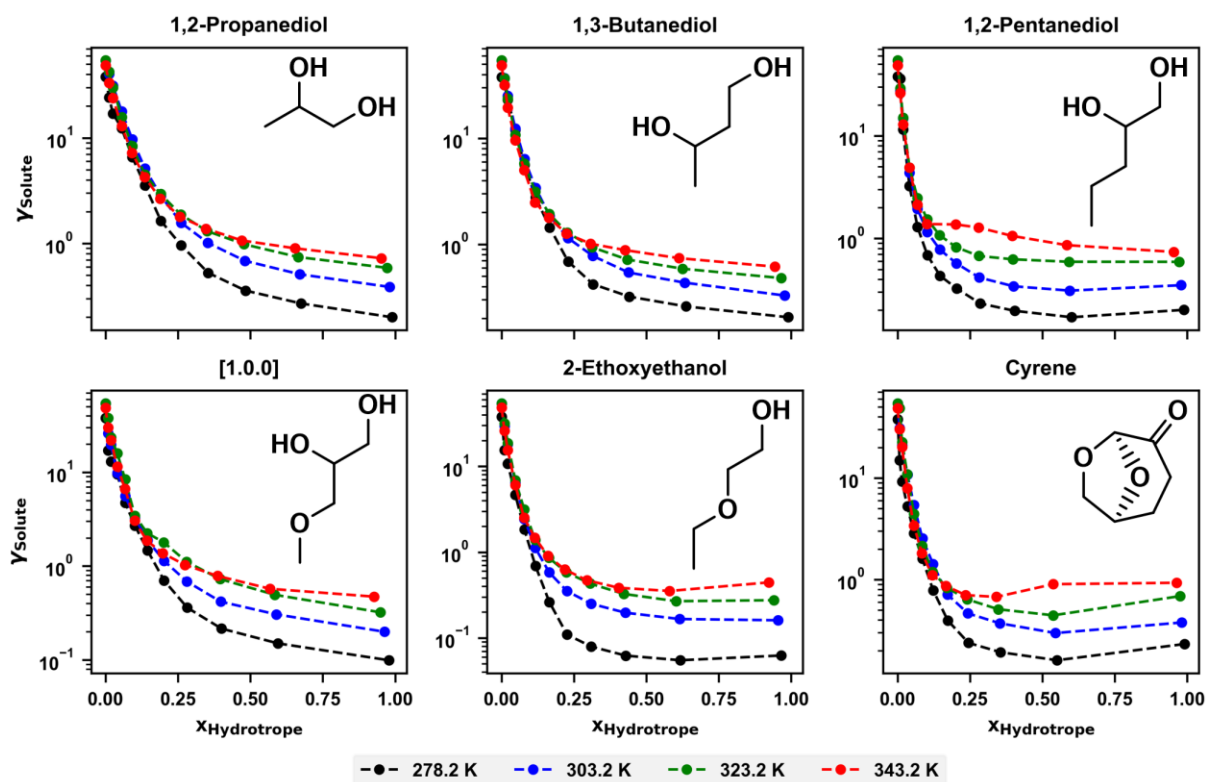


Figure S4. Activity coefficients of syringic acid in aqueous hydrotrope solutions as a function of the mole fraction of the hydrotrope in the ternary water/hydrotrope/solute system. Each panel depicts different hydrotropes, circles represent experimental data measured in this work, and colors represent different temperatures. Lines are simple visual aids. The chemical structures of the hydrotropes are also shown.

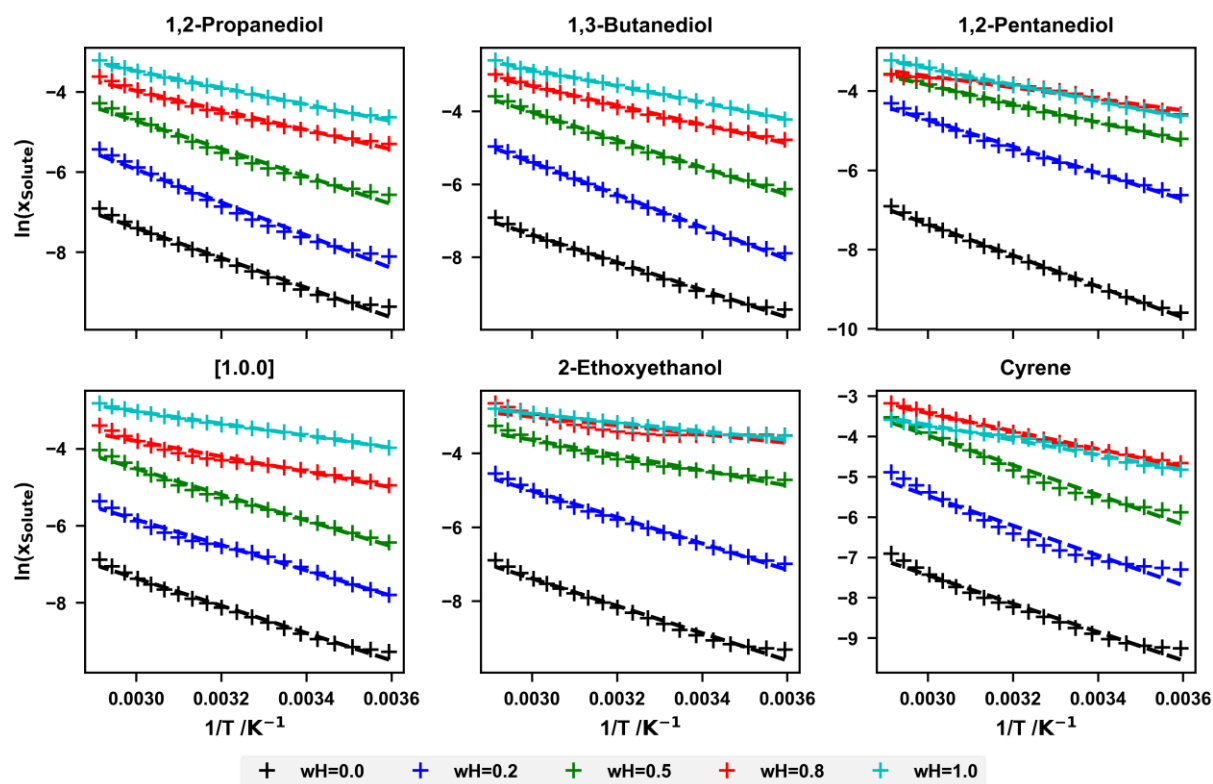


Figure S5. The logarithm of the syringic acid solubility (mole fraction) in aqueous hydrotrope solutions as a function of the inverse of temperature. Each panel depicts different hydrotropes, plus symbols represent GP-predicted data, dashed lines are linear polynomials fitting the data, and colors represent different hydrotrope weight fractions.

2. Tables

Table S1. Fitted coefficients for the polynomial correlations $\rho[g/mL] = A \cdot T^2[K] + B \cdot T[K] + C$ – used in this work to estimate densities for water and all pure hydrotropes, along with the corresponding coefficient of determination and reference for the original data.

Compound	A	B	C	R ²	Ref.
Water	$-4.125 \cdot 10^{-6}$	$2.217 \cdot 10^{-3}$	$7.026 \cdot 10^{-1}$	$9.995 \cdot 10^{-1}$	[1]
1,2-Propanediol	$-9.839 \cdot 10^{-7}$	$-1.424 \cdot 10^{-4}$	1.163	$9.996 \cdot 10^{-1}$	[2–4]
1,3-Butanediol	$-4.745 \cdot 10^{-6}$	$2.306 \cdot 10^{-3}$	$7.344 \cdot 10^{-1}$	$9.970 \cdot 10^{-1}$	[2,5]
1,2-Pentanediol	$-8.578 \cdot 10^{-7}$	$-2.199 \cdot 10^{-4}$	1.109	$9.994 \cdot 10^{-1}$	[4,6]
[1.0.0] ^{a)}	0	$-8.08 \cdot 10^{-4}$	1.352	1.000	[7]
2-Ethoxyethanol	$-7.413 \cdot 10^{-7}$	$-4.733 \cdot 10^{-4}$	1.167	1.000	[8]
Cyrene	$1.838 \cdot 10^{-7}$	$-1.093 \cdot 10^{-3}$	1.557	1.000	[9]

^{a)}Polynomial coefficients extracted directly from reference.

Table S2. Experimental solubility of syringic acid (g/L) in pure solvents at different temperatures and atmospheric pressure. Experimental standard deviations, derived from three independent measurements for each data point, are included in parentheses. Mole fraction, temperate, and pressure uncertainties of 0.001, 0.5 K, and 0.05, respectively.

T /K	Water	1,2-Propanediol	1,3-Butanediol	1,2-Pentanediol	[1.0.0]	2-Ethoxyehtanol	Cyrene
278.2	0.632 (0.018)	29.158 (1.333)	23.217 (0.577)	19.932 (0.190)	45.290 (0.159)	71.977 (1.130)	18.282 (0.429)
288.2	0.763 (0.003)	33.220 (0.842)	31.571 (0.447)	24.030 (0.343)	59.763 (0.238)	73.090 (0.992)	21.277 (0.518)
303.2	1.462 (0.004)	48.618 (0.889)	46.997 (0.516)	37.110 (1.111)	72.669 (0.421)	89.785 (0.489)	36.420 (1.387)
323.2	3.297 (0.020)	71.110 (1.270)	71.547 (0.397)	49.157 (1.203)	100.222 (0.959)	115.458 (1.190)	44.910 (0.340)
333.2	4.616 (0.045)	88.214 (0.405)	81.667 (1.465)	73.510 (0.284)	115.317 (2.790)	129.140 (0.648)	54.488 (0.361)
343.2	7.555 (0.059)	114.532 (0.397)	111.221 (0.159)	79.067 (2.619)	137.202 (0.959)	142.814 (1.440)	67.409 (0.099)

Table S3. Experimental solubility of syringic acid (g/L) in binary mixtures of water and hydrotrope at different hydrotrope compositions (weight fraction) and different temperatures at atmospheric pressure. Experimental standard deviations, derived from three independent measurements for each data point, are included in parentheses. Mole fraction, temperate, and pressure uncertainties of 0.001, 0.5 K, and 0.05, respectively.

w_H	T /K	1,2-Propanediol	1,3-Butanediol	1,2-Pentanediol	[1.0.0]	2-Ethoxyethanol	Cyrene
0.05	278.2	0.953 (0.038)	0.723 (0.110)	0.636 (0.000)	1.350 (0.050)	1.480 (0.050)	1.550 (0.010)
	303.2	1.891 (0.052)	2.058 (0.018)	2.745 (0.23)	2.918 (0.042)	2.568 (0.037)	2.480 (0.059)
	323.2	4.074 (0.095)	4.676 (0.034)	5.881 (0.008)	4.570 (0.20)	5.430 (0.130)	3.560 (0.450)
	343.2	10.586 (0.195)	11.021 (0.397)	13.322 (0.206)	11.720 (0.140)	13.450 (0.210)	11.650 (0.320)
0.10	278.2	1.306 (0.268)	0.954 (0.044)	1.905 (0.147)	1.700 (0.120)	2.050 (0.010)	2.420 (0.020)
	303.2	2.348 (0.004)	2.896 (0.012)	4.885 (0.075)	3.711 (0.010)	3.975 (0.067)	3.520 (0.079)
	323.2	5.539 (0.056)	6.956 (0.060)	10.830 (0.270)	7.010 (0.110)	8.750 (0.210)	7.410 (0.520)
	343.2	14.194 (0.135)	17.194 (0.127)	25.443 (0.524)	15.420 (0.070)	21.410 (0.20)	16.820 (0.650)
0.20	278.2	1.658 (0.000)	1.671 (0.022)	6.105 (0.179)	2.140 (0.130)	4.270 (0.320)	3.960 (0.010)
	303.2	3.785 (0.036)	5.355 (0.026)	14.775 (0.008)	6.846 (0.118)	10.185 (0.063)	6.320 (0.198)
	323.2	9.629 (0.190)	13.810 (0.690)	29.472 (0.698)	9.550 (0.230)	21.350 (0.350)	14.170 (0.590)
	343.2	23.793 (0.675)	31.335 (0.032)	58.753 (2.952)	26.720 (1.040)	48.280 (0.130)	39.030 (1.230)
0.30	278.2	2.828 (0.103)	3.237 (0.030)	13.670 (0.889)	3.920 (0.240)	9.750 (0.030)	6.680 (0.190)
	303.2	6.316 (0.067)	9.363 (0.044)	29.607 (0.29)	10.939 (0.442)	23.830 (0.454)	11.550 (0.595)
	323.2	16.431 (0.127)	23.120 (0.381)	51.295 (1.881)	16.340 (0.360)	41.100 (1.850)	31.500 (0.330)
	343.2	38.473 (0.190)	53.040 (1.873)	115.037 (0.794)	41.360 (0.080)	99.480 (1.760)	80.360 (1.900)
0.40	278.2	4.749 (0.248)	5.870 (0.325)	22.682 (0.429)	6.20 (0.520)	22.880 (0.430)	10.730 (0.060)
	303.2	10.791 (0.071)	15.589 (0.127)	43.686 (0.262)	16.678 (0.053)	45.491 (0.989)	22.033 (0.040)
	323.2	27.392 (1.278)	37.592 (0.214)	72.007 (2.920)	35.241 (1.340)	80.340 (4.630)	57.350 (1.450)
	343.2	57.771 (0.040)	92.366 (2.063)	151.568 (4.841)	78.430 (0.950)	144.070 (2.080)	130.190 (1.590)
0.50	278.2	9.183 (0.242)	9.916 (0.000)	31.256 (2.047)	10.040 (0.140)	51.900 (0.660)	19.460 (0.020)

	303.2	17.351 (0.032)	25.028 (0.032)	55.801 (0.127)	25.340 (0.085)	75.015 (0.697)	34.790 (0.396)
	323.2	37.148 (0.349)	53.23 (0.571)	88.438 (0.238)	47.350 (0.808)	110.450 (3.190)	89.780 (2.090)
	343.2	80.694 (0.29)	111.782 (1.270)	---	110.320 (0.020)	195.640 (0.320)	182.600 (5.870)
0.60	278.2	13.748 (0.286)	17.923 (2.539)	35.588 (1.476)	18.170 (1.630)	102.523 (0.730)	33.150 (0.130)
	303.2	27.250 (0.571)	34.881 (0.238)	64.729 (0.040)	36.138 (0.147)	104.150 (1.010)	59.310 (0.793)
	323.2	50.437 (0.032)	68.265 (0.000)	98.314 (0.635)	51.342 (0.613)	137.340 (1.120)	110.340 (1.870)
	343.2	103.309 (1.508)	133.779 (0.000)	118.544 (11.309)	128.840 (0.820)	234.010 (1.130)	200.890 (3.170)
0.70	278.2	21.481 (0.524)	24.730 (2.452)	41.301 (3.746)	29.620 (1.520)	118.110 (0.640)	46.100 (0.150)
	303.2	36.195 (0.762)	43.344 (0.476)	73.680 (0.873)	50.220 (0.119)	121.621 (0.827)	75.760 (1.387)
	323.2	61.952 (1.841)	78.730 (0.397)	100.054 (1.190)	68.798 (0.476)	154.340 (0.366)	120.310 (3.490)
	343.2	114.756 (2.143)	140.850 (0.794)	107.330 (7.574)	143.430 (1.590)	258.360 (4.470)	208.690 (0.950)
0.80	278.2	26.515 (0.881)	26.481 (0.595)	39.258 (0.984)	39.970 (3.070)	123.340 (1.340)	45.890 (0.100)
	303.2	44.690 (0.603)	50.644 (0.595)	72.108 (0.238)	66.254 (0.366)	126.522 (2.886)	76.260 (1.585)
	323.2	68.887 (1.936)	83.949 (0.476)	87.652 (2.222)	84.660 (0.850)	165.420 (0.160)	121.560 (3.240)
	343.2	123.959 (0.238)	134.116 (1.428)	104.431 (7.380)	152.450 (0.100)	260.120 (1.280)	180.250 (1.430)
0.90	278.2	28.350 (1.333)	25.572 (0.310)	34.410 (3.016)	43.810 (3.230)	110.430 (1.590)	41.040 (0.970)
	303.2	48.394 (0.317)	49.354 (0.198)	60.773 (1.190)	69.210 (0.162)	117.917 (1.296)	71.218 (0.343)
	323.2	73.511 (0.286)	80.470 (0.000)	71.098 (0.397)	94.798 (3.115)	158.580 (1.920)	105.349 (4.284)
	343.2	119.863 (0.000)	126.148 (0.635)	98.090 (1.428)	160.450 (0.970)	230.250 (7.030)	106.170 (1.380)

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