

SUPPORTING INFORMATION

CORRELATING CHEMICO-PHYSICAL FEATURES OF THYMOL-BASED DEEP EUTECTIC SOLVENTS WITH ASTAXANTHIN EXTRACTION PERFORMANCES

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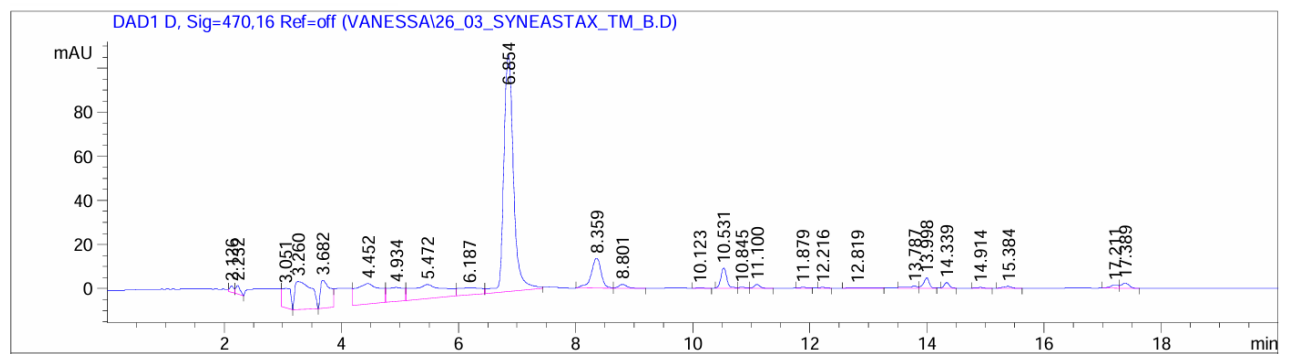
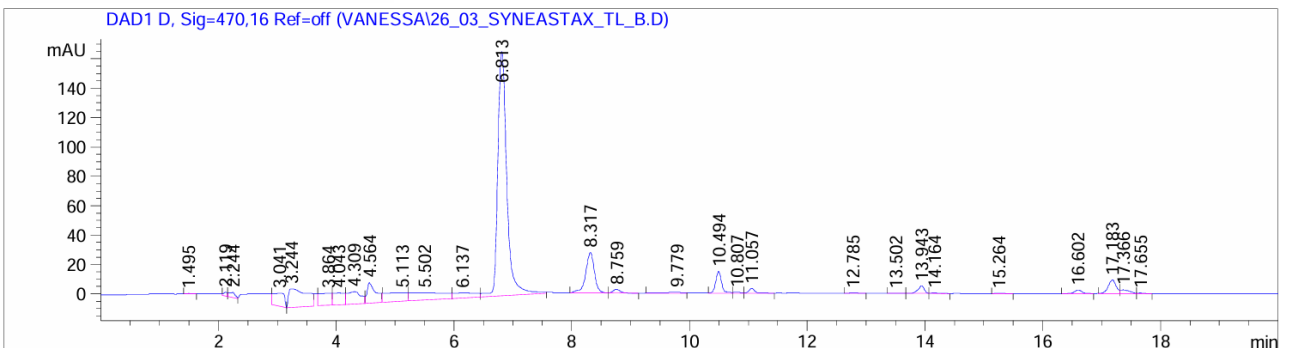
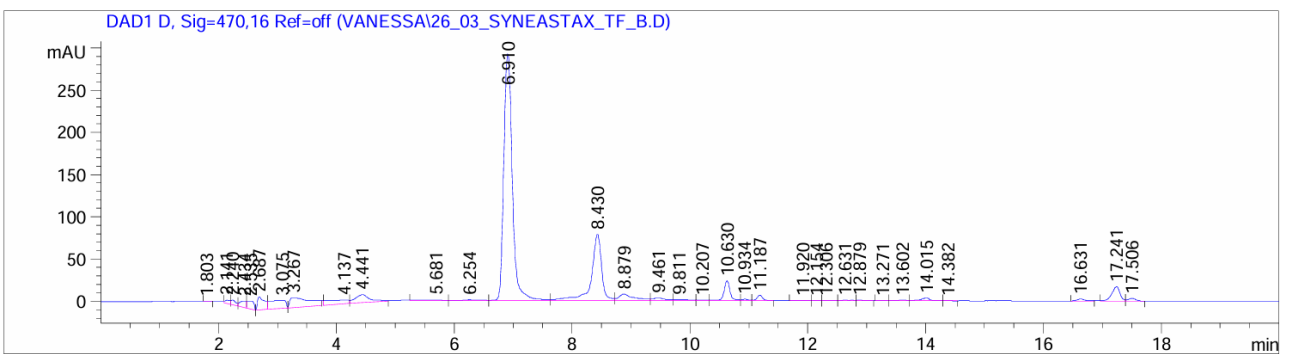
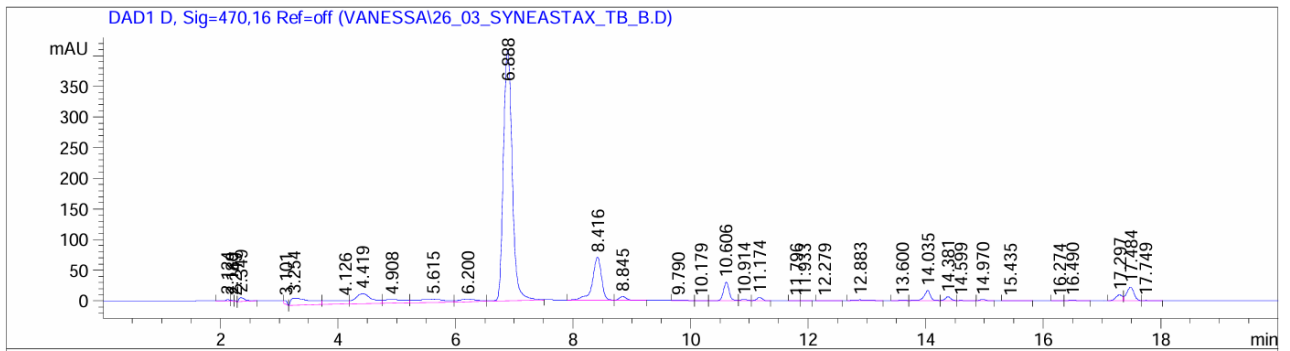
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Figure S1. HPLC chromatograms of extracts from cyanobacteria using DESs



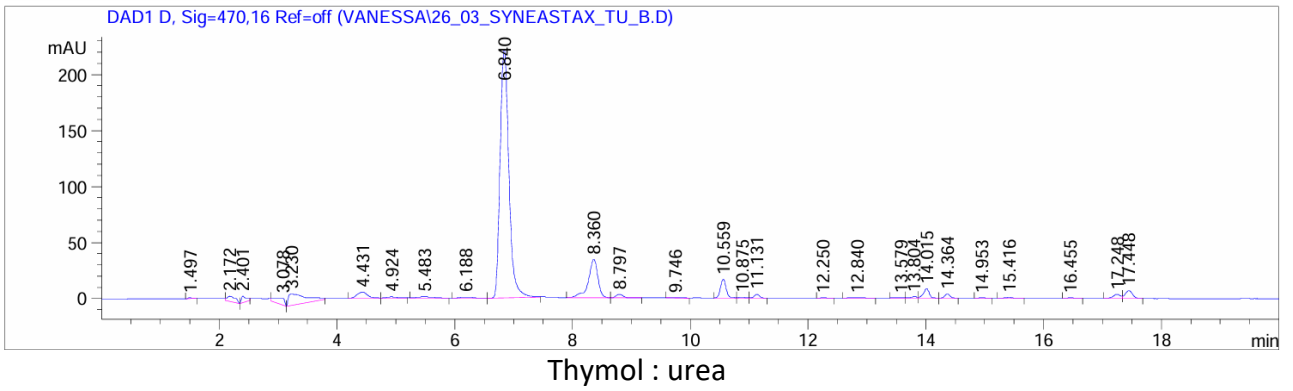
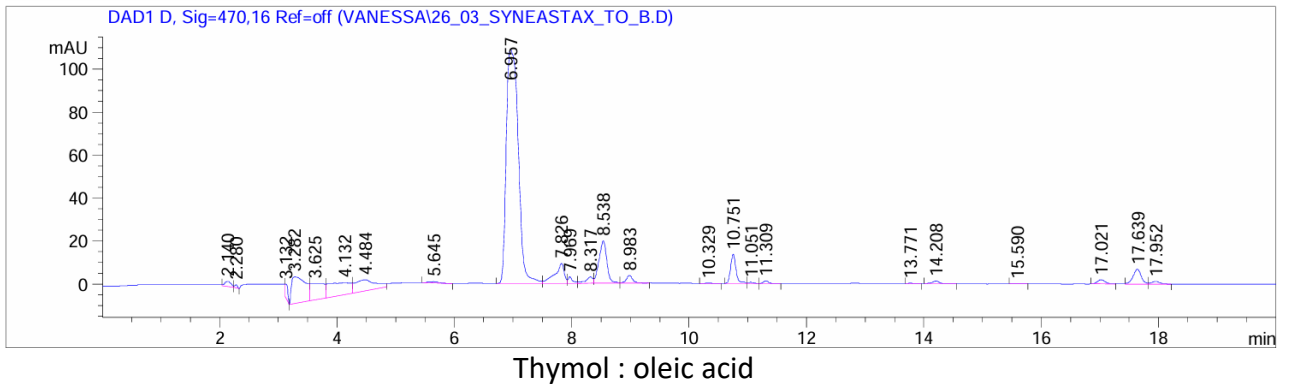


Figure S2. Nile-Red UV-Vis spectra in DESs for polarity measures

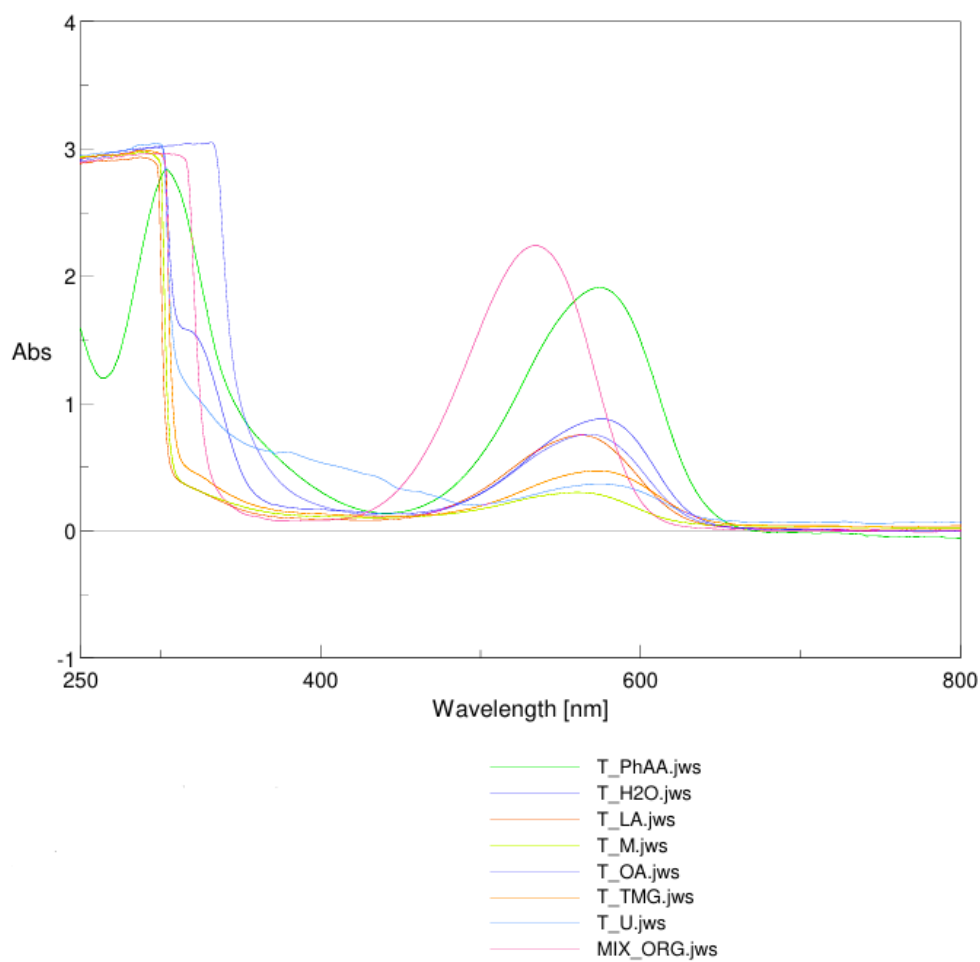
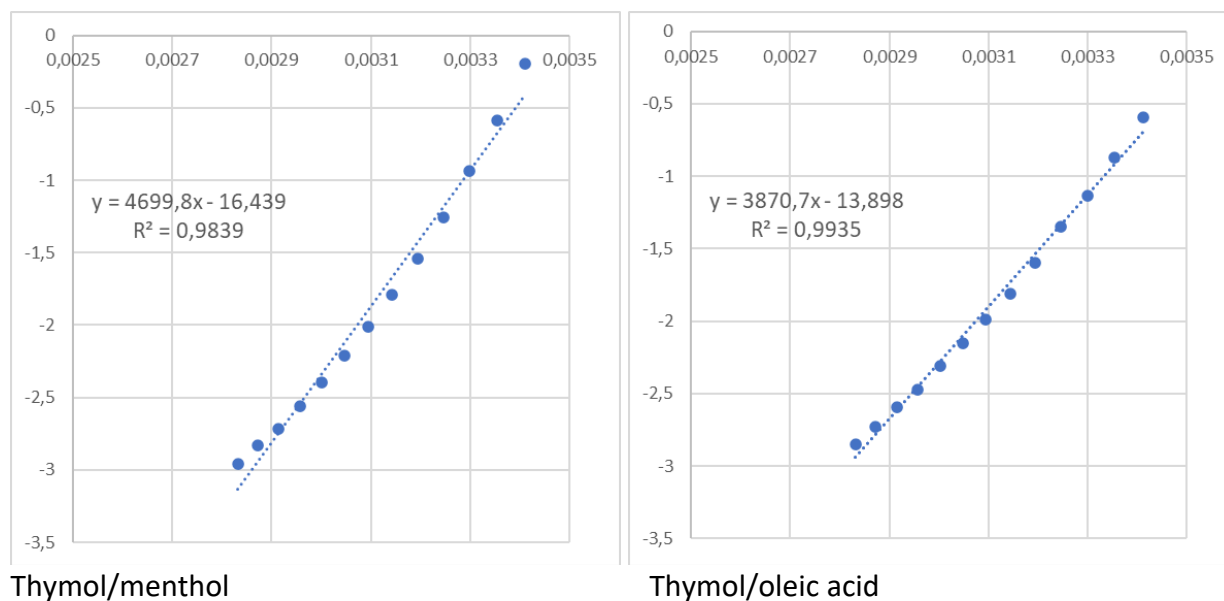
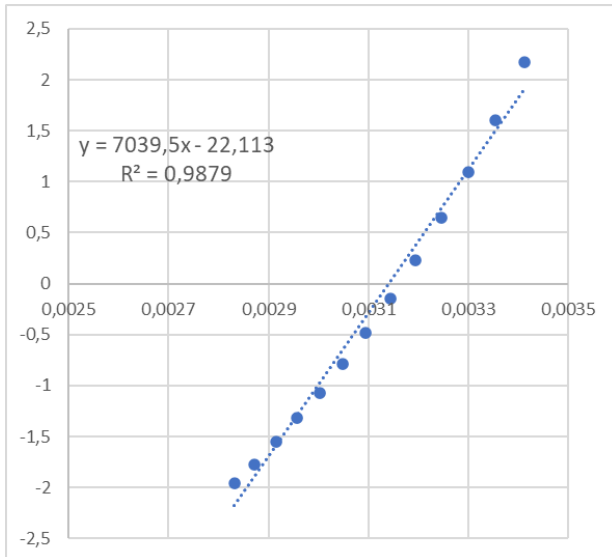


Table S1. Values of viscosity of DESs

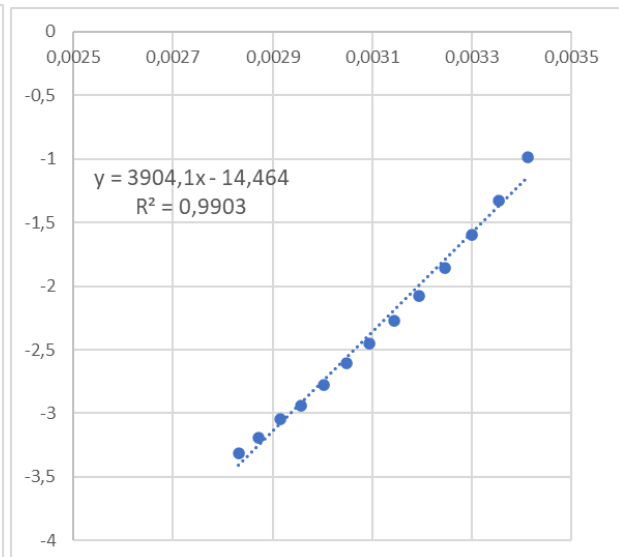
T (K)	VISCOSITY (POISE)						
	T/M	T/OA	T/TMG	T/PhAA	T/H2O	T/U	T/LA
303,15	0,393	0,322	2,996	0,202	0,196	0,196	0,124
308,15	0,284	0,260	1,902	0,156	0,151	0,151	0,101
313,15	0,214	0,203	1,260	0,126	0,119	0,119	0,084
318,15	0,167	0,164	0,862	0,103	0,097	0,097	0,070
323,15	0,134	0,137	0,616	0,086	0,077	0,077	0,060
328,15	0,110	0,116	0,455	0,074	0,065	0,065	0,051
333,15	0,091	0,099	0,343	0,062	0,055	0,055	0,044
338,15	0,077	0,085	0,268	0,053	0,047	0,047	0,039
343,15	0,066	0,075	0,212	0,048	0,041	0,041	0,034
348,15	0,059	0,065	0,170	0,041	0,036	0,036	0,030
353,15	0,052	0,058	0,142	0,036	0,032	0,032	0,027

Figure S3. Arrhenius plots (ln of viscosity vs. Temperature⁻¹) of DESs

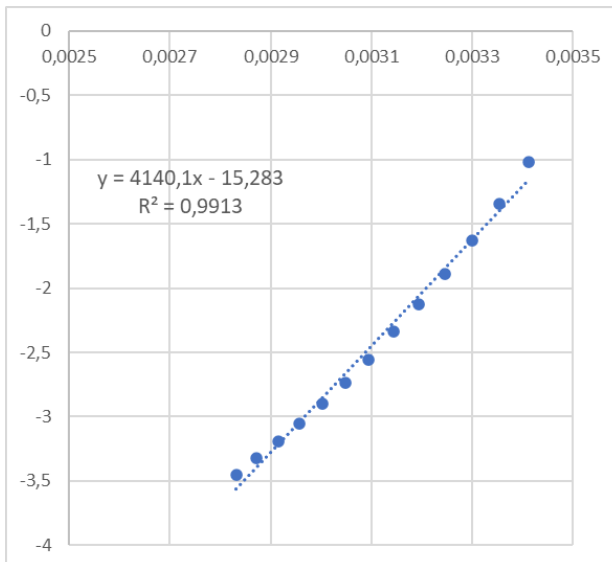




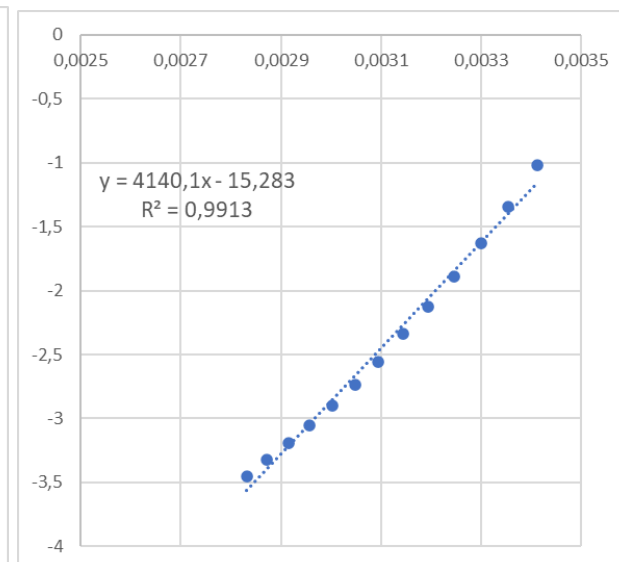
Thymol/betaine



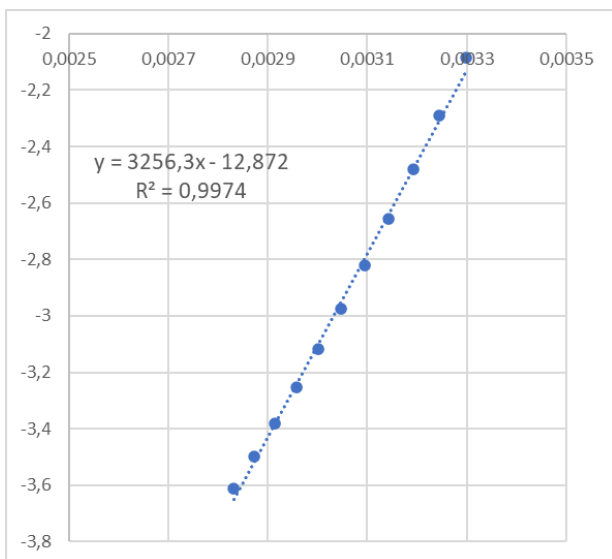
Thymol/Phenylacetic acid



Thymol/Water



Thymol/Urea



Thymol/Lauric acid

Tables S4. Correlation between the properties analyzed in the present study. All the liquids (top); excluding T/LA ES (middle); excluding T/LA ES and excluding T/TMG DES (bottom). Extraction = extraction yield (wt%); Solubility = Astaxanthin solubility (wt%); Polarity = Polarity (E_{NR} , kcal mol⁻¹); $\Sigma|\Delta\delta|$ = HBD-HBA intimacy (a.u.); Prep. Time = preparation time (h); Visc. 303 K = Viscosity at the temperature of 303 K; Visc. 323 K (Poise) = Viscosity at the temperature of 323 K (Poise); Ea Visc. = Activation Energy of Viscosity (kJ mol⁻¹); Density = Density (g mL⁻¹); Mol. Vol. = Molar Volume (cm³ mol⁻¹); Therm. st. = Thermal Stability after 72 hours (%); Light st. = light Stability after 72 hours (%). Squares coloured following a colour progressive scale made with conditional formatting in Microsoft Excel: red – lower values, white – medium values, blue – higher values.

All the liquids

	Extraction	Solubility	Polarity	$\Sigma \Delta\delta $	Prep. time	Visc 303 K	Visc 323 K	Ea Visc.	Density	Mol. Vol.	Therm. st.	Light st.
Extraction	1.00	0.25	0.51	0.37	0.34	0.16	0.21	0.21	0.04	0.09	0.42	0.03
Solubility	0.25	1.00	0.14	0.32	0.15	0.45	0.45	0.32	0.08	0.12	0.03	0.09
Polarity	0.51	0.14	1.00	0.90	0.59	0.01	0.01	0.02	0.41	0.55	0.01	0.05
$\Sigma \Delta\delta $	0.37	0.32	0.90	1.00	0.60	0.00	0.00	0.01	0.42	0.56	0.00	0.01
Prep. time	0.34	0.15	0.59	0.60	1.00	0.06	0.09	0.01	0.05	0.27	0.02	0.14
Visc 303 K	0.16	0.45	0.01	0.00	0.06	1.00	0.99	0.90	0.20	0.09	0.26	0.35
Visc 323 K	0.21	0.45	0.01	0.00	0.09	0.99	1.00	0.90	0.20	0.07	0.28	0.32
Ea Visc.	0.21	0.32	0.02	0.01	0.01	0.90	0.90	1.00	0.25	0.23	0.47	0.18
Density	0.04	0.08	0.41	0.42	0.05	0.20	0.20	0.25	1.00	0.55	0.03	0.07
Mol. Vol.	0.09	0.12	0.55	0.56	0.27	0.09	0.07	0.23	0.55	1.00	0.18	0.03
Therm. stab.	0.42	0.03	0.01	0.00	0.02	0.26	0.28	0.47	0.03	0.18	1.00	0.01
Light stab.	0.03	0.09	0.05	0.01	0.14	0.35	0.32	0.18	0.07	0.03	0.01	1.00

Excluding ES T/LA

	Extraction	Solubility	Polarity	$\Sigma \Delta\delta $	Prep. time	Visc 303 K	Visc 323 K	Ea Visc.	Density	Mol. Vol.	Therm. st.	Light st.
Extraction	1.00	0.44	0.78	0.82	0.54	0.13	0.17	0.15	0.27	0.42	0.41	0.01
Solubility	0.44	1.00	0.09	0.22	0.09	0.68	0.70	0.73	0.00	0.03	0.26	0.04
Polarity	0.78	0.09	1.00	0.94	0.54	0.00	0.00	0.00	0.37	0.54	0.16	0.14
$\Sigma \Delta\delta $	0.82	0.22	0.94	1.00	0.56	0.02	0.03	0.03	0.23	0.41	0.18	0.08
Prep. time	0.54	0.09	0.54	0.56	1.00	0.12	0.16	0.09	0.00	0.18	0.22	0.09
Visc 303 K	0.13	0.68	0.00	0.02	0.12	1.00	0.99	0.95	0.17	0.04	0.24	0.51
Visc 323 K	0.17	0.70	0.00	0.03	0.16	0.99	1.00	0.93	0.15	0.02	0.24	0.49
Ea Visc.	0.15	0.73	0.00	0.03	0.09	0.95	0.93	1.00	0.10	0.08	0.35	0.42
Density	0.27	0.00	0.37	0.23	0.00	0.17	0.15	0.10	1.00	0.31	0.13	0.43
Mol. Vol.	0.42	0.03	0.54	0.41	0.18	0.04	0.02	0.08	0.31	1.00	0.00	0.28
Therm. stab.	0.41	0.26	0.16	0.18	0.22	0.24	0.24	0.35	0.13	0.00	1.00	0.16
Light stab.	0.01	0.04	0.14	0.08	0.09	0.51	0.49	0.42	0.43	0.28	0.16	1.00

Excluding ES T/LA and excluding T/TMG

	Extraction	Solubility	Polarity	$\Sigma \Delta\delta $	Prep. time	Visc 303 K	Visc 323 K	Ea Visc.	Density	Mol. Vol.	Therm. st.	Light st.
Extraction	1.00	0.55	0.94	0.86	0.51	0.95	0.89	0.20	0.60	0.63	0.35	0.22
Solubility	0.55	1.00	0.43	0.49	0.01	0.57	0.39	0.34	0.63	0.39	0.08	0.85
Polarity	0.94	0.43	1.00	0.97	0.67	0.98	0.91	0.19	0.39	0.54	0.28	0.17
$\Sigma \Delta\delta $	0.86	0.49	0.97	1.00	0.59	0.97	0.85	0.25	0.32	0.46	0.20	0.25
Prep. time	0.51	0.01	0.67	0.59	1.00	0.54	0.67	0.00	0.03	0.30	0.15	0.01
Visc 303 K	0.95	0.57	0.98	0.97	0.54	1.00	0.89	0.25	0.47	0.55	0.26	0.28
Visc 323 K	0.89	0.39	0.91	0.85	0.67	0.89	1.00	0.03	0.30	0.79	0.12	0.18
Ea Visc.	0.20	0.34	0.19	0.25	0.00	0.25	0.03	1.00	0.39	0.01	0.44	0.17
Density	0.60	0.63	0.39	0.32	0.03	0.47	0.30	0.39	1.00	0.26	0.54	0.28
Mol. Vol.	0.63	0.39	0.54	0.46	0.30	0.55	0.79	0.01	0.26	1.00	0.01	0.27
Therm. stab.	0.35	0.08	0.28	0.20	0.15	0.26	0.12	0.44	0.54	0.01	1.00	0.01
Light stab.	0.22	0.85	0.17	0.25	0.01	0.28	0.18	0.17	0.28	0.27	0.01	1.00