

## Supplementary Materials

### *Using COSMO-RS in the designing and screening of different eutectic solvents for the extraction of carbaryl*

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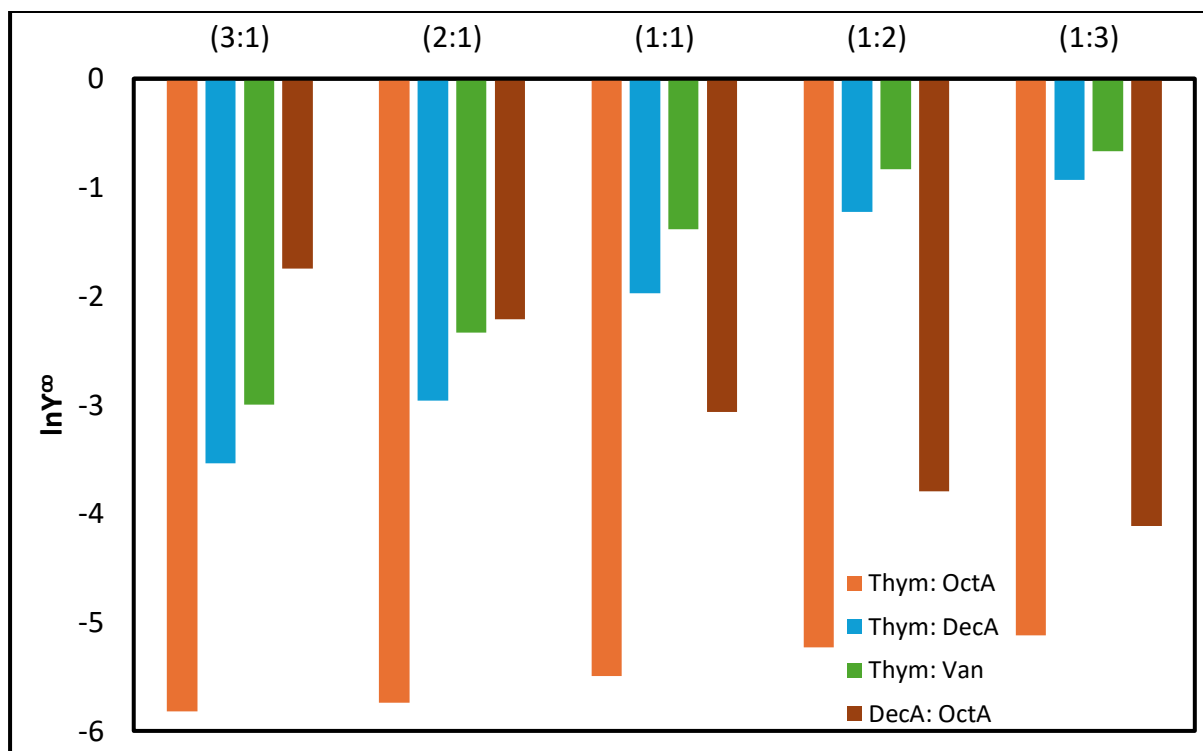
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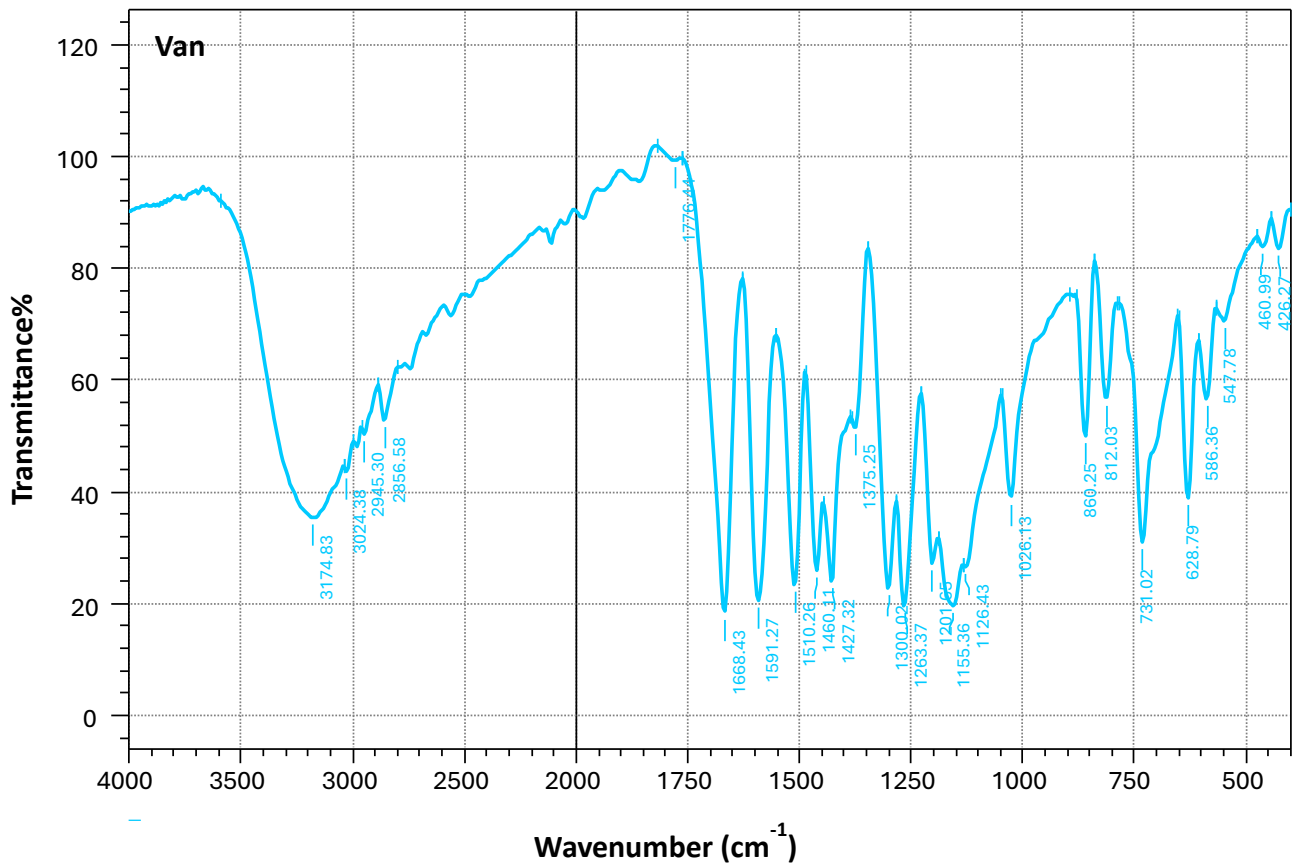
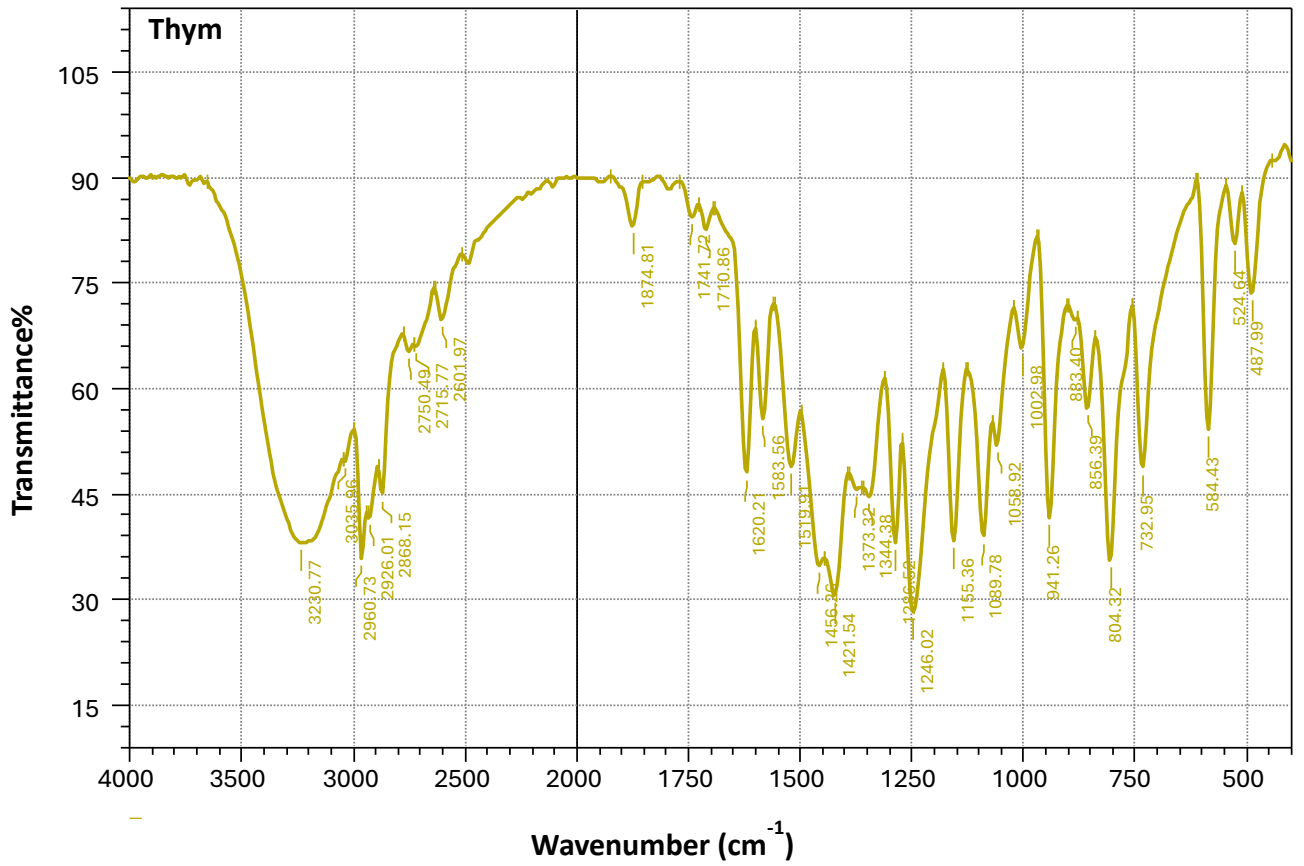
<sup>1</sup> These authors are considered co-first authors because they contributed equally to this work.

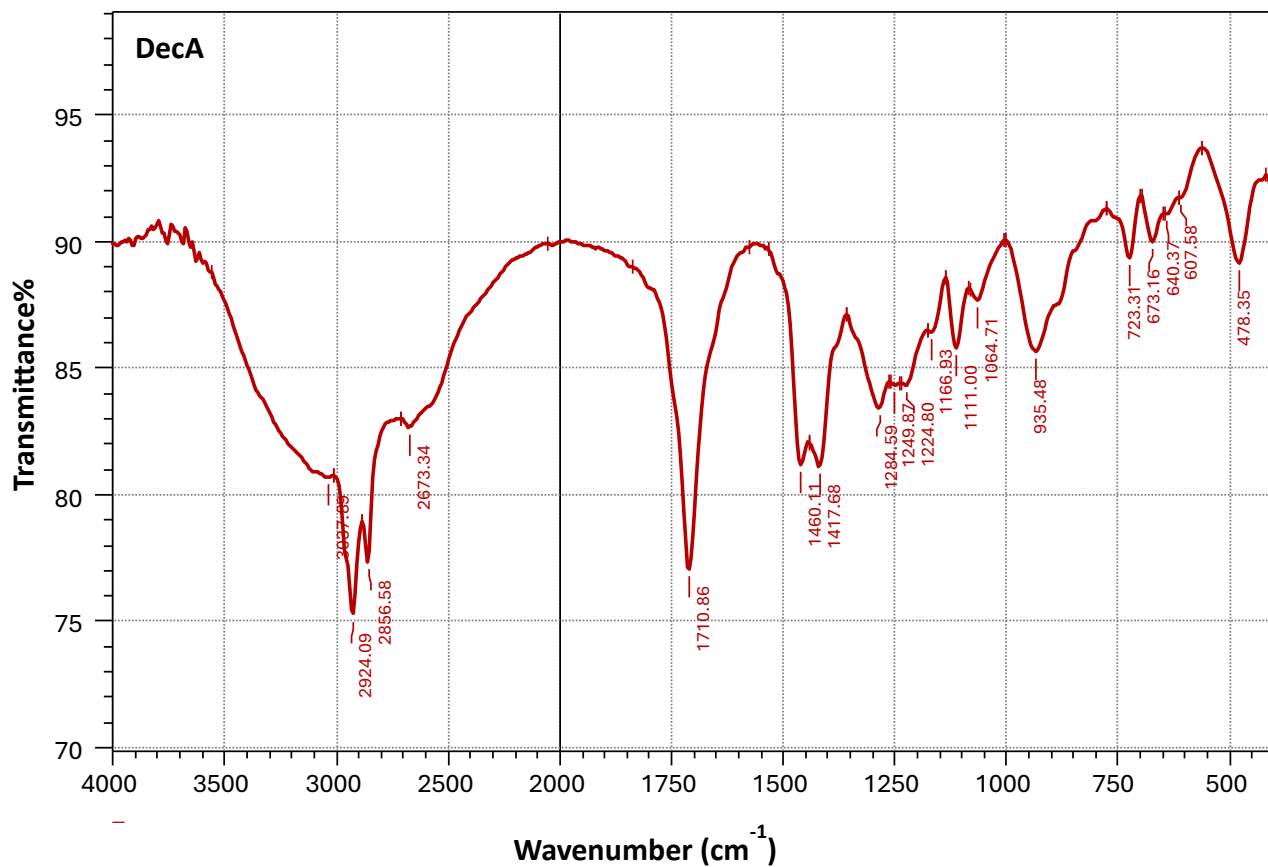
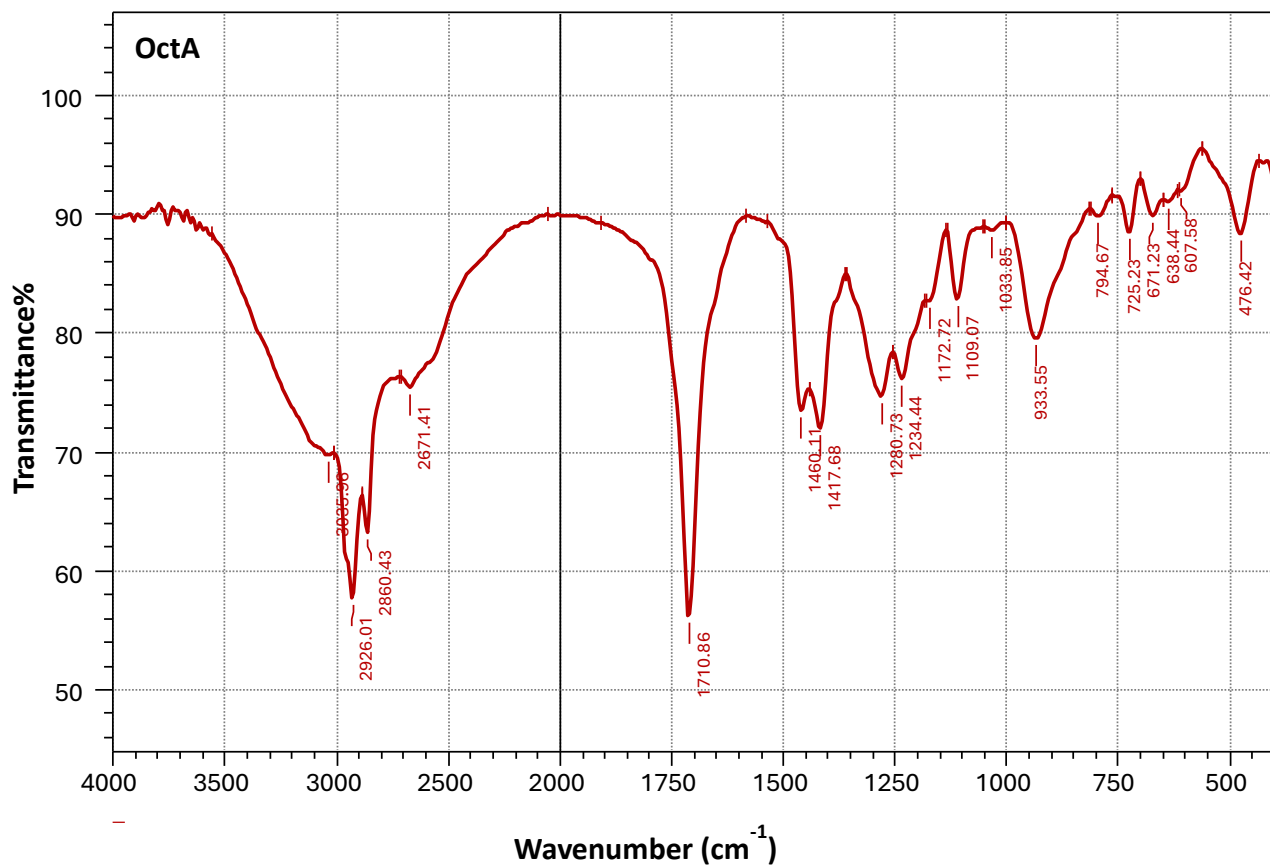
**Table S1.** Preparation conditions of different ESs at equimolar composition in this research work.

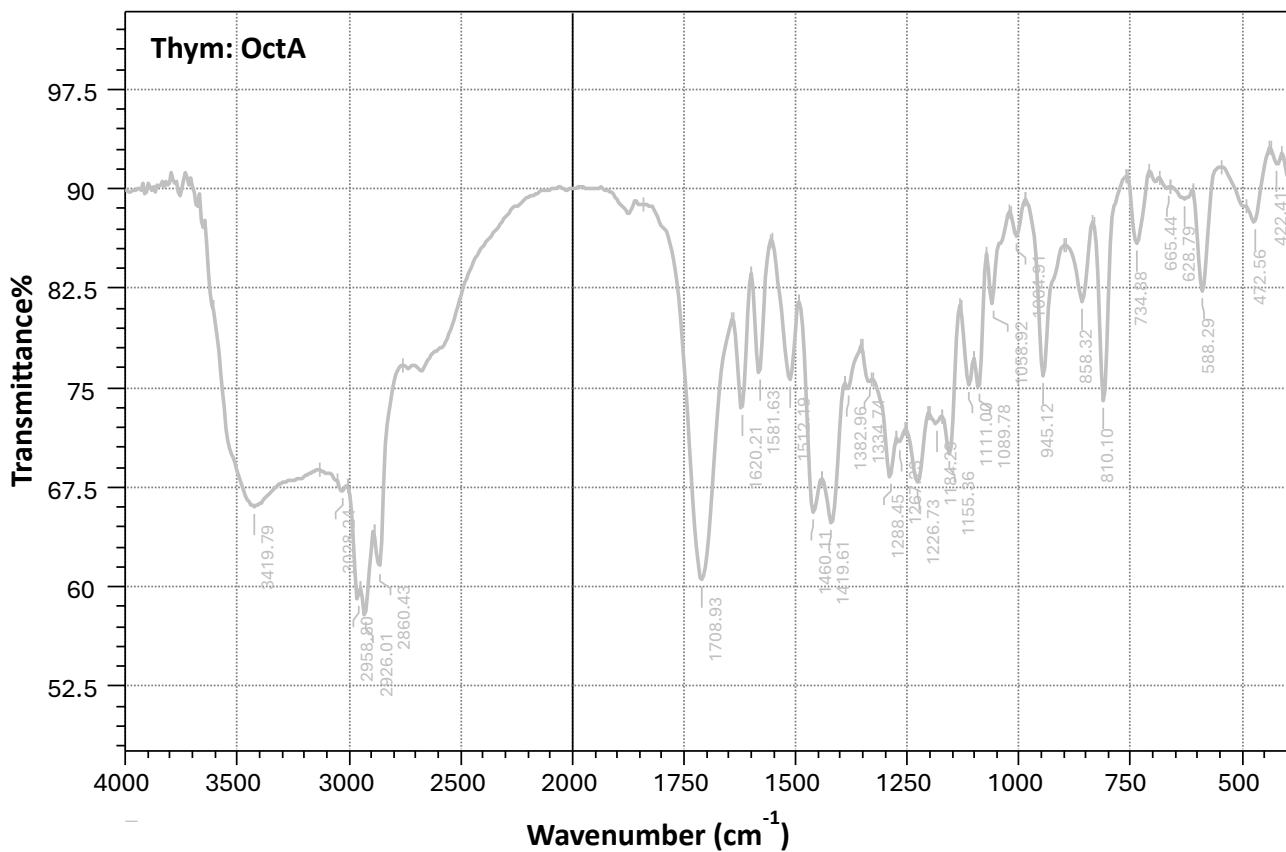
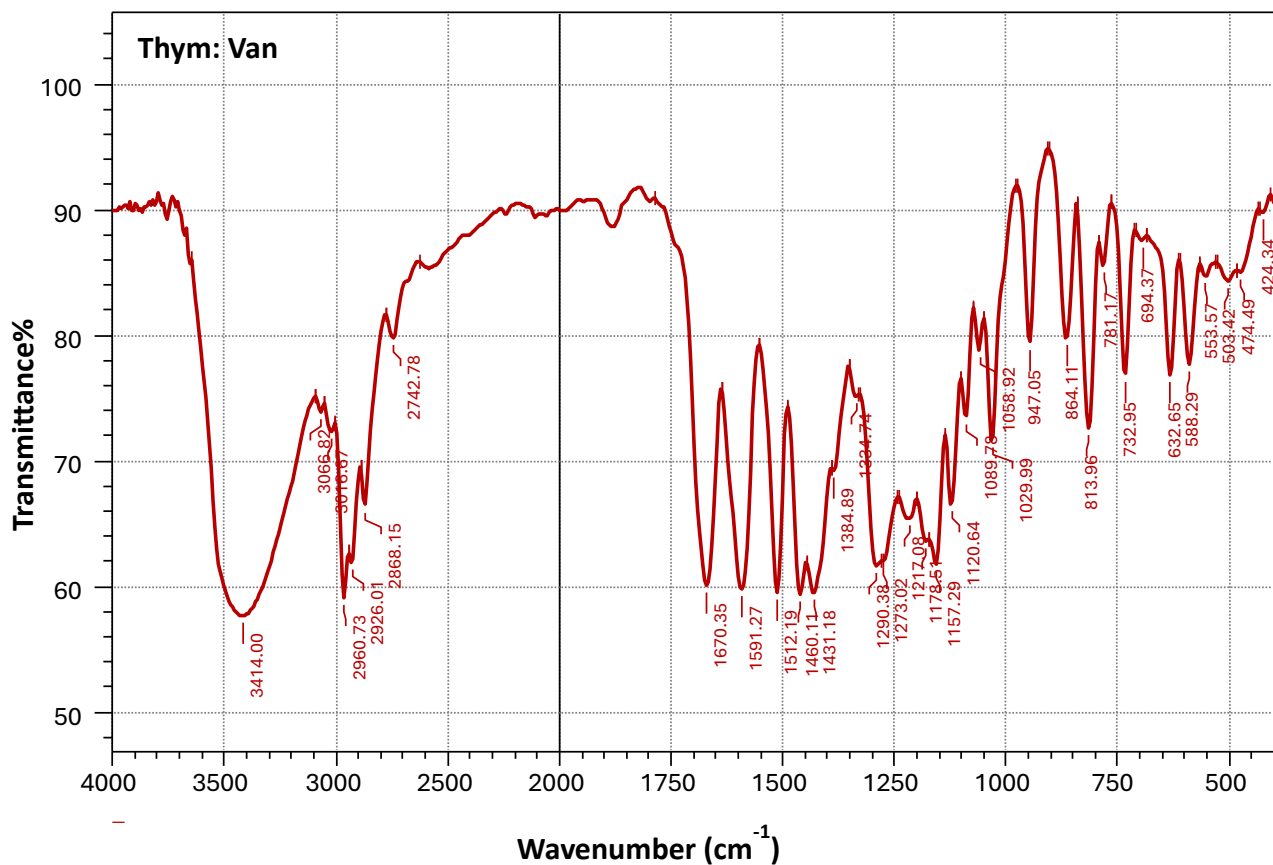
HBA	HBD	$\gamma^\infty$	Preparation temperature (°C)	Stability
Thym	AcetA	-1.96	80	Stable
	OxA	-5.49	60	X
	MalA	-2.62	80	X
	OctA	-2.18	80	Stable
	DecA	-1.98	80	Stable
	4-NP	-4.78	80	X
	4-CP	-5.30	80	X
	Van	-1.38	80	Stable
DecA	AcetA	-0.648	60	Stable
	OxA	-3.07	60	X
	MalA	-1.22	60	X
	OctA	-0.427	60	Stable
	4-NP	-2.26	60	Stable
	4-CP	-2.01	60	Stable
	Van	-0.888	80	X
CitA	OxA	-3.09	80	X
	MalA	-1.82	80	X
	OctA	-1.52	80	X
	4-NP	-2.71	60	X
	4-CP	-2.60	60	X



**Fig. S1.** Predicted  $\ln Y^{\infty}$  of ESs at different compositions of HBAs and HBDs.







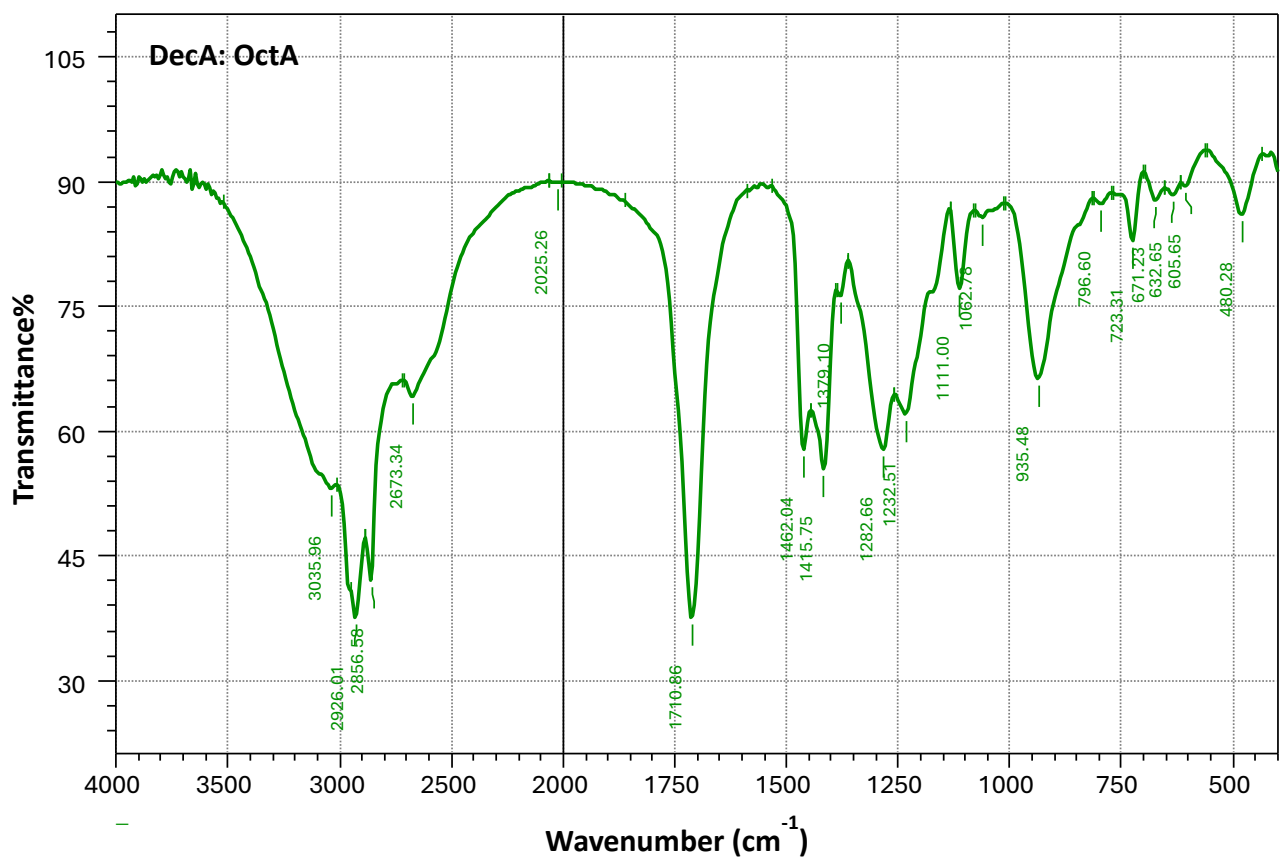
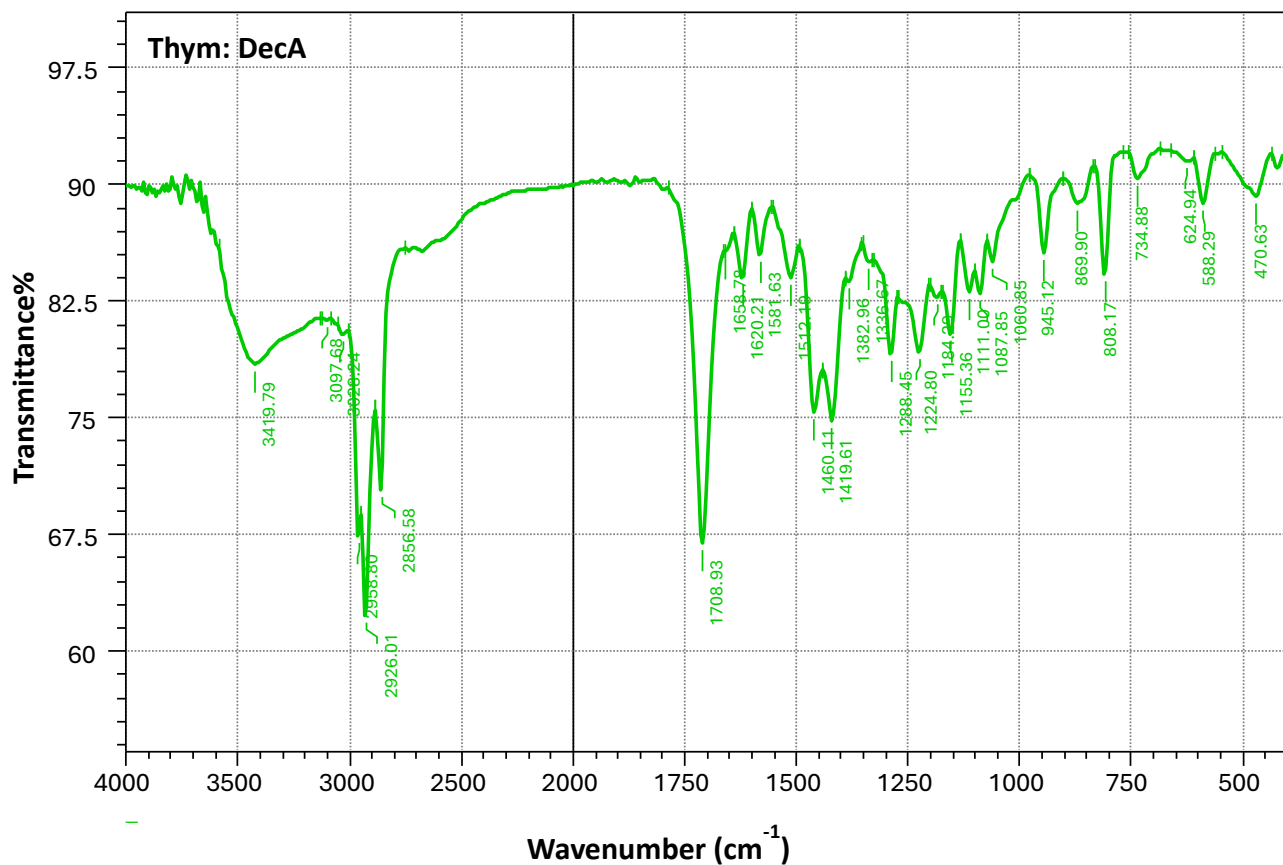
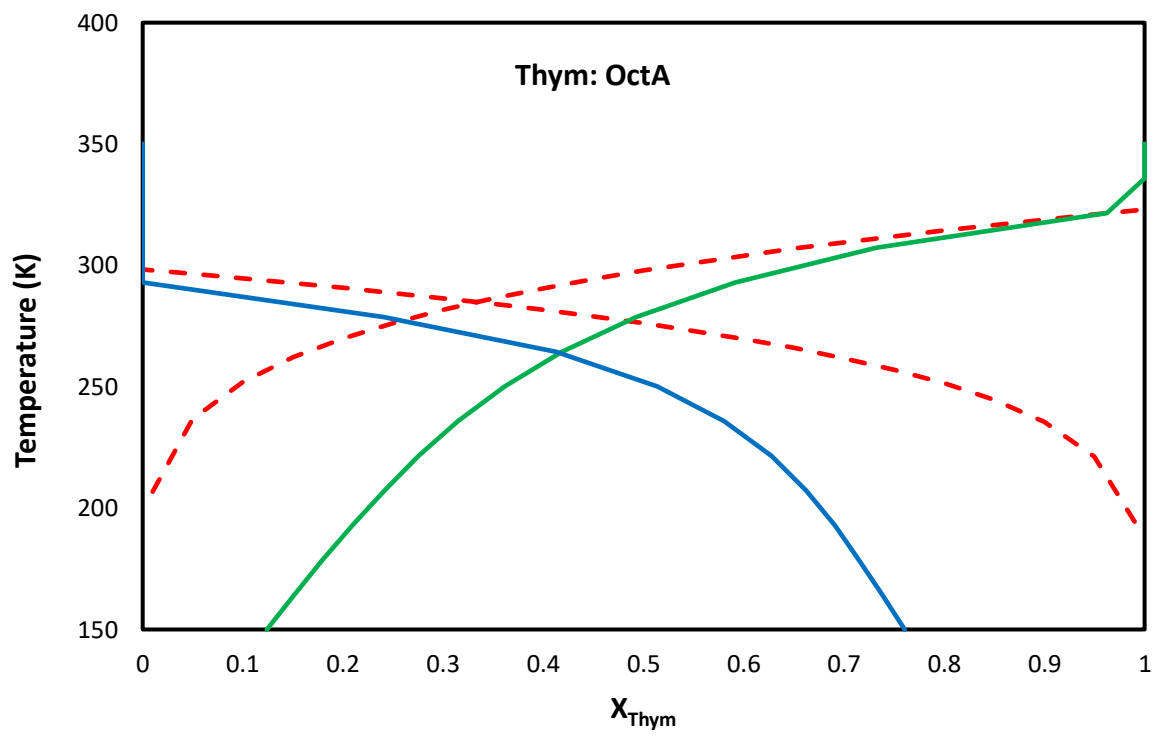
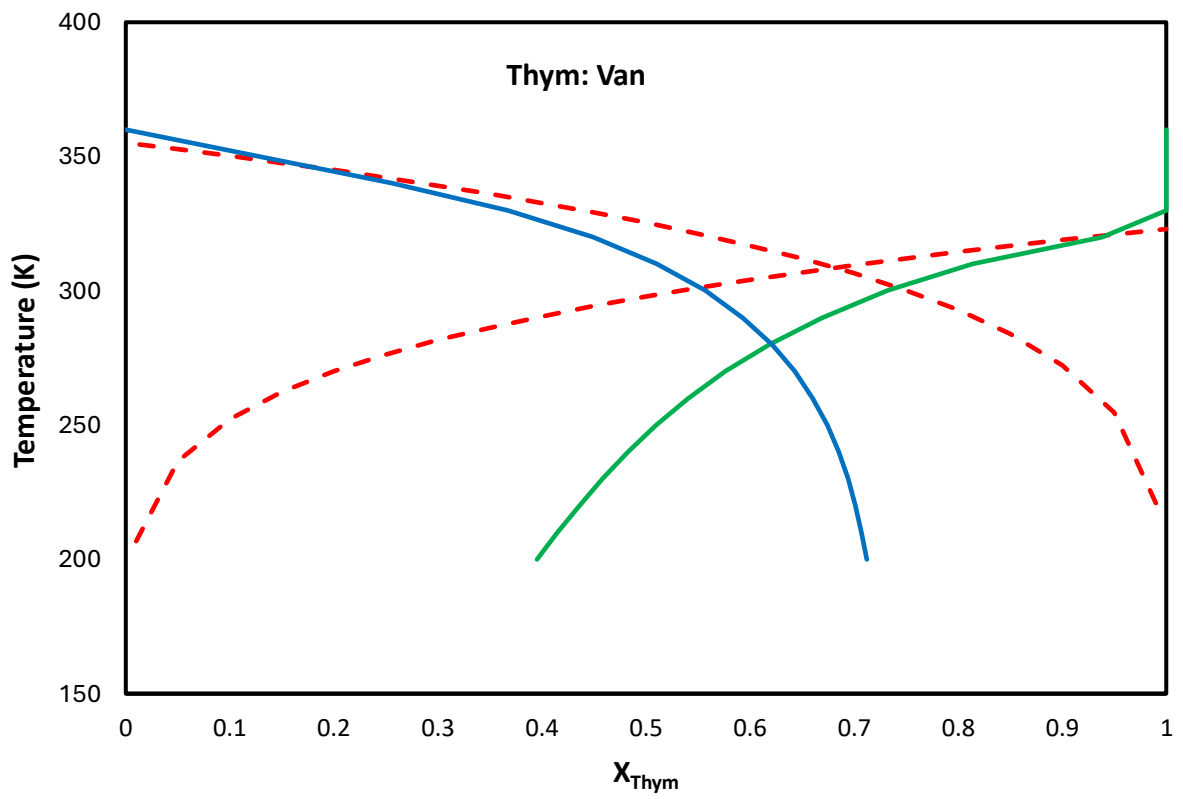
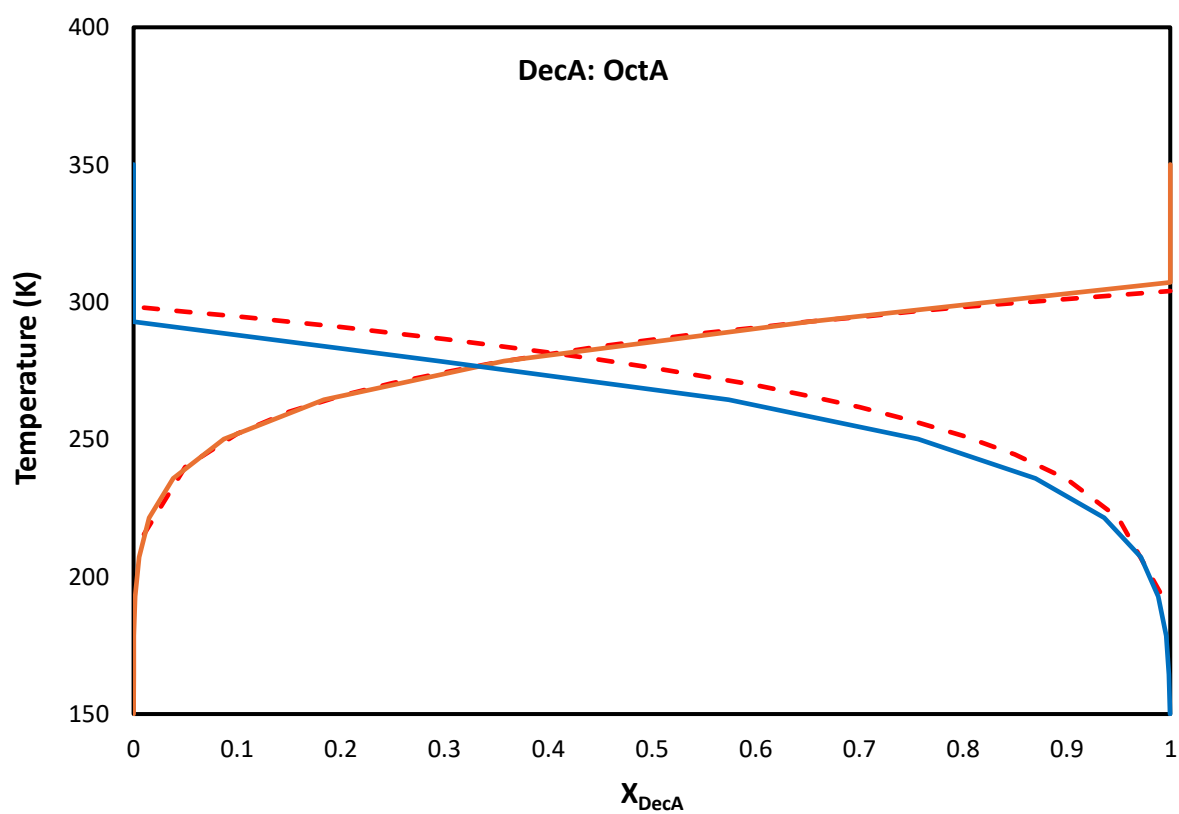
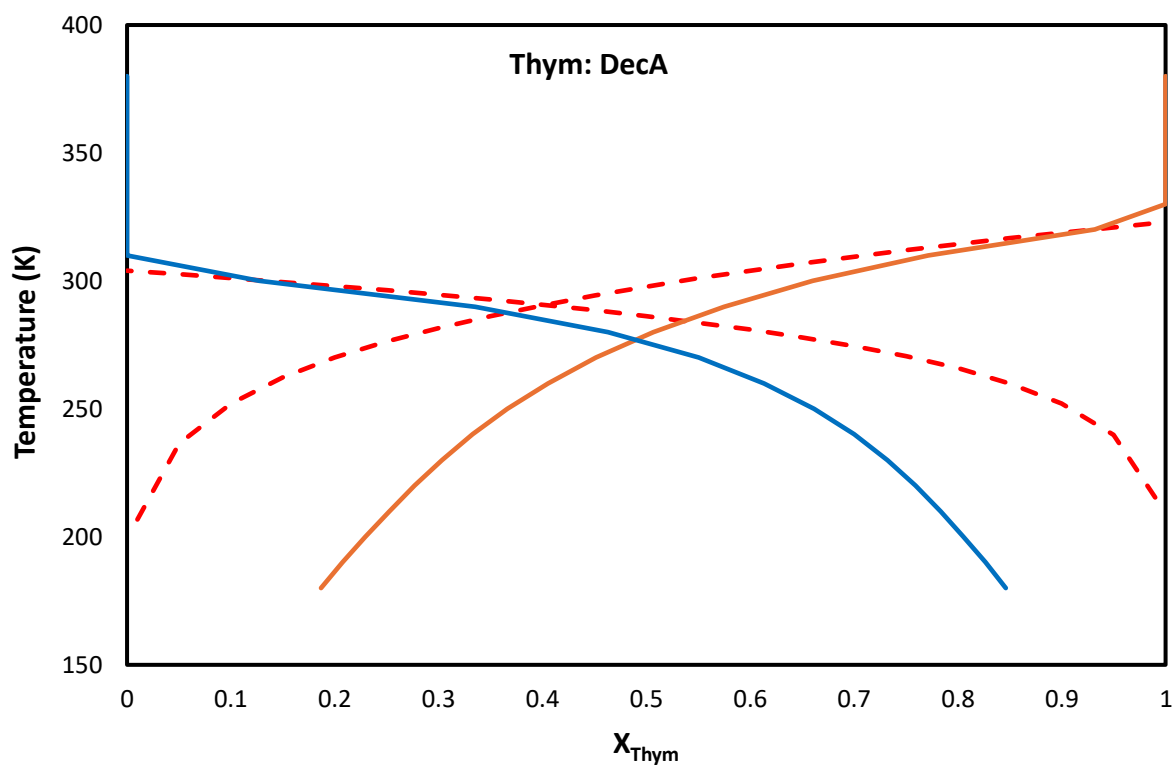


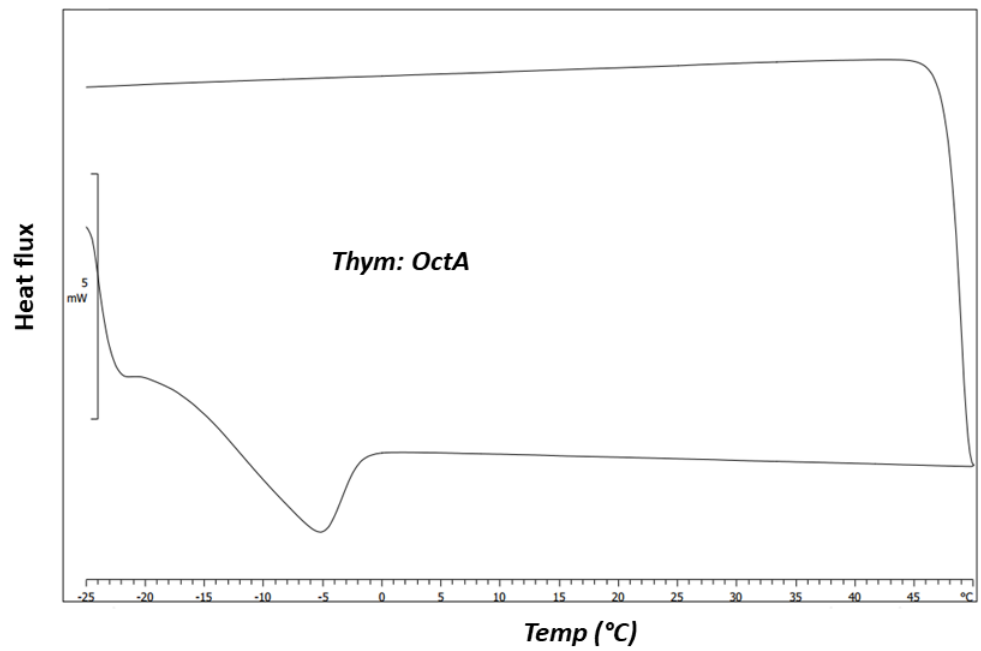
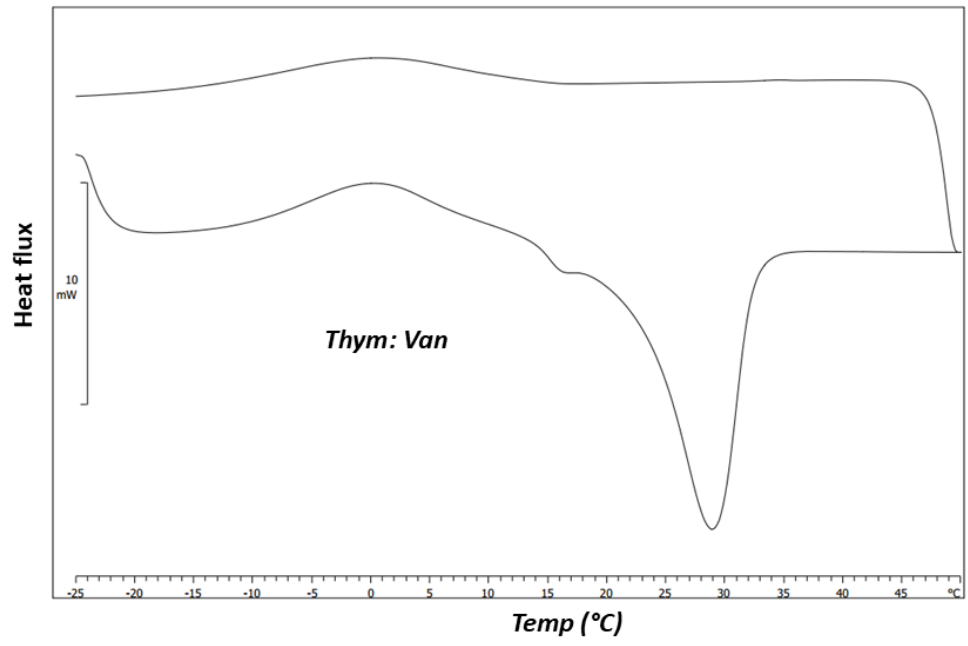
Fig. S2. FTIR spectra of HBAs, HBDs, and ESs.

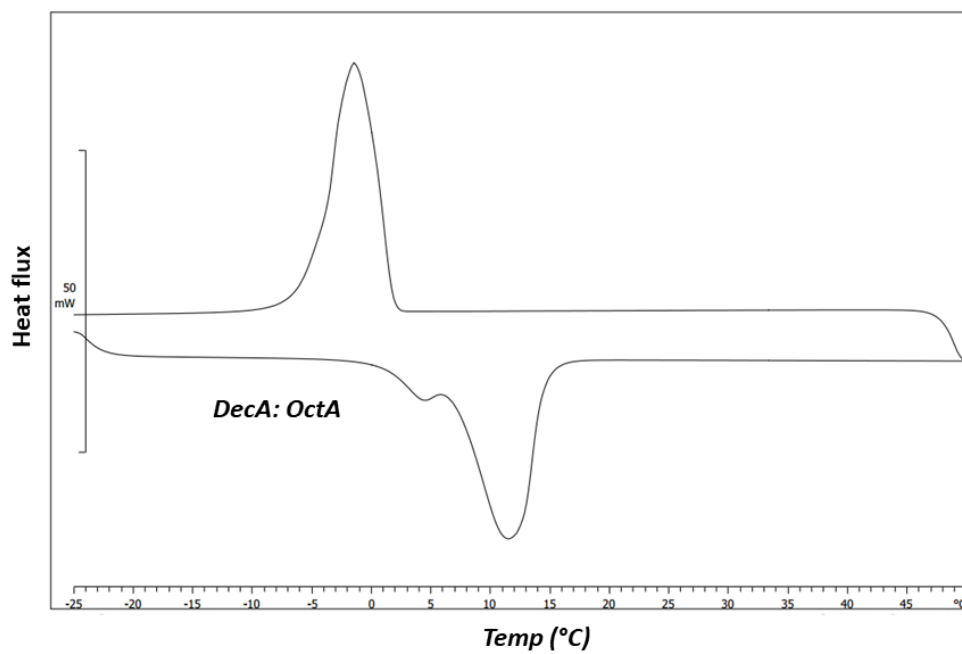
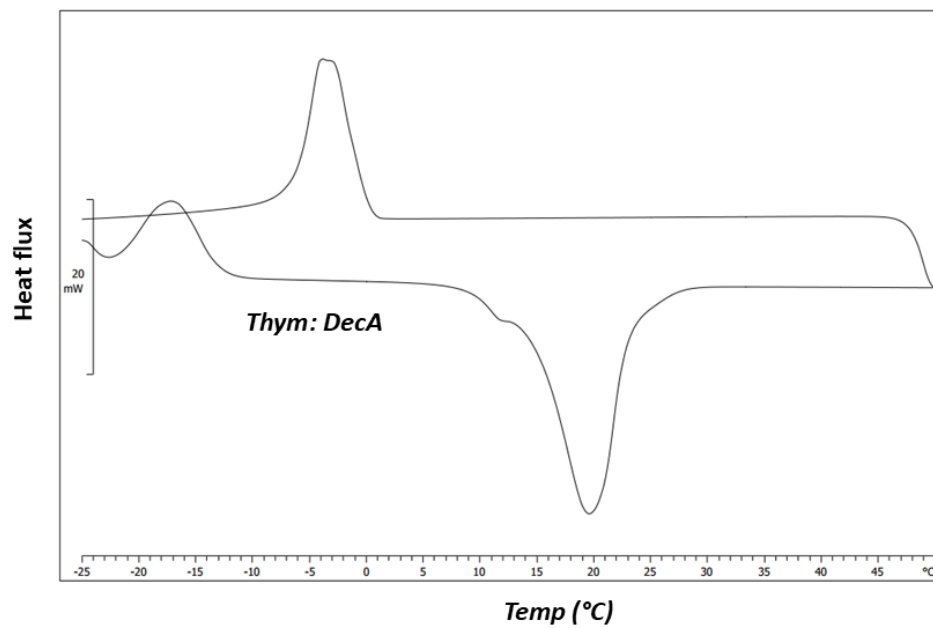




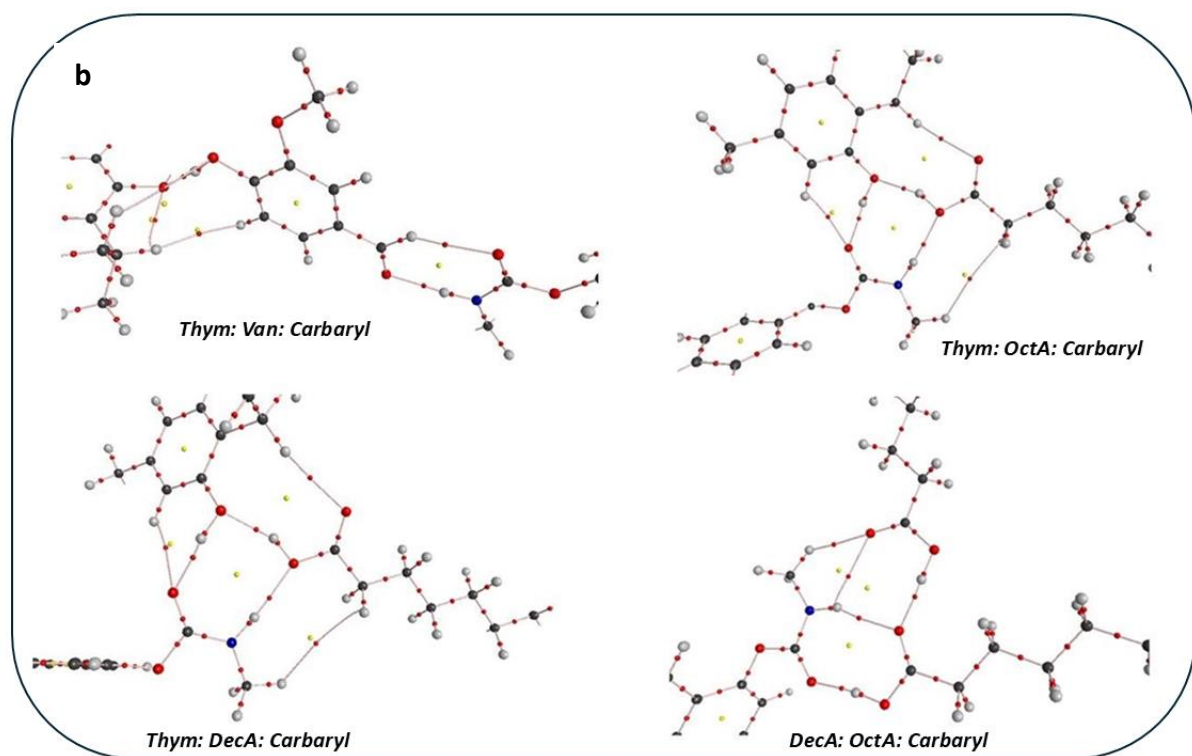
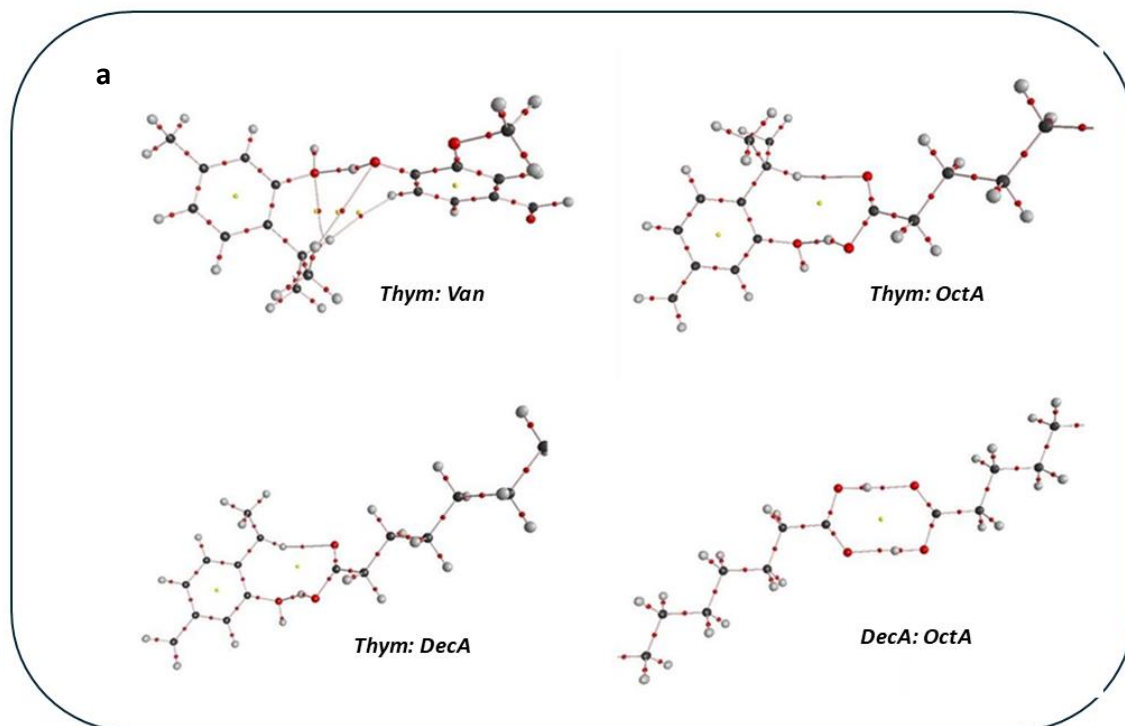


**Fig. S3.** Predicted solid-liquid equilibrium phase diagrams using COSMO-RS. Solid lines represent the COSMO-RS calculations, and dashed lines represent ideal solubility curves.





**Fig. S4.** DSC thermograms of ESs at a 1:1 molar ratio of the parent components.



**Fig. S5.** Molecular graphs of (a) ESs including BCPs (red) and RCPs (yellow) and (b) the complexes formed between ESs and carbaryl.