

## Electronic Supplementary Information (ESI)

# Rapid Dissolution of High Concentration Poly(3-hydroxybutyrate) using Neoteric Biosolvent: Experiment and Molecular Dynamics Simulation

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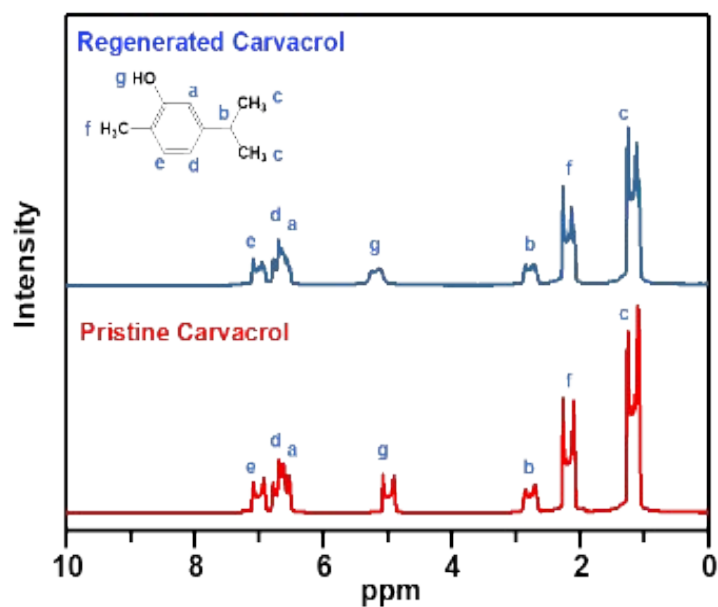
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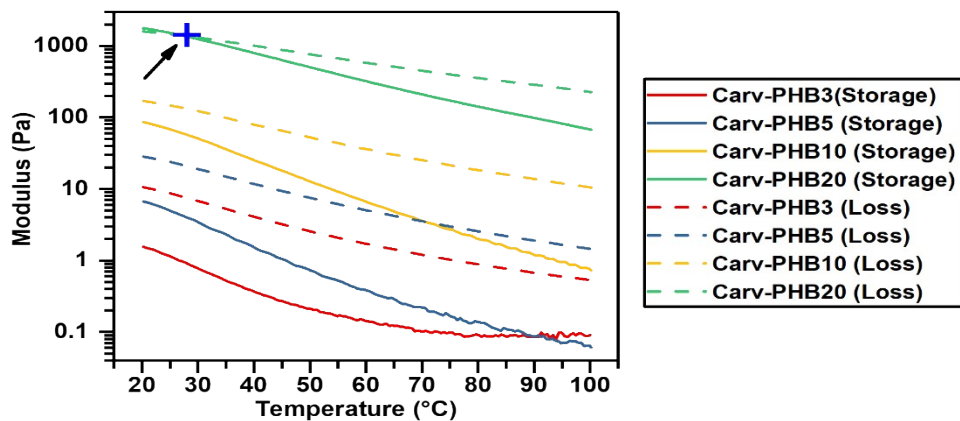
Number of Tables: 3



**Figure S1.** <sup>1</sup>H NMR spectra for pristine carvacrol (bottom) and recovered/regenerated carvacrol (top).

**Table S1.** Activation energies of selected Carv-PHBx samples

Samples	Activation energy	
	(kJ/mol)	R
Carv-PHB3	35.63±0.30	0.993
Carv-PHB5	35.82±0.23	0.996
Carv-PHB10	36.58±0.18	0.998
Carv-PHB20	27.26±0.16	0.997



**Figure S2.** Storage modulus ( $G'$ ) and Loss modulus ( $G''$ ) of carvacrol/PHB samples as a function of temperature.

**Table S2.** Composition of bioadhesive formulation (Carv-PHB\_Adh)

Ingredient	(~% w/w)
PHB	22.3
Gum rosin	17.8
Natural Beeswax	4.5
Carvacrol	55.4
<b>Total</b>	<b>100</b>

**Table S3.** H-bond densities obtained using Molecular Dynamic (MD) simulation for Carv-PHBx samples

Samples	Total H-bonds density		Carv-Carv H bonds		PHB-Carv H bonds		PHB-PHB H bonds		Diffusion coefficient ( $1 \times 10^5 \text{ cm}^2/\text{s}$ )		H bond breaking (20-100 °C)
	20 °C	100 °C	20 °C	100 °C	20 °C	100 °C	20 °C	100 °C	20 °C	100 °C	
Carv-PHB1	493	291	479	280	14	11	0	0	0.033	0.92	202
Carv-PHB3	517	309	475	276	42	31	1	2	0.03	0.76	208
Carv-PHB5	532	325	463	271	67	51	2	3	0.026	0.69	207
Carv-PHB10	581	372	427	254	150	111	4	7	0.014	0.54	209
Carv-PHB20	651	472	383	220	245	236	22	17	0.0081	0.37	179