Thymol as starting material for the development of a biobased material with enhanced antimicrobial activity: synthesis, characterization, and potential application

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Supporting Information

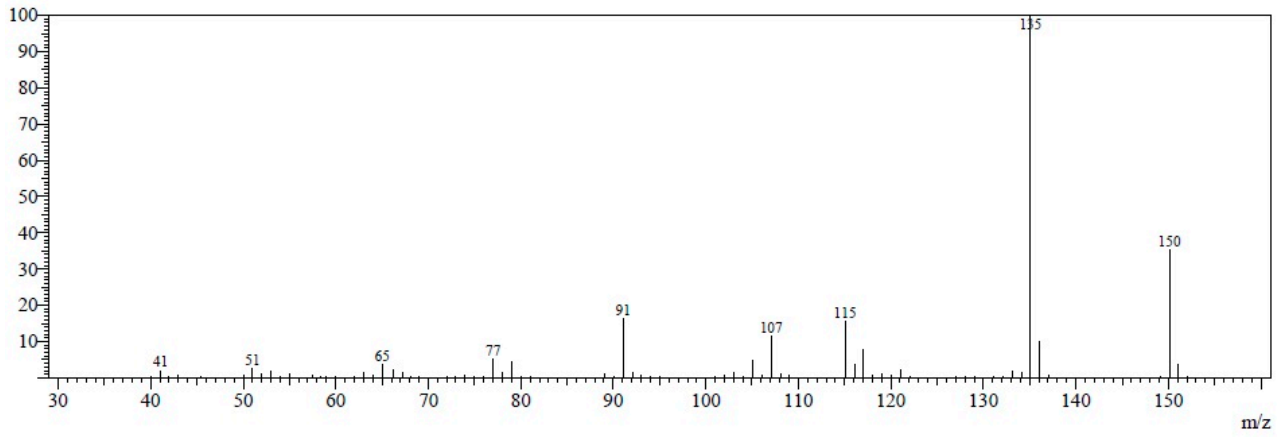


Figure S1. LREIMS (70eV) data of thymol extracted from thyme essential oil.

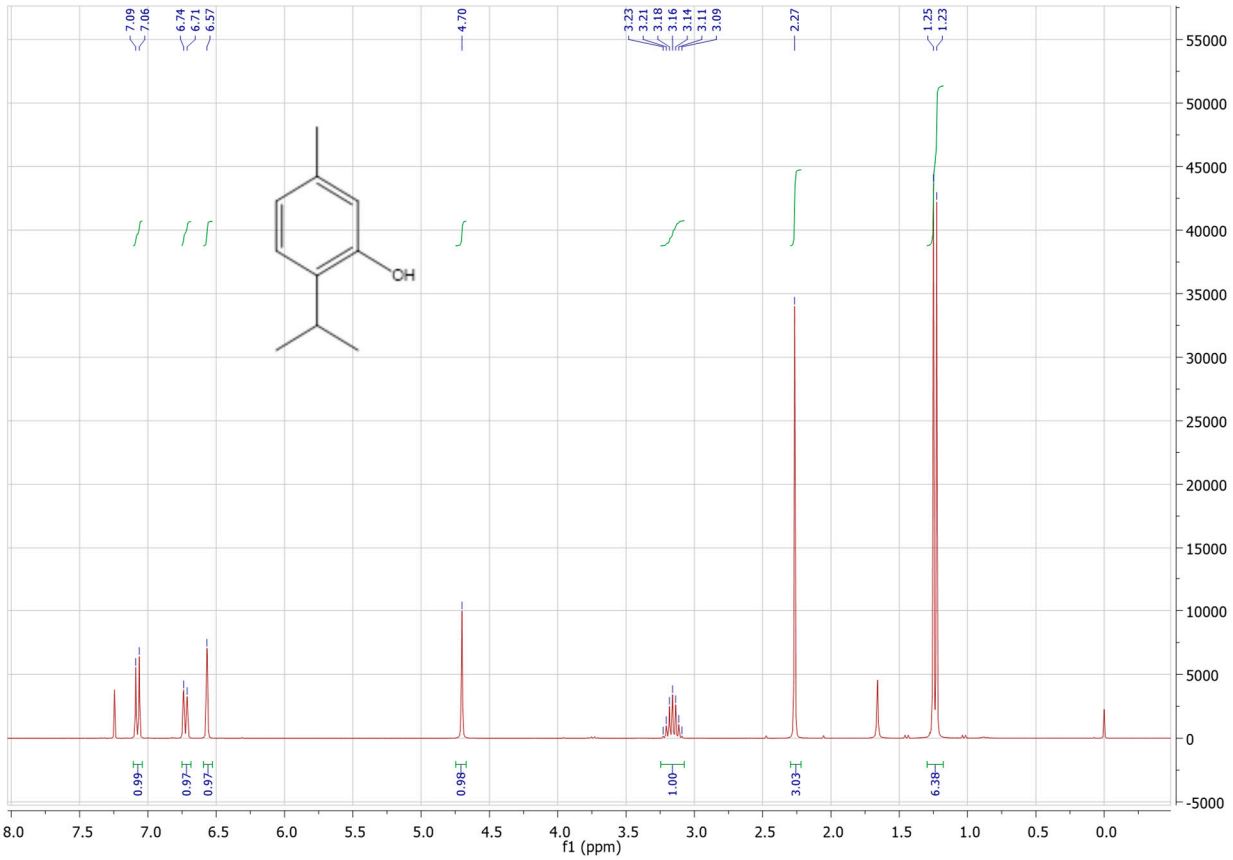


Figure S2. ^{1}H NMR spectrum of thymol (δ, $CDCl_3$, 300 MHz).

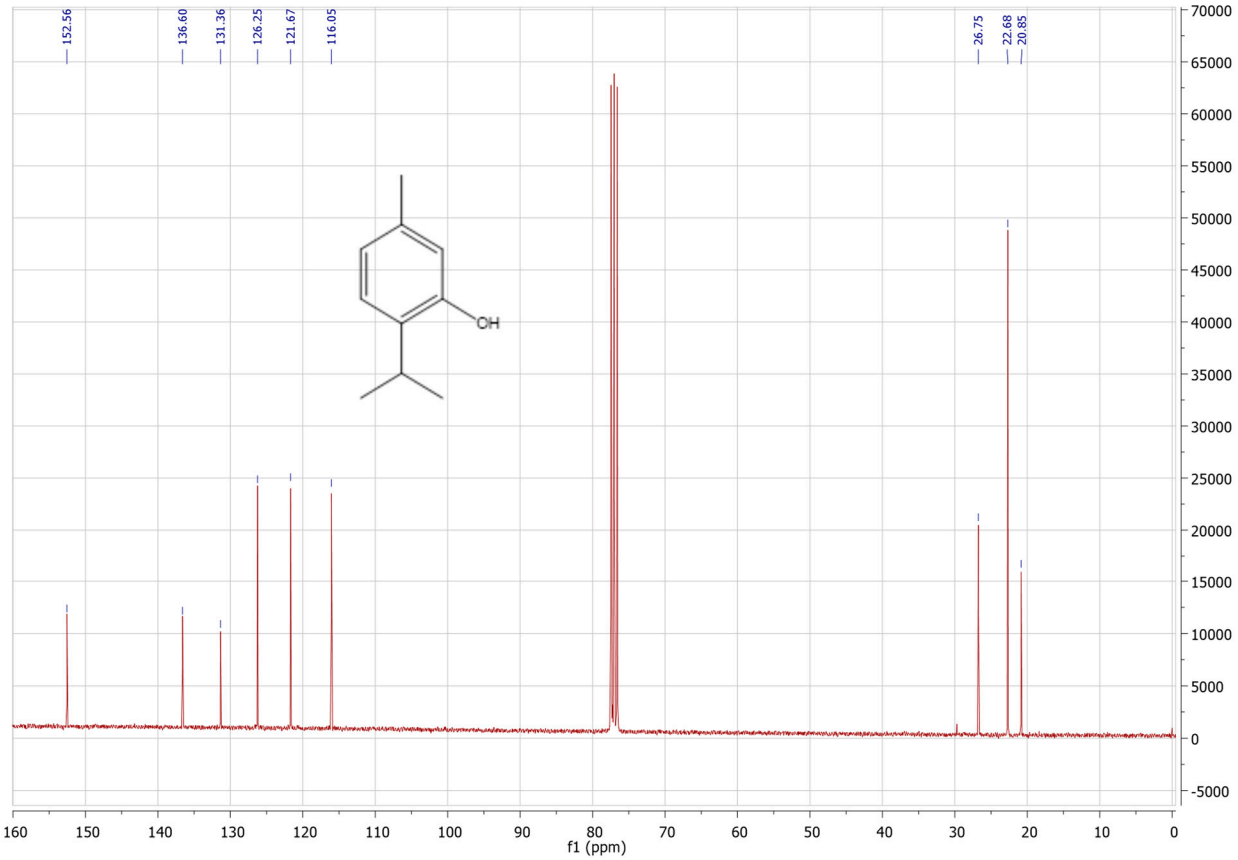


Figure S3. ^{13}C NMR spectrum of thymol (δ, $CDCl_3$, 75 MHz).

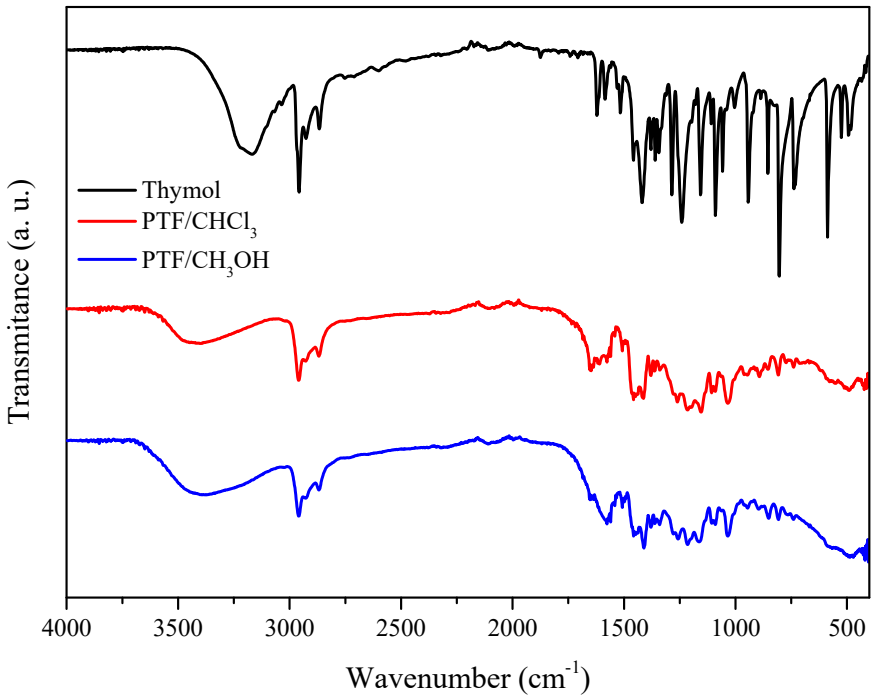


Figure S4. Infrared spectra for thymol (black), PTF/$CHCl_3$ (red) and PTF/CH_3OH (blue).

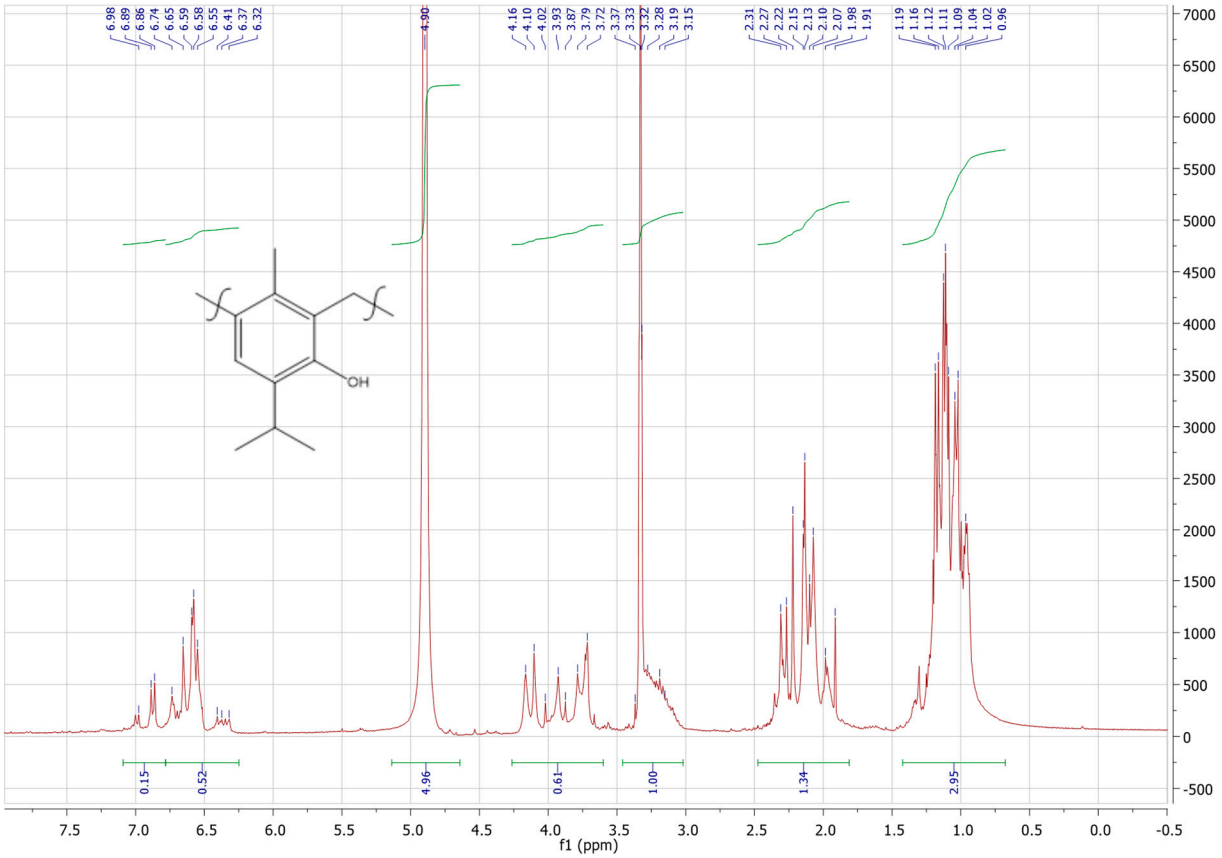


Figure S5. ^{1}H NMR spectrum of PTF (δ, CD_3OD, 300 MHz).

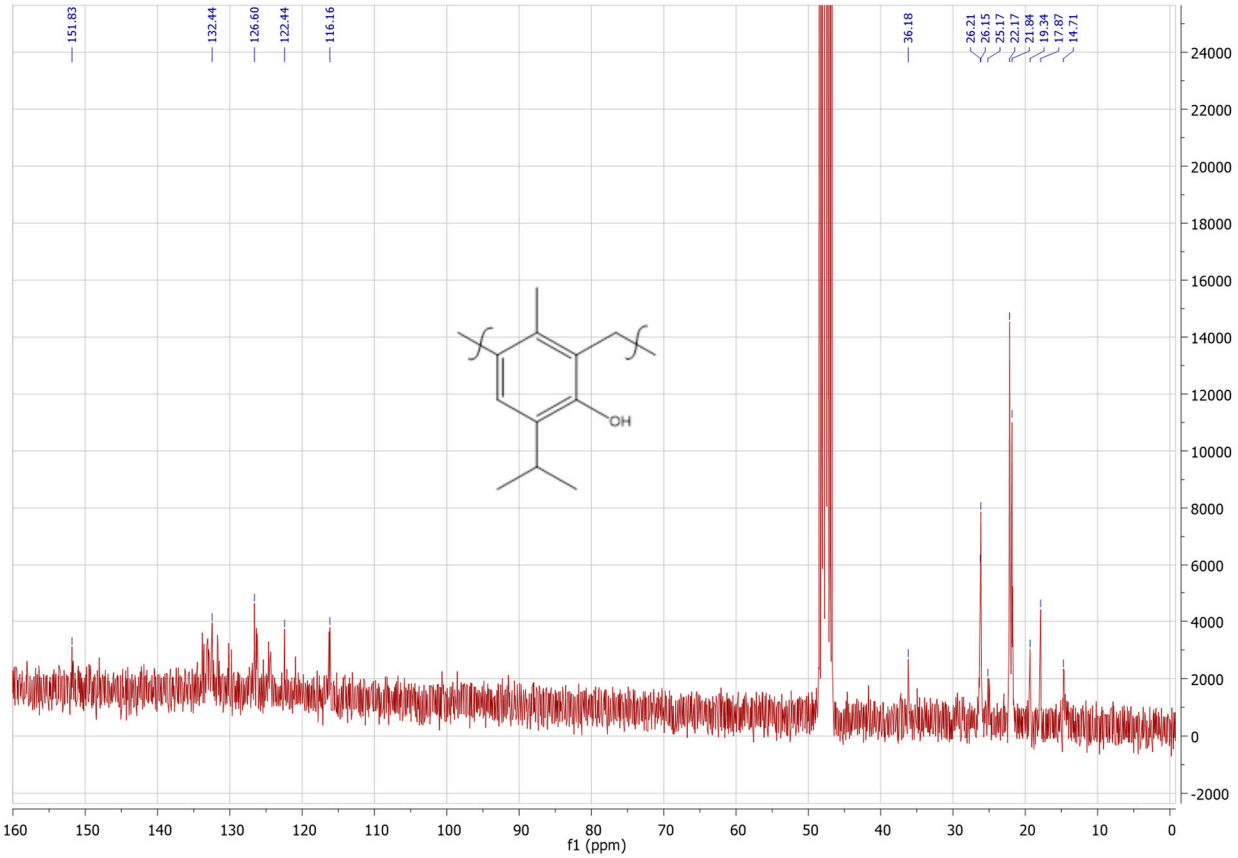


Figure S6. ^{13}C NMR spectrum of PTF (δ, CD_3OD, 75 MHz).

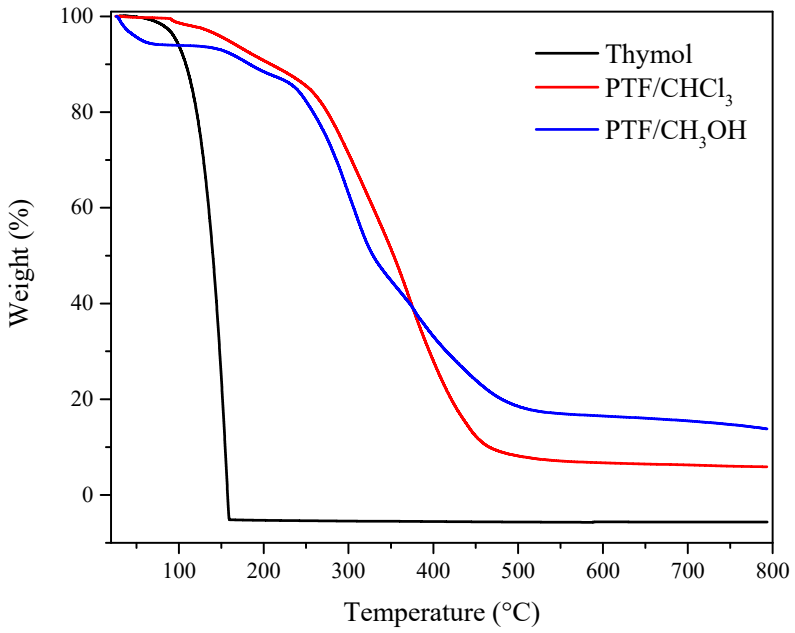


Figure S7. TG curves for thymol (black), PTF/$CHCl_3$ (red) and PTF/CH_3OH (blue), ranging from 20 to 800 °C at 10 °C.min^{-1} and inert nitrogen atmosphere at 50 mL.min^{-1}.

Table S1: Fluorescent signal of the metabolism of resazurin to resofurin, comparing different concentrations of thymol, PTF/$CHCl_3$, and PTF/CH_3OH.

µg.mL^{-1}	*Thymol*	*PTF/$CHCl_3$*	*PTF/CH_3OH*	*Control*
500.00	507 ± 176	590 ± 190	338 ± 100	1542 ± 378
250.00	1483 ± 252	1264 ± 185	922 ± 422	
125.00	1734 ± 299	1370 ± 166	1377 ± 258	
62.50	1945 ± 371	1699 ± 140	1410 ± 190	
31.25	1795 ± 539	1607 ± 229	1418 ± 250	
15.63	2354 ± 436	2017 ± 90	2011 ± 47	
7.81	2035 ± 289	1897 ± 93	1820 ± 86	
3.91	2639 ± 356	2540 ± 117	2918 ± 329	

Table S2: Colorimetric quantification of biomass, comparing different concentrations of thymol, PTF/$CHCl_3$, and PTF/CH_3OH.

µg.mL^{-1}	*Thymol*	*PTF/$CHCl_3$*	*PTF/CH_3OH*	*Control*
500.00	0.14 ± 0.02	0.15 ± 0.02	0.18 ± 0.06	0.16 ± 0.05
250.00	0.15 ± 0.03	0.20 ± 0.01	0.15 ± 0.02	
125.00	0.15 ± 0.02	0.16 ± 0.02	0.14 ± 0.01	
62.50	0.13 ± 0.02	0.13 ± 0.01	0.20 ± 0.01	
31.25	0.11 ± 0.02	0.11 ± 0.01	0.15 ± 0.01	
15.63	0.10 ± 0.02	0.12 ± 0.03	0.12 ± 0.04	
7.81	0.12 ± 0.03	0.12 ± 0.01	0.16 ± 0.00	
3.91	0.14 ± 0.04	0.15 ± 0.03	0.18 ± 0.00	