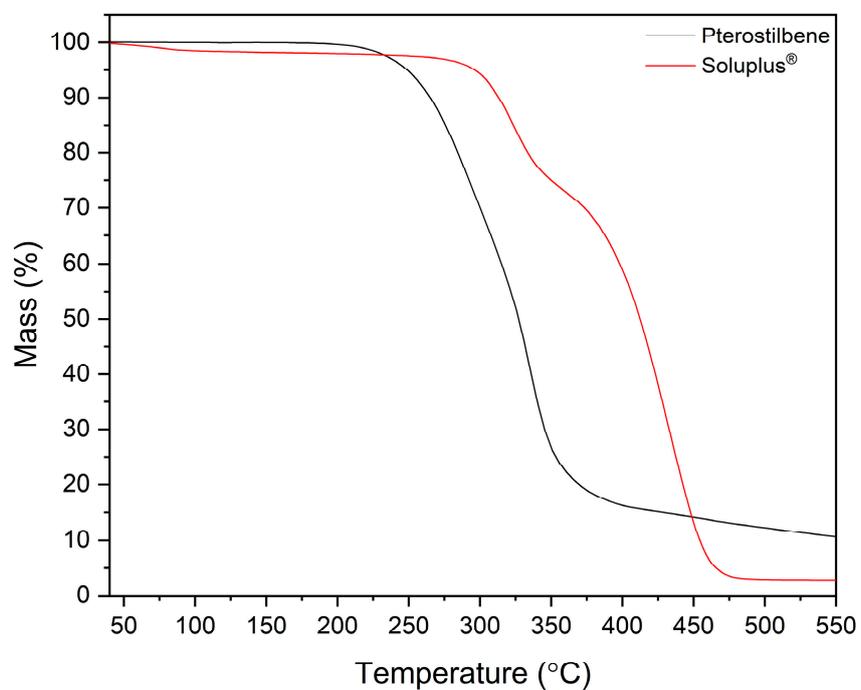
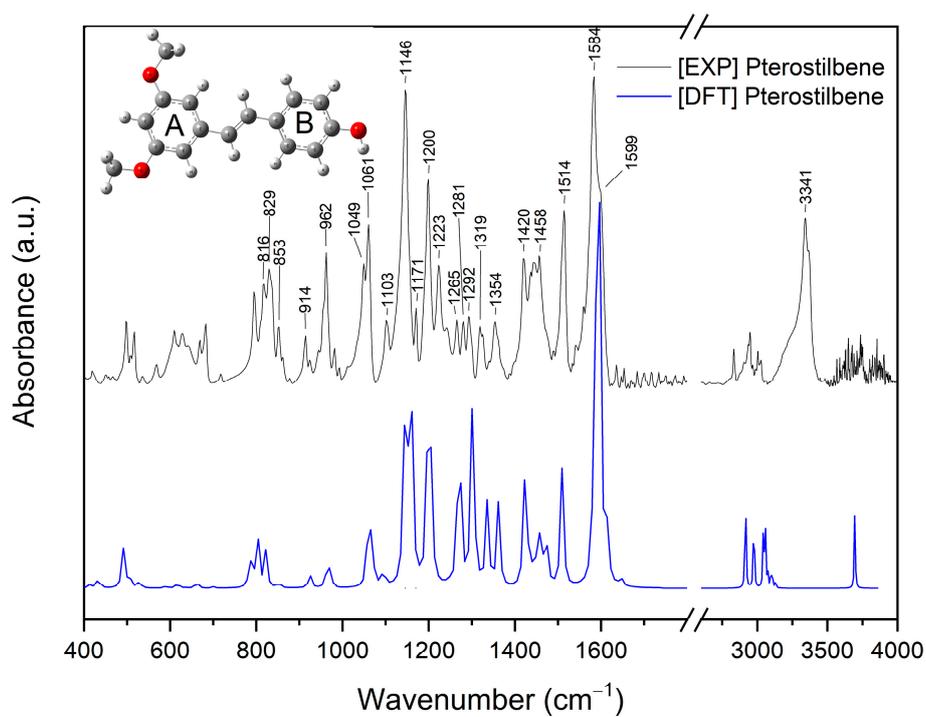


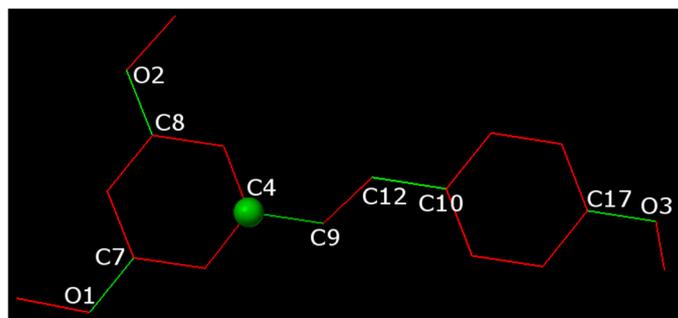
Supplementary Materials



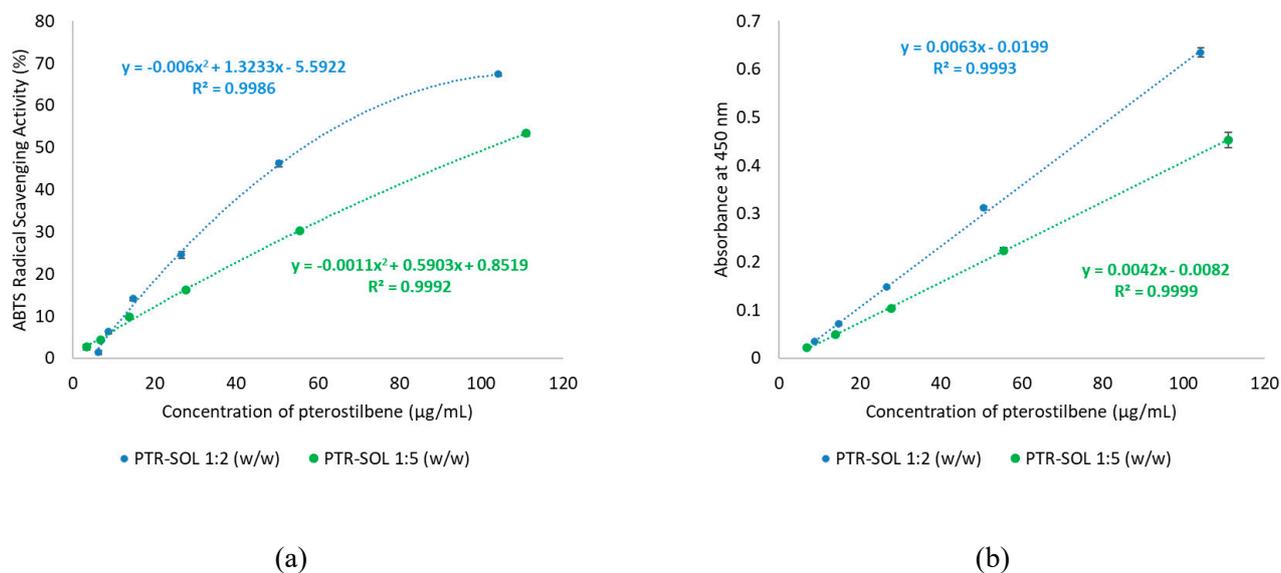
**Figure S1.** TG analysis of pterostilbene and Soluplus®.



**Figure S2.** Experimental (EXP) and calculation (DFT) IR absorption spectra of pterostilbene at room temperature.



**Figure S3.** Torsion tree of pterostilbene. The “root” of the torsion tree is shown as a green sphere. The rotatable and non-rotatable bonds are shown as a green line and red line, respectively.



**Figure S4.** Antioxidant activity of PTR-SOL 1:2 w/w and PTR-SOL 1:5 w/w (a) ABTS radical scavenging activity in relation to the pterostilbene concentration; (b) Cupric ion ( $\text{Cu}^{2+}$ ) reducing activity in relation to the pterostilbene concentration.

**Table S1.** Selected characteristic theoretical (DFT) and experimental (EXP) bonds (in  $\text{cm}^{-1}$ ) of pterostilbene (PTR). Assignments of PTR bands made based on DFT calculations with application of 6-31G(d,p) basis set.

Pterostilbene		Band assignment
DFT	EXP	
787	816	2-CHw + CHt at benzene ring B
805	829	CHt at benzene ring A + 4'-ang 6'-CHw
822	853	6-, 5'- and 6'-CHw
926	914	5' and 6'-CHt
970	962	CHw at main chain
1066	1049	C-C-Cs in benzene ring A + 2-, 4-, 6-CHb + 5-OCs
	1061	
1092	1103	2-, 4-CHb + 3-OCs
1144	1146	2- and 6-CHb
1161	1171	2'- and 5'-CHb + 4'-OHb
1205	1200	3- and 5-COCas
	1223	
1205	1265	2-, 4-, 6-CHb + CHb at main chain + 2'-, 3'-CHb
1301	1281	C-C-Cb in benzene ring A
	1292	
1335	1319	2'- 5'-, 6'-CHb + C-C-Cas in benzene ring B + 4'-OHb
1362	1354	CHw in 3- and 5-OCH <sub>3</sub> group + def. benzene ring A + CHb at main chain
1422	1420	CHw in 3- and 5-OCH <sub>3</sub> group + 2-, 4-, 6-CHb
1475	1458	CHb and CHw in 3- and 5-OCH <sub>3</sub> group
1509	1514	2'-, 3'-, 5'- and 6'-CHb + C-C-Cs in benzene ring B
1597	1584	2-, 4-, 6-CHb + C-C-Cas in benzene ring A
1614	1599	C=Cs in in benzene ring B
2919	2853	CH <sub>3</sub> s in 5-OCH <sub>3</sub> group
2972	2942	CH <sub>2</sub> s in 5-OCH <sub>3</sub> group
3041	3005	CH <sub>3</sub> s in 3-OCH <sub>3</sub> group
3059	3028	CHs at benzene ring B and at main chain
3694	3341	4'-OHs

Legend: s - stretching, t - twisting, w - wagging, def. - deformation. Carbon atom numbers and localization of benzene ring A and B were described in Figure 6a.

**Table S2.** Selected characteristic bonds (in  $\text{cm}^{-1}$ ) of pterostilbene (PTR), Soluplus<sup>®</sup> (SOL), and systems of PTR-SOL (ratio 1:2, and 1:5). Assignments of PTR bands made based on DFT calculations, and SOL based on literature.

PTR	SOL	PTR-SOL 1:2 w/w	PTR-SOL 1:5 w/w	Band assignment
816		–	–	2-CHw + CHt at benzene ring B
829		–	–	CHt at benzene ring A + 4'- ang 6'-CHw
	841	835	839	*
853		–	–	6-, 5'- and 6'-CHw
914		–	–	5' and 6'-CHt
962		↓	–	CHw at main chain
	974	–	↓	*
	1020	↓	↓	*
1049		↓	–	
1061		1063↓	–	C-C-Cs in benzene ring A + 2-, 4-, 6-CHb + 5-OCs
1103		↓	–	2-, 4-CHb + 3-OCs
1146		1148↓	1150↓	2- and 6-CHb
1171		↓	↓	2'- and 5'-CHb + 4'-OHb
	1196	1200	1200	
1200		–	–	
1223		–	–	3- and 5-COCas
	1234	↓	↓	C-O-C s in the ether groups [1]
1265		↓	–	2-, 4-, 6-CHb + CHb at main chain + 2'-, 3'-CHb
1281		↓	–	
1292		↓	–	C-C-Cb in benzene ring A
1319		–	–	2'- 5'-, 6'-CHb + C-C-Cas in benzene ring B + 4'-OHb
1354		–	–	CHw in 3- and 5-OCH <sub>3</sub> group + def. benzene ring A + CHb at main chain
1420		–	–	CHw in 3- and 5-OCH <sub>3</sub> group + 2-, 4-, 6-CHb
	1420	1423	1422	*
	1437	1443	1441	*
1458		–	–	CHb and CHw in 3- and 5-OCH <sub>3</sub> group
	1458	↓	↓	*
	1475	1477↓	1477↓	C-O-C s in the ether groups [1]
1514		↓	↓	2'-, 3'-, 5'- and 6'-CHb + C-C-Cs in benzene ring B
1584		1586↓	1587↓	2-, 4-, 6-CHb + C-C-Cas in benzene ring A
1599		+	+	C=Cs in in benzene ring B
	1634	↓	↓	C=O stretching in tertiary amide [2,3] in the caprolactam [4] or C(O)N [5]
	1734	↓	+	C=O stretching in the ester [2,3] or OC(O)CH <sub>3</sub> [5]
2833		2837↓	–	CH <sub>3</sub> s in 5-OCH <sub>3</sub> group
	2859	↓	+	C-H stretching [3]
	2926	2930	↑	aliphatic -CH stretching [3]
2949		–	–	CH <sub>2</sub> s in 5-OCH <sub>3</sub> group
3005		–	–	CH <sub>3</sub> s in 3-OCH <sub>3</sub> group
3028		–	–	CHs at benzene ring B and at main chain
3341		+	–	4'-OHs
3370		+	–	

Legend: ↓ - decrease in peak intensity, ↑ - increase in peak intensity, + - a band is observed in this range, -- a band is not observed in this range, \* - no information in the literature, s - stretching, t - twisting, w - wagging, def. – deformation. Carbon atom numbers and localization of benzene ring A and B were described in Figure 6a.

**Table S3.** Validation parameters of HPLC-DAD methods for concentration determination of pterostilbene

Pterostilbene	
Parameter	PTR dissolved in acetonitrile; Injection volume 10 $\mu$ L
Linearity range ( $\text{mg}\cdot\text{mL}^{-1}$ )	0.002-0.0006
Correlation coefficient (r)	1.00
a $\pm$ S <sub>a</sub>	16 778 474 262.6 $\pm$ 183692326.8
b $\pm$ S <sub>b</sub>	- 687 544.89 $\pm$ 227956.1827 insignificant ( $\alpha=0.05$ )
LOD ( $\text{mg}\cdot\text{mL}^{-1}$ )	0.000060
LOQ ( $\text{mg}\cdot\text{mL}^{-1}$ )	0.00020
Retention Time	4.275