



SUPPLEMENTARY MATERIAL TO
**Quantitative structure–retention relationship model for
predicting retention indices of constituents of essential oils of
Thymus vulgaris (Lamiaceae)**

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TABLE S-I. The model descriptors

Compound	log <i>RI</i>	<i>piPC02</i>	<i>ChiA_B(p)</i>	<i>SM2_B(s)</i>	<i>Mor15u</i>
α -Thujene	2.9782	3.0910	0.2770	4.0010	0.0380
β -Pinene	2.9965	3.0450	0.2760	4.0620	-0.0990
β -Myrcene	3.0026	2.8330	0.2990	4.2640	-0.2090
<i>o</i> -Cymene	3.0224	3.1570	0.2820	4.1530	-0.0340
1,8-cineole	3.0253	3.0450	0.2870	4.1650	-0.5370
<i>cis</i> - β -Terpineol	3.0370	2.9440	0.2950	4.5530	-0.3410
Terpinolene	3.0426	3.0450	0.2900	4.0490	-0.3850
Linalool	3.0481	2.8900	0.3010	4.6160	-0.3950
Isopulegol	3.0550	2.8900	0.3000	4.5510	-0.7510
Camphor	3.0652	3.1780	0.2750	4.6470	0.2260
Isoborneol	3.0785	3.0910	0.2820	4.4790	0.1290
Thymol methyl ether	3.0983	3.3140	0.2900	4.4190	0.7360
Verbenone	3.1031	3.2580	0.2710	4.6890	-0.1530
Dihydrocarvone	3.1116	2.9960	0.2920	4.7080	-0.7890
Thymol	3.1399	3.2770	0.2840	4.6130	-0.3090
Eugenol	3.1464	3.3140	0.2950	4.8060	0.8050
β -Caryophyllene	3.1667	3.4010	0.2830	4.4520	-0.5860
α -Bergamotene	3.1644	3.4340	0.2830	4.4110	-0.6540
Germacrene D	3.1787	3.2960	0.2940	4.4990	-1.2250
γ -Elemene	3.1804	3.4010	0.2820	4.5670	-0.7370
β -Bisabolene	3.1867	3.3320	0.2930	4.4910	-0.8340
δ -cadinene	3.1906	3.4340	0.2850	4.3990	-1.2070
Caryophyllene oxide	3.2009	3.4970	0.2790	4.5700	-1.0600
Spathulenol	3.2063	3.5260	0.2750	4.7900	-0.3710
Aromadendrene oxide	3.2101	3.5260	0.2780	4.4750	-0.8480
Muurolol	3.2177	3.4010	0.2880	4.7500	-1.3860
Bisabolol	3.2201	3.3670	0.2950	4.7810	-1.0370

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