**SUPPLEMENTARY MATERIAL**

**Quantitative structure-retention relationship model for predicting retention indices of constituents of essential oils of *Thymus vulgaris Lamiaceae***

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Table S-II.The model descriptors

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Nom** | **log IR** | **piPC02** | **ChiA\_B(p)** | **SM2\_B(s)** | **Mor15u** |
| alpha-Thujene | 2.9782 | 3.0910 | 0.2770 | 4.0010 | 0.0380 |
| beta-Pinene | 2.9965 | 3.0450 | 0.2760 | 4.0620 | -0.0990 |
| beta-Myrcene | 3.0026 | 2.8330 | 0.2990 | 4.2640 | -0.2090 |
| o-Cymene | 3.0224 | 3.1570 | 0.2820 | 4.1530 | -0.0340 |
| 1,8-cineole | 3.0253 | 3.0450 | 0.2870 | 4.1650 | -0.5370 |
| cis-beta-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 |
| beta-Caryophyllene | 3.1667 | 3.4010 | 0.2830 | 4.4520 | -0.5860 |
| alpha-Bergamotene | 3.1644 | 3.4340 | 0.2830 | 4.4110 | -0.6540 |
| Germacrene D | 3.1787 | 3.2960 | 0.2940 | 4.4990 | -1.2250 |
| gamma-Elemene | 3.1804 | 3.4010 | 0.2820 | 4.5670 | -0.7370 |
| beta-Bisabolene | 3.1867 | 3.3320 | 0.2930 | 4.4910 | -0.8340 |
| Delta-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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