[**Exploring 3D-QSPR models of human skin permeability for a diverse dataset of chemical compounds**](javascript:void(0))

Soheila Rezaei1, 2, Hassan Behnejad1, Jahan. B Ghasemi2[[1]](#footnote-1)

*1Department of Physical Chemistry, School of Chemistry, University College of Science, University of Tehran, Tehran 14155, Iran.*

*2Department of Analytical Chemistry, School of Chemistry, University College of Science, University of Tehran, Tehran 14155, Iran.*

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| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Table 1S.** Name of chemical compounds and experimental calculation skin permeability, compared with Predicted Results for five models | | | | | | | | |
| **Train set** | | | **Pred.** **Pka(cm/s)** | | | | | |
| **Compounds** | **Exp.**  **Pka(cm/s)** | **MW** | **PLS** | **FFD-PLS** | **GA-PLS** | **SPA-PLS** | **GA-SVM** | **GA-SVM** |
| 1,1,1-trichloropropanone | 5.18 | 161.4 | 4.5 | 4.95 | 4.64 | 5.06 | 4.81 | 5.07 |
| 1,1-dichloropropanone | 4.92 | 126.97 | 4.44 | 5.04 | 4.76 | 4.89 | 5.03 | 5.04 |
| 1-hexyl-2-pyrrolidone | 5.21 | 169.3 | 5.03 | 5.18 | 5.34 | 5.46 | 5.32 | 5.3 |
| 1-methoxy-2-propanol | 6.40 | 90.14 | 6.32 | 6.14 | 6.18 | 6.01 | 6.28 | 6.29 |
| 1-octyl-2-azacycloheptanone | 4.84 | 225.42 | 5.14 | 5.34 | 5.3 | 5.35 | 5.31 | 5.46 |
| 2,4,6-trichlorophenol | 4.78 | 197.44 | 5.38 | 5.56 | 4.91 | 4.97 | 4.89 | 4.89 |
| 2,4-dichlorophenol | 6.74 | 163 | 5.26 | 7.1 | 4.92 | 4.96 | 4.82 | 4.89 |
| 2-amino-4-nitrophenol | 5.90 | 154.14 | 6.86 | 5.13 | 6.94 | 6.65 | 6.85 | 6.7 |
| 2-butanone | 5.04 | 72.12 | 4.74 | 5.58 | 4.84 | 4.98 | 5.22 | 5.3 |
| 2-chlorophenol | 7.16 | 128.56 | 5.64 | 6.1 | 5.6 | 5.49 | 5.44 | 5.15 |
| 2-ethoxyethanol | 8.03 | 90.14 | 6.71 | 6.65 | 6.72 | 6.89 | 7.04 | 7.05 |
| 2-hydroxypropyl nicotinate | 4.76 | 181.21 | 7.22 | 5.39 | 7.02 | 7.27 | 6.45 | 7.67 |
| 2-naphthol | 6.86 | 144.18 | 5.21 | 6.94 | 5.07 | 5.35 | 5.1 | 5.33 |
| 2-nitro-p-phenylenediamine | 5.28 | 153.16 | 6.76 | 5.43 | 6.88 | 6.92 | 6.75 | 6.75 |
| 2-phenylethanol | 5.00 | 122.18 | 5.17 | 5.31 | 5.06 | 4.99 | 5.17 | 5.17 |
| 3,4-xylenol | 5.81 | 122.18 | 5.18 | 7.1 | 5.09 | 5.4 | 5.02 | 5.19 |
| 3-nitrophenol | 6.11 | 139.12 | 6.87 | 7.12 | 6.6 | 6.38 | 6.36 | 5.92 |
| 4-amino-2-nitrophenol | 5.00 | 154.14 | 6.54 | 5.44 | 6.45 | 6.23 | 6.25 | 6.12 |
| 4-bromophenol | 4.65 | 173.01 | 5.17 | 5.34 | 5.17 | 4.97 | 5.11 | 4.73 |
| 4-chloro-3,5-dimethylphenol | 6.23 | 156.62 | 5.09 | 5.55 | 5.1 | 5.4 | 5.05 | 5.08 |
| 4-chloro-m-phenylenediamine | 5.73 | 142.6 | 6.38 | 5.34 | 6.6 | 6.1 | 6.34 | 6.12 |
| 4-chlorophenol | 6.26 | 128.56 | 5.04 | 6.12 | 4.87 | 4.86 | 4.9 | 4.89 |
| 4-cyanophenol | 6.90 | 119.13 | 4.73 | 6.45 | 4.81 | 5.01 | 5.16 | 5.62 |
| 4-hydroxybenzyl alcohol | 6.16 | 124.15 | 5.79 | 6.6 | 5.73 | 6.02 | 5.79 | 6.22 |
| 4-hydroxyphenylacetamide | 5.81 | 151.18 | 6.55 | 7.01 | 7.03 | 7.11 | 6.79 | 7.01 |
| 4-hydroxyphenylacetic acid | 5.38 | 152.16 | 6.42 | 5.39 | 6.53 | 6.91 | 6.28 | 6.83 |
| 4-nitrophenol | 7.30 | 139.12 | 6.73 | 6.77 | 6.6 | 6.39 | 6.44 | 5.92 |
| 4-propoxyphenol | 6.08 | 152.21 | 5.02 | 6.1 | 4.78 | 5.07 | 4.98 | 5.27 |
| 5-fluorouracil | 6.20 | 130.09 | 7.2 | 7 | 7.3 | 7.79 | 7.34 | 7.41 |
| acetic acid | 5.22 | 60.06 | 6.14 | 5.33 | 6.39 | 6.63 | 6.52 | 6.44 |
| acetylsalicylic acid | 4.69 | 180.17 | 6.4 | 5.05 | 6.2 | 5.72 | 5.84 | 5.81 |
| amylobarbital | 4.79 | 226.31 | 6.91 | 5.13 | 7.16 | 6.12 | 6.77 | 6.31 |
| Aniline | 4.35 | 93.14 | 6.11 | 5 | 5.89 | 5.82 | 5.39 | 5.33 |
| Anisole | 7.46 | 108.15 | 4.72 | 6.96 | 4.8 | 4.66 | 4.91 | 4.63 |
| aspartic acid | 5.34 | 133.12 | 8 | 5.54 | 7.67 | 7.39 | 7.63 | 7.7 |
| Atenolol | 5.35 | 266.38 | 7.18 | 5.71 | 7.07 | 6.97 | 7.24 | 7.24 |
| Barbital | 7.15 | 184.22 | 7.21 | 7.94 | 7.3 | 7.43 | 7.03 | 7.4 |
| benzaldehyde | 6.30 | 106.13 | 4.72 | 6.96 | 4.77 | 4.59 | 4.84 | 4.68 |
| Benzene | 6.35 | 78.12 | 5.3 | 6.22 | 5.24 | 5.13 | 4.89 | 4.69 |
| benzenetriol | 4.35 | 126.12 | 7.66 | 4.53 | 7.4 | 7.69 | 7.53 | 7.52 |
| benzyl alcohol | 7.27 | 108.15 | 5.31 | 7.04 | 5.1 | 5.24 | 5.06 | 5.45 |
| benzyl nicotinate | 6.00 | 213.25 | 6.21 | 5.99 | 6.12 | 5.92 | 5.77 | 5.46 |
| betamethasone | 5.34 | 392.51 | 7.77 | 5.54 | 7.93 | 7.61 | 7.72 | 7.26 |
| Betaxolol | 6.41 | 307.48 | 7.25 | 6.11 | 7.45 | 7.05 | 6.87 | 6.41 |
| bromochloroacetic acid | 5.97 | 173.39 | 6.29 | 6.27 | 6.28 | 6.62 | 6.35 | 6.46 |
| bromochloroacetonitrile | 6.51 | 154.39 | 4.44 | 6.28 | 4.3 | 4.04 | 4.34 | 4.32 |
| bromodichloromethane | 4.56 | 163.82 | 4.68 | 4.64 | 4.66 | 4.58 | 4.47 | 4.27 |
| butobarbital | 4.35 | 212.28 | 7.18 | 4.74 | 7.37 | 7.34 | 7.16 | 7.38 |
| butoxyethanol | 6.21 | 118.2 | 5.68 | 5.54 | 5.93 | 5.76 | 6.11 | 5.89 |
| butyl nicotinate | 7.87 | 179.24 | 5.16 | 6.6 | 5.31 | 4.92 | 5.45 | 5.42 |
| butyl p-aminobenzoate | 7.68 | 193.27 | 4.58 | 7.69 | 4.18 | 4.72 | 4.72 | 4.72 |
| butyric acid | 5.60 | 88.12 | 6.22 | 5.07 | 6.25 | 6.19 | 6.3 | 6.3 |
| Catechol | 7.75 | 110.12 | 6.3 | 8.18 | 6.4 | 5.87 | 6.18 | 5.96 |
| chloral hydrate | 6.14 | 165.4 | 6.04 | 6.37 | 5.86 | 5.57 | 5.86 | 5.86 |
| chloroacetic acid | 4.33 | 94.5 | 6.4 | 4.54 | 5.98 | 6.1 | 6.13 | 6.36 |
| chloroacetonitrile | 6.28 | 75.50 | 4.64 | 6.31 | 4.65 | 4.44 | 4.65 | 4.67 |
| chlorodibromomethane | 4.38 | 208.27 | 4.71 | 4.5 | 4.75 | 4.69 | 4.47 | 4.37 |
| Chloroform | 7.00 | 119.37 | 4.64 | 6.43 | 4.65 | 4.58 | 4.42 | 4.24 |
| chlorpheniramine | 7.05 | 274.82 | 6.04 | 6 | 6.23 | 5.63 | 6.1 | 6.1 |
| codeine | 5.95 | 299.4 | 7.32 | 5.13 | 7.28 | 7.22 | 7.06 | 7.76 |
| cortexolone | 5.78 | 346.51 | 7.31 | 5.92 | 7.42 | 7.24 | 7.56 | 7.47 |
| corticosterone | 6.00 | 346.51 | 7.27 | 5.86 | 7.15 | 7.32 | 7.24 | 7.19 |
| coumarin | 6.28 | 146.15 | 4.76 | 5.69 | 5.03 | 5.34 | 5.1 | 5.45 |
| cyclobarbitone | 5.35 | 236.3 | 7.3 | 5.34 | 7.33 | 7.31 | 6.9 | 6.76 |
| dexamethasone | 5.26 | 392.51 | 8.08 | 5.79 | 7.98 | 7.99 | 7.86 | 7.86 |
| dibromoacetic acid | 6.54 | 217.84 | 6.26 | 5.93 | 6.23 | 5.96 | 6.07 | 6.25 |
| dibromoacetonitrile | 5.68 | 198.84 | 3.99 | 6.3 | 4.1 | 4.19 | 4.43 | 4.38 |
| dichloroacetic acid | 6.08 | 128.94 | 6.18 | 5.6 | 6.18 | 6.48 | 6.24 | 6.17 |
| dichloroacetonitrile | 6.19 | 109.94 | 4.29 | 6.18 | 4.19 | 4.07 | 4.27 | 4.27 |
| diclofenac | 5.33 | 296.16 | 6.74 | 6.36 | 6.72 | 6.64 | 6.59 | 6.89 |
| diethylene glycol mono n-butyl ether acetate | 6.48 | 204.3 | 5.89 | 7.56 | 5.9 | 6.2 | 6.14 | 6.94 |
| dimethylethylamine | 6.94 | 73.16 | 4.99 | 7.24 | 5.33 | 5.11 | 5.4 | 5.12 |
| ephedrine | 7.03 | 165.26 | 5.84 | 6.4 | 6.19 | 5.39 | 5.89 | 5.71 |
| estradiol | 5.48 | 272.42 | 5.66 | 6.22 | 5.41 | 5.82 | 5.79 | 6.02 |
| estrone | 7.81 | 270.4 | 6 | 7.1 | 5.85 | 6.56 | 6.11 | 6.11 |
| ethacrynic acid | 7.19 | 303.15 | 7.02 | 7.97 | 6.86 | 6.92 | 7.21 | 7.27 |
| ethanol | 6.30 | 46.08 | 6.33 | 7.03 | 6.43 | 6.36 | 6.39 | 6.17 |
| ethyl ether | 6.76 | 74.14 | 5.5 | 7.39 | 5.48 | 5.5 | 5.73 | 5.46 |
| ethyl nicotinate | 5.30 | 151.18 | 5.48 | 7.12 | 5.7 | 5.19 | 5.69 | 5.63 |
| ethyl p-aminobenzoate | 5.82 | 165.21 | 4.9 | 6.91 | 5.27 | 5.31 | 5.15 | 5.15 |
| ethylene glycol mono isopropyle ether | 7.23 | 104.17 | 6.27 | 6.94 | 6.28 | 6.39 | 6.44 | 6.42 |
| ethylene glycol mono n-propyl ether | 6.61 | 104.17 | 5.94 | 7.28 | 6.29 | 6.23 | 6.46 | 6.5 |
| etodolac | 6.51 | 287.39 | 6.47 | 5.96 | 6.41 | 5.99 | 6.33 | 5.79 |
| fentanyl | 6.78 | 336.52 | 5.98 | 6.84 | 5.77 | 5.76 | 5.97 | 5.97 |
| flufenamic acid | 6.55 | 281.25 | 6.38 | 7.13 | 6.54 | 6.47 | 6.3 | 6.3 |
| flurbiprofen | 7.22 | 244.28 | 5.97 | 6.81 | 5.96 | 5.88 | 6.05 | 5.44 |
| flurbiprofen glucoside | 4.84 | 406.44 | 7.38 | 5.32 | 7.21 | 6.98 | 7.08 | 6.59 |
| flurbiprofen mannoside | 6.15 | 406.44 | 7.37 | 6.61 | 7.25 | 7.05 | 7.05 | 7.05 |
| griseofulvin | 7.59 | 352.79 | 6.42 | 6.92 | 6.45 | 6.76 | 6.33 | 6.55 |
| haloperidol | 8.38 | 375.9 | 6.84 | 7.63 | 6.74 | 6.63 | 6.92 | 6.92 |
| hexanoic acid | 6.48 | 116.18 | 5.73 | 6.96 | 5.69 | 5.72 | 5.61 | 5.59 |
| histidine | 6.08 | 155.18 | 7.19 | 6.08 | 7.19 | 7.6 | 7.07 | 7.7 |
| hydrocortisone | 5.99 | 362.51 | 7.58 | 5.51 | 7.64 | 7.92 | 7.64 | 7.74 |
| hydrocortisone hemipimelate | 7.33 | 504.68 | 6.56 | 7.9 | 6.58 | 6.32 | 6.56 | 6.41 |
| hydrocortisone hemisuccinate | 7.94 | 462.59 | 7.13 | 7.11 | 7.41 | 6.94 | 7.14 | 6.87 |
| hydrocortisone hexanoate | 5.99 | 460.67 | 6.15 | 5.7 | 6.08 | 6.1 | 6.45 | 5.44 |
| hydrocortisone methylpimelate | 5.26 | 518.71 | 6.1 | 6.19 | 6.22 | 6.01 | 6.61 | 5.93 |
| hydrocortisone methylsuccinate | 5.19 | 476.62 | 6.36 | 5.84 | 6.61 | 6.47 | 6.79 | 7.04 |
| hydrocortisone N,N-dimethylsuccinate | 6.64 | 489.67 | 7.1 | 6.77 | 7.53 | 7.33 | 7.62 | 7.41 |
| hydrocortisone pimelamate | 6.10 | 503.7 | 6.71 | 6.52 | 6.31 | 6.85 | 6.5 | 6.52 |
| hydroquinone | 4.70 | 110.12 | 6.08 | 5.65 | 6.08 | 6.45 | 6.17 | 6.4 |
| hydroxypregnenolone | 5.31 | 332.53 | 7.35 | 5.68 | 7.19 | 7.35 | 6.89 | 6.86 |
| hydroxyprogesterone | 5.54 | 330.51 | 6.98 | 5.46 | 6.85 | 6.9 | 6.87 | 6.89 |
| ibuprofen mannoside | 5.78 | 368.47 | 7.12 | 5.47 | 6.97 | 6.47 | 6.91 | 6.44 |
| indomethacin | 5.36 | 357.81 | 6.96 | 5.5 | 6.61 | 7 | 6.95 | 7.11 |
| iso-thymol | 6.90 | 150.24 | 5.22 | 5.5 | 5.16 | 5.2 | 4.95 | 5.03 |
| ketoprofen | 8.96 | 254.3 | 6.81 | 7.79 | 6.64 | 6.67 | 6.3 | 6.26 |
| ketoprofen mannoside | 5.31 | 416.46 | 7.34 | 5.38 | 7.46 | 7.62 | 7.36 | 7.48 |
| L-alanyl-L-tryptophan | 5.64 | 275.34 | 8.07 | 5.68 | 8.11 | 7.74 | 8.27 | 8.27 |
| levodopa | 6.07 | 197.21 | 7.6 | 6.48 | 7.74 | 7.76 | 7.63 | 7.63 |
| levosimendan | 7.37 | 280.32 | 6.8 | 6.57 | 6.42 | 6 | 6.59 | 6.59 |
| lidocaine | 4.67 | 234.38 | 6.67 | 5.42 | 6.88 | 6.07 | 6.19 | 5.97 |
| linolenic acid | 7.18 | 278.48 | 5.98 | 5.51 | 5.88 | 6 | 5.88 | 5.98 |
| lysine | 7.91 | 146.22 | 7.56 | 8.04 | 7.59 | 7.95 | 7.47 | 7.44 |
| mannitol | 6.38 | 182.2 | 7.54 | 6 | 7.65 | 7.82 | 7.63 | 7.83 |
| meperidine | 6.05 | 247.37 | 5.92 | 6.5 | 5.97 | 5.5 | 5.88 | 5.88 |
| methanol | 5.41 | 32.05 | 6.67 | 6.19 | 6.48 | 6.61 | 6.71 | 6.78 |
| methyl 4-hydroxyphenylacetate | 8.37 | 166.19 | 5.41 | 8.08 | 5.34 | 5.21 | 5.37 | 5.15 |
| methyl p-aminobenzoate | 6.63 | 151.18 | 5.19 | 6.33 | 5.44 | 5.59 | 5.3 | 5.21 |
| metoprolol | 6.21 | 267.41 | 6.53 | 5.88 | 6.66 | 6.86 | 6.75 | 6.75 |
| naproxen | 3.64 | 230.28 | 6.31 | 4.84 | 6.16 | 6.57 | 6.06 | 6.21 |
| naproxen glucoside | 8.96 | 392.44 | 7.4 | 8.3 | 7.43 | 7.54 | 7.6 | 7.78 |
| naproxen mannoside | 8.25 | 392.44 | 7.54 | 7.32 | 7.67 | 8 | 7.59 | 7.81 |
| n-butanol | 8.56 | 74.14 | 5.96 | 6.2 | 5.63 | 5.98 | 5.45 | 5.55 |
| n-decanol | 4.83 | 158.32 | 5.09 | 5.94 | 4.78 | 4.91 | 4.81 | 4.81 |
| n-hexyl nicotinate | 7.08 | 207.3 | 5.55 | 6.63 | 5.64 | 5.64 | 5.42 | 5.42 |
| nicotine | 6.55 | 162.26 | 5.6 | 5.9 | 5.51 | 5.82 | 5.45 | 5.65 |
| nimesulide | 5.68 | 308.34 | 6.03 | 6.13 | 6.3 | 6.18 | 6.01 | 6.44 |
| n-nonanol | 6.41 | 144.29 | 5.17 | 6.21 | 4.99 | 4.86 | 4.89 | 4.81 |
| n-pentanol | 7.05 | 88.17 | 5.44 | 5.93 | 5.51 | 5.98 | 5.71 | 6.02 |
| o-cresol | 7.38 | 108.15 | 5.54 | 6.61 | 5.44 | 5.67 | 5.36 | 5.47 |
| octylparaben | 5.62 | 250.37 | 5.82 | 5.91 | 5.99 | 5.84 | 5.72 | 5.7 |
| o-phenylenediamine | 6.30 | 108.16 | 6.56 | 6.05 | 6.49 | 6.39 | 5.99 | 6.6 |
| ouabain | 5.26 | 584.73 | 7.48 | 6.19 | 8 | 8.51 | 8.45 | 8.85 |
| oxprenolol | 6.60 | 265.39 | 6.48 | 6.45 | 6.55 | 5.85 | 6.46 | 6.26 |
| p-cresol | 6.02 | 108.15 | 5.26 | 6.62 | 5.35 | 5.28 | 5.29 | 5.15 |
| p-ethylphenol | 8.38 | 122.18 | 5.06 | 6.36 | 4.74 | 4.91 | 4.97 | 5.12 |
| phenol | 6.94 | 94.12 | 5.77 | 6.51 | 5.66 | 5.59 | 5.61 | 5.62 |
| phloroglucinol | 5.33 | 126.12 | 6.74 | 5.88 | 6.54 | 6.33 | 6.35 | 6.18 |
| piroxicam | 7.73 | 331.38 | 6.92 | 6.61 | 6.85 | 6.76 | 6.54 | 7.26 |
| p-n-butylphenol | 5.80 | 150.24 | 4.67 | 6.35 | 4.43 | 5.05 | 4.78 | 4.78 |
| p-phenylenediamine | 5.37 | 108.16 | 6.39 | 6 | 6.52 | 6.6 | 6.31 | 6.58 |
| prednisolone | 5.23 | 360.49 | 8.04 | 6.19 | 7.87 | 7.97 | 7.8 | 8.02 |
| pregnenolone | 6.03 | 316.53 | 6.4 | 6.02 | 6.51 | 6.82 | 6.49 | 6.27 |
| progesterone | 5.00 | 314.51 | 5.91 | 6.17 | 6.12 | 6.54 | 6.27 | 6.27 |
| propranolol | 7.31 | 259.38 | 6.83 | 6.14 | 6.87 | 6.12 | 6.58 | 6.16 |
| propylparaben | 8.59 | 180.22 | 5.43 | 6.4 | 5.61 | 5.97 | 5.52 | 5.52 |
| pyrogallol | 5.05 | 126.12 | 6.66 | 5.98 | 6.45 | 6.39 | 6.35 | 6.43 |
| raffinose | 5.28 | 504.5 | 7.65 | 6.01 | 7.9 | 8.01 | 8.26 | 8.39 |
| ranitidine | 7.30 | 314.46 | 7.16 | 6.09 | 7.03 | 6.86 | 7.23 | 7.5 |
| resorcinol | 7.98 | 110.12 | 6.66 | 6.36 | 6.56 | 6.53 | 6.52 | 6.69 |
| scopolamine | 6.44 | 303.39 | 6.99 | 6.04 | 6.89 | 6.9 | 6.38 | 7.19 |
| sufentanil | 5.18 | 386.61 | 6.42 | 6.18 | 6.21 | 6.71 | 6.18 | 6.35 |
| testosterone | 6.44 | 288.47 | 5.78 | 6.11 | 5.85 | 5.75 | 6.1 | 6.03 |
| theophylline | 4.68 | 180.19 | 6.07 | 6 | 6.41 | 6.39 | 6.06 | 6.46 |
| toluene | 6.90 | 92.15 | 4.95 | 6.43 | 4.75 | 4.34 | 4.49 | 4.07 |
| triamcinolone | 5.44 | 394.48 | 8.3 | 6.18 | 8.27 | 8.42 | 8.24 | 8.53 |
| triamcinolone acetonide | 8.24 | 434.55 | 7.68 | 6.5 | 7.72 | 8.02 | 7.71 | 8.14 |
| triglycol nicotinate | 6.28 | 255.3 | 7.38 | 6.23 | 7.99 | 8.42 | 7.73 | 8.45 |
| Test Set | | | | | | | | |
| 1-octyl-2-pyrrolidone | 4.78 | 197.36 | 4.77 | 5.67 | 5.61 | 4.7 | 4.75 | 5.58 |
| 4-chloro-3-methylphenol | 5 | 142.59 | 5.11 | 5.4 | 5.22 | 5.15 | 5.1 | 4.93 |
| 5-aminolevulinic acid | 5.7 | 131.15 | 7.2 | 6.37 | 7.87 | 7.33 | 7.24 | 8 |
| Acyclovir | 7.59 | 225.24 | 7.97 | 7.66 | 7.12 | 8.1 | 7.81 | 6.92 |
| Aldosterone | 7.35 | 360.49 | 7.07 | 7.19 | 7.34 | 6.87 | 6.92 | 7.37 |
| aminopyrine | 7.51 | 231.33 | 5.37 | 6.82 | 5.35 | 5.88 | 5.73 | 5.43 |
| benzoic acid | 4.3 | 122.13 | 5.88 | 4.75 | 5.59 | 5.44 | 5.31 | 5.44 |
| betamethasone 17-valerate | 4.61 | 476.64 | 7.61 | 5.91 | 7.73 | 7.2 | 7.14 | 7.15 |
| bromoacetic acid | 6.07 | 138.95 | 6.3 | 6.08 | 6.01 | 5.96 | 6.09 | 5.96 |
| Bromoform | 4.26 | 252.72 | 4.87 | 4.75 | 4.84 | 4.83 | 4.56 | 4.55 |
| butyl paraben | 7.08 | O-N | 5.1 | 7.64 | 5.55 | 4.98 | 5.38 | 5.53 |
| Caffeine | 6.65 | 194.22 | 5.31 | 6.96 | 5.33 | 5.61 | 5.39 | 7.46 |
| cortexone | 6.05 | 330.51 | 7.59 | 6.1 | 7.7 | 7.46 | 7.49 | 6.98 |
| cortisone | 7.38 | 360.49 | 7.68 | 6.72 | 7.74 | 7.71 | 7.6 | 7.93 |
| cytarabine | 5.74 | 243.25 | 6.79 | 5.62 | 6.92 | 7.23 | 7.18 | 8.76 |
| diazinon | 6.91 | 304.39 | 4.65 | 5.96 | 5.2 | 4.89 | 4.96 | 5.16 |
| dipropylene glycol mono methyl ether | 6.44 | 148.23 | 6.32 | 5.97 | 6.26 | 6.39 | 6.24 | 6.18 |
| ethylene glycol mono methyl ether acetate | 7.73 | 118.15 | 5.31 | 6.72 | 5.44 | 5.51 | 5.62 | 5.87 |
| famotidine | 6.78 | 337.51 | 7.73 | 6.98 | 7.49 | 7.68 | 7.8 | 7.71 |
| heptanoic acid | 7.74 | 130.21 | 5.7 | 7.64 | 5.74 | 5.29 | 5.52 | 5.19 |
| hydrocortisone hydroxyhexanoate | 6.86 | 476.67 | 6.93 | 5.48 | 7.05 | 7.06 | 7.17 | 6.85 |
| hydrocortisone propionate | 7.89 | 418.58 | 7.58 | 7.44 | 7.49 | 7.35 | 7.33 | 6.61 |
| hydrocortisone succinamate | 7.7 | 461.61 | 7.07 | 7.24 | 7.42 | 7.46 | 7.18 | 7.44 |
| hydromorphone | 5.66 | 285.37 | 6.97 | 5.3 | 6.75 | 7.13 | 6.55 | 7.44 |
| ibuprofen | 6.55 | 206.31 | 5.79 | 5.34 | 6.39 | 5.9 | 5.82 | 6.02 |
| ibuprofen glucoside | 4.78 | 368.47 | 6.95 | 5.39 | 6.42 | 6.66 | 6.94 | 6.41 |
| isoquinoline | 5.59 | 129.17 | 4.95 | 6.24 | 5.03 | 5.3 | 5.13 | 5.21 |
| ketoprofen glucoside | 6.37 | 416.46 | 8.27 | 6.48 | 7.91 | 7.91 | 7.72 | 7.5 |
| ketorolac | 5.01 | 255.29 | 7.02 | 5.33 | 7.16 | 6.52 | 6.44 | 6.86 |
| m-cresol | 6.38 | 108.15 | 5.4 | 5.47 | 5.75 | 5.33 | 5.41 | 5.52 |
| methyl 4-hydroxybenzoate | 6.37 | 152.16 | 5.71 | 6.47 | 5.62 | 5.63 | 5.45 | 5.56 |
| methyl nicotinate | 7.61 | 137.15 | 5.23 | 6.2 | 4.99 | 5.55 | 5.61 | 5.32 |
| methyl salicylate | 7.86 | 152.16 | 6.25 | 6.83 | 6.11 | 6.09 | 5.87 | 5.9 |
| methyltriglycol nicotinate | 5.82 | 269.33 | 6.97 | 5.98 | 7.16 | 7.23 | 7.07 | 6.9 |
| morphine | 7.12 | 285.37 | 7.08 | 5.62 | 6.87 | 7.29 | 7.15 | 8.95 |
| n-heptanol | 5 | 116.23 | 5.22 | 5.97 | 4.96 | 5.34 | 5.17 | 4.9 |
| n-hexanol | 7.71 | 102.2 | 5.38 | 6.5 | 5.74 | 5.69 | 5.77 | 5.84 |
| nicorandil | 8.08 | 211.2 | 6.46 | 6.54 | 7.34 | 6.59 | 6.37 | 6.38 |
| nizatidine | 6.5 | 331.52 | 7 | 6.62 | 8.1 | 7.61 | 7.38 | 7.99 |
| n-octanol | 4.23 | 130.26 | 4.86 | 5.82 | 5.26 | 5.04 | 5.11 | 5.37 |
| nortriptyline | 4.54 | 263.41 | 6.59 | 6.19 | 6.44 | 6.48 | 6.42 | 6.2 |
| n-propanol | 6.9 | 60.11 | 5.77 | 6.61 | 5.84 | 5.92 | 5.96 | 5.67 |
| octanoic acid | 8.86 | 144.24 | 5.3 | 6.56 | 5.37 | 5.07 | 5.55 | 5.68 |
| oleic acid | 7.65 | 282.52 | 6.43 | 6.23 | 6.52 | 6.18 | 6.19 | 6.43 |
| o-t-butylphenol | 8.35 | 150.24 | 5.86 | 6.67 | 6.12 | 6.14 | 5.75 | 5.82 |
| pentanoic acid | 8.14 | 102.15 | 6.01 | 6.55 | 5.84 | 6.03 | 6.05 | 6.03 |
| phenobarbital | 5.5 | 232.26 | 6.99 | 6.19 | 6.43 | 7.14 | 6.89 | 6.86 |
| salicylic acid | 4.59 | 138.13 | 6.22 | 5.99 | 5.64 | 6.08 | 5.83 | 5.74 |
| sucrose | 6.48 | 342.34 | 7.6 | 6 | 7.8 | 7.7 | 7.74 | 8.35 |
| thymol | 6.11 | 150.24 | 5.44 | 6.18 | 5.43 | 5.45 | 5.32 | 5.26 |
| trichloroacetic acid | 4.86 | 163.38 | 5.84 | 5.99 | 5.43 | 5.37 | 5.43 | 5.82 |
| urea | 7.45 | 60.07 | 6.11 | 6.21 | 6.45 | 6.61 | 7.07 | 6.62 |

1. Corresponding author. Tel.: +98 21 61112726; Email address:[*Jahan.ghasemi@ut.ac.ir*](mailto:Jahan.ghasemi@ut.ac.ir) *(J.B. Ghasemi).* [↑](#footnote-ref-1)