

Table S1. Biological properties of APIs (n = 129).

| API | B1 | B2 | B3 | BB _{vivo} | CNS+/- | LactMed | LLL H | log U/D 7.2 | M/P | M/P _{code} | PB | PB _{code} | PhCharge |
|----------------------|-------|-------|--------|--------------------|--------|---------|-------|----------------|-------|---------------------|-------|--------------------|----------|
| acebutolol | 0.09 | -0.86 | -0.83 | | 0 | 2 | 3 | -2.2 | 9.65 | 4 | 0.26 | 5 | 1 |
| aceclofenac | -0.44 | -0.66 | 1.11 | | | | | -4.6 | | | 0.99 | 1 | -1 |
| acenocumarol | -1.07 | -1.20 | 0.68 | | 1 | 1 | | -2.7 | | | 0.987 | 1 | -1 |
| acetylsalicylic acid | -4.75 | -0.47 | -13.67 | | 1 | 2 | 3 | -3.72 | 1.08 | 3 | 0.995 | 1 | -1 |
| aciclovir | -1.71 | -1.21 | -1.39 | -0.836 | | 1 | 2 | -2.09 | 2.35 | 4 | 0.21 | 5 | 0 |
| alprazolam | 0.29 | -0.06 | 1.68 | 0.019 | 1 | 1 | 3 | -4.83 | 0.18 | 1 | 0.8 | 4 | 0 |
| amiodarone | 0.60 | -0.14 | 0.84 | | 1 | 2 | | -2.17 | 8.8 | 4 | 0.96 | 2 | 1 |
| amlodipine | -0.09 | -1.05 | -1.42 | | 0 | 1 | 3 | -1.77 | | | 0.975 | 2 | 1 |
| amoxicillin | -2.23 | -1.99 | -0.74 | | 0 | 1 | 1 | -4.76 | 0.028 | 1 | 0.2 | 5 | 0 |
| astemizol | -0.31 | -0.05 | -0.31 | | 1 | | | -1.48 | 4.4 | 4 | 0.967 | 2 | 1 |
| atorvastatin | 0.37 | -1.24 | 0.11 | | 0 | | 3 | -2.91 | | | 0.98 | 1 | -1 |
| atropine | -0.34 | -0.25 | 0.19 | -0.060 | 1 | | 3 | -2.78 | | | 0.18 | 5 | 1 |
| azithromycin | 0.51 | -2.33 | 0.56 | | 0 | 1 | 2 | -1.39 | | | 0.29 | 5 | 2 |
| betaxolol | 0.29 | -0.26 | -0.17 | | 0 | 2 | 3 | -2.23 | 2.75 | 4 | 0.5 | 5 | 1 |
| bilastine | -0.70 | -0.71 | 0.39 | | | | | -0.61 | | | 0.87 | 3 | 0 |
| biperiden | 0.55 | 0.17 | 0.69 | | 1 | | | -2.06 | | | 0.6 | 4 | 1 |
| bisoprolol | -0.42 | -0.41 | 0.40 | | 0 | | 3 | -2.22 | | | 0.3 | 5 | 1 |
| bromazepam | -0.27 | -0.32 | 0.63 | | 1 | | | -4.19 | | | 0.7 | 4 | 0 |
| bromocriptine | -0.93 | -1.34 | 1.58 | -1.100 | 0 | 0 | | -0.76 | | | 0.93 | 3 | 0 |
| buspirone | -0.71 | -0.57 | -0.08 | 0.480 | 1 | 1 | 3 | -0.52 | | | 0.95 | 2 | 1 |
| caffeine | -0.81 | -0.31 | -1.20 | -0.022 | 1 | 2 | 2 | -6.68 | 0.661 | 2 | 0.3 | 5 | 0 |
| capecitabine | -1.57 | -1.38 | -0.40 | | 1 | | | -1.79 | | | 0.6 | 4 | 0 |
| captopril | 0.18 | -0.37 | -0.52 | | 1 | 1 | 2 | -3.61 | 0.031 | 1 | 0.275 | 5 | -1 |
| carbamazepine | -4.80 | -0.19 | -14.67 | -0.070 | 1 | 2 | 2 | -6.74 | 0.558 | 2 | 0.76 | 4 | 0 |
| carbegoline | -0.88 | -0.60 | -0.52 | | 1 | | 4 | -2.21 | | | 0.41 | 5 | 2 |
| carvedilol | -0.17 | -0.66 | -1.69 | | 0 | | 3 | -1.04 | | | 0.98 | 1 | 1 |
| cefuroxime | -3.12 | -2.64 | -1.71 | | 0 | 0 | 2 | -4.61 | | | 0.5 | 5 | -1 |
| celecoxib | 0.29 | -0.70 | -0.16 | | 1 | 1 | 2 | -2.48 | 0.41 | 2 | 0.97 | 2 | 0 |

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|---------------------------|-------|-------|-------|--------|---|---|---|-------|-------|---|-------|---|----|
| celiprolol | 0.07 | -0.91 | -0.89 | | | | | -2.3 | | | 0.275 | 5 | 1 |
| cephalexin | -0.06 | 0.03 | -1.32 | | 0 | 1 | 1 | -4.08 | 0.012 | 1 | 0.14 | 5 | 0 |
| cetirizine | -0.32 | -0.30 | 0.39 | -2.150 | 1 | 1 | 2 | -3.74 | | | 0.93 | 3 | 0 |
| chloramphenikol | -1.61 | -1.30 | -0.79 | | 0 | 1 | 4 | -3.83 | 0.6 | 2 | 0.55 | 4 | 0 |
| chlorpromazine | 0.24 | 0.04 | 1.22 | 0.950 | 1 | 1 | 3 | -2.21 | 0.4 | 2 | 0.9 | 3 | 1 |
| chlortalidone | -1.70 | -1.34 | -0.98 | | 1 | 1 | 4 | -2.37 | 0.062 | 1 | 0.75 | 4 | 0 |
| cimetidine | -1.64 | -1.28 | -0.96 | -1.420 | 0 | 1 | 1 | -0.13 | 1.7 | 4 | 0.17 | 5 | 1 |
| ciprofloxacin | -0.14 | -0.62 | -1.59 | | | 1 | 3 | -0.36 | 2.15 | 4 | 0.3 | 5 | 0 |
| cisapride | -0.79 | -0.83 | 0.46 | | 1 | 1 | | -0.27 | 0.045 | 1 | 0.975 | 2 | 1 |
| clarithromycin | -2.57 | -2.38 | -0.67 | | 0 | 1 | 1 | -0.96 | 0.25 | 1 | 0.7 | 4 | 1 |
| clindamycin | 0.38 | -1.15 | 0.13 | | 0 | 1 | 2 | -1.53 | 0.3 | 1 | 0.93 | 3 | 1 |
| clobazam | -0.67 | -0.10 | -1.37 | 0.350 | 1 | 1 | 3 | -1.39 | 0.25 | 1 | 0.85 | 3 | -1 |
| clonidine | -0.36 | -0.04 | -0.53 | 0.150 | 1 | 2 | 3 | -0.9 | 2 | 4 | 0.3 | 5 | 1 |
| clorazepate | -0.95 | -1.09 | 0.71 | | 1 | 2 | 3 | -1.9 | 0.2 | 1 | 0.975 | 2 | -1 |
| clozapine | 0.36 | 0.50 | 0.22 | | 1 | | 3 | -0.13 | 2.79 | 4 | 0.99 | 1 | 1 |
| cypheptadine | -0.09 | 0.10 | -0.09 | | 1 | | 3 | -1.75 | | | 0.975 | 2 | 1 |
| desloratidine | -0.22 | 0.15 | -0.63 | | 1 | 1 | 2 | -3.07 | | | 0.845 | 4 | 1 |
| diazepam | 0.11 | 0.02 | 0.84 | 0.346 | 1 | 2 | 3 | -3.8 | 0.19 | 1 | 0.98 | 1 | 0 |
| digoxin | -2.46 | -2.70 | 0.67 | -1.230 | 0 | 1 | 2 | -6.3 | 0.7 | 2 | 0.25 | 5 | 0 |
| dihydroergotamine | -0.18 | -1.34 | -1.72 | | 0 | | 4 | -0.02 | | | 0.93 | 3 | 1 |
| diphenhydramin | 0.27 | 0.35 | 0.38 | | 1 | 1 | 2 | -1.56 | | | 0.985 | 1 | 1 |
| doxazosin | 0.46 | -1.42 | 0.41 | | 1 | 1 | 4 | -0.68 | | | 0.98 | 1 | 1 |
| doxycycline | -2.83 | -2.36 | -1.60 | | 0 | 1 | 3 | -0.47 | 0.34 | 1 | 0.9 | 3 | 0 |
| drotaverine | -0.81 | -0.24 | -1.42 | | 1 | | | -1.03 | | | 0.875 | 3 | 1 |
| enalapril | -0.93 | -0.99 | 0.49 | | 0 | 1 | 2 | -4.05 | 0.02 | 1 | 0.55 | 4 | -1 |
| epplerone | -0.73 | -0.72 | 0.32 | | 1 | | 3 | | | | 0.5 | 5 | 0 |
| escitalopram | 0.27 | -0.03 | -0.23 | | 1 | 1 | 2 | -2.37 | 2.2 | 4 | 0.56 | 4 | 1 |
| estradiol benzoate | -0.97 | -1.07 | 1.44 | | | | 3 | | | | 0.95 | 2 | 0 |
| estrone | -0.87 | -1.02 | 0.77 | | | | | -3.05 | | | 0.95 | 2 | 0 |
| famotidine | -3.55 | -3.26 | -1.22 | | 1 | 1 | 1 | -0.73 | 1.5 | 4 | 0.175 | 5 | 1 |
| fexofenadine | -0.48 | -0.75 | 1.24 | -0.980 | 0 | 1 | 2 | -0.27 | | | 0.65 | 4 | 0 |

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|-------------------------------|-------|-------|-------|--------|---|---|---|-------|-------|---|-------|---|----|
| fluoxetine | 0.43 | 0.21 | 0.30 | | 1 | 2 | 2 | -2.85 | 0.68 | 2 | 0.945 | 2 | 1 |
| flupenthixol | 0.18 | -0.29 | 2.00 | | 1 | 1 | | -0.15 | 1.15 | 3 | 0.95 | 2 | 1 |
| furosemide | -1.84 | -1.55 | -0.79 | | 0 | | 3 | -4.16 | | | 0.95 | 2 | -1 |
| gliclazide | -0.86 | -0.84 | 0.29 | | 1 | | | -1.13 | | | 0.94 | 3 | -1 |
| haloperidol | -0.26 | -0.10 | -0.01 | 1.340 | 1 | 1 | 3 | -0.84 | 0.64 | 2 | 0.92 | 3 | 1 |
| hydrocortisone acetate | -0.12 | -0.42 | 1.44 | | | | 2 | -5.22 | | | 0.95 | 2 | 0 |
| hydroxyzine | -0.21 | -0.03 | -0.05 | 0.285 | 1 | 1 | 1 | -0.58 | | | 0.93 | 3 | 1 |
| ibuprofen | 0.17 | -0.05 | 1.25 | -0.180 | 1 | 1 | 1 | -2.79 | 0 | 1 | 0.95 | 2 | -1 |
| indomethacin | -1.02 | -0.47 | -1.38 | -1.260 | 1 | 1 | 3 | -3.24 | 0.47 | 2 | 0.97 | 2 | -1 |
| ketoprofen | 0.53 | -0.32 | 0.62 | | 1 | 1 | | -2.97 | | | 0.99 | 1 | -1 |
| ketotifen | -0.54 | -0.23 | -0.54 | | 1 | 0 | 3 | -1.64 | | | 0.75 | 4 | 1 |
| lamotrigine | -0.99 | -0.90 | 0.03 | 0.480 | 1 | 2 | 3 | -1.81 | 0.513 | 2 | 0.55 | 4 | 0 |
| levocetirizine | -0.12 | -0.30 | 1.08 | | 1 | 1 | 3 | -3.74 | | | 0.915 | 3 | 0 |
| levofloxacin | -0.85 | -0.63 | -0.36 | | | 1 | 3 | -2.01 | 0.95 | 3 | 0.31 | 5 | -1 |
| loperamide | 0.25 | -0.15 | 1.84 | 0.770 | 0 | | 2 | -0.56 | | | 0.97 | 2 | 1 |
| loratadine | -0.44 | -0.13 | -0.52 | | 1 | 1 | 1 | -2.93 | 1.2 | 4 | 0.98 | 1 | 0 |
| lorazepam | -0.25 | -0.44 | 1.05 | 0.440 | 1 | 1 | 3 | -3.6 | 0.205 | 1 | 0.87 | 3 | 0 |
| medazepam | 0.56 | 0.30 | 1.48 | | 1 | | | -1.02 | | | 0.99 | 1 | |
| meloxicam | -2.05 | -1.63 | -1.25 | | 0 | | 3 | -2.7 | | | 0.99 | 1 | -1 |
| methyldopa | -1.62 | -1.11 | -1.40 | | 0 | 1 | 2 | -1.63 | 0.265 | 1 | 0.2 | 5 | 0 |
| mianserin | 0.19 | 0.44 | -0.20 | 0.990 | 1 | 1 | | -1.06 | 2.2 | 4 | 0.9 | 3 | 0 |
| midazolam | 0.28 | 0.14 | 1.04 | 0.398 | 1 | 1 | 2 | -1.17 | 0.785 | 2 | 0.97 | 2 | 0 |
| mirtazapine | 0.03 | 0.24 | -0.09 | 0.530 | 1 | 1 | 3 | -0.9 | 1.1 | 3 | 0.85 | 3 | 0 |
| montelukast | 0.77 | -0.58 | 1.40 | | 1 | 1 | 3 | -2.44 | | | 0.99 | 1 | -1 |
| naproxen | -0.10 | -0.20 | 0.83 | | 1 | 1 | 4 | -2.36 | 0.16 | 1 | 0.99 | 1 | -1 |
| nebivolol | -0.02 | -0.59 | -1.18 | | 1 | | 3 | -1.45 | | | 0.98 | 1 | 1 |
| olanzapine | -1.34 | -0.80 | -1.45 | | | 1 | 2 | -0.13 | 0.38 | 1 | 0.175 | 5 | 1 |
| oxazepam | -0.33 | -0.44 | 0.79 | 0.580 | 1 | 1 | 3 | -3.74 | 0.1 | 1 | 0.85 | 3 | 0 |
| oxybutinin | 0.63 | -0.25 | 0.96 | | 1 | | 3 | -1.04 | | | 0.92 | 3 | 1 |
| pantoprazole | -0.15 | -0.83 | -1.61 | | 0 | 1 | 1 | -1.13 | | | 0.98 | 1 | 0 |

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|-----------------------|-------|-------|-------|--------|---|---|---|-------|-------|---|-------|---|----|
| paracetamol | -0.79 | -0.24 | -1.33 | -0.463 | 1 | 1 | 1 | -2.66 | 0.84 | 3 | 0.25 | 5 | 0 |
| paroxetine | 0.06 | -0.09 | -0.91 | | 1 | 1 | 2 | -2.48 | 0.675 | 2 | 0.94 | 3 | 1 |
| pergolide | -0.17 | -0.16 | 0.48 | 0.300 | 1 | | | -0.78 | | | 0.9 | 3 | 1 |
| perindopril | -0.97 | -0.99 | 0.37 | | 0 | 1 | 3 | -4.05 | | | 0.15 | 5 | -1 |
| phenytoin | -0.61 | -0.38 | -0.30 | -0.096 | 1 | 1 | 2 | -0.88 | 0.29 | 1 | 0.9 | 3 | 0 |
| pindolol | -0.05 | -0.37 | -1.28 | | 1 | 1 | 3 | -2.34 | | | 0.4 | 5 | 1 |
| piroxicam | -1.30 | -1.18 | -0.13 | | 0 | 1 | 2 | -2.7 | 0.02 | 1 | 0.99 | 1 | -1 |
| prednisolone | -0.96 | -0.97 | 0.34 | | 1 | | 2 | -5.26 | 0.13 | 1 | 0.9 | 3 | 0 |
| progesterone | -0.08 | -0.20 | 0.90 | | | 1 | 3 | | | | 0.975 | 2 | 0 |
| promazine | 0.16 | 0.04 | 0.96 | 0.880 | 1 | | | -2.23 | | | 0.94 | 3 | 1 |
| promethazine | -0.36 | 0.04 | -0.77 | | 1 | | 2 | -1.78 | | | 0.93 | 3 | 1 |
| propafenone | 0.42 | -0.39 | 0.27 | | 0 | 1 | 2 | -2.11 | | | 0.97 | 2 | 1 |
| propranolol | -0.05 | -0.12 | 0.74 | 1.110 | 1 | 1 | 2 | -2.3 | 0.396 | 1 | 0.9 | 3 | 1 |
| quetiapine | -0.52 | -0.63 | 0.76 | | 1 | 1 | 2 | -0.46 | | | 0.83 | 4 | 1 |
| quinapril | 0.40 | -0.99 | 0.18 | | 0 | 1 | 2 | -3.81 | 0.12 | 1 | 0.97 | 2 | -1 |
| risperidone | -0.68 | -0.44 | -0.35 | -0.020 | 1 | 1 | 3 | -0.87 | 0.26 | 1 | 0.88 | 3 | 1 |
| rizatriptan | -0.78 | -0.40 | -0.80 | 0.780 | 1 | | 3 | -2.29 | | | 0.14 | 5 | 1 |
| rosuvastatin | 0.32 | -1.71 | -0.08 | | 0 | 1 | 3 | -2.95 | | | 0.88 | 3 | -1 |
| roxitromicin | 0.58 | -2.92 | 0.79 | | 0 | 1 | | -0.96 | 0.04 | 1 | 0.96 | 2 | 1 |
| rupatadine | -0.04 | 0.08 | 0.15 | | | | | -0.25 | | | 0.985 | 1 | 1 |
| sertraline | 0.39 | 0.35 | 0.18 | | 1 | 1 | 2 | -2.27 | 1.85 | 4 | 0.98 | 1 | 1 |
| sildenafil | -0.08 | -1.20 | -1.40 | | 1 | 1 | 3 | -1.17 | | | 0.96 | 2 | 0 |
| simvastatin | -0.27 | -0.62 | 1.55 | | 1 | | 3 | -6.29 | | | 0.95 | 2 | 0 |
| spironolactone | -0.62 | -0.82 | 1.00 | | 1 | | 2 | | 0.615 | 2 | 0.9 | 3 | 0 |
| sulpiride | -1.42 | -1.21 | -0.43 | | 1 | 2 | 2 | -1.77 | | | 0.4 | 5 | 1 |
| telmisartan | 0.33 | -0.46 | 3.03 | | 1 | | 4 | -3.34 | | | 0.995 | 1 | -1 |
| temazepam | -0.17 | -0.30 | 0.91 | | 1 | 1 | 3 | -4.46 | 0.14 | 1 | 0.96 | 2 | 0 |
| theophylline | -1.09 | -0.56 | -1.32 | -0.341 | 1 | 1 | 3 | -1.4 | 0.697 | 2 | 0.4 | 5 | 0 |
| thioridazine | -0.07 | -0.37 | 1.43 | 0.285 | 1 | | 4 | -2.64 | | | 0.95 | 2 | 1 |
| tolterodine | 0.63 | 0.17 | 0.96 | | 1 | | 3 | -3.48 | | | 0.963 | 2 | 1 |
| trazodone | -0.06 | -0.13 | 0.74 | | 1 | 1 | 2 | -0.32 | 0.53 | 2 | 0.92 | 3 | 1 |

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|-----------------------|-------|-------|-------|--------|---|---|---|-------|------|---|-------|---|----|
| tropicamid | 0.14 | -0.31 | -0.67 | | 1 | | 3 | -1.88 | | | 0.45 | 5 | 0 |
| valproic acid | 0.54 | -0.05 | 0.64 | | 1 | 1 | 4 | -2.38 | 0.05 | 1 | 0.85 | 3 | -1 |
| valsartan | -0.93 | -1.25 | 1.28 | | 0 | | 3 | -3.64 | | | 0.955 | 2 | -1 |
| venlafaxine | 0.36 | 0.02 | 0.05 | | 1 | 1 | 3 | -2.07 | 3.32 | 4 | 0.27 | 5 | 1 |
| verapamil | -0.72 | -0.48 | -0.38 | -0.470 | 1 | 1 | 2 | -1.77 | 0.6 | 2 | 0.9 | 3 | 1 |
| zolmitriptane | -0.86 | -0.37 | -1.17 | | 1 | | 3 | -2.32 | | | 0.25 | 5 | 1 |
| zolpidem | -0.29 | -0.05 | -0.24 | -0.480 | 1 | 1 | 3 | -0.43 | 0.15 | 1 | 0.92 | 3 | 0 |
| zopiclone | -0.87 | -0.92 | 0.49 | | 0 | | 2 | -0.5 | 0.51 | 2 | 0.45 | 5 | 0 |
| zuclopenthixol | 0.12 | -0.29 | 1.82 | | 1 | 1 | 3 | -0.17 | 0.37 | 1 | 0.985 | 1 | 1 |

Table S2. Physicochemical properties of APIs (n = 129).

| API | a/b/n code ¹ | DM | eH | eH-eL | eL ² | HA | HD | log D | log P | MW ³ | pKa | PSA ⁴ | Sa ³ | V ³ |
|----------------------|----------------------------|------|-------|-------|-----------------|----|----|-------|-------|-----------------|-------|------------------|-----------------|----------------|
| acebutolol | 1 | 2.65 | -9.19 | -8.68 | -5.11 | 5 | 3 | 0.26 | -0.33 | 3.36 | 9.4 | 8.77 | 6.33 | 3.29 |
| aceclofenac | -1 | 1.93 | -8.85 | -8.58 | -2.68 | 5 | 2 | 0.44 | 3.54 | 3.54 | 2.6 | 7.56 | 4.44 | 2.84 |
| acenocumarol | -1 | 8.94 | -9.74 | -8.27 | -14.71 | 7 | 1 | 0.34 | 2.68 | 3.53 | 4.5 | 10.94 | 4.66 | 2.96 |
| acetylsalicylic acid | -1 | 5.18 | -9.78 | -9.08 | -6.93 | 4 | 1 | -1.89 | 1.30 | 1.80 | 3.48 | 6.36 | 3.05 | 1.52 |
| aciclovir | 0 | 5.69 | -8.76 | -8.27 | -4.89 | 8 | 4 | -1.76 | -1.45 | 2.25 | 5.11 | 10.98 | 3.59 | 1.86 |
| alprazolam | 0 | 6.16 | -9.51 | -9.36 | -1.42 | 4 | 0 | 2.5 | 4.68 | 3.09 | 2.37 | 3.81 | 2.94 | 2.69 |
| amiodarone | 1 | 5.30 | -7.46 | -4.11 | -33.48 | 3 | 0 | 6.94 | 3.01 | 6.45 | 9.37 | 4.27 | 5.21 | 4.46 |
| amlodipine | 1 | 2.88 | -8.66 | -8.32 | -3.35 | 5 | 2 | 2.59 | -1.51 | 4.09 | 8.97 | 9.99 | 5.92 | 3.62 |
| amoxicillin | -1 | 4.32 | -9.20 | -8.87 | -3.31 | 8 | 5 | -2.43 | -0.15 | 3.65 | 2.44 | 15.83 | 4.88 | 3.07 |
| astemizol | 1 | 1.71 | -7.83 | -7.52 | -3.07 | 5 | 1 | 4.08 | 0.71 | 4.59 | 8.68 | 3.74 | 6.02 | 4.22 |
| atorvastatin | -1 | 2.22 | -9.00 | -8.86 | -1.40 | 5 | 4 | 1.11 | 1.54 | 5.63 | 4.29 | 11.18 | 6.75 | 5.21 |
| atropine | 1 | 2.48 | -9.42 | -9.46 | 0.41 | 4 | 1 | -0.94 | 1.71 | 2.89 | 9.98 | 4.98 | 4.24 | 2.79 |
| azithromycin | 1 | | | 0.00 | | 13 | 5 | 3.18 | 2.44 | | 8.59 | 18.01 | | |
| betaxolol | 1 | 1.20 | -8.98 | -9.42 | 4.43 | 4 | 2 | 0.93 | 1.00 | 3.07 | 9.43 | 5.07 | 5.89 | 3.15 |
| bilastine | 0 | 2.69 | -8.82 | -8.70 | -1.22 | 6 | 2 | 1.97 | 2.10 | 4.64 | 6.59 | 7.85 | 6.65 | 4.54 |
| biperiden | 1 | 2.30 | -9.16 | -9.48 | 3.22 | 2 | 1 | 1.68 | 2.71 | 3.11 | 9.26 | 2.35 | 4.11 | 3.20 |
| bisoprolol | 1 | 1.93 | -9.09 | -9.42 | 3.27 | 5 | 2 | 0.4 | 2.13 | 3.25 | 9.42 | 6.00 | 7.05 | 3.31 |
| bromazepam | 0 | 2.87 | -9.13 | -9.02 | -1.07 | 4 | 1 | 1.65 | 2.59 | 3.16 | 11.39 | 5.44 | 2.67 | 2.36 |
| bromocriptine | 0 | 4.25 | -8.92 | -7.96 | -9.58 | 10 | 3 | 5.07 | 4.48 | 6.69 | 6.44 | 11.82 | 6.06 | 5.64 |
| buspirone | 0 | 4.32 | -8.74 | -8.58 | -1.56 | 7 | 0 | 3.35 | 1.18 | 3.86 | 7.72 | 6.96 | 5.19 | 3.71 |
| caffeine | 0 | 3.92 | -9.00 | -8.47 | -5.36 | 6 | 0 | -0.13 | -1.06 | 1.94 | 0.52 | 5.35 | 3.41 | 1.68 |
| capecitabine | -1 | 4.97 | -9.72 | -8.38 | -13.37 | 9 | 3 | -0.73 | 0.53 | 3.59 | 5.41 | 12.07 | 5.37 | 3.04 |
| captopril | -1 | 1.87 | -9.35 | -9.45 | 1.05 | 3 | 2 | -3.15 | 0.30 | 2.17 | 3.59 | 5.76 | 3.63 | 1.92 |
| carbamazepine | 0 | 3.25 | -9.05 | -8.53 | -5.19 | 3 | 2 | 2.67 | 2.10 | 2.36 | 13.94 | 4.63 | 2.85 | 2.19 |
| carbegoline | 1 | 3.58 | -8.39 | -8.15 | -2.38 | 7 | 2 | -0.19 | 0.29 | 4.24 | 9.41 | 7.17 | 6.41 | 4.10 |
| carvedilol | 0 | 3.15 | -8.56 | -8.35 | -2.09 | 5 | 3 | 3.29 | -2.04 | 4.20 | 8.24 | 7.57 | 5.49 | 3.97 |
| cefuroxime | -1 | 2.73 | -8.76 | -7.44 | -13.17 | 4 | 12 | 2.91 | -2.08 | 4.24 | 2.59 | 19.91 | 4.26 | 3.75 |
| celecoxib | 0 | 4.09 | -9.93 | -8.51 | -14.21 | 3 | 1 | 4.21 | 1.02 | 3.81 | 9.68 | 7.80 | 5.10 | 2.97 |

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|---------------------------|----|-------|--------|--------|--------|----|---|-------|-------|--------|-------|-------|------|------|
| celiprolol | 1 | 2.01 | -9.24 | -8.78 | -4.56 | 5 | 3 | 0.22 | -0.45 | 3.65 | 9.5 | 9.09 | 6.62 | 3.59 |
| cephalexin | -1 | 5.35 | -9.59 | -8.97 | -6.25 | 5 | 3 | -2.44 | -1.31 | 3.47 | 3.12 | 3.25 | 4.24 | 2.95 |
| cetirizine | -1 | 3.56 | -8.97 | -8.75 | -2.20 | 5 | 1 | -1.13 | 2.11 | 3.75 | 3.46 | 5.30 | 5.01 | 3.37 |
| chloramphenikol | 0 | -9.08 | -10.34 | -9.01 | -13.37 | 7 | 3 | 1.02 | -0.25 | 3.23 | 11.03 | 11.54 | 4.50 | 2.44 |
| chlorpromazine | 1 | 7.13 | -6.83 | -6.90 | 0.74 | 2 | 0 | 3.26 | 3.77 | 3.19 | 9.41 | 3.18 | 3.04 | 2.62 |
| chlortalidone | 0 | 4.04 | -9.45 | -8.68 | -7.73 | 6 | 4 | -0.74 | -0.63 | 3.19 | 9.57 | 11.79 | 3.79 | 2.51 |
| cimetidine | 0 | 11.01 | -8.75 | -8.48 | -2.76 | 6 | 3 | -0.25 | -0.59 | 2.52 | 7.07 | 11.42 | 2.94 | 2.29 |
| ciprofloxacin | 0 | 6.93 | -8.72 | -7.94 | -7.85 | 6 | 2 | -0.85 | -1.85 | 331.35 | 7.56 | 7.29 | 4.25 | 2.84 |
| cisapride | 0 | 1.68 | -8.72 | -8.54 | -1.86 | 7 | 3 | 2.6 | 2.25 | 4.66 | 7.47 | 8.61 | 6.66 | 4.11 |
| clarithromycin | 0 | | | 0.00 | | 14 | 4 | 2.33 | 3.16 | | 8.16 | 18.29 | | |
| clindamycin | 1 | | | 0.00 | | 7 | 4 | 0.48 | 1.59 | | 8.73 | 10.58 | | |
| clobazam | 0 | 4.18 | -9.21 | -8.66 | -5.52 | 4 | 0 | 1.59 | -1.40 | 3.01 | 8.59 | 4.03 | 4.02 | 2.58 |
| clonidine | 0 | 3.51 | -8.90 | -8.48 | -4.25 | 3 | 2 | -0.68 | 0.28 | 2.30 | 8.1 | 3.64 | 3.10 | 1.86 |
| clorazepate | -1 | 3.51 | -9.12 | -9.01 | -1.13 | 6 | 4 | 1.55 | 2.75 | 3.15 | 5.3 | 10.22 | 2.91 | 2.57 |
| clozapine | 0 | 1.13 | -8.78 | -8.51 | -2.69 | 1 | 0 | 4.86 | 1.77 | 2.87 | 7.33 | 0.32 | 3.81 | 2.90 |
| cypheptadine | 1 | 1.98 | -8.63 | -8.83 | 2.03 | 3 | 1 | 2.44 | 1.16 | 2.65 | 8.95 | 2.76 | 3.89 | 2.66 |
| desloratidine | 1 | 3.04 | -9.13 | -8.83 | -2.94 | 2 | 1 | 4.1 | 0.07 | 3.11 | 10.27 | 2.49 | 3.75 | 2.88 |
| diazepam | 0 | 3.57 | -9.06 | -8.96 | -1.00 | 3 | 0 | 2.91 | 3.01 | 2.85 | 3.4 | 3.27 | 2.80 | 2.50 |
| digoxin | 0 | 5.58 | -8.45 | -7.28 | -11.68 | 14 | 6 | 0.85 | 2.67 | 7.81 | 13.5 | 20.31 | 7.66 | 7.05 |
| dihydroergotamine | 0 | 3.90 | -8.60 | -8.50 | -1.05 | 6 | 3 | 2.05 | -2.11 | 4.78 | 7.22 | 11.82 | 5.13 | 4.33 |
| diphenhydramin | 1 | 0.52 | -9.18 | -9.41 | 2.36 | 2 | 0 | 2.29 | 2.09 | 2.55 | 8.76 | 1.25 | 4.92 | 2.65 |
| doxazosin | 0 | 4.02 | -8.67 | -7.54 | -11.34 | 9 | 1 | 0.6 | 2.14 | 4.09 | 6.52 | 12.27 | 4.93 | 3.46 |
| doxycycline | 0 | 11.15 | -9.00 | -7.85 | -11.51 | 10 | 7 | -3.32 | -1.86 | 4.44 | 7.67 | 18.16 | 4.43 | 3.68 |
| drotaverine | 0 | 3.56 | -8.36 | -7.99 | -3.63 | 5 | 1 | 6.12 | -1.51 | 3.98 | 6.17 | 4.90 | 6.39 | 3.89 |
| enalapril | -1 | 3.46 | -9.37 | -9.38 | 0.20 | 7 | 2 | -2.35 | 2.30 | 3.75 | 3.15 | 9.59 | 4.19 | 3.48 |
| eplerenone | | 3.20 | -10.28 | -10.00 | -2.81 | 6 | 0 | 1.05 | 1.96 | 4.15 | | 7.89 | 4.43 | 3.73 |
| escitalopram | 1 | 2.57 | -9.21 | -8.37 | -8.44 | 3 | 0 | 0.39 | 0.87 | 3.24 | 9.57 | 3.63 | 5.46 | 3.08 |
| estradiol benzoate | 0 | 5.95 | -10.11 | -9.97 | -1.40 | 4 | 0 | 2.51 | 4.20 | 3.73 | | 6.04 | 4.77 | 3.58 |
| estrone | 0 | 5.76 | -10.17 | -9.95 | -2.21 | 6 | 1 | 2.53 | 2.86 | 4.02 | 10.25 | 9.77 | 4.73 | 3.67 |
| famotidine | 0 | 1.01 | -8.55 | -7.97 | -5.85 | 9 | 8 | -1.02 | -1.11 | 3.36 | 7.93 | 23.78 | 4.85 | 2.69 |
| fexofenadine | 0 | 2.61 | -8.98 | -8.75 | -2.28 | 5 | 3 | 2.3 | 3.81 | 5.02 | 6.93 | 8.10 | 6.27 | 4.87 |

| | | | | | | | | | | | | | | |
|-------------------------------|----|------|--------|--------|--------|---|---|-------|-------|------|-------|-------|------|------|
| fluoxetine | 1 | 4.43 | -9.41 | -9.02 | -3.95 | 2 | 1 | 1.56 | 1.93 | 3.09 | 10.05 | 2.13 | 4.99 | 2.71 |
| flupenthixol | 0 | 4.80 | -7.61 | -6.76 | -8.51 | 3 | 1 | 4.42 | 5.33 | 4.30 | 7.05 | 5.20 | 5.85 | 3.65 |
| furosemide | -1 | 3.27 | -8.92 | -7.90 | -10.23 | 7 | 4 | -0.12 | -0.24 | 3.11 | 3.04 | 13.10 | 4.19 | 2.42 |
| gliclazide | -1 | 5.31 | -9.38 | -8.30 | -10.80 | 6 | 2 | -0.28 | 1.90 | 3.23 | 6.07 | 8.69 | 4.91 | 2.86 |
| haloperidol | 0 | 2.85 | -9.22 | -8.75 | -4.64 | 3 | 1 | 2.11 | 1.31 | 3.76 | 8.04 | 4.05 | 5.29 | 3.37 |
| hydrocortisone acetate | 0 | 4.23 | -10.14 | -10.06 | -0.86 | 4 | 0 | 4.53 | 4.20 | 3.73 | 12.42 | 6.04 | 4.77 | 3.58 |
| hydroxyzine | 0 | 1.27 | -8.81 | -8.75 | -0.65 | 4 | 1 | 2 | 1.23 | 3.75 | 6.62 | 3.59 | 5.48 | 3.54 |
| ibuprofen | -1 | 1.91 | -9.39 | -9.58 | 1.92 | 2 | 1 | 0.8 | 3.83 | 2.06 | 4.41 | 3.73 | 2.52 | 2.42 |
| indomethacin | -1 | 2.98 | -8.69 | -8.12 | -5.75 | 5 | 1 | -0.16 | -1.43 | 3.58 | 3.96 | 6.36 | 4.94 | 3.05 |
| ketoprofen | -1 | 4.50 | -9.96 | -9.56 | -3.99 | 3 | 1 | -0.25 | 2.56 | 2.54 | 4.23 | 5.44 | 4.07 | 2.36 |
| ketotifen | 1 | 4.07 | -9.08 | -8.07 | -10.10 | 2 | 0 | 3.28 | 0.26 | 3.09 | 8.84 | 4.86 | 3.89 | 2.87 |
| lamotrigine | 0 | 2.75 | -8.22 | -7.66 | -5.61 | 5 | 4 | -0.19 | 1.38 | 2.56 | 5.39 | 9.07 | 3.15 | 1.93 |
| levocetizine | -1 | 1.73 | -9.00 | -8.83 | -1.67 | 5 | 1 | -1.13 | 3.48 | 3.89 | 3.46 | 5.30 | 5.59 | 3.55 |
| levofloxacin | -1 | 7.21 | -8.72 | -7.88 | -8.37 | 7 | 1 | 0.65 | 0.62 | 3.61 | 5.19 | 7.33 | 4.75 | 3.06 |
| loperamide | 0 | 4.65 | -8.52 | -8.50 | -0.23 | 4 | 1 | 3.53 | 5.01 | 4.77 | 7.76 | 4.38 | 4.89 | 4.33 |
| loratadine | 0 | 2.90 | -9.02 | -8.36 | -6.59 | 4 | 0 | 5.94 | 0.30 | 3.69 | 4.27 | 4.24 | 4.93 | 3.31 |
| lorazepam | 0 | 6.40 | -7.77 | -7.65 | -1.17 | 4 | 2 | 2.47 | 3.42 | 3.21 | 10.8 | 6.17 | 2.58 | 2.53 |
| medazepam | 0 | 4.08 | -8.34 | -8.28 | -0.59 | 2 | 0 | 4.42 | 4.29 | 3.30 | 6.18 | 1.56 | 2.80 | 2.49 |
| meloxicam | -1 | 5.35 | -7.64 | -6.38 | -12.59 | 7 | 2 | -0.09 | -1.16 | 3.51 | 4.5 | 13.62 | 4.03 | 2.71 |
| methyldopa | 0 | 1.56 | -9.07 | -9.34 | 2.75 | 5 | 5 | -2.38 | -1.46 | 2.11 | 5.57 | 10.38 | 3.34 | 1.85 |
| mianserin | 1 | 0.56 | -8.66 | -8.93 | 2.68 | 2 | 0 | 2.76 | 0.94 | 2.64 | 8.26 | 0.65 | 3.65 | 2.64 |
| midazolam | 0 | 3.03 | -9.24 | -9.11 | -1.28 | 3 | 0 | 3.92 | 3.41 | 3.26 | 6.03 | 2.53 | 3.04 | 2.76 |
| mirtazapine | 0 | 1.76 | -8.79 | -8.81 | 0.19 | 3 | 0 | 1.97 | 1.16 | 2.65 | 8.1 | 1.94 | 3.57 | 2.60 |
| montelukast | -1 | 3.34 | -7.46 | -6.83 | -6.36 | 4 | 2 | 5.19 | 4.13 | 5.88 | 4.76 | 7.04 | 7.27 | 5.47 |
| naproxen | -1 | 1.92 | -9.10 | -8.82 | -2.79 | 3 | 1 | 0.47 | 2.99 | 2.30 | 4.84 | 4.65 | 3.89 | 2.15 |
| nebivolol | 1 | 2.46 | -9.05 | -8.94 | -1.07 | 5 | 3 | 2.4 | -1.03 | 4.05 | 8.65 | 7.10 | 5.05 | 3.53 |
| olanzapine | 0 | 7.55 | -9.20 | -8.41 | -7.85 | 6 | 1 | -1.48 | -1.56 | 3.28 | 7.33 | 8.41 | 6.19 | 3.01 |
| oxazepam | 0 | 3.38 | -9.09 | -8.98 | -1.06 | 4 | 2 | 2.32 | 2.91 | 2.87 | 10.94 | 6.17 | 2.72 | 2.72 |
| oxybutinin | 0 | 1.02 | -9.18 | -9.11 | -0.66 | 3 | 1 | 5.53 | 3.24 | 3.57 | 8.24 | 4.98 | 5.82 | 3.61 |
| pantoprazole | 0 | 7.25 | -9.09 | -8.19 | -9.03 | 6 | 1 | 1.5 | -1.89 | 3.83 | 8.33 | 8.63 | 5.08 | 3.01 |
| paracetamol | 0 | 3.28 | -8.58 | -8.65 | 0.73 | 3 | 2 | 0.34 | -1.32 | 1.51 | 9.86 | 4.93 | 3.03 | 1.39 |

| | | | | | | | | | | | | | | |
|-----------------------|----|-------|--------|--------|--------|----|---|-------|-------|------|-------|-------|------|------|
| paroxetine | 1 | 2.12 | -9.00 | -9.04 | 0.34 | 4 | 1 | 1.19 | -0.49 | 3.31 | 9.68 | 3.97 | 4.12 | 2.99 |
| pergolide | 0 | 1.93 | -8.35 | -8.50 | 1.51 | 2 | 1 | 2.29 | 2.29 | 3.14 | 7.98 | 4.43 | 4.50 | 3.09 |
| perindopril | -1 | 6.26 | -9.78 | -10.07 | 2.88 | 7 | 2 | -0.01 | 2.06 | 3.68 | 3.15 | 9.59 | 5.43 | 3.52 |
| phenytoin | 0 | 2.98 | -9.84 | -9.55 | -2.94 | 4 | 2 | 2.48 | 0.73 | 2.52 | 6.32 | 5.82 | 3.32 | 2.26 |
| pindolol | 1 | 3.19 | -8.47 | -8.53 | 0.63 | 3 | 3 | 0.19 | -1.23 | 2.48 | 9.54 | 5.73 | 4.60 | 2.44 |
| piroxicam | -1 | 11.24 | -8.63 | -8.84 | 2.05 | 7 | 2 | -2.14 | 1.07 | 3.33 | 4.5 | 10.80 | 2.66 | 2.50 |
| prednisolone | 0 | 3.68 | -10.01 | -9.54 | -4.70 | 5 | 3 | 1.49 | 2.01 | 3.46 | 12.46 | 9.48 | 3.96 | 3.14 |
| progesterone | | 5.88 | -9.29 | -9.03 | -2.60 | 3 | 1 | 6.24 | 3.12 | 3.77 | | 4.65 | 4.54 | 3.60 |
| promazine | 1 | 2.86 | -7.54 | -7.15 | -3.93 | 2 | 0 | 2.67 | 3.25 | 2.84 | 9.43 | 3.18 | 2.93 | 2.53 |
| promethazine | 1 | 3.40 | -7.83 | -7.76 | -0.65 | 2 | 0 | 3.2 | -0.20 | 2.84 | 8.98 | 3.18 | 4.36 | 2.76 |
| propafenone | 1 | 2.97 | -8.77 | -8.59 | -1.75 | 4 | 2 | 2.06 | 1.86 | 3.29 | 9.31 | 5.86 | 5.36 | 3.28 |
| propranolol | 1 | 1.53 | -8.36 | -7.79 | -5.71 | 3 | 2 | 1.27 | 2.80 | 2.59 | 9.5 | 4.15 | 3.09 | 2.56 |
| quetiapine | 0 | 1.57 | -8.68 | -7.95 | -7.24 | 5 | 1 | 1.55 | 2.84 | 3.84 | 6.74 | 7.36 | 5.42 | 3.55 |
| quinapril | -1 | 5.13 | -9.50 | -9.59 | 0.91 | 5 | 2 | 0.85 | 1.69 | 4.39 | 3.39 | 9.59 | 6.10 | 4.10 |
| risperidone | 0 | 3.42 | -8.93 | -8.06 | -8.76 | 6 | 0 | 2.27 | 0.63 | 4.10 | 8.07 | 6.19 | 4.91 | 3.73 |
| rizatriptan | 1 | 1.76 | -8.14 | -7.45 | -6.90 | 4 | 1 | 2.68 | -0.27 | 3.12 | 9.49 | 5.91 | 4.26 | 2.90 |
| rosuvastatin | -1 | 5.66 | -9.19 | -8.13 | -10.63 | 8 | 3 | -2.63 | 1.18 | 4.82 | 4.25 | 14.09 | 6.89 | 4.12 |
| roxitromicin | 0 | | | 0.00 | | 16 | 5 | 2.9 | 2.90 | | 8.16 | 21.69 | | |
| rupatadine | 0 | 1.61 | -8.99 | -8.35 | -6.43 | 3 | 0 | 5.97 | 1.63 | 4.15 | 6.95 | 2.90 | 4.97 | 3.94 |
| sertraline | 1 | 2.87 | -9.19 | -9.09 | -0.94 | 1 | 1 | 2.77 | 1.68 | 3.06 | 9.47 | 1.20 | 4.21 | 2.72 |
| sildenafil | 0 | 5.84 | -8.91 | -9.86 | 9.47 | 8 | 1 | 2.27 | -1.47 | 4.75 | 6.03 | 10.91 | 6.47 | 4.20 |
| simvastatin | 0 | 5.78 | -9.10 | -9.33 | 2.25 | 5 | 1 | 4.41 | 4.43 | 4.19 | 13.49 | 7.28 | 5.71 | 4.10 |
| spironolactone | | 1.67 | -9.76 | -8.96 | -7.98 | 4 | 0 | 3.12 | 3.33 | 4.17 | | 8.57 | 4.94 | 3.82 |
| sulpiride | 1 | 3.65 | -7.89 | -6.22 | -16.74 | 7 | 3 | -1.12 | 0.48 | 3.41 | 8.97 | 11.01 | 5.08 | 3.02 |
| telmisartan | -1 | 0.71 | -8.56 | -8.02 | -5.48 | 6 | 1 | 4.76 | 7.39 | 5.01 | 3.86 | 6.31 | 6.39 | 4.69 |
| temazepam | 0 | 2.48 | -9.17 | -9.09 | -0.83 | 4 | 1 | 2.15 | 3.15 | 3.01 | 11.66 | 5.29 | 2.84 | 2.53 |
| theophylline | 0 | 3.47 | -9.10 | -8.53 | -5.77 | 6 | 1 | -0.2 | -1.31 | 1.80 | 8.6 | 6.93 | 3.02 | 1.50 |
| thioridazine | 0 | 0.98 | -7.92 | -7.65 | -2.68 | 2 | 0 | 3.94 | 4.18 | 3.71 | 9.84 | 5.71 | 4.89 | 3.50 |
| tolterodine | 1 | 2.18 | -8.95 | -9.17 | 2.20 | 2 | 1 | 2.94 | 3.24 | 3.25 | 10.68 | 2.35 | 5.73 | 3.44 |
| trazodone | 0 | 3.41 | -8.50 | -7.88 | -6.21 | 6 | 0 | 1.58 | 2.80 | 3.72 | 7.52 | 4.24 | 5.01 | 3.36 |
| tropicamid | 0 | 4.06 | -9.68 | -9.40 | -2.81 | 3 | 1 | 1.15 | -0.01 | 2.84 | 5.32 | 5.34 | 4.15 | 2.76 |

| | | | | | | | | | | | | | | |
|-----------------------|----|------|--------|--------|-------|---|---|-------|-------|------|------|-------|------|------|
| valproic acid | -1 | 1.93 | -11.19 | -12.19 | 10.01 | 2 | 1 | 0.16 | 2.61 | 1.44 | 4.82 | 3.73 | 3.75 | 5.54 |
| valsartan | -1 | 2.92 | -9.69 | -9.05 | -6.39 | 8 | 2 | 0.05 | 3.88 | 4.22 | 3.56 | 11.21 | 5.46 | 3.92 |
| venlafaxine | 1 | 3.25 | -9.02 | -9.29 | 2.73 | 3 | 1 | 1.07 | 1.44 | 2.77 | 9.27 | 3.27 | 4.44 | 2.85 |
| verapamil | 1 | 5.44 | -8.76 | -8.85 | 0.90 | 6 | 0 | 2.33 | 0.57 | 4.55 | 8.97 | 6.40 | 7.51 | 4.53 |
| zolmitriptane | 1 | 4.09 | -8.73 | -8.57 | -1.57 | 5 | 2 | -0.44 | -1.01 | 2.89 | 9.52 | 5.74 | 4.68 | 2.74 |
| zolpidem | 0 | 6.69 | -8.37 | -8.33 | -0.45 | 4 | 0 | 3.02 | 0.86 | 3.07 | 6.77 | 3.76 | 3.33 | 2.94 |
| zopiclone | 0 | 5.47 | -9.13 | -8.95 | -1.78 | 9 | 0 | -42 | 2.31 | 3.89 | 6.7 | 9.18 | 3.36 | 3.86 |
| zuclopenthixol | 0 | 2.45 | -7.57 | -7.12 | -4.53 | 3 | 1 | 5.06 | 4.97 | 3.97 | 7.03 | 5.20 | 5.58 | 3.55 |

1 – code describing the acid-base properties: (-1) - acids; (0) - neutral drugs; (1) - bases

2 – value multiplied by 10

3 – value divided by 100

4 – value divided by 10

Table S3. Chromatographic data and their derivatives obtained from the NP TLC experiment for 129 APIs.

| API | C _{NP} [*] | NP ^{**} | NP/C | NP/PSA | R _M NP | R _M NP | R _M NP/C | R _M NP/PSA | R _M NP/PB | R _M NP/logP | R _M NP/B2 | NP/B2 | NP/PB | NP/logP |
|----------------------|------------------------------|------------------|------|--------|-------------------|-------------------|---------------------|-----------------------|----------------------|------------------------|----------------------|--------|-------|---------|
| acebutolol | 0.45 | 0.46 | 1.02 | 0.52 | 0.07 | 0.09 | 0.80 | 0.0008 | 0.268 | -0.2110 | -0.081 | -0.54 | 1.77 | -1.39 |
| aceclofenac | 0.89 | 0.90 | 1.01 | 1.19 | -0.95 | -0.91 | 1.05 | -0.0126 | -0.964 | -0.2696 | 1.439 | -1.36 | 0.91 | 0.25 |
| acenocumarol | 0.99 | 0.98 | 0.99 | 0.90 | -1.69 | -2.00 | 0.85 | -0.0154 | -1.712 | -0.6307 | 1.404 | -0.81 | 0.99 | 0.37 |
| acetylsalicylic acid | 0.89 | 0.90 | 1.01 | 1.41 | -0.93 | -0.91 | 1.02 | -0.0146 | -0.935 | -0.7159 | 1.978 | -1.90 | 0.90 | 0.69 |
| aciclovir | 0.73 | 0.73 | 0.99 | 0.66 | -0.42 | -0.43 | 0.97 | -0.0038 | -2.005 | 0.2903 | 0.348 | -0.60 | 3.45 | -0.50 |
| alprazolam | 0.85 | 0.86 | 1.01 | 2.25 | -0.79 | -0.75 | 1.05 | -0.0207 | -0.985 | -0.1685 | 12.466 | -13.60 | 1.08 | 0.18 |
| amiodarone | 0.55 | 0.6 | 1.09 | 1.41 | -0.18 | -0.09 | 2.02 | -0.0041 | -0.183 | -0.0585 | 1.296 | -4.42 | 0.63 | 0.20 |
| amlodipine | 0.56 | 0.56 | 1.00 | 0.56 | -0.10 | -0.10 | 1.00 | -0.0010 | -0.107 | 0.0694 | 0.100 | -0.53 | 0.57 | -0.37 |
| amoxicillin | 0.68 | 0.68 | 1.00 | 0.43 | -0.33 | -0.33 | 1.00 | -0.0021 | -1.637 | 2.1824 | 0.165 | -0.34 | 3.40 | -4.53 |
| astemizol | 0.62 | 0.61 | 0.98 | 1.63 | -0.19 | -0.21 | 0.91 | -0.0052 | -0.201 | -0.2736 | 3.791 | -11.90 | 0.63 | 0.86 |
| atorvastatin | 0.9 | 0.9 | 1.00 | 0.81 | -0.95 | -0.95 | 1.00 | -0.0085 | -0.974 | -0.6196 | 0.769 | -0.72 | 0.92 | 0.58 |
| atropine | 0.27 | 0.26 | 0.96 | 0.52 | 0.45 | 0.43 | 1.05 | 0.0091 | 2.524 | 0.2656 | -1.822 | -1.04 | 1.44 | 0.15 |
| azithromycin | 0.63 | 0.63 | 1.00 | 0.35 | -0.23 | -0.23 | 1.00 | -0.0013 | -0.797 | -0.0947 | 0.099 | -0.27 | 2.17 | 0.26 |
| betaxolol | 0.66 | 0.65 | 0.98 | 1.28 | -0.27 | -0.29 | 0.93 | -0.0053 | -0.538 | -0.2688 | 1.016 | -2.46 | 1.30 | 0.65 |
| bilastine | 0.46 | 0.44 | 0.96 | 0.56 | 0.10 | 0.07 | 1.50 | 0.0013 | 0.120 | 0.0499 | -0.148 | -0.62 | 0.51 | 0.21 |
| biperiden | 0.68 | 0.65 | 0.96 | 2.77 | -0.27 | -0.33 | 0.82 | -0.0115 | -0.448 | -0.0992 | -1.568 | 3.79 | 1.08 | 0.24 |
| bisoprolol | 0.67 | 0.66 | 0.98 | 1.09 | -0.28 | -0.31 | 0.91 | -0.0046 | -0.928 | -0.1307 | 0.675 | -1.59 | 2.18 | 0.31 |
| bromazepam | 0.87 | 0.90 | 1.03 | 1.65 | -0.93 | -0.83 | 1.13 | -0.0171 | -1.329 | -0.3593 | 2.885 | -2.77 | 1.28 | 0.35 |
| bromocriptine | 0.95 | 0.96 | 1.01 | 0.81 | -1.38 | -1.28 | 1.08 | -0.0117 | -1.484 | -0.3081 | 1.027 | -0.71 | 1.03 | 0.21 |
| buspirone | 0.57 | 0.58 | 1.01 | 0.83 | -0.13 | -0.12 | 1.07 | -0.0019 | -0.138 | -0.1113 | 0.231 | -1.01 | 0.61 | 0.49 |
| caffeine | 0.82 | 0.82 | 1.00 | 1.53 | -0.66 | -0.66 | 1.00 | -0.0123 | -2.195 | 0.6213 | 2.130 | -2.65 | 2.73 | -0.77 |
| capecitabine | 0.92 | 0.92 | 1.00 | 0.76 | -1.06 | -1.06 | 1.00 | -0.0088 | -1.768 | -2.0013 | 0.766 | -0.66 | 1.53 | 1.74 |
| captopril | 0.77 | 0.74 | 0.96 | 1.28 | -0.45 | -0.52 | 0.87 | -0.0079 | -1.652 | -1.5142 | 1.212 | -1.97 | 2.69 | 2.47 |
| carbamazepine | 0.95 | 0.95 | 0.99 | 2.04 | -1.24 | -1.28 | 0.97 | -0.0267 | -1.625 | -0.5881 | 6.357 | -4.86 | 1.24 | 0.45 |
| carbegoline | 0.68 | 0.68 | 1.00 | 0.95 | -0.33 | -0.33 | 1.00 | -0.0046 | -0.798 | -1.1288 | 0.546 | -1.13 | 1.66 | 2.34 |
| carvedilol | 0.73 | 0.9 | 1.23 | 1.19 | -0.95 | -0.43 | 2.21 | -0.0126 | -0.974 | 0.4678 | 1.437 | -1.36 | 0.92 | -0.44 |
| cefuroxime | 0.97 | 0.98 | 1.01 | 0.49 | -1.69 | -1.51 | 1.12 | -0.0085 | -3.380 | 0.8126 | 0.641 | -0.37 | 1.96 | -0.47 |
| celecoxib | 0.98 | 0.99 | 1.01 | 1.27 | -2.00 | -1.69 | 1.18 | -0.0256 | -2.057 | -1.9565 | 2.848 | -1.41 | 1.02 | 0.97 |
| celiprolol | 0.45 | 0.46 | 1.02 | 0.51 | 0.07 | 0.09 | 0.80 | 0.0008 | 0.253 | -0.1547 | -0.077 | -0.51 | 1.67 | -1.02 |
| cephalexin | 0.9 | 0.9 | 1.00 | 2.77 | -0.95 | -0.95 | 1.00 | -0.0293 | -6.816 | 0.7284 | -35.766 | 33.73 | 6.43 | -0.69 |

| | | | | | | | | | | | | | | |
|---------------------------|------|------|------|-------|-------|-------|------|---------|--------|---------|---------|--------|------|-------|
| cetirizine | 0.64 | 0.65 | 1.01 | 1.22 | -0.26 | -0.25 | 1.04 | -0.0049 | -0.279 | -0.1229 | 0.861 | -2.14 | 0.69 | 0.31 |
| chloramphenikol | 0.99 | 0.97 | 0.98 | 0.84 | -1.51 | -2.00 | 0.76 | -0.0131 | -2.745 | 6.0386 | 1.162 | -0.75 | 1.76 | -3.88 |
| chlorthalidone | 0.43 | 0.43 | 0.99 | 1.34 | 0.13 | 0.12 | 1.07 | 0.0041 | 0.146 | 0.0348 | 3.408 | 11.03 | 0.47 | 0.11 |
| cimetidine | 0.96 | 0.96 | 0.99 | 0.81 | -1.33 | -1.38 | 0.96 | -0.0113 | -1.769 | 2.1060 | 0.991 | -0.71 | 1.27 | -1.52 |
| ciprofloxacin | 0.64 | 0.67 | 1.05 | 0.59 | -0.31 | -0.25 | 1.23 | -0.0027 | -1.809 | 0.5213 | 0.240 | -0.52 | 3.94 | -1.14 |
| cisapride | 0.11 | 0.11 | 1.00 | 0.15 | 0.91 | 0.91 | 1.00 | 0.0125 | 3.027 | -0.4908 | -1.467 | -0.18 | 0.37 | -0.06 |
| clarithromycin | 0.64 | 0.63 | 0.98 | 0.73 | -0.23 | -0.25 | 0.93 | -0.0027 | -0.237 | -0.1027 | 0.279 | -0.76 | 0.65 | 0.28 |
| clindamycin | 0.99 | 0.99 | 0.99 | 0.54 | -1.82 | -2.00 | 0.91 | -0.0099 | -2.596 | -0.5751 | 0.764 | -0.41 | 1.41 | 0.31 |
| clobazam | 0.69 | 0.66 | 0.96 | 0.62 | -0.29 | -0.35 | 0.83 | -0.0027 | -0.310 | -0.1812 | 0.252 | -0.58 | 0.71 | 0.42 |
| clonidine | 0.95 | 0.95 | 1.00 | 2.36 | -1.28 | -1.28 | 1.00 | -0.0318 | -1.504 | 0.9134 | 13.161 | -9.78 | 1.12 | -0.68 |
| clorazepate | 0.49 | 0.50 | 1.02 | 1.37 | 0.00 | 0.02 | 0.00 | 0.0000 | 0.000 | 0.0000 | 0.000 | -14.00 | 1.67 | 1.79 |
| clozapine | 0.94 | 0.94 | 1.00 | 0.92 | -1.19 | -1.19 | 1.00 | -0.0117 | -1.226 | -0.4345 | 1.099 | -0.86 | 0.96 | 0.34 |
| ciproheptadine | 0.45 | 0.46 | 1.01 | 14.04 | 0.08 | 0.09 | 0.90 | 0.0242 | 0.079 | 0.0443 | 0.158 | 0.92 | 0.46 | 0.26 |
| desloratidine | 0.45 | 0.43 | 0.94 | 1.54 | 0.13 | 0.09 | 1.51 | 0.0048 | 0.135 | 0.1132 | 1.251 | 4.05 | 0.44 | 0.37 |
| diazepam | 0.36 | 0.35 | 0.97 | 1.40 | 0.27 | 0.25 | 1.08 | 0.0108 | 0.318 | 3.8406 | 1.813 | 2.36 | 0.41 | 5.00 |
| digoxin | 0.95 | 0.95 | 0.99 | 2.89 | -1.24 | -1.28 | 0.97 | -0.0378 | -1.260 | -0.4103 | -50.868 | 38.92 | 0.96 | 0.31 |
| dihydroergotamine | 0.80 | 0.77 | 0.96 | 0.38 | -0.51 | -0.60 | 0.85 | -0.0025 | -2.050 | -0.1920 | 0.190 | -0.28 | 3.06 | 0.29 |
| diphenhydramin | 0.72 | 0.75 | 1.04 | 0.63 | -0.48 | -0.41 | 1.16 | -0.0040 | -0.513 | 0.2261 | 0.355 | -0.56 | 0.81 | -0.36 |
| doxazosin | 0.42 | 0.33 | 0.77 | 2.61 | 0.32 | 0.14 | 2.26 | 0.0255 | 0.322 | 0.1519 | 0.913 | 0.94 | 0.33 | 0.16 |
| doxycycline | 0.8 | 0.81 | 1.01 | 0.66 | -0.63 | -0.60 | 1.05 | -0.0051 | -0.643 | -0.2943 | 0.445 | -0.57 | 0.83 | 0.38 |
| drotaverine | 0.06 | 0.05 | 0.75 | 0.02 | 1.33 | 1.19 | 1.11 | 0.0073 | 1.474 | -0.7133 | -0.562 | -0.02 | 0.05 | -0.02 |
| enalapril | 0.61 | 0.59 | 0.97 | 1.21 | -0.16 | -0.19 | 0.81 | -0.0032 | -0.181 | 0.1047 | 0.669 | -2.50 | 0.67 | -0.39 |
| eplerenone | 0.33 | 0.33 | 0.98 | 0.34 | 0.32 | 0.31 | 1.03 | 0.0033 | 0.577 | 0.1380 | -0.321 | -0.33 | 0.59 | 0.14 |
| escitalopram | 0.94 | 0.94 | 1.00 | 1.19 | -1.19 | -1.19 | 1.00 | -0.0151 | -2.390 | -0.6097 | 1.670 | -1.31 | 1.88 | 0.48 |
| estradiol benzoate | 0.42 | 0.42 | 1.00 | 1.16 | 0.14 | 0.14 | 1.00 | 0.0039 | 0.250 | 0.1611 | -4.227 | -12.67 | 0.75 | 0.48 |
| estrone | 0.97 | 0.98 | 1.01 | 1.62 | -1.69 | -1.51 | 1.12 | -0.0280 | -1.779 | -0.4024 | 1.583 | -0.92 | 1.03 | 0.23 |
| famotidine | 0.99 | 0.99 | 1.00 | 1.01 | -2.00 | -2.00 | 1.00 | -0.0204 | -2.101 | -0.6978 | 1.963 | -0.97 | 1.04 | 0.35 |
| fexofenadine | 0.70 | 0.71 | 1.01 | 0.30 | -0.39 | -0.37 | 1.06 | -0.0016 | -2.222 | 0.3503 | 0.119 | -0.22 | 4.06 | -0.64 |
| flouxetine | 0.61 | 0.60 | 0.98 | 0.73 | -0.17 | -0.19 | 0.86 | -0.0021 | -0.257 | -0.0438 | 0.223 | -0.79 | 0.92 | 0.16 |
| flupenthixol | 0.68 | 0.67 | 0.99 | 3.15 | -0.31 | -0.33 | 0.94 | -0.0145 | -0.325 | -0.1594 | -1.487 | 3.24 | 0.71 | 0.35 |
| furosemide | 0.51 | 0.52 | 1.02 | 1.00 | -0.03 | -0.02 | 2.00 | -0.0007 | -0.037 | -0.0065 | 0.122 | -1.82 | 0.55 | 0.10 |
| gliclazide | 0.92 | 0.92 | 1.00 | 0.70 | -1.06 | -1.06 | 1.00 | -0.0081 | -1.117 | 4.4196 | 0.685 | -0.59 | 0.97 | -3.83 |
| gliclazide | 0.95 | 0.95 | 1.00 | 1.09 | -1.28 | -1.28 | 1.00 | -0.0147 | -1.360 | -0.6730 | 1.516 | -1.13 | 1.01 | 0.50 |

| | | | | | | | | | | | | | | |
|-------------------------------|------|------|------|------|-------|-------|------|---------|--------|---------|--------|--------|------|-------|
| haloperidol | 0.66 | 0.65 | 0.98 | 1.59 | -0.26 | -0.29 | 0.90 | -0.0064 | -0.282 | -0.1980 | 2.551 | -6.35 | 0.70 | 0.49 |
| hydrocortisone acetate | 0.96 | 0.96 | 1.00 | 1.59 | -1.38 | -1.38 | 1.00 | -0.0228 | -1.453 | -0.3286 | 3.286 | -2.29 | 1.01 | 0.23 |
| hydroxyzine | 0.55 | 0.55 | 1.00 | 1.53 | -0.09 | -0.09 | 1.00 | -0.0024 | -0.094 | -0.0709 | 3.108 | -19.61 | 0.59 | 0.45 |
| ibuprofen | 0.93 | 0.90 | 0.96 | 2.40 | -0.93 | -1.12 | 0.83 | -0.0249 | -0.980 | -0.2430 | 18.687 | -17.97 | 0.94 | 0.23 |
| indomethacin | 0.88 | 0.90 | 1.02 | 1.42 | -0.95 | -0.87 | 1.10 | -0.0150 | -0.984 | 0.6673 | 2.028 | -1.91 | 0.93 | -0.63 |
| ketoprofen | 0.89 | 0.89 | 1.00 | 1.64 | -0.91 | -0.91 | 1.00 | -0.0167 | -0.917 | -0.3547 | 2.812 | -2.76 | 0.90 | 0.35 |
| ketotifen | 0.34 | 0.36 | 1.06 | 0.74 | 0.25 | 0.29 | 0.87 | 0.0051 | 0.333 | 0.9611 | -1.087 | -1.57 | 0.48 | 1.38 |
| lamotrigine | 0.89 | 0.90 | 1.01 | 0.99 | -0.93 | -0.91 | 1.02 | -0.0103 | -1.692 | -0.6744 | 1.029 | -0.99 | 1.63 | 0.65 |
| levocetizine | 0.63 | 0.64 | 1.02 | 1.21 | -0.25 | -0.23 | 1.08 | -0.0047 | -0.273 | -0.0718 | 0.830 | -2.13 | 0.70 | 0.18 |
| levofloxacin | 0.17 | 0.17 | 0.97 | 0.23 | 0.70 | 0.69 | 1.02 | 0.0096 | 2.272 | 1.1358 | -1.125 | -0.26 | 0.53 | 0.27 |
| loperamide | 0.68 | 0.67 | 0.99 | 1.53 | -0.31 | -0.33 | 0.94 | -0.0070 | -0.317 | -0.0614 | 2.004 | -4.37 | 0.69 | 0.13 |
| loratadine | 0.94 | 0.94 | 1.00 | 2.22 | -1.19 | -1.19 | 1.00 | -0.0282 | -1.219 | -3.9833 | 9.061 | -7.13 | 0.96 | 3.13 |
| lorazepam | 0.94 | 0.94 | 1.00 | 1.52 | -1.19 | -1.19 | 1.00 | -0.0194 | -1.374 | -0.3494 | 2.716 | -2.14 | 1.08 | 0.27 |
| medazepam | 0.91 | 0.94 | 1.03 | 6.03 | -1.19 | -1.00 | 1.19 | -0.0766 | -1.207 | -0.2785 | -4.018 | 3.16 | 0.95 | 0.22 |
| meloxicam | 0.99 | 0.98 | 0.99 | 0.72 | -1.69 | -2.00 | 0.85 | -0.0124 | -1.707 | 1.4571 | 1.035 | -0.60 | 0.99 | -0.84 |
| methyldopa | 0.38 | 0.37 | 0.96 | 0.35 | 0.24 | 0.21 | 1.13 | 0.0023 | 1.202 | -0.1647 | -0.216 | -0.33 | 1.83 | -0.25 |
| mianserin | 0.54 | 0.55 | 1.01 | 8.41 | -0.08 | -0.07 | 1.13 | -0.0121 | -0.087 | -0.0834 | -0.177 | 1.23 | 0.61 | 0.58 |
| midazolam | 0.82 | 0.83 | 1.01 | 3.27 | -0.67 | -0.66 | 1.02 | -0.0267 | -0.694 | -0.1975 | -4.709 | 5.77 | 0.85 | 0.24 |
| mirtazapine | 0.39 | 0.39 | 0.99 | 1.99 | 0.20 | 0.19 | 1.05 | 0.0105 | 0.239 | 0.1754 | 0.858 | 1.62 | 0.45 | 0.33 |
| montelukast | 0.95 | 0.95 | 1.00 | 1.35 | -1.28 | -1.28 | 1.00 | -0.0182 | -1.292 | -0.3096 | 2.206 | -1.64 | 0.96 | 0.23 |
| naproxen | 0.92 | 0.89 | 0.97 | 1.91 | -0.91 | -1.06 | 0.86 | -0.0195 | -0.917 | -0.3037 | 4.598 | -4.51 | 0.90 | 0.30 |
| nebivolol | 0.75 | 0.75 | 1.00 | 1.06 | -0.48 | -0.48 | 1.00 | -0.0067 | -0.487 | 0.4632 | 0.811 | -1.28 | 0.77 | -0.73 |
| olanzapine | 0.28 | 0.29 | 1.02 | 0.34 | 0.40 | 0.41 | 0.97 | 0.0048 | 2.283 | -0.2561 | -0.500 | -0.36 | 1.63 | -0.18 |
| oxazepam | 0.93 | 0.94 | 1.01 | 1.52 | -1.16 | -1.12 | 1.03 | -0.0188 | -1.362 | -0.3979 | 2.631 | -2.12 | 1.10 | 0.32 |
| oxybutinin | 0.68 | 0.66 | 0.97 | 1.33 | -0.29 | -0.33 | 0.88 | -0.0058 | -0.313 | -0.0889 | 1.155 | -2.65 | 0.72 | 0.20 |
| pantoprazole | 0.93 | 0.92 | 0.99 | 1.07 | -1.06 | -1.12 | 0.94 | -0.0123 | -1.082 | 0.5612 | 1.271 | -1.10 | 0.94 | -0.49 |
| paracetamol | 0.93 | 0.94 | 1.01 | 1.90 | -1.16 | -1.12 | 1.03 | -0.0235 | -4.632 | 0.8772 | 4.779 | -3.86 | 3.74 | -0.71 |
| paroxetine | 0.55 | 0.56 | 1.02 | 1.41 | -0.10 | -0.09 | 1.20 | -0.0026 | -0.111 | 0.2137 | 1.183 | -6.33 | 0.60 | -1.14 |
| pergolide | 0.48 | 0.47 | 0.98 | 1.06 | 0.05 | 0.03 | 1.50 | 0.0012 | 0.058 | 0.0228 | -0.322 | -2.90 | 0.52 | 0.21 |
| perindopril | 0.47 | 0.46 | 0.97 | 0.47 | 0.08 | 0.05 | 1.50 | 0.0008 | 0.523 | 0.0381 | -0.079 | -0.46 | 3.03 | 0.22 |
| phenytoin | 0.97 | 0.97 | 1.00 | 1.67 | -1.51 | -1.51 | 1.00 | -0.0259 | -1.677 | -2.0680 | 3.929 | -2.52 | 1.08 | 1.33 |
| pindolol | 0.53 | 0.52 | 0.98 | 0.91 | -0.03 | -0.05 | 0.67 | -0.0006 | -0.087 | 0.0283 | 0.094 | -1.41 | 1.30 | -0.42 |
| piroxicam | 0.98 | 0.98 | 1.00 | 0.91 | -1.69 | -1.69 | 1.00 | -0.0157 | -1.707 | -1.5796 | 1.432 | -0.83 | 0.99 | 0.92 |

| | | | | | | | | | | | | | | |
|-----------------------|------|------|------|------|-------|-------|------|---------|--------|---------|--------|--------|------|--------|
| prednisolone | 0.94 | 0.94 | 0.99 | 0.99 | -1.16 | -1.19 | 0.97 | -0.0122 | -1.287 | -0.5761 | 1.193 | -0.96 | 1.04 | 0.47 |
| progesterone | 0.96 | 0.96 | 1.00 | 2.06 | -1.38 | -1.38 | 1.00 | -0.0297 | -1.416 | -0.4424 | 6.989 | -4.86 | 0.98 | 0.31 |
| promazine | 0.39 | 0.37 | 0.95 | 1.16 | 0.23 | 0.19 | 1.19 | 0.0073 | 0.246 | 0.0711 | 6.000 | 9.61 | 0.39 | 0.11 |
| promethazine | 0.43 | 0.42 | 0.98 | 1.32 | 0.14 | 0.12 | 1.15 | 0.0044 | 0.151 | -0.7009 | 3.639 | 10.90 | 0.45 | -2.10 |
| propafenone | 0.57 | 0.59 | 1.04 | 1.01 | -0.16 | -0.12 | 1.29 | -0.0027 | -0.163 | -0.0850 | 0.405 | -1.51 | 0.61 | 0.32 |
| propranolol | 0.54 | 0.50 | 0.93 | 1.21 | 0.00 | -0.07 | 0.00 | 0.0000 | 0.000 | 0.0000 | 0.000 | -4.28 | 0.56 | 0.18 |
| quetiapine | 0.68 | 0.68 | 1.00 | 0.92 | -0.33 | -0.33 | 1.00 | -0.0044 | -0.394 | -0.1153 | 0.519 | -1.08 | 0.82 | 0.24 |
| quinapril | 0.44 | 0.44 | 1.00 | 0.46 | 0.10 | 0.10 | 1.00 | 0.0011 | 0.108 | 0.0620 | -0.106 | -0.45 | 0.45 | 0.26 |
| risperidone | 0.29 | 0.29 | 0.98 | 0.46 | 0.40 | 0.39 | 1.03 | 0.0064 | 0.454 | 0.6341 | -0.900 | -0.64 | 0.32 | 0.45 |
| rizatriptan | 0.20 | 0.20 | 0.98 | 0.33 | 0.62 | 0.60 | 1.02 | 0.0104 | 4.398 | -2.2806 | -1.544 | -0.49 | 1.39 | -0.72 |
| rosuvastatin | 0.9 | 0.89 | 0.99 | 0.63 | -0.91 | -0.95 | 0.95 | -0.0064 | -1.032 | -0.7695 | 0.532 | -0.52 | 1.01 | 0.75 |
| roxitromicin | 0.91 | 0.92 | 1.01 | 0.42 | -1.06 | -1.00 | 1.06 | -0.0049 | -1.105 | -0.3658 | 0.363 | -0.31 | 0.96 | 0.32 |
| rupatadine | 0.42 | 0.43 | 1.02 | 1.48 | 0.12 | 0.14 | 0.87 | 0.0042 | 0.124 | 0.0751 | 1.480 | 5.20 | 0.44 | 0.26 |
| sertraline | 0.53 | 0.53 | 1.00 | 4.41 | -0.05 | -0.05 | 1.00 | -0.0043 | -0.053 | -0.0311 | -0.147 | 1.49 | 0.54 | 0.32 |
| sildenafil | 0.69 | 0.67 | 0.97 | 0.61 | -0.31 | -0.35 | 0.89 | -0.0028 | -0.320 | 0.2092 | 0.256 | -0.56 | 0.70 | -0.46 |
| simvastatin | 0.19 | 0.17 | 0.89 | 0.23 | 0.69 | 0.63 | 1.09 | 0.0095 | 0.725 | 0.1554 | -1.114 | -0.27 | 0.18 | 0.04 |
| spironolactone | 0.98 | 0.96 | 0.97 | 1.11 | -1.33 | -1.69 | 0.78 | -0.0155 | -1.474 | -0.3984 | 1.609 | -1.16 | 1.06 | 0.29 |
| sulpiride | 0.27 | 0.26 | 0.96 | 0.24 | 0.45 | 0.43 | 1.05 | 0.0041 | 1.136 | 0.9464 | -0.374 | -0.21 | 0.65 | 0.54 |
| telmisartan | 0.90 | 0.90 | 0.99 | 1.42 | -0.93 | -0.95 | 0.98 | -0.0148 | -0.935 | -0.1259 | 2.013 | -1.94 | 0.90 | 0.12 |
| temazepam | 0.94 | 0.94 | 0.99 | 1.77 | -1.16 | -1.19 | 0.97 | -0.0219 | -1.206 | -0.3676 | 3.867 | -3.12 | 0.97 | 0.30 |
| theophylline | 0.86 | 0.87 | 1.01 | 1.25 | -0.81 | -0.79 | 1.02 | -0.0116 | -2.017 | 0.6158 | 1.436 | -1.54 | 2.16 | -0.66 |
| thioridazine | 0.47 | 0.43 | 0.91 | 0.75 | 0.12 | 0.05 | 2.35 | 0.0021 | 0.129 | 0.0293 | -0.334 | -1.17 | 0.45 | 0.10 |
| tolterodine | 0.1 | 0.08 | 0.80 | 0.34 | 1.06 | 0.95 | 1.11 | 0.0452 | 1.101 | 0.3274 | 6.186 | 0.47 | 0.08 | 0.02 |
| trazodone | 0.71 | 0.72 | 1.01 | 1.69 | -0.40 | -0.39 | 1.03 | -0.0094 | -0.434 | -0.1427 | 3.044 | -5.45 | 0.78 | 0.26 |
| tropicamid | 0.85 | 0.86 | 1.01 | 1.61 | -0.79 | -0.75 | 1.05 | -0.0148 | -1.752 | 78.8370 | 2.561 | -2.79 | 1.91 | -86.00 |
| valproic acid | 0.69 | 0.67 | 0.97 | 1.80 | -0.31 | -0.35 | 0.89 | -0.0082 | -0.362 | -0.1178 | 6.176 | -13.45 | 0.79 | 0.26 |
| valsartan | 0.89 | 0.91 | 1.02 | 0.81 | -0.98 | -0.91 | 1.08 | -0.0087 | -1.025 | -0.2523 | 0.786 | -0.73 | 0.95 | 0.23 |
| venlafaxine | 0.36 | 0.37 | 1.03 | 1.13 | 0.23 | 0.25 | 0.93 | 0.0071 | 0.856 | 0.1605 | 9.712 | 15.55 | 1.37 | 0.26 |
| verapamil | 0.54 | 0.53 | 0.97 | 0.82 | -0.04 | -0.07 | 0.62 | -0.0007 | -0.048 | -0.0763 | 0.091 | -1.10 | 0.58 | 0.92 |
| zolmitriptane | 0.31 | 0.29 | 0.94 | 0.51 | 0.39 | 0.35 | 1.12 | 0.0068 | 1.555 | -0.3850 | -1.049 | -0.78 | 1.16 | -0.29 |
| zolpidem | 0.86 | 0.88 | 1.02 | 2.34 | -0.87 | -0.79 | 1.10 | -0.0230 | -0.941 | -1.0062 | 15.802 | -16.07 | 0.96 | 1.02 |
| zopiclone | 0.96 | 0.96 | 1.00 | 1.05 | -1.38 | -1.38 | 1.00 | -0.0150 | -3.067 | -0.5975 | 1.498 | -1.04 | 2.13 | 0.42 |
| zuclopenthixol | 0.47 | 0.47 | 1.00 | 0.90 | 0.05 | 0.05 | 1.00 | 0.0010 | 0.053 | 0.0105 | -0.183 | -1.65 | 0.48 | 0.09 |

* R_f value from the non-impregnated NP plate (control)

** R_f value from the NP plate impregnated with 2 mg/mL BSA solution

Table S4. Chromatographic data and their derivatives obtained from the RP TLC experiment for 129 APIs.

| API | C _{RP} [*] | RP ^{**} | RP/C | RP/PSA | R _M RP | R _M RP | R _M RP/C | R _M RP/PSA | R _M RP/PB | R _M RP/logP | R _M RP/B2 | RP/B2 | RP/PB | RP/logP |
|----------------------|------------------------------|------------------|------|--------|-------------------|-------------------|---------------------|-----------------------|----------------------|------------------------|----------------------|--------|-------|---------|
| acebutolol | 0.78 | 0.82 | 1.05 | 0.94 | -0.55 | -0.66 | 1.20 | -0.01 | -2.533 | 1.996 | 0.770 | -0.96 | 3.15 | -2.48 |
| aceclofenac | 0.93 | 0.93 | 1.00 | 1.23 | -1.12 | -1.12 | 1.00 | -0.01 | -1.135 | -0.317 | 1.694 | -1.40 | 0.94 | 0.26 |
| acenocumarol | 0.93 | 0.92 | 0.99 | 0.84 | -1.12 | -1.06 | 0.94 | -0.01 | -1.075 | -0.396 | 0.881 | -0.76 | 0.93 | 0.34 |
| acetylsalicylic acid | 0.98 | 0.99 | 1.01 | 1.56 | -1.69 | -2.00 | 1.18 | -0.03 | -2.006 | -1.535 | 4.241 | -2.10 | 0.99 | 0.76 |
| aciclovir | 0.99 | 0.98 | 0.99 | 0.89 | -2.00 | -1.69 | 0.85 | -0.02 | -8.049 | 1.166 | 1.397 | -0.81 | 4.67 | -0.68 |
| alprazolam | 0.80 | 0.78 | 0.98 | 2.05 | -0.60 | -0.55 | 0.91 | -0.01 | -0.687 | -0.117 | 8.692 | -12.33 | 0.98 | 0.17 |
| amiodarone | 0.33 | 0.34 | 1.03 | 0.80 | 0.31 | 0.29 | 0.94 | 0.01 | 0.300 | 0.096 | -2.120 | -2.50 | 0.35 | 0.11 |
| amlodipine | 0.61 | 0.68 | 1.11 | 0.68 | -0.19 | -0.33 | 1.69 | 0.00 | -0.336 | 0.217 | 0.311 | -0.65 | 0.70 | -0.45 |
| amoxilcillin | 0.99 | 0.98 | 0.99 | 0.62 | -2.00 | -1.69 | 0.85 | -0.01 | -8.451 | 11.268 | 0.851 | -0.49 | 4.90 | -6.53 |
| astemizol | 0.65 | 0.62 | 0.95 | 1.66 | -0.27 | -0.21 | 0.79 | -0.01 | -0.220 | -0.299 | 4.149 | -12.10 | 0.64 | 0.87 |
| atorvastatin | 0.80 | 0.89 | 1.11 | 0.80 | -0.60 | -0.91 | 1.51 | -0.01 | -0.927 | -0.590 | 0.731 | -0.72 | 0.91 | 0.58 |
| atropine | 0.73 | 0.72 | 0.99 | 1.45 | -0.43 | -0.41 | 0.95 | -0.01 | -2.279 | -0.240 | 1.645 | -2.89 | 4.00 | 0.42 |
| azithromycin | 0.24 | 0.24 | 1.00 | 0.13 | 0.50 | 0.50 | 1.00 | 0.00 | 1.726 | 0.205 | -0.214 | -0.10 | 0.83 | 0.10 |
| betaxolol | 0.27 | 0.25 | 0.93 | 0.49 | 0.43 | 0.48 | 1.10 | 0.01 | 0.954 | 0.477 | -1.804 | -0.95 | 0.50 | 0.25 |
| bilastine | 0.76 | 0.72 | 0.95 | 0.92 | -0.50 | -0.41 | 0.82 | -0.01 | -0.471 | -0.195 | 0.579 | -1.02 | 0.83 | 0.34 |
| biperiden | 0.87 | 0.85 | 0.98 | 3.62 | -0.83 | -0.75 | 0.91 | -0.03 | -1.256 | -0.278 | -4.393 | 4.96 | 1.42 | 0.31 |
| bisoprolol | 0.57 | 0.56 | 0.98 | 0.93 | -0.12 | -0.10 | 0.86 | 0.00 | -0.349 | -0.049 | 0.254 | -1.36 | 1.87 | 0.26 |
| bromazepam | 0.83 | 0.81 | 0.98 | 1.49 | -0.69 | -0.63 | 0.91 | -0.01 | -0.900 | -0.243 | 1.952 | -2.51 | 1.16 | 0.31 |
| bromocriptine | 0.69 | 0.70 | 1.01 | 0.59 | -0.35 | -0.37 | 1.06 | 0.00 | -0.396 | -0.082 | 0.274 | -0.52 | 0.75 | 0.16 |
| buspirone | 0.70 | 0.69 | 0.99 | 0.99 | -0.37 | -0.35 | 0.94 | 0.00 | -0.366 | -0.294 | 0.613 | -1.22 | 0.73 | 0.58 |
| caffeine | 0.91 | 0.90 | 0.99 | 1.68 | -1.00 | -0.95 | 0.95 | -0.02 | -3.181 | 0.900 | 3.087 | -2.91 | 3.00 | -0.85 |
| capecitabine | 0.90 | 0.89 | 0.99 | 0.74 | -0.95 | -0.91 | 0.95 | -0.01 | -1.513 | -1.713 | 0.656 | -0.64 | 1.48 | 1.68 |
| captopril | 0.99 | 0.99 | 1.00 | 1.72 | -2.00 | -2.00 | 1.00 | -0.03 | -7.257 | -6.652 | 5.325 | -2.64 | 3.60 | 3.30 |
| carbamazepine | 0.83 | 0.84 | 1.01 | 1.81 | -0.69 | -0.72 | 1.05 | -0.02 | -0.948 | -0.343 | 3.707 | -4.32 | 1.11 | 0.40 |
| carbegoline | 0.68 | 0.68 | 1.00 | 0.95 | -0.33 | -0.33 | 1.00 | 0.00 | -0.798 | -1.129 | 0.546 | -1.13 | 1.66 | 2.34 |
| carvedilol | 0.59 | 0.61 | 1.03 | 0.81 | -0.16 | -0.19 | 1.23 | 0.00 | -0.198 | 0.095 | 0.292 | -0.92 | 0.62 | -0.30 |
| cefuroxime | 0.88 | 0.87 | 0.99 | 0.44 | -0.87 | -0.83 | 0.95 | 0.00 | -1.651 | 0.397 | 0.313 | -0.33 | 1.74 | -0.42 |
| celecoxib | 0.75 | 0.75 | 1.00 | 0.96 | -0.48 | -0.48 | 1.00 | -0.01 | -0.492 | -0.468 | 0.681 | -1.07 | 0.77 | 0.74 |
| celiprolol | 0.75 | 0.79 | 1.05 | 0.87 | -0.48 | -0.58 | 1.21 | -0.01 | -2.092 | 1.279 | 0.634 | -0.87 | 2.87 | -1.76 |
| cephalexin | 0.99 | 0.99 | 1.00 | 3.04 | -2.00 | -2.00 | 1.00 | -0.06 | -14.255 | 1.523 | -74.799 | 37.11 | 7.07 | -0.76 |

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|---------------------------|------|------|------|-------|-------|-------|------|-------|---------|--------|---------|--------|------|-------|
| cetirizine | 0.83 | 0.82 | 0.99 | 1.55 | -0.69 | -0.66 | 0.96 | -0.01 | -0.708 | -0.312 | 2.187 | -2.72 | 0.88 | 0.39 |
| chloramphenikol | 0.89 | 0.89 | 1.00 | 0.77 | -0.91 | -0.91 | 1.00 | -0.01 | -1.651 | 3.632 | 0.699 | -0.69 | 1.62 | -3.56 |
| chlorthalidone | 0.49 | 0.50 | 1.02 | 1.57 | 0.02 | 0.00 | 0.00 | 0.00 | 0.000 | 0.000 | 0.000 | 12.98 | 0.56 | 0.13 |
| cimetidine | 0.91 | 0.92 | 1.01 | 0.78 | -1.00 | -1.06 | 1.06 | -0.01 | -1.414 | 1.684 | 0.792 | -0.69 | 1.23 | -1.46 |
| ciprofloxacin | 0.88 | 0.87 | 0.99 | 0.76 | -0.87 | -0.83 | 0.95 | -0.01 | -4.856 | 1.399 | 0.645 | -0.68 | 5.12 | -1.47 |
| cisapride | 0.38 | 0.21 | 0.55 | 0.29 | 0.21 | 0.58 | 2.71 | 0.01 | 1.918 | -0.311 | -0.929 | -0.34 | 0.70 | -0.11 |
| clarithromycin | 0.65 | 0.62 | 0.95 | 0.72 | -0.27 | -0.21 | 0.79 | 0.00 | -0.218 | -0.094 | 0.256 | -0.75 | 0.64 | 0.28 |
| clindamycin | 0.83 | 0.78 | 0.94 | 0.43 | -0.69 | -0.55 | 0.80 | 0.00 | -0.785 | -0.174 | 0.231 | -0.33 | 1.11 | 0.25 |
| clobazam | 0.25 | 0.25 | 1.00 | 0.24 | 0.48 | 0.48 | 1.00 | 0.00 | 0.513 | 0.300 | -0.417 | -0.22 | 0.27 | 0.16 |
| clonidine | 0.79 | 0.80 | 1.01 | 1.99 | -0.58 | -0.60 | 1.05 | -0.01 | -0.708 | 0.430 | 6.197 | -8.23 | 0.94 | -0.57 |
| clorazepate | 0.73 | 0.68 | 0.93 | 1.87 | -0.43 | -0.33 | 0.76 | -0.01 | -1.091 | -1.169 | 9.165 | -19.04 | 2.27 | 2.43 |
| clozapine | 0.81 | 0.81 | 1.00 | 0.79 | -0.63 | -0.63 | 1.00 | -0.01 | -0.646 | -0.229 | 0.579 | -0.74 | 0.83 | 0.29 |
| clozapine | 0.57 | 0.57 | 1.00 | 17.59 | -0.12 | -0.12 | 1.00 | -0.04 | -0.124 | -0.069 | -0.247 | 1.15 | 0.58 | 0.32 |
| cypheptadine | 0.45 | 0.47 | 1.04 | 1.70 | 0.09 | 0.05 | 0.60 | 0.00 | 0.054 | 0.045 | 0.497 | 4.48 | 0.48 | 0.41 |
| desloratidine | 0.58 | 0.58 | 1.00 | 2.33 | -0.14 | -0.14 | 1.00 | -0.01 | -0.166 | -2.003 | -0.945 | 3.91 | 0.69 | 8.29 |
| diazepam | 0.77 | 0.77 | 1.00 | 2.36 | -0.52 | -0.52 | 1.00 | -0.02 | -0.535 | -0.174 | -21.613 | 31.71 | 0.79 | 0.26 |
| digoxin | 0.84 | 0.85 | 1.01 | 0.42 | -0.72 | -0.75 | 1.05 | 0.00 | -3.013 | -0.282 | 0.279 | -0.31 | 3.40 | 0.32 |
| dihydroergotamine | 0.78 | 0.78 | 1.00 | 0.66 | -0.55 | -0.55 | 1.00 | 0.00 | -0.591 | 0.261 | 0.409 | -0.58 | 0.84 | -0.37 |
| diphenhydramin | 0.58 | 0.54 | 0.93 | 4.33 | -0.14 | -0.07 | 0.50 | -0.01 | -0.071 | -0.033 | -0.200 | 1.55 | 0.55 | 0.26 |
| doxazosin | 0.75 | 0.73 | 0.97 | 0.59 | -0.48 | -0.43 | 0.91 | 0.00 | -0.441 | -0.202 | 0.305 | -0.52 | 0.74 | 0.34 |
| doxycycline | 0.08 | 0.09 | 1.13 | 0.05 | 1.06 | 1.00 | 0.95 | 0.01 | 1.116 | -0.540 | -0.426 | -0.04 | 0.10 | -0.05 |
| drotaverine | 0.55 | 0.58 | 1.05 | 1.18 | -0.09 | -0.14 | 1.61 | 0.00 | -0.160 | 0.093 | 0.593 | -2.46 | 0.66 | -0.38 |
| enalapril | 0.60 | 0.58 | 0.97 | 0.60 | -0.18 | -0.14 | 0.80 | 0.00 | -0.255 | -0.061 | 0.142 | -0.59 | 1.05 | 0.25 |
| eplerenone | 0.84 | 0.85 | 1.01 | 1.08 | -0.72 | -0.75 | 1.05 | -0.01 | -1.507 | -0.384 | 1.053 | -1.19 | 1.70 | 0.43 |
| escitalopram | 0.55 | 0.52 | 0.95 | 1.43 | -0.09 | -0.03 | 0.40 | 0.00 | -0.062 | -0.040 | 1.048 | -15.68 | 0.93 | 0.60 |
| estradiol benzoate | 0.63 | 0.62 | 0.98 | 1.03 | -0.23 | -0.21 | 0.92 | 0.00 | -0.224 | -0.051 | 0.199 | -0.58 | 0.65 | 0.15 |
| estrone | 0.79 | 0.77 | 0.97 | 0.79 | -0.58 | -0.52 | 0.91 | -0.01 | -0.552 | -0.183 | 0.516 | -0.76 | 0.81 | 0.27 |
| famotidine | 0.98 | 0.99 | 1.01 | 0.42 | -1.69 | -2.00 | 1.18 | -0.01 | -11.404 | 1.798 | 0.613 | -0.30 | 5.66 | -0.89 |
| fexofenadine | 0.85 | 0.86 | 1.01 | 1.06 | -0.75 | -0.79 | 1.05 | -0.01 | -1.213 | -0.207 | 1.053 | -1.15 | 1.32 | 0.23 |
| fluoxetine | 0.54 | 0.73 | 1.35 | 3.43 | -0.07 | -0.43 | 6.20 | -0.02 | -0.457 | -0.224 | -2.088 | 3.53 | 0.77 | 0.38 |
| flupenthixol | 0.66 | 0.66 | 1.00 | 1.27 | -0.29 | -0.29 | 1.00 | -0.01 | -0.303 | -0.054 | 1.010 | -2.31 | 0.69 | 0.12 |
| furosemide | 0.96 | 0.96 | 1.00 | 0.73 | -1.38 | -1.38 | 1.00 | -0.01 | -1.453 | 5.751 | 0.891 | -0.62 | 1.01 | -4.00 |
| gliclazide | 0.83 | 0.80 | 0.96 | 0.92 | -0.69 | -0.60 | 0.87 | -0.01 | -0.640 | -0.317 | 0.714 | -0.95 | 0.85 | 0.42 |

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|-------------------------------|------|------|------|------|-------|-------|------|-------|--------|--------|--------|--------|------|-------|
| haloperidol | 0.61 | 0.64 | 1.05 | 1.58 | -0.19 | -0.25 | 1.29 | -0.01 | -0.272 | -0.191 | 2.458 | -6.30 | 0.70 | 0.49 |
| hydrocortisone acetate | 0.82 | 0.82 | 1.00 | 1.36 | -0.66 | -0.66 | 1.00 | -0.01 | -0.693 | -0.157 | 1.568 | -1.95 | 0.86 | 0.20 |
| hydroxyzine | 0.62 | 0.59 | 0.95 | 1.64 | -0.21 | -0.16 | 0.74 | 0.00 | -0.170 | -0.129 | 5.637 | -21.04 | 0.63 | 0.48 |
| ibuprofen | 0.83 | 0.81 | 0.98 | 2.17 | -0.69 | -0.63 | 0.91 | -0.02 | -0.663 | -0.164 | 12.645 | -16.27 | 0.85 | 0.21 |
| indomethacin | 0.88 | 0.87 | 0.99 | 1.37 | -0.87 | -0.83 | 0.95 | -0.01 | -0.851 | 0.577 | 1.754 | -1.85 | 0.90 | -0.61 |
| ketoprofen | 0.91 | 0.86 | 0.95 | 1.58 | -1.00 | -0.79 | 0.78 | -0.01 | -0.796 | -0.308 | 2.441 | -2.66 | 0.87 | 0.34 |
| ketotifen | 0.75 | 0.74 | 0.99 | 1.52 | -0.48 | -0.45 | 0.95 | -0.01 | -0.606 | -1.747 | 1.977 | -3.22 | 0.99 | 2.85 |
| lamotrigine | 0.87 | 0.86 | 0.99 | 0.95 | -0.83 | -0.79 | 0.95 | -0.01 | -1.433 | -0.571 | 0.872 | -0.95 | 1.56 | 0.62 |
| levocetizine | 0.83 | 0.83 | 1.00 | 1.57 | -0.69 | -0.69 | 1.00 | -0.01 | -0.753 | -0.198 | 2.287 | -2.76 | 0.91 | 0.24 |
| levofloxacin | 0.27 | 0.30 | 1.11 | 0.41 | 0.43 | 0.37 | 0.85 | 0.01 | 1.187 | 0.594 | -0.588 | -0.48 | 0.97 | 0.48 |
| loperamide | 0.75 | 0.77 | 1.03 | 1.76 | -0.48 | -0.52 | 1.10 | -0.01 | -0.541 | -0.105 | 3.419 | -5.02 | 0.79 | 0.15 |
| loratadine | 0.68 | 0.68 | 1.00 | 1.60 | -0.33 | -0.33 | 1.00 | -0.01 | -0.334 | -1.091 | 2.482 | -5.16 | 0.69 | 2.27 |
| lorazepam | 0.83 | 0.83 | 1.00 | 1.35 | -0.69 | -0.69 | 1.00 | -0.01 | -0.792 | -0.201 | 1.565 | -1.89 | 0.95 | 0.24 |
| medazepam | 0.66 | 0.65 | 0.98 | 4.17 | -0.29 | -0.27 | 0.93 | -0.02 | -0.272 | -0.063 | -0.904 | 2.19 | 0.66 | 0.15 |
| meloxicam | 0.95 | 0.95 | 1.00 | 0.70 | -1.28 | -1.28 | 1.00 | -0.01 | -1.292 | 1.102 | 0.783 | -0.58 | 0.96 | -0.82 |
| methyldopa | 0.85 | 0.86 | 1.01 | 0.83 | -0.75 | -0.79 | 1.05 | -0.01 | -3.942 | 0.540 | 0.708 | -0.77 | 4.30 | -0.59 |
| mianserin | 0.55 | 0.55 | 1.00 | 8.49 | -0.09 | -0.09 | 1.00 | -0.01 | -0.097 | -0.093 | -0.197 | 1.24 | 0.61 | 0.59 |
| midazolam | 0.66 | 0.66 | 1.00 | 2.61 | -0.29 | -0.29 | 1.00 | -0.01 | -0.297 | -0.084 | -2.014 | 4.62 | 0.68 | 0.19 |
| mirtazapine | 0.58 | 0.58 | 1.00 | 2.99 | -0.14 | -0.14 | 1.00 | -0.01 | -0.165 | -0.121 | -0.591 | 2.45 | 0.68 | 0.50 |
| montelukast | 0.70 | 0.69 | 0.99 | 0.98 | -0.37 | -0.35 | 0.94 | 0.00 | -0.351 | -0.084 | 0.599 | -1.19 | 0.70 | 0.17 |
| naproxen | 0.88 | 0.87 | 0.99 | 1.87 | -0.87 | -0.83 | 0.95 | -0.02 | -0.834 | -0.276 | 4.181 | -4.41 | 0.88 | 0.29 |
| nebivolol | 0.40 | 0.40 | 1.00 | 0.56 | 0.18 | 0.18 | 1.00 | 0.00 | 0.180 | -0.171 | -0.299 | -0.68 | 0.41 | -0.39 |
| olanzapine | 0.53 | 0.50 | 0.94 | 0.59 | -0.05 | 0.00 | 0.00 | 0.00 | 0.000 | 0.000 | 0.000 | -0.63 | 2.86 | -0.32 |
| oxazepam | 0.83 | 0.84 | 1.01 | 1.36 | -0.69 | -0.72 | 1.05 | -0.01 | -0.847 | -0.247 | 1.637 | -1.91 | 0.99 | 0.29 |
| oxybutinin | 0.29 | 0.24 | 0.83 | 0.48 | 0.39 | 0.50 | 1.29 | 0.01 | 0.544 | 0.155 | -2.008 | -0.96 | 0.26 | 0.07 |
| pantoprazole | 0.85 | 0.83 | 0.98 | 0.96 | -0.75 | -0.69 | 0.91 | -0.01 | -0.703 | 0.364 | 0.825 | -0.99 | 0.85 | -0.44 |
| paracetamol | 0.92 | 0.92 | 1.00 | 1.86 | -1.06 | -1.06 | 1.00 | -0.02 | -4.243 | 0.804 | 4.378 | -3.80 | 3.68 | -0.70 |
| paroxetine | 0.60 | 0.67 | 1.12 | 1.69 | -0.18 | -0.31 | 1.75 | -0.01 | -0.327 | 0.628 | 3.474 | -7.57 | 0.71 | -1.37 |
| pergolide | 0.55 | 0.53 | 0.96 | 1.20 | -0.09 | -0.05 | 0.60 | 0.00 | -0.058 | -0.023 | 0.322 | -3.27 | 0.59 | 0.23 |
| perindopril | 0.57 | 0.58 | 1.02 | 0.60 | -0.12 | -0.14 | 1.15 | 0.00 | -0.935 | -0.068 | 0.142 | -0.59 | 3.87 | 0.28 |
| phenytoin | 0.87 | 0.86 | 0.99 | 1.48 | -0.83 | -0.79 | 0.95 | -0.01 | -0.876 | -1.080 | 2.052 | -2.24 | 0.96 | 1.18 |
| pindolol | 0.76 | 0.78 | 1.03 | 1.36 | -0.50 | -0.55 | 1.10 | -0.01 | -1.374 | 0.447 | 1.488 | -2.11 | 1.95 | -0.63 |
| piroxicam | 0.58 | 0.60 | 1.03 | 0.56 | -0.14 | -0.18 | 1.26 | 0.00 | -0.178 | -0.165 | 0.149 | -0.51 | 0.61 | 0.56 |

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|-----------------------|------|------|------|------|-------|-------|------|-------|--------|--------|---------|--------|------|--------|
| prednisolone | 0.87 | 0.88 | 1.01 | 0.93 | -0.83 | -0.87 | 1.05 | -0.01 | -0.961 | -0.430 | 0.892 | -0.91 | 0.98 | 0.44 |
| progesterone | 0.71 | 0.68 | 0.96 | 1.46 | -0.39 | -0.33 | 0.84 | -0.01 | -0.336 | -0.105 | 1.658 | -3.44 | 0.70 | 0.22 |
| promazine | 0.51 | 0.51 | 1.00 | 1.60 | -0.02 | -0.02 | 1.00 | 0.00 | -0.018 | -0.005 | -0.451 | 13.24 | 0.54 | 0.16 |
| promethazine | 0.49 | 0.47 | 0.96 | 1.48 | 0.02 | 0.05 | 3.00 | 0.00 | 0.056 | -0.261 | 1.355 | 12.20 | 0.51 | -2.35 |
| propafenone | 0.56 | 0.61 | 1.09 | 1.04 | -0.10 | -0.19 | 1.85 | 0.00 | -0.200 | -0.104 | 0.498 | -1.56 | 0.63 | 0.33 |
| propranolol | 0.64 | 0.63 | 0.98 | 1.52 | -0.25 | -0.23 | 0.93 | -0.01 | -0.257 | -0.083 | 1.978 | -5.39 | 0.70 | 0.23 |
| quetiapine | 0.73 | 0.69 | 0.95 | 0.94 | -0.43 | -0.35 | 0.80 | 0.00 | -0.419 | -0.122 | 0.551 | -1.09 | 0.83 | 0.24 |
| quinapril | 0.57 | 0.56 | 0.98 | 0.58 | -0.12 | -0.10 | 0.86 | 0.00 | -0.108 | -0.062 | 0.106 | -0.57 | 0.58 | 0.33 |
| risperidone | 0.62 | 0.58 | 0.94 | 0.94 | -0.21 | -0.14 | 0.66 | 0.00 | -0.159 | -0.223 | 0.316 | -1.31 | 0.66 | 0.92 |
| rizatriptan | 0.72 | 0.77 | 1.07 | 1.30 | -0.41 | -0.52 | 1.28 | -0.01 | -3.748 | 1.944 | 1.316 | -1.93 | 5.50 | -2.85 |
| rosuvastatin | 0.92 | 0.88 | 0.96 | 0.62 | -1.06 | -0.87 | 0.82 | -0.01 | -0.983 | -0.733 | 0.507 | -0.52 | 1.00 | 0.75 |
| roxitromicin | 0.80 | 0.79 | 0.99 | 0.36 | -0.60 | -0.58 | 0.96 | 0.00 | -0.599 | -0.198 | 0.197 | -0.27 | 0.82 | 0.27 |
| rupatadine | 0.55 | 0.52 | 0.95 | 1.79 | -0.09 | -0.03 | 0.40 | 0.00 | -0.035 | -0.021 | -0.420 | 6.29 | 0.53 | 0.32 |
| sertraline | 0.49 | 0.48 | 0.98 | 3.99 | 0.02 | 0.03 | 2.00 | 0.00 | 0.035 | 0.021 | 0.098 | 1.35 | 0.49 | 0.29 |
| sildenafil | 0.77 | 0.76 | 0.99 | 0.70 | -0.52 | -0.50 | 0.95 | 0.00 | -0.521 | 0.341 | 0.417 | -0.63 | 0.79 | -0.52 |
| simvastatin | 0.66 | 0.65 | 0.98 | 0.89 | -0.29 | -0.27 | 0.93 | 0.00 | -0.283 | -0.061 | 0.435 | -1.05 | 0.68 | 0.15 |
| spironolactone | 0.78 | 0.77 | 0.99 | 0.90 | -0.55 | -0.52 | 0.95 | -0.01 | -0.583 | -0.158 | 0.636 | -0.93 | 0.86 | 0.23 |
| sulpiride | 0.85 | 0.86 | 1.01 | 0.78 | -0.75 | -0.79 | 1.05 | -0.01 | -1.971 | -1.642 | 0.649 | -0.71 | 2.15 | 1.79 |
| telmisartan | 0.87 | 0.85 | 0.98 | 1.35 | -0.83 | -0.75 | 0.91 | -0.01 | -0.757 | -0.102 | 1.630 | -1.84 | 0.85 | 0.12 |
| temazepam | 0.79 | 0.79 | 1.00 | 1.49 | -0.58 | -0.58 | 1.00 | -0.01 | -0.599 | -0.183 | 1.922 | -2.64 | 0.82 | 0.25 |
| theophylline | 0.94 | 0.93 | 0.99 | 1.34 | -1.19 | -1.12 | 0.94 | -0.02 | -2.808 | 0.858 | 2.000 | -1.66 | 2.33 | -0.71 |
| thioridazine | 0.40 | 0.40 | 1.00 | 0.70 | 0.18 | 0.18 | 1.00 | 0.00 | 0.185 | 0.042 | -0.481 | -1.09 | 0.42 | 0.10 |
| tolterodine | 0.45 | 0.43 | 0.96 | 1.83 | 0.09 | 0.12 | 1.40 | 0.01 | 0.127 | 0.038 | 0.714 | 2.51 | 0.45 | 0.13 |
| trazodone | 0.76 | 0.74 | 0.97 | 1.75 | -0.50 | -0.45 | 0.91 | -0.01 | -0.494 | -0.162 | 3.461 | -5.64 | 0.80 | 0.26 |
| tropicamid | 0.83 | 0.83 | 1.00 | 1.55 | -0.69 | -0.69 | 1.00 | -0.01 | -1.530 | 68.863 | 2.237 | -2.70 | 1.84 | -83.00 |
| valproic acid | 0.04 | 0.04 | 1.00 | 0.11 | 1.38 | 1.38 | 1.00 | 0.04 | 1.624 | 0.529 | -27.715 | -0.80 | 0.05 | 0.02 |
| valsartan | 0.97 | 0.96 | 0.99 | 0.86 | -1.51 | -1.38 | 0.91 | -0.01 | -1.445 | -0.356 | 1.108 | -0.77 | 1.01 | 0.25 |
| venlafaxine | 0.61 | 0.65 | 1.07 | 1.99 | -0.19 | -0.27 | 1.38 | -0.01 | -0.996 | -0.187 | -11.296 | 27.31 | 2.41 | 0.45 |
| verapamil | 0.86 | 0.86 | 1.00 | 1.34 | -0.79 | -0.79 | 1.00 | -0.01 | -0.876 | -1.383 | 1.656 | -1.81 | 0.96 | 1.51 |
| zolmitriptane | 0.86 | 0.86 | 1.00 | 1.50 | -0.79 | -0.79 | 1.00 | -0.01 | -3.153 | 0.781 | 2.126 | -2.32 | 3.44 | -0.85 |
| zolpidem | 0.76 | 0.77 | 1.01 | 2.05 | -0.50 | -0.52 | 1.05 | -0.01 | -0.570 | -0.610 | 9.583 | -14.06 | 0.84 | 0.90 |
| zopiclone | 0.84 | 0.83 | 0.99 | 0.90 | -0.72 | -0.69 | 0.96 | -0.01 | -1.530 | -0.298 | 0.748 | -0.90 | 1.84 | 0.36 |
| zuclopenthixol | 0.62 | 0.60 | 0.97 | 1.15 | -0.21 | -0.18 | 0.83 | 0.00 | -0.179 | -0.035 | 0.618 | -2.10 | 0.61 | 0.12 |

* R_f value from the non-impregnated RP plate (control)

** R_f value from the RP plate impregnated with 2 mg/mL BSA solution

Table S5. Chromatographic data obtained for 129 compounds from HPLC_{HSA} and HPLC_{IAM} experiments and their derivatives.

| API | k _{HSA} | log k _{HSA} | log k _{HSA} /B2 | log k _{HSA} /log P | log k _{HSA} /PB | log k _{HSA} /PSA | k _{IAM} | log k _{IAM} | log k _{IAM} /B2 | log k _{IAM} /log P | log k _{IAM} /PB | log k _{IAM} /PSA |
|----------------------|------------------|----------------------|-----------------------------|--------------------------------|-----------------------------|------------------------------|------------------|----------------------|-----------------------------|--------------------------------|-----------------------------|------------------------------|
| acebutolol | 1.13 | 0.05 | -0.06 | -0.16 | 0.20 | 0.001 | 5.06 | 0.70 | -0.82 | -2.13 | 2.71 | 0.01 |
| aceclofenac | 55.89 | 1.75 | -2.64 | 0.49 | 1.76 | 0.023 | 2.63 | 0.42 | -0.63 | 0.12 | 0.42 | 0.01 |
| acenocumarol | 18.58 | 1.27 | -1.05 | 0.47 | 1.29 | 0.012 | 0.53 | -0.27 | 0.23 | -0.10 | -0.28 | 0.00 |
| acetylsalicylic acid | 0.31 | -0.51 | 1.08 | -0.39 | -0.51 | -0.008 | 0.03 | -1.52 | 3.22 | -1.17 | -1.52 | -0.02 |
| aciclovir | 0.19 | -0.72 | 0.60 | 0.50 | -3.43 | -0.007 | 0.09 | -1.04 | 0.86 | 0.72 | -4.94 | -0.01 |
| alprazolam | 0.89 | -0.05 | 0.80 | -0.01 | -0.06 | -0.001 | 3.14 | 0.50 | -7.85 | 0.11 | 0.62 | 0.01 |
| amiodarone | 124.01 | 2.09 | -15.41 | 0.70 | 2.18 | 0.049 | 99.63 | 2.00 | -14.71 | 0.66 | 2.08 | 0.05 |
| amlodipine | 5.45 | 0.74 | -0.70 | -0.49 | 0.75 | 0.007 | 98.90 | 2.00 | -1.90 | -1.32 | 2.05 | 0.02 |
| amoxicillin | 0.94 | -0.03 | 0.01 | 0.18 | -0.13 | 0.000 | 0.05 | -1.32 | 0.66 | 8.80 | -6.60 | -0.01 |
| astemizol | 13.32 | 1.12 | -21.95 | 1.58 | 1.16 | 0.030 | 26.27 | 1.42 | -27.70 | 2.00 | 1.47 | 0.04 |
| atorvastatin | 3.48 | 0.54 | -0.44 | 0.35 | 0.55 | 0.005 | 8.28 | 0.92 | -0.74 | 0.60 | 0.94 | 0.01 |
| atropine | 1.23 | 0.09 | -0.36 | 0.05 | 0.50 | 0.002 | 3.91 | 0.59 | -2.38 | 0.35 | 3.29 | 0.01 |
| azithromycin | 0.23 | -0.64 | 0.27 | -0.26 | -2.20 | -0.004 | 0.06 | -1.20 | 0.51 | -0.49 | -4.14 | -0.01 |
| betaxolol | 1.59 | 0.20 | -0.76 | 0.20 | 0.40 | 0.004 | 15.60 | 1.19 | -4.51 | 1.19 | 2.39 | 0.02 |
| bilastine | 0.67 | -0.17 | 0.25 | -0.08 | -0.20 | -0.002 | 0.55 | -0.26 | 0.36 | -0.12 | -0.30 | 0.00 |
| biperiden | 0.58 | -0.24 | -1.38 | -0.09 | -0.39 | -0.010 | 41.47 | 1.62 | 9.43 | 0.60 | 2.70 | 0.07 |
| bisoprolol | 1.07 | 0.03 | -0.07 | 0.01 | 0.10 | 0.000 | 6.74 | 0.83 | -2.01 | 0.39 | 2.76 | 0.01 |
| bromazepam | 0.63 | -0.20 | 0.62 | -0.08 | -0.29 | -0.004 | 2.21 | 0.34 | -1.07 | 0.13 | 0.49 | 0.01 |
| bromocriptine | 8.09 | 0.91 | -0.68 | 0.20 | 0.98 | 0.008 | 12.69 | 1.10 | -0.82 | 0.25 | 1.19 | 0.01 |
| buspirone | 0.89 | -0.05 | 0.09 | -0.04 | -0.05 | -0.001 | 7.00 | 0.84 | -1.49 | 0.72 | 0.89 | 0.01 |
| caffeine | 0.23 | -0.64 | 2.06 | 0.60 | -2.13 | -0.012 | 0.18 | -0.75 | 2.44 | 0.71 | -2.51 | -0.01 |
| capecitabine | 0.3 | -0.52 | 0.38 | -0.99 | -0.87 | -0.004 | 1.11 | 0.04 | -0.03 | 0.08 | 0.07 | 0.00 |
| captopril | 0.15 | -0.82 | 2.20 | -2.75 | -3.00 | -0.014 | 0.01 | -2.19 | 5.83 | -7.28 | -7.95 | -0.04 |
| carbamazepine | 1.09 | 0.04 | -0.19 | 0.02 | 0.05 | 0.001 | 1.50 | 0.18 | -0.91 | 0.08 | 0.23 | 0.00 |
| carbegoline | 3.23 | 0.51 | -0.85 | 1.76 | 1.24 | 0.007 | 17.05 | 1.23 | -2.05 | 4.25 | 3.00 | 0.02 |
| carvedilol | 14.5 | 1.16 | -1.75 | -0.57 | 1.19 | 0.015 | 0.00 | | | | | |
| cefuroxime | 0.23 | -0.64 | 0.24 | 0.31 | -1.28 | -0.003 | 1.69 | 0.23 | -0.09 | -0.11 | 0.45 | 0.00 |

| | | | | | | | | | | | | |
|---------------------------|-------|-------|--------|-------|-------|--------|-------|-------|--------|-------|-------|-------|
| celecoxib | 13.42 | 1.13 | -1.61 | 1.11 | 1.16 | 0.014 | 50.01 | 1.70 | -2.42 | 1.67 | 1.75 | 0.02 |
| celiprolol | 1.12 | 0.05 | -0.05 | -0.11 | 0.18 | 0.001 | 5.87 | 0.77 | -0.85 | -1.71 | 2.80 | 0.01 |
| cephalexin | 0.16 | -0.80 | -29.83 | 0.61 | -5.68 | -0.024 | 0.00 | | | | | |
| cetirizine | 1.55 | 0.19 | -0.63 | 0.09 | 0.20 | 0.004 | 1.05 | 0.02 | -0.07 | 0.01 | 0.02 | 0.00 |
| chloramphenikol | 0.61 | -0.21 | 0.17 | 0.86 | -0.39 | -0.002 | 1.08 | 0.03 | -0.03 | -0.13 | 0.06 | 0.00 |
| chlorpromazine | 13.33 | 1.12 | 29.20 | 0.30 | 1.25 | 0.035 | 58.85 | 1.77 | 45.94 | 0.47 | 1.97 | 0.06 |
| chlortalidone | 0.85 | -0.07 | 0.05 | 0.11 | -0.09 | -0.001 | 1.32 | 0.12 | -0.09 | -0.19 | 0.16 | 0.00 |
| cimetidine | 0.67 | -0.17 | 0.14 | 0.29 | -1.02 | -0.002 | 0.26 | -0.58 | 0.45 | 0.98 | -3.41 | -0.01 |
| ciprofloxacin | 0.19 | -0.72 | 1.17 | 0.39 | -2.40 | -0.010 | 1.22 | 0.09 | -0.14 | -0.05 | 0.29 | 0.00 |
| cisapride | 4.88 | 0.69 | -0.83 | 0.31 | 0.71 | 0.008 | 57.99 | 1.76 | -2.13 | 0.78 | 1.81 | 0.02 |
| clarithromycin | 0.82 | -0.09 | 0.04 | -0.03 | -0.12 | 0.000 | 0.10 | -1.02 | 0.43 | -0.32 | -1.45 | -0.01 |
| clindamycin | 1.34 | 0.13 | -0.11 | 0.08 | 0.14 | 0.001 | 11.34 | 1.05 | -0.92 | 0.66 | 1.13 | 0.01 |
| clobazam | 1.01 | 0.00 | -0.04 | 0.00 | 0.01 | 0.000 | 2.58 | 0.41 | -4.23 | -0.29 | 0.48 | 0.01 |
| clonidine | 1.35 | 0.13 | -3.65 | 0.47 | 0.43 | 0.004 | 2.83 | 0.45 | -12.66 | 1.61 | 1.51 | 0.01 |
| clorazepate | 3.99 | 0.60 | -0.55 | 0.22 | 0.62 | 0.006 | 4.88 | 0.69 | -0.63 | 0.25 | 0.71 | 0.01 |
| clozapine | 6.84 | 0.84 | 1.69 | 0.47 | 0.84 | 0.258 | 50.94 | 1.71 | 3.45 | 0.96 | 1.72 | 0.53 |
| cypheptadine | 9.7 | 0.99 | 9.40 | 0.85 | 1.01 | 0.036 | 23.79 | 1.38 | 13.12 | 1.19 | 1.41 | 0.05 |
| desloratidine | 5.97 | 0.78 | 5.23 | 11.09 | 0.92 | 0.031 | 50.45 | 1.70 | 11.48 | 24.33 | 2.02 | 0.07 |
| diazepam | 3.57 | 0.55 | 22.76 | 0.18 | 0.56 | 0.017 | 5.08 | 0.71 | 29.07 | 0.23 | 0.72 | 0.02 |
| digoxin | 0.21 | -0.68 | 0.25 | -0.25 | -2.71 | -0.003 | 3.69 | 0.57 | -0.21 | 0.21 | 2.27 | 0.00 |
| dihydroergotamine | 0.23 | -0.64 | 0.47 | 0.30 | -0.69 | -0.005 | 0.00 | | | | | |
| diphenhydramin | 1.88 | 0.27 | 0.79 | 0.13 | 0.28 | 0.022 | 3.66 | 0.56 | 1.62 | 0.27 | 0.57 | 0.05 |
| doxazosin | 5.51 | 0.74 | -0.52 | 0.35 | 0.76 | 0.006 | 0.22 | -0.66 | 0.46 | -0.31 | -0.67 | -0.01 |
| doxycycline | 1.68 | 0.23 | -0.10 | -0.12 | 0.25 | 0.001 | 1.76 | 0.24 | -0.10 | -0.13 | 0.27 | 0.00 |
| drotaverine | 1.91 | 0.28 | -1.19 | -0.19 | 0.32 | 0.006 | 31.24 | 1.49 | -6.33 | -0.99 | 1.71 | 0.03 |
| enalapril | 0.34 | -0.47 | 0.47 | -0.20 | -0.85 | -0.005 | 0.05 | -1.29 | 1.31 | -0.56 | -2.35 | -0.01 |
| eplerenone | 0.21 | -0.68 | 0.95 | -0.35 | -1.36 | -0.009 | 1.54 | 0.19 | -0.26 | 0.10 | 0.38 | 0.00 |
| escitalopram | 2.84 | 0.45 | -13.67 | 0.52 | 0.81 | 0.013 | 32.08 | 1.51 | -45.42 | 1.73 | 2.69 | 0.04 |
| estradiol benzoate | | | 0.00 | 0.00 | 0.00 | | 6.92 | 0.84 | -0.79 | 0.20 | 0.88 | 0.01 |
| estrone | 11.01 | 1.04 | -1.02 | 0.36 | 1.10 | 0.011 | 29.40 | 1.47 | -1.44 | 0.51 | 1.55 | 0.02 |
| famotidine | 0.99 | 0.00 | 0.00 | 0.00 | -0.02 | 0.000 | 0.26 | -0.58 | 0.18 | 0.53 | -3.33 | 0.00 |

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|-------------------------------|-------|-------|--------|-------|-------|--------|-------|-------|--------|-------|-------|-------|
| fexofenadine | 1.07 | 0.03 | -0.04 | 0.01 | 0.05 | 0.000 | 1.08 | 0.03 | -0.04 | 0.01 | 0.05 | 0.00 |
| fluoxetine | 6.06 | 0.78 | 3.78 | 0.41 | 0.83 | 0.037 | 66.64 | 1.82 | 8.82 | 0.94 | 1.93 | 0.09 |
| flupenthixol | 15.36 | 1.19 | -4.16 | 0.22 | 1.25 | 0.023 | 51.21 | 1.71 | -5.99 | 0.32 | 1.80 | 0.03 |
| furosemide | 11.66 | 1.07 | -0.69 | -4.44 | 1.12 | 0.008 | 0.28 | -0.56 | 0.36 | 2.32 | -0.59 | 0.00 |
| gliclazide | 9.69 | 0.99 | -1.17 | 0.52 | 1.05 | 0.011 | 0.28 | -0.55 | 0.66 | -0.29 | -0.59 | -0.01 |
| haloperidol | 4.8 | 0.68 | -6.70 | 0.52 | 0.74 | 0.017 | 23.74 | 1.38 | -13.53 | 1.05 | 1.50 | 0.03 |
| hydrocortisone acetate | 0.66 | -0.18 | 0.43 | -0.04 | -0.19 | -0.003 | 2.82 | 0.45 | -1.07 | 0.11 | 0.47 | 0.01 |
| hydroxyzine | 3.69 | 0.57 | -20.22 | 0.46 | 0.61 | 0.016 | 13.82 | 1.14 | -40.67 | 0.93 | 1.23 | 0.03 |
| ibuprofen | 65.66 | 1.82 | -36.49 | 0.47 | 1.91 | 0.049 | 0.86 | -0.07 | 1.34 | -0.02 | -0.07 | 0.00 |
| indomethacin | 64.78 | 1.81 | -3.85 | -1.27 | 1.87 | 0.028 | 1.08 | 0.03 | -0.07 | -0.02 | 0.03 | 0.00 |
| ketoprofen | 24.32 | 1.39 | -4.29 | 0.54 | 1.40 | 0.025 | 0.20 | -0.71 | 2.19 | -0.28 | -0.72 | -0.01 |
| ketotifen | 5.83 | 0.77 | -3.33 | 2.94 | 1.02 | 0.016 | 22.04 | 1.34 | -5.85 | 5.17 | 1.79 | 0.03 |
| lamotrigine | 1.08 | 0.03 | -0.04 | 0.02 | 0.06 | 0.000 | 0.71 | -0.15 | 0.16 | -0.11 | -0.27 | 0.00 |
| levocetizine | 1.77 | 0.25 | -0.82 | 0.07 | 0.27 | 0.005 | 3.82 | 0.58 | -1.93 | 0.17 | 0.64 | 0.01 |
| levofloxacin | 3.94 | 0.60 | -0.95 | 0.96 | 1.92 | 0.008 | 0.90 | -0.04 | 0.07 | -0.07 | -0.14 | 0.00 |
| loperamide | 4.47 | 0.65 | -4.24 | 0.13 | 0.67 | 0.015 | 0.00 | | | | | |
| loratadine | 10.54 | 1.02 | -7.76 | 3.41 | 1.04 | 0.024 | 11.76 | 1.07 | -8.12 | 3.57 | 1.09 | 0.03 |
| lorazepam | 2.21 | 0.34 | -0.78 | 0.10 | 0.40 | 0.006 | 9.04 | 0.96 | -2.17 | 0.28 | 1.10 | 0.02 |
| medazepam | 17.86 | 1.25 | 4.21 | 0.29 | 1.26 | 0.080 | 34.65 | 1.54 | 5.18 | 0.36 | 1.56 | 0.10 |
| meloxicam | 63.54 | 1.80 | -1.10 | -1.55 | 1.82 | 0.013 | 0.49 | -0.31 | 0.19 | 0.27 | -0.31 | 0.00 |
| methyldopa | 0.36 | -0.44 | 0.40 | 0.30 | -2.22 | -0.004 | 0.10 | -1.02 | 0.91 | 0.70 | -5.08 | -0.01 |
| mianserin | 6.39 | 0.81 | 1.82 | 0.86 | 0.90 | 0.124 | 21.72 | 1.34 | 3.02 | 1.42 | 1.49 | 0.21 |
| midazolam | 3.22 | 0.51 | 3.55 | 0.15 | 0.52 | 0.020 | 5.69 | 0.76 | 5.28 | 0.22 | 0.78 | 0.03 |
| mirtazapine | 2.96 | 0.47 | 1.99 | 0.41 | 0.55 | 0.024 | 5.83 | 0.77 | 3.23 | 0.66 | 0.90 | 0.04 |
| montelukast | 0.19 | -0.72 | 1.24 | -0.17 | -0.73 | -0.010 | 99.10 | 2.00 | -3.44 | 0.48 | 2.02 | 0.03 |
| naproxen | 90.08 | 1.95 | -9.90 | 0.65 | 1.97 | 0.042 | 0.31 | -0.51 | 2.59 | -0.17 | -0.52 | -0.01 |
| nebivolol | 7.49 | 0.87 | -1.49 | -0.85 | 0.89 | 0.012 | 0.00 | | | | | |
| olanzapine | 4.83 | 0.68 | -0.86 | -0.44 | 3.91 | 0.008 | 20.31 | 1.31 | -1.64 | -0.84 | 7.47 | 0.02 |
| oxazepam | 1.65 | 0.22 | -0.49 | 0.07 | 0.26 | 0.004 | 4.78 | 0.68 | -1.54 | 0.23 | 0.80 | 0.01 |
| oxybutinin | 4.01 | 0.60 | -2.42 | 0.19 | 0.66 | 0.012 | 49.68 | 1.70 | -6.80 | 0.52 | 1.84 | 0.03 |
| pantoprazole | 2.09 | 0.32 | -0.38 | -0.17 | 0.33 | 0.004 | 2.19 | 0.34 | -0.41 | -0.18 | 0.35 | 0.00 |

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|-----------------------|-------|-------|-------|-------|-------|--------|--------|-------|--------|-------|-------|-------|
| paracetamol | 0.28 | -0.55 | 2.28 | 0.42 | -2.21 | -0.011 | 0.32 | -0.49 | 2.03 | 0.37 | -1.97 | -0.01 |
| paroxetine | 5.96 | 0.78 | -8.76 | -1.58 | 0.82 | 0.020 | 115.77 | 2.06 | -23.31 | -4.21 | 2.20 | 0.05 |
| pergolide | 0.07 | -1.15 | 7.12 | -0.50 | -1.28 | -0.026 | 0.00 | | | | | |
| perindopril | 0.49 | -0.31 | 0.31 | -0.15 | -2.07 | -0.003 | 0.18 | -0.76 | 0.77 | -0.37 | -5.05 | -0.01 |
| phenytoin | 1.63 | 0.21 | -0.55 | 0.29 | 0.24 | 0.004 | 1.78 | 0.25 | -0.65 | 0.34 | 0.28 | 0.00 |
| pindolol | 1.65 | 0.22 | -0.59 | -0.18 | 0.54 | 0.004 | 6.09 | 0.78 | -2.12 | -0.64 | 1.96 | 0.01 |
| piroxicam | 32.92 | 1.52 | -1.29 | 1.42 | 1.53 | 0.014 | 0.16 | -0.79 | 0.67 | -0.74 | -0.80 | -0.01 |
| prednisolone | 0.52 | -0.28 | 0.29 | -0.14 | -0.32 | -0.003 | 2.84 | 0.45 | -0.47 | 0.23 | 0.50 | 0.00 |
| progesterone | 5.7 | 0.76 | -3.83 | 0.24 | 0.78 | 0.016 | 34.99 | 1.54 | -7.82 | 0.49 | 1.58 | 0.03 |
| promazine | 8.9 | 0.95 | 24.65 | 0.29 | 1.01 | 0.030 | 0.10 | -1.02 | -26.48 | -0.31 | -1.08 | -0.03 |
| promethazine | 5.35 | 0.73 | 18.91 | -3.64 | 0.78 | 0.023 | 14.96 | 1.17 | 30.50 | -5.87 | 1.26 | 0.04 |
| propafenone | 3.23 | 0.51 | -1.31 | 0.27 | 0.52 | 0.009 | 66.74 | 1.82 | -4.68 | 0.98 | 1.88 | 0.03 |
| propranolol | 3.48 | 0.54 | -4.64 | 0.19 | 0.60 | 0.013 | 28.09 | 1.45 | -12.40 | 0.52 | 1.61 | 0.03 |
| quetiapine | 2.48 | 0.39 | -0.63 | 0.14 | 0.48 | 0.005 | 17.02 | 1.23 | -1.95 | 0.43 | 1.48 | 0.02 |
| quinapril | 3.1 | 0.49 | -0.50 | 0.29 | 0.51 | 0.005 | 1.22 | 0.09 | -0.09 | 0.05 | 0.09 | 0.00 |
| risperidone | 2.11 | 0.32 | -0.73 | 0.51 | 0.37 | 0.005 | 4.83 | 0.68 | -1.54 | 1.09 | 0.78 | 0.01 |
| rizatriptan | 2.06 | 0.31 | -0.79 | -1.16 | 2.24 | 0.005 | 2.53 | 0.40 | -1.01 | -1.49 | 2.88 | 0.01 |
| rosuvastatin | 1.96 | 0.29 | -0.17 | 0.25 | 0.33 | 0.002 | 0.96 | -0.02 | 0.01 | -0.02 | -0.02 | 0.00 |
| roxitromicin | 1.03 | 0.01 | 0.00 | 0.00 | 0.01 | 0.000 | 0.00 | | | | | |
| rupatadine | 12.38 | 1.09 | 13.22 | 0.67 | 1.11 | 0.038 | 9.29 | 0.97 | 11.71 | 0.59 | 0.98 | 0.03 |
| sertraline | 13.19 | 1.12 | 3.16 | 0.67 | 1.14 | 0.093 | 42.89 | 1.63 | 4.60 | 0.97 | 1.67 | 0.14 |
| sildenafil | 1.62 | 0.21 | -0.17 | -0.14 | 0.22 | 0.002 | 14.26 | 1.15 | -0.96 | -0.79 | 1.20 | 0.01 |
| simvastatin | 8.72 | 0.94 | -1.52 | 0.21 | 0.99 | 0.013 | 13.21 | 1.12 | -1.81 | 0.25 | 1.18 | 0.02 |
| spironolactone | 0.82 | -0.09 | 0.10 | -0.03 | -0.10 | -0.001 | 13.38 | 1.13 | -1.37 | 0.34 | 1.25 | 0.01 |
| sulpiride | 1.45 | 0.16 | -0.13 | 0.34 | 0.40 | 0.001 | 1.66 | 0.22 | -0.18 | 0.46 | 0.55 | 0.00 |
| telmisartan | 22.51 | 1.35 | -2.93 | 0.18 | 1.36 | 0.021 | 4.68 | 0.67 | -1.45 | 0.09 | 0.67 | 0.01 |
| temazepam | 1.26 | 0.10 | -0.33 | 0.03 | 0.10 | 0.002 | 6.74 | 0.83 | -2.77 | 0.26 | 0.86 | 0.02 |
| theophylline | 0.22 | -0.66 | 1.17 | 0.50 | -1.64 | -0.009 | 0.12 | -0.94 | 1.67 | 0.72 | -2.35 | -0.01 |
| thioridazine | 18.57 | 1.27 | -3.46 | 0.30 | 1.34 | 0.022 | 47.61 | 1.68 | -4.58 | 0.40 | 1.77 | 0.03 |
| tolterodine | 2.9 | 0.46 | 2.70 | 0.14 | 0.48 | 0.020 | 0.21 | -0.68 | -3.95 | -0.21 | -0.70 | -0.03 |
| trazodone | 2.22 | 0.35 | -2.64 | 0.12 | 0.38 | 0.008 | 9.30 | 0.97 | -7.38 | 0.35 | 1.05 | 0.02 |

| | | | | | | | | | | | | |
|-----------------------|-------|-------|--------|-------|-------|--------|-------|-------|-------|-------|-------|-------|
| tropicamid | 0.15 | -0.82 | 2.68 | 82.39 | -1.83 | -0.015 | 1.06 | 0.03 | -0.09 | -2.68 | 0.06 | 0.00 |
| valproic acid | 4.46 | 0.65 | -13.04 | 0.25 | 0.76 | 0.017 | 0.08 | -1.09 | 21.90 | -0.42 | -1.28 | -0.03 |
| valsartan | 48.78 | 1.69 | -1.35 | 0.44 | 1.77 | 0.015 | 0.08 | -1.10 | 0.88 | -0.28 | -1.15 | -0.01 |
| venlafaxine | 1.05 | 0.02 | 0.89 | 0.01 | 0.08 | 0.001 | 8.25 | 0.92 | 38.52 | 0.64 | 3.40 | 0.03 |
| verapamil | 2.22 | 0.35 | -0.73 | 0.61 | 0.38 | 0.005 | 11.97 | 1.08 | -2.26 | 1.89 | 1.20 | 0.02 |
| zolmitriptane | 1.7 | 0.23 | -0.62 | -0.23 | 0.92 | 0.004 | 3.30 | 0.52 | -1.40 | -0.51 | 2.07 | 0.01 |
| zolpidem | 1.77 | 0.25 | -4.53 | 0.29 | 0.27 | 0.007 | 2.60 | 0.42 | -7.58 | 0.48 | 0.45 | 0.01 |
| zopiclone | 0.76 | -0.12 | 0.13 | -0.05 | -0.26 | -0.001 | 0.91 | -0.04 | 0.04 | -0.02 | -0.09 | 0.00 |
| zuclopenthixol | 16.18 | 1.21 | -4.24 | 0.24 | 1.23 | 0.023 | 48.73 | 1.69 | -5.92 | 0.34 | 1.71 | 0.03 |

Table S6. Biological properties for APIs from the external group (n = 38). An external API group (n = 38) was assembled at a later time than previous one (n = 129).

| API | B1 | B2 | B3 | BB _{vivo} | CNS+/- | LactMed | LLL H | log U/D 7.2 | M/P | PB | PhCharge |
|---------------------|-------|-------|-------|--------------------|--------|---------|-------|----------------|------|------|----------|
| acetazolamid | -1.60 | -1.29 | 0.52 | | 1 | 1 | 2 | -0.24 | 0.28 | 0.98 | -1 |
| amitriptyline | 0.76 | 0.50 | -0.45 | 0.89 | 1 | 1 | 2 | -1.98 | 0.92 | 0.95 | 1 |
| bupivacaine | 0.16 | 0.03 | 1.25 | | 1 | 1 | 2 | -0.93 | 0.37 | 0.95 | 1 |
| chloroquine | 0.39 | 0.10 | 0.89 | | 1 | 1 | 2 | -3.27 | 2.65 | 0.55 | 2 |
| citalopram | 0.13 | -0.03 | -0.23 | | 1 | 2 | 2 | -2.37 | 1.03 | 0.80 | 1 |
| clomipramine | 0.79 | 0.44 | -0.28 | | 1 | 1 | 2 | -2.26 | 1.13 | 0.98 | 1 |
| colchicine | -0.93 | -0.78 | -1.99 | | 1 | 2 | 4 | | 0.95 | 0.39 | 0 |
| diltiazem | -0.02 | -0.40 | -1.22 | | 1 | 1 | 3 | -1.74 | 0.99 | 0.75 | 1 |
| doxepin | 0.54 | 0.35 | -0.18 | | 1 | 1 | 5 | -2.20 | 1.37 | 0.76 | 1 |
| duloxetine | 0.56 | 0.21 | -0.65 | | 1 | 1 | 3 | -2.82 | 0.78 | 0.90 | 1 |
| eletriptan | -0.19 | -0.30 | -0.84 | | 1 | 1 | 3 | -3.15 | 0.25 | 0.85 | 1 |
| ethambutol | -0.86 | -0.49 | -0.52 | | 0 | 1 | 2 | -2.39 | 1.00 | 0.25 | 1 |
| ethanol | -0.19 | 0.22 | -0.67 | -0.16 | 1 | 2 | 3 | | 0.95 | 0.00 | 0 |
| fluvoxamine | -0.14 | -0.36 | 0.68 | | 1 | 1 | 2 | -2.19 | 1.33 | 0.79 | 1 |
| gabapentin | -0.63 | -0.47 | -0.19 | | 1 | 1 | 2 | -0.29 | 1.00 | 0.03 | 0 |
| gentamycin | -3.13 | -2.65 | -2.40 | | 0 | 1 | 2 | -2.57 | 0.36 | 0.15 | 5 |
| hydrochlorothiazide | -1.62 | -1.35 | -2.29 | | 0 | 1 | 2 | -1.75 | 0.38 | 0.68 | 0 |
| itraconazole | -0.66 | -1.07 | 3.68 | | 0 | 1 | 2 | -0.73 | 1.14 | 1.00 | 0 |
| ketorolac | -0.33 | -0.40 | 0.23 | | 1 | 1 | 2 | -2.91 | 0.03 | 0.99 | -1 |
| levetiracetam | -0.93 | -0.47 | -1.02 | | 1 | 1 | 3 | | 1.00 | 0.10 | 0 |
| lincomycin | -1.62 | -1.47 | -0.43 | | 0 | | 2 | -1.58 | 0.15 | 0.70 | 1 |
| mesalazine | -0.99 | -0.79 | -1.55 | | 0 | 1 | 3 | -5.30 | 2.69 | 0.43 | -1 |
| minoxidil | -1.00 | -0.95 | -0.18 | | 1 | | 3 | -1.66 | 0.82 | 0.00 | 0 |
| nitrendipine | -0.92 | -1.22 | -1.09 | | 0 | 1 | 2 | -4.41 | 0.30 | 0.99 | 0 |
| ofloxacin | -0.66 | -0.63 | -1.97 | | 0 | 1 | 2 | -2.01 | 1.26 | 0.32 | -1 |

| | | | | | | | | | | | |
|-------------------------|-------|-------|-------|--|---|---|---|-------|------|------|----|
| oxcarbamazepine | -0.55 | -0.47 | -0.87 | | 1 | | 3 | -6.53 | 0.50 | 0.40 | 0 |
| pefloxacin | -0.52 | -0.48 | -1.44 | | 0 | | | -7.04 | 0.96 | 0.25 | -1 |
| pregabalin | -0.63 | -0.47 | -0.22 | | 1 | 1 | 3 | -0.57 | 0.55 | 0.00 | 0 |
| primidone | -0.60 | -0.38 | -0.31 | | 1 | 2 | 3 | -5.06 | 0.72 | 0.70 | 0 |
| propylthiouracil | -0.29 | -0.11 | -0.31 | | 1 | 1 | 2 | -0.43 | 0.17 | 0.82 | 0 |
| quinine | -0.11 | -0.18 | -0.07 | | 1 | 1 | 2 | -2.08 | 0.23 | 0.70 | 1 |
| rifampicin | -2.81 | -2.98 | -0.67 | | 0 | 1 | 2 | -2.24 | 0.40 | 0.89 | 1 |
| rimantadine | 0.26 | 0.13 | 0.43 | | 1 | | 3 | -3.56 | 2.00 | 0.40 | 1 |
| timolol | -0.85 | -0.73 | -0.06 | | 0 | 1 | 2 | -2.15 | 0.80 | 0.10 | 1 |
| tinidazole | -1.35 | -1.02 | -0.65 | | 1 | 1 | 3 | -4.90 | 1.14 | 0.12 | 0 |
| tramadol | 0.01 | 0.02 | -0.67 | | 1 | 1 | 2 | -2.41 | 2.30 | 0.20 | 1 |
| trimethoprim | -1.33 | -1.14 | -1.90 | | 1 | 1 | 2 | -0.30 | 1.25 | 0.44 | 1 |
| warfarin | -0.33 | -0.47 | -0.44 | | 1 | 0 | 2 | -2.70 | 0.00 | 0.99 | -1 |

Table S7. Physicochemical properties for APIs from the external group (n = 38).

| API | a/b/n code ¹ | DM | eH | eH-eL | eL ² | HA | HD | log D | log P | MW ³ | pKa | PSA ⁴ | Sa ³ | V ³ |
|--------------------|----------------------------|------|-------|--------|-----------------|----|----|-------|-------|-----------------|-------|------------------|-----------------|----------------|
| acetazolamid | 0 | 0.89 | -9.06 | -9.13 | 0.69 | 5 | 2 | -0.55 | -0.26 | 2.22 | 7.44 | 11.50 | 4.69 | 2.9 |
| amitriptyline | 1 | 6.42 | -9.9 | -8.20 | -17.01 | 1 | 0 | 3.15 | 4.41 | 2.77 | 9.18 | 0.32 | 3.61 | 1.56 |
| bupivacaine | 0 | 3.02 | -9.03 | -9.37 | 3.37 | 2 | 1 | 2.80 | 3.31 | 2.88 | 8.13 | 3.23 | 4.78 | 3.02 |
| chloroquine | 1 | 4.4 | -8.6 | -8.03 | -5.71 | 3 | 1 | 1.87 | 4.41 | 3.20 | 10.47 | 2.82 | 5.94 | 3.11 |
| citalopram | 1 | 2.83 | -7.98 | -8.86 | 8.83 | 3 | 0 | 0.39 | 3.48 | 3.24 | 9.57 | 3.63 | 5.88 | 3.14 |
| clomipramine | 1 | 1.53 | -8.49 | -8.65 | 1.56 | 2 | 0 | 3.50 | 4.94 | 3.15 | 9.46 | 0.65 | 5.11 | 3.05 |
| colchicine | 0 | 5.95 | -9.11 | -8.52 | -5.91 | 6 | 1 | 0.92 | 1.07 | 3.99 | | 8.31 | 5.47 | 3.61 |
| diltiazem | 1 | 2.43 | -8.71 | -8.52 | -1.86 | 4 | 0 | 2.10 | 4.73 | 4.15 | 8.94 | 5.91 | 6.17 | 3.96 |
| doxepin | 1 | 0.31 | -9.11 | -9.03 | -0.81 | 2 | 0 | 2.08 | 3.84 | 2.79 | 9.40 | 1.25 | 4.69 | 2.81 |
| duloxetine | 1 | 0.96 | -9.01 | -8.63 | -3.82 | 2 | 1 | 1.24 | 4.81 | 2.97 | 10.02 | 2.13 | 4.56 | 2.84 |
| eletriptan | 1 | 4.88 | -8.5 | -7.90 | -5.96 | 3 | 1 | 0.36 | 2.98 | 3.83 | 10.35 | 5.32 | 4.69 | 3.57 |
| ethambutol | 1 | 1.11 | -9.11 | -11.45 | 23.39 | 4 | 4 | -2.21 | -0.29 | 2.04 | 9.59 | 6.45 | 4.95 | 2.18 |
| ethanol | 0 | | | | | 1 | 1 | -0.19 | -0.18 | 0.46 | | 2.02 | | |
| flvoxamine | 1 | 3.9 | -9.69 | -8.87 | -8.25 | 4 | 1 | 1.15 | 3.71 | 3.18 | 9.39 | 5.68 | 5.89 | 2.79 |
| gabapentin | 0 | 1.56 | -9.35 | -10.19 | 8.36 | 3 | 2 | -1.31 | 1.08 | 1.71 | 7.50 | 6.33 | 2.38 | 1.7 |
| gentamycin | 1 | 4.31 | -9.34 | -11.20 | 18.62 | 12 | 8 | -7.81 | -2.04 | 4.78 | 9.77 | 19.97 | 4.71 | 4.25 |
| hydrochlorotiazide | 0 | 7.27 | -9.64 | -8.46 | -11.83 | 5 | 3 | -0.09 | -0.02 | 2.98 | 8.95 | 11.84 | 3.85 | 2.01 |
| itraconazole | 0 | 6.11 | -8.42 | -7.65 | -7.7 | 9 | 0 | 4.26 | 4.53 | 6.73 | 6.47 | 10.08 | 8.43 | 6.15 |
| ketorolac | -1 | 2.14 | -9.19 | -8.83 | -3.63 | 3 | 1 | -0.95 | 2.68 | 2.55 | 4.29 | 5.93 | 3.87 | 2.39 |
| levetiracetam | 0 | 5.71 | -9.8 | -10.45 | 6.49 | 2 | 1 | -0.67 | -0.88 | 1.70 | | 6.34 | 3.09 | 1.62 |
| lincomycin | 1 | 3.92 | -8.5 | -8.50 | 0.04 | 8 | 5 | -0.48 | 0.72 | 4.07 | 8.78 | 12.60 | 6.35 | 3.89 |
| mesalazine | -1 | 3.8 | -8.18 | -8.06 | -1.23 | 4 | 3 | -2.61 | 0.74 | 1.53 | 1.90 | 8.36 | 2.49 | 1.28 |
| minoxidil | 0 | 4.2 | -8.07 | -8.10 | 0.29 | 5 | 2 | 0.65 | 1.62 | 2.09 | 5.54 | 9.36 | 3.16 | 1.96 |
| nitrendipine | 0 | 6.92 | -9.09 | -8.00 | -10.94 | 5 | 1 | 3.50 | 3.81 | 3.60 | 2.79 | 11.05 | 5.3 | 2.98 |
| ofloxacin | -1 | 4.68 | -8.72 | -7.82 | -8.97 | 7 | 1 | -0.65 | 1.85 | 3.61 | 5.19 | 7.33 | 4.74 | 3.07 |
| oxcarbamazepine | 0 | 3.46 | -9.31 | -8.84 | -4.73 | 2 | 1 | 1.25 | 1.66 | 2.52 | 13.73 | 6.34 | 3.02 | 2.26 |
| pefloxacin | -1 | 9.41 | -9.01 | -7.97 | -10.45 | 6 | 1 | 0.52 | 1.92 | 3.33 | 0.16 | 6.41 | 4.66 | 2.91 |
| pregabalin | 0 | 1.67 | -9.53 | -10.46 | 9.29 | 3 | 2 | -1.38 | 1.09 | 1.59 | 7.77 | 6.33 | 3.54 | 1.65 |

| | | | | | | | | | | | | | | |
|-------------------------|----|------|--------|--------|--------|----|---|-------|-------|------|-------|-------|------|------|
| primidone | 0 | 2.84 | -9.78 | -9.77 | -0.15 | 2 | 2 | 0.40 | 0.83 | 2.18 | 12.26 | 5.82 | 3.19 | 2.02 |
| propylthiouracil | 0 | 5.57 | -9.2 | -7.93 | -12.71 | 1 | 2 | 1.18 | 1.15 | 1.70 | 7.63 | 4.11 | 3.32 | 1.51 |
| quinine | 1 | 1.73 | -9.55 | -9.54 | -0.14 | 4 | 1 | 1.58 | 2.82 | 3.24 | 9.28 | 4.56 | 4.22 | 3.06 |
| rifampicin | -1 | | | | | 14 | 6 | -0.46 | 2.05 | 8.23 | 4.96 | 22.02 | | |
| rimantadine | 1 | 1.22 | -9.33 | -12.28 | 29.54 | 1 | 1 | 0.08 | 3.31 | 1.79 | 10.76 | 2.60 | 2.43 | 1.91 |
| timolol | 1 | 3.06 | -9.17 | -8.05 | -11.24 | 7 | 2 | -1.39 | 1.28 | 3.16 | 9.35 | 7.97 | 4.95 | 2.88 |
| tinidazole | 0 | 2.34 | -10.52 | -9.24 | -12.82 | 5 | 0 | -0.27 | -0.29 | 2.47 | 2.30 | 9.78 | 4.41 | 2 |
| tramadol | 1 | | | | | 3 | 1 | 0.36 | 2.32 | 2.63 | 9.61 | 3.27 | | |
| trimethoprim | 0 | 2.09 | -8.8 | -8.68 | -1.22 | 7 | 2 | 0.58 | 0.59 | 2.90 | 6.90 | 10.55 | 4.14 | 2.63 |
| warfarin | -1 | 4.12 | -7.38 | -6.05 | -13.35 | 3 | 1 | -0.90 | 3.13 | 3.08 | 4.50 | 6.36 | 4.01 | 2.76 |

1 – code describing the acid-base properties: (-1) - acids; (0) - neutral drugs; (1) - bases

2 – value multiplied by 10

3 – value divided by 100

4 – value divided by 10

Table S8. Chromatographic data and their derivatives obtained from the NP TLC and RP TLC experiment for the external group of APIs (n = 38).

| API | C _{NP} [*] | NP ^{**} | NP/C | NP/PSA | C _{RP} [*] | RP ^{**} | RP/C | RP/PSA | NP/B2 | RP/B2 | NP/PB | RP/PB | NP/logP | RP/logP |
|--------------------|------------------------------|------------------|------|--------|------------------------------|------------------|------|--------|--------|---------|--------|--------|---------|---------|
| acetazolamid | 0.94 | 0.94 | 1.00 | 0.817 | 0.97 | 0.96 | 0.99 | 0.834 | -0.727 | -0.742 | 0.959 | 0.980 | -3.615 | -3.692 |
| amitriptyline | 0.32 | 0.31 | 0.97 | 9.568 | 0.67 | 0.63 | 0.94 | 19.444 | 0.626 | 1.272 | 0.326 | 0.663 | 0.070 | 0.143 |
| bupivacaine | 0.67 | 0.67 | 1.00 | 2.072 | 0.74 | 0.75 | 1.01 | 2.319 | 22.666 | 25.372 | 0.705 | 0.789 | 0.202 | 0.227 |
| chloroquine | 0.17 | 0.17 | 1.00 | 0.604 | 0.40 | 0.30 | 0.75 | 1.065 | 1.763 | 3.111 | 0.309 | 0.545 | 0.039 | 0.068 |
| citalopram | 0.30 | 0.29 | 0.97 | 0.800 | 0.62 | 0.60 | 0.97 | 1.655 | -8.745 | -18.094 | 0.363 | 0.750 | 0.083 | 0.172 |
| clomipramine | 0.33 | 0.32 | 0.97 | 4.938 | 0.59 | 0.59 | 1.00 | 9.105 | 0.722 | 1.331 | 0.327 | 0.602 | 0.065 | 0.119 |
| colchicine | 0.79 | 0.77 | 0.97 | 0.927 | 0.91 | 0.91 | 1.00 | 1.095 | -0.984 | -1.163 | 1.974 | 2.333 | 0.720 | 0.850 |
| diltiazem | 0.49 | 0.49 | 1.00 | 0.829 | 0.76 | 0.72 | 0.95 | 1.219 | -1.230 | -1.808 | 0.653 | 0.960 | 0.104 | 0.152 |
| doxepin | 0.30 | 0.31 | 1.03 | 2.486 | 0.58 | 0.54 | 0.93 | 4.330 | 0.892 | 1.554 | 0.411 | 0.715 | 0.081 | 0.141 |
| duloxetine | 0.32 | 0.33 | 1.03 | 1.552 | 0.57 | 0.53 | 0.93 | 2.493 | 1.595 | 2.562 | 0.367 | 0.589 | 0.069 | 0.110 |
| eletriptan | 0.29 | 0.28 | 0.97 | 0.527 | 0.62 | 0.62 | 1.00 | 1.166 | -0.922 | -2.041 | 0.329 | 0.729 | 0.094 | 0.208 |
| ethambutol | 0.19 | 0.21 | 1.11 | 0.325 | 0.97 | 0.95 | 0.98 | 1.472 | -0.433 | -1.957 | 0.840 | 3.800 | -0.724 | -3.276 |
| ethanol | | | | | | | | | | | | | | |
| fluvoxamine | 0.34 | 0.32 | 0.94 | 0.563 | 0.62 | 0.62 | 1.00 | 1.091 | -0.883 | -1.711 | 0.408 | 0.790 | 0.086 | 0.167 |
| gabapentin | 0.91 | 0.91 | 1.00 | 1.437 | 0.66 | 0.66 | 1.00 | 1.042 | -1.952 | -1.416 | 30.333 | 22.000 | 0.843 | 0.611 |
| gentamycin | 0.96 | 0.94 | 0.98 | 0.471 | 0.91 | 0.90 | 0.99 | 0.451 | -0.355 | -0.340 | 6.267 | 6.000 | -0.461 | -0.441 |
| hydrochlorotiazide | 0.96 | 0.96 | 1.00 | 0.811 | 0.97 | 0.96 | 0.99 | 0.811 | -0.713 | -0.713 | 1.414 | 1.414 | -48.000 | -48.000 |
| itraconazole | 0.96 | 0.97 | 1.01 | 0.962 | 0.86 | 0.84 | 0.98 | 0.833 | -0.910 | -0.788 | 0.972 | 0.842 | 0.214 | 0.185 |
| ketorolac | 0.92 | 0.91 | 0.99 | 1.535 | 0.96 | 0.96 | 1.00 | 1.619 | -2.265 | -2.389 | 0.919 | 0.970 | 0.340 | 0.358 |
| levetiracetam | 0.92 | 0.92 | 1.00 | 1.451 | 0.92 | 0.92 | 1.00 | 1.451 | -1.968 | -1.968 | 9.200 | 9.200 | -1.045 | -1.045 |
| lincomycin | 0.91 | 0.91 | 1.00 | 0.722 | 0.94 | 0.94 | 1.00 | 0.746 | -0.620 | -0.640 | 1.300 | 1.343 | 1.264 | 1.306 |
| mesalazine | 0.94 | 0.93 | 0.99 | 1.113 | 0.99 | 0.97 | 0.98 | 1.161 | -1.178 | -1.228 | 2.163 | 2.256 | 1.257 | 1.311 |
| minoxidil | 0.43 | 0.42 | 0.98 | 0.449 | 0.80 | 0.82 | 1.03 | 0.876 | -0.442 | -0.862 | | | 0.259 | 0.506 |
| nitrendipine | 0.97 | 0.97 | 1.00 | 0.878 | 0.86 | 0.86 | 1.00 | 0.779 | -0.795 | -0.705 | 0.980 | 0.869 | 0.255 | 0.226 |
| ofloxacin | 0.24 | 0.23 | 0.96 | 0.314 | 0.54 | 0.50 | 0.93 | 0.682 | -0.367 | -0.799 | 0.719 | 1.563 | 0.124 | 0.270 |
| oxcarbamazepine | 0.91 | 0.90 | 0.99 | 1.420 | 0.91 | 0.91 | 1.00 | 1.435 | -1.926 | -1.947 | 2.250 | 2.275 | 0.542 | 0.548 |
| pefloxacin | 0.30 | 0.29 | 0.97 | 0.452 | 0.76 | 0.70 | 0.92 | 1.092 | -0.606 | -1.463 | 1.160 | 2.800 | 0.151 | 0.365 |
| pregabalin | 0.76 | 0.76 | 1.00 | 1.200 | 0.41 | 0.41 | 1.00 | 0.648 | -1.630 | -0.880 | | | 0.697 | 0.376 |

| | | | | | | | | | | | | | | |
|-------------------------|------|------|------|-------|------|------|------|-------|--------|--------|-------|-------|--------|--------|
| primidone | 0.90 | 0.93 | 1.03 | 1.598 | 0.93 | 0.97 | 1.04 | 1.667 | -2.421 | -2.525 | 1.329 | 1.386 | 1.120 | 1.169 |
| propylthiouracil | 0.94 | 0.94 | 1.00 | 2.285 | 0.93 | 0.93 | 1.00 | 2.261 | -8.462 | -8.372 | 1.146 | 1.134 | 0.817 | 0.809 |
| quinine | 0.30 | 0.29 | 0.97 | 0.636 | 0.66 | 0.64 | 0.97 | 1.404 | -1.590 | -3.508 | 0.414 | 0.914 | 0.103 | 0.227 |
| rifampicin | 0.73 | 0.77 | 1.05 | 0.350 | 0.95 | 0.94 | 0.99 | 0.427 | -0.259 | -0.316 | 0.865 | 1.056 | 0.376 | 0.459 |
| rimantadine | 0.92 | 0.92 | 1.00 | 3.536 | 0.95 | 0.95 | 1.00 | 3.651 | 7.040 | 7.270 | 2.300 | 2.375 | 0.278 | 0.287 |
| timolol | 0.34 | 0.32 | 0.94 | 0.401 | 0.97 | 0.97 | 1.00 | 1.216 | -0.439 | -1.331 | 3.200 | 9.700 | 0.250 | 0.758 |
| tinidazole | 0.89 | 0.88 | 0.99 | 0.900 | 0.94 | 0.93 | 0.99 | 0.951 | -0.865 | -0.914 | 7.333 | 7.750 | -3.034 | -3.207 |
| tramadol | 0.31 | 0.31 | 1.00 | 0.948 | 0.63 | 0.64 | 1.02 | 1.957 | 13.025 | 26.891 | 1.550 | 3.200 | 0.134 | 0.276 |
| trimethoprim | 0.57 | 0.59 | 1.04 | 0.559 | 0.84 | 0.83 | 0.99 | 0.787 | -0.517 | -0.727 | 1.341 | 1.886 | 1.000 | 1.407 |
| warfarin | 0.99 | 0.99 | 1.00 | 1.557 | 0.87 | 0.83 | 0.95 | 1.305 | -2.104 | -1.764 | 1.000 | 0.838 | 0.316 | 0.265 |

* R_f value from the non-impregnated NP or RP plate (control)

** R_f value from the NP or RP plate impregnated with 2 mg/mL BSA solution

Table S9. Chromatographic data from HPLC_{HSA} and HPLC_{IAM} experiments and their derivatives obtained for 38 external APIs.

| API | k _{HSA} | log k _{HSA} | log k _{HSA} /B2 | log k _{HSA} /PB | log k _{HSA} /log P | k _{IAM} | log k _{IAM} |
|--------------------|------------------|----------------------|--------------------------|--------------------------|-----------------------------|------------------|----------------------|
| acetazolamid | 0.74 | -0.13 | -0.575 | 0.760 | -2.863 | 2.90 | 0.46 |
| amitriptyline | 5.87 | 0.77 | 11.854 | 6.178 | 1.331 | 1.56 | 0.19 |
| bupivacaine | 1.18 | 0.07 | 40.084 | 1.247 | 0.358 | 3.02 | 0.48 |
| chloroquine | 18.05 | 1.26 | 187.127 | 32.812 | 4.092 | 3.11 | 0.49 |
| citalopram | 2.67 | 0.43 | -80.418 | 3.333 | 0.766 | 3.14 | 0.50 |
| clomipramine | 9.09 | 0.96 | 20.510 | 9.278 | 1.841 | 3.05 | 0.48 |
| colchicine | 0.28 | -0.55 | -0.362 | 0.726 | 0.265 | 3.61 | 0.56 |
| diltiazem | 1.74 | 0.24 | -4.362 | 2.316 | 0.367 | 3.96 | 0.60 |
| doxepin | 4.25 | 0.63 | 12.220 | 5.624 | 1.106 | 2.81 | 0.45 |
| duloxetine | 8.16 | 0.91 | 39.435 | 9.063 | 1.696 | 2.84 | 0.45 |
| eletriptan | 3.78 | 0.58 | -12.429 | 4.441 | 1.267 | 3.57 | 0.55 |
| ethambutol | 1.73 | 0.24 | -3.557 | 6.906 | -5.953 | 2.18 | 0.34 |
| ethanol | 0.02 | -1.76 | 0.078 | | -0.097 | 0.01 | -2.09 |
| fluvoxamine | 0.25 | -0.60 | -0.696 | 0.321 | 0.068 | 2.79 | 0.45 |
| gabapentin | 0.15 | -0.84 | -0.312 | 4.843 | 0.135 | 1.70 | 0.23 |
| gentamycin | 1.50 | 0.18 | -0.568 | 10.028 | -0.737 | 4.25 | 0.63 |
| hydrochlorotiazide | 0.61 | -0.22 | -0.452 | 0.897 | -30.451 | 2.01 | 0.30 |
| itraconazole | 9.65 | 0.98 | -9.055 | 9.668 | 2.130 | 6.15 | 0.79 |
| ketorolac | 9.65 | 0.98 | -24.017 | 9.747 | 3.601 | 2.39 | 0.38 |
| levetiracetam | 0.07 | -1.16 | -0.149 | 0.696 | -0.079 | 1.62 | 0.21 |
| lincomycin | 0.82 | -0.08 | -0.560 | 1.175 | 1.142 | 3.89 | 0.59 |
| mesalazine | 0.18 | -0.73 | -0.234 | 0.430 | 0.250 | 1.28 | 0.11 |
| minoxidil | 0.40 | -0.40 | -0.422 | | 0.248 | 1.96 | 0.29 |
| nitrendipine | 3.55 | 0.55 | -2.906 | 3.581 | 0.931 | 2.98 | 0.47 |
| ofloxacin | 6.62 | 0.82 | -10.566 | 20.673 | 3.576 | 3.07 | 0.49 |
| oxcarbamazepine | 0.40 | -0.40 | -0.846 | 0.988 | 0.238 | 2.26 | 0.35 |
| pefloxacin | 12.43 | 1.09 | -25.980 | 49.720 | 6.474 | 2.91 | 0.46 |
| pregabalin | 0.14 | -0.87 | -0.291 | | 0.124 | 1.65 | 0.22 |

| | | | | | | | |
|-------------------------|-------|-------|---------|--------|--------|------|------|
| primidone | 0.22 | -0.66 | -0.569 | 0.312 | 0.263 | 2.02 | 0.31 |
| propylthiouracil | 0.33 | -0.48 | -2.950 | 0.400 | 0.285 | 1.51 | 0.18 |
| quinine | 2.59 | 0.41 | -14.194 | 3.699 | 0.918 | 3.06 | 0.49 |
| rifampicin | 0.03 | -1.53 | -0.010 | 0.034 | 0.015 | 8.37 | 0.92 |
| rimantadine | 0.16 | -0.80 | 1.222 | 0.399 | 0.048 | 1.91 | 0.28 |
| timolol | 0.13 | -0.88 | -0.179 | 1.304 | 0.102 | 2.88 | 0.46 |
| tinidazole | 0.12 | -0.92 | -0.118 | 0.997 | -0.413 | 2.00 | 0.30 |
| tramadol | 1.08 | 0.03 | 45.221 | 5.381 | 0.464 | 3.90 | 0.59 |
| trimethoprim | 0.85 | -0.07 | -0.749 | 1.943 | 1.449 | 2.63 | 0.42 |
| warfarin | 13.86 | 1.14 | -29.454 | 14.001 | 4.428 | 2.76 | 0.44 |