Compound Name Class PCID Water Solubility Caco2 Permeability Intestinal Absorption (%) Skin Permeability P-gp Substrate CYP3A4 Substrate CYP Inhibitors BBB Permeability Total Clearance AMES Toxicity hERG I Inhibitor hERG II Inhibitor Hepatotoxicity

Acetyl tyrosine ethyl ester Amino acid 2004 -2.089 0.453 82.974 -2.922 No No None -0.249 0.645 Yes No No No

N(alpha)-Benzyloxycarbonyl-Lleucine Amino acid 74840 -2.701 0.946 91.584 -2.728 Yes No None -0.131 0.598 No No No No

8-Desoxygartanin Xanthone 392450 -4.075 1.139 90.497 -2.735 Yes Yes CYP1A2;CYP2C19;CYP2C9 -0.87 0.329 Yes No Yes Yes

Lophophorine Alkaloids 442315 -1.499 1.876 92.43 -2.647 No Yes CYP2D6 0.262 0.926 No No No No

L-trans-5-Hydroxy-2piperidinecarboxylic acid Piperidines 151730 -0.102 0.492 70.428 -2.735 No No None -0.75 0.666 No No No No

Candimine Alkaloids 441588 -3.395 0.806 64.066 -3.235 Yes Yes None -0.286 0.687 Yes No No Yes

5-(2-Methylpropyl)tetrahydro2-oxo-3-furancarboxylic acid Lactone 131751114 -1.397 0.721 83.985 -2.735 No No None -0.211 0.331 No No No No

Diethyl (2R "3R)-2-methyl-3hydroxysuccinate,Carboxylic ester" 440395 -0.162 0.836 87.543 -3.519 No No None -0.412 0.997 No No No No

1-O-Sinapoyl-β-D-glucose Glycosides 5280406 -1.961 0.172 47.505 -2.744 Yes No None -1.308 0.71 No No No No

Epifisetinidol-(4beta->8)catechin Flavonoids 14332863 -2.892 -0.094 72.79 -2.735 Yes No None -1.66 -0.04 No No Yes No

4-(3-Pyridyl)-3-butenoic acid Pyridine 5478892 -1.248 1.217 96.679 -2.722 No No None -0.013 0.329 No No No No

Justicidin A Lignin 159982 -5.226 1.272 99.247 -2.733 No Yes CYP1A2;CYP2C19;CYP2C9 -0.968 0.39 Yes No Yes No

N-Acetyl-DL-methionine Amino acid 6180 -0.81 0.647 84.272 -2.725 No No None -0.276 0.304 No No No No

"1alpha,2alpha,4betaH,6alpha,8R)-p-Menthane-2,6,8,9-tetrol, " Terpenoid 85290815 -1.251 0.406 54.506 -3.685 No No None -0.772 1.327 No No No No

Methyl o-methoxyhippuric acid Carboxylic acid 531541 -1.75 0.524 85.712 -3.162 No No None -0.227 0.341 No No No No

Di-4-coumaroylputrescine Cinnamic acids 44241258 -3.661 0.196 67.759 -2.788 Yes Yes CYP2C19;CYP2C9;CYP3A4 -0.731 0.459 No No Yes Yes

Convicine Glycoside 88000 -2.389 -0.557 18.305 -2.735 No No None -1.142 0.564 No No No Yes

8-Deoxy-11 "13dihydroxygrosheimin,Terpenoid" 5260103 -2.645 0.524 68.497 -4.038 No No None 0.013 0.378 Yes No No No

Suberylglycine Carboxylic acid 6453952 -1.403 -0.504 19.486 -2.735 No No None -0.924 0.662 No No No No

Schizonepetoside E Terpenoid 46173963 -2.236 0.39 39.736 -2.812 Yes No None -1.074 1.335 No No No No

2-Hexyl-1 3-dioxan-5-ol Dioxane 74361 -2.003 1.707 93.821 -2.896 No No None 0.58 1.426 No No No Yes

Kanokoside A Glycoside 10457683 -2.942 0.354 67.366 -2.738 Yes No None -1.572 1.085 No No No No

N-Feruloyltyramine Coumaric Acids 5280537 -3.292 0.925 90.23 -2.806 Yes Yes CYP1A2;CYP2C19;CYP3A4 -0.715 0.27 No No Yes Yes

2-[3-Ethyl-5-(4methoxyphenyl)-1H-pyrazol-4yl]phenol Phenol 257428 -3.192 1.252 93.703 -2.735 Yes Yes CYP1A2;CYP2C19;CYP2C9;CYP3A4 0.319 0.436 No No Yes No

Indole-3-carbinol Indole 3712 -1.874 1.586 92.085 -2.602 No No CYP1A2 0.439 0.515 No No No Yes

Moschamine Amines 5969616 -3.739 -0.1 78.363 -2.737 Yes Yes CYP1A2;CYP2C19;CYP2C9 -1.022 0.462 No No Yes Yes

6-Hydroxypentadecanedioic acid Lipid 131751198 -2.704 0.614 27.495 -2.735 No No None -1.159 1.684 No No No No

Kolanone Benzophenones 6439598 -5.33 0.72 91.763 -2.743 Yes Yes CYP3A4 0.409 0.863 No No No No

5-Oxoavermectin''1b'' aglycone Lactones 11953976 -5.666 0.911 90.148 -3.545 Yes Yes None -0.7 0.422 No No No No

7(14)-Bisabolene-2 3 10 11tetrol Sesquiterpenoid 73816843 -1.942 0.612 93.226 -3.742 No No None -0.962 1.335 No No No No

1-Methoxy-1-(2 4 5trimethoxyphenyl)-2-propanol Alkylbenzene 131751190 -1.751 1.271 94.27 -3.082 No No None -0.804 0.795 Yes No No No

3-Oxo-12 18-ursadien-28-oic acid Terpenoids 14707579 -3.201 1.26 100 -2.735