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**Table L Observed and predicted melting point values of the dataset studied.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Substances Set** | **MPobs**  (°C) | **MPpred I**  (°C) | **MPpred II MPpred III**  (°C) (\*C) | | **MPpred IV**  (°C) |
| buramate | 40 | 80.0 | 116.2 | 139.1 | 111.7 |
| fenpiprane | 41 | 87.5 | 94.5 | 73.2 | 85.0 |
| trimipramine | 45 | 127.5 | 125.8 | 109.5 | 120.9 |
| phencarbamide | 48 | 63.5 | 154.9 | 71.7 | 96.7 |
| banactyzine | 51 | 132.9 | 121.0 | 103.4 | 119.1 |
| ethopropazine | 53 | 103.9 | 109.4 | 107.3 | 106.9 |
| xibenolol | 57 | 90.4 | 112.0 | 65.5 | 89.3 |
| prometazine | 60 | 136.4 | 122.6 | 119.0 | 126.0 |
| gemfibrozil | 61 | 76.2 | 125.8 | 75.3 | 92.4 |
| isosorbide | 61 | 213.6 | 141.3 | 209.6 | 188.2 |
| fluanisone | 67.5 | 108.2 | 133.2 | 101.2 | 114.2 |
| penbutolol | 68 | 78.4 | 95.6 | 68.5 | 80.9 |
| ranitidine | 69 | 119.4 | 119.0 | 115.2 | 117.9 |
| propoxyphene | 75 | 83.6 | 107.1 | 69.2 | 86.6 |
| novonal | 75 | 63.3 | 109.4 | 73.2 | 82.0 |
| phenadoxone | 75 | 89.0 | 102.1 | 93.0 | 94.7 |
| ibuprofen | 75 | 109.4 | 124.9 | 103.9 | 112.7 |
| mebutamate | 77 | 106.0 | 139.0 | 121.3 | 122.1 |
| moxaverine | 78 | 123.9 | 117.4 | 134.9 | 125.4 |
| etisazol | 78 | 135.8 | 130.1 | 142.7 | 136.2 |
| nabumetone | 80 | 126.5 | 108.3 | 119.1 | 118.0 |
| cloranolol | 82 | 73.9 | 117.4 | 70.3 | 87.2 |
| pentifylline | 82 | 150.2 | 111.5 | 149.6 | 137.1 |
| fentanyl | 83 | 90.8 | 146.4 | 98.9 | 112.0 |
| zipeprol | 83 | 109.0 | 140.6 | 106.9 | 118.8 |
| anileridine | 83 | 114.6 | 101.8 | 119.8 | 112.1 |
| amphetaminil | 85 | 96.0 | 100.3 | 98.4 | 98.3 |
| piprozolin | 86 | 124.6 | 150.7 | 121.8 | 132.4 |
| econazole | 86.8 | 126.2 | 155.0 | 124.2 | 135.1 |
| chloroquine | 87 | 80.3 | 116.3 | 72.6 | 89.7 |
| methdilazine | 87 | 145.3 | 116.9 | 134.5 | 132.2 |
| noxythiolin | 88 | 125.2 | 158.3 | 107.1 | 130.2 |
| tulobuterol | 89 | 88.6 | 109.5 | 78.5 | 92.2 |
| acetorphan | 89 | **111.0** | 108.7 | 116.7 | 112.1 |
| zotepine | 90 | **141.4** | 120.4 | 129.8 | 130.5 |
| vinylbital | 90 | **127.2** | 139.2 | 140.4 | 135.6- |
| phenindamine | 91 | 148.1 | 161.5 | 143.6 | 151.1 |
| carisoprodol | 92 | 67.8 | 143.3 | 95.7 | 102.3 |
| alc1ofenac | 92 | 123.5 | 121.7 | 128.1 | 124.4 |
| maprotiline | 92 | 126.3 | 106.6 | 130.1 | 121.0 |
| tolindate | 94 | 68.3 | 168.2 | 94.3 | 110.3 |
| perphenazine | 94 | 136.3 | 165.6 | 137.5 | 146.5 |
| ketoprofen | 94 | 145.9 | 158.8 | 152.7 | 152.5 |
| thenaldine | 95 | 107.0 | 109.4 | 112.6 | 109.7 |
| alibendol | 95 | 146.1 | 110.8 | 148.9 | 135.3 |
| tamoxi fen | 96 | 92.2 | 106.7 | 93.8 | 97.6 |
| tropicamide | 96 | 110.6 | 141.8 | 121.2 | 124.5 |

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|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| limaprost | te | 97 | 125.4 | 102.2 | 105.1 | 110.9 |
| metaproterenol | tr | 100 | 93.1 | 113.0 | 126.4 | 110.8 |
| medmain | tr | 100 | 123.6 | 117.7 | 131.0 | 124.1 |
| plafibride | te | 100 | 149.1, | 135.7 | 136.9 | 140.6 |
| acetylpheneturide | tr | 100 | 127.1 | 123.6 | 150.0 | 133.6 |
| phenocoll | tr | 100.5 | 143.1 | 114.6 | 140.0 | 132.6 |
| hycanthone | te | 100.6 | 145.7 | 171.9 | 162.6 | 160.1 |
| piperidione | tr | 102 | 120.8 | 151.6 | 120.7 | 131.0 |
| isoxsuprine | tr | 102.5 | 94.6 | 93.0 | 94.6 | 94.1 |
| meprobamate | te | 104 | 109.9 | 164.1 | 126.5 | 133.5 |
| diphemethoxidine | tr | 106 | 113.8 | 132.1 | 106.5 | 117.5 |
| pipobroman | tr | 106 | 114.5 | 163.6 | 109.2 | 129.1 |
| mepiprazole | tr | 106 | 127.1 | 119.1 | 138.1 | 128.1 |
| zidovudine | te | 106 | 143.5 | 115.9 | 238.8 | 166.1 |
| bupivacaine | tr | 107 | 84.0 | 104.6 | 83.5 | 90.7 |
| cetoxime | te | 107 | 125.9 | 154.2 | 125.9 | 135.3 |
| toremifene | tr | 108 | 93.0 | 158.1 | 93.8 | 115.0 |
| acecarbromal | kr | 109 | 145.2 | 125.3 | 133.1 | 134.5 |
| celiprolol | tr | 110 | 85.3 | 163.6 | 99.2 | 116.0 |
| flurbiprofen | te | 110 | 132.8 | 106.0 | 132.4 | 123.7 |
| amphotalide | tr | 113 | 143.3 | 130.3 | 146.0 | 139.9 |
| valnoctamide | te | 113.5 | 71.6 | 97.4 | 67.9 | 79.0 |
| isbogrel | te | 114 | 104.1 | 148.4 | 110.8 | 121.1 |
| ifenprodil | tr | 114 | 131.2 | 101.5 | 112.7 | 115.1 |
| atropin | tr | 114 | 117.9 | 180.0 | 121.5 | 139.8 |
| detomidine | tr | 114 | 133.7 | 153.0 | 138.5 | 141.7 |
| bamipine | tr | 115 | 88.3 | 159.0 | 86.1 | 111.1 |
| flupirtine | tr | 115 | 141.3 | 121.1 | 152.6 | 138.3 |
| ipriflavone | te | 115 | 176.4 | 143.1 | 177.5 | 165.7 |
| flumetramide | tr | 115.5 | 103.8 | 155.4 | 151.4 | 136.9 |
| dibenzepin | tr | 116 | 132.5 | 124.7 | 153.5 | 136.9 |
| valsartan | tr | 116 | 159.5 | 135.5 | 159.8 | 151.6 |
| pericyazine | te | 116 | 152.2 | 140.5 | 160.8 | 151.2 |
| fadrozole | te | 117 | 173.7 | 145.4 | 177.3 | 165.5 |
| moperone | tr | 118 | 151.4 | 133.8 | 104.1 | 129.8 |
| flutoprazepam | tr | 118 | 166.2 | 167.1 | 159.9 | 164.4 |
| morphazinamide | te | 118.5 | 175.4 | 152.6 | 166.0 | 164.7 |
| acebutolol | tr | 119 | 108.3 | 105.1 | 101.5 | 105.0 |
| terbutaline | te | 119 | 120.4 | 152.2 | 120.2 | 131.0 |
| pirozadil | tr | 119 | 152.0 | 120.2 | 174.3 | 148.8 |
| chlophedianol | tr | 120 | 95.7 | 115.3 | 84.1 | 98.4 |
| pridinol | tr | 120 | 91.9 | 143.8 | 86.5 | 107.4 |
| antazoline | tr | 120 | 102.5 | 126.9 | 103.7 | 111.0 |
| vinconate | te | 120 | 243.1 | 148.1 | 197.1 | 196.1 |
| capobenic acid | tr | 121 | 111.9 | 148.4 | 116.8 | 125.7 |
| difenpiramide | tr | 122 | 119.4 | 157.1 | 140.1 | 138.9 |
| propizepine | te | 122 | 111.7 | 121.4 | 170.7 | 134.6 |
| benzoic acid | tr | 122.4 | 135.7 | 179.3 | 167.2 | 160.7 |
| bamethan | te | 123.5 | 70.9 | 96.3 | 88.4 | 85.2 |
| nadolol | tr | 124 | 159.7 | 136.7 | 123.4 | 139.9 |

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|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| benzarone | tr | 124.3 | 185.5 | 186.0 | 184.4 | 185.3 |
| lofexidine | tr | 126 | 132.4 | 158.9 | 106.0 | 132.5 |
| mecloqualone | te | 126 | 187.1 | 144.3 | 182.4 | 171.3 |
| seratrodast | tr | 128 | 168.5 | 134.4 | 108.0 | 137.0 |
| simetride | te | 128 | 103.5 | 138.7 | 133.9 | 125.4 |
| febantel | tr | 129 | 121.3 | 132.0 | 175.6 | 143.0 |
| clonidine | tr | 130 | 112.8 | 152.4 | 130.0 | 131.7 |
| xylometazoline | te | 131 | 93.5 | 148.7 | 86.5 | 109.5 |
| thozalinone | tr | 133 | 145.5 | 142.1 | 145.8 | 144.5 |
| erytromycin | tr | 135 | 159.3 | 129.0 | 152.6 | 147.0 |
| mephenytoin | te | 136 | 128.0 | 132.9 | 135.7 | 132.2 |
| aminorex | tr | 136 | 155.3 | 110.0 | 157.0 | 140.8 |
| praziquantel | tr | 136 | 179.7 | 165.0 | 170.9 | 171.8 |
| ipsapirone | te | 137 | 169.7 | 151.0 | 170.4 | 163.7 |
| butalbital | tr | 138 | 142.8 | 157.8 | 140.3 | 146.9 |
| zafirlukast | tr | 138 | 177.1 | 165.4 | 193.5 | 178.7 |
| alizapride | tr | 139 | 192.9 | 182.0 | 189.3 | 188.1 |
| phenazopyridine | te | 139 | 183.5 | 145.7 | 193.4 | 174.2 |
| alpidem | tr | 140 | 115.6 | 155.4 | 132.3 | 134.4 |
| erythrocentaurin | te | 140 | 185.6 | 149.6 | 184.1 | 173.1 |
| cimetidine | tr | 141 | 147.7 | 125.2 | 137.3 | 136.8 |
| ethinylestradiol | tr | 141 | 102.6 | 124.0 | 179.2 | 135.2 |
| letosteine | tr | 142 | 163.5 | 153.5 | 106.0 | 141.0 |
| proglumide | te | 142 | 103.9 | 127.1 | 118.7 | 116.6 |
| fexofenadine | te | 142 | 115.0 | 144.2 | 120.4 | 126.5 |
| carbaryl | tr | 142 | 174.6 | 137.5 | 162.2 | 158.1 |
| acetylsalicylic acid | tr | 142.4 | 144.6 | 156.6 | 176.4 | 159.2 |
| ahistan | tr | 144 | 171.4 | 127.8 | 156.1 | 151.8 |
| carbutamide | tr | 144 | 137.3 | 178.2 | 158.4 | 158.0 |
| doxofylline | te | 144 | 181.2 | 158.4 | 220.0 | 186.5 |
| felodipin | tr | 145 | 100.5 | 143.2 | 138.8 | 127.5 |
| atenolol | tr | 146 | 132.0 | 142.2 | 113.2 | 129.1 |
| sertaconazole | tr | 146 | 148.8 | 155.3 | 138.5 | 147.5 |
| ketoconazol | te | 146 | 191.3 | 152.3 | 184.4 | 176.0 |
| metoclopramide | tr | 146.5 | 109.7 | 138.2 | 109.8 | 119.2 |
| pyrinoline | te | 146.5 | 174.5 | 155.9 | 178.5 | 169.6 |
| clotrimazole | tr | 147 | 143.2 | 138.3 | 153.6 | 145.0 |
| haloperidol | tr | 148 | 152.1 | 132.3 | 105.4 | 130.0 |
| thialbarbital | tr | 148 | 152.2 | 146.9 | 134.1 | 144.4 |
| salacetamide | te | 148 | 166.8 | 165.5 | 172.6 | 168.3 |
| dimecrotic acid | te | 149 | 176.3 | 133.8 | 147.4 | 152.5 |
| morazone | tr | 149 | 141.1 | 121.0 | 149.6 | 137.2 |
| aceclofenac | tr | 149 | 158.4 | 177.6 | 154.3 | 163.4 |
| astemizole | te | 149.1 | 148.6 | 143.4 | 167.5 | 153.2 |
| abecamil | tr | 150 | 222.2 | 181.4 | 198.0 | 200.5 |
| acemetacin | tr | 150 | 184.9 | 201.8 | 203.5 | 196.7 |
| felbamate | tr | 151 | 166.9 | 154.0 | 165.3 | 162.1 |
| mafenide | te | 151 | 234.3 | 130.6 | 195.4 | 186.8 |
| ujothion | te | 152 | 140.2 | 152.3 | 134.2 | 142.2 |
| naproxen | tr | 152 | 161.8 | 153.6 | 155.3 | 156.9 |

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|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| glymidine | tr | 152 | 105.8 | 174.4 | 160.5 | 146.9 |
| bufexamac | tr | 153 | 152.3 | 147.5 | 116.0 | 138.6 |
| florfenicol | tr | 153 | 158.1 | 168.5 | 147.9 | 158.2 |
| testosterone | te | 153 | 180.2 | 203.4 | 181.9 | 188.5 |
| taurolidine | tr | 154 | 185.1 | 189.7 | 189.0 | 187.9 |
| vamicamide | te | 156 | 146.4 | 143.3 | 105.2 | 131.6 |
| ketobemidone | tr | 156 | 160.5 | 169.3 | 106.5 | 145.4 |
| amobarbital | te | 156 | 116.7 | 168.1 | 131.8 | 138.8 |
| erdosteine | tr | 156 | 161.1 | 116.7 | 135.9 | 137.9 |
| benzetimide | te | 156 | 122.1 | 151.9 | 146.3 | 140.1 |
| urapidil | tr | 156 | 171.7 | 127.9 | 147.3 | 149.0 |
| metizoline | tr | 156 | 163.3 | 130.5 | 148.6 | 147.4 |
| omeprazole | tr | 156 | 148.5 | 144.0 | 162.8 | 151.8 |
| phenallymal | tr | 156 | 151.6 | 160.3 | 176.1 | 162.7 |
| moricizine | te | 156 | 201.5 | 204.9 | 187.5 | 198.0 |
| zileuton | te | 157 | 186.1 | 182.1 | 186.9 | 185.0 |
| succisulfone | tr | 157 | 188.7 | 201.3 | 191.4 | 193.8 |
| salicylic acid | tr | 157 | 181.5 | 210.8 | 194.6 | 195.6 |
| dapiprazole | tr | 158 | 121.6 | 107.7 | 155.0 | 128.1 |
| lidoflazine | te | 159 | 140.8 | 126.4 | 100.3 | 122.5 |
| amidephrine | tr | 159 | 122.2 | 163.6 | 146.0 | 143.9 |
| adrafinil | tr | 159 | 130.0 | 173.8 | 153.4 | 152.4 |
| azacyclonol | tr | 160 | 111.4 | 118.9 | 115.5 | 115.3 |
| bucetin | te | 160 | 168.1 | 146.0 | 124.5 | 146.2 |
| methallatal | tr | 160 | 125.2 | 124.4 | 127.1 | 125.5 |
| benzydamine | tr | 160 | 135.7 | 146.8 | 127.3 | 136.6 |
| oxaprozin | te | 160.5 | 110.9 | 132.5 | 175.0 | 139.5 |
| warfarin | tr | 161 | 186.9 | 221.6 | 191.7 | 200.0 |
| propranolol | tr | 162 | 155.2 | 162.1 | 108.5 | 141.9 |
| torsemide | te | 163 | 179.1 | 135.4 | 163.9 | 159.5 |
| famotidine | tr | 163 | 150.3 | 127.3 | 176.7 | 151.4 |
| tyramine | tr | 164 | 163.4 | 154.1 | 132.1 | 149.8 |
| tolrestat | tr | 164 | 138.5 | 158.6 | 143.2 | 146.8 |
| modafinil | tr | 164 | 151.9 | 168.0 | 144.2 | 154.7 |
| halazepam | te | 164 | 174.1 | 146.2 | 162.6 | 161.0 |
| guanoxan | tr | 164 | 195.1 | 181.6 | 186.6 | 187.8 |
| Metralindole | te | 164 | 210.7 | 204.0 | 196.0 | 203.6 |
| lorazepam | tr | 166 | 186.2 | 183.5 | 199.1 | 189.6 |
| fosfosal | te | 168 | 230.5 | 230.6 | 247.4 | 236.2 |
| sumatriptan | te | 169 | 164.1 | 148.6 | 142.9 | 151.9 |
| acetaminophen | tr | 169 | 174.3 | 164.2 | 152.7 | 163.7 |
| glyburide | tr | 169 | 177.9 | 171.0 | 156.7 | 168.5 |
| pindolol | tr | 170 | 156.0 | 138.6 | 139.2 | 144.6 |
| tolazamide | te | 170 | 151.7 | 175.8 | 157.2 | 161.6 |
| benperidol | tr | 170 | 151.1 | 141.8 | 161.7 | 151.6 |
| metopimazine | tr | 170 | 173.8 | 153.7 | 178.9 | 168.8 |
| isoniazid | tr | 171.4 | 195.6 | 210.3 | 197.0 | 201.0 |
| heptabarbital | te | 174 | 177.0 | 117.9 | 155.8 | 150.2 |
| piposulfan | tr | 175 | 182.2 | 156.4 | 171.9 | 170.1 |
| amisometradine | tr | 175 | 184.8 | 169.3 | 174.4 | 176.2 |

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| --- | --- | --- | --- | --- | --- | --- |
| mephobarbital | te | 176 | 149.6 | 138.6 | 156.9 | 148.4 |
| acifran | tr | 176 | 183.4 | 180.7 | 187.0 | 183.7 |
| propallylonal | tr | 177 | 200.7 | 167.7 | 146.9 | 171.7 |
| ximoprofen | te | 178 | 153.3 | 169.1 | 144.3 | 155.6 |
| sulpiride | tr | 178 | 180.6 | 158.7 | 158.0 | 165.7 |
| zomepirac | tr | 178 | 189.0 | 160.2 | 166.4 | 171.9 |
| nomifensine | te | 179 | 147.3 | 173.0 | 139.2 | 153.2 |
| dextromoramide | tr | 180 | 114.8 | 105.0 | 109.6 | 109.8 |
| molindone | tr | 180 | 149.6 | 107.0 | 162.1 | 139.6 |
| sulthiame | te | 180 | 182.4 | 130.1 | 187.3 | 166.6 |
| irbesartan | tr | 180 | 175.9 | 114.7 | 192.2 | 160.9 |
| letrozole | tr | 181 | 229.2 | 131.2 | 198.4 | 186.3 |
| amphenidone | te | 182.5 | 183.8 | 166.2 | 183.9 | 177.9 |
| zoxazolamine | tr | 184 | 191.3 | 162.9 | 224.4 | 192.8 |
| haloxazolam | tr | 185 | 187.6 | 173.9 | 187.6 | 183.0 |
| bezafibrate | tr | 186 | 157.1 | 149.8 | 133.5 | 146.8 |
| oxazolam | te | 186 | 218.7 | 128.1 | 183.0 | 176.6 |
| acetoaminosalol | tr | 187 | 178.4 | 148.9 | 173.0 | 166.8 |
| acetohexamide | te | 188 | 176.9 | 176.8 | 166.4 | 173.4 |
| verazide | te | 189 | 170.5 | 140.5 | 165.3 | 158.8 |
| glisoxepid | tr | 189 | 133.8 | 153.6 | 178.5 | 155.3 |
| pyrazinamide | tr | 189 | 191.7 | 161.3 | 211.5 | 188.2 |
| spiperone | tr | 190 | 169.7 | 178.2 | 146.7 | 164.9 |
| carbamazepine | tr | 190 | 209.3 | 170.8 | 212.4 | 197.5 |
| glibornuride | te | 192 | 119.0 | 159.4 | 168.4 | 148.9 |
| clebopride | tr | 194 | 132.9 | 139.1 | 151.4 | 141.1 |
| acediasulfone | tr | 194 | 183.9 | 152.8 | 192.9 | 176.5 |
| hymecromone | te | 194 | 185.1 | 164.8 | 222.0 | 190.6 |
| aceglutamide | tr | 197 | 154.5 | 169.6 | 154.5 | 159.5 |
| zopolrestat | tr | 197 | 160.5 | 163.9 | 223.8 | 182.8 |
| probenecid | te | 198 | 177.3 | 169.1 | 127.6 | 158.0 |
| piroxicam | tr | 198 | 214.2 | 160.8 | 221.4 | 198.8 |
| furonazide | tr | 199 | 222.9 | 156.3 | 185.2 | 188.1 |
| ursodiol | te | 203 | 121.6 | 149.0 | 167.0 | 145.9 |
| caroxazone | tr | 203 | 197.8 | 178.8 | 194.0 | 190.2 |
| oxazepam | tr | 205 | 185.3 | 125.7 | 202.3 | 171.1 |
| lonidamine | te | 207 | 193.3 | 111.0 | 189.4 | 164.6 |
| indoramin | tr | 208 | 145.0 | 159.0 | 163.8 | 155.9 |
| albendazole | tr | 208 | 156.3 | 176.5 | 165.6 | 166.1 |
| vigabatrin | te | 209 | 128.6 | 179.4 | 118.6 | 142.2 |
| buprenorphine | tr | 209 | 193.6 | 168.9 | 201.2 | 187.9 |
| albutoin | tr | 210 | 114.0 | 136.5 | 100.1 | 116.9 |
| methetion | te | 210 | 92.7 | 148.6 | 140.4 | 127.2 |
| griseofulvin | tr | 219 | 200.9 | 195.7 | 206.5 | 201.1 |
| tirofiban | te | 223 | 179.0 | 117.9 | 115.9 | 137.6 |
| hydrocortisone | tr | 223 | 207.8 | 197.5 | 209.9 | 205.0 |
| Melengestroleacetate | tr | 224 | 224.5 | 182.1 | 183.9 | 196.8 |
| delavirdine | tr | 226 | 200.9 | 215.8 | 187.1 | 201.3 |
| acitretin | tr | 228 | 117.8 | 155.8 | 119.7 | 131.1 |
| apazone | te | 228 | 135.3 | 178.1 | 173.9 | 162.4 |

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| --- | --- | --- | --- | --- | --- | --- |
| oxibendazole | tr | 230 | 190.1 | 211.6 | 184.9 | 195.5 |
| ondansetron | te | 231 | 246.8 | 154.7 | 190.6 | 197.4 |
| ubenimex | te | 233 | 134.4 | 165.4 | 138.4 | 146.1 |
| phenopyrazone | tr | 233 | 169.0 | 102.3 | 167.7 | 146.4 |
| diaveridine | tr | 233 | 165.4 | 117.2 | 168.9 | 150.5 |
| chlorazanil | tr | 233 | 166.5 | 152.1 | 175.3 | 164.6 |
| sulfamerazine | tr | 234 | 196.8 | 188.6 | 191.7 | 192.4 |
| yohimbine | te | 234 | 186.2 | 180.6 | 239.8' | 202.2 |
| lotrifen | tr | 238 | 199.7 | 194.4 | 199.2 | 197.8 |
| zolimidine | te | 242 | 166.1 | 149.4 | 179.1 | 164.9 |
| clometacin | tr | 242 | 187.8 | 196.0 | 190.9 | 191.5 |
| velnacrine | tr | 245 | 197.4 | 186.0 | 195.0 | 192.8 |
| arprinocid | tr | 245 | 198.5 | 182.8 | 210.7 | 197.3 |
| metolazone | te | 252 | 201.5 | 183.2 | 200.7 | 195.1 |
| flumequine | tr | 253 | 225.6 | 216.1 | 219.1 | 220.3 |
| aciclovir | tr | 255 | 237.1 | 182.1 | 242.0 | 220.4 |
| skfl 05657 | te | 257 | 197.7 | 180.7 | 184.1 | 187.5 |
| ciprofloxacin | tr | 266 | 213.9 | 202.5 | 219.9 | 212.1 |
| hydrochlorothiazide | tr | 267 | 258.5 | 196.4 | 253.5 | 236.1 |
| ibafloxacin | tr | 269 | 222.8 | 189.5 | 212.3 | 208.2 |
| pazufloxacin | te | 269 | 243.0 | 190.2 | 249.0 | 227.4 |
| theophylline | tr | 270 | 253.5 | 210.9 | 242.9 | 235.8 |
| acefylline | te | 271 | 254.8 | 182.9 | 241.7 | 226.5 |
| hydroflumethiazide | tr | 272 | 257.4 | 234.2 | 252.3 | 248.0 |
| moxesterol | tr | 280 | 193.5 | 228.2 | 184.5 | 202.1 |
| primidone | te | 281 | 200.3 | 146.3 | 149.1 | 165.3 |
| prazosin | tr | 285 | 227.4 | 184.1 | 226.9 | 212.8 |
| acedapsone | tr | 289 | 175.3 | 136.6 | 171.5 | 161.1 |
| phenytoin | te | 295 | 189.2 | 133.9 | 173.0 | 165.3 |
| orotic acid | tr | 345 | 275.9 | 263.2 | 298.4 | 279.2 |

The dataset is presented as training (tr) and test (te) sets. **Mpobs and** Mppred denotes observed

and predicted mp, respectively. Model I is based on 2D descriptors, model II on 3D descriptors, model III on both 2D and 3D descriptors and model IV is the averaged consensus of

the three developed models.