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# 基于支持向量机方法的 HERG 钾离子通道抑制剂分类模型

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# Classification Models for HERGPotassiumChannel Inhibitors Based on the Support Vector Machine Approach

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**表 S1** 训练集 367 个化合物及实验 $IC_{50}$ ($\mu mol \cdot L^{-1}$)值，治疗范围，细胞系

**Table S1** 367 compounds in training set with their experimental HERG $IC_{50}$ value ($\mu mol \cdot L^{-1}$), therapeutic area, cell line

| No. | Name | Class | $IC_{50}$ ($\mu mol \cdot L^{-1}$) | Cell |
|---|---|---|---|---|
| 001 | Acetylmethadone | Analgesic | 3.0 | HEK |
| 002 | Alfuzosin | Alpha1 antagonist | 83.3 | CHO |
| 003 | Almokalant | Antiarrhythmic | 0.005 | VM |
| 004 | Alosetron | Antiemetic | 3.2 | HEK |
| 005 | Ambasilide | Anti-arrhythmic | 3.6 | HEK |
| 006 | Amiodarone | Antiarrhythmic | 1 | HERG/L |
| 007 | Amitriptyline | Antidepressant | 10 | CHO |
| 008 | Amlodipine | Ca-channel blocker | 3 | AT-1 |
| 009 | Amsacrine | Antineoplastic | 0.2094 | HEK |
| 010 | Apomorphine | Dopamine receptor agonist | 2.4 | CHO |
| 011 | Aprinidine | Anti-arrhythmic | 0.23 | COS |
| 012 | Artemisin | Antimalarial | 110 | HEK |
| 013 | Astemizole | Antihistamine | 0.0115 | HEK |
| 014 | Azimilide | Antiarrhythmic | 1.41 | HEK |
| 015 | BMCL20031829_01 | Antipsychotic | 0.088 | CHO |
| 016 | BMCL20031829_02 | Antipsychotic | 0.01 | CHO |
| 017 | BMCL20031829_03 | Antipsychotic | 0.007 | CHO |
| 018 | BMCL20031829_04 | Antipsychotic | 0.579 | CHO |
| 019 | BMCL20031829_05 | Antipsychotic | 75 | CHO |
| 020 | BMCL20031829_06 | Antipsychotic | 0.137 | CHO |
| 021 | BMCL20031829_07 | Antipsychotic | 0.131 | CHO |
| 022 | BMCL20031829_08 | Antipsychotic | 0.036 | CHO |
| 023 | BMCL20031829_09 | Antipsychotic | >10 | CHO |
| 024 | BMCL20031829_10 | Antipsychotic | 0.0062 | CHO |
| 025 | BMCL20031829_11 | Antipsychotic | 0.46 | CHO |
| 026 | BMCL20031829_12 | Antipsychotic | >10 | CHO |
| 027 | BMCL20031829_13 | Antipsychotic | 0.0235 | CHO |
| 028 | BMCL20031829_14 | Antipsychotic | 0.204 | CHO |
| 029 | BMCL20031829_15 | Antipsychotic | 0.011 | CHO |
| 030 | BMCL20031829_16 | Antipsychotic | 26 | CHO |
| 031 | BMCL20031829_17 | Antipsychotic | 1.48 | CHO |
| 032 | BMCL20031829_18 | Antipsychotic | 4.55 | CHO |
| 033 | BMCL20031829_19 | Antipsychotic | 1.947 | CHO |
| 034 | BMCL20031829_20 | Antipsychotic | 15.7 | CHO |
| 035 | BMCL20031829_21 | Antipsychotic | 2.2 | CHO |
| 036 | BMCL20031829_22 | Antipsychotic | 3.5 | CHO |
| 037 | BMCL20031829_23 | Antipsychotic | >10 | CHO |
| 038 | BMCL20051225_3hS | Calcium-sensing receptor antagonist | 1.24 | HEK |
| 039 | BMCL20061207_01 | 5-HT2C receptor agonists | 2.5 | CHO |
| 040 | BMCL20061207_13 | 5-HT2C receptor agonists | 21.0 | CHO |
| 041 | BMCL20061207_18 | 5-HT2C receptor agonists | >30 | CHO |
| 042 | BMCL20061207_7a | 5-HT2C receptor agonists | 40 | CHO |
| 043 | BMCL20061775_14 | KSP inhibitor | >10 | CHO |
| 044 | BMCL20061775_15 | KSP inhibitor | 1.3 | CHO |
| 045 | BMCL20061775_16 | KSP inhibitor | 2.2 | CHO |
| 046 | BMCL20061775_17 | KSP inhibitor | 2.4 | CHO |
| 047 | BMCL20061775_20 | KSP inhibitor | 1.5 | CHO |
| 048 | BMCL20061775_21 | KSP inhibitor | 25.0 | CHO |
| 049 | BMCL20061775_22 | KSP inhibitor | 11.0 | CHO |
| 050 | BMCL20061780_01 | KSP inhibitor | 3.5 | CHO |

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|---|---|---|---|---|
| 051 | BMCL20061780_02 | KSP inhibitor | 1.3 | CHO |
| 052 | BMCL20061780_14 | KSP inhibitor | 7.8 | CHO |
| 053 | BMCL20061780_15 | KSP inhibitor | 8.5 | CHO |
| 054 | BMCL20061780_16 | KSP inhibitor | 5.6 | CHO |
| 055 | BMCL20061780_17 | KSP inhibitor | 18.0 | CHO |
| 056 | BMCL20061780_18 | KSP inhibitor | 7.8 | CHO |
| 057 | BMCL20061780_19 | KSP inhibitor | 33.0 | CHO |
| 058 | BMCL20061780_20 | KSP inhibitor | 15.0 | CHO |
| 059 | BMCL20061780_21 | KSP inhibitor | 6.6 | CHO |
| 060 | BMCL20064262_01 | MCH receptor-1 antagonist | 0.052 | CHO |
| 061 | BMCL20064262_02 | MCH receptor-1 antagonist | << 1.0 | CHO |
| 062 | BMCL20064262_03 | MCH receptor-1 antagonist | << 1.0 | CHO |
| 063 | BMCL20064262_05 | MCH receptor-1 antagonist | << 1.0 | CHO |
| 064 | BMCL20064262_06 | MCH receptor-1 antagonist | <<1.0 | CHO |
| 065 | BMCL20064262_26 | MCH receptor-1 antagonist | 0.69 | CHO |
| 066 | BMCL20064262_33 | MCH receptor-1 antagonist | << 1.0 | CHO |
| 067 | BMCL20064262_34 | MCH receptor-1 antagonist | << 1.0 | CHO |
| 068 | BMCL20064311_12c | GlyT1 inhibitor | 1.8 | CHO |
| 069 | BMCL20064311_27 | GlyT1 inhibitor | 1.4 | CHO |
| 070 | BMCL20064311_28 | GlyT1 inhibitor | >24.0 | CHO |
| 071 | BMCL20064633_01 | CCR5 antagonist | << 1.0 | HEK |
| 072 | BMCL20064633_03 | CCR5 antagonist | << 1.0 | HEK |
| 073 | BMCL20064633_06 | CCR5 antagonist | << 1.0 | HEK |
| 074 | BMCL20064633_07 | CCR5 antagonist | << 1.0 | HEK |
| 075 | BMCL20064633_08 | CCR5 antagonist | << 1.0 | HEK |
| 076 | BMCL20065507_01 | Factor Xa inhibitor | <<1.0 | HEK |
| 077 | BMCL20065507_02 | Factor Xa inhibitor | <<1.0 | HEK |
| 078 | BMCL20065507_03 | Factor Xa inhibitor | <<1.0 | HEK |
| 079 | BMCL20065507_05 | Factor Xa inhibitor | <<1.0 | HEK |
| 080 | BMCL20065507_06 | Factor Xa inhibitor | >10 | HEK |
| 081 | BMCL20065507_08 | Factor Xa inhibitor | >10 | HEK |
| 082 | BMCL20065507_10 | Factor Xa inhibitor | >10 | HEK |
| 083 | BMCL20065507_11 | Factor Xa inhibitor | <<1.0 | HEK |
| 084 | BMCL20065507_12 | Factor Xa inhibitor | >10 | HEK |
| 085 | BMCL20065507_13 | Factor Xa inhibitor | <<1.0 | HEK |
| 086 | BMCL20065507_14 | Factor Xa inhibitor | >10 | HEK |
| 087 | BMCL20065507_15 | Factor Xa inhibitor | <<1.0 | HEK |
| 088 | BMCL20065507_16 | Factor Xa inhibitor | >10 | HEK |
| 089 | BMCL20065507_17 | Factor Xa inhibitor | <<1.0 | HEK |
| 090 | BMCL20065507_20 | Factor Xa inhibitor | <<1.0 | HEK |
| 091 | BMCL20065507_23 | Factor Xa inhibitor | >10 | HEK |
| 092 | BMCL20065507_25 | Factor Xa inhibitor | <<1.0 | HEK |
| 093 | BMCL20065507_26 | Factor Xa inhibitor | <<1.0 | HEK |
| 094 | BMCL20065507_27 | Factor Xa inhibitor | >10 | HEK |
| 095 | BMCL20065507_28 | Factor Xa inhibitor | <<1.0 | HEK |
| 096 | BMCL20065507_29 | Factor Xa inhibitor | >10 | HEK |
| 097 | BMCL20065507_30 | Factor Xa inhibitor | >10 | HEK |
| 098 | BMCL20065507_31 | Factor Xa inhibitor | <<1.0 | HEK |
| 099 | BMCL20065507_32 | Factor Xa inhibitor | >10 | HEK |
| 100 | BMCL20065507_33 | Factor Xa inhibitor | <<1.0 | HEK |
| 101 | BMCL20065507_34 | Factor Xa inhibitor | >10 | HEK |
| 102 | BMCL20065507_35 | Factor Xa inhibitor | <<1.0 | HEK |
| 103 | BMCL20065507_36 | Factor Xa inhibitor | >10 | HEK |
| 104 | BMCL20065507_38 | Factor Xa inhibitor | >10 | HEK |
| 105 | BMCL20065507_40 | Factor Xa inhibitor | >10 | HEK |
| 106 | BMCL20065855_06 | Kv1.5 blocker | >30 | HEK |
| 107 | BMCL20065855_29 | Kv1.5 blocker | >30 | HEK |
| 108 | BMCL20065859_08i | Kv1.5 blocker | 21.0 | HEK |

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|---|---|---|---|---|
| 109 | BRL_32872 | Anti-arrhythmic | 0.0198 | HEK |
| 110 | Benzoylecgonine | Ergot alkaloids | 4000 | HEK |
| 111 | Bepridil | Antiemetic | 0.023 | HEK |
| 112 | Berberine | Alkaloid | 3.1 | HEK |
| 113 | Bisindolylmaleimide I | Kinase C Inhibitor | 1 | HEK |
| 114 | Bupivacaine | Analgesic | 25 | HEK |
| 115 | Buprenorphine | Analgesic | 7.5 | HEK |
| 116 | Carvedilol | Beta-blocker | 10.42 | XO |
| 117 | Cetirizine | Antihistamine | 30 | HEK |
| 118 | Chloroquine | Antimalarial | 2.5 | HEK |
| 119 | Chlorpheniramine | Antihistamine | 21.0 | HEK |
| 120 | Chlorpromazine | Antipsychotic | 1.47 | CHO |
| 121 | Chromanol 293B | Antiarrhythmic | 6.6 | HEK |
| 122 | Ciprofloxacin | Antibiotic | 966 | CHO |
| 123 | Cisapride | Prokinetic | 0.027 | HEK |
| 124 | Citalopram | Antidepressant | 3.97 | HEK |
| 125 | Clarithromycin | Antibiotic | 32.9 | HEK |
| 126 | Clobutinol | Antitussive | 2.9 | HEK |
| 127 | Clofilium | Anti-arrhythmic | 0.0126 | HEK |
| 128 | Clomiphene | Anti-estrogen agent | 0.18 | HEK |
| 129 | Clotrimazol | Antimycotic | 3 | HEK |
| 130 | Clozapine | Antipsychotic | 0.256 | HEK |
| 131 | Clozapine N-oxide | Antipsychotic | 133.3 | HEK |
| 132 | Cocaethyline | Anesthetic | 1.2 | HEK |
| 133 | Cocaine | Local anesthetic | 7.2 | HEK |
| 134 | Cyamemazine | Antipsychotic | 0.87 | HEK |
| 135 | D-703 | Antiemetic | 0.182 | HEK |
| 136 | Desbutylhalofantrine | Antimalarial | 0.0717 | HEK |
| 137 | Desipramine | Antiemetic | 1.39 | HEK |
| 138 | Desmethylastemizole | Antihistamine | 0.001 | HEK |
| 139 | Desmethylclozapine | Antipsychotic | 4.49 | HEK |
| 140 | Desmethylolanzapine | Antipsychotic | 14.2 | HEK |
| 141 | Diltiazem | Ca-channel blocker | 17.3 | HEK |
| 142 | Diphenhydramine | Antihistamine | 2.6 | HEK |
| 143 | Disopyramide | Antiarrhythmic | 92 | HERG/L |
| 144 | Dofetilide | Antiarrhythmic | 0.0103 | HEK |
| 145 | Dolasetron | Antiemetic | 5.95 | HEK |
| 146 | Domperidone | Prokinetic | 0.162 | CHO |
| 147 | Doxazosin | Alpha1-blocker | 0.5851 | HEK |
| 148 | Droperidol | Antipsychotic | 0.0322 | HEK |
| 149 | E-4031 | Antiarrhythmic | 0.012 | HEK |
| 150 | Ebastine | Antihistamine | 0.331 | GP/VM |
| 151 | EGIS-7229 (S-21407) | Antiarrhythmic | 6.6 | HEK |
| 152 | EMD-60263 | Ca-sensitizing agent | 6.6 | HEK |
| 153 | EMD-60417 | Antiarrhythmic | 1.32 | HEK |
| 154 | EMD-66398 | Antiarrhythmic | 0.89 | HEK |
| 155 | EMD-66430 | Antiarrhythmic | 1.12 | HEK |
| 156 | Encainide | Antiarrhythmic | 6 | Feline/VM |
| 157 | Epinastine | Antihistamine | 165 | XO |
| 158 | ER-118585 | PDE5 inhibitor | 0.0407 | HEK |
| 159 | Erythromycin | Antibiotic | 115 | HEK |
| 160 | Erythromycylamine | Antibiotic | 273.9 | HEK |
| 161 | Fentanyl | Opiate | 1.8 | HEK |
| 162 | Fexofenadine | Antihistamine | 21.57 | HEK |
| 163 | Flecainide | Antiarrhythmic | 3.91 | HEK |
| 164 | Fluoxetine | Antidepressant | 0.46 | HEK |
| 165 | Gatifloxacin | Antibiotic | 130 | HEK |
| 166 | Glibenclamide | Sulfonylurea | 74 | Neuroblastoma |

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|---|---|---|---|---|
| 167 | Glimepiride | Sulfonylurea | 74 | HEK |
| 168 | Granisetron | Antiemetic | 3.73 | HEK |
| 169 | Grepafloxacin | Antibiotic | 50 | HEK |
| 170 | Halofantrine | Antimalarial | 0.0308 | HEK |
| 171 | Haloperidol | Antipsychotic | 0.019 | HEK |
| 172 | Hesperitin | Flavonoide | 288.8 | XO |
| 173 | Hydrodolasetron MDL-74156 | 5-HT3 antogonist | 12.1 | CHO |
| 174 | Ibutilide | Antiarrhythmic | 0.015 | HERG/L |
| 175 | Imipramine | Antidepressant | 3.4 | HEK |
| 176 | IQB-9302 Ciprocaine | Local anesthetic | 20 | HEK |
| 177 | JMC20051725_8l | Protein kinase C-ß inhibitor | << 1.0 | HEK |
| 178 | JMC20051725_8f | Protein kinase C-ß inhibitor | 0.028 | HEK |
| 179 | JMC20051725_8i | Protein kinase C-ß inhibitor | << 1.0 | HEK |
| 180 | JMC20051725_8m | Protein kinase C-ß inhibitor | << 1.0 | HEK |
| 181 | JMC20056174_10c | Prostaglandin D2 receptor CRTH2 antagonists | >50.0 | CHO |
| 182 | JMC20062143_12 | VEGFR-2 inhibitor | 18.0 | CHO |
| 183 | JMC20062143_14 | VEGFR-2 inhibitor | 18.0 | CHO |
| 184 | JMC20062143_15 | VEGFR-2 inhibitor | 20.0 | CHO |
| 185 | JMC20063614_32 | α-Amino amide dipeptidyl peptidase IV inhibitor | 16.0 | HEK |
| 186 | JMC20063753_21d | MCH receptor-1 antagonist | 1.8 | CHO |
| 187 | JMC20063766_14 | Vascular endothelial growth factor receptor-2 inhibitor | 16.6 | HEK |
| 188 | JMC20066569_01 | MCH receptor | 1.4 | HEK |
| 189 | JMC20066569_02 | MCH receptor | 11.5 | HEK |
| 190 | JMC20066569_17 | MCH receptor | 63.7 | HEK |
| 191 | JMC20066569_18 | MCH receptor | 3.6 | HEK |
| 192 | JMC20066569_19 | MCH receptor | 7.4 | HEK |
| 193 | JMC20066569_20 | MCH receptor | 2.5 | HEK |
| 194 | JMC20066569_21 | MCH receptor | 3.6 | HEK |
| 195 | JMC20066569_22 | MCH receptor | 15.1 | HEK |
| 196 | JMC20066569_23 | MCH receptor | 5.0 | HEK |
| 197 | JMC20066569_30 | MCH receptor | 4.0 | HEK |
| 198 | JMC20066569_31 | MCH receptor | 6.7 | HEK |
| 199 | JMC20066569_34 | MCH receptor | 10.5 | HEK |
| 200 | JMC20066569_35 | MCH receptor | 15.9 | HEK |
| 201 | JMC20066569_36 | MCH receptor | 6.2 | HEK |
| 202 | JMC20066569_40 | MCH receptor | 19.9 | HEK |
| 203 | JMC20066569_42 | MCH receptor | 5.6 | HEK |
| 204 | JMC20066569_43 | MCH receptor | 13.5 | HEK |
| 205 | JMC20066569_44 | MCH receptor | 12.2 | HEK |
| 206 | JMC20066569_46 | MCH receptor | 10.4 | HEK |
| 207 | JMC20066569_47 | MCH receptor | 5.4 | HEK |
| 208 | JMC20066569_49 | MCH receptor | 21.2 | HEK |
| 209 | JMC20066569_51 | MCH receptor | 14.7 | HEK |
| 210 | JMC20066569_52 | MCH receptor | 8.5 | HEK |
| 211 | JMC20066569_53 | MCH receptor | 20.3 | HEK |
| 212 | JMC20066569_54 | MCH receptor | 47.7 | HEK |
| 213 | Josamycin | Antibiotic | 102.4 | HEK |
| 214 | Ketanserin | Antiemetic | 0.107 | HEK |
| 215 | Ketoconazole | Antimycotic | 1.9 | HEK |
| 216 | LAAM | Opiate agonist | 2.2 | HEK |
| 217 | Levofloxacin | Antibiotic | 915 | CHO |
| 218 | Lidoflazine | Antiemetic | 0.016 | HEK |
| 219 | Lopinavir | Antiviral | 8.6 | HEK |
| 220 | Loratadine | Antihistamine | 2.3 | HEK |
| 221 | Losartan | Diuretic | 7.76 | HEK |
| 222 | Lumefantrine | Antimalarial | 8.1 | HEK |

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|---|---|---|---|---|
| 223 | LY-97241/UK-06711-13 | Antiarrhythmic | 0.0016 | CHO |
| 224 | Maprotiline | Antidepressant | 5.2 | HEK |
| 225 | Mefloquine | Antimalarial | 2.56 | HEK |
| 226 | Mesoridazine | Antipsychotic | 0.435 | HEK |
| 227 | Methadone | Analgesic | 9.8 | HEK |
| 228 | Methoxyverapamil( D-600) | Antiemetic | 6.6 | HEK |
| 229 | Methylecgonidine | Ergot alkaloids | 170 | HEK |
| 230 | Mibefradil | Antiemetic | 1.43 | COS |
| 231 | Mizolastine | Antihistamine | 0.441 | HEK |
| 232 | MK-499 | Antiarrhythmic | 0.021 | HEK |
| 233 | Morin | Flavonoide | 111.4 | HEK |
| 234 | Mosapride | Prokinetic | 7.75 | HEK |
| 235 | Moxifloxacin | Antibiotic | 129 | HEK |
| 236 | Naringenin | Flavonoide | 36.5 | HEK |
| 237 | N-Desbutyllumefantrine | Antimalarial | 5.5 | HEK |
| 238 | NIP-142 | Antiarrhythmic agent | 44.0 | HEK |
| 239 | NPS-2143 | Calcium-sensing receptor antagonist | 0.190 | HEK |
| 240 | Nelfinavir | Antiviral | 11.5 | HEK |
| 241 | Nicotine | Stimulant | 244.8 | HEK |
| 242 | Nifedipine | Ca-channel blocker | 615 | HEK |
| 243 | Nitrendipine | Ca-channel blocker | 115 | HEK |
| 244 | Norastemizole | Antihistamine | 0.028 | HEK |
| 245 | Norfluoxetine | Antidepressant | 2.30 | HEK |
| 246 | Norverapamil | Antiemetic | 3.15 | HEK |
| 247 | OPC-18790 | Antipsychotic | 0.96 | HEK |
| 248 | Ofloxacin | Antibiotic | 1420 | CHO |
| 249 | Olanzapine | Antipsychotic | 0.181 | HEK |
| 250 | Oleandomycin | Antibiotic | 339.6 | HEK |
| 251 | Ondansetron | Antiemetic | 0.81 | HEK |
| 252 | Oxybutynin | Antimuscarinic | 25.0 | HEK |
| 253 | PNU-0068611A | Antiarrhythmic | 0.0808 | XO |
| 254 | Paliperidone or 9-hydroxyrisperidone | Antipsychotic | 1.3 | HEK |
| 255 | Pentobarbital | Antiepileptic | 130 | HEK |
| 256 | Pergolide LY_141B | Dopamine receptor agonist | 0.12 | CHO |
| 257 | Perhexilene | Antiemetic | 7.8 | CHO |
| 258 | Phenobarbital | Antiepileptic | 3000 | HEK |
| 259 | Phenytoin | Antiepileptic | 240 | HEK |
| 260 | Pilsicainide | $Na^+$ Channel Blocker | 20.4 | HEK |
| 261 | Pimozide | Antipsychotic | 0.001 | HEK |
| 262 | Prazosin | Alpha1-blocker | 1.57 | HEK |
| 263 | Procainamide | Antiarrhythmic | 139 | HEK |
| 264 | Propoxyphene | Analgesic | 2.75 | HEK |
| 265 | Propranolol | Beta-blocker | 15 | AT-1 |
| 266 | Prucalopride | Prokinetic | 5.70 | HEK |
| 267 | Pyrilamine | Antihistamine | 1.1 | HEK |
| 268 | Quetiapine | antipsychotic | 5.765 | HEK |
| 269 | Quinidine | Antiarrhythmic | 1.068 | HEK |
| 270 | Ranolazine | Antianginal | 11.5 | VM |
| 271 | Risperidone | Antipsychotic | 0.163 | HEK |
| 272 | Ropinirole | Dopamine receptor agonist | 1.20 | CHO |
| 273 | Roxithromycin | Antibiotic | 36.5 | HEK |
| 274 | Saquinavir | Antiviral | 15.3 | HEK |
| 275 | Sertindole | Antipsychotic | 0.0126 | HEK |
| 276 | Sildenafil | PDE5 inhibitor | 100 | HEK |
| 277 | Sotalol | Antiarrhythmic | 269 | HEK |
| 278 | Sparfloxacin | Antibiotic | 18 | CHO |

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| 279 | Spironolactone | Diuretic | 23 | CHO |
| 280 | Sulfamethoxazole | Sulfonamid | 10000 | HEK |
| 281 | Tadalafil | PDE5 inhibitor | 100 | HEK |
| 282 | Tamoxifen | Antineoplastic | 1 | HEK |
| 283 | Tamsulosin | Alpha1-blocker | 104.8 | CHO |
| 284 | Terazosin | Alpha1-blocker | 17.7 | HEK |
| 285 | Terfenadine | Antihistamine | 0.0084 | HEK |
| 286 | Terikalant | Antiarrhythmic | 0.25 | XO |
| 287 | Terodiline | Antiarrhythmic | 5.75 | HEK |
| 288 | Thioridazine | Antipsychotic | 0.096 | HEK |
| 289 | Tolterodine | Muscarinic antagonist | 0.017 | CHO |
| 290 | Trazodone | Antidepressant | 2.9 | HEK |
| 291 | Trimebutine | Local anesthetic | 90 | HEK |
| 292 | Trimethaphan | antihypertensive | 10 | AT-1 |
| 293 | Trimethoprim | Antiinfective | 240 | HEK |
| 294 | UK-064962-01 | Antiarrhythmic | 0.2732 | XO |
| 295 | UK-064963-01 | Antiarrhythmic | 0.3287 | XO |
| 296 | UK-068097 | Antiarrhythmic | 0.9920 | XO |
| 297 | UK-068522 | Antiarrhythmic | 2.590 | XO |
| 298 | UK-068523 | Antiarrhythmic | 0.081 | XO |
| 299 | UK-068526-01 | Antiarrhythmic | 0.044 | XO |
| 300 | Valproic acid | Anticonvulsant | 20 | AT-1 |
| 301 | Vardenafil | PDE5 inhibitor | 12.8 | HEK |
| 302 | Verapamil | Antiemetic | 0.136 | HEK |
| 303 | Vesnarinone | Antipsychotic | 1.1 | HEK |
| 304 | WAY-123398 | Antiarrhythmic | 0.019 | Feline VM |
| 305 | Ziprasidone | Antipsychotic | 0.125 | HEK |
| 306 | JMC_20042405_1 | HIV-1 inhibitor | 1.1 | HEK |
| 307 | JMC_20042405_30 | HIV-1 inhibitor | 5.8 | HEK |
| 308 | JMC_20046655-6 | Growth hormone secretagogue receptor antagonist | 6.1 | CHO |
| 309 | JMC_20055888-7 | MCH receptor 1 antagonist | 2.25 | HEK |
| 310 | JMC20066439_25 | Dipepzidyl peptidase IV inhibitor | > 300 | HEK |
| 311 | JMC_doi061118e_15 | CCR8 antagonist | Ki>10 | HEK |
| 312 | JMC20066954_8b | Kv1.5 antagonist | 33.5 | Displacement [$^{35}$S]MK-0499/HEK |
| 313 | JMC20066954_8c | | 62 | |
| 314 | JMC20066954_8d | | 1.65 | |
| 315 | JMC20066954_8e | | 10 | |
| 316 | JMC20066954_8f | | 135 | |
| 317 | JMC20066954_8h | | 16 | |
| 318 | JMC20066954_12 | | 20.5 | |
| 319 | JMC20066954_13 | | 15 | |
| 320 | JMC20066954_19 | | >30 | |
| 321 | JMC20065954_16 | | 21 | |
| 322 | JMC20067450_6b | Dopamine D4 agonist | 14.5% | % inhibition @ 3µg/ml / HEK |
| 323 | JMC20067450_7a | | 45% | |
| 324 | JMC20066946_08 | Leukocyte function associated antigen-1 antagonist | 24% | % inhibition @ 30µM / HEK |
| 325 | BMC_doi200612028_21b | MCH-R1 antagonist | 8.1 | HEK |
| 326 | BMC_doi200612028_21e | | 3.3 | |
| 327 | BMC_doi200612028_21j | | 1.7 | |
| 328 | BMCL_doi200611065_01 | MCH-R1 antagonist | 15.1 | Displacement of [$^{3}$H]-dofetilide /HEK |
| 329 | BMCL_doi200611065_06 | | 5.28 | |
| 330 | BMCL_doi200611065_07 | | 1.37 | |
| 331 | BMCL_doi200611065_08 | | 6.08 | |
| 332 | BMCL_doi200611065_09 | | 2.53 | |
| 333 | BMCL_doi200611065_10 | | 34.6 | |
| 334 | BMCL_doi200611065_11 | | 26.7 | |
| 335 | BMCL_doi200611065_12 | | 20 | |

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|---|---|---|---|---|
| 336 | BMCL_doi200611065_13 | | 25 | |
| 337 | BMCL_doi200611065_14 | | 85.2 | |
| 338 | BMCL_doi200611065_16 | | 5.79 | |
| 339 | BMCL_doi200611065_17 | | 85.8 | |
| 340 | BMCL_doi200611065_18 | | 47.4 | |
| 341 | BMCL_doi200611065_19 | | 51.1 | |
| 342 | BMCL_doi200611065_r16_1 | | 47.7 | |
| 343 | BMCL_doi200611065_r16_2 | | 60.7 | |
| 344 | CP122721 | | 1.8 | |
| 345 | BMCL20060811_01b | | 0.24 | |
| 346 | BMCL20060811_01c | | 0.36 | |
| 347 | BMCL20060811_01d | | 1.4 | |
| 348 | BMCL20060811_04 | | 4.8 | |
| 349 | BMCL20060811_05a | NK1 antagonist | 0.27 | Displacement [$^{35}$S]MK-0499/HEK |
| 350 | BMCL20060811_05b | | 0.42 | |
| 351 | BMCL20060811_05c | | 0.19 | |
| 352 | BMCL20060811_05d | | >6 | |
| 353 | BMCL20060811_05e | | 5.8 | |
| 354 | BMCL20060811_05f | | >5 | |
| 355 | BMCL20060811_05g | | >6 | |
| 356 | PNU_282987 | | 57% | |
| 357 | PHA_543613 | | 29% | |
| 358 | BMC20068219_01h | | 2% | |
| 359 | BMC20068219_01i | | <1% | |
| 360 | BMC20068219_01k | | 71% | |
| 361 | BMC20068219_01o | α7 nicotinic acetylcholine receptor agonist | 5% | % inhibition @ 20μM / HEK |
| 362 | BMC20068219_02a | | 18% | |
| 363 | BMC20068219_02c | | 35% | |
| 364 | BMC20068219_02e | | 60% | |
| 365 | BMC20068219_09a | | 16% | |
| 366 | BMC20068219_09c | | 41% | |
| 367 | BMC20068219_18a | | 19% | |

**表 S2** 外部测试集 97 个化合物及实验 $IC_{50}$ ($\mu mol \cdot L^{-1}$)值

**Table S2** 97 compounds in external testing set with their experiment HERG $IC_{50}$ values ($\mu mol \cdot L^{-1}$)

| No. | Compound | Class | $IC_{50}$($\mu mol \cdot L^{-1}$) | Ref. |
|---|---|---|---|---|
| 01 | BMC2009731-20 | | 0.19 | |
| 02 | BMC2009731-24 | | 0.078 | |
| 03 | BMC2009731-25 | | 0.1 | |
| 04 | BMC2009731-26 | | 1.3 | |
| 05 | BMC2009731-27 | | 2.0 | |
| 06 | BMC2009731-28 | | 1.8 | |
| 07 | BMC2009731-29 | | 2.7 | |
| 08 | BMC2009731-34 | | 0.47 | |
| 09 | BMC2009731-35 | | 1.2 | |
| 10 | BMC2009731-36 | | 1.7 | |
| 11 | BMC2009731-37 | | 1.6 | |
| 12 | BMC2009731-38 | | 0.84 | |
| 13 | BMC2009731-43 | | 3.1 | |
| 14 | BMC2009731-44 | | 0.13 | |
| 15 | BMC2009731-45 | VEGFR-2 | 1.1 | 16 |
| 16 | BMC2009731-48 | inhibitor | 4.9 | |
| 17 | BMC2009731-52 | | 0.63 | |
| 18 | BMC2009731-53 | | 4.1 | |
| 19 | BMC2009731-54 | | 0.40 | |
| 20 | BMC2009731-56 | | 0.075 | |
| 21 | BMC2009731-57 | | 0.048 | |
| 22 | BMC2009731-58 | | 0.079 | |
| 23 | BMC2009731-59 | | 0.017 | |
| 24 | BMC2009731-60 | | 0.39 | |
| 25 | BMC2009731-61 | | 0.11 | |
| 26 | BMC2009731-62 | | 0.12 | |
| 27 | BMC2009731-63 | | 0.43 | |
| 28 | BMC2009731-65 | | 0.27 | |
| 29 | BMC2009731-66 | | 0.23 | |
| 30 | BMC2009731-68 | | 2.0 | |
| 31 | BMCL20075558-07 | HERG | 2.6 | 17 |
| 32 | BMCL20075558-08 | | 2.4 | |
| 33 | BMCL20075558-09 | | 1.6 | |
| 34 | BMCL20075558-10 | | 7.4 | |
| 35 | BMCL20075558-11 | | 3.1 | |
| 36 | BMCL20075558-12 | | 8.6 | |
| 37 | BMCL20075558-18a | | 16 | |
| 38 | BMCL20075558-18b | | 3.3 | |
| 39 | BMCL20075558-18c | | 10 | |

| | | | | |
|---|---|---|---|---|
| 40 | BMCL20075558-18d | | <1.5 | |
| 41 | BMCL20075558-18f | | 11 | |
| 42 | BMCL20084859-01 | | 0.092 | |
| 43 | BMCL20084859-02 | | 0.041 | |
| 44 | BMCL20084859-03 | | 0.903 | |
| 45 | BMCL20084859-04 | | 0.082 | |
| 46 | BMCL20084859-05 | | 2.34 | |
| 47 | BMCL20084859-06 | | 0.120 | |
| 48 | BMCL20084859-07 | | 0.297 | |
| 49 | BMCL20084859-08 | | 0.710 | |
| 50 | BMCL20084859-09 | | 0.100 | |
| 51 | BMCL20084859-10 | | 0.052 | |
| 52 | BMCL20084859-11 | | 0.029 | |
| 53 | BMCL20084859-12 | | 0.031 | |
| 54 | BMCL20084859-13 | | >33 | |
| 55 | BMCL20084859-14 | | 0.043 | |
| 56 | BMCL20084859-15 | | 9.65 | |
| 57 | BMCL20084859-16 | | 1.5 | |
| 58 | BMCL20084859-17 | | 0.048 | |
| 59 | BMCL20084859-18 | | 0.078 | |
| 60 | BMCL20084859-19 | | 0.927 | |
| 61 | BMCL20084859-20 | MCH-R1 | 0.347 | 18 |
| 62 | BMCL20084859-21 | antagonists | 2.14 | |
| 63 | BMCL20084859-22 | | 0.109 | |
| 64 | BMCL20084859-23 | | 0.636 | |
| 65 | BMCL20084859-24 | | 3.05 | |
| 66 | BMCL20084859-25 | | 0.029 | |
| 67 | BMCL20084859-26 | | 0.042 | |
| 68 | BMCL20084859-27 | | 0.111 | |
| 69 | BMCL20084859-28 | | 2.26 | |
| 70 | BMCL20084859-29 | | 0.104 | |
| 71 | BMCL20084859-30 | | 1.25 | |
| 72 | BMCL20084859-31 | | 0.169 | |
| 73 | BMCL20084859-32 | | 0.313 | |
| 74 | BMCL20084859-33 | | 0.303 | |
| 75 | BMCL20084859-34 | | 0.269 | |
| 76 | BMCL20084859-35 | | 0.020 | |
| 77 | BMCL20084859-36 | | 0.113 | |
| 78 | BMCL20084859-37 | | 0.037 | |
| 79 | BMCL20084859-38 | | 0.025 | |
| 80 | BMCL20084859-39 | | 0.066 | |
| 81 | BMCL20084859-40 | | 0.026 | |
| 82 | BMCL20085554-3 | HERG binding | 49.9 | 19 |

| | | | | |
|---|---|---|---|---|
| 83 | BMCL20085554-13 | 0.68 | | |
| 84 | BMCL20085554-9a | >94.5 | | |
| 85 | BMCL20085554-9b | 71.5 | | |
| 86 | BMCL20085554-9e | 31.8 | | |
| 87 | BMCL20085554-10a | 6.96 | | |
| 88 | BMCL20085554-10b | 0.74 | | |
| 89 | BMCL20085554-10c | 2.7 | | |
| 90 | BMCL20085554-10d | 0.96 | | |
| 91 | BMCL20085554-10e | 8.95 | | |
| 92 | BMCL20085554-10f | 23.0 | | |
| 93 | BMCL20085554-14 | 18.6 | | |
| 94 | BMCL20085554-15 | 34.0 | | |
| 95 | BMCL20085554-16 | 13.6 | | |
| 96 | BMCL20085554-17 | 36.6 | | |
| 97 | BMCL20085554-18 | 50.1 | | |

表 S3 三个模型所筛选的分子描述符

**Table S3** Molecular descriptors selected by the three models

| Model | Type | Descripor |
|---|---|---|
| Model I (42) | Charge descriptors | number of rotatable bonds |
| | Topological indices | sum of E-State of atom type $ssCH_2$ , sum of E-State of atom type aaCH, sum of E-State of atom type dssC, sum of E-State of atom type aasC, sum of E-State of atom type aaO, sum of E-State of all C atoms, average E-State values, ALOGP weighted Moreau-Broto lagged 1, ALOGP weighted Moreau-Broto lagged 3, ALOGP weighted Moreau-Broto lagged 9, E-State weighted Moreau-Broto lagged 5, Polarizability weighted Moreau-Broto lagged 0, ALOGP weighted Geary lagged 6, BCUT 4th highest of E-State |
| | Geometrical molecular descriptors | Radius of gyration, unweighted 2nd MS-WHIM Skewness over VDW surface, unweighted 2nd MS-WHIM Kurtosis over VDW surface, P-MEP weighted 1st MS-WHIM Kurtosis over VDW surface, P-MEP weighted 3rd MS-WHIM Kurtosis over VDW surface, N-MEP weighted 1st MS-WHIM Kurtosis over VDW surface, N-MEP-weighted 1st MS-WHIM Kurtosis by SAS surface, partial positive surface area, total polar surface area, ALOGP weighted RDF g(2.0), atomic charge weighted RDF g(5.5), polarizability weighted RDF g(11.5), polarizability weighted RDF g(13.0), polarizability weighted RDF g(14.0), unweighted 3D-MoRSE-Signal I(6.0), 3D-MoRSE-Signal I(11.0) weighted by atomic mass, 3D-MoRSE-Signal I(16.0) weighted by atomic mass, 3D-MoRSE-Signal I(10.0) weighted by VDW, unweighted H-GETAWAY HATS6 , unweighted H-GETAWAY HATS8, unweighted H-GETAWAY H6, unweighted H-GETAWAY H8 , H-GETAWAY HATS weighted by VDW, H-GETAWAY HATS1 weighted by E-State, H-GETAWAY HATS weighted by E-State, unweighted R-GETAWAY R3 , R-GETAWAY R2 weighted by VDW |
| | Topological indices | topological charge index G4, sum of E-State of atom type aaCH, sum of E-State of atom type sOH, ALOGP weighted Moreau-Broto lagged 1, E-State weighted Moreau-Broto lagged 5, E-State weighted Moreau-Broto lagged 6, ALOGP weighted Geary lagged 1, polarizability weighted Geary lagged 5, BCUT 2th lowest of ALOGP, BCUT 5th lowest of ALOGP, BCUT 5th highest of E-State, BCUT 5th lowest of polarizability |
| Model II (25) | Geometrical molecular descriptors | unweighted 1st MS-WHIM Skewness by SAS surface, PSA for O atom, Polar Surface Area, ALOGP weighted RDF g(8.0), atomic charge weighted RDF g(2.5), E-State weighted RDF g(1.0), 3D-MoRSE-Signal I(10.0) weighted by atomic mass, 3D-MoRSE-Signal I(16.0) weighted by atomic mass, 3D-MoRSE-Signal I(25.0) weighted by E-State, 3D-MoRSE-Signal I(30.0) weighted by E-State, Electronegativity weighted H-GETAWAY H0, E-State weighted H-GETAWAY HATS7, atomic mass-weighted R-GETAWAY R5 |

| | | |
|---|---|---|
| | Charge descriptors | $0^{th}$ Electronic-topological descriptors $1^{th}$ Electronic-topological descriptors, the global topological charge index J, |
| | Topological indices | sum of Estate of atom type sssCH, sum of Estate of atom type dssC, sum of Estate of atom type aasC, sum of Estate of atom type aaO, ALOGP weighted Moreau-Broto lagged 3, ALOGP weighted Moreau-Broto lagged 5 , ALOGP weighted Moreau-Broto lagged 9, atomic charge weighted moran lagged 1, ALOGP weighted Geary 5, atomic charge weighted Geary 10, E-State weighted Geary 7, polarizability mass weighted Geary 3, BCUT 1th lowest of ALOGP, radius of gyration, 2nd MS-WHIM kurtosis over VDW surface |
| Model III (40) | Geometrical Molecular Descriptors | total variance of the surface potential weighted by SAS surface*1000, total polar surface area, RSAM index, ALOGP weighted RDF g(8.0), polarizability weighted RDF g(14.0), 2nd directional WHIM shape weighted by atomic mass, WHIM size D weighted by E-State, unweighted 3D-MoRSE-Signal I( 6.0), unweighted 3D-MoRSE-Signal I(12.0), unweighted 3D-MoRSE-Signal I(16.0), unweighted 3D-MoRSE-Signal I(22.0), 3D-MoRSE-Signal I(10.0) weighted by atomic mass, 3D-MoRSE-Signal I(10.0) weighted by VDW, 3D-MoRSE-Signal I(25.0) weighted by E-State, atomic mass weighted H-GETAWAY H6, VDW weighted H-GETAWAY H0, Electronegativity weighted H-GETAWAY HATS0, E-State weighted H-GETAWAY HATS7, E-State weighted H-GETAWAY H1, unweighted R-GETAWAY R3, E-State weighted R-GETAWAY R+5, E-State weighted R-GETAWAY R+7 |

**表 S4** 1559 个分子描述符

**Table S4** Full list of 1559 molecular descriptors

| | |
|---|---|
| 1 | Number of Atoms |
| 2 | Number of Heavy atoms |
| 3 | Number of H atoms |
| 4 | Number of B atoms |
| 5 | Number of C atoms |
| 6 | Number of N atoms |
| 7 | Number of O atoms |
| 8 | Number of F atoms |
| 9 | Number of P atoms |
| 10 | Number of S atoms |
| 11 | Number of Cl atoms |
| 12 | Number of Br atoms |
| 13 | Number of I atoms |
| 14 | Number of Bonds |
| 15 | Number of non-H Bonds |
| 16 | Number of rings |
| 17 | Molecular weight |
| 18 | Average molecular weight |
| 19 | Number of H-bond donnor |
| 20 | Number of H-bond acceptor |
| 21 | Sanderson electronegativity sum |
| 22 | Number of rotable bonds |
| 23 | Dipole moment (in Debye) |
| 24 | Total absolute atomic charge |
| 25 | Total squared atomic charge |
| 26 | Charge Polarization |
| 27 | Topological electronic index TE |
| 28 | Topological electronic index CTE |
| 29 | Maximum negative charges |
| 30 | Maximum positive charges |
| 31 | Local dipol index |
| 32 | Total negative charges |
| 33 | Total positive charges |
| 34 | Submolecular Polarity Parameter |
| 35 | Second-order submolecular polarity parameter |
| 36 | Relative positive charge |
| 37 | Relative negative charge |
| 38 | 0th Electronic-topological |
| 39 | 1th Electronic-topological |
| 40 | 2th Electronic-topological |
| 41 | Electron charge density connectivity index |

42 Hydrophobic alogp
43 Molecular polarizability
44 Schultz molecular topological index
45 Gutman molecular topological index
46 Topological charge index G1
47 Topological charge index G2
48 Topological charge index G3
49 Topological charge index G4
50 Topological charge index G5
51 Mean topological charge index J1
52 Mean topological charge index J2
53 Mean topological charge index J3
54 Mean topological charge index J4
55 Mean topological charge index J5
56 Global topological charge index J
57 Wiener index
58 Mean Wiener index
59 Harary index
60 Gravitational topological index
61 Molecular path count of length 1
62 Molecular path count of length 2
63 Molecular path count of length 3
64 Molecular path count of length 4
65 Molecular path count of length 5
66 Molecular path count of length 6
67 Total path count
68 Sum of Estate of atom type sLi
69 Sum of Estate of atom type ssBe
70 Sum of Estate of atom type ssssBe
71 Sum of Estate of atom type ssBH
72 Sum of Estate of atom type sssB
73 Sum of Estate of atom type ssssB
74 Sum of Estate of atom type sCH3
75 Sum of Estate of atom type dCH2
76 Sum of Estate of atom type ssCH2
77 Sum of Estate of atom type tCH
78 Sum of Estate of atom type dsCH
79 Sum of Estate of atom type aaCH
80 Sum of Estate of atom type sssCH
81 Sum of Estate of atom type ddC
82 Sum of Estate of atom type tsC
83 Sum of Estate of atom type dssC
84 Sum of Estate of atom type aasC

85 Sum of Estate of atom type aaaC
86 Sum of Estate of atom type sssC
87 Sum of Estate of atom type sNH3
88 Sum of Estate of atom type sNH2
89 Sum of Estate of atom type ssNH2
90 Sum of Estate of atom type dNH
91 Sum of Estate of atom type ssNH
92 Sum of Estate of atom type aaNH
93 Sum of Estate of atom type tN
94 Sum of Estate of atom type sssNH
95 Sum of Estate of atom type dsN
96 Sum of Estate of atom type aaN
97 Sum of Estate of atom type sssN
98 Sum of Estate of atom type ddsN
99 Sum of Estate of atom type aasN
100 Sum of Estate of atom type aOH
101 Sum of Estate of atom type sOH
102 Sum of Estate of atom type dO
103 Sum of Estate of atom type ssO
104 Sum of Estate of atom type aaO
105 Sum of Estate of atom type F
106 Sum of Estate of atom type ssSiH2
107 Sum of Estate of atom type ssSiH2
108 Sum of Estate of atom type sssSiH
109 Sum of Estate of atom type ssssSi
110 Sum of Estate of atom type sPH2
111 Sum of Estate of atom type ssPH
112 Sum of Estate of atom type sssP
113 Sum of Estate of atom type dsssP
114 Sum of Estate of atom type ssssP
115 Sum of Estate of atom type sSH
116 Sum of Estate of atom type dS
117 Sum of Estate of atom type ssS
118 Sum of Estate of atom type aaS
119 Sum of Estate of atom type dssS
120 Sum of Estate of atom type ddssS
121 Sum of Estate of atom type sCl
122 Sum of Estate of atom type sGeH3
123 Sum of Estate of atom type ssGeH2
124 Sum of Estate of atom type sssGeH
125 Sum of Estate of atom type ssssGe
126 Sum of Estate of atom type sAsH2
127 Sum of Estate of atom type ssAsH

128 Sum of Estate of atom type sssAs
129 Sum of Estate of atom type sssdAs
130 Sum of Estate of atom type ssssAs
131 Sum of Estate of atom type sSeH
132 Sum of Estate of atom type dSe
133 Sum of Estate of atom type ssSe
134 Sum of Estate of atom type aaSe
135 Sum of Estate of atom type dssSe
136 Sum of Estate of atom type ddssSe
137 Sum of Estate of atom type sBr
138 Sum of Estate of atom type sSnH3
139 Sum of Estate of atom type ssSnH2
140 Sum of Estate of atom type sssSnH
141 Sum of Estate of atom type ssssSn
142 Sum of Estate of atom type sI
143 Sum of Estate of atom type sPbH3
144 Sum of Estate of atom type ssPbH2
145 Sum of Estate of atom type sssPbH
146 Sum of Estate of atom type ssssPb
147 Sum of Estate of atom type unknown
148 Sum of Estate of all heavy atoms
149 Sum of Estate of all C atoms
150 Sum of Estate of all halogen atoms
151 Sum of Estate of all hetero atoms
152 Sum of Estate of H-bond acceptors
153 Average of Estate values
154 Maximum of Estate values
155 Minimum of Estate values
156 Sum of H Estate of atom type HsOH
157 Sum of H Estate of atom type HdNH
158 Sum of H Estate of atom type HsSH
159 Sum of H Estate of atom type HsNH2
160 Sum of H Estate of atom type HssNH
161 Sum of H Estate of atom type HaaNH
162 Sum of H Estate of atom type HsNH3p
163 Sum of H Estate of atom type HssNH2p
164 Sum of H Estate of atom type HsssNHp
165 Sum of H Estate of atom type HtCH
166 Sum of H Estate of atom type HdCH2
167 Sum of H Estate of atom type HdsCH
168 Sum of H Estate of atom type HaaCH
169 Sum of H Estate of atom type HCHnX
170 Sum of H Estate of atom type HCsats

171 Sum of H Estate of atom type HCsatu
172 Sum of H Estate of atom type Havin
173 Sum of H Estate of atom type Hother
174 Sum of H Estate of atom type Hmisc
175 Sum of H Estate of H-bond donors
176 Xu index
177 Modified Xu Index
178 Balaban Index J
179 Platt Number
180 Log of Superpendentic index
181 First Zagreb Index(M1)
182 Second Zagreb Index(M2)
183 First Modified Zagreb Index
184 Second Modified Zagreb Index
185 Quadratic index(Q)
186 0th edge connectivity index
187 Edge connectivity index
188 Extened edge connectivity inndex
189 2th spectral moment
190 3th spectral moment
191 4th spectral moment
192 5th spectral moment
193 6th spectral moment
194 7th spectral moment
195 8th spectral moment
196 9th spectral moment
197 10th spectral moment
198 Atomic mass weighted Moreau-Broto lagged 0
199 Atomic mass weighted Moreau-Broto lagged 1
200 Atomic mass weighted Moreau-Broto lagged 2
201 Atomic mass weighted Moreau-Broto lagged 3
202 Atomic mass weighted Moreau-Broto lagged 4
203 Atomic mass weighted Moreau-Broto lagged 5
204 Atomic mass weighted Moreau-Broto lagged 6
205 Atomic mass weighted Moreau-Broto lagged 7
206 Atomic mass weighted Moreau-Broto lagged 8
207 Atomic mass weighted Moreau-Broto lagged 9
208 Atomic mass weighted Moreau-Broto lagged 10
209 Electronegativity weighted Moreau-Broto lagged 0
210 Electronegativity weighted Moreau-Broto lagged 1
211 Electronegativity weighted Moreau-Broto lagged 2
212 Electronegativity weighted Moreau-Broto lagged 3
213 Electronegativity weighted Moreau-Broto lagged 4

214 Electronegativity weighted Moreau-Broto lagged 5
215 Electronegativity weighted Moreau-Broto lagged 6
216 Electronegativity weighted Moreau-Broto lagged 7
217 Electronegativity weighted Moreau-Broto lagged 8
218 Electronegativity weighted Moreau-Broto lagged 9
219 Electronegativity weighted Moreau-Broto lagged 10
220 VDW radius weighted Moreau-Broto lagged 0
221 VDW radius weighted Moreau-Broto lagged 1
222 VDW radius weighted Moreau-Broto lagged 2
223 VDW radius weighted Moreau-Broto lagged 3
224 VDW radius weighted Moreau-Broto lagged 4
225 VDW radius weighted Moreau-Broto lagged 5
226 VDW radius weighted Moreau-Broto lagged 6
227 VDW radius weighted Moreau-Broto lagged 7
228 VDW radius weighted Moreau-Broto lagged 8
229 VDW radius weighted Moreau-Broto lagged 9
230 VDW radius weighted Moreau-Broto lagged 10
231 ALOGP weighted Moreau-Broto lagged 0
232 ALOGP weighted Moreau-Broto lagged 1
233 ALOGP weighted Moreau-Broto lagged 2
234 ALOGP weighted Moreau-Broto lagged 3
235 ALOGP weighted Moreau-Broto lagged 4
236 ALOGP weighted Moreau-Broto lagged 5
237 ALOGP weighted Moreau-Broto lagged 6
238 ALOGP weighted Moreau-Broto lagged 7
239 ALOGP weighted Moreau-Broto lagged 8
240 ALOGP weighted Moreau-Broto lagged 9
241 ALOGP weighted Moreau-Broto lagged 10
242 Atomic charge weighted Moreau-Broto lagged 0
243 Atomic charge weighted Moreau-Broto lagged 1
244 Atomic charge weighted Moreau-Broto lagged 2
245 Atomic charge weighted Moreau-Broto lagged 3
246 Atomic charge weighted Moreau-Broto lagged 4
247 Atomic charge weighted Moreau-Broto lagged 5
248 Atomic charge weighted Moreau-Broto lagged 6
249 Atomic charge weighted Moreau-Broto lagged 7
250 Atomic charge weighted Moreau-Broto lagged 8
251 Atomic charge weighted Moreau-Broto lagged 9
252 Atomic charge weighted Moreau-Broto lagged 10
253 E-State weighted Moreau-Broto lagged 0
254 E-State weighted Moreau-Broto lagged 1
255 E-State weighted Moreau-Broto lagged 2
256 E-State weighted Moreau-Broto lagged 3

257 E-State weighted Moreau-Broto lagged 4
258 E-State weighted Moreau-Broto lagged 5
259 E-State weighted Moreau-Broto lagged 6
260 E-State weighted Moreau-Broto lagged 7
261 E-State weighted Moreau-Broto lagged 8
262 E-State weighted Moreau-Broto lagged 9
263 E-State weighted Moreau-Broto lagged 10
264 Polarizability mass weighted Moreau-Broto lagged 0
265 Polarizability mass weighted Moreau-Broto lagged 1
266 Polarizability mass weighted Moreau-Broto lagged 2
267 Polarizability mass weighted Moreau-Broto lagged 3
268 Polarizability mass weighted Moreau-Broto lagged 4
269 Polarizability mass weighted Moreau-Broto lagged 5
270 Polarizability mass weighted Moreau-Broto lagged 6
271 Polarizability mass weighted Moreau-Broto lagged 7
272 Polarizability mass weighted Moreau-Broto lagged 8
273 Polarizability mass weighted Moreau-Broto lagged 9
274 Polarizability weighted Moreau-Broto lagged 10
275 Atomic mass weighted Moran lagged 1
276 Atomic mass weighted Moran lagged 2
277 Atomic mass weighted Moran lagged 3
278 Atomic mass weighted Moran lagged 4
279 Atomic mass weighted Moran lagged 5
280 Atomic mass weighted Moran lagged 6
281 Atomic mass weighted Moran lagged 7
282 Atomic mass weighted Moran lagged 8
283 Atomic mass weighted Moran lagged 9
284 Atomic mass weighted Moran lagged 10
285 Electronegativity weighted Moran lagged 1
286 Electronegativity weighted Moran lagged 2
287 Electronegativity weighted Moran lagged 3
288 Electronegativity weighted Moran lagged 4
289 Electronegativity weighted Moran lagged 5
290 Electronegativity weighted Moran lagged 6
291 Electronegativity weighted Moran lagged 7
292 Electronegativity weighted Moran lagged 8
293 Electronegativity weighted Moran lagged 9
294 Electronegativity weighted Moran lagged 10
295 VDW weighted Moran lagged 1
296 VDW weighted Moran lagged 2
297 VDW weighted Moran lagged 3
298 VDW weighted Moran lagged 4
299 VDW weighted Moran lagged 5

300 VDW weighted Moran lagged 6
301 VDW weighted Moran lagged 7
302 VDW weighted Moran lagged 8
303 VDW weighted Moran lagged 9
304 VDW weighted Moran lagged 10
305 ALOGP weighted Moran lagged 1
306 ALOGP weighted Moran lagged 2
307 ALOGP weighted Moran lagged 3
308 ALOGP weighted Moran lagged 4
309 ALOGP weighted Moran lagged 5
310 ALOGP weighted Moran lagged 6
311 ALOGP weighted Moran lagged 7
312 ALOGP weighted Moran lagged 8
313 ALOGP weighted Moran lagged 9
314 ALOGP weighted Moran lagged 10
315 Atomic charge weighted Moran lagged 1
316 Atomic charge weighted Moran lagged 2
317 Atomic charge weighted Moran lagged 3
318 Atomic charge weighted Moran lagged 4
319 Atomic charge weighted Moran lagged 5
320 Atomic charge weighted Moran lagged 6
321 Atomic charge weighted Moran lagged 7
322 Atomic charge weighted Moran lagged 8
323 Atomic charge weighted Moran lagged 9
324 Atomic charge weighted Moran lagged 10
325 E-State weighted Moran lagged 1
326 E-State weighted Moran lagged 2
327 E-State weighted Moran lagged 3
328 E-State weighted Moran lagged 4
329 E-State weighted Moran lagged 5
330 E-State weighted Moran lagged 6
331 E-State weighted Moran lagged 7
332 E-State weighted Moran lagged 8
333 E-State weighted Moran lagged 9
334 E-State weighted Moran lagged 10
335 Polarizability mass weighted Moran lagged 1
336 Polarizability mass weighted Moran lagged 2
337 Polarizability mass weighted Moran lagged 3
338 Polarizability mass weighted Moran lagged 4
339 Polarizability mass weighted Moran lagged 5
340 Polarizability mass weighted Moran lagged 6
341 Polarizability mass weighted Moran lagged 7
342 Polarizability mass weighted Moran lagged 8

343 Polarizability mass weighted Moran lagged 9
344 Polarizability mass weighted Moran lagged 10
345 Atomic mass weighted Geary lagged 1
346 Atomic mass weighted Geary lagged 2
347 Atomic mass weighted Geary lagged 3
348 Atomic mass weighted Geary lagged 4
349 Atomic mass weighted Geary lagged 5
350 Atomic mass weighted Geary lagged 6
351 Atomic mass weighted Geary lagged 7
352 Atomic mass weighted Geary lagged 8
353 Atomic mass weighted Geary lagged 9
354 Atomic mass weighted Geary lagged10
355 Electronegativity weighted Geary lagged 1
356 Electronegativity weighted Geary lagged 2
357 Electronegativity weighted Geary lagged 3
358 Electronegativity weighted Geary lagged 4
359 Electronegativity weighted Geary lagged 5
360 Electronegativity weighted Geary lagged 6
361 Electronegativity weighted Geary lagged 7
362 Electronegativity weighted Geary lagged 8
363 Electronegativity weighted Geary lagged 9
364 Electronegativity weighted Geary lagged10
365 VDW weighted Geary lagged 1
366 VDW weighted Geary lagged 2
367 VDW weighted Geary lagged 3
368 VDW weighted Geary lagged 4
369 VDW weighted Geary lagged 5
370 VDW weighted Geary lagged 6
371 VDW weighted Geary lagged 7
372 VDW weighted Geary lagged 8
373 VDW weighted Geary lagged 9
374 VDW weighted Geary lagged10
375 ALOGP weighted Geary lagged 1
376 ALOGP weighted Geary lagged 2
377 ALOGP weighted Geary lagged 3
378 ALOGP weighted Geary lagged 4
379 ALOGP weighted Geary lagged 5
380 ALOGP weighted Geary lagged 6
381 ALOGP weighted Geary lagged 7
382 ALOGP weighted Geary lagged 8
383 ALOGP weighted Geary lagged 9
384 ALOGP weighted Geary lagged10
385 Atomic charge weighted Geary lagged 1

386 Atomic charge weighted Geary lagged 2
387 Atomic charge weighted Geary lagged 3
388 Atomic charge weighted Geary lagged 4
389 Atomic charge weighted Geary lagged 5
390 Atomic charge weighted Geary lagged 6
391 Atomic charge weighted Geary lagged 7
392 Atomic charge weighted Geary lagged 8
393 Atomic charge weighted Geary lagged 9
394 Atomic charge weighted Geary lagged10
395 E-State weighted Geary lagged 1
396 E-State weighted Geary lagged 2
397 E-State weighted Geary lagged 3
398 E-State weighted Geary lagged 4
399 E-State weighted Geary lagged 5
400 E-State weighted Geary lagged 6
401 E-State weighted Geary lagged 7
402 E-State weighted Geary lagged 8
403 E-State weighted Geary lagged 9
404 E-State weighted Geary lagged10
405 Polarizability mass weighted Geary lagged 1
406 Polarizability mass weighted Geary lagged 2
407 Polarizability mass weighted Geary lagged 3
408 Polarizability mass weighted Geary lagged 4
409 Polarizability mass weighted Geary lagged 5
410 Polarizability mass weighted Geary lagged 6
411 Polarizability mass weighted Geary lagged 7
412 Polarizability mass weighted Geary lagged 8
413 Polarizability mass weighted Geary lagged 9
414 E-State weighted Geary lagged10
415 0th Kier-Hall connectivity index
416 1th Kier-Hall connectivity index
417 2th Kier-Hall connectivity index
418 Mean Randic Connectivity index
419 Simple topological index by Narumi
420 Harmonic topological index by Narumi
421 Geometric topological index by Narumi
422 Arithmetic topological index by Narumi
423 0th valence connectivity index
424 1th valence connectivity index
425 2th valence connectivity index
426 0th order delta chi index
427 1th order delta chi index
428 2th order delta chi index

429 Poligini index
430 0th Solvation connectivity index
431 1th Solvation connectivity index
432 2th Solvation connectivity index
433 Electron charge density index
434 1th order Kier shape index
435 2th order Kier shape index
436 3th order Kier shape index
437 1th order Kappa alpha shape index
438 2th order Kappa alpha shape index
439 3th order Kappa alpha shape index
440 Kier Molecular Flexibility Index
441 Topological radius
442 Topological diameter
443 Graph-theoretical shape coefficient
444 Eccentricity
445 Average atom eccentricity
446 Mean eccentricity deviation
447 Average distance degree
448 Mean distance degree deviation
449 Unipolarity
450 Rouvary index Irouv
451 Centralization
452 Variation
453 Dispersion
454 Log of PRS INDEX
455 RDSQ ondex
456 RDCHI index
457 BCUT 1th highest eigenvalue by mass
458 BCUT 2th highest eigenvalue by mass
459 BCUT 3th highest eigenvalue by mass
460 BCUT 4th highest eigenvalue by mass
461 BCUT 5th highest eigenvalue by mass
462 BCUT 1th lowest eigenvalue of mass
463 BCUT 2th lowest eigenvalue of mass
464 BCUT 3th lowest eigenvalue of mass
465 BCUT 4th lowest eigenvalue of mass
466 BCUT 5th lowest eigenvalue of mass
467 BCUT 1th highest eigenvalue by electronegativity
468 BCUT 2th highest eigenvalue by electronegativity
469 BCUT 3th highest eigenvalue by electronegativity
470 BCUT 4th highest eigenvalue by electronegativity
471 BCUT 5th highest eigenvalue by electronegativity

472 BCUT 1th lowest eigenvalue by electronegativity
473 BCUT 2th lowest eigenvalue by electronegativity
474 BCUT 3th lowest eigenvalue by electronegativity
475 BCUT 4th lowest eigenvalue by electronegativity
476 BCUT 5th lowest eigenvalue by electronegativity
477 BCUT 1th highest eigenvalue by VDW radius
478 BCUT 2th highest eigenvalue by VDW radius
479 BCUT 3th highest eigenvalue by VDW radius
480 BCUT 4th highest eigenvalue by VDW radius
481 BCUT 5th highest eigenvalue by VDW radius
482 BCUT 1th lowest eigenvalue by VDW radius
483 BCUT 2th lowest eigenvalue by VDW radius
484 BCUT 3th lowest eigenvalue by VDW radius
485 BCUT 4th lowest eigenvalue by VDW radius
486 BCUT 5th lowest eigenvalue by VDW radius
487 BCUT 1th highest eigenvalue by atomic charges
488 BCUT 2th highest eigenvalue by atomic charges
489 BCUT 3th highest eigenvalue by atomic charges
490 BCUT 4th highest eigenvalue by atomic charges
491 BCUT 5th highest eigenvalue by atomic charges
492 BCUT 1th lowest eigenvalue by atomic charges
493 BCUT 2th lowest eigenvalue by atomic charges
494 BCUT 3th lowest eigenvalue by atomic charges
495 BCUT 4th lowest eigenvalue by atomic charges
496 BCUT 5th lowest eigenvalue by atomic charges
497 BCUT 1th highest eigenvalue by ALOGP
498 BCUT 2th highest eigenvalue by ALOGP
499 BCUT 3th highest eigenvalue by ALOGP
500 BCUT 4th highest eigenvalue by ALOGP
501 BCUT 5th highest eigenvalue by ALOGP
502 BCUT 1th lowest eigenvalue by ALOGP
503 BCUT 2th lowest eigenvalue by ALOGP
504 BCUT 3th lowest eigenvalue by ALOGP
505 BCUT 4th lowest eigenvalue by ALOGP
506 BCUT 5th lowest eigenvalue by ALOGP
507 BCUT 1th highest eigenvalue by E-State
508 BCUT 2th highest eigenvalue by E-State
509 BCUT 3th highest eigenvalue by E-State
510 BCUT 4th highest eigenvalue by E-State
511 BCUT 5th highest eigenvalue by E-State
512 BCUT 1th lowest eigenvalue by E-State
513 BCUT 2th lowest eigenvalue by E-State
514 BCUT 3th lowest eigenvalue by E-State

515 BCUT 4th lowest eigenvalue by E-State
516 BCUT 5th lowest eigenvalue by E-State
517 BCUT 1th highest eigenvalue by polarizability
518 BCUT 2th highest eigenvalue by polarizability
519 BCUT 3th highest eigenvalue by polarizability
520 BCUT 4th highest eigenvalue by polarizability
521 BCUT 5th highest eigenvalue by polarizability
522 BCUT 1th lowest eigenvalue by polarizability
523 BCUT 2th lowest eigenvalue by polarizability
524 BCUT 3th lowest eigenvalue by polarizability
525 BCUT 4th lowest eigenvalue by polarizability
526 BCUT 5th lowest eigenvalue by polarizability
527 3D Wiener Index
528 Gravitational 3D index
529 Radius of gyration
530 Principal moments of Inertia,IA=
531 Principal moments of Inertia,IB=
532 Principal moments of Inertia,IC=
533 Ovality from VDW
534 0th moment over VDW volume
535 2th invariant moment over VDW volume(*0.01)
536 2th moment shape index overVDW volume
537 4th invariant moment over VDW volume(*0.001)
538 4th moment shape index over VDW volume
539 6th invariant moment over VDW volume(*0.0001)
540 6th moment shape index over VDW volume
541 0th order moment overVDW surface
542 2th order invariant moment overVDW surface
543 2th order moment shape index overVDW surface
544 4th order invariant moment overVDW surface
545 4th order moment shape index overVDW surface
546 6th order invariant moment overVDW surface
547 6th order moment shape index overVDW surface
548 Minimum MEP at VDW surface
549 Maximum MEP at VDW surface
550 Local polarity of molecule by VDW surface
551 Total variance of the surface potential*1000 at VDW surface
552 1st MS-WHIM Variance over VDW surface
553 2nd MS-WHIM Variance over VDW surface
554 3rd MS-WHIM Variance over VDW surface
555 1st MS-WHIM eigenvalue proportion over VDW surface
556 2nd MS-WHIM eigenvalue proportion over VDW surface
557 The MS-WHIM accentric factor over VDW surface

558 1st MS-WHIM skewness over VDW surface
559 2nd MS-WHIM skewness over VDW surface
560 3rd MS-WHIM skewness over VDW surface
561 1st MS-WHIM kurtosis over VDW surface(*1.0e-4)
562 2nd MS-WHIM kurtosis over VDW surface(*1.0e-4)
563 3rd MS-WHIM kurtosis over VDW surface(*1.0e-4)
564 1st MS-WHIM Variance over VDW surface
565 2nd MS-WHIM Variance over VDW surface
566 3rd MS-WHIM Variance over VDW surface
567 1st MS-WHIM eigenvalue proportion over VDW surface
568 2nd MS-WHIM eigenvalue proportion over VDW surface
569 The MS-WHIM accentric factor over VDW surface
570 1st MS-WHIM skewness over VDW surface
571 2nd MS-WHIM skewness over VDW surface
572 3rd MS-WHIM skewness over VDW surface
573 1st MS-WHIM kurtosis over VDW surface(*1.0e-4)
574 2nd MS-WHIM kurtosis over VDW surface(*1.0e-4)
575 3rd MS-WHIM kurtosis over VDW surface(*1.0e-4)
576 1st MS-WHIM Variance over VDW surface
577 2nd MS-WHIM Variance over VDW surface
578 3rd MS-WHIM Variance over VDW surface
579 1st MS-WHIM eigenvalue proportion over VDW surface
580 2nd MS-WHIM eigenvalue proportion over VDW surface
581 The MS-WHIM accentric factor over VDW surface
582 1st MS-WHIM skewness over VDW surface
583 2nd MS-WHIM skewness over VDW surface
584 3rd MS-WHIM skewness over VDW surface
585 1st MS-WHIM kurtosis over VDW surface(*1.0e-4)
586 2nd MS-WHIM kurtosis over VDW surface(*1.0e-4)
587 3rd MS-WHIM kurtosis over VDW surface(*1.0e-4)
588 Ovality from SAS
589 0th moment over SAS volume
590 2th invariant moment over SAS volume(*0.01)
591 2th moment shape index overSAS volume
592 4th invariant moment over SAS volume(*0.001)
593 4th moment shape index over SAS volume
594 6th invariant moment over SAS volume(*0.0001)
595 6th moment shape index over SAS volume
596 0th order moment overSAS surface
597 2th order invariant moment overSAS surface
598 2th order moment shape index overSAS surface
599 4th order invariant moment overSAS surface
600 4th order moment shape index overSAS surface

601 6th order invariant moment overSAS surface
602 6th order moment shape index overSAS surface
603 Minimum MEP at SAS surface
604 Maximum MEP at SAS surface
605 Local polarity of molecule by SAS surface
606 Total variance of the surface potential*1000 at SAS surface
607 1st MS-WHIM Variance over SAS surface
608 2nd MS-WHIM Variance over SAS surface
609 3rd MS-WHIM Variance over SAS surface
610 1st MS-WHIM eigenvalue proportion over SAS surface
611 2nd MS-WHIM eigenvalue proportion over SAS surface
612 The MS-WHIM accentric factor over SAS surface
613 1st MS-WHIM skewness over SAS surface
614 2nd MS-WHIM skewness over SAS surface
615 3rd MS-WHIM skewness over SAS surface
616 1st MS-WHIM kurtosis over SAS surface(*1.0e-4)
617 2nd MS-WHIM kurtosis over SAS surface(*1.0e-4)
618 3rd MS-WHIM kurtosis over SAS surface(*1.0e-4)
619 1st MS-WHIM Variance over SAS surface
620 2nd MS-WHIM Variance over SAS surface
621 3rd MS-WHIM Variance over SAS surface
622 1st MS-WHIM eigenvalue proportion over SAS surface
623 2nd MS-WHIM eigenvalue proportion over SAS surface
624 The MS-WHIM accentric factor over SAS surface
625 1st MS-WHIM skewness over SAS surface
626 2nd MS-WHIM skewness over SAS surface
627 3rd MS-WHIM skewness over SAS surface
628 1st MS-WHIM kurtosis over SAS surface(*1.0e-4)
629 2nd MS-WHIM kurtosis over SAS surface(*1.0e-4)
630 3rd MS-WHIM kurtosis over SAS surface(*1.0e-4)
631 1st MS-WHIM Variance over SAS surface
632 2nd MS-WHIM Variance over SAS surface
633 3rd MS-WHIM Variance over SAS surface
634 1st MS-WHIM eigenvalue proportion over SAS surface
635 2nd MS-WHIM eigenvalue proportion over SAS surface
636 The MS-WHIM accentric factor over SAS surface
637 1st MS-WHIM skewness over SAS surface
638 2nd MS-WHIM skewness over SAS surface
639 3rd MS-WHIM skewness over SAS surface
640 1st MS-WHIM kurtosis over SAS surface(*1.0e-4)
641 2nd MS-WHIM kurtosis over SAS surface(*1.0e-4)
642 3rd MS-WHIM kurtosis over SAS surface(*1.0e-4)
643 PNSA1

644 PPSA1
645 PNSA2
646 PPSA2
647 PNSA3
648 PPSA3
649 DPSA1
650 DPSA2
651 DPSA3
652 TPSA
653 TASA
654 RASA
655 RPSA
656 FNSA1
657 FNSA2
658 FNSA3
659 FPSA1
660 FPSA2
661 FPSA3
662 WNSA1
663 WNSA2
664 WNSA3
665 WPSA1
666 WPSA2
667 WPSA3
668 RPCS
669 RNCS
670 PSA for N atoms
671 PSA for O atoms
672 PSA for H on N,O atoms
673 Polar Surface Area(PSA)
674 RSHM index
675 RSAM index
676 Sum of absolute charge for N,O
677 HDCA index
678 FHDCA index
679 Un-weighted RDF g( 0.0000)
680 Un-weighted RDF g( 0.5000)
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708 Atomic mass weighted RDF g( 0.0000)
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853 E-State weighted RDF g( 0.0000)
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882 Polarizability weighted RDF g( 0.0000)
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909 Polarizability weighted RDF g( 13.5000)
910 Polarizability weighted RDF g( 14.0000)
911 1st directional WHIM size by Un-weighted
912 2nd directional WHIM size by Un-weighted
913 3rd directional WHIM size by Un-weighted
914 1st directional WHIM shape by Un-weighted
915 2nd directional WHIM shape by Un-weighted
916 3rd directional WHIM shape by Un-weighted
917 1st directional WHIM density by Un-weighted
918 2nd directional WHIM density by Un-weighted
919 3rd directional WHIM density by Un-weighted
920 Global WHIM T by Un-weighted
921 Global WHIM A by Un-weighted
922 Global WHIM V by Un-weighted
923 Global WHIM G by Un-weighted
924 Global WHIM D by Un-weighted
925 1st directional WHIM size by Atomic mass
926 2nd directional WHIM size by Atomic mass
927 3rd directional WHIM size by Atomic mass
928 1st directional WHIM shape by Atomic mass
929 2nd directional WHIM shape by Atomic mass
930 3rd directional WHIM shape by Atomic mass
931 1st directional WHIM density by Atomic mass
932 2nd directional WHIM density by Atomic mass
933 3rd directional WHIM density by Atomic mass
934 Global WHIM T by Atomic mass
935 Global WHIM A by Atomic mass
936 Global WHIM V by Atomic mass
937 Global WHIM G by Atomic mass
938 Global WHIM D by Atomic mass
939 1st directional WHIM size by VDW radius
940 2nd directional WHIM size by VDW radius
941 3rd directional WHIM size by VDW radius
942 1st directional WHIM shape by VDW radius
943 2nd directional WHIM shape by VDW radius
944 3rd directional WHIM shape by VDW radius

945 1st directional WHIM density by VDW radius
946 2nd directional WHIM density by VDW radius
947 3rd directional WHIM density by VDW radius
948 Global WHIM T by VDW radius
949 Global WHIM A by VDW radius
950 Global WHIM V by VDW radius
951 Global WHIM G by VDW radius
952 Global WHIM D by VDW radius
953 1st directional WHIM size by Electronegativity
954 2nd directional WHIM size by Electronegativity
955 3rd directional WHIM size by Electronegativity
956 1st directional WHIM shape by Electronegativity
957 2nd directional WHIM shape by Electronegativity
958 3rd directional WHIM shape by Electronegativity
959 1st directional WHIM density by Electronegativity
960 2nd directional WHIM density by Electronegativity
961 3rd directional WHIM density by Electronegativity
962 Global WHIM T by Electronegativity
963 Global WHIM A by Electronegativity
964 Global WHIM V by Electronegativity
965 Global WHIM G by Electronegativity
966 Global WHIM D by Electronegativity
967 1st directional WHIM size by POlarizability
968 2nd directional WHIM size by POlarizability
969 3rd directional WHIM size by POlarizability
970 1st directional WHIM shape by POlarizability
971 2nd directional WHIM shape by POlarizability
972 3rd directional WHIM shape by POlarizability
973 1st directional WHIM density by POlarizability
974 2nd directional WHIM density by POlarizability
975 3rd directional WHIM density by POlarizability
976 Global WHIM T by POlarizability
977 Global WHIM A by POlarizability
978 Global WHIM V by POlarizability
979 Global WHIM G by POlarizability
980 Global WHIM D by POlarizability
981 1st directional WHIM size by E-State
982 2nd directional WHIM size by E-State
983 3rd directional WHIM size by E-State
984 1st directional WHIM shape by E-State
985 2nd directional WHIM shape by E-State
986 3rd directional WHIM shape by E-State
987 1st directional WHIM density by E-State

988 2nd directional WHIM density by E-State
989 3rd directional WHIM density by E-State
990 Global WHIM T by E-State
991 Global WHIM A by E-State
992 Global WHIM V by E-State
993 Global WHIM G by E-State
994 Global WHIM D by E-State
995 3D-MoRSE-Signal I( 1.0) by Un-
996 3D-MoRSE-Signal I( 2.0) by Un-
997 3D-MoRSE-Signal I( 3.0) by Un-
998 3D-MoRSE-Signal I( 4.0) by Un-
999 3D-MoRSE-Signal I( 5.0) by Un-
1000 3D-MoRSE-Signal I( 6.0) by Un-
1001 3D-MoRSE-Signal I( 7.0) by Un-
1002 3D-MoRSE-Signal I( 8.0) by Un-
1003 3D-MoRSE-Signal I( 9.0) by Un-
1004 3D-MoRSE-Signal I(10.0) by Un-
1005 3D-MoRSE-Signal I(11.0) by Un-
1006 3D-MoRSE-Signal I(12.0) by Un-
1007 3D-MoRSE-Signal I(13.0) by Un-
1008 3D-MoRSE-Signal I(14.0) by Un-
1009 3D-MoRSE-Signal I(15.0) by Un-
1010 3D-MoRSE-Signal I(16.0) by Un-
1011 3D-MoRSE-Signal I(17.0) by Un-
1012 3D-MoRSE-Signal I(18.0) by Un-
1013 3D-MoRSE-Signal I(19.0) by Un-
1014 3D-MoRSE-Signal I(20.0) by Un-
1015 3D-MoRSE-Signal I(21.0) by Un-
1016 3D-MoRSE-Signal I(22.0) by Un-
1017 3D-MoRSE-Signal I(23.0) by Un-
1018 3D-MoRSE-Signal I(24.0) by Un-
1019 3D-MoRSE-Signal I(25.0) by Un-
1020 3D-MoRSE-Signal I(26.0) by Un-
1021 3D-MoRSE-Signal I(27.0) by Un-
1022 3D-MoRSE-Signal I(28.0) by Un-
1023 3D-MoRSE-Signal I(29.0) by Un-
1024 3D-MoRSE-Signal I(30.0) by Un-
1025 3D-MoRSE-Signal I(31.0) by Un-
1026 3D-MoRSE-Signal I(32.0) by Un-
1027 3D-MoRSE-Signal I( 1.0) by Atomic mass
1028 3D-MoRSE-Signal I( 2.0) by Atomic mass
1029 3D-MoRSE-Signal I( 3.0) by Atomic mass
1030 3D-MoRSE-Signal I( 4.0) by Atomic mass

1031 3D-MoRSE-Signal I( 5.0) by Atomic mass
1032 3D-MoRSE-Signal I( 6.0) by Atomic mass
1033 3D-MoRSE-Signal I( 7.0) by Atomic mass
1034 3D-MoRSE-Signal I( 8.0) by Atomic mass
1035 3D-MoRSE-Signal I( 9.0) by Atomic mass
1036 3D-MoRSE-Signal I(10.0) by Atomic mass
1037 3D-MoRSE-Signal I(11.0) by Atomic mass
1038 3D-MoRSE-Signal I(12.0) by Atomic mass
1039 3D-MoRSE-Signal I(13.0) by Atomic mass
1040 3D-MoRSE-Signal I(14.0) by Atomic mass
1041 3D-MoRSE-Signal I(15.0) by Atomic mass
1042 3D-MoRSE-Signal I(16.0) by Atomic mass
1043 3D-MoRSE-Signal I(17.0) by Atomic mass
1044 3D-MoRSE-Signal I(18.0) by Atomic mass
1045 3D-MoRSE-Signal I(19.0) by Atomic mass
1046 3D-MoRSE-Signal I(20.0) by Atomic mass
1047 3D-MoRSE-Signal I(21.0) by Atomic mass
1048 3D-MoRSE-Signal I(22.0) by Atomic mass
1049 3D-MoRSE-Signal I(23.0) by Atomic mass
1050 3D-MoRSE-Signal I(24.0) by Atomic mass
1051 3D-MoRSE-Signal I(25.0) by Atomic mass
1052 3D-MoRSE-Signal I(26.0) by Atomic mass
1053 3D-MoRSE-Signal I(27.0) by Atomic mass
1054 3D-MoRSE-Signal I(28.0) by Atomic mass
1055 3D-MoRSE-Signal I(29.0) by Atomic mass
1056 3D-MoRSE-Signal I(30.0) by Atomic mass
1057 3D-MoRSE-Signal I(31.0) by Atomic mass
1058 3D-MoRSE-Signal I(32.0) by Atomic mass
1059 3D-MoRSE-Signal I( 1.0) by Atomic number
1060 3D-MoRSE-Signal I( 2.0) by Atomic number
1061 3D-MoRSE-Signal I( 3.0) by Atomic number
1062 3D-MoRSE-Signal I( 4.0) by Atomic number
1063 3D-MoRSE-Signal I( 5.0) by Atomic number
1064 3D-MoRSE-Signal I( 6.0) by Atomic number
1065 3D-MoRSE-Signal I( 7.0) by Atomic number
1066 3D-MoRSE-Signal I( 8.0) by Atomic number
1067 3D-MoRSE-Signal I( 9.0) by Atomic number
1068 3D-MoRSE-Signal I(10.0) by Atomic number
1069 3D-MoRSE-Signal I(11.0) by Atomic number
1070 3D-MoRSE-Signal I(12.0) by Atomic number
1071 3D-MoRSE-Signal I(13.0) by Atomic number
1072 3D-MoRSE-Signal I(14.0) by Atomic number
1073 3D-MoRSE-Signal I(15.0) by Atomic number

1074 3D-MoRSE-Signal I(16.0) by Atomic number
1075 3D-MoRSE-Signal I(17.0) by Atomic number
1076 3D-MoRSE-Signal I(18.0) by Atomic number
1077 3D-MoRSE-Signal I(19.0) by Atomic number
1078 3D-MoRSE-Signal I(20.0) by Atomic number
1079 3D-MoRSE-Signal I(21.0) by Atomic number
1080 3D-MoRSE-Signal I(22.0) by Atomic number
1081 3D-MoRSE-Signal I(23.0) by Atomic number
1082 3D-MoRSE-Signal I(24.0) by Atomic number
1083 3D-MoRSE-Signal I(25.0) by Atomic number
1084 3D-MoRSE-Signal I(26.0) by Atomic number
1085 3D-MoRSE-Signal I(27.0) by Atomic number
1086 3D-MoRSE-Signal I(28.0) by Atomic number
1087 3D-MoRSE-Signal I(29.0) by Atomic number
1088 3D-MoRSE-Signal I(30.0) by Atomic number
1089 3D-MoRSE-Signal I(31.0) by Atomic number
1090 3D-MoRSE-Signal I(32.0) by Atomic number
1091 3D-MoRSE-Signal I( 1.0) by VDW
1092 3D-MoRSE-Signal I( 2.0) by VDW
1093 3D-MoRSE-Signal I( 3.0) by VDW
1094 3D-MoRSE-Signal I( 4.0) by VDW
1095 3D-MoRSE-Signal I( 5.0) by VDW
1096 3D-MoRSE-Signal I( 6.0) by VDW
1097 3D-MoRSE-Signal I( 7.0) by VDW
1098 3D-MoRSE-Signal I( 8.0) by VDW
1099 3D-MoRSE-Signal I( 9.0) by VDW
1100 3D-MoRSE-Signal I(10.0) by VDW
1101 3D-MoRSE-Signal I(11.0) by VDW
1102 3D-MoRSE-Signal I(12.0) by VDW
1103 3D-MoRSE-Signal I(13.0) by VDW
1104 3D-MoRSE-Signal I(14.0) by VDW
1105 3D-MoRSE-Signal I(15.0) by VDW
1106 3D-MoRSE-Signal I(16.0) by VDW
1107 3D-MoRSE-Signal I(17.0) by VDW
1108 3D-MoRSE-Signal I(18.0) by VDW
1109 3D-MoRSE-Signal I(19.0) by VDW
1110 3D-MoRSE-Signal I(20.0) by VDW
1111 3D-MoRSE-Signal I(21.0) by VDW
1112 3D-MoRSE-Signal I(22.0) by VDW
1113 3D-MoRSE-Signal I(23.0) by VDW
1114 3D-MoRSE-Signal I(24.0) by VDW
1115 3D-MoRSE-Signal I(25.0) by VDW
1116 3D-MoRSE-Signal I(26.0) by VDW

1117 3D-MoRSE-Signal I(27.0) by VDW
1118 3D-MoRSE-Signal I(28.0) by VDW
1119 3D-MoRSE-Signal I(29.0) by VDW
1120 3D-MoRSE-Signal I(30.0) by VDW
1121 3D-MoRSE-Signal I(31.0) by VDW
1122 3D-MoRSE-Signal I(32.0) by VDW
1123 3D-MoRSE-Signal I( 1.0) by Electronegativity
1124 3D-MoRSE-Signal I( 2.0) by Electronegativity
1125 3D-MoRSE-Signal I( 3.0) by Electronegativity
1126 3D-MoRSE-Signal I( 4.0) by Electronegativity
1127 3D-MoRSE-Signal I( 5.0) by Electronegativity
1128 3D-MoRSE-Signal I( 6.0) by Electronegativity
1129 3D-MoRSE-Signal I( 7.0) by Electronegativity
1130 3D-MoRSE-Signal I( 8.0) by Electronegativity
1131 3D-MoRSE-Signal I( 9.0) by Electronegativity
1132 3D-MoRSE-Signal I(10.0) by Electronegativity
1133 3D-MoRSE-Signal I(11.0) by Electronegativity
1134 3D-MoRSE-Signal I(12.0) by Electronegativity
1135 3D-MoRSE-Signal I(13.0) by Electronegativity
1136 3D-MoRSE-Signal I(14.0) by Electronegativity
1137 3D-MoRSE-Signal I(15.0) by Electronegativity
1138 3D-MoRSE-Signal I(16.0) by Electronegativity
1139 3D-MoRSE-Signal I(17.0) by Electronegativity
1140 3D-MoRSE-Signal I(18.0) by Electronegativity
1141 3D-MoRSE-Signal I(19.0) by Electronegativity
1142 3D-MoRSE-Signal I(20.0) by Electronegativity
1143 3D-MoRSE-Signal I(21.0) by Electronegativity
1144 3D-MoRSE-Signal I(22.0) by Electronegativity
1145 3D-MoRSE-Signal I(23.0) by Electronegativity
1146 3D-MoRSE-Signal I(24.0) by Electronegativity
1147 3D-MoRSE-Signal I(25.0) by Electronegativity
1148 3D-MoRSE-Signal I(26.0) by Electronegativity
1149 3D-MoRSE-Signal I(27.0) by Electronegativity
1150 3D-MoRSE-Signal I(28.0) by Electronegativity
1151 3D-MoRSE-Signal I(29.0) by Electronegativity
1152 3D-MoRSE-Signal I(30.0) by Electronegativity
1153 3D-MoRSE-Signal I(31.0) by Electronegativity
1154 3D-MoRSE-Signal I(32.0) by Electronegativity
1155 3D-MoRSE-Signal I( 1.0) by Polarizability
1156 3D-MoRSE-Signal I( 2.0) by Polarizability
1157 3D-MoRSE-Signal I( 3.0) by Polarizability
1158 3D-MoRSE-Signal I( 4.0) by Polarizability
1159 3D-MoRSE-Signal I( 5.0) by Polarizability

1160 3D-MoRSE-Signal I( 6.0) by Polarizability
1161 3D-MoRSE-Signal I( 7.0) by Polarizability
1162 3D-MoRSE-Signal I( 8.0) by Polarizability
1163 3D-MoRSE-Signal I( 9.0) by Polarizability
1164 3D-MoRSE-Signal I(10.0) by Polarizability
1165 3D-MoRSE-Signal I(11.0) by Polarizability
1166 3D-MoRSE-Signal I(12.0) by Polarizability
1167 3D-MoRSE-Signal I(13.0) by Polarizability
1168 3D-MoRSE-Signal I(14.0) by Polarizability
1169 3D-MoRSE-Signal I(15.0) by Polarizability
1170 3D-MoRSE-Signal I(16.0) by Polarizability
1171 3D-MoRSE-Signal I(17.0) by Polarizability
1172 3D-MoRSE-Signal I(18.0) by Polarizability
1173 3D-MoRSE-Signal I(19.0) by Polarizability
1174 3D-MoRSE-Signal I(20.0) by Polarizability
1175 3D-MoRSE-Signal I(21.0) by Polarizability
1176 3D-MoRSE-Signal I(22.0) by Polarizability
1177 3D-MoRSE-Signal I(23.0) by Polarizability
1178 3D-MoRSE-Signal I(24.0) by Polarizability
1179 3D-MoRSE-Signal I(25.0) by Polarizability
1180 3D-MoRSE-Signal I(26.0) by Polarizability
1181 3D-MoRSE-Signal I(27.0) by Polarizability
1182 3D-MoRSE-Signal I(28.0) by Polarizability
1183 3D-MoRSE-Signal I(29.0) by Polarizability
1184 3D-MoRSE-Signal I(30.0) by Polarizability
1185 3D-MoRSE-Signal I(31.0) by Polarizability
1186 3D-MoRSE-Signal I(32.0) by Polarizability
1187 3D-MoRSE-Signal I( 1.0) by E-State
1188 3D-MoRSE-Signal I( 2.0) by E-State
1189 3D-MoRSE-Signal I( 3.0) by E-State
1190 3D-MoRSE-Signal I( 4.0) by E-State
1191 3D-MoRSE-Signal I( 5.0) by E-State
1192 3D-MoRSE-Signal I( 6.0) by E-State
1193 3D-MoRSE-Signal I( 7.0) by E-State
1194 3D-MoRSE-Signal I( 8.0) by E-State
1195 3D-MoRSE-Signal I( 9.0) by E-State
1196 3D-MoRSE-Signal I(10.0) by E-State
1197 3D-MoRSE-Signal I(11.0) by E-State
1198 3D-MoRSE-Signal I(12.0) by E-State
1199 3D-MoRSE-Signal I(13.0) by E-State
1200 3D-MoRSE-Signal I(14.0) by E-State
1201 3D-MoRSE-Signal I(15.0) by E-State
1202 3D-MoRSE-Signal I(16.0) by E-State

1203 3D-MoRSE-Signal I(17.0) by E-State
1204 3D-MoRSE-Signal I(18.0) by E-State
1205 3D-MoRSE-Signal I(19.0) by E-State
1206 3D-MoRSE-Signal I(20.0) by E-State
1207 3D-MoRSE-Signal I(21.0) by E-State
1208 3D-MoRSE-Signal I(22.0) by E-State
1209 3D-MoRSE-Signal I(23.0) by E-State
1210 3D-MoRSE-Signal I(24.0) by E-State
1211 3D-MoRSE-Signal I(25.0) by E-State
1212 3D-MoRSE-Signal I(26.0) by E-State
1213 3D-MoRSE-Signal I(27.0) by E-State
1214 3D-MoRSE-Signal I(28.0) by E-State
1215 3D-MoRSE-Signal I(29.0) by E-State
1216 3D-MoRSE-Signal I(30.0) by E-State
1217 3D-MoRSE-Signal I(31.0) by E-State
1218 3D-MoRSE-Signal I(32.0) by E-State
1219 H-GETAWAY Geometric Mean HGM
1220 H-GETAWAY Mean Information Content HIC
1221 H-GETAWAY ATS0 by Un-weighted
1222 H-GETAWAY ATS1 by Un-weighted
1223 H-GETAWAY ATS2 by Un-weighted
1224 H-GETAWAY ATS3 by Un-weighted
1225 H-GETAWAY ATS4 by Un-weighted
1226 H-GETAWAY ATS5 by Un-weighted
1227 H-GETAWAY ATS6 by Un-weighted
1228 H-GETAWAY ATS7 by Un-weighted
1229 H-GETAWAY ATS8 by Un-weighted
1230 H-GETAWAY ATS by Un-weighted
1231 H-GETAWAY HATS0 by Un-weighted
1232 H-GETAWAY HATS1 by Un-weighted
1233 H-GETAWAY HATS2 by Un-weighted
1234 H-GETAWAY HATS3 by Un-weighted
1235 H-GETAWAY HATS4 by Un-weighted
1236 H-GETAWAY HATS5 by Un-weighted
1237 H-GETAWAY HATS6 by Un-weighted
1238 H-GETAWAY HATS7 by Un-weighted
1239 H-GETAWAY HATS8 by Un-weighted
1240 H-GETAWAY HATS by Un-weighted
1241 H-GETAWAY H0 by Un-weighted
1242 H-GETAWAY H1 by Un-weighted
1243 H-GETAWAY H2 by Un-weighted
1244 H-GETAWAY H3 by Un-weighted
1245 H-GETAWAY H4 by Un-weighted

1246 H-GETAWAY H5 by Un-weighted
1247 H-GETAWAY H6 by Un-weighted
1248 H-GETAWAY H7 by Un-weighted
1249 H-GETAWAY H8 by Un-weighted
1250 H-GETAWAY HT by Un-weighted
1251 H-GETAWAY ATS0 by Atomic mass
1252 H-GETAWAY ATS1 by Atomic mass
1253 H-GETAWAY ATS2 by Atomic mass
1254 H-GETAWAY ATS3 by Atomic mass
1255 H-GETAWAY ATS4 by Atomic mass
1256 H-GETAWAY ATS5 by Atomic mass
1257 H-GETAWAY ATS6 by Atomic mass
1258 H-GETAWAY ATS7 by Atomic mass
1259 H-GETAWAY ATS8 by Atomic mass
1260 H-GETAWAY ATS by Atomic mass
1261 H-GETAWAY HATS0 by Atomic mass
1262 H-GETAWAY HATS1 by Atomic mass
1263 H-GETAWAY HATS2 by Atomic mass
1264 H-GETAWAY HATS3 by Atomic mass
1265 H-GETAWAY HATS4 by Atomic mass
1266 H-GETAWAY HATS5 by Atomic mass
1267 H-GETAWAY HATS6 by Atomic mass
1268 H-GETAWAY HATS7 by Atomic mass
1269 H-GETAWAY HATS8 by Atomic mass
1270 H-GETAWAY HATS by Atomic mass
1271 H-GETAWAY H0 by Atomic mass
1272 H-GETAWAY H1 by Atomic mass
1273 H-GETAWAY H2 by Atomic mass
1274 H-GETAWAY H3 by Atomic mass
1275 H-GETAWAY H4 by Atomic mass
1276 H-GETAWAY H5 by Atomic mass
1277 H-GETAWAY H6 by Atomic mass
1278 H-GETAWAY H7 by Atomic mass
1279 H-GETAWAY H8 by Atomic mass
1280 H-GETAWAY HT by Atomic mass
1281 H-GETAWAY ATS0 by Atomic number
1282 H-GETAWAY ATS1 by Atomic number
1283 H-GETAWAY ATS2 by Atomic number
1284 H-GETAWAY ATS3 by Atomic number
1285 H-GETAWAY ATS4 by Atomic number
1286 H-GETAWAY ATS5 by Atomic number
1287 H-GETAWAY ATS6 by Atomic number
1288 H-GETAWAY ATS7 by Atomic number

1289 H-GETAWAY ATS8 by Atomic number
1290 H-GETAWAY ATS by Atomic number
1291 H-GETAWAY HATS0 by Atomic number
1292 H-GETAWAY HATS1 by Atomic number
1293 H-GETAWAY HATS2 by Atomic number
1294 H-GETAWAY HATS3 by Atomic number
1295 H-GETAWAY HATS4 by Atomic number
1296 H-GETAWAY HATS5 by Atomic number
1297 H-GETAWAY HATS6 by Atomic number
1298 H-GETAWAY HATS7 by Atomic number
1299 H-GETAWAY HATS8 by Atomic number
1300 H-GETAWAY HATS by Atomic number
1301 H-GETAWAY H0 by Atomic number
1302 H-GETAWAY H1 by Atomic number
1303 H-GETAWAY H2 by Atomic number
1304 H-GETAWAY H3 by Atomic number
1305 H-GETAWAY H4 by Atomic number
1306 H-GETAWAY H5 by Atomic number
1307 H-GETAWAY H6 by Atomic number
1308 H-GETAWAY H7 by Atomic number
1309 H-GETAWAY H8 by Atomic number
1310 H-GETAWAY HT by Atomic number
1311 H-GETAWAY ATS0 by VDW
1312 H-GETAWAY ATS1 by VDW
1313 H-GETAWAY ATS2 by VDW
1314 H-GETAWAY ATS3 by VDW
1315 H-GETAWAY ATS4 by VDW
1316 H-GETAWAY ATS5 by VDW
1317 H-GETAWAY ATS6 by VDW
1318 H-GETAWAY ATS7 by VDW
1319 H-GETAWAY ATS8 by VDW
1320 H-GETAWAY ATS by VDW
1321 H-GETAWAY HATS0 by VDW
1322 H-GETAWAY HATS1 by VDW
1323 H-GETAWAY HATS2 by VDW
1324 H-GETAWAY HATS3 by VDW
1325 H-GETAWAY HATS4 by VDW
1326 H-GETAWAY HATS5 by VDW
1327 H-GETAWAY HATS6 by VDW
1328 H-GETAWAY HATS7 by VDW
1329 H-GETAWAY HATS8 by VDW
1330 H-GETAWAY HATS by VDW
1331 H-GETAWAY H0 by VDW

1332 H-GETAWAY H1 by VDW
1333 H-GETAWAY H2 by VDW
1334 H-GETAWAY H3 by VDW
1335 H-GETAWAY H4 by VDW
1336 H-GETAWAY H5 by VDW
1337 H-GETAWAY H6 by VDW
1338 H-GETAWAY H7 by VDW
1339 H-GETAWAY H8 by VDW
1340 H-GETAWAY HT by VDW
1341 H-GETAWAY ATS0 by Electronegativity
1342 H-GETAWAY ATS1 by Electronegativity
1343 H-GETAWAY ATS2 by Electronegativity
1344 H-GETAWAY ATS3 by Electronegativity
1345 H-GETAWAY ATS4 by Electronegativity
1346 H-GETAWAY ATS5 by Electronegativity
1347 H-GETAWAY ATS6 by Electronegativity
1348 H-GETAWAY ATS7 by Electronegativity
1349 H-GETAWAY ATS8 by Electronegativity
1350 H-GETAWAY ATS by Electronegativity
1351 H-GETAWAY HATS0 by Electronegativity
1352 H-GETAWAY HATS1 by Electronegativity
1353 H-GETAWAY HATS2 by Electronegativity
1354 H-GETAWAY HATS3 by Electronegativity
1355 H-GETAWAY HATS4 by Electronegativity
1356 H-GETAWAY HATS5 by Electronegativity
1357 H-GETAWAY HATS6 by Electronegativity
1358 H-GETAWAY HATS7 by Electronegativity
1359 H-GETAWAY HATS8 by Electronegativity
1360 H-GETAWAY HATS by Electronegativity
1361 H-GETAWAY H0 by Electronegativity
1362 H-GETAWAY H1 by Electronegativity
1363 H-GETAWAY H2 by Electronegativity
1364 H-GETAWAY H3 by Electronegativity
1365 H-GETAWAY H4 by Electronegativity
1366 H-GETAWAY H5 by Electronegativity
1367 H-GETAWAY H6 by Electronegativity
1368 H-GETAWAY H7 by Electronegativity
1369 H-GETAWAY H8 by Electronegativity
1370 H-GETAWAY HT by Electronegativity
1371 H-GETAWAY ATS0 by Polarizability
1372 H-GETAWAY ATS1 by Polarizability
1373 H-GETAWAY ATS2 by Polarizability
1374 H-GETAWAY ATS3 by Polarizability

1375 H-GETAWAY ATS4 by Polarizability
1376 H-GETAWAY ATS5 by Polarizability
1377 H-GETAWAY ATS6 by Polarizability
1378 H-GETAWAY ATS7 by Polarizability
1379 H-GETAWAY ATS8 by Polarizability
1380 H-GETAWAY ATS by Polarizability
1381 H-GETAWAY HATS0 by Polarizability
1382 H-GETAWAY HATS1 by Polarizability
1383 H-GETAWAY HATS2 by Polarizability
1384 H-GETAWAY HATS3 by Polarizability
1385 H-GETAWAY HATS4 by Polarizability
1386 H-GETAWAY HATS5 by Polarizability
1387 H-GETAWAY HATS6 by Polarizability
1388 H-GETAWAY HATS7 by Polarizability
1389 H-GETAWAY HATS8 by Polarizability
1390 H-GETAWAY HATS by Polarizability
1391 H-GETAWAY H0 by Polarizability
1392 H-GETAWAY H1 by Polarizability
1393 H-GETAWAY H2 by Polarizability
1394 H-GETAWAY H3 by Polarizability
1395 H-GETAWAY H4 by Polarizability
1396 H-GETAWAY H5 by Polarizability
1397 H-GETAWAY H6 by Polarizability
1398 H-GETAWAY H7 by Polarizability
1399 H-GETAWAY H8 by Polarizability
1400 H-GETAWAY HT by Polarizability
1401 H-GETAWAY ATS0 by E-State
1402 H-GETAWAY ATS1 by E-State
1403 H-GETAWAY ATS2 by E-State
1404 H-GETAWAY ATS3 by E-State
1405 H-GETAWAY ATS4 by E-State
1406 H-GETAWAY ATS5 by E-State
1407 H-GETAWAY ATS6 by E-State
1408 H-GETAWAY ATS7 by E-State
1409 H-GETAWAY ATS8 by E-State
1410 H-GETAWAY ATS by E-State
1411 H-GETAWAY HATS0 by E-State
1412 H-GETAWAY HATS1 by E-State
1413 H-GETAWAY HATS2 by E-State
1414 H-GETAWAY HATS3 by E-State
1415 H-GETAWAY HATS4 by E-State
1416 H-GETAWAY HATS5 by E-State
1417 H-GETAWAY HATS6 by E-State

1418 H-GETAWAY HATS7 by E-State
1419 H-GETAWAY HATS8 by E-State
1420 H-GETAWAY HATS by E-State
1421 H-GETAWAY H0 by E-State
1422 H-GETAWAY H1 by E-State
1423 H-GETAWAY H2 by E-State
1424 H-GETAWAY H3 by E-State
1425 H-GETAWAY H4 by E-State
1426 H-GETAWAY H5 by E-State
1427 H-GETAWAY H6 by E-State
1428 H-GETAWAY H7 by E-State
1429 H-GETAWAY H8 by E-State
1430 H-GETAWAY HT by E-State
1431 R-GETAWAY RARS
1432 R-GETAWAY RCON
1433 R-GETAWAY REIG
1434 R-GETAWAY R1 by Un-weighted
1435 R-GETAWAY R2 by Un-weighted
1436 R-GETAWAY R3 by Un-weighted
1437 R-GETAWAY R4 by Un-weighted
1438 R-GETAWAY R5 by Un-weighted
1439 R-GETAWAY R6 by Un-weighted
1440 R-GETAWAY R7 by Un-weighted
1441 R-GETAWAY R8 by Un-weighted
1442 R-GETAWAY RT by Un-weighted
1443 R-GETAWAY R+1 by Un-weighted
1444 R-GETAWAY R+2 by Un-weighted
1445 R-GETAWAY R+3 by Un-weighted
1446 R-GETAWAY R+4 by Un-weighted
1447 R-GETAWAY R+5 by Un-weighted
1448 R-GETAWAY R+6 by Un-weighted
1449 R-GETAWAY R+7 by Un-weighted
1450 R-GETAWAY R+8 by Un-weighted
1451 R-GETAWAY RT+ by Un-weighted
1452 R-GETAWAY R1 by Atomic mass
1453 R-GETAWAY R2 by Atomic mass
1454 R-GETAWAY R3 by Atomic mass
1455 R-GETAWAY R4 by Atomic mass
1456 R-GETAWAY R5 by Atomic mass
1457 R-GETAWAY R6 by Atomic mass
1458 R-GETAWAY R7 by Atomic mass
1459 R-GETAWAY R8 by Atomic mass
1460 R-GETAWAY RT by Atomic mass

1461 R-GETAWAY R+1 by Atomic mass
1462 R-GETAWAY R+2 by Atomic mass
1463 R-GETAWAY R+3 by Atomic mass
1464 R-GETAWAY R+4 by Atomic mass
1465 R-GETAWAY R+5 by Atomic mass
1466 R-GETAWAY R+6 by Atomic mass
1467 R-GETAWAY R+7 by Atomic mass
1468 R-GETAWAY R+8 by Atomic mass
1469 R-GETAWAY RT+ by Atomic mass
1470 R-GETAWAY R1 by Atomic number
1471 R-GETAWAY R2 by Atomic number
1472 R-GETAWAY R3 by Atomic number
1473 R-GETAWAY R4 by Atomic number
1474 R-GETAWAY R5 by Atomic number
1475 R-GETAWAY R6 by Atomic number
1476 R-GETAWAY R7 by Atomic number
1477 R-GETAWAY R8 by Atomic number
1478 R-GETAWAY RT by Atomic number
1479 R-GETAWAY R+1 by Atomic number
1480 R-GETAWAY R+2 by Atomic number
1481 R-GETAWAY R+3 by Atomic number
1482 R-GETAWAY R+4 by Atomic number
1483 R-GETAWAY R+5 by Atomic number
1484 R-GETAWAY R+6 by Atomic number
1485 R-GETAWAY R+7 by Atomic number
1486 R-GETAWAY R+8 by Atomic number
1487 R-GETAWAY RT+ by Atomic number
1488 R-GETAWAY R1 by VDW
1489 R-GETAWAY R2 by VDW
1490 R-GETAWAY R3 by VDW
1491 R-GETAWAY R4 by VDW
1492 R-GETAWAY R5 by VDW
1493 R-GETAWAY R6 by VDW
1494 R-GETAWAY R7 by VDW
1495 R-GETAWAY R8 by VDW
1496 R-GETAWAY RT by VDW
1497 R-GETAWAY R+1 by VDW
1498 R-GETAWAY R+2 by VDW
1499 R-GETAWAY R+3 by VDW
1500 R-GETAWAY R+4 by VDW
1501 R-GETAWAY R+5 by VDW
1502 R-GETAWAY R+6 by VDW
1503 R-GETAWAY R+7 by VDW

1504 R-GETAWAY R+8 by VDW
1505 R-GETAWAY RT+ by VDW
1506 R-GETAWAY R1 by Electronegativity
1507 R-GETAWAY R2 by Electronegativity
1508 R-GETAWAY R3 by Electronegativity
1509 R-GETAWAY R4 by Electronegativity
1510 R-GETAWAY R5 by Electronegativity
1511 R-GETAWAY R6 by Electronegativity
1512 R-GETAWAY R7 by Electronegativity
1513 R-GETAWAY R8 by Electronegativity
1514 R-GETAWAY RT by Electronegativity
1515 R-GETAWAY R+1 by Electronegativity
1516 R-GETAWAY R+2 by Electronegativity
1517 R-GETAWAY R+3 by Electronegativity
1518 R-GETAWAY R+4 by Electronegativity
1519 R-GETAWAY R+5 by Electronegativity
1520 R-GETAWAY R+6 by Electronegativity
1521 R-GETAWAY R+7 by Electronegativity
1522 R-GETAWAY R+8 by Electronegativity
1523 R-GETAWAY RT+ by Electronegativity
1524 R-GETAWAY R1 by Polarizability
1525 R-GETAWAY R2 by Polarizability
1526 R-GETAWAY R3 by Polarizability
1527 R-GETAWAY R4 by Polarizability
1528 R-GETAWAY R5 by Polarizability
1529 R-GETAWAY R6 by Polarizability
1530 R-GETAWAY R7 by Polarizability
1531 R-GETAWAY R8 by Polarizability
1532 R-GETAWAY RT by Polarizability
1533 R-GETAWAY R+1 by Polarizability
1534 R-GETAWAY R+2 by Polarizability
1535 R-GETAWAY R+3 by Polarizability
1536 R-GETAWAY R+4 by Polarizability
1537 R-GETAWAY R+5 by Polarizability
1538 R-GETAWAY R+6 by Polarizability
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1541 R-GETAWAY RT+ by Polarizability
1542 R-GETAWAY R1 by E-State
1543 R-GETAWAY R2 by E-State
1544 R-GETAWAY R3 by E-State
1545 R-GETAWAY R4 by E-State
1546 R-GETAWAY R5 by E-State

1547 R-GETAWAY R6 by E-State

1548 R-GETAWAY R7 by E-State

1549 R-GETAWAY R8 by E-State

1550 R-GETAWAY RT by E-State

1551 R-GETAWAY R+1 by E-State

1552 R-GETAWAY R+2 by E-State

1553 R-GETAWAY R+3 by E-State

1554 R-GETAWAY R+4 by E-State

1555 R-GETAWAY R+5 by E-State

1556 R-GETAWAY R+6 by E-State

1557 R-GETAWAY R+7 by E-State

1558 R-GETAWAY R+8 by E-State

1559 R-GETAWAY RT+ by E-State

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