机器学习方法用于建立乙酰胆碱酯酶抑制剂的分类模型

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Classification Models for Acetylcholinesterase Inhibitors Based on Machine Learning Methods

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Table S1 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] 1st Electronic-topological

[40] 2nd 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)

[229] Moreau-Broto autocorrelation of lag 9 weighted by vdW radius

[230] Moreau-Broto autocorrelation of lag 10 weighted by vdW radius

[231] Moreau-Broto autocorrelation of lag 0 weighted by atom AlogP

[232] Moreau-Broto autocorrelation of lag 1 weighted by atom AlogP

[233] Moreau-Broto autocorrelation of lag 2 weighted by atom AlogP

[234] Moreau-Broto autocorrelation of lag 3 weighted by atom AlogP

[235] Moreau-Broto autocorrelation of lag 4 weighted by atom AlogP

[236] Moreau-Broto autocorrelation of lag 5 weighted by atom AlogP

[237] Moreau-Broto autocorrelation of lag 6 weighted by atom AlogP

[238] Moreau-Broto autocorrelation of lag 7 weighted by atom AlogP

[239] Moreau-Broto autocorrelation of lag 8 weighted by atom AlogP

[240] Moreau-Broto autocorrelation of lag 9 weighted by atom AlogP

[241] Moreau-Broto autocorrelation of lag 10 weighted by atom AlogP

[242] Moreau-Broto autocorrelation of lag 0 weighted by atomic charge

[243] Moreau-Broto autocorrelation of lag 1 weighted by atomic charge

[244] Moreau-Broto autocorrelation of lag 2 weighted by atomic charge

[245] Moreau-Broto autocorrelation of lag 3 weighted by atomic charge

[246] Moreau-Broto autocorrelation of lag 4 weighted by atomic charge

[247] Moreau-Broto autocorrelation of lag 5 weighted by atomic charge

[248] Moreau-Broto autocorrelation of lag 6 weighted by atomic charge

[249] Moreau-Broto autocorrelation of lag 7 weighted by atomic charge

[250] Moreau-Broto autocorrelation of lag 8 weighted by atomic charge

[251] Moreau-Broto autocorrelation of lag 9 weighted by atomic charge

[252] Moreau-Broto autocorrelation of lag 10 weighted by atomic charge

[253] Moreau-Broto autocorrelation of lag 0 weighted by E-State indices

[254] Moreau-Broto autocorrelation of lag 1 weighted by E-State indices

[255] Moreau-Broto autocorrelation of lag 2 weighted by E-State indices

[256] Moreau-Broto autocorrelation of lag 3 weighted by E-State indices

[257] Moreau-Broto autocorrelation of lag 4 weighted by E-State indices

[258] Moreau-Broto autocorrelation of lag 5 weighted by E-State indices

[259] Moreau-Broto autocorrelation of lag 6 weighted by E-State indices

[260] Moreau-Broto autocorrelation of lag 7 weighted by E-State indices

[261] Moreau-Broto autocorrelation of lag 8 weighted by E-State indices

[262] Moreau-Broto autocorrelation of lag 9 weighted by E-State indices

[263] Moreau-Broto autocorrelation of lag 10 weighted by E-State indices

[264] Moreau-Broto autocorrelation of lag 0 weighted by polarizability

[265] Moreau-Broto autocorrelation of lag 1 weighted by polarizability

[266] Moreau-Broto autocorrelation of lag 2 weighted by polarizability

[267] Moreau-Broto autocorrelation of lag 3 weighted by polarizability

[268] Moreau-Broto autocorrelation of lag 4 weighted by polarizability

[269] Moreau-Broto autocorrelation of lag 5 weighted by polarizability

[270] Moreau-Broto autocorrelation of lag 6 weighted by polarizability

[271] Moreau-Broto autocorrelation of lag 7 weighted by polarizability

[272] Moreau-Broto autocorrelation of lag 8 weighted by polarizability

[273] Moreau-Broto autocorrelation of lag 9 weighted by polarizability

[274] Moreau-Broto autocorrelation of lag 10 weighted by polarizability

[275] Moran autocorrelation of lag 1 weighted by atomic mass

[276] Moran autocorrelation of lag 2 weighted by atomic mass

[277] Moran autocorrelation of lag 3 weighted by atomic mass

[278] Moran autocorrelation of lag 4 weighted by atomic mass

[279] Moran autocorrelation of lag 5 weighted by atomic mass

[280] Moran autocorrelation of lag 6 weighted by atomic mass

[281] Moran autocorrelation of lag 7 weighted by atomic mass

[282] Moran autocorrelation of lag 8 weighted by atomic mass

[283] Moran autocorrelation of lag 9 weighted by atomic mass

[284] Moran autocorrelation of lag 10 weighted by atomic mass

[285] Moran autocorrelation of lag 1 weighted by electronegativity

[286] Moran autocorrelation of lag 2 weighted by electronegativity

[287] Moran autocorrelation of lag 3 weighted by electronegativity

[288] Moran autocorrelation of lag 4 weighted by electronegativity

[289] Moran autocorrelation of lag 5 weighted by electronegativity

[290] Moran autocorrelation of lag 6 weighted by electronegativity

[291] Moran autocorrelation of lag 7 weighted by electronegativity

[292] Moran autocorrelation of lag 8 weighted by electronegativity

[293] Moran autocorrelation of lag 9 weighted by electronegativity

[294] Moran autocorrelation of lag 10 weighted by electronegativity

[295] Moran autocorrelation of lag 1 weighted by vdW radius

[296] Moran autocorrelation of lag 2 weighted by vdW radius

[297] Moran autocorrelation of lag 3 weighted by vdW radius

[298] Moran autocorrelation of lag 4 weighted by vdW radius

[299] Moran autocorrelation of lag 5 weighted by vdW radius

[300] Moran autocorrelation of lag 6 weighted by vdW radius

[301] Moran autocorrelation of lag 7 weighted by vdW radius

[302] Moran autocorrelation of lag 8 weighted by vdW radius

[303] Moran autocorrelation of lag 9 weighted by vdW radius

[304] Moran autocorrelation of lag 10 weighted by vdW radius

[305] Moran autocorrelation of lag 1 weighted by atom AlogP

[306] Moran autocorrelation of lag 2 weighted by atom AlogP

[307] Moran autocorrelation of lag 3 weighted by atom AlogP

[308] Moran autocorrelation of lag 4 weighted by atom AlogP

[309] Moran autocorrelation of lag 5 weighted by atom AlogP

[310] Moran autocorrelation of lag 6 weighted by atom AlogP

[311] Moran autocorrelation of lag 7 weighted by atom AlogP

[312] Moran autocorrelation of lag 8 weighted by atom AlogP

[313] Moran autocorrelation of lag 9 weighted by atom AlogP

[314] Moran autocorrelation of lag 10 weighted by atom AlogP

[315] Moran autocorrelation of lag 1 weighted by atomic mass

[316] Moran autocorrelation of lag 2 weighted by atomic mass

[317] Moran autocorrelation of lag 3 weighted by atomic mass

[318] Moran autocorrelation of lag 4 weighted by atomic mass

[319] Moran autocorrelation of lag 5 weighted by atomic mass

[320] Moran autocorrelation of lag 6 weighted by atomic mass

[321] Moran autocorrelation of lag 7 weighted by atomic mass

[322] Moran autocorrelation of lag 8 weighted by atomic mass

[323] Moran autocorrelation of lag 9 weighted by atomic mass

[324] Moran autocorrelation of lag 10 weighted by atomic mass

[325] Moran autocorrelation of lag 1 weighted by E-State indices

[326] Moran autocorrelation of lag 2 weighted by E-State indices

[327] Moran autocorrelation of lag 3 weighted by E-State indices

[328] Moran autocorrelation of lag 4 weighted by E-State indices

[329] Moran autocorrelation of lag 5 weighted by E-State indices

[330] Moran autocorrelation of lag 6 weighted by E-State indices

[331] Moran autocorrelation of lag 7 weighted by E-State indices

[332] Moran autocorrelation of lag 8 weighted by E-State indices

[333] Moran autocorrelation of lag 9 weighted by E-State indices

[334] Moran autocorrelation of lag 10 weighted by E-State indices

[335] Moran autocorrelation of lag 1 weighted by atomic polarizability

[336] Moran autocorrelation of lag 2 weighted by atomic polarizability

[337] Moran autocorrelation of lag 3 weighted by atomic polarizability

[338] Moran autocorrelation of lag 4 weighted by atomic polarizability

[339] Moran autocorrelation of lag 5 weighted by atomic polarizability

[340] Moran autocorrelation of lag 6 weighted by atomic polarizability

[341] Moran autocorrelation of lag 7 weighted by atomic polarizability

[342] Moran autocorrelation of lag 8 weighted by atomic polarizability

[343] Moran autocorrelation of lag 9 weighted by atomic polarizability

[344] Moran autocorrelation of lag 10 weighted by atomic polarizability

[345] Geary autocorrelation of lag 1 weighted by atomic mass

[346] Geary autocorrelation of lag 2 weighted by atomic mass

[347] Geary autocorrelation of lag 3 weighted by atomic mass

[348] Geary autocorrelation of lag 4 weighted by atomic mass

[349] Geary autocorrelation of lag 5 weighted by atomic mass

[350] Geary autocorrelation of lag 6 weighted by atomic mass

[351] Geary autocorrelation of lag 7 weighted by atomic mass

[352] Geary autocorrelation of lag 8 weighted by atomic mass

[353] Geary autocorrelation of lag 9 weighted by atomic mass

[354] Geary autocorrelation of lag 10 weighted by atomic mass

[355] Geary autocorrelation of lag 1 weighted by electronegativity

[356] Geary autocorrelation of lag 2 weighted by electronegativity

[357] Geary autocorrelation of lag 3 weighted by electronegativity

[358] Geary autocorrelation of lag 4 weighted by electronegativity

[359] Geary autocorrelation of lag 5 weighted by electronegativity

[360] Geary autocorrelation of lag 6 weighted by electronegativity

[361] Geary autocorrelation of lag 7 weighted by electronegativity

[362] Geary autocorrelation of lag 8 weighted by electronegativity

[363] Geary autocorrelation of lag 9 weighted by electronegativity

[364] Geary autocorrelation of lag 10 weighted by electronegativity

[365] Geary autocorrelation of lag 1 weighted by vdW radius

[366] Geary autocorrelation of lag 2 weighted by vdW radius

[367] Geary autocorrelation of lag 3 weighted by vdW radius

[368] Geary autocorrelation of lag 4 weighted by vdW radius

[369] Geary autocorrelation of lag 5 weighted by vdW radius

[370] Geary autocorrelation of lag 6 weighted by vdW radius

[371] Geary autocorrelation of lag 7 weighted by vdW radius

[372] Geary autocorrelation of lag 8 weighted by vdW radius

[373] Geary autocorrelation of lag 9 weighted by vdW radius

[374] Geary autocorrelation of lag 10 weighted by vdW radius

[375] Geary autocorrelation of lag 1 weighted by atom AlogP

[376] Geary autocorrelation of lag 2 weighted by atom AlogP

[377] Geary autocorrelation of lag 3 weighted by atom AlogP

[378] Geary autocorrelation of lag 4 weighted by atom AlogP

[379] Geary autocorrelation of lag 5 weighted by atom AlogP

[380] Geary autocorrelation of lag 6 weighted by atom AlogP

[381] Geary autocorrelation of lag 7 weighted by atom AlogP

[382] Geary autocorrelation of lag 8 weighted by atom AlogP

[383] Geary autocorrelation of lag 9 weighted by atom AlogP

[384] Geary autocorrelation of lag 10 weighted by atom AlogP

[385] Geary autocorrelation of lag 1 weighted by atomic charge

[386] Geary autocorrelation of lag 2 weighted by atomic charge

[387] Geary autocorrelation of lag 3 weighted by atomic charge

[388] Geary autocorrelation of lag 4 weighted by atomic charge

[389] Geary autocorrelation of lag 5 weighted by atomic charge

[390] Geary autocorrelation of lag 6 weighted by atomic charge

[391] Geary autocorrelation of lag 7 weighted by atomic charge

[392] Geary autocorrelation of lag 8 weighted by atomic charge

[393] Geary autocorrelation of lag 9 weighted by atomic charge

[394] Geary autocorrelation of lag 10 weighted by atomic charge

[395] Geary autocorrelation of lag 1 weighted by E-State indices

[396] Geary autocorrelation of lag 2 weighted by E-State indices

[397] Geary autocorrelation of lag 3 weighted by E-State indices

[398] Geary autocorrelation of lag 4 weighted by E-State indices

[399] Geary autocorrelation of lag 5 weighted by E-State indices

[400] Geary autocorrelation of lag 6 weighted by E-State indices

[401] Geary autocorrelation of lag 7 weighted by E-State indices

[402] Geary autocorrelation of lag 8 weighted by E-State indices

[403] Geary autocorrelation of lag 9 weighted by E-State indices

[404] Geary autocorrelation of lag 10 weighted by E-State indices

[405] Geary autocorrelation of lag 1 weighted by atomic polarizability

[406] Geary autocorrelation of lag 2 weighted by atomic polarizability

[407] Geary autocorrelation of lag 3 weighted by atomic polarizability

[408] Geary autocorrelation of lag 4 weighted by atomic polarizability

[409] Geary autocorrelation of lag 5 weighted by atomic polarizability

[410] Geary autocorrelation of lag 6 weighted by atomic polarizability

[411] Geary autocorrelation of lag 7 weighted by atomic polarizability

[412] Geary autocorrelation of lag 8 weighted by atomic polarizability

[413] Geary autocorrelation of lag 9 weighted by atomic polarizability

[414] Geary autocorrelation of lag 10 weighted by atomic polarizability

[415] 0th Kier-Hall connectivity index

[416] 1st Kier-Hall connectivity index

[417] 2nd 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] 1st valence connectivity index

[425] 2nd valence connectivity index

[426] 0th order delta chi index

[427] 1st order delta chi index

[428] 2nd order delta chi index

[429] Poligini index

[430] 0th Solvation connectivity index

[431] 1st Solvation connectivity index

[432] 2nd Solvation connectivity index

[433] Electron charge density index

[434] 1st order Kier shape index

[435] 2nd order Kier shape index

[436] 3rd order Kier shape index

[437] 1st order Kappa alpha shape index

[438] 2nh order Kappa alpha shape index

[439] 3rd 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 index

[456] RDCHI index

[457] First highest eigenvalue of BCUT descriptors weighted by atomic mass

[458] Second highest eigenvalue of BCUT descriptors weighted by atomic mass

[459] Third highest eigenvalue of BCUT descriptors weighted by atomic mass

[460] Forth highest eigenvalue of BCUT descriptors weighted by atomic mass

[461] Fifth highest eigenvalue of BCUT descriptors weighted by atomic mass

[462] First lowest eigenvalue of BCUT descriptors weighted by atomic mass

[463] Second lowest eigenvalue of BCUT descriptors weighted by atomic mass

[464] Third lowest eigenvalue of BCUT descriptors weighted by atomic mass

[465] Forth lowest eigenvalue of BCUT descriptors weighted by atomic mass

[466] Fifth lowest eigenvalue of BCUT descriptors weighted by atomic mass

[467] First highest eigenvalue of BCUT descriptors weighted by electronegativity

[468] Second highest eigenvalue of BCUT descriptors weighted by electronegativity

[469] Third highest eigenvalue of BCUT descriptors weighted by electronegativity

[470] Forth highest eigenvalue of BCUT descriptors weighted by electronegativity

[471] Fifth highest eigenvalue of BCUT descriptors weighted by electronegativity

[472] First lowest eigenvalue of BCUT descriptors weighted by electronegativity

[473] Second lowest eigenvalue of BCUT descriptors weighted by electronegativity

[474] Third lowest eigenvalue of BCUT descriptors weighted by electronegativity

[475] Forth lowest eigenvalue of BCUT descriptors weighted by electronegativity

[476] Fifth lowest eigenvalue of BCUT descriptors weighted by electronegativity

[477] First highest eigenvalue of BCUT descriptors weighted by vdW radius

[478] Second highest eigenvalue of BCUT descriptors weighted by vdW radius

[479] Third highest eigenvalue of BCUT descriptors weighted by vdW radius

[480] Forth highest eigenvalue of BCUT descriptors weighted by vdW radius

[481] Fifth highest eigenvalue of BCUT descriptors weighted by vdW radius

[482] First lowest eigenvalue of BCUT descriptors weighted by vdW radius

[483] Second lowest eigenvalue of BCUT descriptors weighted by vdW radius

[484] Third lowest eigenvalue of BCUT descriptors weighted by vdW radius

[485] Forth lowest eigenvalue of BCUT descriptors weighted by vdW radius

[486] Fifth lowest eigenvalue of BCUT descriptors weighted by vdW radius

[487] First highest eigenvalue of BCUT descriptors weighted by atomic charge

[488] Second highest eigenvalue of BCUT descriptors weighted by atomic charge

[489] Third highest eigenvalue of BCUT descriptors weighted by atomic charge

[490] Forth highest eigenvalue of BCUT descriptors weighted by atomic charge

[491] Fifth highest eigenvalue of BCUT descriptors weighted by atomic charge

[492] First lowest eigenvalue of BCUT descriptors weighted by atomic charge

[493] Second lowest eigenvalue of BCUT descriptors weighted by atomic charge

[494] Third lowest eigenvalue of BCUT descriptors weighted by atomic charge

[495] Forth lowest eigenvalue of BCUT descriptors weighted by atomic charge

[496] Fifth lowest eigenvalue of BCUT descriptors weighted by atomic charge

[497] First highest eigenvalue of BCUT descriptors weighted by atom AlogP

[498] Second highest eigenvalue of BCUT descriptors weighted by atom AlogP

[499] Third highest eigenvalue of BCUT descriptors weighted by atom AlogP

[500] Forth highest eigenvalue of BCUT descriptors weighted by atom AlogP

[501] Fifth highest eigenvalue of BCUT descriptors weighted by atom AlogP

[502] First lowest eigenvalue of BCUT descriptors weighted by atom AlogP

[503] Second lowest eigenvalue of BCUT descriptors weighted by atom AlogP

[504] Third lowest eigenvalue of BCUT descriptors weighted by atom AlogP

[505] Forth lowest eigenvalue of BCUT descriptors weighted by atom AlogP

[506] Fifth lowest eigenvalue of BCUT descriptors weighted by atom AlogP

[507] First highest eigenvalue of BCUT descriptors weighted by E-State indices

[508] Second highest eigenvalue of BCUT descriptors weighted by E-State indices

[509] Third highest eigenvalue of BCUT descriptors weighted by E-State indices

[510] Forth highest eigenvalue of BCUT descriptors weighted by E-State indices

[511] Fifth highest eigenvalue of BCUT descriptors weighted by E-State indices

[512] First lowest eigenvalue of BCUT descriptors weighted by E-State indices

[513] Second lowest eigenvalue of BCUT descriptors weighted by E-State indices

[514] Third lowest eigenvalue of BCUT descriptors weighted by E-State indices

[515] Forth lowest eigenvalue of BCUT descriptors weighted by E-State indices

[516] Fifth lowest eigenvalue of BCUT descriptors weighted by E-State indices

[517] First highest eigenvalue of BCUT descriptors weighted by polarizability

[518] Second highest eigenvalue of BCUT descriptors weighted by polarizability

[519] Third highest eigenvalue of BCUT descriptors weighted by polarizability

[520] Forth highest eigenvalue of BCUT descriptors weighted by polarizability

[521] Fifth highest eigenvalue of BCUT descriptors weighted by polarizability

[522] First lowest eigenvalue of BCUT descriptors weighted by polarizability

[523] Second lowest eigenvalue of BCUT descriptors weighted by polarizability

[524] Third lowest eigenvalue of BCUT descriptors weighted by polarizability

[525] Forth lowest eigenvalue of BCUT descriptors weighted by polarizability

[526] Fifth lowest eigenvalue of BCUT descriptors weighted 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] 2nd invariant moment over vdW volume(*0.01)

[536] 2nd moment shape index over vdW 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 over vdW surface

[542] 2nd order invariant moment over vdW surface

[543] 2nd order moment shape index over vdW surface

[544] 4th order invariant moment over vdW surface

[545] 4th order moment shape index over vdW surface

[546] 6th order invariant moment over vdW surface

[547] 6th order moment shape index over vdW 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] Un-weighted 1st MS-WHIM Variance over vdW surface

[553] Un-weighted 2nd MS-WHIM Variance over vdW surface

[554] Un-weighted 3rd MS-WHIM Variance over vdW surface

[555] Un-weighted 1st MS-WHIM eigenvalue proportion over vdW surface

[556] Un-weighted 2nd MS-WHIM eigenvalue proportion over vdW surface

[557] Un-weighted The MS-WHIM accentric factor over vdW surface

[558] Un-weighted 1st MS-WHIM skewness over vdW surface

[559] Un-weighted 2nd MS-WHIM skewness over vdW surface

[560] Un-weighted 3rd MS-WHIM skewness over vdW surface

[561] Un-weighted 1st MS-WHIM kurtosis over vdW surface

[562] Un-weighted 2nd MS-WHIM kurtosis over vdW surface

[563] Un-weighted 3rd MS-WHIM kurtosis over vdW surface

[564] Positive MEP weighted 1st MS-WHIM Variance over vdW surface

[565] Positive MEP weighted 2nd MS-WHIM Variance over vdW surface

[566] Positive MEP weighted 3rd MS-WHIM Variance over vdW surface

[567] Positive MEP weighted 1st MS-WHIM eigenvalue proportion over vdW surface

[568] Positive MEP weighted 2nd MS-WHIM eigenvalue proportion over vdW surface

[569] Positive MEP weighted the MS-WHIM accentric factor over vdW surface

[570] Positive MEP weighted 1st MS-WHIM skewness over vdW surface

[571] Positive MEP weighted 2nd MS-WHIM skewness over vdW surface

[572] Positive MEP weighted 3rd MS-WHIM skewness over vdW surface

[573] Positive MEP weighted 1st MS-WHIM kurtosis over vdW surface

[574] Positive MEP weighted 2nd MS-WHIM kurtosis over vdW surface

[575] Positive MEP weighted 3rd MS-WHIM kurtosis over vdW surface

[576] Negative MEP weighted 1st MS-WHIM Variance over vdW surface

[577] Negative MEP weighted 2nd MS-WHIM Variance over vdW surface

[578] Negative MEP weighted 3rd MS-WHIM Variance over vdW surface

[579] Negative MEP weighted 1st MS-WHIM eigenvalue proportion over vdW surface

[580] Negative MEP weighted 2nd MS-WHIM eigenvalue proportion over vdW surface

[581] Negative MEP weighted the MS-WHIM accentric factor over vdW surface

[582] Negative MEP weighted 1st MS-WHIM skewness over vdW surface

[583] Negative MEP weighted 2nd MS-WHIM skewness over vdW surface

[584] Negative MEP weighted 3rd MS-WHIM skewness over vdW surface

[585] Negative MEP weighted 1st MS-WHIM kurtosis over vdW surface

[586] Negative MEP weighted 2nd MS-WHIM kurtosis over vdW surface

[587] Negative MEP weighted 3rd MS-WHIM kurtosis over vdW surface

[588] Ovality from SAS

[589] 0th moment over SAS volume

[590] 2nd invariant moment over SAS volume

[591] 2nd moment shape index over SAS volume

[592] 4th invariant moment over SAS volume

[593] 4th moment shape index over SAS volume

[594] 6th invariant moment over SAS volume

[595] 6th moment shape index over SAS volume

[596] 0th order moment over SAS surface

[597] 2nd order invariant moment over SAS surface

[598] 2nd order moment shape index over SAS surface

[599] 4th order invariant moment over SAS surface

[600] 4th order moment shape index over SAS surface

[601] 6th order invariant moment over SAS surface

[602] 6th order moment shape index over SAS 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] Un-weighted 1st MS-WHIM Variance over SAS surface

[608] Un-weighted 2nd MS-WHIM Variance over SAS surface

[609] Un-weighted 3rd MS-WHIM Variance over SAS surface

[610] Un-weighted MS-WHIM eigenvalue proportion over SAS surface

[611] Un-weighted 2nd MS-WHIM eigenvalue proportion over SAS surface

[612] Un-weighted the MS-WHIM accentric factor over SAS surface

[613] Un-weighted 1st MS-WHIM skewness over SAS surface

[614] Un-weighted 2nd MS-WHIM skewness over SAS surface

[615] Un-weighted 3rd MS-WHIM skewness over SAS surface

[616] Un-weighted 1st MS-WHIM kurtosis over SAS surface

[617] Un-weighted 2nd MS-WHIM kurtosis over SAS surface

[618] Un-weighted 3rd MS-WHIM kurtosis over SAS surface

[619] Positive MEP weighted 1st MS-WHIM Variance over SAS surface

[620] Positive MEP weighted 2nd MS-WHIM Variance over SAS surface

[621] Positive MEP weighted 3rd MS-WHIM Variance over SAS surface

[622] Positive MEP weighted 1st MS-WHIM eigenvalue proportion over SAS surface

[623] Positive MEP weighted 2nd MS-WHIM eigenvalue proportion over SAS surface

[624] Positive MEP weighted the MS-WHIM accentric factor over SAS surface

[625] Positive MEP weighted 1st MS-WHIM skewness over SAS surface

[626] Positive MEP weighted 2nd MS-WHIM skewness over SAS surface

[627] Positive MEP weighted 3rd MS-WHIM skewness over SAS surface

[628] Positive MEP weighted 1st MS-WHIM kurtosis over SAS surface

[629] Positive MEP weighted 2nd MS-WHIM kurtosis over SAS surface

[630] Positive MEP weighted 3rd MS-WHIM kurtosis over SAS surface

[631] Negative MEP weighted 1st MS-WHIM Variance over SAS surface

[632] Negative MEP weighted 2nd MS-WHIM Variance over SAS surface

[633] Negative MEP weighted 3rd MS-WHIM Variance over SAS surface

[634] Negative MEP weighted 1st MS-WHIM eigenvalue proportion over SAS surface

[635] Negative MEP weighted 2nd MS-WHIM eigenvalue proportion over SAS surface

[636] Negative MEP weighted the MS-WHIM accentric factor over SAS surface

[637] Negative MEP weighted 1st MS-WHIM skewness over SAS surface

[638] Negative MEP weighted 2nd MS-WHIM skewness over SAS surface

[639] Negative MEP weighted 3rd MS-WHIM skewness over SAS surface

[640] Negative MEP weighted 1st MS-WHIM kurtosis over SAS surface

[641] Negative MEP weighted 2nd MS-WHIM kurtosis over SAS surface

[642] Negative MEP weighted 3rd MS-WHIM kurtosis over SAS surface

[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)

[681] Un-weighted RDF g(1.0000)

[682] Un-weighted RDF g(1.5000)

[683] Un-weighted RDF g(2.0000)

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[700] Un-weighted RDF g(10.5000)

[701] Un-weighted RDF g(11.0000)

[702] Un-weighted RDF g(11.5000)

[703] Un-weighted RDF g(12.0000)

[704] Un-weighted RDF g(12.5000)

[705] Un-weighted RDF g(13.0000)

[706] Un-weighted RDF g(13.5000)

[707] Un-weighted RDF g(14.0000)

[708] RDF descriptors g(0.0000) weighted by atomic mass

[709] RDF descriptors g(0.5000) weighted by atomic mass

[710] RDF descriptors g(1.0000) weighted by atomic mass

[711] RDF descriptors g(1.5000) weighted by atomic mass

[712] RDF descriptors g(2.0000) weighted by atomic mass

[713] RDF descriptors g(2.5000) weighted by atomic mass

[714] RDF descriptors g(3.0000) weighted by atomic mass

[715] RDF descriptors g(3.5000) weighted by atomic mass

[716] RDF descriptors g(4.0000) weighted by atomic mass

[717] RDF descriptors g(4.5000) weighted by atomic mass

[718] RDF descriptors g(5.0000) weighted by atomic mass

[719] RDF descriptors g(5.5000) weighted by atomic mass

[720] RDF descriptors g(6.0000) weighted by atomic mass

[721] RDF descriptors g(6.5000) weighted by atomic mass

[722] RDF descriptors g(7.0000) weighted by atomic mass

[723] RDF descriptors g(7.5000) weighted by atomic mass

[724] RDF descriptors g(8.0000) weighted by atomic mass

[725] RDF descriptors g(8.5000) weighted by atomic mass

[726] RDF descriptors g(9.0000) weighted by atomic mass

[727] RDF descriptors g(9.5000) weighted by atomic mass

[728] RDF descriptors g(10.0000) weighted by atomic mass

[729] RDF descriptors g(10.5000) weighted by atomic mass

[730] RDF descriptors g(11.000) weighted by atomic mass

[731] RDF descriptors g(11.5000) weighted by atomic mass

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[733] RDF descriptors g(12.5000) weighted by atomic mass

[734] RDF descriptors g(13.0000) weighted by atomic mass

[735] RDF descriptors g(13.5000) weighted by atomic mass

[736] RDF descriptors g(14.0000) weighted by atomic mass

[737] RDF descriptors g(0.0000) weighted by vdW radius

[738] RDF descriptors g(0.5000) weighted by vdW radius

[739] RDF descriptors g(1.0000) weighted by vdW radius

[740] RDF descriptors g(1.5000) weighted by vdW radius

[741] RDF descriptors g(2.0000) weighted by vdW radius

[742] RDF descriptors g(2.5000) weighted by vdW radius

[743] RDF descriptors g(3.0000) weighted by vdW radius

[744] RDF descriptors g(3.5000) weighted by vdW radius

[745] RDF descriptors g(4.0000) weighted by vdW radius

[746] RDF descriptors g(4.5000) weighted by vdW radius

[747] RDF descriptors g(5.0000) weighted by vdW radius

[748] RDF descriptors g(5.5000) weighted by vdW radius

[749] RDF descriptors g(6.0000) weighted by vdW radius

[750] RDF descriptors g(6.5000) weighted by vdW radius

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[752] RDF descriptors g(7.5000) weighted by vdW radius

[753] RDF descriptors g(8.0000) weighted by vdW radius

[754] RDF descriptors g(8.5000) weighted by vdW radius

[755] RDF descriptors g(9.0000) weighted by vdW radius

[756] RDF descriptors g(9.5000) weighted by vdW radius

[757] RDF descriptors g(10.0000) weighted by vdW radius

[758] RDF descriptors g(10.5000) weighted by vdW radius

[759] RDF descriptors g(11.000) weighted by vdW radius

[760] RDF descriptors g(11.5000) weighted by vdW radius

[761] RDF descriptors g(12.0000) weighted by vdW radius

[762] RDF descriptors g(12.5000) weighted by vdW radius

[763] RDF descriptors g(13.0000) weighted by vdW radius

[764] RDF descriptors g(13.5000) weighted by vdW radius

[765] RDF descriptors g(14.0000) weighted by vdW radius

[766] RDF descriptors g(0.0000) weighted by electronegativity

[767] RDF descriptors g(0.5000) weighted by electronegativity

[768] RDF descriptors g(1.0000) weighted by electronegativity

[769] RDF descriptors g(1.5000) weighted by electronegativity

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[777] RDF descriptors g(5.5000) weighted by electronegativity

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[779] RDF descriptors g(6.5000) weighted by electronegativity

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[788] RDF descriptors g(11.000) weighted by electronegativity

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[794] RDF descriptors g(14.0000) weighted by electronegativity

[795] RDF descriptors g(0.0000) weighted by atom AlogP

[796] RDF descriptors g(0.5000) weighted by atom AlogP

[797] RDF descriptors g(1.0000) weighted by atom AlogP

[798] RDF descriptors g(1.5000) weighted by atom AlogP

[799] RDF descriptors g(2.0000) weighted by atom AlogP

[800] RDF descriptors g(2.5000) weighted by atom AlogP

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[802] RDF descriptors g(3.5000) weighted by atom AlogP

[803] RDF descriptors g(4.0000) weighted by atom AlogP

[804] RDF descriptors g(4.5000) weighted by atom AlogP

[805] RDF descriptors g(5.0000) weighted by atom AlogP

[806] RDF descriptors g(5.5000) weighted by atom AlogP

[807] RDF descriptors g(6.0000) weighted by atom AlogP

[808] RDF descriptors g(6.5000) weighted by atom AlogP

[809] RDF descriptors g(7.0000) weighted by atom AlogP

[810] RDF descriptors g(7.5000) weighted by atom AlogP

[811] RDF descriptors g(8.0000) weighted by atom AlogP

[812] RDF descriptors g(8.5000) weighted by atom AlogP

[813] RDF descriptors g(9.0000) weighted by atom AlogP

[814] RDF descriptors g(9.5000) weighted by atom AlogP

[815] RDF descriptors g(10.0000) weighted by atom AlogP

[816] RDF descriptors g(10.5000) weighted by atom AlogP

[817] RDF descriptors g(11.000) weighted by atom AlogP

[818] RDF descriptors g(11.5000) weighted by atom AlogP

[819] RDF descriptors g(12.0000) weighted by atom AlogP

[820] RDF descriptors g(12.5000) weighted by atom AlogP

[821] RDF descriptors g(13.0000) weighted by atom AlogP

[822] RDF descriptors g(13.5000) weighted by atom AlogP

[823] RDF descriptors g(14.0000) weighted by atom AlogP

[824] RDF descriptors g(0.0000) weighted by atomic charge

[825] RDF descriptors g(0.5000) weighted by atomic charge

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[829] RDF descriptors g(2.5000) weighted by atomic charge

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[833] RDF descriptors g(4.5000) weighted by atomic charge

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[852] RDF descriptors g(14.0000) weighted by atomic charge

[853] RDF descriptors g(0.0000) weighted by E-State indices

[854] RDF descriptors g(0.5000) weighted by E-State indices

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[878] RDF descriptors g(12.5000) weighted by E-State indices

[879] RDF descriptors g(13.0000) weighted by E-State indices

[880] RDF descriptors g(13.5000) weighted by E-State indices

[881] RDF descriptors g(14.0000) weighted by E-State indices

[882] RDF descriptors g(0.0000) weighted by polarizability

[883] RDF descriptors g(0.5000) weighted by polarizability

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[885] RDF descriptors g(1.5000) weighted by polarizability

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[889] RDF descriptors g(3.5000) weighted by polarizability

[890] RDF descriptors g(4.0000) weighted by polarizability

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[908] RDF descriptors g(13.0000) weighted by polarizability

[909] RDF descriptors g(13.5000) weighted by polarizability

[910] RDF descriptors g(14.0000) weighted by polarizability

[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 indices

[982] 2nd directional WHIM size by E-State indices

[983] 3rd directional WHIM size by E-State indices

[984] 1st directional WHIM shape by E-State indices

[985] 2nd directional WHIM shape by E-State indices

[986] 3rd directional WHIM shape by E-State indices

[987] 1st directional WHIM density by E-State indices

[988] 2nd directional WHIM density by E-State indices

[989] 3rd directional WHIM density by E-State indices

[990] Global WHIM T by E-State indices

[991] Global WHIM A by E-State indices

[992] Global WHIM V by E-State indices

[993] Global WHIM G by E-State indices

[994] Global WHIM D by E-State indices

[995] Unweighted 3D-MoRSE Signal I(1.0)

[996] Unweighted 3D-MoRSE Signal I(2.0)

[997] Unweighted 3D-MoRSE Signal I(3.0)

[998] Unweighted 3D-MoRSE Signal I(4.0)

[999] Unweighted 3D-MoRSE Signal I(5.0)

[1000] Unweighted 3D-MoRSE Signal I(6.0)

[1001] Unweighted 3D-MoRSE Signal I(7.0)

[1002] Unweighted 3D-MoRSE Signal I(8.0)

[1003] Unweighted 3D-MoRSE Signal I(9.0)

[1004] Unweighted 3D-MoRSE Signal I(10.0)

[1005] Unweighted 3D-MoRSE Signal I(11.0)

[1006] Unweighted 3D-MoRSE Signal I(12.0)

[1007] Unweighted 3D-MoRSE Signal I(13.0)

[1008] Unweighted 3D-MoRSE Signal I(14.0)

[1009] Unweighted 3D-MoRSE Signal I(15.0)

[1010] Unweighted 3D-MoRSE Signal I(16.0)

[1011] Unweighted 3D-MoRSE Signal I(17.0)

[1012] Unweighted 3D-MoRSE Signal I(18.0)

[1013] Unweighted 3D-MoRSE Signal I(19.0)

[1014] Unweighted 3D-MoRSE Signal I(20.0)

[1015] Unweighted 3D-MoRSE Signal I(21.0)

[1016] Unweighted 3D-MoRSE Signal I(22.0)

[1017] Unweighted 3D-MoRSE Signal I(23.0)

[1018] Unweighted 3D-MoRSE Signal I(24.0)

[1019] Unweighted 3D-MoRSE Signal I(25.0)

[1020] Unweighted 3D-MoRSE Signal I(26.0)

[1021] Unweighted 3D-MoRSE Signal I(27.0)

[1022] Unweighted 3D-MoRSE Signal I(28.0)

[1023] Unweighted 3D-MoRSE Signal I(29.0)

[1024] Unweighted 3D-MoRSE Signal I(30.0)

[1025] Unweighted 3D-MoRSE Signal I(31.0)

[1026] Unweighted 3D-MoRSE Signal I(32.0)

[1027] 3D-MoRSE-Signal I(1.0) weighted by atomic mass

[1028] 3D-MoRSE-Signal I(2.0) weighted by atomic mass

[1029] 3D-MoRSE-Signal I(3.0) weighted by atomic mass

[1030] 3D-MoRSE-Signal I(4.0) weighted by atomic mass

[1031] 3D-MoRSE-Signal I(5.0) weighted by atomic mass

[1032] 3D-MoRSE-Signal I(6.0) weighted by atomic mass

[1033] 3D-MoRSE-Signal I(7.0) weighted by atomic mass

[1034] 3D-MoRSE-Signal I(8.0) weighted by atomic mass

[1035] 3D-MoRSE-Signal I(9.0) weighted by atomic mass

[1036] 3D-MoRSE-Signal I(10.0) weighted by atomic mass

[1037] 3D-MoRSE-Signal I(11.0) weighted by atomic mass

[1038] 3D-MoRSE-Signal I(12.0) weighted by atomic mass

[1039] 3D-MoRSE-Signal I(13.0) weighted by atomic mass

[1040] 3D-MoRSE-Signal I(14.0) weighted by atomic mass

[1041] 3D-MoRSE-Signal I(15.0) weighted by atomic mass

[1042] 3D-MoRSE-Signal I(16.0) weighted by atomic mass

[1043] 3D-MoRSE-Signal I(17.0) weighted by atomic mass

[1044] 3D-MoRSE-Signal I(18.0) weighted by atomic mass

[1045] 3D-MoRSE-Signal I(19.0) weighted by atomic mass

[1046] 3D-MoRSE-Signal I(20.0) weighted by atomic mass

[1047] 3D-MoRSE-Signal I(21.0) weighted by atomic mass

[1048] 3D-MoRSE-Signal I(22.0) weighted by atomic mass

[1049] 3D-MoRSE-Signal I(23.0) weighted by atomic mass

[1050] 3D-MoRSE-Signal I(24.0) weighted by atomic mass

[1051] 3D-MoRSE-Signal I(25.0) weighted by atomic mass

[1052] 3D-MoRSE-Signal I(26.0) weighted by atomic mass

[1053] 3D-MoRSE-Signal I(27.0) weighted by atomic mass

[1054] 3D-MoRSE-Signal I(28.0) weighted by atomic mass

[1055] 3D-MoRSE-Signal I(29.0) weighted by atomic mass

[1056] 3D-MoRSE-Signal I(30.0) weighted by atomic mass

[1057] 3D-MoRSE-Signal I(31.0) weighted by atomic mass
[1058] 3D-MoRSE-Signal I(32.0) weighted by atomic mass
[1059] 3D-MoRSE-Signal I(1.0) weighted by atomic number
[1060] 3D-MoRSE-Signal I(2.0) weighted by atomic number
[1061] 3D-MoRSE-Signal I(3.0) weighted by atomic number
[1062] 3D-MoRSE-Signal I(4.0) weighted by atomic number
[1063] 3D-MoRSE-Signal I(5.0) weighted by atomic number
[1064] 3D-MoRSE-Signal I(6.0) weighted by atomic number
[1065] 3D-MoRSE-Signal I(7.0) weighted by atomic number
[1066] 3D-MoRSE-Signal I(8.0) weighted by atomic number
[1067] 3D-MoRSE-Signal I(9.0) weighted by atomic number
[1068] 3D-MoRSE-Signal I(10.0) weighted by atomic number
[1069] 3D-MoRSE-Signal I(11.0) weighted by atomic number
[1070] 3D-MoRSE-Signal I(12.0) weighted by atomic number
[1071] 3D-MoRSE-Signal I(13.0) weighted by atomic number
[1072] 3D-MoRSE-Signal I(14.0) weighted by atomic number
[1073] 3D-MoRSE-Signal I(15.0) weighted by atomic number
[1074] 3D-MoRSE-Signal I(16.0) weighted by atomic number
[1075] 3D-MoRSE-Signal I(17.0) weighted by atomic number
[1076] 3D-MoRSE-Signal I(18.0) weighted by atomic number
[1077] 3D-MoRSE-Signal I(19.0) weighted by atomic number
[1078] 3D-MoRSE-Signal I(20.0) weighted by atomic number
[1079] 3D-MoRSE-Signal I(21.0) weighted by atomic number
[1080] 3D-MoRSE-Signal I(22.0) weighted by atomic number
[1081] 3D-MoRSE-Signal I(23.0) weighted by atomic number
[1082] 3D-MoRSE-Signal I(24.0) weighted by atomic number
[1083] 3D-MoRSE-Signal I(25.0) weighted by atomic number
[1084] 3D-MoRSE-Signal I(26.0) weighted by atomic number
[1085] 3D-MoRSE-Signal I(27.0) weighted by atomic number
[1086] 3D-MoRSE-Signal I(28.0) weighted by atomic number
[1087] 3D-MoRSE-Signal I(29.0) weighted by atomic number
[1088] 3D-MoRSE-Signal I(30.0) weighted by atomic number
[1089] 3D-MoRSE-Signal I(31.0) weighted by atomic number
[1090] 3D-MoRSE-Signal I(32.0) weighted by atomic number
[1091] 3D-MoRSE-Signal I(1.0) weighted by vdW radius
[1092] 3D-MoRSE-Signal I(2.0) weighted by vdW radius
[1093] 3D-MoRSE-Signal I(3.0) weighted by vdW radius
[1094] 3D-MoRSE-Signal I(4.0) weighted by vdW radius
[1095] 3D-MoRSE-Signal I(5.0) weighted by vdW radius
[1096] 3D-MoRSE-Signal I(6.0) weighted by vdW radius
[1097] 3D-MoRSE-Signal I(7.0) weighted by vdW radius
[1098] 3D-MoRSE-Signal I(8.0) weighted by vdW radius
[1099] 3D-MoRSE-Signal I(9.0) weighted by vdW radius
[1100] 3D-MoRSE-Signal I(10.0) weighted by vdW radius
[1101] 3D-MoRSE-Signal I(11.0) weighted by vdW radius
[1102] 3D-MoRSE-Signal I(12.0) weighted by vdW radius

[1103] 3D-MoRSE-Signal I(13.0) weighted by vdW radius
[1104] 3D-MoRSE-Signal I(14.0) weighted by vdW radius
[1105] 3D-MoRSE-Signal I(15.0) weighted by vdW radius
[1106] 3D-MoRSE-Signal I(16.0) weighted by vdW radius
[1107] 3D-MoRSE-Signal I(17.0) weighted by vdW radius
[1108] 3D-MoRSE-Signal I(18.0) weighted by vdW radius
[1109] 3D-MoRSE-Signal I(19.0) weighted by vdW radius
[1110] 3D-MoRSE-Signal I(20.0) weighted by vdW radius
[1111] 3D-MoRSE-Signal I(21.0) weighted by vdW radius
[1112] 3D-MoRSE-Signal I(22.0) weighted by vdW radius
[1113] 3D-MoRSE-Signal I(23.0) weighted by vdW radius
[1114] 3D-MoRSE-Signal I(24.0) weighted by vdW radius
[1115] 3D-MoRSE-Signal I(25.0) weighted by vdW radius
[1116] 3D-MoRSE-Signal I(26.0) weighted by vdW radius
[1117] 3D-MoRSE-Signal I(27.0) weighted by vdW radius
[1118] 3D-MoRSE-Signal I(28.0) weighted by vdW radius
[1119] 3D-MoRSE-Signal I(29.0) weighted by vdW radius
[1120] 3D-MoRSE-Signal I(30.0) weighted by vdW radius
[1121] 3D-MoRSE-Signal I(31.0) weighted by vdW radius
[1122] 3D-MoRSE-Signal I(32.0) weighted by vdW radius
[1123] 3D-MoRSE-Signal I(1.0) weighted by electronegativity
[1124] 3D-MoRSE-Signal I(2.0) weighted by electronegativity
[1125] 3D-MoRSE-Signal I(3.0) weighted by electronegativity
[1126] 3D-MoRSE-Signal I(4.0) weighted by electronegativity
[1127] 3D-MoRSE-Signal I(5.0) weighted by electronegativity
[1128] 3D-MoRSE-Signal I(6.0) weighted by electronegativity
[1129] 3D-MoRSE-Signal I(7.0) weighted by electronegativity
[1130] 3D-MoRSE-Signal I(8.0) weighted by electronegativity
[1131] 3D-MoRSE-Signal I(9.0) weighted by electronegativity
[1132] 3D-MoRSE-Signal I(10.0) weighted by electronegativity
[1133] 3D-MoRSE-Signal I(11.0) weighted by electronegativity
[1134] 3D-MoRSE-Signal I(12.0) weighted by electronegativity
[1135] 3D-MoRSE-Signal I(13.0) weighted by electronegativity
[1136] 3D-MoRSE-Signal I(14.0) weighted by electronegativity
[1137] 3D-MoRSE-Signal I(15.0) weighted by electronegativity
[1138] 3D-MoRSE-Signal I(16.0) weighted by electronegativity
[1139] 3D-MoRSE-Signal I(17.0) weighted by electronegativity
[1140] 3D-MoRSE-Signal I(18.0) weighted by electronegativity
[1141] 3D-MoRSE-Signal I(19.0) weighted by electronegativity
[1142] 3D-MoRSE-Signal I(20.0) weighted by electronegativity
[1143] 3D-MoRSE-Signal I(21.0) weighted by electronegativity
[1144] 3D-MoRSE-Signal I(22.0) weighted by electronegativity
[1145] 3D-MoRSE-Signal I(23.0) weighted by electronegativity
[1146] 3D-MoRSE-Signal I(24.0) weighted by electronegativity
[1147] 3D-MoRSE-Signal I(25.0) weighted by electronegativity
[1148] 3D-MoRSE-Signal I(26.0) weighted by electronegativity

[1149] 3D-MoRSE-Signal I(27.0) weighted by electronegativity

[1150] 3D-MoRSE-Signal I(28.0) weighted by electronegativity

[1151] 3D-MoRSE-Signal I(29.0) weighted by electronegativity

[1152] 3D-MoRSE-Signal I(30.0) weighted by electronegativity

[1153] 3D-MoRSE-Signal I(31.0) weighted by electronegativity

[1154] 3D-MoRSE-Signal I(32.0) weighted by electronegativity

[1155] 3D-MoRSE-Signal I(1.0) weighted by polarizability

[1156] 3D-MoRSE-Signal I(2.0) weighted by polarizability

[1157] 3D-MoRSE-Signal I(3.0) weighted by polarizability

[1158] 3D-MoRSE-Signal I(4.0) weighted by polarizability

[1159] 3D-MoRSE-Signal I(5.0) weighted by polarizability

[1160] 3D-MoRSE-Signal I(6.0) weighted by polarizability

[1161] 3D-MoRSE-Signal I(7.0) weighted by polarizability

[1162] 3D-MoRSE-Signal I(8.0) weighted by polarizability

[1163] 3D-MoRSE-Signal I(9.0) weighted by polarizability

[1164] 3D-MoRSE-Signal I(10.0) weighted by polarizability

[1165] 3D-MoRSE-Signal I(11.0) weighted by polarizability

[1166] 3D-MoRSE-Signal I(12.0) weighted by polarizability

[1167] 3D-MoRSE-Signal I(13.0) weighted by polarizability

[1168] 3D-MoRSE-Signal I(14.0) weighted by polarizability

[1169] 3D-MoRSE-Signal I(15.0) weighted by polarizability

[1170] 3D-MoRSE-Signal I(16.0) weighted by polarizability

[1171] 3D-MoRSE-Signal I(17.0) weighted by polarizability

[1172] 3D-MoRSE-Signal I(18.0) weighted by polarizability

[1173] 3D-MoRSE-Signal I(19.0) weighted by polarizability

[1174] 3D-MoRSE-Signal I(20.0) weighted by polarizability

[1175] 3D-MoRSE-Signal I(21.0) weighted by polarizability

[1176] 3D-MoRSE-Signal I(22.0) weighted by polarizability

[1177] 3D-MoRSE-Signal I(23.0) weighted by polarizability

[1178] 3D-MoRSE-Signal I(24.0) weighted by polarizability

[1179] 3D-MoRSE-Signal I(25.0) weighted by polarizability

[1180] 3D-MoRSE-Signal I(26.0) weighted by polarizability

[1181] 3D-MoRSE-Signal I(27.0) weighted by polarizability

[1182] 3D-MoRSE-Signal I(28.0) weighted by polarizability

[1183] 3D-MoRSE-Signal I(29.0) weighted by polarizability

[1184] 3D-MoRSE-Signal I(30.0) weighted by polarizability

[1185] 3D-MoRSE-Signal I(31.0) weighted by polarizability

[1186] 3D-MoRSE-Signal I(32.0) weighted by polarizability

[1187] 3D-MoRSE-Signal I(1.0) weighted by E-State indices

[1188] 3D-MoRSE-Signal I(2.0) weighted by E-State indices

[1189] 3D-MoRSE-Signal I(3.0) weighted by E-State indices

[1190] 3D-MoRSE-Signal I(4.0) weighted by E-State indices

[1191] 3D-MoRSE-Signal I(5.0) weighted by E-State indices

[1192] 3D-MoRSE-Signal I(6.0) weighted by E-State indices

[1193] 3D-MoRSE-Signal I(7.0) weighted by E-State indices

[1194] 3D-MoRSE-Signal I(8.0) weighted by E-State indices

[1195] 3D-MoRSE-Signal I(9.0) weighted by E-State indices

[1196] 3D-MoRSE-Signal I(10.0) weighted by E-State indices

[1197] 3D-MoRSE-Signal I(11.0) weighted by E-State indices

[1198] 3D-MoRSE-Signal I(12.0) weighted by E-State indices

[1199] 3D-MoRSE-Signal I(13.0) weighted by E-State indices

[1200] 3D-MoRSE-Signal I(14.0) weighted by E-State indices

[1201] 3D-MoRSE-Signal I(15.0) weighted by E-State indices

[1202] 3D-MoRSE-Signal I(16.0) weighted by E-State indices

[1203] 3D-MoRSE-Signal I(17.0) weighted by E-State indices

[1204] 3D-MoRSE-Signal I(18.0) weighted by E-State indices

[1205] 3D-MoRSE-Signal I(19.0) weighted by E-State indices

[1206] 3D-MoRSE-Signal I(20.0) weighted by E-State indices

[1207] 3D-MoRSE-Signal I(21.0) weighted by E-State indices

[1208] 3D-MoRSE-Signal I(22.0) weighted by E-State indices

[1209] 3D-MoRSE-Signal I(23.0) weighted by E-State indices

[1210] 3D-MoRSE-Signal I(24.0) weighted by E-State indices

[1211] 3D-MoRSE-Signal I(25.0) weighted by E-State indices

[1212] 3D-MoRSE-Signal I(26.0) weighted by E-State indices

[1213] 3D-MoRSE-Signal I(27.0) weighted by E-State indices

[1214] 3D-MoRSE-Signal I(28.0) weighted by E-State indices

[1215] 3D-MoRSE-Signal I(29.0) weighted by E-State indices

[1216] 3D-MoRSE-Signal I(30.0) weighted by E-State indices

[1217] 3D-MoRSE-Signal I(31.0) weighted by E-State indices

[1218] 3D-MoRSE-Signal I(32.0) weighted by E-State indices

[1219] H-GETAWAY Geometric Mean HGM

[1220] H-GETAWAY Mean Information Content HIC

[1221] unweighted H-GETAWAY ATS0

[1222] unweighted H-GETAWAY ATS1

[1223] unweighted H-GETAWAY ATS2

[1224] unweighted H-GETAWAY ATS3

[1225] unweighted H-GETAWAY ATS4

[1226] unweighted H-GETAWAY ATS5

[1227] unweighted H-GETAWAY ATS6

[1228] unweighted H-GETAWAY ATS7

[1229] unweighted H-GETAWAY ATS8

[1230] unweighted H-GETAWAY ATS

[1231] unweighted H-GETAWAY HATS0

[1232] unweighted H-GETAWAY HATS1

[1233] unweighted H-GETAWAY HATS2

[1234] unweighted H-GETAWAY HATS3

[1235] unweighted H-GETAWAY HATS4

[1236] unweighted H-GETAWAY HATS5

[1237] unweighted H-GETAWAY HATS6

[1238] unweighted H-GETAWAY HATS7

[1239] unweighted H-GETAWAY HATS8

[1240] unweighted H-GETAWAY HATS

[1241] unweighted H-GETAWAY H0

[1242] unweighted H-GETAWAY H1

[1243] unweighted H-GETAWAY H2

[1244] unweighted H-GETAWAY H3

[1245] unweighted H-GETAWAY H4

[1246] unweighted H-GETAWAY H5

[1247] unweighted H-GETAWAY H6

[1248] unweighted H-GETAWAY H7

[1249] unweighted H-GETAWAY H8

[1250] unweighted H-GETAWAY HT

[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 radius
[1312] H-GETAWAY ATS1 by vdW radius
[1313] H-GETAWAY ATS2 by vdW radius
[1314] H-GETAWAY ATS3 by vdW radius
[1315] H-GETAWAY ATS4 by vdW radius
[1316] H-GETAWAY ATS5 by vdW radius
[1317] H-GETAWAY ATS6 by vdW radius
[1318] H-GETAWAY ATS7 by vdW radius
[1319] H-GETAWAY ATS8 by vdW radius
[1320] H-GETAWAY ATS by vdW radius
[1321] H-GETAWAY HATS0 by vdW radius
[1322] H-GETAWAY HATS1 by vdW radius
[1323] H-GETAWAY HATS2 by vdW radius
[1324] H-GETAWAY HATS3 by vdW radius
[1325] H-GETAWAY HATS4 by vdW radius
[1326] H-GETAWAY HATS5 by vdW radius
[1327] H-GETAWAY HATS6 by vdW radius
[1328] H-GETAWAY HATS7 by vdW radius
[1329] H-GETAWAY HATS8 by vdW radius
[1330] H-GETAWAY HATS by vdW radius
[1331] H-GETAWAY H0 by vdW radius
[1332] H-GETAWAY H1 by vdW radius

[1333] H-GETAWAY H2 by vdW radius

[1334] H-GETAWAY H3 by vdW radius

[1335] H-GETAWAY H4 by vdW radius

[1336] H-GETAWAY H5 by vdW radius

[1337] H-GETAWAY H6 by vdW radius

[1338] H-GETAWAY H7 by vdW radius

[1339] H-GETAWAY H8 by vdW radius

[1340] H-GETAWAY HT by vdW radius

[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 indices

[1402] H-GETAWAY ATS1 by E-State indices

[1403] H-GETAWAY ATS2 by E-State indices

[1404] H-GETAWAY ATS3 by E-State indices

[1405] H-GETAWAY ATS4 by E-State indices

[1406] H-GETAWAY ATS5 by E-State indices

[1407] H-GETAWAY ATS6 by E-State indices

[1408] H-GETAWAY ATS7 by E-State indices

[1409] H-GETAWAY ATS8 by E-State indices

[1410] H-GETAWAY ATS by E-State indices

[1411] H-GETAWAY HATS0 by E-State indices

[1412] H-GETAWAY HATS1 by E-State indices

[1413] H-GETAWAY HATS2 by E-State indices

[1414] H-GETAWAY HATS3 by E-State indices

[1415] H-GETAWAY HATS4 by E-State indices

[1416] H-GETAWAY HATS5 by E-State indices

[1417] H-GETAWAY HATS6 by E-State indices

[1418] H-GETAWAY HATS7 by E-State indices

[1419] H-GETAWAY HATS8 by E-State indices

[1420] H-GETAWAY HATS by E-State indices

[1421] H-GETAWAY H0 by E-State indices

[1422] H-GETAWAY H1 by E-State indices

[1423] H-GETAWAY H2 by E-State indices

[1424] H-GETAWAY H3 by E-State indices

[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 radius
[1489] R-GETAWAY R2 by vdW radius
[1490] R-GETAWAY R3 by vdW radius
[1491] R-GETAWAY R4 by vdW radius
[1492] R-GETAWAY R5 by vdW radius
[1493] R-GETAWAY R6 by vdW radius
[1494] R-GETAWAY R7 by vdW radius
[1495] R-GETAWAY R8 by vdW radius
[1496] R-GETAWAY RT by vdW radius
[1497] R-GETAWAY R+1 by vdW radius
[1498] R-GETAWAY R+2 by vdW radius
[1499] R-GETAWAY R+3 by vdW radius
[1500] R-GETAWAY R+4 by vdW radius
[1501] R-GETAWAY R+5 by vdW radius
[1502] R-GETAWAY R+6 by vdW radius
[1503] R-GETAWAY R+7 by vdW radius
[1504] R-GETAWAY R+8 by vdW radius
[1505] R-GETAWAY RT+ by vdW radius
[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

[1539] R-GETAWAY R+7 by Polarizability

[1540] R-GETAWAY R+8 by Polarizability

[1541] R-GETAWAY RT+ by Polarizability

[1542] R-GETAWAY R1 by E-State indices

[1543] R-GETAWAY R2 by E-State indices

[1544] R-GETAWAY R3 by E-State indices

[1545] R-GETAWAY R4 by E-State indices

[1546] R-GETAWAY R5 by E-State indices

[1547] R-GETAWAY R6 by E-State indices

[1548] R-GETAWAY R7 by E-State indices

[1549] R-GETAWAY R8 by E-State indices

[1550] R-GETAWAY RT by E-State indices

[1551] R-GETAWAY R+1 by E-State indices

[1552] R-GETAWAY R+2 by E-State indices

[1553] R-GETAWAY R+3 by E-State indices

[1554] R-GETAWAY R+4 by E-State indices

[1555] R-GETAWAY R+5 by E-State indices

[1556] R-GETAWAY R+6 by E-State indices

[1557] R-GETAWAY R+7 by E-State indices

[1558] R-GETAWAY R+8 by E-State indices

[1559] GETAWAY RT+ by E-State indices

表 S2 筛选出的 37 个分子描述符
Table S2 Selected Molecular descriptors

SN	Descriptions	Type
1	0th Electronic-topological	Charge descriptors
2	Hydrophobic alogp	Physical chemistry properties descriptors
3	Sum of H Estate of atom type HCsats	Topological descriptors
4	ALOGP weighted Moreau-Broto lagged 2	
5	ALOGP weighted Moreau-Broto lagged 8	
6	Atomic mass weighted moran lagged 4	
7	ALOGP weighted moran lagged 4	
8	E-State weighted moran lagged 1	
9	Polarizability mass weighted moran lagged 3	
10	ALOGP weighted Geary 4	
11	Atomic charge weighted Geary10	
12	E-State weighted Geary 1	
13	Polarizability mass weighted Geary 3	
14	1st MS-WHIM skewness over VDW surface	Geometrical molecular descriptors
15	PPSA3	
16	DPSA1	
17	FNSA1	
18	Un-weighted RDF g(6.0000)	
19	Un-weighted RDF g(8.5000)	
20	Un-weighted RDF g(11.0000)	
21	ALOGP weighted RDF g(5.5000)	
22	ALOGP weighted RDF g(6.5000)	
23	Polarizability weighted RDF g(3.5000)	
24	Polarizability weighted RDF g(5.5000)	
25	Global WHIM D by Atomic mass	
26	3rd directional WHIM density by VDW radius	
27	3D-MoRSE-Signal I(6.0) by Un-	
28	3D-MoRSE-Signal I(14.0) by Un-	
29	3D-MoRSE-Signal I(29.0) by Un-	
30	3D-MoRSE-Signal I(18.0) by Atomic mass	
31	3D-MoRSE-Signal I(30.0) by Atomic mass	
32	H-GETAWAY H1 by Atomic mass	
33	H-GETAWAY H5 by Atomic mass	
34	R-GETAWAY R7 by Un-weighted	
35	R-GETAWAY R+2 by E-State	
36	R-GETAWAY R+6 by E-State	
37	R-GETAWAY R+8 by E-State	

表**S3**　SVM模型y-scrambling验证结果[a]
Table S3　the results of y-scrambling test on SVM model

No. permutation	Step[b] (Number of Descriptors)	Prediction for positive	Prediction for negati	Average of Q （%）
		Average of SE(%)	Average of SP (%)	
1	564	70.5	26.0	53.2
	295	77.1	23.5	56.3
	53	78.7	46.0	66.0
2	564	70.5	32.0	55.5
	295	72.4	33.5	57.3
	42	75.9	48.0	65.1
3	564	75.6	24.0	55.5
	295	75.6	23.0	55.2
	50	77.5	46.0	65.3
4	564	74.9	30.0	57.5
	295	72.4	28.5	55.3
	55	74.9	47.0	64.1
5	564	71.4	24.0	53.0
	295	73.3	28.5	55.9
	54	74.0	43.5	62.1
6	564	74.6	27.5	56.3
	295	75.9	27.5	57.1
	54	76.2	50.0	66.0
7	564	68.9	34.0	55.3
	295	69.2	35.5	56.1
	39	76.8	53.0	67.6
8	564	73.0	26.0	54.8
	295	76.5	22.0	55.3
	53	78.1	47.0	66.0
9	564	74.3	27.5	56.1
	295	73.7	30.5	56.9
	55	79.4	47.0	66.8
10	564	74.3	25.5	55.3
	295	77.8	22.0	56.1
	57	79.4	41.0	64.5
11	564	73.7	30.0	56.7
	295	73.3	30.5	56.7
	38	77.5	47.5	65.8
12	564	71.1	22.0	52.0
	295	73.0	20.0	52.4
	34	73.7	51.0	64.9
13	564	72.1	23.0	53.0
	295	74.9	24.0	55.2
	56	74.0	46.5	63.3
14	564	72.1	25.5	54.0
	295	73.3	24.0	54.2

	49	72.7	48.0	63.1
15	564	75.9	22.5	55.2
	295	79.7	23.0	57.7
	58	75.9	49.5	65.6
16	564	68.6	22.5	50.7
	295	70.5	21.0	51.3
	43	76.5	46.0	64.7
17	564	74.9	30.5	57.7
	295	74.9	31.5	58.1
	47	75.9	52.0	66.6
18	564	77.1	30.0	58.8
	295	75.6	32.5	58.8
	58	82.5	48.0	69.1
19	564	75.2	30.0	57.7
	295	76.2	28.0	57.5
	39	77.8	50.0	67.0
20	564	72.7	16.0	50.7
	295	74.9	16.0	52.0
	51	75.2	43.0	62.7
21	564	72.1	31.5	56.3
	295	71.4	36.0	57.7
	56	75.6	47.0	64.5
22	564	74.0	32.5	57.9
	295	75.9	29.0	57.7
	58	79.0	46.5	66.4
23	564	74.0	32.0	57.7
	295	75.2	29.5	57.5
	57	79.4	43.0	65.3
24	564	71.4	31.0	55.8
	295	70.2	32.0	55.4
	49	76.8	48.0	65.6
25	564	70.8	25.5	53.2
	295	74.3	25.5	55.3
	58	75.6	48.0	64.9
26	564	72.4	25.5	54.2
	295	73.7	28.0	55.9
	51	75.6	42.0	62.5
27	564	72.7	37.0	58.8
	295	72.7	34.5	57.9
	59	77.8	48.5	66.4
28	564	75.2	32.0	58.5
	295	75.6	33.5	59.2
	44	77.5	51.5	67.4
29	564	72.1	26.0	54.2
	295	78.1	21.5	56.1
	49	75.9	45.0	63.9

30	564	73.3	31.5	57.1
	295	73.3	32.0	57.3
	58	80.3	43.5	66.0

a) average prediction accuracies obtained from 5-fold cross validation, b) steps(preprocessing; ranking and backward selection;

Monte Carlo simulated annealing)