Supporting Information

JRgui: A Python Program of Joback and Reid Method

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1. A list of molecular descriptors available in JRgui

The PDF version of RDKit documentation (http://www.rdkit.org/RDKit_Docs.current.pdf, created on October 8th, 2017) summarizes a list of available descriptors (pages 63-65). In addition to those, the eleven physical properties predicted by JR method, and crystalline/amorphous solubility by General Solubility Equations (1 for original GSE; 2 for modified version) are exported. Finally a list of 85 fragment descriptors is also calculated (fr_Al_COO to fr_urea, last 85 columns in output csv file) and summarized in Table S1.

Table S1: The 85 molecular descriptors for describing fragments of molecule. (see also FragmentDescriptors.csv in the RDKit installation folder.)

Oxygen (15)	
fr_Al_OH	Number of aliphatic hydroxyl groups
fr_Ar_OH	Number of aromatic hydroxyl groups
fr_methoxy	Number of methoxy groups -OCH3
fr_oxime	Number of oxime groups
fr_ester	Number of esters
fr_Al_COO	Number of aliphatic carboxylic acids
fr_Ar_COO	Number of Aromatic carboxylic acide
fr_C_O	Number of carbonyl O
fr_C_O_noCOO	Number of carbonyl O, excluding COOH
fr_COO	Number of carboxylic acids
fr_COO2	Number of carboxylic acids
fr_ketone	"Number of ketones"
fr_ether	Number of ether oxygens (including phenoxy)
fr_phenol	Number of phenols
fr_aldehyde	Number of aldehydes
Nitrogen (27)	
fr_quatN	Number of quarternary nitrogens
fr_NH2	Number of Primary amines
fr_NH1	Number of Secondary amines
fr_NH0	Number of Tertiary amines
fr_Ar_N	Number of aromatic nitrogens
fr_ArN	Number of N functional groups attached to aromatics
fr_Ar_NH	Number of aromatic amines
fr_aniline	Number of anilines
fr_Imine	Number of Imines
fr_nitrile	Number of nitriles
fr_hdrzine	Number of hydrazine groups
fr_hdrzone	Number of hydrazone groups" Includes cyclic hydrazones
fr_nitroso	Number of nitroso groups
fr_N_O	Number of hydroxylamine groups
fr_nitro	Number of nitro groups
fr_azo	Number of azo groups
fr_diazo	Number of diazo groups
fr_azide	Number of azide groups
fr_amide	Number of amides
fr_priamide	Number of primary amides
fr_amidine	Number of amidine groups
fr_guanido	Number of guanidine groups
fr_Nhpyrrole	Number of H-pyrrole nitrogens
fr_imide	Number of imide groups
fr_isocyan	Number of isocyanates
fr_isothiocyan	Number of isothiocyanates
fr_thiocyan	Number of thiocyanates

Halogens (2)	
fr_halogen	Number of halogens
fr_alkyl_halide	Number of alkyl halides
Sulfurs (5)	
fr_sulfide	Number of thioether
fr_SH	Number of thiol groups
fr_sulfone	Number of sulfone groups
fr_sulfonamd	Number of sulfonamides
fr_prisulfonamd	Number of primary sulfonamides
Miscellaneous Functional Groups (19)	
fr_barbitur	Number of barbiturate groups
fr_urea	Number of urea groups
fr_term_acetylene	Number of terminal acetylenes
fr_imidazole	Number of imidazole rings
fr_furan	Number of furan rings
fr_thiophene	Number of thiophene rings
fr_thiazole	Number of thiazole rings
fr_oxazole	Number of oxazole rings
fr_pyridine	Number of pyridine rings
fr_piperdine	Number of piperdine rings
fr_piperzine	Number of piperzine rings
fr_morpholine	Number of morpholine rings
fr_lactam	Number of beta lactams
fr_lactone	Number of cyclic esters (lactones
fr_tetrazole	Number of tetrazole rings
fr_epoxide	Number of epoxide rings
fr_unbrch_alkane	Number of unbranched alkanes of at least 4 members (excludes halogenated alkanes)
fr_bicyclic	Bicyclic
fr_benzene	Number of benzene rings
Phosphates (2)	
fr_phos_acid	Number of phosphoric acid groups
fr_phos_ester	Number of phosphoric ester groups
Topliss Metabolism (15)	
fr_nitro_arom	Number of nitro benzene ring substituents
fr_nitro_arom_nonortho	Number of non-ortho nitro benzene ring substituents
fr_dihydropyridine	Number of dihydropyridines
fr_phenol_noOrthoHbond	Number of phenolic OH excluding ortho intramolecular Hbond substituents
fr_Al_OH_noTert	Number of aliphatic hydroxyl groups excluding tert-OH
fr_benzodiazepine	Number of benzodiazepines with no additional fused rings
fr_para_hydroxylation	Number of para-hydroxylation sites
fr_allylic_oxid	Number of allylic oxidation sites excluding steroid dienone
fr_aryl_methyl	Number of aryl methyl sites for hydroxylation
fr_Ndealkylation1	Number of XCCNR groups
fr_Ndealkylation2	Number of tert-alicyclic amines (no heteroatoms)
fr_alkyl_carbamate	Number of alkyl carbamates (subject to hydrolysis)
fr_ketone_Topliss	Number of ketones excluding diaryl
fr_ArN	Number of N functional groups attached to aromatics
fr_HOCCN	Number of C(OH)CCN-Ctert-alkyl or C(OH)CCNcyclic