8 Supplementary Material

Abbreviations	***Module***	***Name***	***Constructor***	***Description***
ABC	$ABCIndex$	ABC	$ABCIndex()$	$atom-bond\ connectivity\_index$
Top_dia	$Topological\ Index$	$Diameter$	$Diameter()$	$topological\_diameter$
Top_Shape	$Topological\ Index$	$TopoShapeIndex$	$TopologicalShapeIndex()$	$topological\_shape\_index$
$Walk\_C$	$WalkCount$	$MWC01$	$WalkCount(1, False, False)$	$walk\_count\_(leg-1)$
Top_Charge	$Topological\ Charge$	$GGI1$	$TopologicalCharge(`raw', 1)$	$1-ordered\ raw\ topological\_charge$
Top_PSA	$TopoPSA$	$TopoPSA(NO)$	$TopoPSA(True)$	$topological\_polar\ surface\_area\ (use\_only\_nitrogen\ and\_oxygen)$
S_log	$SLogP$	$SLogP$	$SLogP()$	$Wildman-Crippen\_LogP$
R_B_C	$RotatableBond$	$nRot$	$RotatableBondsCount()$	$rotatable\_bonds\_count$
$Wiener$	$WienerIndex$	$WPath$	$WienerIndex(False)$	$Wiener\_index$
$Z1$	$ZagrebIndex$	$Zagreb1$	$ZagrebIndex(1, 1)$	$Zagreb\_index\ (version\_1)$
$Z2$	$ZagrebIndex$	$Zagreb2$	$ZagrebIndex(2, 1)$	$Zagreb\_index\ (version\_2)$
$mZagreb2$	$ZagrebIndex$	$mZagreb2$	$ZagrebIndex(2, -1)$	$modified\_Zagreb\ index\_(version\_2)$
$Acid\_Base$	$AcidBase$	$nAcid$	$AcidicGroupCount()$	$acidic\ group\ count$
$Arom\_atic$	$Aromatic$	$nAromAtom$	$AromaticAtomsCount()$	$aromatic\ atoms\ count$
$Arom\_atic\_1$	$Aromatic$	$nAromBond$	$AromaticBondsCount()$	$aromatic\ bonds\ count$
$Atom\_Count$	$AtomCount$	$nAtom$	$AtomCount(`Atom')$	$number\ of\ all\ atoms$
$Atom\_Count\_1$	$AtomCount$	$nHeavyAtom$	$AtomCount(`HeavyAtom')$	$number\ of\ heavy\ atoms$
$Atom\_Count\_2$	$AtomCount$	$nSpiro$	$AtomCount(`Spiro')$	$number\ of\ spiro\ atoms$
$Atom\_Count\_3$	$AtomCount$	$nBridgehead$	$AtomCount(`Bridgehead')$	$number\ of\ bridgehead\ atoms$
$Atom\_Count\_4$	$AtomCount$	$nHetero$	$AtomCount(`Hetero')$	$number\ of\ hetero\ atoms$
$Atom\_Count\_5$	$AtomCount$	nX	$AtomCount(`X')$	$number\ of\ halogen\ atoms$
$Auto\_correlation$	$Autocorrelation$	$ATS0m$	$ATS(0, `m')$	$moreau-broto\ autocorrelation\ of\ lag\ 0\ weighted\ by\ mass$
$Auto\_correlation\_1$	$Autocorrelation$	$AATS0m$	$AATS(0, `m')$	$averaged\ moreau-broto\ autocorrelation\ of\ lag\ 0\ weighted\ by\ mass$
$Auto\_correlation\_2$	$Autocorrelation$	$ATSC0m$	$ATSC(0, `m')$	$centered\ moreau-broto\ autocorrelation\ of\ lag\ 0\ weighted\ by\ mass$
$Auto\_correlation\_3$	$Autocorrelation$	$AATSC0m$	$AATSC(0, `m')$	$averaged\ and\ centered\ moreau-broto\ autocorrelation\ of\ lag\ 0\ weighted\ by\ mass$
$Auto\_correlation\_4$	$Autocorrelation$	$MATS1m$	$MATS(1, `m')$	$moran\ coefficient\ of\ lag\ 1\ weighted\ by\ mass$

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Auto correlation_5	*Autocorrelation*	*GATS1m*	*GATS*(1, '*m*')	*geary coefficient oflag 1 weighted by mass*
Balaban_J	*BalabanJ*	*BalabanJ*	*BalabanJ*()	*Balaban's J index*
Bertz_CT	*BertzCT*	*BertzCT*	*BertzCT*()	*Bertz CT*
Bond_Count	*BondCount*	*nBonds*	*BondCount*('*any*', *False*)	*number of all bonds in non − kekulized structure*
Carbon_Types	*CarbonTypes*	*C1SP3*	*CarbonTypes*(1, 3)	*SP3 carbon bound to 1 other carbon*
Constitutional	*Constitutional*	*Sv*	*ConstitutionalSum*('*v*')	*sum of constitutional weighted by vdw volume*
Constitutional_1	*Constitutional*	*Mv*	*ConstitutionalMean*('*v*')	*mean of constitutional weighted by vdw volume*
Eccentric Connectivity Index	*Eccentric Connectivity Index*	*ECIndex*	*EccentricConnectivityIndex*()	*eccentric connectivity index*
E_State	*EState*	*NsLi*	*AtomTypeEState*('*count*', '*sLi*')	*number of sLi*
Fragment Complexity	*Fragment Complexity*	*fragCpx*	*FragmentComplexity*()	*fragment complexity*
Frame_work	*Framework*	*fMF*	*Framework*()	*molecular framework ratio*
Hydrogen Bond	*HydrogenBond*	*nHBAcc*	*HBondAcceptor*()	*number of hydrogen bond acceptor*
Hydrogen Bond_1	*HydrogenBond*	*nHBDon*	*HBondDonor*()	*number of hydrogen bond donor*
Information Content	*Information Content*	*IC0*	*InformationContent*(0)	$0 - ordered$ *neighborhood information content*
Information Content 1	*Information Content*	*IC1*	*InformationContent*(1)	1 *ordered neighborhood information content*
Information Content 2	*Information Content*	*IC2*	*InformationContent*(2)	$2 - ordered$ *neighborhood information content*
Information Content 4	*Information Content*	*IC4*	*InformationContent*(4)	$4 - ordered$ *neighborhood information content*
Information Content_5	*Information Content*	*IC5*	*InformationContent*(5)	$5 - ordered$ *neighborhood information content*
Information Content_6	*Information Content*	*IC6*	*InformationContent*(6)	$6 - ordered$ *neighborhood information content*
Lip_inski	*Lipinski*	*Lipinski*	*Lipinski*()	*Lipinski rule of five*
Lip_inski_1	*Lipinski*	*GhoseFilter*	*GhoseFilter*()	*Ghose filter*
Log_S	*LogS*	*FilterItLogS*	*LogS*()	$Filter - it$ *LogS*
McGowan Volume	*McGowan Volume*	*VMcGowan*	*McGowanVolume*()	*McGowan volume*
Moe_Type	*MoeType*	*LabuteASA*	*LabuteASA*()	*Labute's Approximate Surface Area*
Moe_Type_1	*MoeType*	*PEOE_VSA1*	*PEOE_VSA*(1)	*MOE_Charge_VSA_Descriptor*1 $(-inf < x < -0.30)$
Moe_Type_2	*MoeType*	*PEOE_VSA2*	*PEOE_VSA*(2)	*MOE_Charge_VSA_Descriptor*2 $(-0.30 <= x < -0.25)$
Moe_Type_3	*MoeType*	*PEOE_VSA3*	*PEOE_VSA*(3)	*MOE_Charge_VSA_Descriptor*3 $(-0.25 <= x < -0.20)$
Moe_Type_4	*MoeType*	*PEOE_VSA4*	*PEOE_VSA*(4)	*MOE_Charge_VSA_Descriptor*4 $(-0.20 <= x < -0.15)$
Moe_Type_5	*MoeType*	*PEOE_VSA5*	*PEOE_VSA*(5)	*MOE_Charge_VSA_Descriptor*5 $(-0.15 <= x < -0.10)$
Path_Count	*PathCount*	*MPC2*	*PathCount*(2, *False*, *False*, *False*)	$1 - ordered$ *path count*
Polariz_ability	*Polarizability*	*apol*	*APol*(*False*)	*atomic polarizability*
Polariz_ability_1	*Polarizability*	*bpol*	*BPol*(*False*)	*bond polarizability*
Ring_Count	*RingCount*	*nRing*	*RingCount*(*None*, *False*, *False*, *None*, *None*)	*ring count*
MW	*Weight*	*MW*	*Weight*(*True*, *False*)	*exact molecular weight*