MYCOTOXINS:MOLECULAR MODELING & CLASSIFICATION

P.URBANIAK

ABSTRACT

Mycotoxins are known for their heigh toxicity.In that study
1) We modelize conformations of 28 mycotoxins with Prochemist, a molecular modeling & Qsar package using the wavelet transform as a novel descriptor
2) and classify the 28 molecules according to their wavelet coefficients with the molecular machine,an unsupervised data classifier.

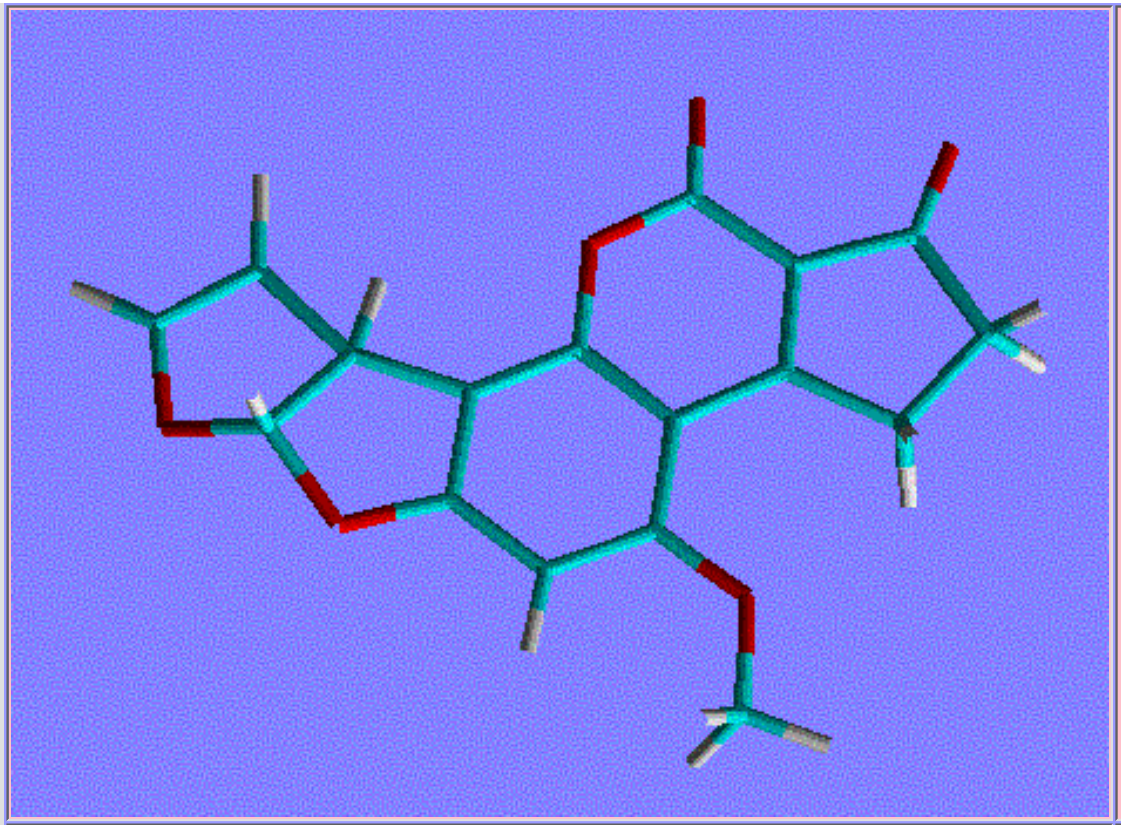
The full set

Molecules_Name	Formula	MW
Mycotoxin 81	C22H1807	394.374
Insariotoxin	C24H34O9	466.521
Trans-Zearalenone	C18H22O5	318.364
Mycotoxin HT 2	C22H32O8	424.485
Zenone	C18H22O5	318.364
TR-2 Mycotoxin	C22H27N3O6	429.466
Secalonic acid D-	C32H30O14	638.572
Afbi	C17H12O6	312.274
Aflatoxin B1	C17H12O6	312.274
T-2 Toxin	C24H34O9	466.521

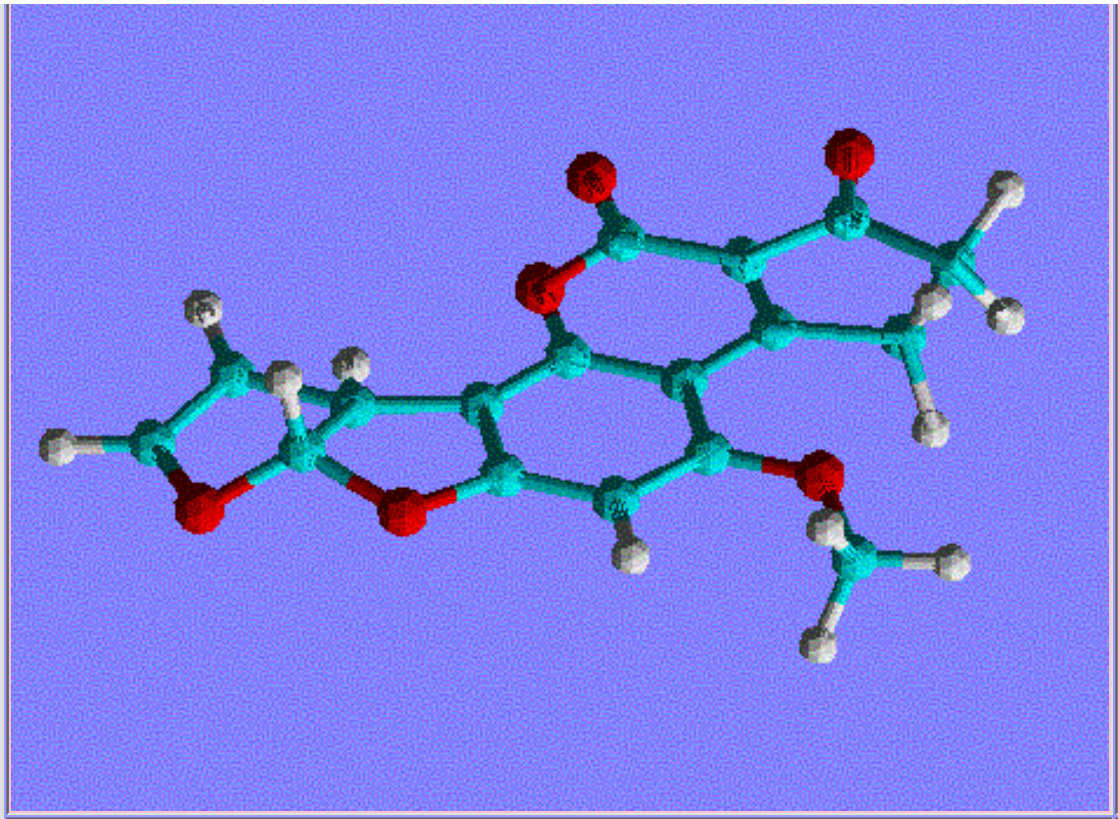
Sterigmatocysin	C18H12O6	324.284
Tenuazonic Acid	C10H15No3	197.231
Citrinin	C13H14O5	250.247
Penicillic acid	C8H10O4	170.163
Patulin	C7H6O4	154.12
Antimycin A1	C27H38N2O9	534.599
Cytochalasin D	C30H37No6	507.618
Trichodermin	C17H24O4	292.37
Phalloidine	C35H48N8O11S	788.869
Alpha-amanitin	C39H54N10O14S	918.971
Phomin	C29H37NO5	479.608
Trichoderonin	C17H24O4	292.37
Trichodermin	C17H24O4	292.37
Trichodermol	C15H22O3	250.333
Pramuscimol	C5H8N2O5	176.127
Cytochalasin	C30H37NO6	507.618
Gliotoxin	C13H14N2O4S2	326.393
Phalloidine	C35H48N8O11S	788.869
Muscimol	C4H6N2O2	114.103
Alpha-Amanitin	C39H54N10O14S	918.971
Ibotenic Acid-	C5H6N2O4	158.112

PART I:Aflatoxin Molecular Modeling

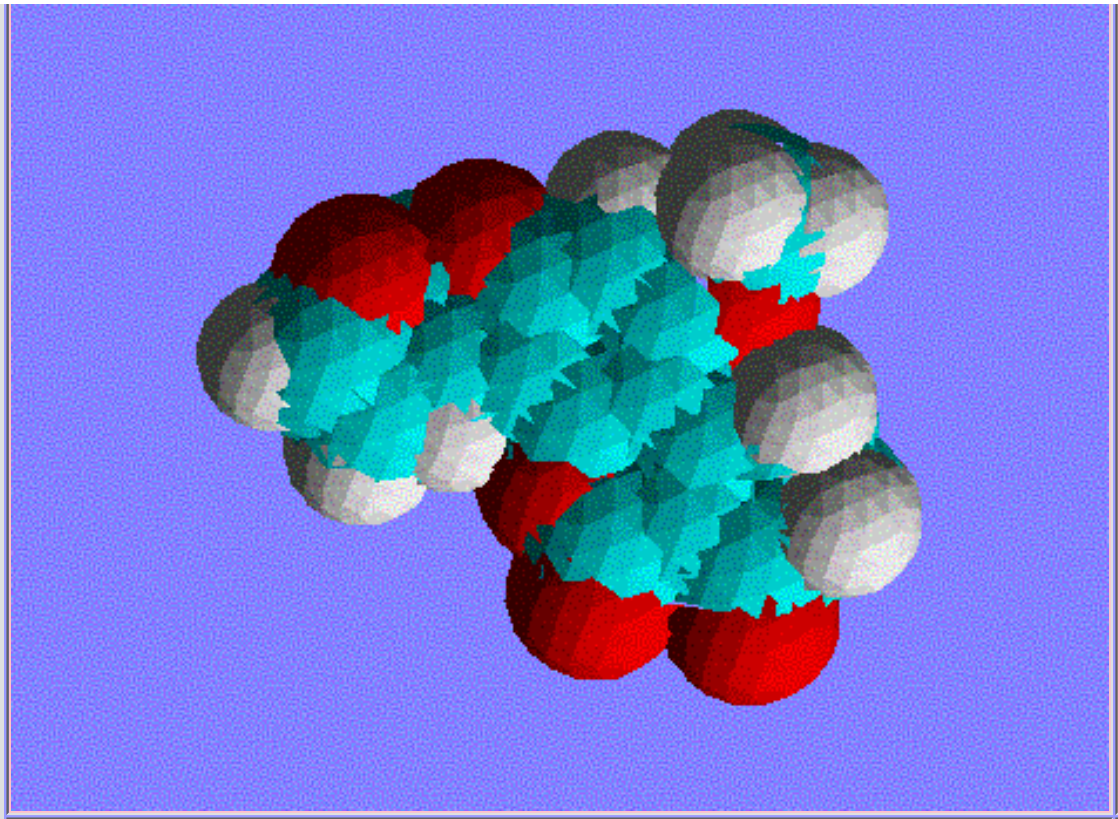
Image	View



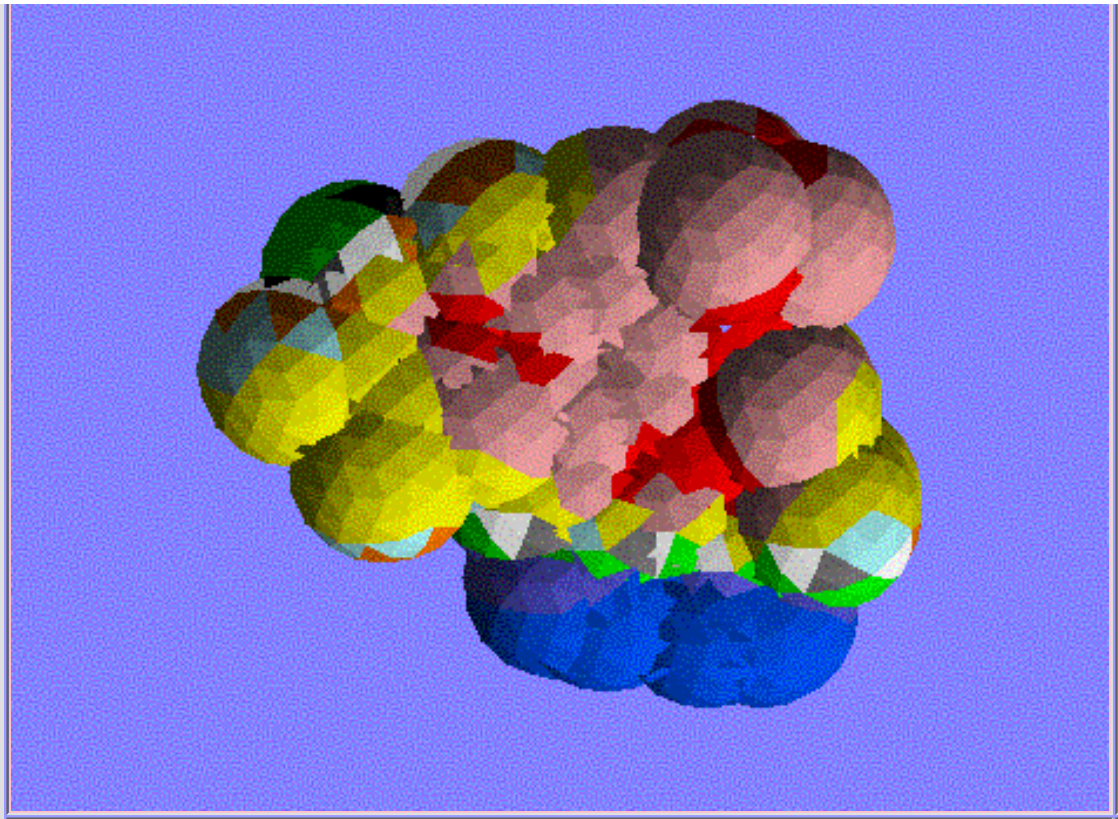
Stick(Prochemist 6.4)



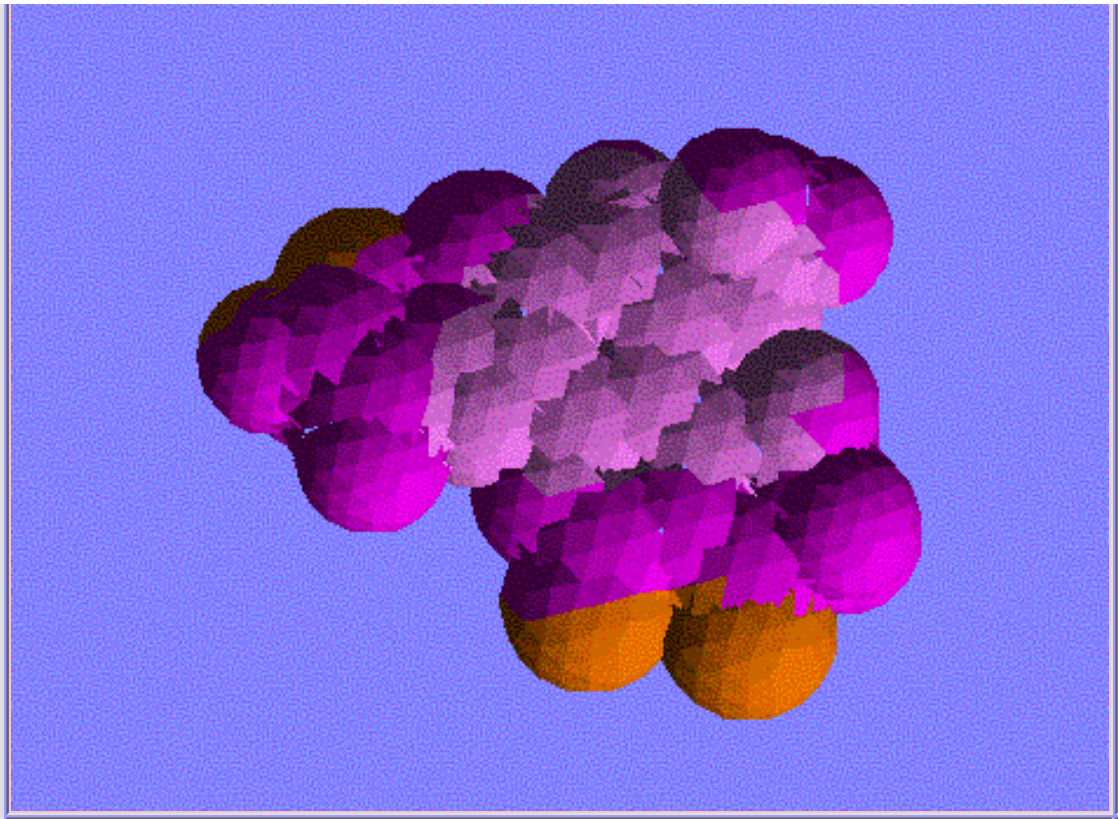
Ball & Stick(Type dependent radius)



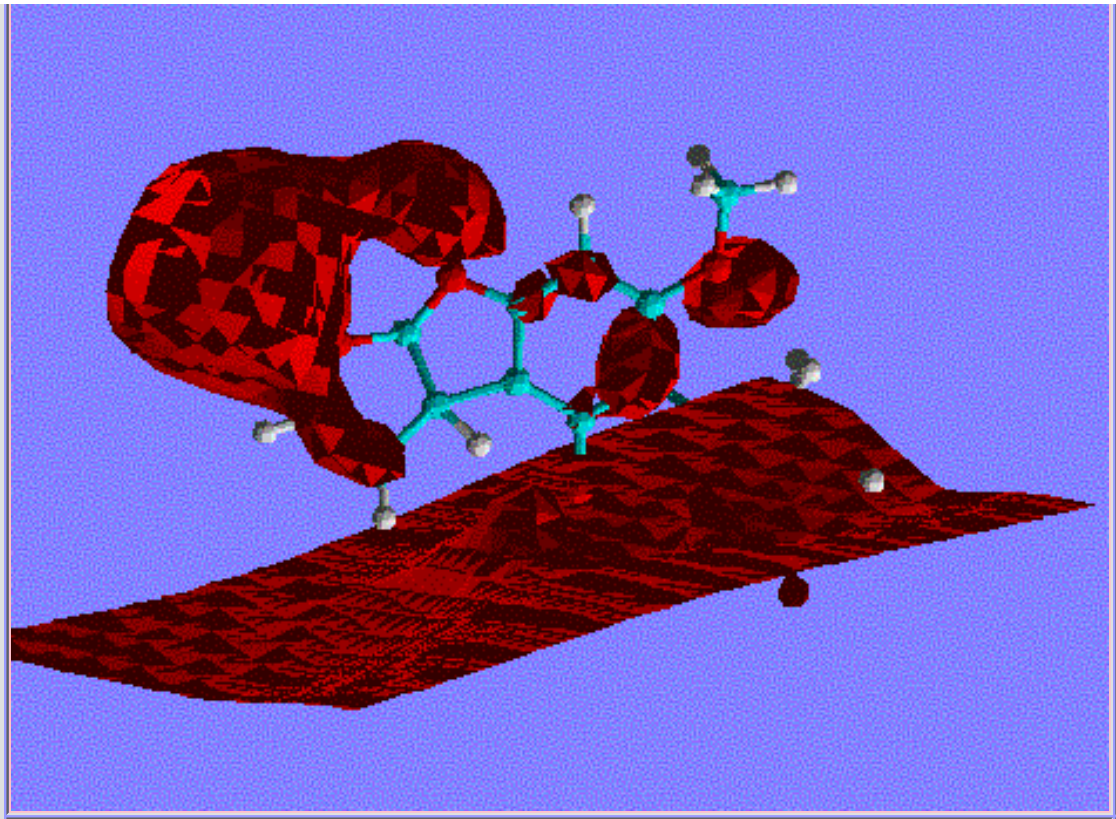
Van Der Walls Surface



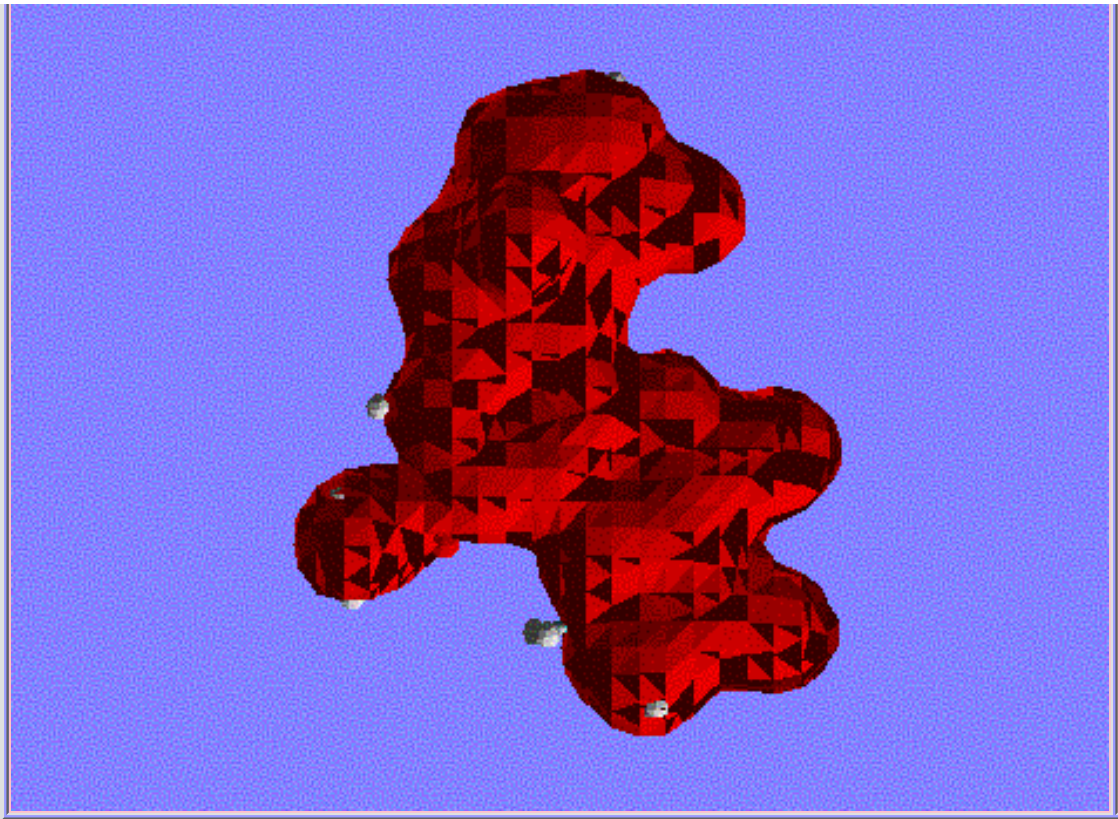
Electrostatic Potential(Charge=2Ang)



Molecular Lipophilic Potential(Equation $fi/_{(1+di)}$

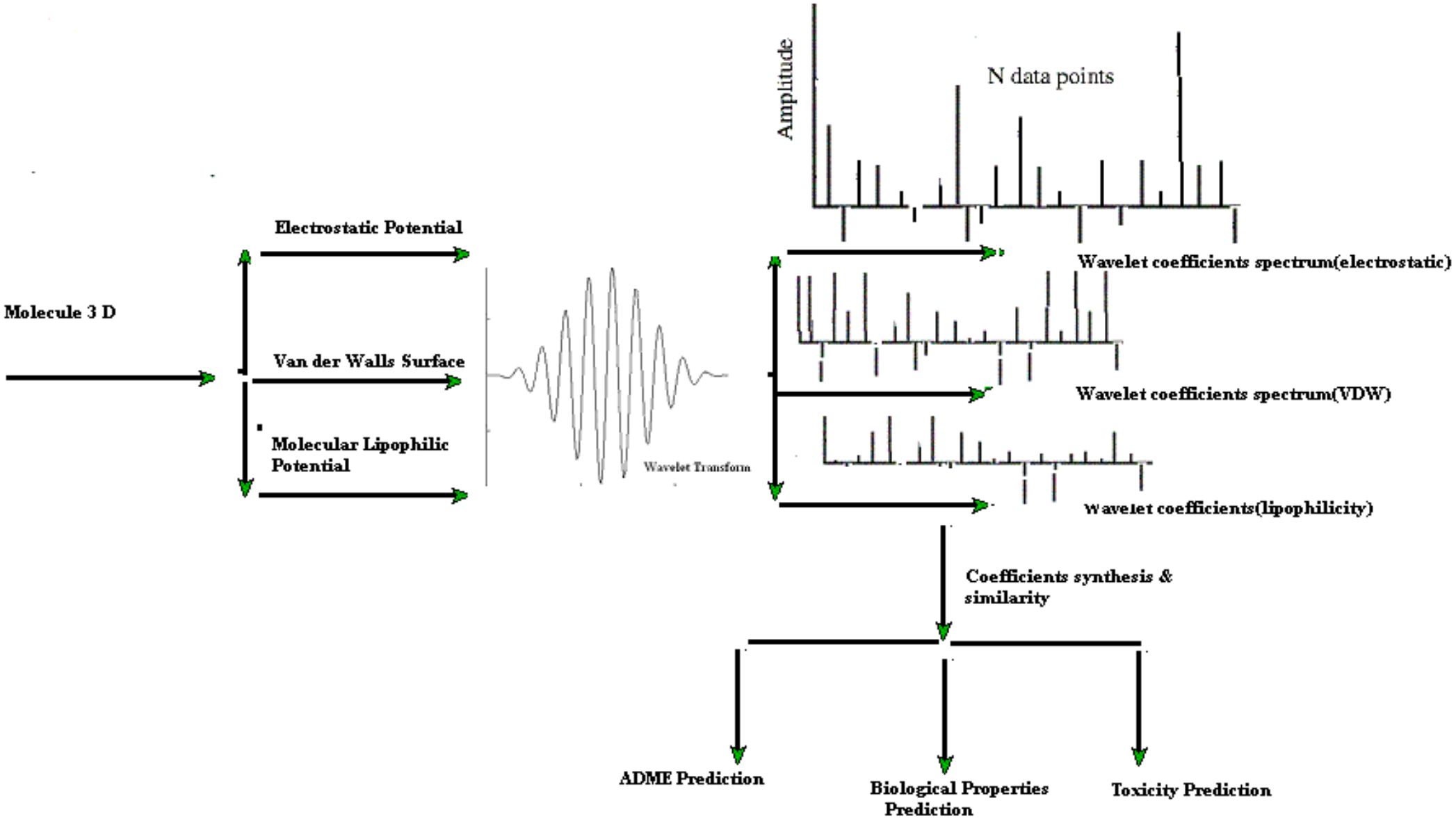


Electrostatic Potential :isovalue E>10 ev



Electronic Density(Mopac 6.0 Pm3/Force/Gradient 1.0)

PART II Wavelet Transform



ProChemist 6.4

(ADME= Absorption Distribution Metabolism Elimination)

PART IIIClassification

HOME:

Last revised:24/11/2005