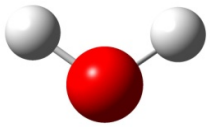
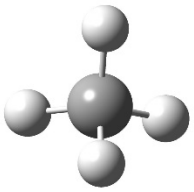
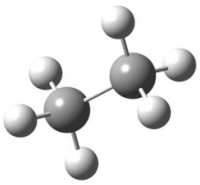
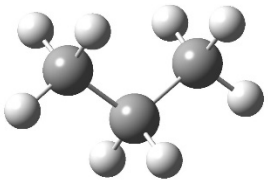
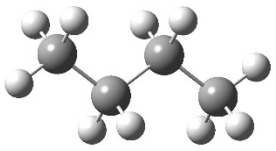
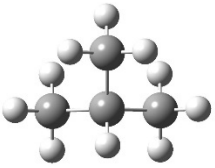
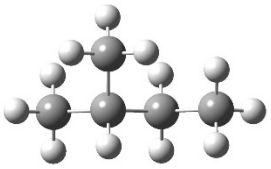
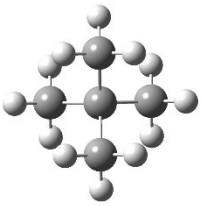
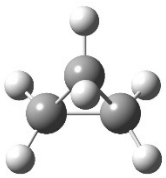
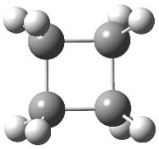
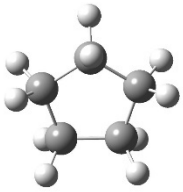
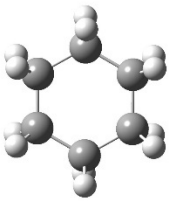
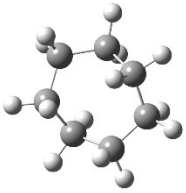
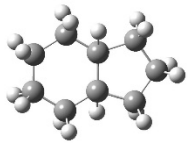
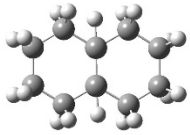
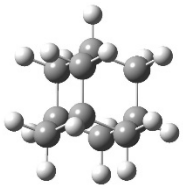
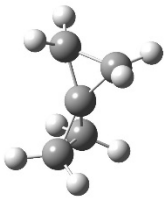
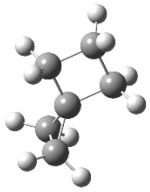
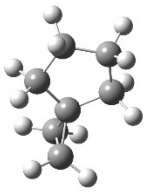
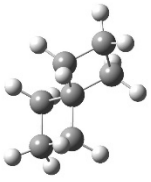
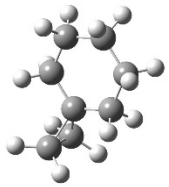
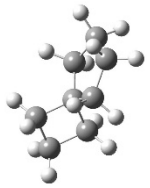
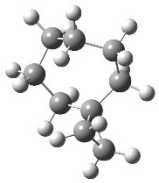
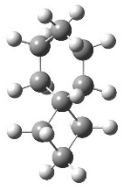
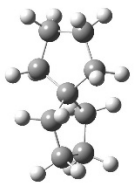
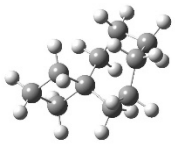
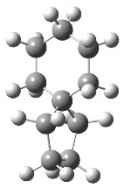
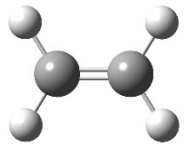
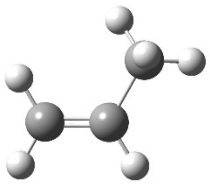
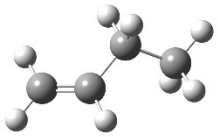
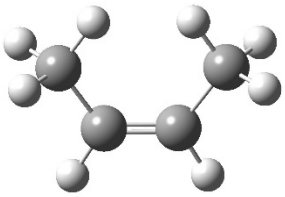
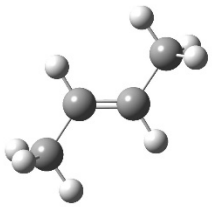
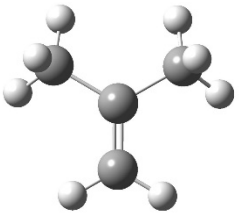
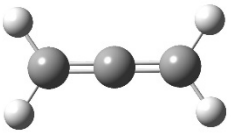
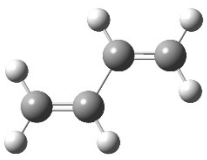
Fragment Molecules

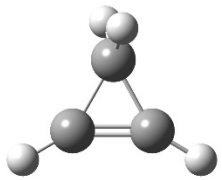
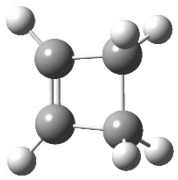
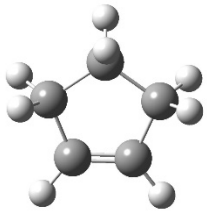
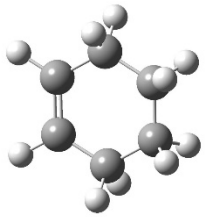
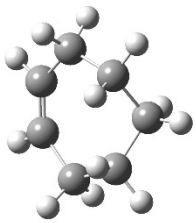
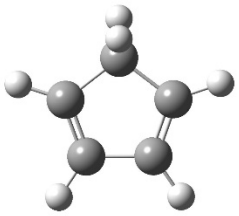
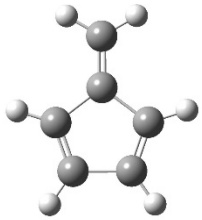
Prio	*Abbreviation*	*Name*	*Chemical name*	*Structure Diagram*
Smallest (basic) Fragment Molecule				
1	H20	Water	Water	
Alkanes				
2	Me	Methane	Methane	
5	Et	Ethane	Ethane	
8	Pr	Propane	Propane	
9	Bu	Butane	Butane	
	IsoBu	Isobutane	Isobutane	

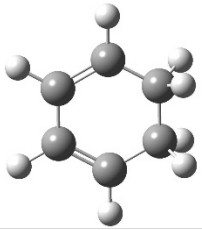
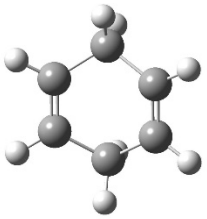
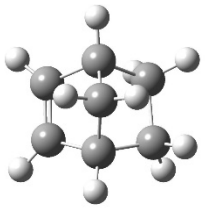
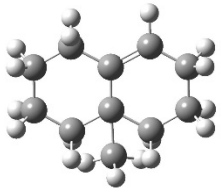
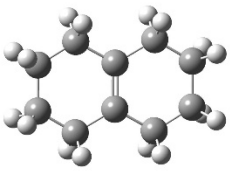
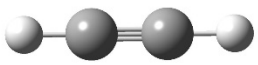
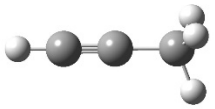
	IsoPe	Isopentane	Isopentane	
	NeoPe	Neopentane	Neopentane	
Cycloalkanes				
	CycPr	Cyclopropane	Cyclopropane	
	CycBu	Cyclobutane	Cyclobutane	
	CycPe	Cyclopentane	Cyclopentane	
	CycHex	Cyclohexane	Cyclohexane	
	CycHep	Cycloheptane	Cycloheptane	

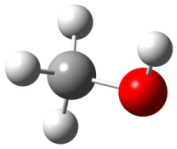
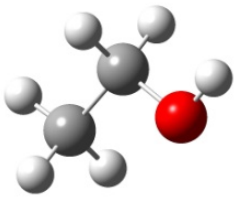
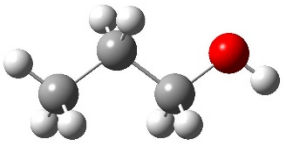
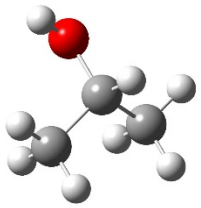
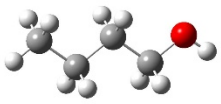
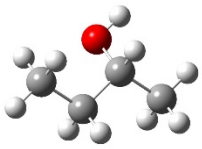
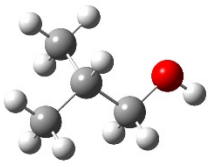
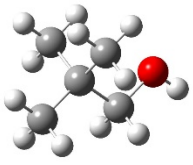
	Hydrindane	Hydrindane	Hydrindane	
	Decalin	Decalin	Decalin	
	Adamantane	Adamantane	Adamantane	
Spiro compounds				
	Spiro22Pe	Spiropentane22	Spiro(2.2)pentane	
	Spiro23Hex	Spirohexane23	Spiro(2.3)hexane	
	Spiro24Hep	Spiroheptane24	Spiro(2.4)heptane	
	Spiro33Hep	Spiroheptane33	Spiro(3.3)heptane	

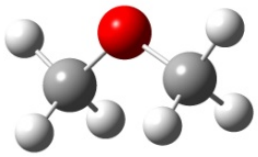
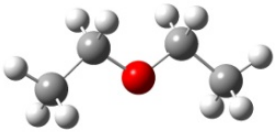
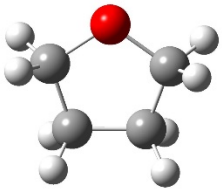
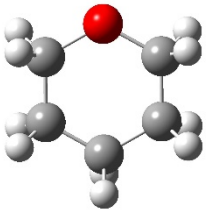
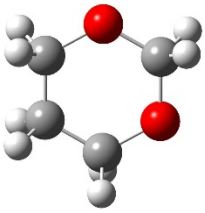
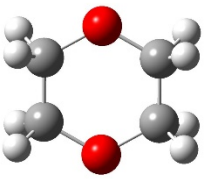
	Spiro25Oct	Spirooctane25	Spiro(2.5)octane	
	Spiro34Oct	Spirooctane34	Spiro(3.4)octane	
	Spiro26Non	Spirononane26	Spiro(2.6)nonane	
	Spiro35Non	Spirononane35	Spiro(3.5)nonane	
	Spiro44Non	Spirononane44	Spiro(4.4)nonane	
	Spiro36Dec	Spirodecane36	Spiro(3.6)decane	
	Spiro45Dec	Spirodecane45	Spiro(4.5)decane	
Alkenes				

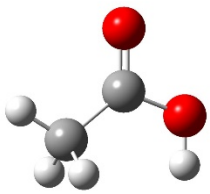
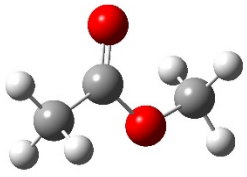
	Ethene	Ethene	Ethene	
	Propene	Propene	1-Propene	
	Butene	Butene	1-Butene	
10	CisButene	CisButene	(Z)-2-Butene	
	TrButene	TransButene	(E)-2-Butene	
	IsoButene	IsoButene	2-Methylpropene	
	Propadiene	Propadiene	Propadiene	
	Butadiene	Butadiene	Buta-1,3-diene	

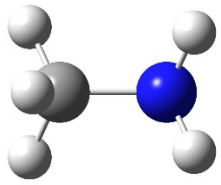
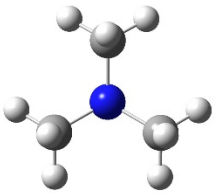
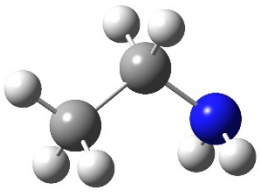
Cycloalkenes				
	CycPropene	Cyclopropene	Cyclopropene	
	CycButene	Cyclobutene	Cyclobutene	
	CycPentene	Cyclopentene	Cyclopentene	
	CycHexene	Cyclohexene	Cyclohexene	
	CycHeptene	Cycloheptene	Cycloheptene	
	CycPentDi	Cyclopentadiene	Cyclopentadiene	
	Fulvene	Fulvene	5-Methylene-1,3-cyclopen-tadiene	

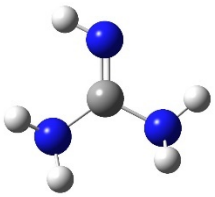
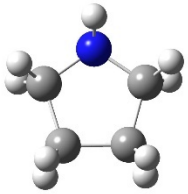
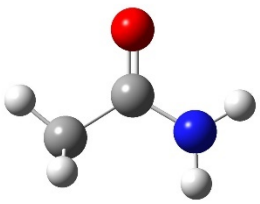
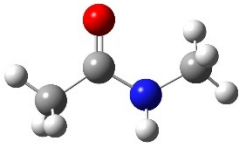
	CycHexDi13	Cyclohexadiene13	1,3-Cyclohexadiene	
	CycHexDi14	Cyclohexadiene14	1,4-Cyclohexadiene	
	Norbornene	Norbornene	Norbornene	
	MeOcthNaph	MethylOcatahydronaphtha-lene	4a-methyl-1,2,3,4,4a,5,6,7-ocatahydronaphthalene	
	OctHydNaph	Ocatahydronaphthalene	Ocatahydronaphthalene	
Alkynes				
	Ethyne	Ethyne	Ethyne	
	Propyne	Propyne	Propyne	
Alcohols				

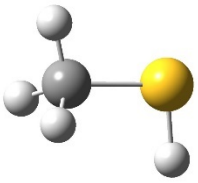
3	MeOH	Methanol	Methanol	
6	EtOH	Ethanol	Ethanol	
11	PrOH	Propanol	1-Propanol	
	Pr2OH	Propanol2	2-Propanol	
	BuOH	Butanol	1-Butanol	
	Bu2OH	Butanol2	2-Butanol	
	IsoBuOH	Isobutanol	2-Methyl-1-propanol	
	TBuOH	TertButanol	2-Methyl-2-propanol	

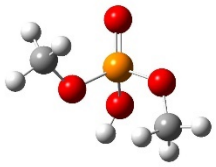
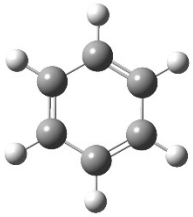
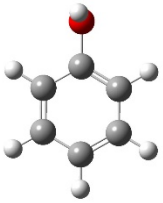
Ethers				
4	Me2O	Dimethylether	Methoxymethane	
7	Et2O	Diethylether	Ethoxyethane	
	EtMeO	Ethylmethylether	Methoxyethane	
Cyclic Ethers				
	THF	Tetrahydrofuran	Tetrahydrofuran	
	THP	Tetrahydropyran	Tetrahydropyran	
	Dioxane13	Dioxane13	1,3-Dioxane	
	Dioxane14	Dioxane14	1,4-Dioxane	
Aldehydes				
	HCHO	Formaldehyde	Formaldehyde	
	AcCHO	Acetaldehyde	Ethanal	
	PrCHO	Propionaldehyde	Propanal	

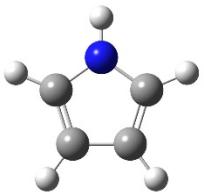
	ButCHO	Butyraldehyde	Butanal	
	CrotCHO	Crotonaldehyde	(E)-2-Butenal	
	SCHO	Thioformaldehyde	Thioformaldehyde	
	BuOHCHO	AcetAldol	3-Hydroxybutanal	
Ketones				
	AcCO	Acetone	2-Propanone	
	ButCO	Butanone2	2-Butanone	
	MeVinCO	Methylvinylketone	3-Buten-2-on	
	AcAcCO	Acetylacetone	2,4-Pentadione	
Cyclic Ketones				
	CycHexCO	Cyclohexanone	Cyclohexanone	
	OQuinone	OrthoQuinone	1,2-Benzoquinone	
	PQuinone	ParaQuinone	1,4-Benzoquinone	
	Camphor	Camphor	Camphor	
Carboxylic Acids				
	FCOOH	FormicAcid	Formic Acid	
	FCOON	FormicAcidN	Formic Acid (-)	
12	HAc	AceticAcid	Acetic Acid	
	HAcN	AceticAcidN	Acetic Acid (-)	
	PrCOOH	PropanoicAcid	Propanoic Acid	
	PrCOON	PropanoicAcidN	Propanoic Acid (-)	
Carboxylic Acid Ester				
13	MeAc	MethylAcetate	Methyl Acetate	
	EtAc	EthylAcetate	Ethyl acetate	
	EtAcAc	Ethyl acetoacetate	Ethyl 3-oxobutanoate	
	Butyrolact	Butyrolactone	γ-Butyrolactone	
	Valerolact	Valerolactone	δ-Valerolactone	
Carboxylic Acid Anhydrides				
	AcCOOAc	AceticAnhydride	Acetic Anhydride	
	ProCOOPr	PropionicAnhydride	Propionic Anhydride	

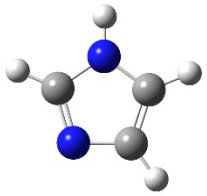
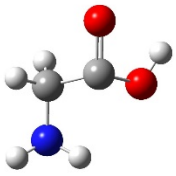
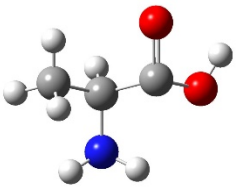
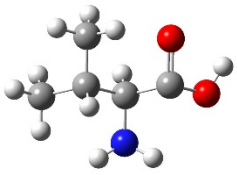
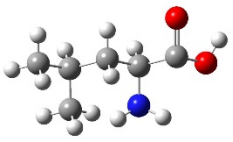
	AcCOOPro	AceticPropanoicAnhydride	Acetic Propanoic Anhydride	
	AcCOOBut	AceticButyicAnhydride	Acetic Butyic Anhydride	
	SuccCOO	SuccinicAnhydride	Succinic Anhydride	
	MaleicCOO	MaleicAnhydride	Maleic Anhydride	
(Cyclic) Sugars				
	Glucose	Glucose	α-D-Glucopyranose	
	Ribose	Ribose	α-D-Ribofuranose	
	DeORibose	Deoxyribose	2-Deoxy-D-ribose	
	Fructose	Fructose	D-fructofuranose	
Nitrogen Compounds				
	NH3	Ammonia	Ammonia	
	NH4P	Ammonium	Ammonium (+)	
	NitricAcid	NitricAcid	Nitric acid	
	NO3N	Nitrate	Nitrate	
Amines				
14	MeNH2	Methylamine	Methanamine	
	MeNH2P	MethylamineP	Methanamine (+)	
	DiMeNH	Dimethylamine	Dimethylamine	
	DiMeNHP	DimethylamineP	Dimethylamine (+)	
15	TriMeN	Trimethylamine	N,N-Dimethylmethanamine	
	TriMeNP	TrimethylamineP	N,N-Dimethylmethanamine (+)	
16	EtNH2	Ethylamine	Ethanamine	
	EtNH2P	EthylamineP	Ethanamine (+)	
	EtMeNH	Ethylmethylamine	N-Methylethanamine	
	EtMeNHP	EthylmethylamineP	N-Methylethanamine (+)	
	DiEtNH	Diethylamine	N-Ethylethanamine	
	DiEtNHP	DiethylamineP	N-Ethylethanamine (+)	

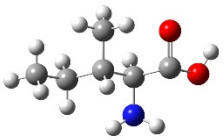
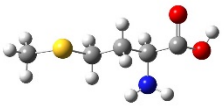
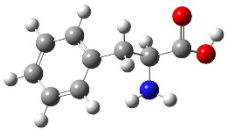
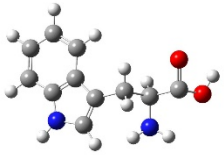
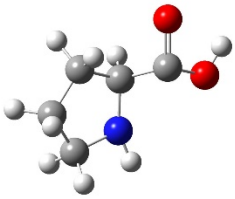
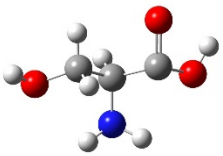
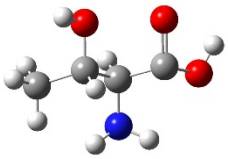
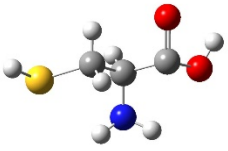
	PrNH2	Propylamine	1-Propanamine	
	PrNH2P	PropylamineP	1-Propanamine (+)	
	IsoPrNH2	Isopropylamine	2-Propanamine	
	IsoPrNH2P	IsopropylamineP	2-Propanamine (+)	
	BuNH2	Butylamine	1-Butanamine	
	BuNH2P	ButylamineP	1-Butanamine (+)	
	Bu2NH2	Butylamine2	2-Butanamine	
	Bu2NH2P	Butylamine2P	2-Butanamine (+)	
	IsoBuNH2	Isobutylamine	2-Methyl-1-propanamine	
	IsoBuNH2P	IsobutylamineP	2-Methyl-1-propanamine (+)	
	TertBuNH2	TertButylamine	2-Amino-2-methylpropane	
	TertBuNH2P	TertButylamineP	2-Amino-2-methylpropane (+)	
17	Guanidine	Guanidine	Guanidine	
	GuanidineP	GuanidineP	Guanidine (+)	
Cyclic Amines				
18	Azolid	Azolidine	Pyrrolidine	
	AzolidP	AzolidineP	Pyrrolidine (+)	
	Quinuclid	Quinuclidine	Quinuclidine	
	QuinuclidP	QuinuclidineP	Quinuclidine (+)	
	Urotropine	Urotropine	Urotropine	
Carboxylic Acid Amides				
19	AcNH2	Acetamide	Acetamide	
20	MeAcNH	Methylacetamide	N-Methyl acetamide	

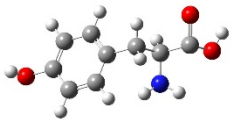
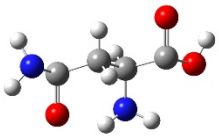
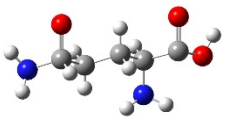
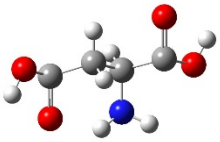
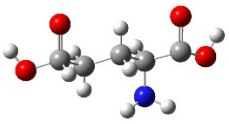
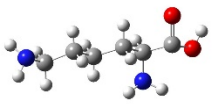
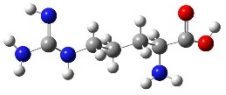
Heterocyclic Compounds				
	Oxazoline	Oxazoline	Oxazoline	
	Succinimid	Succinimide	Succinimide	
Sulfur Compounds				
	H2SO4	SulfuricAcid	Sulfuric acid	
	MeSO3	MethylSulfuricAcid	(Mono)MethylSulfuric acid	
Thiols				
21	MeSH	Methanethiol	Methanethiol	
	MeSHN	MethanethiolN	Methanethiol (-)	
	EtSH	Ethanethiol	Ethanethiol	
	EtSHN	EthanethiolN	Ethanethiol (-)	
	PrSH	Propanethiol	1-Propanethiol	
	PrSHN	PropanethiolN	1-Propanethiol (-)	
	Pr2SH	Propanethiol2	2-Propanthiol	
	Pr2SHN	Propanethiol2N	2-Propanthiol (-)	
	Buten2SH	Butenthiol2	But-2-en-1-thiol	
	Buten2SHN	Butenthiol2N	But-2-en-1-thiol (-)	
Thioether				
	Me2S	Dimethylsulfide	Dimethyl sulfide	
	Et2S	Diethylsulfide	Diethyl sulfide	
	EtMeS	Ethylmethylsulfide	Ethyl methyl sulfide	
Cyclic Thioether				
	Trithiane	Trithiane	1,3,5-Trithiane	
Thioester				
	MeOS	Methylthioacetate	Methyl thioacetate	
	EtOS	Ethylpropanethioate	Ethyl propanethioate	
Thio acids				
	ThioAcAc	ThioaceticAcid	Thioacetic acid	
	ThioAcAcN	ThioaceticAcidN	Thioacetic acid (-)	
Phosphorus Compounds				

22	DMP	Dimethylphosphate	Dimethyl phosphate	
	DMPN	DimethylphosphateN	Dimethyl phosphate (-)	
	MePDeORib	MethylphosphateDe oxyribose	Methylphosphate deoxyri-bose	
	PO4	PhosphoricAcid	Phosphoric acid	
	PO4N	PhosphoricAcidN	Phosphoric acid (3-)	
Aromatic Compounds				
With C only				
23	Ph	Benzene	Benzene	
	MePh	Toluene	Toluene	
	Indane	Indane	Indane	
	Indene	Indene	Indene	
	Naphthalen	Naphthalene	Naphthalene	
	Anthracene	Anthracene	Anthracene	
	Phenanth	Phenanthrene	Phenanthrene	
	Tetracene	Tetracene	Tetracene	
	Fluorene	Fluorene	Fluorene	
	Acenapht	Acenaphthene	Acenaphtene	
	PhAnthrac	Benzanthracene	Benzanthracene	
	Tetralin	Tetralin	Tetralin	
	Pyrene	Pyrene	Pyrene	
With additional O only				
24	PhOH	Phenol	Phenol	
	PhOHN	Phenol	Phenol (-)	
	PhCHO	Benzaldehyde	Benzaldehyde	
	PhCOMe	Acetophenone	1-Phenylethanone	
	PhCOPh	Benzophenone	Benzophenone	
	Antquinone	Anthraquinone	Anthraquinone	
	Cumarin	Cumarin	Cumarin	
	Naphquinon	Naphthoquinone	1,4-Naphthoquinone	

	Naphthol1	Naphthol1	1-Naphthol	
	Naphthol2	Naphthol2	2-Naphthol	
	Phthalide	Phthalide	Phthalide	
	Vanillin	Vanillin	Vanillin	
With N only				
	PhNH2	Aniline	Aniline	
	PhNH2P	Aniline	Aniline (+)	
	Benzidine	Benzidine	Benzidine	
	BenzidineP	BenzidineP	Benzidine (2+)	
	Carbazole	Carbazole	Carbazole	
	CarbazoleP	CarbazoleP	Carbazole (+)	
With O, N etc.				
	PhCONH2	Benzamide	Benzamide	
	PhNO2	Nitrobenzene	Nitrobenzene	
	Phthalimid	Phthalimide	Phthalimide	
	PhthalimiP	Phthalimide	Phthalimide (+)	
	Phenothiaz	Phenothiazine	Phenothiazine	
	PhenothiaP	PhenothiazineP	Phenothiazine (+)	
Heteroaromatic Compounds				
Single 0				
	Furan	Furan	Furan	
	Furfural	Furfural	Furfural	
Single N				
25	Pyrrole	Pyrrole	Pyrrole	
	PyrroleP	PyrroleP	Pyrrole (+)	
	Pyridine	Pyridine	Pyridine	
	PyridineP	PyridineP	Pyridine (+)	
	Indole	Indole	Indole	
	IndoleP	IndoleP	Indole (+)	
	Quinoline	Quinoline	Quinoline	
	QuinolineP	QuinolineP	Quinoline (+)	
	Isoquino	Isoquinoline	Isoquinoline	
	IsoquinoP	IsoquinolineP	Isoquinoline (+)	
	Quinaldine	Quinaldine	Quinaldine	
	QuinaldinP	QuinaldineP	Quinaldine (+)	
Multiple N				

26	Imidazole	Imidazole	1H-Imidazole	
	ImidazoleP	ImidazoleP	1H-Imidazole (+)	
	Pyrazine	Pyrazine	Pyrazine	
	PyrazineP	PyrazineP	Pyrazine (2+)	
	Pyrimidine	Pyrimidine	Pyrimidine	
	PyrimidinP	PyrimidineP	Pyrimidine (2+)	
	Pyridazine	Pyridazine	Pyridazine	
	PyridazinP	PyridazineP	Pyridazine (2+)	
	Triazine	Triazine	1,3,5-Triazine	
	TriazineP	TriazineP	1,3,5-Triazine (3+)	
	Acridine	Acridine	Acridine	
	AcridineP	AcridineP	Acridine (+)	
Single S				
	Thiophene	Thiophene	Thiophene	
Amino acids				
	Gly	Glycine	Glycine	
	Ala	Alanine	Alanine	
	Val	Valine	Valine	
	Leu	Leucine	Leucine	

	Ile	Isoleucine	Isoleucine	
	Met	Methionine	Methionine	
	Phe	Phenylalanine	Phenylalanine	
	Trp	Tryphtophan	Tryphtophan	
	Pro	Proline	Proline	
	Ser	Serine	Serine	
	Thr	Threonine	Threonine	
	Cys	Cysteine	Cysteine	

	Tyr	Tyrosine	Tyrosine	
	Asn	Asparagine	Asparagine	
	Gln	Glutamine	Glutamine	
	Asp	Aspartate	Aspartate	
	Glu	Glutamate	Glutamate	
	Lys	Lysine	Lysine	
	Arg	Arginine	Arginine	
	His	Histidine	Histidine	

Amino acid sidechains				
	GlySC	GlycineSideChain	Glycine side chain	
	AlaSC	AlanineSideChain	Alanine side chain	
	ValSC	ValineSideChain	Valine side chain	
	LeuSC	LeucineSideChain	Leucine side chain	
	IleSC	IsoleucineSideChain	Isoleucine side chain	
	MetSC	MethionineSideChain	Methionine side chain	
	PheSC	PhenylalanineSideChain	Phenylalanine side chain	
	TrpSC	TryphtophanSideChain	Tryphtophan side chain	
	ProSC	ProlineSideChain	Proline side chain	
	SerSC	SerineSideChain	Serine side chain	
	ThrSC	ThreonineSideChain	Threonine side chain	
	CysSC	CysteineSideChain	Cysteine side chain	
	TyrSC	TyrosineSideChain	Tyrosine side chain	
	AsnSC	AsparagineSideChain	Asparagine side chain	
	GlnSC	GlutamineSideChain	Glutamine side chain	
	AspSC	AspartateSideChain	Aspartate side chain	
	GluSC	GlutamateSideChain	Glutamate side chain	
	LysSC	LysineSideChain	Lysine side chain	
	ArgSC	ArginineSideChain	Arginine side chain	
	HisSC	HistidineSideChain	Histidine side chain	
DNA/RNA				
	T	Thymine	Thymine	
	C	Cytosine	Cytosine	
	U	Uracil	Uracil	
	A	Adenine	Adenine	
	G	Guanine	Guanine	
… to be discussed				
	PeroxAc	PeroxyaceticAcid	PeroxyaceticAcid	
	PeroxAcN	PeroxyaceticAcidN	PeroxyaceticAcid (-)	
	PeroxbenAc	PeroxybenzoicAcid	PeroxybenzoicAcid	
	PeroxbenAc	PeroxybenzoicAcid	PeroxybenzoicAcid	
	PeroxAc	PeroxyaceticAcid	PeroxyaceticAcid	
	PeroxbenAc	PeroxybenzoicAcid	PeroxybenzoicAcid	
	ZnAc	ZincAcetate	Zinc diacetate	
	N2	Nitrogen	Nitrogen	
	O2	Oxygen	Oxygen	

Force Fields

Source: Tinker - Software Tools for Molecular Design, Current Major Version: Tinker 8.4, Release Date: February 2018, Minor Version: 8.4.4 (April 16, 2018)

- AMOEBA-2009 (amoeba09.prm)
- MM3-2000 (mm3.prm)
- MMFF94 (mmff.prm)
- OPLS-AA (oplsaa.prm)
- SMOOTH-AA (smoothaa.prm)

Project

Modelling of molecule-pair repulsions a(ij) according to priority for **26** prioritized fragment molecules:

- Minimal set for LogP simulations: H2O, Me, MeOH (Prio 1-3)
- Minimal set for C10E4/H2O simulations: H2O, Me, MeOH, Me2O, Et (Prio 1-5)
- Minimal set for protein-membrane simulations: **26** prioritized fragment molecules (Prio 1-26)