

Supplementary Materials: Extended Functional Groups (EFG): An Efficient Set for Chemical Characterization and Structure-Activity Relationship Studies of Chemical Compounds

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Group names of extended functional groups (EFGs) available as part of the ToxAlerts tool (<http://ochem.eu/alerts>).

Visual depictions of the corresponding EFG can be found online in ToxAlerts tool. LS and HS correspondingly denote low and high specificity functional group patterns (for the explanation please refer to the main article or ToxAlerts tool).

Chemistry of the Elements

- Alkali metals
- Alkaline earth metals
- Transition metals
- Lanthanoids
- Actinoids
- Post-transition metals
- Metalloids
- Nonmetals

- Tetragens (carbon group)
- Pnictogens (nitrogen group)
- Chalcogens (oxygen group)
- Halogens
- Noble gases

- Organic and inorganic cations and anions
 - Any cations
 - Any anions

Chemistry of ORGANIC Compounds

Hydrocarbons

- Alkenes
- Alkadienes
 - Cumulated alkadienes (1,2-alkadienes)
 - Conjugated alkadienes (1,3-alkadienes)
 - Isolated alkadienes (1,4-alkadienes)
- Alkynes
- Arenes

HYDROCARBON Halogen derivatives

- Hydrocarbon Halogen Derivatives with Csp³-Hal Bonds
 - Alkyl halides
 - Alkyl fluorides
 - Alkyl chlorides
 - Alkyl bromides
 - Alkyl iodides

Allyl halides

- Allyl fluorides
- Allyl chlorides
- Allyl bromides
- Allyl iodides

Benzyl halides

- Benzyl fluorides
- Benzyl chlorides
- Benzyl bromides
- Benzyl iodides

Gem-Dihalides *

Gem-Trihalides **

- * Belong formally to carbonyl derivatives
- ** Belong formally to carboxyl derivatives

Hydrocarbon halogen derivatives with Csp²-Hal bonds

Vinyl halides

- Vinyl fluorides
- Vinyl chlorides
- Vinyl bromides
- Vinyl iodides

Aryl halides

- Aryl fluorides
- Aryl chlorides
- Aryl bromides
- Aryl iodides

Hydrocarbon halogen derivatives with Csp-Hal bonds

Alkynyl halides

- Alkynyl fluorides
- Alkynyl chlorides
- Alkynyl bromides
- Alkynyl iodides

*Hydrocarbon Hydroxyl and Thiol Derivatives*Hydrocarbon hydroxyl derivatives with Csp³-O(S) bonds

Alcohols

- Primary alcohols
- Secondary alcohols
- Tertiary alcohols

Thiols

- Alkylthiols

1,2-Diols

1,2-Dithiols

1,2-Aminoalcohols

1,2-Aminothiols

Ethers

- Dialkylethers
- Alkylarylethers
- Diarylethers

Thioethers

- Dialkylthioethers

- Alkylarylthioethers
- Diarylthioethers
- Hydroperoxides
- Peroxides
- Disulfides

Hydrocarbon Hydroxyl Derivatives with Csp²-O(S) Bonds

- Enols
- Thioenols
- Enoethers
- Thioenolethers
- Enediols
- Enethiodiols
- Phenols
- Thiophenols
- Diphenols
 - 1,2-Diphenols
 - 1,3-Diphenols
 - 1,4-Diphenols
- Dithiophenols
 - 1,2-Dithiophenols
 - 1,3-Dithiophenols
 - 1,4-Dithiophenols
- Aminophenols
 - 1,2-Aminophenols
 - 1,3-Aminophenols
 - 1,4-Aminophenols
- Aminothiophenols
 - 1,2-Aminothiophenols
 - 1,3-Aminothiophenols
 - 1,4-Aminothiophenols

Hydrocarbon Hydroxyl Derivatives with Csp-O(S) Bonds

- Alkynyl alcohols
- Alkynyl thiols

(THIO)Carbonyl Compounds and Their Derivatives

Carbonyl compounds: aldehydes and ketones

- Aldehydes
- Ketones
- Quinones

Thiocarbonyl compounds: thioaldehydes and thioketones

- Thioaldehydes
- Thioketones
- Thioquinones

(Thio)carbonyl compounds derivatives

- Carbonyl hydrates
- Hemiacetals/Hemiketals
- Acetals/Ketals
- Thioacetals/Thioketals

- Imines
- Hydrazones
- Oximes
 - Oxime ethers
- Semicarbazones
- Thiosemicarbazones

- Ketenes
- Ketene acetal derivatives

(THIO)Carboxylic Acid Derivatives

- Carboxylic acid derivatives
 - Carboxylic acids
 - Carboxylic acid salts
 - Carboxylic acid esters
 - Lactones
 - Carboxylic acid anhydrides
 - Acyl halides
 - Acyl fluorides
 - Acyl chlorides
 - Acyl bromides
 - Acyl iodides
 - Carboxylic acid amides
 - Carboxylic acid primary amides
 - Carboxylic acid secondary amides
 - Carboxylic acid tertiary amides
 - Lactams
 - Carboxylic acid imides
 - Carboxylic acid unsubstituted imides
 - Carboxylic acid substituted imides
 - Carboxylic acid hydrazides
 - Carboxylic acid azides
 - Hydroxamic acids
 - Imido esters
 - Imidoyl halides
 - Carboxylic acid amidines
 - Carboxylic acid amidrazones
 - Nitriles
 - Isonitriles
 - Acyl cyanides
 - α -Substituted carboxylic acids
 - α -Aminoacids
 - α -Hydroxyacids
 - α -Oxoacids
 - α,β -Unsaturated carboxylic acids

- Orthocarboxylic acid derivatives
 - Carboxylic acid orthoesters
 - Carboxylic acid amide acetals

- Thiocarboxylic acid derivatives
 - Thiocarboxylic acids

- Thiocarboxylic acid esters
 - Thiolactones
- Thiocarboxylic acid amides
 - Thiolactams
- Imidothioesters

(THIO)Carbonic Acid Derivatives

- Carbonic acid derivatives
 - Carbonic acid esters
 - Carbonic acid monoesters
 - Carbonic acid diesters
 - Carbonic acid ester halides
 - Ureas
 - Isoureas
 - Guanidines
 - Semicarbazides
 - Carbodiimides
 - Cyanates
 - Isocyanates

- Thiocarbonic acid derivatives
 - Thiocarbonic acid esters
 - Thiocarbonic acid monoesters
 - Thiocarbonic acid diesters
 - Thiocarbonic acid ester halides
 - Thioureas
 - Isothioureas
 - Thiosemicarbazides
 - Isothiocyanates
 - Thiocyanates

(THIO)Carbamic acid derivatives

- Carbamic acid derivatives
 - Carbamic acid
 - Carbamic acid esters (urethanes)
 - Carbamic acid halides

- Thiocarbamic acid derivatives
 - Thiocarbamic acid esters
 - Thiocarbamic acid halides

Organonitrogen compounds

- Amines
 - Primary amines
 - Primary aliphatic amines
 - Primary aromatic amines
 - Secondary amines
 - Secondary aliphatic amines
 - Secondary mixed amines (aryl alkyl)
 - Secondary aromatic amines
 - Tertiary amines

- Tertiary aliphatic amines
- Tertiary mixed amines (aryl alkyl)
- Tertiary aromatic amines
- Quaternary ammonium salts
- 1,2-Diamines
- 1,2-Aminoalcohols
- 1,2-Aminothiols
- Aminals
- Hemiaminals
- Thiohemiaminals
- Aminophenols
 - 1,2-Aminophenols
 - 1,3-Aminophenols
 - 1,4-Aminophenols
- Aminothiophenols
 - 1,2-Aminothiophenols
 - 1,3-Aminothiophenols
 - 1,4-Aminothiophenols
- Enamines
- Hydroxylamines
- Hydrazine derivatives
- Azo compounds
- Azides
- Diazonium salts
- Nitroso compounds
- Nitro compounds
- N-Oxides
- Nitrites
- Nitrates

(Organo)sulfur COMPOUNDS

Sulfur (VI) Compounds

- Sulfuric acid derivatives
 - Sulfuric acid
 - Sulfuric acid esters
 - Sulfuric acid monoesters
 - Sulfuric acid diesters
 - Sulfuric acid amide esters
 - Sulfuric acid amides
 - Sulfuric acid diamides

Sulfuryl halides

- Sulfonic acid derivatives
 - Sulfonic acids
 - Sulfonic acid esters
 - Sulfonamides
 - Sulfonyl halides

Sulfones

Sulfur (IV) Compounds

- Sulfinic acid derivatives

- Sulfinic acids
- Sulfinic acid esters
- Sulfinic acid halides
- Sulfinic acid amides

Sulfoxides

Sulfur (II) Compounds

- Sulfenic acid derivatives
 - Sulfenic acids
 - Sulfenic acid esters
 - Sulfenic acid halides
 - Sulfenic acid amides

(Organo)phosphorus Compounds

Phosphorus (V) compounds

- Phosphoric acid derivatives
 - Phosphoric acid
 - Phosphoric acid esters
 - Phosphoric acid halides
 - Phosphoric acid amides

- Phosphonic acid derivatives
 - Phosphonic acids
 - Phosphonic acid esters
 - Phosphonic acid amides

Phosphinoxides

- Thiophosphoric acid derivatives
 - Thiophosphoric acids
 - Thiophosphoric acid esters
 - Thiophosphoric acid halides
 - Thiophosphoric acid amides

Phosphorus (III) compounds

Phosphines

Organoboron Compounds

- Boronic acids
- Boronic acid esters

Organometallic Compounds

- Organolithium compounds
- Organomagnesium compounds
- Other organometallic compounds

Heterocyclic Compounds

- Any heterocyclic ring
 - Aromatic heterocyclic compounds
 - Five-membered heterocycles
 - Six-membered heterocycles
 - Oxohetarenes

Thioxohetarenes

Iminohetarenes

Three-membered heterocycles (LS)

Three-membered heterocycles with one heteroatom (LS)

Saturated three-membered heterocycles with one heteroatom (LS)

Unsaturated three-membered heterocycles with one heteroatom (LS)

Three-membered heterocycles with two heteroatoms (LS)

Saturated three-membered heterocycles with two heteroatoms (LS)

Unsaturated three-membered heterocycles with two heteroatoms (LS)

Three-membered heterocycles with three heteroatoms (LS)

Saturated three-membered heterocycles with three heteroatoms (LS)

Unsaturated three-membered heterocycles with three heteroatoms (LS)

Three-membered heterocycles (HS)

Three-membered heterocycles with one heteroatom (HS)

Saturated three-membered heterocycles with one heteroatom (HS)

Aziridines (HS)

Oxiranes (HS)

Thiiranes (HS)

Unsaturated three-membered heterocycles with one heteroatom (HS)

Azirines (HS)

1H-Azirines (HS)

2H-Azirines (HS)

Oxirenes (HS)

Thiirenes (HS)

Three-membered heterocycles with two heteroatoms (HS)

Saturated three-membered heterocycles with two heteroatoms (HS)

Diaziridines (HS)

Dioxiranes (HS)

Oxaziridines (HS)

Thiaziridines (HS)

Unsaturated three-membered heterocycles with two heteroatoms (HS)

Diazirenes (HS)

1H-Diazirenes (HS)

3H-Diazirenes (HS)

Oxazirenes (HS)

Thiazerenes (HS)

Three-membered heterocycles with three heteroatoms (HS)

Saturated three-membered heterocycles with three heteroatoms (HS)

Triaziridines (HS)

Trioxiranes (HS)

Trithiiranes (HS)

Oxadiaziridines (HS)

Dioxaziridines (HS)

Thiodiaziridines (HS)

Dithiaziridines (HS)

Unsaturated three-membered heterocycles with three heteroatoms (HS)

1H-Triazirene (HS)

Oxadiazirenes (HS)

Thiodiazirenes (HS)

Four-membered heterocycles (HS)

Four-membered heterocycles with one heteroatom (LS)

- Unsaturated four-membered heterocycles with one heteroatom (LS)
- Saturated four-membered heterocycles with one heteroatom (LS)
- Four-membered heterocycles with two heteroatoms (LS)
 - Saturated four-membered heterocycles with two heteroatoms (LS)
 - Unsaturated four-membered heterocycles with two heteroatoms (LS)
- Four-membered heterocycles with three heteroatoms (LS)
 - Saturated four-membered heterocycles with three heteroatoms (LS)
 - Unsaturated four-membered heterocycles with three heteroatoms (LS)
- Four-membered heterocycles with four heteroatoms (LS)
 - Saturated four-membered heterocycles with four heteroatoms (LS)
 - Unsaturated four-membered heterocycles with four heteroatoms (LS)
- Four-membered heterocycles with one heteroatom (HS)
 - Saturated four-membered heterocycles with one heteroatom (HS)
 - Azetidines (HS)
 - Oxetanes (HS)
 - Thietanes (HS)
 - Unsaturated four-membered heterocycles with one heteroatom (HS)
 - Azetines (HS)
 - 1-Azetines (HS)
 - 2-Azetines (HS)
 - Azetes (HS)
 - Oxetenes (HS)
 - Thietenes (HS)
- Four-membered heterocycles with two heteroatoms (HS)
 - Saturated four-membered heterocycles with two heteroatoms (HS)
 - Diazetidines (HS)
 - 1,2-Diazetidines (HS)
 - 1,3-Diazetidines (HS)
 - Dioxetanes (HS)
 - 1,2-Dioxetanes (HS)
 - 1,3-Dioxetanes (HS)
 - Dithietanes (HS)
 - 1,2-Dithietanes (HS)
 - 1,3-Dithietanes (HS)
 - Unsaturated four-membered heterocycles with two heteroatoms (HS)
 - Diazetines (HS)
 - Dioxetenes (HS)
 - Dithietenes (HS)
- Five-membered heterocycles (LS)
 - Five-membered heterocycles with one heteroatom (LS)
 - Saturated five-membered heterocycles with one heteroatom (LS)
 - Unsaturated five-membered heterocycles with one heteroatom (LS)
 - Aromatic five-membered heterocycles with one heteroatom (LS)
 - Five-membered heterocycles with two heteroatoms (LS)
 - Saturated five-membered heterocycles with two heteroatoms (LS)
 - Unsaturated five-membered heterocycles with two heteroatoms (LS)
 - Aromatic five-membered heterocycles with two heteroatoms (LS)
 - Five-membered heterocycles with three heteroatoms (LS)
 - Saturated five-membered heterocycles with three heteroatoms (LS)
 - Unsaturated five-membered heterocycles with three heteroatoms (LS)
 - Aromatic five-membered heterocycles with three heteroatoms (LS)
 - Five-membered heterocycles with four heteroatoms (LS)

- Saturated five-membered heterocycles with four heteroatoms (LS)
- Unsaturated five-membered heterocycles with four heteroatoms (LS)
- Aromatic five-membered heterocycles with four heteroatoms (LS)
- Five-membered heterocycles with five heteroatoms (LS)
 - Saturated five-membered heterocycles with five heteroatoms (LS)
 - Unsaturated five-membered heterocycles with five heteroatoms (LS)
 - Aromatic five-membered heterocycles with five heteroatoms (LS)
- Five-membered heterocycles (HS)
 - Five-membered heterocycles with one heteroatom (HS)
 - Saturated five-membered heterocycles with one heteroatom (HS)
 - Pyrrolidines (HS)
 - Tetrahydrofurans (HS)
 - Tetrahydrothiophenes (HS)
 - Unsaturated five-membered heterocycles with one heteroatom (HS)
 - Pyrrolines (HS)
 - 1-Pyrrolines (HS)
 - 2-Pyrrolines (HS)
 - 3-Pyrrolines (HS)
 - Dihydrofurans (HS)
 - 2,3-Dihydrofurans (HS)
 - 2,5-Dihydrofurans (HS)
 - Dihydrothiophenes (HS)
 - 2,3-Dihydrothiophenes (HS)
 - 2,5-Dihydrothiophenes (HS)
 - Aromatic five-membered heterocycles with one heteroatom (HS)
 - Pyrroles (HS)
 - Furans (HS)
 - Thiophenes (HS)
 - Indoles
 - Benzofurans
 - Benzothiophenes
 - Five-membered heterocycles with two heteroatoms (HS)
 - Saturated five-membered heterocycles with two heteroatoms (HS)
 - Diazolidines (HS)
 - Pyrazolidines (HS)
 - Imidazolidines (HS)
 - Dioxolanes (HS)
 - 1,2-Dioxolanes (HS)
 - 1,3-Dioxolanes (HS)
 - Dithiolanes (HS)
 - 1,2-Dithiolanes (HS)
 - 1,3-Dithiolanes (HS)
 - Unsaturated five-membered heterocycles with two heteroatoms (HS)
 - Pyrazolines (HS)
 - 1-Pyrazolines (HS)
 - 2-Pyrazolines (HS)
 - Imidazolines (HS)
 - 2-Imidazolines (HS)
 - 3-Imidazolines (HS)
 - 4-Imidazolines (HS)
 - Dioxolenes (HS)
 - 1,2-Dioxolenes (HS)

- 1,3-Dioxolenes (HS)
- Dithiolenes (HS)
 - 1,2-Dithiolenes (HS)
 - 1,3-Dithiolenes (HS)
- Aromatic five-membered heterocycles with two heteroatoms (HS)
 - Diazoles (HS)
 - Pyrazoles (HS)
 - Imidazoles (HS)
 - Oxazoles (HS)
 - 1,2-Oxazoles (HS)
 - 1,3-Oxazoles (HS)
 - Thiazoles (HS)
 - 1,2-Thiazoles (HS)
 - 1,3-Thiazoles (HS)
- Five-membered heterocycles with three heteroatoms (HS)
 - Saturated five-membered heterocycles with three heteroatoms (HS)
 - Triazolidines (HS)
 - 1,2,3-Triazolidines (HS)
 - 1,2,4-Triazolidines (HS)
 - Trioxolanes (HS)
 - 1,2,3-Trioxolanes (HS)
 - 1,2,4-Trioxolanes (HS)
 - Trithiolanes (HS)
 - 1,2,3-Trithiolanes (HS)
 - 1,2,4-Trithiolanes (HS)
 - Unsaturated five-membered heterocycles with three heteroatoms (HS)
 - 1,2,3-Triazolines (HS)
 - 1,2,4-Triazolines (HS)
 - 1,2,3-Trioxoles (HS)
 - 1,2,3-Trithioles (HS)
 - Aromatic five-membered heterocycles with three heteroatoms (HS)
 - Triazoles (HS)
 - 1,2,3-Triazoles (HS)
 - 1,2,4-Triazoles (HS)
 - Oxadiazoles (HS)
 - 1,2,3-Oxadiazoles (HS)
 - 1,2,4-Oxadiazoles (HS)
 - 1,2,5-Oxadiazoles (furazanes) (HS)
 - 1,3,4-Oxadiazoles (HS)
 - Five-membered heterocycles with four heteroatoms (HS)
 - Saturated five-membered heterocycles with four heteroatoms (HS)
 - Tetrazolidines (HS)
 - Tetraoxolanes (HS)
 - Tetrathiolanes (HS)
 - Unsaturated five-membered heterocycles with four heteroatoms (HS)
 - Aromatic five-membered heterocycles with four heteroatoms (HS)
 - Tetrazoles (HS)
 - Oxatriazoles (HS)
 - 1,2,3,4-Oxatriazoles (HS)
 - 1,2,3,5-Oxatriazoles (HS)
 - Thiatriazoles (HS)
 - 1,2,3,4-Thiatriazoles (HS)
 - 1,2,3,5-Thiatriazoles (HS)

Five-membered heterocycles with five heteroatoms (HS)
Saturated five-membered heterocycles with five heteroatoms (HS)
Pentazolidines (HS)
Pentaoxolanes (HS)
Pentathiolanes (HS)
Unsaturated five-membered heterocycles with five heteroatoms (HS)
Aromatic five-membered heterocycles with five heteroatoms (HS)
Pentazoles

Six-membered heterocycles (LS)

Six-membered heterocycles with one heteroatom (LS)
Saturated six-membered heterocycles with one heteroatom (LS)
Unsaturated six-membered heterocycles with one heteroatom (LS)
Aromatic six-membered heterocycles with one heteroatom (LS)
Six-membered heterocycles with two heteroatoms (LS)
Saturated six-membered heterocycles with two heteroatoms (LS)
Unsaturated six-membered heterocycles with two heteroatoms (LS)
Aromatic six-membered heterocycles with two heteroatoms (LS)
Six-membered heterocycles with three heteroatoms (LS)
Saturated six-membered heterocycles with three heteroatoms (LS)
Unsaturated six-membered heterocycles with three heteroatoms (LS)
Aromatic six-membered heterocycles with three heteroatoms (LS)
Six-membered heterocycles with four heteroatoms (LS)
Saturated six-membered heterocycles with four heteroatoms (LS)
Unsaturated six-membered heterocycles with four heteroatoms (LS)
Aromatic six-membered heterocycles with four heteroatoms (LS)
Six-membered heterocycles with five heteroatoms (LS)
Saturated six-membered heterocycles with five heteroatoms (LS)
Unsaturated six-membered heterocycles with five heteroatoms (LS)
Aromatic six-membered heterocycles with five heteroatoms (LS)
Six-membered heterocycles with six heteroatoms (LS)
Saturated six-membered heterocycles with six heteroatoms (LS)
Unsaturated six-membered heterocycles with six heteroatoms (LS)
Aromatic six-membered heterocycles with six heteroatoms (LS)

Six-membered heterocycles (HS)

Six-membered heterocycles with one heteroatom (HS)
Saturated six-membered heterocycles with one heteroatom (HS)
Piperidines (HS)
Tetrahydropyrans (HS)
Tetrahydrothiopyrans (HS)
Unsaturated six-membered heterocycles with one heteroatom (HS)
Tetrahydropyridines (HS)
Dihydropyridines (HS)
Pyrans (HS)
Thiopyrans (HS)
Aromatic six-membered heterocycles with one heteroatom (HS)
Pyridines (HS)
Six-membered heterocycles with two heteroatoms (HS)
Saturated six-membered heterocycles with two heteroatoms (HS)
Hexahydrodiazines
Dioxanes
Dithianes
Morpholines

- Unsaturated six-membered heterocycles with two heteroatoms (HS)
 - Tetrahydrodiazines (HS)
 - Dihydrodiazines (HS)
 - Dioxines (HS)
 - Dithiines (HS)
- Aromatic six-membered heterocycles with two heteroatoms (HS)
 - Pyridazines (HS)
 - Pyrimidines (HS)
 - Pyrazines (HS)
- Six-membered heterocycles with three heteroatoms (HS)
 - Saturated six-membered heterocycles with three heteroatoms (HS)
 - Hexahydrotriazines (HS)
 - Trioxanes (HS)
 - Trithianes (HS)
 - Unsaturated six-membered heterocycles with three heteroatoms (HS)
 - Aromatic six-membered heterocycles with three heteroatoms (HS)
 - Triazines (HS)
- Six-membered heterocycles with four heteroatoms (HS)
 - Saturated six-membered heterocycles with four heteroatoms (HS)
 - Hexahydrotetrazines (HS)
 - Tetroxanes (HS)
 - Tetrathianes (HS)
 - Unsaturated six-membered heterocycles with four heteroatoms (HS)
 - Dihydrotetrazines (HS)
 - Tetrahydrotetrazines (HS)
 - Aromatic six-membered heterocycles with four heteroatoms (HS)
 - Tetrazines (HS)
- Six-membered heterocycles with five heteroatoms (HS)
 - Saturated six-membered heterocycles with five heteroatoms (HS)
 - Hexahydropentazines (HS)
 - Pentoxanes (HS)
 - Pentathianes (HS)
 - Unsaturated six-membered heterocycles with five heteroatoms (HS)
 - Aromatic six-membered heterocycles with five heteroatoms (HS)
 - Pentazines
- Six-membered heterocycles with six heteroatoms (HS)
 - Saturated six-membered heterocycles with six heteroatoms (HS)
 - Unsaturated six-membered heterocycles with six heteroatoms (HS)
 - Aromatic six-membered heterocycles with six heteroatoms (HS)
 - Hexazines