

Algaecides - Kills or prevents the growth of algae

NAME	OTHER TRADE NAMES	EMP FORMULA	MOLAR MASS
Caprylic Acid	Octanoic Acid	C8H16O2	144.21
Endothall	Endothal	C8H10O5	186.16
Bromine Monochloride	Bromine Chloride	BrCl	115.36
Dichlone	Quintar	C10H4Cl2O2	227.04
Fluorenlol	9h-fluoren-9-ol		182.22
Diuron	Duran DCMU	C9H10Cl2N2O	233.09
Chloropicrin	Chlorpikrin	CCL3NO2	164.37
Phosphine	Phosphane	PH3	33.998
Ethroprop	Rovokil	C8H19O2PS2	242.3
Deet	Diethyltoluamide	C4H13N3	191.27
Antifouling	Parasol	CUH4O2	99.58
Miconazole	Monistat	C18H14Cl4N2O	416.1
Azoxystrobin	Amistar	C22H17N3O5	403.4
Tributyltin (TBT)	Tributylstannanyl	C12H27Sn	290.1

Biocide – Kills living organisms

Benzalkonium Chloride	BZK	C6H5CH2N(CH3)2	170.6592
Nimbin	Neem oil	C30H36O9	540.6

Fungicide – Kills Fungi

Iprodion	Rovral Chipco Green	C13H13Cl2N3O3	330.17
Dicarboximide	Pyrodone	C17H25NO2	275.4
Strobilurin (Qol)	Strobilurin	C25H30O7	442.5
Azole	Pyrrole	C4H5N	67.09
Anilinopyrimidine	N-phenylpyrimidin-2-amine	C10H9N3	171.2

Herbicide – Kills unwanted plants

Solanine	Alpha-solanine	C45H73NO15	868.1
Vinegar	Acetic Acid	C2H4O2	60.05
Monolinuron	Monamex Gramonol Aresin	C9H11ClN2O	214.65
Linuron	Methoxydiuron, Afalon	C9H10Cl2N2O2	249.09

Understanding and Predicting Human Made and Distributed Environmental Toxins on a Molecular Level

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There are a wide range of chemicals and chemical mixtures that humans use to control plants, animals and insects. Many of these are poisons and can attack a number of physiological systems. Algaecides, Antifouling agents, Antimicrobials, Attractants, Biopesticides, Biocides, Disinfectants and sanitizers, Fungicides, Fumigants, Herbicides, Insecticides, Miticides, Microbial pesticides, Molluscicides, Nematicides; Ovicides, Pheromones, Repellents, Rodenticides as well as some chemical defenses used by plants. Six biological parameters are calculated for dozens of these molecules. (GPCR ligand, Ion channel modulator, Kinase inhibitor, Nuclear receptor ligand, Protease inhibitor, Enzyme inhibitor) to help understand what impact they might have on humans and other mammals. For example, G protein-coupled receptors (GPCRs), have several names including G protein-linked receptors (GPLR). They are a family of protein receptors located on the cell membrane that detect molecular species that can initiate or impact cellular responses. G protein-coupled receptors have been correlated with a large number of diseases including cancer, antibiotics, HIV and Alzheimer's, are a target of one third of all medicinal drugs currently being utilized. This presentation will identify the best and the worst of chemicals used and make a suggestion for each to lower their negative impact.

Insecticide – Kills insects

Histamine	2-(1h-imidazol-5-yl)ethanamine	C5H9N3	111.15
Resmethrin,	Benzofuroline Abamectinum	C22H26O3	338.44
Abamectin	Agrimek	C95H142O28	1732.1
Azamethiphos	Azamethiophos	C9H10ClN2O5PS	324.67
Malathion	Carbofos Maldison Mercaptothion Ortho Malathion	C10H19O6PS2	330.36
Nicotine	L-nicotine	C10H14N2	162.23
Ddt	Clofenotane	C14H9Cl5	354.5
Aldrin	Aldrosol, Kortofin, Tatzinho	C12H8Cl6	364.9
Ethroprop	Ethoprophos	C8H19O2PS2	242.3

Miticide – Kills mites and lice

Neem	Salannin, Azadriactin	C34H44O9	596.7
Permethrin	Nix	C21H20Cl2O3	391.28

Nematicide – Kills nematodes

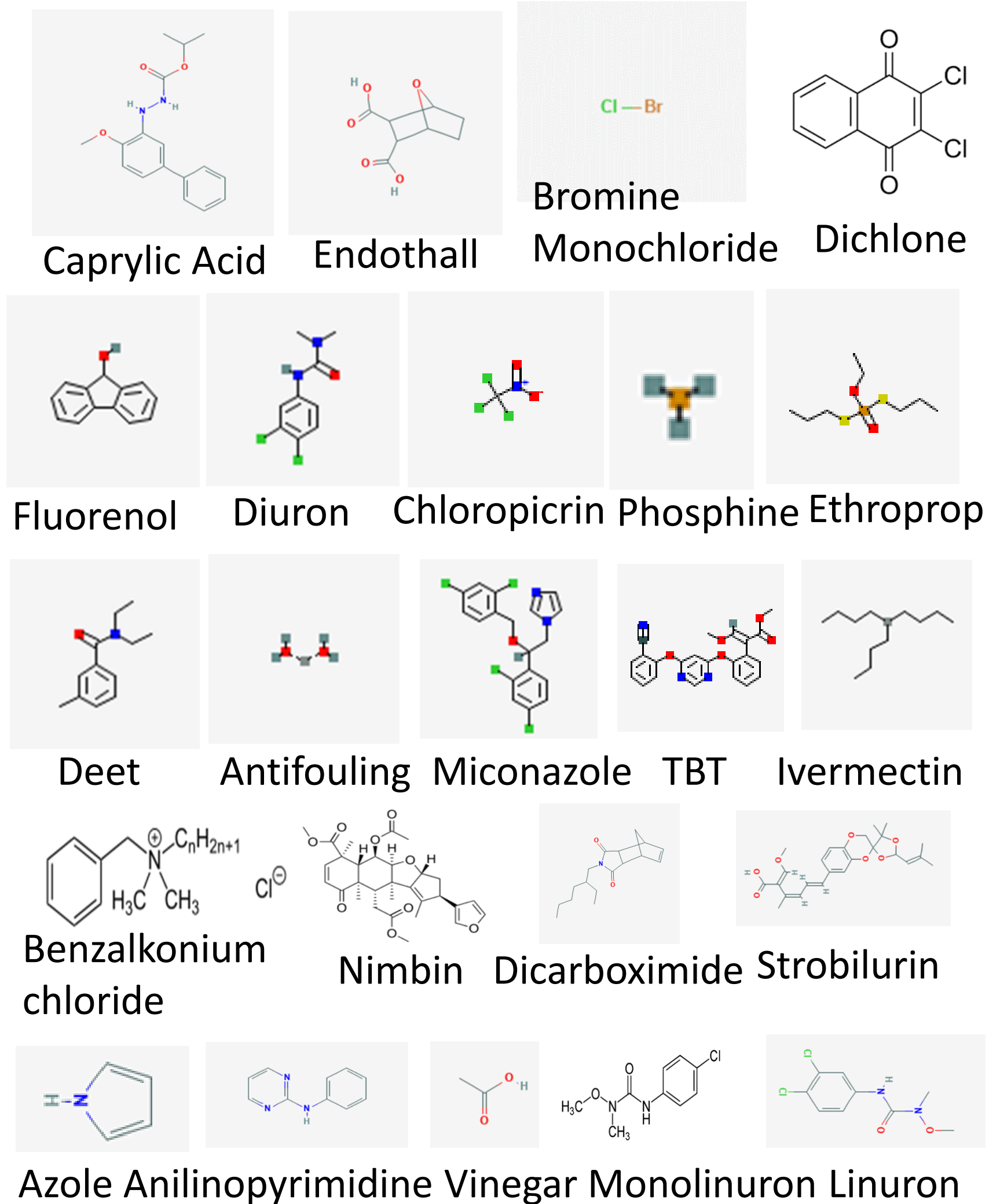
Dibromochloropropane	DBCP And Nematocide	C3H5Br2Cl	236.33
Flumethrin	Bayticol And Bayvarol	C23H22Cl2FNO3	510.4

Pesticide – Kills pests

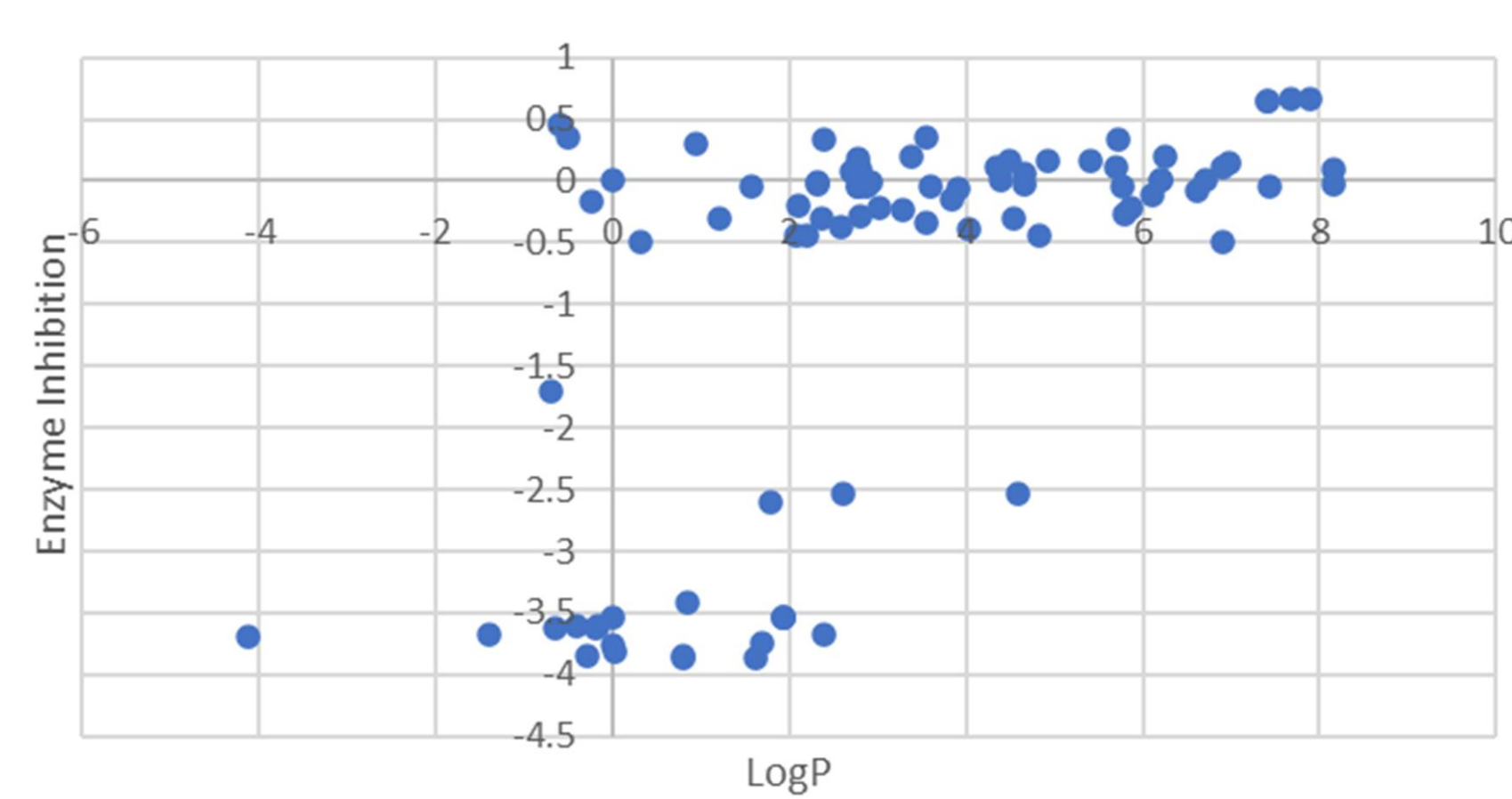
Pentachlorophenol	Dowicide 7 Pentacon Penwar Sinituho Penta	C6HCl5O	266.34
Dienochlorine	Pentac	C10Cl10	474.61
Acequinocyl	Piton	C24H32O4	384,51
Pyrinuron	Pyriminil	C13H12N4O3	272.26
Warfarin	Coumadin	C19H16O4	308.3
Aluminium Phosphide	Phostoxin	AIP	57.9553
Vitamin D2	Viosterol	C28H44O	396.6
Calciferols	Drisdol	C28H44O	396.65

Rodenticide – Kills Rodents

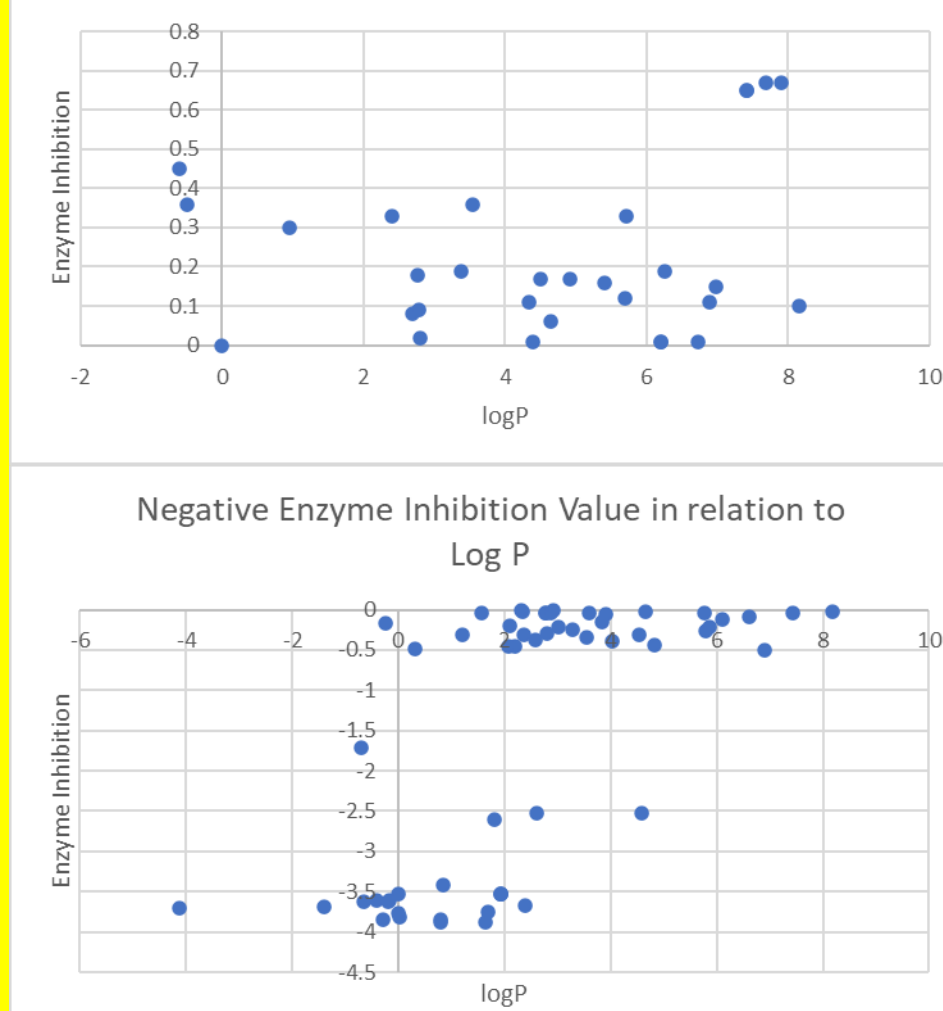
Permethrin	Dibromochloropropane	Flumethrin
Pentachlorophenol	Dienochlorine	Acequinocyl
Pyrinuron	Warfarin	Aluminium phosphide
Vitamin D2	Calciferols	



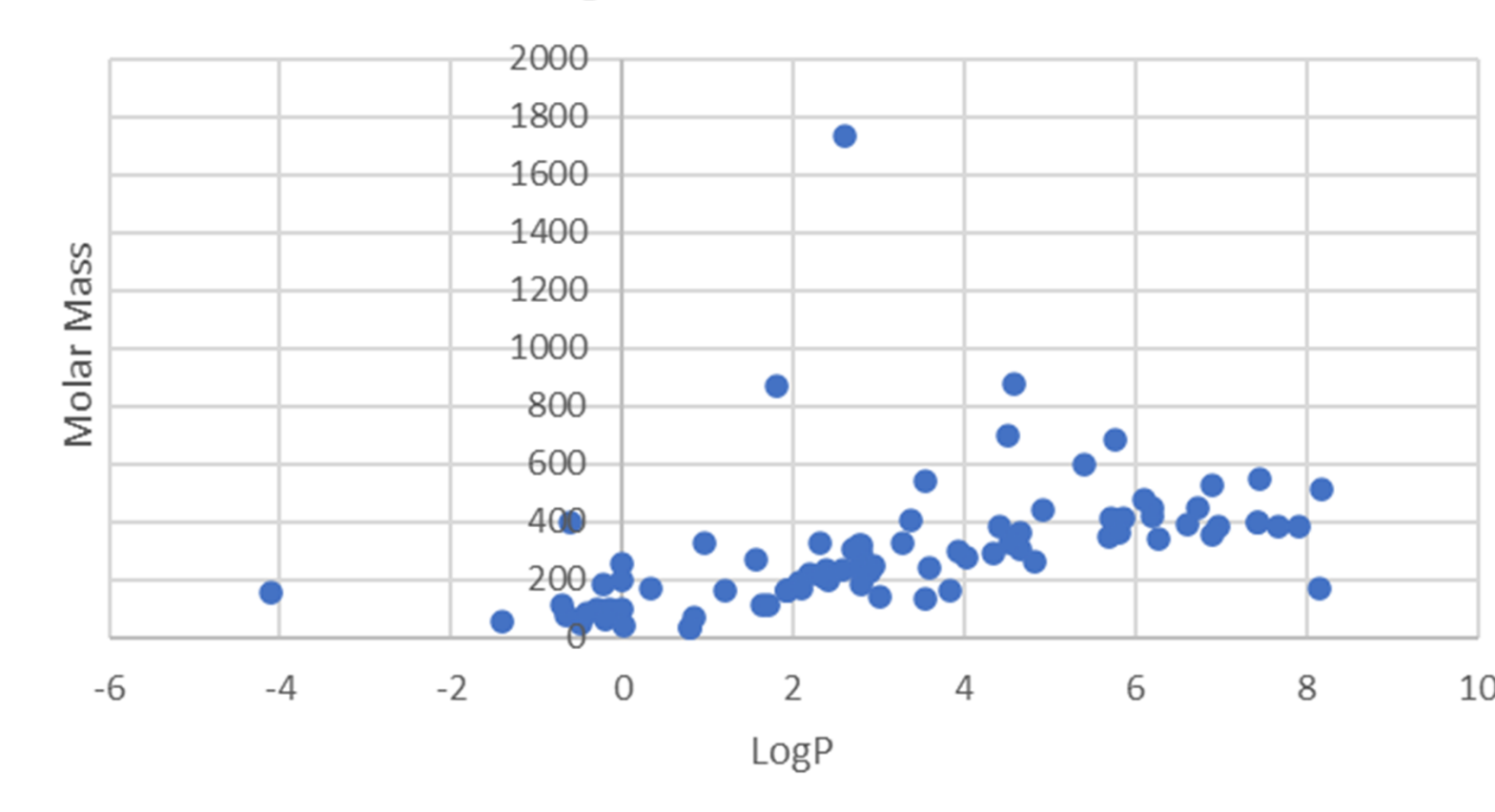
LogP VS. Enzyme Inhibition



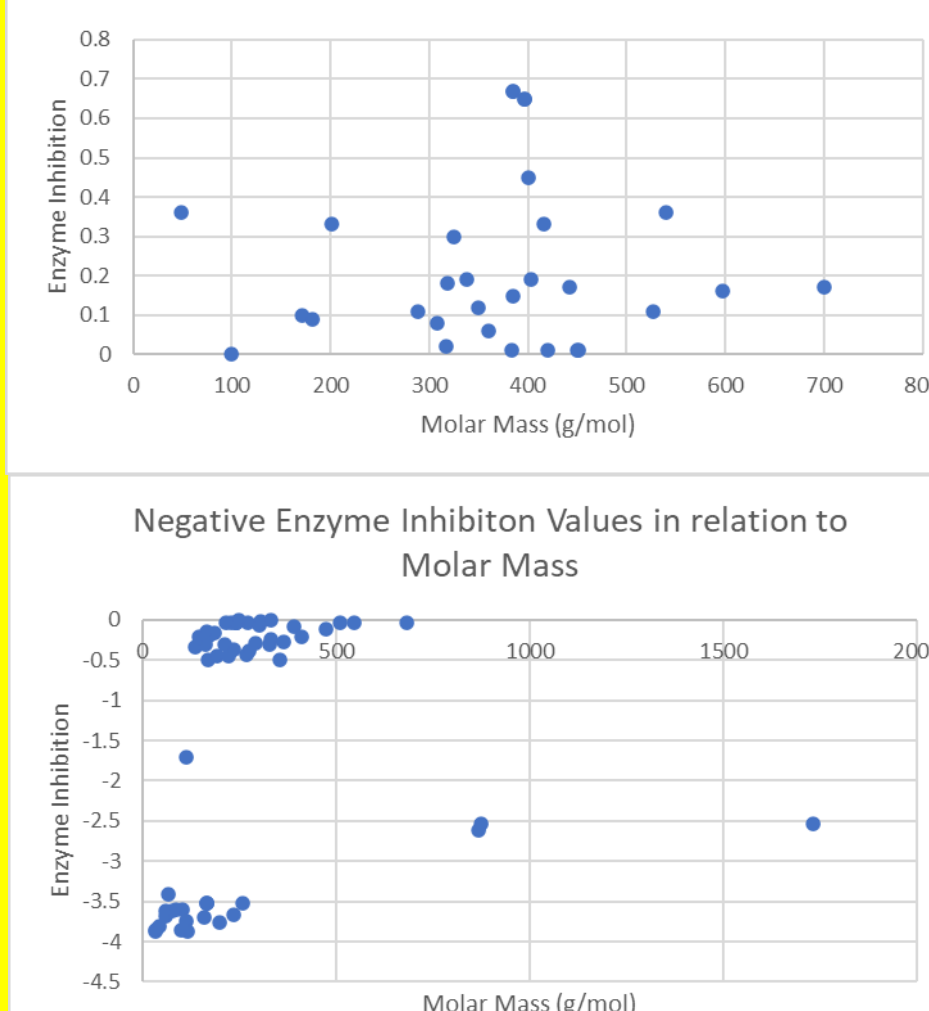
Positive Enzyme Inhibition Values in relation to Log P



LogP Vs. Molar Mass



Positive Enzyme Inhibition Values in relation to Molar Mass



Molar Mass Vs. Enzyme Inhibition

