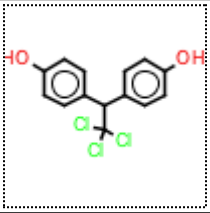
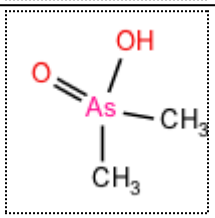
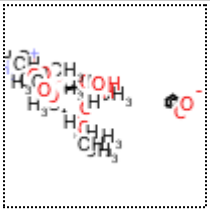
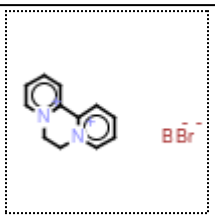
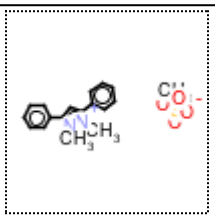
Excluded molecules due to failed descriptors calculation

Knime report *powered by Birt*

"Chemical Structure"	"INCHI_KEY"	"SMILES"	"preferred_name"	"casrn"	"ERROR"
	IUGDILGOLSSKNE-UHFFFAOYSA	C(C(C1C=CC(=CC=1)(Cl)(Cl)Cl	HPTE	2971-36-0	Calculation of Dipole failed:CalcDipole: 1.0: Unable to retrieve required 3D coordinates
	OGGXGZAMXPVRFZ-UHFFFAOYSA	C[As](=O)(C)O	Cacodylic acid	75-60-5	@WARNING: No polarizability increment available for As
	GCKZANITAMOIAR-XWVCPFKXSA	O=C([C@@](C=C6C)([H])[C@@]/4(O)[C@]([C@@H]6O)([H])OCC4=C/C=C/[C@@H]5C)O[C@@H](C3)C[C@@]2(O[C@([C@@]([H])(C)CC)([H])[C@@H](C)C=C2)O[C@]3([H])C=C(C)/[C@H]5O[C@H]1C[C(OC)[C@@H](O[C@H]7C[C@H](OC)[C@@H]([NH2+]C)[C@H](C)O7)[C@H](C)O1.O=C([O-])C8=C	Emamectin benzoate	155569-91-8	Calculation failed after multiple attemts. Exemplary error: org.openscience.cdk.ex CPSA: org.openscience.cdk.ex Molecule must have 3D coordinates
	ODPOAESBSUKMHI-UHFFFAOYSA	[N+]1(C=CC=C2)=C2C3=+](C=CC=C3)CC1.[Br-].[Br-]	Diquat dibromide	85-00-7	Calculation failed after multiple attemts. Exemplary error: org.openscience.cdk.ex CPSA: org.openscience.cdk.ex Molecule must have 3D coordinates
	XQEMNBNCQVQXM-UHFFFAOYSA	C[N+]1=C(C2=CC=CC=C(OC)=O	Difenzoquat metilsulfate	43222-48-6	Calculation failed after multiple attemts. Exemplary error: org.openscience.cdk.ex CPSA: org.openscience.cdk.ex Molecule must have 3D coordinates

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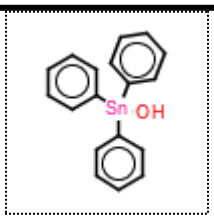
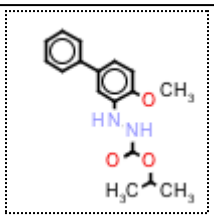
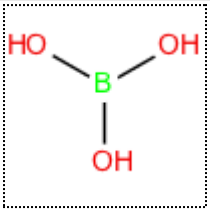
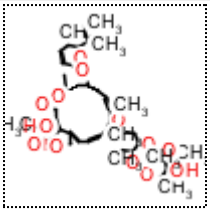
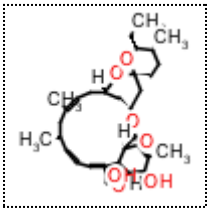
	BFWMWWXRWVJX UHFFFAOYSA	O[Sn] (C1=CC=CC=C1) (C2=CC=CC=C2)C3=(	Fentin	76-87-9	Calculation failed after multiple attemts. Exemplary error: org.openscience.cdk.ex vabc: org.openscience.cdk.ex Unsupported element.
	VHLKTXFWDRXILV UHFFFAOYSA	O=C(NNC1=C(OC)C=	Bifenazate	149877-41-8	External application of task ChemaxonDescriptors crashed (non zero exit code 143) and did not provide results
	KGBXLFKZBHKPEV UHFFFAOYSA	OB(O)O	Boric acid	10043-35-3	inob(o)o alogps - can't do structures without carbons
	RRZXIRBKKLTSOM VRFQAOMKSA	CO[C@H]1C[C@@H (O[C@@H](C) [C@@H]1O)O[C@@H (OC)C[C@@H] (O[C@H]2C)O[C@@ (OC(=O)[C@@H]4/ C=C(/C)[C@@H](O) [C@H]5OC/ C(=CC=C[C@@H]3C [C@@]45O)C[C@]6(/ C=C[C@H](C)[C@H] (O6)[C@@H] (C)CC)O7	Abamectin	71751-41-2	org.openscience.cdk.ex CPSA: org.openscience.cdk.ex Molecule must have 3D coordinates
	VOZIAWLUULBIPN- LRBNAKOISA	O=C2O[C@H]4C[C@ (O[C@]5(O[C@H] (CC)[C@@H] (C)CC5)C4)([H])C/ C=C(C)/C[C@@H] (C)/C=C/ C=C1CO[C@@]3([H] [C@@](O)/1[C@] ([H])2C=C(C) [C@H]3O	Milbemectin (mixture)	51596-11-3	org.openscience.cdk.ex CPSA: org.openscience.cdk.ex Molecule must have 3D coordinates