***Supplementary File 1***

Openeye’s FILTER algorithm parameters

MAX\_COUNT\_FORMAL\_CRG 4 "Maximum number of formal charges"

MAX\_XLOGP 1.0 "Maximum XLogP"

MIN\_SOLUBILITY soluble "Minimum solubility"

MAX\_LIPINSKI 3 "Maximum number of Lipinski violations"

PSA\_USE\_SandP false "Count S and P as polar atoms"

MIN\_2D\_PSA 100.0 "Minimum 2-Dimensional (SMILES) Polar Surface Area"

MAX\_2D\_PSA 250.0 "Maximum 2-Dimensional (SMILES) Polar Surface Area"

RULE 1 acid

RULE 1 acid\_chloride

RULE 1 acid\_halide

RULE 1 alkyl\_phosphate

RULE 1 alkylating\_agent

RULE 1 amide

RULE 1 amine

RULE 1 amino\_acid

RULE 1 carboxylic\_acid

RULE 1 cation\_C\_Cl\_I\_P\_or\_S

RULE 1 disulfide

RULE 1 hydroxylamine

RULE 1 nitro

RULE 1 N\_P\_S\_Halides

RULE 1 organometallic

RULE 1 phosphoric\_acid

RULE 1 phosphoric\_ester

RULE 1 sulfinimine

RULE 1 sulfinylthio

RULE 1 sulfonamide

RULE 1 thiocarbonyl

RULE 1 thioester

RULE 1 thiol

RULE 1 thiourea