

**Supplementary Table Legend**

Supplementary\_Table\_01\_Database\_description

Supplementary\_Table\_02\_Annnotated-Compound\_Pubchem

Supplementary\_Table\_03\_Annnotated-SE\_Pubchem

Supplementary\_Table\_04\_Annnotated-Compound\_Annotations

Supplementary\_Table\_05\_Annnotated-Compound\_Annotation\_Relations

Supplementary\_Table\_06\_Annnotated-SE\_Annotations

Supplementary\_Table\_07\_Annotation\_Prediction\_analysis

Supplementary\_Table\_08\_Threshold\_0.1\_Predictions

Supplementary\_Table\_09\_Annnotated+Threshold\_0.1\_Predictions