**Original**

O=C([O-])c1cc(=O)[nH]c(=O)[nH]1.O=C([O-])c1cc(=O)[nH]c(=O)[nH]1.[Zn+2]

cleanup = True

Chart, radar chart

Description automatically generated

addH = True

Chart, radar chart

Description automatically generated

**Remove Zn2+, with Chembl structure pipeline**

O=C([O-])c1cc(=O)[nH]c(=O)[nH]1.O=C([O-])c1cc(=O)[nH]c(=O)[nH]1

cleanup = True

Shape, radar chart

Description automatically generated with medium confidence

addH = True

Chart, radar chart

Description automatically generated

**Remove Zn2+, without Chembl structure pipeline**

O=C([O-])c1cc(=O)[nH]c(=O)[nH]1.O=C([O-])c1cc(=O)[nH]c(=O)[nH]1

cleanup = False

Chart, radar chart

Description automatically generated

addH = True

Chart, radar chart

Description automatically generated

Node Features

**Original**

O=C([O-])c1cc(=O)[nH]c(=O)[nH]1.O=C([O-])c1cc(=O)[nH]c(=O)[nH]1.[Zn+2]

Node features

[[ 15 15 58 66 66 15 15 66 58 15 66 66 15 15 58 58 66 15 15 107 66 15 66]

[ 3 2 2 1 1 3 3 1 2 3 1 1 3 3 2 2 1 2 3 0 1 3 1]

[ 0 0 0 0 0 0 0 -1 0 0 0 -1 0 0 0 0 0 0 0 2 0 0 0]

[ 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 1 3 3 3]

[ 0 1 1 0 0 1 1 0 1 1 0 0 1 1 1 1 0 1 1 0 0 0 0]

[ 0 1 1 0 0 0 0 0 1 0 0 0 0 0 1 1 0 1 0 0 0 0 0]

[ 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]

[ 0 1 1 0 0 1 1 0 1 1 0 0 1 1 1 1 0 1 1 0 0 0 0]

[ 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]]

**Remove Zn2+, without Chembl structure pipeline**

O=C([O-])c1cc(=O)[nH]c(=O)[nH]1.O=C([O-])c1cc(=O)[nH]c(=O)[nH]1

Node features

[[66 15 66 15 15 58 66 15 66 15 58 15 15 58 66 66 15 15 66 58 15 66]

[ 1 3 1 3 3 2 1 3 1 2 2 3 2 2 1 1 3 3 1 2 3 1]

[ 0 0 0 0 0 0 -1 0 0 0 0 0 0 0 0 0 0 0 -1 0 0 0]

[ 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3]

[ 0 1 0 1 1 1 0 0 0 1 1 0 1 1 0 0 1 1 0 1 1 0]

[ 0 0 0 0 0 1 0 0 0 1 1 0 1 1 0 0 0 0 0 1 0 0]

[ 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]

[ 0 1 0 1 1 1 0 0 0 1 1 0 1 1 0 0 1 1 0 1 1 0]

[ 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0]]