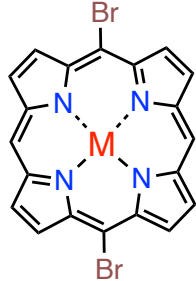
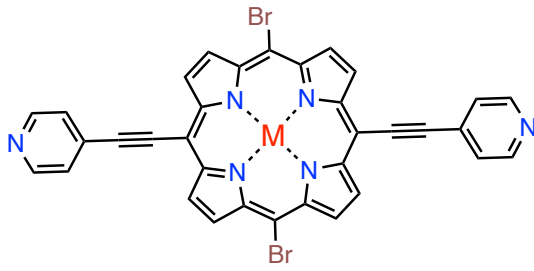
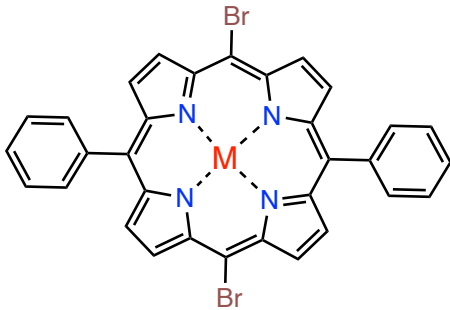
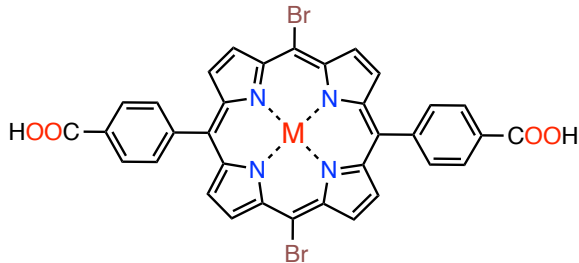
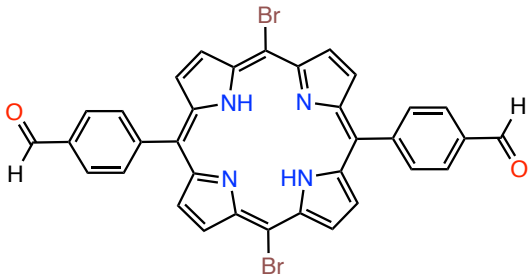


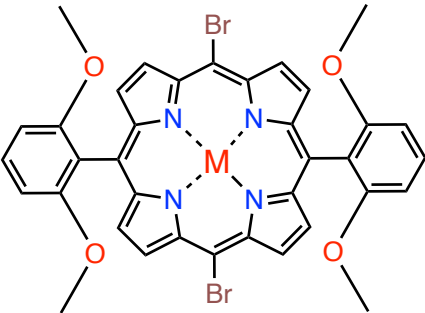
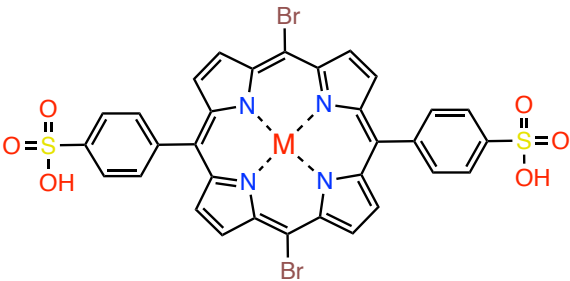
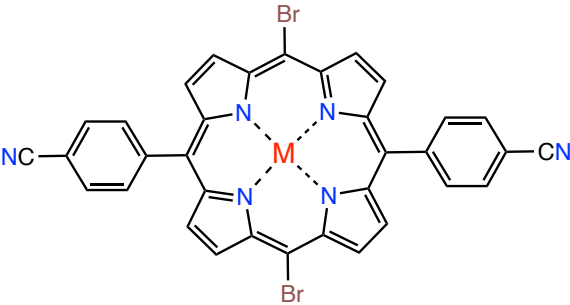
Substituted Functional Groups

No.FG	Smiles string for metal-based one	
1. H	<chem>BrC1=C2C=C/C(N2)=C/C(C=C3)=NC3=C(Br)C4=CC=C(N4)C=C5C=CC1=N5</chem>	
2. Py	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC=NC=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=NC=C6)=C7C=CC1=N/7</chem>	
3. 1,2-dihydropyridine (DHP)	<chem>Br/C1=C2C=C/C(N2)=C(C3=CCNC=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CCN=C=C6)=C7C=CC1=N/7</chem>	

<p>4. 4-ethynylpyridine (C2Py)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C#CC3=CC=NC=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C#CC6=CC=NC=C6)=C7C=CC1=N/7</chem>	
<p>5. Ph</p>	<chem>Br/C1=C2C=C/C(N2)=C(C(C=C/3)=NC3=C(C4=CC=C(/C(C5=CC=CC=C5)=C6C=CC1=N/6)N4)\Br)\C7=CC=CC=C7</chem>	
<p>6. benzoic acid p-CP</p>	<chem>Br/C1=C2C=C/C(N2)=C(C(C=C/3)=NC3=C(C4=CC=C(/C(C5=CC=C(C(O)=O)C=C5)=C6C=CC1=N/6)N4)\Br)\C7=CC=C(C(O)=O)C=C7</chem>	


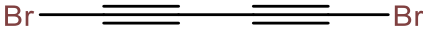
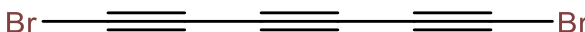
7. m-CP	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC(C(O)=O)=CC=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=CC(C(O)=O)=C6)=C7C=CC1=N/7</chem>	
8. phenol (PhOH)	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC=C(O)C=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=C(O)C=C6)=C7C=CC1=N/7</chem>	
9. benzene-1,2,3-triol (Ph3OH)	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC(O)=C(O)C(O)=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC(O)=C(O)C(O)=C6)=C7C=CC1=N/7</chem>	

<p>10. benzaldehyde (PhCHO)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC=C(C([H])=O)C=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=C(C([H])=O)C=C6)=C7C=CC1=N/7</chem>	
<p>11. <i>m</i>-xylene Ar(Ph2Me)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C(C=C/3)=NC3=C(C4=CC=C(/C(C5=CC(C)=CC(C)=C5)=C6C=CC1=N/6)N4)\Br)\C7=CC(C)=CC(C)=C7</chem>	
<p>12. mesitylene Ar(Ph3Me)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C3=C(C)C=C(C)C=C3C)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=C(C)C=C(C)C=C6C)=C7C=CC1=N/7</chem>	

<p>13. 1,3-dimethoxybenzene Ar(Ph2OMe)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C(C=C/3)=NC3=C(C4=CC=C(/C(C5=C(OC)C=CC=C5OC)=C6C=C(C1=N/6)N4)\Br)\C7=C(OC)C=CC=C7OC</chem>	
<p>14. benzenesulfonic acid (BSA)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC=C(S(=O)(O)=O)C=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=C(S(=O)(O)=O)C=C6)=C7C=CC1=N/7</chem>	
<p>15. benzonitrile (PhCN)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC=C(C#N)C=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=C(C#N)C=C6)=C7C=CC1=N/7</chem>	

<p>16. <i>N,N</i>-dimethylaniline (DMA) /<i>N</i>-methylaniline (NMA)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC=C(NC)C=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=C(NC)C=C6)=C7C=CC1=N/7</chem>	
<p>17. Aniline (PhNH₂)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC=C(N)C=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=C(N)C=C6)=C7C=CC1=N/7</chem>	
<p>18. Nitrobenzene (PhNO₂)</p>	<chem>Br/C1=C2C=C/C(N2)=C(C3=CC=C([N+])([O-])=O)C=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=C([N+])([O-])=O)C=C6)=C7C=CC1=N/7</chem>	

Linker

Linker label	Smiles string	Structure
C2	<chem>C(#CBr)Br</chem>	
C4	<chem>C(#CBr)C#CBr</chem>	
C6	<chem>C(#CC#CBr)C#CBr</chem>	
C8	<chem>BrC#CC#CC#CC#CBr</chem>	