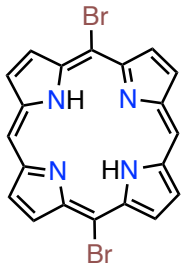
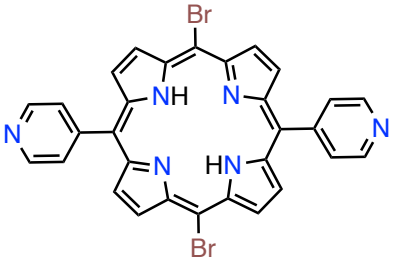
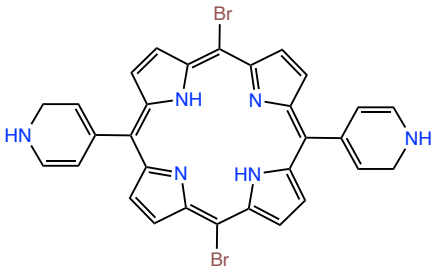
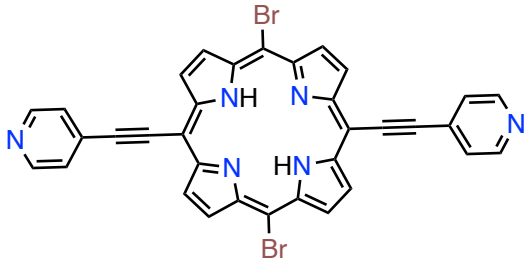
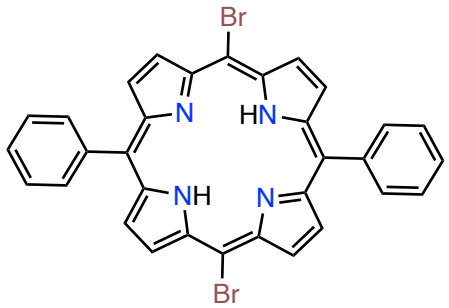
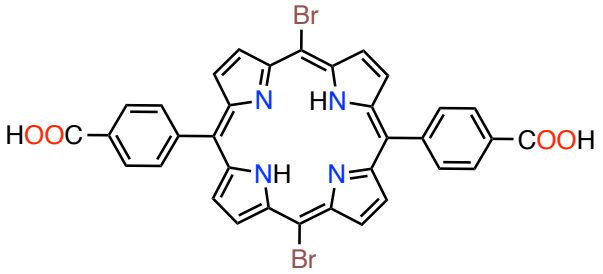
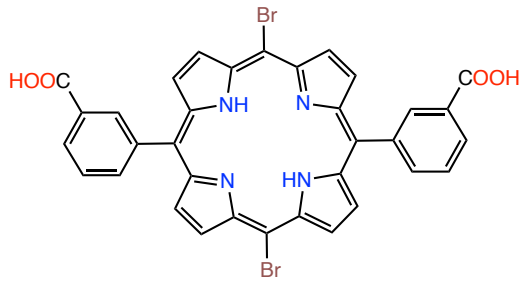
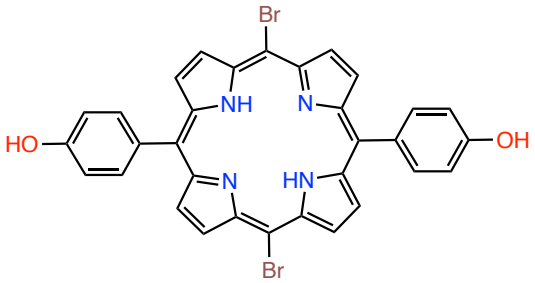
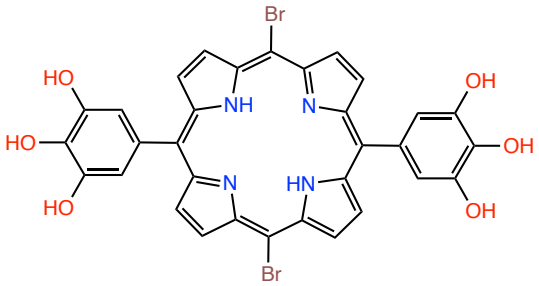
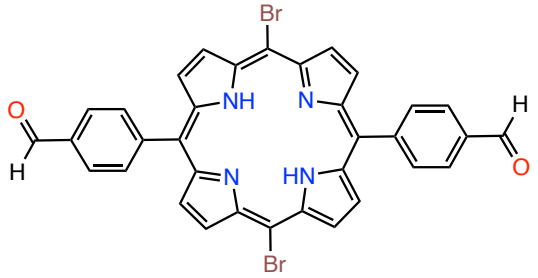
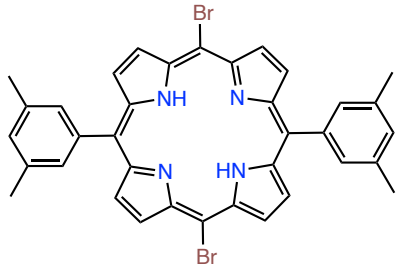
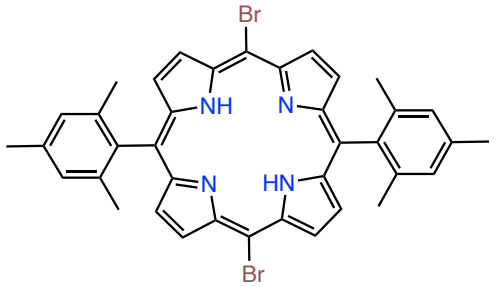
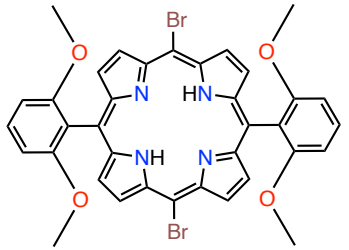
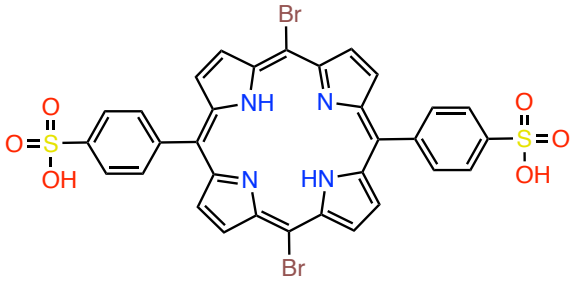
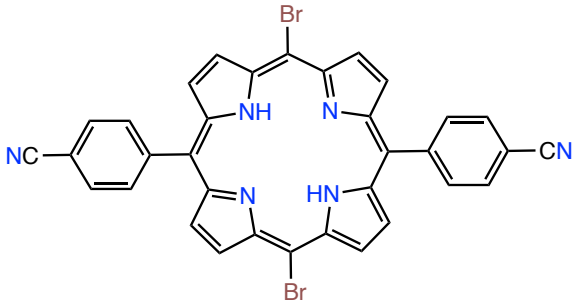
Substituted Functional Groups

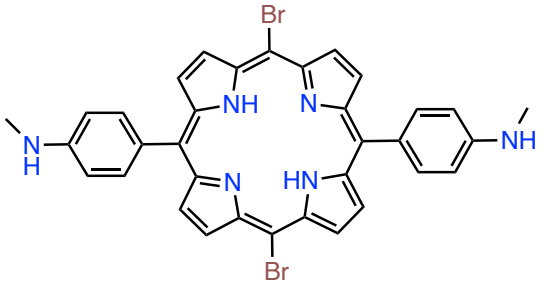
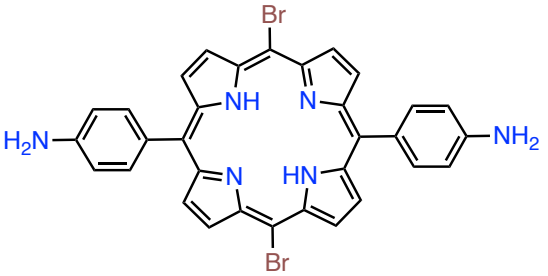
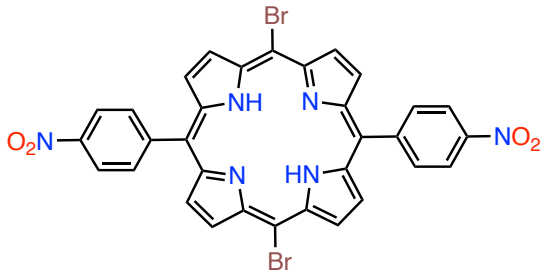
No.FG	Smiles string for free-based one	Structure
1. H	BrC1=C2C=C/C(N2)=C/C(C=C3)=NC3=C(Br)C4=CC=C(N4)C=C5C=CC1=N5	
2. Py	Br/C1=C2C=C/C(N2)=C(C3=CC=NC=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=NC=C6)=C7C=CC1=N/7	
3. 1,2-dihydropyridine (DHP)	Br/C1=C2C=C/C(N2)=C(C3=CCNC=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CCNC=C6)=C7C=CC1=N/7	

4. 4-ethynylpyridine (C2Py)	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	
5. Ph	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	
6. benzoic acid (p-CP)	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	

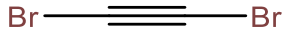
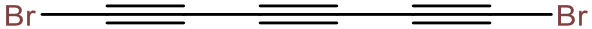
7. m-CP	Br/C1=C2C=C/C(N2)=C(C3=CC(C(O)=O)=CC=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=CC(C(O)=O)=C6)=C7C=CC1=N/7	
8. phenol (PhOH)	Br/C1=C2C=C/C(N2)=C(C3=CC=C(O)C=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC=C(O)C=C6)=C7C=CC1=N/7	
9. benzene-1,2,3-triol (Ph3OH)	Br/C1=C2C=C/C(N2)=C(C3=CC(O)=C(O)C(O)=C3)/C(C=C/4)=NC4=C(Br)/C5=CC=C(N5)/C(C6=CC(O)=C(O)C(O)=C6)=C7C=C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

10. benzaldehyde (PhCHO)	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	
11. *m*-xylene Ar(Ph2Me)	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	
12. mesitylene Ar(Ph3Me)	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	

13. 1,3-dimethoxybenzene Ar(Ph2OMe)	Br/C1=C2C=C/C(N2)=C(C(C=C/3)=NC3=C(C4=CC=C(/C(C5=C(OC)C=CC=C5OC)=C6C=CC1=N/6)N4)\Br)\C7=C(OC)C=CC=C7OC	
14. benzenesulfonic acid (BSA)	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	
15. benzonitrile (PhCN)	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	

16. *N*-methylaniline (NMA)	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	
17. Aniline (PhNH2)	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	
18. Nitrobenzene (PhNO2)	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	

Linker

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