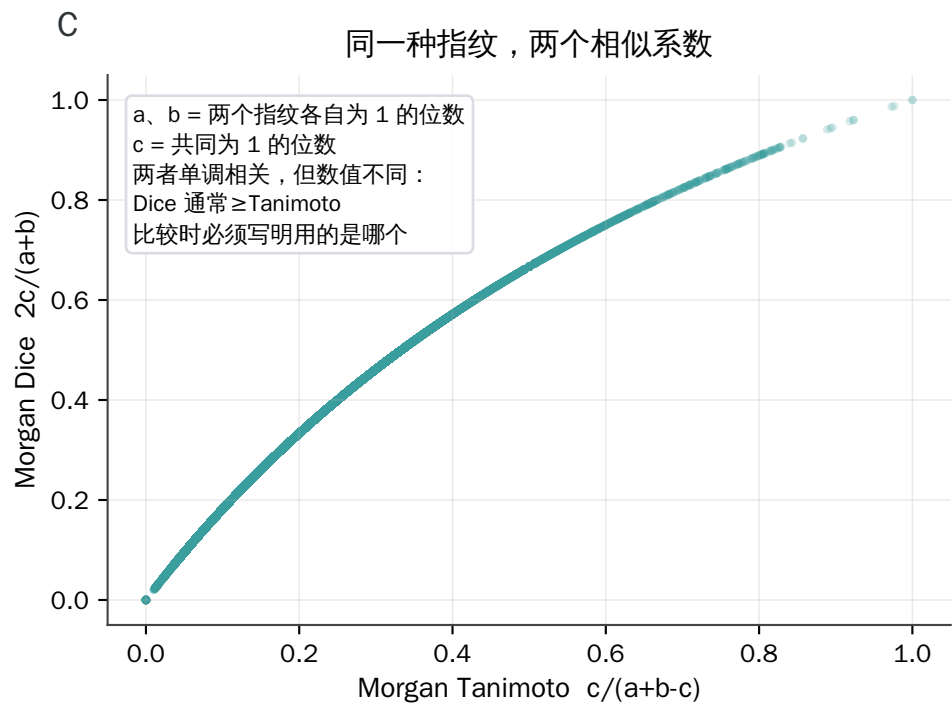
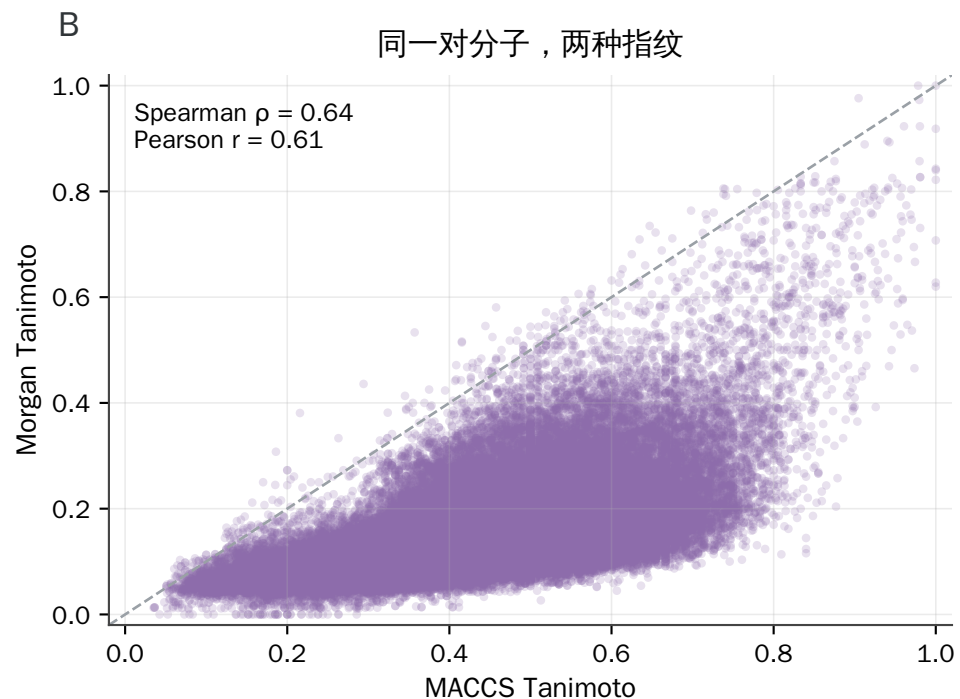
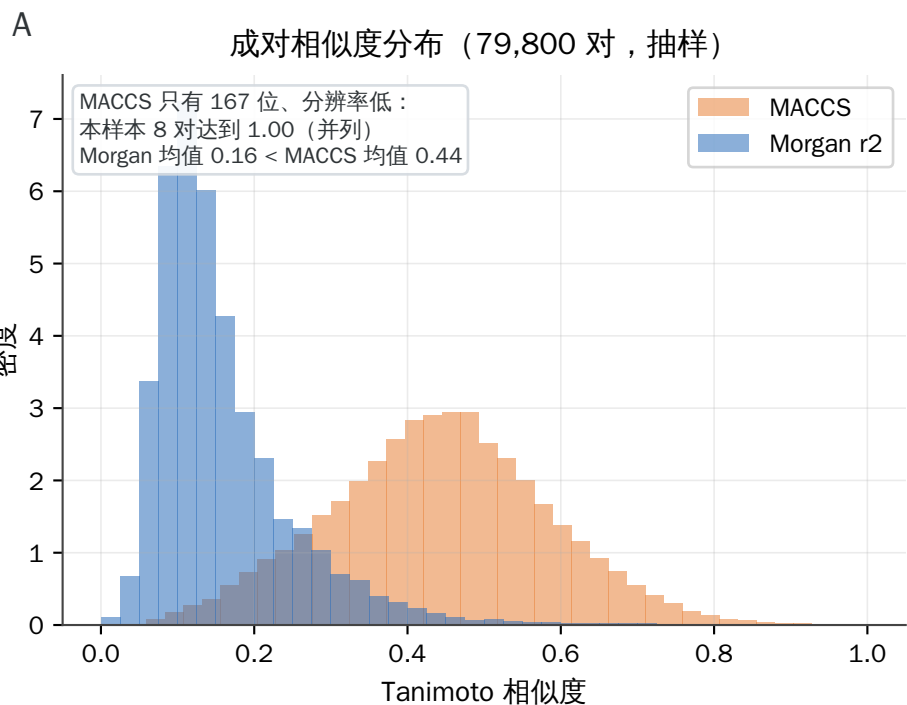


指纹相似性：表示决定排序



D gefitinib 的近邻：换指纹 → 换名单

MACCS 近邻		Morgan r2 近邻	
CHEMBL14699	1.00	CHEMBL14699	0.92
CHEMBL25610	1.00	CHEMBL299672	0.86
CHEMBL384699	1.00	CHEMBL291514	0.84
CHEMBL24137	1.00	CHEMBL57758	0.78
CHEMBL385479	1.00	CHEMBL2425092	0.78
CHEMBL56142	0.97	CHEMBL384699	0.78
CHEMBL99024	0.95	CHEMBL300791	0.77
CHEMBL291514	0.95	CHEMBL56142	0.77

前 8 名中只有 4 个重合 → 相似性依赖表示