

legend: \$RMSE/MAE/R^2\$

	maximum absorption wavelength	maximum emission wavelength
group by	alone: 34.461/19.472/0.877 both peaks:	alone: 45.489/28.923/0.754 both peaks: 44.013/27.212/0.77
smiles	38.617/19.973/0.845	
random	alone: 17.53/9.418/0.968 both peaks: 17.989/10.228/0.967	alone: 23.644/14.608/0.937 both peaks: 23.999/15.105/0.935
scaffold	alone: 30.167/21.226/0.905 both peaks: 31.049/23.227/0.9	alone: 41.404/31.308/0.825 both peaks: 38.486/29.621/0.849