

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

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