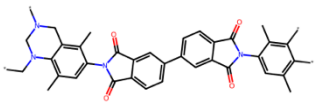
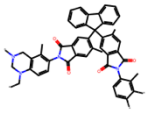
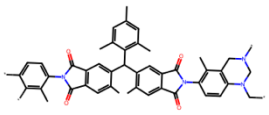
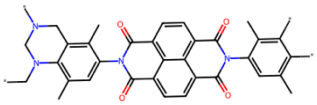
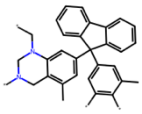
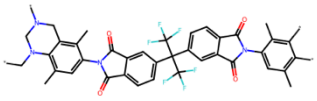
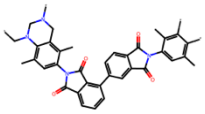
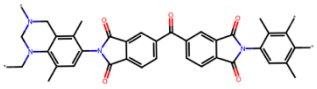
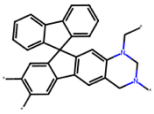
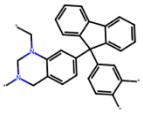
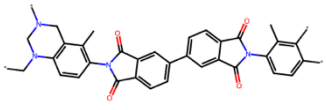
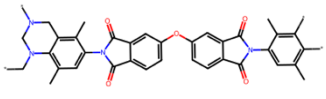
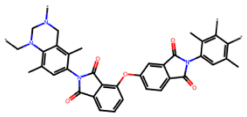
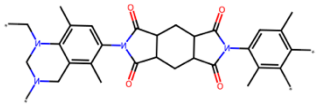
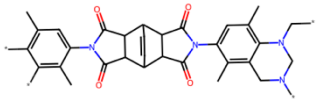
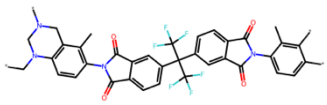
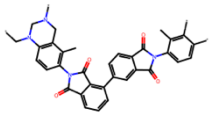
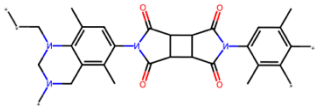
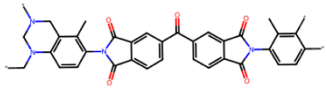
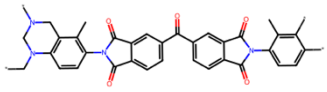
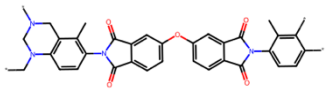
Predicted fractional free volume (FFV) of PIMs

Note: This RF model predicted the FFV of the PIM structure in this work to be approximately 0.40, positioning it within the top 20% among a series of PIMs.

Index	SMILES	Repeat units	Predicted FFV
1	*CN1CN(*)Cc2c(C)c(N3C(=O)c4ccc(-c5ccc6c(c5)C(=O)N(c5cc(C)c(*)c(*)c5C)C6=O)cc4C3=O)cc(C)c21		0.40550893
2	*CN1CN(*)Cc2c1ccc(N1C(=O)c3cc(C)c(C4(c5cc6c(cc5C)C(=O)N(c5ccc(*)c(*)c5C)C6=O)c5ccccc5-c5ccccc54)cc3C1=O)c2C		0.40217199
3	*CN1CN(*)Cc2c1ccc(N1C(=O)c3cc(C)c(C(c4cc5c(cc4C)C(=O)N(c4ccc(*)c(*)c4C)C5=O)c4c(C)cc(C)cc4C)cc3C1=O)c2C		0.39995992
4 (This work)	*CN1CN(*)Cc2c(C)c(N3C(=O)c4ccc5c6c(ccc(c46)C3=O)C(=O)N(c3cc(C)c(*)c(*)c3C)C5=O)cc(C)c21		0.39931013
5	*CN1CN(*)Cc2c(C)cc(C3(c4cc(*)c(*)c(C)c4)c4ccccc4-c4ccccc43)cc21		0.39914182
6	*CN1CN(*)Cc2c(C)c(N3C(=O)c4ccc(C(c5ccc6c(c5)C(=O)N(c5cc(C)c(*)c(*)c5C)C6=O)(C(F)(F)F)C(F)(F)F)cc4C3=O)cc(C)c21		0.39881561
7	*CN1CN(*)Cc2c(C)c(N3C(=O)c4cccc(-c5ccc6c(c5)C(=O)N(c5cc(C)c(*)c(*)c5C)C6=O)c4C3=O)cc(C)c21		0.39667466
8	*CN1CN(*)Cc2c(C)c(N3C(=O)c4ccc(C(=O)c5ccc6c(c5)C(=O)N(c5cc(C)c(*)c(*)c5C)C6=O)cc4C3=O)cc(C)c21		0.39617291
9	*CN1CN(*)Cc2cc3c(cc21)C1(c2ccccc2-c2ccccc21)c1cc(*)c(*)cc1-3		0.39494237
10	*CN1CN(*)Cc2ccc(C3(c4ccc(*)c(*)c4)c4ccccc4-c4ccccc43)cc21		0.39436355
11	*CN1CN(*)Cc2c1ccc(N1C(=O)c3ccc(-c4ccc5c(c4)C(=O)N(c4ccc(*)c(*)c4C)C5=O)cc3C1=O)c2C		0.39416606
12	*CN1CN(*)Cc2c(C)c(N3C(=O)c4ccc(Oc5ccc6c(c5)C(=O)N(c5cc(C)c(*)c(*)c5C)C6=O)cc4C3=O)cc(C)c21		0.39357151

13	*CN1CN(*)Cc2c(C)c(N3C(=O)c4cccc(Oc5ccc6c(c5)C(=O)N(c5cc(C)c(*)c(*)c5C)C6=O)c4C3=O)cc(C)c21		0.39126067
14	*CN1CN(*)Cc2c(C)c(N3C(=O)C4CC5C(=O)N(c6cc(C)c(*)c(*)c6C)C(=O)C5CC4C3=O)cc(C)c21		0.39091107
15	*CN1CN(*)Cc2c(C)c(N3C(=O)C4C5C(=O)N(c6cc(C)c(*)c(*)c6C)C(=O)C5C4C3=O)cc(C)c21		0.39051714
16	*CN1CN(*)Cc2c1ccc(N1C(=O)c3ccc(C(c4ccc5c(c4)C(=O)N(c4ccc(*)c(*)c4C)C5=O)(C(F)(F)F)C(F)(F)F)cc3C1=O)c2C		0.3900206
17	*CN1CN(*)Cc2c1ccc(N1C(=O)c3cccc(-c4ccc5c(c4)C(=O)N(c4ccc(*)c(*)c4C)C5=O)c3C1=O)c2C		0.38929529
18	*CN1CN(*)Cc2c(C)c(N3C(=O)C4C5C=CC(C6C(=O)N(c7cc(C)c(*)c(*)c7C)C(=O)C56)C4C3=O)cc(C)c21		0.38691941
19	*CN1CN(*)Cc2c1ccc(N1C(=O)c3ccc(C(=O)c4ccc5c(c4)C(=O)N(c4ccc(*)c(*)c4C)C5=O)cc3C1=O)c2C		0.38526852
20	*CN1CN(*)Cc2c1ccc(N1C(=O)c3cccc(Oc4ccc5c(c4)C(=O)N(c4ccc(*)c(*)c4C)C5=O)c3C1=O)c2C		0.38371944
21	*CN1CN(*)Cc2c1ccc(N1C(=O)c3ccc(Oc4ccc5c(c4)C(=O)N(c4ccc(*)c(*)c4C)C5=O)cc3C1=O)c2C		0.38238191