Table 1. CSP structure rankings[‡] with different PCM models for the crystal structures predicted in this study.

PCM model	CSD Refcode								
ε[§]	DHURAC10	PAHYON01	URACIL	QOPYOK	BCOCHY	BEPNIT01	ADUQOF*	DAFFIZ01*	YOPKOE*
1	1	1	5	3	4	9	1	2	3
2	1	1	2	3	4	9	1	2	4
3	1	1	1	4	4	9	1	2	4
4	1	1	1	4	4	9	1	2	4
8	1	1	1	4	4	10	1	2	4
11	1	1	1	4	2	10	1	2	4
80	1	1	1	4	2	12	1	2	4

[‡] A structure ranking of 1 indicates that the experimental structure was predicted as global energy minimum. [§] Dielectric constant used for the PCM calculation. ε = 1 is the gas phase calculation. [*] Rankings were done on chiral space groups only since these are chiral molecules crystallising in enantiopure crystal structures.