Supplementary information for

β-Cyclodextrin dimethylformamide 12.5 hydrate: a deeper insight into *β*-cyclodextrin crystal packing

Rubén Granero-García and Francesca P. A. Fabbiani*

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Section S1 Structure coordinates of *β*-CD·DMF 12.5 hydrate from invariom refinement used in the CLPCRY calculation.

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Section S2 $P2_1$ structures used in the XPAC calculation with unit-cell parameters, guest and number of water molecules of hydration. Structures highlighted in grey are those in which the *a* axis is longer than the *c* axis. In all the cases the *b* axis is the shortest axis, with the exception of the refcode highlighted in yellow.

	a **/Å**	***b*** **/Å**	***c*** **/Å**	***β*** **/°**	**V /Å³**	**Guest**	**Hydration number**
ARUXIU	15.1711(3)	10.16870(10)	20.9862(4)	110.92	3024.13	formic acid	7.7
ARUXOA	15.263(4)	10.157(2)	21.044(5)	110.698(4)	3051.81	acetic acid	7.7
BCDEXD03	21.283(5)	10.322(1)	15.092(5)	112.41(1)	3065.07		12.26
BCDEXD04	21.161(7)	10.254(1)	15.110(7)	111.91(2)	3041.83		11.56
BCDEXD05	21.233(5)	10.294(1)	15.103(4)	112.22(1)	3055.96		11.89
BCDEXD10	21.29(2)	10.33(1)	15.10(2)	112.3(5)	3072.51		12
BOBPEN	21.25(3)	10.28(2)	15.30(2)	113.25(9)	3070.86	hydrogen iodide	8
BOBPIR	21.03(3)	10.11(2)	15.33(2)	111.02(9)	3042.47	methanol	6.5
BUVSEQ01	21.080(7)	10.197(1)	15.131(6)	111.58(2)	3024.47		11.19
DEBGOG	15.356(3)	10.101(2)	21.287(3)	112.81(1)	3043.63	benzyl alcohol	5
DEWCOY	15.4244(16)	10.1574(11)	20.557(2)	110.074(2)	3025.04	benzamide	6
DIRVOP	15.285(3)	10.345(2)	20.118(2)	102.14(1)	3109.98	hexamethylenetetramine	6
GUXZOO	15.1220(4)	10.3350(2)	20.9150(3)	109.575(3)	3079.8	*m*-aminophenol	7.5
HAQNUK	15.274(12)	10.178(8)	20.961(16)	110.251(7)	3057.14	1,4-dioxane	7
IZALEB	15.0678(9)	10.2126(6)	20.9653(13)	111.7473(12)	2996.55	nicotinic acid	7.65
KIJSEC	15.1977(7)	10.1763(5)	20.6943(6)	109.239(4)	3021.76	succinic acid	7
KOBRIC	15.223(5)	10.578(3)	20.204(6)	108.37(7)	3087.64	potassium hydroxide	8
KUTKOZ	21.199(12)	9.973(3)	15.271(8)	110.87(3)	3016.74	1,4-butanediol	6.25
LADBAV	15.15(2)	10.343(15)	20.93(3)	109.69(4)	3087.89	pentanedioic acid	4.2
LADQOX	20.82(1)	10.366(6)	14.968(9)	110.12(4)	3033.26	diaqua-dichloro-copper(II)	8.9
MIFHAK	15.231(3)	10.068(3)	21.117(3)	110.16(5)	3039.81	squaric acid	6.65
NUFVEQ	20.8314(9)	10.2937(6)	15.2155(8)	110.733(2)	3051.4	pyrazinamide	5.5
NUFVIU	20.95040(10)	10.2493(2)	15.1424(3)	108.7630(10)	3078.69	piperazine	7.2
PIJGIY	21.212(1)	10.021(3)	15.208(1)	111.47(3)	3008.38	ethylene glycol	8
PIJGOE	21.322(6)	9.954(1)	15.251(6)	111.20(1)	3017.8	glycerol	7.2
POBRON	20.857(6)	10.158(1)	15.140(6)	110.94(1)	2995.79		9.35
POBRON01	15.107(7)	10.242(3)	20.911(8)	110.27(3)	3035.1		9
POVSIC	20.042(6)	10.378(2)	15.123(9)	102.30(2)	3073.32	*trans*-cyclohexane-1,4-diol	5.4
SUJDAD	20.8353(4)	9.93970(10)	15.2043(3)	110.630(2)	2946.85		10.41
TUSHUL	15.1667(5)	10.1850(3)	20.9694(7)	110.993(2)	3024.2		7.5
UPULEX	20.7890	10.2084	15.1091	110.8250	2997.01	4-aminobenzoic acid	10
VACZIJ	15.1550(3)	10.2850(2)	20.9056(5)	109.86	3064.74	dimethylsulfoxide	7.35
VOJLIQ	15.2196(10)	10.2279(7)	20.9321(14)	110.9270(10)	3043.45	*p*-aminobenzoic acid	5
XEGTAF	10.601(4)	26.402(9)	15.586(6)	93.145(6)	4355.76	6'-Methoxycinchonan-9-ol	16.5
YIYSII	21.310	9.987	15.247	111.85	3011.8	diethanolamine	6.4
YIYSOO	21.451	10.014	15.240	111.25	3051.12	1,5-pentanediol	6.2
ZIGZIY	20.988(9)	10.092(2)	15.223(10)	110.30(6)	3024.13	but-2-yne-1,4-diol	7
β-CD·DMF	15.500(3)	9.794(2)	21.689(5)	90.138(3)	3292.5(12)	dimethylformamide	12.5

Section S3 Hydrogen-bond distances (in Å) and angles (in °) in the structure of *β*-CD·DMF 12.5 hydrate.

H bond	*D*–H	H···*A*	*D*···*A*	*D*–H···*A*
O2_1—H2O_1…O3_9^{1_545}	0.84	1.95	2.785(6)	173.5
O3_1—H3O_1…O2_7	0.84	1.98	2.816(5)	177.7
O6_1—H6O_1…O7_9	0.84	1.81	2.643(11)	170.8
O6'_1—H6O'_1…O8'_9^{2_646}	0.84	2.10	2.92(6)	169
O2_2—H2O_2…O1_8^{1_545}	0.84	1.92	2.707(6)	154.4
O3_2—H3O_2…O2_1	0.84	2.10	2.791(5)	138.6
O6_2—H6O_2…O4_9	0.84	1.95	2.733(6)	154.0
O2_3—H2O_3…O2_9	0.84	1.82	2.638(5)	162.5
O3_3—H3O_3…O2_2	0.84	2.01	2.828(5)	163.9
O6_3—H6O_3…O9_9	0.84	1.93	2.743(9)	161.6
O6_3—H6O_3…O9'_9	0.84	1.97	2.784(18)	162.6
O2_4—H2O_4…O10_9	0.84	2.03	2.711(9)	137.7
O2_4—H2O_4…O10'_9	0.84	1.90	2.691(8)	155.6
O3_4—H3O_4…O2_9	0.84	1.90	2.723(5)	165.3
O6_4—H6O_4…O1_9	0.84	1.86	2.688(6)	166.9
O2_5—H2O_5…O6_6^{2_645}	0.84	1.94	2.776(5)	173.6
O3_5—H3O_5…O2_4	0.84	1.86	2.689(5)	168.3
O6_5—H6O_5…O3_6^{2_655}	0.84	2.01	2.835(5)	169.4
O2_6—H2O_6…O3_7	0.84	2.08	2.916(5)	171.1
O3_6—H3O_6…O2_5	0.84	2.04	2.875(5)	174.2
O6_6—H6O_6…O2_7^{1_565}	0.84	2.40	3.188(5)	156.0
O2_7—H2O_7…O6_9^{1_545}	0.84	1.94	2.733(6)	158.2
O3_7—H3O_7…O3_5^{2_645}	0.84	1.90	2.743(5)	177.9
O6_7—H6O_7…O6_4^{1_455}	0.84	1.98	2.786(5)	161.9
O1_9—H1A_9…O3_1^{1_665}	0.84(3)	1.93(3)	2.766(5)	173(6)
O1_9—H1B_9…O2_3^{1_565}	0.85(3)	1.87(4)	2.652(5)	151(6)
O2_9—H2A_9…O6_9^{1_645}	0.86(3)	1.96(4)	2.721(6)	147(6)
O2_9—H2B_9…O6_5^{1_545}	0.87(3)	1.86(4)	2.686(5)	157(6)
O3_9—H3A_9…O6_3^{2_656}	0.91(3)	1.90(4)	2.776(6)	161(6)
O3_9—H3B_9…O11'_9	0.90(3)	2.04(4)	2.93(2)	170(7)
O3_9—H3B_9…O11"_9	0.90(3)	1.90(4)	2.770(9)	162(7)
O4_9—H4A_9…O3_2^{2_656}	0.86(3)	2.03(3)	2.842(6)	159(7)
O5_9—H5A_9…O6_4^{1_455}	0.89(3)	1.84(4)	2.685(6)	156(7)
O5_9—H5B_9…O6_1	0.86(3)	1.96(5)	2.676(7)	139(7)
O6_9—H6A_9…O6_7	0.88(3)	1.87(3)	2.748(6)	176(7)
O6_9—H6B_9…O10'_9^{2_655}	0.88(3)	1.73(4)	2.549(9)	153(7)
O6_9—H6B_9…O10"_9^{2_655}	0.88(3)	2.09(4)	2.931(9)	159(7)
O7_9—H7A_9…O12_9^{2_556}	0.87(3)	2.05(13)	2.552(19)	116(11)
O7_9—H7A_9…O12'_9^{2_556}	0.87(3)	1.91(7)	2.739(18)	159(14)
O7_9—H7B_9…O12"_9	0.86(3)	2.39(16)	2.832(18)	112(13)
O8_9—H8A_9…O6_2^{2_656}	0.85(7)	2.10(8)	2.819(13)	143(7)
O8_9—H8B_9…O2_2^{1_565}	0.87(11)	2.17(11)	3.007(12)	163(11)
O8'_9—H8A_9…O6_2^{2_656}	0.91(7)	2.10(8)	2.78(2)	131(6)
O8'_9—H8B'_9…O7_9^{2_656}	0.87(6)	1.63(10)	2.30(2)	131(16)
O9_9—H9A_9…O5_9^{1_655}	0.85(5)	2.01(5)	2.832(10)	162(5)
O9_9—H9B_9…O11"_9^{2_646}	0.86(3)	2.07(7)	2.829(13)	147(10)
O9'_9—H9A_9…O5_9^{1_655}	0.89(6)	2.01(5)	2.762(18)	141(5)
O9'_9—H9B'_9…O8_9	0.89(14)	2.31(18)	3.14(2)	157(17)

Section S4 Results of the CLPDIM calculation.

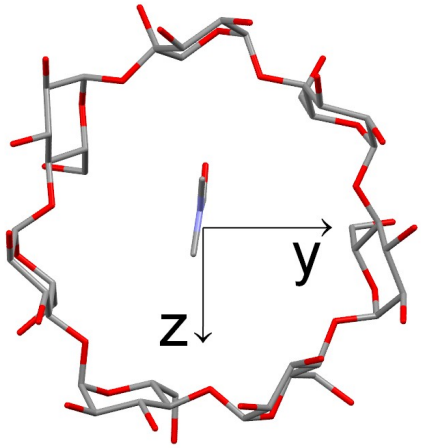

Figure S4.1 Cartesian reference system used in the CLPDIM calculation.

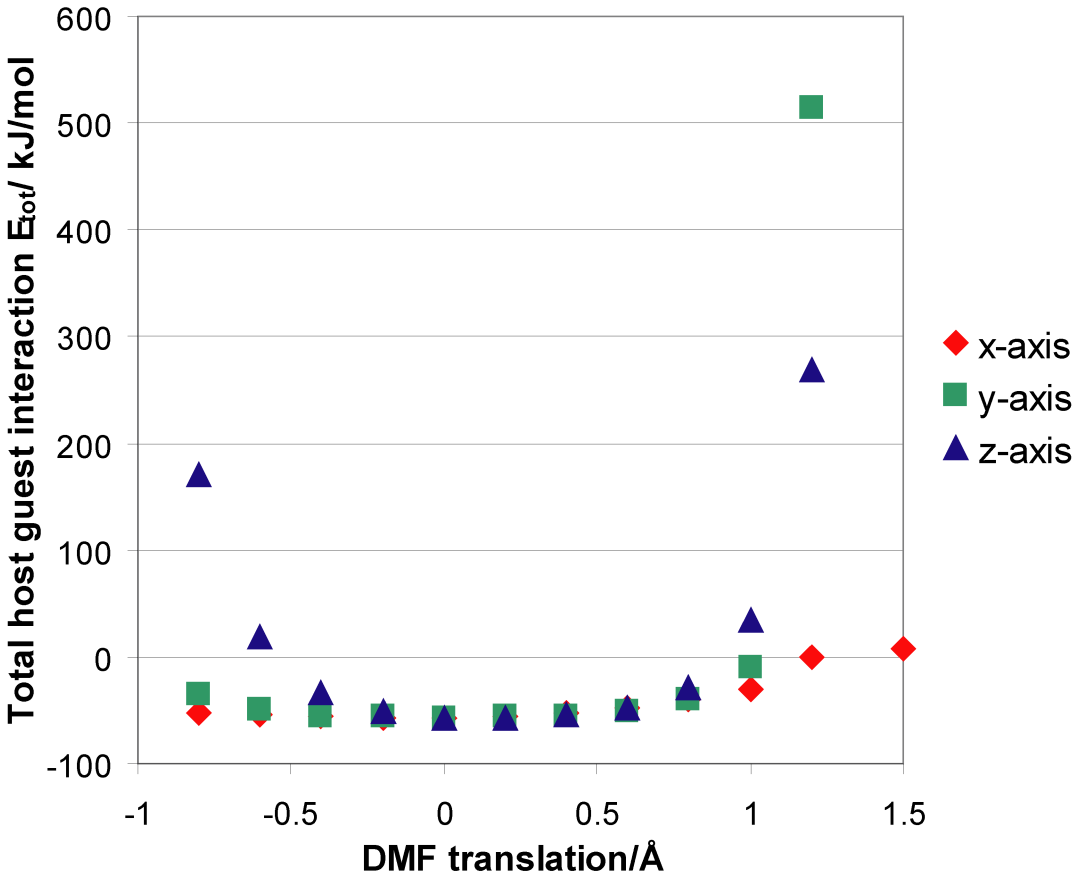

Figure S4.2 Total host-guest interaction energies for translations (along the *x*-, *y*- and *z*-axes) of the DMF with respect to the β-CD cavity, as illustrated in Figure S4.1. The point of zero translation corresponds to the the host-guest geometry observed experimentally.

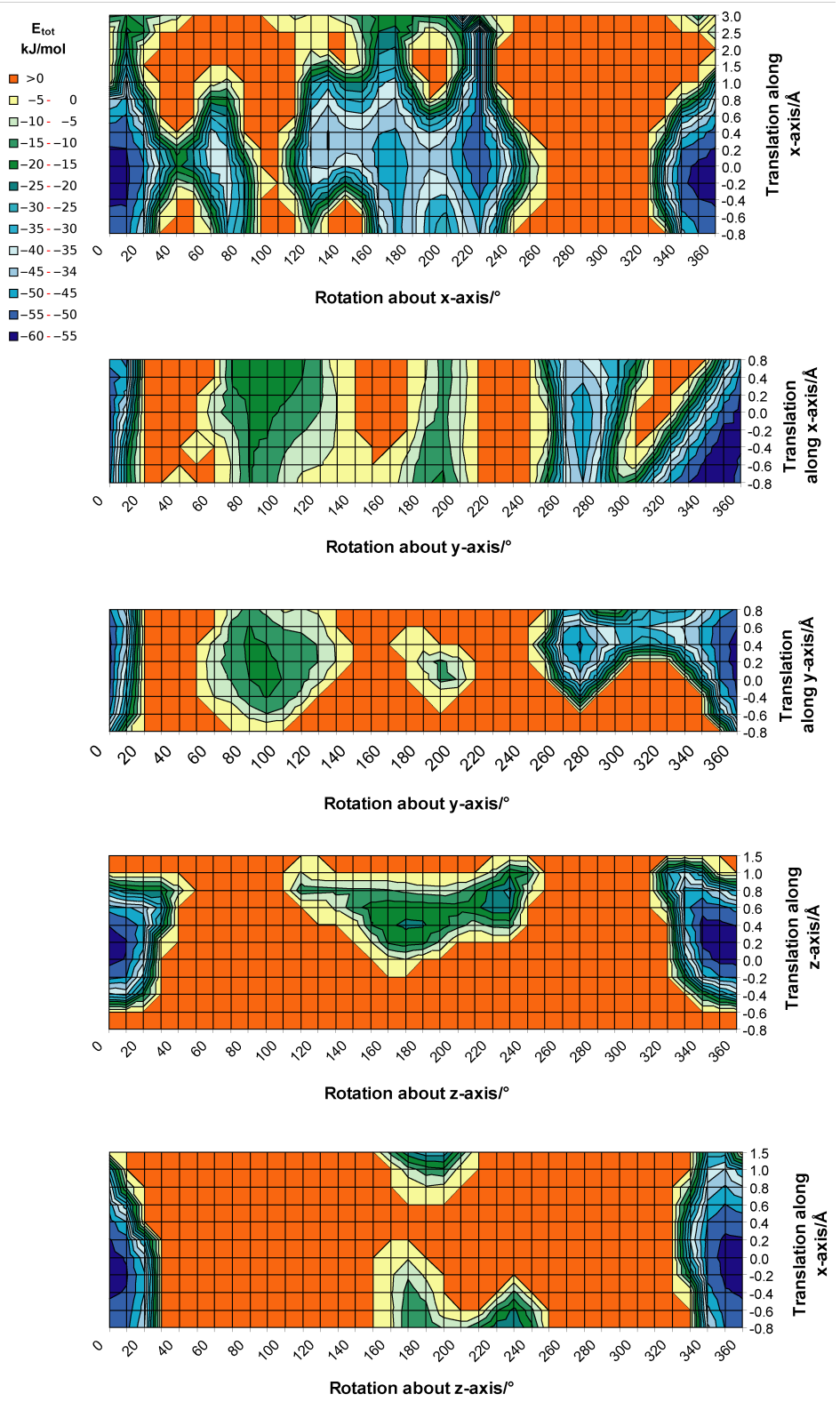

Figure S4.3 Total host-guest interaction energies for the combination of translations and rotations (along and about the *x*-, *y*- and *z*-axes) of the DMF with respect to the *β*-CD. Energy values are colour coded.

Section S5 Complete data from the XPAC calculation.

Parameters for each comparison:

SCA X D n p δ(a) δ(p)	

SCA	Number of dimensions in which there is a similarity (No, 1D, 2D or 3D)
X	Dissimilarity index
D	Stretch parameter (in Å)
n	Number of neighbours
p	Number of points per molecule
δ(a)	Mean difference between angles (in °)
δ(a)	Mean difference between interplanar angles (in °)

	ARUXIU	ARUXOA	BCDEXD03	BCDEXD04	BCDEXD05	BCDEXD10	BOBPEN	BOBPIR	BUVSEQ01	DEBGOG	DEWCOY	DIRVOP
ARUXIU												
ARUXOA	3D 0.6 0.1 14 21 0.3 0.6											
BCDEXD03	3D 1.3 0.1 12 21 0.7 1.1	3D 1.5 0.1 12 21 0.7 1.3										
BCDEXD04	3D 0.8 0.1 12 21 0.4 0.7	3D 1.1 0.1 12 21 0.5 1	3D 0.6 0.1 12 21 0.3 0.5									
BCDEXD05	3D 1.1 0.1 12 21 0.5 1	3D 1.3 0.1 12 21 0.6 1.1	3D 0.4 0 12 21 0.2 0.3	3D 0.3 0 12 21 0.2 0.3								
BCDEXD10	3D 1.6 0.1 12 21 0.7 1.4	3D 1.7 0.1 12 21 0.8 1.5	3D 0.6 0 12 21 0.2 0.6	3D 0.9 0 12 21 0.4 0.8	3D 0.7 0 12 21 0.2 0.6							
BOBPEN	3D 3.1 0.1 14 21 1.3 2.9	3D 3 0.1 14 21 1.2 2.7	3D 3.8 0.1 12 21 1.5 3.5	3D 3.5 0.1 12 21 1.4 3.2	3D 3.7 0.1 12 21 1.4 3.4	3D 4 0.1 12 21 1.5 3.6						
BOBPIR	3D 1 0.1 14 21 0.5 0.9	3D 1 0.1 14 21 0.4 0.9	3D 2.1 0.2 12 21 1.1 1.8	3D 1.6 0.2 12 21 0.8 1.4	3D 1.9 0.2 12 21 0.9 1.6	3D 2.3 0.2 12 21 1.1 2	3D 3 0.2 14 21 1.3 2.7					
BUVSEQ01	3D 0.6 0 14 21 0.2 0.5	3D 0.9 0.1 14 21 0.4 0.8	3D 0.9 0.1 12 21 0.5 0.8	3D 0.4 0 12 21 0.2 0.4	3D 0.7 0.1 12 21 0.4 0.6	3D 1.2 0.1 12 21 0.5 1.1	3D 3.4 0.1 14 21 1.3 3.1	3D 1.4 0.1 14 21 0.7 1.2				
DEBGOG	3D 2.1 0.2 14 21 1 1.9	3D 2.1 0.1 14 21 1 1.9	3D 3.3 0.3 12 21 1.6 2.8	3D 2.8 0.3 12 21 1.4 2.5	3D 3.1 0.3 12 21 1.5 2.7	3D 3.5 0.3 12 21 1.7 3	3D 3.5 0.2 14 21 1.6 3	3D 1.5 0.1 14 21 0.7 1.3	3D 2.5 0.2 14 21 1.2 2.2			
DEWCOY	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -		
DIRVOP	1D 7.2 0.2 2 21 4.5 5.6	1D 7.4 0.2 2 21 4.7 5.8	1D 7 0 2 21 4.4 5.5	1D 7.1 0.1 2 21 4.4 5.5	1D 7.1 0.1 2 21 4.4 5.5	1D 7.3 0 2 21 4.5 5.7	1D 7.8 0.1 2 21 4.9 6.1	1D 7.7 0.2 2 21 4.7 6.1	1D 7.1 0.1 2 21 4.4 5.6	1D 7.8 0.2 2 21 4.8 6.2	No - - - - - -	
GUXZOO	3D 1.3 0.1 12 21 0.7 1.1	3D 1.4 0.1 12 21 0.7 1.3	3D 0.4 0 12 21 0.1 0.4	3D 0.7 0.1 12 21 0.3 0.6	3D 0.5 0 12 21 0.2 0.4	3D 0.7 0 12 21 0.2 0.6	3D 3.8 0.1 12 21 1.5 3.5	3D 2.1 0.2 12 21 1.1 1.8	3D 1 0.1 12 21 0.5 0.8	3D 3.3 0.3 12 21 1.6 2.8	No - - - - - -	1D 7.1 0 2 21 4.4 5.6
HAQNUK	3D 1.2 0.1 14 21 0.5 1.1	3D 1 0 14 21 0.4 0.9	3D 1.2 0.1 12 21 0.6 1.1	3D 1.1 0.1 12 21 0.5 1	3D 1.2 0.1 12 21 0.5 1	3D 1.5 0.1 12 21 0.7 1.3	3D 3.3 0.1 14 21 1.3 3	3D 1.7 0.1 14 21 0.7 1.6	3D 1.1 0.1 14 21 0.5 1	3D 2.9 0.2 14 21 1.3 2.6	No - - - - - -	1D 7.3 0.2 2 21 4.6 5.7
IZALEB	3D 1 0.1 14 21 0.4 0.9	3D 1.2 0.1 14 21 0.5 1.1	3D 0.8 0.1 12 21 0.4 0.7	3D 0.6 0.1 12 21 0.2 0.6	3D 0.6 0.1 12 21 0.3 0.6	3D 1.1 0.1 12 21 0.5 1	3D 3.6 0.1 14 21 1.4 3.2	3D 1.8 0.2 14 21 0.8 1.6	3D 0.7 0.1 14 21 0.3 0.6	3D 2.9 0.3 14 21 1.4 2.5	No - - - - - -	1D 7.1 0.1 2 21 4.4 5.5
KIJSEC	3D 2.5 0.1 14 21 1 2.3	3D 2.2 0.1 14 21 0.9 2	3D 2.3 0.1 12 21 1 2.1	3D 2.4 0.1 12 21 1 2.2	3D 2.4 0.1 12 21 0.9 2.2	3D 2.6 0.1 12 21 1 2.3	3D 3.3 0.1 14 21 1.3 3.1	3D 2.9 0.2 14 21 1.2 2.6	3D 2.5 0.1 14 21 1 2.3	3D 3.8 0.3 14 21 1.7 3.4	No - - - - - -	1D 7.3 0.2 2 21 4.8 5.5
KOBRIC	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -
KUTKOZ	3D 2 0.1 14 21 0.8 1.8	3D 1.9 0.1 14 21 0.7 1.8	3D 2.7 0.2 12 21 1.2 2.4	3D 2.3 0.2 12 21 1 2.1	3D 2.5 0.2 12 21 1.1 2.3	3D 2.8 0.2 12 21 1.2 2.5	3D 3.7 0.2 14 21 1.5 3.3	3D 1.3 0.1 14 21 0.5 1.2	3D 2.2 0.1 14 21 0.9 2	3D 2 0.1 14 21 0.9 1.8	No - - - - - -	1D 8.2 0.4 2 21 4.9 6.6
LADBAV	3D 1.6 0.1 12 21 0.7 1.4	3D 1.6 0.1 12 21 0.7 1.4	3D 1.1 0 12 21 0.4 1	3D 1.2 0.1 12 21 0.5 1.1	3D 1.1 0 12 21 0.4 1	3D 1.2 0 12 21 0.4 1.2	3D 4 0.1 12 21 1.5 3.7	3D 2.2 0.2 12 21 1.1 1.9	3D 1.4 0.1 12 21 0.6 1.2	3D 3.3 0.3 12 21 1.6 2.9	No - - - - - -	1D 7.3 0 2 21 4.5 5.7
LADQOX	3D 1.8 0.1 12 21 0.8 1.6	3D 2.1 0.2 12 21 1 1.8	3D 1 0.1 12 21 0.5 0.9	3D 1.2 0.1 12 21 0.5 1.1	3D 1.1 0.1 12 21 0.5 1	3D 1.3 0.1 12 21 0.6 1.1	3D 4.3 0.1 12 21 1.7 4	3D 2.6 0.2 12 21 1.2 2.3	3D 1.4 0.1 12 21 0.7 1.3	3D 3.6 0.3 12 21 1.8 3.2	No - - - - - -	1D 6.7 0 2 21 4.1 5.3
MIFHAK	3D 1.6 0.1 14 21 0.7 1.5	3D 1.2 0.1 14 21 0.5 1.1	3D 1.8 0.1 12 21 0.8 1.6	3D 1.7 0.1 12 21 0.7 1.5	3D 1.8 0.1 12 21 0.8 1.6	3D 1.9 0.1 12 21 0.9 1.7	3D 3.5 0.1 14 21 1.5 3.2	3D 1.9 0.1 14 21 0.7 1.7	3D 1.7 0.1 14 21 0.7 1.5	3D 2.9 0.2 14 21 1.2 2.6	No - - - - - -	1D 7.8 0.3 2 21 4.9 6
NUFVEQ	3D 1.1 0 12 21 0.5 1	3D 1.2 0.1 12 21 0.5 1.1	3D 1 0.1 12 21 0.5 0.8	3D 0.9 0.1 12 21 0.4 0.7	3D 0.9 0.1 12 21 0.4 0.8	3D 1.3 0.1 12 21 0.6 1.1	3D 3.6 0.1 12 21 1.3 3.3	3D 1.7 0.1 12 21 0.8 1.5	3D 0.9 0 12 21 0.4 0.8	3D 2.8 0.2 12 21 1.3 2.4	No - - - - - -	1D 7.2 0.1 2 21 4.5 5.7
NUFVIU	3D 1.8 0.2 12 21 0.9 1.6	3D 1.8 0.2 12 21 0.9 1.5	3D 0.9 0.1 12 21 0.4 0.8	3D 1.2 0.1 12 21 0.6 1.1	3D 1.1 0.1 12 21 0.5 0.9	3D 1.2 0.1 12 21 0.5 1.1	3D 3.8 0.1 12 21 1.5 3.5	3D 2.5 0.2 12 21 1.2 2.1	3D 1.5 0.1 12 21 0.7 1.3	3D 3.6 0.3 12 21 1.8 3.1	No - - - - - -	1D 7 0.1 2 21 4.4 5.5
PIJGIY	3D 1.1 0.1 14 21 0.4 1	3D 0.9 0.1 14 21 0.3 0.8	3D 2.1 0.2 12 21 0.9 1.9	3D 1.6 0.1 12 21 0.6 1.5	3D 1.9 0.1 12 21 0.8 1.7	3D 2.2 0.1 12 21 0.9 2	3D 3 0.1 14 21 1.3 2.7	3D 0.7 0.1 14 21 0.4 0.6	3D 1.4 0.1 14 21 0.5 1.3	3D 1.9 0.2 14 21 0.9 1.6	No - - - - - -	1D 7.8 0.3 2 21 4.8 6.2
PIJGOE	3D 1.3 0.1 14 21 0.5 1.2	3D 1.1 0.1 14 21 0.4 1	3D 2.2 0.2 12 21 1 2	3D 1.8 0.2 12 21 0.8 1.6	3D 2 0.2 12 21 0.9 1.8	3D 2.3 0.2 12 21 1 2.1	3D 3.2 0.2 14 21 1.4 2.8	3D 1.1 0.1 14 21 0.5 1	3D 1.6 0.1 14 21 0.6 1.5	3D 2.1 0.2 14 21 0.9 1.8	No - - - - - -	1D 7.9 0.4 2 21 4.8 6.2
POBRON	3D 0.7 0 14 21 0.3 0.7	3D 1.2 0.1 14 21 0.5 1.1	3D 1.7 0.2 12 21 0.8 1.4	3D 1.2 0.1 12 21 0.5 1	3D 1.4 0.1 12 21 0.7 1.2	3D 1.8 0.2 12 21 0.9 1.6	3D 3.4 0.2 14 21 1.3 3.1	3D 1.2 0.1 14 21 0.6 1.1	3D 0.8 0.1 14 21 0.4 0.7	3D 2.1 0.2 14 21 1 1.9	No - - - - - -	1D 7.2 0.2 2 21 4.4 5.7
POBRON01	3D 0.8 0.1 12 21 0.4 0.7	3D 1 0.1 12 21 0.5 0.9	3D 0.7 0.1 12 21 0.3 0.6	3D 0.4 0 12 21 0.1 0.4	3D 0.5 0 12 21 0.2 0.5	3D 0.9 0.1 12 21 0.4 0.8	3D 3.6 0.1 12 21 1.4 3.2	3D 1.6 0.2 12 21 0.8 1.4	3D 0.5 0 12 21 0.2 0.5	3D 2.8 0.3 12 21 1.4 2.4	No - - - - - -	1D 7.1 0.1 2 21 4.4 5.6
POVSIC	1D 7.3 0.2 2 21 4.4 5.8	1D 9.8 0.6 4 21 4.9 8.5	1D 9.4 0.5 4 21 4.6 8.2	1D 7.1 0.1 2 21 4.3 5.7	1D 9.5 0.5 4 21 4.7 8.2	1D 9.7 0.5 4 21 4.8 8.4	1D 9.8 0.5 4 21 4.8 8.4	1D 7.8 0.3 2 21 4.6 6.2	1D 7.2 0.2 2 21 4.3 5.7	1D 10.3 0.6 4 21 5.3 8.8	No - - - - - -	3D 1.9 0.1 14 21 0.8 1.7
SUJDAD	3D 1.4 0.1 14 21 0.6 1.2	3D 1.5 0.1 14 21 0.6 1.4	3D 2.5 0.2 12 21 1.2 2.2	3D 2 0.2 12 21 0.9 1.8	3D 2.3 0.2 12 21 1.1 2	3D 2.7 0.2 12 21 1.3 2.4	3D 3.1 0.2 14 21 1.4 2.8	3D 0.8 0.1 14 21 0.3 0.8	3D 1.7 0.1 14 21 0.8 1.5	3D 1.7 0.2 14 21 0.7 1.5	No - - - - - -	1D 7.7 0.4 2 21 4.7 6.2
TUSHUL	3D 0.3 0 14 21 0.1 0.3	3D 0.8 0.1 14 21 0.3 0.7	3D 1.3 0.1 12 21 0.6 1.1	3D 0.8 0.1 12 21 0.4 0.7	3D 1.1 0.1 12 21 0.5 0.9	3D 1.5 0.1 12 21 0.7 1.3	3D 3.2 0.1 14 21 1.3 2.9	3D 1.1 0.1 14 21 0.5 0.9	3D 0.6 0 14 21 0.2 0.5	3D 2.2 0.2 14 21 1.1 2	No - - - - - -	1D 7.2 0.2 2 21 4.5 5.7
UPULEX	1D 18.4 0.1 2 21 7.4 16.8	1D 18.9 0.2 2 21 7.5 17.3	1D 18 0 2 21 7.7 16.3	1D 18.1 0 2 21 7.5 16.5	1D 18.1 0 2 21 7.6 16.4	1D 18.3 0 2 21 7.8 16.6	1D 19 0.1 2 21 9.7 16.3	1D 18.7 0.2 2 21 7.3 17.3	1D 18.2 0 2 21 7.4 16.6	1D 19.1 0.1 2 21 9.8 16.5	No - - - - - -	No - - - - - -
VACZIJ	3D 1.3 0.1 12 21 0.6 1.2	3D 1.4 0.1 12 21 0.6 1.2	3D 0.6 0.1 12 21 0.3 0.5	3D 0.7 0 12 21 0.3 0.7	3D 0.6 0 12 21 0.2 0.5	3D 0.9 0 12 21 0.4 0.8	3D 3.8 0.1 12 21 1.4 3.5	3D 2 0.2 12 21 1 1.8	3D 1 0.1 12 21 0.4 0.9	3D 3.2 0.3 12 21 1.5 2.8	No - - - - - -	1D 7 0.1 2 21 4.4 5.5
VOJLIQ	3D 0.6 0 14 21 0.3 0.5	3D 0.6 0 14 21 0.3 0.6	3D 1.2 0.1 12 21 0.7 1	3D 0.8 0.1 12 21 0.4 0.7	3D 1 0.1 12 21 0.6 0.9	3D 1.5 0.1 12 21 0.7 1.3	3D 3.2 0.1 14 21 1.3 2.9	3D 1.1 0.1 14 21 0.5 1	3D 0.6 0.1 14 21 0.3 0.6	3D 2.2 0.2 14 21 1 1.9	No - - - - - -	1D 7.3 0.1 2 21 4.5 5.7
XEGTAF	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	1D 8.8 0.4 2 21 5.7 6.7	No - - - - - -
YIYSII	3D 1.7 0.1 14 21 0.6 1.6	3D 1.6 0.1 14 21 0.5 1.5	3D 2.4 0.2 12 21 0.9 2.2	3D 2.1 0.1 12 21 0.7 1.9	3D 2.2 0.1 12 21 0.8 2.1	3D 2.5 0.1 12 21 0.9 2.3	3D 3.3 0.1 14 21 1.3 3	3D 1.5 0.1 14 21 0.6 1.3	3D 2 0.1 14 21 0.7 1.8	3D 2.4 0.2 14 21 1.2 2.1	No - - - - - -	1D 7.9 0.4 2 21 4.9 6.3
YIYSOO	3D 2.3 0.1 14 21 0.9 2.1	3D 2 0.1 14 21 0.7 1.8	3D 2.8 0.2 12 21 1.1 2.6	3D 2.6 0.2 12 21 1 2.4	3D 2.7 0.2 12 21 1.1 2.5	3D 2.9 0.2 12 21 1.1 2.7	3D 3.7 0.2 14 21 1.5 3.3	3D 1.7 0.1 14 21 0.7 1.5	3D 2.4 0.1 14 21 0.9 2.3	3D 2.4 0.2 14 21 1.1 2.1	No - - - - - -	1D 8.6 0.3 2 21 5.2 6.8
ZIGZIY	3D 2 0.1 14 21 0.9 1.8	3D 2 0.1 14 21 0.8 1.8	3D 2.7 0.2 12 21 1.3 2.3	3D 2.4 0.2 12 21 1.1 2.1	3D 2.6 0.2 12 21 1.2 2.2	3D 2.8 0.2 12 21 1.4 2.5	3D 3.7 0.2 14 21 1.7 3.2	3D 1.4 0 14 21 0.6 1.3	3D 2.2 0.1 14 21 1 1.9	3D 2 0.1 14 21 0.7 1.8	No - - - - - -	1D 8 0.3 2 21 4.9 6.3
β-CD·DMF	1D 8 0.4 4 21 4 6.9	1D 8.3 0.4 4 21 4.2 7.1	1D 7.9 0.6 4 21 4 6.8	1D 7.9 0.5 4 21 4 6.8	1D 7.9 0.5 4 21 4 6.8	1D 8 0.6 4 21 4.1 6.8	2D 10.4 0.5 6 21 5.5 8.8	1D 8.4 0.4 4 21 4.2 7.2	1D 7.9 0.4 4 21 4 6.8	1D 8.6 0.3 4 21 4.3 7.4	No - - - - - -	2D 8.9 0.4 8 21 4.2 7.7

	GUXZOO	HAQNUK	IZALEB	KIJSEC	KOBRIC	KUTKOZ	LADBAV	LADQOX	MIFHAK	NUFVEQ	NUFVIU	PIJGIY
HAQNUK	3D 1.3 0.1 12 21 0.6 1.1											
IZALEB	3D 0.8 0.1 12 21 0.4 0.7	3D 1 0.1 14 21 0.5 0.9										
KIJSEC	3D 2.4 0.1 12 21 1 2.2	3D 1.8 0.1 14 21 0.7 1.7	3D 2.3 0.1 14 21 0.9 2.1									
KOBRIC	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -								
KUTKOZ	3D 2.7 0.2 12 21 1.2 2.4	3D 2.5 0.1 14 21 0.9 2.3	3D 2.6 0.2 14 21 1 2.4	3D 3.6 0.2 14 21 1.4 3.3	No - - - - - -							
LADBAV	3D 1 0 12 21 0.3 0.9	3D 1.5 0.1 12 21 0.6 1.3	3D 1.2 0.1 12 21 0.5 1.1	3D 2.6 0.1 12 21 1 2.4	No - - - - - -	3D 2.7 0.2 12 21 1.2 2.4						
LADQOX	3D 1 0.1 12 21 0.5 0.8	3D 1.9 0.2 12 21 0.9 1.7	3D 1.2 0.1 12 21 0.6 1.1	3D 2.9 0.1 12 21 1.3 2.6	No - - - - - -	3D 3.3 0.2 12 21 1.4 2.9	3D 1.4 0.1 12 21 0.6 1.3					
MIFHAK	3D 1.8 0.1 12 21 0.8 1.6	3D 1.3 0.1 14 21 0.5 1.2	3D 1.8 0.1 14 21 0.8 1.6	3D 2.1 0.1 14 21 0.9 1.9	No - - - - - -	3D 2.2 0.1 14 21 0.8 2	3D 1.9 0.1 12 21 0.8 1.7	3D 2.5 0.2 12 21 1.1 2.2				
NUFVEQ	3D 1 0.1 12 21 0.5 0.8	3D 1 0.1 12 21 0.4 0.9	3D 0.7 0.1 12 21 0.4 0.6	3D 2.3 0.1 12 21 0.9 2.2	No - - - - - -	3D 2.6 0.1 12 21 1 2.3	3D 1.3 0.1 12 21 0.6 1.1	3D 1.4 0.1 12 21 0.8 1.2	3D 1.8 0.1 12 21 0.7 1.6			
NUFVIU	3D 0.9 0.1 12 21 0.4 0.8	3D 1.5 0.1 12 21 0.7 1.3	3D 1.4 0.1 12 21 0.6 1.2	3D 2.1 0.1 12 21 0.9 1.9	No - - - - - -	3D 2.9 0.2 12 21 1.3 2.6	3D 1.3 0.1 12 21 0.5 1.2	3D 1.4 0.1 12 21 0.7 1.2	3D 1.8 0.1 12 21 0.9 1.6	3D 1.4 0.1 12 21 0.7 1.2		
PIJGIY	3D 2.1 0.1 12 21 0.9 1.9	3D 1.6 0.1 14 21 0.6 1.5	3D 1.8 0.1 14 21 0.7 1.7	3D 2.8 0.1 14 21 1.1 2.5	No - - - - - -	3D 1.3 0.1 14 21 0.5 1.1	3D 2.1 0.1 12 21 0.9 1.9	3D 2.7 0.2 12 21 1.1 2.4	3D 1.6 0 14 21 0.6 1.5	3D 1.8 0.1 12 21 0.7 1.7	3D 2.3 0.2 12 21 1 2.1	
PIJGOE	3D 2.2 0.2 12 21 1 2	3D 1.8 0.1 14 21 0.7 1.6	3D 2 0.2 14 21 0.8 1.9	3D 2.8 0.2 14 21 1.1 2.5	No - - - - - -	3D 1.2 0 14 21 0.5 1.1	3D 2.2 0.2 12 21 1 2	3D 2.8 0.2 12 21 1.2 2.5	3D 1.4 0.1 14 21 0.5 1.3	3D 2.1 0.1 12 21 0.8 1.9	3D 2.4 0.2 12 21 1.1 2.1	3D 0.7 0.1 14 21 0.3 0.7
POBRON	3D 1.6 0.2 12 21 0.8 1.4	3D 1.7 0.1 14 21 0.7 1.5	3D 1.2 0.1 14 21 0.5 1.1	3D 3 0.1 14 21 1.2 2.7	No - - - - - -	3D 2.1 0.1 14 21 0.8 1.9	3D 1.9 0.1 12 21 0.9 1.7	3D 1.9 0.2 12 21 0.9 1.7	3D 2.2 0.1 14 21 0.9 2	3D 1.4 0.1 12 21 0.6 1.2	3D 2.2 0.2 12 21 1 1.9	3D 1.5 0.1 14 21 0.6 1.4
POBRON01	3D 0.6 0.1 12 21 0.3 0.5	3D 1.1 0.1 12 21 0.5 1	3D 0.6 0.1 12 21 0.2 0.6	3D 2.4 0.1 12 21 1 2.2	No - - - - - -	3D 2.3 0.2 12 21 0.9 2.1	3D 1.1 0.1 12 21 0.4 1	3D 1.2 0.1 12 21 0.6 1.1	3D 1.6 0.1 12 21 0.7 1.4	3D 0.8 0.1 12 21 0.4 0.7	3D 1.2 0.1 12 21 0.6 1.1	3D 1.6 0.1 12 21 0.6 1.5
POVSIC	1D 9.5 0.5 4 21 4.6 8.2	1D 9.7 0.6 4 21 4.8 8.4	1D 7.1 0.2 2 21 4.3 5.7	1D 9.4 0.6 4 21 4.7 8.1	No - - - - - -	1D 10.7 0.7 4 21 5.3 9.3	1D 9.7 0.5 4 21 4.8 8.4	1D 6.7 0 2 21 4 5.4	1D 10.2 0.6 4 21 5.1 8.8	1D 7.3 0.1 2 21 4.4 5.8	1D 9.2 0.5 4 21 4.4 8	1D 10.2 0.7 4 21 5.1 8.8
SUJDAD	3D 2.5 0.2 12 21 1.2 2.2	3D 2.3 0.2 14 21 0.9 2.1	3D 2.2 0.2 14 21 1 1.9	3D 3.4 0.2 14 21 1.4 3.1	No - - - - - -	3D 1.3 0.1 14 21 0.5 1.2	3D 2.7 0.2 12 21 1.2 2.4	3D 3 0.2 12 21 1.3 2.6	3D 2.3 0.1 14 21 0.9 2.1	3D 2.2 0.1 12 21 1 2	3D 2.9 0.3 12 21 1.4 2.5	3D 1.1 0.1 14 21 0.5 1
TUSHUL	3D 1.3 0.1 12 21 0.6 1.1	3D 1.3 0.1 14 21 0.5 1.1	3D 1 0.1 14 21 0.4 0.9	3D 2.6 0.1 14 21 1 2.3	No - - - - - -	3D 1.9 0.1 14 21 0.8 1.8	3D 1.6 0.1 12 21 0.7 1.4	3D 1.8 0.1 12 21 0.8 1.6	3D 1.6 0.1 14 21 0.7 1.5	3D 1.1 0 12 21 0.5 0.9	3D 1.8 0.2 12 21 0.9 1.5	3D 1.2 0.1 14 21 0.5 1.1
UPULEX	1D 18.1 0 2 21 7.7 16.4	1D 18.8 0.2 2 21 7.7 17.2	1D 18.3 0 2 21 7.6 16.7	1D 18.6 0 2 21 9.5 16	No - - - - - -	1D 19.5 0.2 2 21 9.9 16.8	1D 18.5 0 2 21 7.8 16.8	1D 17.6 0.1 2 21 7.3 16	1D 19.1 0.1 2 21 9.7 16.5	1D 18.4 0.1 2 21 7.6 16.8	1D 17.9 0 2 21 7.8 16.1	1D 18.9 0.1 2 21 7.5 17.4
VACZIJ	3D 0.6 0 12 21 0.3 0.5	3D 1.1 0.1 12 21 0.5 1	3D 0.8 0.1 12 21 0.3 0.7	3D 2.3 0.1 12 21 0.9 2.1	No - - - - - -	3D 2.7 0.2 12 21 1.1 2.4	3D 1.1 0 12 21 0.4 1	3D 1.1 0.1 12 21 0.6 0.9	3D 1.8 0.1 12 21 0.8 1.6	3D 0.7 0.1 12 21 0.3 0.7	3D 0.9 0.1 12 21 0.4 0.8	3D 2 0.1 12 21 0.8 1.9
VOJLIQ	3D 1.2 0.1 12 21 0.7 1	3D 1 0 14 21 0.4 0.9	3D 0.8 0.1 14 21 0.4 0.7	3D 2.3 0.1 14 21 0.9 2.1	No - - - - - -	3D 2.1 0.1 14 21 0.8 1.9	3D 1.4 0.1 12 21 0.7 1.2	3D 1.8 0.1 12 21 0.9 1.5	3D 1.6 0.1 14 21 0.6 1.4	3D 0.8 0 12 21 0.3 0.7	3D 1.7 0.2 12 21 0.9 1.4	3D 1.3 0.1 14 21 0.5 1.2
XEGTAF	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	1D 6.6 0.4 2 21 2.1 6.2	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -
YIYSII	3D 2.4 0.1 12 21 0.9 2.2	3D 2.1 0.1 14 21 0.6 2	3D 2.3 0.1 14 21 0.8 2.1	3D 3 0.1 14 21 1.1 2.8	No - - - - - -	3D 1.3 0.1 14 21 0.6 1.2	3D 2.4 0.1 12 21 0.9 2.2	3D 3.1 0.2 12 21 1.2 2.8	3D 2 0 14 21 0.7 1.9	3D 2.2 0.1 12 21 0.8 2.1	3D 2.5 0.2 12 21 1 2.3	3D 1.3 0 14 21 0.4 1.2
YIYSOO	3D 2.8 0.2 12 21 1.1 2.6	3D 2.5 0.1 14 21 0.9 2.3	3D 2.8 0.2 14 21 1.1 2.6	3D 3.3 0.2 14 21 1.3 3.1	No - - - - - -	3D 1.1 0.1 14 21 0.5 1	3D 2.8 0.2 12 21 1.1 2.5	3D 3.5 0.3 12 21 1.4 3.2	3D 1.9 0.1 14 21 0.6 1.8	3D 2.7 0.2 12 21 1 2.5	3D 2.9 0.2 12 21 1.2 2.7	3D 1.4 0.1 14 21 0.5 1.2
ZIGZIY	3D 2.7 0.2 12 21 1.3 2.3	3D 2.5 0.1 14 21 1.1 2.3	3D 2.5 0.2 14 21 1.1 2.2	3D 3.6 0.2 14 21 1.5 3.2	No - - - - - -	3D 1.7 0.1 14 21 0.6 1.6	3D 2.7 0.2 12 21 1.3 2.3	3D 3.1 0.2 12 21 1.5 2.8	3D 2.4 0.1 14 21 1 2.2	3D 2.5 0.1 12 21 1.1 2.2	3D 3 0.2 12 21 1.5 2.5	3D 1.6 0.1 14 21 0.7 1.4
β-CD·DMF	1D 7.9 0.6 4 21 4 6.8	1D 8.3 0.5 4 21 4.2 7.1	1D 7.9 0.4 4 21 4 6.8	2D 10 0.4 6 21 5.4 8.4	No - - - - - -	1D 8.7 0.3 4 21 4.4 7.5	1D 8.1 0.6 4 21 4.1 7	1D 7.5 0.5 4 21 3.7 6.4	1D 8.4 0.4 4 21 4.3 7.2	1D 8.1 0.5 4 21 4.1 6.9	1D 7.9 0.6 4 21 4 6.8	1D 8.5 0.4 4 21 4.3 7.3

	PIJGOE	POBRON	POBRON01	POVSIC	SUJDAD	TUSHUL	UPULEX	VACZIJ	VOJLIQ	XEGTAF	YIYSII	YIYSOO	ZIGZIY	β-CD·DMF
POBRON	3D 1.7 0.1 14 21 0.7 1.5													
POBRON01	3D 1.8 0.2 12 21 0.7 1.6	3D 1.2 0.1 12 21 0.5 1												
POVSIC	1D 10.3 0.7 4 21 5.1 8.8	1D 7.2 0.2 2 21 4.3 5.8	1D 7.2 0.1 2 21 4.3 5.7											
SUJDAD	3D 1.2 0.1 14 21 0.5 1.1	3D 1.4 0.1 14 21 0.6 1.3	3D 2 0.2 12 21 0.9 1.8	3D 7.8 0.4 2 21 4.5 6.4										
TUSHUL	3D 1.4 0.1 14 21 0.6 1.3	3D 0.7 0 14 21 0.3 0.7	3D 0.8 0.1 12 21 0.4 0.7	1D 7.3 0.2 2 21 4.4 5.8	3D 1.4 0.1 14 21 0.6 1.2									
UPULEX	1D 18.9 0.1 2 21 7.5 17.4	1D 18 0 2 21 7.2 16.5	1D 18.2 0 2 21 7.5 16.6	No - - - - - -	1D 18.3 0.1 2 21 7.1 16.9	1D 18.4 0.1 2 21 7.4 16.8								
VACZIJ	3D 2.2 0.2 12 21 0.9 2	3D 1.6 0.1 12 21 0.7 1.4	3D 0.7 0 12 21 0.3 0.6	1D 9.4 0.5 4 21 4.6 8.1	3D 2.5 0.2 12 21 1.1 2.2	3D 1.3 0.1 12 21 0.6 1.1	1D 18.1 0 2 21 7.6 16.4							
VOJLIQ	3D 1.6 0.1 14 21 0.6 1.4	3D 1.1 0.1 14 21 0.5 0.9	3D 0.8 0.1 12 21 0.4 0.6	1D 7.3 0.2 2 21 4.4 5.8	3D 1.7 0.1 14 21 0.7 1.5	3D 0.7 0 14 21 0.3 0.6	1D 18.5 0.1 2 21 7.5 16.9	3D 1.1 0.1 12 21 0.5 1						
XEGTAF	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -	No - - - - - -					
YIYSII	3D 1.2 0 14 21 0.5 1.1	3D 2 0.1 14 21 0.8 1.9	3D 2 0.1 12 21 0.7 1.9	1D 10.3 0.7 4 21 5.1 8.9	3D 1.7 0.1 14 21 0.8 1.5	3D 1.7 0.1 14 21 0.6 1.6	1D 19.1 0.2 2 21 9.7 16.4	3D 2.4 0.1 12 21 0.8 2.2	3D 1.9 0.1 14 21 0.6 1.7	No - - - - - -				
YIYSOO	3D 1.4 0 14 21 0.5 1.3	3D 2.6 0.2 14 21 1 2.4	3D 2.5 0.2 12 21 0.9 2.3	1D 11.1 0.6 4 21 5.5 9.6	3D 2 0.1 14 21 0.8 1.8	3D 2.3 0.1 14 21 0.9 2.1	1D 19.5 0.2 2 21 9.8 16.8	3D 2.8 0.2 12 21 1.1 2.6	3D 2.3 0.1 14 21 0.8 2.1	No - - - - - -	3D 1.5 0.1 14 21 0.6 1.4			
ZIGZIY	3D 1.8 0.1 14 21 0.7 1.7	3D 2.2 0.1 14 21 0.9 2	3D 2.3 0.2 12 21 1.1 2	1D 10.7 0.6 4 21 5.5 9.1	3D 1.6 0.1 14 21 0.6 1.5	3D 2 0.1 14 21 0.9 1.8	1D 18.9 0.1 2 21 7.4 17.4	3D 2.8 0.2 12 21 1.3 2.4	3D 2 0.1 14 21 0.8 1.8	No - - - - - -	3D 2.2 0.1 14 21 0.9 2	3D 2 0.1 14 21 0.8 1.8		
β-CD·DMF	1D 8.4 0.3 4 21 4.2 7.2	1D 7.8 0.3 4 21 3.9 6.8	1D 7.9 0.5 4 21 4 6.8	2D 9.4 0.4 8 21 4.4 8.3	1D 8.3 0.2 4 21 4.1 7.2	1D 8 0.4 4 21 4 6.9	No - - - - - -	1D 7.8 0.5 4 21 4 6.7	1D 8.2 0.4 4 21 4.1 7	No - - - - - -	1D 8.6 0.4 4 21 4.4 7.3	1D 9 0.4 4 21 4.6 7.8	1D 8.8 0.3 4 21 4.3 7.7	