SUPPLEMENTARY MATERIAL

Theoretical studies of interactions in cyprodinil–α-cyclodextrin and cyprodinil–β-cyclodextrin systems

Jakub T. Hołaj-Krzak ✉

Institute of Technology and Life Sciences – National Research Institute, Falenty, 3 Hrabska Avenue, 05-090 Raszyn, Poland

Table S1. Selected empirical structural parameters (bond lengths, *R*; angles, *α*; dihedral angles, *β*) of isolated cyprodinil molecules (C^0)

R		***α***		***β***	
bond	**value pm)**	**bond**	**value (°)**	**bond**	**value (°)**
N1–C2	134.1	N1–C2–N7	119.36	N1–C2–N7–C8	−8.01
C2–N7	136.6	C2–N7–C8	130.96	N1–C2–N7–H7a	172.01
C8–N7	140.4	C2–N7–H7a	114.55	C2–N7–C8–C9	−8.84
N7–H7a	88.0	C8–N7–H7a	114.50	H7a–N7–C8–C9	171.15

Source: own elaboration based on JEON *et al.* (2015).

Table S2. Selected empirical structural parameters (bond lengths, *R*; angles, *α*; dihedral angles, *β*) of isolated α-cyclodextrin molecules (α-CD)

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
O1–C2	137.8	C6–O1–C2	112.16	C6–O1–C2–O7	57.04
	141.8		115.16		56.99
	141.1		114.51		58.73
	144.9		113.20		54.95
	139.0		116.34		54.07
	142.5		112.34		57.26
C2–O7	143.7	O1–C2–C3	111.66	O7–C2–C3–O8	55.54
	141.2		110.16		58.58
	140.2		110.30		56.45
	138.8		106.25		59.84
	144.4		108.29		62.53
	140.3		110.01		59.95

cont. Tab. S2

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
C3–O8	141.1	O1–C2–O7	111.88	C2–C3–O8–H8a	−0.04
	137.8		110.48		179.70
	142.0		111.62		179.69
	143.1		110.93		–
	147.2		111.86		−0.53
	145.2		112.20		0.06
C4–O9	141.2	C3–C4–C5	109.96	O8–C3–C4–O9	68.56
	144.0		113.12		69.03
	143.1		109.52		64.98
	146.3		111.10		70.41
	145.8		107.94		59.05
	139.1		106.21		67.17
O8–H8a	82.1	C3–O8–H8a	109.48	C3–C4–O9–H9a	119.03
	82.0		109.45		−55.57
	81.9		109.44		179.97
	–		–		179.80
	81.8		109.51		120.63
	82.0		109.47		−179.75
O9–H9a	82.0	C4–O9–H9a	109.55	O9–C4–C5–O10	−69.00
	82.1		109.30		−72.39
	82.2		109.52		−73.67
	82.0		109.47		−72.95
	82.1		109.54		−71.03
	82.1		109.43		−71.05
C5–O10	140.1	C5–C6–O1	108.74	O10–C5–C6–C11	71.93
	144.2		109.97		78.41
	143.8		110.10		73.14
	143.1		111.14		78.26
	148.3		107.63		72.52
	142.8		111.71		73.04

cont. Tab. S2

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
C6–O1	144.7	C6–C5–O10	109.64	O10–C5–C6–O1	−175.19
	144.7		109.64		−163.23
	144.9		107.20		−168.04
	144.6		110.69		−168.88
	142.5		108.62		−168.56
	140.3		110.73		−166.71
C11–O12	144.6	C11–C6–O1	103.51	O1–C6–C11–O12	116.76
	144.0		104.82		−61.99
	143.7		105.81		−57.34
	150.2		100.62		−68.90
	144.1		108.91		61.54
	143.4		106.16		−56.94
O12–H12a	–	C11–O12–H12a	–	C6–C11–O12–H12a	–
	82.1		109.40		−179.86
	–		–		–
	–		–		–
	82.0		109.25		−58.51
	82.0		109.39		−59.83

Source: own elaboration based on SHA *et al.* (2016).

Table S3. Selected empirical structural parameters (bond lengths, *R*; angles, *α*; dihedral angles, *β*) of isolated β-cyclodextrin molecules (β-CD)

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
O1–C2	141.0	C6–O1–C2	114.20	C6–O1–C2–O7	57.96
	141.7		112.89		61.04
	140.1		114.57		59.38
	139.4		114.18		56.24
	143.1		113.30		61.63
	142.5		113.87		59.01
	140.8		114.68		58.14

cont. Tab. S3

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
C2–O7	142.6	O1–C2–C3	110.45	O7–C2–C3–O8	56.80
	143.5		111.17		52.70
	141.7		111.19		58.43
	142.7		109.75		59.26
	141.1		109.52		58.32
	140.8		109.20		57.05
	141.7		109.72		58.95
C3–O8	142.8	O1–C2–O7	110.34	C2–C3–O8–H8a	–
	144.2		109.76		–
	143.4		111.58		–
	142.5		110.73		–
	144.7		110.16		–
	145.2		111.24		–
	144.1		111.70		–
C4–O9	143.1	C3–C4–C5	109.38	O8–C3–C4–O9	66.75
	145.8		110.41		65.44
	143.5		106.10		62.87
	143.8		110.04		61.80
	142.8		109.42		60.59
	144.2		109.21		64.57
	144.1		109.42		63.21
O8–H8a	–	C3–O8–H8a	–	C3–C4–O9–H9a	–
	–		–		–
	–		–		–
	–		–		–
	–		–		–
	–		–		–
	–		–		–

cont. Tab. S3

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
O9–H9a	–	C4–O9–H9a	–	O9–C4–C5–O10	−67.02
	–		–		−64.96
	–		–		−66.72
	–		–		−67.29
	–		–		−62.94
	–		–		−63.71
	–		–		−69.17
C5–O10	144.0	C5–C6–O1	107.43	O10–C5–C6–C11	73.48
	145.2		107.26		62.25
	156.3		103.24		68.53
	144.6		110.54		73.41
	141.3		110.69		64.37
	143.5		107.73		67.23
	142.3		109.80		74.78
C6–O1	146.6	C6–C5–O10	108.94	O10–C5–C6–O1	−173.47
	145.5		109.34		−178.01
	145.1		101.62		−175.17
	141.8		108.16		−169.62
	144.0		110.30		−176.58
	145.3		109.80		−175.89
	146.8		107.94		−168.59
C11–O12	140.3	C11–C6–O1	104.17	O1–C6–C11–O12	70.95
	125.9		106.48		70.50
	143.1		105.57		−62.90
	140.5		105.83		64.72
	139.4		106.00		−70.97
	142.1		105.69		−61.08
	142.8		104.85		−60.79

cont. Tab. S3

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
O12–H12a	–	C11–O12–H12a	–	C6–C11–O12–H12a	–
	–		–		–
	–		–		–
	–		–		–
	–		–		–
	–		–		–
	–		–		–

Source: own elaboration based on LINDNER and SAENGER (1982).

Table S4. Selected theoretical structural parameters (bond lengths, *R*; angles, *α*; dihedral angles, *β*) of isolated molecules and cyprodinil ions (C^0, C^- C^+) [B3LYP/6-311++G(2d,2p)]

Parameter	**Value of parameter for**		
	C^0	**C^-**	**C^+**
***R* (pm)**			
N1–C2	133.4	138.0	130.6
C2–N7	137.4	132.2	150.2
C8–N7	140.0	136.9	149.1
N7–H7a	100.7	–	102.2
N7–H7b	–	–	102.1
***α* (°)**			
N1–C2–N7	120.63	122.84	114.14
C2–N7–C8	133.09	124.87	114.83
C2–N7–H7a	111.33	–	107.03
C8–N7–H7a	115.58	–	109.53
C2–N7–H7b	–	–	107.57
C8–N7–H7b	–	–	109.25
H7a–N7–H7b	–	–	108.44
***β* (°)**			
N1–C2–N7–C8	0.00	−12.81	88.46
N1–C2–N7–H7a	179.99	–	−149.74
N1–C2–N7–H7b	–	–	−33.38
C2–N7–C8–C9	0.01	−33.19	−95.41
H7a–N7–C8–C9	−179.99	–	144.16
H7b–N7–C8–C9	–	–	25.51

Source: own study.

Table S5. Selected theoretical structural parameters (bond lengths, *R*; angles, *α*; dihedral angles, *β*) of isolated α-cyclodextrin (α-CD) molecules [B3LYP/6-31++G(d,p)]

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
O1–C2	141.3	C6–O1–C2	114.49	C6–O1–C2–O7	55.19
	141.5		114.83		57.85
	142.5		114.63		59.15
	140.8		113.73		58.11
	142.9		114.69		57.08
	141.2		113.65		57.86
C2–O7	140.5	O1–C2–C3	108.23	O7–C2–C3–O8	55.92
	141.0		108.95		58.97
	140.4		109.35		59.85
	142.6		112.25		58.21
	139.7		108.36		59.62
	142.3		111.97		59.40
C3–O8	143.9	O1–C2–O7	112.18	C2–C3–O8–H8a	95.70
	142.9		111.16		−170.72
	142.6		111.45		−169.57
	141.6		111.08		−59.85
	142.1		111.69		−163.49
	141.2		110.71		−48.07
C4–O9	142.7	C3–C4–C5	112.05	O8–C3–C4–O9	64.92
	142.5		110.72		62.15
	142.1		110.87		62.94
	141.5		110.61		65.71
	143.2		112.37		59.03
	141.6		110.33		65.01
O8–H8a	96.6	C3–O8–H8a	109.66	C3–C4–O9–H9a	−60.98
	96.9		107.09		179.11
	96.9		107.22		175.35
	97.2		108.47		−178.46
	96.9		107.95		71.37
	97.4		109.53		−177.31

cont. Tab. S5

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
O9–H9a	96.8	C4–O9–H9a	107.93	O9–C4–C5–O10	−69.07
	97.4		108.32		−69.07
	97.7		109.27		−74.06
	97.4		108.79		−68.34
	96.9		109.83		−67.08
	97.3		108.71		−67.64
C5–O10	142.6	C5–C6–O1	110.69	O10–C5–C6–C11	74.12
	143.7		109.92		70.08
	143.6		111.63		73.78
	143.7		108.66		65.67
	142.3		111.34		76.29
	144.4		108.29		64.65
C6–O1	144.0	C6–C5–O10	111.00	O10–C5–C6–O1	−166.18
	144.2		110.34		−168.79
	144.4		108.24		−164.86
	144.6		109.50		−173.15
	145.0		110.46		−163.87
	144.5		109.82		−174.25
C11–O12	143.1	C11–C6–O1	106.65	O1–C6–C11–O12	70.68
	143.0		107.99		−73.18
	142.7		107.57		−70.44
	142.1		108.08		−87.62
	142.2		106.40		71.17
	142.5		108.09		−88.81
O12–H12a	96.5	C11–O12–H12a	108.77	C6–C11–O12–H12a	173.29
	96.5		108.27		−162.29
	96.5		109.04		−179.70
	97.1		107.93		−89.50
	96.7		109.95		−70.61
	97.1		107.45		−80.66

Source: own study.

Table S6. Selected theoretical structural parameters (bond lengths, *R*; angles, *α*; dihedral angles, *β*) of isolated β-cyclodextrin (β-CD) molecules [B3LYP/6-31++G(d,p)]

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
O1–C2	141.7	C6–O1–C2	115.93	C6–O1–C2–O7	63.49
	143.1		114.23		59.01
	141.3		115.22		56.67
	141.5		115.68		63.10
	141.3		114.64		60.65
	141.3		114.54		58.61
	141.0		115.10		60.65
C2–O7	141.2	O1–C2–C3	108.58	O7–C2–C3–O8	56.38
	140.2		108.44		55.89
	141.1		108.62		59.71
	140.8		109.61		53.21
	141.3		109.77		55.29
	141.3		109.34		58.17
	141.6		109.35		58.59
C3–O8	142.6	O1–C2–O7	111.51	C2–C3–O8–H8a	−167.63
	141.8		110.74		−175.30
	142.8		111.64		−170.44
	142.6		111.70		−171.24
	143.0		110.91		−174.77
	143.1		111.03		−172.75
	143.0		111.49		−168.19
C4–O9	141.9	C3–C4–C5	109.86	O8–C3–C4–O9	59.55
	142.0		110.85		63.40
	142.6		112.04		63.33
	142.3		109.85		61.43
	142.2		110.19		64.11
	142.2		110.92		63.72
	142.1		110.35		61.40

cont. Tab. S6

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
O8–H8a	97.0	C3–O8–H8a	107.02	C3–C4–O9–H9a	−178.93
	96.9		106.45		−166.53
	96.9		107.89		174.89
	97.0		106.73		−169.16
	96.9		106.80		167.28
	96.9		106.83		165.25
	97.0		107.02		168.65
O9–H9a	97.9	C4–O9–H9a	109.68	O9–C4–C5–O10	−68.37
	97.7		109.29		−67.89
	96.9		108.09		−70.18
	97.6		109.19		−64.87
	97.6		109.46		−67.41
	97.7		109.32		−71.53
	97.8		109.52		−71.49
C5–O10	142.9	C5–C6–O1	109.94	O10–C5–C6–C11	69.04
	143.4		108.08		62.88
	144.0		110.42		78.30
	143.2		108.28		63.61
	143.5		108.94		64.61
	143.3		110.57		70.90
	143.1		111.00		71.68
C6–O1	144.6	C6–C5–O10	109.58	O10–C5–C6–O1	−173.15
	144.6		109.78		−178.75
	144.1		113.91		−162.86
	144.2		109.84		−177.33
	144.4		111.06		−174.34
	144.1		111.05		−167.94
	144.2		109.50		−167.40

cont. Tab. S6

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
C11–O12	142.2	C11–C6–O1	105.36	O1–C6–C11–O12	62.61
	143.3		106.06		58.82
	142.9		105.03		−80.16
	142.4		106.91		80.24
	143.0		108.32		−71.56
	142.9		107.78		−71.03
	142.8		107.46		−70.74
O12–H12a	96.7	C11–O12–H12a	107.30	C6–C11–O12–H12a	−58.51
	96.7		106.59		−60.64
	96.4		109.46		155.60
	97.1		109.59		100.01
	96.5		108.17		−155.88
	96.5		108.82		−175.42
	96.5		108.92		−176.99

Source: own study.

Table S7. Selected theoretical structural parameters (bond lengths, *R*; angles, *α*; dihedral angles, *β*) of systems consisting of a molecule and cyprodinil ions with α-cyclodextrin (G4MP2)

Parameter	**C^0@α-CD**	**C^-@α-CD**	**C^+@α-CD**
***R* (pm)**			
N1–C2	133.7	135.7	131.4
C2–N7	137.6	135.4	147.4
C8–N7	138.9	138.4	147.7
N7–H7a	101.8	–	103.0
N7–H7b	–	–	106.3
O1–C2	141.4	141.2	140.4
	141.0	141.2	140.3
	142.0	142.8	140.7
	140.0	141.2	139.9
	142.0	142.6	142.4
	140.4	140.2	140.9

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
C2–O7	139.6	139.7	140.2
	140.5	140.2	141.2
	139.7	139.0	140.7
	142.3	141.0	141.1
	139.2	139.5	138.8
	141.8	142.5	141.4
C3–O8	142.0	142.1	143.3
	142.3	142.4	142.5
	142.0	141.8	143.2
	141.1	140.1	142.4
	141.6	140.8	141.2
	140.4	141.0	140.3
C4–O9	142.6	142.5	141.9
	141.6	141.7	141.6
	141.2	141.4	141.0
	140.6	141.1	143.2
	142.6	140.9	143.4
	141.7	140.5	140.9
O8–H8a	96.6	96.6	96.3
	96.7	96.7	96.6
	96.6	96.6	96.8
	96.8	97.7	97.5
	96.6	99.6	96.4
	97.2	97.0	97.0
O9–H9a	96.8	97.2	96.4
	97.1	97.2	97.1
	97.3	97.3	97.6
	97.1	96.9	98.5
	96.6	100.0	96.6
	97.2	97.7	96.7

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
C5–O10	141.8	141.0	142.1
	143.0	142.6	142.6
	142.7	142.8	142.3
	143.0	143.8	142.2
	141.3	142.3	142.4
	143.6	142.4	144.2
C6–O1	143.1	143.2	143.4
	144.1	144.2	144.0
	143.9	143.6	144.4
	144.0	143.5	144.1
	144.4	144.3	144.0
	143.8	144.1	143.5
C11–O12	142.3	142.7	142.2
	141.5	141.5	142.2
	141.9	142.1	141.6
	141.3	141.6	141.4
	141.5	141.9	141.0
	142.0	142.1	142.1
O12–H12a	96.1	96.1	96.2
	96.6	96.7	96.1
	96.1	96.1	96.1
	96.8	96.8	96.7
	96.4	96.4	96.7
	96.8	97.0	96.8
N7–H7a···O8	–	–	–
	–	–	–
	–	–	–
	–	–	282.0
	–	–	–
	312.9	–	–

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
N7···H9a–O9	–	–	–
	–	–	–
	–	–	–
	–	–	–
	–	276.4	–
	–	–	–
N7–H7b···O9	–	–	–
	–	–	–
	–	–	–
	–	–	266.4
	–	–	–
	–	–	–
***α* (°)**			
N1–C2–N7	120.41	121.84	113.99
C2–N7–C8	131.59	123.13	114.18
C2–N7–H7a	112.17	–	110.12
C8–N7–H7a	115.94	–	110.48
C2–N7–H7b	–	–	108.17
C8–N7–H7b	–	–	110.21
H7a–N7–H7b	–	–	103.08
C6–O1–C2	113.61	113.05	114.35
	114.31	114.01	115.16
	114.18	113.69	115.16
	113.66	112.87	113.94
	114.29	113.01	114.51
	113.67	112.49	113.44
O1–C2–C3	108.15	108.30	108.75
	109.20	108.88	109.56
	109.21	108.47	109.72
	112.74	111.88	111.45
	108.50	110.80	108.37
	111.55	112.45	112.08

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
O1–C2–O7	111.61	111.43	111.90
	110.95	111.03	110.86
	111.39	111.53	111.29
	110.72	109.78	112.10
	111.75	109.70	111.78
	109.64	108.71	110.84
C3–C4–C5	111.85	110.15	112.37
	110.62	110.72	110.43
	110.85	111.11	110.42
	110.39	110.72	111.35
	112.17	111.09	112.86
	109.76	110.19	110.41
C3–O8–H8a	107.40	106.30	108.97
	105.42	105.03	105.70
	106.18	106.13	105.18
	107.69	109.80	108.73
	106.82	110.58	107.91
	109.65	108.76	108.78
C4–O9–H9a	109.19	108.25	107.18
	108.44	108.16	107.96
	108.61	108.44	109.12
	108.22	107.88	109.78
	109.02	107.41	108.34
	108.50	107.65	108.13
C5–C6–O1	110.93	111.52	110.87
	109.31	109.69	110.20
	111.73	111.48	112.00
	108.92	108.32	108.66
	111.18	111.09	110.39
	109.09	109.98	107.49

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
C6–C5–O10	110.02	109.24	111.12
	109.47	108.56	110.62
	108.62	108.62	108.28
	109.37	110.08	109.35
	110.20	109.02	110.55
	109.91	106.73	110.92
C11–C6–O1	106.47	106.54	106.34
	107.87	108.13	107.70
	107.62	107.82	107.35
	108.08	108.11	108.71
	106.27	106.39	106.59
	107.94	108.73	108.36
C11–O12–H12a	109.03	108.88	108.29
	107.05	107.07	107.90
	108.19	107.86	108.49
	107.34	107.03	107.89
	109.07	108.79	110.17
	106.99	107.42	107.79
N7–H7a···O9	–	–	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–
	167.51	–	–
N7···H9a–O9	–	–	–
	–	–	–
	–	–	–
	–	–	–
	–	166.85	–
	–	–	–

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
N7–H7a···O8	–	–	–
	–	–	–
	–	–	–
	–	–	129.42
	–	–	–
	–	–	–
N7–H7b···O9	–	–	–
	–	–	–
	–	–	–
	–	–	170.01
	–	–	–
	–	–	–
β **(°)**			
N1–C2–N7–C8	−1.97	−12.57	77.20
N1–C2–N7–H7a	−175.30	–	−157.84
N1–C2–N7–H7b	–	–	−45.88
C2–N7–C8–C9	−7.31	−37.94	−109.18
H7a–N7–C8–C9	165.82	–	126.05
H7b–N7–C8–C9	–	–	12.79
C6–O1–C2–O7	54.05	54.96	54.74
	56.61	55.84	58.78
	57.46	56.23	59.76
	58.68	56.77	55.34
	55.84	57.07	55.61
	56.68	56.25	57.00
O7–C2–C3–O8	60.17	62.55	54.99
	58.67	59.79	58.92
	61.06	61.57	59.50
	58.30	60.66	58.06
	59.70	61.59	58.96
	64.28	65.02	58.06

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
C2–C3–O8–H8a	−169.99	−167.01	85.21
	−165.73	−162.01	−167.44
	−163.03	−159.79	−157.11
	−64.08	−53.15	−45.13
	−160.09	−146.68	−162.54
	−50.03	−68.28	−46.16
O8–C3–C4–O9	63.57	58.67	65.28
	61.73	60.90	61.27
	62.06	62.06	59.59
	65.38	65.67	65.98
	57.69	66.16	60.08
	58.75	65.20	65.36
C3–C4–O9–H9a	−109.44	−114.16	−55.75
	−175.98	−170.83	175.47
	171.27	174.09	170.03
	−179.56	−177.22	−177.90
	75.42	−67.60	61.33
	172.80	−172.28	−175.78
O9–C4–C5–O10	−70.17	−67.81	−69.26
	−68.86	−70.06	−68.53
	−73.66	−74.21	−72.83
	−67.95	−68.30	−68.44
	−65.68	−67.26	−66.16
	−64.31	−72.49	−65.54
O10–C5–C6–C11	72.26	68.74	74.56
	68.42	69.04	71.31
	74.80	74.12	74.88
	66.31	65.23	67.40
	74.23	71.44	75.57
	66.87	69.09	62.15

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
O10–C5–C6–O1	−167.15	−169.78	−165.42
	−170.78	−169.69	−168.16
	−163.98	−164.53	−164.35
	−172.88	−174.03	−172.10
	−165.60	−167.71	−164.19
	−171.86	−168.61	−176.46
O1–C6–C11–O12	65.27	64.02	72.83
	−95.84	−95.25	−75.02
	−70.29	−69.76	−69.19
	−91.31	−90.51	−93.33
	68.99	70.09	77.49
	−95.22	−101.87	−86.97
C6–C11–O12–H12a	−175.21	177.44	−174.69
	−106.65	−107.55	−167.80
	−175.53	−172.88	−174.87
	−89.05	−87.45	−92.85
	−68.01	−58.18	−63.94
	−80.34	−70.57	−70.48
N7–H7a···O9–C4	–	–	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–
	−25.61	–	–
C2–N7···H9a–O9	–	–	–
	–	–	–
	–	–	–
	–	–	–
	–	136.45	–
	–	–	–

cont. Tab. S7

Parameter	C^0@α-CD	C^-@α-CD	C^+@α-CD
N7–H7a···O8–C3	–	–	–
	–	–	–
	–	–	–
	–	–	9.27
	–	–	–
	–	–	–
N7–H7b···O9–C4	–	–	–
	–	–	–
	–	–	–
	–	–	0.07
	–	–	–
	–	–	–

Source: own study.

Table S8. Selected theoretical structural parameters (bond lengths, *R*; angles, *α*; dihedral angles, *β*) of systems consisting of a molecule and cyprodinil ions with β-cyclodextrin (G4MP2)

Parameter	C^0@β-CD	C^-@β-CD	C^+@β-CD
	***R* (pm)**		
N1–C2	133.4	135.0	131.2
C2–N7	138.1	135.5	148.7
C8–N7	141.2	139.6	148.5
N7–H7a	101.8	106.2	106.4
N7–H7b	–	–	102.2
O1–C2	141.0	141.6	140.0
	142.3	143.9	141.5
	140.7	141.8	141.7
	141.7	141.6	142.0
	140.8	140.6	140.9
	140.8	140.8	140.7
	140.5	140.7	140.0

cont. Tab. S8

Parameter	C^0@β-CD	C^-@β-CD	C^+@β-CD
C2–O7	140.4	140.0	141.6
	139.7	138.2	139.5
	140.7	141.8	139.5
	139.7	140.3	139.4
	140.7	140.8	140.7
	140.6	140.5	140.8
	141.2	140.7	141.7
C3–O8	141.9	141.8	142.3
	141.2	140.9	143.6
	142.4	137.2	141.6
	141.9	142.3	141.6
	142.4	142.7	142.3
	142.6	142.6	142.6
	142.3	142.3	142.5
C4–O9	141.2	141.3	141.0
	141.1	141.9	141.0
	142.5	141.8	142.4
	141.5	139.0	141.8
	141.4	141.2	141.3
	141.4	141.4	141.3
	141.3	141.3	141.2
O8–H8a	96.7	96.6	96.8
	96.6	96.6	97.3
	96.7	–	96.4
	96.7	97.2	96.6
	96.6	96.7	96.6
	96.6	96.6	96.6
	96.6	96.6	96.6
O9–H9a	97.5	97.5	97.7
	97.4	97.2	98.0
	96.7	96.3	96.4
	97.4	106.0	97.0
	97.2	97.7	97.1
	97.3	97.4	97.2
	97.4	97.4	97.4

cont. Tab. S8

Parameter	C^0@β-CD	C^-@β-CD	C^+@β-CD
C5–O10	142.1	142.4	141.7
	142.7	143.3	141.6
	143.2	145.1	143.8
	142.4	141.2	143.3
	142.9	141.8	143.4
	142.5	142.1	142.6
	142.4	142.3	142.2
C6–O1	144.0	143.8	144.4
	144.0	143.5	144.5
	143.3	142.5	143.6
	144.0	144.6	143.5
	144.2	144.7	143.9
	143.5	143.7	143.5
	143.4	143.4	143.5
C11–O12	141.5	141.3	141.6
	142.7	142.3	142.5
	142.1	142.4	142.2
	141.4	142.0	141.2
	141.8	141.6	141.8
	142.2	142.3	142.1
	142.1	142.2	141.9
O12–H12a	96.4	96.5	96.4
	96.3	96.5	96.2
	96.1	96.1	96.5
	96.8	96.8	96.7
	96.6	96.9	96.5
	96.1	96.1	96.1
	96.1	96.1	96.1
N7–H7a···O9	–	–	–
	–	–	–
	302.0	–	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–

cont. Tab. S8

Parameter	C0@β-CD	C−@β-CD	C+@β-CD
N7–H7a···O8	–	–	–
	–	–	271.9
	–	268.7	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–
α **(°)**			
N1–C2–N7	120.52	121.36	113.47
C2–N7–C8	131.40	130.92	115.31
C2–N7–H7a	111.93	114.67	108.92
C8–N7–H7a	114.63	114.39	111.07
C2–N7–H7b	–	–	105.29
C8–N7–H7b	–	–	108.23
H7a–N7–H7b	–	–	107.60
C6–O1–C2	115.02	115.55	115.15
	114.08	113.72	114.78
	114.76	113.66	115.42
	114.92	114.43	115.12
	114.21	114.06	114.21
	114.02	113.93	114.10
	114.78	114.57	115.09
O1–C2–C3	108.62	108.10	109.29
	108.88	107.09	107.41
	109.82	111.53	107.93
	109.63	110.21	109.26
	110.14	110.51	110.02
	109.53	109.53	109.62
	109.21	109.16	109.53

cont. Tab. S8

Parameter	C0@β-CD	C−@β-CD	C+@β-CD
O1–C2–O7	111.27	111.48	111.03
	110.74	111.15	112.15
	111.26	108.38	111.43
	111.43	110.84	111.52
	110.58	110.76	110.39
	110.83	110.96	110.70
	111.37	111.51	111.31
C3–C4–C5	109.75	109.76	109.64
	111.22	110.68	109.96
	111.92	113.81	112.24
	109.92	108.76	109.73
	109.92	109.58	109.98
	110.97	110.98	110.93
	110.10	110.13	110.05
C3–O8–H8a	105.62	106.05	105.35
	105.29	105.04	103.17
	108.61	–	107.83
	105.49	102.77	106.09
	105.58	104.90	105.89
	105.69	105.39	105.81
	106.25	105.94	106.18
C4–O9–H9a	108.74	108.99	108.83
	109.01	108.17	109.30
	106.76	106.41	106.90
	108.39	107.53	108.42
	108.79	109.02	108.91
	108.49	108.40	108.64
	108.81	108.73	108.96
C5–C6–O1	109.68	109.86	109.72
	108.05	108.25	108.88
	109.49	108.63	108.56
	108.57	109.34	108.54
	107.58	107.81	107.71
	110.64	110.76	110.77
	111.35	111.03	111.66

cont. Tab. S8

Parameter	C0@β-CD	C−@β-CD	C+@β-CD
C6–C5–O10	109.07	109.90	108.74
	110.36	109.93	109.95
	114.97	115.36	116.25
	109.24	107.34	109.23
	111.98	111.66	111.66
	110.19	110.08	109.98
	109.63	109.82	109.29
C11–C6–O1	105.08	104.81	105.22
	105.69	105.55	106.16
	105.19	105.13	102.67
	107.02	107.52	106.85
	108.43	108.76	108.37
	107.97	108.06	107.91
	107.59	107.71	107.47
C11–O12–H12a	105.80	105.66	106.10
	106.21	105.77	107.47
	108.38	108.04	106.39
	108.90	108.05	108.64
	106.16	105.93	106.45
	108.00	107.67	108.26
	108.07	107.78	108.29
N7–H7a···O9	–	–	–
	–	–	–
	159.46	–	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–
N7–H7a···O8	–		–
	–	–	171.94
	–	171.88	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–

cont. Tab. S8

Parameter	C0@β-CD	C−@β-CD	C+@β-CD
	β **[°]**		
N1–C2–N7–C8	8.53	2.01	103.41
N1–C2–N7–H7a	171.04	−179.55	−130.96
N1–C2–N7–H7b	–	–	−15.81
C2–N7–C8–C9	−8.24	−4.33	−109.48
H7a–N7–C8–C9	−170.39	177.23	126.00
H7b–N7–C8–C9	–	–	8.09
C6–O1–C2–O7	62.08	62.57	62.96
	58.00	56.27	58.60
	56.25	56.33	55.10
	61.47	64.05	60.71
	59.12	60.05	58.71
	57.03	57.22	57.08
	59.55	59.62	60.15
O7–C2–C3–O8	56.34	56.70	55.42
	55.10	58.80	56.65
	58.02	58.03	58.78
	54.89	54.38	55.55
	54.95	55.10	55.24
	58.88	58.99	59.03
	59.99	59.46	59.86
C2–C3–O8–H8a	−161.95	−160.38	−162.62
	−170.25	−165.95	−158.64
	157.73	–	−166.78
	−163.96	−157.42	−167.26
	−169.89	−165.74	−172.17
	−168.17	−165.14	−169.99
	−161.55	−160.01	−163.14
O8–C3–C4–O9	58.61	58.46	58.45
	64.17	60.99	56.83
	67.01	66.10	63.00
	60.98	58.16	61.10
	64.24	63.30	64.58
	63.63	63.25	63.61
	60.04	60.26	59.84

cont. Tab. S8

Parameter	C0@β-CD	C−@β-CD	C+@β-CD
C3–C4–O9–H9a	−170.16	−176.74	−170.50
	−170.11	−160.72	−172.69
	164.19	177.22	179.22
	−167.98	−168.72	−161.86
	170.91	171.32	171.78
	162.25	166.16	159.85
	166.11	168.10	165.18
O9–C4–C5–O10	−67.54	−67.56	−67.61
	−67.87	−67.53	−67.91
	−66.25	−66.01	−65.10
	−66.01	−66.27	−65.68
	−64.52	−64.29	−65.22
	−71.33	−71.51	−71.60
	−71.24	−70.78	−71.67
O10–C5–C6–C11	65.78	68.19	65.00
	63.81	63.90	65.41
	76.55	72.57	77.67
	64.13	60.42	64.55
	62.34	61.70	62.74
	71.36	71.28	71.78
	72.51	71.21	73.51
O10–C5–C6–O1	−175.98	−174.29	−176.32
	−177.76	−178.25	−175.57
	−165.14	−168.85	−167.50
	−176.28	−178.65	−176.37
	−177.24	−177.46	−176.90
	−167.51	−167.42	−167.11
	−166.59	−167.91	−165.60
O1–C6–C11–O12	59.55	60.49	59.93
	60.79	58.84	62.60
	−80.07	−83.51	−67.64
	82.21	85.58	79.89
	−85.98	−86.15	−86.62
	−71.69	−69.71	−72.84
	−71.28	−70.48	−71.37

cont. Tab. S8

Parameter	C0@β-CD	C−@β-CD	C+@β-CD
C6–C11–O12–H12a	−55.30	−49.60	−61.04
	−60.27	−48.87	−74.75
	169.70	165.78	59.97
	96.89	89.08	93.79
	−102.23	−97.21	−103.98
	−173.81	−161.97	−178.85
	−173.25	−165.99	−175.33
N7–H7a···O9–C4	–	–	–
	–	–	–
	−55.54	–	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–
N7–H7a···O8–C3	–	–	–
	–	–	151.15
	–	126.82	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–

Source: own study.