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
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

cont. Tab. S2

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
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
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

cont. Tab. S2

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
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
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

cont. Tab. S3

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
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	–
	–		–		–
	–		–		–
	–		–		–
	–		–		–
	–		–		–
	–		–		–
O9–H9a	–	C4–O9–H9a	–	O9–C4–C5–O10	−67.02
	–		–		−64.96
	–		–		−66.72
	–		–		−67.29
	–		–		−62.94
	–		–		−63.71
	–		–		−69.17

cont. Tab. S3

R		***α***		***β***	
bond	**value (pm)**	**angle**	**value (°)**	**dihedral angle**	**value (°)**
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
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	**Value of parameter for**		
	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	Value of parameter for		
	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	Value of parameter for		
	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	Value of parameter for		
	C^0@α-CD	C^-@α-CD	C^+@α-CD
N7···H9a–O9	–	–	–
	–	–	–
	–	–	–
	–	–	–
	–	276.4	–
	–	–	–
N7–H7b···O9	–	–	–
	–	–	–
	–	–	–
	–	–	266.4
	–	–	–
	–	–	–
α **(°)**			
N1–C2–N7	120.63	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
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	Value of parameter for		
	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	Value of parameter for		
	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	Value of parameter for		
	C^0@α-CD	**C^-@α-CD**	**C^+@α-CD**
N7–H7a···O8	–	–	–
	–	–	–
	–	–	–
	–	–	129.42
	–	–	–
	–	–	–
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
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
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

cont. Tab. S7

Parameter	Value of parameter for		
	C^0@α-CD	**C^-@α-CD**	**C^+@α-CD**
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
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

cont. Tab. S7

Parameter	Value of parameter for		
	C^0@α-CD	**C^-@α-CD**	**C^+@α-CD**
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	–
	–	–	–
N7–H7a···O8–C3	–	–	–
	–	–	–
	–	–	–
	–	–	9.27
	–	–	–
	–	–	–

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	Value of parameter for		
	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
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

cont. Tab. S8

Parameter	Value of parameter for		
	C^0@β-CD	C^-@β-CD	C^+@β-CD
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
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

cont. Tab. S8

Parameter	Value of parameter for		
	C^0@β-CD	C^-@β-CD	C^+@β-CD
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	–	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–
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

cont. Tab. S8

Parameter	Value of parameter for		
	C^0@β-CD	**C^-@β-CD**	**C^+@β-CD**
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
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

cont. Tab. S8

Parameter	Value of parameter for		
	C^0@β-CD	**C^-@β-CD**	**C^+@β-CD**
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
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	–	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–

cont. Tab. S8

Parameter	Value of parameter for		
	C^0@β-CD	**C^-@β-CD**	**C^+@β-CD**
N7–H7a···O8	–		–
	–	–	171.94
	–	171.88	–
	–	–	–
	–	–	–
	–	–	–
	–	–	–
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

cont. Tab. S8

Parameter	Value of parameter for		
	C^0@β-CD	**C^-@β-CD**	**C^+@β-CD**
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
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

cont. Tab. S8

Parameter	Value of parameter for		
	C^0@β-CD	**C^-@β-CD**	**C^+@β-CD**
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
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.