Electronic supplementary information (ESI)

Experimental and Computational Crystal Structure Landscape Study of Nigerloxin: a Fungal Metabolite from *Aspergillus niger*

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Tables

Table S1 ESPD derived atomic charges used in CSP run for nigerloxin and water molecule.

Molecule	Atom Number	q_{espd}
Nigerloxin	O1	-0.3272
	O2	-0.5151
	O3	-0.5145
	O4	-0.5466
	O5	-0.5361
	N1	-0.8741
	C2	0.2065
	C3	-0.4630
	C4	0.6425
	C5	-0.0444
	C6	0.3872
	C7	0.7870
	C8	0.8764
	C9	-0.3383
	C10	0.0082
	C11	-0.1325
	H1N	0.4458
	H5A	0.4412
	H9	0.2059
	H10	0.1116
	H11A	0.0567
	H11B	0.0615
	H11C	0.0611
Water	O7	-0.7924
	H7A	0.3962
	H7B	0.3962

Table S2 Unit cell parameters and packing energies for the top 50 predicted crystal structures for nigerloxin (Z' = 1).

Rank	Space group	a (Å)	b (Å)	c (Å)	Σ (°)	T (°)	Y (°)	V (Å^3)	ρ (g/cm^3)	Packing energy (kcal/mol)
1	$P2_1/c$	5.35	19.12	9.09	90	99.9	90	915	1.60	-39.42
2	$C2/c$	19.50	5.07	20.25	90	108.2	90	1900	1.55	-37.42
3	$P1$	5.25	9.74	10.08	71.3	87.4	78.1	478	1.54	-37.40
4	$P2_12_12_1$	5.48	6.58	26.95	90	90	90	972	1.51	-35.59
5	$Pbcn$	26.92	8.55	8.54	90	90	90	1964	1.50	-34.56
6	$R3$	23.66	23.66	9.69	90	90	120.0	4698	1.41	-34.56
7	$P2/c$	12.11	4.31	18.95	90	94.7	90	986	1.49	-34.24
8	$Pccn$	8.50	28.35	8.33	90	90.0	90	2007	1.46	-33.35
9	$P2_12_12$	8.48	24.07	4.89	90	90.0	90	999	1.47	-33.00
10	$C2/c$	10.21	19.04	9.84	90	98.2	90	1892	1.55	-36.47
11	$P2_12_12_1$	7.29	9.39	14.42	90	90.0	90	986	1.49	-35.56
12	$P2_1$	9.23	4.91	11.22	90	93.3	90	507	1.45	-34.43
13	$Pnnm$	8.73	18.95	6.26	90	90.0	90	1035	1.42	-32.98
14	$I2$	10.29	4.07	23.42	90	93.6	90	978	1.50	-34.27
15	$Pbca$	7.85	14.83	17.87	90	90.0	90	2080	1.41	-33.75
16	$Pnma$	8.54	6.22	18.27	90	90.0	90	970	1.51	-34.15
17	$Pna2_1$	16.67	12.29	5.01	90	90.0	90	1027	1.43	-33.60
18	$C2/c$	24.99	4.35	18.89	90	111.9	90	1906	1.54	-35.76
19	$P2_12_12_1$	4.76	13.13	15.74	90	90.0	90	984	1.49	-33.92

20	*P*na2$_1$	9.35	19.06	5.74	90	90.0	90	1022	1.44	-34.01
21	*P*bca	8.48	12.91	18.45	90	90.0	90	2021	1.45	-33.12
22	*P*na2$_1$	8.52	24.16	4.89	90	90.0	90	1006	1.46	-33.00
23	*P*2$_1$/n	10.28	5.02	19.13	90	98.1	90	977	1.50	-37.23
24	*P*2$_1$/n	14.06	5.00	14.14	90	97.7	90	986	1.49	-35.87
25	*I*2/a	19.07	5.17	21.12	90	107.7	90	1982	1.48	-35.25
26	C2/m	12.85	6.53	13.53	90	102.9	90	1106	1.33	-33.14
27	*P*2$_1$/n	10.69	7.39	13.19	90	99.4	90	1028	1.43	-34.85
28	*P*2$_1$2$_1$2$_1$	4.40	14.46	15.87	90	90.0	90	1009	1.46	-33.37
29	*C*2/c	8.17	19.12	12.39	90	92.4	90	1934	1.52	-35.55
30	*P*n	5.71	15.24	5.81	90	96.6	90	502	1.46	-34.53
31	*P*2$_1$/n	5.90	15.19	10.73	90	100.3	90	946	1.55	-34.85
32	*P*2/n	10.07	4.13	23.26	90	92.2	90	966	1.52	-33.54
33	*C*2/c	12.85	13.18	12.89	90	103.8	90	2120	1.39	-34.83
34	*P*2$_1$2$_1$2$_1$	4.47	11.46	19.06	90	90.0	90	977	1.50	-33.03
35	*P*2/n	9.65	5.16	19.96	90	98.2	90	983	1.49	-33.60
36	*P*2$_1$/n	5.73	6.22	27.93	90	90.6	90	995	1.48	-34.77
37	*P*2$_1$/n	5.58	31.57	5.82	90	97.5	90	1016	1.45	-34.72
38	*I*2/a	20.61	4.00	24.95	90	109.4	90	1940	1.51	-34.46
39	*P*2$_1$	6.26	5.75	14.41	90	96.0	90	515	1.43	-34.13
40	*I*2	15.10	4.53	15.67	90	113.0	90	987	1.49	-33.01
41	*C*2/c	11.12	15.19	11.95	90	110.7	90	1888	1.56	-34.44
42	*P*2$_1$/n	7.54	6.92	19.93	90	96.4	90	1035	1.42	-34.72
43	*P*2$_1$	6.53	5.87	12.88	90	90.1	90	493	1.49	-33.88
44	*C*2/c	12.93	13.15	12.58	90	103.6	90	2078	1.41	-33.70
45	*C*2/c	17.41	5.23	22.90	90	102.8	90	2032	1.45	-33.36
46	*C*2/c	25.12	4.81	17.00	90	100.4	90	2021	1.45	-33.36
47	*I*2/a	9.91	20.22	10.79	90	99.6	90	2132	1.38	-34.17
48	*P*2$_1$/c	6.65	19.20	7.36	90	91.2	90	939	1.56	-34.62
49	*C*2/c	15.87	7.58	16.67	90	94.6	90	1998	1.47	-34.01
50	*C*2/c	13.45	18.27	8.52	90	104.2	90	2030	1.45	-33.87

CSP protocol: (1) Packing (2) Clustering, (3) Geometry Optimization and (4) Clustering.
List of space groups used in prediction: *P*2$_1$/c, *P*1, *P*2$_1$2$_1$2$_1$, *C*2/c, *P*2$_1$, *P*bca, *P*na21, *P*nma, *C*c, *P*1, *P*bcn, *C*2, *P*ca21, *P*2$_1$/m, *P*2/c, *C*2/m, *R*3, *P*2$_1$2$_1$2, *P*c, *P*ccn

(1) ---- Packing parameters ----

Search algorithm	: MC Simulated Annealing
Maximum number of steps	: 7000
Explore torsions	: No
Pre-optimize structures	: No
Steps to accept before cooling	: 12
Minimum move factor	: 0.1000E-08
Heating factor	: 0.02500
Maximum temperature	: 100000.0 K
Minimum temperature	: 300.0 K

(2) ---- Cluster analysis parameters ----

Cluster grouping	: Forcefield type
Cutoff	: 7.000
Number of bins	: 140
Tolerance	: 0.1300
Maximum number of clusters	: All clusters

(3)---- Geometry optimization parameters ----

Algorithm	: Smart
Convergence tolerance:	
Energy	: 0.0001 kcal/mol
Force	: 0.005 kcal/mol/A
Stress	: 0.005 GPa
Displacement	: 5e-005 A
Maximum number of iterations	: 5000
External pressure	: 0 GPa
Motion groups rigid	: YES
Optimize cell	: YES

---- Energy parameters ----

Forcefield	: Dreiding
Electrostatic terms:	
Summation method	: Ewald

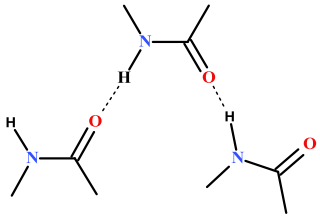
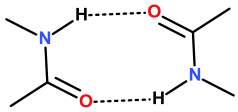
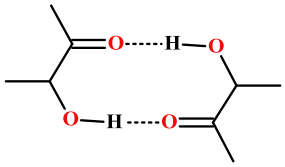
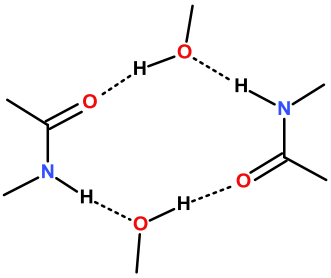
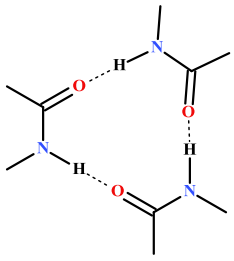
Accuracy	: 0.0001 kcal/mol
Buffer width	: 0.5 A
van der Waals terms:	
Summation method	: Ewald
Accuracy	: 0.0001 kcal/mol
Repulsive cutoff	: 6 A
Buffer width	: 0.5 A
(4) ---- Polymorph Clustering parameters ----	
Cluster grouping	: Forcefield type
Cutoff	: 7.000
Number of bins	: 140
Tolerance	: 0.2100
Maximum number of clusters	: All clusters

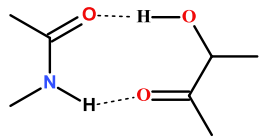
Table S3 Unit cell parameters and packing energies for the top 50 predicted crystal structures for nigerloxin monohydrate.

Rank	Space group	a (Å)	b (Å)	c (Å)	Σ (°)	T (°)	Y (°)	V (Å^3)	ρ (g/cm^3)	Packing energy (kcal/mol)
1	*P*1	5.24	8.61	12.19	99.0	100.0	104.5	513	1.55	-53.19
2	*P*1	5.32	8.56	12.25	97.8	98.2	104.5	525	1.51	-52.56
3	$P2_1/c$	10.29	5.28	20.25	90	94.7	90	1097	1.45	-52.20
4	$P2_1/n$	5.15	24.85	8.43	90	102.0	90	1054	1.51	-52.13
5	$P2_1/n$	7.24	5.26	27.16	90	93.6	90	1032	1.54	-52.05
6	$P2_1/c$	12.03	8.85	10.18	90	108.9	90	1025	1.55	-51.98
7	*P*1	5.91	6.95	12.97	84.8	86.9	87.0	529	1.50	-51.69
8	$P2_1/c$	6.20	6.41	26.19	90	93.0	90	1039	1.53	-51.66
9	*P*1	6.08	6.70	13.37	104.0	95.2	92.0	525	1.51	-51.61
10	$P2_1/n$	5.36	20.09	10.37	90	97.5	90	1108	1.43	-51.55
11	$P2_1/n$	5.23	24.46	8.68	90	105.3	90	1070	1.49	-51.45
12	*P*1	6.31	6.96	12.43	100.3	93.0	96.7	532	1.49	-51.42
13	*P*bca	8.86	9.95	23.72	90	90	90	2091	1.52	-51.33
14	***C*2/c**	**26.54**	**8.85**	**9.03**	**90**	**94.6**	**90**	**2115**	**1.50**	**-51.28**
15	$P2_1/n$	5.52	27.80	7.06	90	91.1	90	1084	1.47	-51.15
16	*P*1	5.32	8.78	12.21	107.5	93.5	106.2	515	1.54	-51.09
17	$P2_1/c$	13.74	8.89	8.92	90	104.4	90	1055	1.51	-51.08
18	*I*a	5.75	23.53	8.37	90	97.9	90	1122	1.42	-51.07
19	*P*1	7.74	7.75	8.86	99.6	94.0	96.4	519	1.53	-50.84
20	*P*1	5.99	7.47	12.28	96.1	103.6	98.4	522	1.52	-50.81
21	*P*1	5.01	7.41	14.33	83.3	87.9	83.8	525	1.51	-50.76
22	*P*1	5.19	6.70	15.55	93.5	93.7	95.5	536	1.48	-50.66
23	$P2_1/n$	5.87	29.49	6.27	90	94.0	90	1081	1.47	-50.65
24	*P*1	4.68	7.28	15.77	78.4	89.2	86.1	525	1.51	-50.64
25	*P*1	6.70	8.61	10.35	88.9	79.2	74.3	564	1.41	-50.63
26	*P*1	5.04	7.80	14.43	93.3	97.1	100.5	551	1.44	-50.56
27	$P2_12_12_1$	5.43	6.70	29.61	90	90	90	1078	1.47	-50.56
28	*P*ccn	8.84	30.66	7.91	90	90	90	2144	1.48	-50.50
29	*P*1	4.61	7.26	15.40	87.5	82.5	85.9	509	1.56	-50.46
30	*P*1	7.78	7.92	8.85	89.5	80.2	80.5	530	1.50	-50.46
31	*P*1	5.12	7.48	15.05	86.2	80.5	79.9	559	1.42	-50.40
32	*P*1	5.37	8.86	12.13	83.8	90.0	74.0	552	1.44	-50.39
33	*P*bca	8.87	8.53	28.36	90	90	90	2146	1.48	-50.37
34	$P2_1/c$	8.69	23.63	5.26	90	105.7	90	1040	1.53	-50.37
35	$P2_1/c$	7.59	27.40	5.00	90	94.2	90	1036	1.53	-50.36
36	*P*1	6.84	8.86	9.26	95.8	102.1	102.0	530	1.50	-50.32
37	$P2_1/n$	10.28	8.84	11.53	90	91.5	90	1047	1.52	-50.30
38	*C*2	8.89	8.85	13.97	90	102.7	90	1073	1.48	-50.28
39	$P2_1/c$	5.54	11.45	17.58	90	98.3	90	1104	1.44	-50.26
40	$P2_1/c$	11.33	8.82	10.71	90	99.3	90	1056	1.50	-50.25
41	*P*1	7.10	8.90	9.33	90.4	104.2	110.3	533	1.49	-50.24
42	$P2_1/c$	5.17	30.30	7.12	90	99.8	90	1098	1.45	-50.21

43	$P2_1/n$	5.20	17.38	11.16	90	97.0	90	1001	1.59	-50.13
44	$C2/m$	20.58	6.44	8.63	90	94.8	90	1139	1.39	-50.08
45	$P1$	5.51	7.83	13.09	104.6	101.4	91.2	533	1.49	-50.08
46	$Pbcn$	30.09	8.85	8.17	90	90	90	2175	1.46	-50.08
47	$Pca2_1$	27.33	7.59	4.98	90	90	90	1032	1.54	-49.96
48	$P2_1/n$	5.17	28.12	7.78	90	96.5	90	1123	1.41	-49.95
49	$P2_1/n$	5.11	31.04	6.75	90	95.3	90	90	1.49	-49.94
50	$P1$	5.54	8.83	11.35	103.1	97.0	94.4	534	1.49	-49.90
89	***P21/c***	**10.22**	**8.84**	**12.59**	**90**	**110.7**	**90**	**1064**	**1.49**	**-49.42**

Table S4 Relative occurrences of various supramolecular synthons in CSD.

Query	Growth unit	Total hits
	1A/1B	4413
	0A	2405
	0B	175
	0F	60
	0E	5

	-	1

CSD search criteria: 3D coordinates determined, No disorder, No errors, Not polymeric, No ions, No powder structures, Only organic molecules

Table S5 Radical scavenging/Biological activities for some of the 4-pyranone derivatives from literature.

Assays used	Unit[#]	Kojic acid	Maltol	Nigerloxin
DPPH	ED_{50} (μM)	-	-	66[4, 5]
OH radical	IC_{50} (μg/ml)	-	0.63[3]	-
$ONOO^-$	IC_{50} (μg/ml)	-	1.0[3]	-
Polyphenol oxidase	IC_{50} (μM)	280[1]	-	-
Mushroom tyrosinase	IC_{50} (μM)	26[2]	-	-
Soybean lipoxygenase	IC_{50} (μM)	175[2]	-	79[4]
Rat lens Aldose Reductase	IC_{50} (μM)	-	-	69[4]
Phospho Molebdenum	Equiv. conc.	-	-	3791[5]
ABTS	ED_{50} (μM)	-	-	8.9[5]
FRAP	Equiv. conc.	-	-	14.4[5]

[#] ED_{50} values corresponds to the concentration required for 50% radical scavenging activity compared with the control test in the reaction after certain specific time 30 min 60 min etc. The IC_{50} values corresponds to the concentration of the compound required for 50% inhibition of enzyme activity compared with the control test.

1. J. S. Chen, C. Wei, and M. R. Marshall *J. Agric. Food Chem.*, **1991**, 39, 1897-1901.
2. Y. -C. Chen, Y. Sugiyama, N. Abe, R. Kuruto-Niwa, R. Nozawa, and A. Hirota *Biosci. Biotech. Biochem.* **2005**, 69, 999–1006.
3. K. S. Kang, H. Y.Kim, J. S. Pyo and T. Yokuzawa *Biol. Pharm. Bull.* **2006,** 29, 750–754.
4. K. C. S. Rao, S. Divakar, K. N. Babu, N. G. Karanth, A. P. Sattur *J. Antibiotic*, **2002**, 55, 789–793.
5. B. S. Suresha and K. Srinivasan *Appl. Biochem. Microbiol.* **2013**, 49, 587–591.

Table S6 Relative stabilities of 0-D growth units for nigerloxin calculated at M06x/6-311G++(d,p) level.

Growth Unit	ΔE (kcal/mol)	ΔE/n
0A	-12.49	-6.25
0B	-11.75	-5.88
0C	-4.05	-2.03
0D	unstable	-
0E	-19.81	-6.60
0F	unstable	-

n= number of molecules in the growth unit

Table S7 Growth units identified from CSP study of nigerloxin (Z' = 1) form and their relative frequencies in the top 50 predicted crystal structures.

Growth unit	Synthon Combination	Frequency	Predicted nigerloxin crystal structures (rank) exhibiting the growth unit
1A	-	23	2, 4, 5, 8, 9, 12, 14, 16, 18, 20, 21, 23, 24, 25, 28, 30, 34, 36, 37, 39, 42, 45, 50
0B	-	20	2, 3, 6, 7, 14, 18, 23, 25, 26, 27, 32, 33, 35, 38, 40, 42, 44, 45, 46, 47
0A	-	17	1, 3, 7, 10, 13, 26, 29, 31, 32, 33, 35, 38, 41, 44, 46, 47, 48
0C	-	13	2, 3, 18, 23, 25, 33, 42, 44, 45, 47, 32, 35, 38
1C	-	12	4, 5, 8, 9, 13, 16, 21, 30, 36, 37, 39, 50
0D	-	11	1, 3, 10, 18, 23, 25, 29, 31, 38, 41, 48
1E	0A+0B	10	3, 7, 26, 32, 33, 35, 38, 44, 46, 47
1J	1A+1C	8	5, 8, 9, 16, 21, 30, 37, 50
1I	-	7	1, 10, 19, 29, 31, 41, 48
3A	0B+0C+1A	7	2, 14, 18, 23, 25, 42, 45
2A	0A+0D+1I	7	1, 10, 19, 29, 31, 41, 48
1G	-	5	15, 27, 40, 43, 49
2B	0C+1E	5	3, 26, 33, 44, 47
1H	-	4	11, 17, 20, 28
0F	-	3	15, 43, 49
2C	0F+1G	3	15, 43, 49
2E	1B+1H	3	11, 17
3C	1A+1H	3	20, 28, 34
3D	1A+1C	3	4, 36, 39
1B	-	2	11, 17
1D	-	2	12, 24
2F	0B+1G	2	27, 40
3B	1A+1D	2	12, 24
0E	-	1	6
1F	-	1	22
1K	0A+1C	1	13
2D	0B+0E	1	6

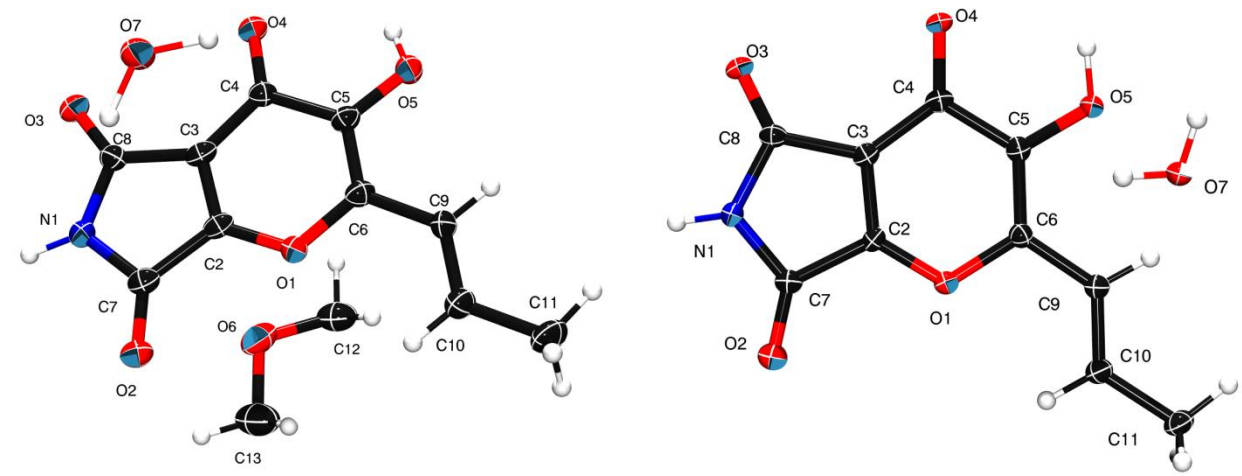
Table S8. Growth units identified from CSP study of nigerloxin monohydrate form and their relative frequencies in the top 50 predicted crystal structures.

Growth Unit	Synthon combination	Frequency	Predicted monohydrate structures (rank) exhibiting the growth unit
1HA	1G+W	29	1, 4, 5, 6, 7, 8, 9, 13, 14, 15, 17, 19, 20, 22, 23, 24, 28, 30, 32, 33, 36, 37, 38, 40, 41, 46, 49
1HB	Unique	2	21, 29
1HC	1G+W	5	2, 11, 12, 48, 50
1HD	1G+W	1	16
1HE	1C+W	2	25
1HF	Unique	2	26, 31
1HG	Unique	2	39, 42
1HH	1G+W	1	43
1HI	1G+W	2	35, 47
1HJ	Unique	1	45
2HA	0B+0C+W	1	10
2HB	0C+W	1	31
2HC	1G+W	1	43
2HD	Unique	1	18
2HE	1G+W	1	34, 44
2HF	1C+W	1	27
3HA	0B+0C+W	1	3

Table S9 Relative frequencies for the higher order supramolecular constructs obtained from 1HA obtained from the CSP of nigerloxin monohydrate.

Supramolecular variant of IHA	Frequency	Predicted monohydrate structures (rank) exhibiting the growth unit
Parallel sheet	14	1, 2, 7, 9, 19, 20, 22, 24, 30, 35, 36, 39, 40, 41
Anti-parallel corrugated sheets	6	4, 13,15, 23, 28, 46,
Anti-parallel sheets	4	14, 17, 33, 38,
Parallel pillared arrangement	2	5, 8,
Parallel corrugated sheets	1	49
Anti-parallel brick wall arrangement	1	32

Figures



(a) **(b)**

Figure S1 ORTEP diagrams representing the asymmetric units of the nigerloxin (a) dioxane water solvate, **1a** and (b) monohydrate form, **1b**. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

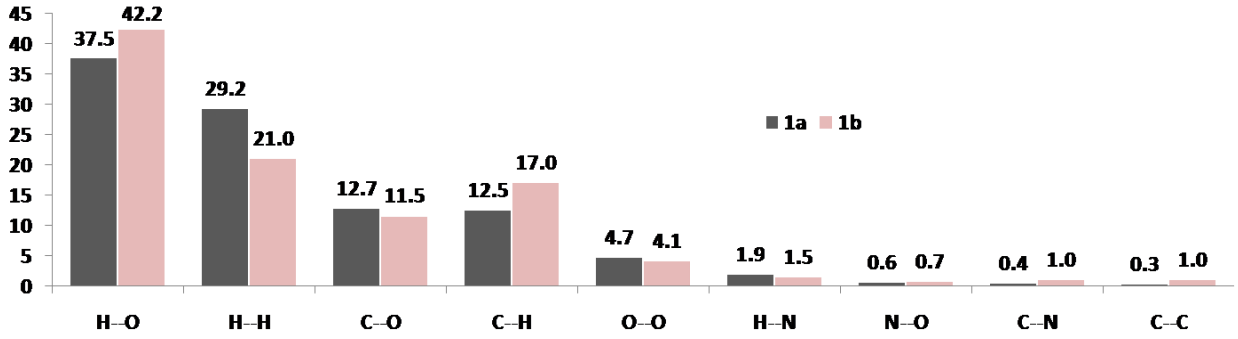


Figure S2 Relative contributions from various types of contacts to the total Hirshfeld surface of nigerloxin molecule in **1a** and **1b**.

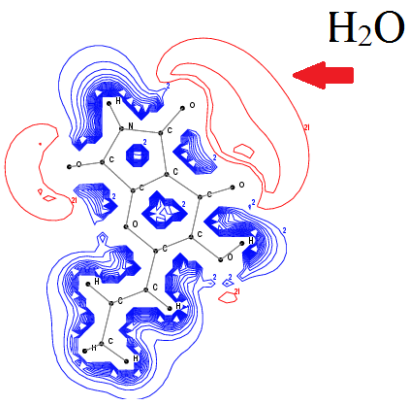


Figure S3 Electrostatic potential map for nigerloxin molecule indicating possible hydration sites. Nulceophilic and electrophilic regions are shown with blue and red contour lines.

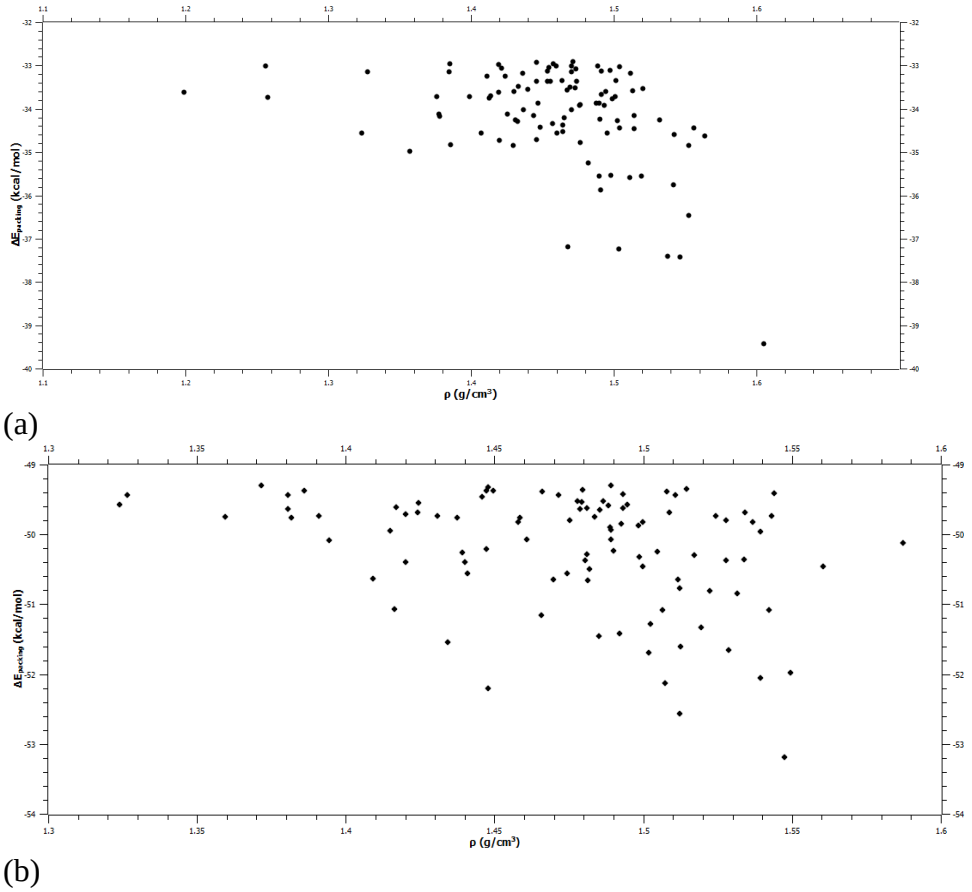


Figure S4 Packing energy versus density plots for top 100 predicted crystal structures for (a) Nigerloxin anhydrous form (Z' = 1) and (b) nigerloxin monohydrate form.

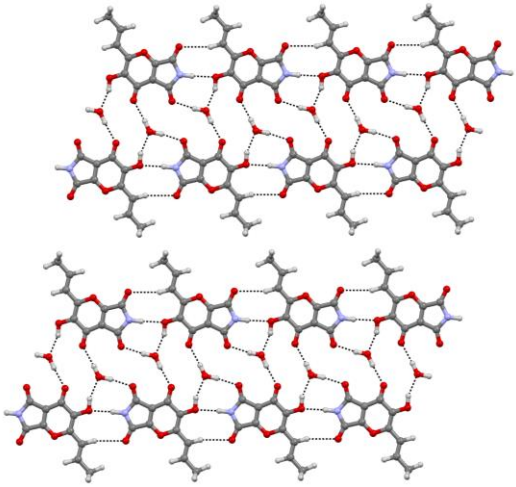
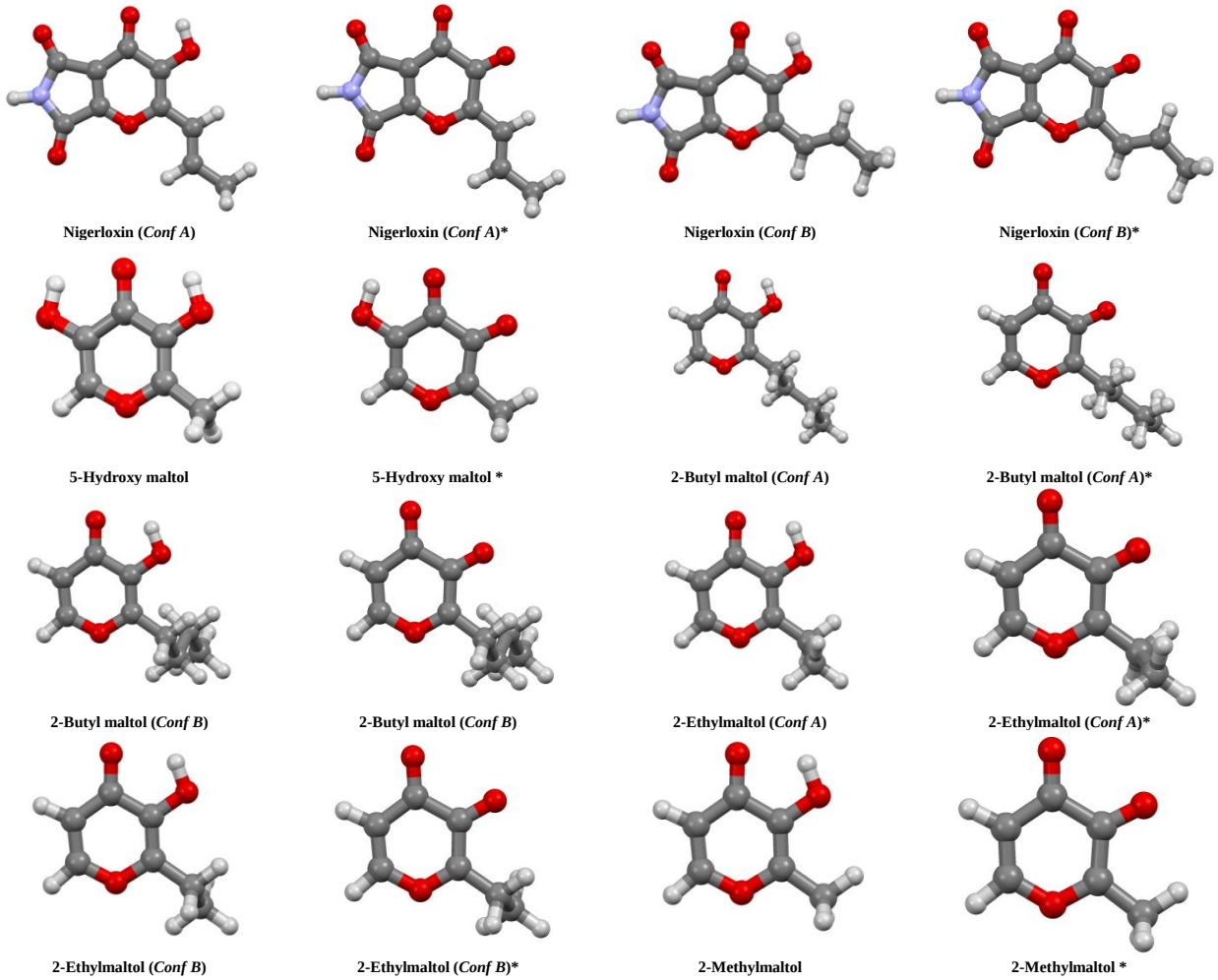
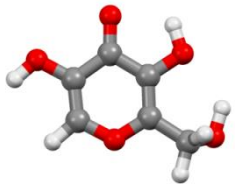
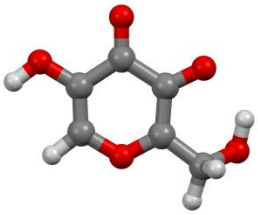


Figure S5 Packing of 1D tapes of nigerloxin and water molecule in the hypothetical desolvated form obtained from **1a** on removing dioxane molecules.

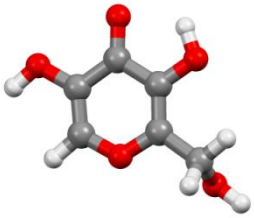




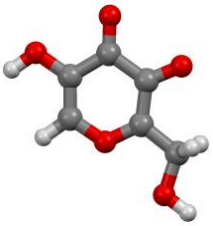
3-Hydroxy kojic acid (*Conf A)*



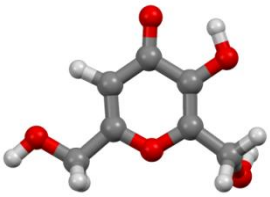
3-Hydroxy kojic acid - *(Conf A)**



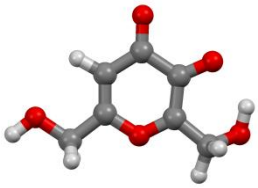
3-Hydroxy kojic acid *(Conf B)*



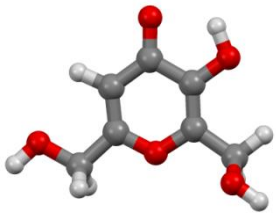
3-Hydroxy kojic acid *(Conf B)**



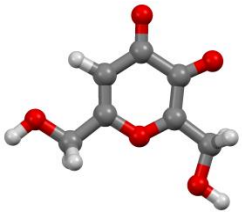
6-Hydroxymethyl kojic acid (*Conf A*)



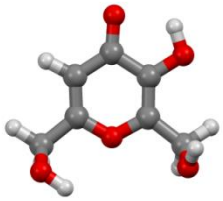
6-hydroxymethyl kojic acid (*Conf A*)*



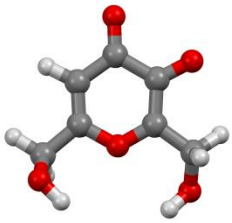
6-Hydroxymethyl kojic acid (*Conf B*)



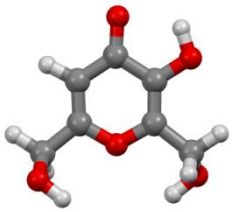
6-Hydroxymethyl kojic acid (*Conf B*)*



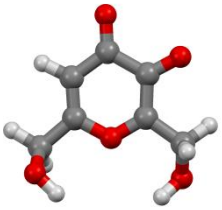
6-Hydroxymethyl kojic acid (*Conf C*)



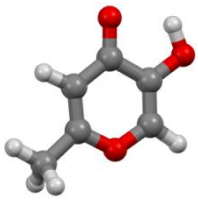
6-Hydroxymethyl kojic acid (*Conf C*)*



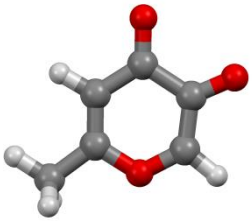
6-Hydroxymethyl kojic acid (*Conf D*)



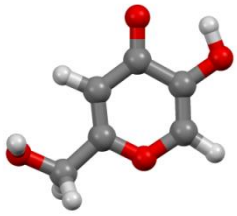
6-Hydroxymethyl kojic acid (*Conf D*)*



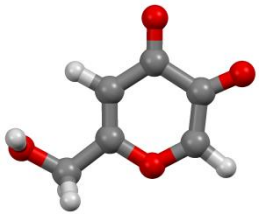
Allomaltol



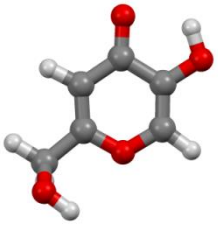
Allomaltol*



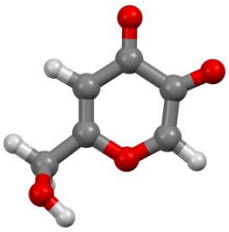
Kojic acid (*Conf A*)



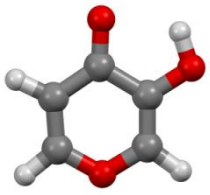
Kojic acid (*Conf A*)*



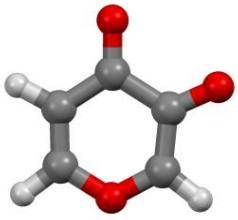
Kojic acid (*Conf B*)



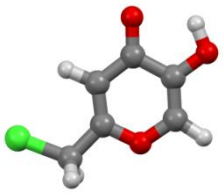
Kojic acid (*Conf B*)*



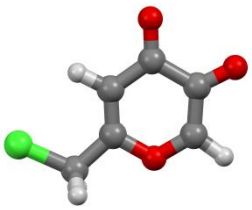
Pyromeconic acid



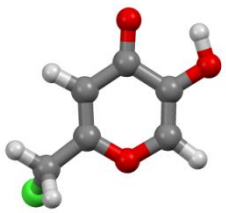
Pyromeconic acid*



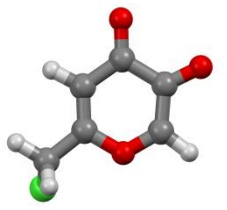
2-Chloro kojic acid (*Conf A*)



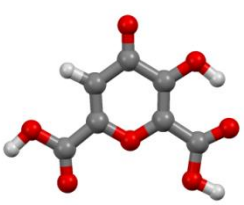
2-Chloro kojic acid (*Conf A*)*

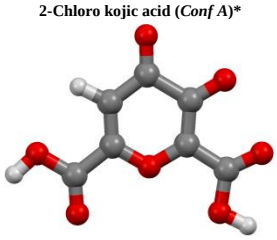


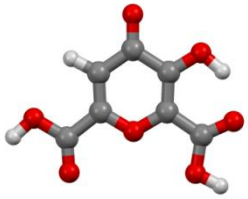
2-Chloro kojic acid (*Conf B*)

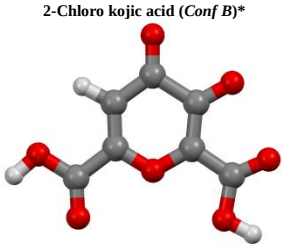


2-Chloro kojic acid (*Conf B*)*









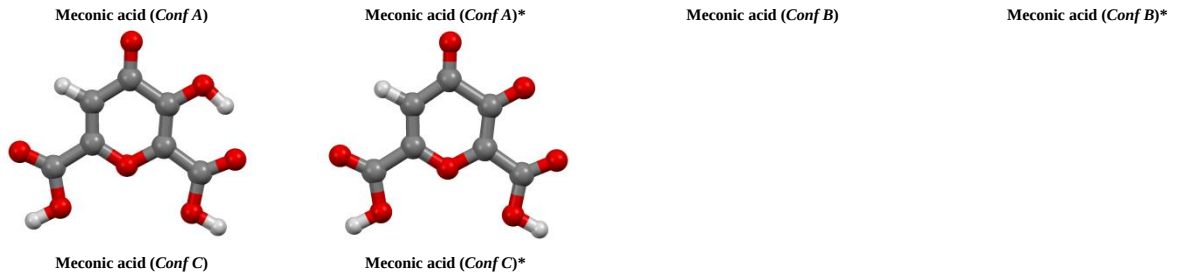


Figure S6 Optimized geometries for the 4H-pyranone derivatives and their oxy-radicals (*).

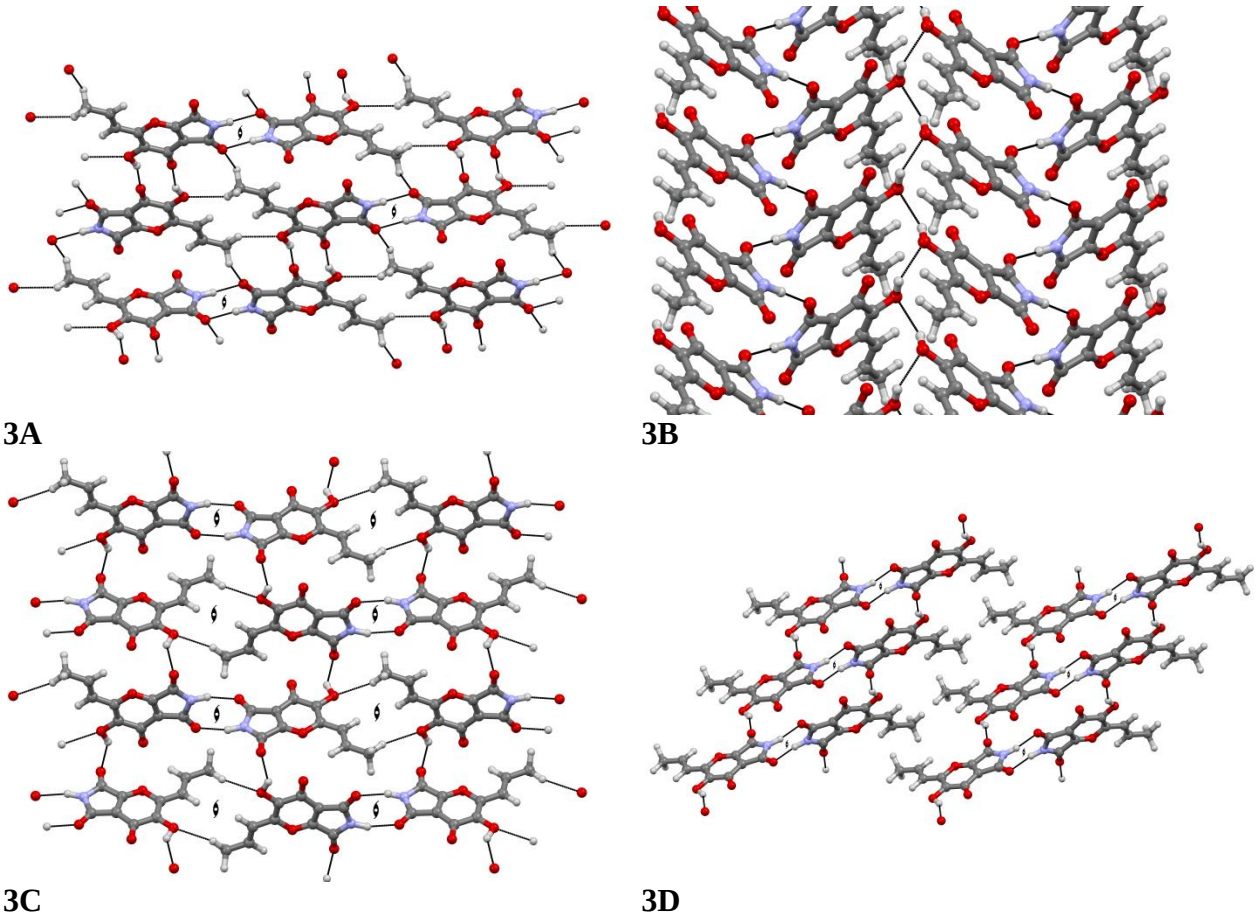
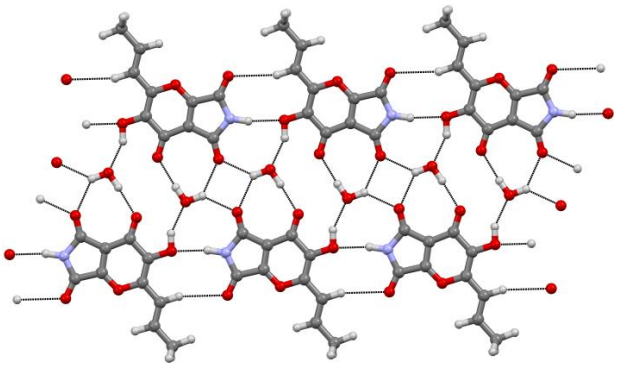
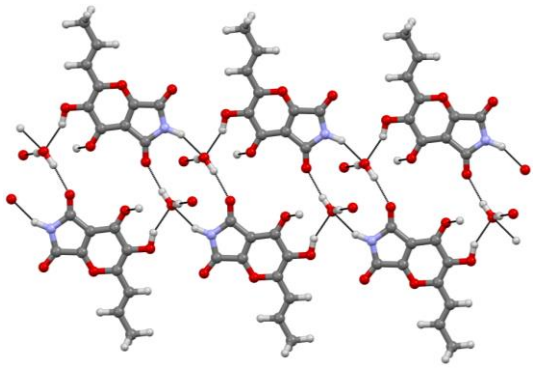


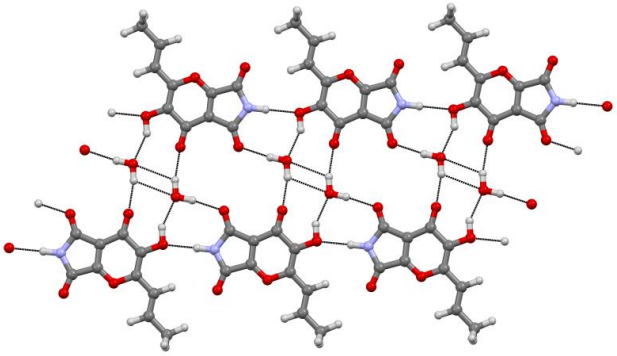
Figure S7 3-D molecular network observed in the CSP generated crystal structure for nigerloxin anhydrate. Symbol "Ò" represents a molecular chain propagating in the direction perpendicular to the plane of paper.



1HA



1HB



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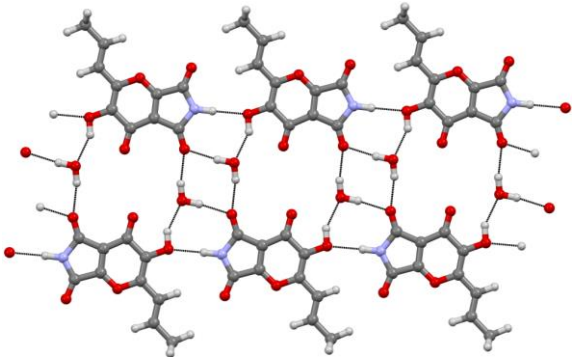
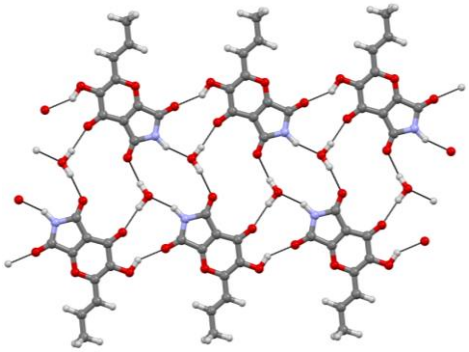
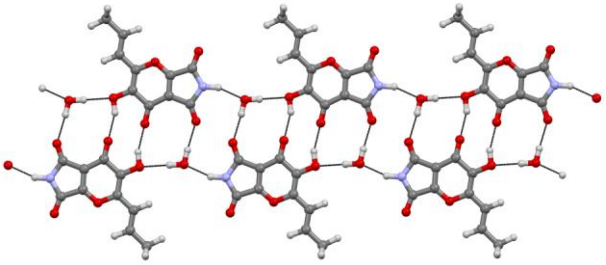


1HD



1HE



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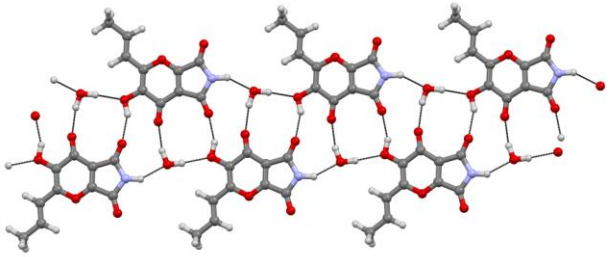
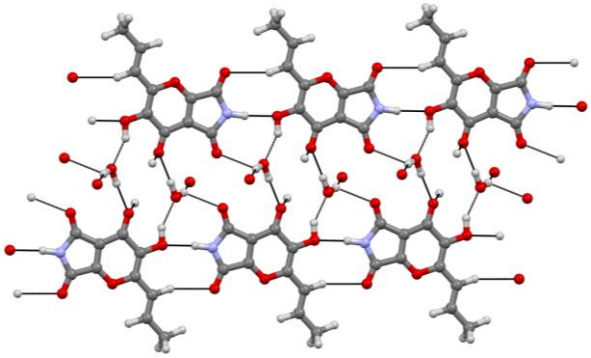
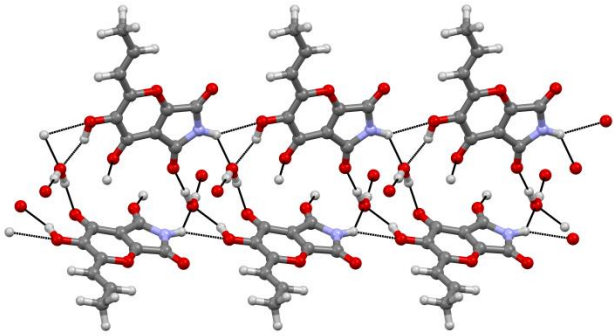


1HG



1HH



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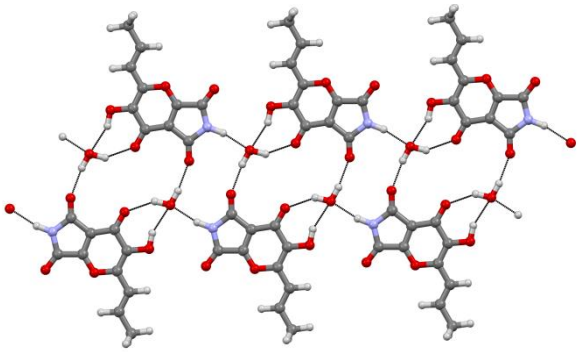

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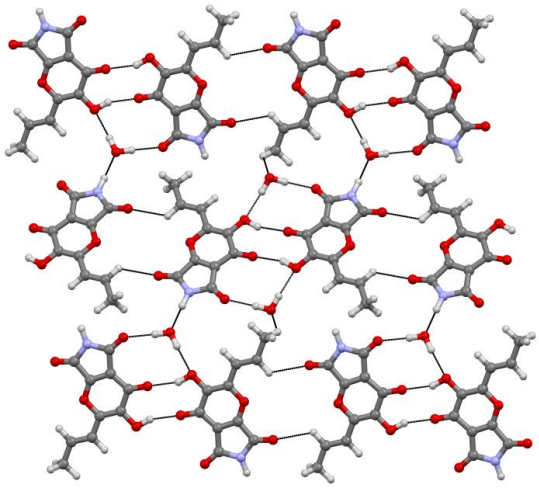

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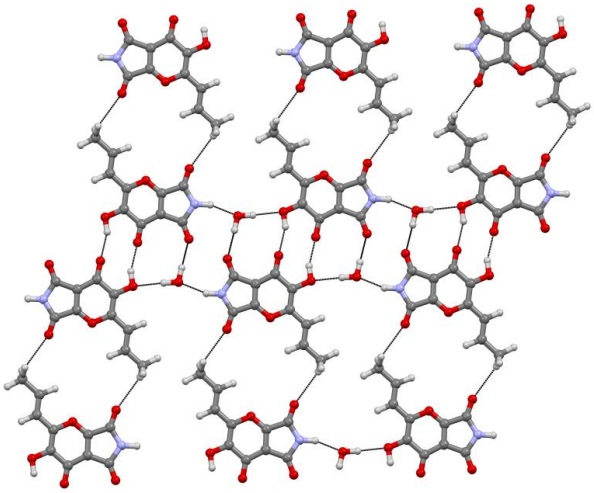

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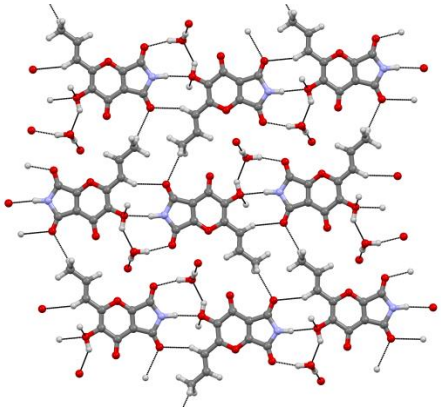

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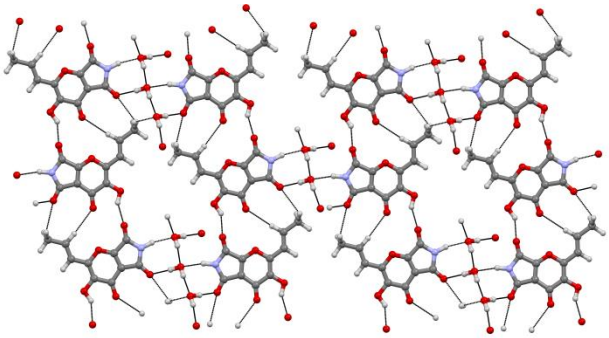

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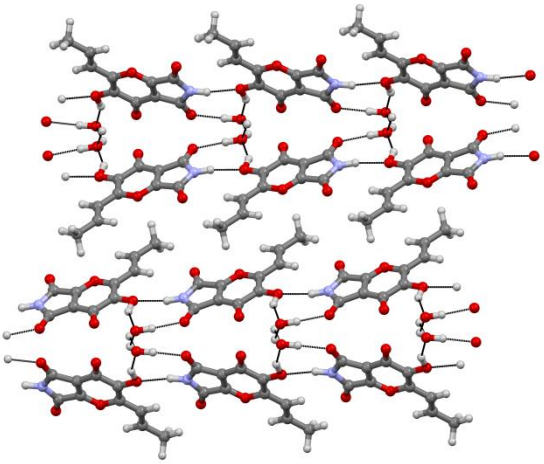

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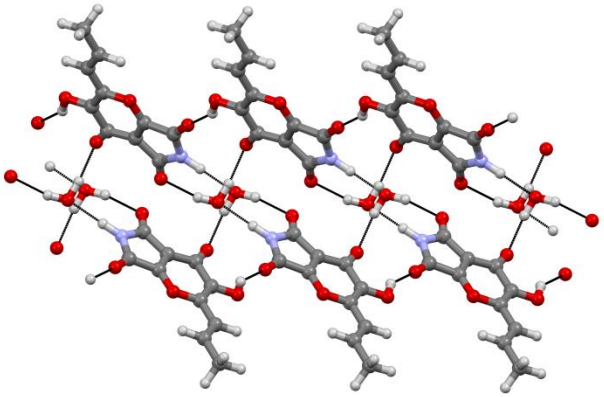

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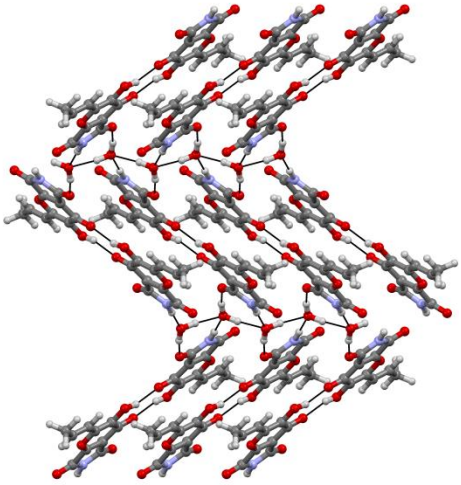

3HA

Figure S8 Growth units identified in the CSP generated crystal structure for nigerloxin monohydrate