Supporting information

Table S1 Interaction energies for selected contacts (kJ/mol)

Crystal	Interaction pair	Contact	E_{ele}	E_{pol}	E_{disp}	E_{rep}	E_{tot}
Oxy-1	Oxy A-Oxy B (asym unit)	O1A-H1A···O3B O1B-H1B···O3A	-46.3	-14.4	-35.8	37.4	-59.1
	Oxy A-Oxy C (asym unit)	C20A-H20H···H15A-C15C	-3.6	-0.3	-24.7	11.7	-16.9
	Oxy B-Oxy C (asym unit)	C1B-H1BA···H20B-C20C	-4.9	-2.1	-42.2	9.5	-39.5
	Oxy B-Oxy D (asym unit)	C20B-H20E···C21D C15B-H15D···H5D-C5D C7B-H7BB···H1DA-C1D	-2.3	-1.5	-45.7	17.7	-31.8
	Oxy C-Oxy D (asym unit)	O1D-H1D···O3C O1C-H1C···O3D C12C-H12A···O3D O1C-H1CB···H12G-C12D	-82.4	-21.2	-36.9	72.1	-68.4
	Oxy B-Oxy D	O2A-H2A···O1C C16C-H16A···O2A	-41.3	-9.7	-18.1	0	-69.1
	Oxy A-Oxy C	O2C-H2C···O1A	-46.7	-14.7	-17.8	0	-79.3
	Oxy A-Oxy A	C19A-H19G···C3A	-4.8	-2.7	-32.2	8.9	-30.8
	Oxy A –Oxy D	C18A-H19I···H19J-C19D	0.2	-0.9	-26.7	7.7	-19.7
	Oxy B-Oxy D	O2B-H2B···O1D C16D-H16G···O2B	-54.7	-13.5	-16.7	0	-84.9
	Oxy B-Oxy D	O2D-H2D···O1B C16B-H16C···O2D	-66.4	-17.7	-16.4	0	-100.5
	Oxy B-Oxy D	C18B-H19F···C21D	-3.2	-1.1	-36.3	11.4	-29.2
	Oxy B-Oxy C	C19B-H19D···H18A-C18C C19B-H19E···H11B-C11C	-5.0	-1.6	-33.7	12.4	-27.9
		C7C-H7CA···H15G-C15D C15C-H15A···H15G-C15D	-4.5	-0.3	-26.4	13.8	-17.4
Oxy-2	Oxy A-Oxy B (asym unit)	O1A-H1A···O3B C20A-H20D···O3B O1B-H1B···O3A	-82.2	-19.2	-36.8	63.2	-75.0
	Oxy B-Oxy D (asym unit)	C5B-H5B···H11H-C11D C9B-H9B···H12H-C12D	-5.1	-1.6	-42.4	13.5	-35.6
	Oxy B-Oxy C (asym unit)	C15B-H15B···C3C C15B-H15B···H5C-C5C	-0.3	-1.4	-45.5	14.4	-32.8
	Oxy C-Oxy D (asym unit)	C21C-H21C···O1D	-12.0	-1.9	-21.2	8.3	26.8
	Oxy A-Oxy D	C9A-H9A···C20D	0.7	-0.5	-28.4	7.3	-20.9
	Oxy A-Oxy-A	O2A-H2A···O1A C16A-H16D···O2A	-60.2	-15.9	-18.7	0	-94.8
	Oxy A-Oxy-D	C19A-H19F···C3D C8A-H8A···O3D	-3.0	-2.5	-28.1	8.5	-25.1
	Oxy A-Oxy B	C15A-H15D···H15A-C15B	-3.5	-0.3	-18.7	8.6	-13.9
	Oxy A-Oxy D	C18A-H18E···H15G-C15D C12A-H12D···H15H-C15D	-1.6	-0.4	-20.1	7.0	-15.1
	Oxy B- Oxy B	O2B-H2B···O1B	-77.2	-18.8	-18.8	0	-114.8

		C16B-H16B···O2B					
	Oxy B-Oxy D	C19B-H19C···C18D	-6.1	-2.7	-31.9	10.4	-30.0
	Oxy B-Oxy C	C18B-H18C···H18I-C18C	0	-0.3	-9.1	2.3	-7.1
	Oxy B-Oxy D	C18B-H18A···O3D	-7.7	-1.7	-10.1	3.2	-16.3
	Oxy B-Oxy A	C6B-H6BB···H21A-C21A	-13.1	-1.7	-10.1	3.6	-21.3
	Oxy B-Oxy D	C15B-H15A···H15D-C15A	-3.0	-0.3	-18.7	8.6	-13.4
	Oxy C-Oxy C	O1C-H1C···O3C	-28.6	-6.6	-9.4	0	-44.6
	Oxy C-Oxy D	O1D-H1D···O1C	-24.6	-5.7	-13.6	0	-43.9
	Oxy C-Oxy D	C19D-H19K···O2C O2D-H2D···H4CB-C4C	-8.2	-1.9	-21.4	6.7	-24.8
		C7C-H7CB···H7DA-C7D	-0.9	-0.4	-26.0	8.0	-19.3
Oxy-acetic	Oxy-acetic acid	O4-H4···O1	-74.6	-14.5	-12.9	45.4	-56.6
	Oxy-Oxy	O2-H2···O3 C21-H21···H4B-C4	-53.6	-14.2	-14.2	0	-82.0
	Oxy-acetic acid	O1-H1···O5	-34.4	-6.3	-10.0	22.5	-28.2
	Oxy-Oxy	C15-H15B···H11A-C11 C19-H19A···H7A-C7 C1-H1B···H7B-C7	-7.3	-2.3	-39.8	13.8	-35.6
	Oxy-Oxy	C4-H4A···O3 C15-H15A···H20-C20	-7.6	-2.7	-28.7	7.4	-31.6
	Oxy-acetic acid	C20-H20A···H23A-C23	0.3	-0.4	-7.4	2.8	-4.7
Metr	Metr A-Metr B (asym unit)	C18A-H18D···C4D C6A-H6AB···C9B C6A-H6AB···C9B C19B-H19B···C4A	-7.2	-1.4	-49.3	17.3	-40.6
	Metr A-Metr A	O1A-H1A···O2A C19A-H19D···O2A C19A-H19F···H2AA-C2A	-40.9	-7.7	-18.0	25.9	-40.7
	Metr A- Metr B	C1B-H1BB···O1A C16A-H16D···C11B	-9.7	-2.3	-31.3	12.4	-30.9
	Metr A-Metr A	C16A- H16C···O2A C16A- H16C···H4A-C4A	-1.6	-1.7	-12.3	6.2	-9.4
	Metr A-Metr B	C15A-H15C···H19C-C19B	0	-0.6	-14.4	4.6	-10.4
	Metr A-Metr A	C15A-H15C···H12A-C12A	2.3	-0.7	-19.9	5.7	-12.6
	Metr A-Metr B	C2A- H2AB···C4B	-7.7	-3.2	-21.3	5.8	-26.4
	Metr A-Metr B	C1A- H1AB···O1B C11A-H11A···H16A-C16B	-4.2	-2.1	-28.7	10.5	-24.5
	Metr B-Metr B	O1B- H1B···O2B C2B- H2BB···O1B O12B- H12B···O2B	-48.9	-9.7	-16.2	29.6	-45.2
	Metr B-Metr B	C4B-H4B···H18A-C18B	-3.6	-1.5	-10.8	3.2	-12.7

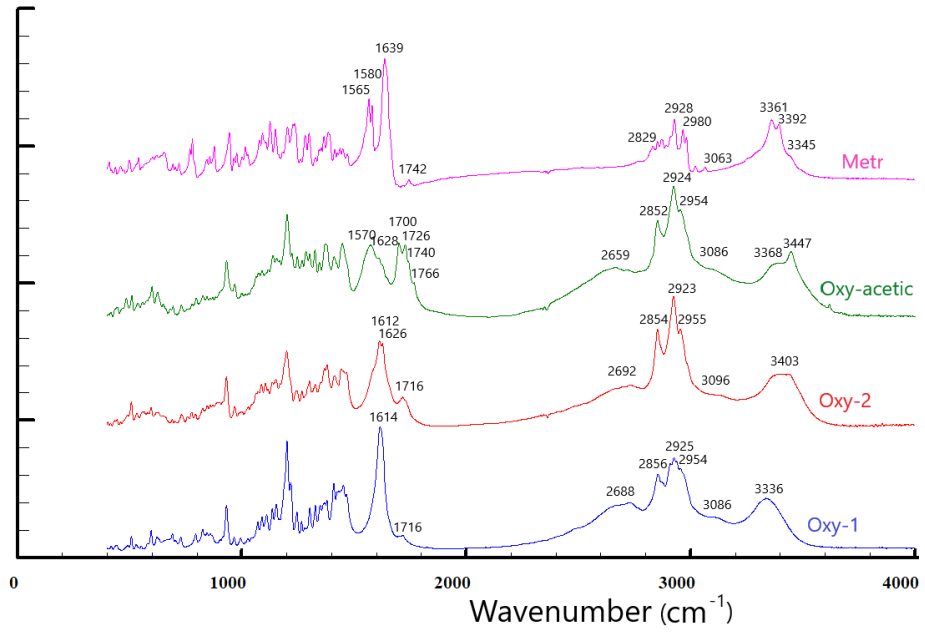
Abbreviations: E_{ele}-electrostatic term; E_{pol}-polarization term; E_{disp}-dispersion term; E_{rep}-dispersion term; E_{tot}-total intermolecular interaction energy

Table S2 Geometry of intermolecular interactions for studied crystal structures (Å, °)

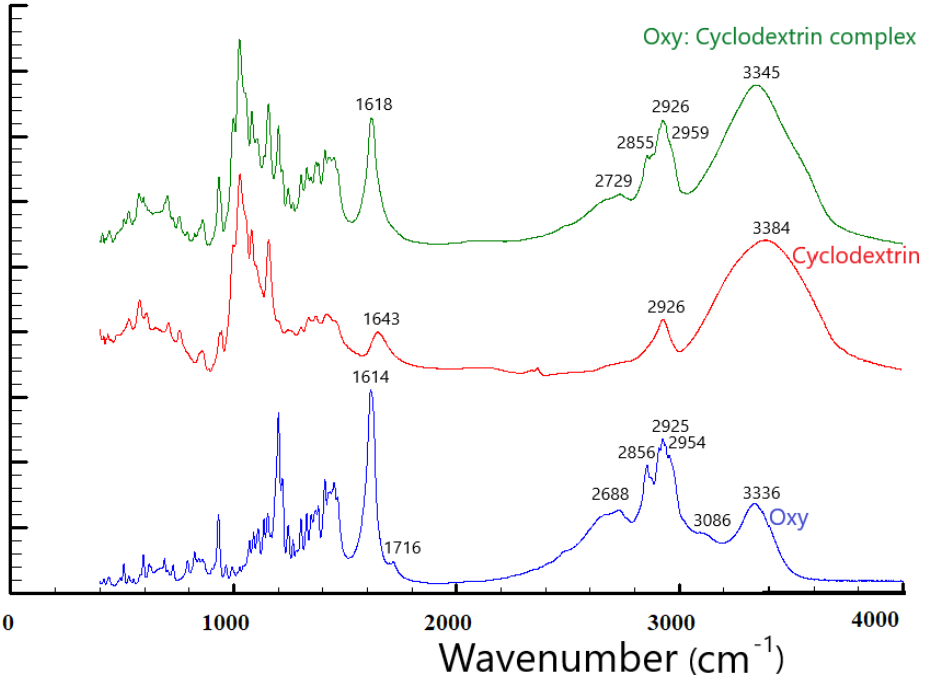
Structure	**D-H···A**	**D-H**	**H···A**	**D···A**	**<(D-H···A)**
Oxy-1	(i) O1A-H1A···O3B	0.823	2.05518(16)	2.8098(2)	152.298(3)
	(i) O1B-H1B···O3A	0.814	1.99974(15)	2.7531(2)	153.725(2)

	C20A-H20H···H15A-C15C	0.960		2.21361(18)	
	C20B-H20E···C21D	0.960	2.8922(3)	3.7303(3)	146.4690(16)
	C15B-H15D···H5D-C5D			2.19370(18)	
	C7B-H7BB···H1DA-C1D			2.3878(2)	
	(i) O1D-H1D···O3C	0.820	1.90749(14)	2.6992(2)	161.994(2)
	(i) O1C-H1C···O3D	0.819	2.96975(14)	2.7114(2)	150.181(3)
	(ii) O2A-H2A···O1C	0.816	1.77336(17)	2.5868(3)	174.0906(7)
	(ii) C16C-H16A···O2A	0.970	2.7021(3)	3.1452(3)	108.342(9)
	(iii) O2C-H2C···O1A	0.824	1.83654(17)	2.6230(3)	159.118(3)
	(iv) O2B-H2B···O1D	0.820	1.88689(18)	2.5870(3)	142.660(4)
	(v) C16D-H16G···O2B	0.970	2.6517(3)	3.1566(3)	112.777(5)
	(vi) O2D-H2D···O1B	0.827	1.76286(17)	2.5878(3)	175.4502
	(vi) C16B-H16C···O2D	0.970	2.6009(2)	3.2623(3)	125.605(5)
	C15C-H15A···H15G-C15D	0.970		2.3133(2)	
Oxy-2	(i) O1A-H1A···O3B	0.817	1.95987(11)	2.77252(15)	172.9784(6)
	(i) O1B-H1B···O3A	0.825	1.97416(10)	2.79317(15)	171.7078(7)
	C5B-H5B···H11H-C11D	0.980/0.970		2.32409(14)	
	C15B-H15B···H5C-C5C	0.970		2.54416(10)	
	(i) C21C-H21C···O1D	0.930	2.45983(15)	3.23776(19)	154.041(9)
	(vii) O2A-H2A···O1A	0.821	1.82200(7)	2.63859(11)	172.9192(5)
	(vii) C16A-H16D···O2A	0.970	2.73326(12)	3.21162(12)	111.0260(8)
	C15A-H15D···H15A-C15B	0.970		2.27015(13)	
	(viii) O2B-H2B···O1B	0.817	1.78115(8)	2.60353(11)	172.5446(5)
	(viii) C16B-H16B···O2B	0.970	2.71829(12)	3.28630(13)	117.9204(13)
	C19B-H19C···C18D	0.960	2.77642(17)	3.5320(2)	136.1621(16)
	C15B-H15A···H15D-C15A	0.970		2.27015(13)	
	(ix) O1C-H1C···O3C	0.825	2.06867(1)	2.87275(16)	164.7665(1)
	(ix) O1D-H1D···O1C	0.828	2.06856(9)	2.86440(12)	161.1981(14)
Oxy-acetic	(x) O1-H1···O5	0. 824	2.04556(7)	2.84518(10)	163.3539(5)
	(xi) O2-H2···O3	0.823	1.82859(8)	2.64782(11)	173.318(4)
	(i) O4-H4···O1	0.826	1.82952(9)	2.65392(13)	175.8624(4)
	C21-H21···H4B-C4	0.930/0.970		2.26982(8)	
	C19-H19A···H7A-C7	0.960/0.970		2.36637(9)	
	C23-H23A···O5	0.960	2.6940(2)	3.4954(3)	141.322(3)
Metr	C18A-H18D···C4D	0.960	2.85576(4)	3.64325(4)	139.9359
	(vi) O1A-H1A···O2A	0. 824	2.07925(3)	2.89537(4)	170.68031(14)
	(viii) C1B-H1BB···O1A	0.970	2.61496(3)	3.42166(4)	140.7613(7)
	C16A-H16D···C11B	0.970	2.81361(5)	3.77175(6)	169.6156(2)
	C15A-H15C···H19C-C19B	0.970/0.960		2.37818(4)	
	C2A- H2AB···C4B	0.970	2.88077(4)	3.66832(5)	138.9892(4)
	(viii) O1B- H1B···O2B	0.844	2.01190(3)	2.84212(4)	167.8053(2)

(i) x,y,z→x,y,z; (ii) x,y,z→-x,-1/2+y,1-z; (iii) x,y,z→-x,-1/2+y,-z; (iv) x,y,z→1-x,1/2+y,-z; (v) x,y,z→1-x,1/2+y,-z; (vi) x,y,z→1-x,-1/2+y,1-z; (vii) x,y,z→2-x, 1/2+y, 1-z; (viii) x,y,z→2-x,-1/2+y,2-z; (ix)x,y,z→3-x,-1/2+y,2-z; (x) x,y,z→x,1-y,1-z; (xi)) x,y,z→1/2-x,-1/2+y,1/2-z



(a)



(b)

Figure S1. FTIR spectra of the four crystal studied (a); spectra of oxymetholone, beta-cyclodextrin and oxymetholone: cyclodextrin complex (b)

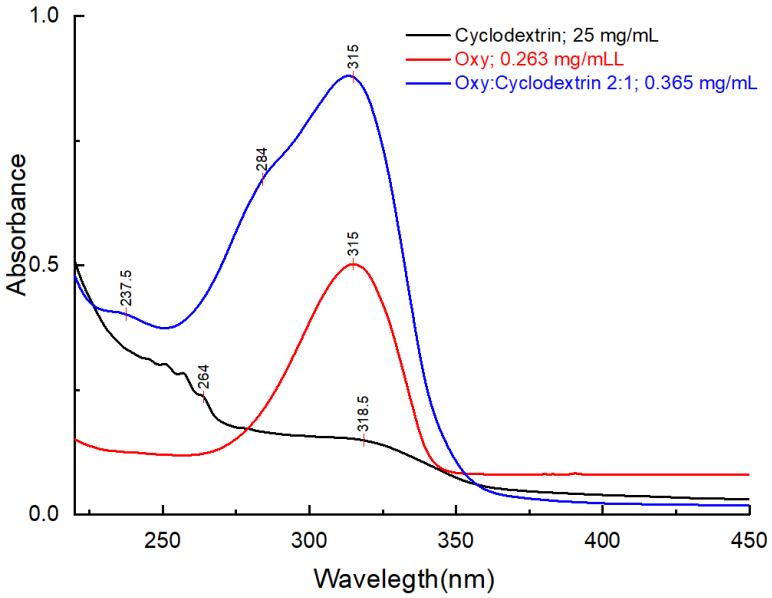


Figure S2. UV spectra of samples