Electronic Supplementary Material (ESI) for RSC Advances.

Nontoxic and Renewable metal-organic framework based on α-cyclodextrin with efficient drug delivery

Jingquan Sha , Xiaohua Zhong, Lianhe Wu, Guodong Liu, Ning Sheng

Key Laboratory of Inorganic Chemistry in Universities of Shandong, Department of Chemistry and Chemical Engineering,Jining University, Qufu, Shandong, 273155, China

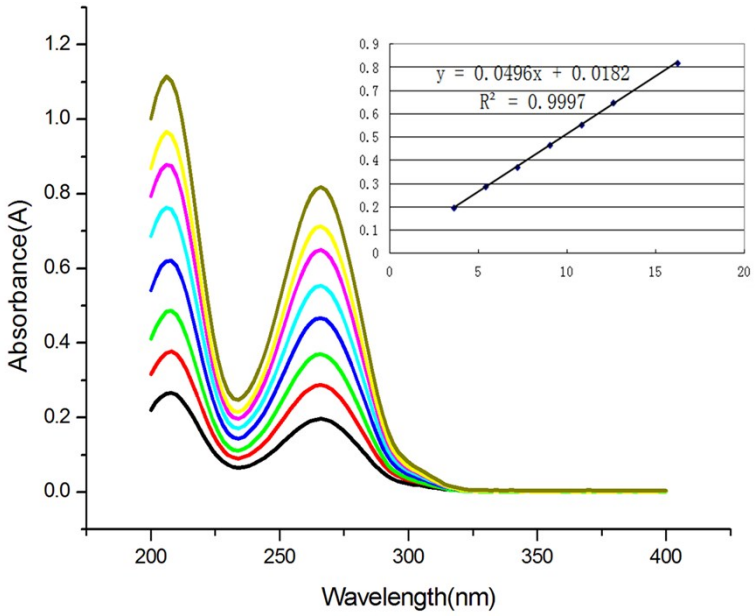

Fig.S1 The UV and standard curve of 5-FU in PBS.

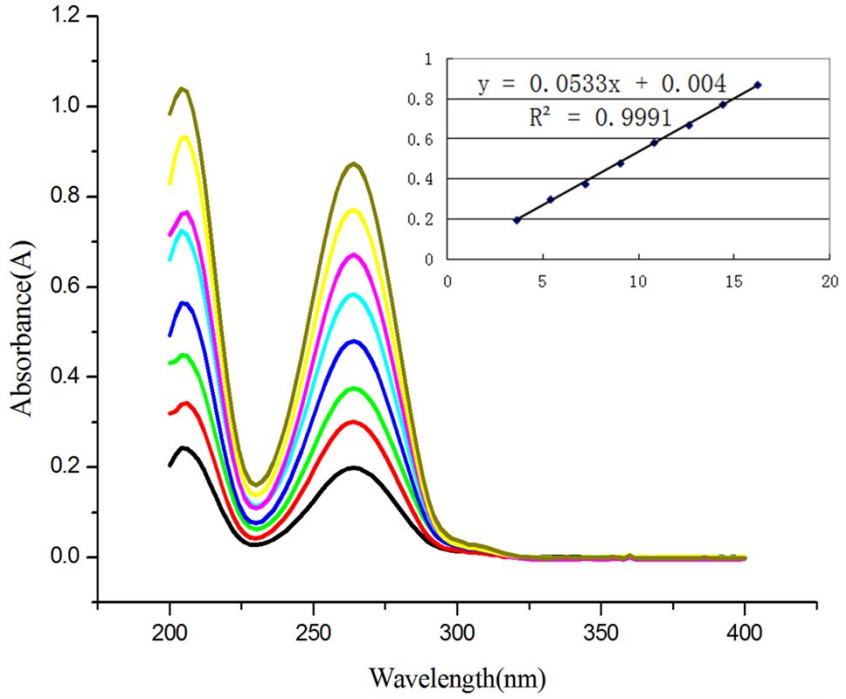

Fig.S2 The UV and standard curve of 5-FU in ethanol.

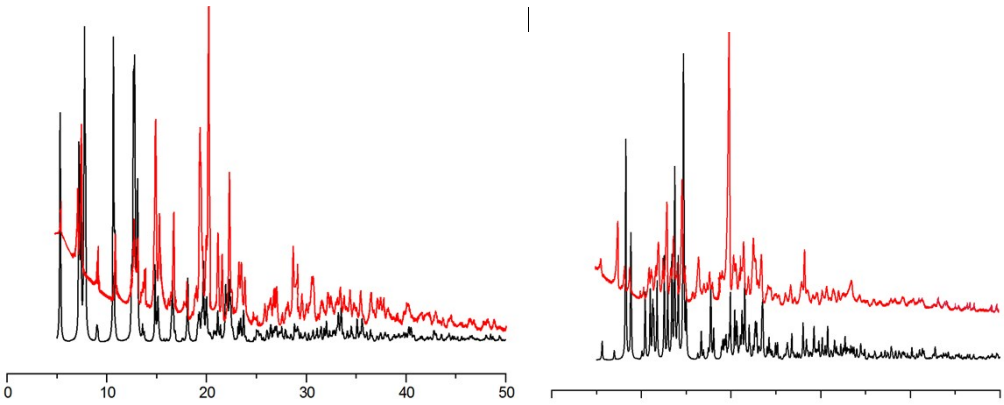

Fig. S3 Experimental (up) and simulated (below) powder X-ray diffraction profiles at room temperature for compounds **1** (left) and **2** (right), indicates that the product possesses high phase purity.

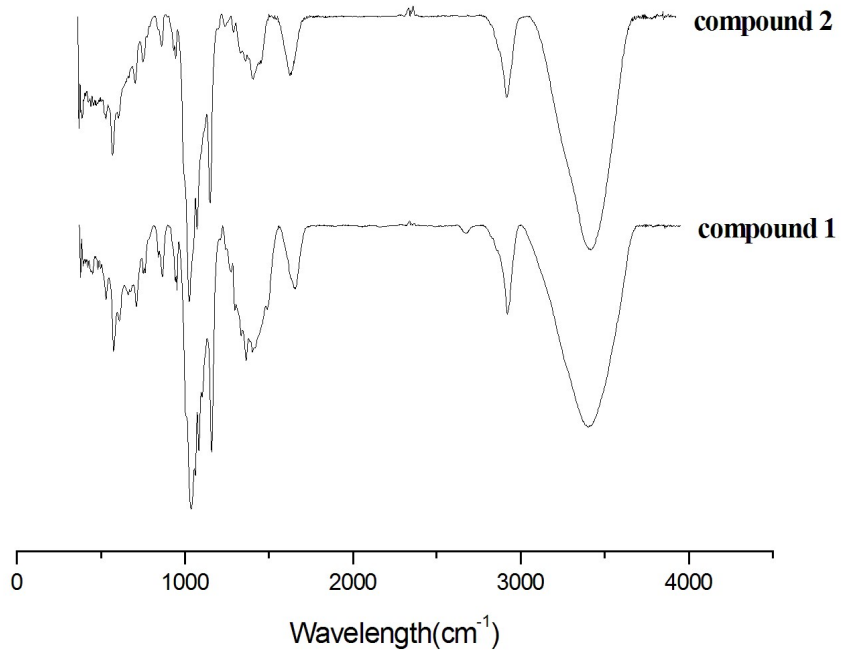

Fig.S4 The IR spectra of compounds **1** and **2**.

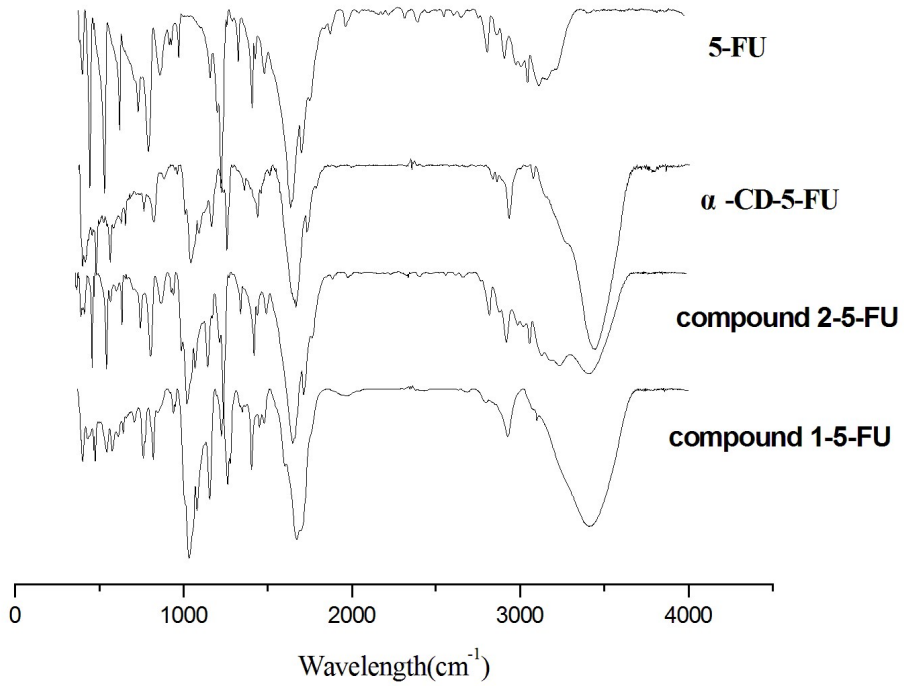

Fig.S5 The IR spectra of 5-FU,**α**-CD-5-FU, compound **1**-5-FU and compound **2**-5-FU.

Table S1 Selected bond length (Å) and bond angle(°) for compound **1**

O(55)-C(95)	1.425(10)	O(68)-C(110)	1.443(7)
O(55)-C(91)	1.456(8)	O(76)-C(119)	1.409(8)
O(57)-C(94)	1.419(9)	O(76)-C(120)	1.449(10)
O(57)-K(1)	3.273(7)	O(37)-C(79)	1.420(9)
O(49)-C(60)	1.433(10)	O(37)-C(82)	1.427(8)
O(49)-K(1)#1	3.207(6)	O(51)-C(125)	1.456(12)
O(49)-H(49)	0.82	O(51)-H(51)	0.82
O(45)-C(55)	1.417(11)	O(38)-C(80)	1.409(13)
O(45)-C(88)	1.450(9)	O(38)-H(38)	0.82
O(30)-C(72)	1.388(10)	O(21)-C(62)	1.426(14)
O(30)-H(30)	0.82	O(21)-H(21)	0.82
O(72)-C(112)	1.409(10)	O(27)-C(68)	1.469(11)
O(72)-K(1)#1	3.097(7)	O(27)-H(27)	0.82
O(72)-H(72)	0.82	O(65)-C(102)	1.439(13)
O(62)-C(100)	1.389(10)	O(65)-H(65)	0.82
O(62)-H(62)	0.82	O(33)-C(74)	1.446(10)
O(71)-C(113)	1.411(10)	O(33)-H(33)	0.82
O(71)-C(109)	1.456(8)	O(80)-C(58)	1.426(13)
O(46)-C(54)	1.317(10)	O(80)-H(80)	0.82
O(46)-K(3)	2.903(6)	C(100)-C(99)	1.469(12)
O(54)-C(90)	1.457(12)	C(100)-C(101)	1.558(10)
O(54)-H(54)	0.82	O(81)-C(114)	1.416(14)
O(75)-C(118)	1.429(10)	O(81)-H(81)	0.82
O(75)-K(3)	2.914(7)	C(94)-C(95)	1.506(12)
O(23)-C(65)	1.427(10)	C(94)-C(93)	1.512(9)
O(23)-K(2)	2.692(6)	C(106)-C(105)	1.507(10)
O(73)-C(113)	1.446(10)	C(106)-C(107)	1.515(10)
O(73)-C(116)	1.457(9)	C(120)-C(121)	1.501(10)
O(47)-C(55)	1.415(8)	C(120)-C(124)	1.568(10)
O(47)-C(56)	1.418(10)	C(117)-C(116)	1.493(11)
O(70)-C(108)	1.421(13)	C(117)-C(118)	1.519(13)
O(70)-H(70)	0.82	C(122)-C(121)	1.494(10)
O(42)-C(85)	1.393(10)	C(122)-C(123)	1.524(10)
O(42)-C(89)	1.474(9)	C(93)-C(92)	1.526(11)
O(42)-H(42)	0.82	C(65)-C(64)	1.520(11)
O(48)-C(59)	1.434(9)	C(65)-C(66)	1.526(8)
O(48)-K(1)#1	2.722(6)	C(116)-C(115)	1.492(13)
O(48)-H(48)	0.82	C(84)-C(82)	1.499(12)
O(77)-C(119)	1.396(11)	C(84)-C(86)	1.539(10)
O(77)-C(115)	1.439(12)	C(55)-C(54)	1.520(11)
O(79)-C(122)	1.403(9)	C(68)-C(69)	1.475(12)
O(79)-K(2)#2	3.256(6)	C(77)-C(76)	1.517(10)

O(79)-H(79)	0.82	C(77)-C(78)	1.522(12)
O(34)-C(79)	1.400(10)	C(108)-C(109)	1.497(12)
O(34)-C(75)	1.434(11)	C(78)-C(79)	1.512(11)
O(26)-C(67)	1.374(10)	C(54)-C(53)	1.566(11)
O(26)-C(70)	1.449(9)	C(54)-K(3)	3.301(8)
O(50)-C(61)	1.411(9)	C(99)-C(96)	1.511(11)
O(50)-C(57)	1.438(11)	C(53)-C(89)	1.502(11)
O(60)-C(101)	1.406(10)	C(71)-C(70)	1.509(11)
O(60)-C(97)	1.427(10)	C(71)-C(72)	1.555(10)
O(52)-C(123)	1.416(9)	C(59)-C(60)	1.473(12)
O(52)-C(124)	1.475(9)	C(59)-C(56)	1.553(10)
O(28)-C(69)	1.427(9)	C(85)-C(86)	1.507(12)
O(28)-C(73)	1.429(10)	C(113)-C(112)	1.514(12)
O(64)-C(105)	1.405(9)	C(67)-C(66)	1.530(12)
O(64)-K(2)	2.660(6)	C(72)-C(73)	1.520(11)
O(63)-C(104)	1.394(9)	C(64)-C(63)	1.506(12)
O(63)-C(101)	1.421(8)	C(105)-C(104)	1.523(9)
O(58)-C(95)	1.416(10)	C(57)-C(58)	1.506(12)
O(58)-C(96)	1.437(10)	C(57)-C(56)	1.529(11)
O(56)-C(93)	1.427(10)	C(89)-C(88)	1.521(11)
O(56)-K(1)	2.741(6)	C(70)-C(69)	1.555(11)
O(59)-C(98)	1.420(12)	C(90)-C(91)	1.487(11)
O(59)-H(59)	0.82	C(87)-C(88)	1.464(12)
O(69)-C(111)	1.433(10)	C(118)-C(119)	1.511(12)
O(69)-K(1)#1	2.711(6)	C(118)-K(3)	3.506(8)
O(69)-H(69)	0.82	C(124)-C(125)	1.483(11)
O(66)-C(107)	1.413(10)	C(91)-C(92)	1.524(10)
O(66)-C(103)	1.448(10)	C(98)-C(97)	1.547(14)
O(22)-C(61)	1.405(9)	C(96)-C(97)	1.559(12)
O(22)-C(64)	1.443(7)	C(82)-C(81)	1.540(10)
O(29)-C(71)	1.392(9)	C(104)-C(103)	1.567(10)
O(29)-K(3)#3	2.687(6)	C(76)-C(75)	1.554(11)
O(29)-H(29)	0.82	C(112)-C(111)	1.529(9)
O(53)-C(123)	1.394(10)	C(111)-C(110)	1.525(10)
O(53)-C(92)	1.436(8)	C(80)-C(81)	1.553(12)
O(74)-C(117)	1.410(10)	C(103)-C(102)	1.507(12)
O(74)-K(3)	2.645(6)	C(62)-C(63)	1.482(12)
O(43)-C(53)	1.437(10)	C(109)-C(110)	1.512(11)
O(43)-K(3)	2.723(6)	C(61)-C(60)	1.528(11)
O(41)-C(86)	1.428(9)	C(74)-C(75)	1.535(11)
O(41)-K(2)#2	3.261(7)	C(115)-C(114)	1.520(14)
O(41)-H(41)	0.82	K(1)-O(69)#4	2.711(6)
O(32)-C(77)	1.457(9)	K(1)-O(48)#4	2.722(6)
O(32)-K(1)	2.673(6)	K(1)-O(72)#4	3.097(7)

O(67)-C(106)	1.435(9)	K(1)-O(49)#4	3.207(6)
O(67)-K(2)	3.190(6)	K(3)-O(29)#5	2.687(6)
O(44)-C(87)	1.425(11)	K(3)-O(61)#5	2.730(6)
O(44)-H(44)	0.82	K(2)-O(40)#6	2.676(6)
O(78)-C(121)	1.466(8)	K(2)-O(78)#6	2.698(6)
O(78)-K(2)#2	2.698(6)	K(2)-O(79)#6	3.255(6)
O(78)-H(78)	0.82	K(2)-O(41)#6	3.261(7)
O(40)-C(84)	1.419(10)	K(2)-C(122)#6	3.540(8)
O(40)-K(2)#2	2.676(6)	O(1W)-H(1O1)	0.8588
O(40)-H(40)	0.82	O(1W)-H(2O1)	0.8517
O(25)-C(66)	1.407(10)	O(2W)-H(1O2)	0.86
O(25)-K(2)	3.129(7)	O(2W)-H(2O2)	0.8596
O(24)-C(67)	1.418(10)	O(3W)-H(1O3)	0.8659
O(24)-C(63)	1.476(8)	O(3W)-H(2O3)	0.853
O(35)-C(78)	1.452(9)	O(4W)-H(1O4)	0.8552
O(35)-K(1)	3.267(6)	O(4W)-H(2O4)	0.8619
O(31)-C(76)	1.423(10)	O(5W)-H(1O5)	0.8615
O(31)-C(73)	1.424(9)	O(5W)-H(2O5)	0.8581
O(31)-H(31)	0.82	O(6W)-H(1O6)	0.8501
O(61)-C(99)	1.467(9)	O(6W)-H(2O6)	0.8526
O(61)-K(3)#3	2.731(6)	O(7W)-H(1O7)	0.8523
O(61)-H(61)	0.82	O(7W)-H(2O7)	0.8499
C(95)-O(55)-C(91)	115.6(5)	O(38)-C(80)-C(81)	112.2(8)
C(94)-O(57)-K(1)	100.4(4)	O(60)-C(97)-C(98)	108.3(7)
C(60)-O(49)-K(1)#1	97.6(4)	O(60)-C(97)-C(96)	108.0(6)
C(60)-O(49)-H(49)	109.5	C(98)-C(97)-C(96)	113.2(7)
K(1)#1-O(49)-H(49)	141.9	O(45)-C(88)-C(87)	107.7(7)
C(55)-O(45)-C(88)	115.9(6)	O(45)-C(88)-C(89)	107.9(6)
C(72)-O(30)-H(30)	109.5	C(87)-C(88)-C(89)	116.2(7)
C(112)-O(72)-K(1)#1	101.8(5)	O(39)-C(81)-C(82)	109.9(6)
C(112)-O(72)-H(72)	109.5	O(39)-C(81)-C(80)	106.9(6)
K(1)#1-O(72)-H(72)	134.2	C(82)-C(81)-C(80)	111.2(7)
C(100)-O(62)-H(62)	109.5	O(66)-C(103)-C(102)	109.3(7)
C(113)-O(71)-C(109)	114.3(5)	O(66)-C(103)-C(104)	110.3(6)
C(54)-O(46)-K(3)	95.5(4)	C(102)-C(103)-C(104)	112.0(6)
C(90)-O(54)-H(54)	109.5	O(25)-C(66)-C(65)	114.2(7)
C(118)-O(75)-K(3)	102.2(4)	O(25)-C(66)-C(67)	112.5(6)
C(65)-O(23)-K(2)	129.9(4)	C(65)-C(66)-C(67)	108.9(7)
C(113)-O(73)-C(116)	121.0(5)	O(65)-C(102)-C(103)	110.4(8)
C(55)-O(47)-C(56)	118.9(5)	O(77)-C(119)-O(76)	112.5(6)
C(108)-O(70)-H(70)	109.5	O(77)-C(119)-C(118)	111.4(7)
C(85)-O(42)-C(89)	121.7(5)	O(76)-C(119)-C(118)	107.2(6)
C(85)-O(42)-H(42)	109.5	O(21)-C(62)-C(63)	108.4(8)
C(89)-O(42)-H(42)	88.1	O(66)-C(107)-O(68)	109.3(7)

C(59)-O(48)-K(1)#1	126.1(4)	O(66)-C(107)-C(106)	111.0(5)
C(59)-O(48)-H(48)	109.5	O(68)-C(107)-C(106)	107.9(6)
K(1)#1-O(48)-H(48)	118.3	O(71)-C(109)-C(108)	106.8(6)
C(119)-O(77)-C(115)	114.1(6)	O(71)-C(109)-C(110)	110.5(6)
C(122)-O(79)-K(2)#2	89.8(4)	C(108)-C(109)-C(110)	113.2(7)
C(122)-O(79)-H(79)	109.5	O(22)-C(61)-O(50)	110.8(6)
K(2)#2-O(79)-H(79)	156.3	O(22)-C(61)-C(60)	108.2(7)
C(79)-O(34)-C(75)	112.2(6)	O(50)-C(61)-C(60)	109.1(6)
C(67)-O(26)-C(70)	119.8(5)	O(49)-C(60)-C(59)	111.1(7)
C(61)-O(50)-C(57)	113.8(6)	O(49)-C(60)-C(61)	111.3(6)
C(101)-O(60)-C(97)	115.7(6)	C(59)-C(60)-C(61)	109.9(8)
C(123)-O(52)-C(124)	111.8(6)	O(33)-C(74)-C(75)	111.2(7)
C(69)-O(28)-C(73)	115.4(5)	O(77)-C(115)-C(116)	110.5(7)
C(105)-O(64)-K(2)	129.4(4)	O(77)-C(115)-C(114)	107.3(8)
C(104)-O(63)-C(101)	119.4(6)	C(116)-C(115)-C(114)	115.1(8)
C(95)-O(58)-C(96)	119.8(6)	O(34)-C(75)-C(74)	108.0(7)
C(93)-O(56)-K(1)	131.9(4)	O(34)-C(75)-C(76)	110.9(6)
C(98)-O(59)-H(59)	109.5	C(74)-C(75)-C(76)	112.2(6)
C(111)-O(69)-K(1)#1	126.7(4)	O(51)-C(125)-C(124)	113.3(7)
C(111)-O(69)-H(69)	109.5	O(53)-C(123)-O(52)	110.8(6)
K(1)#1-O(69)-H(69)	123.5	O(53)-C(123)-C(122)	111.1(6)
C(107)-O(66)-C(103)	114.9(6)	O(52)-C(123)-C(122)	110.3(5)
C(61)-O(22)-C(64)	120.4(6)	O(68)-C(110)-C(109)	109.3(6)
C(71)-O(29)-K(3)#3	142.3(5)	O(68)-C(110)-C(111)	105.2(5)
C(71)-O(29)-H(29)	109.5	C(109)-C(110)-C(111)	115.1(6)
K(3)#3-O(29)-H(29)	101.2	O(24)-C(63)-C(62)	107.5(6)
C(123)-O(53)-C(92)	120.6(6)	O(24)-C(63)-C(64)	108.8(6)
C(117)-O(74)-K(3)	124.9(5)	C(62)-C(63)-C(64)	115.6(7)
C(53)-O(43)-K(3)	116.2(5)	O(34)-C(79)-O(37)	111.6(6)
C(86)-O(41)-K(2)#2	92.2(5)	O(34)-C(79)-C(78)	110.0(5)
C(86)-O(41)-H(41)	109.5	O(37)-C(79)-C(78)	107.5(7)
K(2)#2-O(41)-H(41)	54.4	O(80)-C(58)-C(57)	113.1(8)
C(77)-O(32)-K(1)	129.0(4)	O(81)-C(114)-C(115)	111.9(8)
C(106)-O(67)-K(2)	99.5(4)	O(32)-K(1)-O(69)#4	144.14(18)
C(87)-O(44)-H(44)	109.5	O(32)-K(1)-O(48)#4	86.4(2)
C(121)-O(78)-K(2)#2	123.8(5)	O(69)#4-K(1)-O(48)#4	106.9(2)
C(121)-O(78)-H(78)	109.5	O(32)-K(1)-O(56)	98.4(2)
K(2)#2-O(78)-H(78)	126.1	O(69)#4-K(1)-O(56)	88.6(2)
C(84)-O(40)-K(2)#2	128.2(4)	O(48)#4-K(1)-O(56)	146.16(18)
C(84)-O(40)-H(40)	109.5	O(32)-K(1)-O(72)#4	158.41(16)
K(2)#2-O(40)-H(40)	119.6	O(69)#4-K(1)-O(72)#4	56.90(16)
C(66)-O(25)-K(2)	101.9(5)	O(48)#4-K(1)-O(72)#4	90.22(18)
C(67)-O(24)-C(63)	114.3(6)	O(56)-K(1)-O(72)#4	73.06(19)
C(78)-O(35)-K(1)	96.4(4)	O(32)-K(1)-O(49)#4	73.43(18)

C(76)-O(31)-C(73)	118.3(5)	O(69)#4-K(1)-O(49)#4	86.02(17)
C(76)-O(31)-H(31)	109.5	O(48)#4-K(1)-O(49)#4	57.06(15)
C(73)-O(31)-H(31)	126.4	O(56)-K(1)-O(49)#4	156.18(19)
C(99)-O(61)-K(3)#3	135.4(5)	O(72)#4-K(1)-O(49)#4	121.88(17)
C(99)-O(61)-H(61)	109.5	O(32)-K(1)-O(35)	56.60(15)
K(3)#3-O(61)-H(61)	115.1	O(69)#4-K(1)-O(35)	158.94(18)
C(85)-O(39)-C(81)	112.4(5)	O(48)#4-K(1)-O(35)	72.19(16)
C(107)-O(68)-C(110)	117.5(5)	O(56)-K(1)-O(35)	82.62(16)
C(119)-O(76)-C(120)	117.8(6)	O(72)#4-K(1)-O(35)	102.12(15)
C(79)-O(37)-C(82)	117.5(6)	O(49)#4-K(1)-O(35)	109.35(15)
C(125)-O(51)-H(51)	109.5	O(32)-K(1)-O(57)	85.06(18)
C(80)-O(38)-H(38)	109.5	O(69)#4-K(1)-O(57)	70.36(19)
C(62)-O(21)-H(21)	109.5	O(48)#4-K(1)-O(57)	158.47(16)
C(68)-O(27)-H(27)	109.5	O(56)-K(1)-O(57)	54.98(15)
C(102)-O(65)-H(65)	109.5	O(72)#4-K(1)-O(57)	104.69(17)
C(74)-O(33)-H(33)	109.5	O(49)#4-K(1)-O(57)	101.50(15)
C(58)-O(80)-H(80)	109.5	O(35)-K(1)-O(57)	118.29(16)
O(62)-C(100)-C(99)	113.9(6)	O(74)-K(3)-O(29)#5	152.3(2)
O(62)-C(100)-C(101)	110.3(6)	O(74)-K(3)-O(43)	104.8(2)
C(99)-C(100)-C(101)	108.4(6)	O(29)#5-K(3)-O(43)	99.2(2)
C(114)-O(81)-H(81)	109.5	O(74)-K(3)-O(61)#5	90.0(2)
O(57)-C(94)-C(95)	111.6(6)	O(29)#5-K(3)-O(61)#5	80.45(19)
O(57)-C(94)-C(93)	113.1(6)	O(43)-K(3)-O(61)#5	139.4(2)
C(95)-C(94)-C(93)	110.8(6)	O(74)-K(3)-O(46)	86.56(19)
O(58)-C(95)-O(55)	111.1(6)	O(29)#5-K(3)-O(46)	93.37(19)
O(58)-C(95)-C(94)	109.7(6)	O(43)-K(3)-O(46)	60.6(2)
O(55)-C(95)-C(94)	108.8(6)	O(61)#5-K(3)-O(46)	159.5(2)
O(67)-C(106)-C(105)	109.0(6)	O(74)-K(3)-O(75)	60.94(19)
O(67)-C(106)-C(107)	111.6(6)	O(29)#5-K(3)-O(75)	139.8(2)
C(105)-C(106)-C(107)	110.6(6)	O(43)-K(3)-O(75)	77.07(18)
O(76)-C(120)-C(121)	108.6(6)	O(61)#5-K(3)-O(75)	77.89(17)
O(76)-C(120)-C(124)	107.9(6)	O(46)-K(3)-O(75)	117.36(16)
C(121)-C(120)-C(124)	112.9(5)	O(74)-K(3)-C(54)	108.0(2)
O(74)-C(117)-C(116)	114.8(7)	O(29)#5-K(3)-C(54)	78.85(19)
O(74)-C(117)-C(118)	107.8(6)	O(43)-K(3)-C(54)	46.8(2)
C(116)-C(117)-C(118)	108.5(7)	O(61)#5-K(3)-C(54)	159.27(19)
O(79)-C(122)-C(121)	110.4(6)	O(46)-K(3)-C(54)	23.40(18)
O(79)-C(122)-C(123)	111.6(5)	O(75)-K(3)-C(54)	119.59(18)
C(121)-C(122)-C(123)	107.3(6)	O(74)-K(3)-C(118)	42.47(19)
O(56)-C(93)-C(94)	107.4(6)	O(29)#5-K(3)-C(118)	147.1(2)
O(56)-C(93)-C(92)	110.5(6)	O(43)-K(3)-C(118)	97.21(19)
C(94)-C(93)-C(92)	108.6(6)	O(61)#5-K(3)-C(118)	68.64(18)
O(23)-C(65)-C(64)	111.0(6)	O(46)-K(3)-C(118)	119.52(17)
O(23)-C(65)-C(66)	106.9(6)	O(75)-K(3)-C(118)	23.48(18)

C(64)-C(65)-C(66)	108.1(6)	C(54)-K(3)-C(118)	131.84(18)
O(73)-C(116)-C(115)	108.5(6)	O(64)-K(2)-O(40)#6	143.98(18)
O(73)-C(116)-C(117)	105.7(6)	O(64)-K(2)-O(23)	107.1(2)
C(115)-C(116)-C(117)	114.4(7)	O(40)#6-K(2)-O(23)	92.0(2)
O(40)-C(84)-C(82)	109.5(7)	O(64)-K(2)-O(78)#6	94.8(2)
O(40)-C(84)-C(86)	107.9(6)	O(40)#6-K(2)-O(78)#6	86.3(2)
C(82)-C(84)-C(86)	109.6(7)	O(23)-K(2)-O(78)#6	143.74(18)
O(47)-C(55)-O(45)	110.5(6)	O(64)-K(2)-O(25)	89.39(18)
O(47)-C(55)-C(54)	108.5(6)	O(40)#6-K(2)-O(25)	75.43(19)
O(45)-C(55)-C(54)	113.7(6)	O(23)-K(2)-O(25)	57.23(15)
O(27)-C(68)-C(69)	113.3(7)	O(78)#6-K(2)-O(25)	153.74(17)
O(32)-C(77)-C(76)	108.6(6)	O(64)-K(2)-O(67)	56.65(15)
O(32)-C(77)-C(78)	108.3(6)	O(40)#6-K(2)-O(67)	155.97(19)
C(76)-C(77)-C(78)	111.7(6)	O(23)-K(2)-O(67)	90.02(17)
O(70)-C(108)-C(109)	113.0(7)	O(78)#6-K(2)-O(67)	78.02(19)
O(35)-C(78)-C(79)	111.8(6)	O(25)-K(2)-O(67)	124.81(18)
O(35)-C(78)-C(77)	109.0(6)	O(64)-K(2)-O(79)#6	75.30(17)
C(79)-C(78)-C(77)	108.3(6)	O(40)#6-K(2)-O(79)#6	75.81(17)
O(46)-C(54)-C(55)	116.9(7)	O(23)-K(2)-O(79)#6	157.45(17)
O(46)-C(54)-C(53)	112.5(7)	O(78)#6-K(2)-O(79)#6	55.69(15)
C(55)-C(54)-C(53)	106.3(6)	O(25)-K(2)-O(79)#6	100.84(15)
O(46)-C(54)-K(3)	61.1(4)	O(67)-K(2)-O(79)#6	108.87(16)
C(55)-C(54)-K(3)	164.5(5)	O(64)-K(2)-O(41)#6	157.06(17)
C(53)-C(54)-K(3)	87.7(5)	O(40)#6-K(2)-O(41)#6	55.98(15)
O(61)-C(99)-C(100)	107.1(6)	O(23)-K(2)-O(41)#6	77.01(18)
O(61)-C(99)-C(96)	109.7(6)	O(78)#6-K(2)-O(41)#6	72.15(17)
C(100)-C(99)-C(96)	116.2(6)	O(25)-K(2)-O(41)#6	110.79(17)
O(43)-C(53)-C(89)	110.0(7)	O(67)-K(2)-O(41)#6	101.40(15)
O(43)-C(53)-C(54)	109.2(6)	O(79)#6-K(2)-O(41)#6	109.87(16)
C(89)-C(53)-C(54)	112.7(7)	O(64)-K(2)-C(122)#6	64.15(19)
O(29)-C(71)-C(70)	111.7(7)	O(40)#6-K(2)-C(122)#6	94.86(19)
O(29)-C(71)-C(72)	107.8(5)	O(23)-K(2)-C(122)#6	171.1(2)
C(70)-C(71)-C(72)	111.6(6)	O(78)#6-K(2)-C(122)#6	42.71(16)
O(48)-C(59)-C(60)	109.6(7)	O(25)-K(2)-C(122)#6	119.32(16)
O(48)-C(59)-C(56)	107.7(5)	O(67)-K(2)-C(122)#6	85.97(16)
C(60)-C(59)-C(56)	111.6(7)	O(79)#6-K(2)-C(122)#6	23.35(15)
O(42)-C(85)-O(39)	110.0(6)	O(41)#6-K(2)-C(122)#6	111.55(18)
O(42)-C(85)-C(86)	110.2(6)	H(1O1)-O(1W)-H(2O1)	106.7
O(39)-C(85)-C(86)	110.7(6)	H(1O2)-O(2W)-H(2O2)	105.9
O(71)-C(113)-O(73)	108.7(6)	H(1O3)-O(3W)-H(2O3)	106
O(71)-C(113)-C(112)	109.8(7)	H(1O4)-O(4W)-H(2O4)	106.2
O(73)-C(113)-C(112)	110.3(6)	H(1O5)-O(5W)-H(2O5)	105.9
O(26)-C(67)-O(24)	112.1(7)	H(1O6)-O(6W)-H(2O6)	107.4
O(26)-C(67)-C(66)	108.9(7)	H(1O7)-O(7W)-H(2O7)	107.5

O(24)-C(67)-C(66)	109.9(6)	C(125)-C(124)-C(120)	112.7(6)
O(30)-C(72)-C(73)	111.7(6)	O(60)-C(101)-O(63)	109.7(6)
O(30)-C(72)-C(71)	112.2(6)	O(60)-C(101)-C(100)	110.3(6)
C(73)-C(72)-C(71)	109.0(6)	O(63)-C(101)-C(100)	109.5(6)
O(22)-C(64)-C(63)	108.0(6)	O(55)-C(91)-C(90)	105.7(6)
O(22)-C(64)-C(65)	104.4(6)	O(55)-C(91)-C(92)	109.9(5)
C(63)-C(64)-C(65)	113.0(6)	C(90)-C(91)-C(92)	116.6(7)
O(64)-C(105)-C(106)	108.6(6)	O(59)-C(98)-C(97)	110.3(8)
O(64)-C(105)-C(104)	109.3(5)	O(58)-C(96)-C(99)	107.8(6)
C(106)-C(105)-C(104)	111.2(6)	O(58)-C(96)-C(97)	110.8(6)
O(50)-C(57)-C(58)	106.4(7)	C(99)-C(96)-C(97)	112.0(6)
O(50)-C(57)-C(56)	110.5(6)	O(31)-C(73)-O(28)	108.4(6)
C(58)-C(57)-C(56)	113.5(7)	O(31)-C(73)-C(72)	110.4(6)
O(47)-C(56)-C(57)	107.3(6)	O(28)-C(73)-C(72)	111.1(6)
O(47)-C(56)-C(59)	107.6(6)	O(37)-C(82)-C(84)	105.1(6)
C(57)-C(56)-C(59)	113.1(6)	O(37)-C(82)-C(81)	108.9(6)
O(42)-C(89)-C(53)	108.0(6)	C(84)-C(82)-C(81)	112.5(6)
O(42)-C(89)-C(88)	108.4(6)	O(53)-C(92)-C(91)	108.4(5)
C(53)-C(89)-C(88)	115.3(7)	O(53)-C(92)-C(93)	106.1(6)
O(26)-C(70)-C(71)	104.5(6)	C(91)-C(92)-C(93)	114.6(6)
O(26)-C(70)-C(69)	110.0(6)	O(63)-C(104)-C(105)	108.9(6)
C(71)-C(70)-C(69)	112.5(7)	O(63)-C(104)-C(103)	108.0(6)
O(54)-C(90)-C(91)	109.5(7)	C(105)-C(104)-C(103)	113.0(5)
O(44)-C(87)-C(88)	111.7(7)	O(78)-C(121)-C(122)	108.6(6)
O(75)-C(118)-C(119)	111.3(7)	O(78)-C(121)-C(120)	109.5(5)
O(75)-C(118)-C(117)	114.3(7)	C(122)-C(121)-C(120)	113.0(7)
C(119)-C(118)-C(117)	111.0(6)	O(31)-C(76)-C(77)	107.0(6)
O(75)-C(118)-K(3)	54.3(4)	O(31)-C(76)-C(75)	108.4(6)
C(119)-C(118)-K(3)	164.4(6)	C(77)-C(76)-C(75)	111.0(6)
C(117)-C(118)-K(3)	82.7(4)	O(72)-C(112)-C(113)	113.6(7)
O(28)-C(69)-C(68)	103.8(6)	O(72)-C(112)-C(111)	108.5(6)
O(28)-C(69)-C(70)	108.1(6)	C(113)-C(112)-C(111)	107.5(6)
C(68)-C(69)-C(70)	115.7(7)	O(69)-C(111)-C(110)	109.9(6)
O(52)-C(124)-C(125)	105.2(6)	O(69)-C(111)-C(112)	108.4(6)
O(52)-C(124)-C(120)	108.8(6)	C(110)-C(111)-C(112)	109.4(6)
O(41)-C(86)-C(84)	110.0(7)	O(41)-C(86)-C(85)	111.8(6)

ymmetry transformations used to generate equivalent atoms: #1 x-1,y,z-1; #2 x,y,z+1; #3 x+1,y,z; #4 x+1,y,z+1; #5 x-1,y,z; #6 x,y,z-1

Table S2 Selected bond length (Å) and bond angle(°) for compound **2**

C(1)-O(10)	1.397(11)	C(20)-C(36)	1.505(16)
C(1)-C(6)	1.502(13)	C(20)-C(31)	1.527(13)
C(1)-C(2)	1.529(14)	C(21)-O(6)	1.43(3)
C(2)-O(9)	1.428(13)	C(22)-O(29)	1.453(14)
C(2)-C(3)	1.558(15)	C(22)-C(37)	1.51(2)
C(3)-O(20)	1.376(12)	C(23)-O(18)	1.38(3)
C(3)-O(13)	1.433(11)	C(23)-O(7)	1.455(14)
O(001)-C(12)	1.429(11)	C(24)-O(14)	1.471(12)
C(5)-O(20)	1.427(14)	C(24)-C(26)	1.524(15)
C(5)-C(8)	1.524(19)	C(25)-O(12)	1.391(12)
C(5)-C(6)	1.581(15)	C(25)-O(29)	1.442(15)
C(6)-O(27)	1.401(12)	C(25)-C(26)	1.532(16)
C(7)-O(27)	1.395(13)	C(26)-O(8)	1.422(12)
C(7)-O(3)	1.437(14)	C(27)-O(23)	1.389(11)
C(7)-C(13)	1.504(17)	C(27)-C(28)	1.519(13)
C(8)-O(11)	1.05(9)	C(28)-O(24)	1.414(10)
C(9)-O(3)	1.409(17)	C(28)-O(22)	1.418(10)
C(9)-C(34)	1.548(17)	C(29)-O(21)	1.456(16)
C(9)-C(35)	1.56(2)	C(29)-C(30)	1.535(13)
C(10)-O(13)	1.439(10)	C(30)-O(22)	1.429(11)
C(10)-C(12)	1.526(12)	C(31)-O(24)	1.436(10)
C(10)-C(30)	1.526(13)	C(31)-C(32)	1.524(13)
C(11)-O(4)	1.432(10)	C(32)-O(26)	1.432(11)
C(11)-C(22)	1.542(16)	C(32)-C(33)	1.516(13)
C(11)-C(24)	1.549(13)	C(33)-O(25)	1.413(14)
C(12)-C(27)	1.522(12)	C(34)-O(17)	1.46(2)
C(13)-O(5)	1.436(12)	C(35)-O(7)	1.398(15)
C(13)-C(19)	1.574(16)	C(36)-O(2)	1.437(14)
C(14)-O(1)	1.397(13)	C(37)-O(28)	1.45(3)
C(14)-O(4)	1.398(12)	C(19)-O(15)	1.385(17)
C(14)-C(33)	1.538(15)	C(19)-C(35)	1.542(17)
C(15)-O(18)	1.424(17)	C(20)-O(1)	1.454(11)
C(15)-C(16)	1.49(3)	C(17)-C(18)	1.51(2)
C(15)-C(21)	1.55(3)	C(18)-O(19)	1.47(3)
C(16)-C(17)	1.46(2)	C(18)-C(23)	1.50(3)
O(10)-C(1)-C(6)	108.1(7)	C(35)-C(19)-C(13)	107.8(10)
O(10)-C(1)-C(2)	110.7(8)	O(1)-C(20)-C(36)	105.8(7)
C(6)-C(1)-C(2)	110.5(8)	O(1)-C(20)-C(31)	110.7(7)
O(9)-C(2)-C(1)	114.0(9)	C(36)-C(20)-C(31)	114.6(9)
O(9)-C(2)-C(3)	108.6(8)	O(6)-C(21)-C(15)	111.6(17)
C(1)-C(2)-C(3)	111.3(8)	O(29)-C(22)-C(37)	101.6(10)

O(20)-C(3)-O(13)	111.8(8)	O(29)-C(22)-C(11)	111.0(9)
O(20)-C(3)-C(2)	111.5(8)	C(37)-C(22)-C(11)	114.4(13)
O(13)-C(3)-C(2)	106.0(7)	O(18)-C(23)-O(7)	112.3(18)
O(20)-C(5)-C(8)	105.8(11)	O(18)-C(23)-C(18)	109.8(11)
O(20)-C(5)-C(6)	109.7(9)	O(7)-C(23)-C(18)	104.6(13)
C(8)-C(5)-C(6)	111.0(9)	O(14)-C(24)-C(26)	109.4(8)
O(27)-C(6)-C(1)	107.1(8)	O(14)-C(24)-C(11)	105.6(8)
O(27)-C(6)-C(5)	110.0(8)	C(26)-C(24)-C(11)	110.8(8)
C(1)-C(6)-C(5)	109.7(7)	O(12)-C(25)-O(29)	111.7(10)
O(27)-C(7)-O(3)	110.5(9)	O(12)-C(25)-C(26)	107.5(8)
O(27)-C(7)-C(13)	109.0(9)	O(29)-C(25)-C(26)	106.2(9)
O(3)-C(7)-C(13)	109.8(10)	O(8)-C(26)-C(24)	110.7(8)
O(11)-C(8)-C(5)	101(4)	O(8)-C(26)-C(25)	105.8(9)
O(3)-C(9)-C(34)	108.3(12)	C(24)-C(26)-C(25)	113.0(9)
O(3)-C(9)-C(35)	111.2(12)	O(23)-C(27)-C(28)	106.9(7)
C(34)-C(9)-C(35)	112.0(14)	O(23)-C(27)-C(12)	113.1(8)
O(13)-C(10)-C(12)	104.5(7)	C(28)-C(27)-C(12)	109.3(7)
O(13)-C(10)-C(30)	110.4(7)	O(24)-C(28)-O(22)	110.4(6)
C(12)-C(10)-C(30)	113.0(7)	O(24)-C(28)-C(27)	108.8(7)
O(4)-C(11)-C(22)	111.7(9)	O(22)-C(28)-C(27)	109.9(7)
O(4)-C(11)-C(24)	103.6(7)	O(21)-C(29)-C(30)	109.1(9)
C(22)-C(11)-C(24)	108.5(9)	O(22)-C(30)-C(10)	110.1(7)
O(001)-C(12)-C(27)	109.0(7)	O(22)-C(30)-C(29)	105.1(8)
O(001)-C(12)-C(10)	110.3(7)	C(10)-C(30)-C(29)	114.9(8)
C(27)-C(12)-C(10)	113.1(7)	O(24)-C(31)-C(32)	107.4(7)
O(5)-C(13)-C(7)	109.2(9)	O(24)-C(31)-C(20)	107.0(7)
O(5)-C(13)-C(19)	110.0(9)	C(32)-C(31)-C(20)	112.2(7)
C(7)-C(13)-C(19)	110.6(10)	O(26)-C(32)-C(33)	108.3(8)
O(1)-C(14)-O(4)	112.7(8)	O(26)-C(32)-C(31)	109.8(7)
O(1)-C(14)-C(33)	110.7(8)	C(33)-C(32)-C(31)	110.5(8)
O(4)-C(14)-C(33)	107.6(8)	O(25)-C(33)-C(32)	109.2(9)
O(18)-C(15)-C(16)	110.4(17)	O(25)-C(33)-C(14)	111.3(9)
O(18)-C(15)-C(21)	106.9(12)	C(32)-C(33)-C(14)	109.0(8)
C(16)-C(15)-C(21)	111.9(15)	O(17)-C(34)-C(9)	111.1(15)
C(17)-C(16)-O(12)	105.4(11)	O(7)-C(35)-C(19)	104.1(10)
C(17)-C(16)-C(15)	115.4(12)	O(7)-C(35)-C(9)	108.9(12)
O(12)-C(16)-C(15)	110.1(13)	C(19)-C(35)-C(9)	112.2(10)
C(16)-C(17)-O(16)	114.7(11)	O(2)-C(36)-C(20)	111.9(8)
C(16)-C(17)-C(18)	109.3(15)	O(28)-C(37)-C(22)	112.5(15)
O(16)-C(17)-C(18)	109.9(16)	C(14)-O(1)-C(20)	114.0(7)
O(19)-C(18)-C(17)	109.3(16)	C(36)-O(2)-H(2)	109.5
O(19)-C(18)-C(23)	115.5(13)	C(9)-O(3)-C(7)	112.9(9)
C(17)-C(18)-C(23)	112.4(17)	C(14)-O(4)-C(11)	117.6(7)
O(15)-C(19)-C(35)	107.9(10)	C(3)-O(13)-C(10)	120.1(7)

Table S3 Inhibitory effect of 5-FU, α-CD and derivatives on tumor cells *in vitro*

Material	DOSE (μg/mL)	OD value	Inhibitory effect (%) smmc7721	IC50 (μg/mL)
α-CD	100	3.770	4.910	9.777
	50	3.836	3.058	
	25	3.899	1.291	
	12.5	3.912	0.926	
	6.25	3.933	0.337	
Compound **1**	100	3.727	7.826	13.940
	50	3.759	6.960	
	25	3.895	3.276	
	12.5	3.882	3.628	
	6.25	3.956	1.625	
Compound **2**	100	3.585	7.692	6.807
	50	3.687	4.809	
	25	3.835	0.622	
	12.5	3.787	1.980	
	6.25	3.847	0.283	
5-Fu	100	1.504	65.149	0.025
	50	1.686	59.662	
	25	1.826	55.442	
	12.5	1.919	52.638	
	6.25	2.140	45.975	