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Supporting information for article:

Cocrystals with tunable luminescence colour self-assembled by a predictable method

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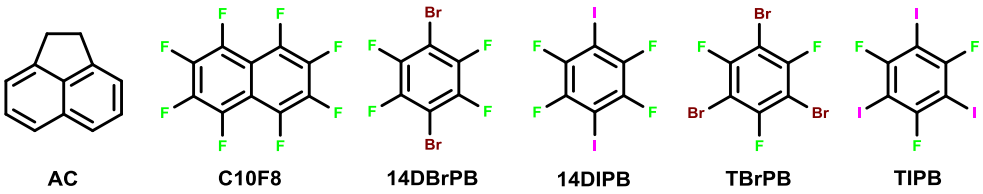
1. Structures of cocrystals



Scheme 1 Structures of selected molecules.

Table S1 Single crystal XRD data and structure refinement.

Reference	AC–C10F8	AC–14DBrPB	AC–14DIPB	AC–TBrPB	AC–TIPB
CCDC no.	1830836	1830835	1830837	1830838	1830839
formula	C22H10F8	C18H10Br2F4	C18H10F4I2	C54H30Br9F9	C24H10F6I6
fw	426.30	462.08	556.06	1568.94	1173.72
Crystal system	monoclinic	monoclinic	triclinic	trigonal	monoclinic
Space group	P1211	P121/n1	P–1	P321	C1c1
a/Å	7.2267(10)	9.1989(14)	5.3366(2)	14.4575(7)	14.2199(4)
b/Å	8.4607(11)	14.436(3)	6.4653(4)	14.4575(7)	45.6676(11)
c/Å	13.509(2)	12.167(3)	12.1051(6)	6.8147(3)	8.9289(3)
α/°	90	90	96.549(4)	90	90
β/°	97.550(15)	101.465(16)	92.853(4)	90	97.688(2)
γ/°	90	90	93.382(4)	120	90
V/Å^3	818.8(2)	1583.6(6)	413.53(4)	1233.57(13)	5746.2(3)
Z	2	4	1	1	8
T/K	100.02(10)	100.02(10)	100.01(10)	100.01(10)	100.00(10)
Refls. collected	3239	8312	2982	7700	25345
Independent reflections	2234	3758	1902	2098	10741
R1 (I > 2σ(I))	0.0602	0.1075	0.0343	0.0491	0.0407
wR(F2) (I > 2σ(I))	0.1470	0.2054	0.0781	0.0965	0.0898
R1 (all data)	0.0708	0.2132	0.0362	0.0552	0.0487
wR(F2) (all data)	0.1579	0.2547	0.0795	0.0991	0.0957

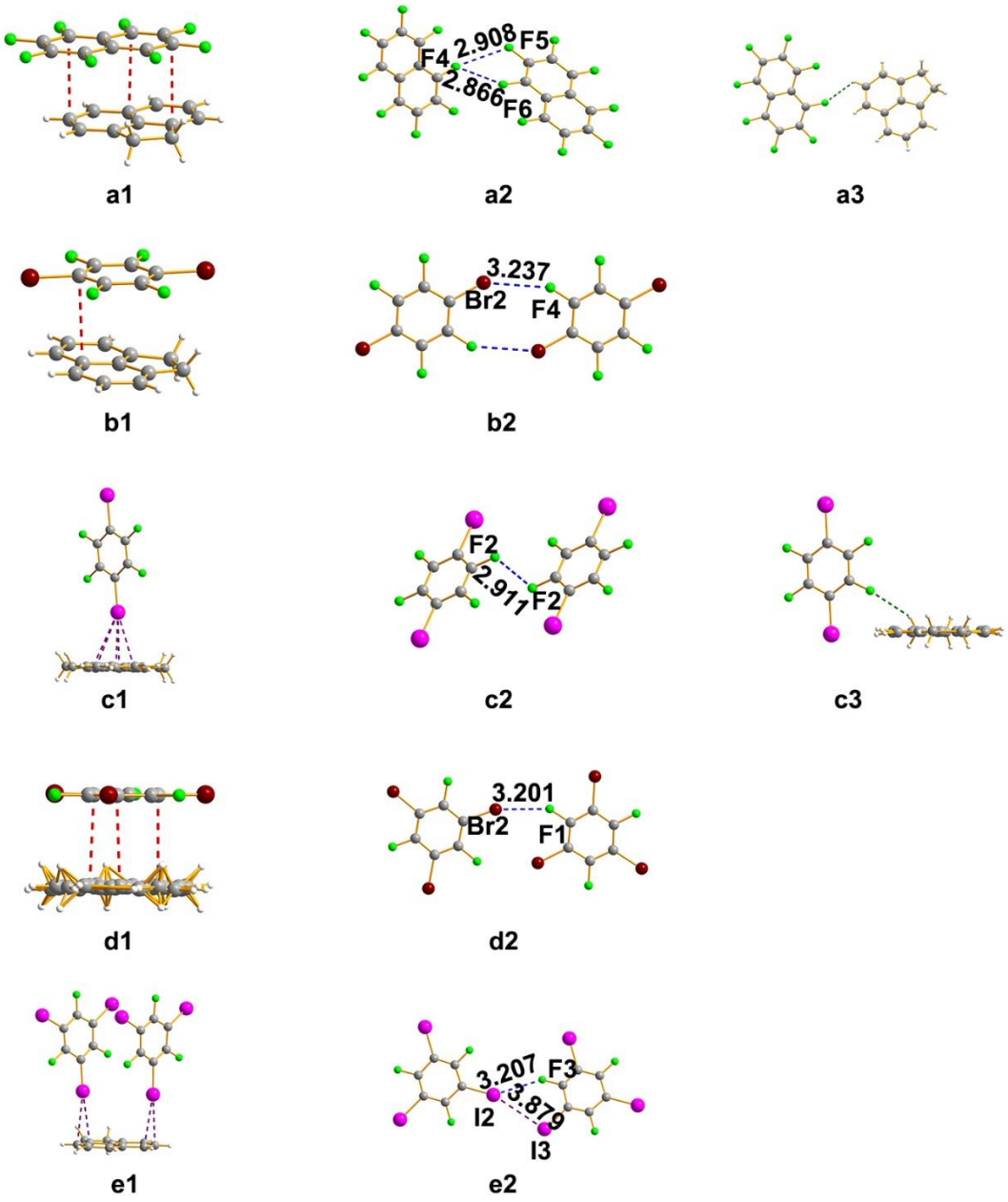


Figure S1 The local structure units and interactions extracted from five cocrystal data. The π–hole···π bond (**a1**), van der Waals F−F contact (**a2**) and C–F···H HB (**a3**) in AC–C10F8 cocrystal. The π–hole···π bond (**b1**) and van der Waals Br–F contact (**b2**) in AC–14DBrPB cocrystal. The C–I···π XB (**c1**), van der Waals F–F contact (**c2**) and C–F···H HB (**c3**) in AC–14DIPB cocrystal. The bonding patterns in AC–TBrPB cocrystal are the same as in AC–14DBrPB cocrystal. The C–I···π XB (**e1**), C–I···I XB (**e2**) and van der Waals F−F contact (**e2**) in AC–TIPB cocrystal. Red dashed line represents π–hole···π bond; purple dashed line represents σ-hole···π bond; blue dashed line represents van der Waals contact; green dashed line represents hydrogen bond.

2. *Phosphorescence spectra of cocrystals*

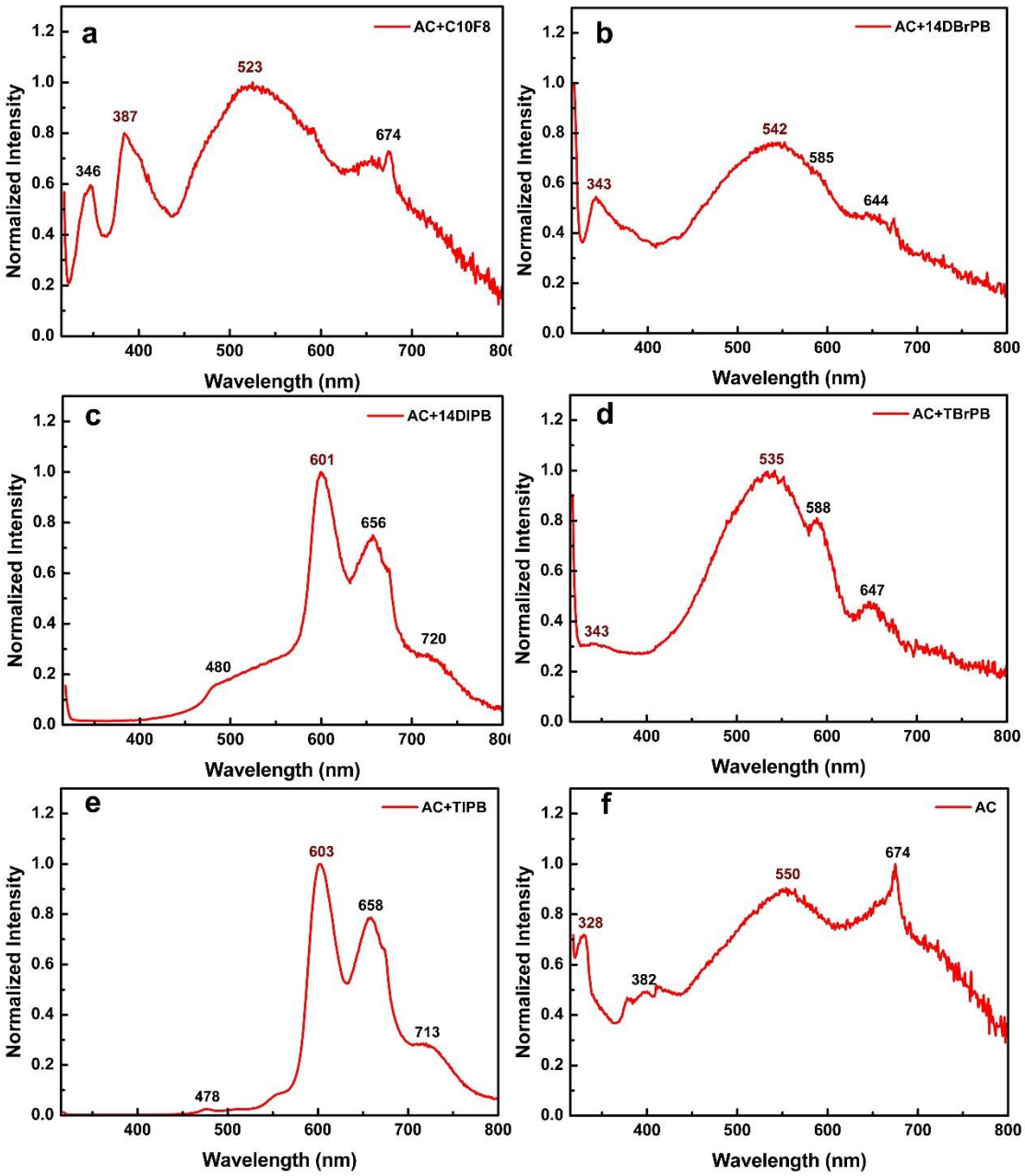


Figure S2 Phosphorescence and delayed fluorescence spectra of the cocrystals measured under phosphorescent mode.

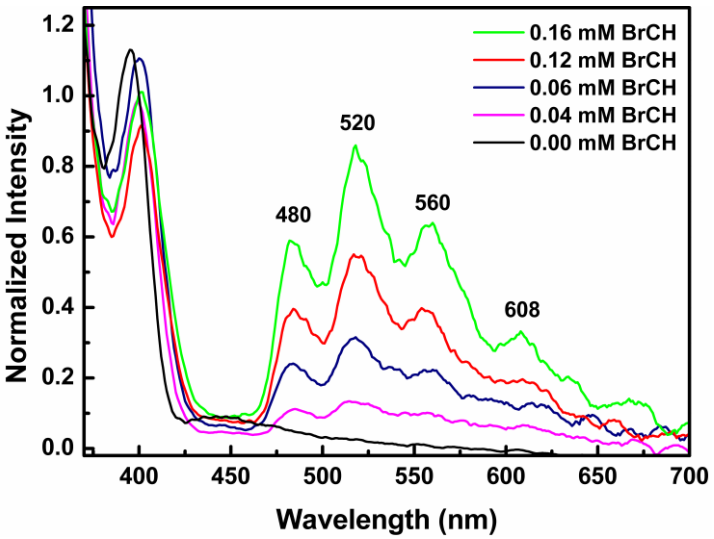


Figure S3 Phosphorescence spectra of AC (black line) induced by bromocyclohexane (BrCH) in β–CD aqueous solution (colorful lines). Conditions: [AC] 5×10^{-5} mol·L^{-1}; [β–CD] 8×10^{-3} mol·L^{-1}; [BrCH] 4×10^{-5}, 6×10^{-5}, 12×10^{-5} and 16×10^{-5} mol·L^{-1} measured under phosphorescent mode.

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