Supplementary Information

X-ray data were collected on a Rigaku AFC12 diffractometer mounted on Rigaku FR-E+ Super Bright Very High Flux rotating anode CCD diffractometer equipped with VariMax very high flux (VHF) optics and Saturn 724+ CCD detector[1]. The crystal structures were solved by direct methods or charge flipping and refined using full matrix least squares (refinement based on F^2) using SHELXL[2]. Where the quality of data has had an effect on the structure, a footnote indicates the approach taken or the cause. Structures previously determined and reported in the literature are included with a citation and for these only pertinent crystal data i.e. unit cell dimensions and space group, are repeated here for the purposes of completeness.

Table S1. Crystal data and refinement details for all compounds compared in this study.

Compound reference	2Br	2Cl-1[3]	2Cl-2[4]	2F-1[5]	2F-2	2I
Chemical formula	$C_8H_7BrO_3$	$C_8H_7ClO_3$	$C_8H_7ClO_3$	$C_8H_7FO_3$	$C_8H_7FO_3$	$C_8H_7IO_3$
Formula Mass	231.05	186.59	186.59	170.14	170.14	278.04
Crystal system	Triclinic	Triclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic
a/ Å	5.708(5)	9.0874(19)	14.1961(7)	8.4238(12)	8.1888(12)	5.805(3)
b/ Å	10.8436(10)	9.805(2)	8.0521(4)	5.4766(7)	10.1998(14)	10.732(6)
c/ Å	14.131(14)	10.830(2)	14.4453(5)	15.959(2)	9.2654(12)	13.969(7)
α/ °	96.952(19)	66.066(14)	90.00	90.00	90.00	96.527(13)
β/ °	93.91(2)	74.371(14)	99.177(3)	95.962(11)	92.709(7)	92.909(13)
γ/ °	90.07(2)	85.606(14)	90.00	90.00	90.00	90.058(13)
Unit cell volume/ Å^3	866.2(11)	848.803	1630.08	732.267	773.02(18)	863.5(8)
Temperature/ K	293(2)				100(2)	100(2)
Space group	$P\bar{1}$	$P\bar{1}$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P\bar{1}$
No. of formula units per unit cell, *Z*	4				4	4
Radiation type	MoK_α				MoK_α	MoK_α
Absorption coefficient, *μ*/ mm^{-1}	4.708				0.127	3.671
No. of reflections measured	3059				9704	10089
No. of unique reflections	3059				1752	3043
R_{int}	0.0000[a]				0.0525	0.0735
Final R_1 values ($I>2\sigma(I)$)	0.0717				0.0602	0.0602
Final wR_2 values ($I>2\sigma(I)$)	0.1576				0.1587	0.1284
Final R_1 values (all data)	0.1070				0.0847	0.0799
Final wR_2 values (all data)	0.1788				0.1743	0.1360
Goodness of fit on F_2	1.204				1.061	1.090
CCDC ID	CCDC 1007650	CSD GUMXAO02	CSD GUMXAO	CSD WESBEB	CCDC 1007651	CCDC 1007652

[a] HKLF5 twin

Compound reference	2Me	3Br-1	3Br-2	3Cl-1[6]	3Cl-2[4]	3Cl-3
Chemical formula	$C_9H_{10}O_3$	$C_8H_7BrO_3$	$C_8H_7BrO_3$	$C_8H_7ClO_3$	$C_8H_7ClO_3$	$C_8H_7ClO_3$
Formula Mass	166.17	231.05	231.05	186.59	186.59	186.59
Crystal system	Triclinic	Monoclinic	Triclinic	Monoclinic	Triclinic	Monoclinic
a/ Å	8.833(5)	8.8529(7)	8.8285(5)	8.6234(12)	8.5962(7)	8.6521(15)
b/ Å	9.263(5)	8.9210(6)	9.3102(7)	10.4812(14)	9.2752(7)	8.9195(15)
c/ Å	10.750(5)	10.7745(8)	10.4698(7)	9.3924(13)	10.3929(8)	10.7309(17)
α/ °	73.230(5)	90.00	92.436(8)	90.00	91.527(6)	90.00
β/ °	81.067(5)	90.568(6)	90.260(8)	93.846(7)	90.339(6)	90.900(6)
γ/ °	77.849(5)	90.00	94.119(8)	90.00	93.360(7)	90.00
Unit cell volume/ Å^3	819.1(7)	850.89(11)	857.54(10)	847.0(2)	826.9	828.0(2)
Temperature/ K	120(2)	100(2)	100(2)			100(2)
Space group	$P\bar{1}$	*P*21/*c*	$P\bar{1}$	*P*21/*c*	$P\bar{1}$	*P*21/*c*
No. of formula units per unit cell, *Z*	2	4	4			4
Radiation type	MoK_α	MoK_α	MoK_α			MoK_α
Absorption coefficient, *μ*/ mm^{-1}	0.101	4.792	4.755			0.421
No. of reflections measured	16751	4482	10931			5526
No. of unique reflections	3744	1949	3907			1895
R_{int}	0.0492	0.0315	0.0646			0.0674
Final R_1 values ($I>2\sigma(I)$)	0.0443	0.0264	0.0516			0.0554
Final wR_2 values ($I>2\sigma(I)$)	0.1082	0.0646	0.0864			0.1217
Final R_1 values (all data)	0.0653	0.0299	0.0984			0.0964
Final wR_2 values (all data)	0.1212	0.0678	0.1005			0.1395
Goodness of fit on F_2	1.052	1.064	1.036			1.050
CCDC ID	CCDC 1007653	CCDC 1007654	CCDC 1007655	CSD FIZPIP00	CSD FIZPEL00	CCDC 10077656

Compound reference	3F$_3$C-1	3F-1	3F-2	3I	3Me-1	4Br
Chemical formula	$C_9H_7F_3O_3$	$C_8H_7FO_3$	$C_8H_7FO_3$	$C_8H_7IO_3$	$C_9H_{10}O_3$	$C_8H_7BrO_3$
Formula Mass	220.15	170.14	170.14	278.04	166.17	231.05
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic	Triclinic	Monoclinic
a/ Å	9.0086(5)	8.1424(6)	5.0748(10)	6.8488(4)	8.5713(5)	19.5315(14)
b/ Å	9.6372(7)	10.2396(7)	5.2814(10)	14.1055(10)	9.3327(7)	9.7410(7)
c/ Å	10.5702(7)	9.3604(6)	15.032(4)	15.0534(10)	10.5393(7)	9.1389(6)
α/ °	86.602(5)	90.00	91.142(7)	104.634(7)	92.391(6)	90.00
β/ °	88.612(5)	91.016(8)	92.370(7)	94.543(7)	94.241(6)	101.132(4)
γ/ °	85.623(4)	90.00	111.420(8)	90.699(6)	90.556(6)	90.00
Unit cell volume/ Å^3	913.22(10)	780.30(9)	374.47(14)	1401.86(16)	839.96(10)	1706.0(2)
Temperature/ K	100(2)	293(2)	100(2)	100(2)	100(2)	100(2)
Space group	$P\bar{1}$	*P*21/*c*	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	*P*21/*c*
No. of formula units per unit cell, *Z*	4	4	2	6	4	8
Radiation type	MoK_α	MoK_α	MoK_α	MoK_α	MoK_α	MoK_α
Absorption coefficient, *μ*/ mm^{-1}	0.158	0.126	0.131	3.391	0.099	4.780
No. of reflections measured	11653	4601	3166	16687	10784	3843
No. of unique reflections	4128	1372	1677	4945	3847	3843
R_{int}	0.0393	0.0899	0.0354	0.0462	0.0558	0.0000[b]
Final R_1 values ($I>2\sigma(I)$)	0.0538	0.1026	0.0616	0.0549	0.0513	0.0847
Final wR_2 values ($I>2\sigma(I)$)	0.1263	0.2744	0.1550	0.1094	0.1174	0.2070
Final R_1 values (all data)	0.0688	0.1836	0.0906	0.0853	0.0798	0.1130
Final wR_2 values (all data)	0.1323	0.3223	0.1666	0.1200	0.1319	0.2205
Goodness of fit on F_2	1.123	1.080	1.116	1.045	1.032	1.161
CCDC ID	CCDC 1007657	CCDC 1007658	CCDC 1008570	CCDC 1007659	CCDC 1007660	CCDC 1007661

[b] HKLF5 twin

Compound reference	4Cl[c]	4F$_3$C	4F[3]	4I	4Me	4MeO-1
Chemical formula	$C_8H_7ClO_3$	$C_9H_7F_3O_3$	$C_8H_7FO_3$	$C_8H_7IO_3$	$C_9H_{10}O_3$	$C_9H_{10}O_4$
Formula Mass	186.59	220.15	170.14	278.04	166.17	182.17
Crystal system	Triclinic	Orthorhombic	Orthorhombic	Triclinic	Orthorhombic	Orthorhombic
a/ Å	4.9711(4)	9.8173(5)	9.4685(9)	4.9583(5)	9.8365(7)	20.805(3)
b/ Å	14.9062(12)	9.6920(5)	16.497(2)	10.3607(11)	9.4215(7)	15.649(3)
c/ Å	16.7920(13)	19.9217(14)	9.7677(8)	17.675(2)	19.2390(15)	5.3033(7)
α/ °	88.109(8)	90.00	90	76.455(5)	90.00	90.00
β/ °	85.871(8)	90.00	90	83.237(6)	90.00	90.00
γ/ °	84.381(9)	90.00	90	88.779(6)	90.00	90.00
Unit cell volume/ Å^3	1234.68(17)	1895.54(19)	1525.73	876.58(16)	1783.0(2)	1726.6(5)
Temperature/ K	100(2)	293(2)		100(2)	100(2)	293(2)
Space group	$P\bar{1}$	*Pbca*	*Pbca*	$P\bar{1}$	*Pbca*	*Pbca*
No. of formula units per unit cell, *Z*	6	8		4	8	8
Radiation type	MoK_α	MoK_α		MoK_α	MoK_α	MoK_α
Absorption coefficient, μ/ mm^{-1}	0.424	0.152		3.616	0.093	0.111
No. of reflections measured	8678	30644		8571	15878	16890
No. of unique reflections	4218	2173		4017	2038	1971
R_{int}	0.1684	0.0735		0.0596	0.1212	0.1451
Final R_1 values ($I>2\sigma(I)$)	0.1238	0.0832		0.0615	0.0710	0.0767
Final wR_2 values ($I>2\sigma(I)$)	0.2195	0.1104		0.1576	0.1594	0.1049
Final R_1 values (all data)	0.3050	0.1612		0.0852	0.1920	0.1957
Final wR_2 values (all data)	0.3039	0.1300		0.1692	0.2198	0.1320
Goodness of fit on F_2	1.010	1.133		1.063	0.996	0.992
CCDC ID	CCDC 1007662	CCDC 1007663	CSD WESBOL	CCDC 1007664	CCDC 1007665	CCDC 1007666

Compound reference	4MeO-2	MA-1[7]	MA-2[8]
Chemical formula	$C_9H_{10}O_4$	$C_8H_8O_3$	$C_8H_8O_3$
Formula Mass	182.17	152.05	152.05
Crystal system	Monoclinic	Orthorhombic	Monoclinic
a/ Å	18.6794(13)	9.669(2)	5.84680(10)
b/ Å	5.1376(2)	16.183(3)	29.2410(4)
c/ Å	9.214(4)	9.953(2)	8.72280(10)
α/ °	90.00	90	90
β/ °	103.682(12)	90	92.1651(8)
γ/ °	90.00	90	90
Unit cell volume/ Å^3	859.1(3)	1557.38	1490.24
Temperature/ K	293(2)		
Space group	*P*21/*c*	*Pbca*	*P*21/*c*
No. of formula units per unit cell, *Z*	4		
Radiation type	MoK_α		
Absorption coefficient, μ/ mm^{-1}	0.112		
No. of reflections measured	18014		
No. of unique reflections	1971		
R_{int}	0.0294		
Final R_1 values ($I>2\sigma(I)$)	0.0336		
Final wR_2 values ($I>2\sigma(I)$)	0.0916		
Final R_1 values (all data)	0.0433		
Final wR_2 values (all data)	0.0958		
Goodness of fit on F_2	1.098		
CCDC ID	CCDC 1007667	CSD DLMAND01	CSD DLMAND02

[c] Poor quality crystal obtained from sublimation was only one available for analysis.

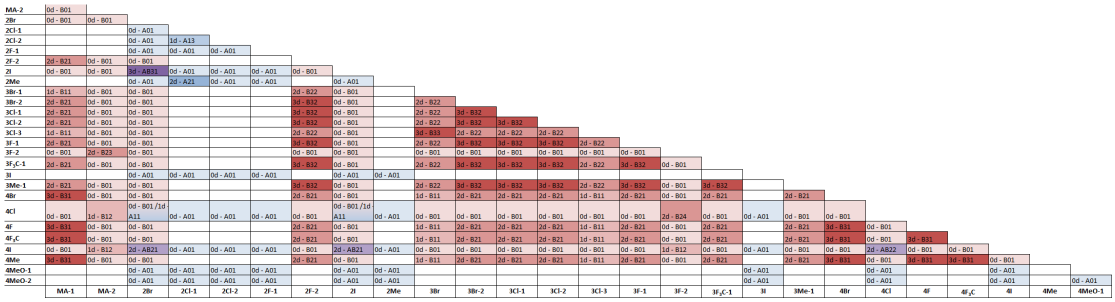

Figure S1. Common supramolecular constructs exhibited by the structures in this study.

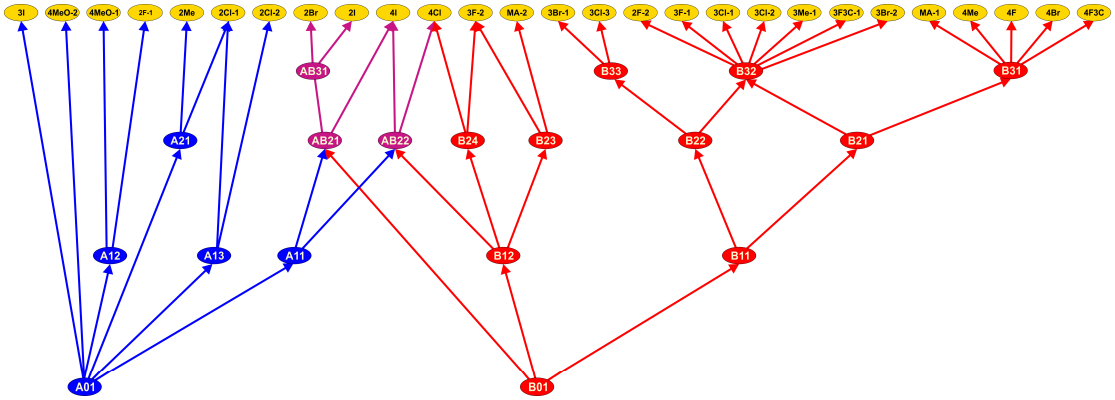

Figure S2. Structural relationship plot showing relationship between supramolecular constructs exhibited by our family of structures.

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