Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A strategy for preparing spirobichroman dianhydride from bisphenol A and its resulting polyimide with low dielectric characteristic

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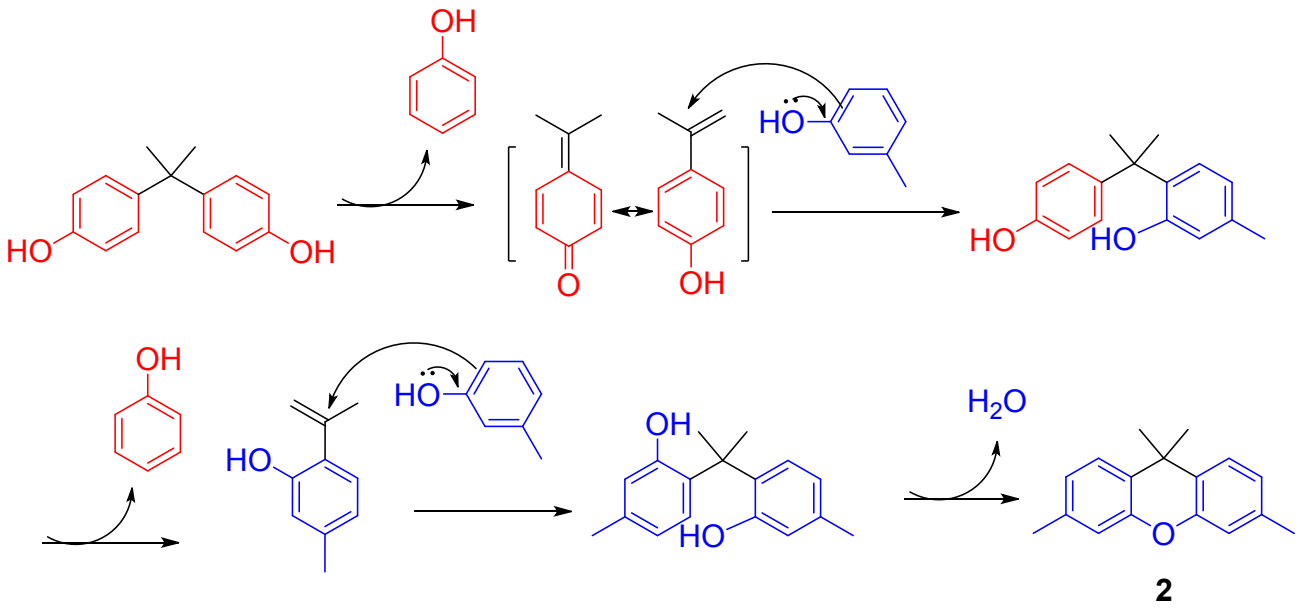
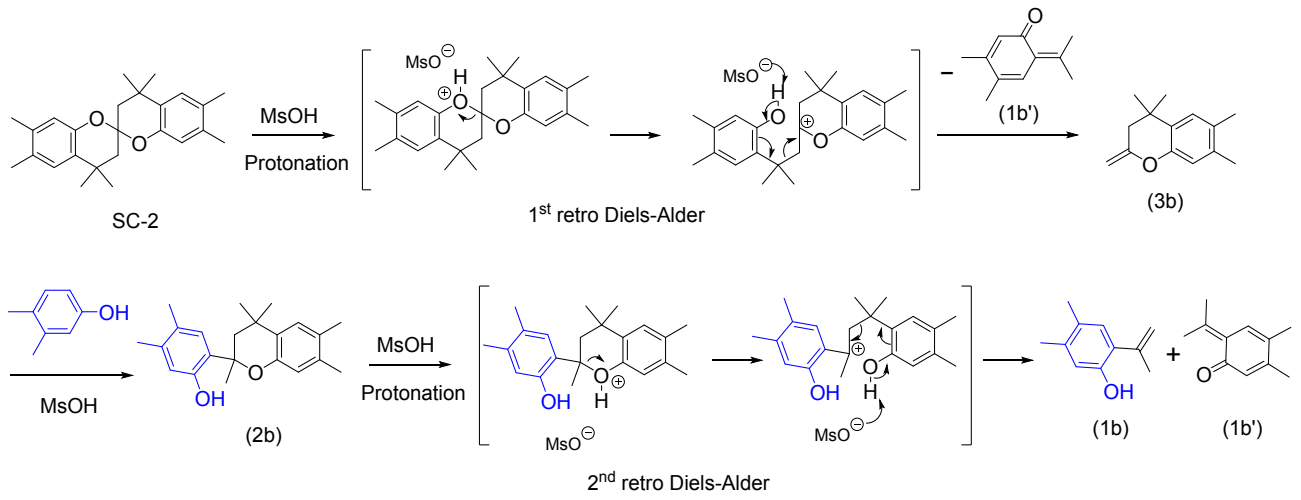


Scheme S1. The transformation of BPA to xanthene **2** in the presence of *m*-cresol.[1]



MsOH=Methanesulfonic acid

Scheme S2. Proposed mechanism on retro Diels-Alder reaction of **OMSBC** in the presence of methanesulfonic acid (MsOH).

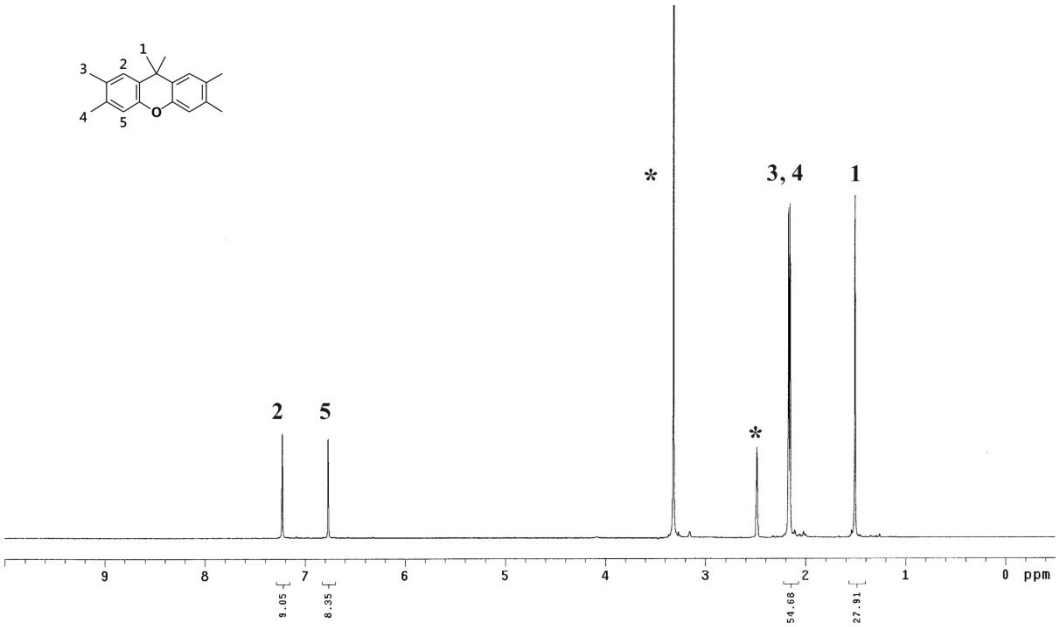


Figure S1. ^{1}H NMR spectrum of **X-2** in DMSO-d_6.

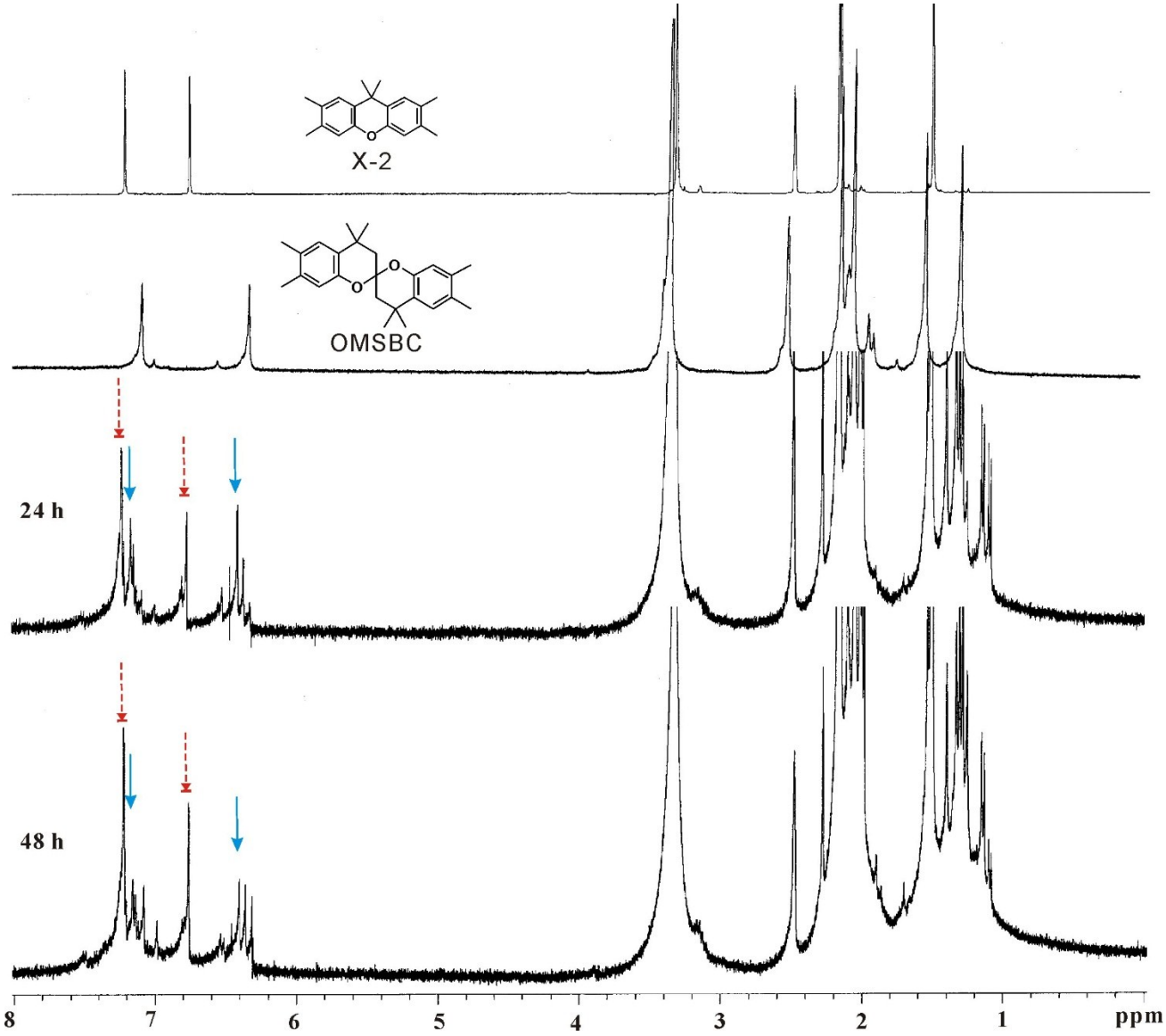


Figure S2. ^{1}H NMR trace for **OMSBC** synthesis after 24 and 48 h in DMSO-d_6.

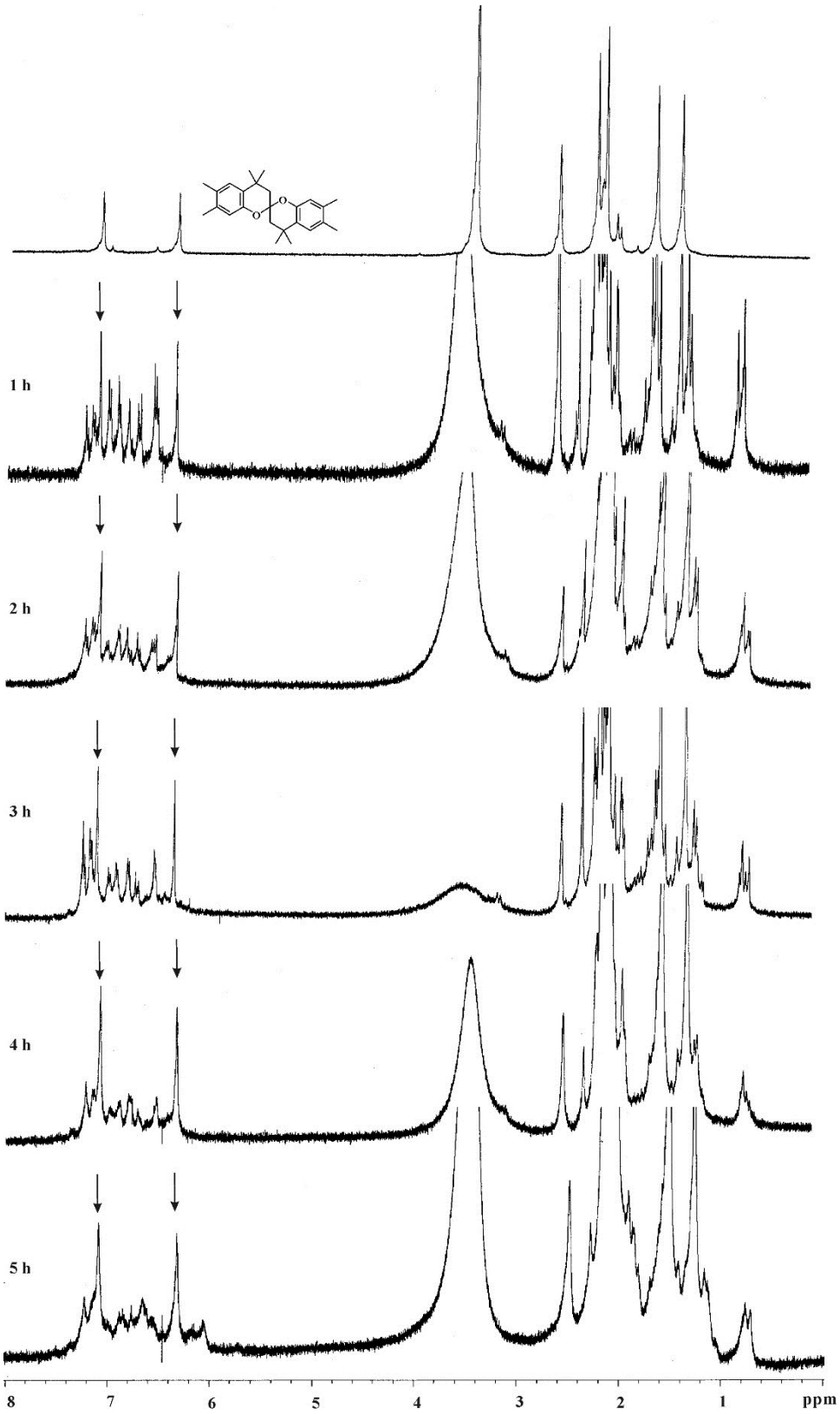


Figure S3. ^{1}H NMR trace for **OMSBC** synthesis after 1-5 h in DMSO-d_6.

Table S1. Crystal data and structure refinement for **SBCDA**.

Identification code	anhydride	
Empirical formula	C25 H20 O8	
Formula weight	448.41	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 26.146(2) Å	α= 90°.
	b = 10.3960(5) Å	β= 127.778(12)°.
	c = 20.1104(16) Å	γ = 90°.
Volume	4320.5(5) $Å^3$	
Z	8	
Density (calculated)	1.379 Mg/m^3	
Absorption coefficient	0.104 mm^{-1}	
F(000)	1872	
Crystal size	0.42 x 0.26 x 0.23 mm^3	
Theta range for data collection	2.83 to 29.30°.	
Index ranges	-33<=h<=29, -13<=k<=7, -26<=l<=25	
Reflections collected	9874	
Independent reflections	4978 [R(int) = 0.0298]	
Completeness to theta = 26.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.99525	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4978 / 0 / 298	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0529, wR2 = 0.1014	
R indices (all data)	R1 = 0.0883, wR2 = 0.1176	
Largest diff. peak and hole	0.263 and -0.219 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **SBCDA**.

U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	2010(1)	1301(1)	218(1)	24(1)
O(2)	2935(1)	-1725(2)	-1027(1)	50(1)
O(3)	3594(1)	-2726(2)	226(1)	45(1)
O(4)	4128(1)	-3316(2)	1584(1)	61(1)
O(5)	-1557(1)	614(2)	-2929(1)	42(1)
O(6)	-1221(1)	-1234(2)	-2172(1)	38(1)
O(7)	-614(1)	-2748(2)	-1183(1)	45(1)
O(8)	1374(1)	682(1)	603(1)	24(1)
C(1)	2455(1)	333(2)	506(1)	21(1)
C(2)	2498(1)	-175(2)	-102(1)	25(1)
C(3)	2945(1)	-1127(2)	152(1)	28(1)
C(4)	3119(1)	-1831(2)	-325(1)	36(1)
C(5)	3738(1)	-2629(2)	1027(2)	42(1)
C(6)	3326(1)	-1597(2)	966(1)	30(1)
C(7)	3285(1)	-1089(2)	1567(1)	28(1)
C(8)	2847(1)	-97(2)	1342(1)	22(1)
C(9)	2804(1)	493(2)	1999(1)	23(1)
C(10)	2378(1)	1702(2)	1638(1)	24(1)
C(11)	1809(1)	1657(2)	714(1)	22(1)
C(12)	1470(1)	2937(2)	387(1)	25(1)
C(13)	848(1)	2946(2)	-528(1)	26(1)
C(14)	483(1)	1690(2)	-711(1)	23(1)
C(15)	-149(1)	1550(2)	-1452(1)	28(1)
C(16)	-470(1)	413(2)	-1610(1)	28(1)
C(17)	-1133(1)	31(2)	-2322(1)	33(1)
C(18)	-651(1)	-1678(2)	-1419(1)	33(1)
C(19)	-182(1)	-609(2)	-1056(1)	25(1)
C(20)	440(1)	-518(2)	-316(1)	24(1)
C(21)	765(1)	640(2)	-154(1)	21(1)
C(22)	3481(1)	914(2)	2773(1)	33(1)
C(23)	2541(1)	-512(2)	2278(1)	30(1)
C(24)	991(1)	3091(2)	-1164(1)	33(1)

C(25)	437(1)	4096(2)	-624(1)	38(1)

Table S3. Bond lengths [Å] and angles [°] for **SBCDA**.

O(1)-C(1)	1.370(2)
O(1)-C(11)	1.4303(19)
O(2)-C(4)	1.185(2)
O(3)-C(4)	1.396(3)
O(3)-C(5)	1.416(3)
O(4)-C(5)	1.186(3)
O(5)-C(17)	1.196(2)
O(6)-C(18)	1.400(2)
O(6)-C(17)	1.399(3)
O(7)-C(18)	1.190(3)
O(8)-C(21)	1.3719(19)
O(8)-C(11)	1.435(2)
C(1)-C(8)	1.404(2)
C(1)-C(2)	1.398(2)
C(2)-C(3)	1.369(3)
C(2)-H(2A)	0.9500
C(3)-C(6)	1.383(3)
C(3)-C(4)	1.481(3)
C(5)-C(6)	1.470(3)
C(6)-C(7)	1.383(2)
C(7)-C(8)	1.394(3)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.521(2)
C(9)-C(23)	1.533(2)
C(9)-C(10)	1.535(3)
C(9)-C(22)	1.541(2)
C(10)-C(11)	1.510(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.509(2)
C(12)-C(13)	1.538(2)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.523(3)
C(13)-C(25)	1.538(3)
C(13)-C(24)	1.544(2)

C(14)-C(21)	1.407(3)
C(14)-C(15)	1.397(2)
C(15)-C(16)	1.369(3)
C(15)-H(15A)	0.9500
C(16)-C(19)	1.381(3)
C(16)-C(17)	1.474(3)
C(18)-C(19)	1.474(3)
C(19)-C(20)	1.381(2)
C(20)-C(21)	1.393(2)
C(20)-H(20A)	0.9500
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800

C(1)-O(1)-C(11)	118.36(13)
C(4)-O(3)-C(5)	110.06(16)
C(18)-O(6)-C(17)	109.65(15)
C(21)-O(8)-C(11)	117.78(13)
O(1)-C(1)-C(8)	123.22(15)
O(1)-C(1)-C(2)	114.29(15)
C(8)-C(1)-C(2)	122.48(17)
C(3)-C(2)-C(1)	117.06(16)
C(3)-C(2)-H(2A)	121.5
C(1)-C(2)-H(2A)	121.5
C(2)-C(3)-C(6)	121.89(16)
C(2)-C(3)-C(4)	130.23(18)
C(6)-C(3)-C(4)	107.88(18)
O(2)-C(4)-O(3)	121.45(19)
O(2)-C(4)-C(3)	131.5(2)

O(3)-C(4)-C(3)	106.99(17)
O(4)-C(5)-O(3)	120.5(2)
O(4)-C(5)-C(6)	132.9(2)
O(3)-C(5)-C(6)	106.53(18)
C(7)-C(6)-C(3)	120.92(18)
C(7)-C(6)-C(5)	130.56(19)
C(3)-C(6)-C(5)	108.52(17)
C(6)-C(7)-C(8)	119.22(17)
C(6)-C(7)-H(7A)	120.4
C(8)-C(7)-H(7A)	120.4
C(1)-C(8)-C(7)	118.37(15)
C(1)-C(8)-C(9)	121.61(16)
C(7)-C(8)-C(9)	120.02(15)
C(23)-C(9)-C(8)	109.34(15)
C(23)-C(9)-C(10)	111.94(14)
C(8)-C(9)-C(10)	109.71(14)
C(23)-C(9)-C(22)	108.64(14)
C(8)-C(9)-C(22)	109.93(14)
C(10)-C(9)-C(22)	107.25(15)
C(11)-C(10)-C(9)	116.05(15)
C(11)-C(10)-H(10A)	108.3
C(9)-C(10)-H(10A)	108.3
C(11)-C(10)-H(10B)	108.3
C(9)-C(10)-H(10B)	108.3
H(10A)-C(10)-H(10B)	107.4
O(1)-C(11)-O(8)	107.62(13)
O(1)-C(11)-C(12)	107.12(14)
O(8)-C(11)-C(12)	110.82(14)
O(1)-C(11)-C(10)	111.12(13)
O(8)-C(11)-C(10)	107.62(13)
C(12)-C(11)-C(10)	112.45(15)
C(11)-C(12)-C(13)	115.79(15)
C(11)-C(12)-H(12A)	108.3
C(13)-C(12)-H(12A)	108.3
C(11)-C(12)-H(12B)	108.3
C(13)-C(12)-H(12B)	108.3
H(12A)-C(12)-H(12B)	107.4
C(14)-C(13)-C(12)	109.34(15)

C(14)-C(13)-C(25)	110.52(15)
C(12)-C(13)-C(25)	107.48(15)
C(14)-C(13)-C(24)	108.48(15)
C(12)-C(13)-C(24)	112.11(14)
C(25)-C(13)-C(24)	108.92(16)
C(21)-C(14)-C(15)	117.99(17)
C(21)-C(14)-C(13)	121.79(15)
C(15)-C(14)-C(13)	120.22(17)
C(16)-C(15)-C(14)	119.57(18)
C(16)-C(15)-H(15A)	120.2
C(14)-C(15)-H(15A)	120.2
C(15)-C(16)-C(19)	121.56(17)
C(15)-C(16)-C(17)	130.32(19)
C(19)-C(16)-C(17)	108.11(18)
O(5)-C(17)-O(6)	121.61(18)
O(5)-C(17)-C(16)	131.2(2)
O(6)-C(17)-C(16)	107.14(18)
O(7)-C(18)-O(6)	120.78(18)
O(7)-C(18)-C(19)	131.9(2)
O(6)-C(18)-C(19)	107.33(18)
C(16)-C(19)-C(20)	121.11(18)
C(16)-C(19)-C(18)	107.72(17)
C(20)-C(19)-C(18)	131.17(19)
C(19)-C(20)-C(21)	117.31(17)
C(19)-C(20)-H(20A)	121.3
C(21)-C(20)-H(20A)	121.3
O(8)-C(21)-C(14)	123.00(16)
O(8)-C(21)-C(20)	114.52(15)
C(14)-C(21)-C(20)	122.45(16)
C(9)-C(22)-H(22A)	109.5
C(9)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(9)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(9)-C(23)-H(23A)	109.5
C(9)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5

C(9)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(13)-C(24)-H(24A)	109.5
C(13)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(13)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(13)-C(25)-H(25A)	109.5
C(13)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(13)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **SBCDA**.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	22(1)	27(1)	24(1)	3(1)	14(1)	5(1)
O(2)	62(1)	55(1)	51(1)	-11(1)	44(1)	-2(1)
O(3)	55(1)	38(1)	64(1)	-1(1)	47(1)	9(1)
O(4)	69(1)	56(1)	78(1)	25(1)	55(1)	35(1)
O(5)	26(1)	57(1)	31(1)	-8(1)	10(1)	-3(1)
O(6)	28(1)	46(1)	38(1)	-15(1)	19(1)	-14(1)
O(7)	48(1)	35(1)	57(1)	-11(1)	34(1)	-17(1)
O(8)	20(1)	21(1)	27(1)	0(1)	12(1)	-3(1)
C(1)	18(1)	19(1)	27(1)	0(1)	14(1)	-4(1)
C(2)	24(1)	27(1)	25(1)	-1(1)	16(1)	-4(1)
C(3)	30(1)	25(1)	36(1)	-6(1)	24(1)	-7(1)
C(4)	40(1)	32(1)	50(1)	-7(1)	35(1)	-4(1)
C(5)	47(1)	34(1)	63(2)	4(1)	42(1)	6(1)
C(6)	31(1)	22(1)	46(1)	2(1)	28(1)	1(1)
C(7)	29(1)	26(1)	33(1)	6(1)	21(1)	4(1)
C(8)	20(1)	21(1)	27(1)	0(1)	15(1)	-4(1)
C(9)	22(1)	22(1)	23(1)	1(1)	13(1)	0(1)
C(10)	23(1)	21(1)	25(1)	-5(1)	15(1)	-5(1)
C(11)	20(1)	19(1)	27(1)	-2(1)	15(1)	-2(1)
C(12)	24(1)	19(1)	32(1)	-1(1)	17(1)	-2(1)
C(13)	21(1)	21(1)	32(1)	2(1)	14(1)	1(1)
C(14)	21(1)	24(1)	28(1)	-2(1)	16(1)	0(1)
C(15)	24(1)	30(1)	29(1)	2(1)	15(1)	2(1)
C(16)	21(1)	34(1)	28(1)	-5(1)	15(1)	-3(1)
C(17)	29(1)	41(1)	34(1)	-12(1)	22(1)	-8(1)
C(18)	32(1)	36(1)	39(1)	-13(1)	26(1)	-11(1)
C(19)	26(1)	26(1)	32(1)	-10(1)	22(1)	-6(1)
C(20)	26(1)	22(1)	31(1)	-3(1)	21(1)	0(1)
C(21)	18(1)	23(1)	26(1)	-4(1)	15(1)	-1(1)
C(22)	25(1)	37(1)	29(1)	0(1)	12(1)	-1(1)
C(23)	35(1)	30(1)	32(1)	5(1)	24(1)	2(1)
C(24)	26(1)	34(1)	32(1)	8(1)	14(1)	-3(1)
C(25)	29(1)	26(1)	46(1)	3(1)	16(1)	5(1)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3)for **SBCDA**.

	x	y	z	U(eq)
H(2A)	2229	127	-666	30
H(7A)	3551	-1412	2126	34
H(10A)	2212	1867	1959	28
H(10B)	2654	2442	1733	28
H(12A)	1776	3566	437	30
H(12B)	1361	3237	755	30
H(15A)	-354	2238	-1843	34
H(20A)	638	-1217	68	28
H(22A)	3767	163	3021	50
H(22B)	3449	1305	3189	50
H(22C)	3659	1543	2601	50
H(23A)	2108	-784	1792	45
H(23B)	2516	-135	2704	45
H(23C)	2831	-1258	2517	45
H(24A)	1252	2361	-1107	50
H(24B)	1228	3893	-1051	50
H(24C)	582	3110	-1737	50
H(25A)	345	4014	-221	57
H(25B)	29	4111	-1198	57
H(25C)	674	4896	-516	57

References

1. Caruso, A. J.; Lee, J. L. *The Journal of Organic Chemistry* **1997,** 62, (4), 1058-1063.