Supporting Material for:

Synthesis and study of mesomorphic properties of unsymmetrical cyclohexanone derived bis-chalcones

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Analytical data of other products:

(2E,6E)-2-(4-butoxybenzylidene)-6-((benzo[d][1,3]dioxol-6-yl)methylene)cyclohexanone

(3a):

Yellow solid (83.45%). ¹H-NMR (400 MHz, CDCl₃): δ 7.77 (s, 1H), 7.72 (s, 1H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.03-7.01 (d, *J* = 7.6 Hz, 1H and one singlet of aromatic H merged with doublet), 6.94 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.02 (s, 2H), 4.01 (t, *J* = 6.8 Hz, 2H), 2.95-2.90 (m, 4H), 1.85-1.76 (m, 4H), 1.55-1.49 (m, 2H), 1.00 (t, *J* = 7.6 Hz, 3H)

IR (KBr): ν 2945, 2865, 1659, 1593, 1555, 1504, 1444, 1246, 1164, 1035, 842 cm^{-1}

Mass (EI): m/z (%) (M+1) 391 (1), 390 (84), 389 (64), 388 (100), 333 (61), 332 (44)

(2*E*,6*E*)-2-(4-hexyloxybenzylidene)-6-((benzo[*d*][1,3]dioxol-6-yl)methylene)cyclohexanone (**3b**):

Yellow solid (78.23%). ^1H -NMR (400 MHz, CDCl_3): δ 7.77 (s, 1H), 7.72 (s, 1H), 7.46 (d, $J = 8.8$ Hz, 2H), 7.03-7.01 (d, $J = 8$ Hz, 1H and one singlet of aromatic H merged with doublet), 6.94 (d, $J = 8.8$ Hz, 2H), 6.87 (d, $J = 8.4$ Hz, 1H), 6.02 (s, 2H), 4.01 (t, $J = 6.4$ Hz, 2H), 2.95-2.90 (m, 4H), 1.84-1.79 (m, 4H), 1.50-1.46 (m, 2H), 1.38-1.35 (m, 4H), 0.94-0.91 (m, 3H)

IR (KBr): ν 2937, 2856, 1654, 1591, 1557, 1507, 1443, 1295, 1248, 1162, 1033, 824 cm^{-1}

Mass (EI): m/z (%) 418 (28), 417 (100), 390 (22), 389 (51), 333 (22), 332 (29)

(2*E*,6*E*)-2-(4-heptyloxybenzylidene)-6-((benzo[*d*][1,3]dioxol-6-yl)methylene)cyclohexanone (**3c**):

Yellow solid (75.08%). ^1H -NMR (400 MHz, CDCl_3): δ 7.77 (s, 1H), 7.72 (s, 1H), 7.46 (d, $J = 8.8$ Hz, 2H), 7.03-7.01 (d, $J = 8$ Hz, 1H and one singlet of aromatic H merged with doublet), 6.94 (d, $J = 8.8$ Hz, 2H), 6.87 (d, $J = 8$ Hz, 1H), 6.02 (s, 2H), 4.01 (t, $J = 6.4$ Hz, 2H), 2.95-2.90 (m, 4H), 1.84-1.77 (m, 4H), 1.51-1.44 (m, 2H), 1.41-1.36 (m, 6H), 0.91 (t, $J = 6.8$ Hz, 3H)

IR (KBr): ν 2935, 2853, 1654, 1590, 1507, 1443, 1297, 1248, 1162, 1035, 923, 823 cm^{-1}

Mass (EI): m/z (%) ($M+1$) 433 (33), 432 (100), 431 (76), 430 (98), 429 (31), 333 (64), 332 (56)

(2*E*,6*E*)-2-(4-decyloxybenzylidene)-6-((benzo[*d*][1,3]dioxol-6-yl)methylene)cyclohexanone (**3e**):

Yellow solid (78.26%). $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 7.77 (s, 1H), 7.72 (s, 1H), 7.46 (d, $J = 8.8$ Hz, 2H), 7.03-7.01 (d, $J = 8$ Hz, 1H and one singlet of aromatic H merged with doublet), 6.94 (d, $J = 8.8$ Hz, 2H), 6.87 (d, $J = 8.4$ Hz, 1H), 6.02 (s, 2H), 4.00 (t, $J = 6.4$ Hz, 2H), 2.93-2.90 (m, 4H), 1.82-1.79 (m, 4H), 1.49-1.44 (m, 2H), 1.34-1.29 (m, 12H), 0.90 (t, $J = 7.2$ Hz, 3H)

IR (KBr): ν 2935, 2849, 1654, 1590, 1506, 1443, 1297, 1249, 1164, 1034, 924, 823 cm^{-1}

Mass (EI): m/z (%) 474 (56), 473 (100), 472 (75), 446 (31), 445 (30), 444 (36), 333 (63), 332 (53)

(2*E*,6*E*)-2-(4-dodecyloxybenzylidene)-6-((benzo[*d*][1,3]dioxol-6-yl)methylene)cyclohexanone (**3f**):

Yellow solid (73.76%). $^1\text{H-NMR}$ (400 MHz, CDCl_3): δ 7.77 (s, 1H), 7.72 (s, 1H), 7.46 (d, $J = 8.8$ Hz, 2H), 7.03-7.01 (d, $J = 8$ Hz, 1H and one singlet of aromatic H merged with doublet), 6.94 (d, $J = 8.8$ Hz, 2H), 6.87 (d, $J = 8.4$ Hz, 1H), 6.02 (s, 2H), 4.00 (t, $J = 6.8$ Hz, 2H), 2.95-2.90 (m, 4H), 1.85-1.77 (m, 4H), 1.55-1.44 (m, 2H), 1.38-1.29 (m, 12H), 0.90 (t, $J = 6.8$, 3H)

IR (KBr): ν 2922, 2850, 1654, 1590, 1505, 1443, 1248, 1164, 1034, 923, 822, 566 cm^{-1}

Mass (EI): m/z (%) 502, 474 (84), 473 (82), 472 (100), 333 (25), 332 (32)

(2E,6E)-2-(4-tetradecyloxybenzylidene)-6-((benzo[d][1,3]dioxol-6-yl)methylene)cyclohexanone (3g):

Yellow solid (70.43%). ¹H-NMR (400 MHz, CDCl₃): δ 7.77 (s, 1H), 7.72 (s, 1H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.03-7.01 (d, *J* = 8 Hz, 1H and one singlet of aromatic H merged with doublet), 6.94 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.02 (s, 2H), 4.00 (t, *J* = 6.8 Hz, 2H), 2.95-2.90 (m, 4H), 1.83-1.79 (m, 4H), 1.49-1.43 (m, 2H), 1.33-1.27 (m, 16H), 0.89 (t, *J* = 6.8 Hz, 3H)

IR (KBr): ν 2920, 2850, 1654, 1592, 1506, 1298, 1249, 1163, 1035, 924, 824 cm⁻¹

Mass (EI): m/z (%) 530 (57), 529 (39), 528 (35), 439 (24), 368 (72), 367 (100), 332 (34)

(2E,6E)-2-(4-hexadecyloxybenzylidene)-6-((benzo[d][1,3]dioxol-6-yl)methylene)cyclohexanone (3h):

Yellow solid (61.85%). ¹H-NMR (400 MHz, CDCl₃): δ 7.77 (s, 1H), 7.72 (s, 1H), 7.46 (d, *J* = 8.8 Hz, 2H), 7.03-7.01 (d, *J* = 8.8 Hz, 1H and one singlet of aromatic H merged with doublet), 6.94 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.4 Hz, 1H), 6.02 (s, 2H), 4.00 (t, *J* = 6.4 Hz, 2H), 2.95-2.91 (m, 4H), 1.85-1.77 (m, 4H), 1.49-1.43 (m, 2H), 1.33-1.27 (m, 24H), 0.89 (t, *J* = 6.8 Hz, 3H)

IR (KBr): ν 3021, 2921, 2850, 1655, 1593, 1506, 1445, 1249, 1163, 1036, 925, 759 cm⁻¹

Mass (EI): m/z (%) 558 (51), 557 (51), 556 (29), 438 (30), 369 (54), 368 (100), 367 (84), 312 (61)

¹H-NMR of compound 3c

¹H-NMR of compound 3d

¹H-NMR of compound 3e

¹H-NMR of compound 3f

¹H-NMR of compound 3g

¹H-NMR of compound 3h

X-ray Crystal Data

Crystal data for compound **3d**

Table 1 Crystal data and structure refinement for **3d**

Empirical Formula	C ₂₉ H ₃₄ O ₄
Formula Weight	446.56
Temperature	293(2)
Wavelength	1.54184
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a/Å 9.2135(3)
	b/Å 11.2936(5)
	c/Å 12.0286(5)
	α /° 86.117(3)
	β /° 74.574(3)
	γ /° 84.317(3)
Volume/Å ³	1199.49(8)
Z	2
(Density calculated)	1.236
Absorption coefficient(μ)	480.0
F(000)	480.0
Crystal size(mm)	0.39 × 0.25 × 0.14
θ range for data collection	7.64 to 146.42°
Reflections collected	11331
Independent reflections	4775[R(int) = 0.0245]
Refinement method	Least Squares minimization
Data / restraints / Parameters	4775/0/299
Goodness of fit on F ²	1.049
Final R indices [I>2sigma(I)]	R ₁ = 0.0463, wR ₂ = 0.1315
R indices (all data)	R ₁ = 0.0524, wR ₂ = 0.1387
Largest difference peak and hole	0.18/-0.19

Table 2: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **1a**. Ueq is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
O24	2716.4(11)	534(1)	609.2(9)	61.0(3)
O33	2323.1(14)	-1213.2(13)	7466.5(10)	77.7(4)
O5	6886.9(13)	-4711.0(12)	11922.4(10)	72.9(3)
O7	8308.6(13)	-4776.0(15)	10030.0(11)	88.2(5)
C11	3922.0(15)	-1537.7(12)	5595.3(11)	48.7(3)
C22	4111.8(15)	-256.2(13)	1883.2(12)	54.0(3)
C18	3072.3(15)	-356.6(12)	3952.9(12)	49.9(3)
C12	3502.7(16)	-1705.5(13)	6884.6(12)	53.1(3)
C14	5815.2(15)	-3242.0(13)	6707.4(12)	54.3(3)
C25	1393.8(15)	1179.3(13)	389.0(12)	54.3(3)
C21	2754.9(15)	295.6(12)	1724.5(12)	50.2(3)
C20	1571.9(16)	560.6(13)	2677.2(13)	57.8(3)
C16	5223.4(16)	-2325.7(13)	4911.6(12)	55.1(3)
C27	372.6(16)	1999.4(13)	-1283.7(13)	56.1(3)
C19	1753.1(17)	244.1(13)	3765.9(13)	57.5(3)
C23	4266.4(15)	-574.9(13)	2969.4(13)	53.2(3)
C29	-554.1(16)	2812.5(14)	-3030.8(13)	56.5(3)
C15	5497.0(17)	-3480.7(13)	5573.0(13)	57.4(3)

C28	745.0(17)	2228.6(15)	-2579.8(13)	60.0(4)
C26	1703.6(16)	1369.2(13)	-898.1(13)	55.7(3)
C10	4249.3(16)	-2405.6(13)	8602.9(12)	54.8(3)
C2	4169.0(18)	-2962.6(14)	10602.3(13)	61.5(4)
C13	4545.6(15)	-2469.7(12)	7453.0(12)	49.5(3)
C8	6935.3(15)	-4158.1(15)	10077.3(13)	57.6(3)
C1	4986.3(16)	-3004.6(12)	9447.6(12)	51.7(3)
C17	3058.4(16)	-717.1(12)	5145.6(12)	52.5(3)
C4	6090.5(16)	-4117.1(13)	11211.3(12)	55.0(3)
C3	4704.9(19)	-3519.9(15)	11502.9(13)	64.2(4)
C9	6438.5(16)	-3614.5(15)	9186.9(13)	59.3(4)
C31	-1384.6(19)	3651.4(16)	-4800.9(14)	66.5(4)
C30	-134.1(18)	3026.4(14)	-4330.8(13)	60.9(4)
C6	8229.8(19)	-5226(2)	11178.3(15)	75.5(5)
C32	-949(3)	3812(2)	-6107.5(17)	83.1(5)

Table 3: Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **1a**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+...+2hka \times b \times U_{12}]$

Atom	U11	U22	U33	U23	U13	U12
O24	49.9(5)	77.5(7)	51.6(6)	2.7(5)	-13.2(4)	10.9(5)
O33	65.9(7)	109.4(10)	49.3(6)	-14.1(6)	-11.5(5)	31.1(6)

O5	62.2(6)	97.6(9)	54.4(6)	11.8(6)	-14.4(5)	2.5(6)
O7	49.7(6)	146.7(13)	58.7(7)	10.4(7)	-10.4(5)	16.1(7)
C11	46.2(6)	53.9(7)	46.1(7)	-7.5(5)	-11.4(5)	-2.3(5)
C22	41.9(6)	64.0(8)	51.5(7)	0.5(6)	-6.8(5)	0.9(5)
C18	50.8(7)	47.0(6)	51.2(7)	-3.8(5)	-12.6(5)	-0.7(5)
C12	48.4(7)	60.5(8)	49.0(7)	-10.5(6)	-10.9(5)	2.9(6)
C14	48.5(7)	60.2(8)	51.0(7)	-2.4(6)	-10.3(6)	3.4(6)
C25	46.7(7)	58.0(8)	57.2(8)	4.0(6)	-15.4(6)	1.4(6)
C21	47.2(7)	50.5(7)	51.3(7)	0.7(5)	-12.2(5)	-0.8(5)
C20	49.5(7)	60.4(8)	58.7(8)	0.4(6)	-12.3(6)	10.9(6)
C16	51.2(7)	63.7(8)	46.8(7)	-7.1(6)	-9.2(5)	5.4(6)
C27	51.3(7)	59.5(8)	54.7(8)	2.7(6)	-13.5(6)	5.0(6)
C19	52.9(7)	58.1(8)	53.3(8)	-5.2(6)	-4.8(6)	11.2(6)
C23	40.8(6)	61.5(8)	55.4(8)	0.0(6)	-11.9(5)	0.7(5)
C29	51.9(7)	59.9(8)	54.3(8)	1.8(6)	-12.3(6)	3.6(6)
C15	57.3(8)	57.2(8)	54.8(8)	-11.3(6)	-11.9(6)	6.9(6)
C28	54.0(8)	66.7(9)	55.4(8)	-0.1(6)	-12.7(6)	8.2(6)
C26	48.4(7)	60.1(8)	56.9(8)	1.2(6)	-14.3(6)	2.6(6)
C10	53.3(7)	58.2(8)	51.4(7)	-7.0(6)	-11.9(6)	0.2(6)
C2	61.5(8)	67.3(9)	51.0(8)	-9.8(6)	-10.6(6)	10.6(7)
C13	46.7(6)	52.8(7)	48.8(7)	-3.7(5)	-11.7(5)	-4.4(5)

C8	42.1(7)	74.1(9)	54.4(8)	-0.5(6)	-9.4(6)	-5.2(6)
C1	52.8(7)	54.7(7)	47.4(7)	-4.6(5)	-12.0(5)	-5.1(5)
C17	51.0(7)	55.4(7)	49.2(7)	-10.0(5)	-10.4(5)	2.5(5)
C4	54.8(7)	61.2(8)	48.9(7)	3.8(6)	-13.2(6)	-8.4(6)
C3	64.5(9)	76.4(10)	44.7(7)	-4.4(6)	-5.7(6)	4.7(7)
C9	46.8(7)	83.9(10)	44.5(7)	-0.5(6)	-6.6(5)	-8.8(6)
C31	64.6(9)	77(1)	61.9(9)	5.4(7)	-25.4(7)	-6.2(8)
C30	62.3(8)	63.4(8)	54.3(8)	-1.3(6)	-15.1(7)	5.7(7)
C6	52.6(8)	104.9(14)	63.9(10)	14.4(9)	-13.3(7)	0.5(8)
C32	93.8(13)	99.0(14)	64.1(11)	8.3(9)	-34.6(10)	-13.6(11)

Table 4 Bond Lengths for exp_675.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O24	C25	1.4338(15)	C25	C26	1.502(2)
O24	C21	1.3595(17)	C21	C20	1.381(2)
O33	C12	1.2282(18)	C20	C19	1.383(2)
O5	C4	1.3707(18)	C16	C15	1.516(2)
O5	C6	1.417(2)	C27	C28	1.514(2)
O7	C8	1.3723(18)	C27	C26	1.5201(18)
O7	C6	1.425(2)	C29	C28	1.5174(19)
C11	C12	1.4987(19)	C29	C30	1.516(2)

C11	C16	1.5064(18)	C10	C13	1.342(2)
C11	C17	1.3414(19)	C10	C1	1.461(2)
C22	C21	1.3944(18)	C2	C1	1.394(2)
C22	C23	1.372(2)	C2	C3	1.394(2)
C18	C19	1.3963(19)	C8	C4	1.380(2)
C18	C23	1.4015(19)	C8	C9	1.360(2)
C18	C17	1.4616(19)	C1	C9	1.409(2)
C12	C13	1.4970(19)	C4	C3	1.353(2)
C14	C15	1.516(2)	C31	C30	1.509(2)
C14	C13	1.5098(18)	C31	C32	1.518(2)

Table 5 Bond Angles for exp_675.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C21	O24	C25	118.36(11)	C14	C15	C16	111.01(12)
C4	O5	C6	105.58(12)	C27	C28	C29	114.83(12)
C8	O7	C6	105.67(12)	C25	C26	C27	113.31(12)
C12	C11	C16	118.07(12)	C13	C10	C1	131.99(14)
C17	C11	C12	116.47(12)	C1	C2	C3	123.12(14)
C17	C11	C16	125.42(13)	C12	C13	C14	118.43(12)
C23	C22	C21	120.83(13)	C10	C13	C12	115.90(12)
C19	C18	C23	116.36(13)	C10	C13	C14	125.67(13)

C19	C18	C17	116.99(12)	O7	C8	C4	109.39(13)
C23	C18	C17	126.64(13)	C9	C8	O7	127.78(14)
O33	C12	C11	120.28(13)	C9	C8	C4	122.79(14)
O33	C12	C13	120.52(13)	C2	C1	C10	116.49(13)
C13	C12	C11	119.20(11)	C2	C1	C9	118.14(13)
C13	C14	C15	111.87(11)	C9	C1	C10	125.37(13)
O24	C25	C26	106.58(11)	C11	C17	C18	131.89(13)
O24	C21	C22	115.64(12)	O5	C4	C8	110.07(13)
O24	C21	C20	124.98(12)	C3	C4	O5	128.48(14)
C20	C21	C22	119.38(13)	C3	C4	C8	121.41(14)
C21	C20	C19	118.97(13)	C4	C3	C2	116.76(14)
C11	C16	C15	111.98(12)	C8	C9	C1	117.77(14)
C28	C27	C26	112.00(12)	C30	C31	C32	113.17(15)
C20	C19	C18	123.07(13)	C31	C30	C29	114.41(13)
C22	C23	C18	121.28(13)	O5	C6	O7	108.49(13)
C30	C29	C28	113.14(12)				

Table 6 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for exp_675.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H22	4922	-410	1245	65
H14A	5957	-3994	7121	65
H14B	6744	-2851	6552	65
H25A	1199	1938	757	65
H25B	520	727	687	65
H20	667	946	2588	69
H16A	6130	-1903	4720	66
H16B	5014	-2505	4195	66
H27A	-479	1516	-1045	67
H27B	80	2752	-908	67
H19	959	441	4403	69
H23	5181	-943	3055	64
H29A	-1388	2310	-2811	68
H29B	-896	3568	-2670	68
H15A	4615	-3930	5723	69
H15B	6349	-3957	5109	69
H28A	1086	1476	-2947	72
H28B	1577	2733	-2807	72

H26A	1965	603	-1250	67
H26B	2568	1836	-1174	67
H10	3420	-1882	8921	66
H2	3222	-2543	10780	74
H17	2313	-301	5694	63
H3	4138	-3483	12267	77
H9	7037	-3644	8431	71
H31A	-1665	4427	-4470	80
H31B	-2263	3196	-4562	80
H30A	730	3499	-4550	73
H30B	171	2265	-4688	73
H6A	8224	-6086	11219	91
H6B	9103	-5025	11411	91
H32A	-787	3047	-6442	125
H32B	-38	4212	-6355	125
H32C	-1747	4280	-6351	125