

Supplementary Information

Multi odd-even effects on cell parameters, melting points, and optical properties of chiral crystal solids based on *S*-naproxen

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Experiment Section

Materials and instruments: The reagents and solvents employed were commercially available and used as received without further purification. Elemental analyses were performed on a Perkin-Elmer 240 elemental analyzer. The FT-IR spectra were recorded from KBr pellets in range 400-4000 cm⁻¹ on a Bruker Tensor27 spectrometer. Fluorescence spectra were taken using Ediburg FLS920 fluorescence spectrophotometer. Uv-Vis spectra for **1-6** were recorded on Hitachi U-3010 spectrometer. CD spectroscopies were performed on a JASCO J-810 spectropolarimeter. Kurtz powder SHG measurements were performed on ground samples of crystalline **1-6** with a synchroscan streak camera (Hamamatsu Model C1587, 8 ps resolution) connected to a polychromator as the detector system, and an optical parametric generator (Spectra Physics, Model: OPA-800C) pumped by a mode-locked Ti: sapphire laser oscillator-amplifier system (Spectra Physics, Model: Hurricane) as the pump source. The powder second-harmonic signals were compared to that of KH₂PO₄ to determine the relative SHG efficiencies of **1-6**.

X-ray Crystallography. Single-crystal X-ray diffraction data for compounds **1-6** were collected on a Bruker CCD APEX diffractometer at room temperature with Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). All the structures were solved by direct methods using the SHELXS program of the SHELXTL package and refined by full-matrix least squares methods with SHELXL.¹ All non-hydrogen atoms were located in successive difference Fourier syntheses, where they were refined with anisotropic thermal parameters on F^2 . Hydrogen atoms were located at geometrically calculated positions and refined with isotropic thermal parameters. The data of the weak interactions were calculated by PLATON.² Crystallographic data and structural refinements for compounds **1-6** are summarized in Table S1.

CCDC reference number 687452, 687453, 687454, 687455, 717531, and 1407685 for **1-6**, respectively. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK; fax: (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

Preparation of naproxen (**1**)

Naproxen (1**).** The *S*-naproxen (1 mmol, 0.230 g) was solved in the mixed solvent of ethanol (5 mL) and water (5 mL). After one week, the colorless needle crystals suitable for X-ray single diffraction were obtained. Yield (90%). M.p. (°C): 155.3-155.4; Elemental analysis found (%) for C₁₄H₁₄O₃ (230.26): C, 73.55; H, 6.63; requires (%): C, 73.03; H, 6.13; IR (KBr, cm⁻¹): 3152 (br), 3001 (w), 2963 (w), 2938 (w), 1925 (w), 1788 (w), 1728 (vs), 1686 (m), 1630 (m), 1604 (s), 1505 (m), 1485 (w), 1453 (w), 1435 (w), 1418 (w), 1394 (m), 1346 (w), 1304 (w), 1264 (s),

1227 (m), 1193 (w), 1158 (m), 1090 (m), 1071 (m), 1028 (s), 963 (w), 925 (w), 895 (m), 855 (m), 818 (s), 793 (m), 741 (w), 673 (m), 641 (m), 599 (w), 569 (w), 528 (w), 484 (m), 472 (m), 422 (m).

Synthesis of naproxen ester derivatives 2-6

Naproxen methyl ester (2). The S-naproxen (10 mmol, 2.300 g) was solved in the mixed solvent of ethanol (3 mL) and water (3 mL). The reaction mixture was refluxed about 4 hours. After the end of reaction, the cool water was added to the mixture. Then, the mixture was filtered under the vacuum pressure and the filtered cake was washed with cool water. The white samples **2** was obtained. Yield (69.92%, 1.708 g). The crystal sample of **2** was solved in the mixed solvents of ethanol solution (ethanol 2 mL and water 2 ml). After one week, the colorless needle crystals suitable to X-ray single diffraction were obtained. M.p. (°C): 89.7-90.2; Elementary Analysis found (%) for C₁₅H₁₆O₃: C, 74.65; H, 6.62; requires (%): C, 73.75; H, 6.60; IR (KBr, cm⁻¹): 3479(w), 3444(w), 2976(m), 2935(w), 2845(w), 2549(w), 2337(m), 1737(vs), 1448(m), 1332(m), 1267(m), 1201(m), 1176(m), 1028(m), 856(m), 823(m); ¹H NMR (400 MHz, d₄-CH₃OH, ppm): 7.73 (dd, J = 8.43, 6.71 Hz, 2H), 7.66 (s, 1H), 7.38 (dd, J = 8.54, 1.65 Hz, 1H), 7.21 (d, J = 2.19 Hz, 1H), 7.12 (dd, J = 8.97, 2.46 Hz, 1H), 3.95-3.85 (m, 4H), 3.66 (s, 3H), 1.54 (d, J = 7.15 Hz, 3H); ¹³C NMR (100 MHz, d₄-CH₃OH, ppm): 175.4, 157.7, 135.6, 133.8, 128.9, 128.7, 126.8, 125.6, 125.4, 118.5, 105.1, 54.2, 51.0, 45.0, 17.5.

Naproxen esters 3-5. The preparation of compounds **3-5** were similar to that of compound **2**.

Naproxene ethyl ester 3: Yield (93.28%, 2.409 g); M.p. (°C): 66.7-68.6; Elementary analysis found (%) for C₁₆H₁₈O₃: C, 74.61; H, 7.04; requires (%): C, 74.39; H, 7.02; IR (KBr, cm⁻¹): 3441(w), 3060 (m), 2980 (s), 2938 (m), 2903 (w), 2843 (w), 2049 (m), 1923 (m), 1731 (vs), 1631 (m), 1605 (vs), 1504 (s), 1482 (m), 1455 (m), 1418 (m), 1392 (s), 1372 (s), 1349 (m), 1326 (s), 1266 (s), 1229 (s), 1182 (m), 1121 (w), 1087 (m), 1070 (m), 1048 (w), 1027 (s), 960 (w), 944 (w), 928 (w), 894 (m), 857 (s), 822 (s), 795 (m), 763 (w), 747 (m), 674 (w), 663 (w), 597 (w), 574 (w), 520 (m), 478 (m), 444 (m), 406 (m); ¹H NMR (400 MHz, d₄-CH₃OH, ppm): 7.81-7.62 (m, 3H), 7.38 (dd, J = 8.53, 1.66 Hz, 1H), 7.21 (d, J = 2.26 Hz, 1H), 7.12 (dd, J = 8.98, 2.49 Hz, 1H), 4.21-4.03 (m, 2H), 3.97-3.82 (m, 4H), 1.54 (d, J = 7.15 Hz, 3H), 1.19 (t, J = 7.12 Hz, 3H); ¹³C NMR (100 MHz, d₄-CH₃OH, ppm): 174.95, 157.66, 135.67, 133.75, 128.90, 128.66, 126.70, 125.55, 125.36, 118.45, 105.06, 60.37, 54.21, 45.13, 17.40, 12.90.

Naproxene n-propyl ester 4: Yield (92.18%, 2.510 g); M.p. (°C): 52.5-53.4; Elementary analysis found (%) for C₁₇H₂₀O₃: C, 74.74; H, 7.38; requires (%): C, 74.97; H, 7.40; IR (KBr, cm⁻¹): 2967 (m), 2936 (m), 1728 (vs), 1633 (m), 1605 (s), 1504 (m), 1485 (m), 1417 (m), 1390 (m), 1374 (m), 1346 (m), 1324 (s), 1270 (s), 1231 (s), 1182 (m),

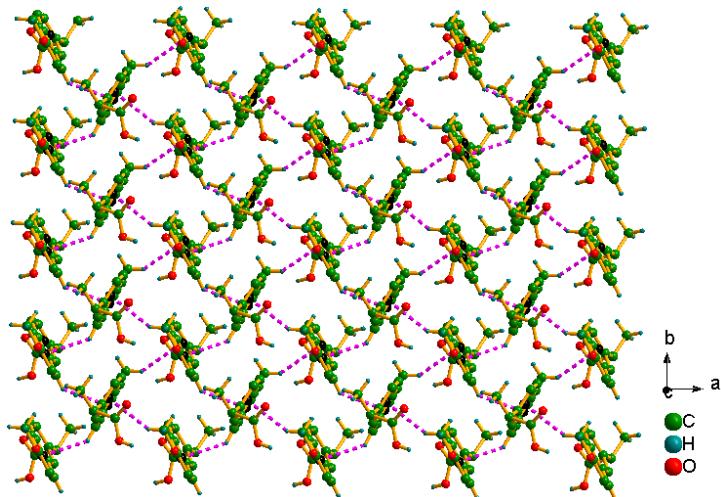
1121 (w), 1097 (m), 1071 (m), 1052 (w), 1028 (s), 1003 (w), 960 (w), 942 (m), 924 (w), 915 (w), 889 (s), 859 (s), 813 (s), 794 (m), 746 (m), 686 (m), 664 (m), 590 (m), 568 (w), 521 (w), 478 (s), 461 (w), 413 (w); ¹H NMR (400 MHz, *d*₄-CH₃OH, ppm): 7.79-7.70 (m, 2H), 7.67 (s, 1H), 7.39 (dd, *J* = 8.56, 1.52 Hz, 1H), 7.21 (d, *J* = 2.24 Hz, 1H), 7.17-7.09 (m, 1H), 4.04 (t, *J* = 6.52 Hz, 2H), 3.90 (d, *J* = 9.98 Hz, 4H), 1.65-1.50 (m, 5H), 0.84 (t, *J* = 7.43 Hz, 3H); ¹³C NMR (100 MHz, *d*₄-CH₃OH, ppm): 176.5, 159.2, 137.2, 135.2, 130.4, 130.1, 128.1, 127.1, 126.8, 119.9, 106.6, 67.4, 55.7, 46.7, 23.0, 18.8, 10.5.

Naproxen *n*-butyl ester 5: Yield (96.32%, 2.758 g); M.p. (°C): 66.0-67.0; Elemental analysis found (%) for C₁₈H₂₂O₃: C, 75.10; H, 7.78; requires (%): C, 75.50; H, 7.74; IR (KBr, cm⁻¹): 3055(w), 2958(m), 2933(w), 2870(w), 2372(w), 2052(w), 1919(w), 1728(vs), 1631(m), 1604(s), 1504(m), 1483(m), 1456(m), 1388(m), 1325(m), 1267(s), 1228(m), 1190(s), 1122(m), 1093(m), 1070(m), 1028(m), 929(m), 854(m), 815(m), 500(m); ¹H NMR (400 MHz, CDCl₃, ppm): 7.75-7.70 (m, 2H), 7.65 (s, 1H), 7.37 (dd, *J* = 8.57, 1.52 Hz, 1H), 7.20 (d, *J* = 2.25 Hz, 1H), 7.18-7.08 (m, 1H), 4.05 (t, *J* = 6.52 Hz, 2H), 3.95-3.82 (m, *J* = 9.96 Hz, 4H), 1.65-1.50 (m, 5H), 1.45-1.39 (m, 2H), 0.85 (t, *J* = 7.43 Hz, 3H); ¹³C NMR (100 MHz, CDCl₃, ppm): 174.75, 157.12, 135.70, 133.66, 129.16, 128.85, 127.00, 126.18, 125.87, 119.23, 105.61, 64.63, 55.26, 45.35, 31.30, 18.53, 13.86, 13.61.

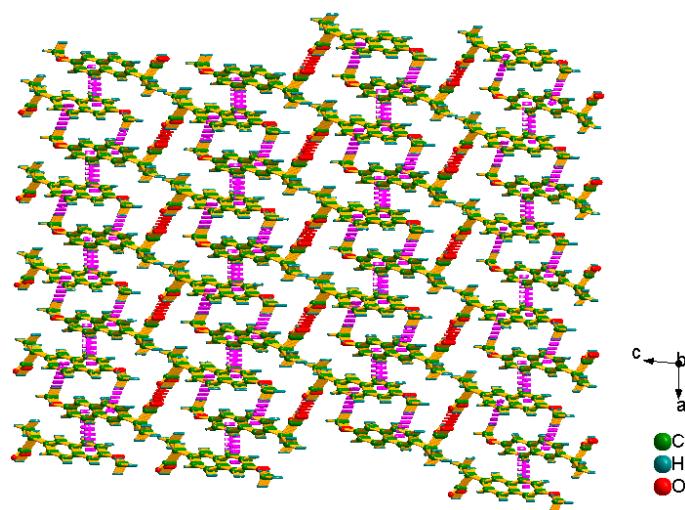
Naproxen *n*-amyl ester 6. Yield (55.55%, 1.669 g); M.p. (°C): 48.4-49.1; Elemental analysis found (%) for C₁₉H₂₄O₃: C, 75.75; H, 8.08; requires (%): C, 75.97; H, 8.05; IR (KBr, cm⁻¹): 3443(br), 3059(w), 2958(s), 2931(s), 2866(m), 2050(w), 1917(w), 1730(vs), 1629(w), 1604(s), 1502(w), 1481(w), 1454(m), 1417(w), 1392(m), 1373(m), 1348(m), 1330(m), 1265(s), 1228(s), 1178(vs), 1120(w), 1089(m), 1028(s), 1001(w), 968(w), 954(w), 923(w), 893(m), 856(s), 821(s), 794(w), 743(w), 731(w), 684(w), 661(w), 575(w), 538(w), 478(m), 426(w), 405(w); ¹H NMR (400 MHz, CDCl₃, ppm): 7.72-7.68 (t, 3H), 7.43-7.41 (dd, *J* = 8.44, 1.34 Hz, 1H), 7.16-7.12 (dd, *J* = 11.69, 2.80 Hz, 2H), 4.09-4.04 (m, 2H), 3.92 (s, 3H), 3.88-3.83 (q, *J* = 7.13 Hz, 1H), 1.61-1.54 (m, 5H), 1.30-1.18 (m, 4H), 0.84-0.81 (t, 3H); ¹³C NMR (100 MHz, CDCl₃, ppm): 174.1, 157.1, 135.3 133.3, 128.7, 128.4, 126.5, 125.8, 125.4, 118.4, 105.1, 70.3, 54.8, 45.0, 27.2, 18.4, 17.9.



(a)

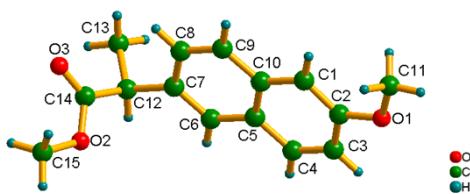


(b)

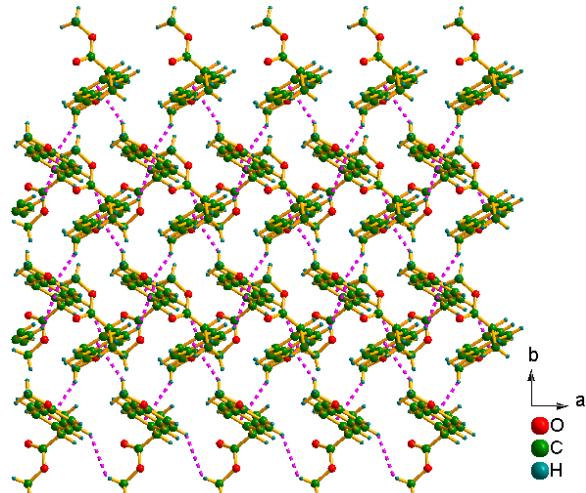


(c)

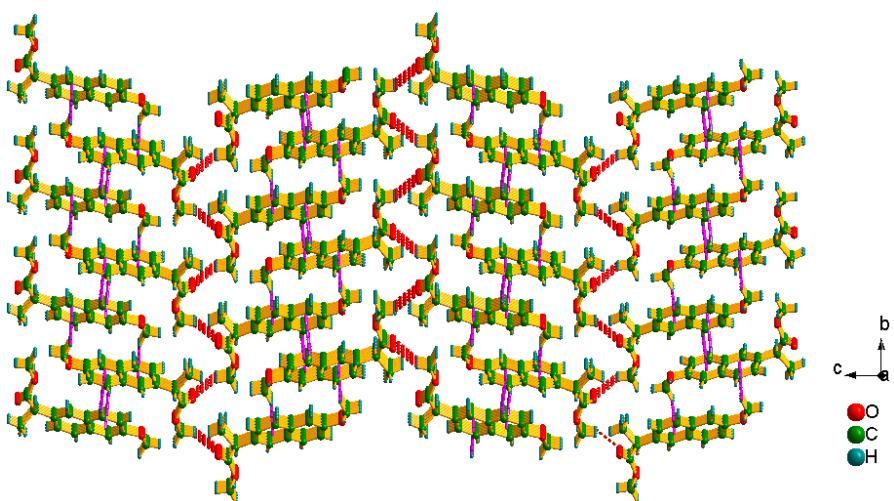
Fig. S1 (a) Ball-stick drawing of **1** in the asymmetric unit. (b) View point of 2D layer extending along the *ab* plane in **1**. (c) Packing diagram of **1** along the *b* axis. The thin purple dashed-lines and red ones represent C-H $\cdots\pi$ packing interactions and hydrogen bonds, respectively.



(a)

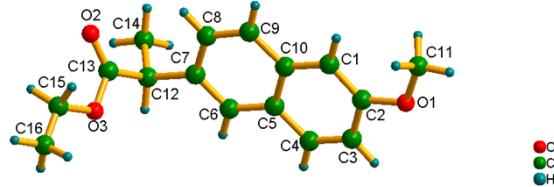


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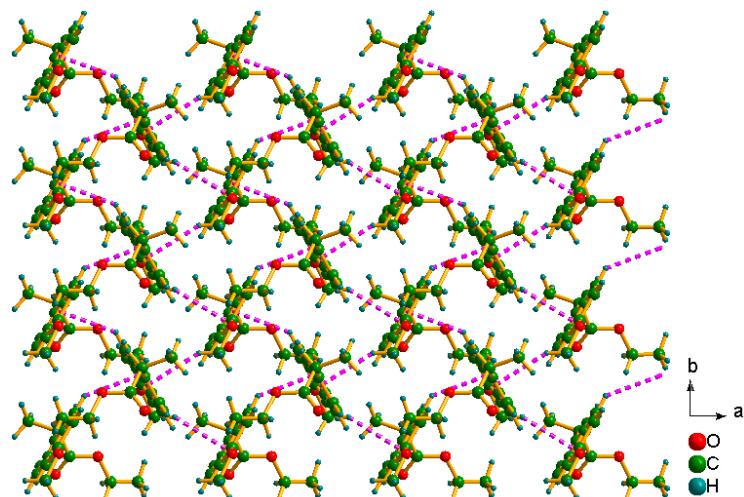


(c)

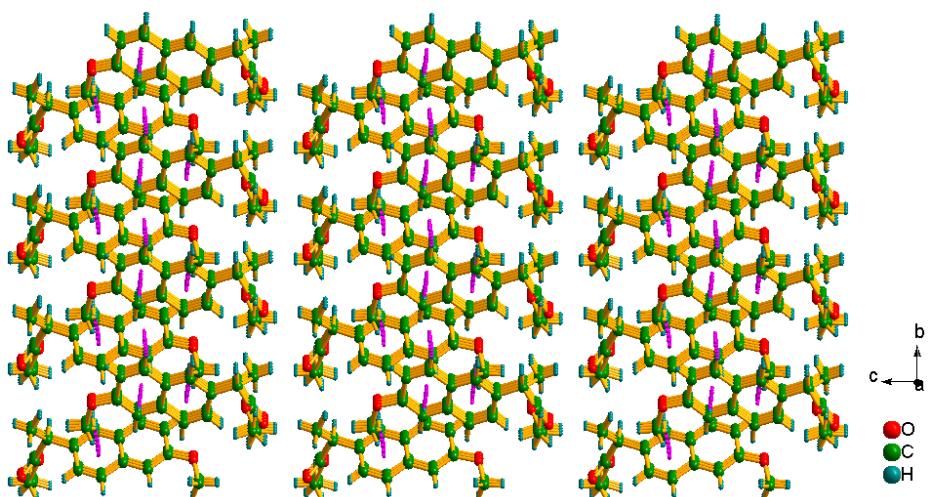
Fig. S2 (a) Ball-stick drawing of **2** in the asymmetric unit. (b) View point of 2D layer extending along the *ab* plane in **2**. (b) Packing diagram of **2** along the *a* axis. The purple dashed-lines and red ones represent C-H $\cdots\pi$ and hydrogen bonds interactions, respectively.



(a)

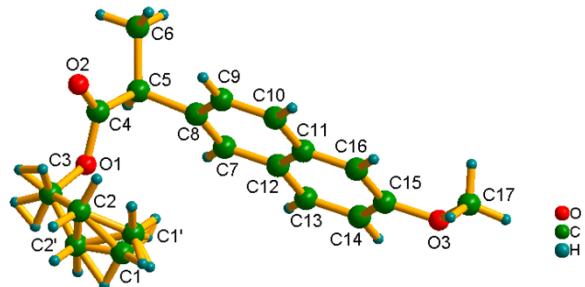


(b)

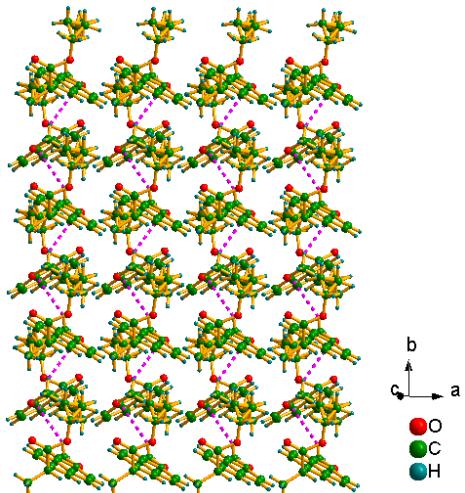


(c)

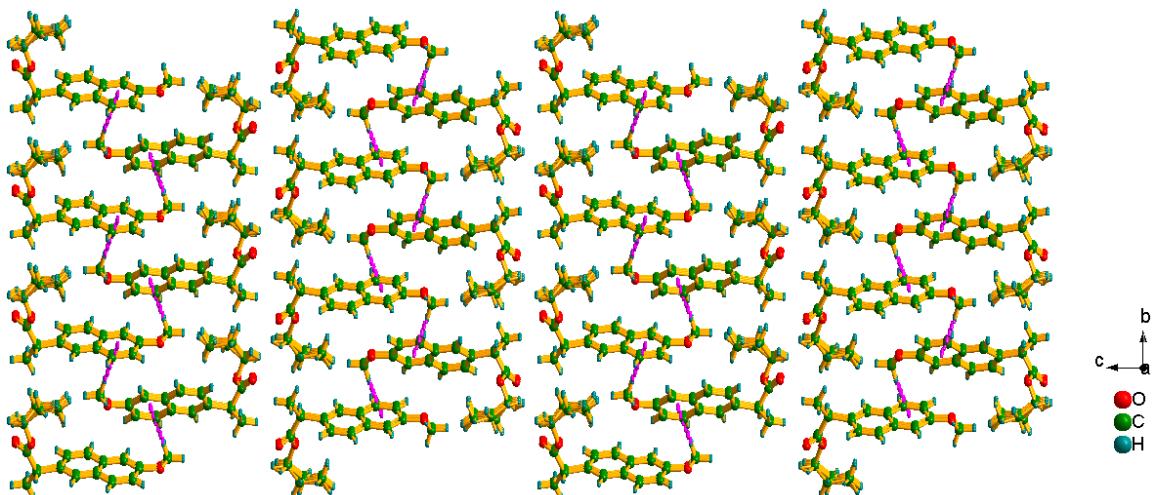
Fig. S3 (a) Ball-stick drawing of **3** in the asymmetric unit. (b) A 2D supramolecular layer in **3** along the *ab* plane. (c) Packing diagram of **3** along the *a* axis. The purple dashed-lines show C-H $\cdots\pi$ packing interactions.



(a)

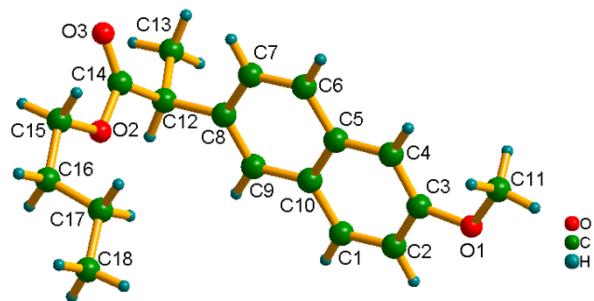


(b)

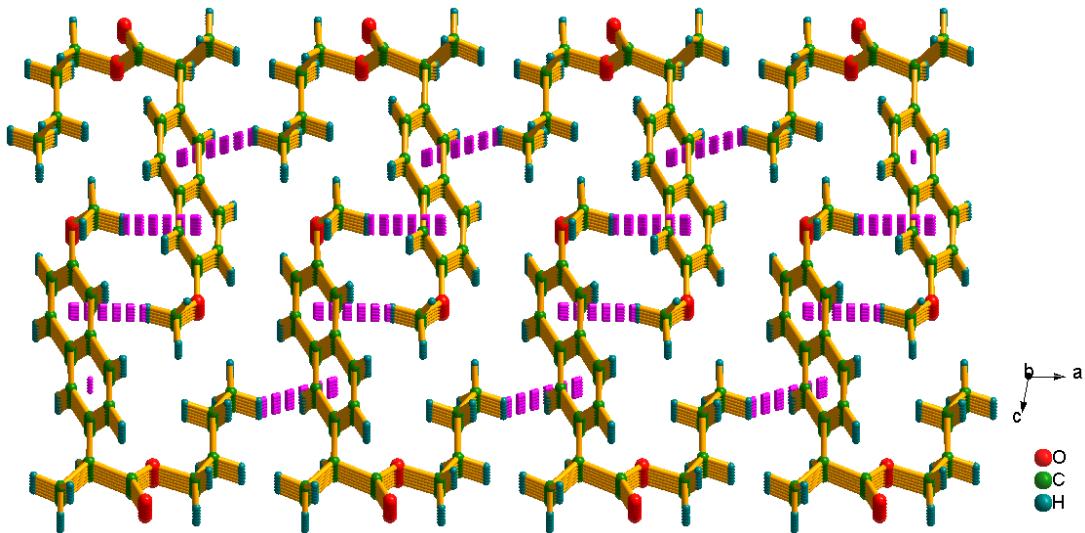


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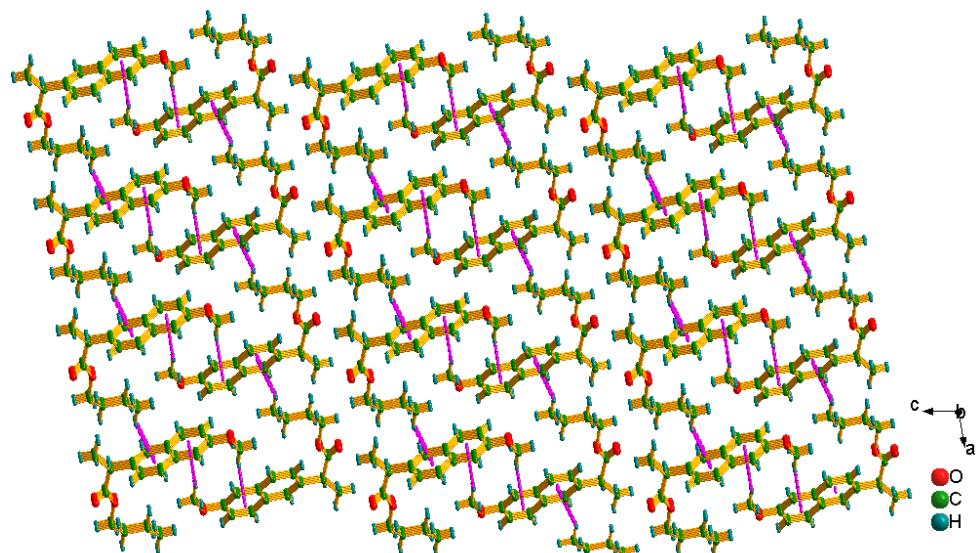
Fig. S4 (a) Ball-stick drawing of **4** in the asymmetric unit. (b) A 2D supramolecular layer in **4**. (c) Packing diagram of **4** along the *a* axis. The red dashed-lines indicate C-H \cdots π packing interactions.



(a)

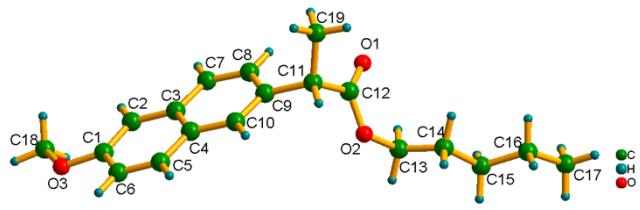


(b)

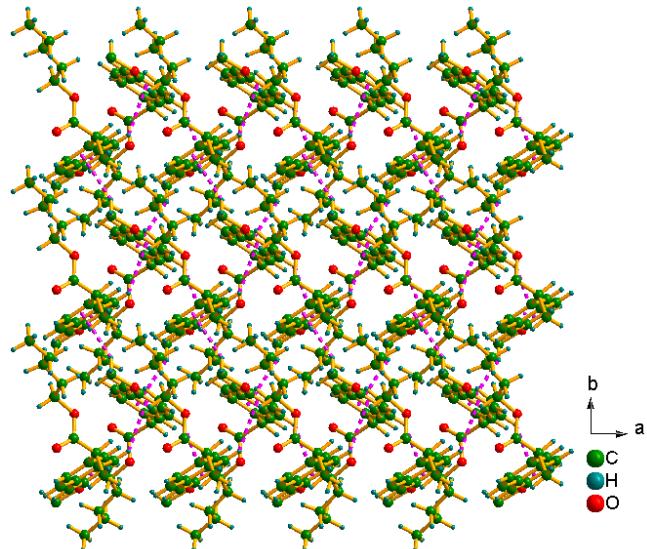


(c)

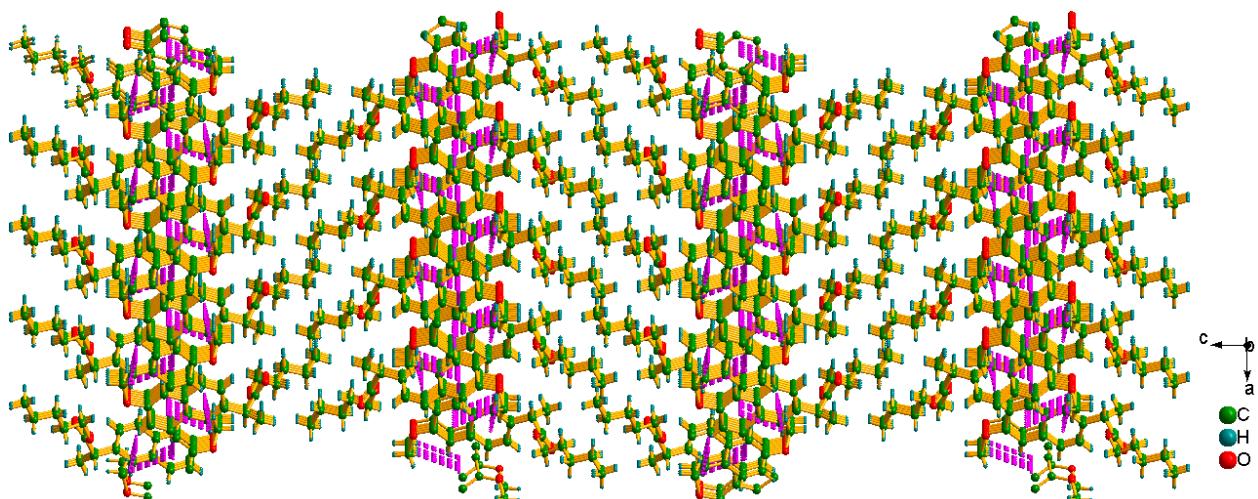
Fig. S5 (a) Ball-stick drawing of **5** in the asymmetric unit. (b) A 2D supramolecular layer in **5** along the *ac* plane. (c) Packing diagram of **5** along the *b* axis. The purple dashed-lines represent C-H $\cdots\pi$ packing interactions.



(a)



(b)



(c)

Fig. S6 (a) Ball-stick drawing of **6** in the asymmetric unit. (b) A 2D supramolecular layer in **6** along the *ab* plane. (c) Packing diagram of **3** along the *b* axis. The purple dashed-lines stand for C-H $\cdots\pi$ packing interactions, respectively.

Table S1 Crystallographic data and structure refinements for **1-6**

	1	2	3	4	5	6
chemical formula	C ₁₄ H ₁₄ O ₃	C ₁₅ H ₁₆ O ₃	C ₁₆ H ₁₈ O ₃	C ₁₇ H ₂₀ O ₃	C ₁₈ H ₂₂ O ₃	C ₁₉ H ₂₄ O ₃
fw	230.25	244.28	258.30	272.33	286.36	300.38
T (K)	298	298	298	298	296	296
λ (Mo K α) (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
crystal system	Monoclinic	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic	Orthorhombic
space group	<i>P</i> 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁	<i>P</i> 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> (Å)	7.87590(10)	5.89120(10)	8.1459(9)	5.6809(12)	8.067(2)	5.806(4)
<i>b</i> (Å)	5.78340(10)	7.9258(2)	5.8321(6)	8.0485(17)	5.7361(15)	8.297(6)
<i>c</i> (Å)	13.3230(2)	28.6878(5)	15.3640(12)	33.742(7)	17.495(5)	37.02(2)
α (degree)	90	90	90	90	90	90.00
β (degree)	93.8770(10)	90	102.919(5)	90	100.528(4)	90.00
γ (degree)	90	90	90	90	90	90.00
<i>V</i> (Å ³)	605.47(2)	1339.50(5)	711.43(12)	1542.8(6)	795.9(4)	1783(2)
<i>Z</i>	2	4	2	4	2	4
Crystal size (mm)	0.05×0.20×0.20	0.20×0.30×0.40	0.06×0.20×0.40	0.10×0.20×0.20	0.10×0.10×0.30	0.10×0.10×0.20
μ (Mo K α) (mm ⁻¹)	0.088	0.084	0.082	0.079	0.080	0.074
ρ (g·cm ⁻³)	1.263	1.211	1.206	1.173	1.195	1.119
GOF	1.02	1.04	1.04	1.07	1.04	1.03

R_1^a ($I > 2\sigma(I)$)	0.0303	0.0410	0.0498	0.0505	0.0509	0.0694
wR_2^b (all data)	0.0853	0.1536	0.1646	0.1551	0.0976	0.2304
Flack	-0.7(12)	0.2(18)	0(3)	2(2)	4.3(15)	0(3)
Reflections collected	3132	7218	3275	13524	7035	9901
Independent reflections	1939	2999	2196	3561	3332	3909
reflections [$I > 2\sigma(I)$]	1825	2232	1387	2430	1512	2470
$F(000)$	244	520	276	584	308	648
R_{int}	0.010	0.016	0.015	0.030	0.050	0.036
θ range	1.5/26.0	1.4/27.4	2.6/26.0	2.4/27.5	2.4/27.6	2.5/27.3
Largest peak and hole [e·Å ⁻³]	-0.11/0.12	-0.19/0.15	-0.14/0.17	-0.16/0.17	-0.14/0.11	-0.20/0.29
CCDC number	687452	687453	687454	687455	717531	1407685

^a $R_1 = \sum |F_o| - |F_c| / \sum |F_o|$. ^b $wR_2 = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$

Table S2 Hydrogen bond geometries in the crystal structures of **1** and **2**

Complex	D–H···A	H···A (Å)	D···A (Å)	D–H···A (°)
1	O(2)–H(2)···O(1) ^a	1.83(3)	2.679(2)	172(3)
2	C(15)–H(15B)···O(3) ^b	2.40	3.217(4)	142

Symmetry codes: ^a-x,-1/2+y,-z, ^b-1-x,1/2+y,-1/2-z.**Table S3** The distance weak packing interactions for compounds **1-6**

Compound	C–H···π	H···π (Å)	C···π (Å)	C–H···π (°)	Average H···π (Å)	Average C···π (Å)
1	C(11)–H(11A)···Cg(2) ^a C(14)–H(14B)···Cg(1) ^b	2.70 2.90	3.4340(16) 3.739(3)	137 146	2.85	3.587
2	C(4)–H(4A)···Cg(1) ^c C(11)–H(11C)···Cg(2) ^d	2.68 2.75	3.4311(18) 3.537(3)	138 140	2.72	3.484
3	C(4)–H(4A)···Cg(1) ^e C(11)–H(11C)···Cg(2) ^f	2.72 2.77	3.479(4) 3.571(5)	139 141	2.75	3.525
4	C17–H17B···Cg(2) ^g	2.86	3.727(7)	151	2.86	3.727
5	C(11)–H(11B)···Cg(1) ^h C(18)–H(18C)···Cg(2) ⁱ	2.77 2.94	3.615(4) 3.740(4)	148 142	2.86	3.678
6	C(5)–H(5A)···Cg(1) ^j C(18)–H(18C)···Cg(2) ^k	2.79 2.81	3.565(4) 3.616(5)	141 143	2.80	3.591

Symmetric codes: ^a-1-x, -1/2+y, -1-z; ^b-x, 1/2+y, -1-z for **1**. ^c-1/2+x, 1/2-y, -z; ^d1/2+x, -1/2-y, -z for **2**. ^e-1-x, 1/2+y, -1-z; ^f-x, -1/2+y, -1-z for **3**. ^g2-x, 1/2+y, 1/2-z for **4**. ^h1-x, 1/2+y, 2-z; ⁱ-1+x, -1+y, z for **5**. ^j1/2+x, 1/2-y, 2-z; ^k-1/2+x, 3/2-y, 2-z for **6**. Cg(1) and Cg(2) represent two phenyl rings in naphthalene groups.**Table S4** The relationships between packing interactions and number of carbon atoms

Compound	Number of carbon atoms*	Stacking interactions	Distances (Å)	Dihedral angles (°)
1	0	Cg(1)…Cg(2) ^a	5.8226(9)	57.69(7)
2	1	Cg(1)…Cg(2) ^b	5.5926(11)	57.86(9)
3	2	Cg(2)…Cg(1) ^c	5.904(2)	1.95(18)
4	3	Cg(1)…Cg(1) ^d Cg(1)…Cg(1) ^e Cg(2)…Cg(2) ^d Cg(2)…Cg(2) ^e	5.6809(13) 5.6809(13) 5.6809(14) 5.6809(14)	0 0 0 0
5	4	Cg(1)…Cg(2) ^c	5.924(2)	1.58(14)
6	5	Cg(2)…Cg(1) ^d	5.851(5)	2.76(15)

*the number of carbon atoms in carbon chain for ester groups. Symmetrical codes and aromatic rings: ^a-X,-1/2+Y,-1-

Z; Cg(1): C(4)-C(5)-C(6)-C(7)-C(12)-C(13); Cg(2): C(7)-C(8)-C(9)-C(10)-C(11)-C(12); ^b-1/2+X,-1/2-Y,-Z;
 Cg(1): C(1)-C(2)-C(3)-C(4)-C(5)-C(10); Cg(2): C(5)-C(6)-C(7)-C(8)-C(9)-C(10); ^cX,-1+Y,Z; Cg(1): C(1)-C(2)-
 C(3)-C(4)-C(5)-C(10); Cg(2): C(5)-C(6)-C(7)-C(8)-C(9)-C(10); ^d-1+X,Y,Z; ^e1+X,Y,Z; Cg(1): C(7)-C(8)-C(9)-
 C(10)-C(11)-C(12); Cg(2): C(11)-C(12)-C(13)-C(14)-C(15)-C(16); ^cX,-1+Y,Z; Cg(1): C(1)-C(2)-C(3)-C(4)-
 C(5)-C(10); Cg(2): C(5)-C(6)-C(7)-C(8)-C(9)-C(10); ^d-1+X,Y,Z; Cg(1): C(1)-C(2)-C(3)-C(4)-C(5)-C(6); Cg(2):
 C(3)-C(4)-C(10)-C(9)-C(8)-C(7).

Table S5 The melting points for compounds **1-6**

Compound	Number of carbon atoms ^a	M.P. (°C)	Average M. P. (°C)
1	0	155.3-155.4	155.1
2	1	89.7-90.2	90.0
3	2	66.7-68.6	67.7
4	3	52.5-53.4	53.0
5	4	66.0-67.0	66.5
6	5	48.4-49.1	48.8

^a the number of carbon atoms in carbon chain for ester groups.

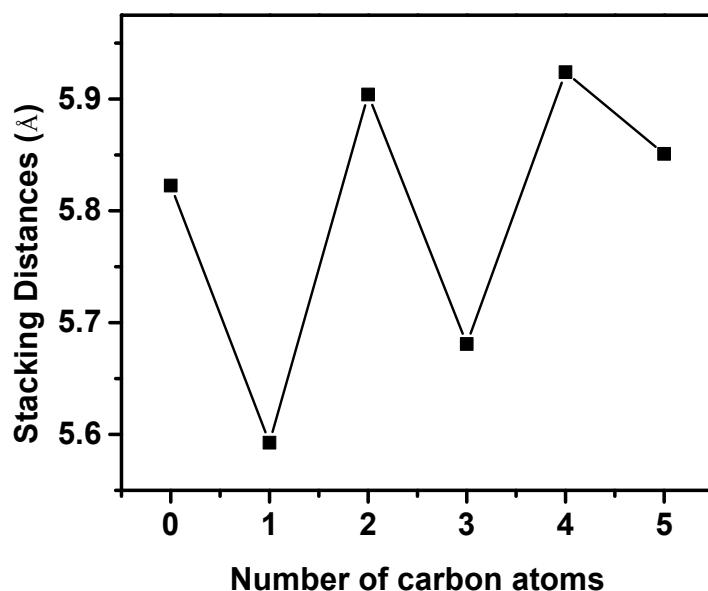


Fig. S7 The alternation of packing interactions

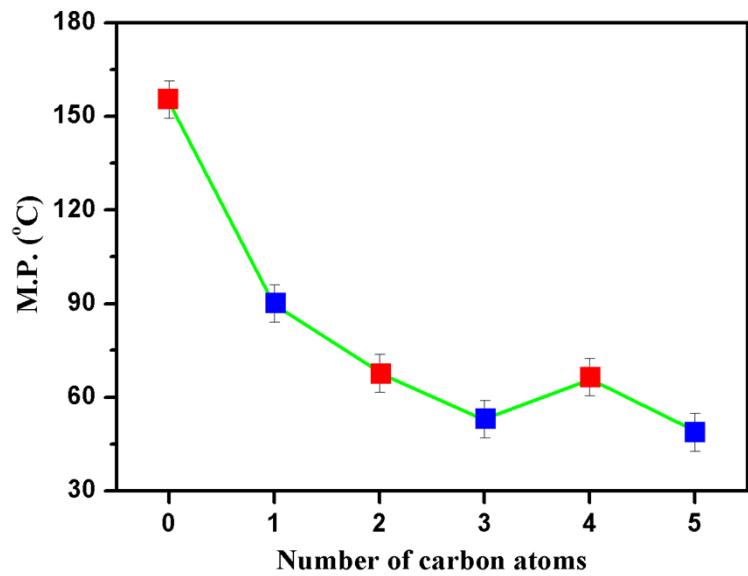


Fig. S8 The relationships between number of carbon atoms and melting points for compounds **1-6**.

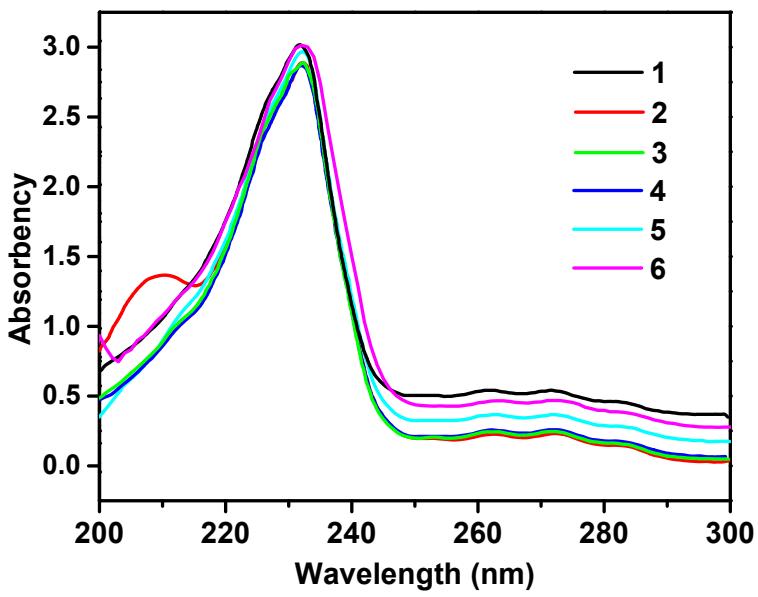


Fig. S9 Uv spectra for compounds **1-6** at 2×10^{-5} M in ethanol solution.

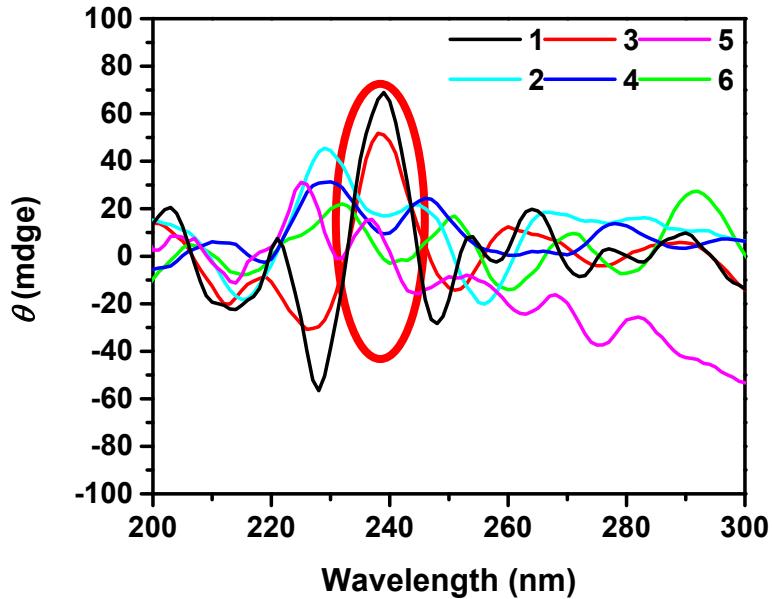


Fig. S10 The odd-even alternation for CD spectra of **1-6**.

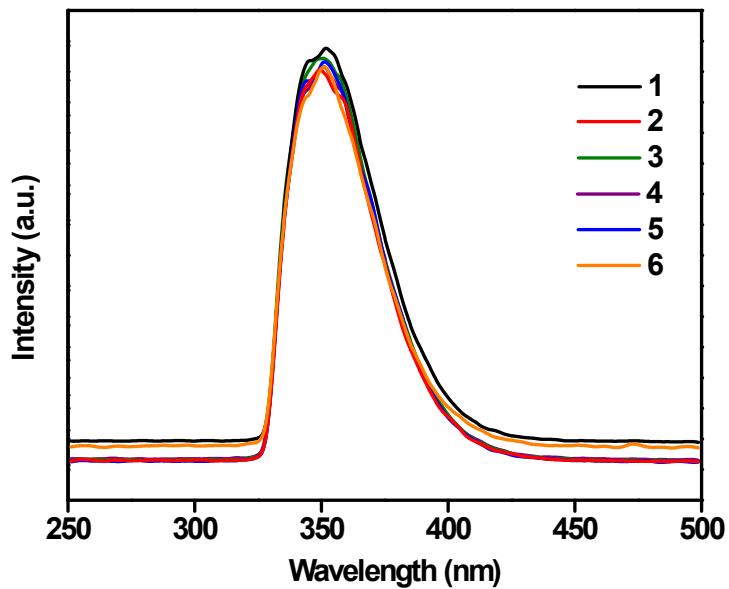


Fig. S11 The luminescent spectra for compounds **1-6** at 2×10^{-5} M in ethanol solvents under room temperature.

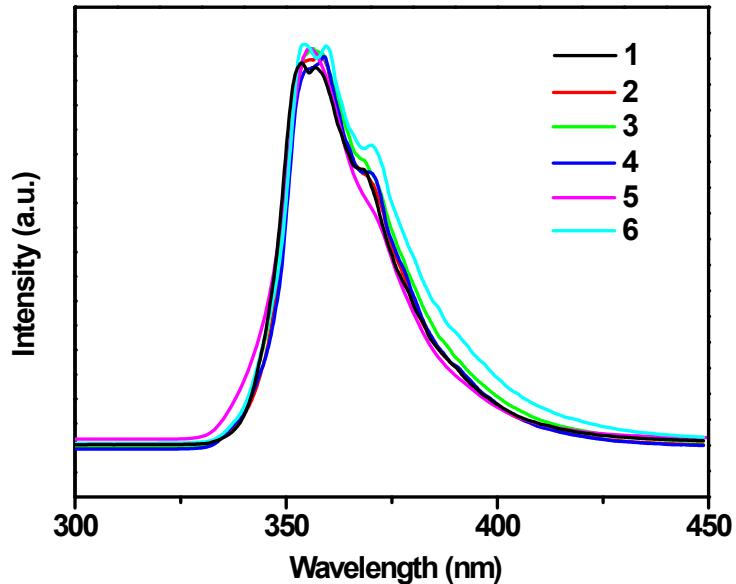


Fig. S12 The solid-state photoluminescent spectra for compounds **1-6** under room temperature.

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