Supplementary Information (SI) for Chemical Science.

Supporting Information

Intramolecular Transamidation Enables One-Pot Synthesis of Three Chiral, Z-Shaped Perilenediimides for Null-Type Supramolecular Polymer Formation

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1. Experimental Procedures

General methods

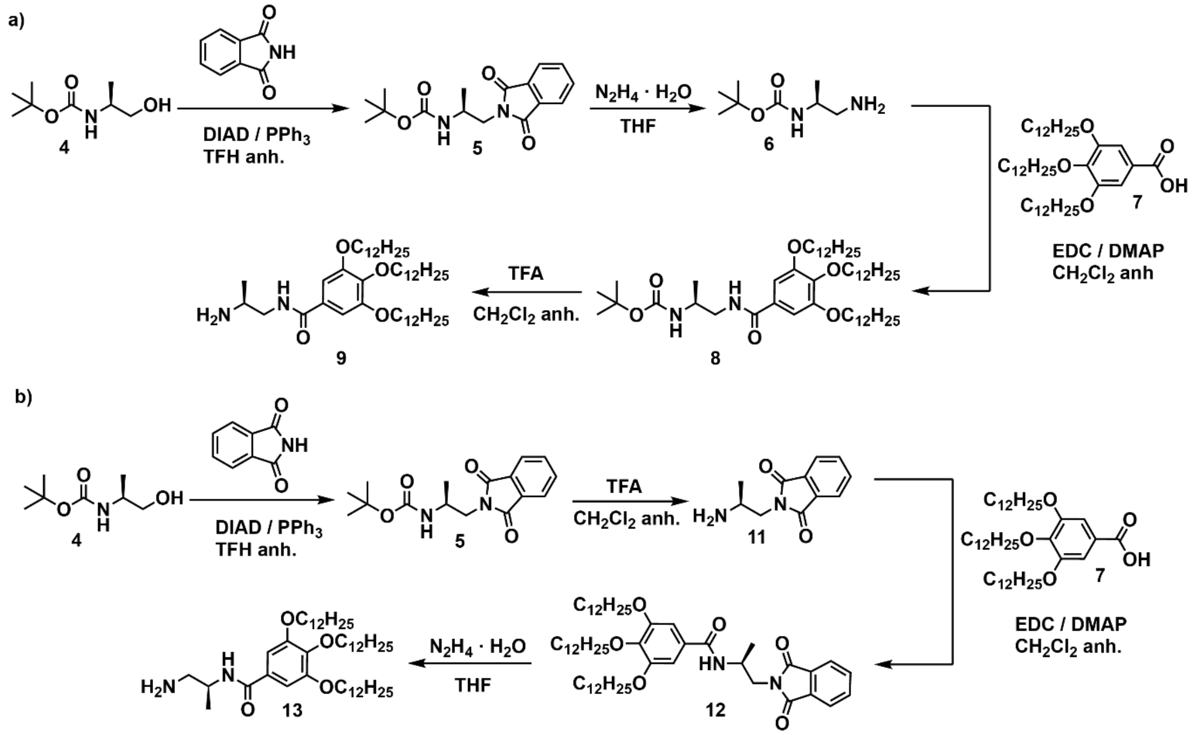
All solvents were dried according to standard procedures. Reagents were used as purchased. All air-sensitive reactions were carried out under argon atmosphere. Flash chromatography was performed using silica gel (Merck, Kieselgel 60, 230-240 mesh or Scharlau 60, 230-240 mesh). Analytical thin layer chromatography (TLC) was performed using aluminium-coated Merck Kieselgel 60 F254 plates. NMR spectra were recorded on a Bruker Avance 300 (^{1}H: 300 MHz; ^{13}C: 75 MHz) spectrometer or on a Bruker AVIII 700MHz (^{1}H: 700 MHz; ^{13}C: 175 MHz), using partially deuterated solvents as internal standards. Coupling constants (J) are denoted in Hz and chemical shifts (δ) in ppm. Multiplicities are denoted as follows: s = singlet, d = doublet, t = triplet, q = quadruplet, m = multiplet, br = broad. FT-IR spectra in film were recorded on a Bruker Tensor 27 (ATR device) spectrometer. UV-Vis spectra were registered on a Jasco-V630 spectrophotometer equipped with a Peltier thermoelectric temperature controller. The spectra were recorded in the continuous mode between 250 and 750 nm, with a wavelength increment of 1 nm, a response time of 4 s, and a bandwidth of 1 nm, by using a quartz cuvette (Hellma). Matrix Assisted Laser Desorption Ionization (coupled to a Time-Of-Flight analyzer) experiments (MALDI-TOF) were recorded on a Bruker REFLEX spectrometer detecting cationic species. AFM measurements were performed under ambient conditions using a MultiMode 8HR SPM from Bruker operating in tapping mode in air with a TESPA-V2 probe. HPLC was performed in an Agilent 1100 equipped with a diode-array detector and with a Chiralpak IA column, using toluene/iPrOH mixture (97/3 or 98/2) as eluent under isocratic conditions (1 mL/min). The integrals were calculated for the maxima of absorption (λ = 489 nm).

Solvent-denaturation model

The Gibbs free energy and the degree of cooperativity of the homopolymerization of Z-PDIs **1-3** have been extracted by applying the SD model in which aliquots of solutions of **1-3** in the good solvent $CHCl_3$ and the bad solvent MCH, keeping constant the total concentration. Fitting the variation of the absorbance versus the molar fraction of $CHCl_3$ and by using the equation $\Delta G' = \Delta G + mf$, being m a parameter that indicates the influence of the good solvent in the energetics of the process and f the molar fraction of the good solvent.[S1[21a]]

Synthetic details and characterization

Synthesis of amines 9 and 13

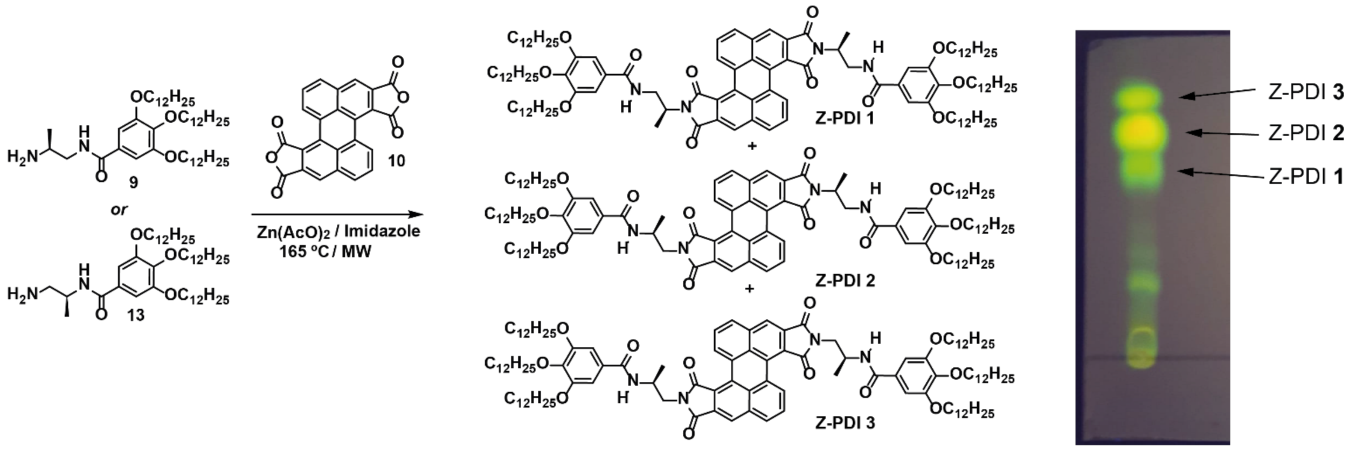


Scheme S1. Synthetic procedure towards the formation of amines **9** (a) and **13** (b).

Compounds **4** - **6**,[S2] **7**,[S3] **8**-**9**,[S2] **10**,[S4] and **11**,[S2] were prepared according to previously reported synthetic procedures and showed identical spectroscopic properties to those reported therein.

Synthesis of Z-PDIs1-3

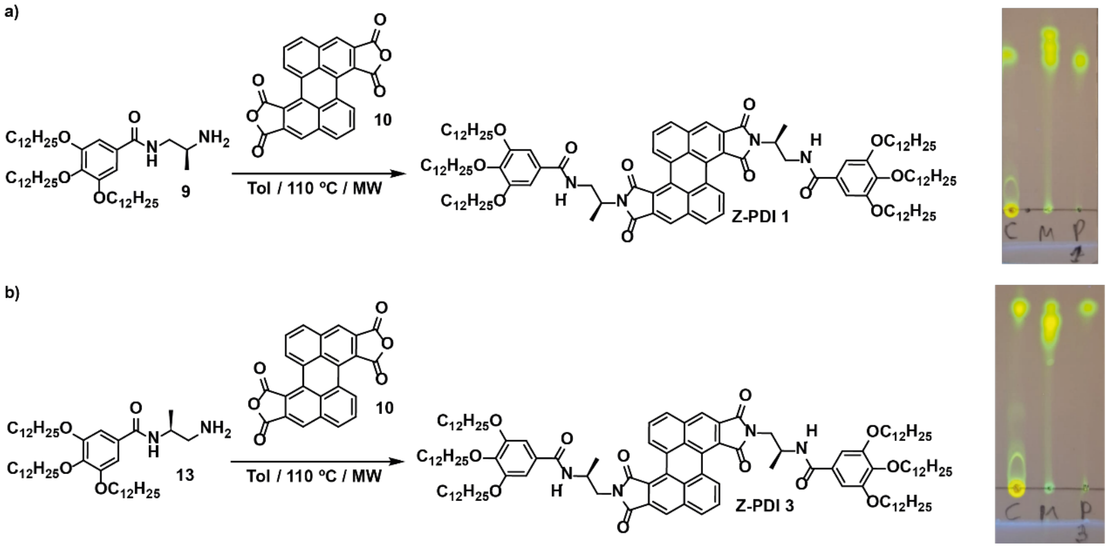
Method A



Scheme S2. Reaction scheme yielding the isomeric mixture of Z-PDIs **1-3**. TLC of the reaction mixture using amine **13** showing the formation of the isomeric mixture of Z-PDIs **1-3** (left).

A mixture of dianhydride **10** (0.030 g, 0.076 mmol, 1 eq.), amine **9** or **13** (0.117 g, 0.160 mmol, 2.1 eq.) and imidazole (0.3 g), were reacted in a microwave vial for 40 minutes at 165°C. After that, the reaction mixture was washed with brine (30 mL) and extracted with CH_2Cl_2 (30 mL). The organic layer was dried with $MgSO_4$, filtered and the solvent evaporated. Purification was performed by column chromatography (silica gel, $CHCl_3$/hexane/Et_2O 65/25/10) to obtain a mixture of Z-PDI **1- 3** with an overall yield of 43 %. In the case of amine **9** the yield of each Z-PDI was: Z-PDI **1** 11% (15 mg) , Z-PDI **2** 23% (32 mg) and Z-PDI **3** 9% (12 mg). In the case of amine **13** the yield of each Z-PDI was: Z-PDI **1** 7% (9 mg), Z-PDI **2** 22% (30 mg) and Z-PDI **3** 12% (16 mg).

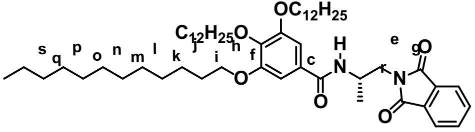
Method B



Scheme S3. Reaction schemes yielding to the formation exclusively of Z-PDI **1** (a) or Z-PDI **3** (b). TLC of the reaction mixture showing the exclusive formation of one of the isomeric Z-PDIs (left). Legend C: reaction mixture, M: mixture of Z-PDIs **1-3**; P1: isolated Z-PDI **1**; P2: isolated Z-PDI **2**.

A mixture of dianhydride **10** (0.030 g, 0.076 mmol, 1 eq.) and amine **9** or **13** (0.117 g, 0.160 mmol, 2.1 eq.) were dissolved in toluene (0.4 mL) and reacted for 4 hours at 110°C in a microwave vial. Then, the reaction mixture (C in the TLC) was washed with brine (30 mL) and extracted with CH_2Cl_2 (30 mL). The organic layer was dried with $MgSO_4$, filtered and the solvent evaporated. Purification was performed by column chromatography (silica gel, $CHCl_3$/hexane/Et_2O 65/25/10) to obtain Z-PDI **1** (37 mg, 27% yield), or Z-PDI **3** (40 mg, 29% yield) as orange solids.

(*S*)-*N*-(1-(1,3-dioxoisoindolin-2-yl)propan-2-yl)-3,4,5-tris(dodecyloxy)benzamide (12)



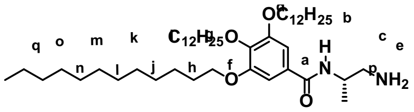
Compound **11** (2.02 g, 2.99 mmol, 1.6 eq.) and hexafluorophosphate benzotriazole tetramethyl uronium (HBTU) (1.13 g, 2.99 mmol, 1.6 eq) were dissolved in CH_2Cl_2 (5 mL) and stirred at room temperature for 30 minutes. Compound **7** (0.57 g, 1.87 mmol, 1 eq.) was dissolved in CH_2Cl_2 (5 mL) and triethylamine (0.52 mL, 0.38 mmol, 1.6 eq.), stirred at room temperature for 30 minutes, and added into compound **9**. The mixture was stirred for 16 hours at room temperature. The crude was washed with brine (50 mL) and extracted with CH_2Cl_2 (30 mL). Purification was performed by column chromatography (silica gel, CH_2Cl_2/EtOAc/MeOH 98/1/1) to obtain a white solid (1.28 g, yield: 79%).

^{1}H NMR (300 MHz, $CDCl_3$) δ: 7.81 (m, 2H, H_a), 7.74 (m, 2H, H_b), 6.97(s, 2H, H_c), 6.81(d, 1H, H_d, *J* = 7.6 Hz), 4.44 (d, 1H, H_e), 4.06 - 3.95 (m, 6H, H_f), 1.88 - 1.68 (m, 6H, H_h), 1.53 - 1.43 (m, 6H, H_i), 1.38 - 1.20 (m, 48H, $H_{j\text{-}q}$), 1.32 (d, 3H, H_r, *J* = 6.5 Hz), 0.87 (m, 9H, H_s).

^{13}C RMN (75 MHz, $CDCl_3$) δ: 169.1, 166.9, 153.1, 140.9, 134.4, 131.9, 129.2, 123.6, 105.4, 76.7, 73.6, 69.2, 46.7, 42.9, 32.1, 30.5, 29.9, 29.8, 29.7, 29.6, 29.5, 26.3, 26.2, 22.8, 18.6, 14.3.

HRMS-MALDI-TOF m/z calcd. $C_{54}H_{88}N_2O_6$ [M] 860.6642, found $[M+H]^+$ 861.6689.

(*S*)-*N*-(1-aminopropan-2-yl)-3,4,5-tris(dodecyloxy)benzamide (13)



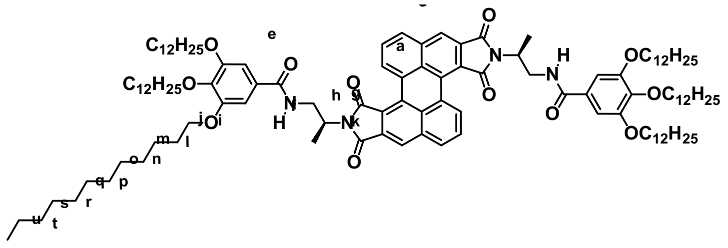
Compound **12** (1.01 g, 1.4 mmol, 1 eq.) was dissolved in THF (7 mL), and hydrazine monohydrate (1.35 mL, 27.8 mmol, 20 eq.) was added dropwise. Then the mixture was heated to reflux and stirred for 48 hours. The reaction was let to cooldown and washed with a 2M NaOH aqueous solution (60 mL) and extracted with CH_2Cl_2 (80 mL). Then, it was dried with $MgSO_4$, filtered and evaporated. Purification was performed by column chromatography (silica gel, CH_2Cl_2/EtOAc/MeOH 84/8/8) to obtain a white solid (0.74 g, yield: 86. %).

^{1}H NMR (300 MHz, $CDCl_3$) δ: 6.98 (s, 2H, H_a), 6.49 (d, 1H, H_b, *J* = 7.9 Hz), 4.16 (m, 1H, H_c), 4.02 - 3.93 (m, 6H, H_d), 2.82 (m, 2H, H_e), 1.85 - 1.62 (m, 6H, H_f), 1.53 - 1.39 (m, 6H, H_g), 1.38 - 1.24 (m, 48H, $H_{h\text{-}o}$), 1.22 (d, 3H, H_p, *J* = 6.8 Hz), 0.87 (m, 9H, H_q).

^{13}C NMR (75 MHz, $CDCl_3$) δ: 167.3, 153.2, 141.3, 129.8, 105.9, 73.6, 69.6, 47.4, 46.9, 32.1, 32.1, 30.5, 29.9, 29.9, 29.9, 29.8, 29.8, 29.7, 29.6, 29.5, 29.52, 26.2, 22.8, 18.4, 14.3.

HRMS-MALDI-TOF m/z calc. $C_{46}H_{87}N_2O_4$ $[M+H]^+$ 731.6666, found $[M+H]^+$ 731.6637.

N,N'-((*2S,2'S*)-(1,3,8,10-tetraoxo-1,3,8,10-tetrahydroanthra[9,1-ef:10,5-e'f']diisoindole-2,9-diyl)bis(propane-2,1-diyl))bis(3,4,5-tris(dodecyloxy)benzamide) (Z-PDI 1)

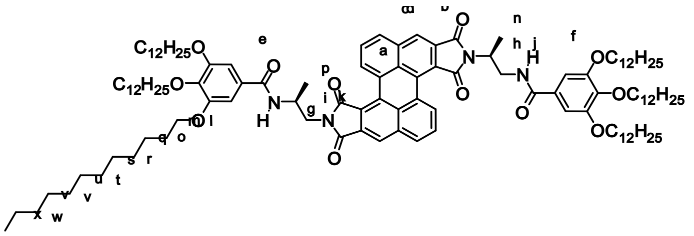


^{1}H NMR (300 MHz, $CDCl_3$) δ: 9.10 (dd, 2H, H_a, *J* = 7.7, 1.1 Hz), 8.28 (s, 2H, H_b), 8.07 (dd, 2H, H_c, *J* = 7.4, 1.1 Hz), 7.83 (t, 2H, H_d, *J* = 7.9Hz), 6.96 (s, 6H, $H_{e,f}$), 4.85 (m, 2H, H_g), 4.26 (m, 2H, H_h), 3.95 (m, 12H, H_i), 3.65 (m, 2H, $H_{h'}$), 1.78 - 1.65 (m, 12H, H_j), 1.60 (d, 6H, H_k, *J* = 7.1 Hz), 1.47 - 1.35 (m, 12H, H_l), 1.34 – 1.18 (m, 96H, $H_{m\text{-}t}$), 0.87 (m, 18H, H_u).

^{13}C NMR (75 MHz, $CDCl_3$) δ: 168.6, 167.9, 167.8, 153.2, 141.2, 134.8, 132.9, 132.7, 132.3, 130.2, 129.4, 129.0, 128.9, 128.6 , 124.2, 122.8, 121.9, 105.7, 73.6, 69.3, 60.5, 32.1, 31.7, 30.4, 29.9, 29.8, 29.7, 29.5, 29.5, 26.2, 22.8, 21.2, 15.8, 14.3, 14.3, 11.6.

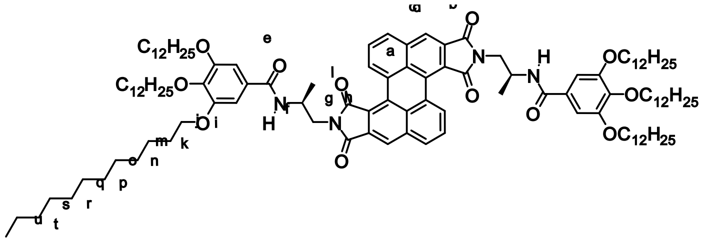
HRMS-MALDI-TOF m/z calc. $C_{116}H_{176}N_4O_{12}Na$ $[M+Na]^+$ 1840.3182, found $[M+Na]^+$ 1840.3185.

3,4,5-tris(dodecyloxy)-*N*-((*S*)-1-(1,3,8,10-tetraoxo-9-((*S*)-1-(3,4,5-tris(dodecyloxy)benzamido)propan-2-yl)-3,8,9,10-tetrahydroanthra[9,1-ef:10,5-e'f']diisoindol-2(1H)-yl)propan-2-yl)benzamide (Z-PDI 2)



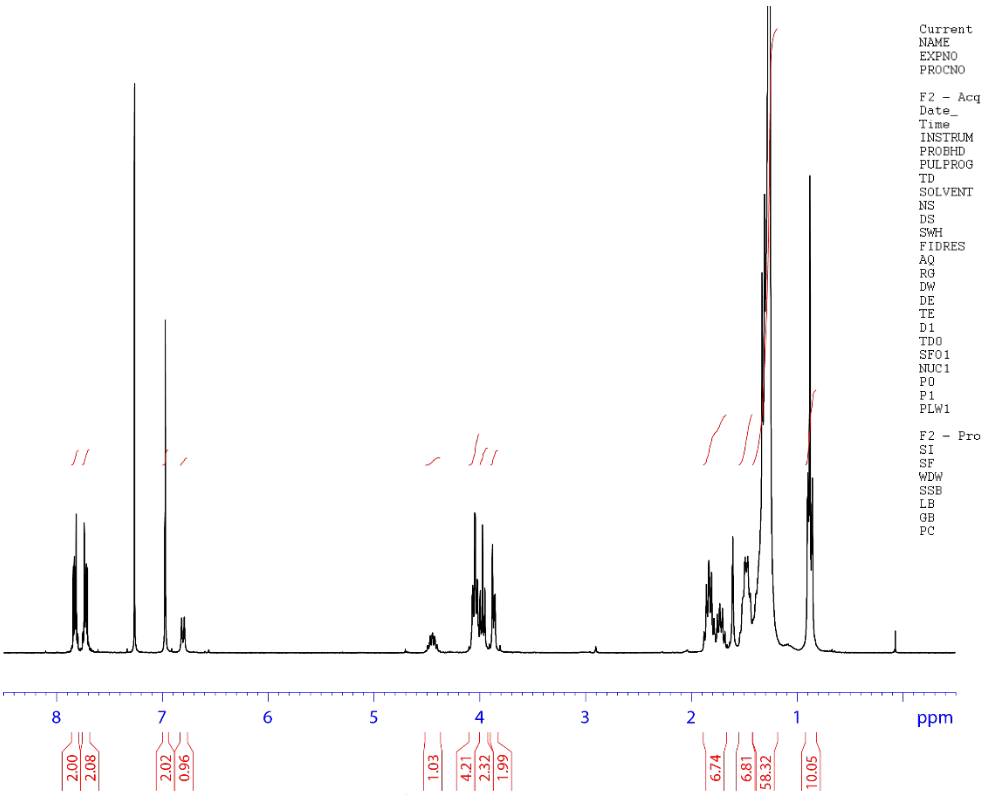
^{1}H NMR (300 MHz, CDCl$_3$) δ: 9.11 (d, 1H, H$_a$, *J* = 7.6 Hz), 9.02 (d, 1H, H$_{a'}$, *J* = 7.6 Hz), 8.29 (s, 1H, H$_b$), 8.28 (s, 1H, H$_{b'}$), 8.07 (d, 2H, H$_c$, *J* = 8.1 Hz), 7.79 (m, 2H, H$_d$), 6.98 (s, 1H, H$_e$), 6.95 (s, 1H, H$_{e'}$), 6.91 (m, 1H, H$_f$), 6.79 (d, 1H, H$_g$, *J* = 7.9 Hz), 4.85 (m, 1H, H$_h$), 4.60 (m, 1H, H$_i$), 4.28 (m, 1H, H$_j$), 3.93 (m, 14H, H$_{k\text{-}l}$), 3.64 (m, 1H, H$_{j'}$), 1.72 (m, 12H, H$_m$), 1.61 (d, 3H, H$_n$, *J* = 7.2 Hz), 1.50 - 1.36 (m, 12H, H$_o$), 1.39 (d, 3H, H$_p$, *J* = 6.7 Hz), 1.35 – 1.13 (m, 96H, H$_{q\text{-}w}$), 0.87 (m, 18H, H$_x$).
^{13}C NMR (175 MHz, CDCl$_3$) δ: 168.7, 168.6, 168.0, 167.9, 167.8, 167.1, 153.1, 141.0, 140.9, 134.8, 133.9, 133.8 133.2, 132.9, 132.7, 132.4, 130.2, 130.1, 129.3, 129.2, 129.1, 129.0, 128.6, 128.5, 124.4, 124.2, 122.9, 105.6, 105.4, 73.6, 69.2, 69.2, 47.7, 46.5, 43.5, 33.8, 32.1, 30.5, 30.4, 30.3, 29.9, 29.9, 29.8, 29.7, 29.6, 29.6, 29.5, 29.5, 29.5, 29.4, 26.8, 26.3, 26.2, 26.2, 23.3, 22.8, 18.8, 15.9, 14.3, 14.3.
HRMS-MALDI-TOF m/z calc. C$_{116}$H$_{176}$N$_4$O$_{12}$Na [M+Na]$^+$ 1840.3182, found [M+Na]$^+$ 1840.3182.

***N*,*N'*-((*2S*,*2'S*)-(1,3,8,10-tetraoxo-1,3,8,10-tetrahydroanthra[9,1-ef:10,5-e'f']diisoindole-2,9-diyl)bis(propane-1,2-diyl))bis(3,4,5-tris(dodecyloxy)benzamide) (Z-PDI 3)**



^{1}H NMR (300 MHz, CDCl$_3$) δ: 9.03 (dd, 2H, H$_a$, *J* = 7.7, 1.1 Hz), 8.28 (s, 2H, H$_b$), 8.06 (d, 2H, H$_c$, *J* = 7.8 Hz), 7.76 (t, 2H, H$_d$, *J* = 7.9 Hz), 6.97 (s, 2H, H$_e$), 6.79 (d, 2H, H$_f$, *J* = 7.7 Hz), 4.60 (m, 2H, H$_g$), 3.96 (m, 16H, H$_{g,i}$), 1.74 (m, 12H, H$_j$), 1.50 – 1.36 (m, 12H, H$_k$), 1.38 (d, 6H, H$_l$, *J* = 6.6 Hz), 1.35 - 1.19 (m, 96H, H$_{m\text{-}t}$), 0.87 (m, 18H, H$_u$).
^{13}C NMR (175 MHz, CDCl$_3$) δ: 168.8, 168.0, 167.1, 153.1, 140.9, 134.8, 133.8, 133.2, 132.7, 132.4, 130.1, 129.2, 129.1, 128.6, 124.4, 122.9, 105.4, 73.6, 69.2, 46.5, 43.6, 37.5, 37.2, 33.8, 33.5, 32.9, 32.1, 31.8, 31.6, 30.4, 30.3, 30.2, 29.9, 29.9, 29.8, 29.7, 29.6, 29.5, 29.5, 29.4, 29.1, 28.1, 27.2, 26.9, 26.3, 26.2, 25.0, 23.6, 23.3, 22.8, 22.6, 19.9, 18.8, 14.3, 14.3, 14.2, 11.6, 11.0, 7.7.
HRMS-MALDI-TOF m/z calc. C$_{116}$H$_{176}$N$_4$O$_{12}$Na [M+Na]$^+$ 1840.3182, found [M+Na]$^+$ 1840.3068.

NMR spectra



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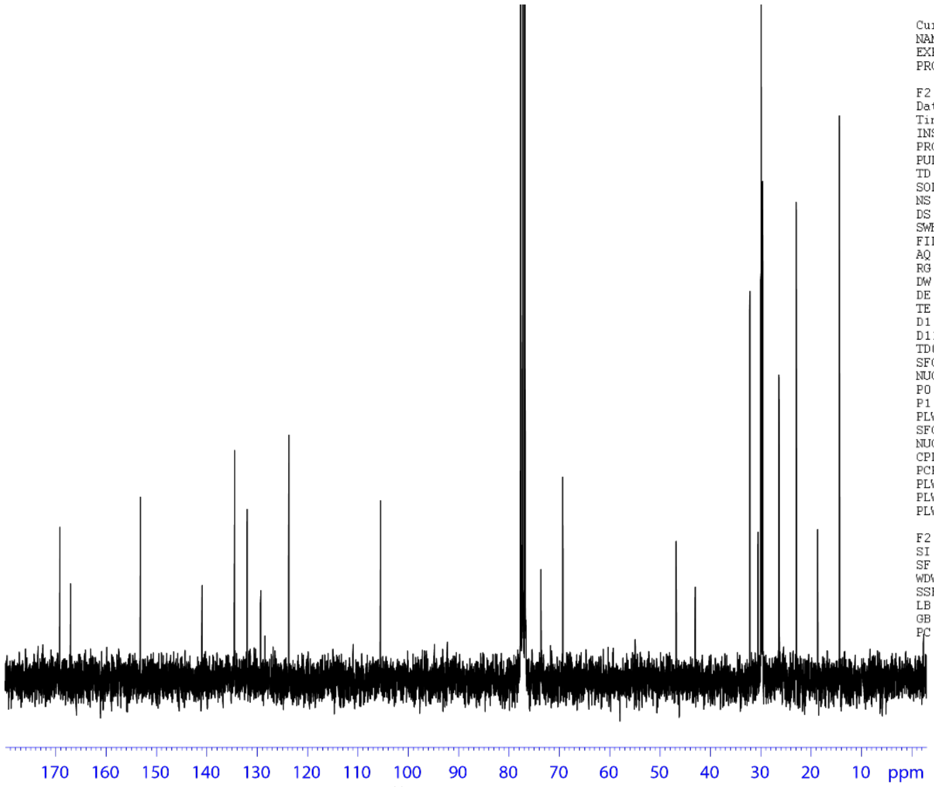
^{1}H-NMR (300 MHz, $CDCl_3$) of compound **12**.



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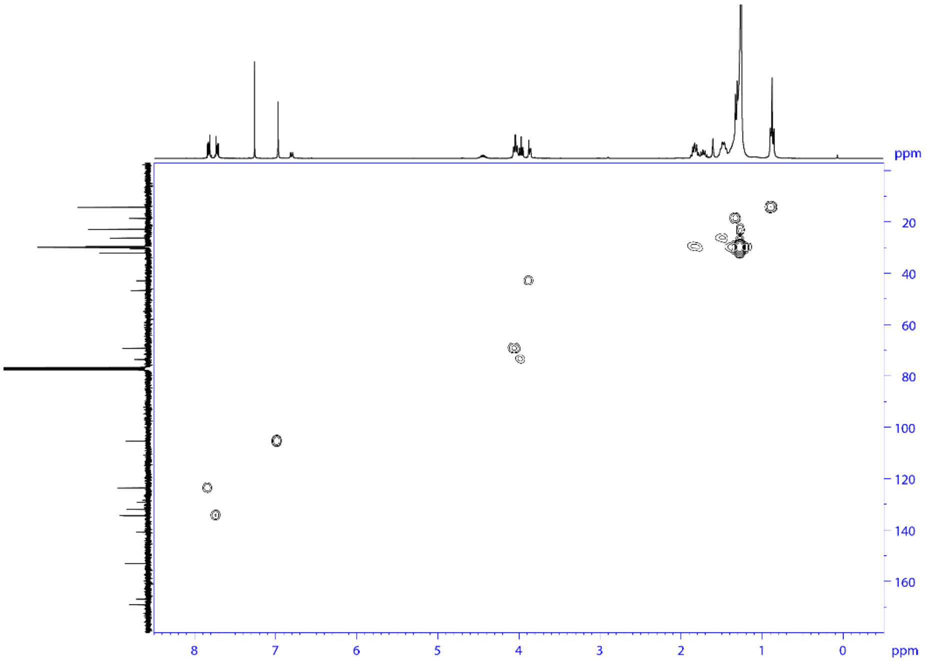
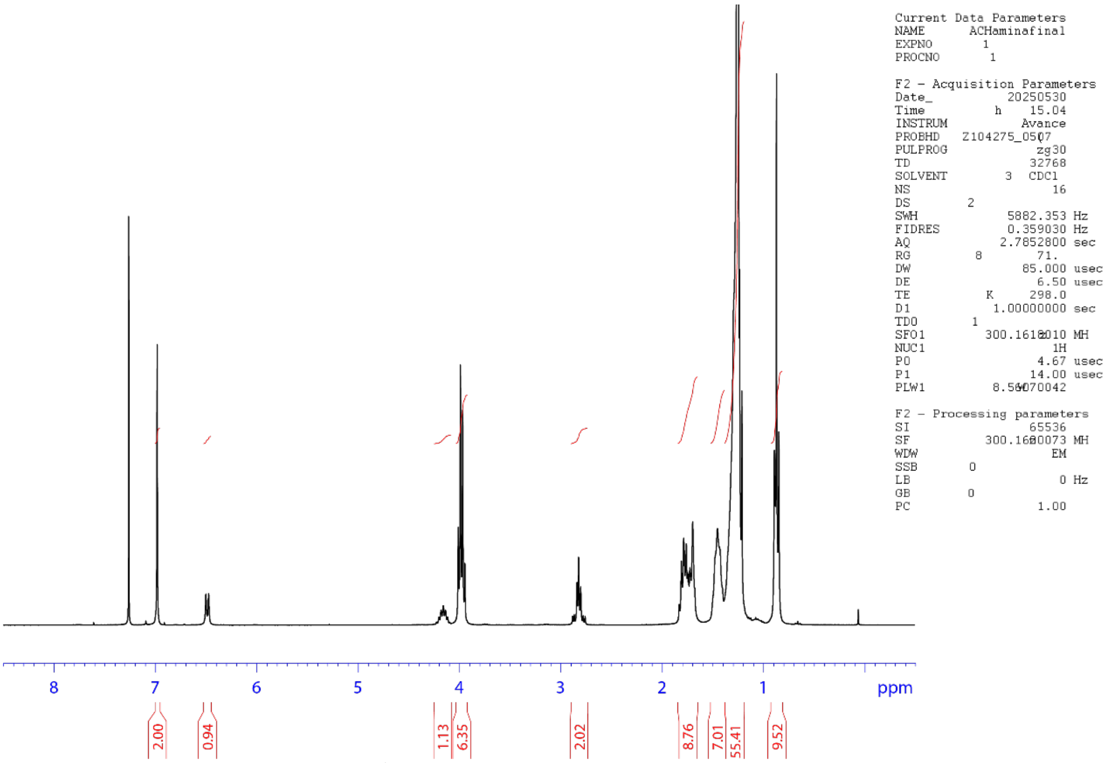
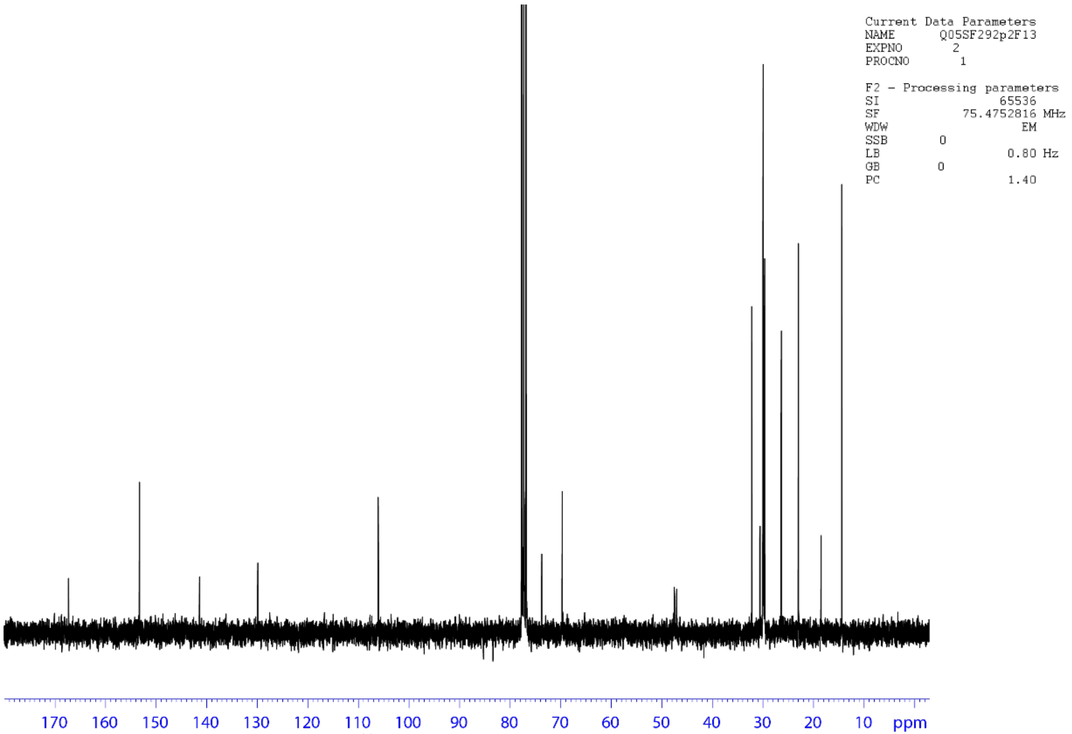
^{13}C-NMR (300 MHz, $CDCl_3$) of compound **12**.



^{1}H, ^{13}C-HMQC (300 MHz, CDCl$_3$) of compound **12**.



^{1}H-NMR (300 MHz, CDCl$_3$) of compound **13**.



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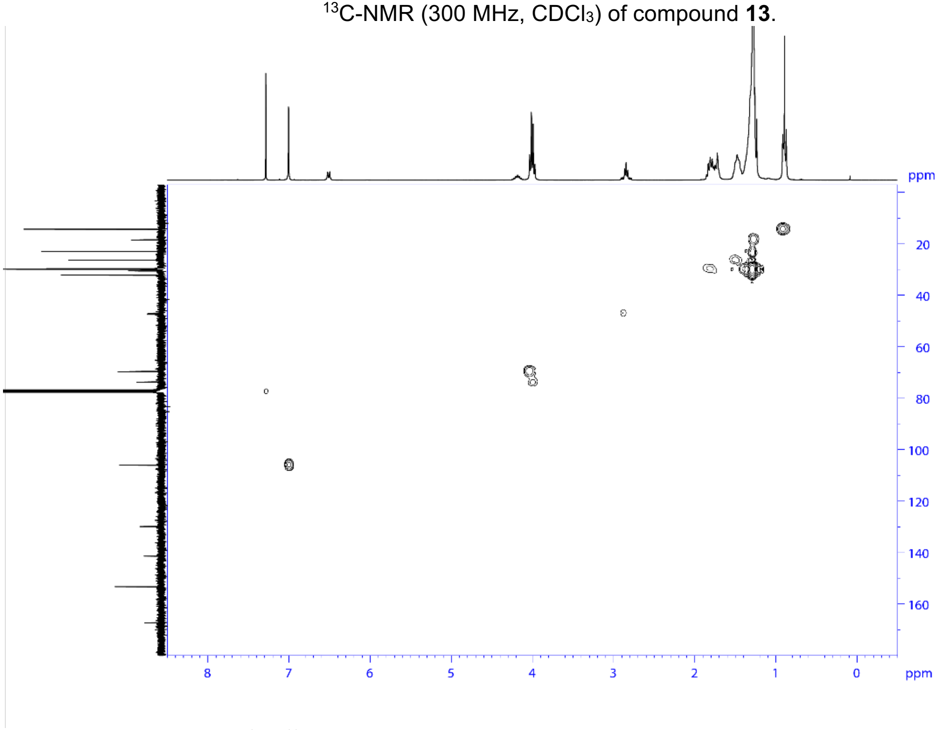
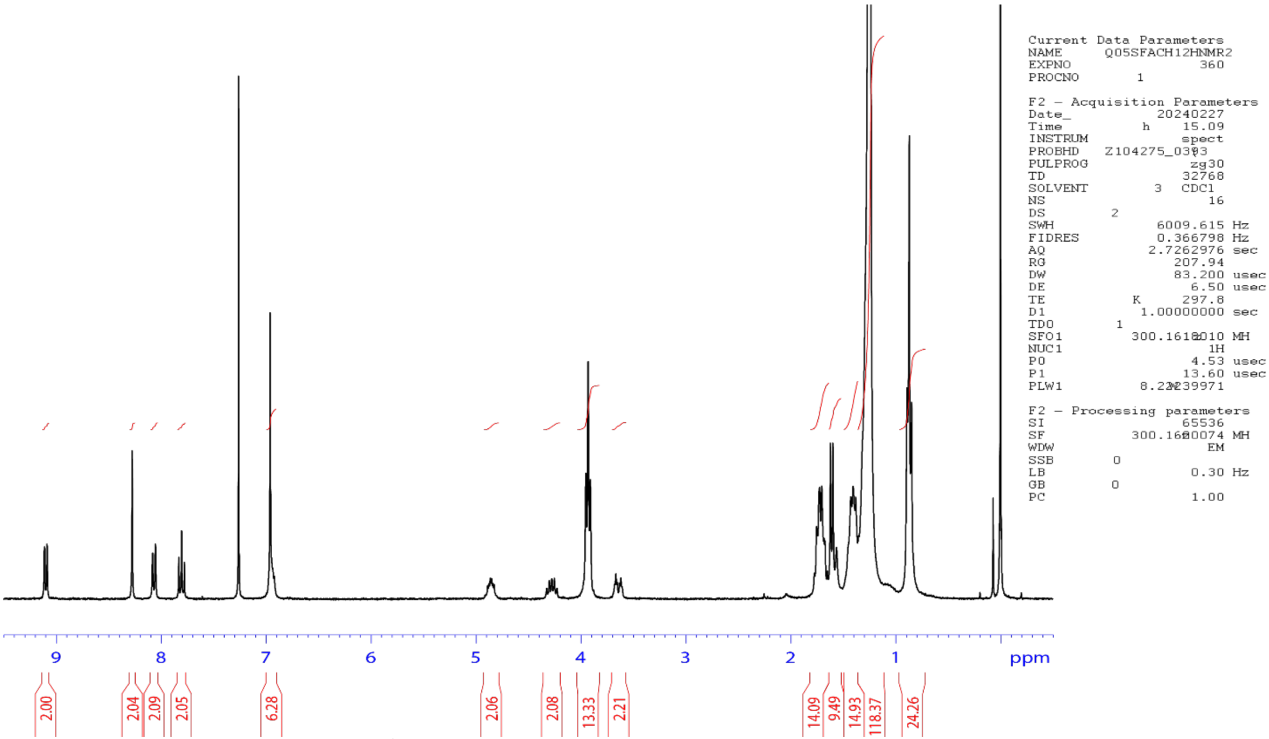
^{13}C-NMR (300 MHz, CDCl$_3$) of compound **13**.



^{1}H, ^{13}C-HMQC (300 MHz, CDCl$_3$) of compound **13**.



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FIDRES             0.366798 Hz
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RG                   207.94
DW                   83.200 usec
DE                     6.50 usec
TE              K     297.8
D1               1.00000000 sec
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P0                     4.53 usec
P1                    13.60 usec
PLW1             8.22239971

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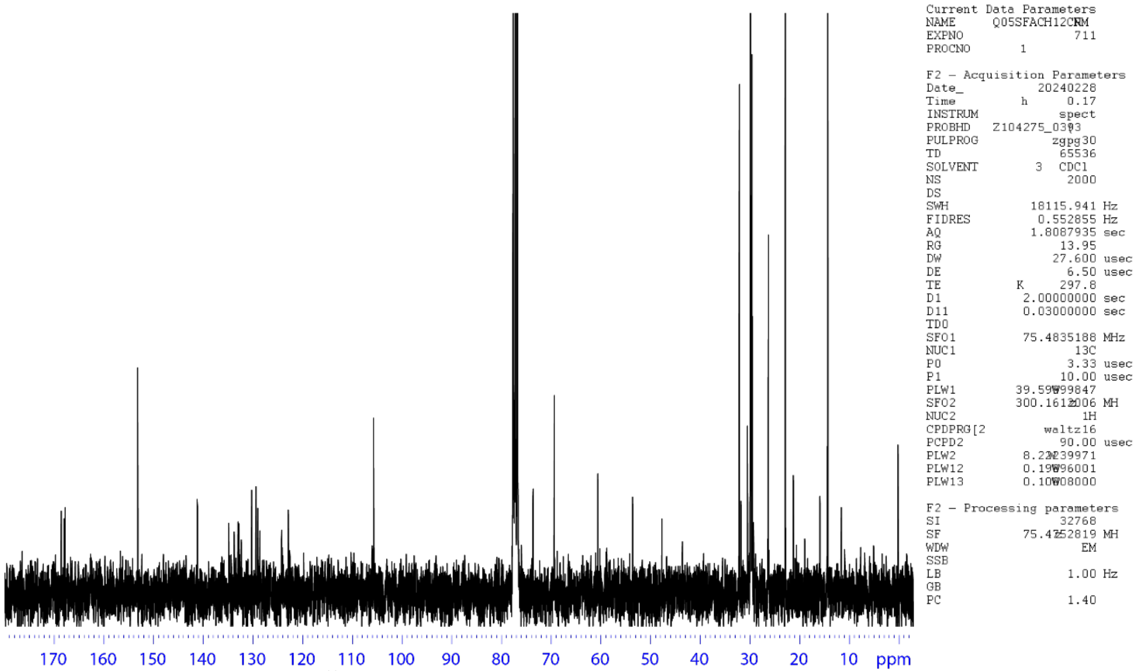
^{1}H-NMR (300 MHz, $CDCl_3$) of compound **Z-PDI 1**.



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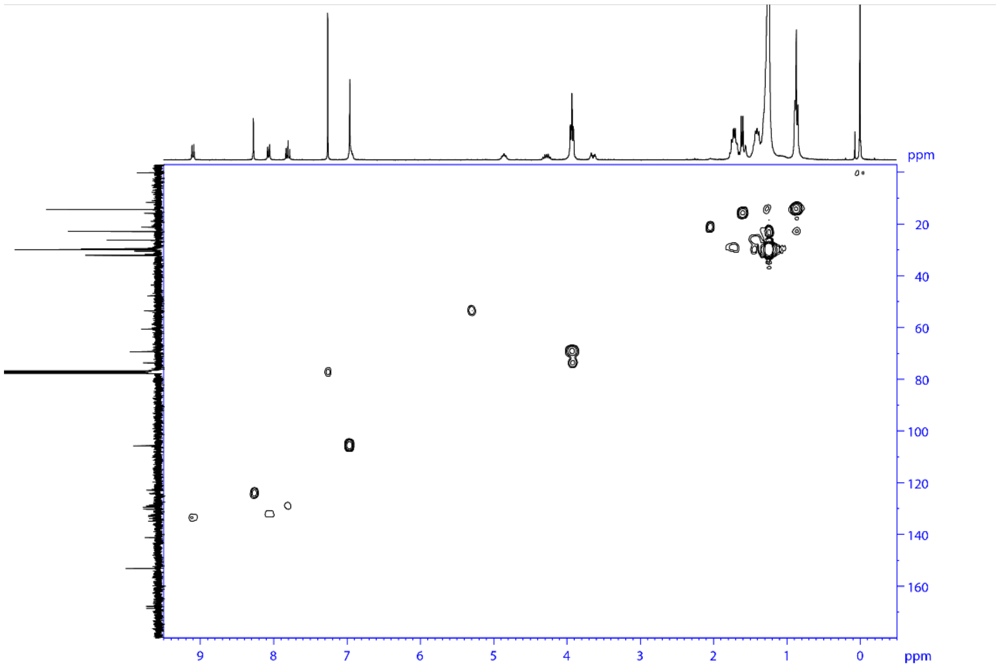
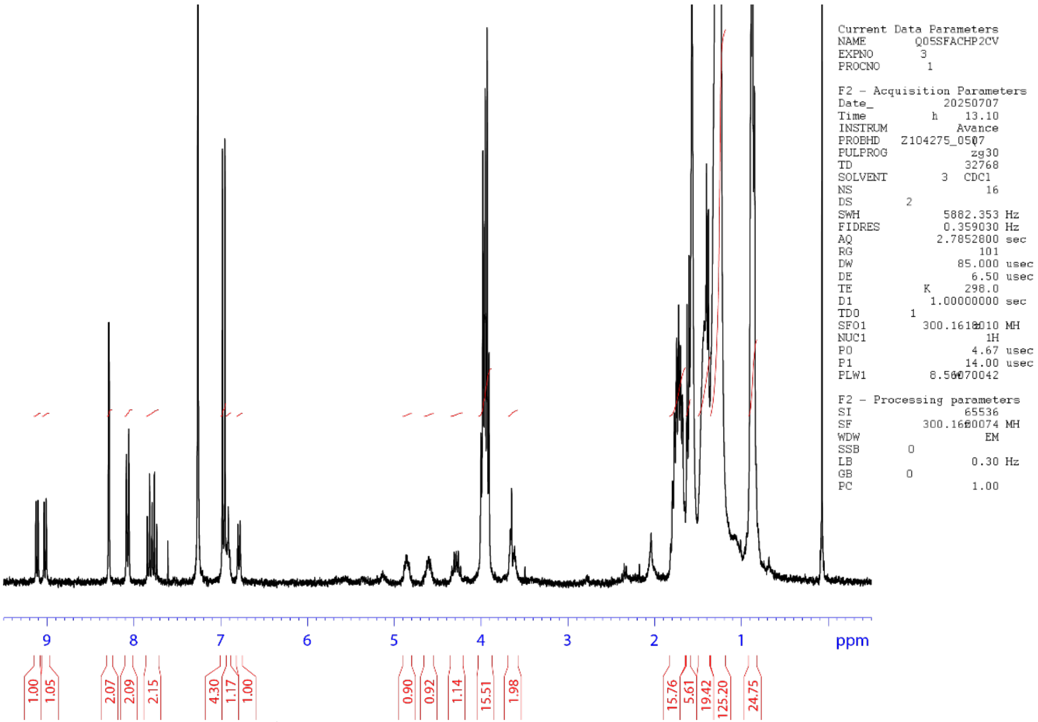
^{13}C-NMR (75 MHz, $CDCl_3$) of compound **Z-PDI 1**.



^1H, ^{13}C-HMQC (300 MHz, $CDCl_3$) of compound **Z-PDI 1**.



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TD                    32768
SOLVENT          3   CDCl
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FIDRES           0.359030 Hz
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RG                      101
DW                   85.000 usec
DE                     6.50 usec
TE             K      298.0
D1             1.00000000 sec
TD0           1
SFO1         300.1618010 MH
NUC1                     1H
P0                     4.67 usec
P1                    14.00 usec
PLW1           8.50070042

F2 - Processing parameters
SI                    65536
SF           300.1600074 MH
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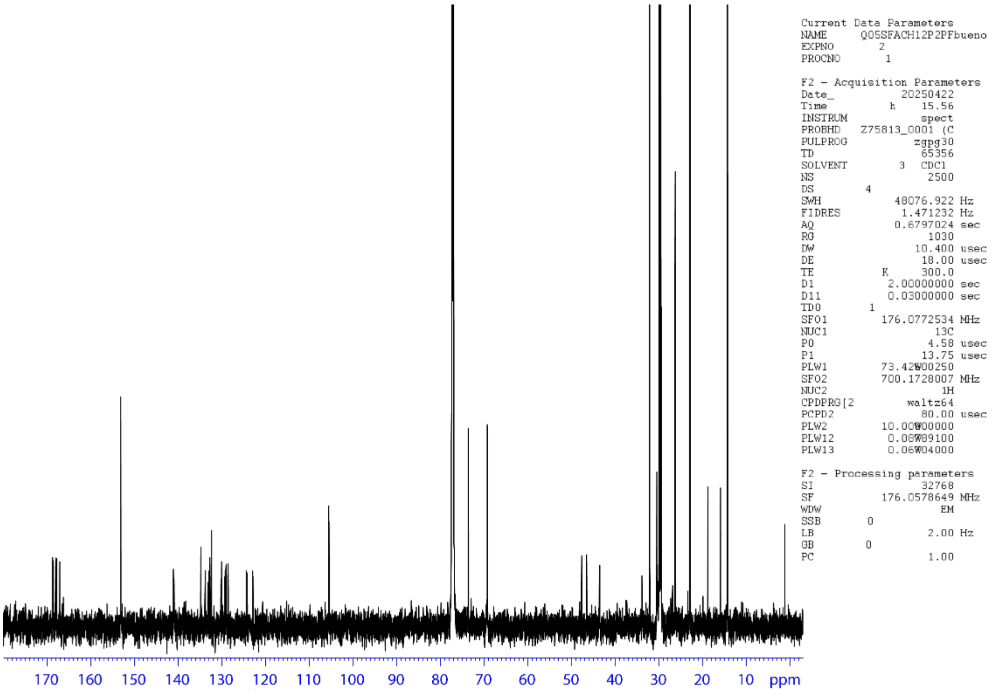
^1H-NMR (300 MHz, $CDCl_3$) of compound **Z-PDI 2**.



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PULPROG             zgpg30
TD                   65356
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DS          4
SWH             48076.922 Hz
FIDRES           1.471232 Hz
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DE                   18.00 usec
TE              K    300.0
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TD0          1
SFO1           176.0772534 MHz
NUC1                   13C
P0                    4.58 usec
P1                   13.75 usec
PLW1           73.42W00250
SFO2           700.1728007 MHz
NUC2                    1H
CPDPRG[2           waltz64
PCPD2                80.00 usec
PLW2           10.00W00000
PLW12           0.08W89100
PLW13           0.06W04000

F2 - Processing parameters
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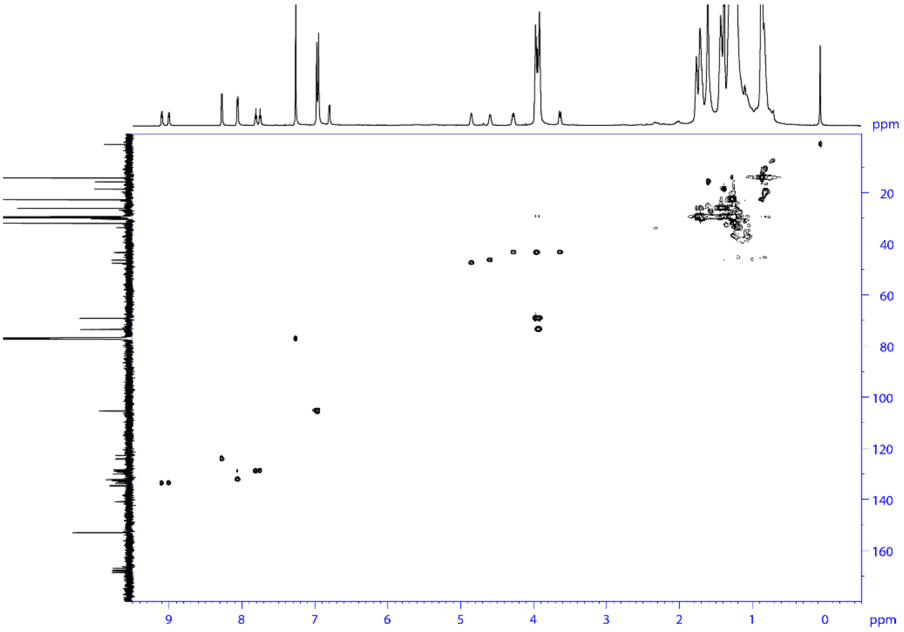
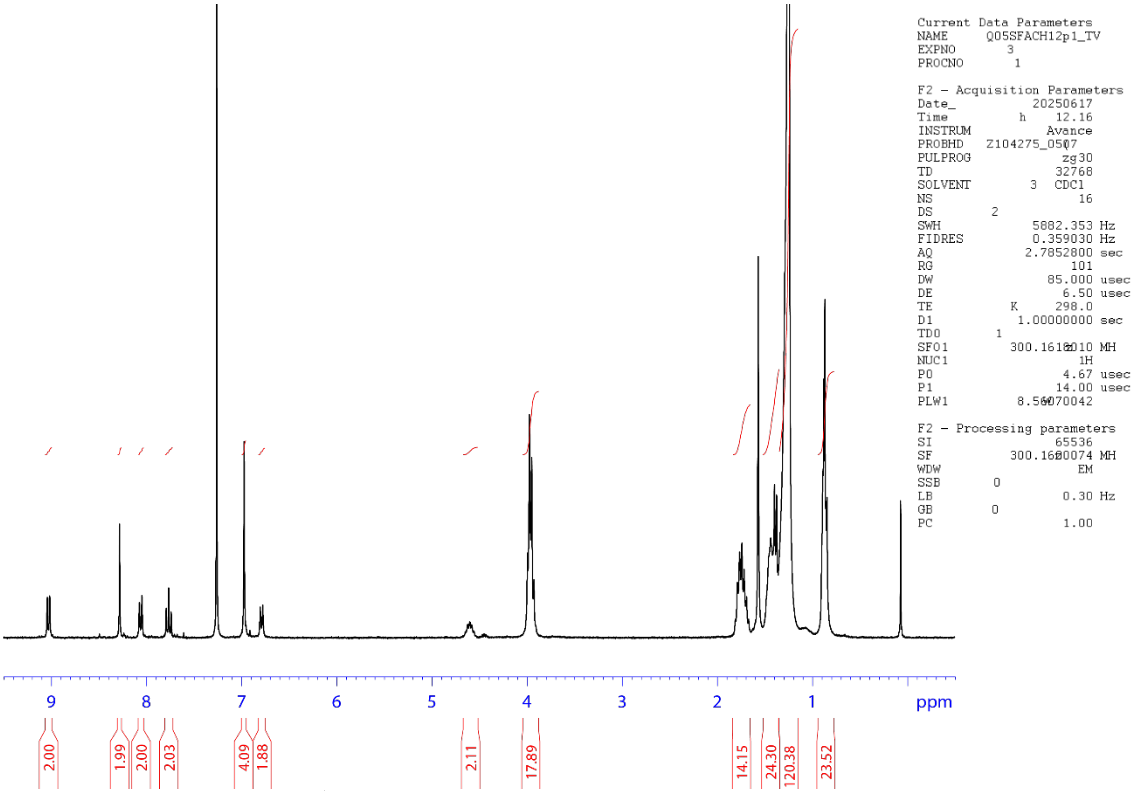
^{13}C-NMR (175 MHz, CDCl$_3$) of compound **Z-PDI 2**.



^{1}H, ^{13}C-HMQC (700 MHz, CDCl$_3$) of compound **Z-PDI 2**.



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PROCNO         1

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PULPROG              zg30
TD                  32768
SOLVENT        3   CDCl
NS                     16
DS           2
SWH              5882.353 Hz
FIDRES           0.359030 Hz
AQ              2.7852800 sec
RG                    101
DW                 85.000 usec
DE                   6.50 usec
TE              K   298.0
D1             1.00000000 sec
TD0           1
SFO1          300.1618010 MH
NUC1                   1H
P0                   4.67 usec
P1                  14.00 usec
PLW1           8.56070042

F2 - Processing parameters
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WDW                    EM
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LB                   0.30 Hz
GB            0
PC                   1.00
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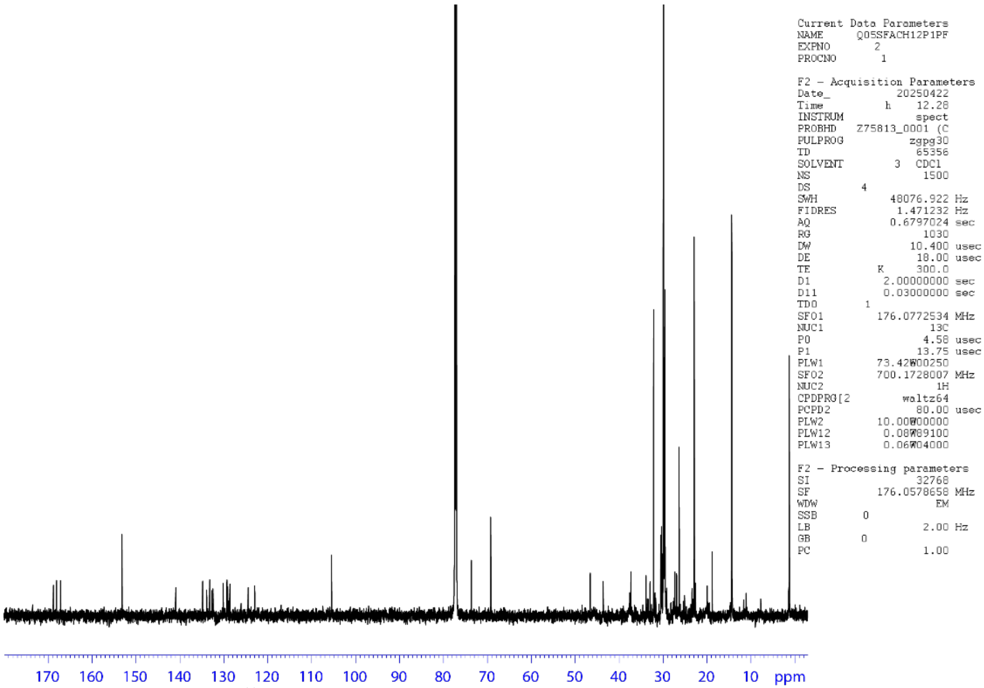
^{1}H-NMR (300 MHz, $CDCl_3$) of compound **Z-PDI 3**.



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PROCNO         1

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PULPROG            zgpg30
TD                  65356
SOLVENT        3   CDCl
NS                   1500
DS           4
SWH             48076.922 Hz
FIDRES           1.471232 Hz
AQ              0.6797024 sec
RG                   1030
DW                 10.400 usec
DE                  18.00 usec
TE              K   300.0
D1             2.00000000 sec
D11            0.03000000 sec
TD0           1
SFO1          176.0772534 MHz
NUC1                  13C
P0                   4.58 usec
P1                  13.75 usec
PLW1          73.42000250
SFO2          700.1728007 MHz
NUC2                   1H
CPDPRG[2          waltz64
PCPD2               80.00 usec
PLW2          10.00000000
PLW12          0.08789100
PLW13          0.06704000

F2 - Processing parameters
SI                  32768
SF            176.0578658 MHz
WDW                    EM
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GB            0
PC                   1.00
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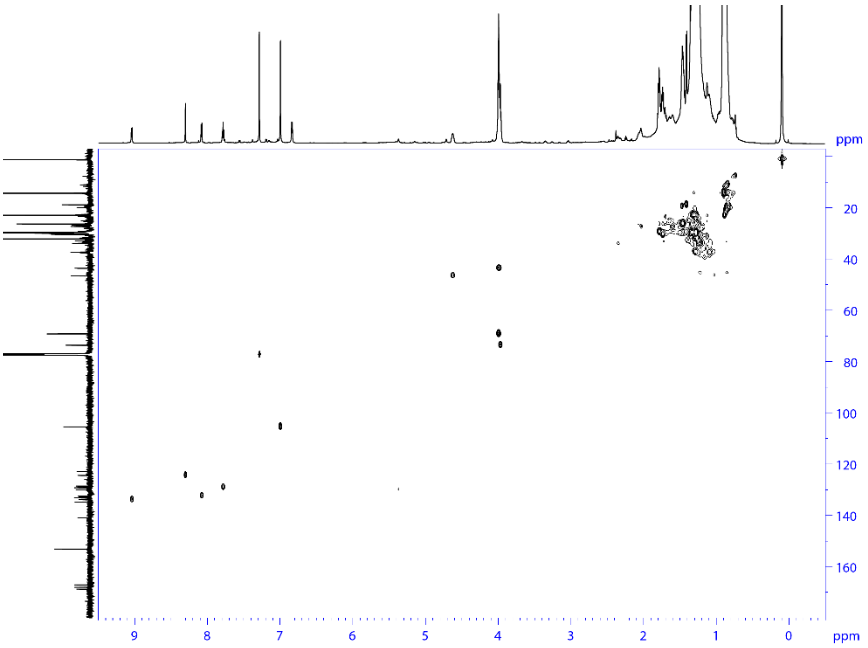
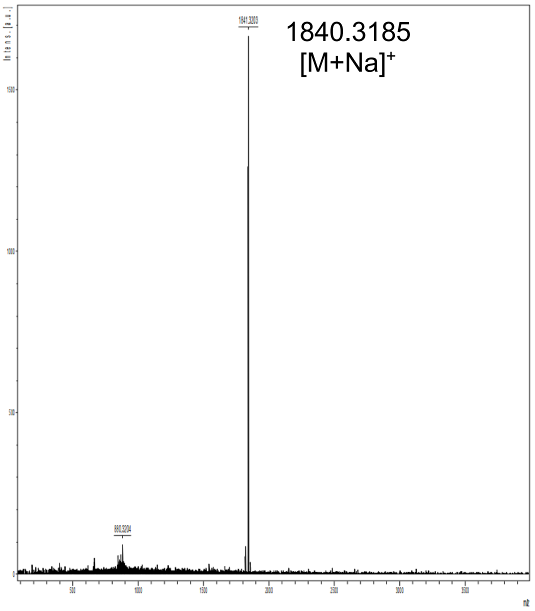
^{13}C-NMR (175 MHz, $CDCl_3$) of compound **Z-PDI 3**.

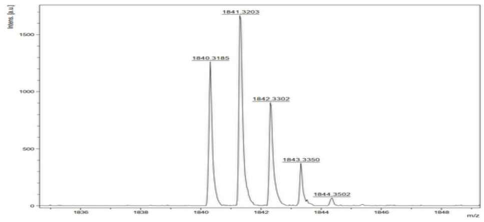


^{1}H, ^{13}C-HMQC (700 MHz, $CDCl_3$) of compound **Z-PDI 3**.

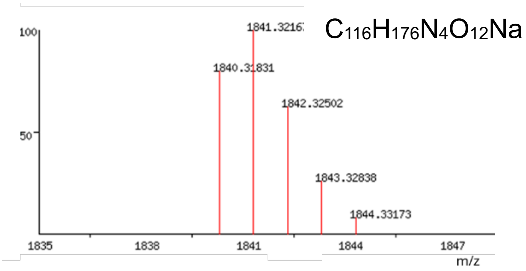
Mass spectra



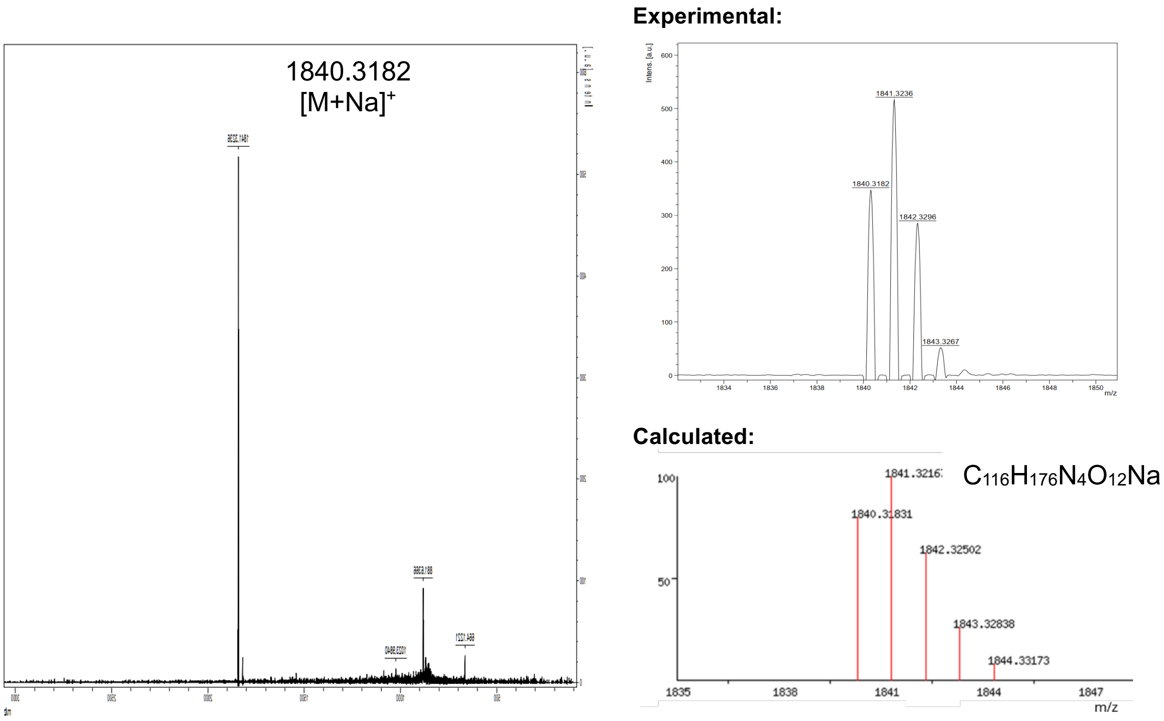
Experimental:



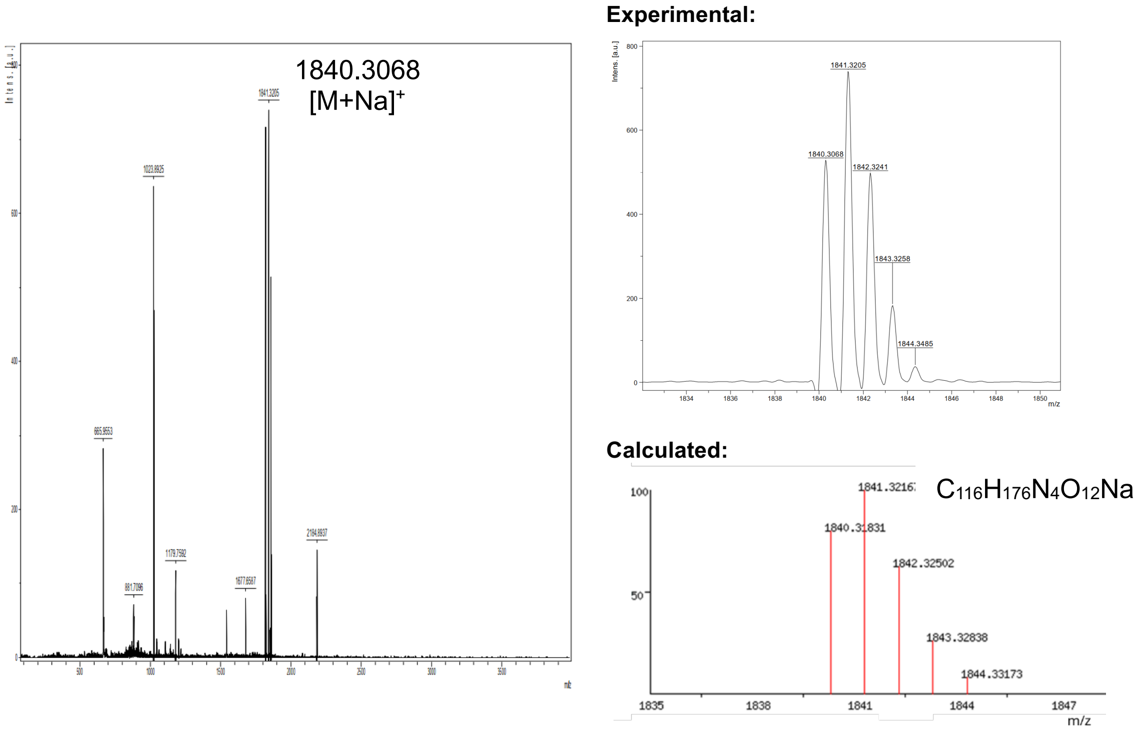
Calculated:



HRMS MALDI-TOF spectrum of PDI **1** (left). At the upright part a zoom of the peak showing the isotopic distribution together with the calculated one (bottom).



HRMS MALDI-TOF spectrum of PDI **2** (left). At the upright part a zoom of the peak showing the isotopic distribution together with the calculated one (bottom).



HRMS MALDI-TOF spectrum of PDI **3** (left). At the upright part a zoom of the peak showing the isotopic distribution together with the calculated one (bottom).

2. Supplementary Figures

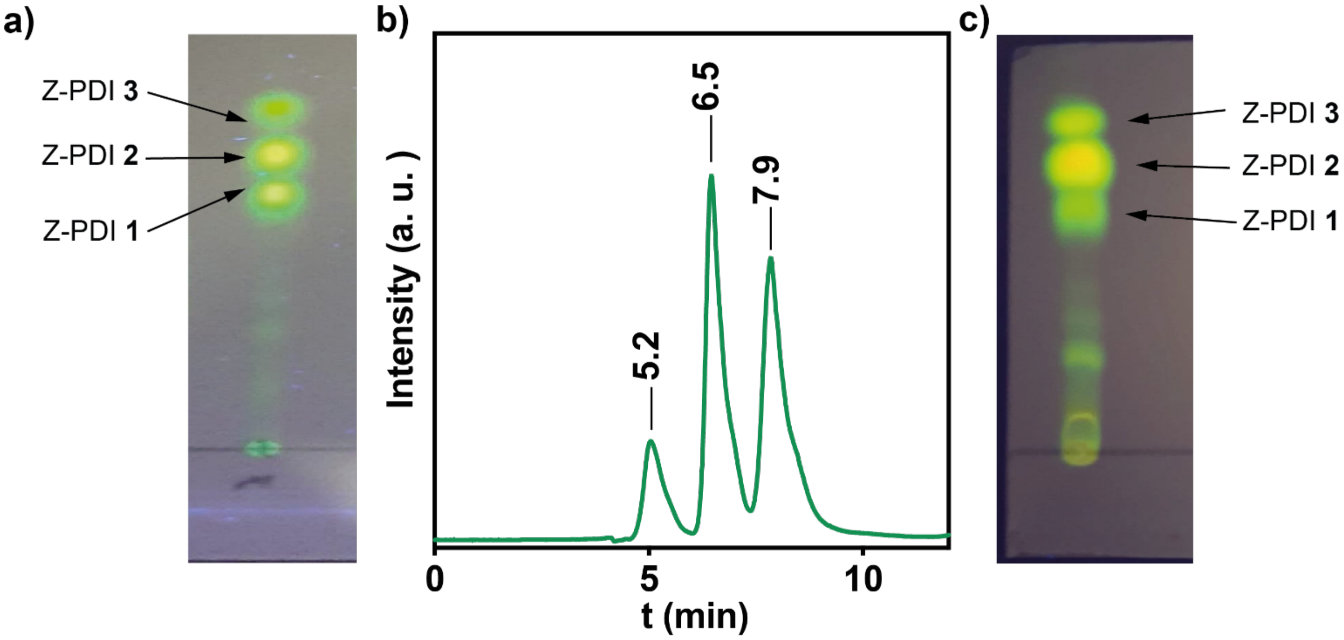


Figure S1. (a) TLC of the reaction mixture obtained by reacting benzamide **9** with dianhydride **10** in the presence of imidazole and $Zn(AcO)_2$ under microwave irradiation at 165 ºC ($CHCl_3$/Hexane/Et_2O 65/25/10). (b) HPLC traces of the three, more apolar greenish spots observed in the TLC shown in panel on a Chiralpack IA column (eluent: toluene/iPrOH 97/3; flow rate: 1 mL/min). (c) TLC of the reaction mixture obtained by reacting benzamide **13** with dianhydride **10** in the presence of imidazole and $Zn(AcO)_2$ under microwave irradiation at 165 ºC ($CHCl_3$/hexane/Et_2O 65/25/10).

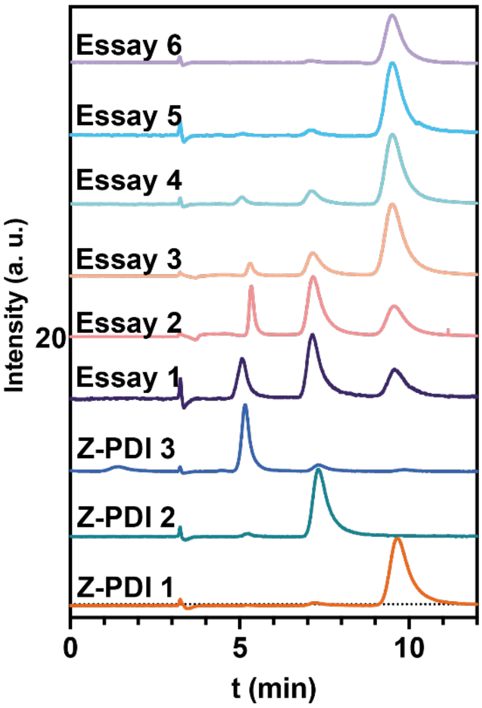


Figure S2. HPLC traces of the isolated Z-PDIs **1-3** and those obtained upon the different reaction conditions collected in Table 1 a ChiralPack IA chiral column (toluene/iPrOH 98/2 as eluent; flow rate 1 mL/min).

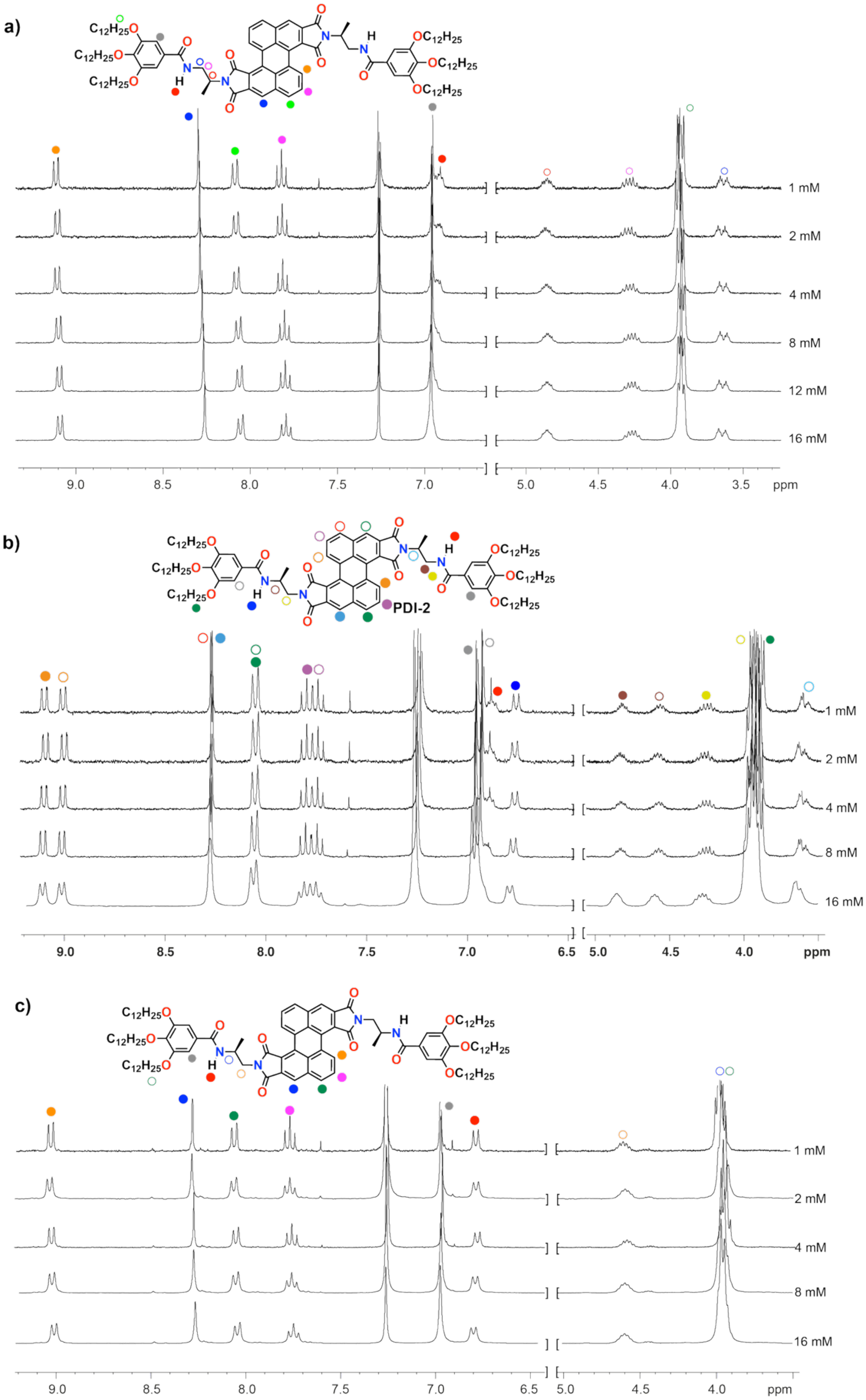


Figure S3. Partial ^{1}H-NMR spectra of Z-PDIs **1-3** recorded at different concentrations showing the aromatic and some of the aliphatic protons ($CDCl_3$, 300 MHz, 298 K). The upper part of the panels displays the chemical structure of the Z-PDIs highlighting the aromatic and the amide protons.

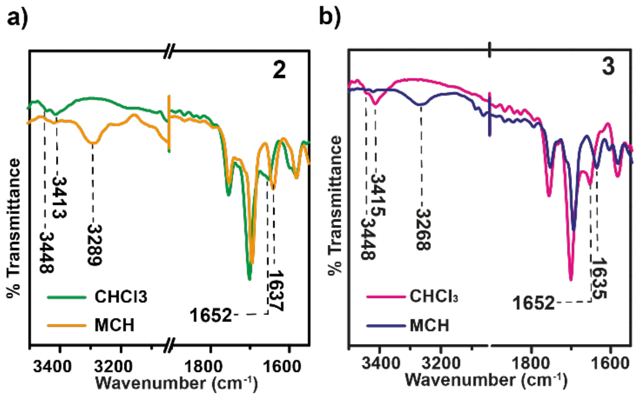


Figure S4. FTIR spectra of Z-PDIs **2** (a) and **3** (b) in CHCl$_3$ and MCH at c_T = 1 mM.

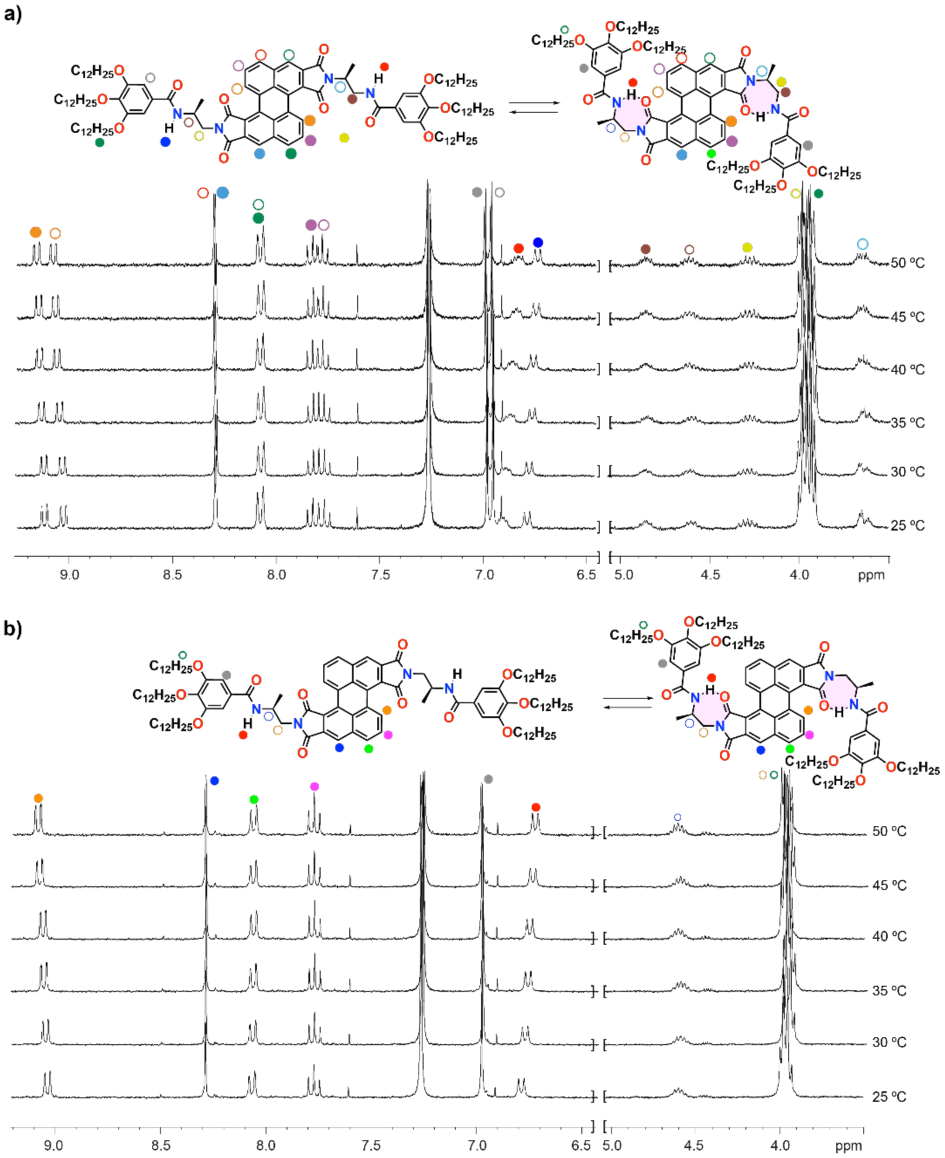


Figure S5. Partial ^{1}H-NMR spectra of Z-PDIs **2** (a) and **3** (b) recorded at different temperatures showing the aromatic and some of the aliphatic protons (CDCl$_3$, 300 MHz, c_T = 1mM). The upper part of the panels displays the chemical structure of the Z-PDIs highlighting the aromatic and the amide protons for both the free and intramolecularly H-bonded species.

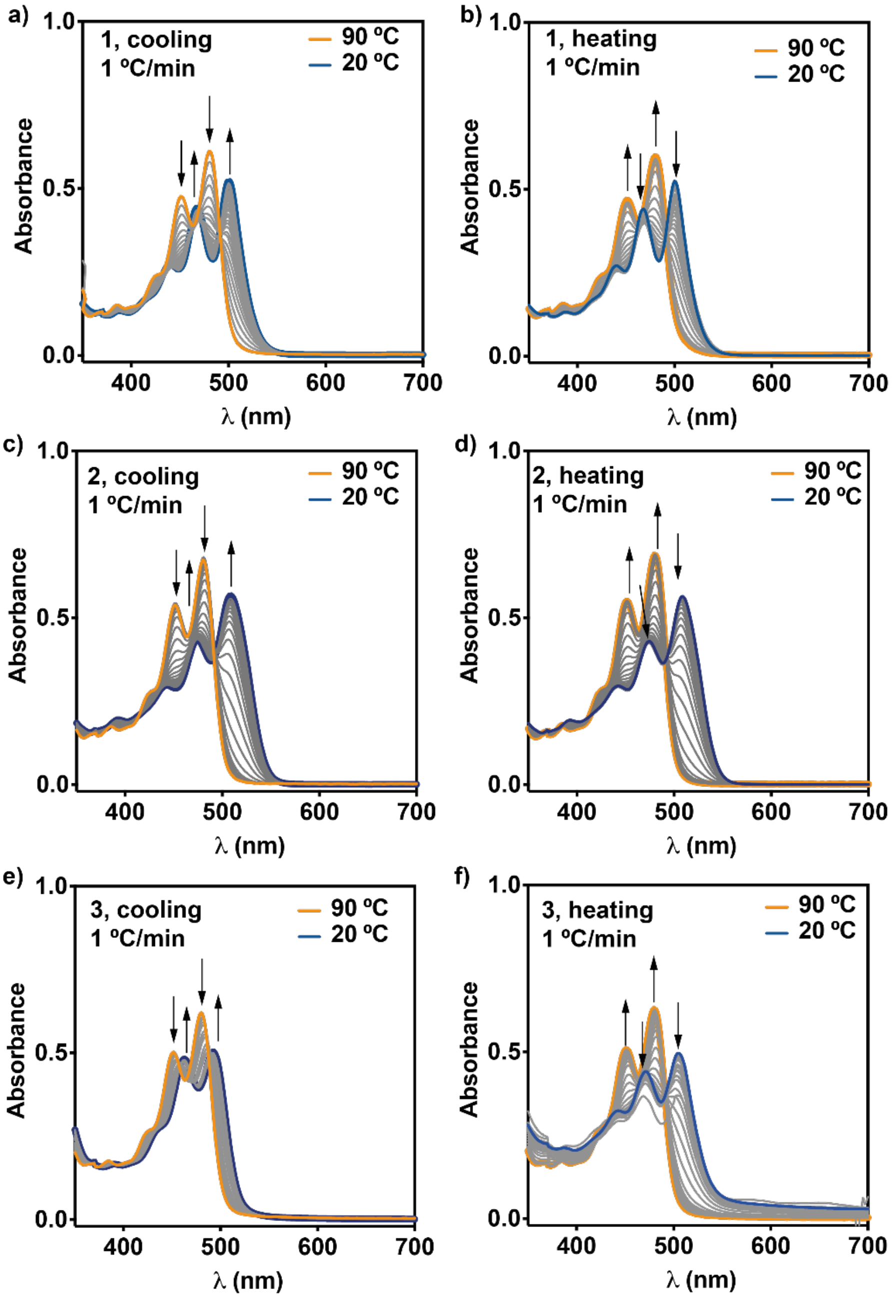


Figure S6. UV-Vis spectra of Z-PDIs **1-3** at different temperatures (c_T = 40 μM, MCH). Arrows indicate the changes observed upon decreasing (a, c, e) or increasing (b, d, f) the temperature.

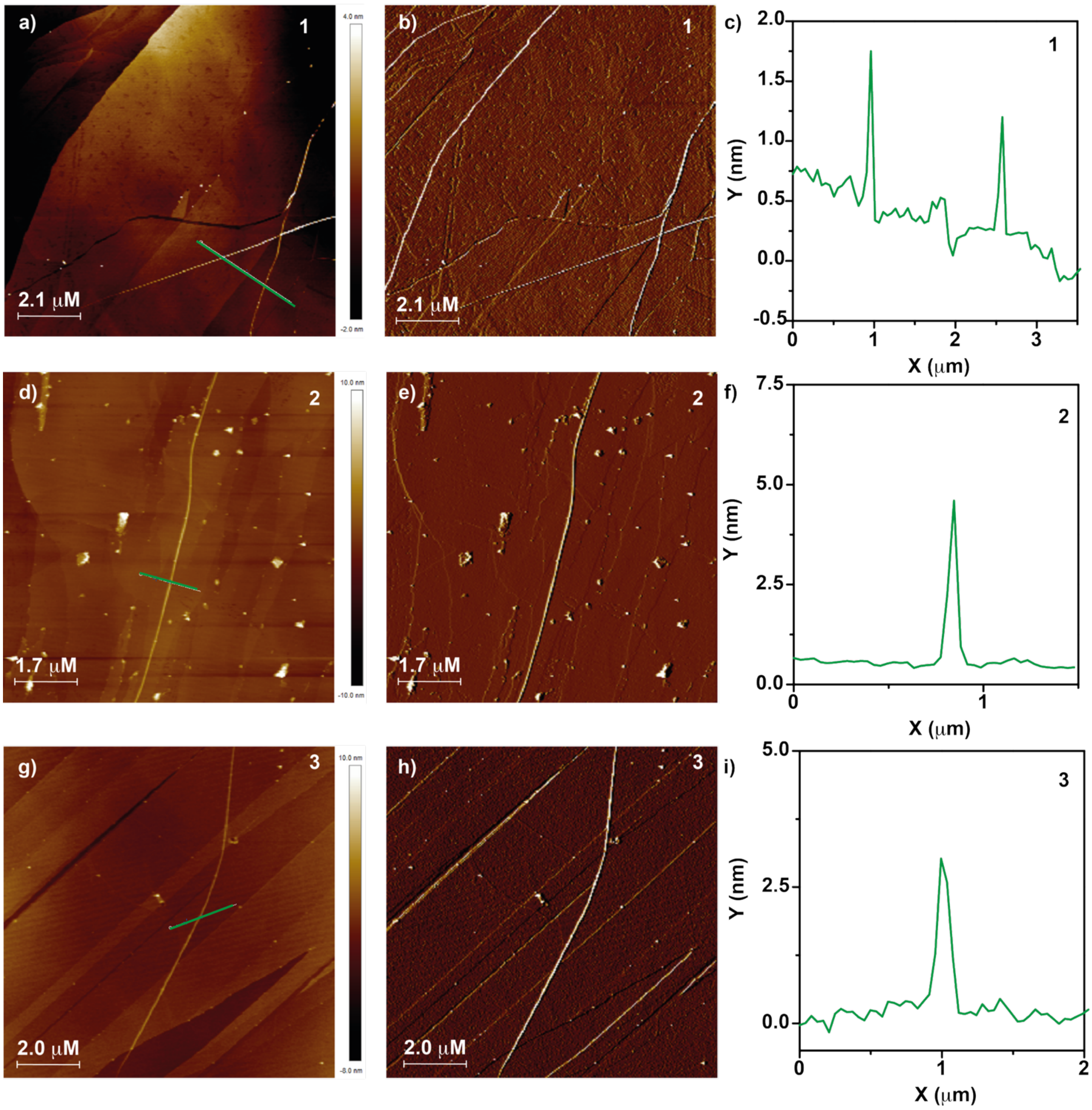


Figure S7. Height (a, d, g) and phase (b, e, h) AFM images of Z-PDIs **1-3**. Panels (c, f, i) show the height profile of the fibrillar structures of Z-PDIs **1-3** along the green line in panels (a, d, g). Experimental conditions: HOPG as surface, c_T = 40 μM; MCH.

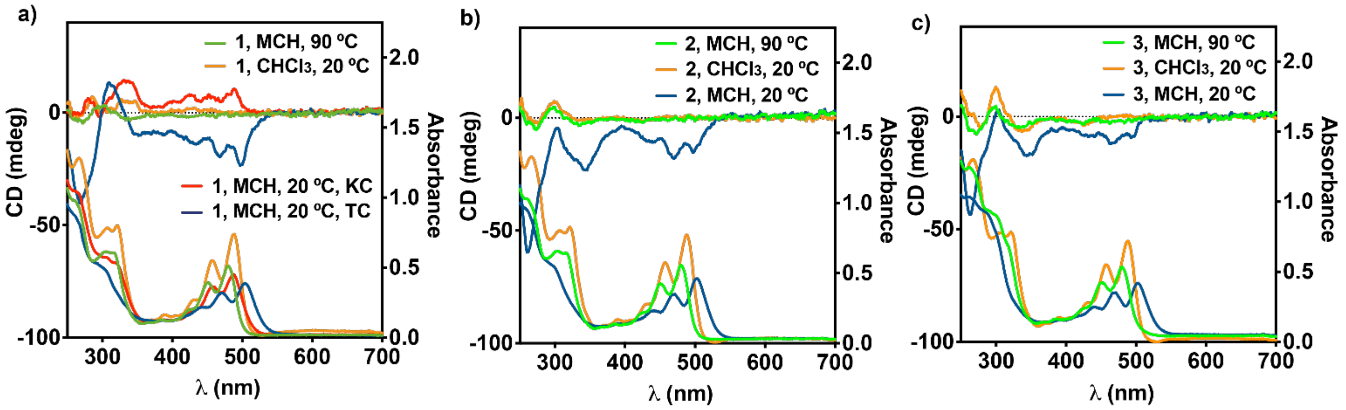


Figure S8. UV-Vis and CD spectra of Z-PDIs **1-3** in different solvents and temperatures (c_T = 40 μM, MCH).

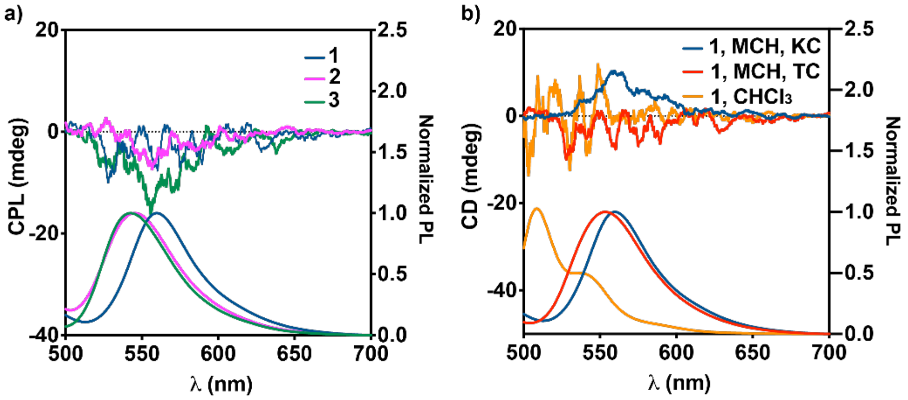


Figure S9. (a) Emission and CPL spectra of Z-PDIs **1-3** in MCH; (b) Emission and CPL spectra of the kinetically (KC) and thermodynamically (TC) controlled aggregates of Z-PDI **1** in MCH and the monomeric species of **1** ($CHCl_3$) (c_T = 40 μM; $\lambda_{exc}(CHCl_3)$ = 457 nm; λ_{exc}(MCH) = 471 nm)

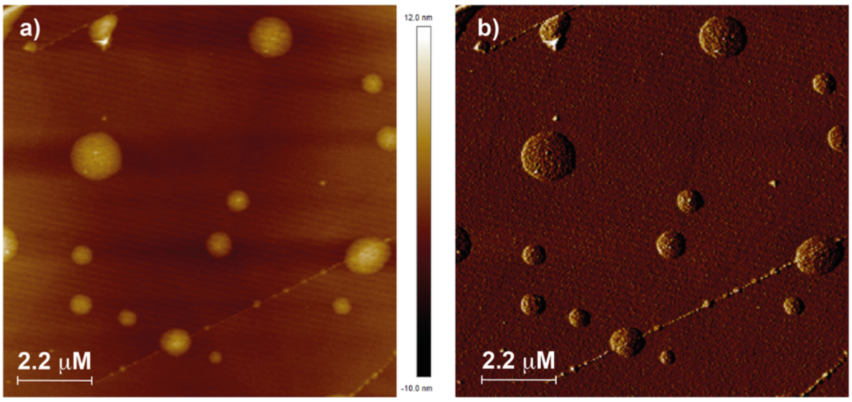


Figure S10. Height (a) and phase (b) AFM images of the kinetically controlled aggregates formed by Z-PDIs **1**. Experimental conditions: HOPG as surface, c_T = 40 μM; MCH.

3. Supporting references

S1 P. A. Korevaar, C. Schaefer, T. F. A. de Greef and E. W. Meijer, *J. Am. Chem. Soc.* 2012, **134**, 13482

S2 H. Nishiwaki, H. Nagaoka, M. Kuriyama, S. Yamauchi andY. Shuto, *Biosci. Biotechnol. Biochem.* 2011, **75**, 780.

S3 S. Ghosh, X.-Q. Li, V. Stepanenko and F. Würthner, *Chem. Eur. J.* 2008, **14**, 11343.

S4 A. J. Schwalb, C. Naranjo, A. Fernández-Alarcón, F. García, E. Ortí, J. Aragó and L. Sánchez, *J. Am. Chem. Soc.* 2025, **147**, 25024