Supporting Information

Syntheses, Charge Separation and Inverted Bulk Heterojunction Solar Cell Application of Phenothiazine-Fullerene Dyads

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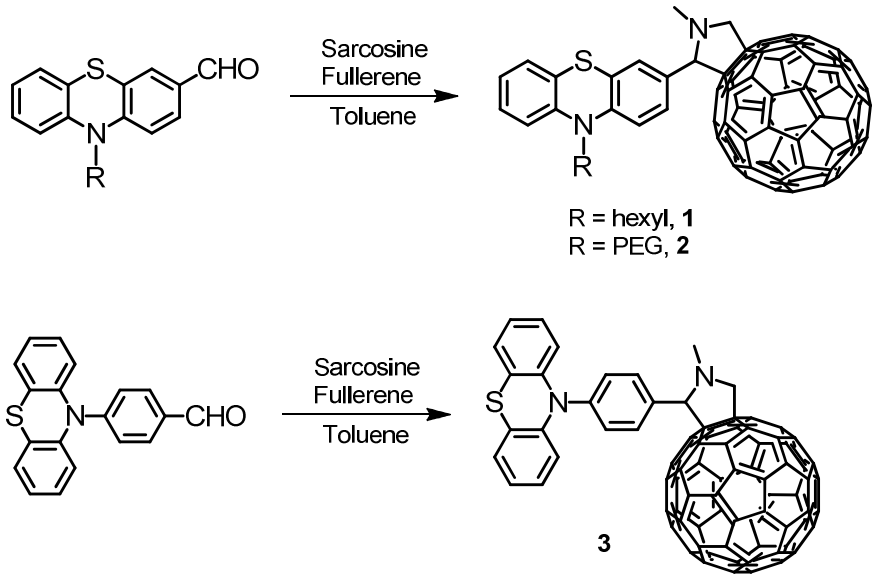

Scheme S1. Synthesis of phenothiazine-fullerene dyads.

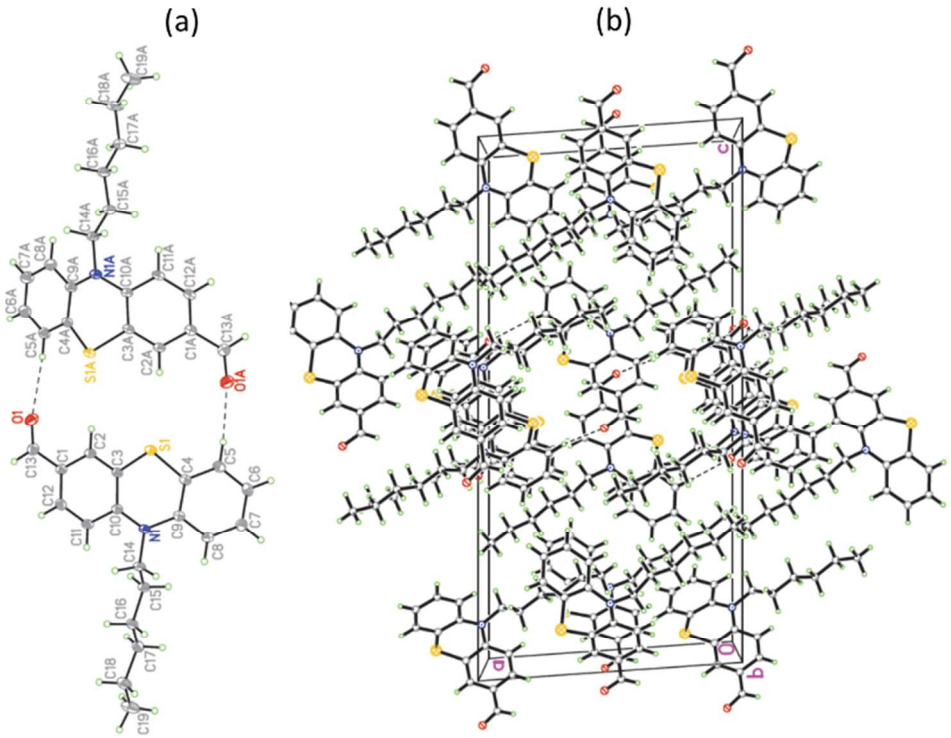

Figure S1. (a) Projection and (b) crystal packing diagrams of 10-hexyl-3-formyl phenothiazine with 50% thermal ellipsoids.

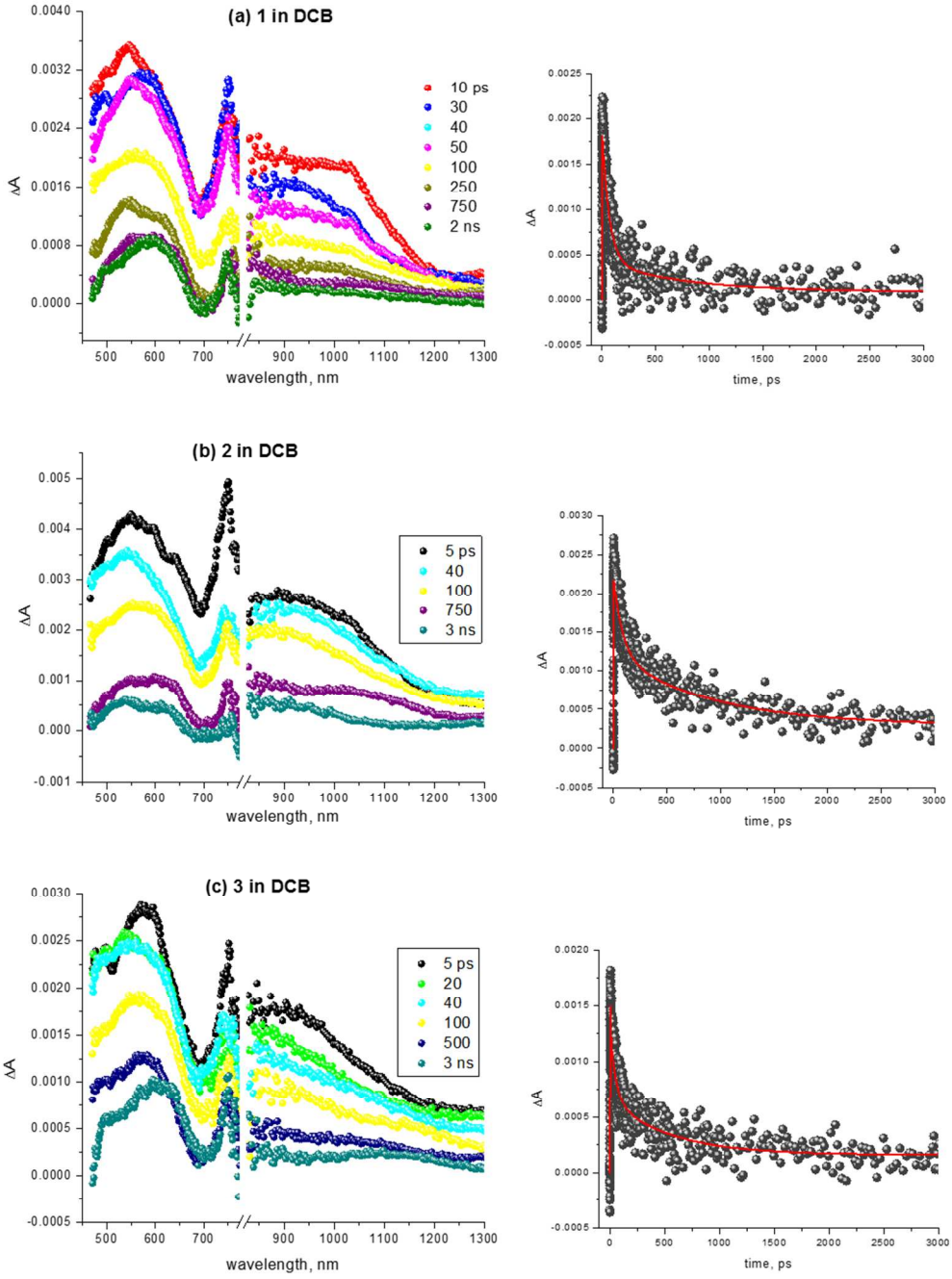

Figure S2. Femtosecond transient absorption spectra (excited at 400 nm of 100 fs laser pulses) at the indicated delay times of dyads **1-3** in Ar-saturated DCB. The right hand side panel shows time profile of the $C_{60}^{\bullet-}$ monitored at 1020 nm.

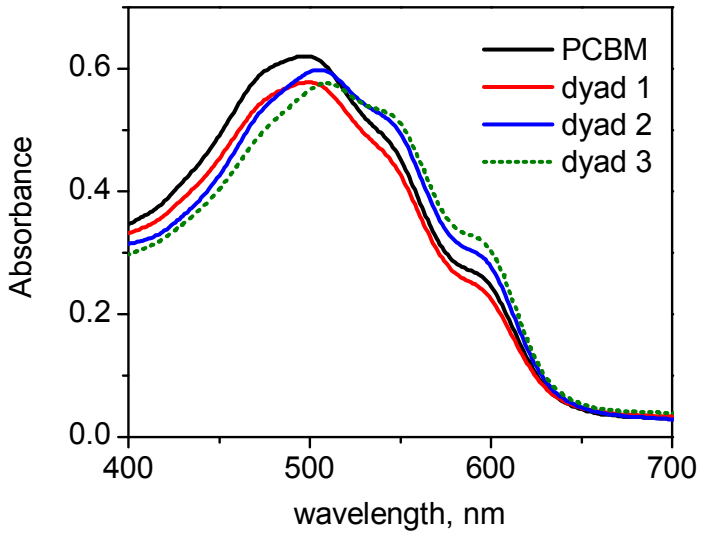

Figure S3. Absorption spectra of the studied OPVs of dyads **1-3** and PCBM reference. P3HT was used as donor material.

Statistical analysis of solar cell data.

The experimental variations of the photovoltaic parameters are presented as standard deviation values (*s*) in the Table 2 after the measured (V_{oc} and I_{sc}) and calculated (*FF* and *PCE*) values. The value of *s* is calculated according to Equation

$$s = \sqrt{\frac{\Sigma_{i=1}^{n}(x_i - \bar{x})^2}{n-1}},$$

where x_i is the value of the measured quantity, $\bar{x}$ is the average of the measured values and *n* is the number of the measured samples. The average power conversion efficiency (PCE) values are considered the most important device parameters.

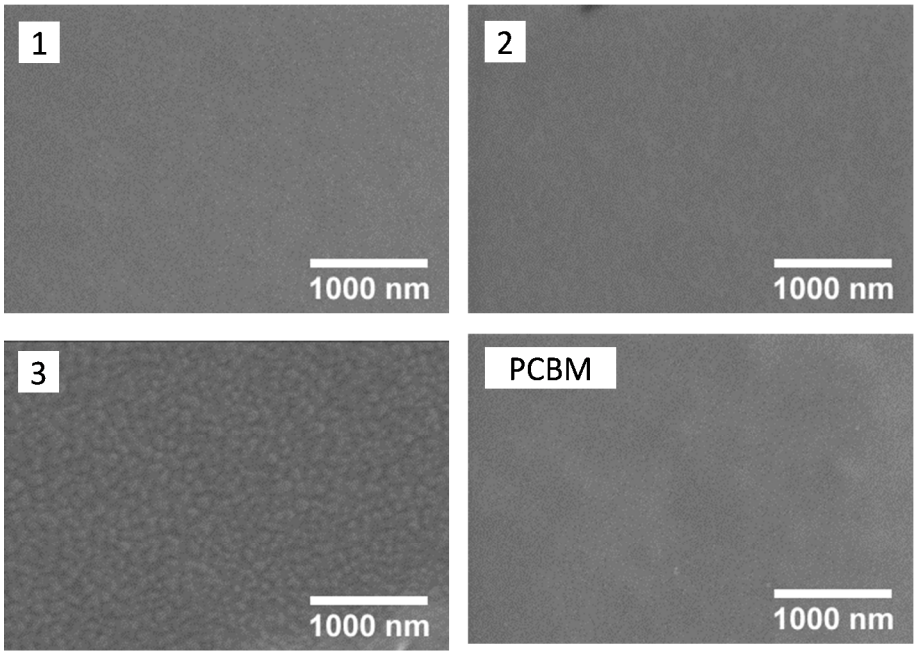

Figure S4. FE-SEM topographical images of BHJ films of dyads **1-3** and PCBM reference with 1 kV acceleration voltage. P3HT was used as donor material.

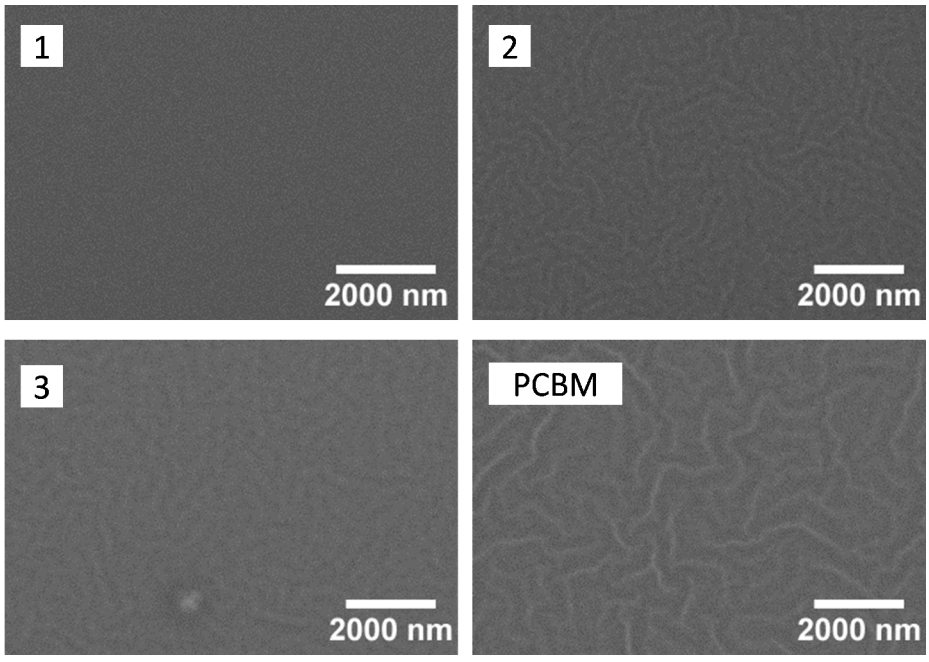

Figure S5. FE-SEM topographical images of BHJ films of dyads **1-3** and PCBM reference with 5 kV acceleration voltage. P3HT was used as donor material.

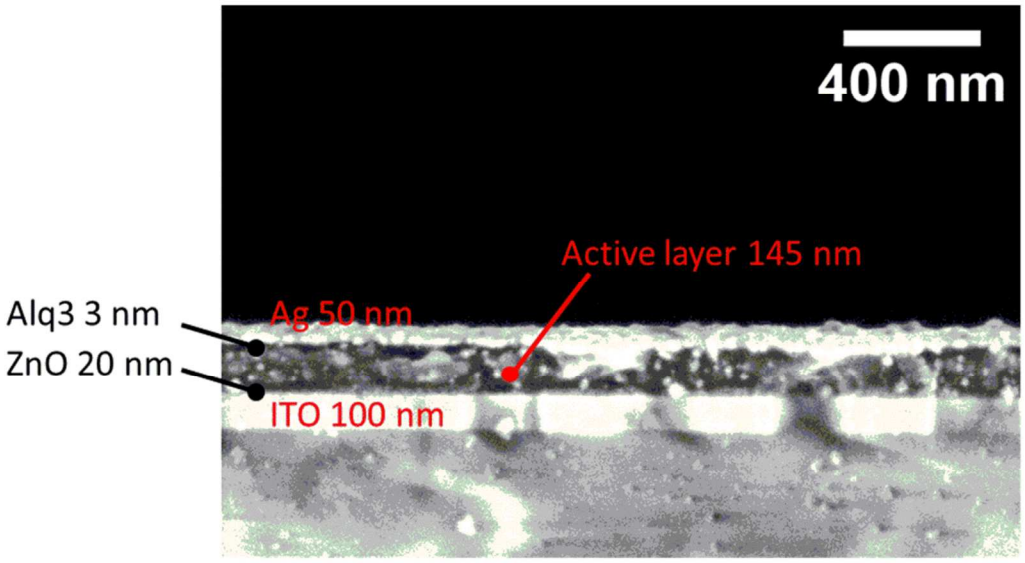

Figure S6. FE-SEM cross-section image of the P3HT:dyad **2** device representing a typical cross profile of the studied solar cells.

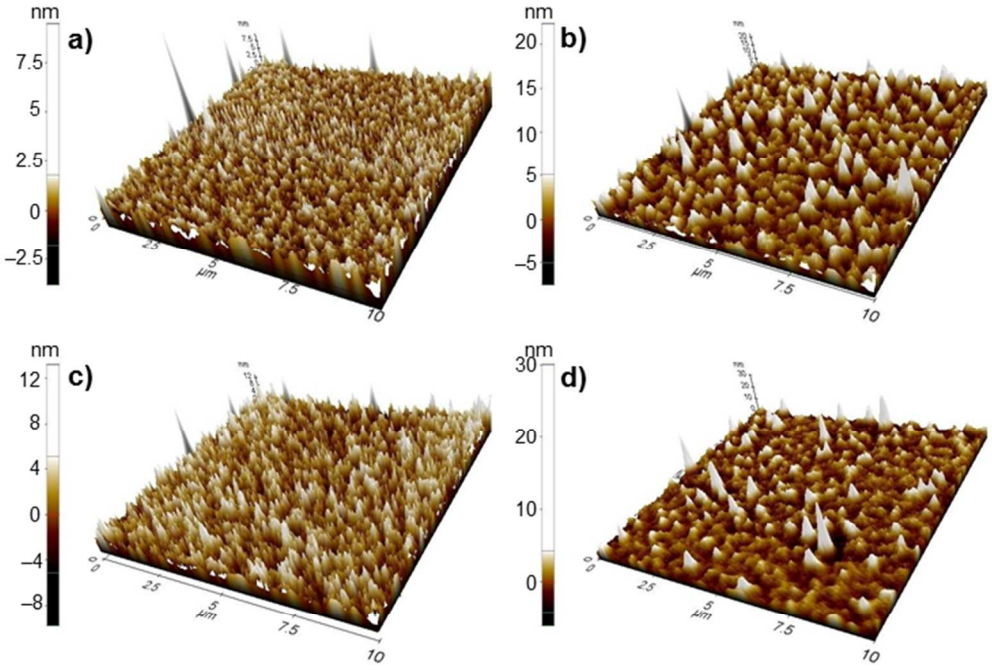

Figure S7. AFM topography images for a) **1**, b) **2**, c) **3**, and d) PCBM containing BHJ films (10 by 10 μm^2 scans).

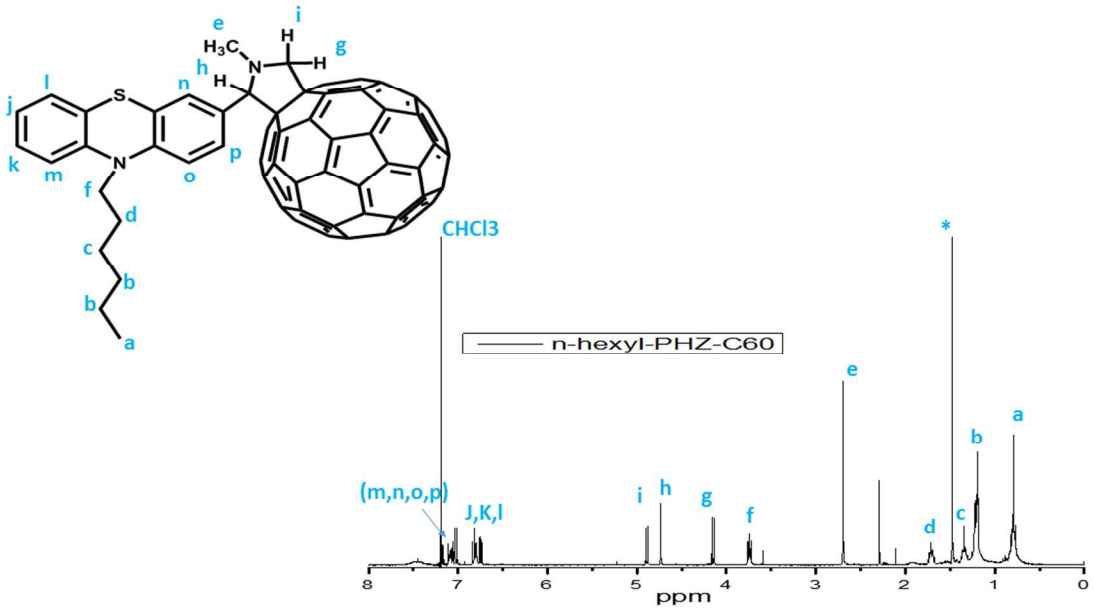

Figure S8. ^{1}H NMR spectrum of dyad **1** in $CDCl_3$.

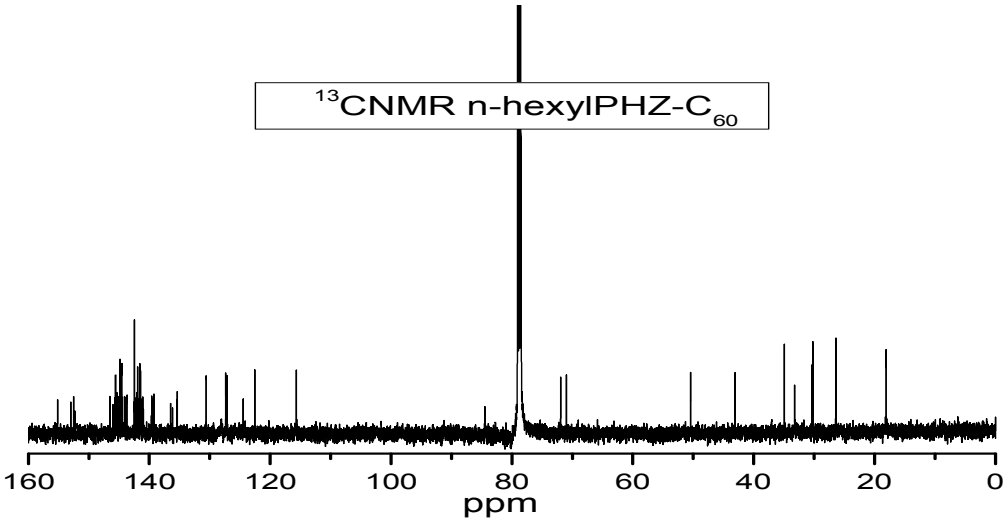

Figure S9. ^{13}C NMR spectrum of dyad **1** in $CDCl_3$.

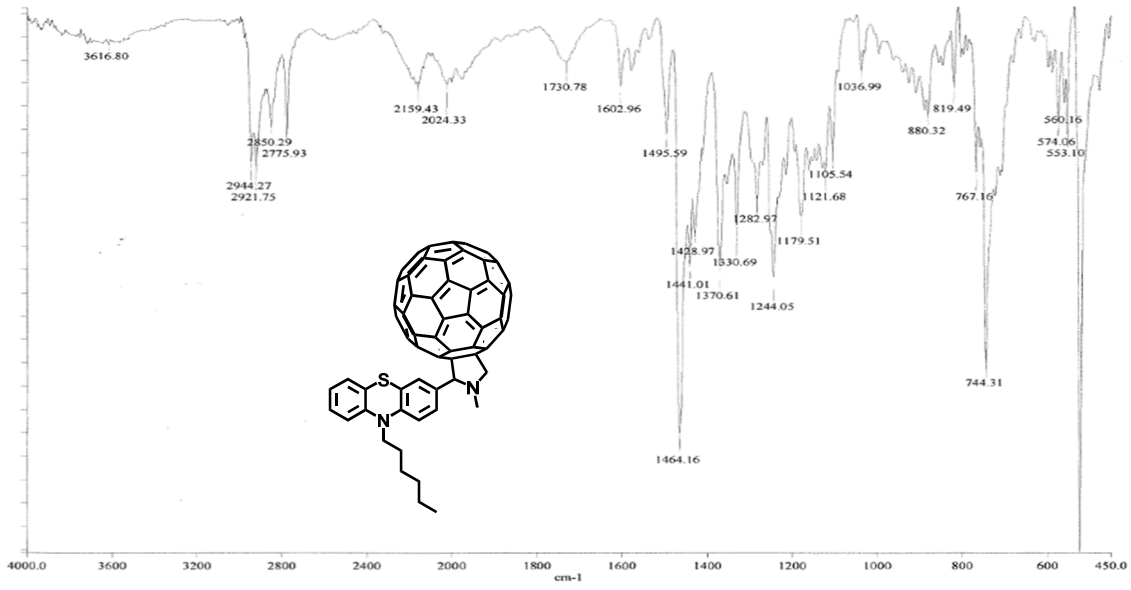

Figure S10. FT-IR spectrum of dyad **1**.

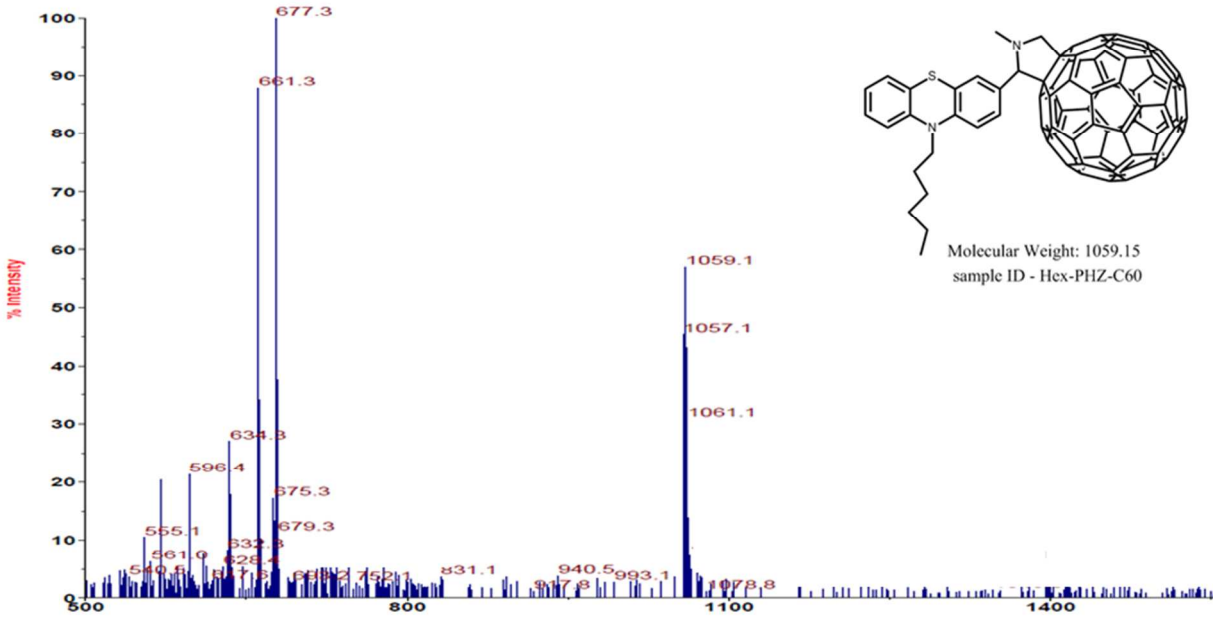

Figure S11. MALDI-mass spectrum of dyad **1**.

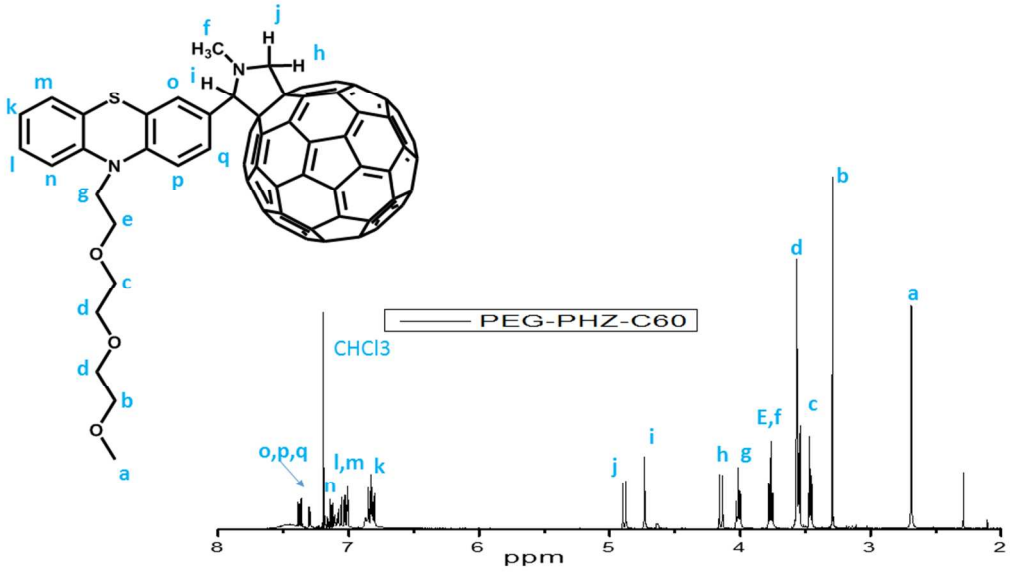

Figure S12. ^{1}H NMR spectrum of dyad **2** in $CDCl_3$.

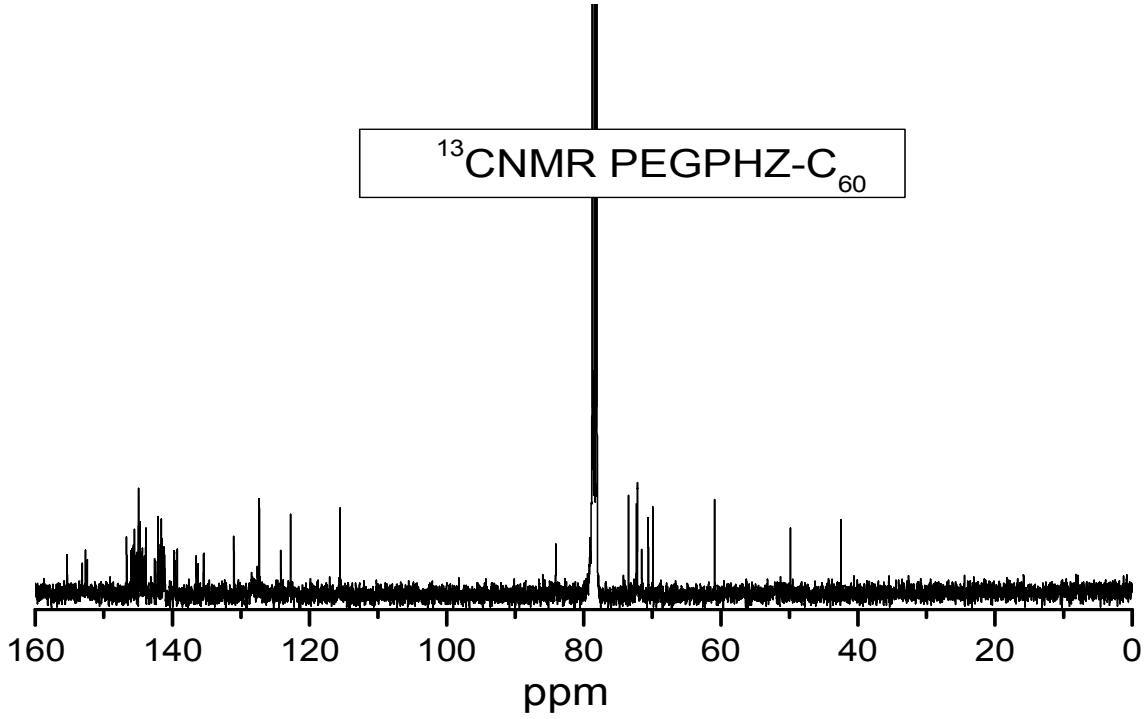

Figure S13. ^{13}C NMR spectrum of dyad **2** in $CDCl_3$.

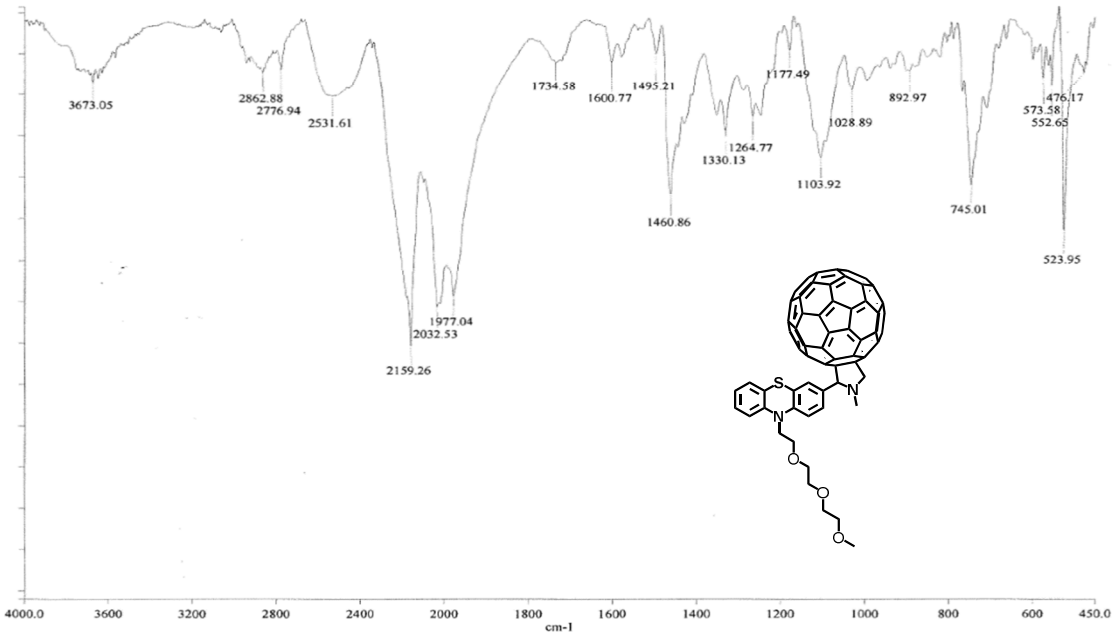

Figure S14. FT-IR spectrum of dyad **2**.

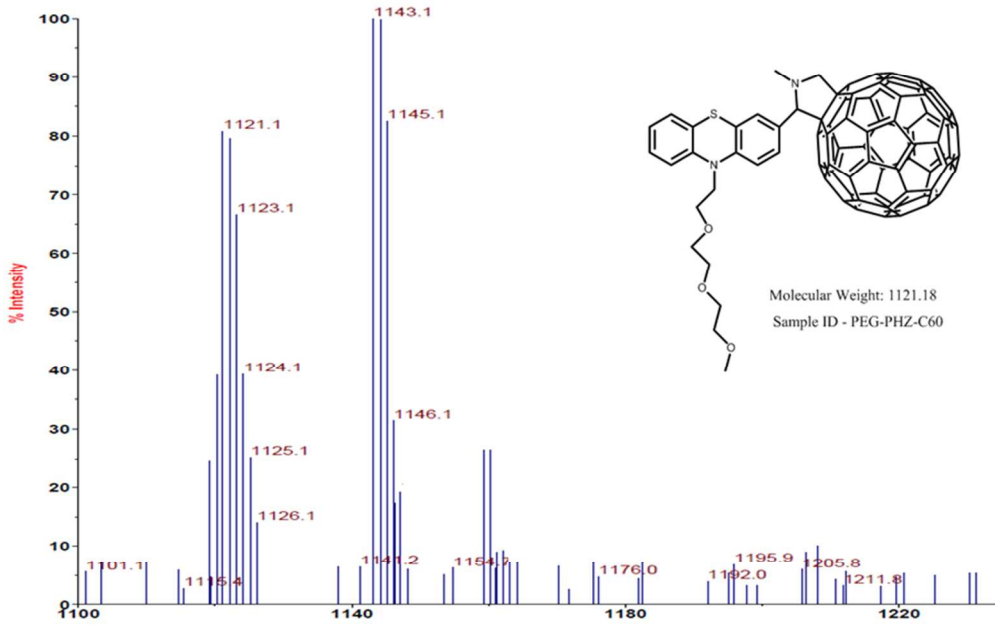

Figure S15. MALDI-mass spectrum of dyad **2**.

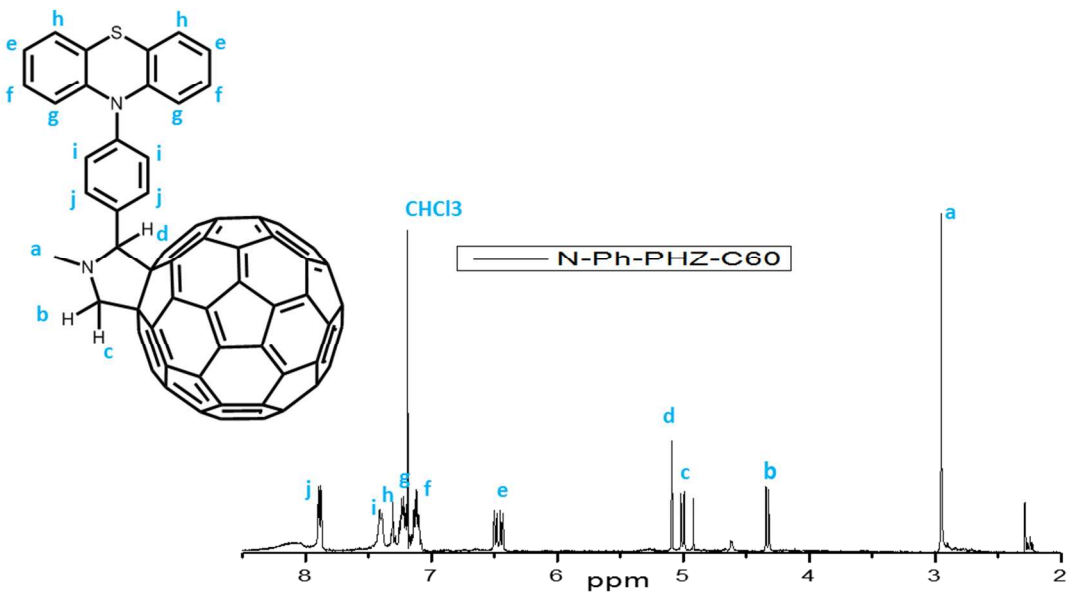

Figure S16. ^{1}H NMR spectrum of dyad **3** in $CDCl_3$.

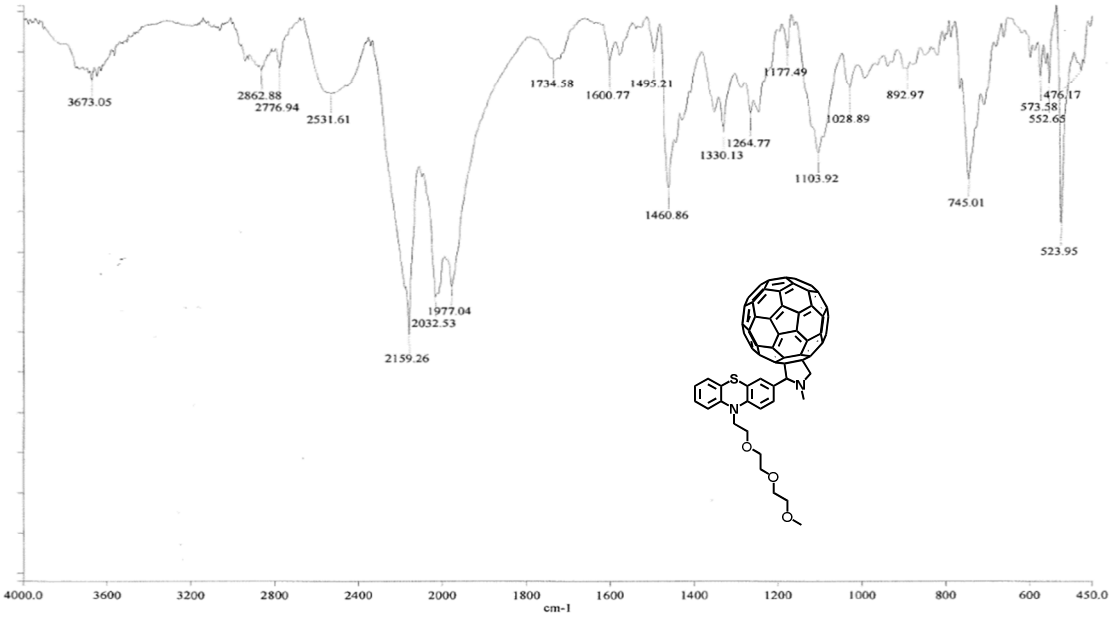

Figure S17. FT-IR spectrum of dyad **3**.

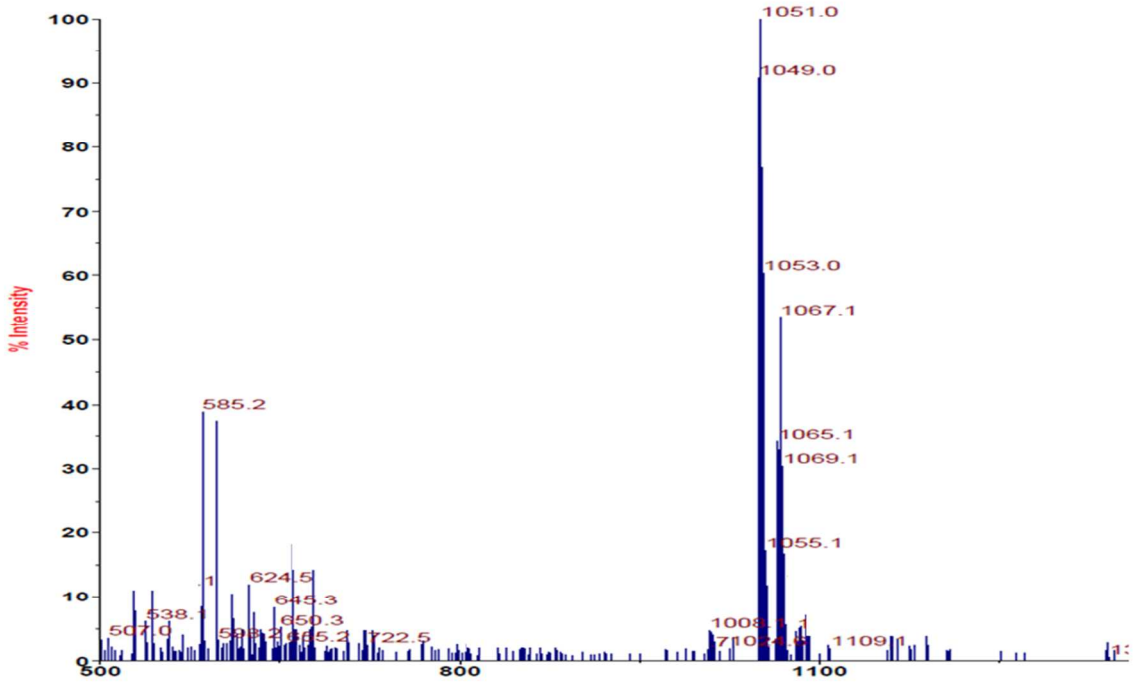

Figure S18. MALDI-mass spectrum of dyad **3**.

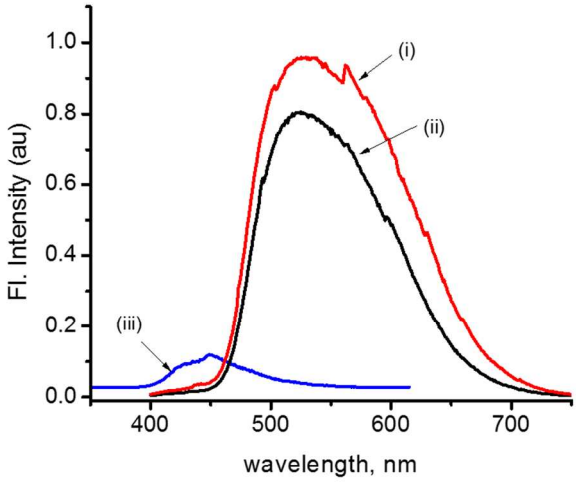

Figure S19. Fluorescence spectrum of (i) (10-hexyl-3-formyl)phenothiazine (λ_{ex} = 387 nm), (ii) (10-triethylene monomethylether-3-formyl)phenothiazine (λ_{ex} = 382 nm), and (iii) 10-(4-formylphenyl)phenothiazine (λ_{ex} = 313 nm) in DCB.

Table S1. Crystal data and structure refinement for 10-hexyl-3-formyl phenothiazine.

Identification code	p21c	
Empirical formula	C19 H21 N O S	
Formula weight	311.43	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 13.8468(13) Å	α= 90°.
	b = 8.3567(8) Å	β= 93.964(2)°.
	c = 28.466(3) Å	γ = 90°.
Volume	3286.0(5) $Å^3$	
Z	8	
Density (calculated)	1.259 Mg/m^3	
Absorption coefficient	0.199 mm^{-1}	
F(000)	1328	
Crystal size	0.26 x 0.15 x 0.11 mm^3	
Theta range for data collection	1.47 to 27.22°.	
Index ranges	-17<=h<=17, -10<=k<=10, -36<=l<=36	
Reflections collected	42803	
Independent reflections	7288 [R(int) = 0.0527]	
Completeness to theta = 27.22°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9781 and 0.9504	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7288 / 0 / 399	
Goodness-of-fit on F^2	1.037	
Final R indices [I>2sigma(I)]	R1 = 0.0794, wR2 = 0.2047	
R indices (all data)	R1 = 0.0960, wR2 = 0.2159	
Largest diff. peak and hole	0.662 and -0.360 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for str0754. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2003(1)	2268(1)	5334(1)	51(1)
N(1)	150(2)	1522(4)	5815(1)	38(1)
C(1)	-246(2)	3522(4)	4456(1)	40(1)
O(1)	232(2)	4492(4)	3723(1)	64(1)
C(2)	673(2)	3096(4)	4645(1)	40(1)
C(3)	807(2)	2456(4)	5088(1)	37(1)
C(4)	1854(2)	774(4)	5755(1)	39(1)
C(5)	2659(3)	-136(5)	5904(1)	46(1)
C(6)	2609(3)	-1198(5)	6276(1)	48(1)
C(7)	1757(3)	-1344(5)	6492(1)	49(1)
C(8)	943(3)	-481(5)	6337(1)	43(1)
C(9)	973(2)	607(4)	5966(1)	38(1)
C(10)	15(2)	2136(4)	5360(1)	36(1)
C(11)	-911(2)	2533(5)	5159(1)	44(1)
C(12)	-1028(3)	3226(5)	4722(1)	46(1)
C(13)	-384(3)	4260(5)	3995(1)	49(1)
C(14)	-670(2)	1589(4)	6116(1)	41(1)
C(15)	-1407(2)	227(4)	6064(1)	43(1)
C(16)	-2271(3)	620(5)	6341(1)	47(1)
C(17)	-3027(3)	-665(5)	6359(2)	53(1)
C(18)	-3882(3)	-123(6)	6634(2)	66(1)
C(19)	-4631(4)	-1350(7)	6688(2)	92(2)
S(1A)	3138(1)	4970(1)	4163(1)	44(1)
N(1A)	4997(2)	5771(4)	3715(1)	41(1)
O(1A)	4769(2)	1112(4)	5511(1)	60(1)
C(1A)	5311(2)	2708(4)	4892(1)	40(1)
C(2A)	4395(2)	3181(4)	4706(1)	39(1)
C(3A)	4295(2)	4205(4)	4331(1)	36(1)
C(4A)	3260(2)	5250(4)	3561(1)	40(1)
C(5A)	2445(3)	5177(5)	3252(1)	49(1)
C(6A)	2496(3)	5561(6)	2783(2)	59(1)

C(7A)	3362(3)	6035(6)	2624(2)	64(1)
C(8A)	4197(3)	6069(5)	2926(1)	54(1)
C(9A)	4162(2)	5702(4)	3402(1)	42(1)
C(10A)	5110(2)	4782(4)	4108(1)	36(1)
C(11A)	6024(2)	4317(5)	4306(1)	42(1)
C(12A)	6114(2)	3310(5)	4688(1)	43(1)
C(13A)	5421(3)	1636(5)	5296(1)	48(1)
C(14A)	5856(2)	6627(4)	3563(1)	43(1)
C(15A)	6521(3)	5679(5)	3260(1)	47(1)
C(16A)	7346(3)	6706(5)	3120(2)	53(1)
C(17A)	8068(3)	5909(5)	2836(1)	50(1)
C(18A)	8888(4)	6870(6)	2694(2)	82(2)
C(19A)	9645(4)	6143(9)	2441(2)	95(2)

Table S3. Bond lengths [Å] and angles [°] for str0754.

S(1)-C(4)	1.753(4)
S(1)-C(3)	1.759(3)
N(1)-C(10)	1.392(4)
N(1)-C(9)	1.415(4)
N(1)-C(14)	1.471(4)
C(1)-C(12)	1.385(5)
C(1)-C(2)	1.393(5)
C(1)-C(13)	1.451(5)
O(1)-C(13)	1.208(5)
C(2)-C(3)	1.372(5)
C(2)-H(2A)	0.9500
C(3)-C(10)	1.412(4)
C(4)-C(5)	1.391(5)
C(4)-C(9)	1.404(5)
C(5)-C(6)	1.385(5)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.375(5)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.385(5)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.396(5)
C(8)-H(8A)	0.9500
C(10)-C(11)	1.408(5)
C(11)-C(12)	1.371(5)
C(11)-H(11A)	0.9500
C(12)-H(12A)	0.9500
C(13)-H(13A)	0.9500
C(14)-C(15)	1.528(5)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.515(5)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.503(5)

C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.532(6)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.474(7)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
S(1A)-C(4A)	1.748(4)
S(1A)-C(3A)	1.760(3)
N(1A)-C(10A)	1.393(4)
N(1A)-C(9A)	1.411(4)
N(1A)-C(14A)	1.477(4)
O(1A)-C(13A)	1.208(5)
C(1A)-C(12A)	1.385(5)
C(1A)-C(2A)	1.399(5)
C(1A)-C(13A)	1.457(5)
C(2A)-C(3A)	1.367(5)
C(2A)-H(2AA)	0.9500
C(3A)-C(10A)	1.416(4)
C(4A)-C(5A)	1.384(5)
C(4A)-C(9A)	1.411(5)
C(5A)-C(6A)	1.379(6)
C(5A)-H(5AA)	0.9500
C(6A)-C(7A)	1.368(6)
C(6A)-H(6AA)	0.9500
C(7A)-C(8A)	1.393(6)
C(7A)-H(7AA)	0.9500
C(8A)-C(9A)	1.392(5)
C(8A)-H(8AA)	0.9500
C(10A)-C(11A)	1.404(5)
C(11A)-C(12A)	1.373(5)
C(11A)-H(11B)	0.9500

C(12A)-H(12B)	0.9500
C(13A)-H(13B)	0.9500
C(14A)-C(15A)	1.528(5)
C(14A)-H(14C)	0.9900
C(14A)-H(14D)	0.9900
C(15A)-C(16A)	1.504(5)
C(15A)-H(15C)	0.9900
C(15A)-H(15D)	0.9900
C(16A)-C(17A)	1.486(5)
C(16A)-H(16C)	0.9900
C(16A)-H(16D)	0.9900
C(17A)-C(18A)	1.471(6)
C(17A)-H(17C)	0.9900
C(17A)-H(17D)	0.9900
C(18A)-C(19A)	1.446(6)
C(18A)-H(18C)	0.9900
C(18A)-H(18D)	0.9900
C(19A)-H(19D)	0.9800
C(19A)-H(19E)	0.9800
C(19A)-H(19F)	0.9800

C(4)-S(1)-C(3)	100.56(16)
C(10)-N(1)-C(9)	122.3(3)
C(10)-N(1)-C(14)	118.0(3)
C(9)-N(1)-C(14)	118.8(3)
C(12)-C(1)-C(2)	118.1(3)
C(12)-C(1)-C(13)	120.8(3)
C(2)-C(1)-C(13)	121.1(3)
C(3)-C(2)-C(1)	121.1(3)
C(3)-C(2)-H(2A)	119.4
C(1)-C(2)-H(2A)	119.4
C(2)-C(3)-C(10)	121.1(3)
C(2)-C(3)-S(1)	117.7(2)
C(10)-C(3)-S(1)	120.8(3)
C(5)-C(4)-C(9)	121.1(3)
C(5)-C(4)-S(1)	118.0(3)

C(9)-C(4)-S(1)	120.7(3)
C(6)-C(5)-C(4)	120.2(3)
C(6)-C(5)-H(5A)	119.9
C(4)-C(5)-H(5A)	119.9
C(7)-C(6)-C(5)	119.2(4)
C(7)-C(6)-H(6A)	120.4
C(5)-C(6)-H(6A)	120.4
C(6)-C(7)-C(8)	121.0(4)
C(6)-C(7)-H(7A)	119.5
C(8)-C(7)-H(7A)	119.5
C(7)-C(8)-C(9)	121.0(3)
C(7)-C(8)-H(8A)	119.5
C(9)-C(8)-H(8A)	119.5
C(8)-C(9)-C(4)	117.4(3)
C(8)-C(9)-N(1)	121.1(3)
C(4)-C(9)-N(1)	121.5(3)
N(1)-C(10)-C(11)	121.7(3)
N(1)-C(10)-C(3)	121.3(3)
C(11)-C(10)-C(3)	116.9(3)
C(12)-C(11)-C(10)	121.1(3)
C(12)-C(11)-H(11A)	119.5
C(10)-C(11)-H(11A)	119.5
C(11)-C(12)-C(1)	121.5(3)
C(11)-C(12)-H(12A)	119.2
C(1)-C(12)-H(12A)	119.2
O(1)-C(13)-C(1)	126.5(4)
O(1)-C(13)-H(13A)	116.7
C(1)-C(13)-H(13A)	116.7
N(1)-C(14)-C(15)	116.9(3)
N(1)-C(14)-H(14A)	108.1
C(15)-C(14)-H(14A)	108.1
N(1)-C(14)-H(14B)	108.1
C(15)-C(14)-H(14B)	108.1
H(14A)-C(14)-H(14B)	107.3
C(16)-C(15)-C(14)	109.5(3)
C(16)-C(15)-H(15A)	109.8

C(14)-C(15)-H(15A)	109.8
C(16)-C(15)-H(15B)	109.8
C(14)-C(15)-H(15B)	109.8
H(15A)-C(15)-H(15B)	108.2
C(17)-C(16)-C(15)	116.1(3)
C(17)-C(16)-H(16A)	108.3
C(15)-C(16)-H(16A)	108.3
C(17)-C(16)-H(16B)	108.3
C(15)-C(16)-H(16B)	108.3
H(16A)-C(16)-H(16B)	107.4
C(16)-C(17)-C(18)	111.7(4)
C(16)-C(17)-H(17A)	109.3
C(18)-C(17)-H(17A)	109.3
C(16)-C(17)-H(17B)	109.3
C(18)-C(17)-H(17B)	109.3
H(17A)-C(17)-H(17B)	107.9
C(19)-C(18)-C(17)	114.9(4)
C(19)-C(18)-H(18A)	108.5
C(17)-C(18)-H(18A)	108.5
C(19)-C(18)-H(18B)	108.5
C(17)-C(18)-H(18B)	108.5
H(18A)-C(18)-H(18B)	107.5
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(4A)-S(1A)-C(3A)	99.58(16)
C(10A)-N(1A)-C(9A)	121.7(3)
C(10A)-N(1A)-C(14A)	118.3(3)
C(9A)-N(1A)-C(14A)	118.4(3)
C(12A)-C(1A)-C(2A)	118.1(3)
C(12A)-C(1A)-C(13A)	120.8(3)
C(2A)-C(1A)-C(13A)	121.1(3)
C(3A)-C(2A)-C(1A)	120.9(3)

C(3A)-C(2A)-H(2AA)	119.6
C(1A)-C(2A)-H(2AA)	119.6
C(2A)-C(3A)-C(10A)	121.4(3)
C(2A)-C(3A)-S(1A)	118.6(2)
C(10A)-C(3A)-S(1A)	119.6(3)
C(5A)-C(4A)-C(9A)	120.5(3)
C(5A)-C(4A)-S(1A)	119.3(3)
C(9A)-C(4A)-S(1A)	120.0(3)
C(6A)-C(5A)-C(4A)	120.8(4)
C(6A)-C(5A)-H(5AA)	119.6
C(4A)-C(5A)-H(5AA)	119.6
C(7A)-C(6A)-C(5A)	119.5(4)
C(7A)-C(6A)-H(6AA)	120.3
C(5A)-C(6A)-H(6AA)	120.3
C(6A)-C(7A)-C(8A)	120.7(4)
C(6A)-C(7A)-H(7AA)	119.6
C(8A)-C(7A)-H(7AA)	119.6
C(9A)-C(8A)-C(7A)	120.8(4)
C(9A)-C(8A)-H(8AA)	119.6
C(7A)-C(8A)-H(8AA)	119.6
C(8A)-C(9A)-C(4A)	117.6(3)
C(8A)-C(9A)-N(1A)	121.6(3)
C(4A)-C(9A)-N(1A)	120.8(3)
N(1A)-C(10A)-C(11A)	122.4(3)
N(1A)-C(10A)-C(3A)	120.9(3)
C(11A)-C(10A)-C(3A)	116.8(3)
C(12A)-C(11A)-C(10A)	121.1(3)
C(12A)-C(11A)-H(11B)	119.4
C(10A)-C(11A)-H(11B)	119.4
C(11A)-C(12A)-C(1A)	121.6(3)
C(11A)-C(12A)-H(12B)	119.2
C(1A)-C(12A)-H(12B)	119.2
O(1A)-C(13A)-C(1A)	125.6(4)
O(1A)-C(13A)-H(13B)	117.2
C(1A)-C(13A)-H(13B)	117.2
N(1A)-C(14A)-C(15A)	116.3(3)

N(1A)-C(14A)-H(14C)	108.2
C(15A)-C(14A)-H(14C)	108.2
N(1A)-C(14A)-H(14D)	108.2
C(15A)-C(14A)-H(14D)	108.2
H(14C)-C(14A)-H(14D)	107.4
C(16A)-C(15A)-C(14A)	110.6(3)
C(16A)-C(15A)-H(15C)	109.5
C(14A)-C(15A)-H(15C)	109.5
C(16A)-C(15A)-H(15D)	109.5
C(14A)-C(15A)-H(15D)	109.5
H(15C)-C(15A)-H(15D)	108.1
C(17A)-C(16A)-C(15A)	116.1(3)
C(17A)-C(16A)-H(16C)	108.3
C(15A)-C(16A)-H(16C)	108.3
C(17A)-C(16A)-H(16D)	108.3
C(15A)-C(16A)-H(16D)	108.3
H(16C)-C(16A)-H(16D)	107.4
C(18A)-C(17A)-C(16A)	117.8(4)
C(18A)-C(17A)-H(17C)	107.9
C(16A)-C(17A)-H(17C)	107.9
C(18A)-C(17A)-H(17D)	107.9
C(16A)-C(17A)-H(17D)	107.9
H(17C)-C(17A)-H(17D)	107.2
C(19A)-C(18A)-C(17A)	120.5(5)
C(19A)-C(18A)-H(18C)	107.2
C(17A)-C(18A)-H(18C)	107.2
C(19A)-C(18A)-H(18D)	107.2
C(17A)-C(18A)-H(18D)	107.2
H(18C)-C(18A)-H(18D)	106.8
C(18A)-C(19A)-H(19D)	109.5
C(18A)-C(19A)-H(19E)	109.5
H(19D)-C(19A)-H(19E)	109.5
C(18A)-C(19A)-H(19F)	109.5
H(19D)-C(19A)-H(19F)	109.5
H(19E)-C(19A)-H(19F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for str0754. 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}
S(1)	28(1)	64(1)	62(1)	14(1)	5(1)	-10(1)
N(1)	29(1)	44(2)	44(2)	-1(1)	10(1)	-3(1)
C(1)	38(2)	36(2)	48(2)	-3(1)	4(1)	-8(1)
O(1)	66(2)	68(2)	59(2)	14(2)	9(1)	-14(2)
C(2)	36(2)	39(2)	46(2)	-4(2)	8(1)	-8(1)
C(3)	29(2)	36(2)	47(2)	-2(1)	6(1)	-5(1)
C(4)	35(2)	40(2)	43(2)	-8(1)	4(1)	-4(1)
C(5)	38(2)	49(2)	50(2)	-8(2)	4(2)	-4(2)
C(6)	46(2)	42(2)	56(2)	-6(2)	-4(2)	5(2)
C(7)	53(2)	49(2)	44(2)	0(2)	-1(2)	0(2)
C(8)	43(2)	47(2)	41(2)	-2(2)	6(1)	-5(2)
C(9)	37(2)	37(2)	40(2)	-7(1)	5(1)	-5(1)
C(10)	34(2)	33(2)	43(2)	-4(1)	6(1)	-9(1)
C(11)	31(2)	49(2)	55(2)	2(2)	9(1)	-8(2)
C(12)	33(2)	45(2)	59(2)	2(2)	1(2)	-4(2)
C(13)	47(2)	45(2)	55(2)	2(2)	0(2)	-9(2)
C(14)	36(2)	41(2)	47(2)	-4(2)	14(1)	-5(1)
C(15)	38(2)	40(2)	51(2)	-2(2)	12(2)	-7(2)
C(16)	38(2)	44(2)	60(2)	1(2)	14(2)	-1(2)
C(17)	44(2)	41(2)	76(3)	5(2)	12(2)	-1(2)
C(18)	43(2)	67(3)	90(3)	-6(2)	18(2)	-4(2)
C(19)	66(3)	85(4)	131(5)	-23(4)	48(3)	-13(3)
S(1A)	29(1)	53(1)	51(1)	1(1)	11(1)	1(1)
N(1A)	32(1)	44(2)	48(2)	-1(1)	11(1)	-8(1)
O(1A)	63(2)	58(2)	61(2)	9(1)	14(1)	-5(1)
C(1A)	35(2)	41(2)	42(2)	-7(1)	6(1)	-3(1)
C(2A)	32(2)	41(2)	46(2)	-5(2)	10(1)	-7(1)
C(3A)	27(2)	40(2)	43(2)	-6(1)	8(1)	-3(1)
C(4A)	34(2)	35(2)	50(2)	-6(1)	5(1)	0(1)
C(5A)	38(2)	47(2)	61(2)	-2(2)	3(2)	-2(2)
C(6A)	48(2)	70(3)	58(2)	0(2)	-5(2)	-4(2)

C(7A)	58(3)	84(3)	49(2)	5(2)	2(2)	-5(2)
C(8A)	49(2)	63(3)	50(2)	5(2)	8(2)	-4(2)
C(9A)	38(2)	40(2)	50(2)	-4(2)	8(1)	-4(1)
C(10A)	31(2)	39(2)	39(2)	-7(1)	9(1)	-6(1)
C(11A)	27(2)	55(2)	46(2)	-7(2)	9(1)	-7(1)
C(12A)	30(2)	53(2)	47(2)	-7(2)	5(1)	-1(2)
C(13A)	51(2)	46(2)	49(2)	-2(2)	3(2)	-3(2)
C(14A)	34(2)	41(2)	55(2)	-2(2)	13(2)	-10(1)
C(15A)	45(2)	43(2)	57(2)	-6(2)	17(2)	-8(2)
C(16A)	42(2)	43(2)	77(3)	0(2)	24(2)	-5(2)
C(17A)	46(2)	56(2)	49(2)	-2(2)	13(2)	-8(2)
C(18A)	58(3)	65(3)	130(5)	-11(3)	52(3)	-9(2)
C(19A)	59(3)	124(5)	107(4)	-21(4)	48(3)	-7(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for str0754.

	x	y	z	U(eq)
H(2A)	1215	3251	4463	48
H(5A)	3244	-30	5751	55
H(6A)	3159	-1817	6380	58
H(7A)	1725	-2049	6753	59
H(8A)	356	-630	6485	52
H(11A)	-1464	2317	5328	53
H(12A)	-1660	3511	4599	55
H(13A)	-1022	4595	3898	59
H(14A)	-1018	2609	6052	49
H(14B)	-407	1618	6449	49
H(15A)	-1619	79	5728	51
H(15B)	-1105	-783	6182	51
H(16A)	-2033	881	6668	56
H(16B)	-2585	1594	6204	56
H(17A)	-2732	-1632	6510	64
H(17B)	-3266	-953	6034	64
H(18A)	-3630	231	6951	79
H(18B)	-4189	815	6472	79
H(19A)	-5166	-884	6850	138
H(19B)	-4351	-2245	6874	138
H(19C)	-4873	-1738	6377	138
H(2AA)	3834	2786	4841	47
H(5AA)	1844	4858	3363	58
H(6AA)	1935	5497	2572	71
H(7AA)	3393	6343	2304	76
H(8AA)	4798	6347	2806	65
H(11B)	6590	4706	4174	51
H(12B)	6742	3018	4814	52
H(13B)	6061	1323	5400	58
H(14C)	6242	6998	3848	52

H(14D)	5631	7590	3385	52
H(15C)	6781	4737	3438	57
H(15D)	6147	5289	2973	57
H(16C)	7072	7630	2938	64
H(16D)	7689	7132	3410	64
H(17C)	8333	4979	3018	60
H(17D)	7720	5485	2547	60
H(18C)	8616	7762	2498	99
H(18D)	9201	7353	2983	99
H(19D)	10006	6979	2287	142
H(19E)	9356	5408	2202	142
H(19F)	10086	5551	2661	142