

Protein Detection by AIE-Active Tetraphenylethene- Based Fluorescent Probes

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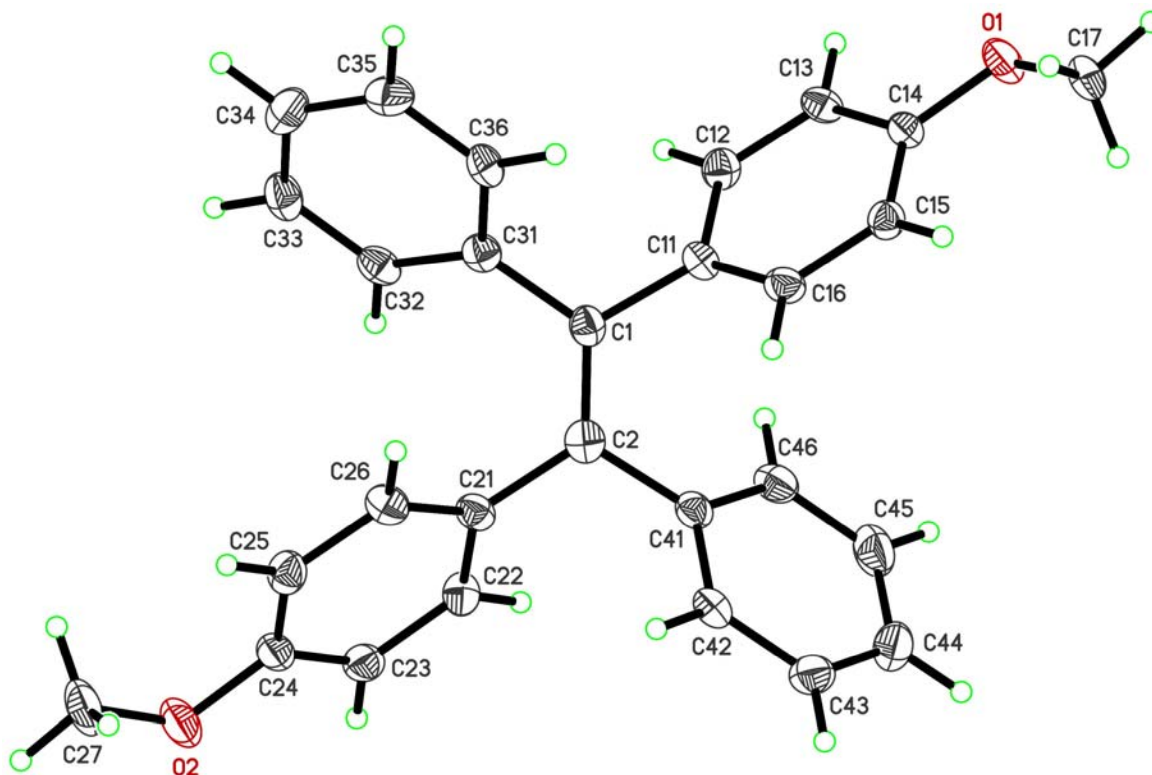


Figure S1. ORTEP drawing of **1** with atom-labeling scheme for Tables S1–S5.

Table S1. Crystal data and structure refinement for TPE derivative **1**

Identification code	dye 1
Empirical formula	C ₂₈ H ₂₄ O ₂
Formula weight	392.47
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)
Unit cell dimensions	a = 9.6751(12) Å α = 90°. b = 10.2214(12) Å β = 96.993(2)°. c = 10.6522(13) Å γ = 90°.
Volume	1045.6(2) Å ³
Z	2
Density (calculated)	1.247 Mg/m ³
Absorption coefficient	0.077 mm ⁻¹
F(000)	416
Crystal size	0.30 x 0.25 x 0.20 mm ³
Theta range for data collection	1.93 to 29.08°.
Index ranges	-12 ≤ h ≤ 12, -13 ≤ k ≤ 13, -14 ≤ l ≤ 12
Reflections collected	9063
Independent reflections	2622 [R(int) = 0.0411]
Completeness to theta = 25.00°	98.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00 and 0.92
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2622 / 1 / 273
Goodness-of-fit on F ²	1.012
Final R indices [I > 2σ(I)]	R1 = 0.0392, wR2 = 0.0891
R indices (all data)	R1 = 0.0498, wR2 = 0.0949
Absolute structure parameter	0.7(15)
Largest diff. peak and hole	0.330 and -0.189 e.Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TPE derivative **1**.U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
O(1)	-220(2)	3320(2)	3706(2)	27(1)
O(2)	10229(2)	9060(2)	1511(2)	33(1)
C(1)	4314(2)	6160(2)	2166(2)	20(1)
C(2)	5558(2)	6294(2)	2876(2)	22(1)
C(11)	3158(2)	5372(2)	2622(2)	21(1)
C(12)	1872(2)	5951(2)	2682(2)	22(1)
C(13)	772(2)	5258(2)	3055(2)	21(1)
C(14)	931(2)	3929(2)	3346(2)	20(1)
C(15)	2198(2)	3318(2)	3263(2)	20(1)
C(16)	3306(2)	4047(2)	2916(2)	22(1)
C(17)	-135(2)	1946(2)	3920(2)	28(1)
C(21)	6783(2)	6985(2)	2442(2)	20(1)
C(22)	7534(2)	7858(2)	3275(2)	23(1)
C(23)	8675(2)	8522(2)	2945(2)	24(1)
C(24)	9101(2)	8341(2)	1763(2)	23(1)
C(25)	8392(2)	7467(2)	920(2)	24(1)
C(26)	7250(2)	6794(2)	1274(2)	23(1)
C(27)	10628(3)	8973(3)	266(3)	39(1)
C(31)	3973(2)	6715(2)	873(2)	20(1)
C(32)	4370(2)	7964(2)	523(2)	22(1)
C(33)	4041(2)	8401(2)	-702(2)	26(1)
C(34)	3289(3)	7628(2)	-1606(2)	29(1)
C(35)	2868(2)	6389(2)	-1267(2)	28(1)
C(36)	3203(2)	5944(2)	-42(2)	23(1)
C(41)	5835(2)	5737(2)	4185(2)	20(1)
C(42)	7009(2)	4943(2)	4467(2)	22(1)
C(43)	7315(2)	4400(2)	5660(2)	28(1)
C(44)	6475(3)	4653(3)	6592(3)	33(1)
C(45)	5324(3)	5460(3)	6325(2)	33(1)
C(46)	5003(2)	5992(2)	5136(2)	25(1)

Table S3. Bond lengths [\AA] and angles [$^\circ$] for TPE derivative **1**

O(1)-C(14)	1.371(2)
O(1)-C(17)	1.423(3)
O(2)-C(24)	1.369(3)
O(2)-C(27)	1.428(3)
C(1)-C(2)	1.348(3)
C(1)-C(31)	1.489(3)
C(1)-C(11)	1.505(3)
C(2)-C(21)	1.500(3)
C(2)-C(41)	1.500(3)
C(11)-C(12)	1.386(3)
C(11)-C(16)	1.394(3)
C(12)-C(13)	1.377(3)
C(13)-C(14)	1.398(3)
C(14)-C(15)	1.388(3)
C(15)-C(16)	1.392(3)
C(21)-C(26)	1.389(3)
C(21)-C(22)	1.398(3)
C(22)-C(23)	1.377(3)
C(23)-C(24)	1.384(3)
C(24)-C(25)	1.387(3)
C(25)-C(26)	1.391(3)
C(31)-C(36)	1.396(3)
C(31)-C(32)	1.397(3)
C(32)-C(33)	1.379(3)
C(33)-C(34)	1.383(3)
C(34)-C(35)	1.391(4)
C(35)-C(36)	1.382(3)
C(41)-C(46)	1.394(3)
C(41)-C(42)	1.398(3)
C(42)-C(43)	1.385(3)

C(43)-C(44)	1.382(4)
C(44)-C(45)	1.388(4)
C(45)-C(46)	1.378(3)
C(14)-O(1)-C(17)	117.38(18)
C(24)-O(2)-C(27)	117.4(2)
C(2)-C(1)-C(31)	124.19(19)
C(2)-C(1)-C(11)	121.42(19)
C(31)-C(1)-C(11)	114.35(18)
C(1)-C(2)-C(21)	124.1(2)
C(1)-C(2)-C(41)	121.93(19)
C(21)-C(2)-C(41)	113.97(18)
C(12)-C(11)-C(16)	118.22(19)
C(12)-C(11)-C(1)	119.53(18)
C(16)-C(11)-C(1)	122.14(19)
C(13)-C(12)-C(11)	121.57(19)
C(12)-C(13)-C(14)	119.7(2)
O(1)-C(14)-C(15)	124.58(18)
O(1)-C(14)-C(13)	115.58(19)
C(15)-C(14)-C(13)	119.8(2)
C(14)-C(15)-C(16)	119.41(19)
C(15)-C(16)-C(11)	121.23(19)
C(26)-C(21)-C(22)	117.2(2)
C(26)-C(21)-C(2)	124.4(2)
C(22)-C(21)-C(2)	118.3(2)
C(23)-C(22)-C(21)	121.6(2)
C(22)-C(23)-C(24)	120.1(2)
O(2)-C(24)-C(23)	116.0(2)
O(2)-C(24)-C(25)	124.2(2)
C(23)-C(24)-C(25)	119.8(2)
C(24)-C(25)-C(26)	119.3(2)

C(21)-C(26)-C(25)	122.0(2)
C(36)-C(31)-C(32)	118.0(2)
C(36)-C(31)-C(1)	118.05(19)
C(32)-C(31)-C(1)	123.9(2)
C(33)-C(32)-C(31)	120.6(2)
C(32)-C(33)-C(34)	121.0(2)
C(33)-C(34)-C(35)	119.0(2)
C(36)-C(35)-C(34)	120.2(2)
C(35)-C(36)-C(31)	121.1(2)
C(46)-C(41)-C(42)	118.6(2)
C(46)-C(41)-C(2)	123.4(2)
C(42)-C(41)-C(2)	117.98(19)
C(43)-C(42)-C(41)	120.5(2)
C(44)-C(43)-C(42)	120.3(2)
C(43)-C(44)-C(45)	119.4(2)
C(46)-C(45)-C(44)	120.6(2)
C(45)-C(46)-C(41)	120.6(2)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for TPE derivative **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
O(1)	19(1)	24(1)	40(1)	4(1)	10(1)	-3(1)
O(2)	25(1)	31(1)	43(1)	7(1)	10(1)	-6(1)
C(1)	21(1)	19(1)	22(1)	1(1)	6(1)	1(1)
C(2)	25(1)	19(1)	23(1)	-2(1)	6(1)	2(1)
C(11)	18(1)	21(1)	23(1)	0(1)	5(1)	-3(1)
C(12)	24(1)	18(1)	24(1)	1(1)	4(1)	1(1)
C(13)	14(1)	23(1)	26(1)	-2(1)	4(1)	2(1)
C(14)	17(1)	23(1)	21(1)	1(1)	2(1)	-4(1)
C(15)	21(1)	19(1)	21(1)	2(1)	3(1)	1(1)
C(16)	16(1)	22(1)	26(1)	1(1)	2(1)	2(1)
C(17)	24(1)	26(1)	33(1)	5(1)	5(1)	-9(1)
C(21)	17(1)	18(1)	26(1)	1(1)	4(1)	1(1)
C(22)	26(1)	22(1)	21(1)	1(1)	5(1)	-2(1)
C(23)	23(1)	21(1)	27(1)	3(1)	-2(1)	-3(1)
C(24)	17(1)	20(1)	33(1)	8(1)	3(1)	2(1)
C(25)	25(1)	26(1)	23(1)	3(1)	7(1)	5(1)
C(26)	21(1)	23(1)	26(1)	-4(1)	4(1)	0(1)
C(27)	30(1)	40(1)	50(2)	15(1)	20(1)	-3(1)
C(31)	19(1)	20(1)	23(1)	-1(1)	5(1)	3(1)
C(32)	18(1)	19(1)	31(1)	-3(1)	5(1)	0(1)
C(33)	26(1)	20(1)	35(1)	5(1)	11(1)	1(1)
C(34)	33(1)	32(1)	23(1)	6(1)	3(1)	6(1)
C(35)	25(1)	32(1)	26(1)	-4(1)	-2(1)	-1(1)
C(36)	23(1)	18(1)	27(1)	1(1)	6(1)	-5(1)
C(41)	19(1)	20(1)	21(1)	-1(1)	2(1)	-5(1)
C(42)	18(1)	22(1)	26(1)	-1(1)	6(1)	-3(1)
C(43)	24(1)	27(1)	32(1)	4(1)	-2(1)	0(1)
C(44)	37(1)	36(1)	25(1)	8(1)	3(1)	-6(1)
C(45)	33(1)	39(1)	29(1)	0(1)	13(1)	-7(1)
C(46)	19(1)	31(1)	26(1)	-3(1)	4(1)	-2(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for TPE derivative **1**

	x	y	z	U(eq)
H(12A)	1747	6848	2460	26
H(13A)	-92	5682	3114	25
H(15A)	2308	2411	3441	24
H(16A)	4179	3633	2879	26
H(17A)	-1027	1626	4147	41
H(17B)	603	1761	4612	41
H(17C)	78	1505	3150	41
H(22A)	7251	7997	4087	27
H(23A)	9171	9107	3530	29
H(25A)	8682	7330	110	29
H(26A)	6777	6187	699	28
H(27A)	11412	9564	194	58
H(27B)	9840	9222	-354	58
H(27C)	10906	8072	104	58
H(32A)	4871	8518	1134	27
H(33A)	4335	9246	-928	31
H(34A)	3063	7938	-2447	35
H(35A)	2350	5847	-1878	34
H(36A)	2903	5099	181	27
H(42A)	7600	4775	3836	26
H(43A)	8108	3852	5839	34
H(44A)	6684	4277	7409	40
H(45A)	4752	5647	6966	39
H(46A)	4207	6537	4964	30