Supplementary Materials

3-[4-(2-Phenylethyl)piperazin-1-yl]-7*H*-benzo[*de*]-anthracen-7-one

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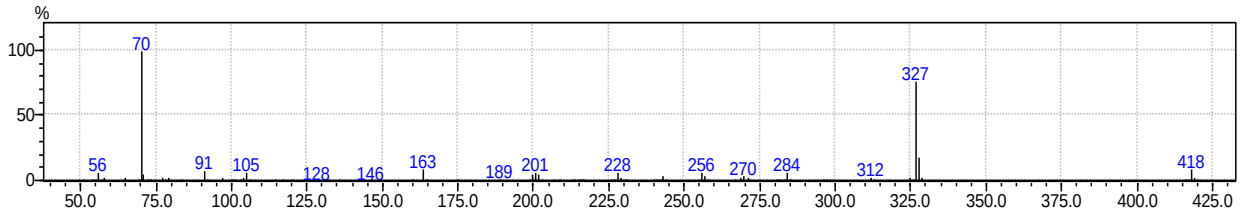

Figure S1. Mass spectrum of 3-[4-(2-phenylethyl)piperazin-1-yl]-7*H*-benzo[*de*]anthracen-7-one.

Table S1. Crystal data and structure refinement for 3-[4-(2-phenylethyl)piperazin-1-yl]-7*H*-benzo[*de*]-anthracen-7-one.

Empirical formula	$C_{29}H_{26}N_2O$
Formula weight	418.52
Temperature/K	120.0(1)
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	8.8957(10)
b/Å	9.41743(14)
c/Å	13.3599(2)
α/°	75.4592(13)
β/°	77.5237(11)
γ/°	87.4987(11)
Volume/Å^3	1057.73(3)
Z	2
ρ_{calc}g/cm^3	1.314
μ/mm^{-1}	0.619
F(000)	444.0
Crystal size/mm^3	0.21 × 0.17 × 0.08
Radiation	CuKα (λ = 1.54184 Å)

2Θ max.range for data collection/°	160.0
Index ranges	$-11 \le h \le 11$, $-12 \le k \le 11$, $-17 \le l \le 13$
Reflections collected	17586
Independent reflections	4554 [R_{int} = 0.0190, R_{sigma} = 0.0163]
Data/restraints/parameters	4554/0/290
Goodness-of-fit on F^2	1.073
Final R indexes [$I > 2\sigma(I)$]	R_1 = 0.0396, wR_2 = 0.1120
Final R indexes [all data]	R_1 = 0.0415, wR_2 = 0.1135
Largest diff. peak/hole / e Å^{-3}	0.62/-0.17

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3). U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	*U*(eq)
C1	1652.3(13)	3806.9(12)	56.7(8)	26.9(2)
C2	1069.2(13)	2391.5(12)	582.2(9)	27.5(2)
C3	1273.3(11)	1716.7(11)	1585.2(8)	23.1(2)
C4	2097.2(13)	2018.8(11)	3195.8(8)	26.2(2)
C5	2878.7(14)	2788.5(12)	3678.4(8)	29.4(2)
C6	3607.3(13)	4118.7(12)	3106.7(9)	27.5(2)
C7	4242.1(12)	6148.2(11)	1506.4(8)	24.6(2)
C8	4662.3(12)	8177.7(12)	-114.8(9)	26.2(2)
C9	4488.9(12)	8830.0(12)	-1129.9(9)	28.1(2)
C10	3698.0(13)	8073.4(12)	-1633.6(9)	28.2(2)
C11	3049.6(12)	6709.6(12)	-1112.8(9)	26.9(2)
C12	3173.0(11)	6039.3(11)	-68.3(8)	22.5(2)
C13	4015.2(11)	6795.3(11)	420.7(8)	23.2(2)

C14	3489.2(12)	4712.3(11)	2070.3(8)	23.1(2)
C15	2670.8(11)	3951.1(11)	1555.2(8)	21.3(2)
C16	2485.6(11)	4590.6(11)	500.4(8)	22.4(2)
C17	2022.1(11)	2542.5(11)	2118.1(8)	22.2(2)
N18	721.6(10)	284.4(9)	2125.8(7)	23.55(19)
C19	1904.8(11)	-812.4(11)	2379.7(8)	24.1(2)
C20	1158.8(12)	-2181.6(11)	3161.3(8)	26.0(2)
N21	57.4(10)	-2827.3(9)	2726.6(7)	24.2(2)
C22	-1093.7(12)	-1733.4(12)	2435.4(9)	27.9(2)
C23	-337.4(13)	-358.4(12)	1655.9(9)	27.7(2)
C24	-638.3(13)	-4143.5(12)	3501.7(8)	27.1(2)
C25	-1551.8(12)	-5067.5(11)	3042.8(8)	25.7(2)
C26	-2334.5(11)	-6375.8(11)	3871.3(8)	23.3(2)
C27	-3440.6(12)	-6177.5(12)	4735.7(8)	26.4(2)
C28	-4202.2(12)	-7361.3(13)	5495.0(9)	29.2(2)
C29	-3861.6(13)	-8776.9(12)	5395.1(9)	30.1(2)
C30	-2749.1(14)	-8992.5(12)	4546.4(9)	31.5(2)
C31	-1989.3(12)	-7804.5(12)	3792.3(9)	27.0(2)
O32	5018.4(10)	6779.5(9)	1925.8(6)	33.8(2)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$). The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	32.6(5)	25.5(5)	24.4(5)	-5.0(4)	-11.0(4)	-2.1(4)
C2	32.2(5)	25.4(5)	28.5(5)	-7.6(4)	-11.8(4)	-4.0(4)
C3	22.6(5)	21.1(5)	26.4(5)	-7.3(4)	-5.0(4)	-0.5(4)

C4	31.6(5)	22.2(5)	24.6(5)	-5.7(4)	-5.5(4)	-0.6(4)
C5	41.3(6)	26.6(5)	22.2(5)	-6.5(4)	-10.7(4)	0.2(4)
C6	35.0(6)	25.3(5)	26.5(5)	-10.2(4)	-11.0(4)	-0.4(4)
C7	26.6(5)	23.5(5)	26.7(5)	-10.7(4)	-6.7(4)	0.7(4)
C8	26.2(5)	23.5(5)	30.2(5)	-9.5(4)	-5.1(4)	-1.4(4)
C9	27.6(5)	23.4(5)	31.0(5)	-4.8(4)	-3.0(4)	-2.2(4)
C10	29.9(5)	26.9(5)	26.1(5)	-2.8(4)	-6.7(4)	0.3(4)
C11	29.7(5)	25.1(5)	27.4(5)	-5.9(4)	-9.5(4)	-0.9(4)
C12	22.2(5)	21.4(5)	24.6(5)	-7.2(4)	-4.9(4)	1.9(4)
C13	23.2(5)	21.4(5)	25.7(5)	-8.1(4)	-4.5(4)	1.7(4)
C14	25.5(5)	21.7(5)	24.4(5)	-8.8(4)	-6.9(4)	1.8(4)
C15	21.3(4)	20.8(5)	23.2(5)	-8.3(4)	-4.9(4)	2.5(4)
C16	23.3(5)	20.9(5)	24.3(5)	-6.8(4)	-6.5(4)	1.4(4)
C17	22.6(5)	21.3(5)	24.3(5)	-8.2(4)	-5.9(4)	2.0(4)
N18	24.1(4)	20.3(4)	28.0(4)	-6.4(3)	-8.2(3)	-1.7(3)
C19	22.8(5)	22.2(5)	28.3(5)	-6.7(4)	-6.9(4)	-0.8(4)
C20	27.3(5)	23.9(5)	28.3(5)	-5.3(4)	-9.9(4)	-3.0(4)
N21	25.6(4)	21.3(4)	26.5(4)	-4.4(3)	-8.2(3)	-3.3(3)
C22	25.3(5)	24.4(5)	35.0(6)	-6.3(4)	-9.3(4)	-2.9(4)
C23	29.1(5)	23.1(5)	33.2(5)	-5.1(4)	-13.4(4)	-2.3(4)
C24	31.1(5)	25.2(5)	25.4(5)	-4.0(4)	-8.6(4)	-5.5(4)
C25	29.2(5)	24.4(5)	24.0(5)	-5.4(4)	-6.5(4)	-4.6(4)
C26	23.2(5)	24.6(5)	24.0(5)	-5.6(4)	-8.8(4)	-2.4(4)
C27	25.9(5)	25.8(5)	29.0(5)	-7.9(4)	-7.4(4)	-0.2(4)
C28	26.0(5)	36.1(6)	25.5(5)	-7.2(4)	-5.0(4)	-3.3(4)

C29	33.2(5)	29.3(5)	26.9(5)	-0.5(4)	-10.1(4)	-9.3(4)
C30	39.5(6)	22.5(5)	34.1(6)	-6.9(4)	-11.0(5)	-2.3(4)
C31	28.4(5)	26.8(5)	27.4(5)	-9.5(4)	-5.4(4)	-1.9(4)
O32	44.1(5)	30.2(4)	31.6(4)	-8.9(3)	-14.1(3)	-9.7(3)

Table S4. Bond Lengths for 3-[4-(2-phenylethyl)piperazin-1-yl]-7*H*-benzo[*de*]anthracen-7-one.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.4042(14)	C14	C15	1.4238(14)
C1	C16	1.3794(14)	C15	C16	1.4288(14)
C2	C3	1.3783(15)	C15	C17	1.4272(14)
C3	C17	1.4435(14)	N18	C19	1.4743(13)
C3	N18	1.4133(13)	N18	C23	1.4643(13)
C4	C5	1.3772(15)	C19	C20	1.5141(14)
C4	C17	1.4151(14)	C20	N21	1.4637(12)
C5	C6	1.3961(15)	N21	C22	1.4628(14)
C6	C14	1.3820(15)	N21	C24	1.4619(13)
C7	C13	1.4792(15)	C22	C23	1.5200(14)
C7	C14	1.4813(14)	C24	C25	1.5292(14)
C7	O32	1.2306(13)	C25	C26	1.5116(13)
C8	C9	1.3800(16)	C26	C27	1.3921(15)
C8	C13	1.3992(14)	C26	C31	1.3918(15)
C9	C10	1.3945(15)	C27	C28	1.3900(15)
C10	C11	1.3816(15)	C28	C29	1.3869(16)
C11	C12	1.4056(15)	C29	C30	1.3855(17)
C12	C13	1.4094(14)	C30	C31	1.3890(15)

C12	C16	1.4711(14)			

Table S5. Bond Angles for 3-[4-(2-phenylethyl)piperazin-1-yl]-7*H*-benzo[*de*]anthracen-7-one.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C16	C1	C2	122.27(10)	C1	C16	C12	122.58(9)
C3	C2	C1	121.61(9)	C1	C16	C15	117.73(9)
C2	C3	C17	118.11(9)	C15	C16	C12	119.69(9)
C2	C3	N18	122.83(9)	C4	C17	C3	122.06(9)
N18	C3	C17	119.01(9)	C4	C17	C15	118.57(9)
C5	C4	C17	121.28(10)	C15	C17	C3	119.34(9)
C4	C5	C6	120.09(10)	C3	N18	C19	115.83(8)
C14	C6	C5	120.54(10)	C3	N18	C23	116.28(8)
C13	C7	C14	117.23(9)	C23	N18	C19	107.95(8)
O32	C7	C13	121.39(10)	N18	C19	C20	110.08(8)
O32	C7	C14	121.37(10)	N21	C20	C19	110.92(8)
C9	C8	C13	120.82(10)	C22	N21	C20	109.25(8)
C8	C9	C10	119.13(10)	C24	N21	C20	109.35(8)
C11	C10	C9	120.60(10)	C24	N21	C22	112.16(8)
C10	C11	C12	121.35(10)	N21	C22	C23	111.10(8)
C11	C12	C13	117.49(9)	N18	C23	C22	109.97(8)
C11	C12	C16	122.13(9)	N21	C24	C25	113.15(8)
C13	C12	C16	120.37(9)	C26	C25	C24	112.25(8)
C8	C13	C7	118.45(9)	C27	C26	C25	120.44(9)
C8	C13	C12	120.55(10)	C31	C26	C25	121.51(9)
C12	C13	C7	121.00(9)	C31	C26	C27	118.05(10)

C6	C14	C7	118.59(9)	C28	C27	C26	121.53(10)
C6	C14	C15	120.55(10)	C29	C28	C27	119.67(10)
C15	C14	C7	120.85(9)	C30	C29	C28	119.46(10)
C14	C15	C16	120.74(9)	C29	C30	C31	120.56(10)
C14	C15	C17	118.68(9)	C30	C31	C26	120.72(10)
C17	C15	C16	120.58(9)				

Table S6. Torsion Angles for 3-[4-(2-phenylethyl)piperazin-1-yl]-7*H*-benzo[*de*]anthracen-7-one.

A	B	C	D	Angle/˚	A	B	C	D	Angle/˚
C1	C2	C3	C17	3.98(16)	C14	C15	C17	C4	5.68(14)
C1	C2	C3	N18	-178.92(9)	C16	C1	C2	C3	1.33(18)
C2	C1	C16	C12	176.53(9)	C16	C12	C13	C7	0.67(15)
C2	C1	C16	C15	-3.63(16)	C16	C12	C13	C8	-179.58(9)
C2	C3	C17	C4	171.31(10)	C16	C15	C17	C3	4.62(15)
C2	C3	C17	C15	-6.82(15)	C16	C15	C17	C4	-173.58(9)
C2	C3	N18	C19	117.14(11)	C17	C3	N18	C19	-65.79(12)
C2	C3	N18	C23	-11.24(15)	C17	C3	N18	C23	165.83(9)
C3	N18	C19	C20	167.19(8)	C17	C4	C5	C6	0.50(17)
C3	N18	C23	C22	-167.70(8)	C17	C15	C16	C1	0.58(15)
C4	C5	C6	C14	3.23(17)	C17	C15	C16	C12	-179.57(8)
C5	C4	C17	C3	176.90(10)	N18	C3	C17	C4	-5.90(15)
C5	C4	C17	C15	-4.96(15)	N18	C3	C17	C15	175.97(8)
C5	C6	C14	C7	178.14(9)	N18	C19	C20	N21	59.75(11)
C5	C6	C14	C15	-2.36(16)	C19	N18	C23	C22	60.18(11)
C6	C14	C15	C16	177.12(9)	C19	C20	N21	C22	-56.89(11)

C6	C14	C15	C17	-2.14(15)	C19	C20	N21	C24	-179.99(8)
C7	C14	C15	C16	-3.39(15)	C20	N21	C22	C23	56.80(11)
C7	C14	C15	C17	177.34(8)	C20	N21	C24	C25	-168.23(9)
C8	C9	C10	C11	2.19(16)	N21	C22	C23	N18	-59.68(11)
C9	C8	C13	C7	179.84(9)	N21	C24	C25	C26	-176.77(8)
C9	C8	C13	C12	0.08(16)	C22	N21	C24	C25	70.42(11)
C9	C10	C11	C12	-0.43(17)	C23	N18	C19	C20	-60.44(10)
C10	C11	C12	C13	-1.47(15)	C24	N21	C22	C23	178.22(8)
C10	C11	C12	C16	179.77(9)	C24	C25	C26	C27	61.82(13)
C11	C12	C13	C7	-178.11(9)	C24	C25	C26	C31	-118.80(11)
C11	C12	C13	C8	1.65(15)	C25	C26	C27	C28	178.49(9)
C11	C12	C16	C1	-1.25(16)	C25	C26	C31	C30	-178.29(9)
C11	C12	C16	C15	178.91(9)	C26	C27	C28	C29	-0.09(15)
C13	C7	C14	C6	-176.40(9)	C27	C26	C31	C30	1.11(15)
C13	C7	C14	C15	4.10(14)	C27	C28	C29	C30	0.92(16)
C13	C8	C9	C10	-2.01(16)	C28	C29	C30	C31	-0.73(17)
C13	C12	C16	C1	-179.97(9)	C29	C30	C31	C26	-0.30(16)
C13	C12	C16	C15	0.20(15)	C31	C26	C27	C28	-0.92(15)
C14	C7	C13	C8	177.50(9)	O32	C7	C13	C8	-2.18(15)
C14	C7	C13	C12	-2.74(14)	O32	C7	C13	C12	177.58(10)
C14	C15	C16	C1	-178.67(9)	O32	C7	C14	C6	3.28(16)
C14	C15	C16	C12	1.18(15)	O32	C7	C14	C15	-176.22(9)
C14	C15	C17	C3	-176.12(9)					

Table S7. Hydrogen Atom Coordinates (Å×104) and Isotropic Displacement Parameters (Å2×103).

Atom	*x*	*y*	*z*	*U*(iso)
H1	1466.51	4239.64	-628.07	32
H2	520.69	1886.64	238.06	33
H4	1598.75	1118.78	3594.09	31
H5	2922.06	2413.73	4401.25	35
H6	4189.08	4619.84	3432.91	33
H8	5228.13	8673.41	224.77	31
H9	4902.93	9782.06	-1481.04	34
H10	3604.15	8499.58	-2341.27	34
H11	2509.21	6214.76	-1467.94	32
H19A	2650.47	-397.95	2686.15	29
H19B	2472.24	-1064.51	1724.61	29
H20A	1963.2	-2906.37	3332.75	31
H20B	620.76	-1931.9	3824.14	31
H22A	-1692.97	-1473.81	3079.35	33
H22B	-1815.45	-2154.42	2114.32	33
H23A	234.24	-607.77	1000.85	33
H23B	-1137.34	362.35	1467.11	33
H24A	-1332.64	-3848.69	4099.71	32
H24B	184.8	-4751.83	3783.3	32
H25A	-2339.62	-4447.37	2725.71	31
H25B	-847.07	-5414.66	2473.08	31
H27	-3680.41	-5210.58	4808.36	32
H28	-4952.18	-7201.56	6079.38	35

H29	-4386.8	-9592.17	5904.54	36
H30	-2503.97	-9960.97	4479.56	38
H31	-1225.59	-7969.05	3216.3	32

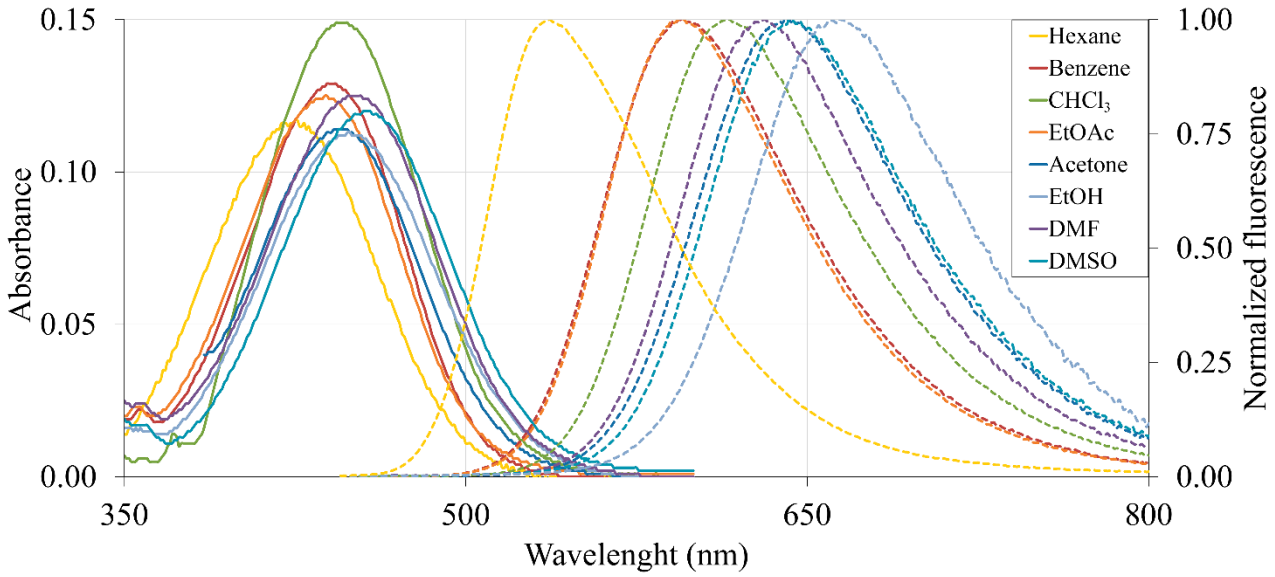

Figure S2. The absorption and emission spectra of dye **2** in various organic solvents.