Supplementary Materials

3-[N-(4-Methoxybenzyl)amino]benzo[*de*]anthracen-7-one

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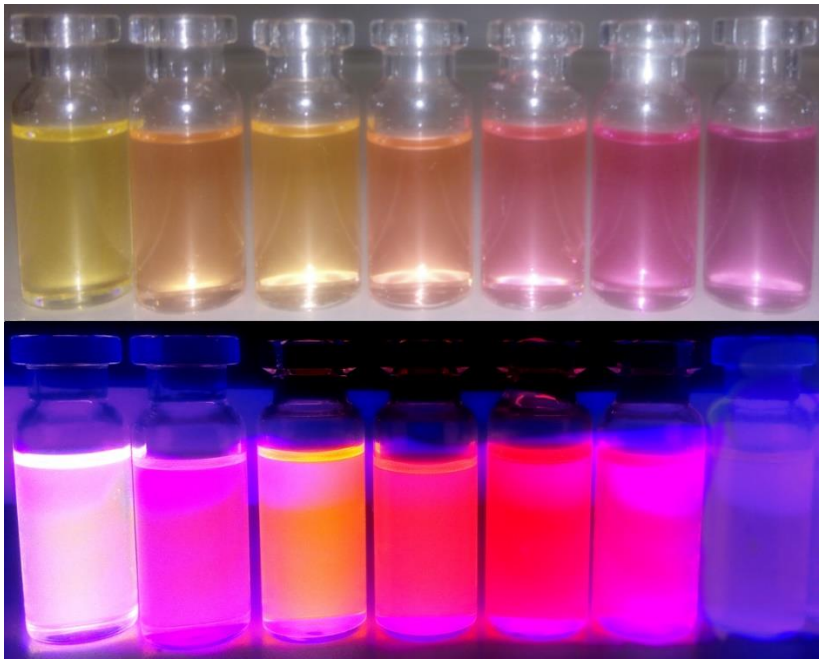


Figure S1. Solutions of synthesized amine **3** in benzene, chloroform, ethyl acetate, acetone, dimethylformamide, dimethyl sulfoxide, and ethanol in visible and UV light (365 nm).

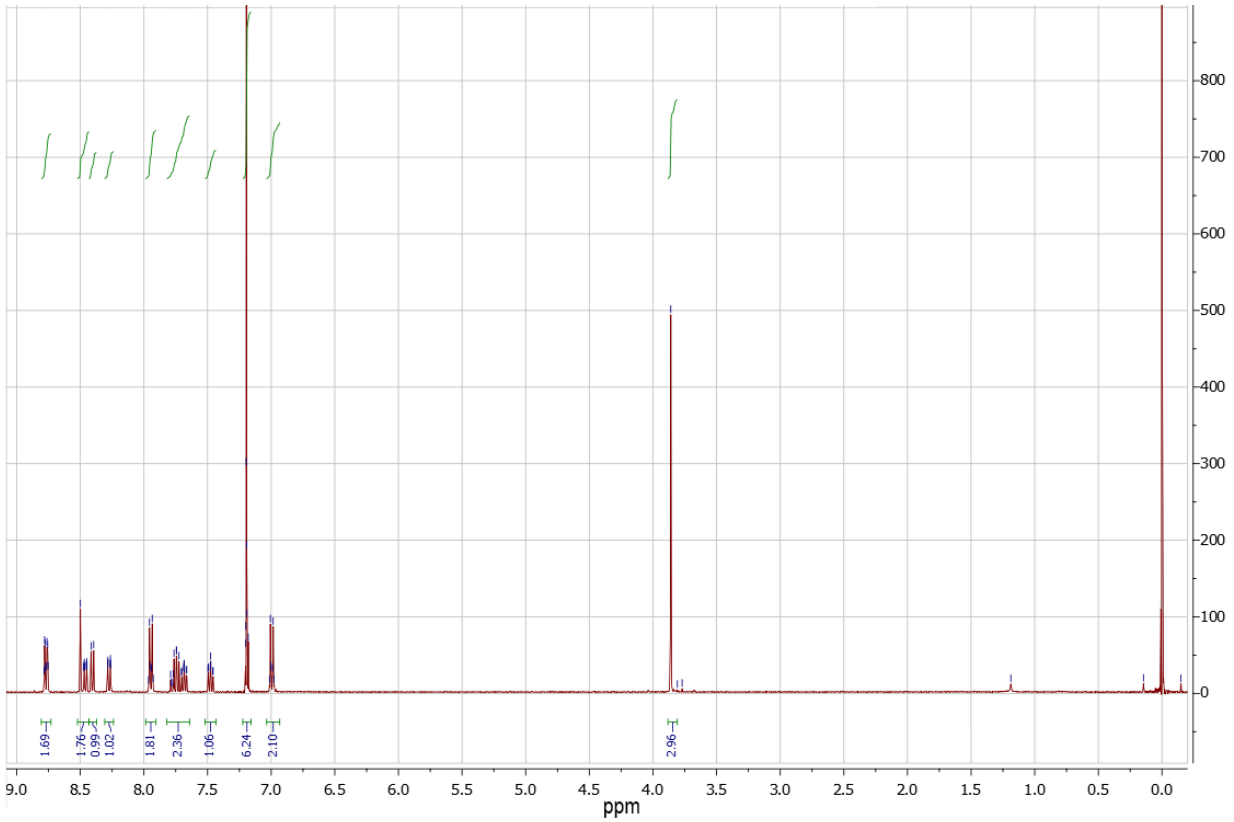


Figure S2. [1]H NMR spectrum of 3-[N-(4-methoxybenzyledene)amino]benzo[*de*]anthracen-7-one (**2**).

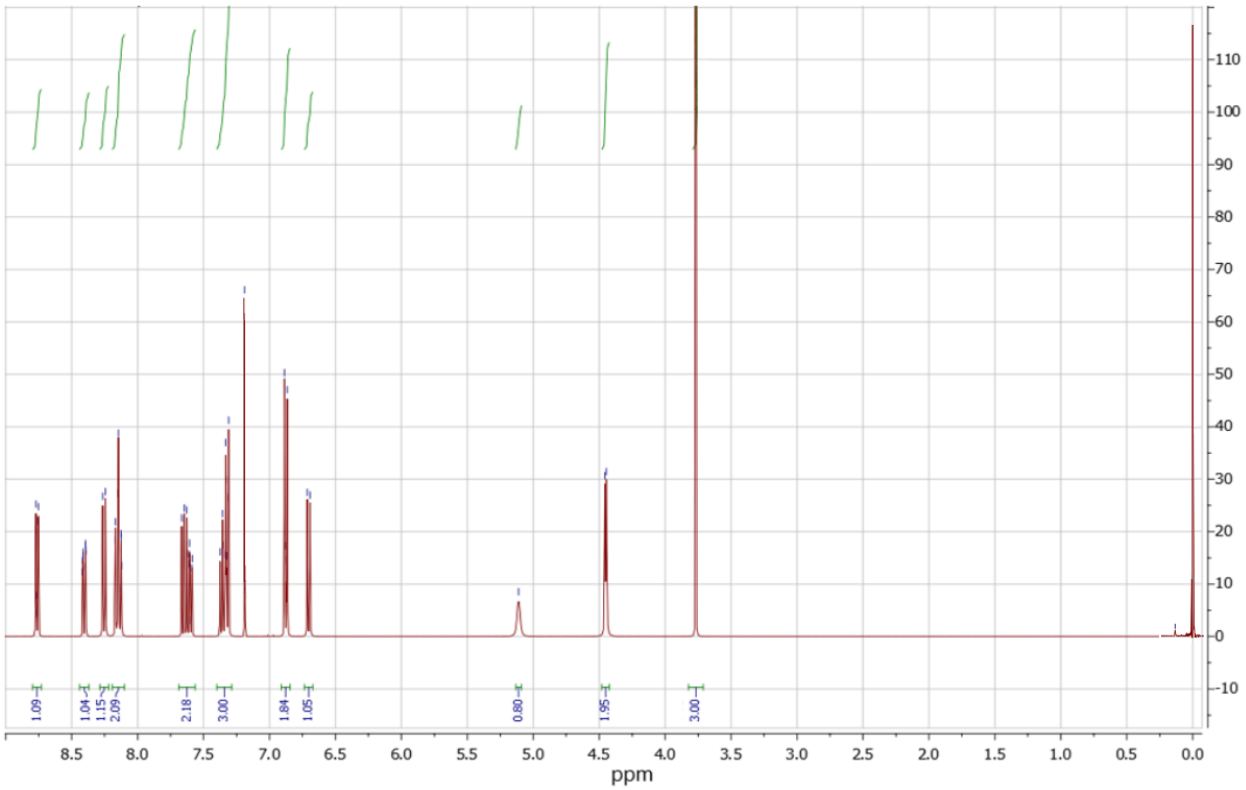


Figure S3. [1]H NMR spectrum of 3-[N-(4-methoxybenzyl)amino]benzo[*de*]anthracen-7-one (**3**).

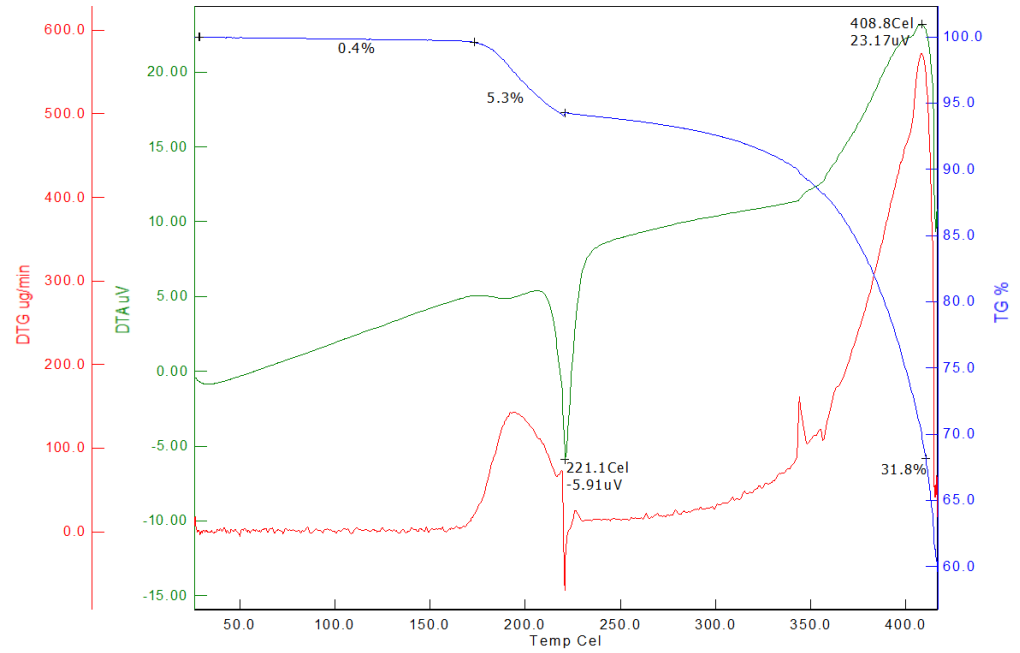


Figure S4. Simultaneous TG-DTA curves for 3-[N-(4-methoxybenzyledene)amino]benzo[*de*]anthracen-7-one (**2**).

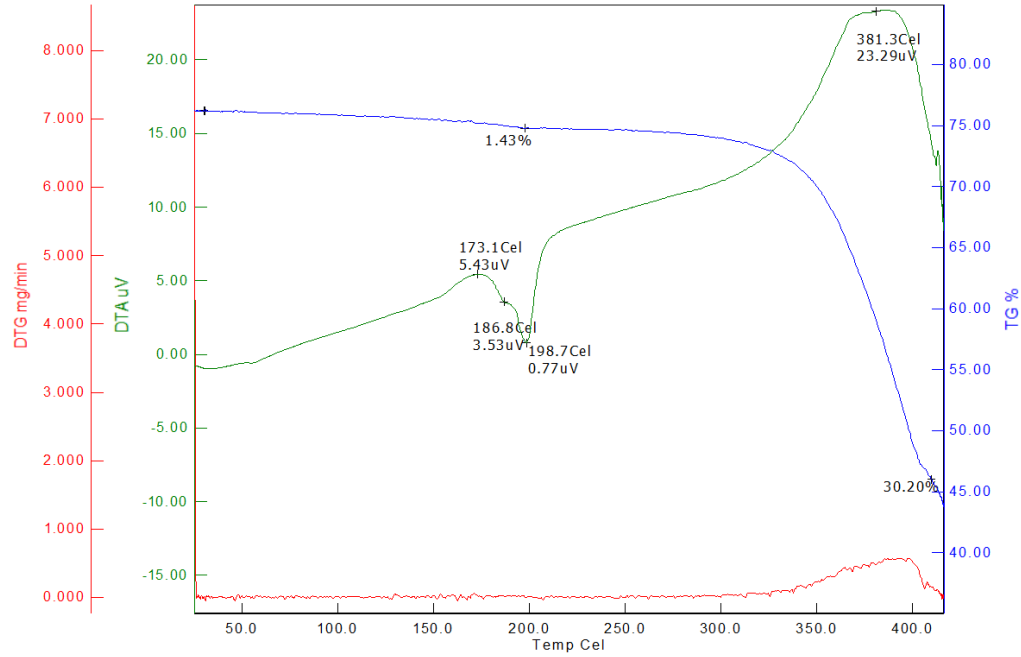


Figure S5. Simultaneous TG-DTA curves for 3-[N-(4-methoxybenzyl)amino]benzo[*de*]anthracen-7-one (**3**).

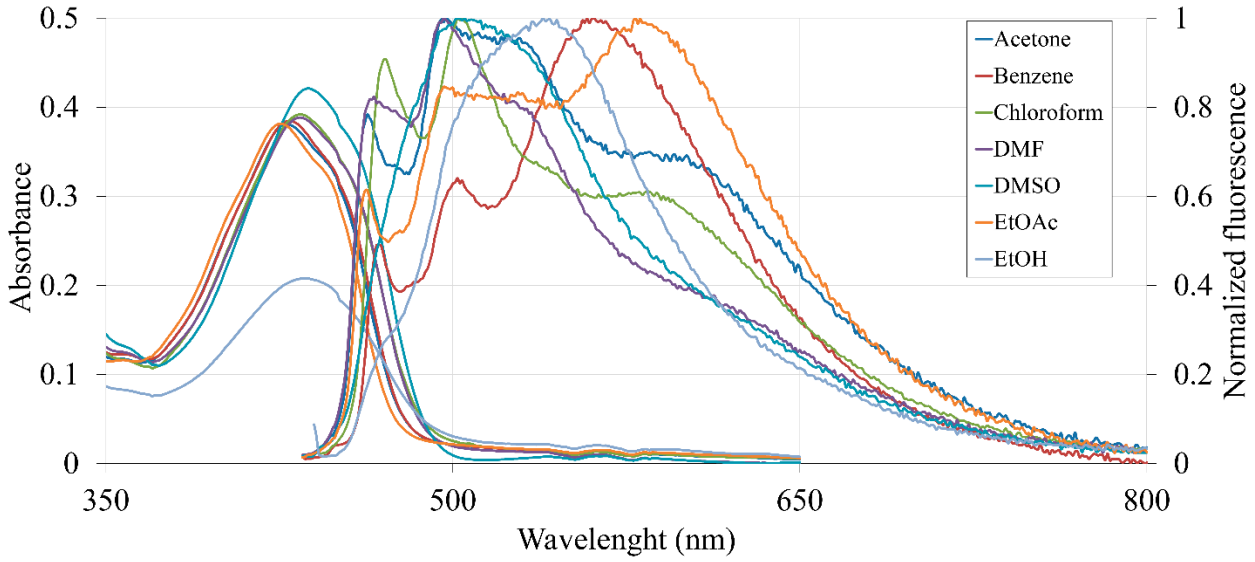


Figure S6. The absorption and emission (λ_{exc}=425 nm) spectra of 3-[N-(4-methoxybenzyledene)amino]-benzo[*de*]anthracen-7-one (**2**) in various organic solvents.

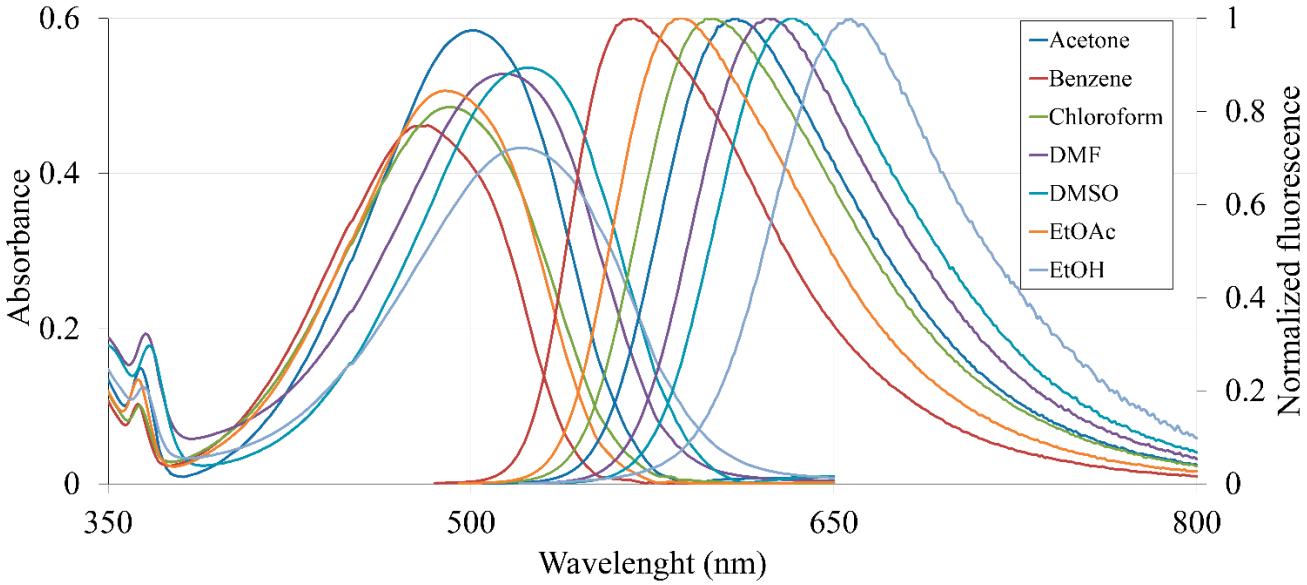


Figure S7. The absorption and emission (λ_{exc}=480 nm) spectra of 3-[N-(4-methoxybenzyl)amino]-benzo[*de*]anthracen-7-one (**3**) in various organic solvents.

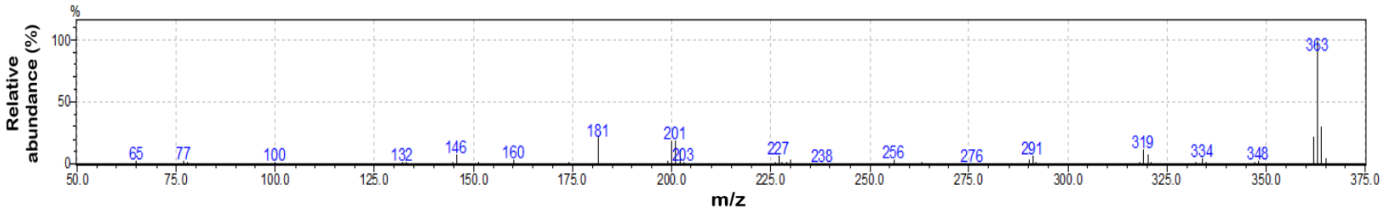


Figure S8. Mass spectrum of 3-[N-(4-methoxybenzyl)amino]benzo[*de*]anthracen-7-one (**3**).

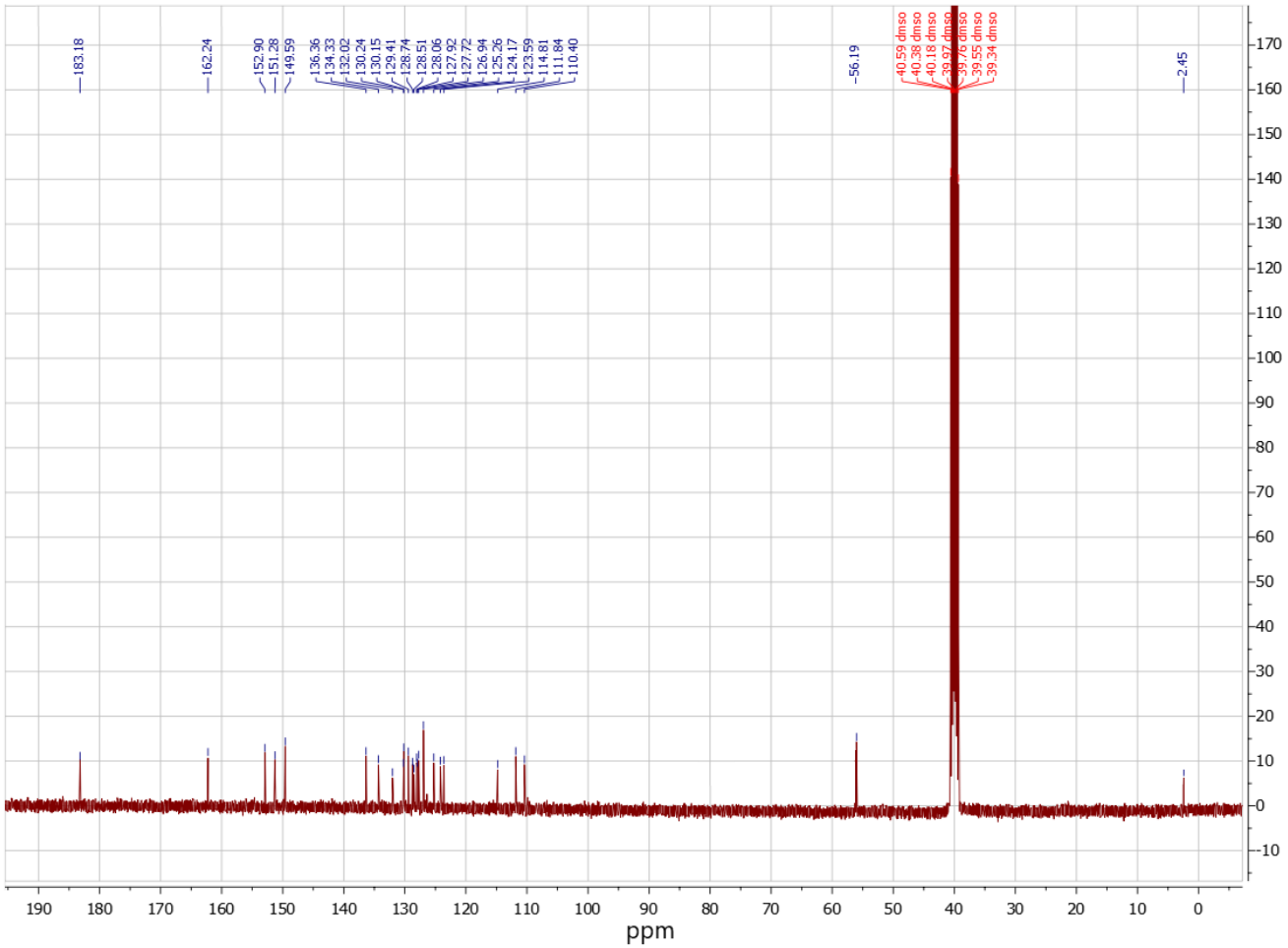


Figure S9. ^{13}C NMR spectrum of 3-[N-(4-methoxybenzyledene)amino]benzo[*de*]anthracen-7-one (**2**).

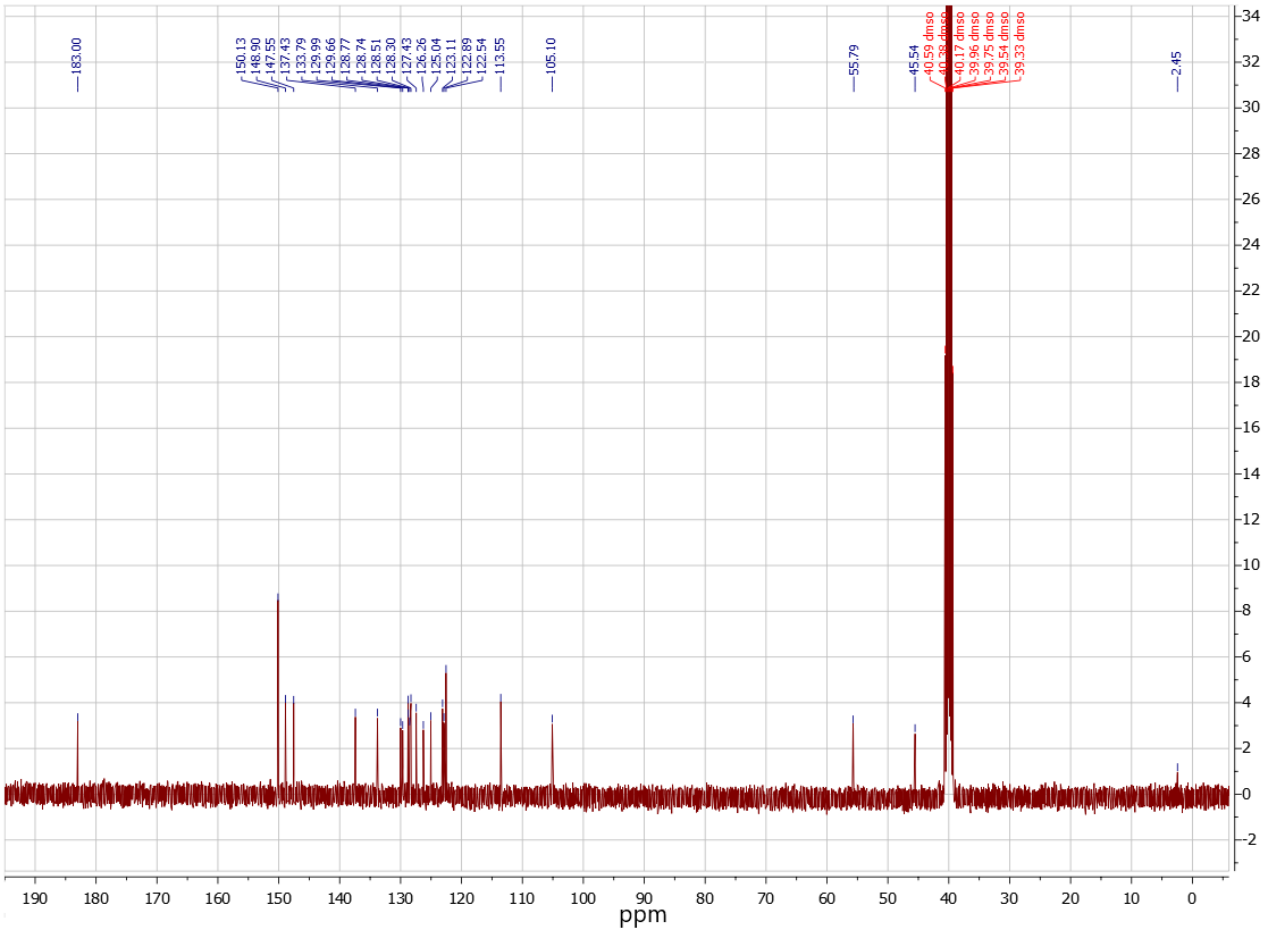
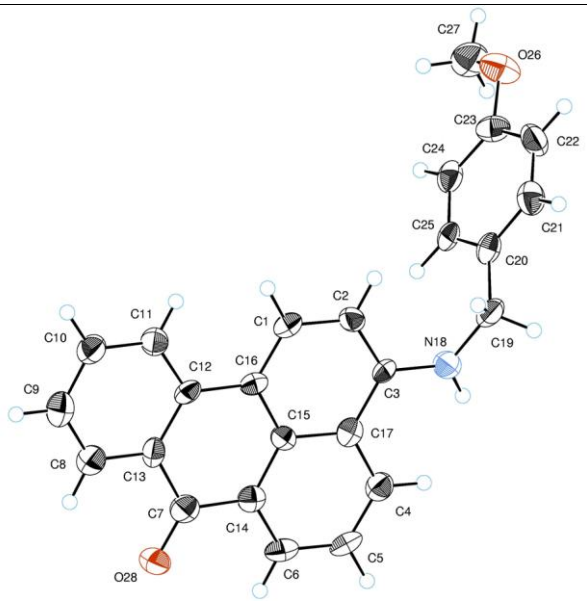


Figure S10. ^{13}C NMR spectrum of 3-[N-(4-methoxybenzyl)amino]benzo[*de*]anthracen-7-one (**3**).

Table S1. Crystal data and structure refinement parameters for 3-[N-(4-methoxybenzyl)amino]benzo[*de*]-anthracen-7-one (**3**).

Parameter	
ORTEP	

Empirical formula	$C_{25}H_{19}NO_2$
Formula weight	365.41
Difractometer	Bruker–Nonius KappaCCD
Radiation	Mo Kα (λ = 0.71073 Å)
Temperature (K)	173 (1)
Crystal size (mm^3)	0.43×0.07×0.02
Crystal system	Monoclinic
Space group	*P* 21
a (Å)	5.1595(4)
b (Å)	13.9950(9)
c (Å)	12.479(1)
β (°)	94.725(3)
Unit cell volume ($Å^3$)	898.01(12)
Molecular multiplicity	2
Calculated density (g/cm^3)	1.351
Absorption coefficient (mm^{-1})	0.086
F(000)	384
$2\theta_{max}$ (°)	57.0
Reflections collected	2812
Number of independent reflections	2361 (R_{int} = 0.0464)
Reflections with $I>2\sigma(I)$	2361
Number of refined parameters	258
Goodness of fit	1.028
R-factors (*R*1 for $I>2\sigma(I)$, and *wR*2 for all data)	0.0664, 0.1182
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.180, –0.229
CCDC deposition number	2106683

Table S2. Bond lengths and angles for 3-[N-(4-methoxybenzyl)amino]benzo[*de*]anthracen-7-one (**3**).

Bond length [Å]		Angle [deg]	
C(1)-C(16)	1.381(6)	C(16)-C(1)-C(2)	121.4(4)
C(1)-C(2)	1.401(6)	C(16)-C(1)-H(1)	119.3
C(1)-H(1)	0.9300	C(2)-C(1)-H(1)	119.3
C(2)-C(3)	1.390(6)	C(3)-C(2)-C(1)	121.7(4)

C(2)-H(2)	0.9300	C(3)-C(2)-H(2)	119.2
C(3)-N(18)	1.362(6)	C(1)-C(2)-H(2)	119.2
C(3)-C(17)	1.436(6)	N(18)-C(3)-C(2)	120.7(4)
C(4)-C(5)	1.353(7)	N(18)-C(3)-C(17)	120.1(4)
C(4)-C(17)	1.395(7)	C(2)-C(3)-C(17)	119.1(4)
C(4)-H(4)	0.9300	C(5)-C(4)-C(17)	120.8(5)
C(5)-C(6)	1.391(7)	C(5)-C(4)-H(4)	119.6
C(5)-H(5)	0.9300	C(17)-C(4)-H(4)	119.6
C(6)-C(14)	1.367(6)	C(4)-C(5)-C(6)	121.3(5)
C(6)-H(6)	0.9300	C(4)-C(5)-H(5)	119.3
C(7)-O(28)	1.243(6)	C(6)-C(5)-H(5)	119.3
C(7)-C(13)	1.471(7)	C(14)-C(6)-C(5)	120.2(5)
C(7)-C(14)	1.482(7)	C(14)-C(6)-H(6)	119.9
C(8)-C(9)	1.374(7)	C(5)-C(6)-H(6)	119.9
C(8)-C(13)	1.384(7)	O(28)-C(7)-C(13)	120.9(4)
C(8)-H(8)	0.9300	O(28)-C(7)-C(14)	121.3(5)
C(9)-C(10)	1.392(7)	C(13)-C(7)-C(14)	117.8(4)
C(9)-H(9)	0.9300	C(9)-C(8)-C(13)	121.0(5)
C(10)-C(11)	1.390(7)	C(9)-C(8)-H(8)	119.5
C(10)-H(10)	0.9300	C(13)-C(8)-H(8)	119.5
C(11)-C(12)	1.403(6)	C(8)-C(9)-C(10)	120.1(5)
C(11)-H(11)	0.9300	C(8)-C(9)-H(9)	120.0
C(12)-C(13)	1.415(7)	C(10)-C(9)-H(9)	120.0
C(12)-C(16)	1.465(6)	C(11)-C(10)-C(9)	119.1(5)
C(14)-C(15)	1.411(6)	C(11)-C(10)-H(10)	120.5
C(15)-C(16)	1.432(6)	C(9)-C(10)-H(10)	120.5
C(15)-C(17)	1.447(6)	C(10)-C(11)-C(12)	122.1(5)
N(18)-C(19)	1.455(6)	C(10)-C(11)-H(11)	118.9
N(18)-H(18)	0.88(5)	C(12)-C(11)-H(11)	118.9
C(19)-C(20)	1.512(7)	C(11)-C(12)-C(13)	117.0(4)
C(19)-H(19A)	0.9700	C(11)-C(12)-C(16)	121.9(4)
C(20)-C(25)	1.382(6)	C(13)-C(12)-C(16)	121.1(4)
C(20)-C(21)	1.398(7)	C(8)-C(13)-C(12)	120.6(5)
C(21)-C(22)	1.365(7)	C(8)-C(13)-C(7)	118.9(4)
C(21)-H(21)	0.9300	C(12)-C(13)-C(7)	120.4(4)
C(22)-C(23)	1.389(8)	C(6)-C(14)-C(15)	120.8(4)
C(22)-H(22)	0.9300	C(6)-C(14)-C(7)	119.0(4)
C(23)-O(26)	1.365(6)	C(15)-C(14)-C(7)	120.2(4)
C(23)-C(24)	1.375(7)	C(14)-C(15)-C(16)	122.0(4)
C(24)-C(25)	1.399(7)	C(14)-C(15)-C(17)	118.1(4)
C(24)-H(24)	0.9300	C(16)-C(15)-C(17)	119.9(4)
C(25)-H(25)	0.9300	C(1)-C(16)-C(15)	119.1(4)
O(26)-C(27)	1.425(7)	C(1)-C(16)-C(12)	122.5(4)
C(27)-H(27A)	0.9600	C(15)-C(16)-C(12)	118.4(4)
C(27)-H(27C)	0.9600	C(4)-C(17)-C(3)	122.5(4)
		C(4)-C(17)-C(15)	118.8(4)
		C(3)-C(17)-C(15)	118.7(4)
		C(3)-N(18)-C(19)	122.8(4)
		C(3)-N(18)-H(18)	117(3)
		C(19)-N(18)-H(18)	119(3)

	N(18)-C(19)-C(20) 116.8(4) N(18)-C(19)-H(19A) 108.1 H(19A)-C(19)-H(19B) 107.3 C(25)-C(20)-C(21) 117.1(5) C(25)-C(20)-C(19) 123.9(5) C(21)-C(20)-C(19) 119.0(4) C(22)-C(21)-C(20) 121.0(4) C(22)-C(21)-H(21) 119.5 C(20)-C(21)-H(21) 119.5 C(21)-C(22)-C(23) 121.5(5) C(23)-C(22)-H(22) 119.2 O(26)-C(23)-C(24) 126.0(5) O(26)-C(23)-C(22) 115.3(5) C(24)-C(23)-C(22) 118.7(5) C(23)-C(24)-C(25) 119.5(5) C(23)-C(24)-H(24) 120.2 C(20)-C(25)-C(24) 122.1(5) C(20)-C(25)-H(25) 118.9 C(23)-O(26)-C(27) 116.4(4) O(26)-C(27)-H(27A) 109.5 H(27B)-C(27)-H(27C) 109.5