Supplementary Content

Coumarin-Pterocarpan Conjugate- A Natural Product Inspired Hybrid Molecular Probe for DNA Recognition

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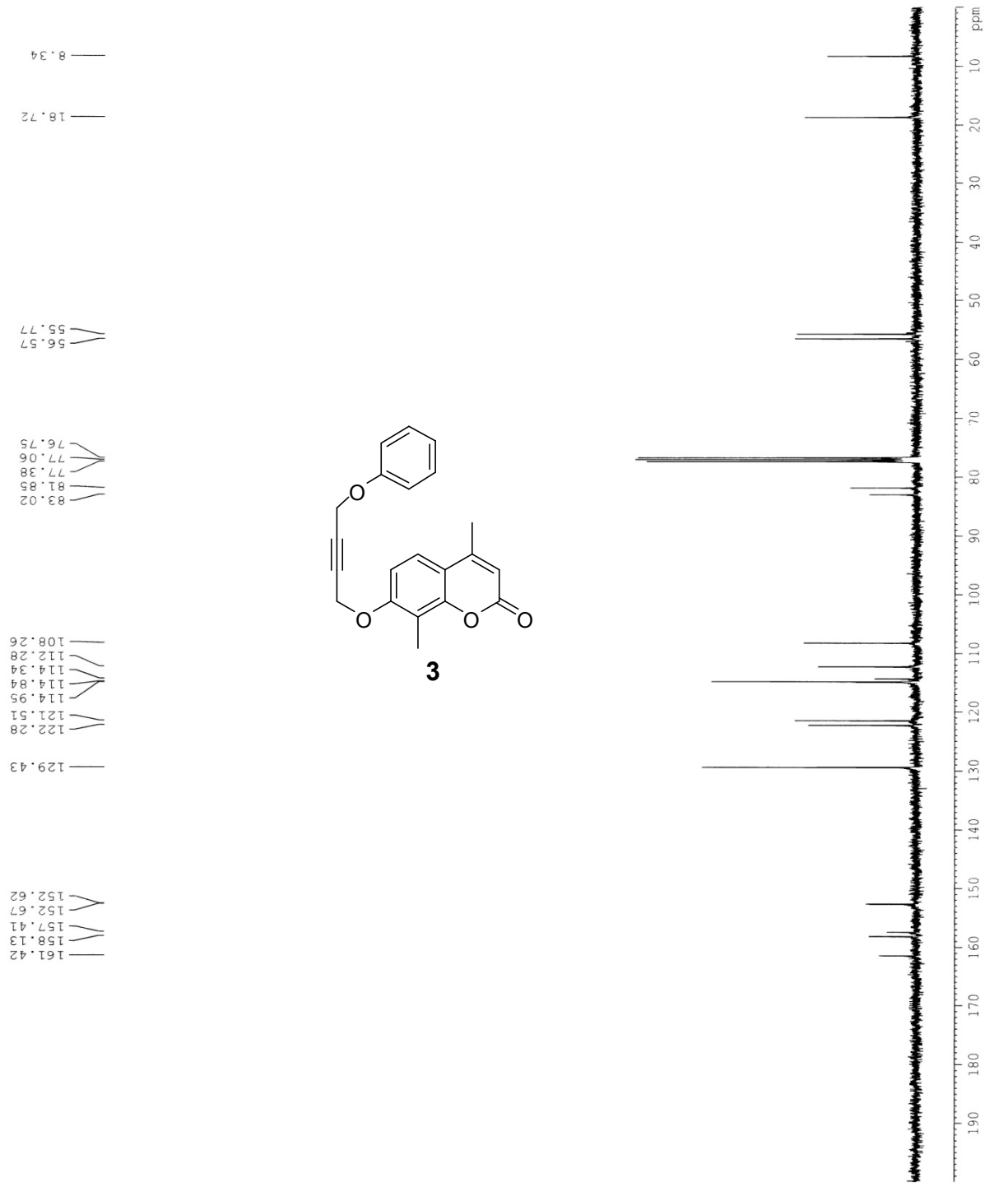
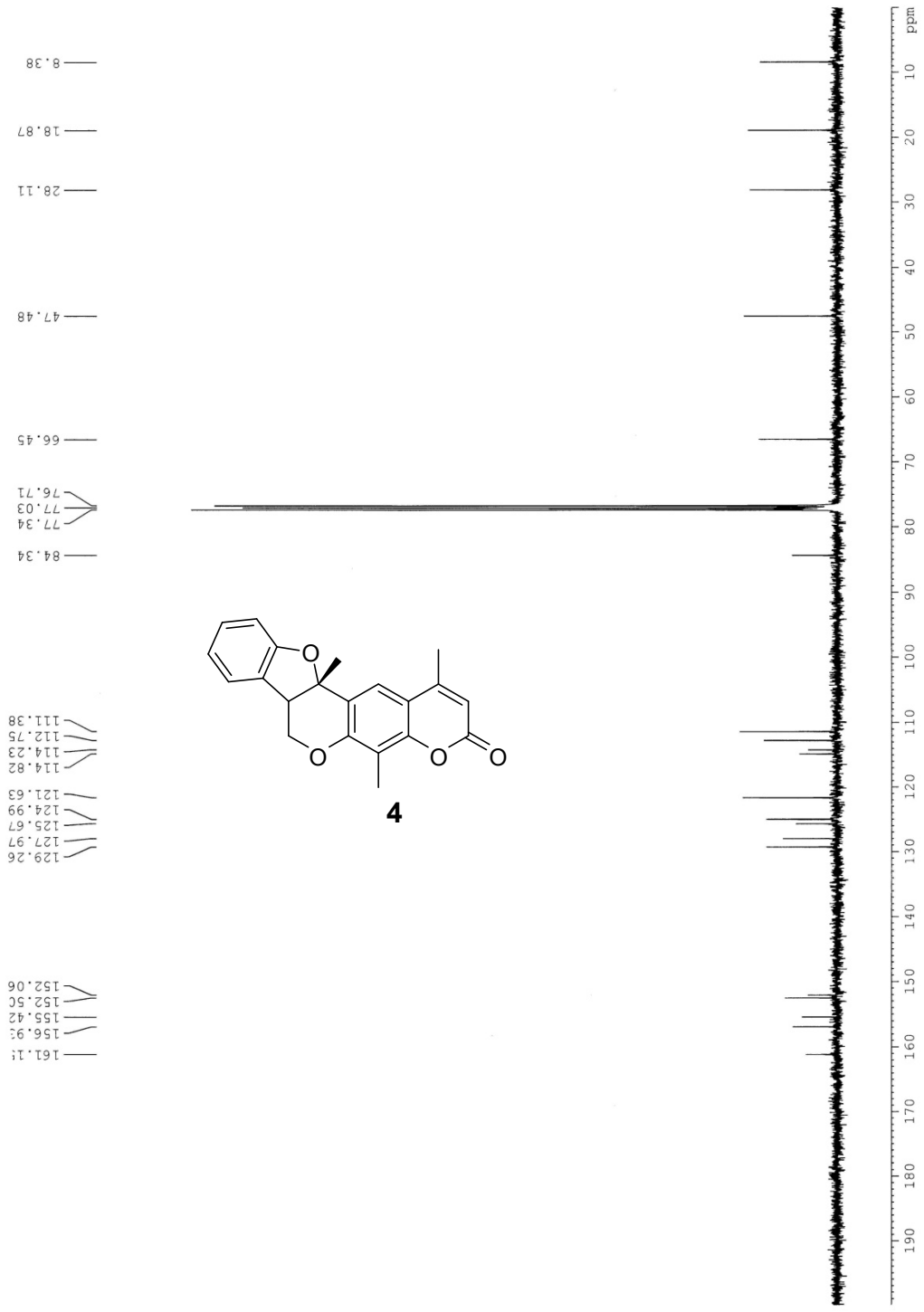
^{1}H NMR spectrum (500 MHz, $CDCl_3$) of compound **3**



1

^{3}C NMR spectrum (100 MHz, $CDCl_3$) of compound **3**

^{1}H NMR spectrum (400 MHz, $CDCl_3$) of compound **4**



4

^{13}C NMR spectrum (100 MHz, $CDCl_3$) of compound **4**

Determination of Molar Extinction coefficiet of compound 4 in buffer & DMSO

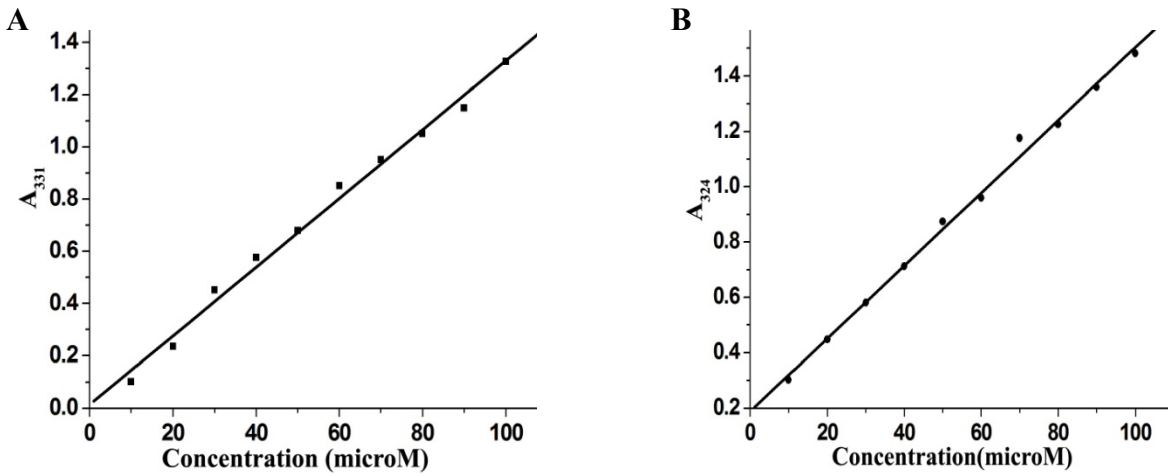
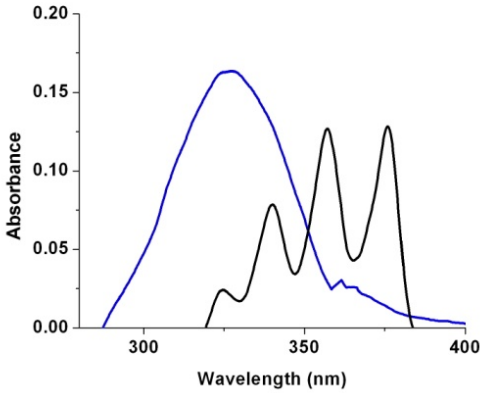
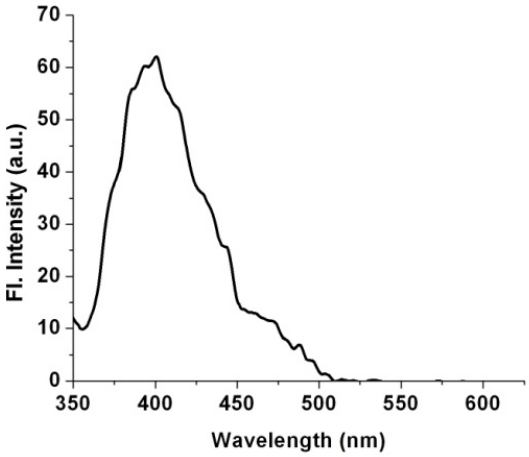


Fig 8. (A) Plot of Absorbance (331nm) vs. Concentration (micro M) for **4** in buffer; (B) Plot of Absorbance (324nm) vs. Concentration (microM) for **4** in DMSO.

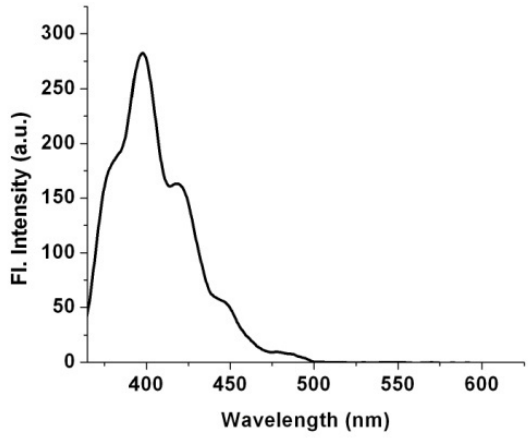
Determination of Quantum Yield of 4



Absorbance spectrum of anthracene in cyclohexane solution (black) and compound 4 in aq sodium cacodylate buffer solution (blue).



Fluorescence spectrum of **4** in aqueous buffer solution (λ_{ex} = 331 nm.)



Fluorescence spectrum of anthracene in cyclohexane solution (λ_{ex} = 356 nm.)

Co-ordinates of standard orientation of **4** obtained from DFT calculation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.227400	-0.156300	-0.325700
2	6	0	0.249900	-1.561000	-0.353500
3	6	0	1.496500	-2.208100	-0.293200
4	6	0	2.713400	-1.502400	-0.254900
5	6	0	2.670600	-0.098000	-0.239800
6	6	0	1.427100	0.550000	-0.258600
7	8	0	3.883800	-2.210300	-0.225900
8	6	0	5.047300	-1.507900	-0.206400
9	6	0	5.081400	-0.030400	-0.197600
10	6	0	3.924000	0.669300	-0.211100
11	6	0	3.948400	2.179400	-0.216000
12	8	0	6.123300	-2.102800	-0.198900
13	6	0	-1.081600	0.598800	-0.439400
14	6	0	-2.306000	-0.354200	-0.480200
15	6	0	-2.007700	-1.658900	0.243200
16	8	0	-0.906600	-2.294000	-0.342900
17	8	0	-1.305900	1.464900	0.680200
18	6	0	-2.654900	1.473700	0.975800
19	6	0	-3.307000	0.451800	0.296400
20	6	0	-3.344200	2.356700	1.806000
21	6	0	-4.726400	2.184100	1.929100
22	6	0	-5.387500	1.158300	1.239900
23	6	0	-4.682300	0.273200	0.417500
24	6	0	-1.089600	1.486100	-1.701400
25	6	0	1.568500	-3.722400	-0.287400
26	1	0	1.381800	1.648800	-0.233600
27	1	0	6.054100	0.486400	-0.184900
28	1	0	4.982600	2.589500	-0.238400
29	1	0	3.426800	2.575600	-1.116400
30	1	0	3.457700	2.580200	0.699500
31	1	0	-2.652400	-0.554700	-1.520000
32	1	0	-2.877500	-2.352600	0.176600
33	1	0	-1.785700	-1.489400	1.322600
34	1	0	-2.815600	3.164800	2.333800
35	1	0	-5.303700	2.868100	2.572400
36	1	0	-6.478300	1.043300	1.350000
37	1	0	-5.191700	-0.542300	-0.118000
38	1	0	-2.072800	1.991000	-1.838900
39	1	0	-0.324100	2.292100	-1.655500
40	1	0	-0.890700	0.880600	-2.615000
41	1	0	0.584500	-4.224600	-0.403500
42	1	0	2.204700	-4.083400	-1.127100
43	1	0	2.010000	-4.079600	0.670800

Fluorescence titration of compound 4 with different nucleotides

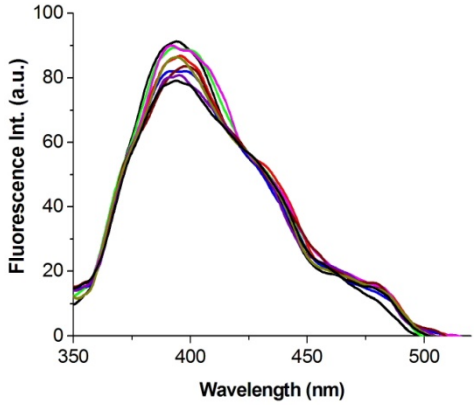


Figure 9. Fluorescence emission of ligand **4** (10 nm) in presence of increasing concentration of AMP (0-10 µM).

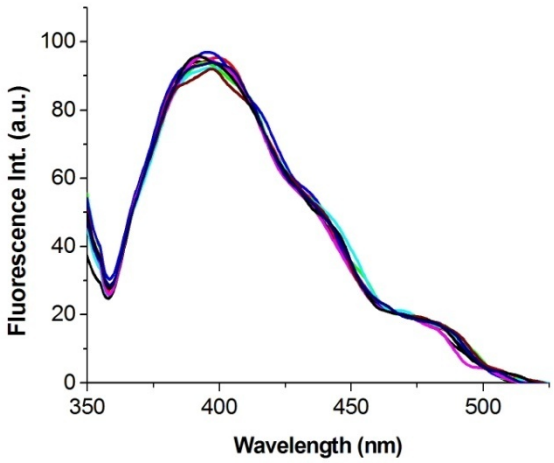


Figure 10. Fluorescence emission of ligand **4** (10 nm) in presence of increasing concentration of CMP (0-10 µM).

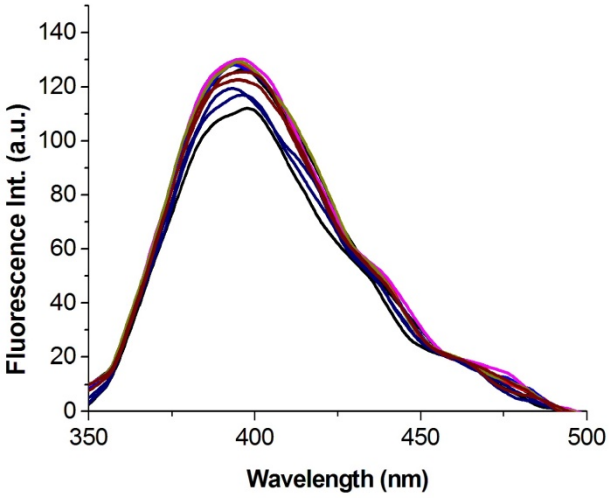


Figure 11. Fluorescence emission of ligand **4** (10 nm) in presence of increasing concentration of GMP (0-10 µM).

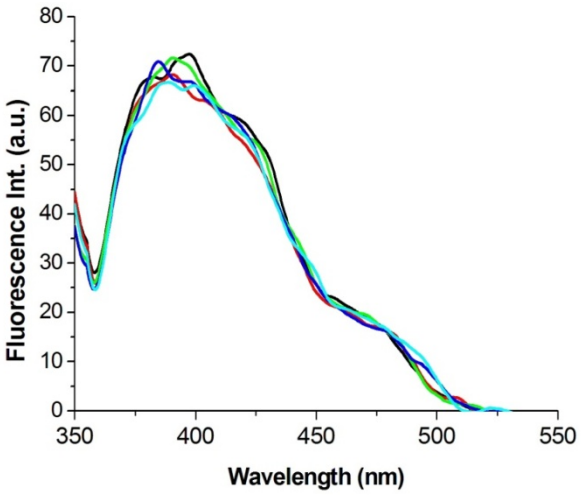


Figure 12. Fluorescence emission of ligand **4** (10 nm) in presence of increasing concentration of TMP (0, 1, 2, 3, 13 μM).

Determination of detection limit of compound 4

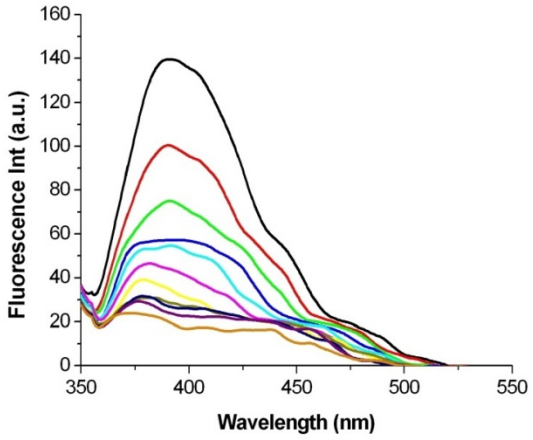


Figure 13. Emission spectra of ligand **4** in presence of ct-DNA with gradual dilution keeping [ligand]/[DNA]= 1:100 ([DNA] = 1000 nm, 500 nM, 250 nM, 125 nM up to 3.9 nM). The most underneath spectra (dark yellow) is due to noise obtained from buffer solution only. For all the spectra λ_{ex} = 331 nm).

Fluorescence titration of compound 4 with a sequence of DNA

Compound **4** (20 nM) was excited at 331 nm and emission spectra were recorded. Then oligonucleotide d(5'-CATGGCCATG-3')$_2$ was added (from 0 to 10 μM) gradually to this solution, mixed thoroughly after each addition and the corresponding emission spectrum was recorded.

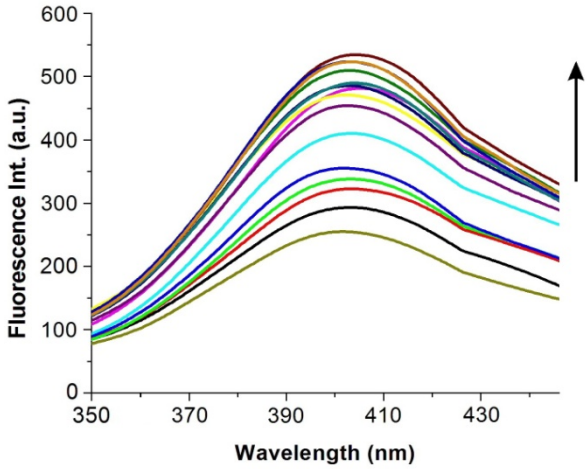


Figure 14. Emission spectra of compound **4** (20 nM) in presence of increasing concentration of d(5'-CATGGCCATG-3')$_2$ up to 10 μM.