Electronic Supplementary Material (ESI) for New Journal of Chemistry. This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2014

## SUPPORTING INFORMATION

### **Carbazole-Corrole and Carbazole-Prophyrin Dyads:**

### Synthesis, Fluorescence and Electrochemical Studies

Naresh Balsukuri<sup>a</sup>, Sudipta Das<sup>a</sup>, Iti Gupta<sup>\*a</sup>

<sup>a</sup>Indian Institute of Gandhinagar, VGEC Campus, Chandkheda, Ahmedabad-382424, India

\* Corresponding author. Tel.: +917932419502; fax: +917923972324; e-mail: iti@iitgn.ac.in

#### **List of Contents**

#### Page No.

S2
S2
<b>S</b> 3
<b>S</b> 3
S4
S4
S5
<b>S</b> 5
<b>S</b> 6
<b>S</b> 7
<b>S</b> 7
<b>S</b> 8
<b>S</b> 9
<b>S</b> 9
<b>S</b> 10
S10
S11
S11
S12
S13
S14
S15
S16
S17



Figure 1. ESI-MS of compound 3



Figure 2.<sup>1</sup>H NMR of compound **3** in CDCl<sub>3</sub>







Figure 4. ESI-MS of compound 4



Figure 5. <sup>1</sup>H NMR of compound **4** in CDCl<sub>3</sub>



Figure 6.<sup>13</sup>CNMR of compound **4** in CDCl<sub>3</sub>



Figure 7. ESI-MS of compound 5



Figure 8.<sup>1</sup>HNMR of compound **5** in CDCl<sub>3</sub>



Figure 9. <sup>13</sup>CNMR of compound **5** in CDCl<sub>3</sub>







Figure 11. <sup>13</sup>CNMR of compound **6** in CDCl<sub>3</sub>



Figure 12. Partial <sup>1</sup>H-NMR and <sup>1</sup>H-<sup>1</sup>H COSY spectra of dyad **6** recorded in CDCl<sub>3</sub>.







Figure 14.<sup>1</sup>HNMR of compound **7** in CDCl<sub>3</sub>



Figure 15.<sup>13</sup>CNMR of compound **7** in CDCl<sub>3</sub>



Figure 16. MALDI-MS of compound 8







Figure 18. <sup>13</sup>CNMR of compound **8** in CDCl<sub>3</sub>



Figure 19. MALDI-MS of compound 9



Figure 20. Comparison of emission spectra of dyad 7 and a 1:1 mixture of N-butylcarbazole and porphyrin 3 in toluene ( $\lambda_{ex} = 300$  nm). The sharp peak at 600 nm is due to the scattering which is observed exactly at the double of excitation wavelength 300 nm (second order diffraction through emission monochromator in the fluorescence instrument).<sup>1</sup>



Figure 21. Comparison of emission spectra of dyad **8** and a 1:1 mixture of N-butylcarbazole and ZnTPP in toluene ( $\lambda_{ex} = 270$  nm). The sharp peak at 600 nm is due to the scattering which is observed exactly at the double of excitation wavelength 300 nm (second order diffraction through emission monochromator in the fluorescence instrument).<sup>1</sup>

# Table 1. Fröster Energy Transfer Calculations of dyad 4 using PhotoChemCAD<sup>2</sup> software

Results of Forster Energy Transfer Calculation

Donor	
Acceptor	
Solvent	
Refractive index (n)	1.490
Orientation factor	1.125
Quantum yield	0.127
Actual distance	15.200
Epsilon	21600.000
Wavelength for epsilon (nm)	300.000
Low wavelength (nm)	310.000
High wavelength (nm)	700.000
J value (cm(6)/mmol)	1.145e-013
Forster distance	37.798
Efficiency (%)	99.579
Fluorescence lifetime (ns)	8.890
Rate of energy transfer (1/s)	2.660e+010

Dexter overlap integral (1/eV) 6.095e-001

## Table 2. Fröster Energy Transfer Calculations of dyad 7 using PhotoChemCAD software

Results of Forster Energy Transfer Calculation	
Donor	
Acceptor	
Solvent	
Refractive index (n)	1. 490
Orientation factor	1.125
Quantum yield	0.127
Actual distance	15.200
Epsilon	18125,000
Wavelength for epsilon (nm)	300.000
Low wavelength (nm)	310.000
High wavelength (nm)	700.000
J value $(cm(6)/mmol)$	9.173e-014
Forster distance	36. 426
Efficiency (%)	99.475
Fluorescence lifetime (ns)	8.890
Rate of energy transfer (1/s)	2.131e+010

Dexter overlap integral (1/eV) 4.437e-001

Table 3. Fröster Energy Transfer Calculations of dyad 8 using PhotoChemCAD software

Results of Forster Energy Transfer Calculation

Donor	
Acceptor	
Solvent	
Refractive index (n)	1.490
Orientation factor	1.125
Quantum yield	0.127
Actual distance	15.200
Epsilon	29655.000
Wavelength for epsilon (nm)	270.000
Low wavelength (nm)	310.000
High wavelength (nm)	700.000
J value (cm(6)/mmol)	8.078e-014
Forster distance	35.663
Efficiency (%)	99.404
Fluorescence lifetime (ns)	8.890
Rate of energy transfer (1/s)	1.876e+010
Dexter overlap integral (1/eV)	3.219e-001

## **Reference:**

1. S. Ik Yang, J. Li, H. Sun Cho, D. Kim, D. F. Bocian, D. Holten and J. S. Lindsey, *Journal of Materials Chemistry*, 2000, **10**, 283-296.

2. Principles of Fluorescence Spectroscopy, J. R. Lakowicz, 3<sup>rd</sup> Edn. Springer, 2006.