SUPLEMENTARY INFORMATION

Charge Separation and Charge Recombination Photophysical Studies in a Series of Perylene-C_{60} Linear and Cyclic Dyads

S. Pla,[a] M. Niemi,[b] L. Martín-Gomis,[a] F. Fernández-Lázaro,[a] H. Lemmetyinen,[b] N. V. Tkachenko[b,*] Á. Sastre-Santos[a,*]

División de Química Orgánica, Instituto de Bioingeniería, Universidad Miguel Hernández, Avda. de la Universidad, s/n, Elche 03202, Spain.

E-mail: asastre@umh.es

N,N'-di-(3-hidroxypropyl)-1,7-(N-pyrrolidinyl)perylene-3,4,9,10-tetracarboxydiimide (PDI-1):

Fig S1 ^{1}H-NMR-($CDCl_3$) of PDI-1

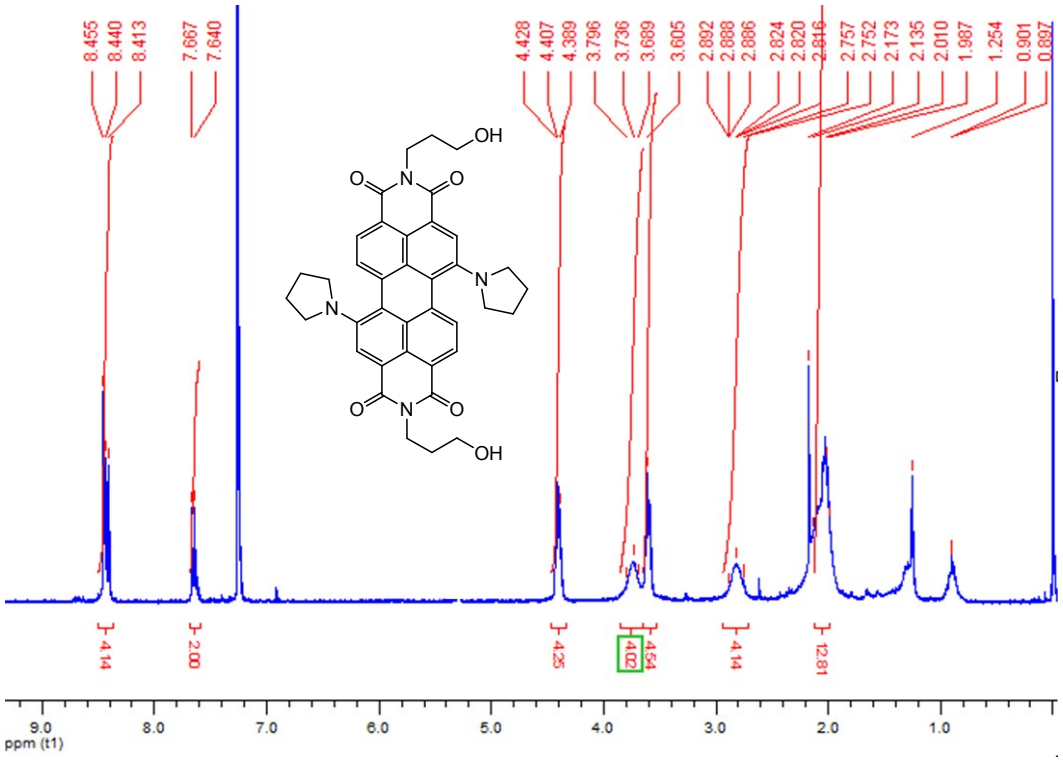


Fig S2 ^{13}C-NMR-$CDCl_3$) of PDI-1

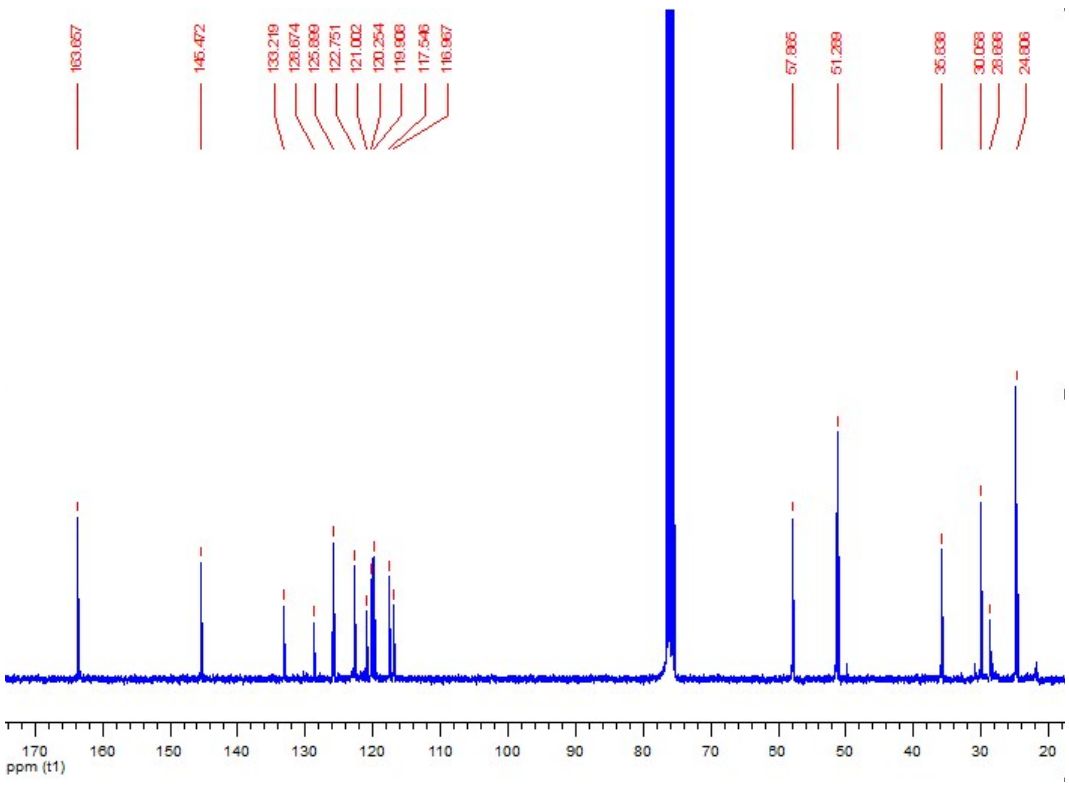


Fig S3 MS of PDI-1

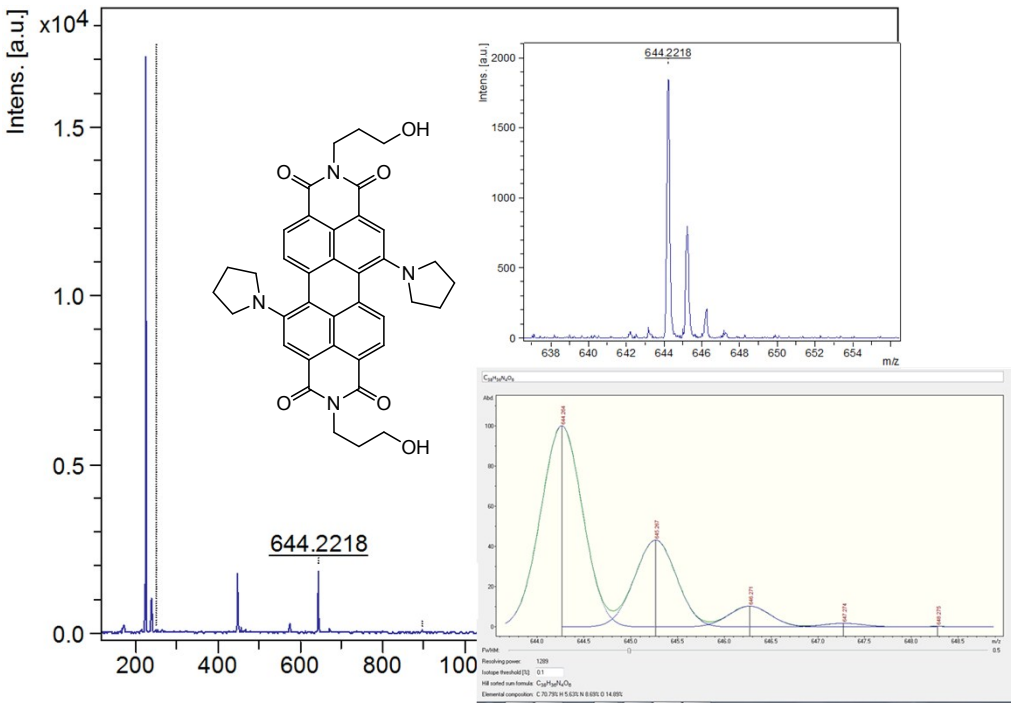


Fig S4 IR spectrum (KBr) of PDI-1

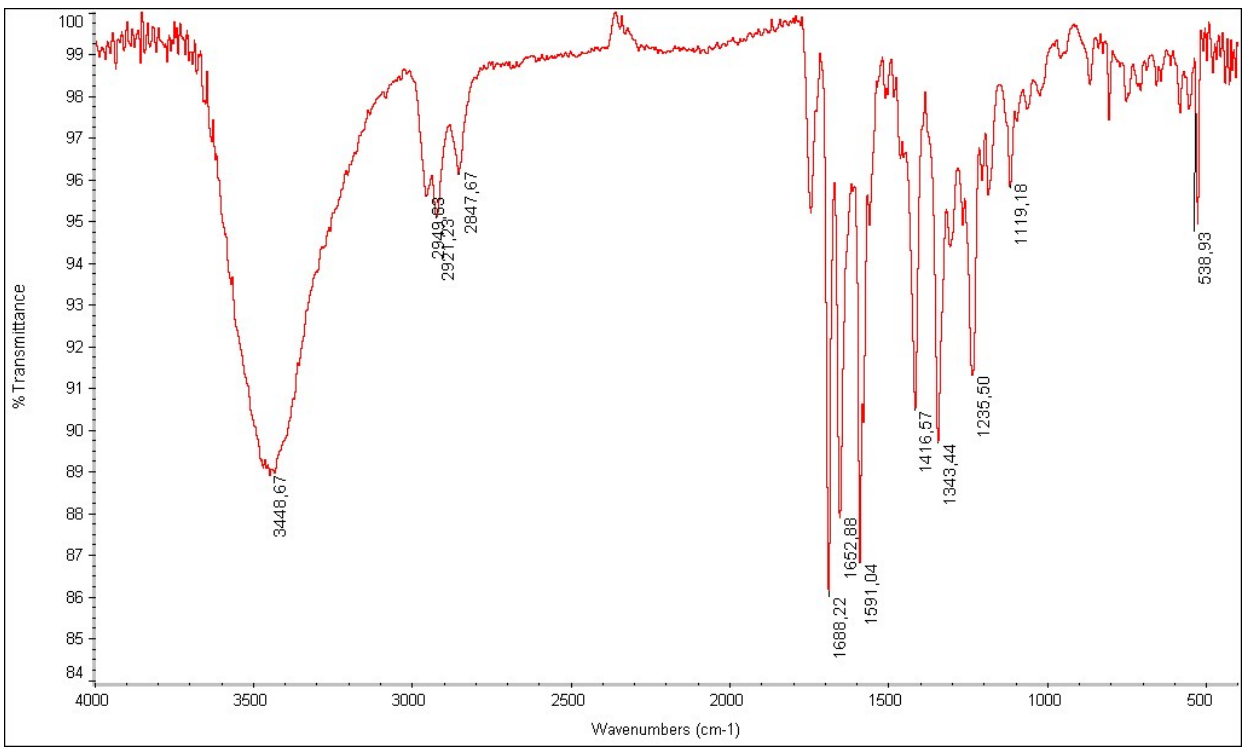
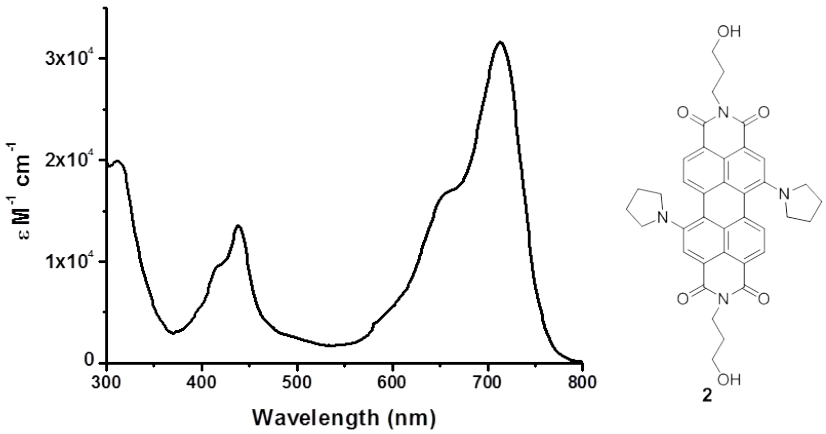


Fig S5 UV-vis spectrum ($CHCl_3$) of PDI-1



N,N'-di-[3-(ethoxycarbonylmethylcarbaloxy)propyl)]-1,7-(N-pyrrolidinyl)perylene-3,4,9,10-tetracarboxydiimide (PDI-2):

Fig S6 ^{1}H-NMR-($CDCl_3$) of PDI-2

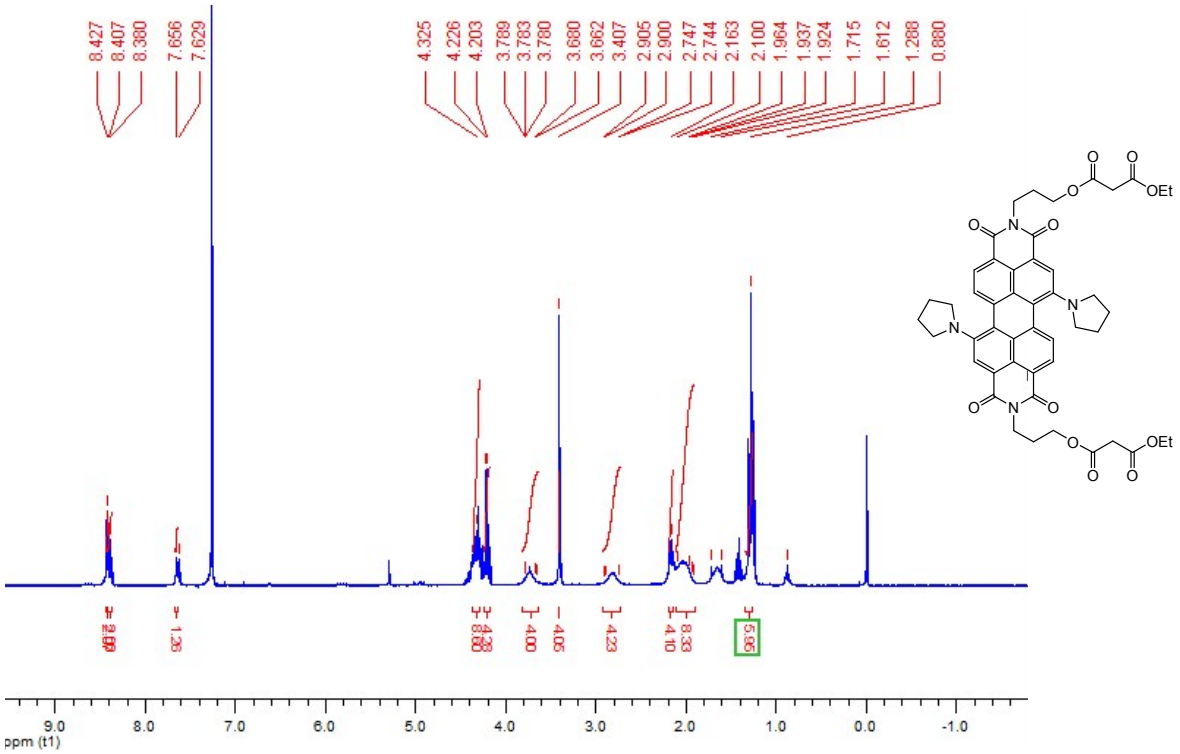


Fig S7 ^{13}C-NMR-$CDCl_3$) of PDI-2

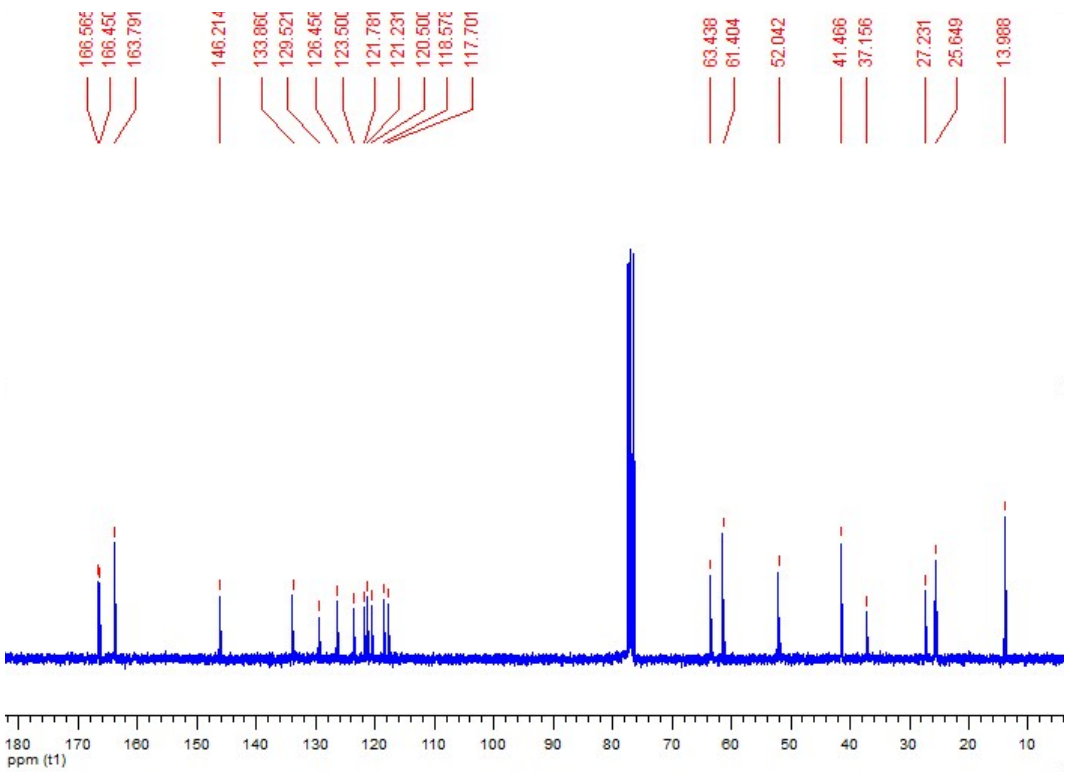


Fig S8 MS of PDI-2

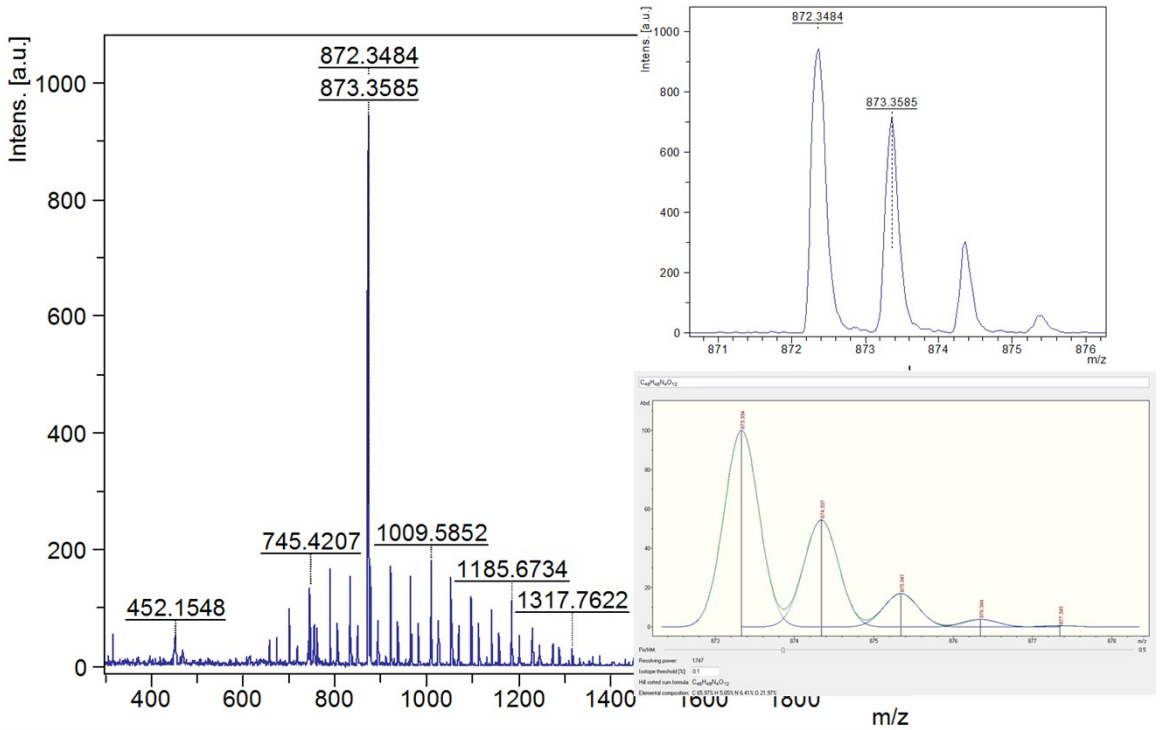


Fig S9 IR spectrum (KBr) of 3

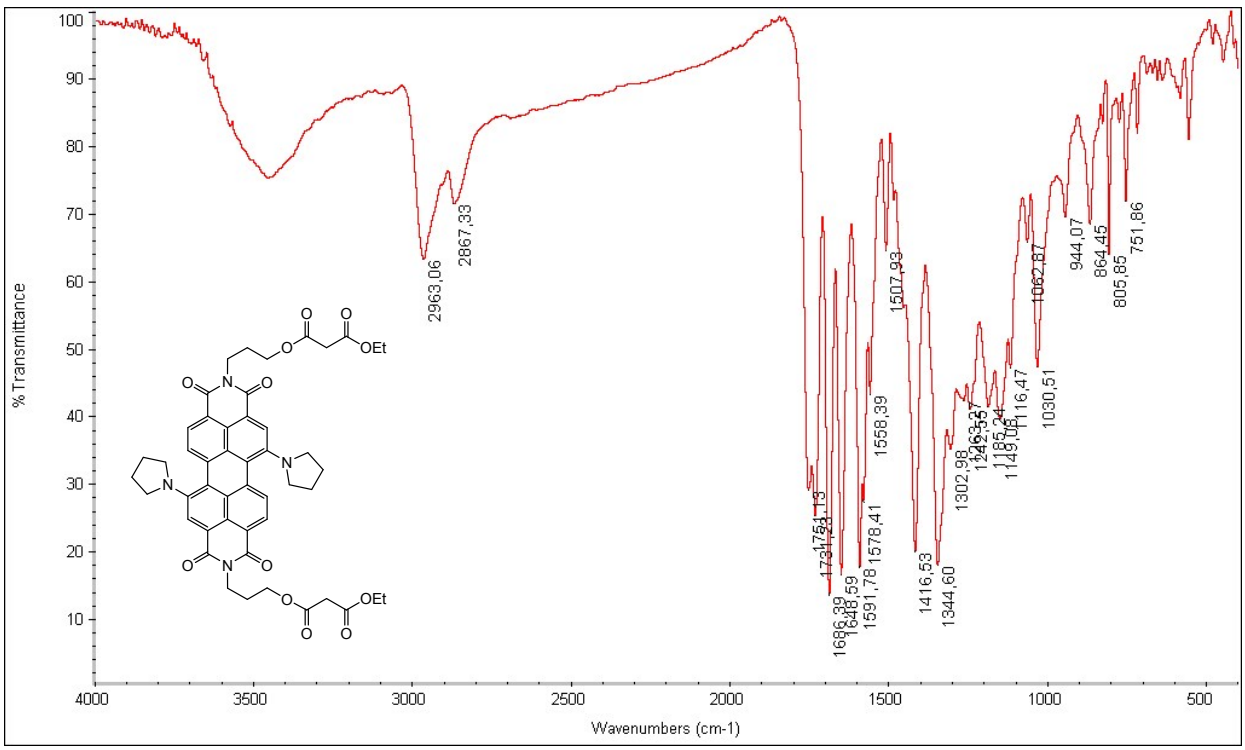
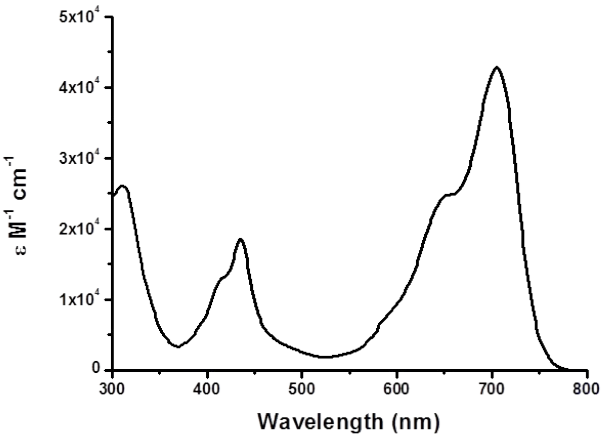
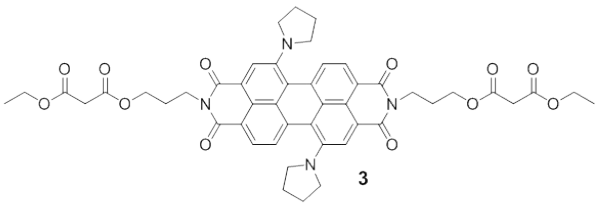


Fig S10 UV-vis spectrum ($CHCl_3$) of PDI-2





DB-3:

Fig S11 ^{1}H-NMR-($CDCl_3$) of DB-3

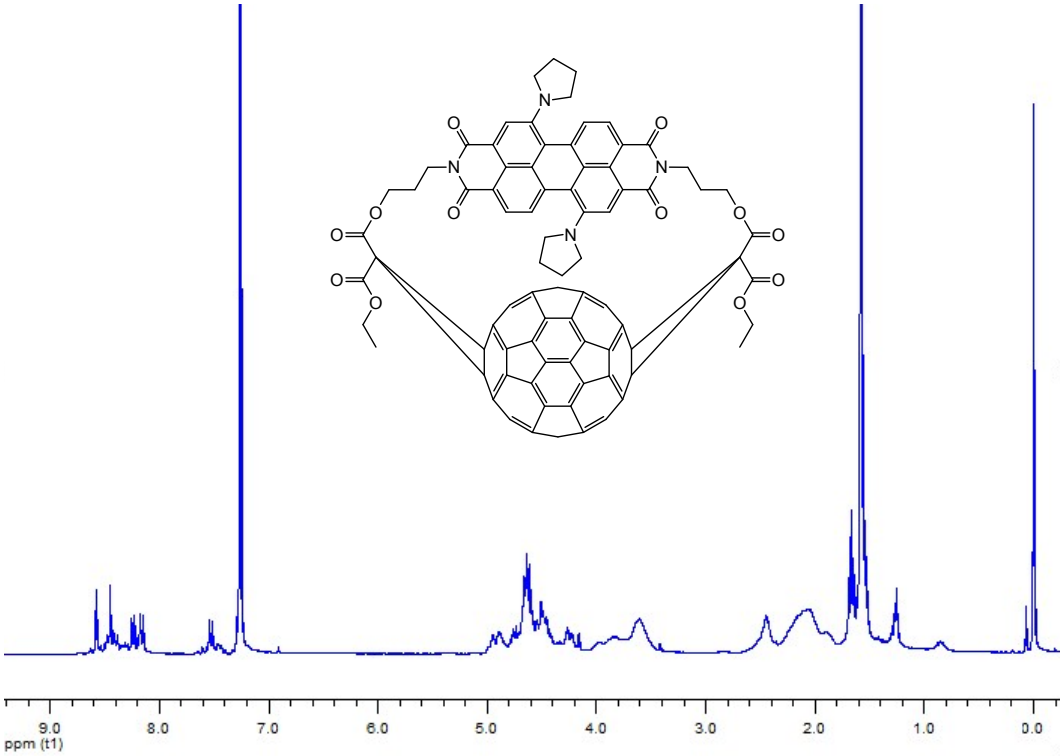


Fig S12 MS of DB-3

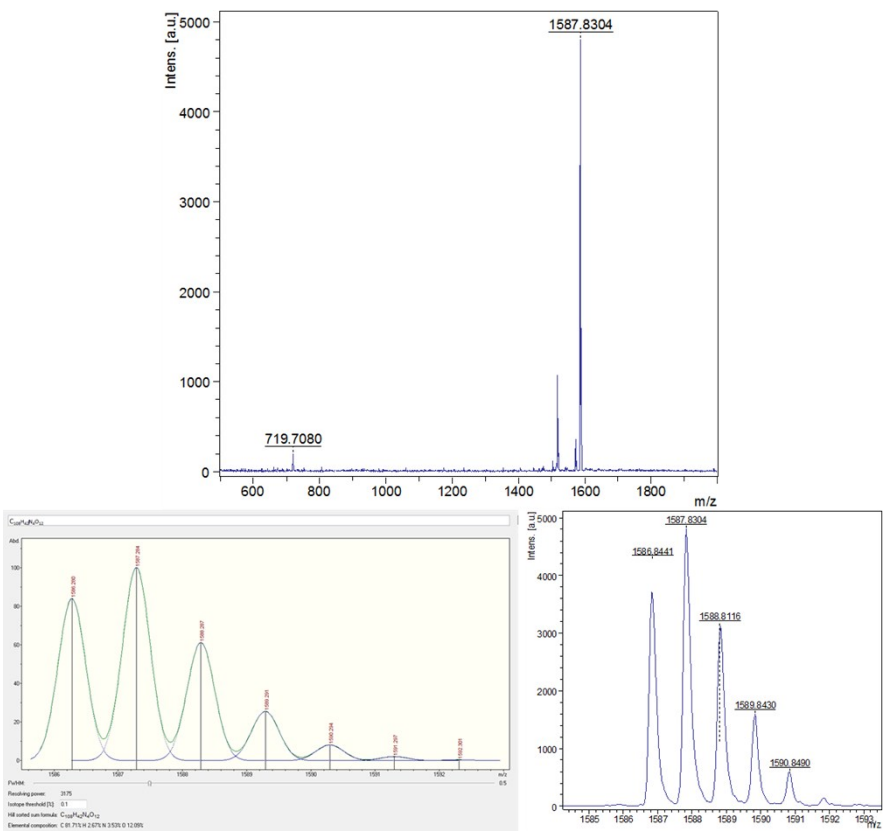


Fig S13 IR spectrum (KBr) of DB-3

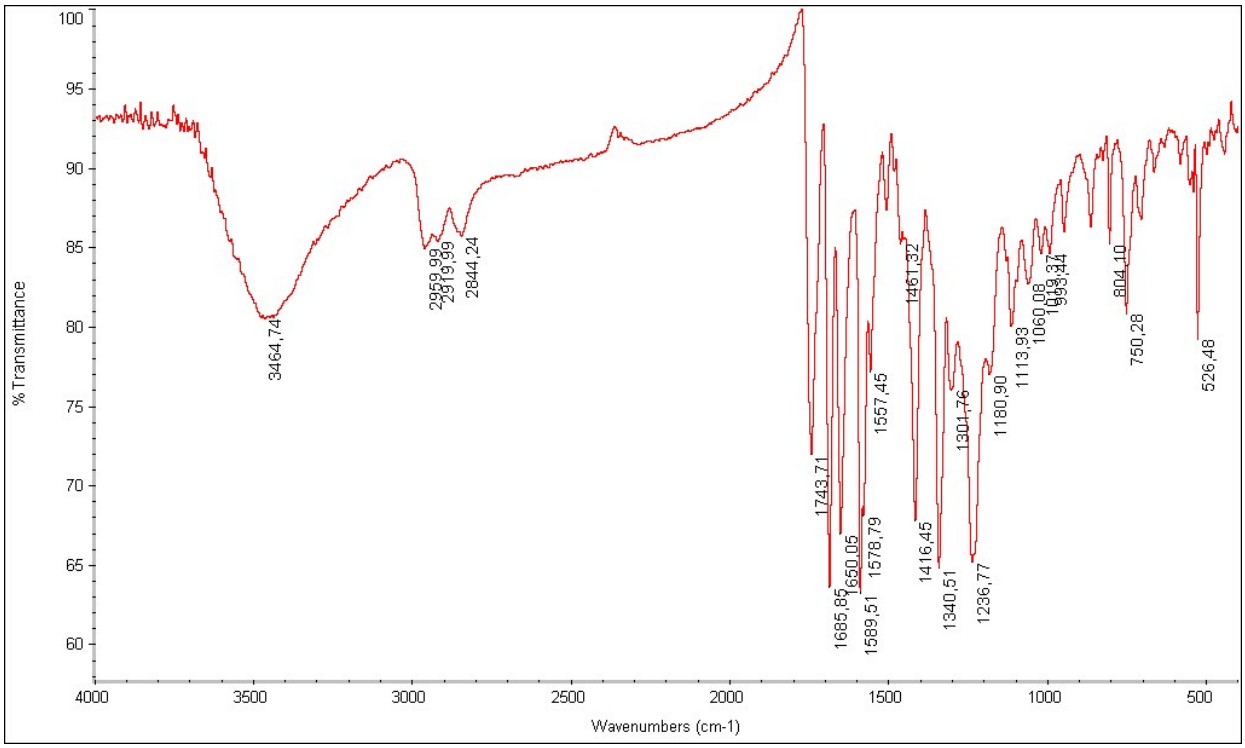
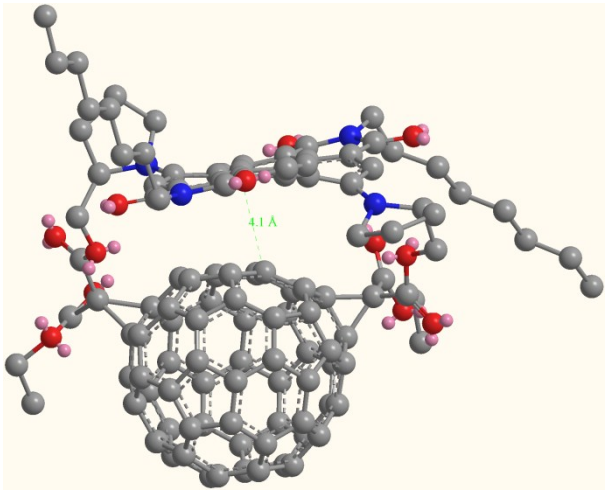
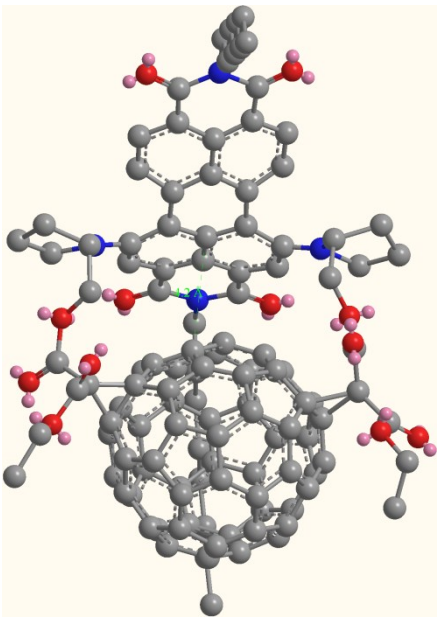


Figure S14. Minimum-energy structures of DB1, DB2 and DB3 dyads were calculated using MM2 (CS-ChemBio 3D)

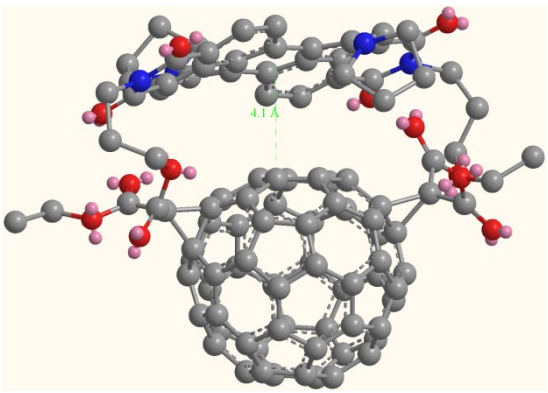
DB1



DB2



DB3



Python code to calculate ET rate constant defined by eq. (4); the function is loaded to gnumeric spreadsheet

```
from Gnumeric import GnumericError, GnumericErrorVALUE
import Gnumeric
import string
import math as m
import numpy as n

# universal constants
k_B = 1.380658e-23 # Boltzmann constant in J/K
h_P = 6.6260755e-34 # Planck constant in J s
h_bar = 1.0545727e-34 # Planck constatn / 2*pi
q_e = 1.602177e-19 # elementary charge in C


def quantum_ET_rate(Velec, dG, Ereorg, Sev, Evib, temp):
	'@FUNCTION=QUANTUM_ET_RATE\n'\
	'@SYNTAX=quantum_ET_rate(Velec, dG, Ereorg, Sev, Evib, temp)\n'\
	'@DESCRIPTION=Calculate electron transfer rate according to semi-quantum theory.\n'\
	'Parameters: Velec - electronic coupling (in eV), dG - ET free energy (in eV),\n'\
	'Ereorg - reorganization energy (in eV), Sev - couplign constant (dimensionless),\n'\
	'Evib - vibration mode energy (in eV), and temp - temperature (in K).\n\n'\
	'@EXAMPLES='\
	'@SEEALSO='

	# prepare to calc sum
	_mult = 1.0
	arg = 4*Ereorg*k_B*temp/q_e
	_E = dG + Ereorg
	_sum = m.exp(-(_E**2)/arg)
	_n = 1
	# calculate sum for 50 vibrational levels
	while _n < 50:
		_mult *= Sev/_n
		_E += Evib
		_sum += _mult*m.exp(-(_E**2)/arg)
		_n += 1
	# and add electronic coupling and other coeff.
	return m.sqrt(m.pi/(Ereorg*q_e*k_B*temp))*((Velec*q_e)**2)*_sum*m.exp(-Sev)/h_bar
```