

Electronic Supplementary Information (ESI)

New thermal stability cyano-substituted D-A- π -A-D structural molecules with aggregation-induced emission and large two-photo absorption cross-sections

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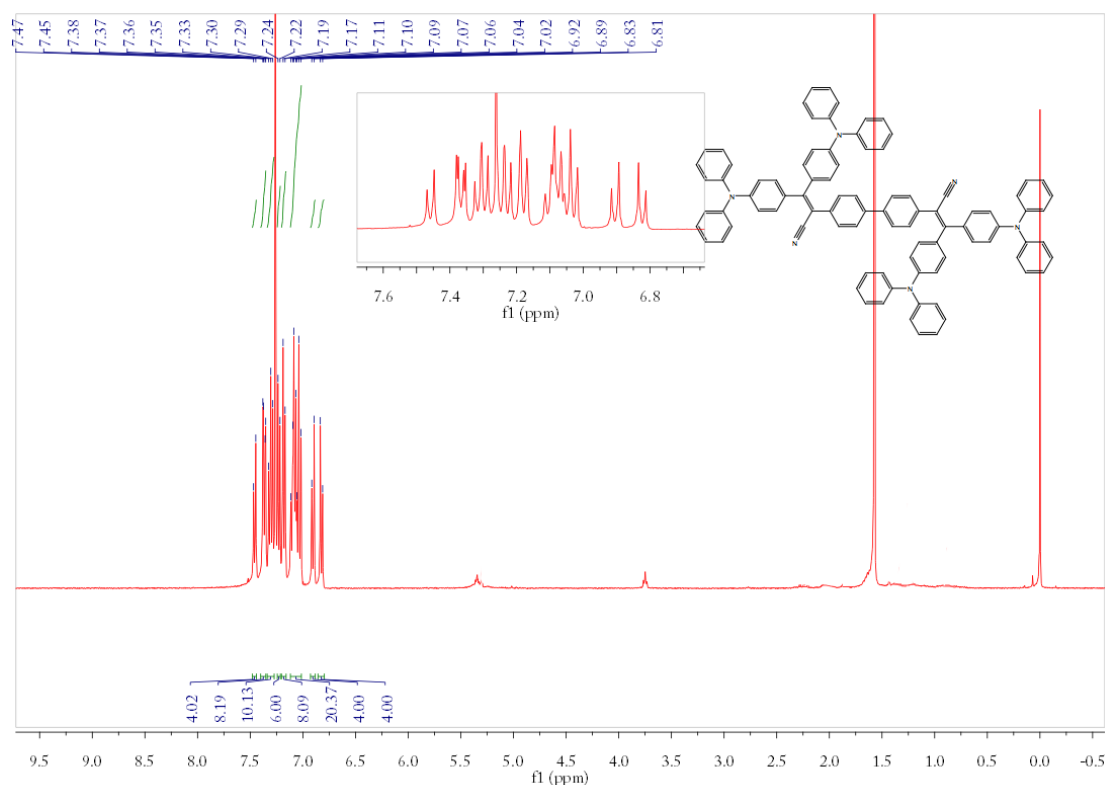


Figure S1. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **4a**.

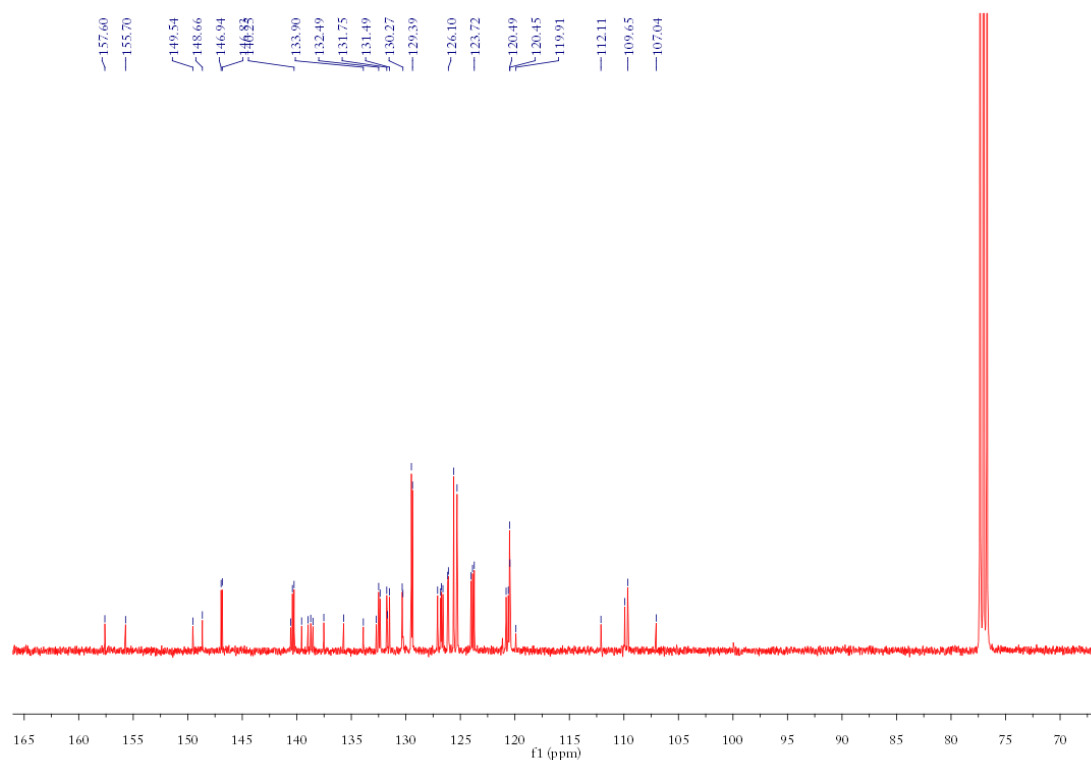


Figure S2. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **4a**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

39 formula(e) evaluated with 4 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-100 H: 0-70 N: 0-6

H-TIAN

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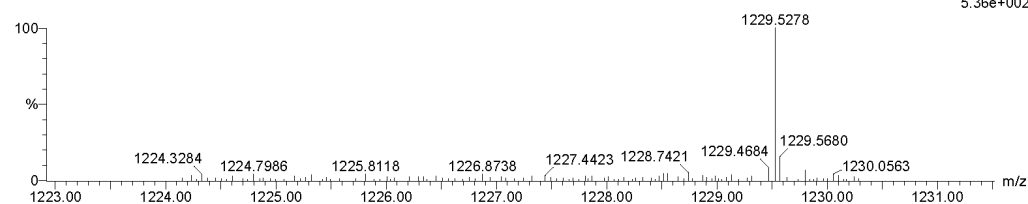
TH-HW-01 95 (3.003) Cm (84:95)

26-Feb-2012

14:15:46

1: TOF MS ES+

5.36e+002



Minimum:

Maximum:

50.0

50.0

-1.5

100.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

i-FIT (Norm)

Formula

1229.5278

1229.5271

0.7

0.6

61.5

91.7

0.0

$\text{C}_{90}\text{H}_{65}\text{N}_6$

Figure S3. ESI-MS spectrum of compound **4a**.

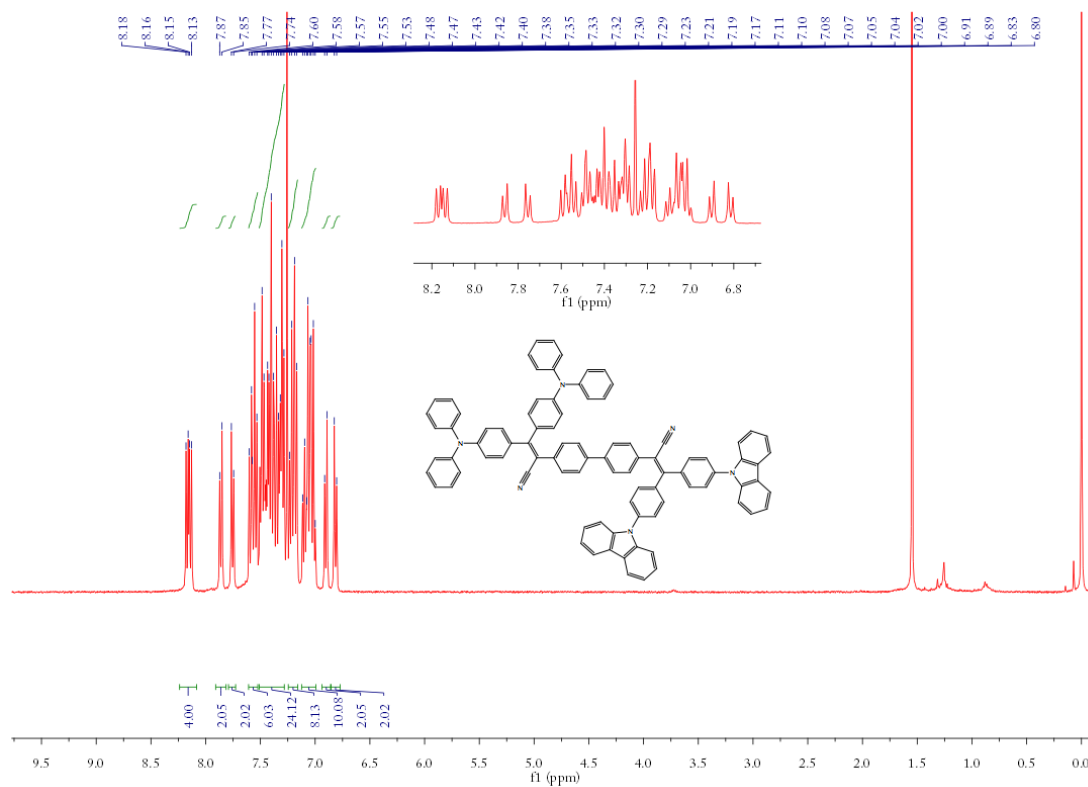


Figure S4. ¹H NMR (400 MHz, CDCl₃) spectrum of compound **4b**.

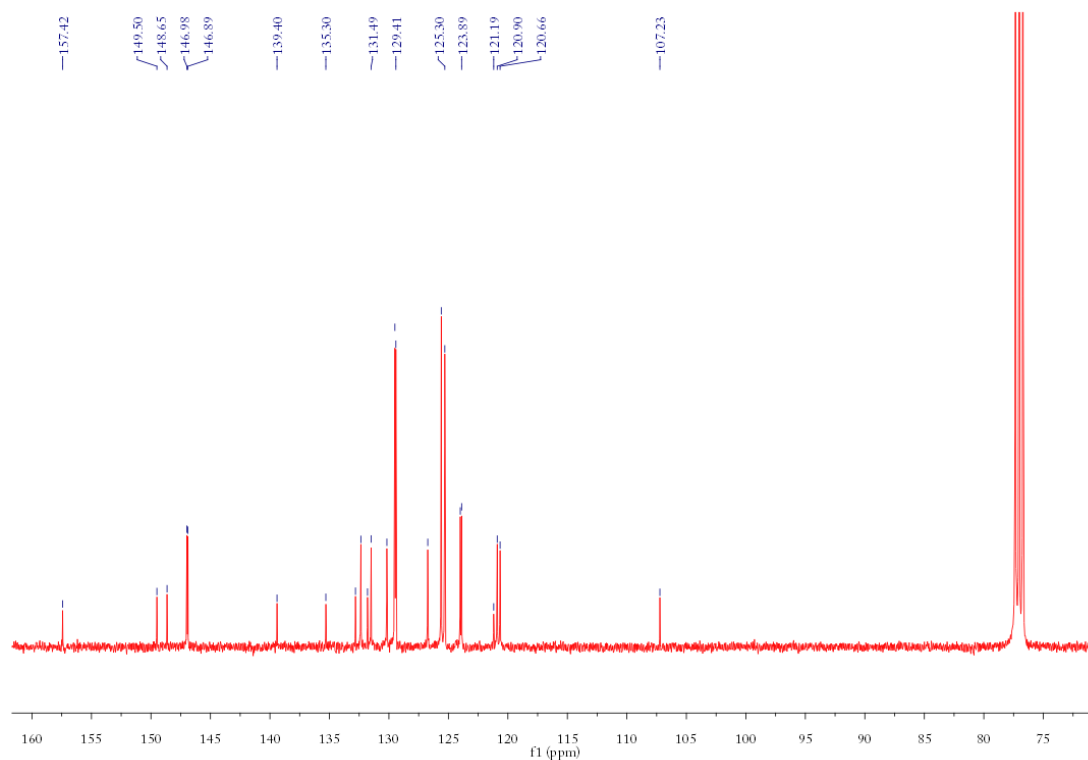


Figure S5. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound **4b**

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-91 H: 0-65 N: 0-6

H-TIAN

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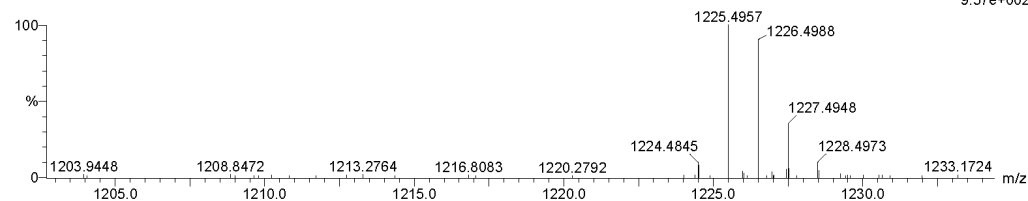
23-Apr-2012

21:51:37

1: TOF MS ES+

9.57e+002

TH-HW-KA 12 (0.445) Cm (9:12)



Minimum: -1.5
Maximum: 50.0 50.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1225.4957	1225.4958	-0.1	-0.1	63.5	41.6	0.0	C90 H61 N6

Figure S6. ESI-MS spectrum of compound **4b**.

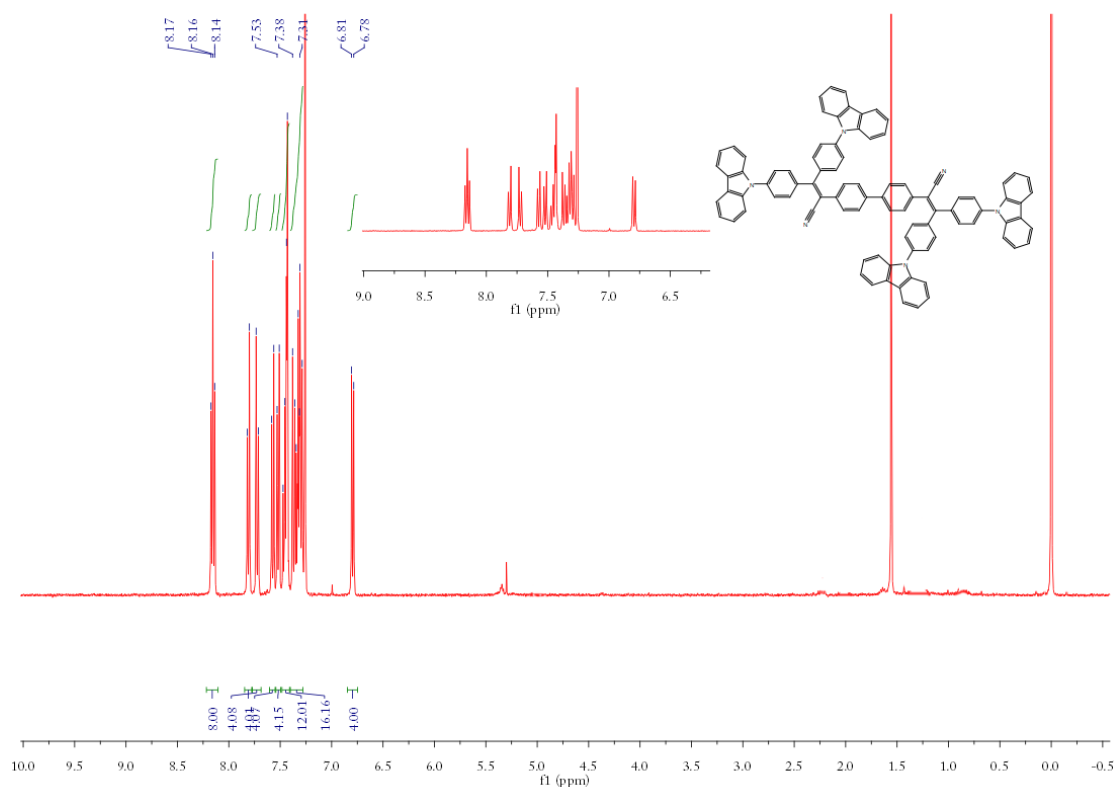


Figure S7. ^1H NMR (400 MHz, CDCl_3) spectrum of compound **4c**.

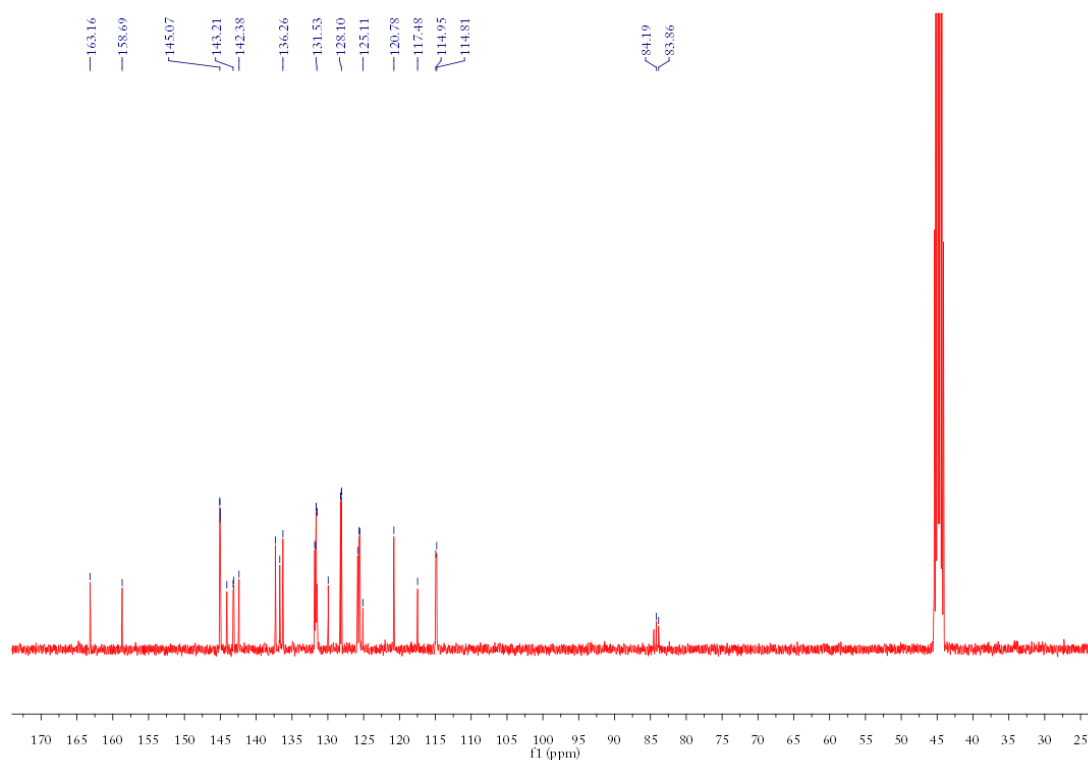


Figure S8. ^{13}C NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **4c**.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

3 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

C: 0-91 H: 0-65 N: 0-6

H-TIAN

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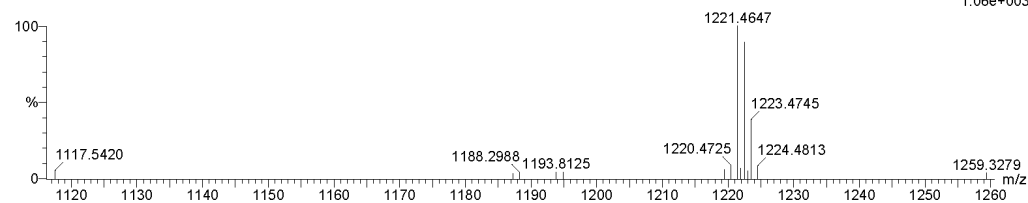
TH-HW-KK 23 (0.790) Cm (21:25)

23-Apr-2012

21:58:18

1: TOF MS ES+

1.06e+003



Minimum: -1.5
Maximum: 50.0 50.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
1221.4647	1221.4645	0.2	0.2	65.5	21.3	0.0	C90 H57 N6

Figure S9. ESI-MS spectrum of compound **4c**.