

**Supporting information:****Charge transfer interactions in a multichromophoric  
hexaarylbenzene containing pyrene and triarylamines**

By Christoph Lambert\*, Julia Ehbets, Dirk Rausch, Markus Steeger

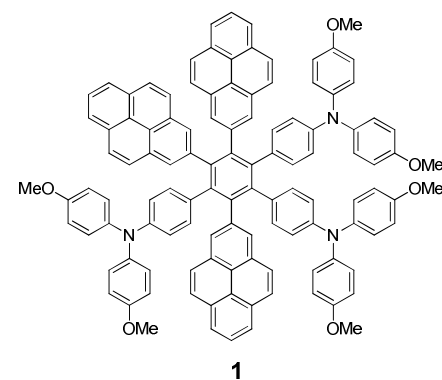
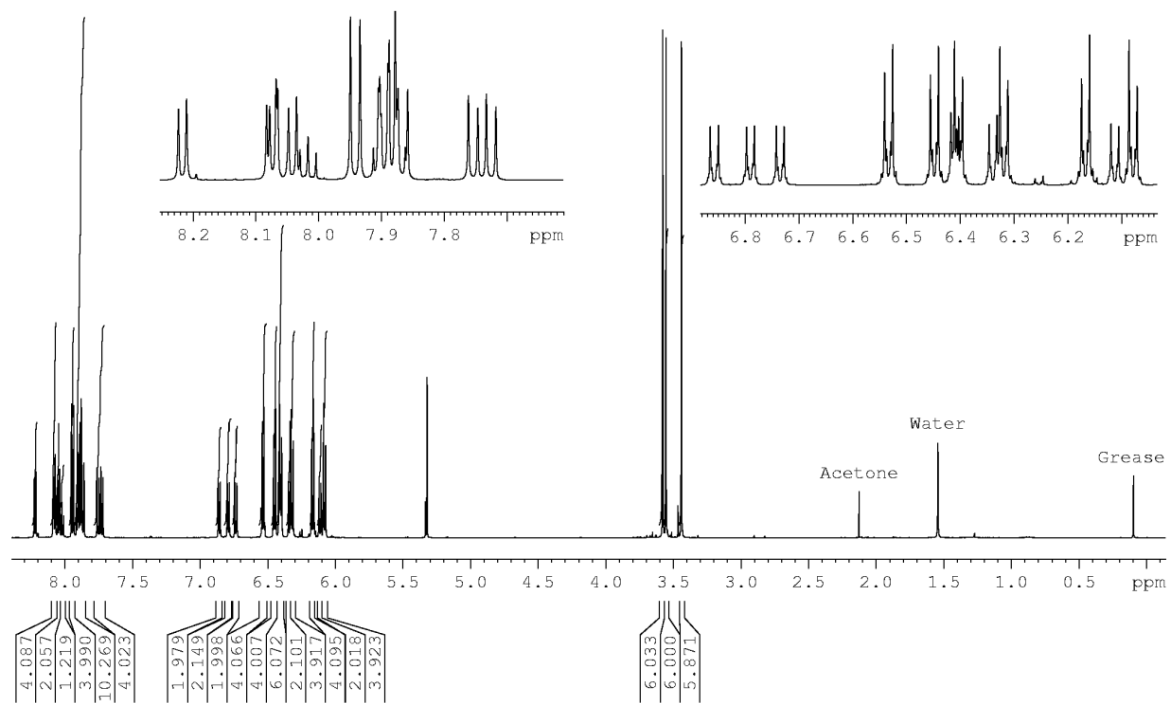
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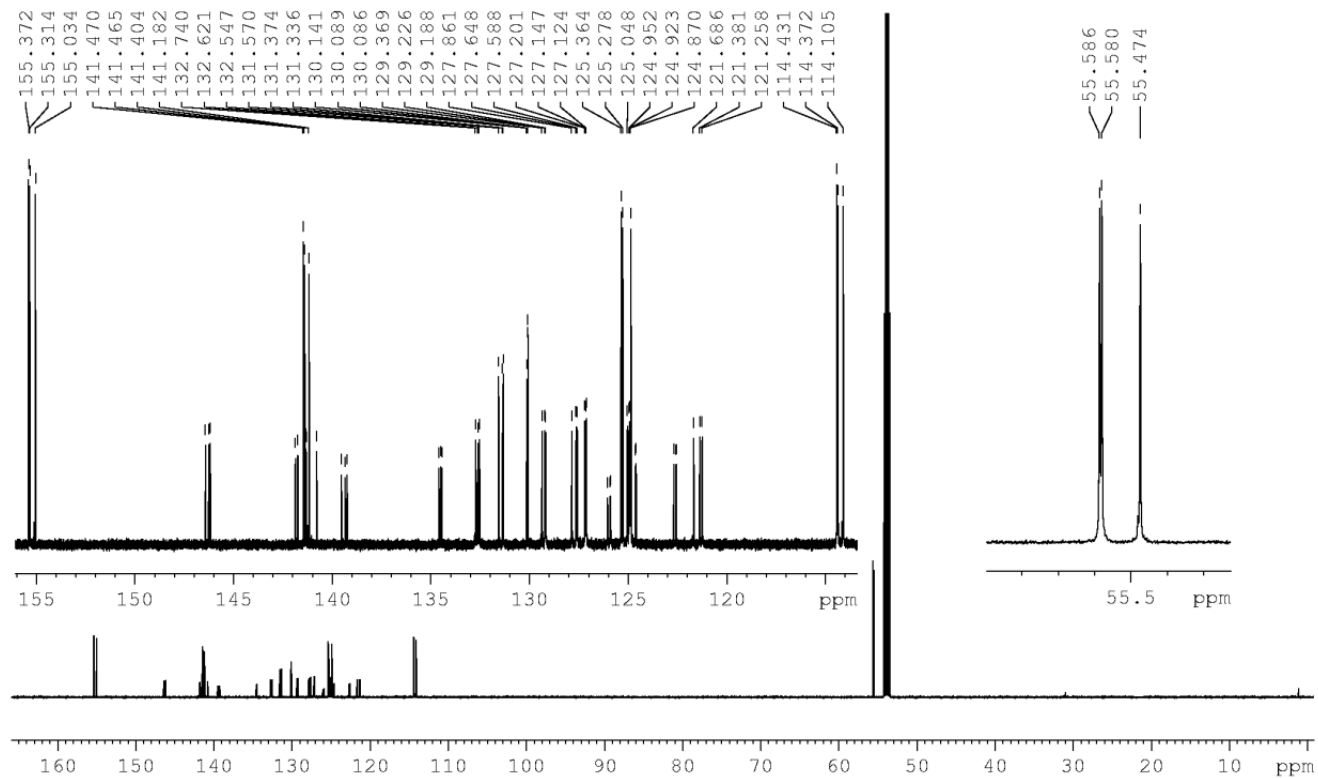
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<sup>1</sup>H-NMR of substance 1



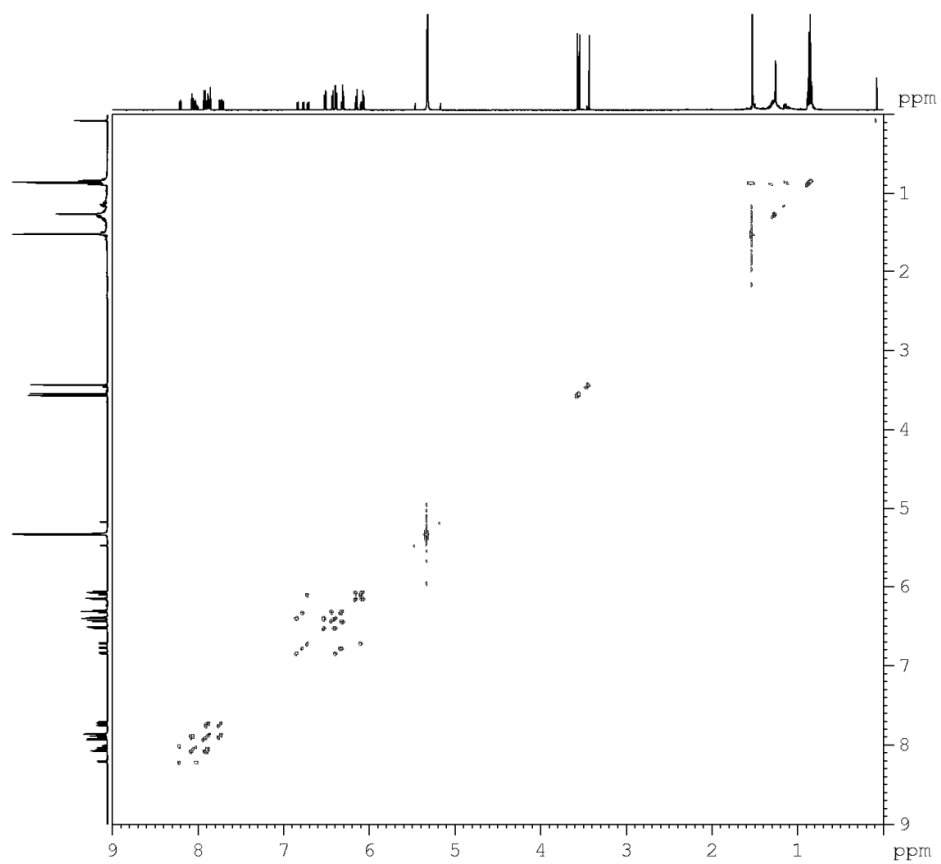
**Figure S1.** <sup>1</sup>H-NMR (600 MHz) of substance **1** in DCM-d<sub>2</sub>.

$^{13}\text{C}$ -NMR of substance 1



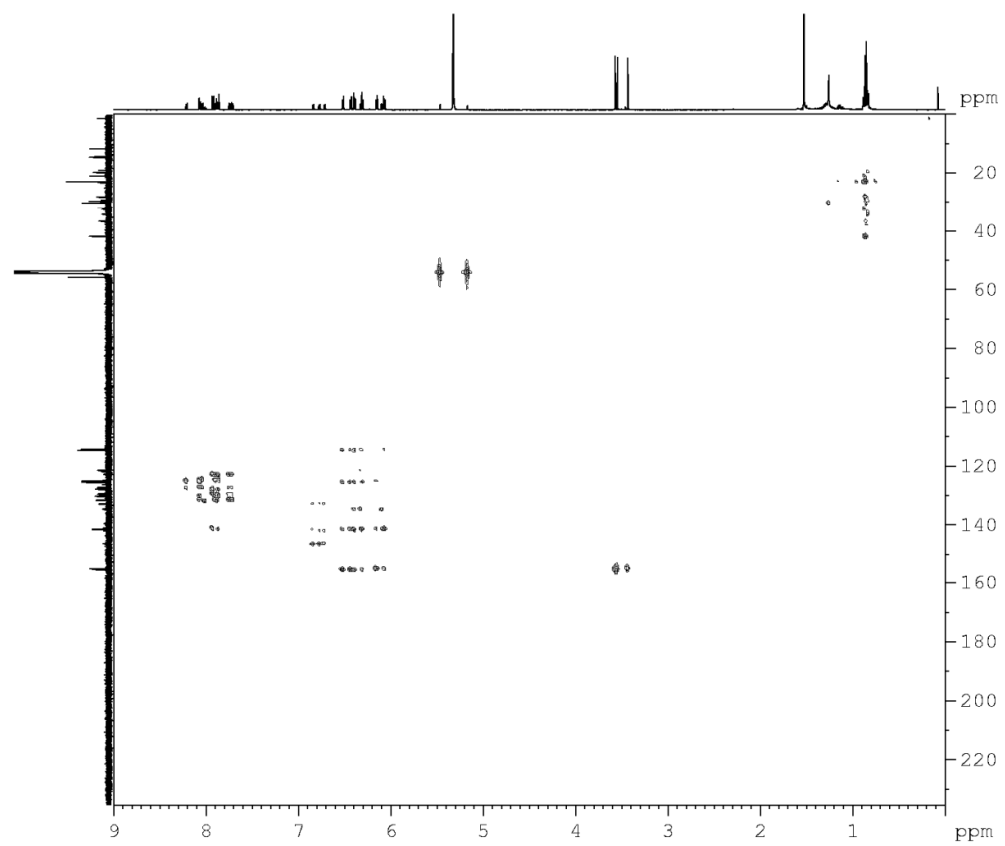
**Figure S2.**  $^{13}\text{C}$ -NMR (151 MHz) of substance 1 in  $\text{DCM-d}_2$ .

COSY substance 1

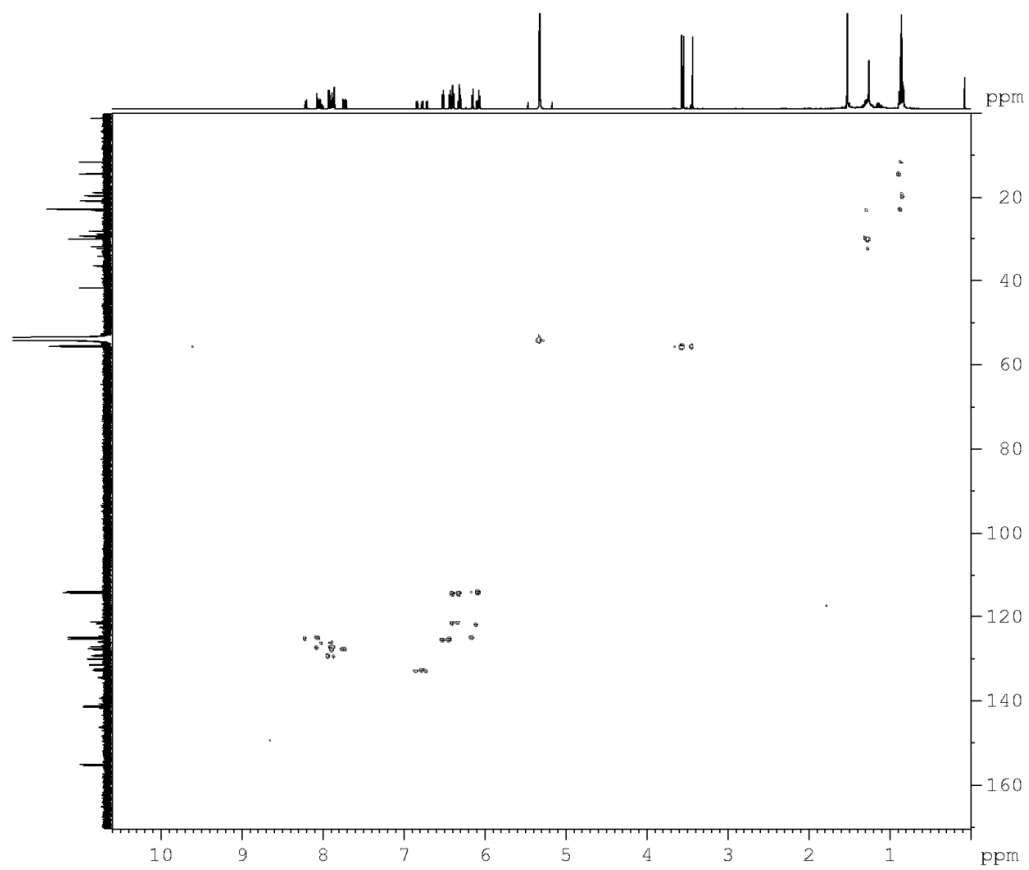


**Figure S3.** COSY of substance **1** in DCM-d<sub>2</sub>.

HMBC substance 1

**Figure S4.** HMBC of substance 1 in DCM-d<sub>2</sub>.

HSQC substance 1



**Figure S5.** HSQC of substance **1** in DCM-d<sub>2</sub>.

## Mass Spectrum Molecular Formula Report

## Analysis Info

Analysis Name D:\Data\Spektren2012\2012\_0129.d  
Method esi\_tune\_pos\_high.m  
Comment Julia Ehbets  
JE23.7-fest  
11 pmol /  $\mu$ l in Aceton

Acquisition Date 26.01.2012 15:11:16  
Operator Administrator  
Instrument microTOF 88

## Acquisition Parameter

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Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	23.0 V	Set Flight Tube	8600 V
				Set Detector TOF	1970 V

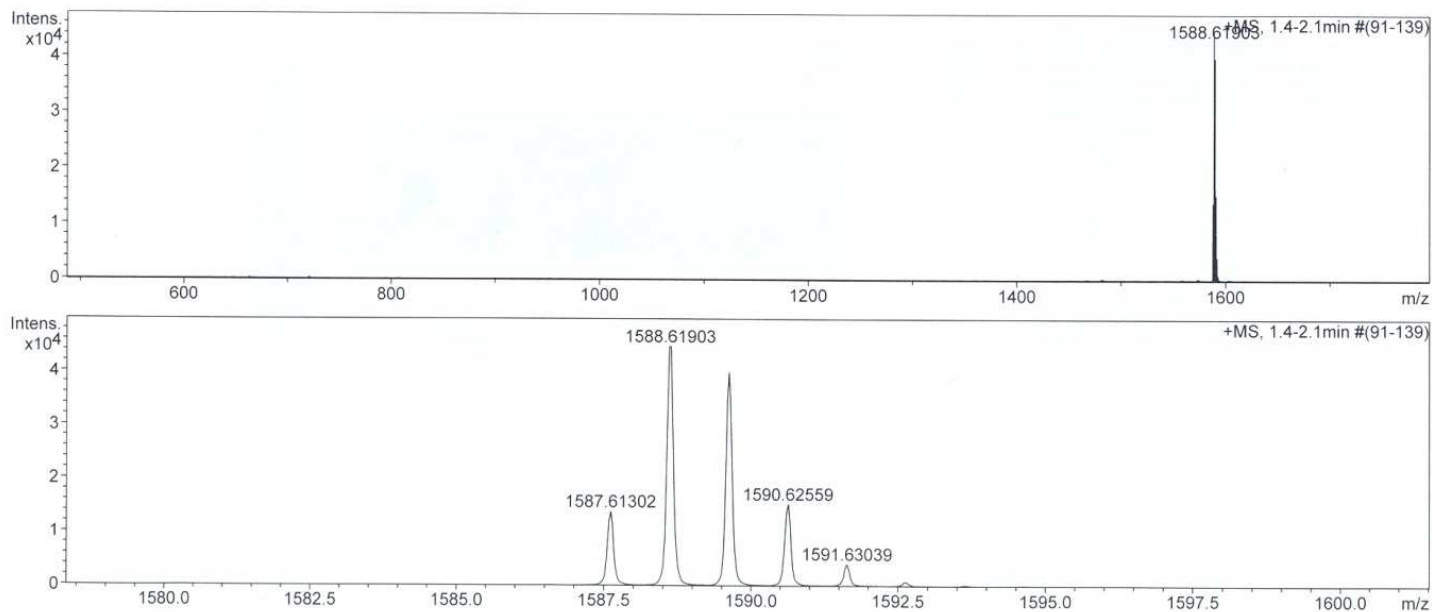
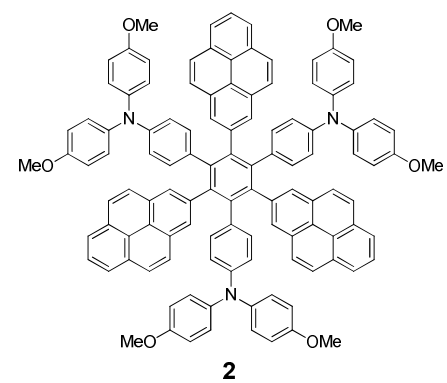
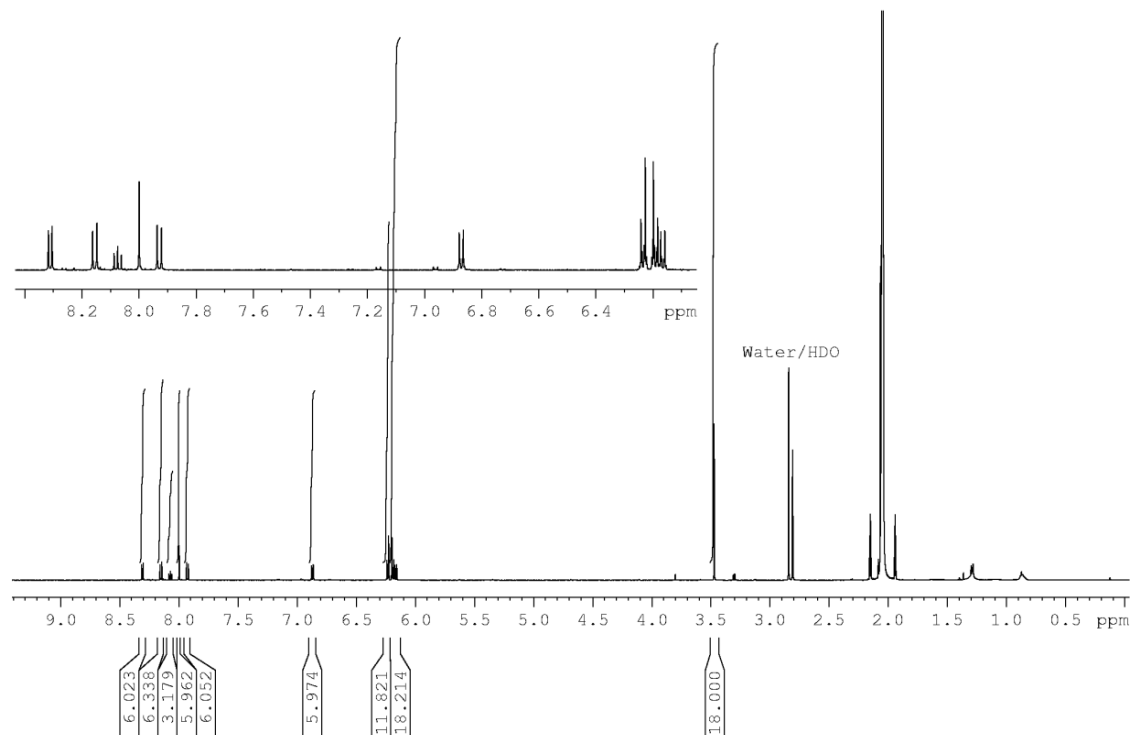


Figure S6. ESI of substance 1.

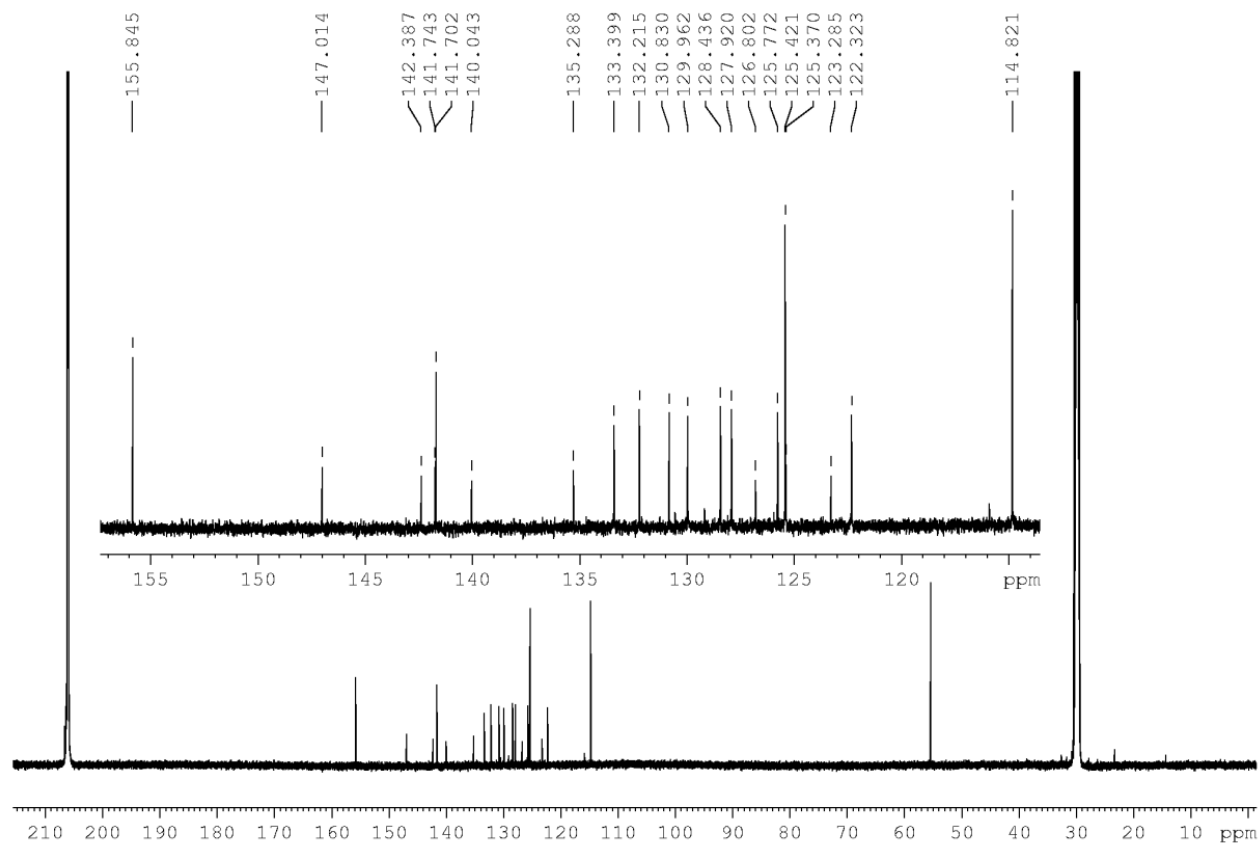


<sup>1</sup>H-NMR of substance 2



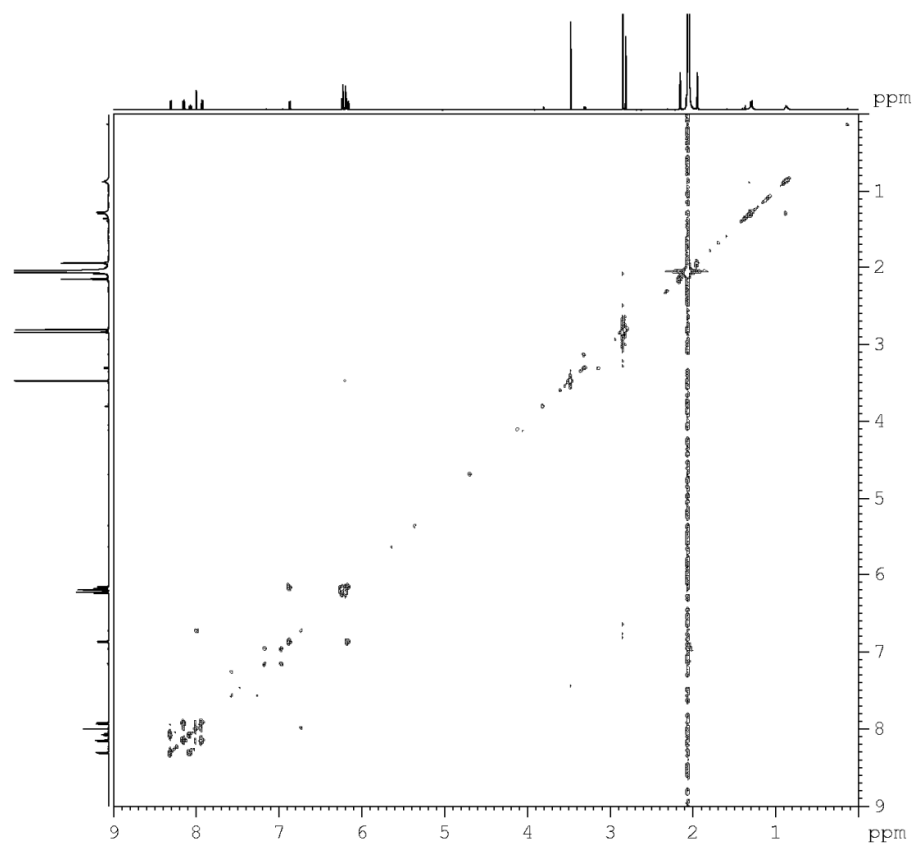
**Figure S7.** <sup>1</sup>H-NMR (600 MHz) of substance **2** in acetone-d<sub>6</sub>.

$^{13}\text{C}$ -NMR of substance 2



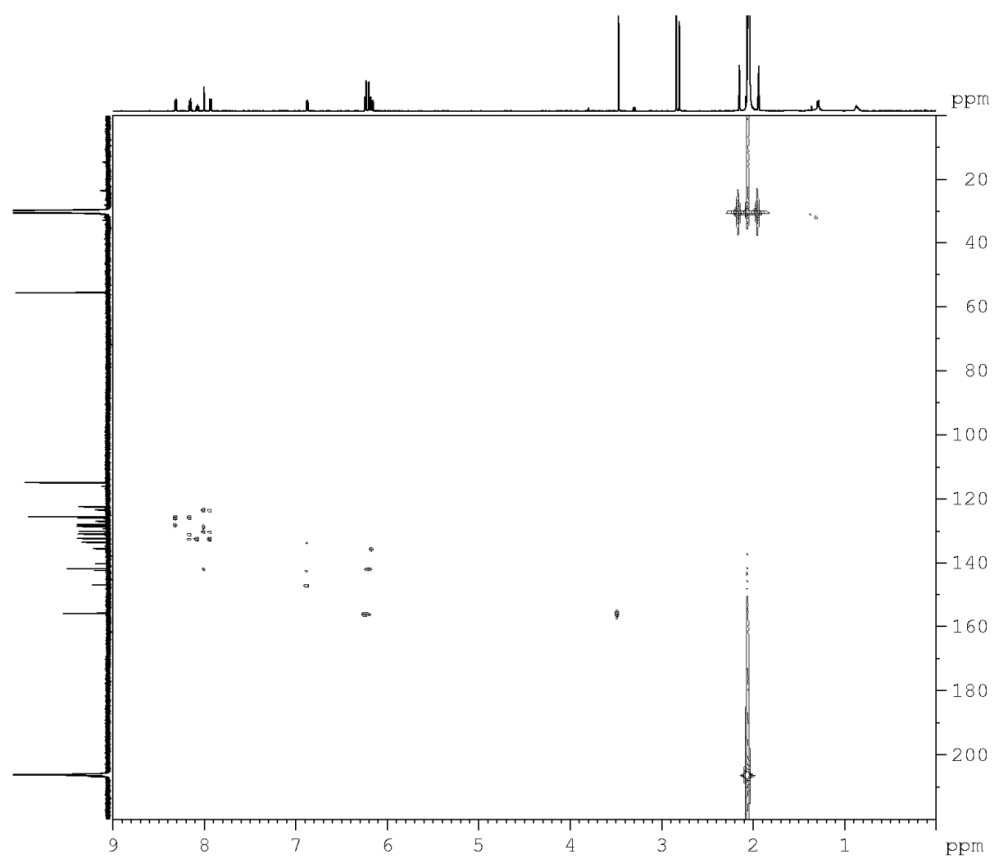
**Figure S8.**  $^{13}\text{C}$ -NMR (151 MHz) of substance 2 in acetone- $\text{d}_6$ .

COSY substance 2



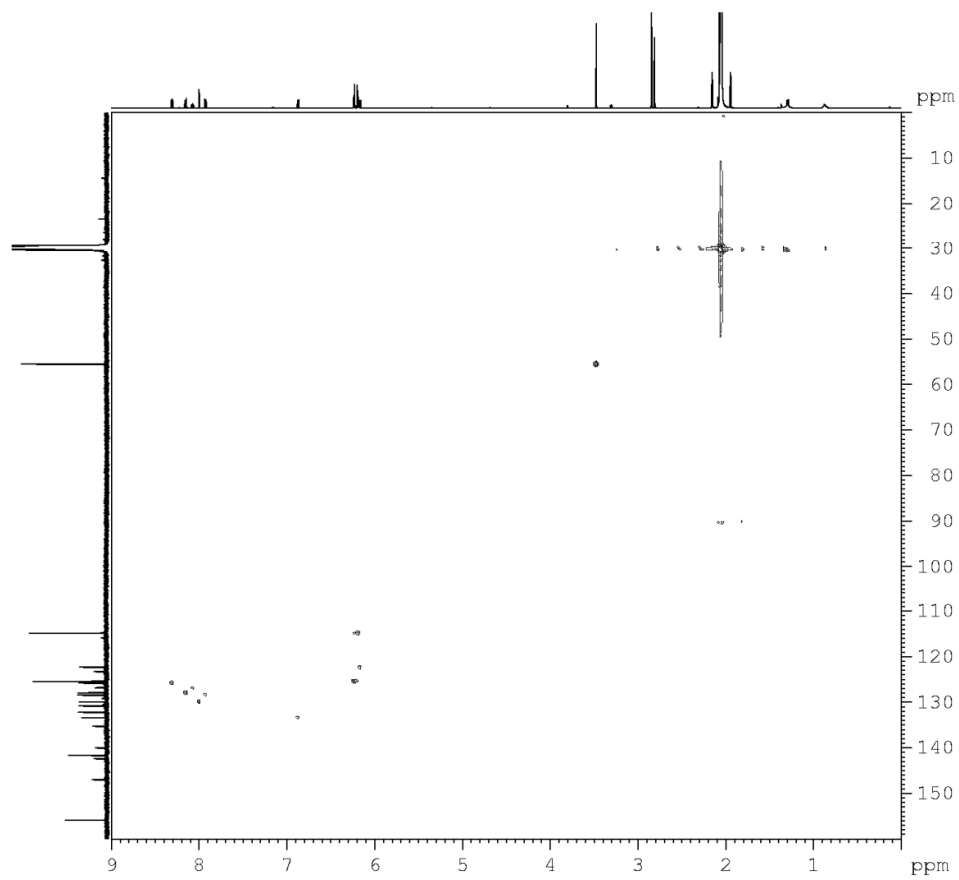
**Figure S9.** COSY of substance **2** in acetone-d<sub>6</sub>.

HMBC substance 2



**Figure S10.** HMBC of substance **2** in acetone-d<sub>6</sub>.

HSQC substance 2



**Figure S11.** HSQC of substance **2** in acetone-d<sub>6</sub>.

## Mass Spectrum Molecular Formula Report

## Analysis Info

Analysis Name D:\Data\Spektren2012\2012\_0117.d  
Method esi\_tune\_pos\_high.m  
Comment Julia Ehbets  
JES  
11 pmol /  $\mu$ l in Aceton

Acquisition Date 24.01.2012 14:36:47  
Operator Administrator  
Instrument micrOTOF 88

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Scan Begin	50 m/z	Hexapole RF	800.0 V	Set Pulsar Push	804 V
Scan End	3000 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	23.0 V	Set Flight Tube	8600 V
				Set Detector TOF	1980 V

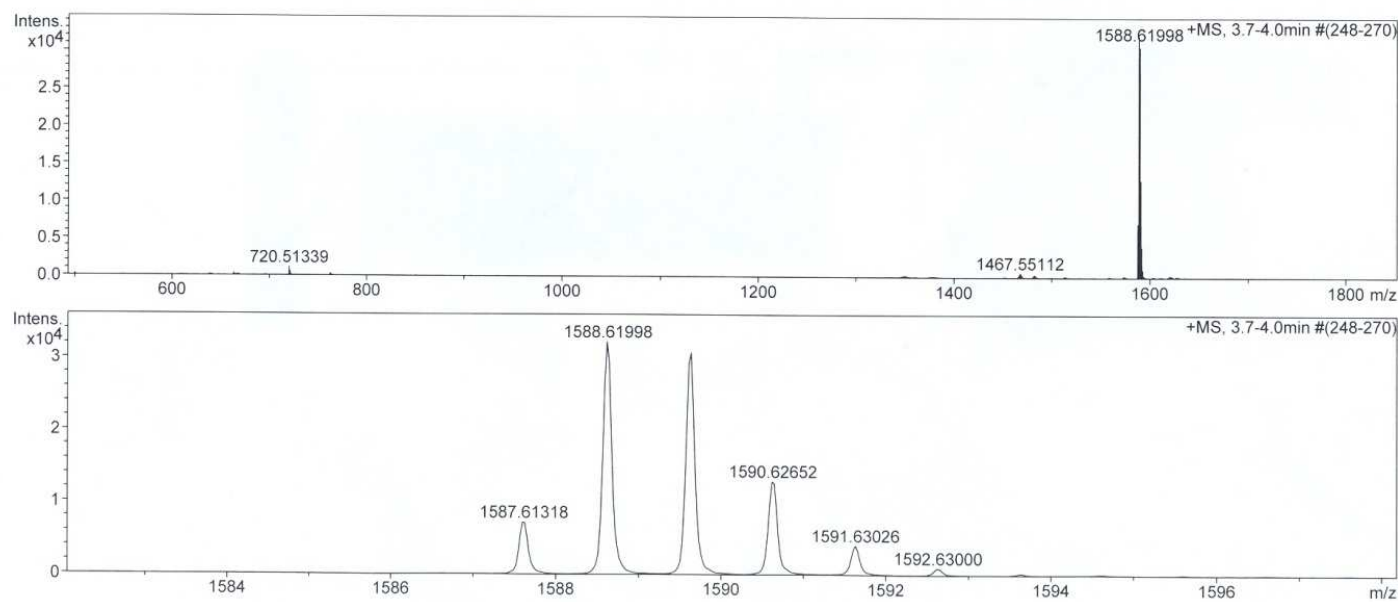
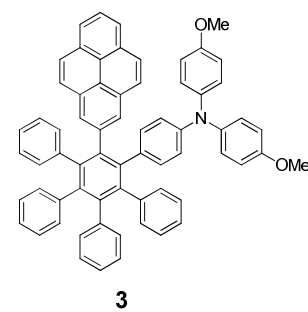
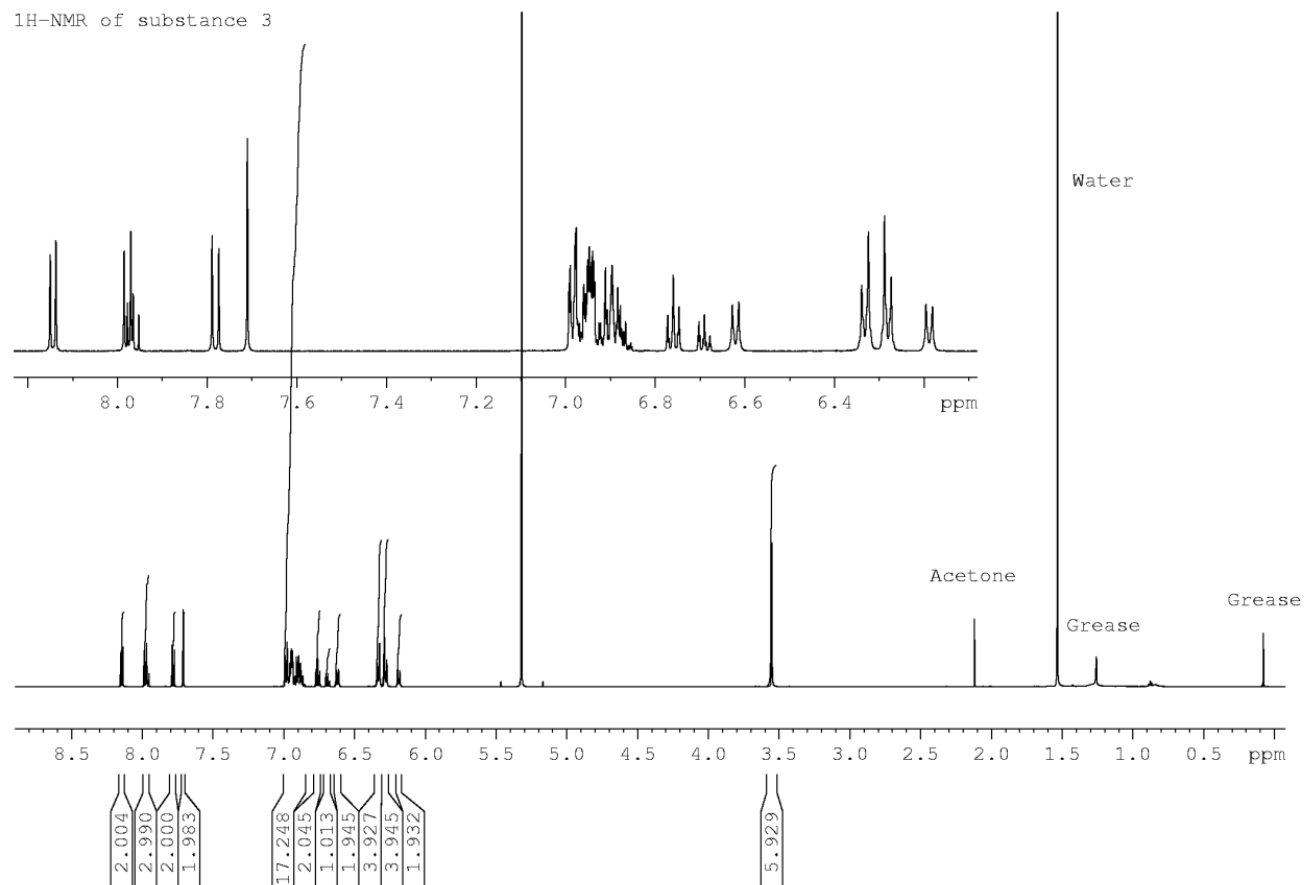
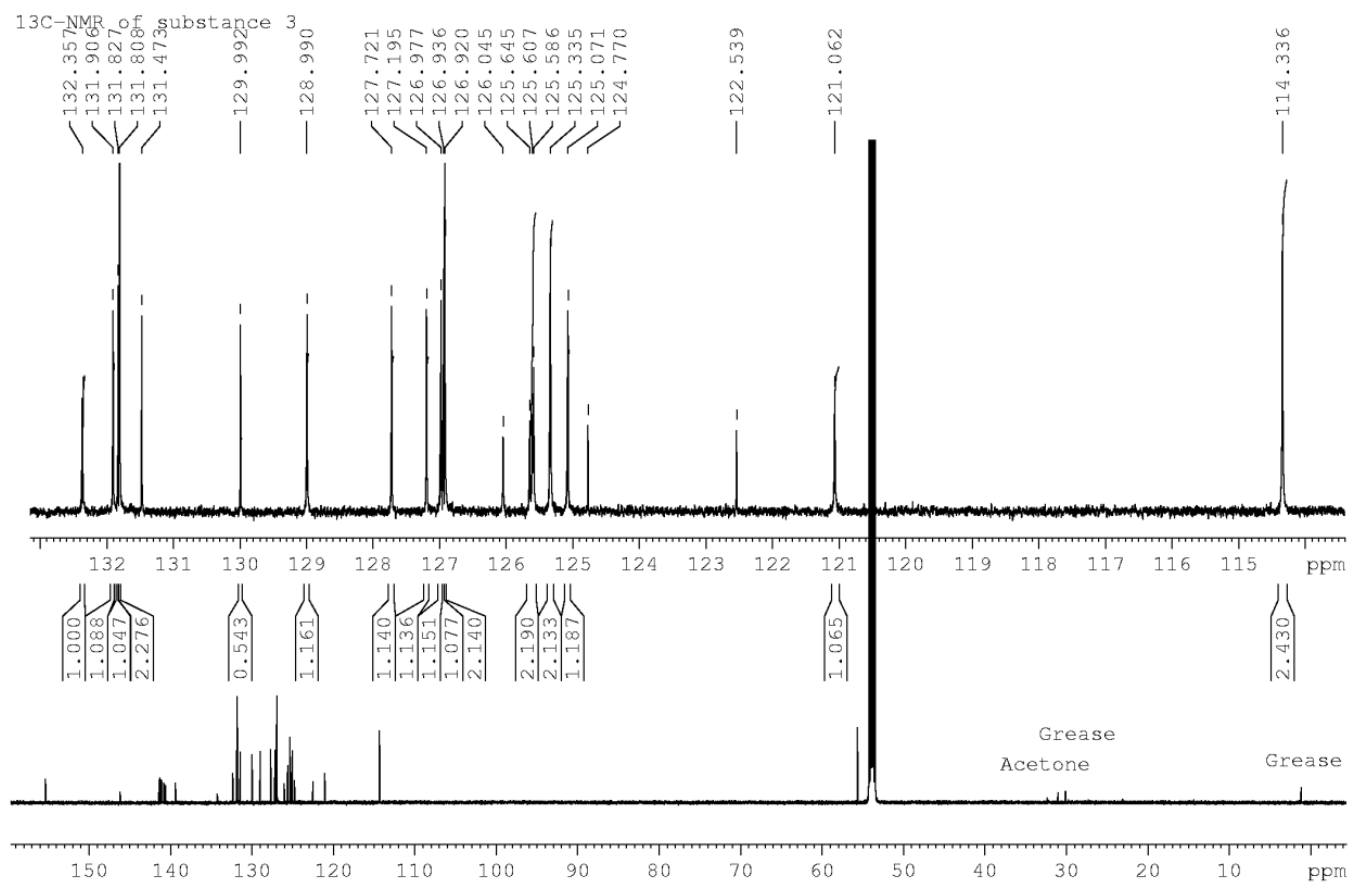


Figure S12. ESI of substance 2.

<sup>1</sup>H-NMR of substance 3



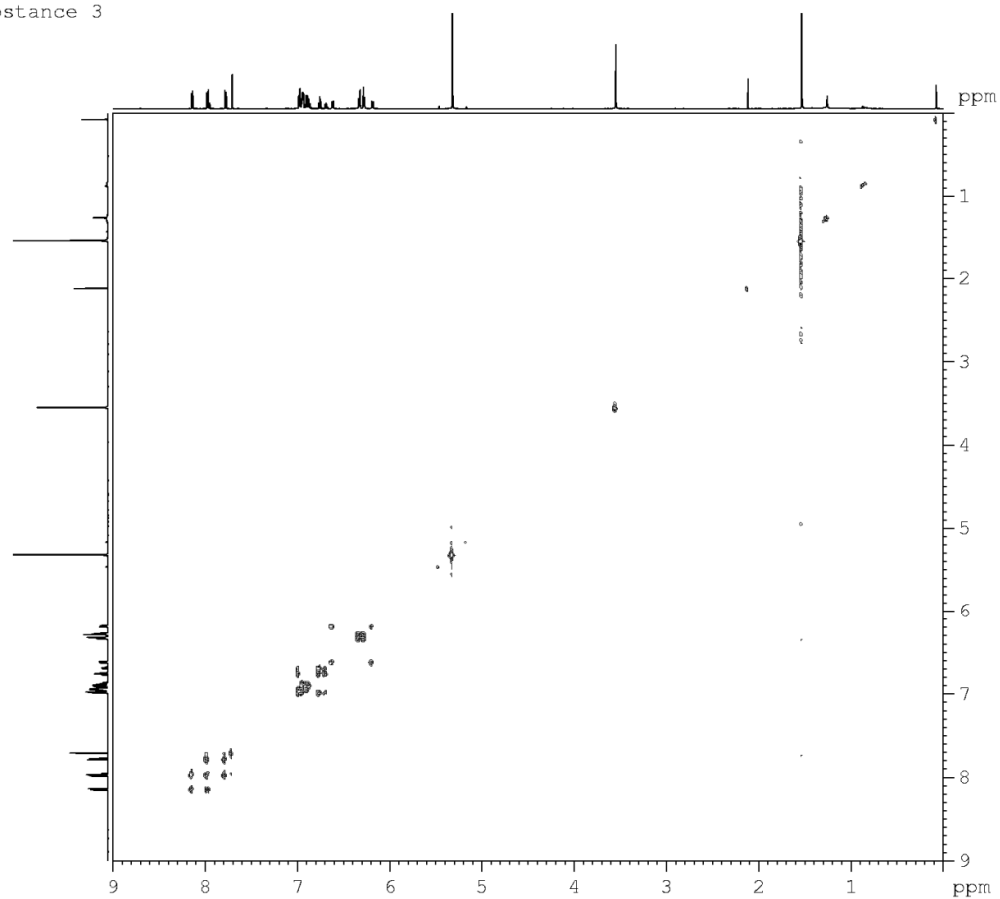
**Figure S13.** <sup>1</sup>H-NMR (600 MHz) of substance **3** in DCM-d<sub>2</sub>.



**Figure S14.** <sup>13</sup>C-NMR (151 MHz) of substance **3** in DCM-d<sub>2</sub>.

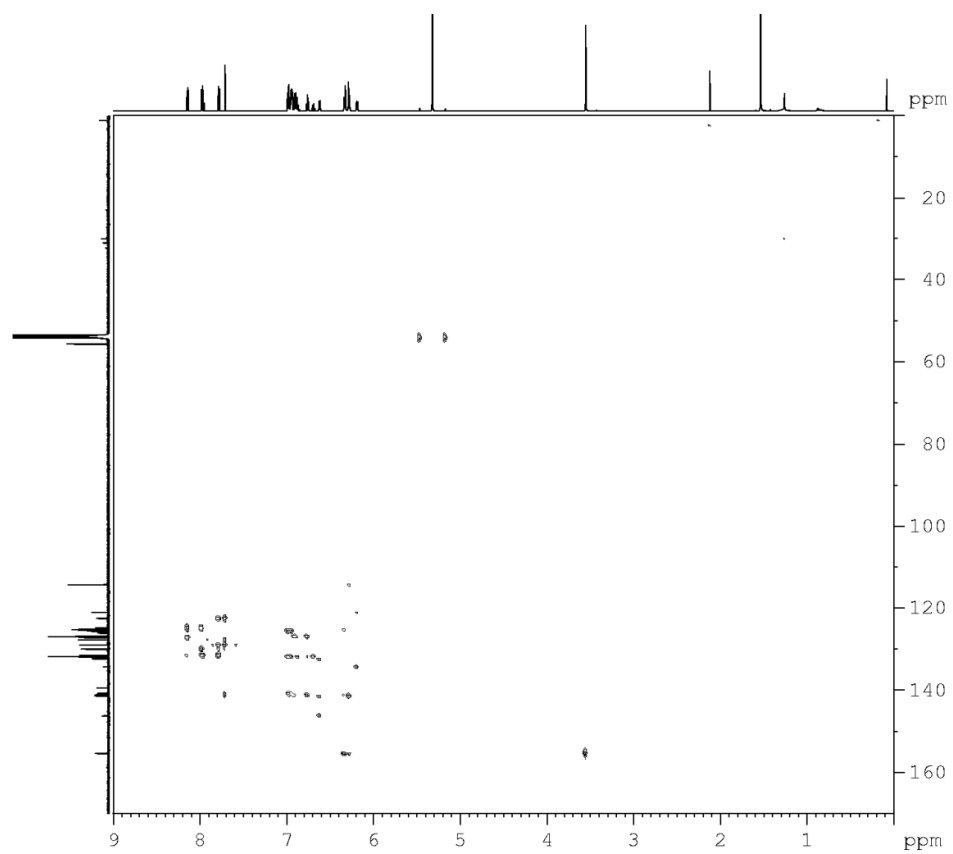


COSY substance 3



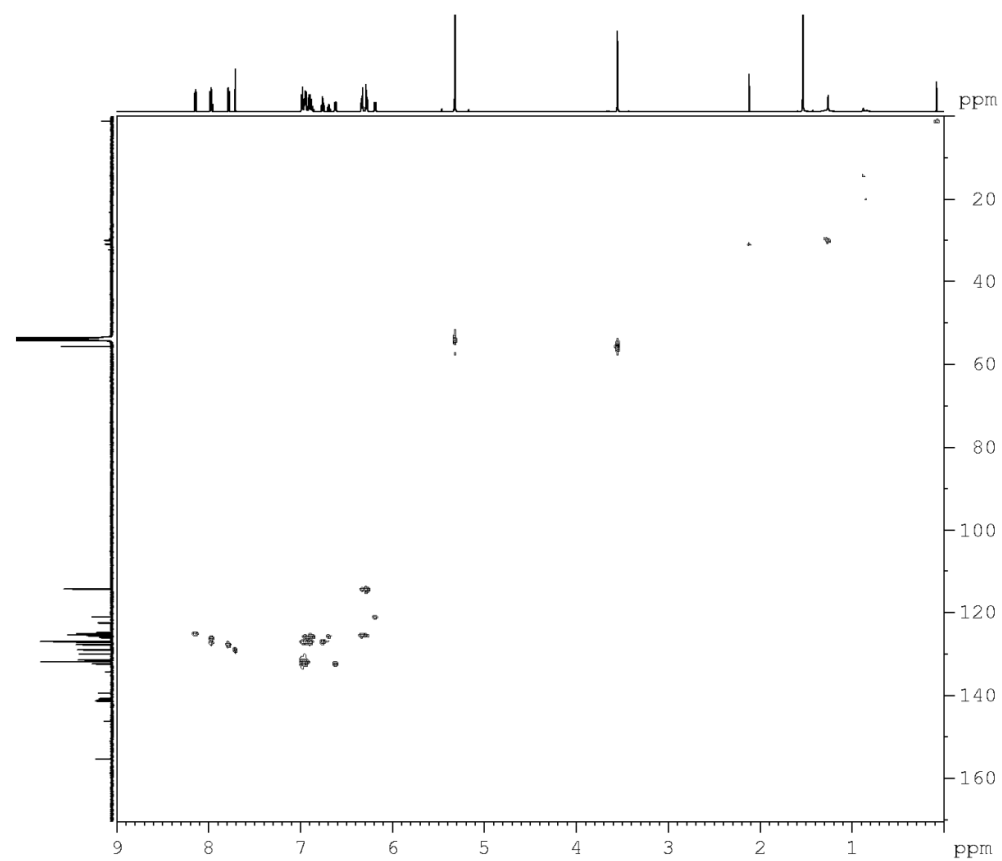
**Figure S15.** COSY of substance **3** in DCM-d<sub>2</sub>.

HMBC substance 3



**Figure S16.** HMBC of substance **3** in DCM-d<sub>2</sub>.

HSQC substance 3



**Figure S17.** HSQC of substance **3** in DCM-d<sub>2</sub>.

## Mass Spectrum Molecular Formula Report

## Analysis Info

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Method esi\_tune\_pos\_wide.m  
Comment Julia Ehbets  
JE25.3-1  
4 pmol /  $\mu$ l in Aceton

Acquisition Date 03.02.2012 10:38:28  
Operator Administrator  
Instrument micrOTOF 88

## Acquisition Parameter

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Scan End	2800 m/z	Skimmer 1	50.0 V	Set Reflector	1700 V
		Hexapole 1	23.0 V	Set Flight Tube	8600 V
				Set Detector TOF	1970 V

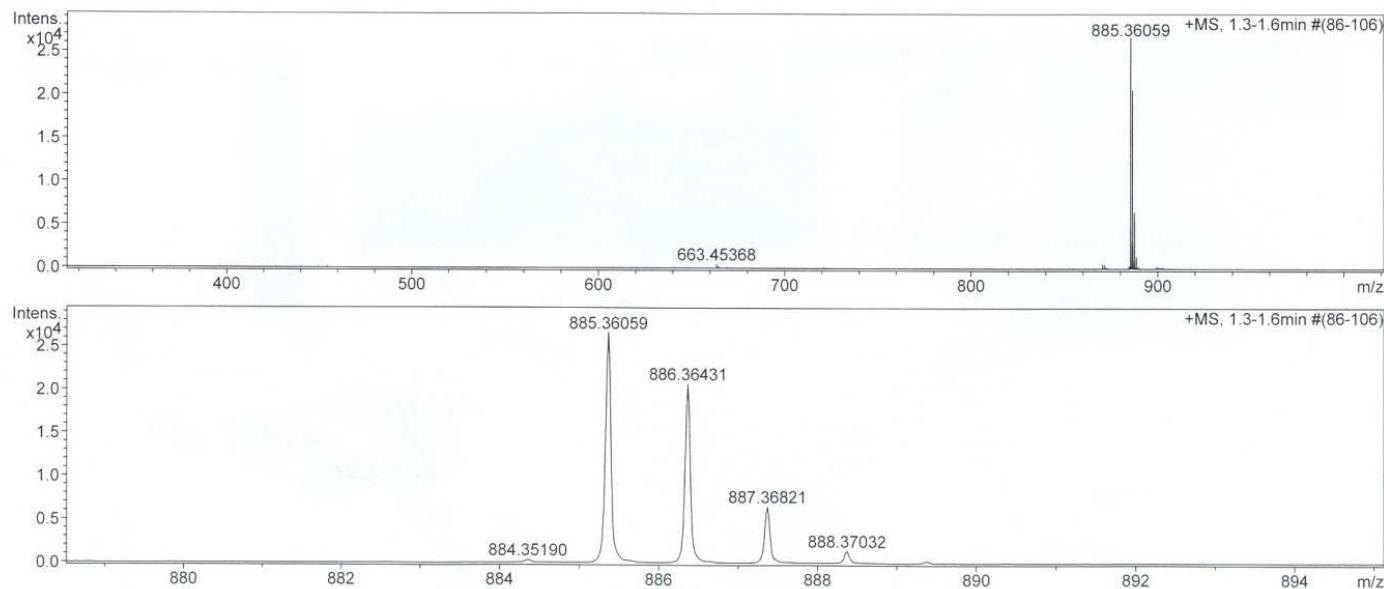
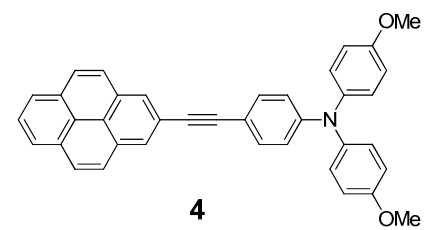
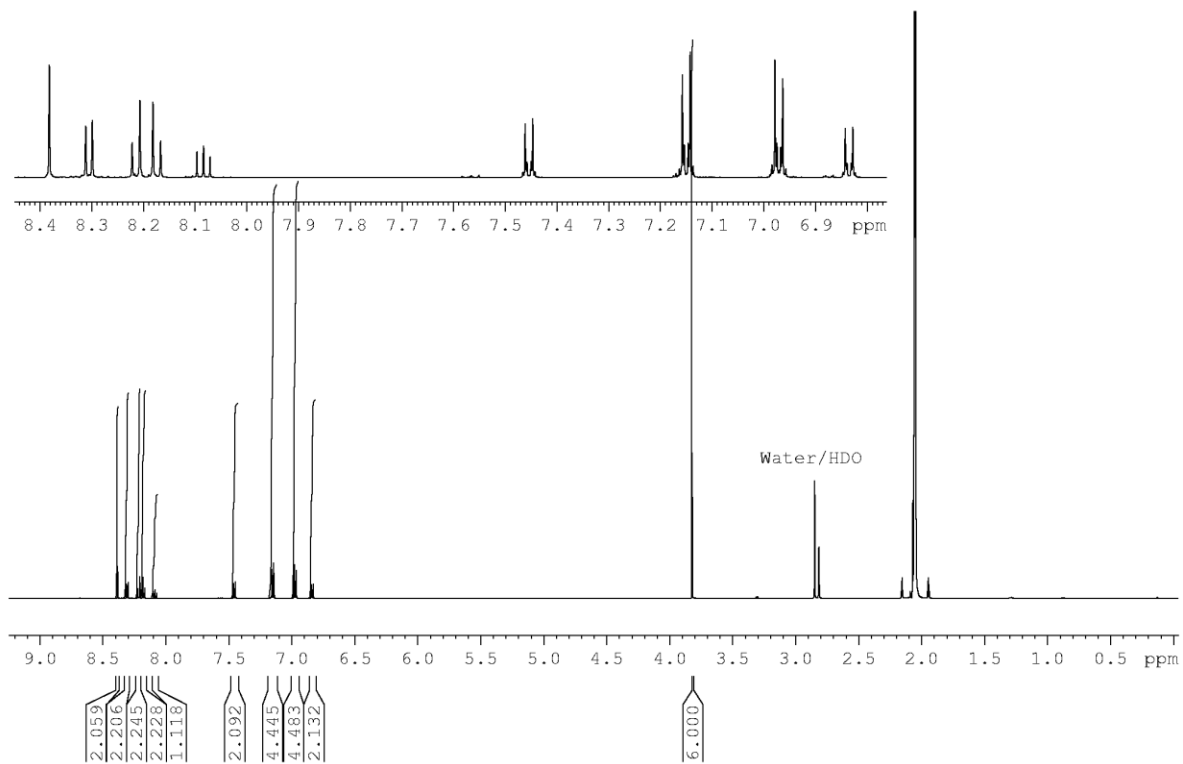


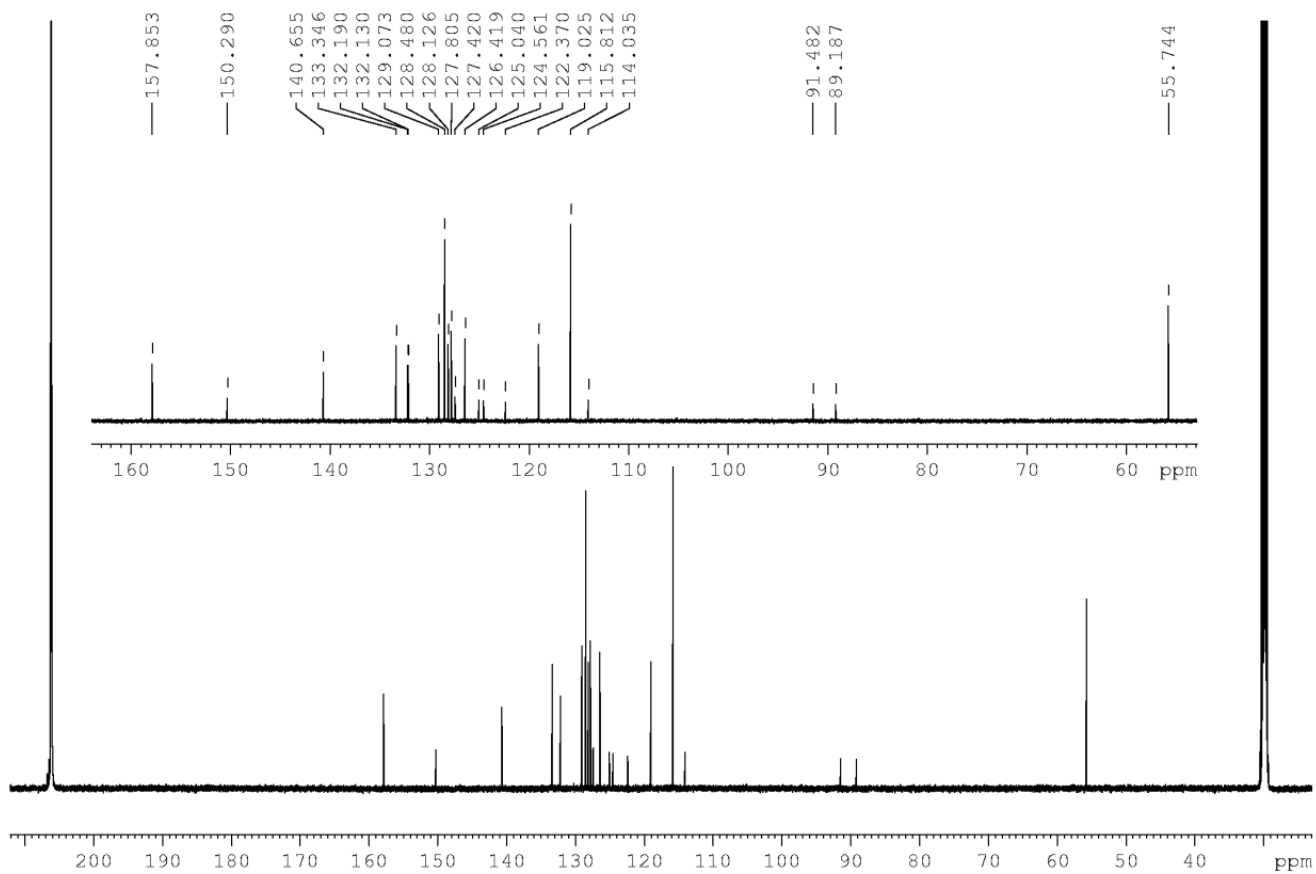
Figure S18. ESI of substance 3.

<sup>1</sup>H-NMR of substance 4



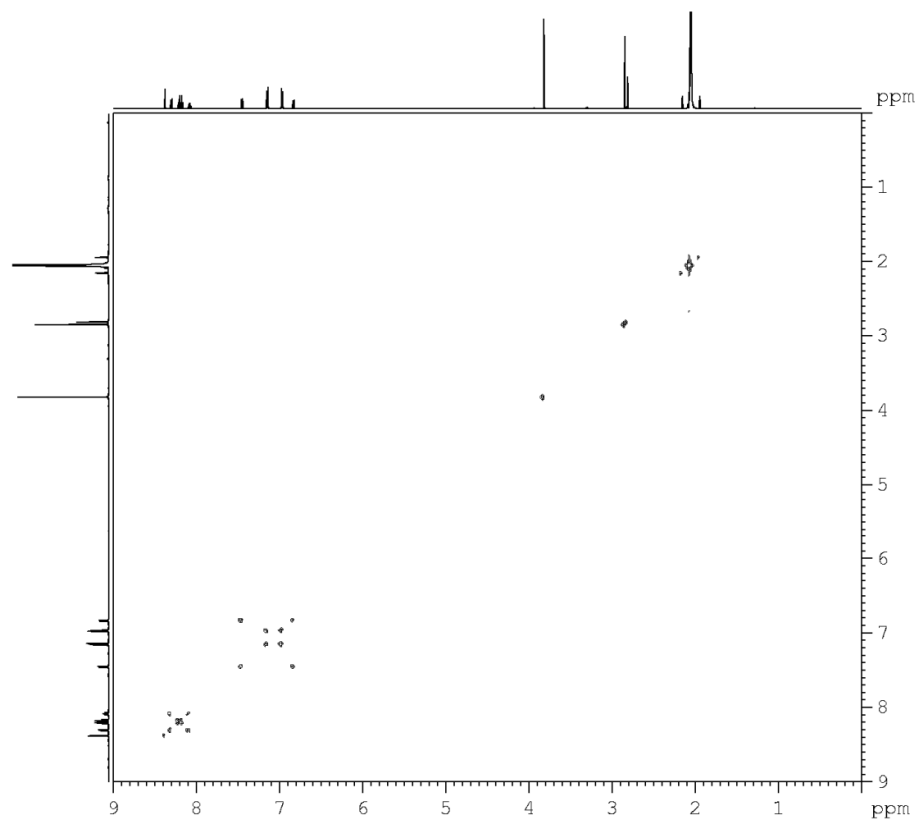
**Figure S19.** <sup>1</sup>H-NMR (600 MHz) of substance **4** in acetone-d<sub>6</sub>.

$^{13}\text{C}$ -NMR of substance 4

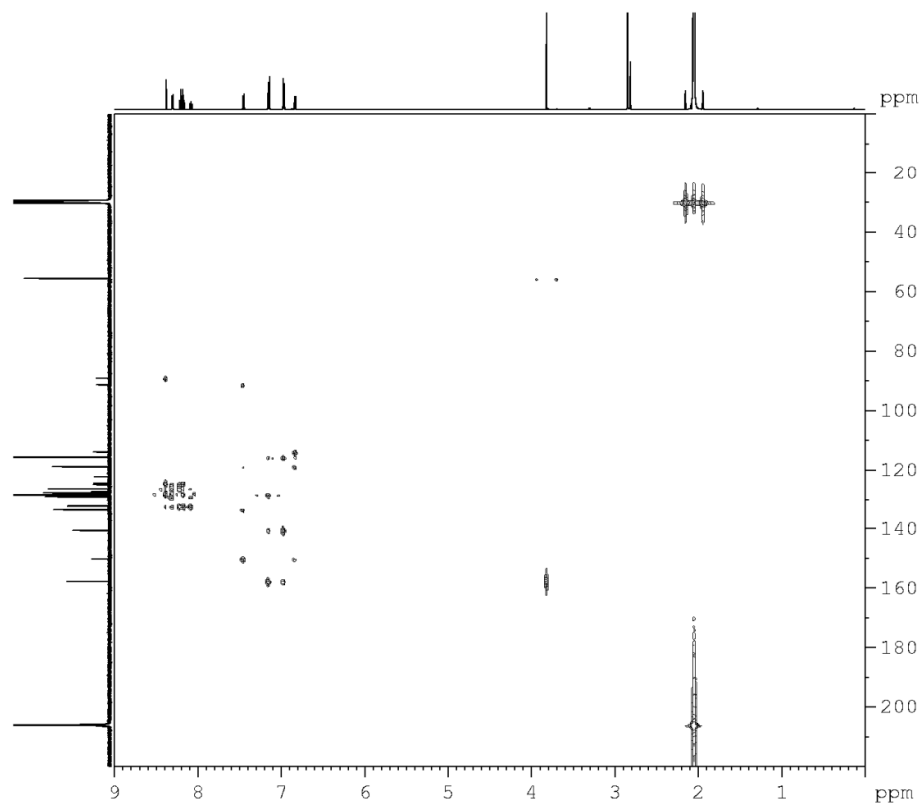


**Figure S20.**  $^{13}\text{C}$ -NMR (151 MHz) of substance 4 in acetone- $\text{d}_6$ .

COSY of substance 4

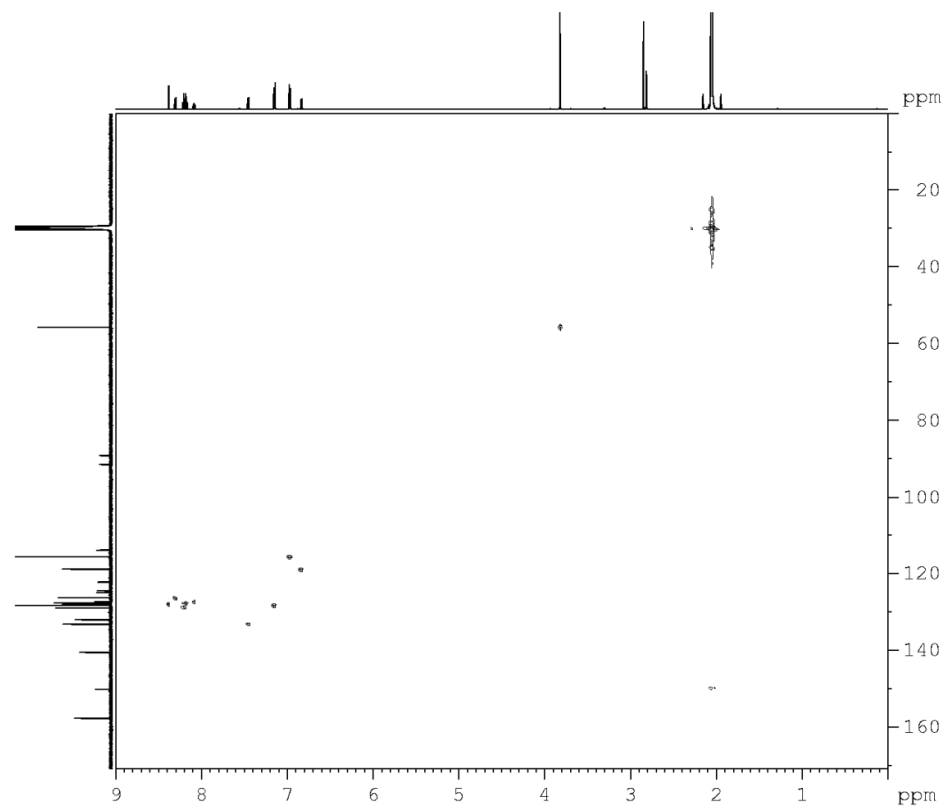
**Figure S21.** COSY of substance **4** in acetone-d<sub>6</sub>.

HMBC substance 4

**Figure S22.** HMBC of substance **4** in acetone-d<sub>6</sub>.



HSQC substance 4



**Figure S23.** HSQC of substance **4** in acetone-d<sub>6</sub>.

## Mass Spectrum Molecular Formula Report

## Analysis Info

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Method esi\_tune\_pos\_wide.m  
Comment Julia Ehbets  
JE8.19VII-2  
2,5 pmol /  $\mu$ l in Aceton

Acquisition Date 19.01.2012 14:59:35  
Operator Administrator  
Instrument micrOTOF 88

## Acquisition Parameter

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Scan End 1650 m/z

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Hexapole RF 350.0 V  
Skimmer 1 50.0 V  
Hexapole 1 23.0 V

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Set Pulsar Push 804 V  
Set Reflector 1700 V  
Set Flight Tube 8600 V  
Set Detector TOF 1970 V

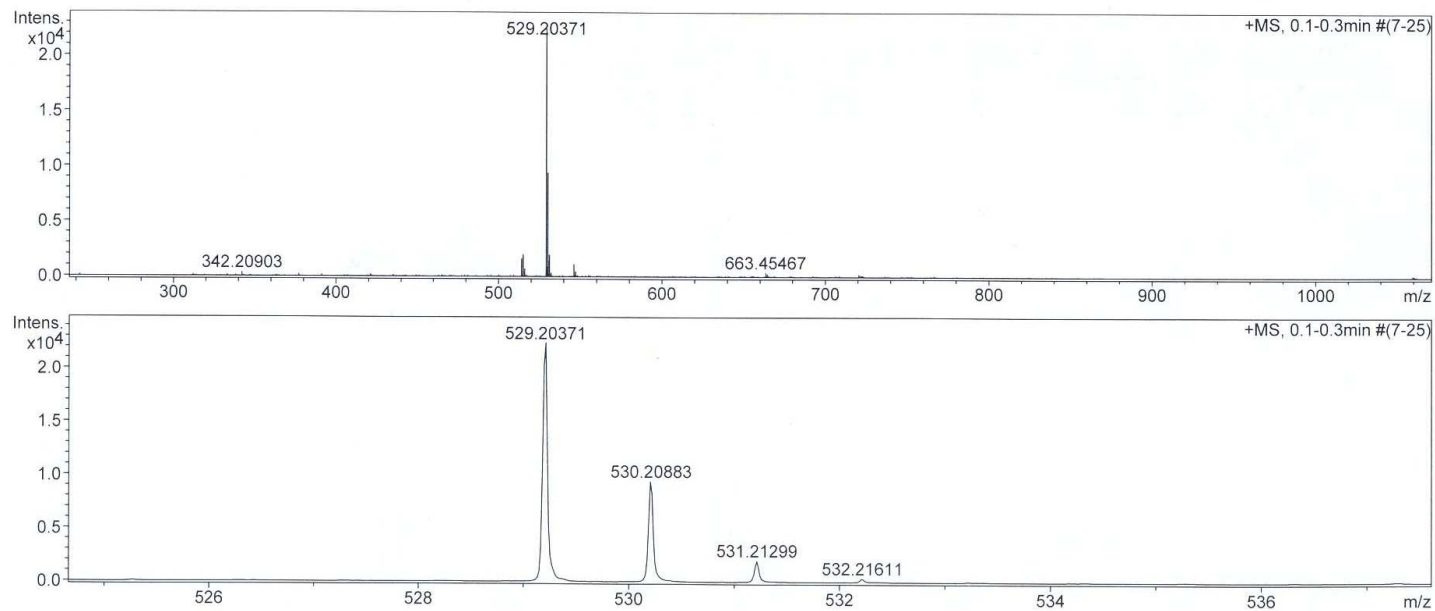
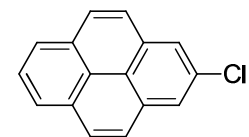
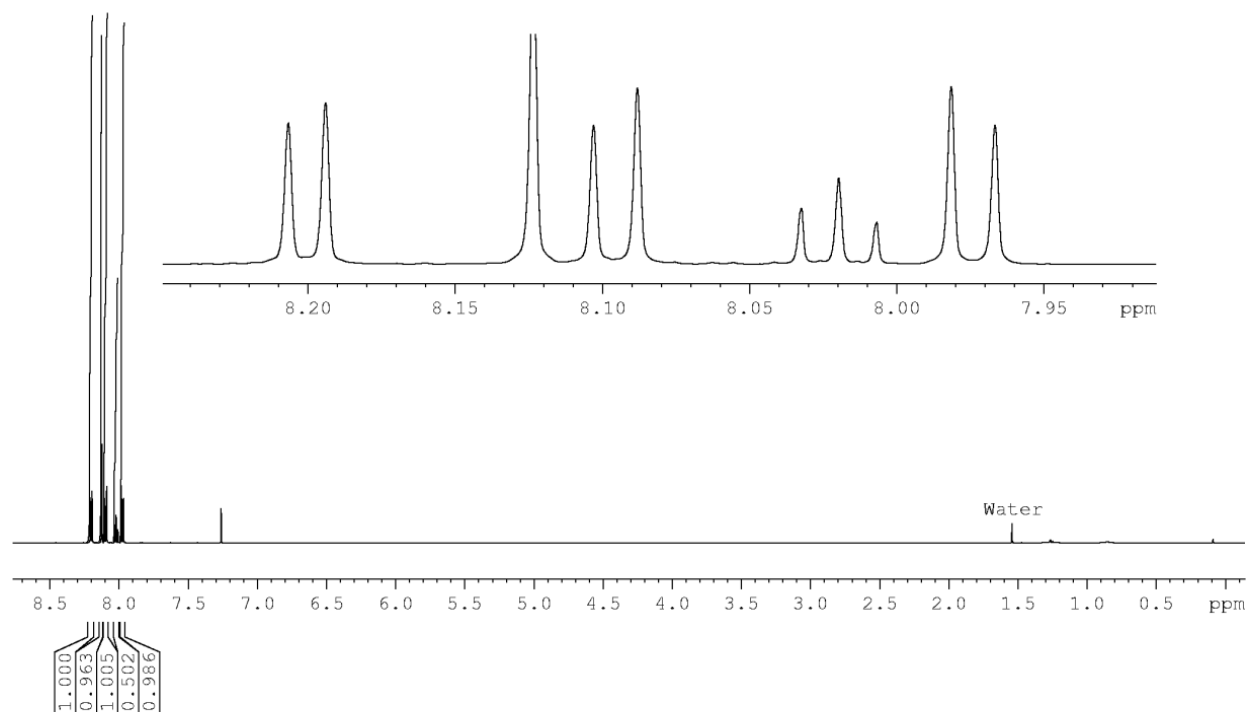


Figure S24. ESI of substance 4.

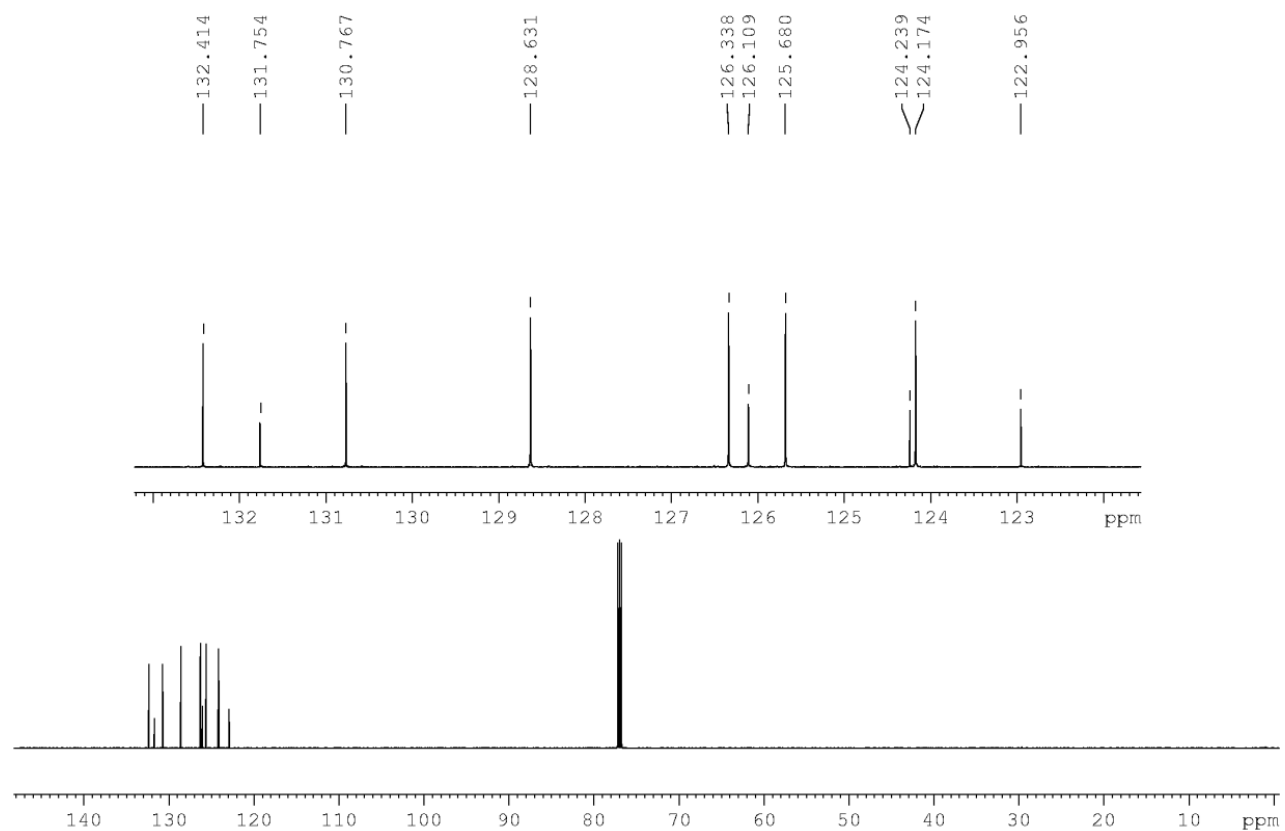
<sup>1</sup>H-NMR of substance 5



**5**

**Figure S25.** <sup>1</sup>H-NMR (600 MHz) of substance **5** in chloroform-d.

$^{13}\text{C}$ -NMR of substance 5



**Figure S26.**  $^{13}\text{C}$ -NMR (151 MHz) of substance 5 in chloroform-d.