

## Electronic Supplementary data

For

### Development of a facile and sensitive fluorimetric derivatization reagent for detecting formaldehyde

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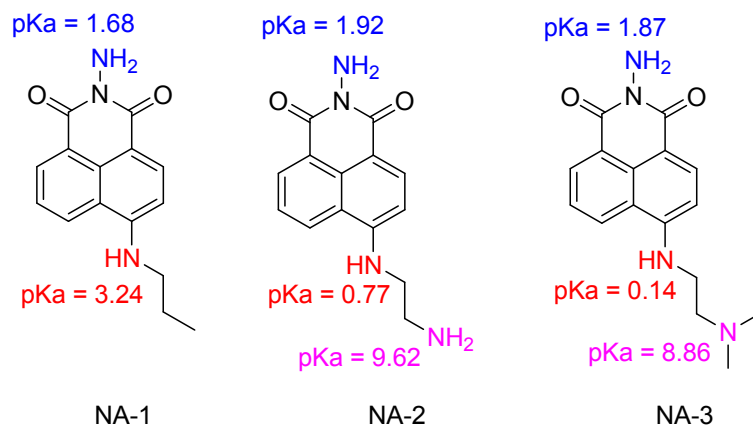


Fig. S1 *pKa* values of amino groups calculated by MarvinSketch software using macro mode and dynamic acid/baseprefix at 298 K

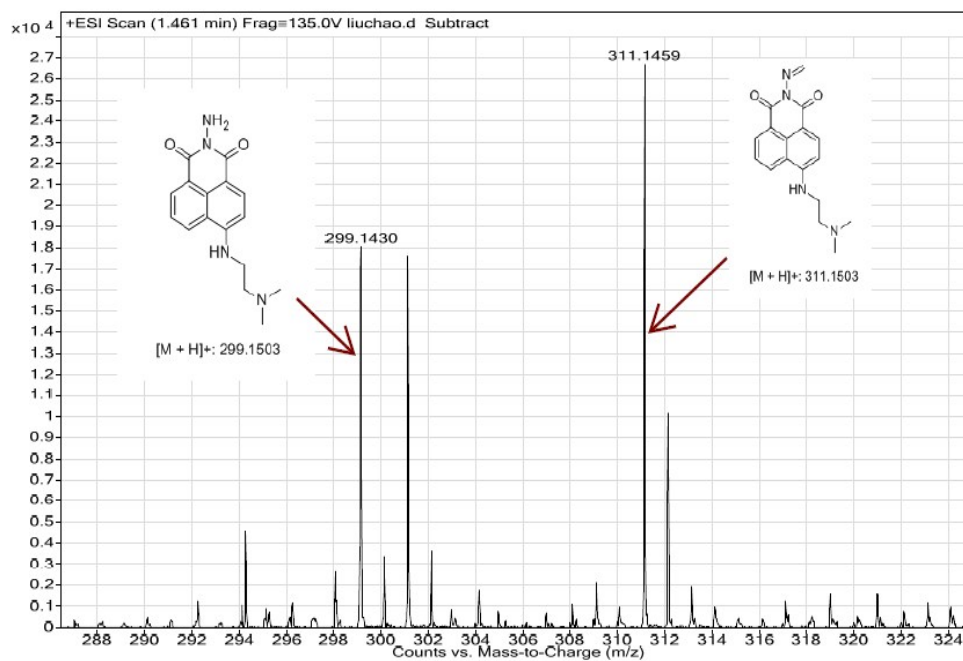


Fig. S2 HRMS spectrum of isolated reaction product of **NA3** and formaldehyde

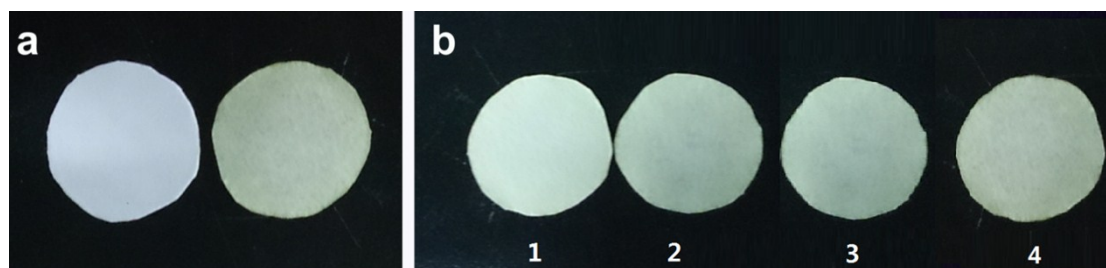


Fig. S3 (a) Photographs of the white filter paper (left) and prepared test paper (right) under natural light, (b) photographs of the test paper in the absence and presence of formaldehyde under natural light. 1, blank; 2, formaldehyde in MeCN (10 % HOAc) solution; 3, formaldehyde in water solution; 4, formaldehyde-contained air condition

Table S1. Detailed comparison of the reagent NA3 with other reported fluorimetric derivatization reagents

reagent	reaction site	$\lambda_{em}/nm$	detection limit / $\mu M.L^{-1}$	reaction time	comment	Ref.
hydralazine	hydrazine	389	0.067	25 min	100 °C	1
AAA	carboxide	368	0.02	10-30 min	in the presence of ammonia	2
FAP-1	amino	662	5.0	2 h	--	3
FP1	amino	650	10.0	3 h	37 °C	4
NPz	hydrazine	540	8.72	4 min	room temperature	5
RFFP	amino	359, 451	18.7	> 3h	--	6
NA3	hydrazine	515	0.104	9min	room temperature	this work

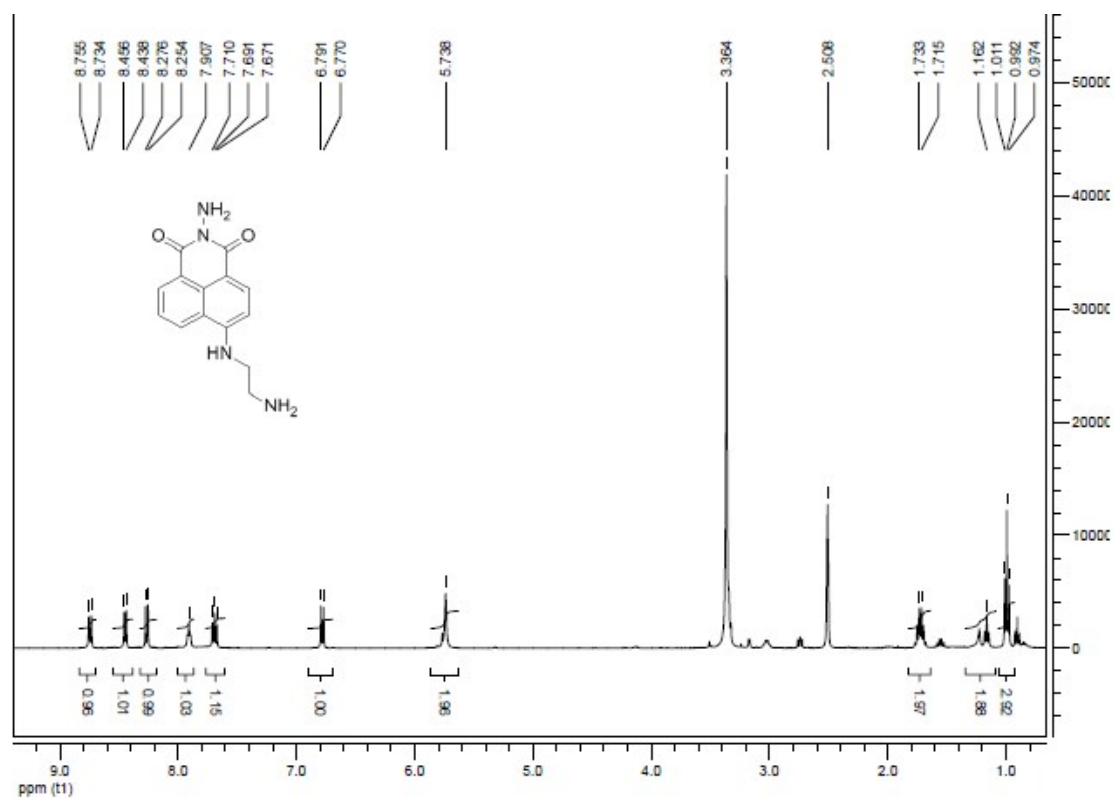


Fig. S4 <sup>1</sup>H-NMR spectrum of NA1

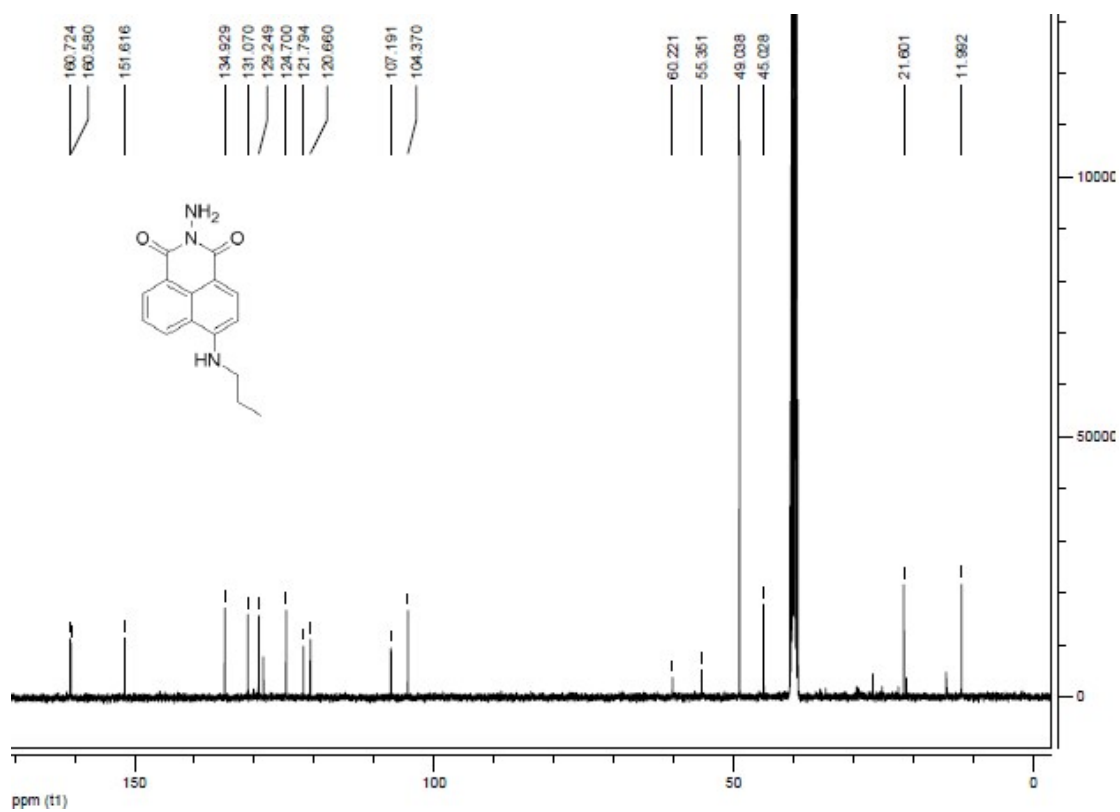


Fig. S5 <sup>13</sup>C-NMR spectrum of NA1

Sample Name	Unavailable	Position	Unavailable	Instrument Name	Unavailable	User Name	Unavailable
Inj Vol	Unavailable	InjPosition	Unavailable	SampleType	Unavailable	IRM Calibration Status	Success
Data Filename	0908-810-1.d	ACQ Method		Comment	Sample information is unavailable	Acquired Time	Unavailable



Fig. S6 HR-ESI-MS spectrum of NA1

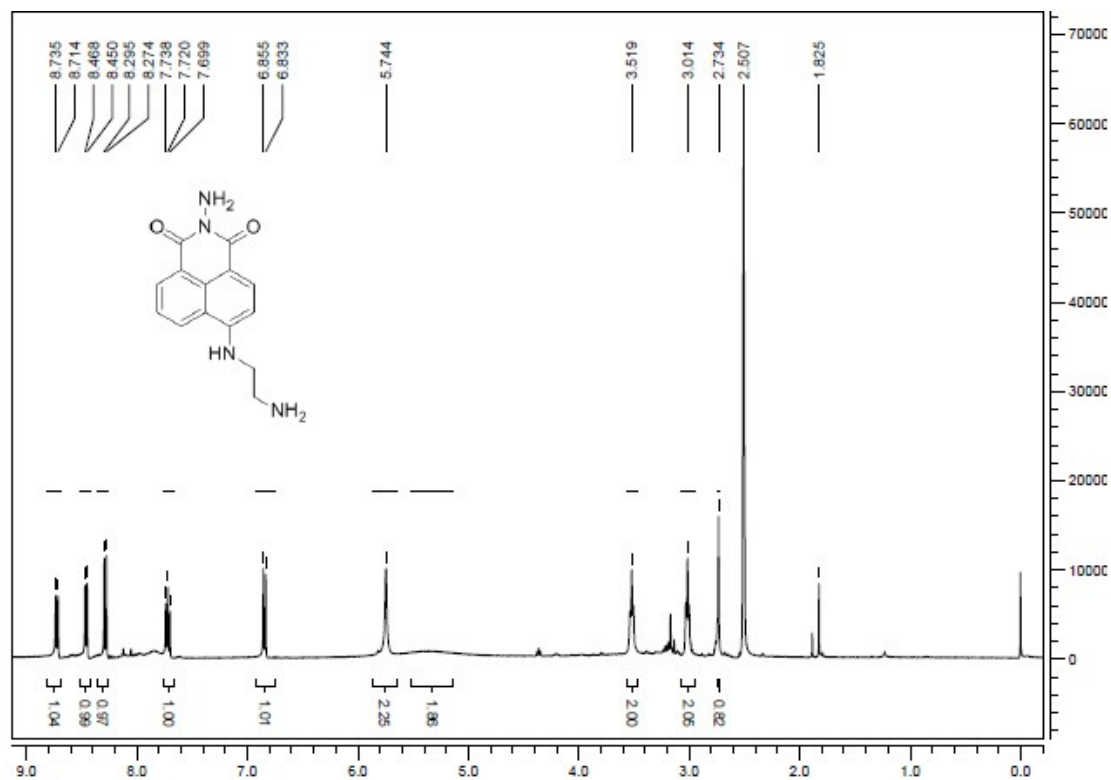


Fig. S7 <sup>1</sup>H-NMR spectrum of NA2

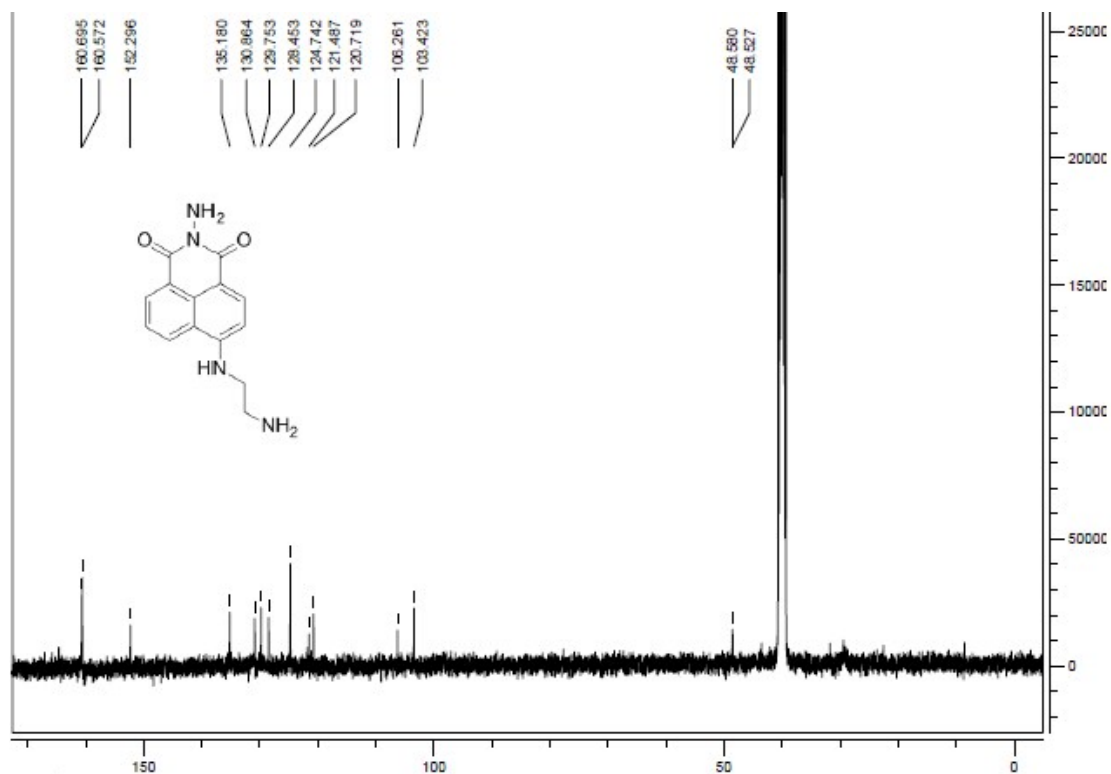


Fig. S8 <sup>13</sup>C-NMR spectrum of NA2

Sample Name	0908-610	Position	F1-68	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	0908-727-1.d	ADQ Method	0103.m	Comment		Acquired Time	9/8/2015 9:44:53 AM

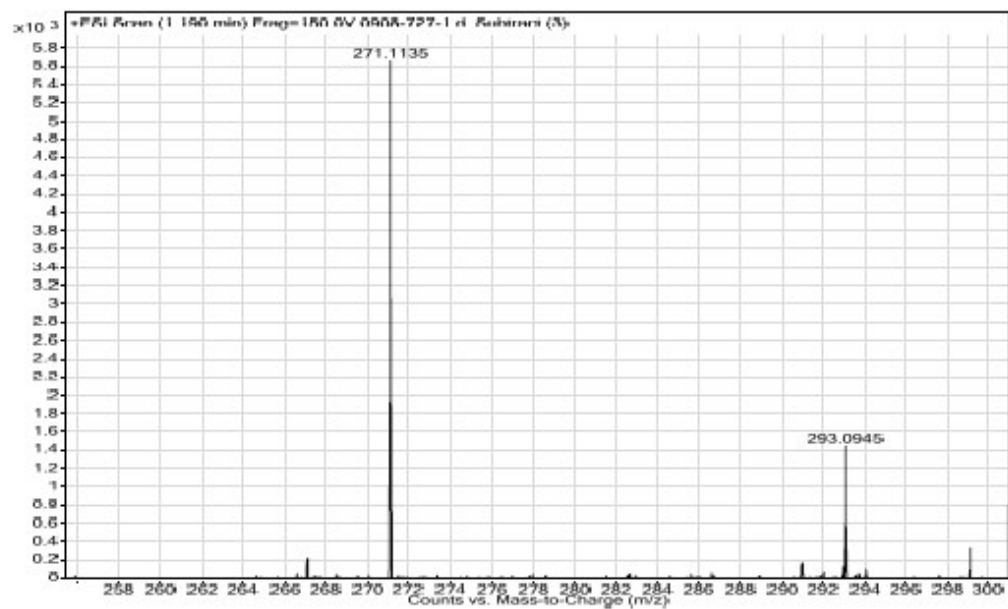


Fig. S9 HR-ESI-MS spectrum of NA2

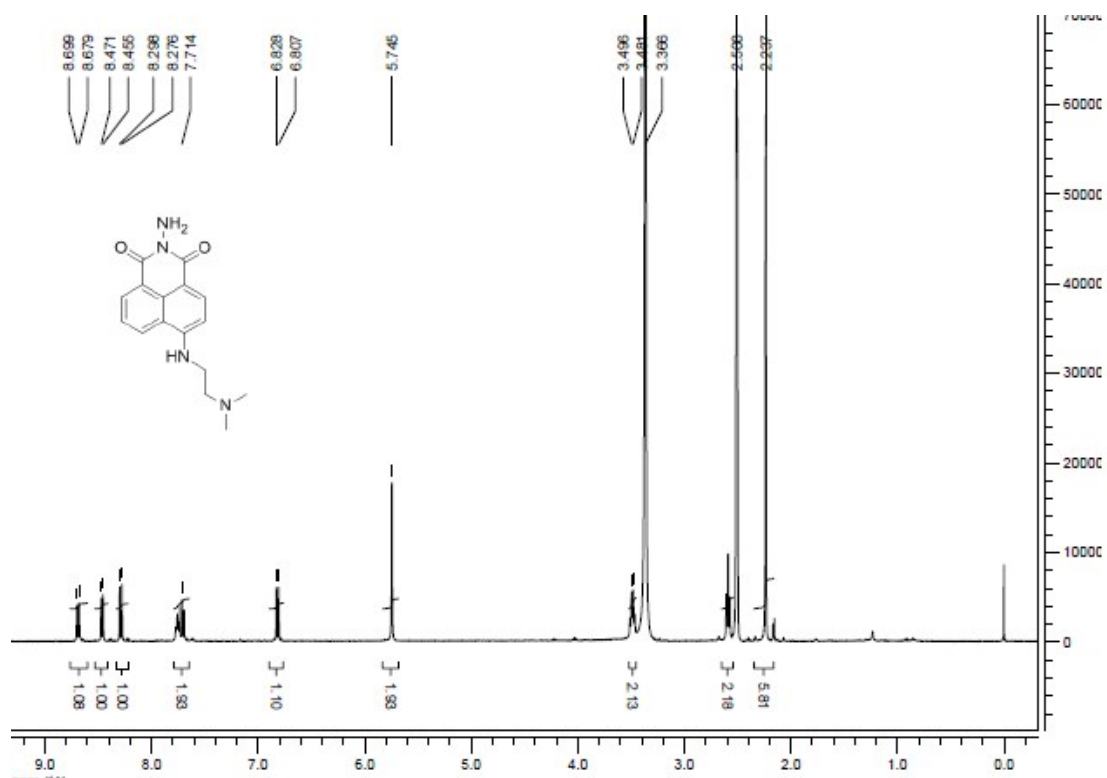


Fig. S10  $^1\text{H-NMR}$  spectrum of NA3

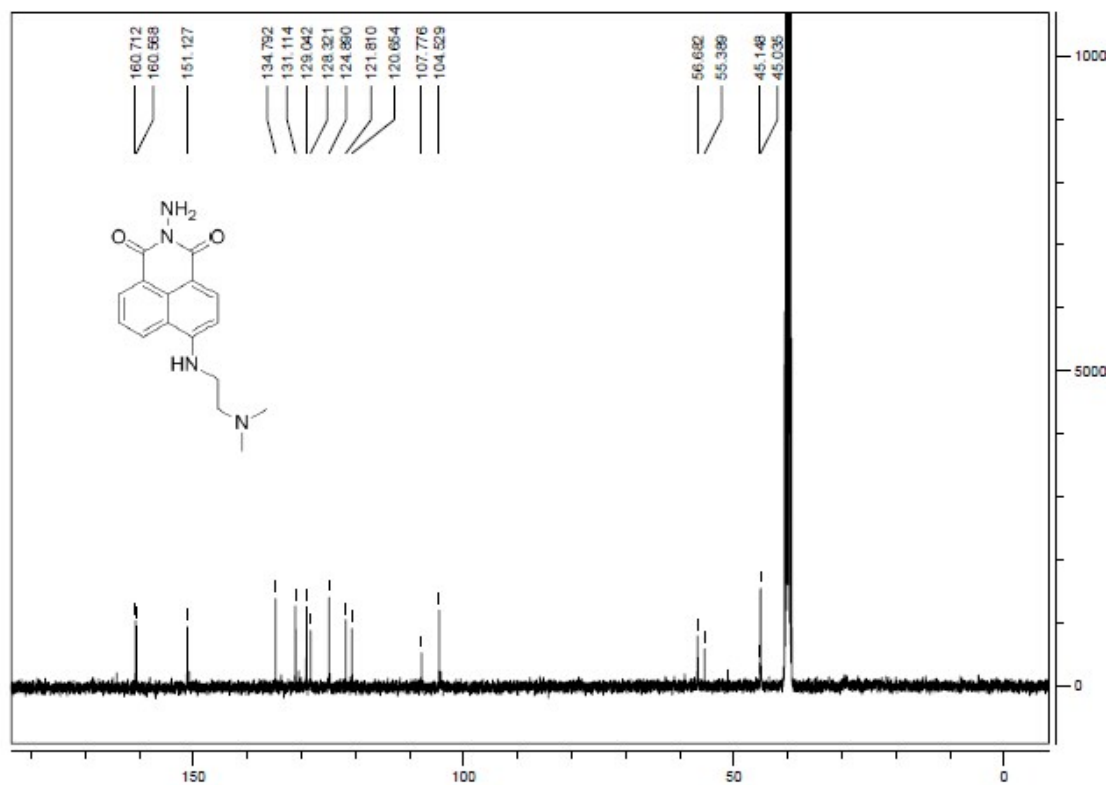
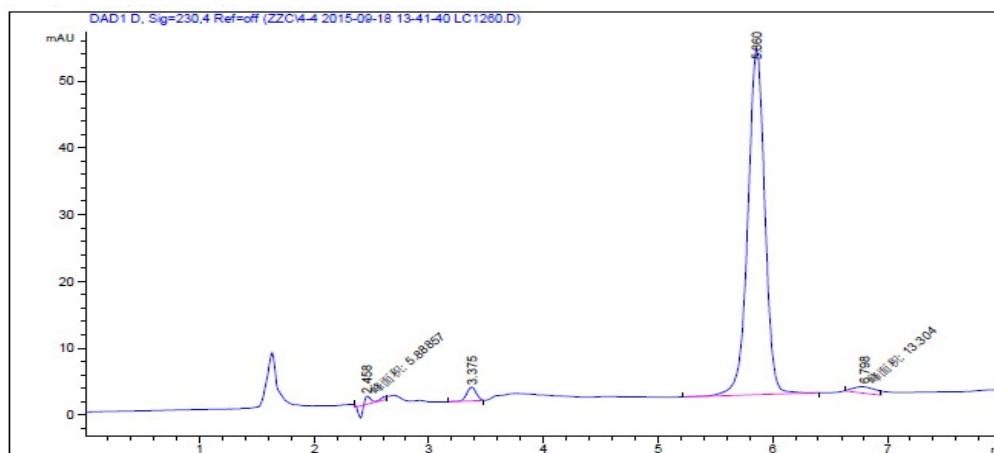


Fig. S11  $^{13}\text{C-NMR}$  spectrum of NA3

Sample Name 0908-808 Position P1-P8 Instrument Name Instrument 1 User Name  
 Inj Vol -1 InjPosition InjPosition SampleType Sample IRM Calibration Status Success  
 Data Filename 0908-808.d ACQ Method 0103.m Comment Acquired Time 9/8/2015 9:33:02 AM



Fig. S12 HR-ESI-MS spectrum of NA3



面积百分比报告

排序 : 信号  
 乘积因子 : 1.0000  
 稀释因子 : 1.0000  
 内标中不使用乘积因子和稀释因子

信号 1: DAD1 D, Sig=230,4 Ref=off

峰 #	保留时间 [min]	类型	峰宽 [min]	峰面积 [mAU*s]	峰高 [mAU]	峰面积 %
1	2.458	MM	0.0834	5.88857	1.17649	1.0458
2	3.375	BB	0.1075	11.62448	2.00891	2.0646
3	5.860	BB	0.1692	532.23035	51.21563	94.5267
4	6.798	MM	0.2345	13.30401	9.45624e-1	2.3629

Fig. S13 HPLC spectrum of NA3



Reference:

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