Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Targetable, Two-Photon Fluorescent Probe for Local Nitric Oxide Capture in the Plasma Membranes of Live Cells and Brain Tissue

Xinfu Zhang,[†] Benlei Wang,[†] Yi Xiao,[†]* Chao Wang,[†] and Ling He[†]

*Corresponding author, E-mail address: xiaoyi@dlut.edu.cn

[†]State Key Laboratory of Fine Chemicals, Dalian University of Technology, Dalian 116024, China

Table of Contents

Figure S1-Figure S9 S2-S5

NMR spectra S6-S112

HRMS of **Mem-NO** S12

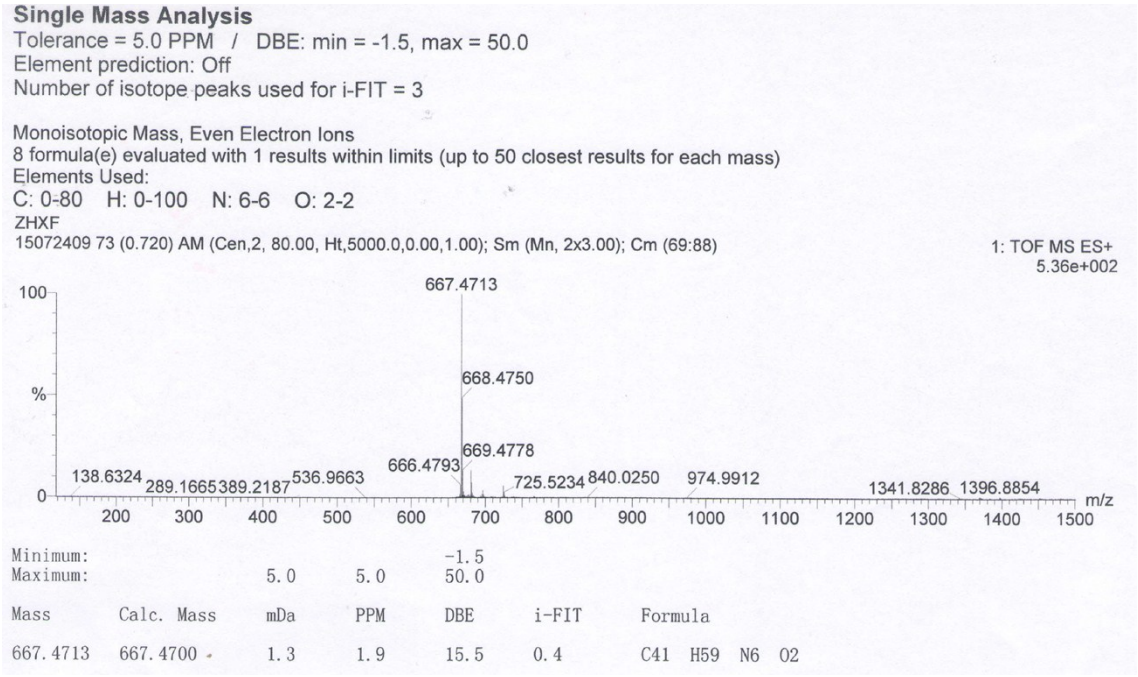


Figure S1. HRMS of **Mem-NOT**, prepared from **Mem-NO** by adding NO solution.

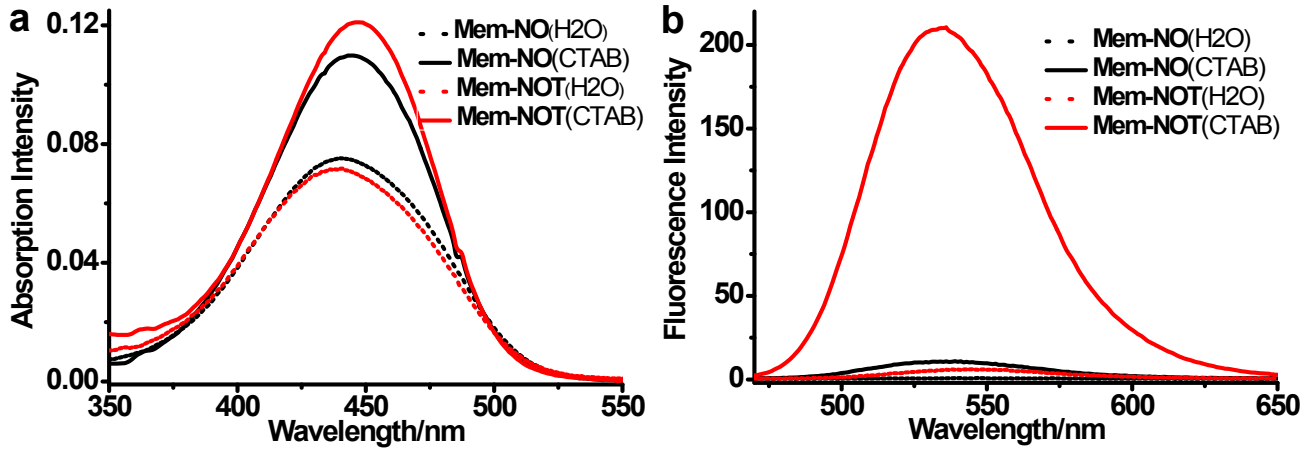


Figure S2. (a) Absorption spectra and (b) fluorescence spectra of **Mem-NO** (5×10^{-5} M) and **Mem-NOT** (5×10^{-5} M) in water and 2 mM CTAB solution.

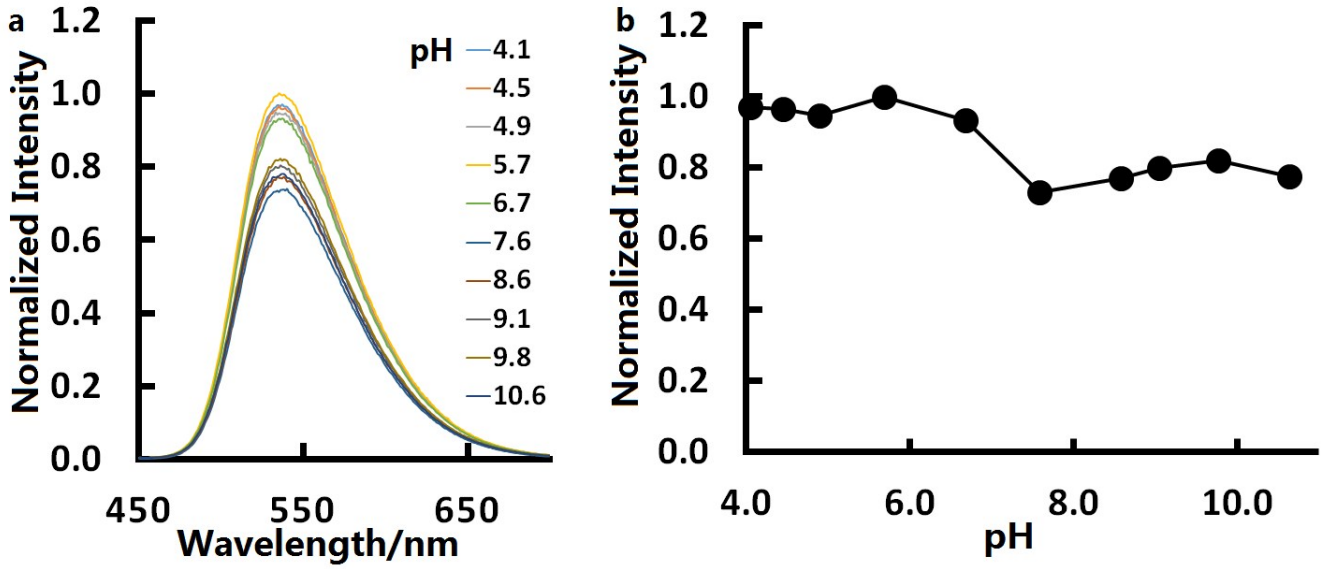


Figure S3: (a) Normalized fluorescence spectrum of **Mem-NO** vs pH; (b) normalized fluorescence intensity at 535 nm vs pH.

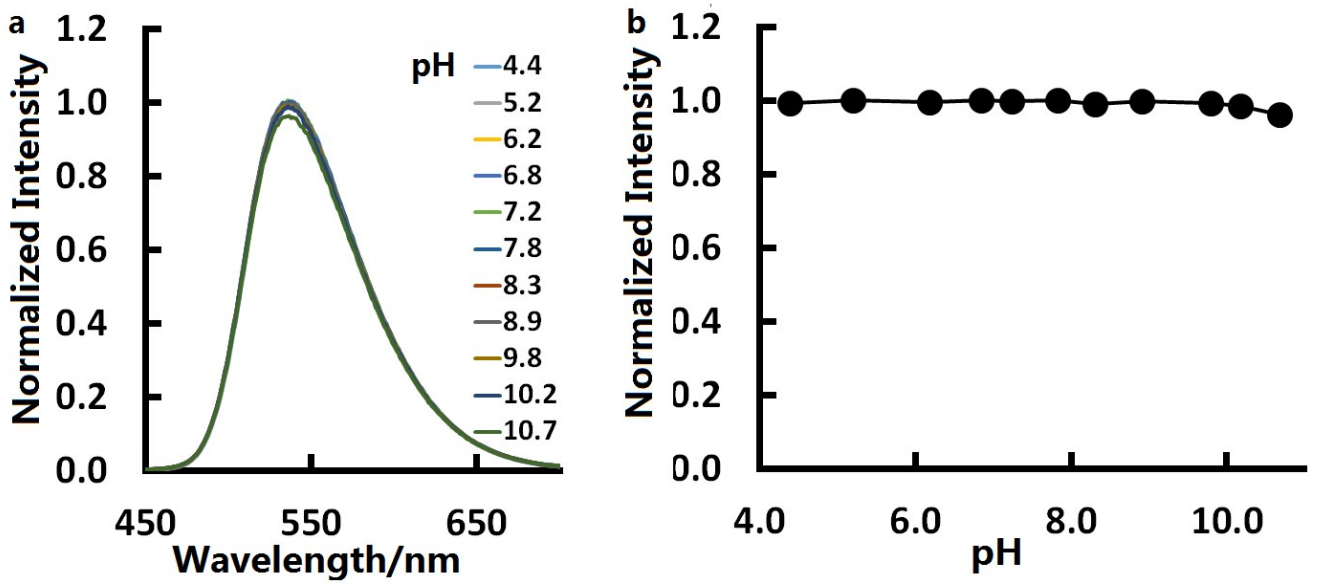


Figure S4: (a) Normalized fluorescence spectrum of **Mem-NOT** vs pH; (b) normalized fluorescence intensity at 535 nm vs pH.

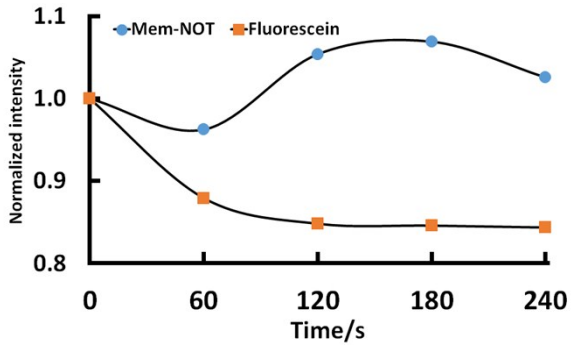


Figure S5. Normalized remaining fluorescence intensity upon various irradiation time.

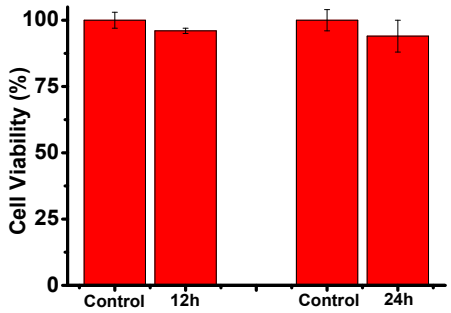


Figure S6. Cell viability of **Mem-NO** (5.0 μM) after incubated for 12 h and 24 h.

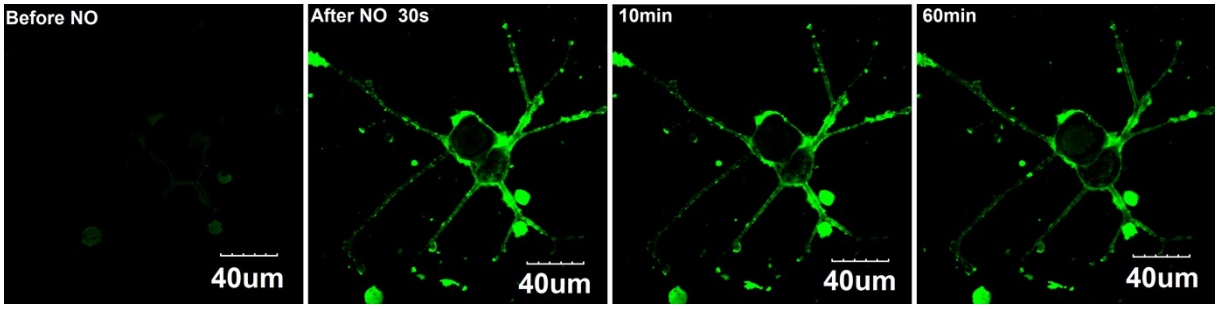


Figure S7. Fluorescence images of neuron cells stained with **Mem-NO** (5 μM, 5 min) before and after adding NO solution.

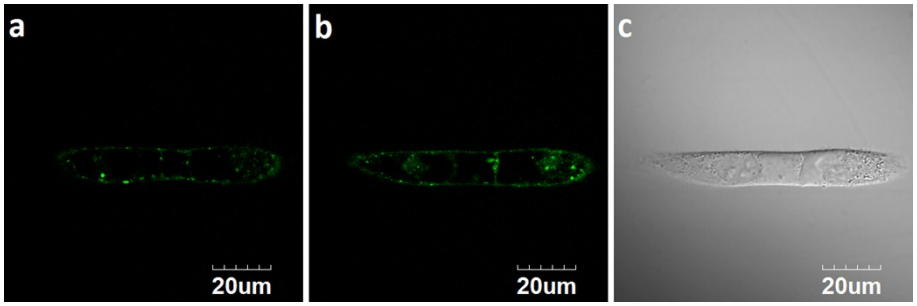


Figure S8. Fluorescence images of HUVEC cells stained with **Mem-NO** further incubated in normal culture medium. (a) is 0 min, (b) is 30 min after the incubation, (c) is bright field.

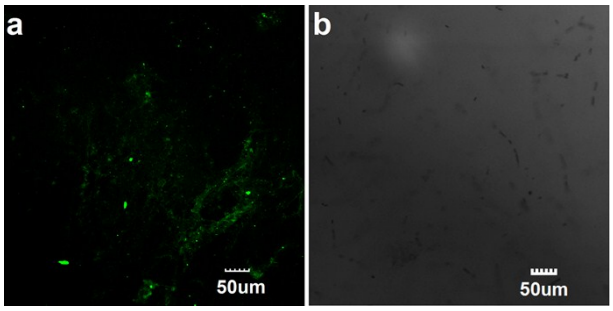
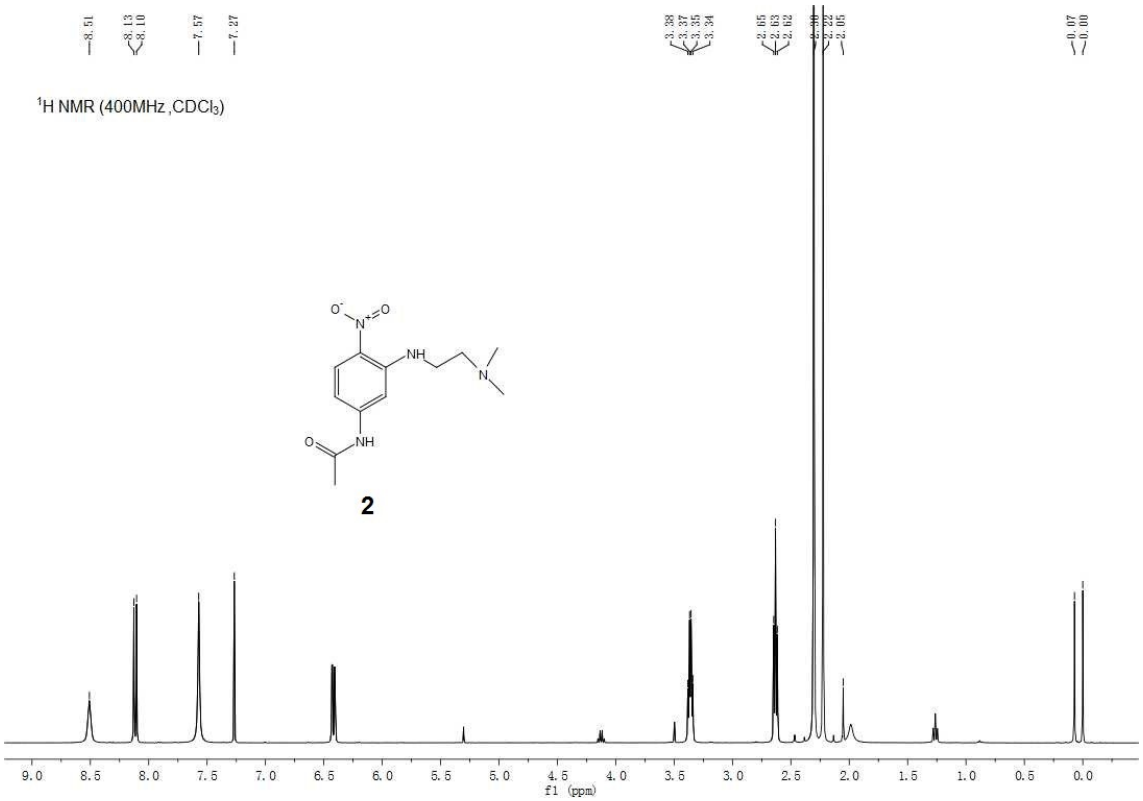
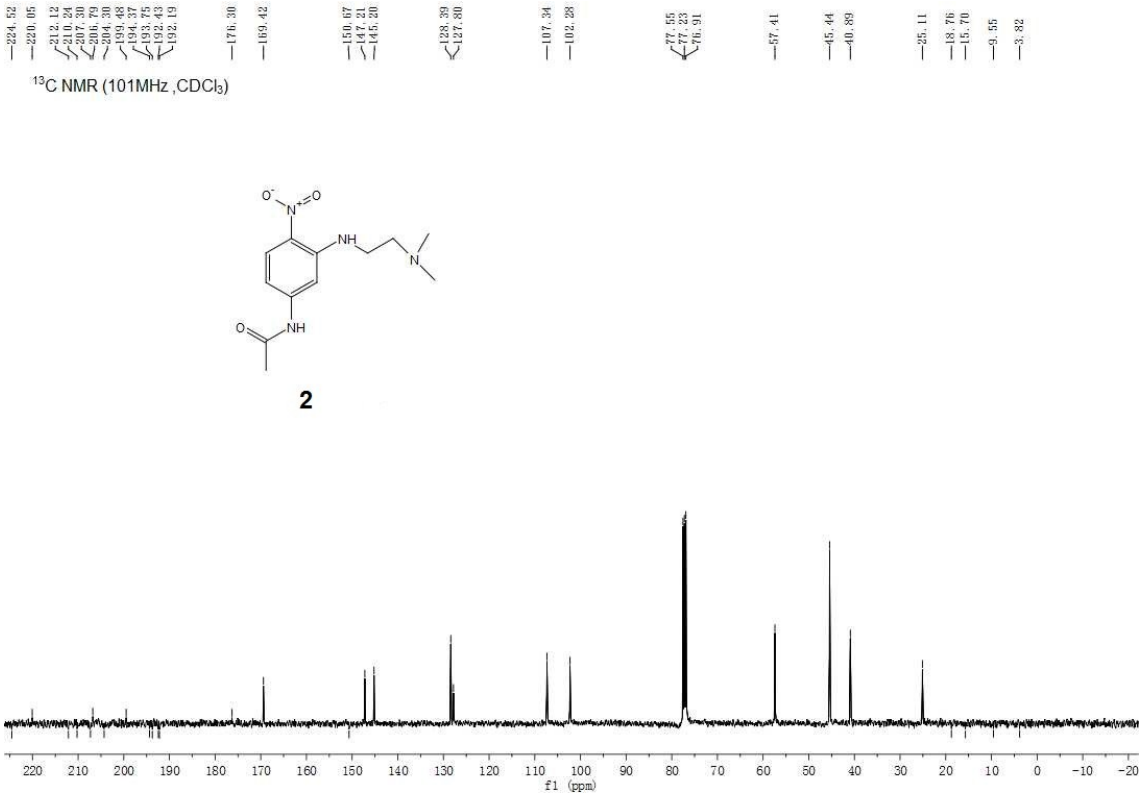
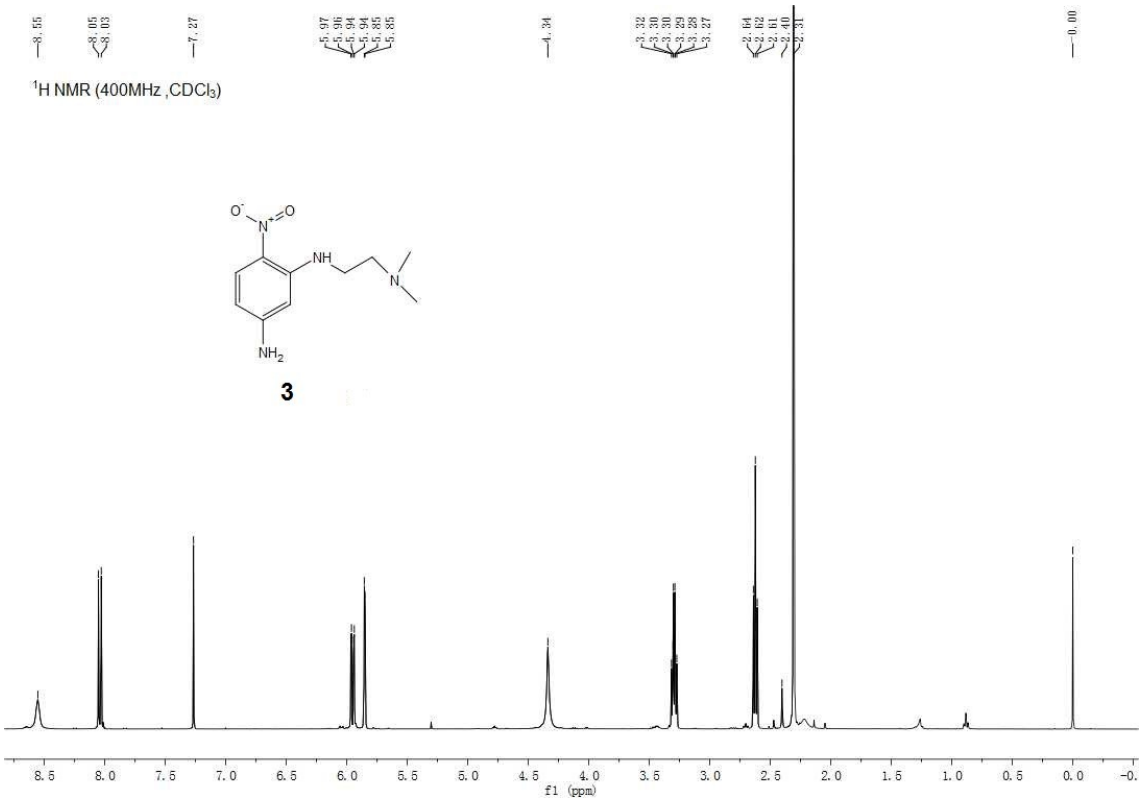


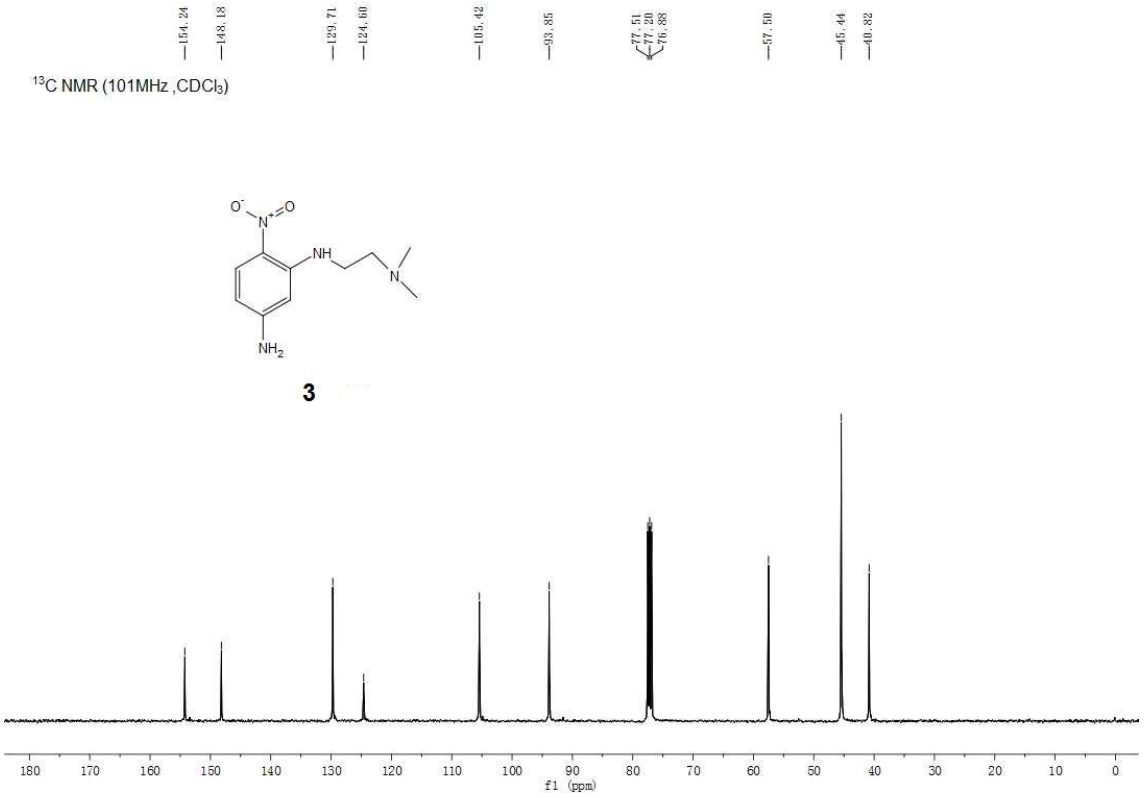
Figure S9. Images of mouse brain slice stained with **Mem-NO** and imaged before DEA NONOate was added. (a) TPM image of the brain slice at a depth of 100 μm. (b) Bright-field image. The TPM image was collected at 520-580 nm upon excitation at 810 nm with fs pulses.

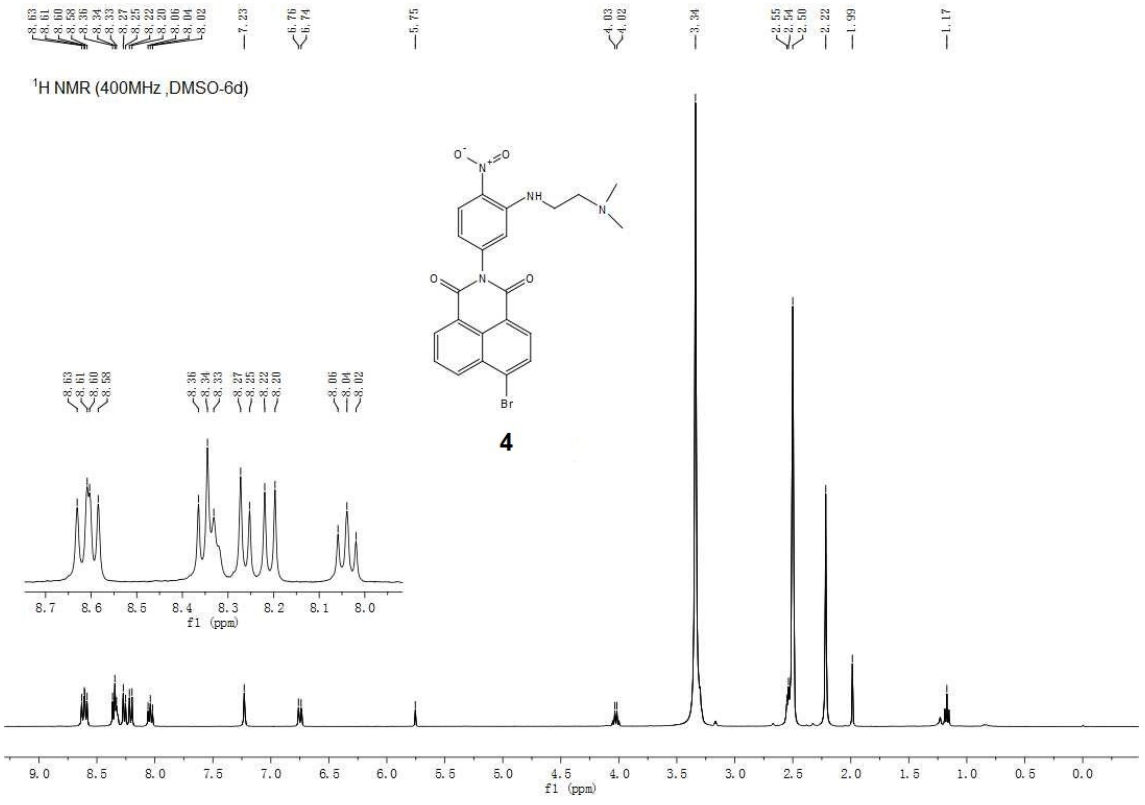
NMR spectra of Compounds

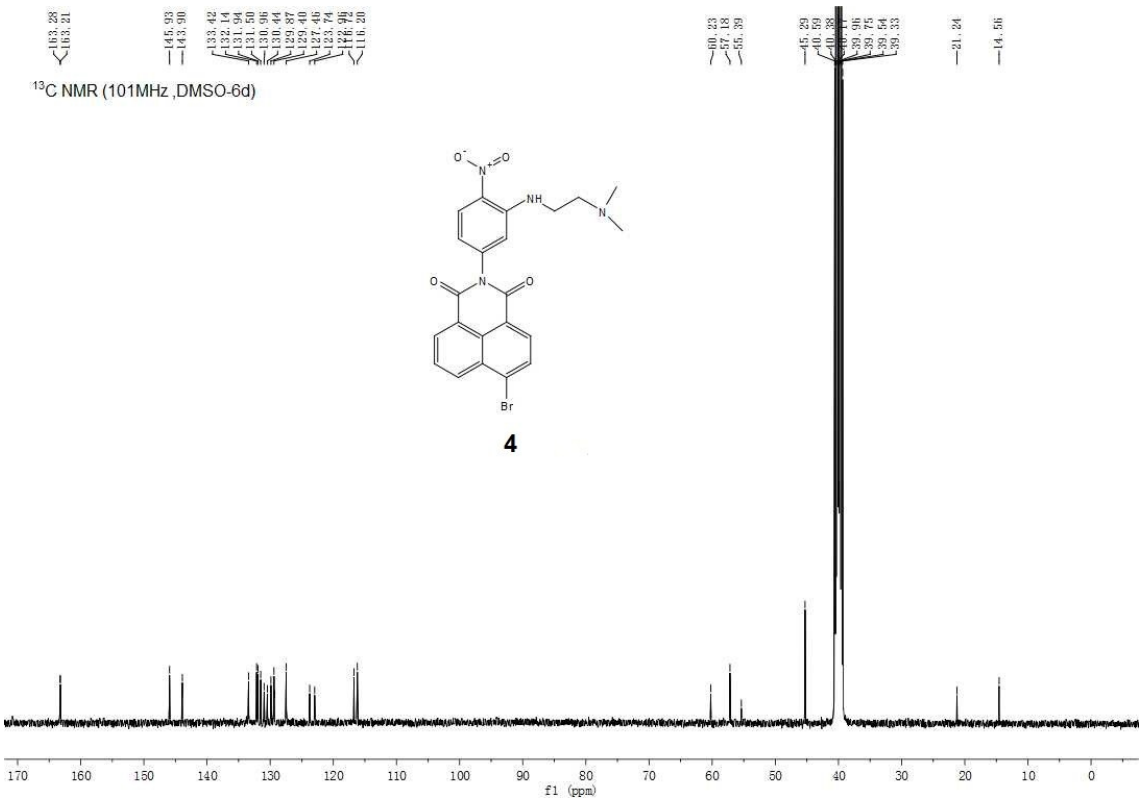




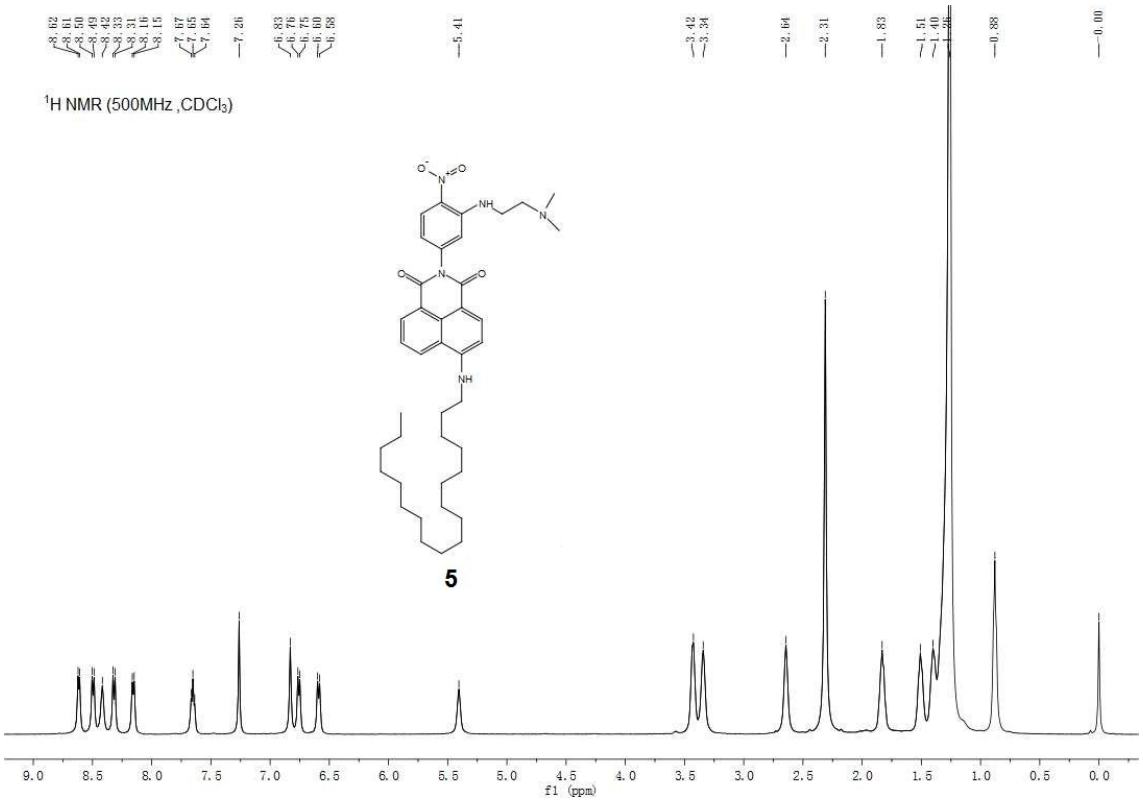

8.55
8.05
8.03
7.27
5.97
5.96
5.94
5.94
5.85
5.85
4.34
3.32
3.30
3.30
3.29
3.28
3.27
2.64
2.62
2.61
2.40
2.31
0.00
^{1}H NMR (400MHz ,CDCl$_3$)
O
N
O
NH
N
NH$_2$
3
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


154.24
148.18
129.71
124.60
105.42
93.85
77.51
77.20
76.88
57.50
45.44
40.82
13C NMR (101MHz ,CDCl3)
NH
N
NH2
3
f1 (ppm)

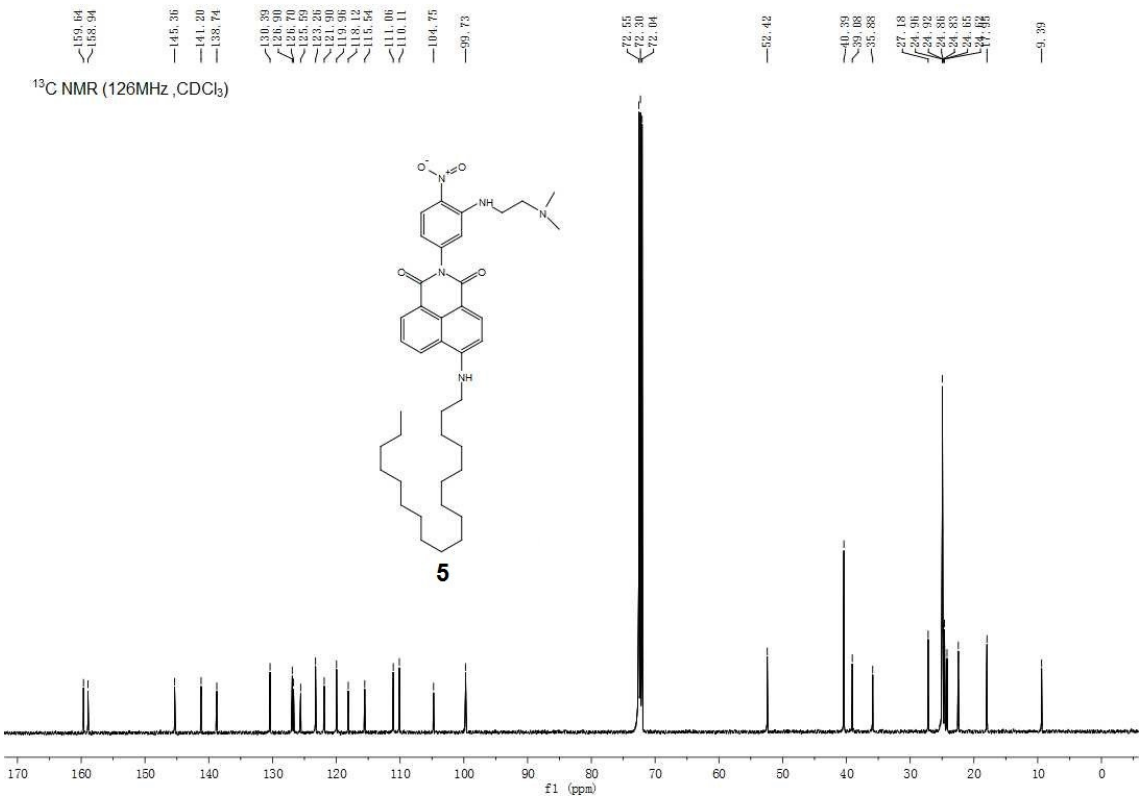

8.63
8.61
8.60
8.58
8.36
8.34
8.33
8.27
8.25
8.22
8.20
8.06
8.04
8.02
7.23
6.76
6.74
5.75
4.03
4.02
3.34
2.55
2.54
2.50
2.22
1.99
1.17
1H NMR (400MHz ,DMSO-6d)
NH
N
O
N
O
Br
4
f1 (ppm)

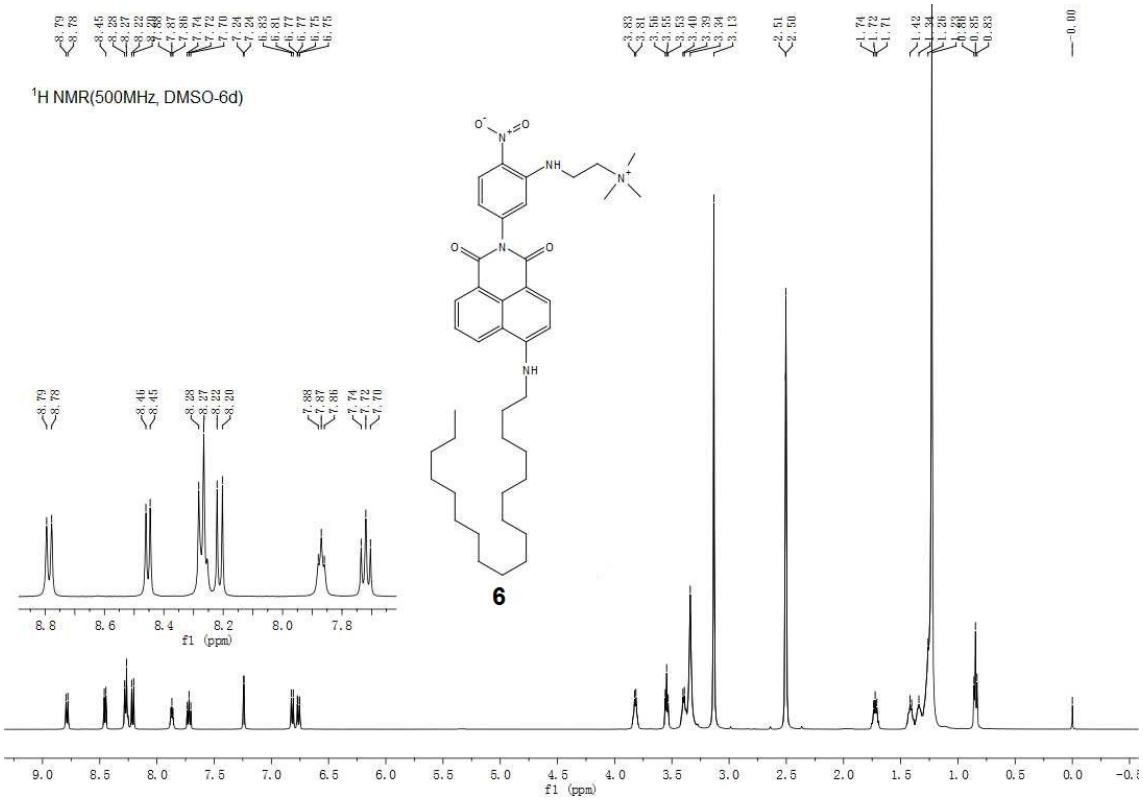

163.28
163.21
145.93
143.90
133.42
132.14
131.94
131.50
130.96
130.44
129.87
129.40
127.46
127.24
123.74
122.96
116.72
116.20
60.23
57.18
55.39
45.29
40.59
40.38
39.96
39.75
39.54
39.33
21.24
14.56
13C NMR (101MHz ,DMSO-6d)
f1 (ppm)

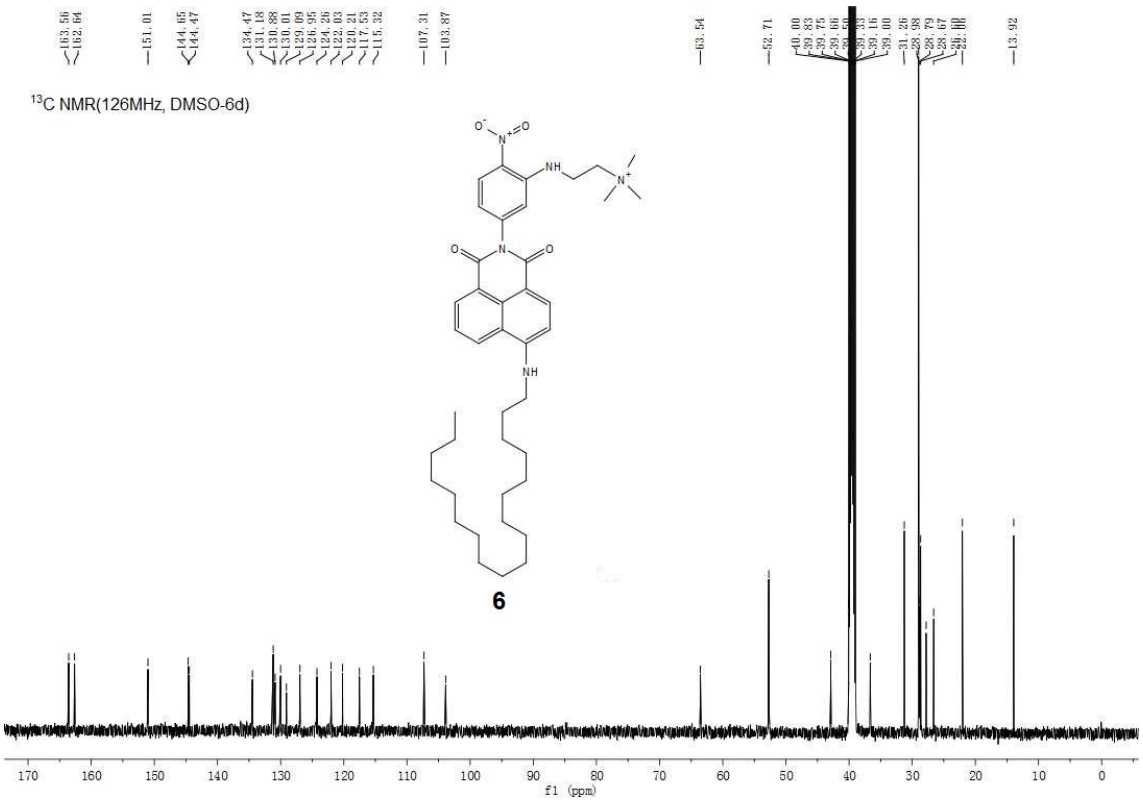
4

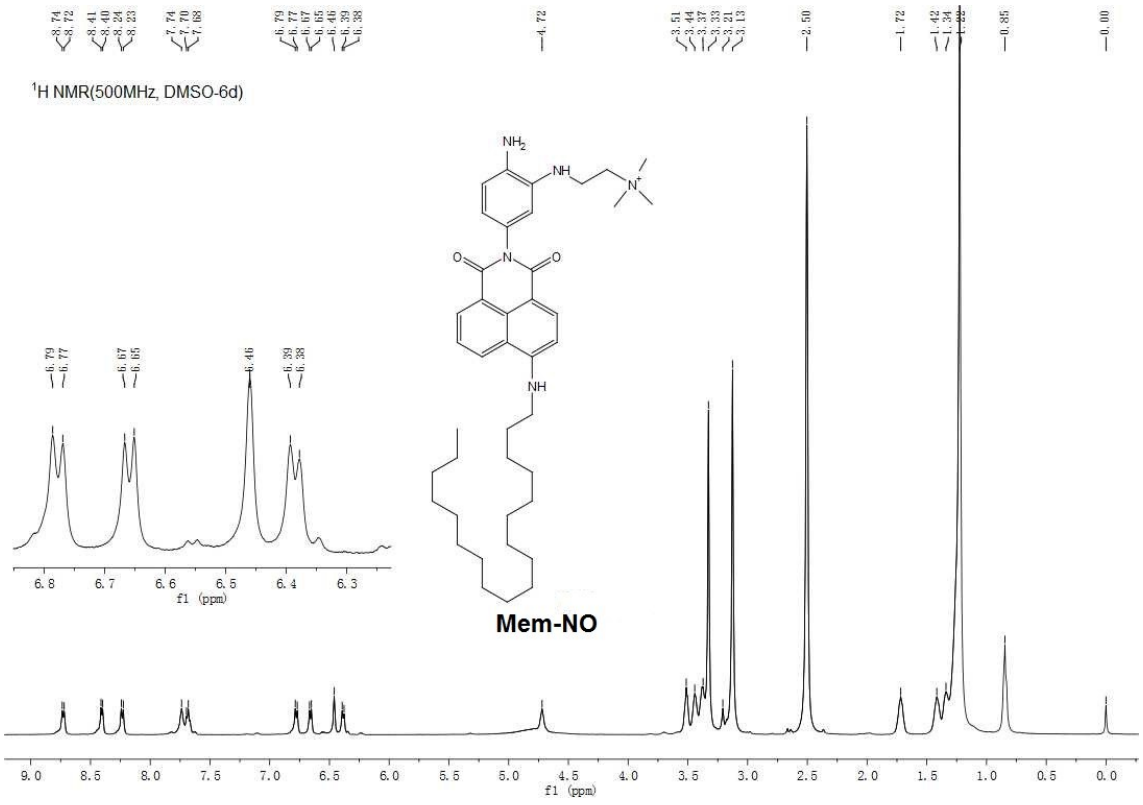

8.62
8.61
8.50
8.49
8.42
8.33
8.31
8.16
8.15
7.67
7.65
7.64
7.26
6.83
6.76
6.75
6.60
6.58
5.41
3.42
3.34
2.64
2.31
1.83
1.51
1.40
0.88
0.00
1H NMR (500MHz ,CDCl3)
f1 (ppm)

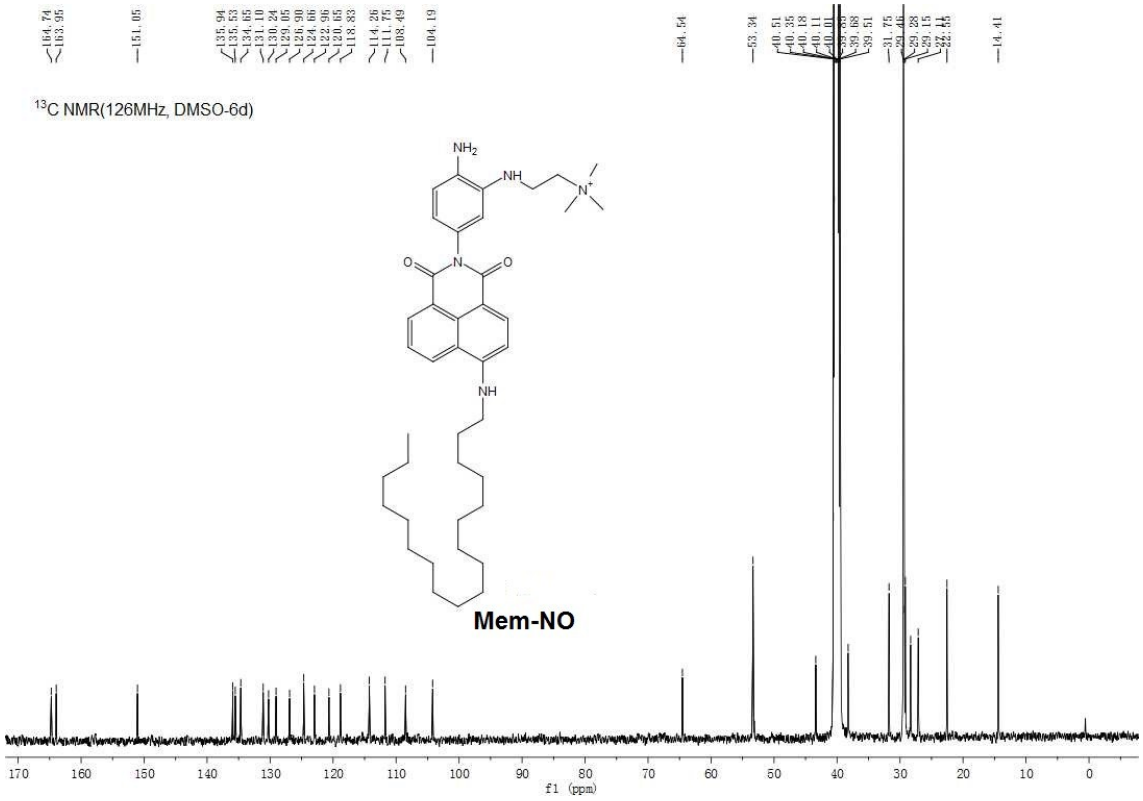
5


159.64
158.94
145.36
141.20
138.74
130.39
126.90
126.70
125.59
123.26
121.00
119.96
118.12
115.54
111.06
110.11
104.75
99.73
72.55
72.30
72.04
52.42
40.39
39.08
35.88
27.18
24.96
24.92
24.86
24.83
24.65
9.39
13C NMR (126MHz ,CDCl3)
5
f1 (ppm)

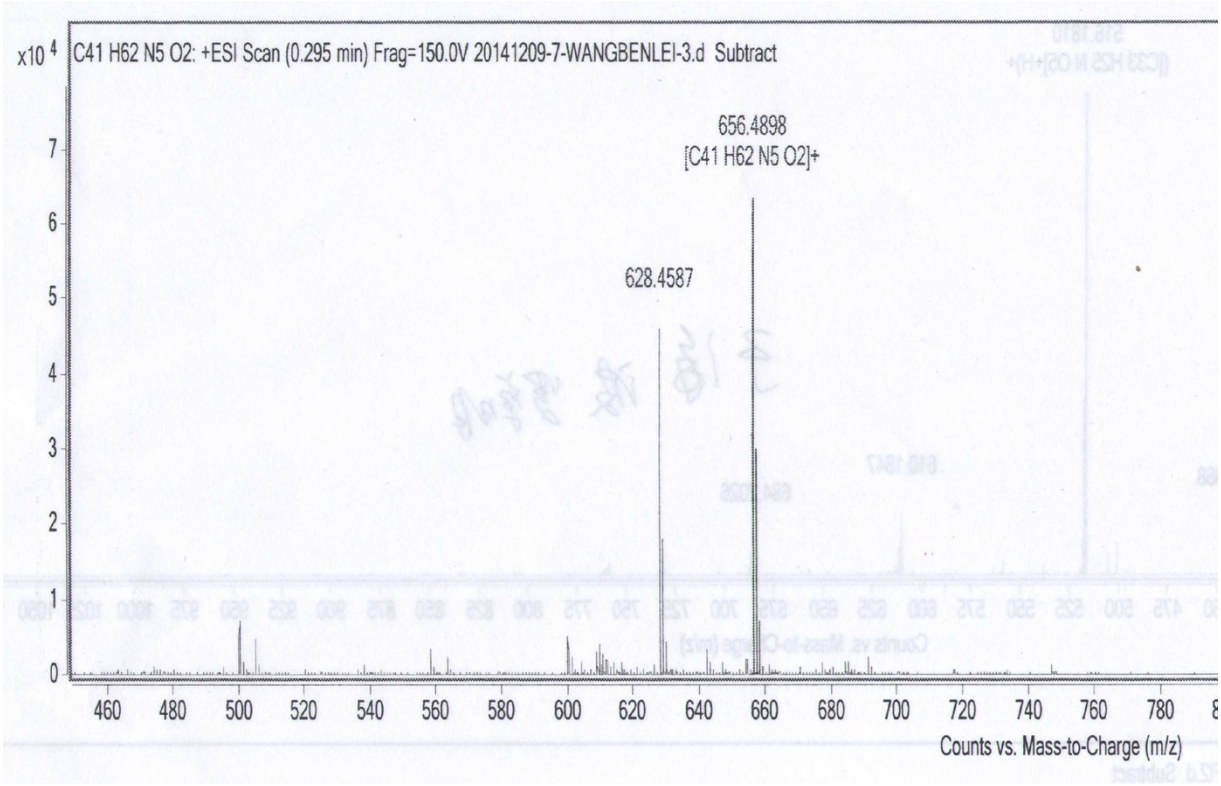

8.79
8.78
8.45
8.28
8.27
8.22
8.20
7.88
7.87
7.86
7.74
7.72
7.70
6.83
6.81
6.77
6.75
3.83
3.81
3.56
3.55
3.53
3.40
3.39
3.34
3.13
2.51
2.50
1.74
1.72
1.71
1.42
1.26
0.85
0.83
0.00
1H NMR(500MHz, DMSO-6d)
6
f1 (ppm)


^{13}C NMR(126MHz, DMSO-6d)
6
f1 (ppm)


^{1}H NMR(500MHz, DMSO-6d)
Mem-NO
f1 (ppm)



HRMS of **Mem-NO**


x10 4
C41 H62 N5 O2: +ESI Scan (0.295 min) Frag=150.0V 20141209-7-WANGBENLEI-3.d Subtract
656.4898
[C41 H62 N5 O2]+
628.4587
7
6
5
4
3
2
1
0
460
480
500
520
540
560
580
600
620
640
660
680
700
720
740
760
780
Counts vs. Mass-to-Charge (m/z)