Electronic Supplementary Information

Near-infrared Fluorescence Probes Detect Reactive Oxygen Species for Keloid Diagnosis

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1. UV/Vis absorption and fluorescence spectra in titration experiments

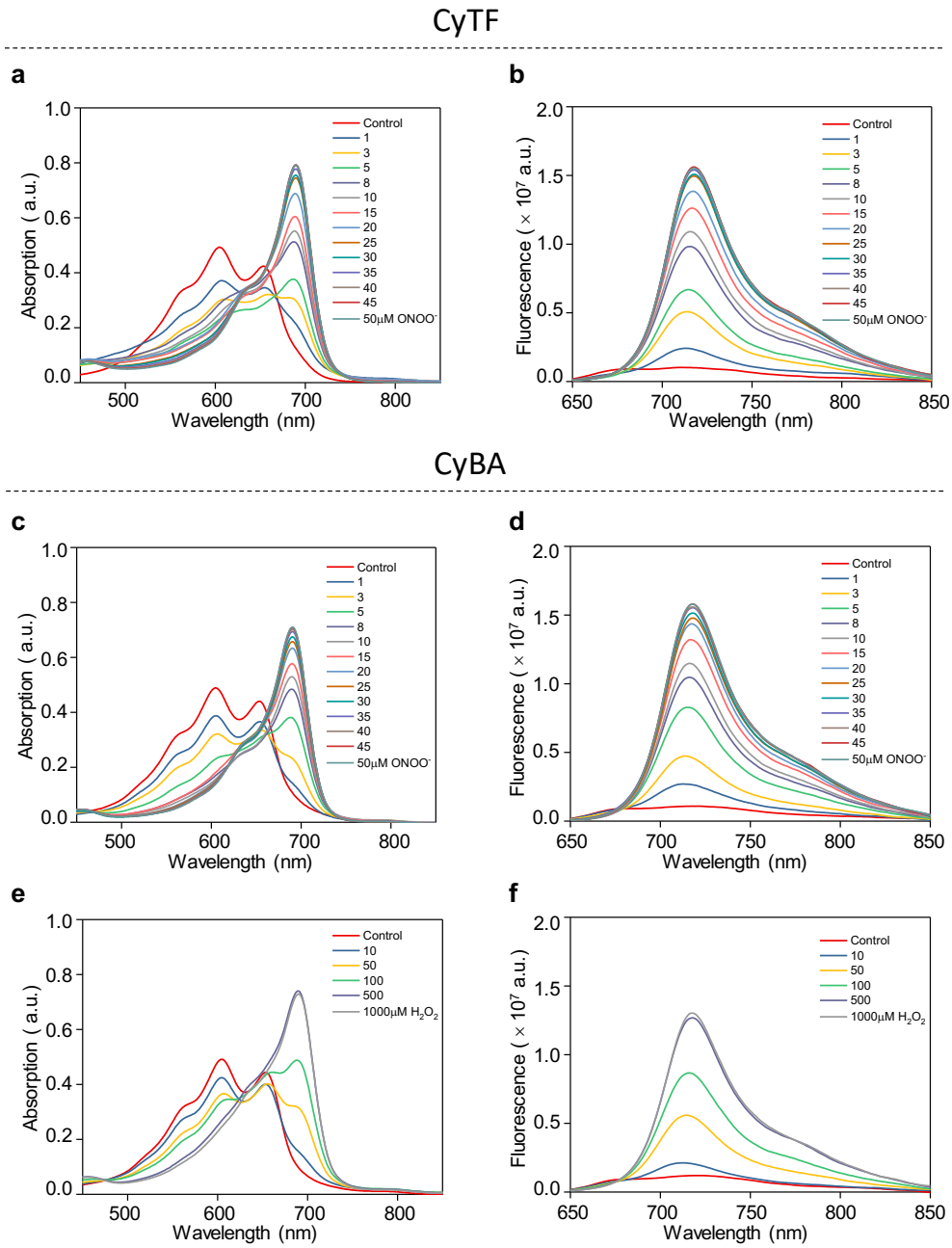


Fig. S1 (a) UV-Vis absorption spectra and (b) fluorescence of CyTF (20 μM) upon titrating different concentrations of $ONOO^-$. (c) UV-Vis absorption and (d) fluorescence of CyBA (20 μM) upon titrating different concentrations of $ONOO^-$. (e) UV-Vis absorption and (f) fluorescence of CyBA (20 μM) upon titrating different concentrations of H_2O_2. Experiments were performed at 25 °C in PBS (1 ×, pH = 7.4) containing 20% DMSO. Excitation: 640 nm.

2. Time-dependent fluorescence spectra

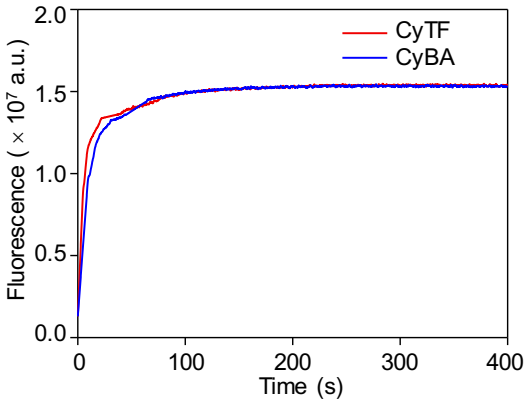


Fig. S2 Time-dependent fluorescence changes of CyTF (20 μM) and CyBA (20 μM) upon addition of 25 μM $ONOO^-$.

3. HPLC experiments

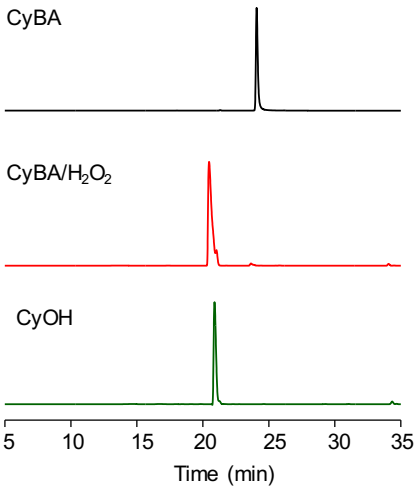


Fig. S3 High performance liquid chromatography (HPLC) traces of the incubation mixture of CyBA in the absence (upper panel) or presence (middle panel) of H_2O_2 (500 μM), and HPLC traces of CyOH in water (lower panel). Wavelength: 600 nm.

4. Cytotoxicity

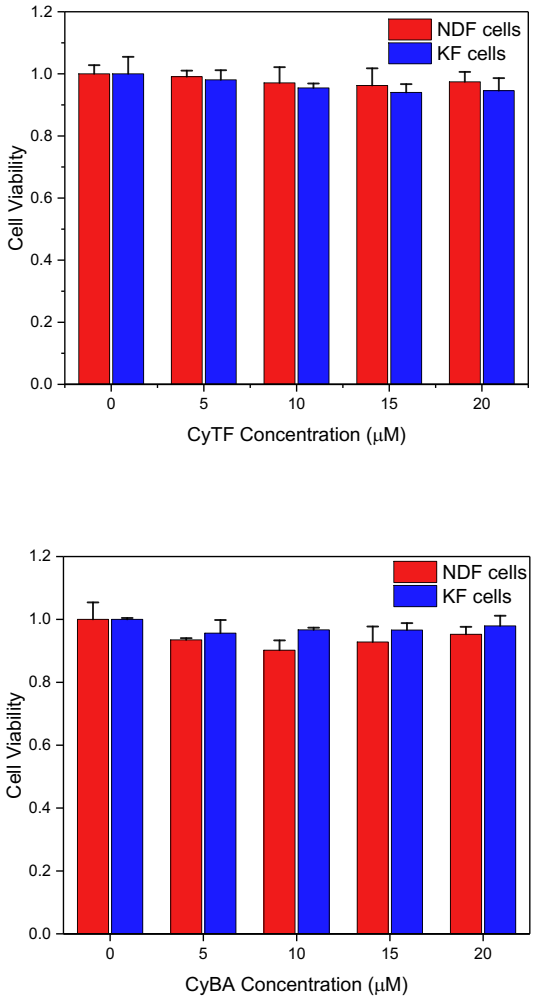


Fig. S4 MTS assay for the relative viability of Normal Dermal Fibroblasts (NDFs) and Keloid-derived fibroblasts (KFs) treated with various concentrations of CyTF and CyBA. Error bars represent the standard deviation of 5 trials.

5. Stability test

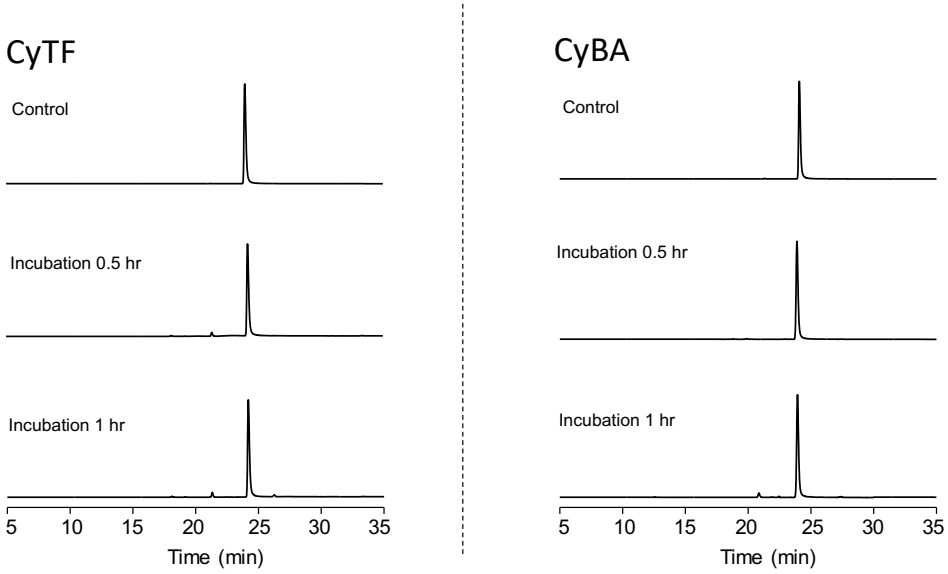
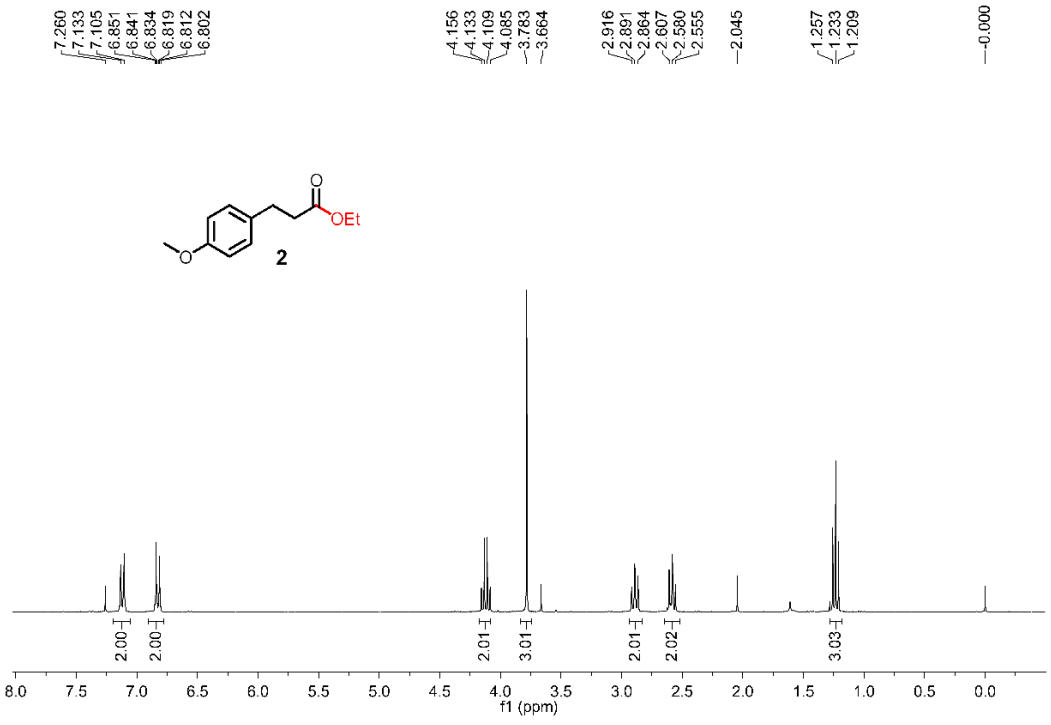


Fig. S5 HPLC traces of 10 μM CyTF and CyBA in DMEM after incubation for 0, 0.5 and 1 h.

6. NMR and MS Data

Compound 2:



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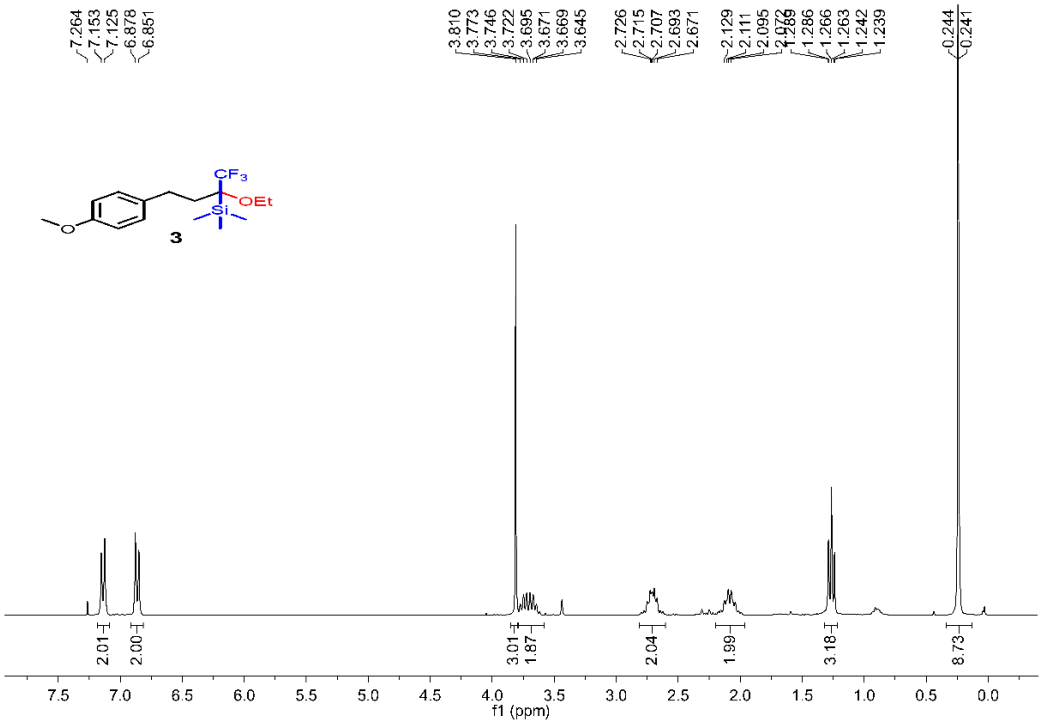

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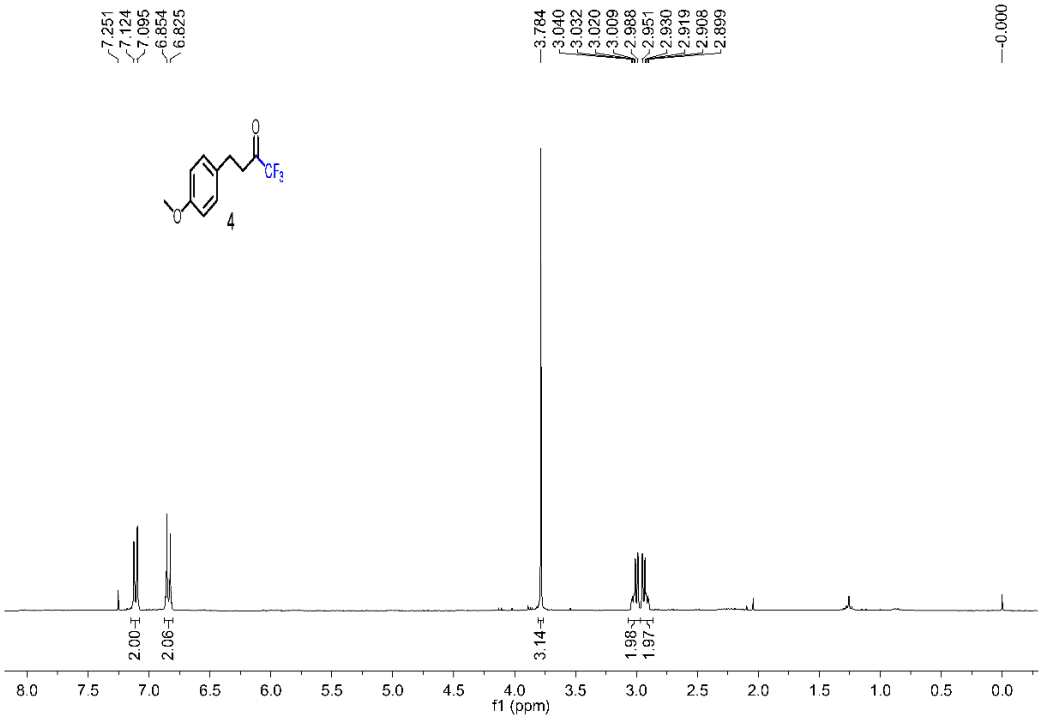
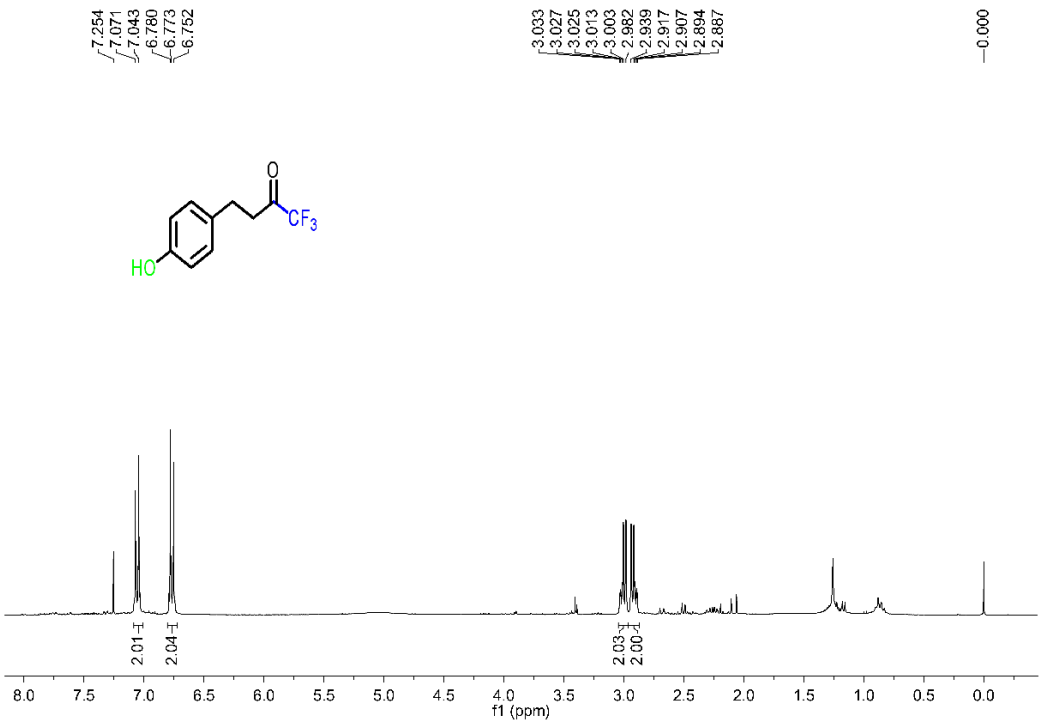
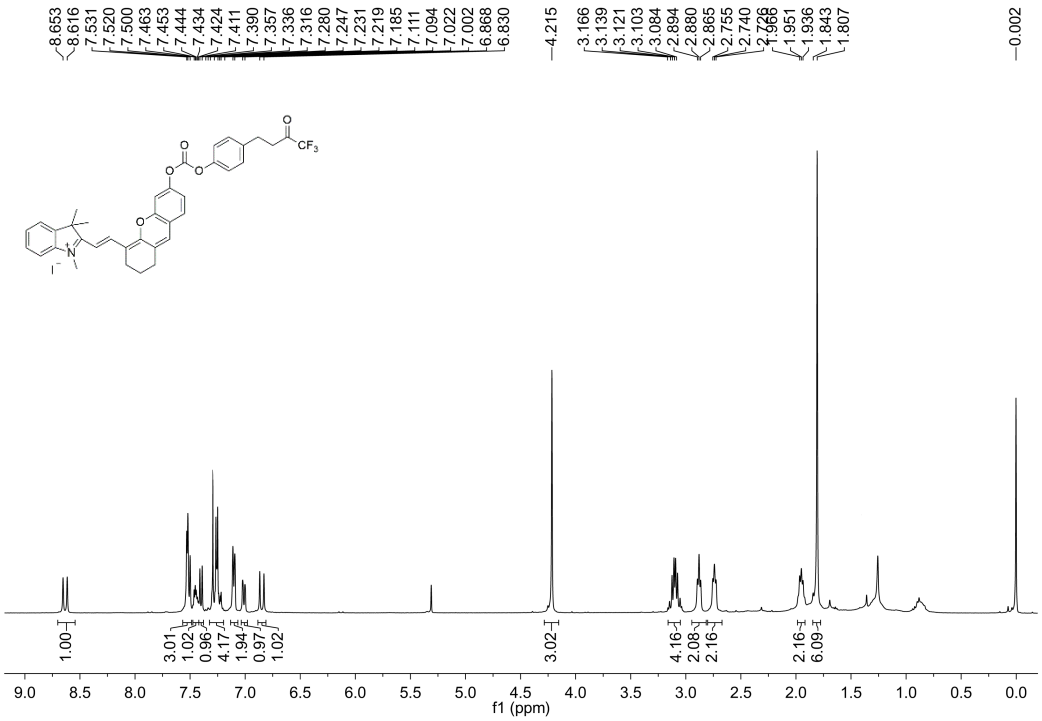
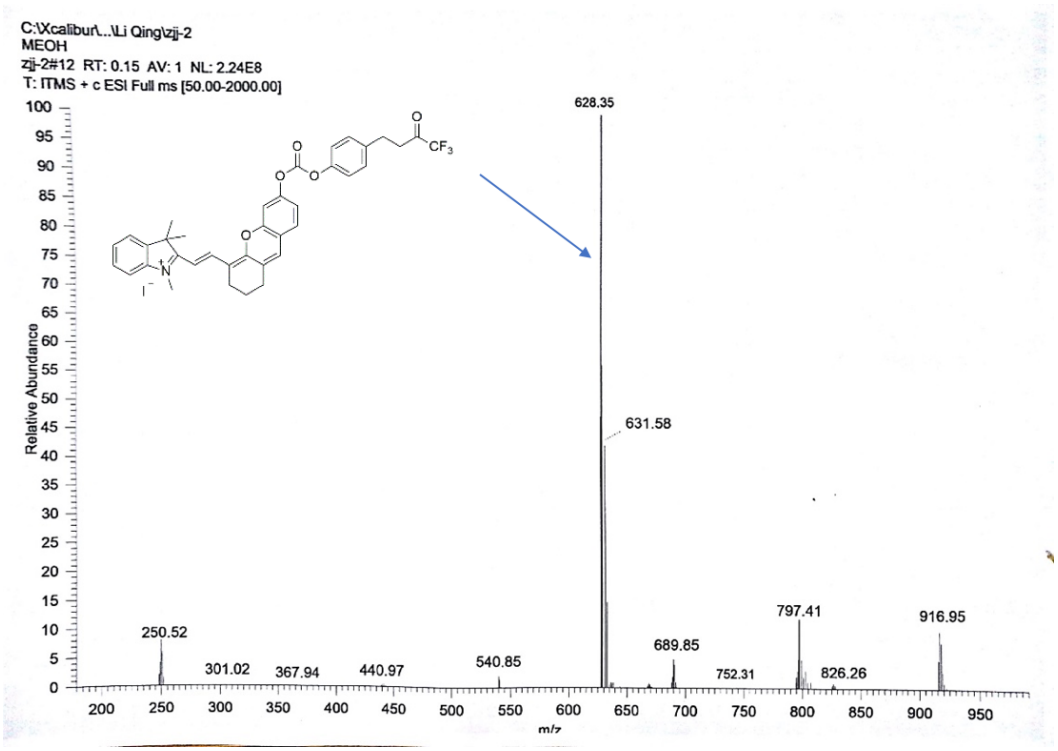


Compound 5:

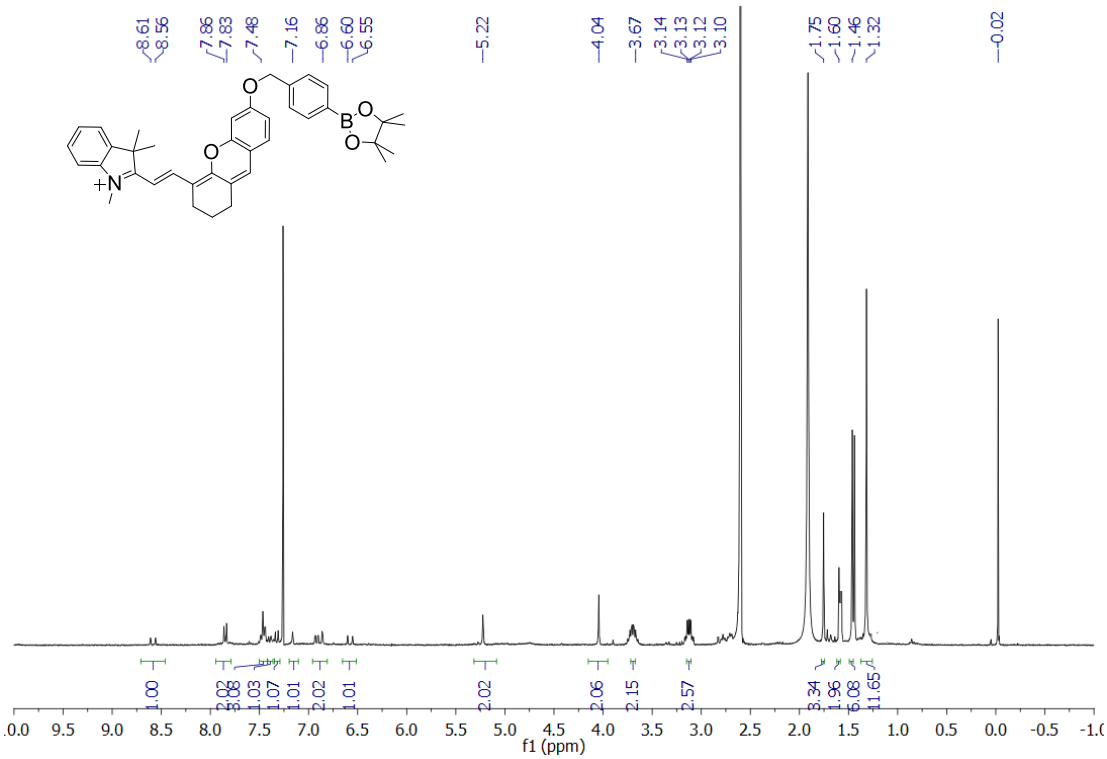


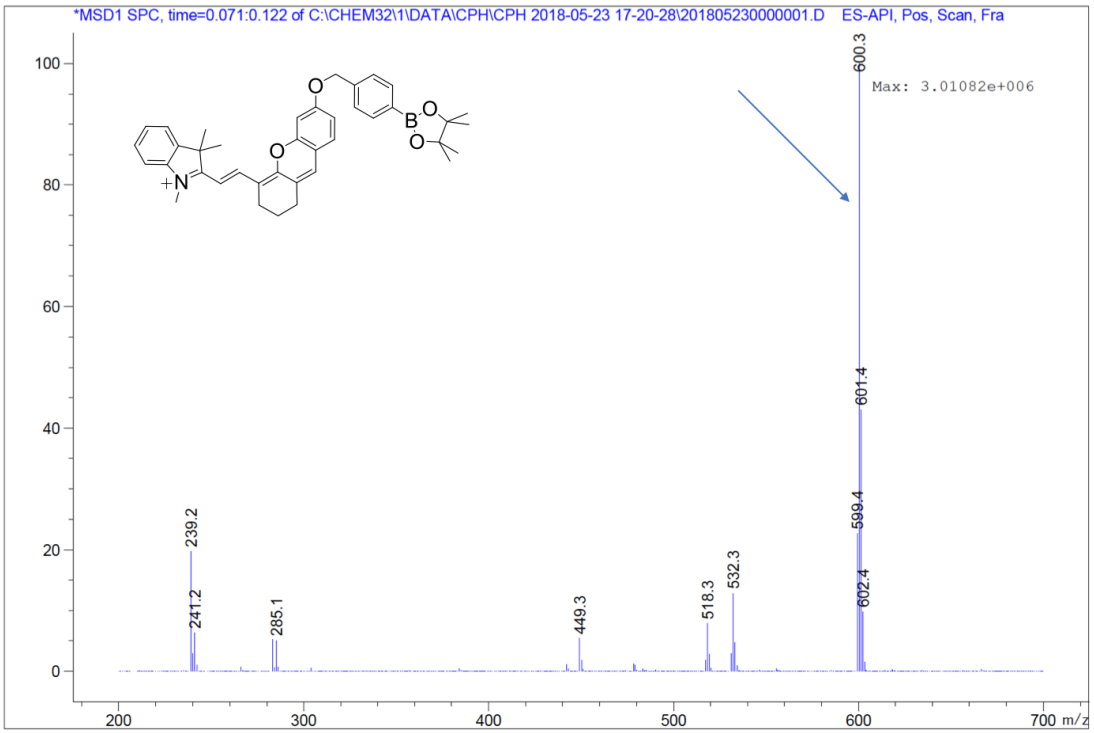
CyTF:




C:\Xcalibur\...\Li Qing\zji-2
MEOH
zji-2#12 RT: 0.15 AV: 1 NL: 2.24E8
T: ITMS + c ESI Full ms [50.00-2000.00]
Relative Abundance
m/z
628.35
631.58
250.52
301.02
367.94
440.97
540.85
689.85
752.31
797.41
826.26
916.95

CyBA:


8.61
8.56
7.86
7.83
7.48
7.16
6.86
6.60
6.55
5.22
4.04
3.67
3.14
3.13
3.12
3.10
1.75
1.60
1.46
1.32
0.02
f1 (ppm)



7. HPLC condition for ROS cleavage experiment and stability test

Time (minute)	Flow (ml/min.)	H_2O %	CH_3CN %
0	1.0	70	30
3	1.0	70	30
35	1.0	30	90
37	1.0	30	90
38	1.0	70	30
40	1.0	70	30