Experimental

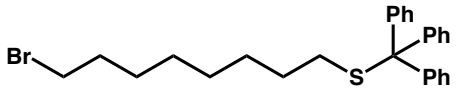
Materials and Instruments

All commercially available compounds were purchased from Sigma Aldrich or Alfa Aesar. All solvents were purchased dry from Sigma Aldrich with a Sure seal system. NMR spectra were recorded on a Bruker AVANCE 400 spectrometer. The chemical shifts (δ) are given in parts per million relative to $CDCl_3$ (7.26 ppm for 1H) $CDCl_3$ (77.16 ppm for ^{13}C). Flash column chromatography was performed using silica gel (particle size 200-300 mesh) or using a Biotage Isolera Spektra system. Particle size and zeta potential were measured with a Zetasizer Nano-ZS (Malvern Instruments Ltd., UK). Flow cytometry was performed on an Attune NxT flow cytometer (Invitrogen). Cell sorting was performed on an Influx cell sorter (BD). The fluorescence of FEDS was measured by a Tecan Infinite M200 microplate reader. Fetal Bovine Serum (FBS), Opti-MEM, Ham's F-12 Nutrient Mix and Dulbecco's Modified Eagle Medium (DMEM) were purchased from Gibco. Accutase was purchased from Invitrogen. NucSpot® Live 488 Nuclear Stains was purchased from Biotium. The Genomic extraction kit and PCR product purification kit were purchased from Qiagen. T7 Endonuclease 1 (T7E1) was purchased from NEB. Rabbit red blood cells were purchased from Hemostat Laboratories. Monoclonal HEK-RT3-4 reporter cells expressing GFP under the control of the P_{tet} promoter, here referred to as "RT HEK", was a generous gift from GenEdit[1]. Primary Ai9 mouse myoblast cells, were also a generous gift from GenEdit[1]. Cas9-NLS and Cas9-mCherry fusion proteins were purchased from the UC Berkeley QB3 MacroLab core facility. CrRNA and tracrRNA were purchased from IDT. The protospacer sequences of crRNA were described as below:

GFP: GCTGAAGCACTGCACGCCAT.

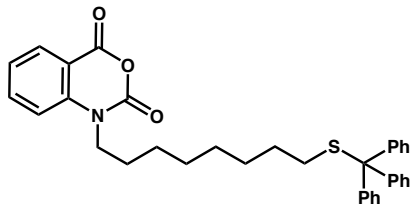
Ai9: AAGTAAAACCTCTACAAATG.

Synthesis of compounds



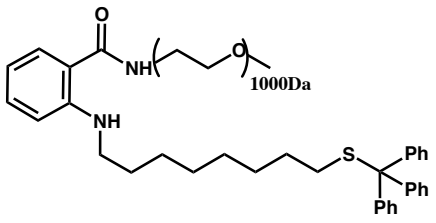
1

Compound **1**. 1,8-dibromooctane (2.76g, 10mmol), triphenylmethanethiol (6.8g, 25mmol) and potassium carbonate (11 g, 80 mmol) were added into acetonitrile (50 mL) in a 250 mL round-bottom flask and stirred at room temperature for 20 h. The solvent was then removed under vacuum. The resulting mixture was then re-dissolved in 150 mL CH_2Cl_2 and washed with water and brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography (hexane/CH_2Cl_2, 9/1) to obtain 1-Tritylthiol-8-bromo-octane (1.9 g, 41%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 7.9 Hz, 6H), 7.30-7.26 (m, 6H), 7.23-7.19 (m, 3H), 3.39 (t, *J* = 6.8 Hz, 2H), 2.14 (t, *J* = 7.3 Hz, 2H), 1.82 (p, *J* = 7.0 Hz, 2H), 1.38 (m, 4H), 1.29-1.09 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.1, 129.6, 127.8, 126.5, 77.4, 77.1, 76.7, 66.4, 34.1, 32.8, 32.0, 29.0, 28.9, 28.6, 28.1. HRMS (EI) m/z calculated for: $[C_{27}H_{31}BrS]^+$: 466.1330. Found: 466.1299 (Δ 0.0031).



2

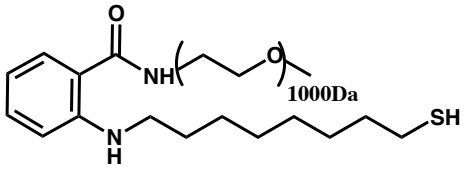
Compound **2**. NaH (90 mg, 2.1 mmol) was slowly added into a DMF solution (10 mL) of isatoic anhydride (0.3 g, 1.9 mmol) at 0°C and stirred for 10 min. To this solution, 1-Tritylthiol-8-bromo-octane (**1**) (0.9 g, 1.9 mmol) was then added dropwise and the resulting mixture was stirred for 24 h at room temperature. The reaction mixture was diluted with 150 mL EtOAc, washed with saturated ammonium chloride solution and brine, dried over anhydrous Na_2SO_4, and filtered. The filtrate was concentrated under reduced pressure and was purified by silica gel column chromatography (hexane/EtOAc, 8/2) to obtain N-(1-tritylthio-)octylisatoic anhydride as a white powder (0.5 g, 48%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.21 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.79 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.51 – 7.38 (m, 6H), 7.36 – 7.28 (m, 7H), 7.28 – 7.21 (m, 3H), 7.18 (d, *J* = 8.5 Hz, 1H), 4.11 – 4.01 (m, 2H), 2.18 (t, *J* = 7.3 Hz, 2H), 1.83 – 1.68 (m, 2H), 1.42 (m, 4H), 1.37 – 1.15 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.7, 147.8, 145.2, 141.5, 137.3, 131.2, 129.7, 127.9, 126.7, 124.0, 114.0, 112.0, 77.5, 77.2, 76.8, 66.5, 45.1, 32.1, 29.1, 29.0, 28.7, 27.0, 26.7. HRMS (ESI) m/z calculated for: $[C_{35}H_{35}NO_3SNa]^+$: 572.2230. Found: 572.2224 (Δ 0.0006).



3

Compound **3**. Amino-PEG_{1000}-OMe (200 mg, 0.2 mmol) and triethylamine (90 µL, 0.64 mmol) were dissolved in DMF (3 mL) and stirred for 10 min at room temperature. N-(1-

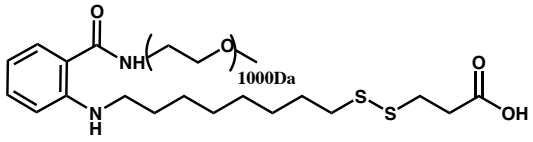
tritylthio-)octylisatoic anhydride (**2**) (110 mg, 0.2 mmol) was then added into the solution and the reaction mixture was stirred at room temperature overnight. The solvent was then removed under reduced pressure and the resulting crude product was purified by silica gel column chromatography (CH_2Cl_2/MeOH, 9/0.5, v/v) to obtain **3** as a viscous colorless oil (290 mg, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.34 (m, 6H), 7.25 – 7.21 (m, 6H), 7.18 – 7.14 (m, 3H), 6.71 (s, 1H), 6.63 (d, *J* = 8.4 Hz, 1H), 6.52 (t, *J* = 7.6 Hz, 1H), 3.62 – 3.57 (m, 88H), 3.51 (dd, *J* = 5.8, 3.6 Hz, 2H), 3.34 (s, 3H), 3.06 (t, *J* = 7.1 Hz, 2H), 2.09 (t, *J* = 7.3 Hz, 2H), 1.59 (p, *J* = 7.2 Hz, 2H), 1.35 – 1.30 (m, 4H), 1.22 – 1.12 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 145.0, 132.7, 129.6, 127.8, 127.6, 126.5, 77.5, 77.2, 76.8, 71.9, 70.6, 70.5, 70.3, 69.8, 66.3, 59.0, 39.3, 32.0, 29.2, 29.0, 28.9, 28.6, 27.1. HRMS (ESI) m/z calculated for n=17: $[C_{69}H_{109}N_2O_{18}S]^+$: 1285.7391. Found: 1285.7427 (Δ 0.0036).



4

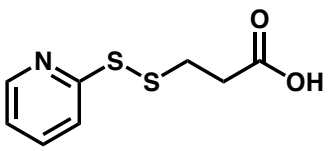
Compound **4**. Compound **3** (290 mg, 0.2 mmol) was dissolved in CH_2Cl_2 (5 mL). TFA (0.8 mL) and Et_3SiH (0.8 mL) were added and the solution was stirred for 2 h at room temperature. The reaction mixture was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography (CH_2Cl_2/MeOH, 9/0.6, v/v) to obtain compound **4** as a viscous colorless oil (180 mg, 74%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.8 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.02 (d, *J* = 8.3 Hz, 1H), 6.83 (t, *J* = 7.4 Hz, 1H), 3.66 – 3.60 (m, 84H), 3.53 (dd, *J* = 5.8, 3.4 Hz, 2H), 3.36 (s, 3H), 3.17 (t, *J* = 7.3 Hz, 2H), 2.53 – 2.47 (m, 2H), 1.71 – 1.65 (m, 2H), 1.60 – 1.53 (m, 2H), 1.43 – 1.28 (m,

9H), 1.24 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.3, 144.7, 136.1, 133.1, 128.0, 100.5, 77.5, 77.4, 77.2, 76.8, 71.9, 70.5, 70.4, 70.2, 69.8, 59.1, 39.6, 34.1, 29.3, 29.0, 28.4, 27.0, 24.7, 23.6. HRMS (ESI) m/z calculated for n=17: $[C_{50}H_{95}N_2O_{18}S]^+$: 1043.6295. Found: 1043.6321 (Δ 0.0026).



FEDS

FEDS. Compound **4** (200.9 mg, 0.16 mmol, 1eq) was added to a solution of 3-(pyridin-2-yldisulfaneyl)propanoic acid (70.6 mg, 0.33mmol, 2.1 eq) and AcOH (317 µL, 0.33g, 5.5mmol, 34 eq) in CH_2Cl_2 (8 mL) and stirred overnight. Acetic acid was removed by co-evaporation with toluene under reduced pressure, the crude product was purified by silica gel column chromatography (DCM/EtOAc 9/1 to DCM/MeOH, 9/1, to DCM/MeOH, 8/2, v/v) to obtain **FEDS** as a viscous colorless oil (194.7mg, 0.14mmol, 87% yield). ^{1}H NMR (400 MHz, Methanol-d_4) δ 7.50 (d, *J* = 7.9 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 1H), 6.71 (d, *J* = 8.4 Hz, 1H), 6.58 (t, *J* = 7.5 Hz, 1H), 3.63 (dd, *J* = 12.2, 5.5 Hz, 87H), 3.54 (t, *J* = 5.9 Hz, 4H), 3.36 (s, 3H), 3.14 (t, *J* = 6.9 Hz, 2H), 2.90 (t, *J* = 7.0 Hz, 2H), 2.70 (dt, *J* = 10.7, 7.2 Hz, 4H), 1.67 (m, *J* = 14.9, 11.0, 7.0 Hz, 4H), 1.41 (m, *J* = 21.6, 6.7 Hz, 8H). ^{13}C NMR (101 MHz, MeOD) δ 172.24, 150.87, 133.78, 129.39, 116.67, 115.76, 112.56, 72.79, 71.39, 71.34, 71.20, 71.16, 70.76, 59.13, 43.95, 40.43, 39.67, 35.24, 34.58, 30.38, 30.27, 30.21, 30.14, 29.35, 28.20. HRMS (ESI) m/z calculated for: n=17, $[C_{53}H_{97}N_2O_{20}S_2]^-$: 1145.6082. Found: 1145.6067 (Δ 0.0015).



5

Compound **5.** 3-mercaptopropanoic acid (1.5 g, 14 mmol) in 10 mL EtOH was added dropwise into 15 mL EtOH solution containing 1,2-di(pyridin-2-yl)disulfane (6.2 g, 28 mmol) and AcOH (0.8 mL) and stirred overnight at room temperature. The reaction mixture was concentrated under reduced pressure and purified by silica gel column chromatography (hexane/EtOAc/AcOH, 50/50/0.5, v/v/v) to obtain **5** as a white powder (1.6 g, 53%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 11.60 (s, 1H), 8.47 (d, J = 4.8 Hz, 1H), 7.96 – 7.48 (m, 2H), 7.16 – 7.10 (m, 1H), 3.03 (t, J = 6.9 Hz, 2H), 2.78 (t, J = 6.9 Hz, 2H). HRMS (ESI) m/z calculated for: $[C_8H_{10}NO_2S_2]^+$: 216.0147. Found: 216.0144 (Δ 0.0003).

Quantum yield measurement

To measure the quantum yield, FEDS was added to the wells of a black Falcon 96 well plate and the absorption at 350 nm and the corresponding fluorescence were measured with a Tecan microplate reader. A plot of absorbance vs integrated fluorescent intensity was made and the slope was calculated. Quinine sulfate was used as standard for quantum yield calculations. The quantum yield was calculated according to the following equation: $\Phi_{FEDS} = \Phi_{ST}(\frac{Slope_{FEDS}}{Slope_{ST}})(\frac{\eta_{FEDS}^2}{\eta_{ST}^2})$, where Φ_{FEDS} and Φ_{ST} are the quantum yield for FEDS and quinine sulfate. $Slope_{FEDS}$ and $Slope_{ST}$ are the slope of the absorbance vs integrated fluorescent intensity plot for FEDS and quinine sulfate and η_{FEDS} and η_{ST} are the refractive index of water and 0.1M sulfuric acid.

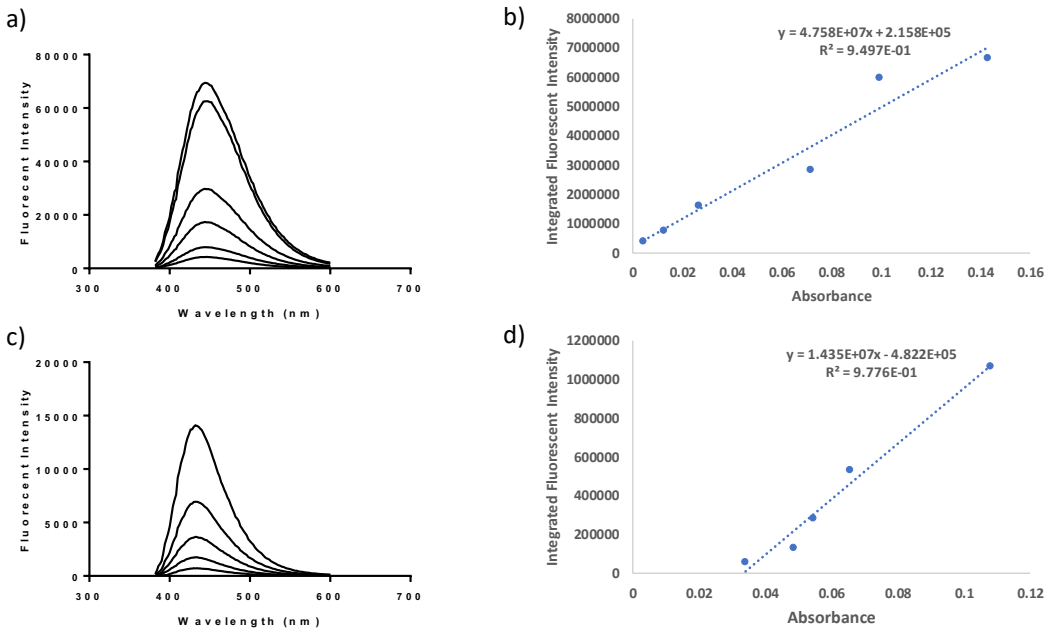


Fig. S1 Quantum yield of FEDS, using quinine sulfate as the standard. Fluorescent intensity of a) FEDS and c) quinine sulfate was measured at different concentrations at an excitation wavelength of 350 nm. Absorbance vs integrated fluorescent intensity was plotted for b) FEDS and d) quinine sulfate at an excitation wavelength of 350 nm.

DLS measurements

DLS experiments were performed with a Zetasizer Nano instrument (Malvern Instruments Ltd., UK) equipped with a 10-mW helium-neon laser (λ = 632.8 nm) and thermoelectric temperature controller at 25 °C. Measurements were taken at a 90° scattering angle. The Cas9 RNP and FEDEX were dissolved in a pH 7.2 10 mM HEPES buffer with a Cas9 RNP concentration of 0.05 mg/mL.

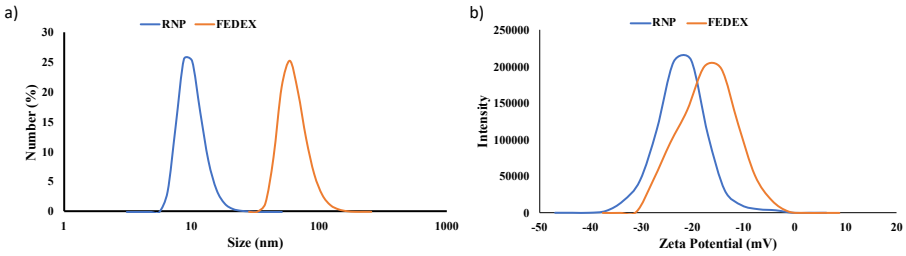


Fig. S2 Size and Zeta Potential of the Cas9 RNP and FEDEX.

Hemolysis assay

Fresh rabbit red blood cells (RBC) were washed three times with 150 mM PBS. The RBCs (10^8) were then suspended in 1 ml of 0.1 M sodium phosphate buffer at the appropriate pH. FEDS and reduced FEDS were dissolved in 0.1 M sodium phosphate buffer, at different concentrations. The hemolysis assay was performed by adding FEDS to 10^8 RBCs suspended in 1 ml of the appropriate pH phosphate buffer. The RBCs were inverted several times for mixing, and incubated in a 37°C water bath for 60 min. The cells were centrifuged at 1000 g for 5 min and the absorbance of the supernatant was measured at 541 nm. To determine a 100% hemolysis, 10^8 RBCs were lysed by suspending them in distilled water. The control was 10^8 RBCs in buffer. All hemolysis experiments were done in triplicate.

Cell culture

HeLa cells and RT HEK cells were cultured in Dulbecco's modified Eagle's medium (DMEM; Invitrogen) supplemented with 10% fetal bovine serum (Gibco), and 1% penicillin−streptomycin (Invitrogen) and maintained at 37 °C in a humidified incubator (Thermo Electron Corporation) containing 5% CO_2. When the cells reached 80% confluency, they were passaged using an Accutase solution (Invitrogen); media was changed every 2 − 3 days.

Ai9 myoblast cells were cultured in Ham's F-12 Nutrient Mix (Gibco) supplemented with 20% fetal bovine serum (Gibco), and 1% penicillin−streptomycin (Invitrogen) and 10 ng/mL of bFGF (Sigma Aldrich) (myoblast growth medium), and maintained at 37 °C in a humidified incubator (Thermo Electron Corporation) containing 5% CO_2. When the cells

reached 80% confluency, they were passaged using an Accutase solution (Invitrogen) and seeded to a Matrigel coated flask. Media was changed every 2 − 3 days.

Flow cytometry

RT HEK cells were seeded in 48 well plates at a density of 20K per well. After 24 hours, 150 μL Opti-MEM (Gibco) containing Cas9 RNP (5 μg Cas9) mixed with 1μL of lipofectamine 2000 and 100 μg of FEDS was added to the RT HEK cells. The cells were transfected for 48 hrs at 37 °C in a humidified incubator containing 5% CO_2 and medium was replaced with fresh DMEM medium supplemented with 10% FBS, 1% penicillin-streptomycin and 1 μg/mL doxycycline. RT HEK cells were detached by Accutase (Invitrogen) and the GFP signals were analysed by Attune NxT flow cytometer (Invitrogen). Gene editing efficiency was determined by the percentage of GFP negative cells as shown in Fig. S3.

Primary Ai9 mouse myoblast cells were seeded in 48 well plates at a density of 20K per well. After 24 hours, 150 μL of Opti-MEM (Gibco) containing Cas9 RNP that targeted the Ai9 STOP cassette (5 μg Cas9) mixed with 1μL of lipofectamine 2000 and 100 μg of FEDS, was added to the Ai9 myoblast cells. The cells were transfected for 24 hrs at 37 °C in a humidified incubator containing 5% CO_2, and the media was replaced with myoblast growth medium and the cells were grown in myoblast growth medium for another 24 hrs. The myoblasts were detached with Accutase (Invitrogen) and the TdTomato signal was analysed with a Attune NxT flow cytometer (Invitrogen). The gene editing efficiency was determined by identifying the percentage of TdTomato positive cells, as shown in Fig. S4.

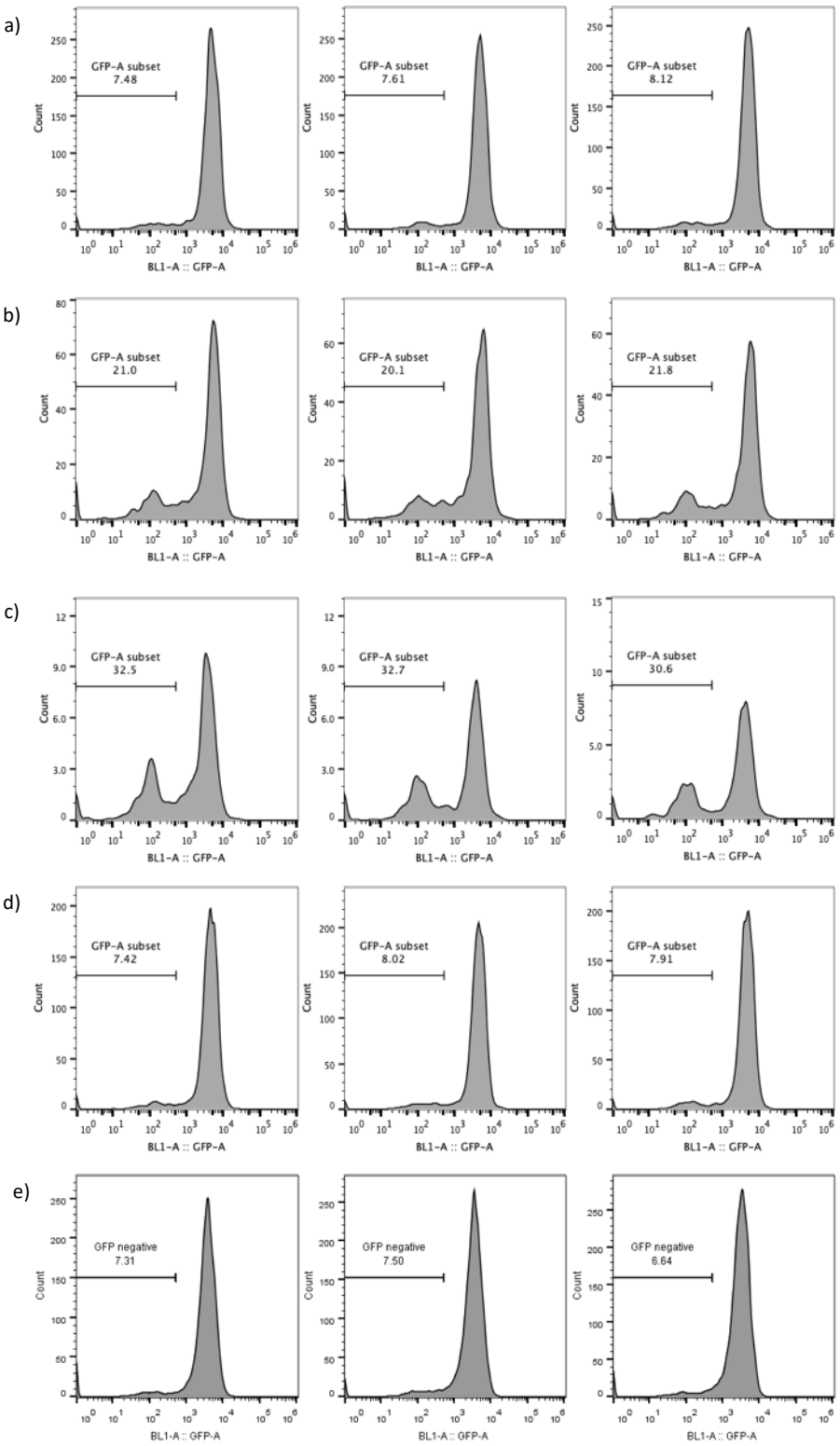


Fig. S3 Gating of GFP negative RT HEK cells. a) Untreated cells, b) cells treated with lipofectamine 2000/RNP, c) cells treated with FEDEX, d) cells treated Cas9 RNP alone, e) cells treated with FEDEX without guide RNA.

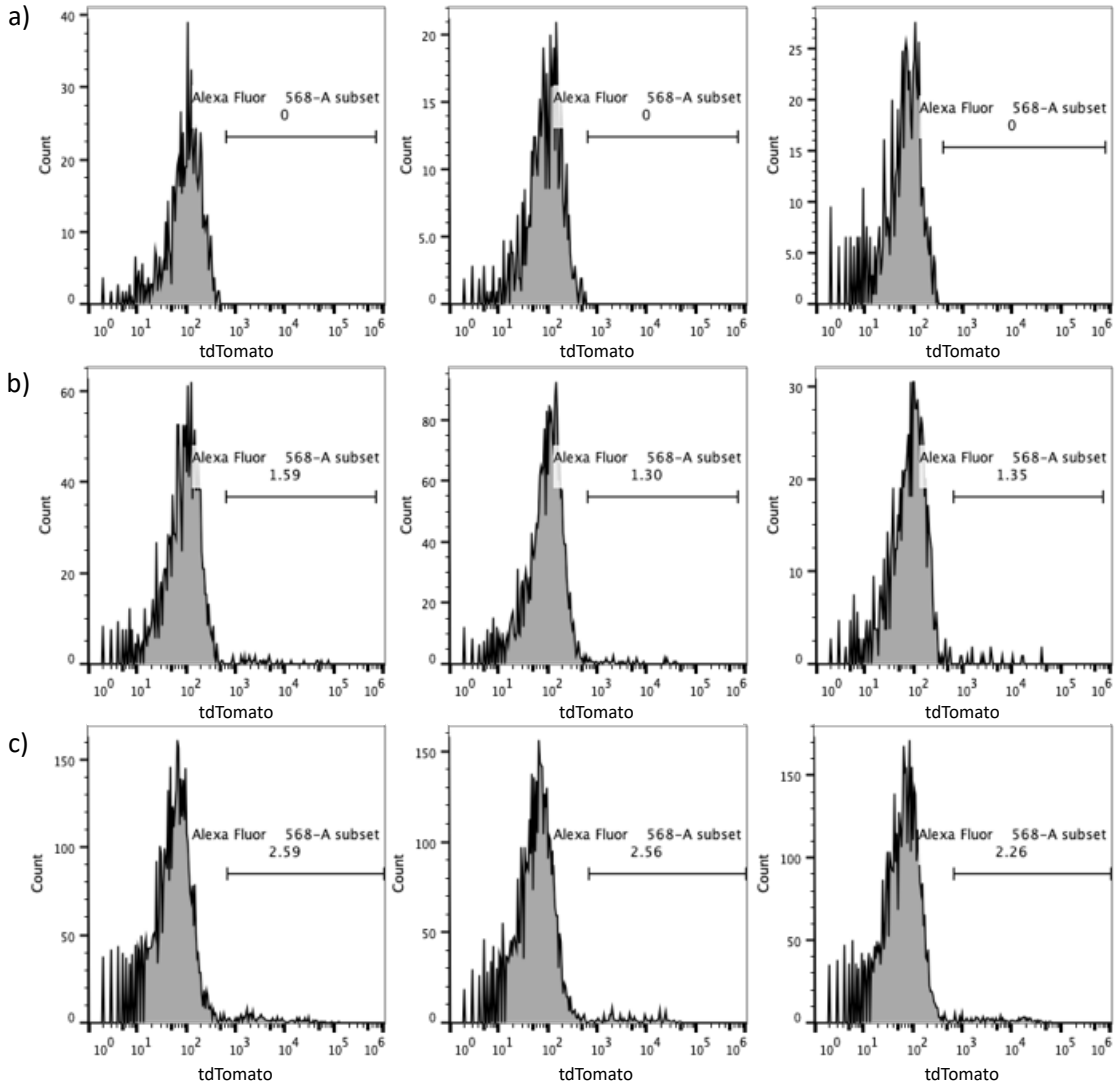


Fig. S4 Gating of tdTomato positive Ai9 myoblast cells. a) Untreated cells, b) cells treated with lipofectamine 2000/Cas9 RNP, c) cells treated with FEDEX.

Cell Viability

HEK 293T cells were seeded in 96 well plates at a density of 5K per well and incubated at 37 °C in a humidified incubator containing 5% CO_2 for 24 hrs. 1 µL of

lipofectamine 2000, 100 μg of FEDS or 1 μL lipofectamine + 100 μg FEDS were added to 100 μL of DMEM medium supplemented with 10% FBS and 1% penicillin-streptomycin and the cells were incubated with the solution for 24 hours. The cells were further washed with PBS and incubated with 100 μL fresh medium containing resazurin (Alamar Blue) (0.01 mg/mL) for another 4 h. The cell viability was then determined by measuring the fluorescence intensity of each well (E_x = 550 nm, E_m = 595 nm) using a microplate reader. Untreated cells and fresh medium were used as controls for a 100% and 0% cell proliferation, respectively. Double concentration (2X) of lipofectamine 2000, FEDS and lipofectamine 2000 + FEDS were also added to the cells for the viability assay.

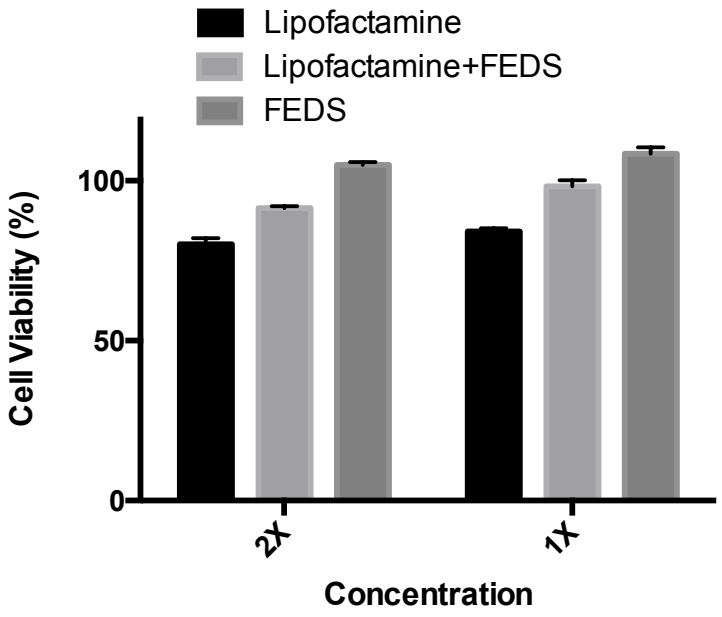


Fig. S5 Cell viability assay of lipofectamine 2000, lipofectamine 2000 + FEDS and FEDS performed at different concentrations. 1X refers to 1 μL lipofectamine 2000 added to a 100 μL media, 100 μg FEDS or 1μL lipofectamine 2000 + 100 μg FEDS added to a 100 μL of media. 2X refers to 2 μL lipofectamine 2000, 200 μg FEDS or 2μL lipofectamine 2000 + 200 μg FEDS added to a 100 μL of media.

Cell internalization studies

The intracellular delivery of FEDEX was investigated using fluorescence microscopy. HeLa cells were cultured in DMEM supplemented with 10% FBS and 1% P/S. Glass cover slides were placed on the bottom of the 6 well plates and the cells (50,000 cells/well) were seeded the day before the addition of FEDEX. FEDEX formulated with Cas9-mCherry RNP was added to the cell cultures and incubated for 4hrs. The cells were washed three times with PBS, stained with the NucSpot Live 488 for nucleus staining and visualized with a fluorescent microscope.

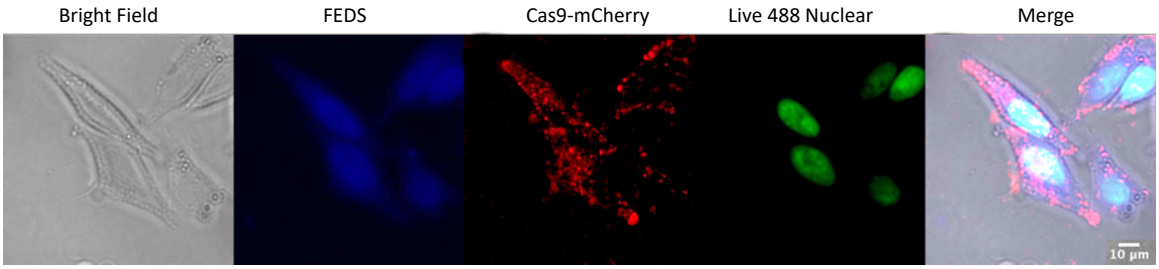


Fig. S6 FEDEX internalization by HeLa cells after 4hrs of incubation. The Cas9-mCherry fusion protein was used to visualize the RNP localization. FEDS was distributed throughout the cells after 4 hrs of incubation.

T7E1 assay

RT HEK cells were seeded in 48 well plates at a density of 20K per well. After 24 hours, 150 µL Opti-MEM (Gibco) containing Cas9 RNP (5 µg Cas9) mixed with 1µL of lipofectamine 2000 and 100 µg of FEDS was added to the RT HEK cells. The cells were transfected for 48 hrs at 37 °C in a humidified incubator containing 5% CO_2 and the medium was replaced with fresh DMEM medium supplemented with 10% FBS, 1% penicillin-streptomycin and 1 µg/mL doxycycline. RT HEK cells were detached by Accutase (Invitrogen) and the cell pellets were collected by centrifugation at 500g for 5 min. Genomic DNA was extracted with a genomic extraction kit (Qiagen) and amplified by PCR following the PCR product purification guidelines provided by Qiagen. The

purified PCR products were further annealed by the following program: 95˚ 5 min, 95->85˚ at 2˚/sec, 85->25˚ at 0.1˚/sec and 4˚ hold. The annealed PCR product were mixed with T7E1 for 15 min at 37˚ according to NEB assay protocol. The digested samples were run on an SDS-PAGE gel (4%-20%, Biorad).

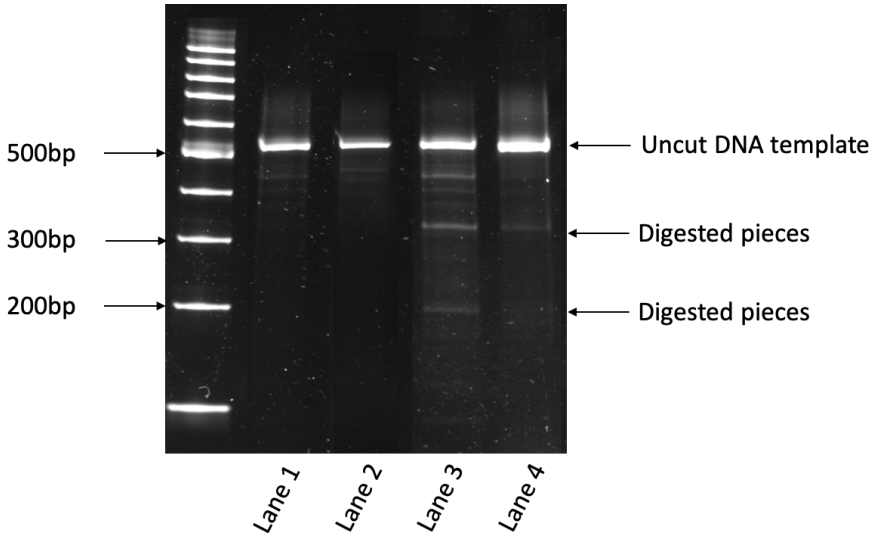


Fig. S7 FEDEX enhances the gene editing efficiency of Cas9 RNP as measured by the T7E1 assay. T7E1 digestion of the PCR product of the GFP gene from control RT HEK cells (without transfection) (Lane 1), RT HEK cells treated with Cas9 RNP alone (Lane 2), RT HEK cells treated with FEDEX (Lane 3) and RT HEK cells treated with lipofectamine 2000/RNP (Lane 4).

Cell Sorting

RT HEK cells were seeded in 48 well plates at a density of 20K per well. After 24 hours, 150 µL Opti-MEM (Gibco) containing Cas9 RNP (5 µg Cas9) mixed with 1µL of lipofectamine 2000 and 100 µg of FEDS was added to RT HEK cells. The cells were transfected for 24 hrs at 37 °C in a humidified incubator containing 5% CO_2 and the medium was replaced with fresh DMEM medium supplemented with 10% FBS, 1% penicillin-streptomycin and 1 µg/mL doxycycline. RT HEK cells were detached by

Accutase (Invitrogen) and sorted with an Influx cell sorter (BD) according to the intensity of FEDS (see Fig. S8). Both FEDS positive and negative cells were collected and cultured for further flow cytometry analysis.

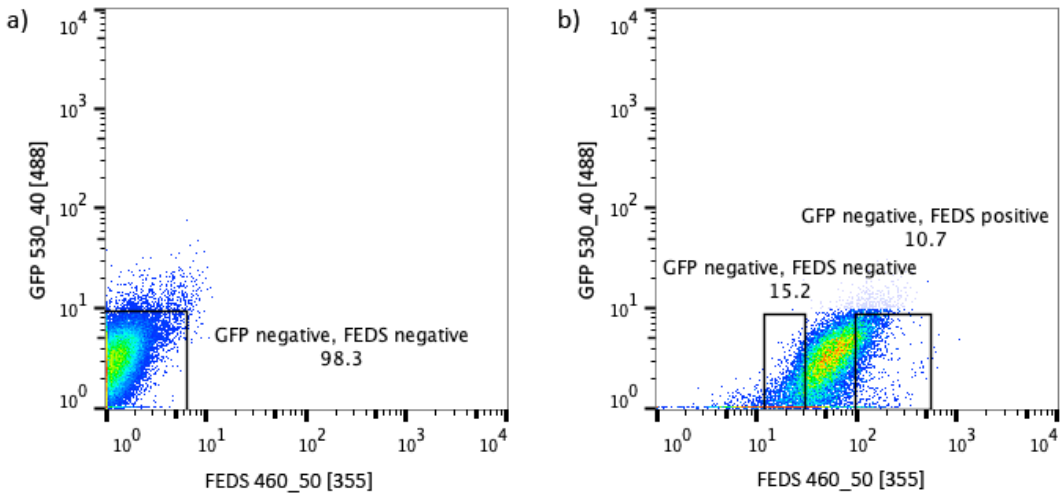
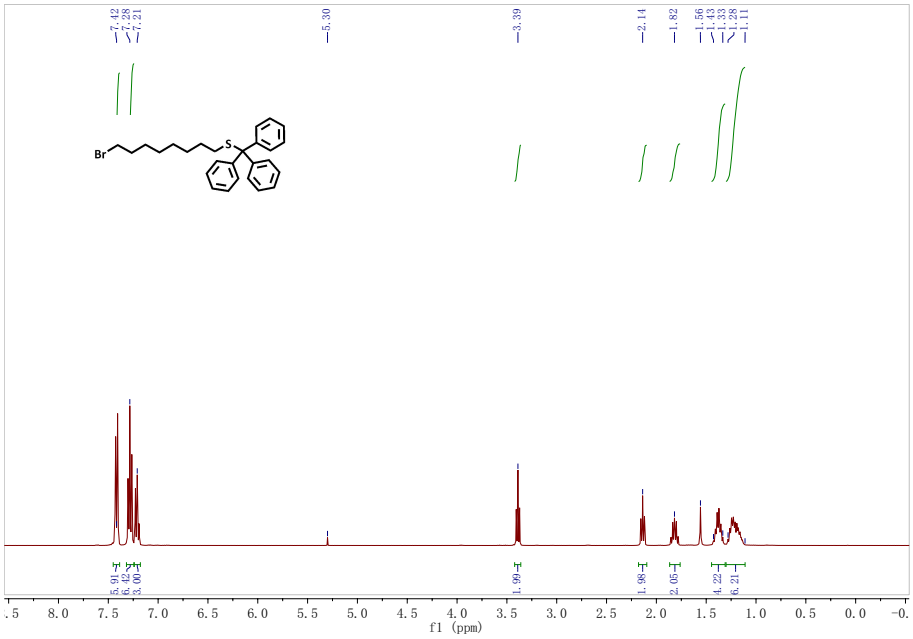


Fig. S8 Gating of RT HEK cells collected after transfection. Cell sorting of RT HEK cells after treatment with a) lipofectamine 2000/Cas9 RNP or b) FEDEX. **a)** GFP (Ex 488 nm, Em 530-540 nm) negative cells were collected for further Dox activation and flow cytometry measurement, after transfection with lipofectamine 2000/RNP. No FEDS signals (Ex 355 nm, Em 450-460 nm) was present in these cells. **b)** FEDS negative RT HEK cells and FEDS positive RT HEK cells were collected respectively for further Dox activation and flow cytometry measurement, after transfection with FEDEX.

Reference

1. H. M. Park, H. Liu, J. Wu, A. Chong, V. Mackley, C. Fellmann, A. Rao, F. Jiang, H. Chu, N. Murthy, and K. Lee, *Nat. Commun.*, 2018, **9**, 3313.

^{1}H NMR and ^{13}C NMR spectrum


7.42
7.28
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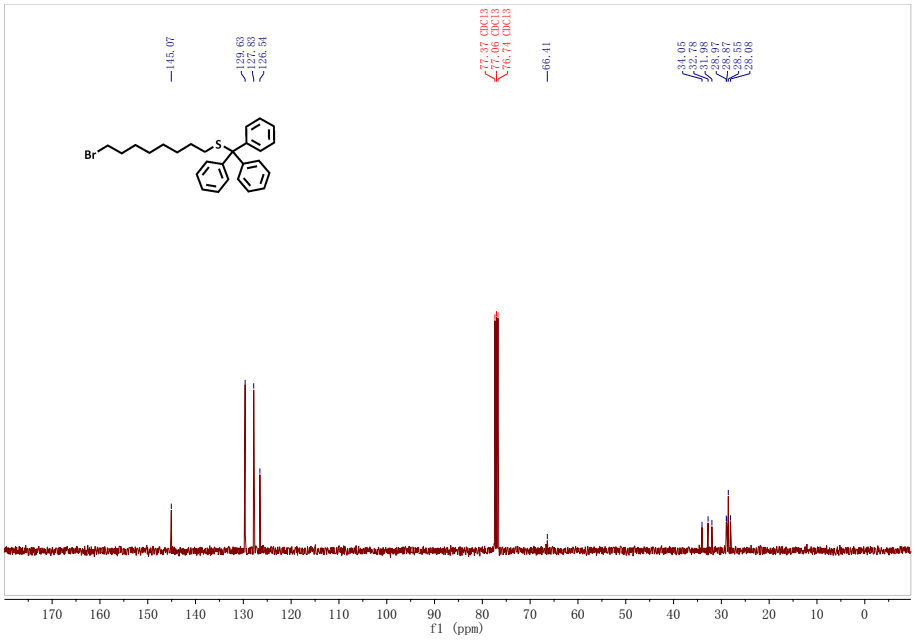
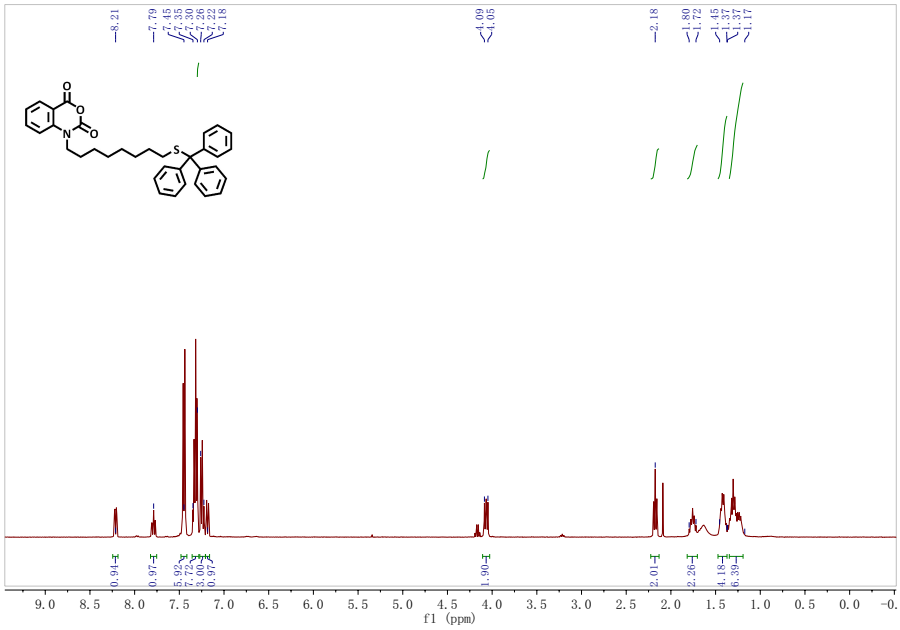
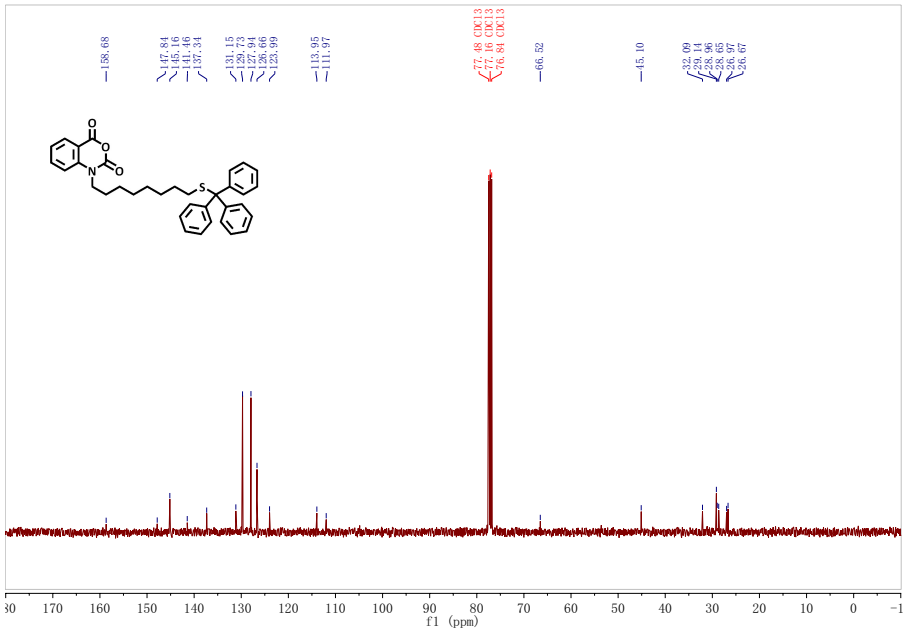
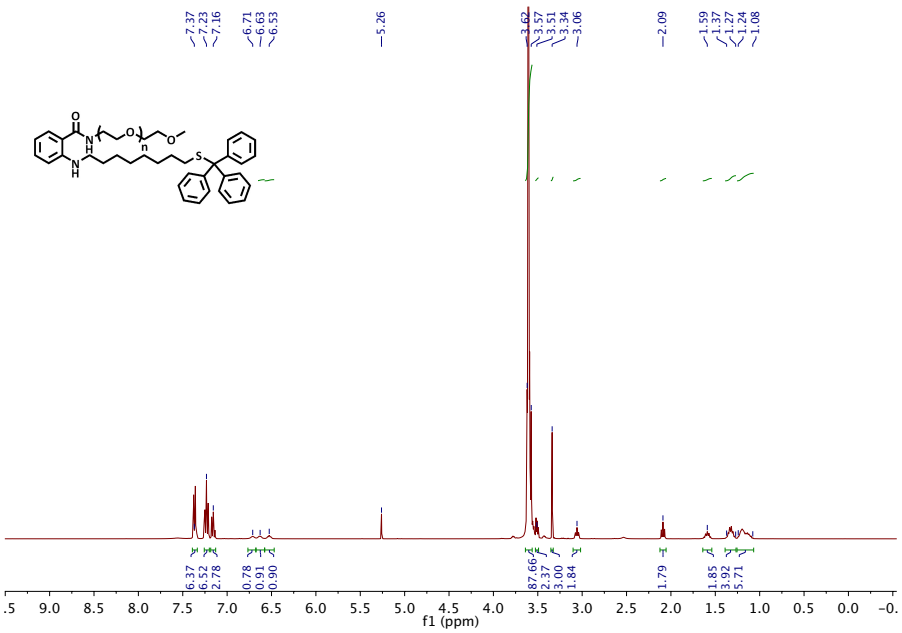
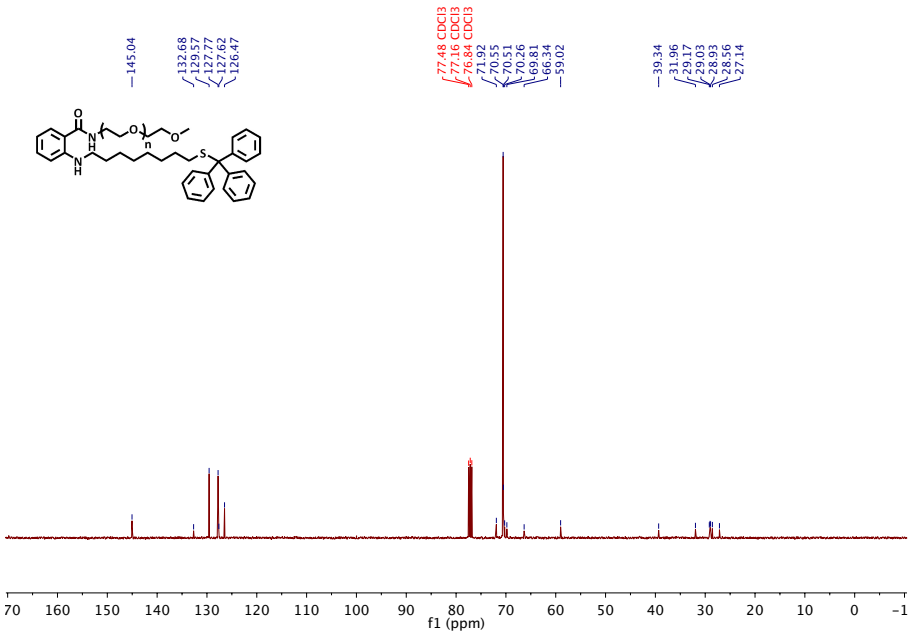
6.21
f1 (ppm)

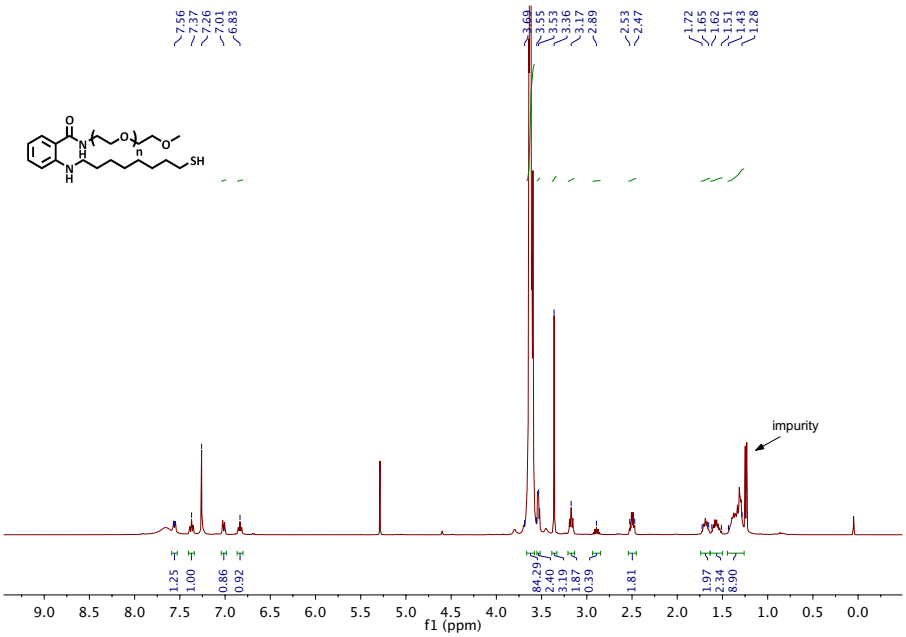

145.07
129.63
127.83
126.54
77.37 CDCl3
77.06 CDCl3
76.74 CDCl3
66.41
34.05
32.78
31.98
28.97
28.87
28.55
28.08
Br
S
f1 (ppm)

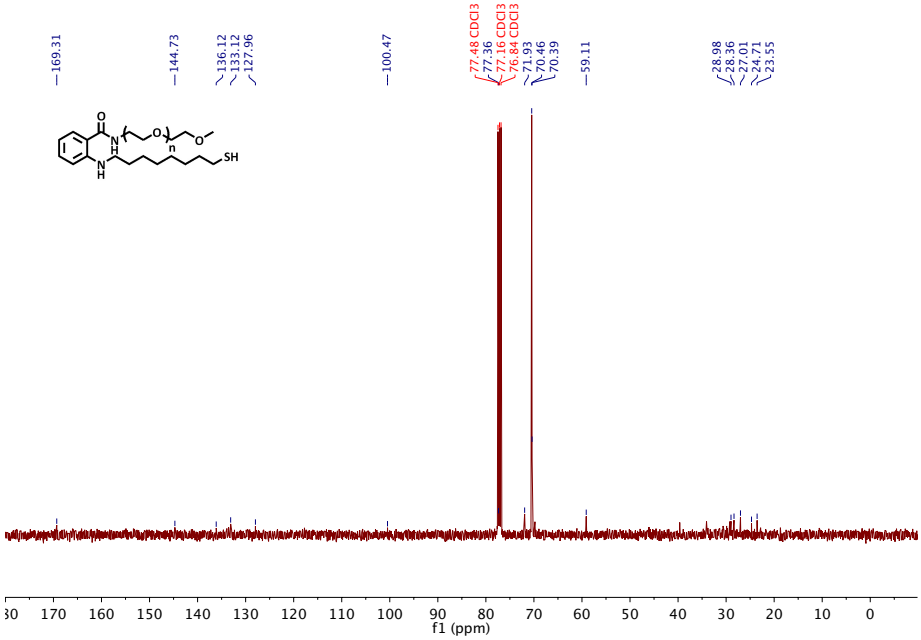

8.21
7.79
7.45
7.35
7.30
7.26
7.22
7.18
4.09
4.05
2.18
1.80
1.72
1.45
1.37
1.17
0.94
0.97
5.92
7.72
3.06
0.97
1.90
2.01
2.26
4.18
6.39
f1 (ppm)

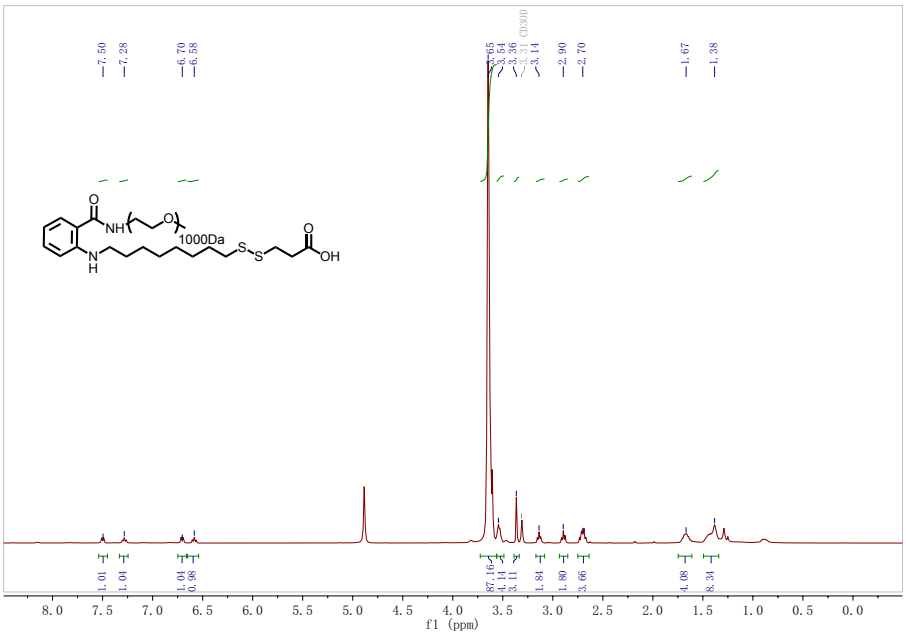

168.68
147.84
145.16
141.46
137.34
131.15
129.73
127.64
126.66
123.99
113.95
111.97
77.48 CDCl3
77.16 CDCl3
76.81 CDCl3
66.52
45.10
29.09
28.14
28.96
28.65
26.97
26.67
f1 (ppm)

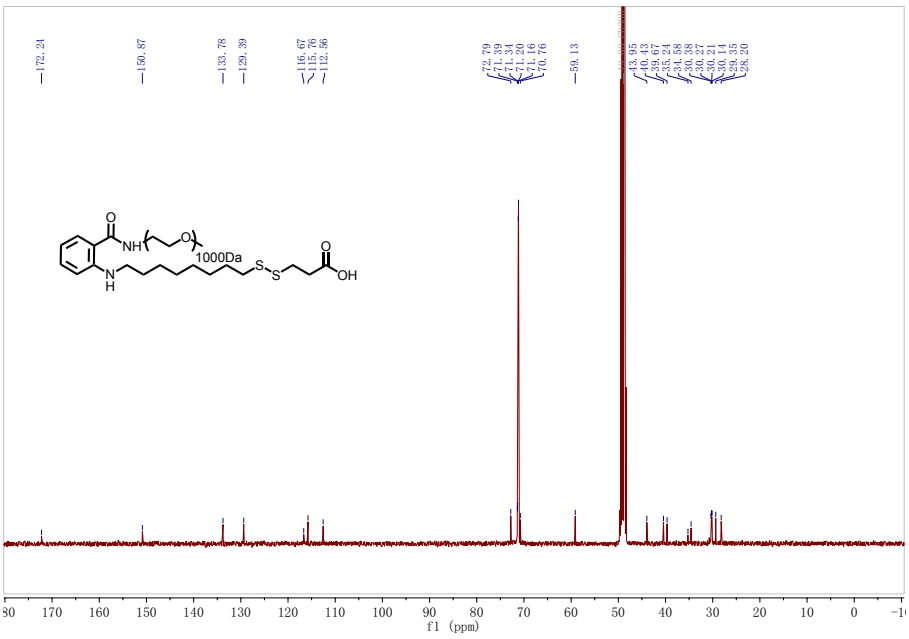

7.37
7.23
7.16
6.71
6.63
6.53
5.26
3.62
3.57
3.51
3.34
3.06
2.09
1.59
1.37
1.27
1.24
1.08
6.37
6.52
2.78
0.78
0.91
0.90
87.66
2.37
3.00
1.84
1.79
1.85
3.92
5.71
f1 (ppm)

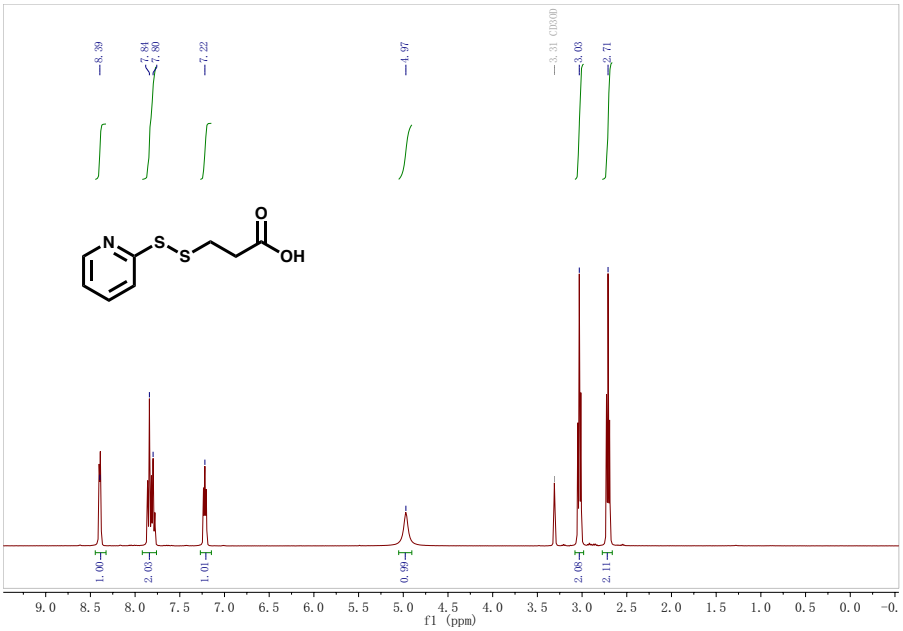

145.04
132.68
129.57
127.77
127.62
126.47
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
71.92
70.55
70.51
70.26
69.81
66.34
59.02
39.34
31.96
29.17
29.03
28.83
28.56
27.14
f1 (ppm)

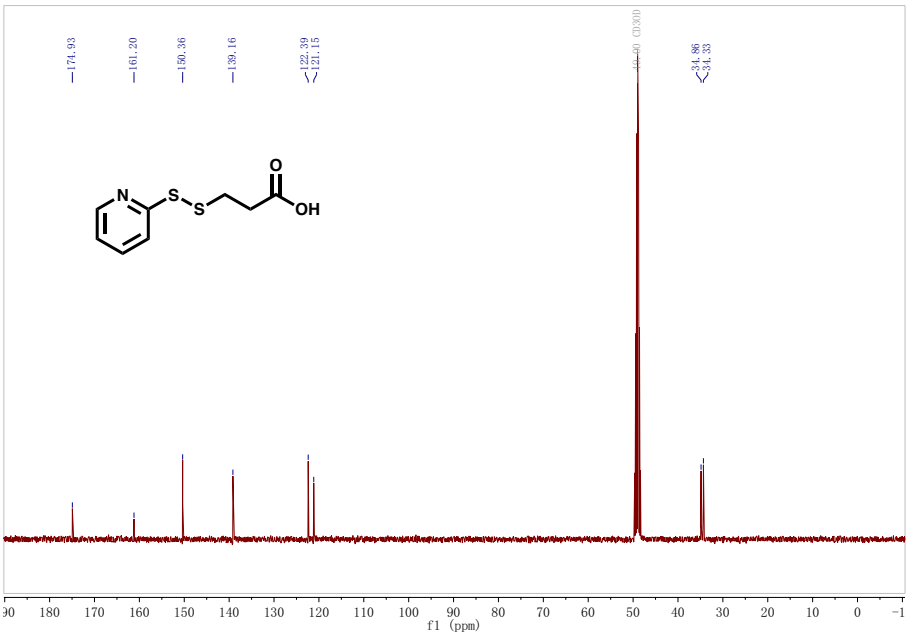

7.56
7.37
7.36
7.01
6.83
3.69
3.55
3.53
3.36
3.17
2.89
2.53
2.47
1.72
1.65
1.62
1.51
1.43
1.28
impurity
1.25
1.00
0.86
0.92
84.29
2.40
3.19
1.87
0.39
1.81
1.97
2.34
8.90
f1 (ppm)


169.31
144.73
136.12
133.12
127.96
100.47
77.48 CDCl3
77.16 CDCl3
76.84 CDCl3
71.93
70.46
70.39
59.11
28.98
28.36
27.01
24.71
23.55
f1 (ppm)


7.50
7.28
6.70
6.58
3.65
3.54
3.36
3.31
3.14
2.90
2.70
1.67
1.38
1.01
1.04
1.04
0.98
87.16
4.14
3.11
1.84
1.80
3.66
4.08
8.34
NH
O
1000Da
S
S
OH
N
H
f1 (ppm)


172.24
150.87
133.78
129.39
116.67
115.76
112.56
72.79
71.39
71.34
71.20
71.16
70.76
69.13
43.95
40.43
39.67
35.24
34.58
30.38
30.27
30.21
30.14
29.35
28.20
NH
O
1000Da
S
S
OH
N
H
f1 (ppm)


8.39
7.84
7.80
7.22
4.97
3.31 CD3OD
3.03
2.71
1.00
2.03
1.01
0.99
2.08
2.11
f1 (ppm)


174.93
161.20
150.36
139.16
122.39
121.15
49.00 CD3OD
34.86
34.33
f1 (ppm)