Electronic Supplementary Information (ESI)

Theranostic system for ratiometric fluorescence monitoring of peptide-guided targeted drug delivery

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1. Absorption and fluorescence spectra

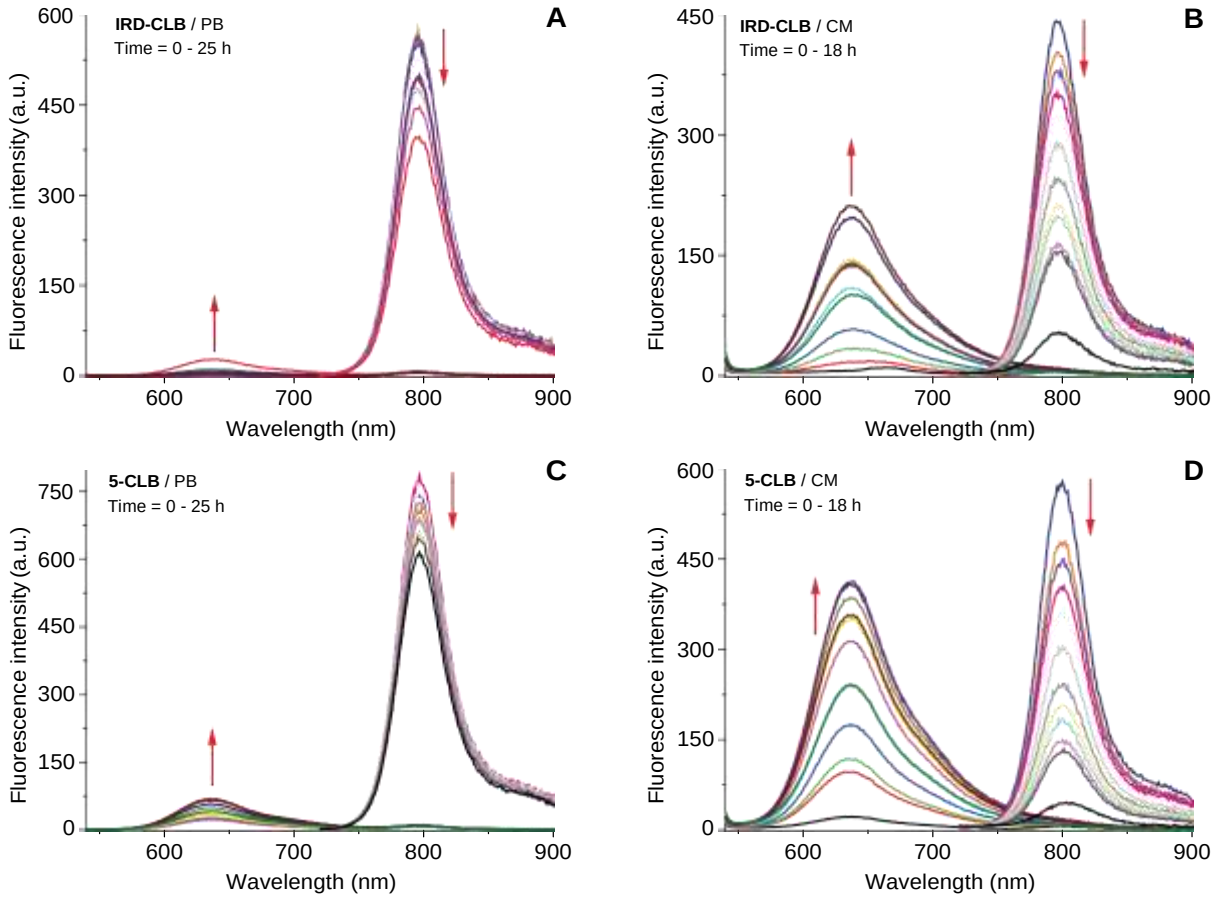


Fig. S1 The time-dependent spectra of **IRD-CLB** (**A**, **B**) and **5-CLB** (**C**, **D**) in PB (**A**, **C**) and CM (**B**, **D**) measured at $T = 25\,^{\circ}C$ after incubation at 37 °C. The excitation wavelength was 532 nm for **RD** (shorter-wavelength emission bands) and 720 nm for **IRD-CLB** and **5-CLB** (longer-wavelength emission bands).

2. NMR, MS and HPLC data

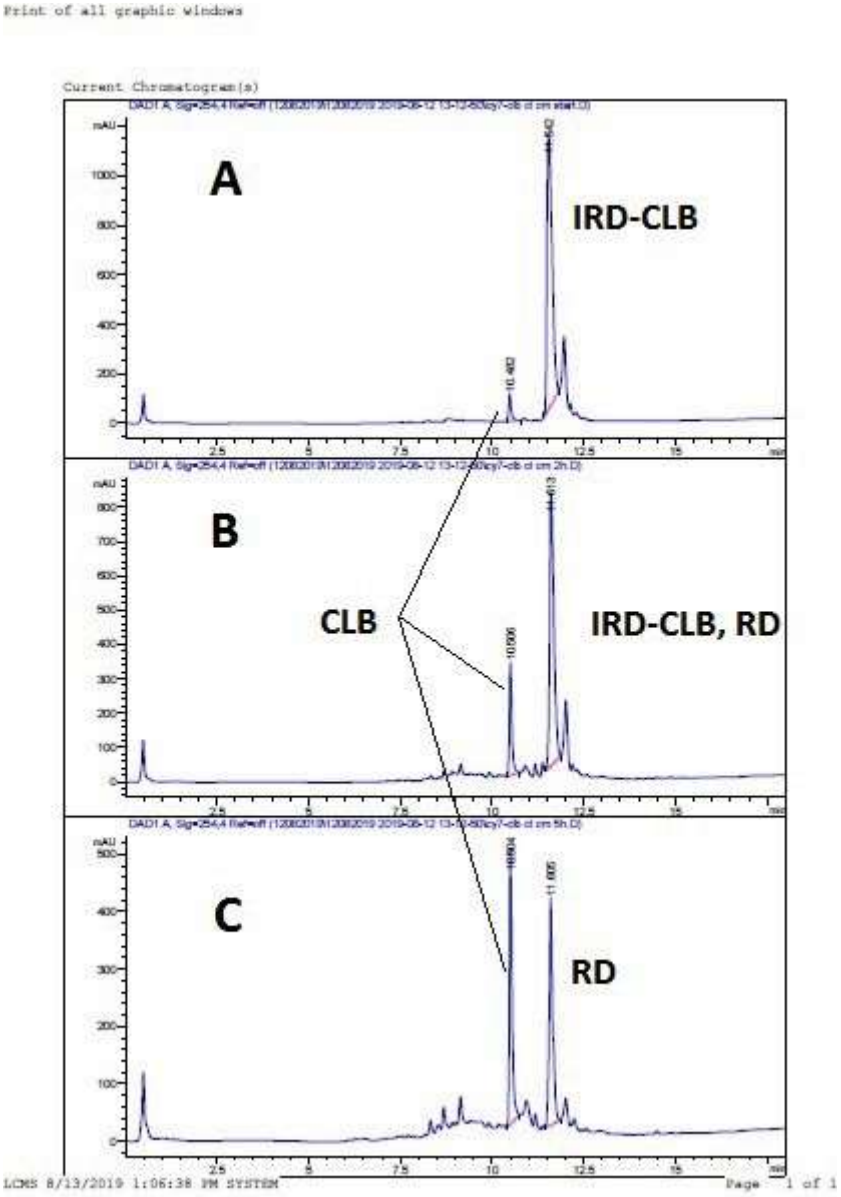


Fig. S2 Cleavage of **IRD-CLB** in CM over time: A - time 0, B - 2 h and C - 5 h.

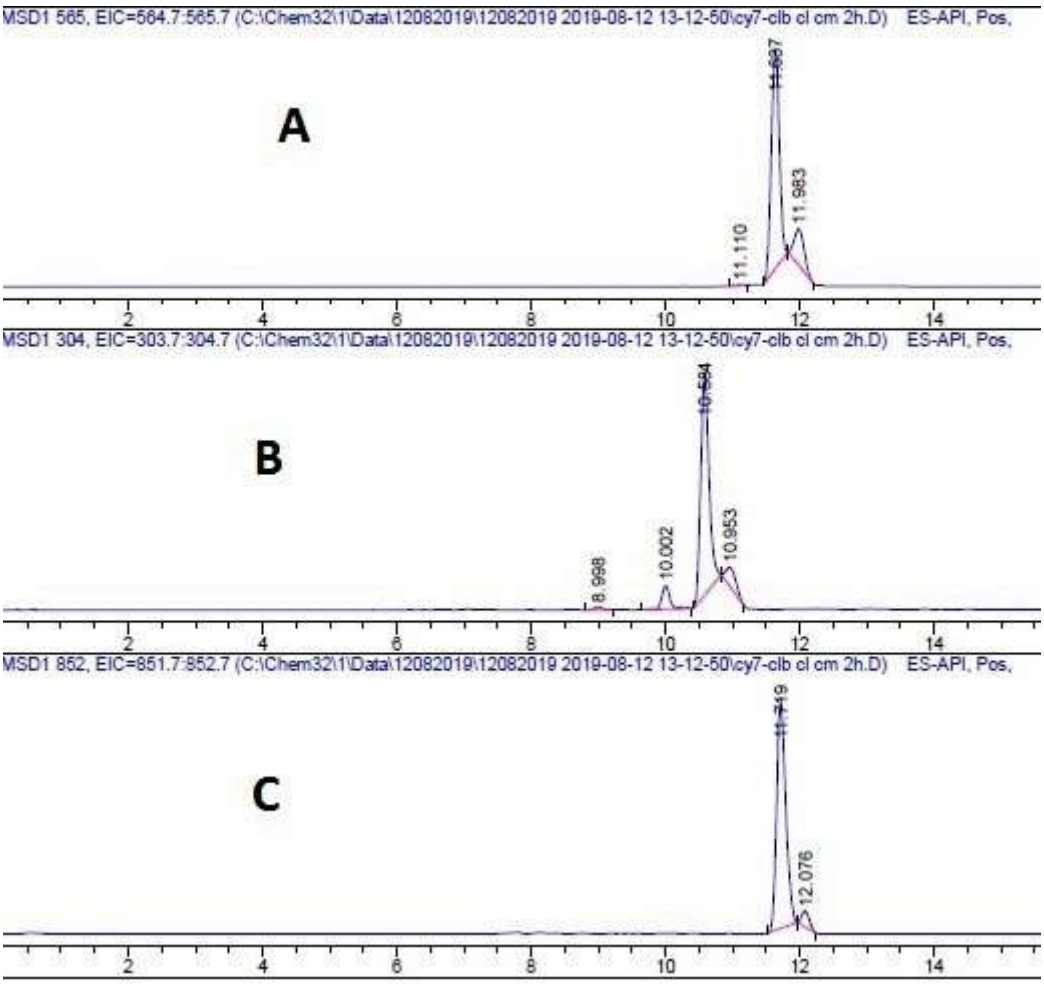


Fig. S3 MS-TIC of A - **RD**, B - **CLB** and C - **IRD-CLB** shown in Fig. S2,B.

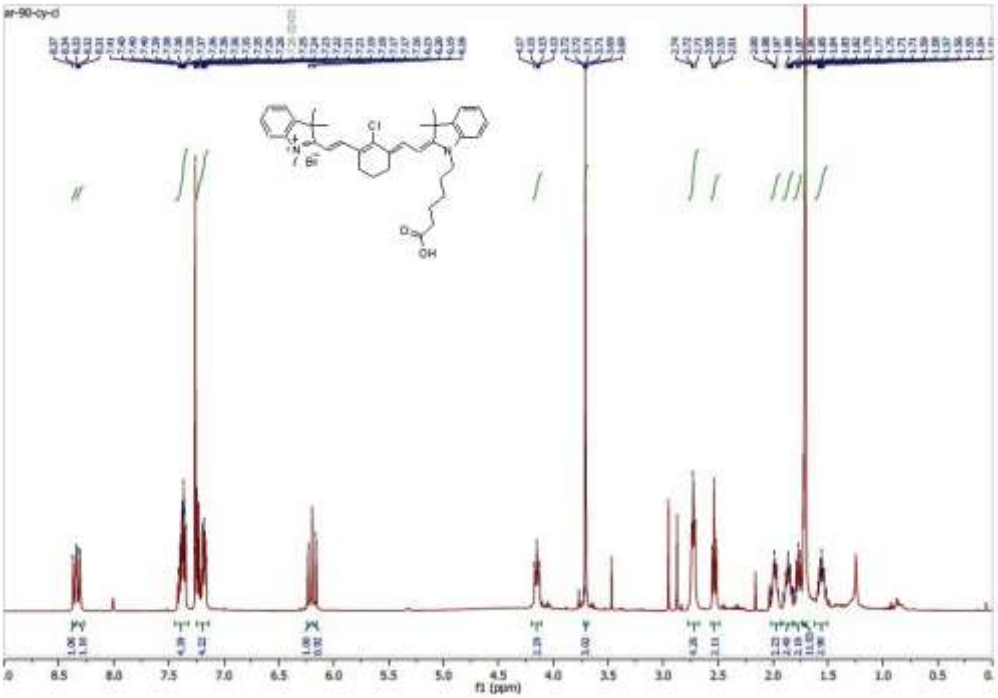


Fig. S4 ^{1}H NMR spectrum of compound **4** (400 MHz, $CDCl_3$).

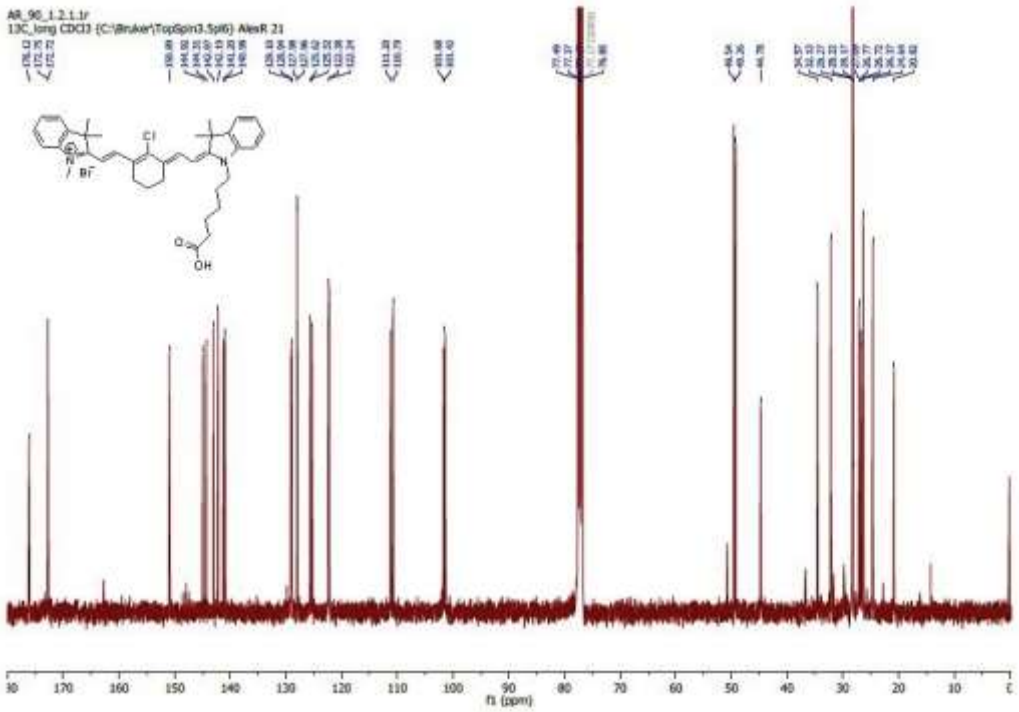


Fig. S5 ^{13}C NMR spectrum of compound **4** (101 MHz, $CDCl_3$).

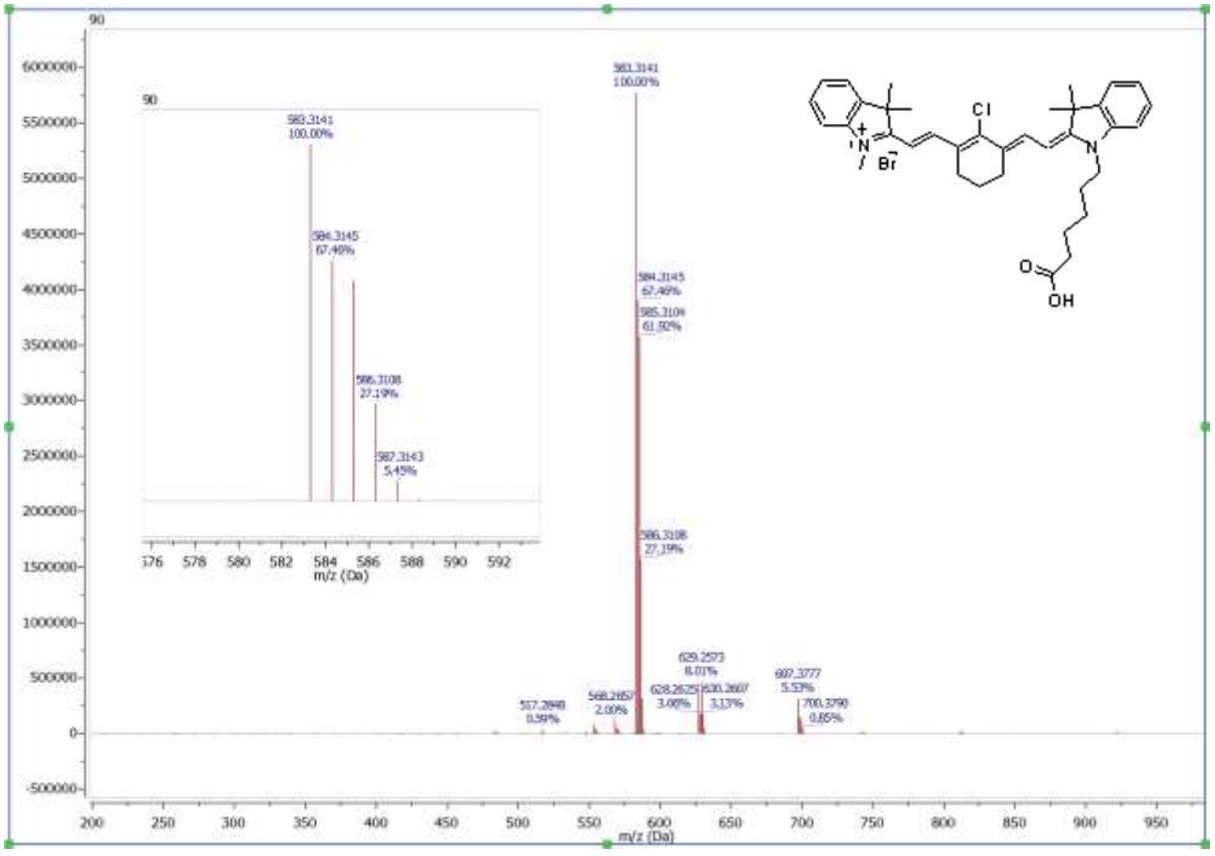


Fig. S6 HRMS spectrum of compound **4.**

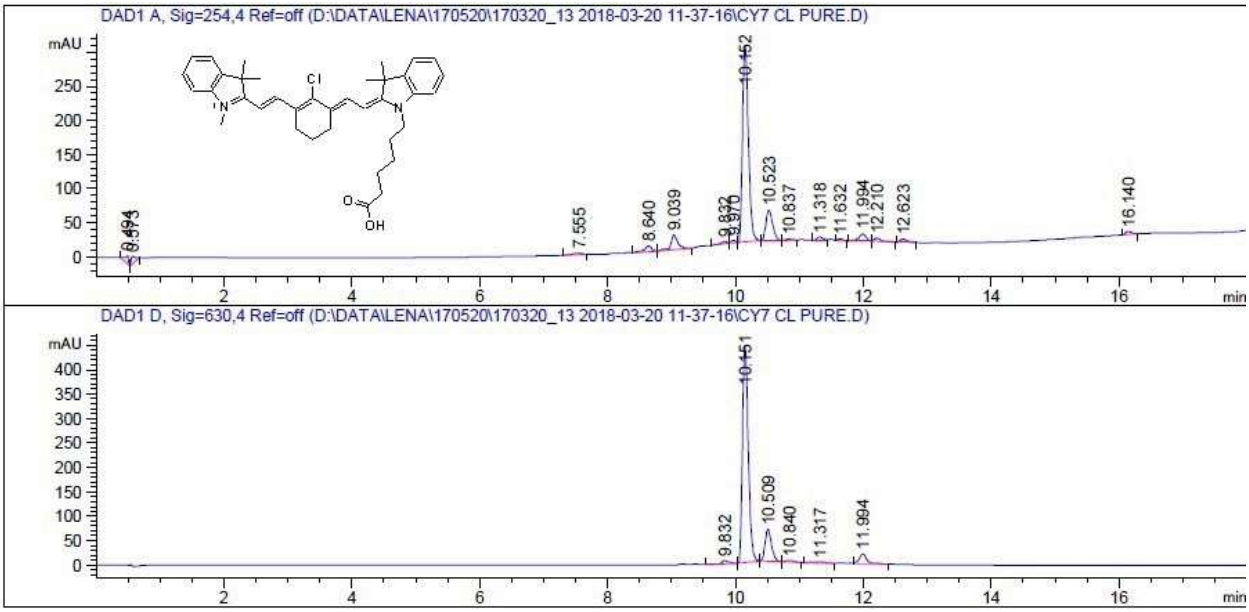


Fig. S7 HPLC chromatogram of compound **4.**

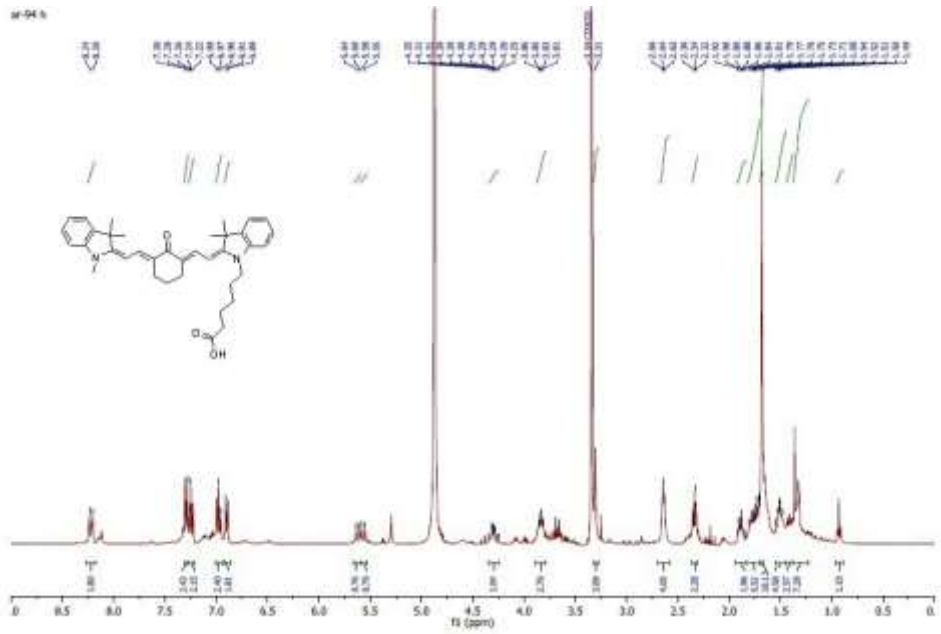


Fig. S8 ^{1}H NMR spectrum of **RD** (400 MHz, MeOD).

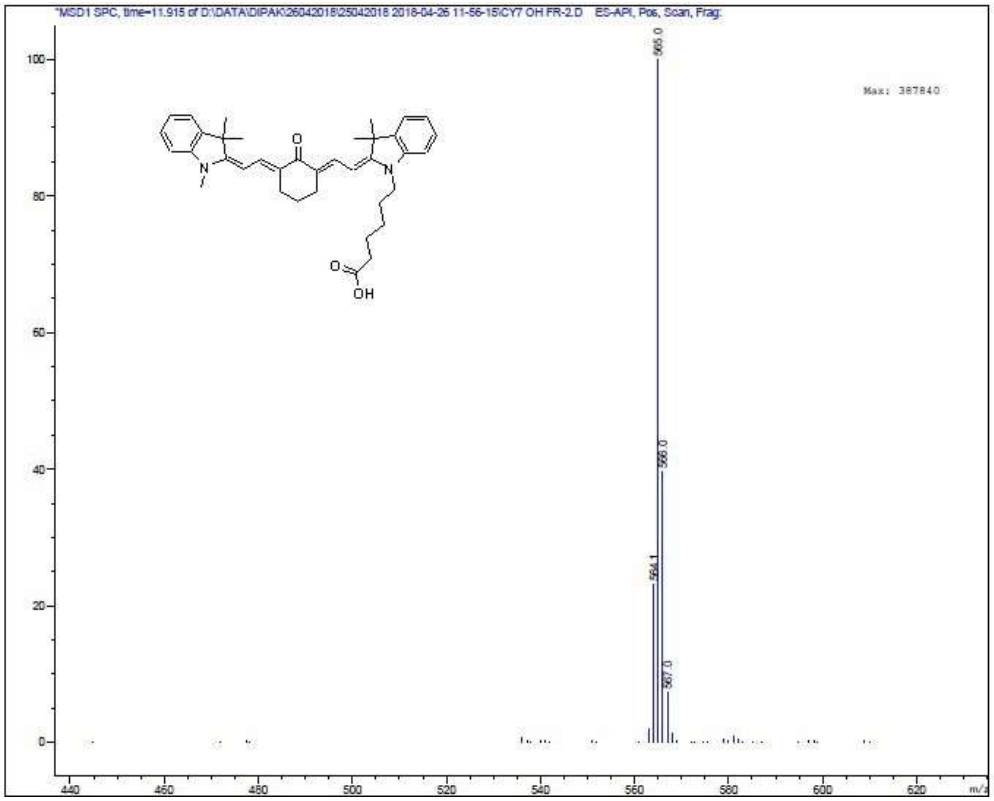


Fig. S9 MS spectrum of **RD.**

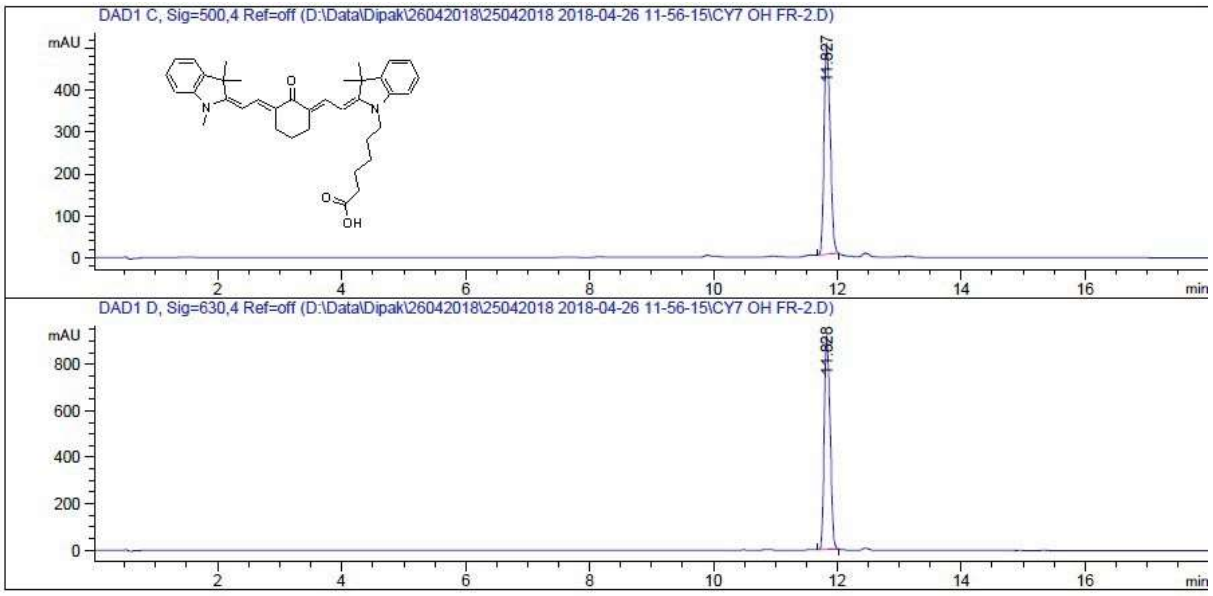


Fig. S10 HPLC chromatogram of **RD.**

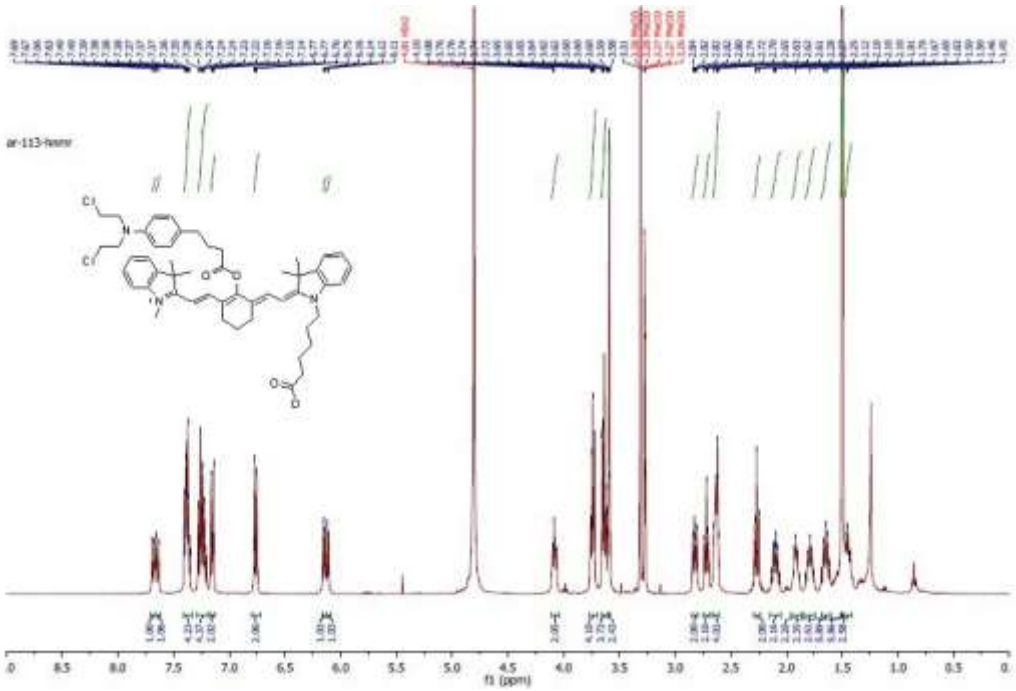


Fig. S11 ^{1}H NMR spectrum of **IRD-CLB** (400 MHz, MeOD).

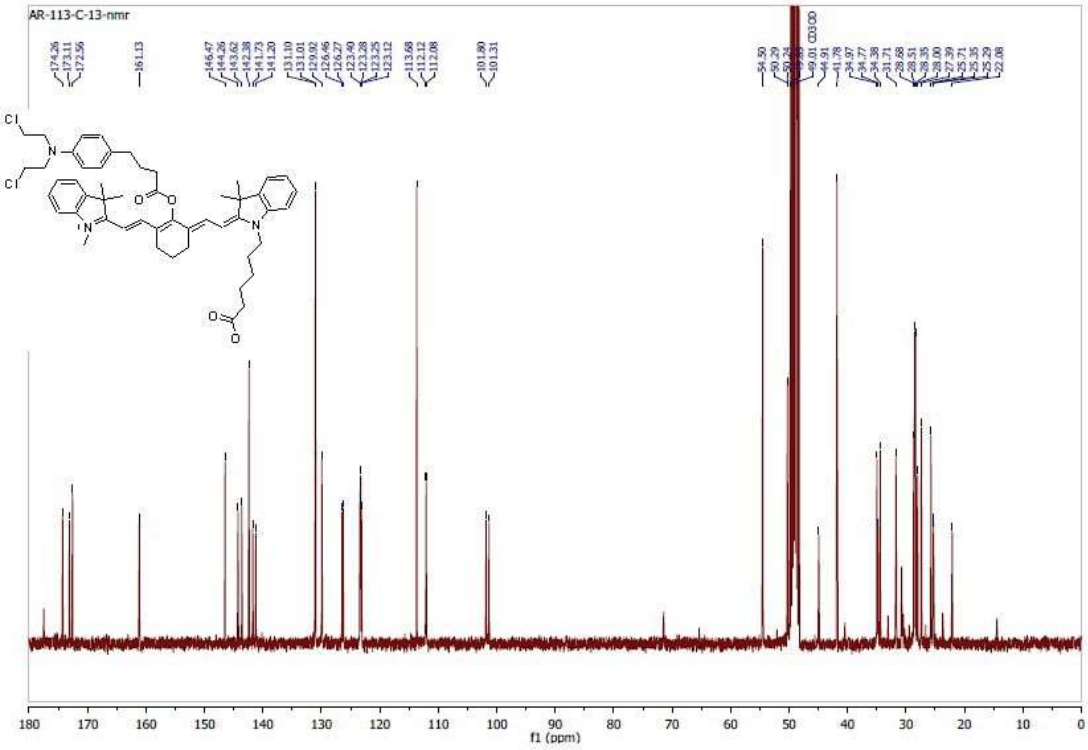


Fig. 12 ^{13}C NMR spectrum of **IRD-CLB** (101 MHz, MeOD).

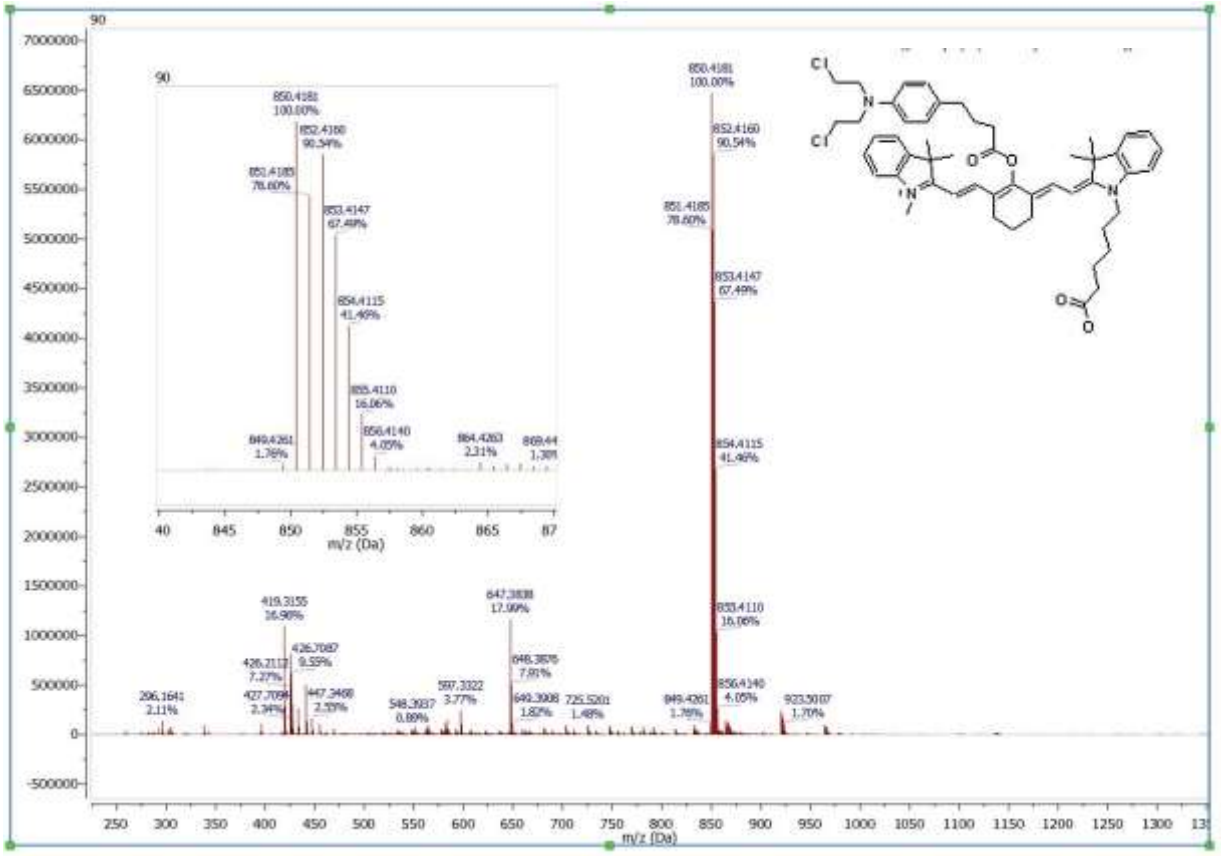


Fig. S13 HRMS spectrum of **IRD-CLB.**

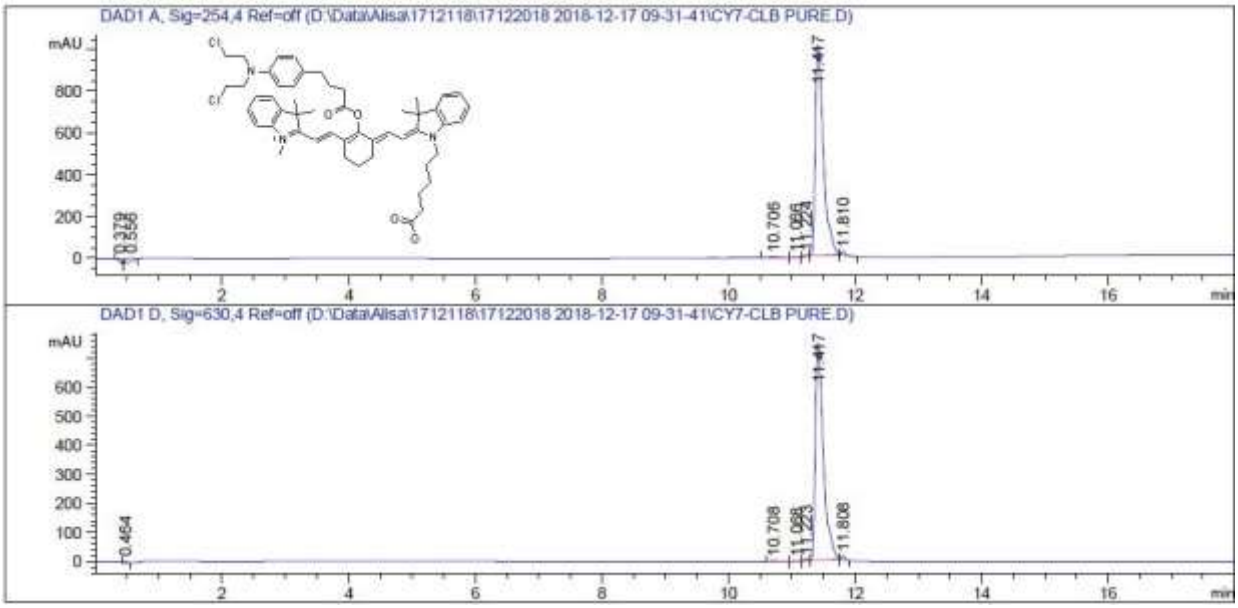


Fig. S14 HPLC chromatogram of **IRD-CLB.**

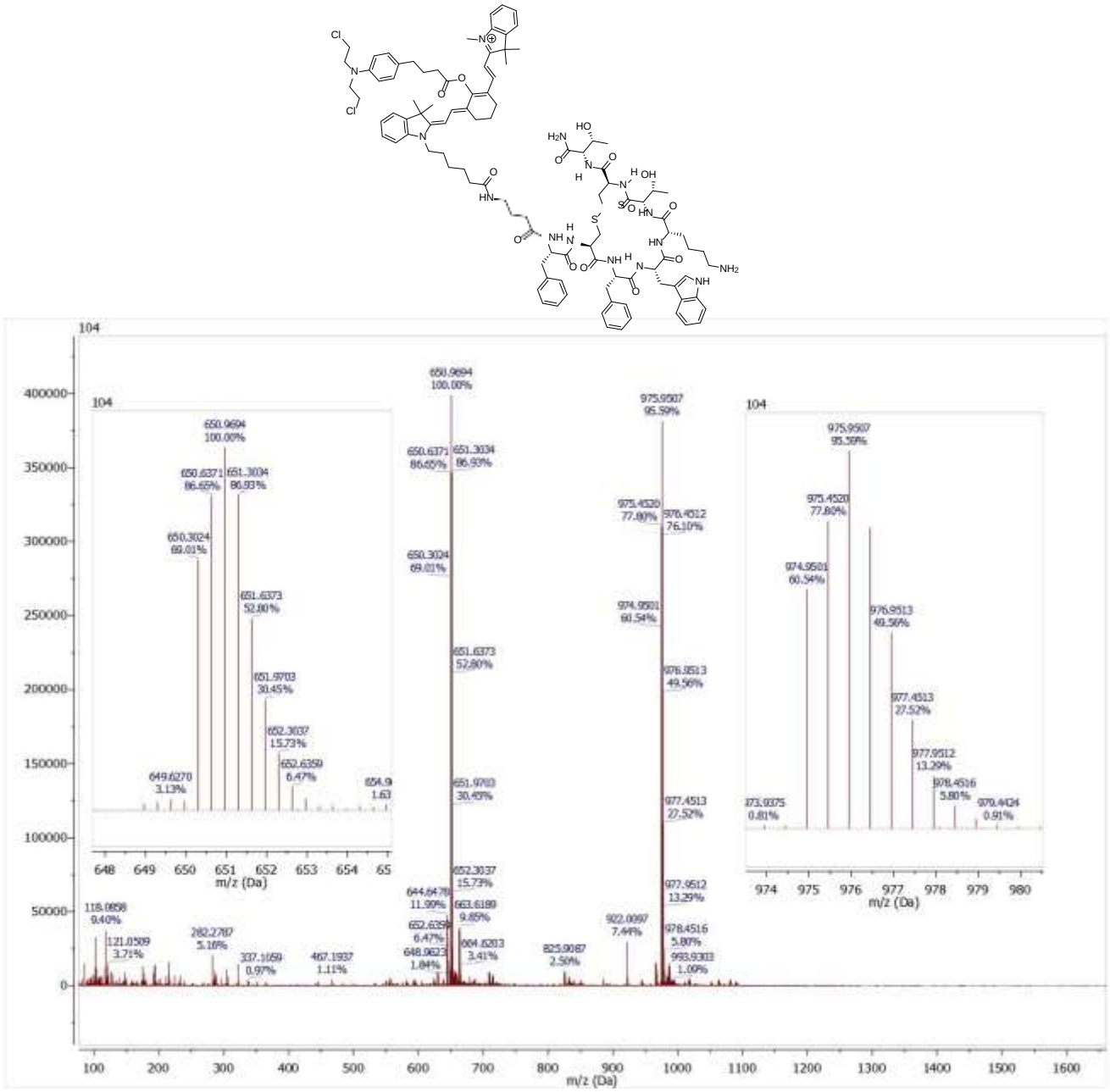
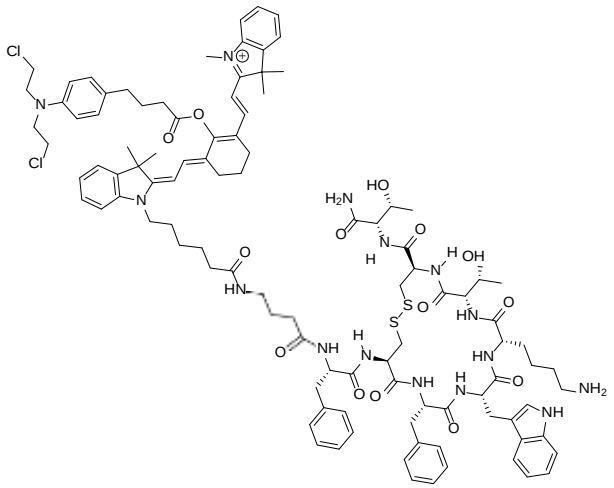
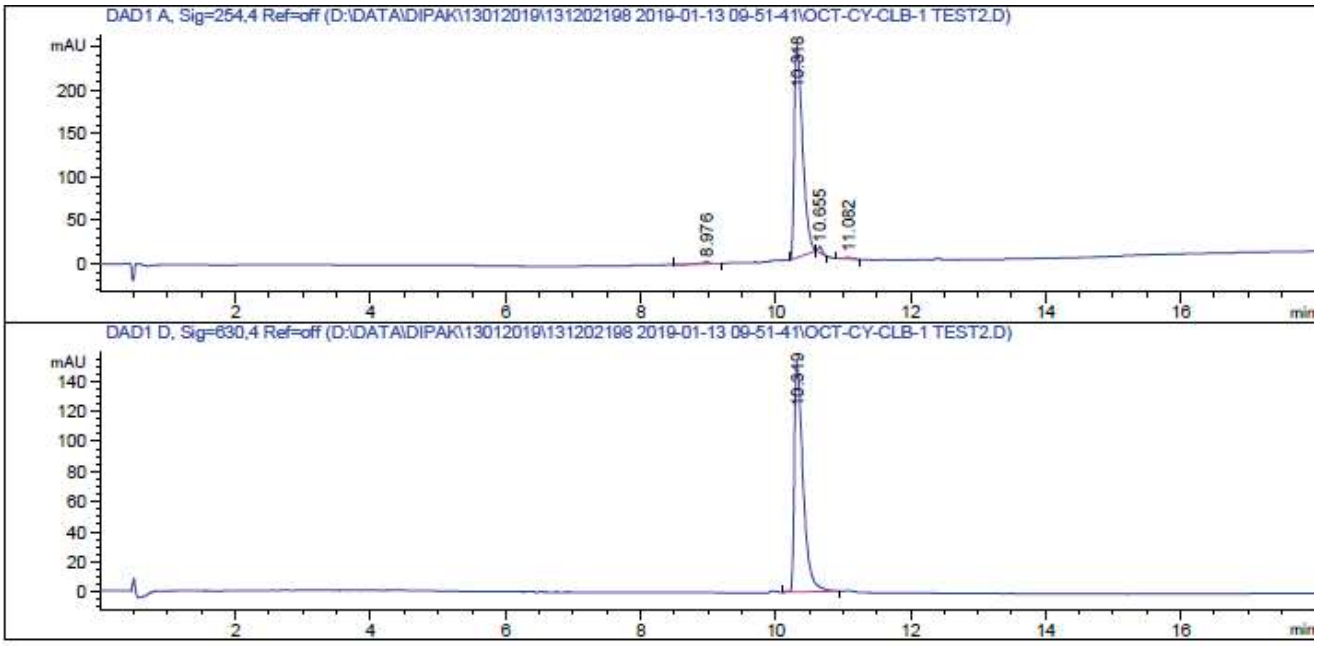


Fig. S15 HRMS spectrum of **5-CLB.**



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                          Area Percent Report
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Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Do not use Multiplier & Dilution Factor with ISTDs


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Peak RetTime Type  Width     Area      Height     Area
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----|-------|----|-------|----------|----------|--------|
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Fig. S16 HPLC chromatogram of **5-CLB.**

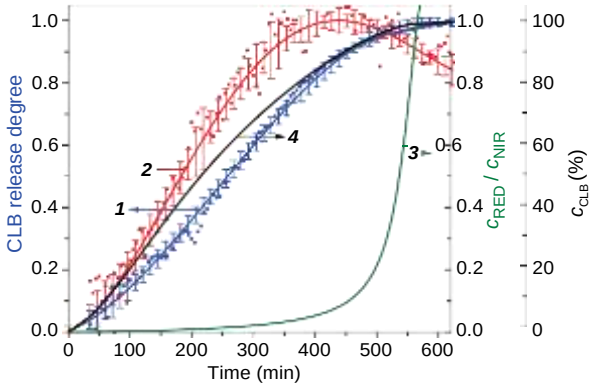

Fig. S17 The change of the **CLB** release degree in Panc-1 cell line over time, which was calculated on the base of the drug cleavage profile (Drug Degree = $c_{CLB}/c_{5\text{-}CLB} = 1 - B_{NIR}$, Fig. 6) as the normalized ratio between the number of the released **CLB** molecules and the number of **5-CLB** conjugates in the sample (mean ± standard error for three independent experiments). 2 – Increase of the relative concentration of **RD** ($c_{RD} = B_{Red}$) (mean ± standard error for three independent experiments). 3 – Ratiometric curve ($c_{RD}/c_{5\text{-}CLB} = B_{Red}/B_{NIR}$). 4 – Relative concentration of free **CLB** molecules calculated as $c_{CLB} = [B_{Red}/(B_{Red} + B_{NIR})] \times 100\%$.

