## **Supporting Information**

# Bioluminescence imaging of carbon monoxide in cancer cells based on a selective deiodination reaction

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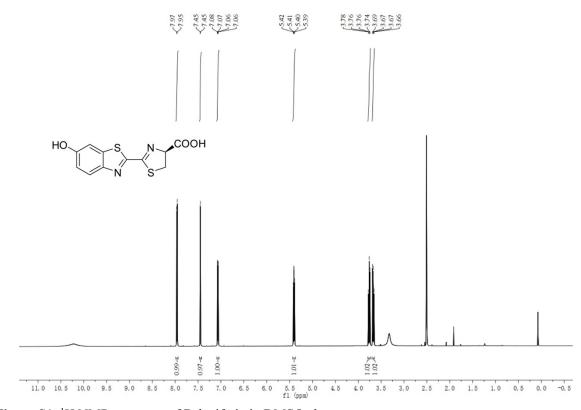
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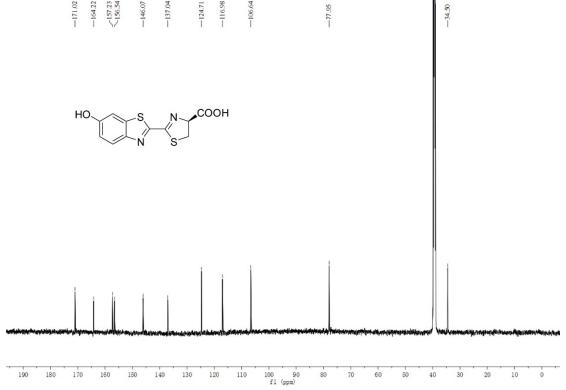
#### 1. Cell culture

HEK 293T cells were purchased from the Committee on Type Culture Collection of Chinese Academy of Sciences. Huh7 (human liver cancers cell line) cells expressing firefly luciferase were supplied by Cellcyto.

#### 2. NMR and MS spectra of D-luciferin



**Figure S1.** <sup>1</sup>H NMR spectrum of D-luciferin in DMSO- $d_6$ .



**Figure S2.**  $^{13}$ C NMR spectrum of D-luciferin in DMSO- $d_6$ .

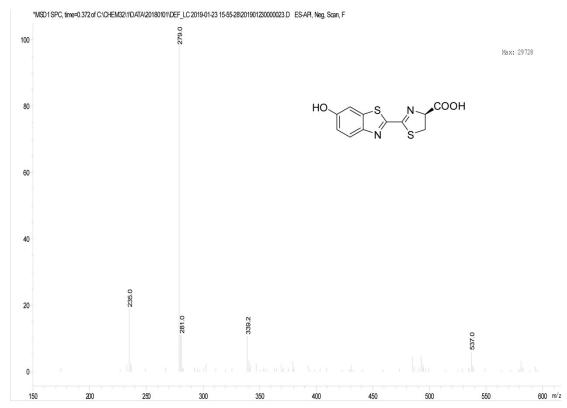


Figure S3. Mass spectrum of D-luciferin.

### 1. NMR and MS spectra of 7'-iodo-luciferin

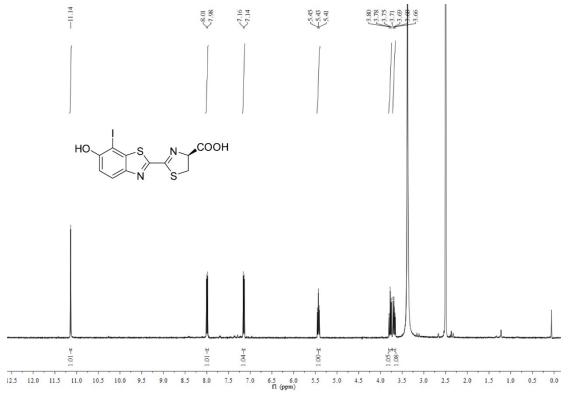
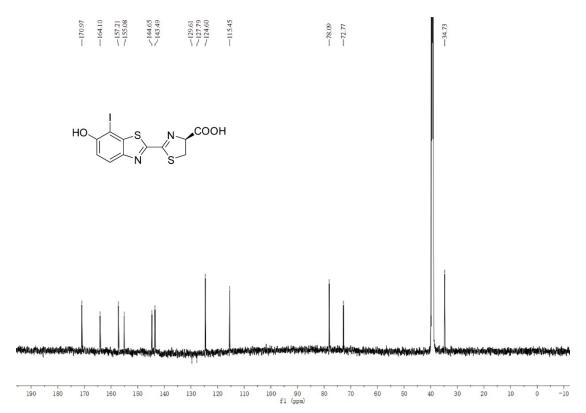


Figure S4. <sup>1</sup>H NMR spectrum of 7'-iodo-luciferin in DMSO- $d_6$ .



**Figure S5.**  $^{13}$ C NMR spectrum of 7'-iodo-luciferin in DMSO- $d_6$ .

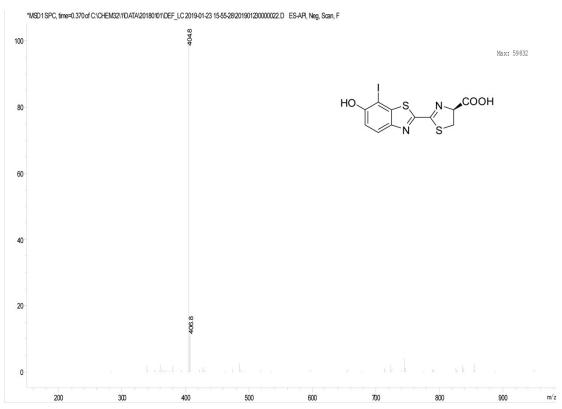


Figure S6. Mass spectrum of 7'-iodo-luciferin.