Supporting Information

# High-Efficiency Dynamic Sensing of Biothiols in Cancer Cells with a Fluorescent β-Cyclodextrin Supramolecular Assembly

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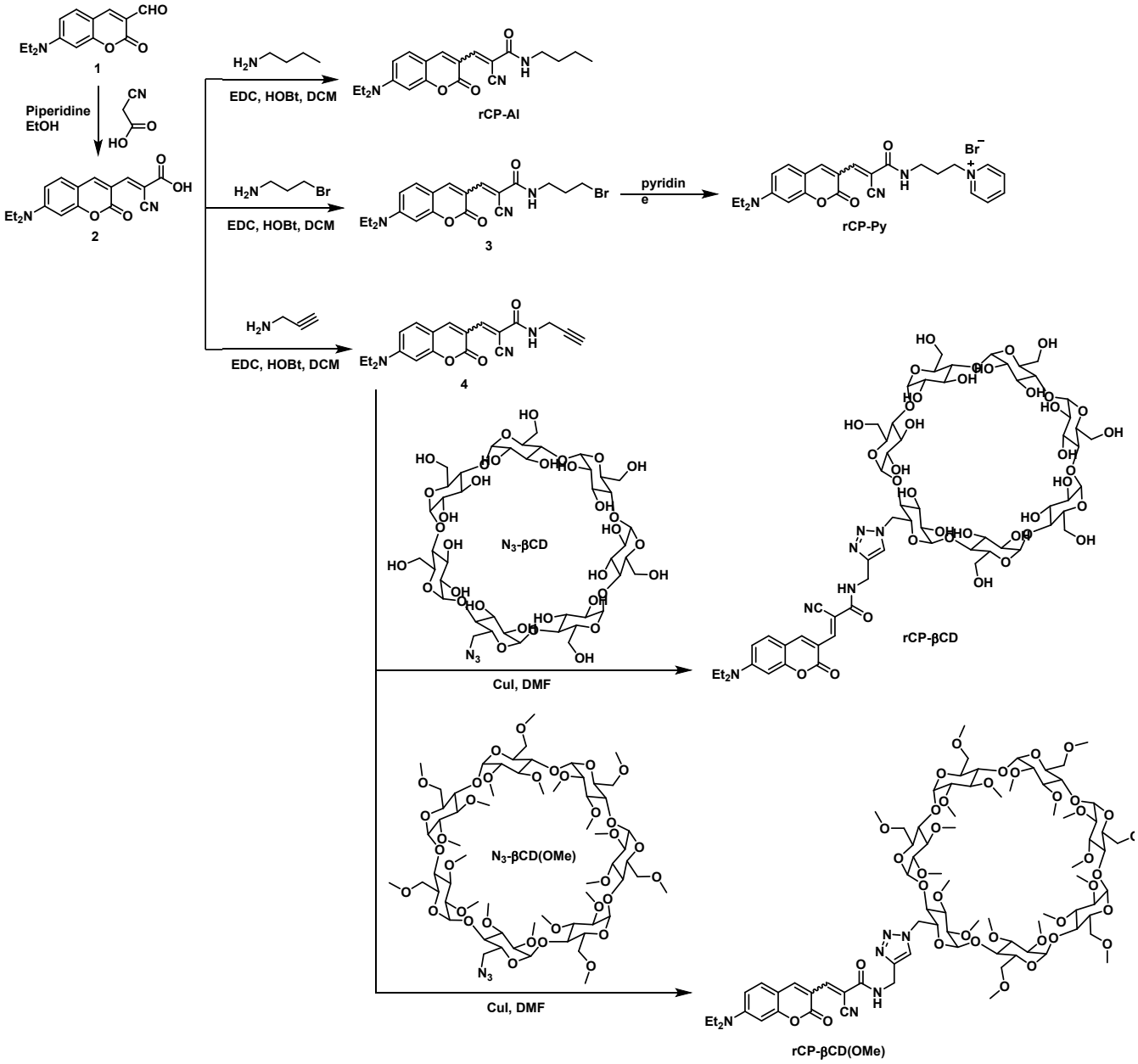
## 1. Synthesis




**Scheme S1**. Synthesis of **rCP-AI**, **rCP-Py**, **rCP-βCD** and **rCP-βCD (OMe)**.

**Compound 1**

Starting compound **1** was synthesized according to the reported procedure. [1]

**Compound 2**

To a solution of compound **1** (200 mg, 0.82 mmol) in absolute ethyl alcohol, 2-cyanoacetic acid (138.9 mg, 1.63 mmol) and piperidine (16.2 μL, 0.16 mmol) were added, and the reaction mixture was refluxed for 6 hours. Cooling to room temperature to obtain a large amount of precipitate, filtered and recrystallized in absolute ethyl alcohol to afford compound **2** (166.4 mg, 65%) as a dark green solid. $^{1}$H NMR (300 MHz, DMSO) δ 13.70 (s, 1H), 8.74 (s, 1H), 8.23 (s, 1H), 7.59 (d, J = 9.1 Hz, 1H), 6.82 (dd, J = 9.1, 2.3 Hz, 1H), 6.63 (d, J = 2.1 Hz, 1H), 3.53 (q, J = 6.9 Hz, 6H), 1.16 (t, J = 7.0 Hz, 6H).

$^{13}$C NMR (75 MHz, $CDCl_3$) δ 164.16, 160.69, 157.96, 153.85, 147.34, 144.31, 132.75, 117.18, 111.17, 110.04, 108.47, 97.08, 45.1, 12.87. HRMS-ESI (m/z): $[M-H]^-$ calcd for $C_{17}H_{16}N_2O_4$: 311.1115; found: 311.1035.

**Compound rCP-AI**

Compound **2** (350 mg, 1.12 mmol), EDC (214.7 mg, 1.12 mmol) and HOBt (151.3 mg, 1.12 mmol) were dissolved in anhydrous DCM and the solution was stirred at room temperature for 30 min. After that, n-butylamine (68.2 mg, 0.93 mmol) in DCM was added, and the reaction mixture was stirred overnight, quenched with water. The aqueous solution was extracted with DCM, and the combined organic phase was washed with brine, dried over $MgSO_4$, filtered and evaporated. The resultant residue was purified by slica column chromatography to afford **rCP-AI** (411.2 mg, 73%) as a red solid.

$^1$H NMR (400 MHz, DMSO) δ 8.67 (s, 1H), 8.36 (s, 1H), 8.12 (s, 1H), 7.59 (d, J = 9.0 Hz, 1H), 6.82 (d, J = 8.3 Hz, 1H), 6.63 (s, 1H), 3.56-3.47 (m, 4H), 3.15-3.24 (m, 2H), 1.55 – 1.42 (m, 2H), 1.29 (dd, J = 14.5, 7.2 Hz, 2H), 1.15 (t, J = 6.8 Hz, 6H), 0.89 (t, J = 7.2 Hz, 3H).
$^{13}$C NMR (100 MHz, DMSO) δ 160.76, 160.15, 157.07, 152.78, 143.59, 143.19, 131.72, 116.68, 110.31, 107.66, 102.99, 99.42, 96.46, 44.44, 30.92, 19.45, 13.58, 12.29. HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{21}H_{25}N_3NaO_3$: 390.1788; found: 390.1791.

**Compound 3**

Compound **2** (400 mg, 1.28 mmol), EDC (245.7 mg, 1.28 mmol) and HOBt (172.9 mg, 1.28 mmol) were dissolved in anhydrous DCM and the solution was stirred at room temperature for 30 min. After that, 3-bromopropylamine hydrobromide (233.8 mg, 1.07 mmol) with two drops of triethylamine in DCM was added, and the reaction mixture was stirred overnight, quenched with water. The aqueous solution was extracted with DCM, and the combined organic phase was washed with brine, dried over $MgSO_4$, filtered and evaporated. The resultant residue was purified by slica column chromatography to afford compound **3** (375.2 mg, 68%) as a red solid.
$^1$H NMR (400 MHz, DMSO) δ 8.68 (s, 1H), 8.49 (s, 1H), 8.14 (s, 1H), 7.60 (d, J = 9.0 Hz, 1H), 6.82 (d, J = 9.0 Hz, 1H), 6.64 (s, 1H), 3.68 – 3.44 (m, 6H), 3.42 – 3.26 (m, 2H), 2.05 (m, 2H), 1.15 (t, J = 7.0 Hz, 6H).
$^{13}$C NMR (100 MHz, DMSO) δ 161.03, 160.07, 157.03, 152.76, 143.72, 143.17, 131.69, 116.57, 110.27, 110.10, 107.60, 102.59, 96.39, 44.38, 38.28, 32.17, 31.95, 12.22. HRMS-ESI (m/z): $[M+Na]^+$ calcd for $C_{20}H_{22}BrN_3O_3$: 454.0839; found: 454.0740.

**Compound rCP-Py**

Compound **3** (200 mg) was dissolved in pyridine and the solution was stirred was stirred at 80 °C for 1 hour. Cooling to room temperature, and added petroleum ether to precipitate solid, filtered and dried to afford compound **rCP-Py** (213 mg, 90%) as a deep rose solid.
$^1$H NMR (400 MHz, DMSO) δ 9.14 (d, J = 5.6 Hz, 2H), 8.69 (s, 1H), 8.62 (t, J = 7.5 Hz, 1H), 8.47 (s, 1H), 8.24 - 8.14 (m, 3H), 7.61 (d, J = 9.0 Hz, 1H), 6.83 (d, J = 8.9 Hz, 1H), 6.64 (s, 1H), 4.66 (t, J = 6.9 Hz, 2H), 3.53 (d, J = 6.9 Hz, 4H), 3.29 (d, J = 5.8 Hz, 2H), 2.26 - 2.14 (t, J = 6.4 Hz, 2H), 1.16 (t, J = 6.8 Hz, 6H).
$^{13}$C NMR (100 MHz, DMSO) δ 161.76, 160.75, 157.71, 153.47, 146.01, 145.42, 144.60, 143.84, 132.45, 128.50, 117.24, 110.99, 110.53, 108.26, 102.67, 97.02, 59.30, 45.04, 37.02, 31.10, 12.87. HRMS-ESI (m/z): $[M]^+$ calcd for $C_{25}H_{27}N_4O_3^+$: 431.2072; found: 431.2081.

**Compound 4**

Compound **2** (300 mg, 0.96 mmol), EDC (184.0 mg, 0.96 mmol) and HOBt (129.7 mg, 0.96 mmol) were dissolved in anhydrous DCM and the solution was stirred at room temperature for 30 min. After that, mono-propargylamine (44.1 mg, 0.80 mmol) in DCM was added, and the reaction mixture was stirred overnight, quenched with water. The aqueous solution was extracted with DMC, and the combined organic phase was washed with brine, dried over $MgSO_4$, filtered and evaporated. The resultant residue was purified by slica column chromatography to afford compound **4** (167.5 mg, 50%) as a red solid.
$^1$H NMR (400 MHz, DMSO) δ 8.86 (t, J = 5.5 Hz, 1H), 8.69 (s, 1H), 8.16 (s, 1H), 7.60 (d, J = 9.1 Hz, 1H), 6.83 (d, J = 9.1, 1H), 6.63 (s, 1H), 3.97 (d, J = 5.5, 2H), 3.52 (q, J = 7.1 Hz, 4H), 3.15 (t, J = 2.4 Hz, 1H), 1.16 (t, J = 7.0 Hz, 6H).
$^{13}$C NMR (100 MHz, DMSO) δ 160.91, 160.10, 157.16, 152.94, 144.29, 143.38, 131.85, 116.50, 110.40, 109.99, 107.71, 101.87, 96.47, 80.68, 72.95, 55.94, 44.48, 29.01, 18.47, 12.29. HRMS-ESI (m/z): $[M+H]^+$ calcd for $C_{20}H_{19}N_3O_3$: 350.1426; found: 350.1506.

**Compound $N_3$-βCD**

Compound **$N_3$-βCD** was synthesized according to the reported procedure. [2]

**Compound rCP-βCD**

Compound **4** (57.5 mg, 0.16 mmol), **$N_3$-βCD** (185.5 mg, 0.16 mmol) and CuI (30.4 mg, 0.16 mmol) were dissolved in anhydrous DMF under nitrogen protection and the solution was stirred at 80 °C for 6 hours. After that, filtered and evaporated, and the resultant residue was purified by silica gel chromatography to afford **rCP-βCD** (160.9 mg, 66%) as a red solid.
$^1$H NMR (400 MHz, DMSO) δ 8.87 (s, 1H), 8.69 (s, 1H), 8.17 (s, 1H), 7.96 (s, 1H), 7.60 (d, J = 7.9 Hz, 1H), 6.82 (d, J = 8.8 Hz, 1H), 6.64 (s, 1H), 5.98 – 5.61 (m, 16H), 4.84 (s, 7H), 4.65 – 4.41 (m, 8H), 3.84 – 3.46 (m, 33H), 1.15 (t, J = 6.3 Hz, 6H).
$^{13}$C NMR (100 MHz, DMSO) δ 161.60, 160.70, 157.71, 153.44. 144.63, 144.41, 143.95, 132.39, 124.88, 117.15, 110.94, 110.72, 108.26, 103.06, 102.40, 97.04, 83.75, 81.99, 73.49, 72.87, 70.50, 70.38, 60.35, 45.02, 26.83, 12.85.
HRMS-MALDI (m/z): $[M+Na]^+$ calcd for $C_{62}H_{88}N_6O_{37}$: 1531.5081; found: 1531.5085.

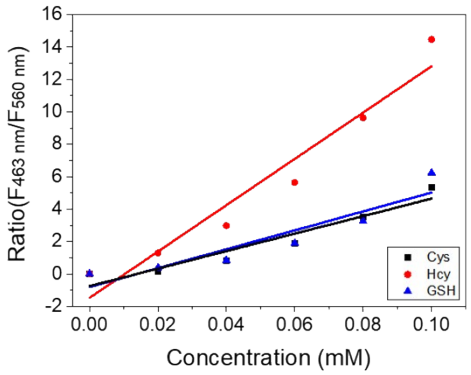
**Compound $N_3$-βCD(OMe)**

Compound **$N_3$-βCD(OMe)** was synthesized according to the reported procedure.[3]

**Compound rCP-βCD(OMe)**

Compound **4** (86.0 mg, 0.25 mmol), **$N_3$-βCD(OMe)** (354.6 mg, 0.25 mmol) and CuI (47.6 mg, 0.25 mmol) were dissolved in anhydrous DMF under nitrogen protection and the solution was stirred at 80 °C for 6 hours. After that, filtered and evaporated, and the resultant residue was purified by silica gel chromatography to afford **rCP-βCD(OMe)** (110 mg, 25%) as a red solid.
$^1$H NMR (400 MHz, $CDCl_3$) δ 8.68 (s, 1H), 8.54 (s, 1H), 7.67 (s, 1H), 7.36 (d, J = 9.0 Hz, 1H), 6.83 (s, 1H), 6.61 (d, J = 9.1 Hz, 1H), 6.44 (s, 1H), 5.27 (s, 1H), 5.17 – 5.06 (m, 5H), 4.87 (m, 1H), 4.78 (m, 1H), 4.64 (m, 1H), 4.11 – 2.98 (m, 104H), 1.23 (s, 6H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 160.81, 160.68, 157.86, 153.26, 146.26, 143.66, 143.37, 131.73, 124.87, 117.57, 111.28, 110.17, 108.51, 100.49, 99.19, 99.07, 98.95, 98.87, 98.08, 97.16, 82.76, 82.00, 81.93, 81.86, 81.73, 81.60, 81.07, 80.32, 80.25, 80.18, 79.93, 79.85, 79.17, 71.29, 71.21, 70.90, 70.78, 70.65, 70.26, 61.75, 61.50, 61.46, 61.40, 61.37, 61.33, 59.23, 59.15, 58.99, 58.90, 58.74, 58.66, 58.55, 58.44, 58.40, 58.37, 45.31, 12.49.
HRMS-MALDI (m/z): $[M+Na]^+$ calcd for $C_{62}H_{88}N_6O_{37}$: 1811.8211; found: 1811.8215.

## 2. UV/vis absorption and fluorescence spectroscopy




$R=0.96$
$y_{Cys}=53.9645x_{Cys}- 0.7476$ $LOD_{Cys}=122$ nM

$R=0.97$
$y_{Hcy}=142.8703x_{Hcy}- 1.4703$ $LOD_{Hcy}=46$ nM

$R=0.93$
$y_{GSH}=58.3367x_{GSH}- 0.8074$ $LOD_{GSH}=113$ nM

**Figure S1.** The line relationship between the fluorescent intensity ratio of the **rCP-βCD** (10 μM at 463 nm and 560 nm) and the concentration of the biothiols in PBS buffer (pH 7.4, 10 mM). Each spectrum was recorded after 3 min. ($\lambda_{ex}$= 405 nm. Slits: 2.5/5 nm; $\lambda_{ex}$= 485 nm. Slits: 5/5 nm)

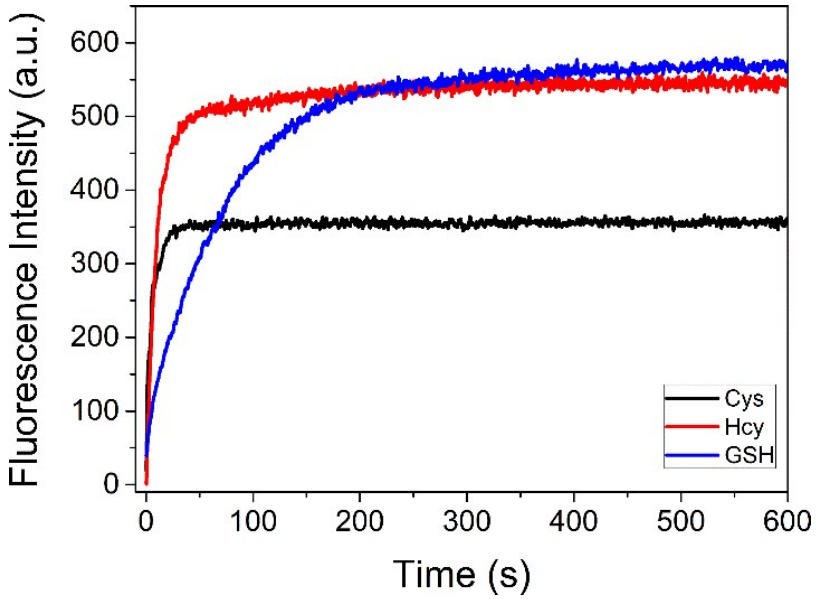



**Figure S2.** Time-dependence of fluorescence emission at 463 nm by **rCP-βCD** upon reaction with biothiols (0.5 mM) ($\lambda_{ex}$ = 405 nm; slits: 2.5/5 nm).

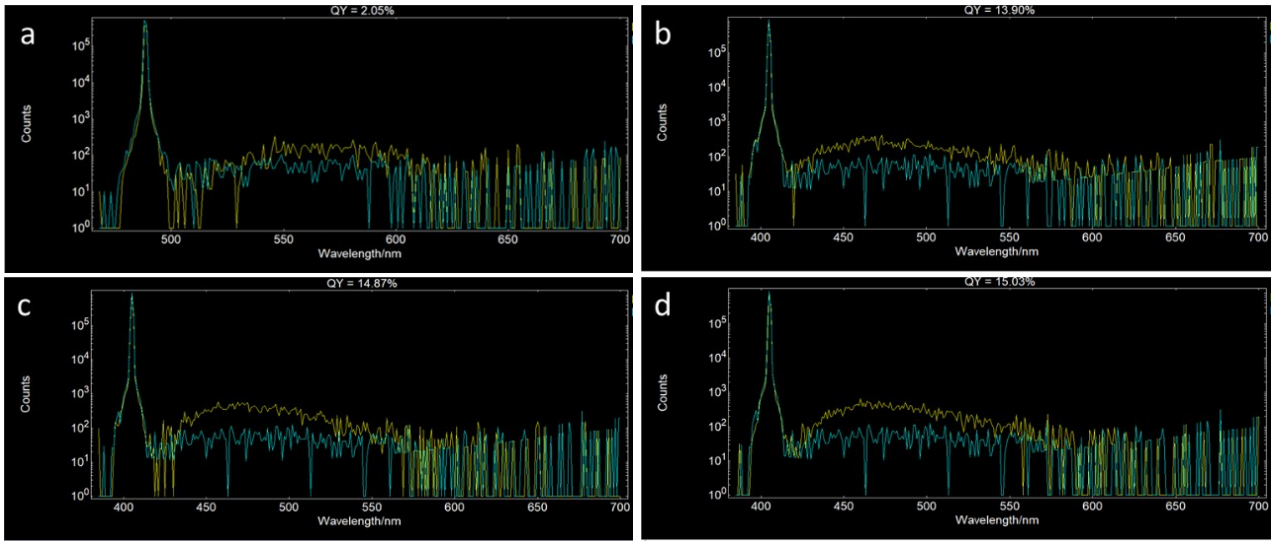



**Figure S3.** Quantum yields for **rCP-βCD** in 560 nm and related **rCP-βCD**+biothiols species in 463 nm in PBS buffer (pH 7.4, 10 mM) (a: **rCP-βCD**; b: **rCP-βCD**+Cys; c: **rCP-βCD**+Hcy; d: **rCP-βCD**+GSH).

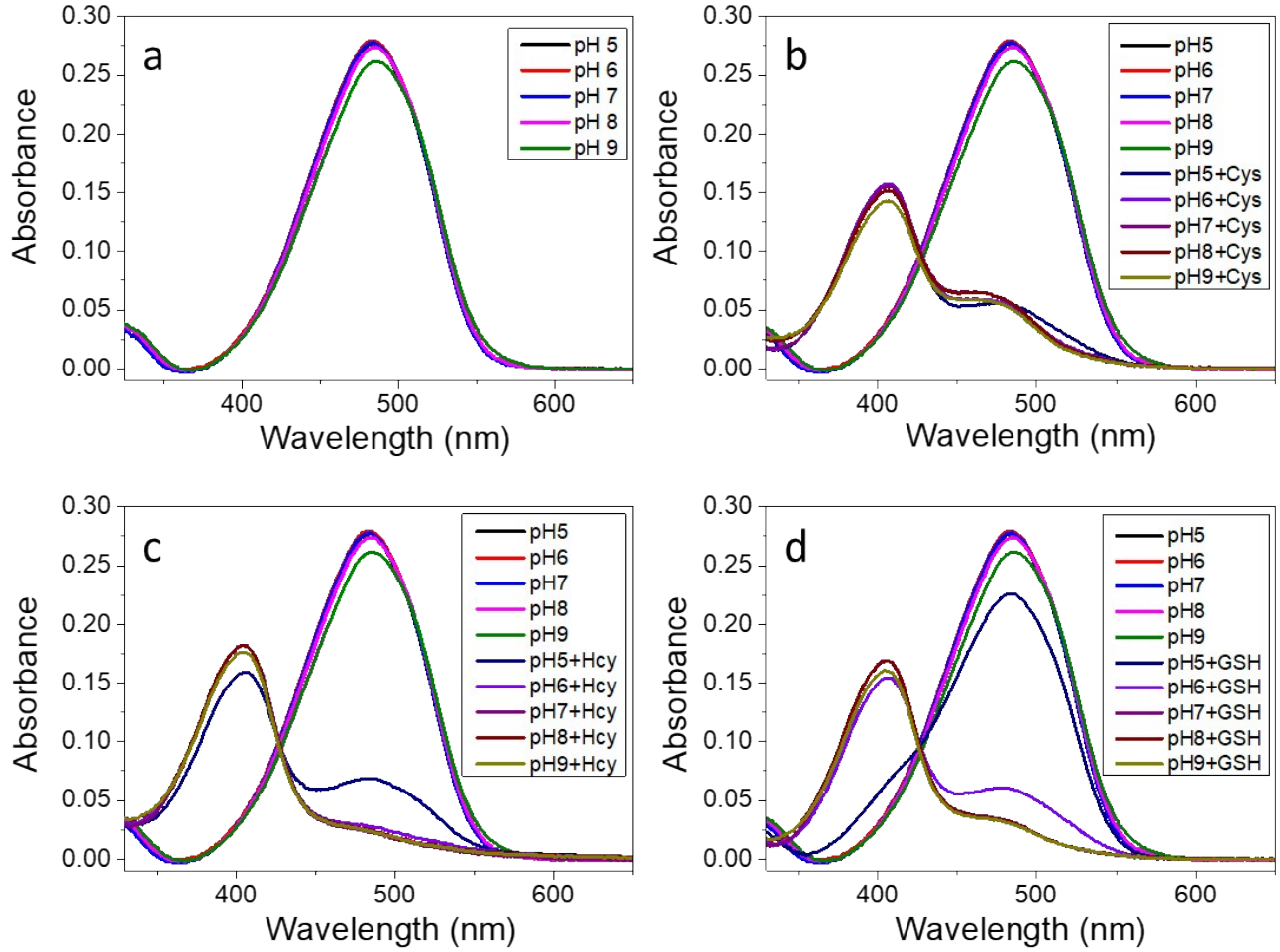



**Figure S4.** UV-vis absorption changes of **rCP-βCD** (10 μM) in the absence or prescence of biothiols (0.5 mM) in PBS buffer (10 mM) at varied pH values (5 - 9). (a) **rCP-βCD**; (b) **rCP-βCD**+Cys; **(c) rCP-βCD**+Hcy; (d) **rCP-βCD**+GSH.

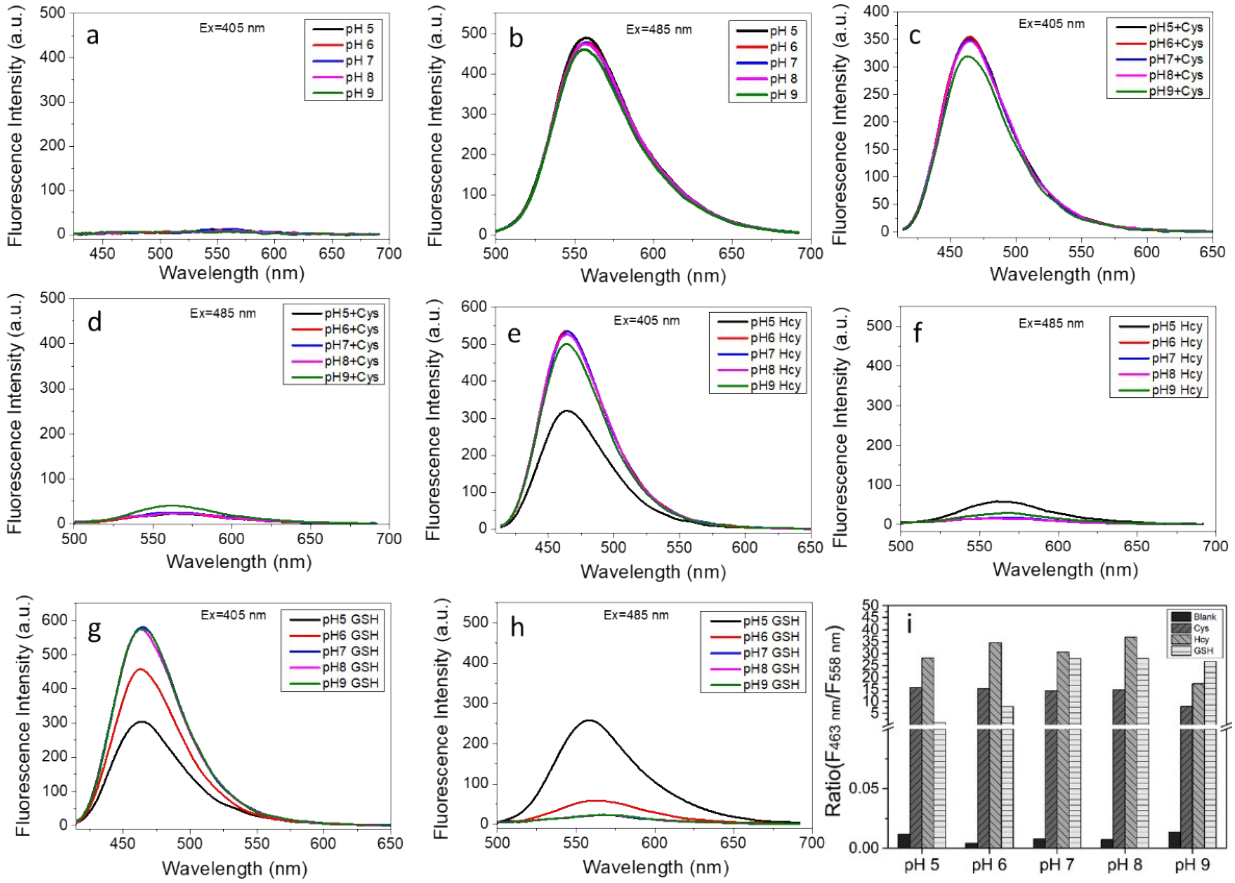



**Figure S5.** Fluorescence spectra changes of **rCP-βCD** (10 μM) with or without the presence of biothiols (0.5 mM) in PBS buffer (10 mM) at varied pH values (5 - 9). (a, b) **rCP-βCD**; (c, d) **rCP-βCD**+Cys; (e, f) **rCP-βCD**+Hcy; (g, h) **rCP-βCD**+GSH. (a, c, e, g: $\lambda_{ex}$ = 405 nm; slits: 2.5/5 nm; b, d, f, h:□$\lambda_{ex}$ = 485 nm; slits: 5/5 nm). (i) Ratios of fluorescence intensities at 463 and 560 nm for **rCP-βCD** in the absence or presence of biothiols (0.5 mM) at various pH values.

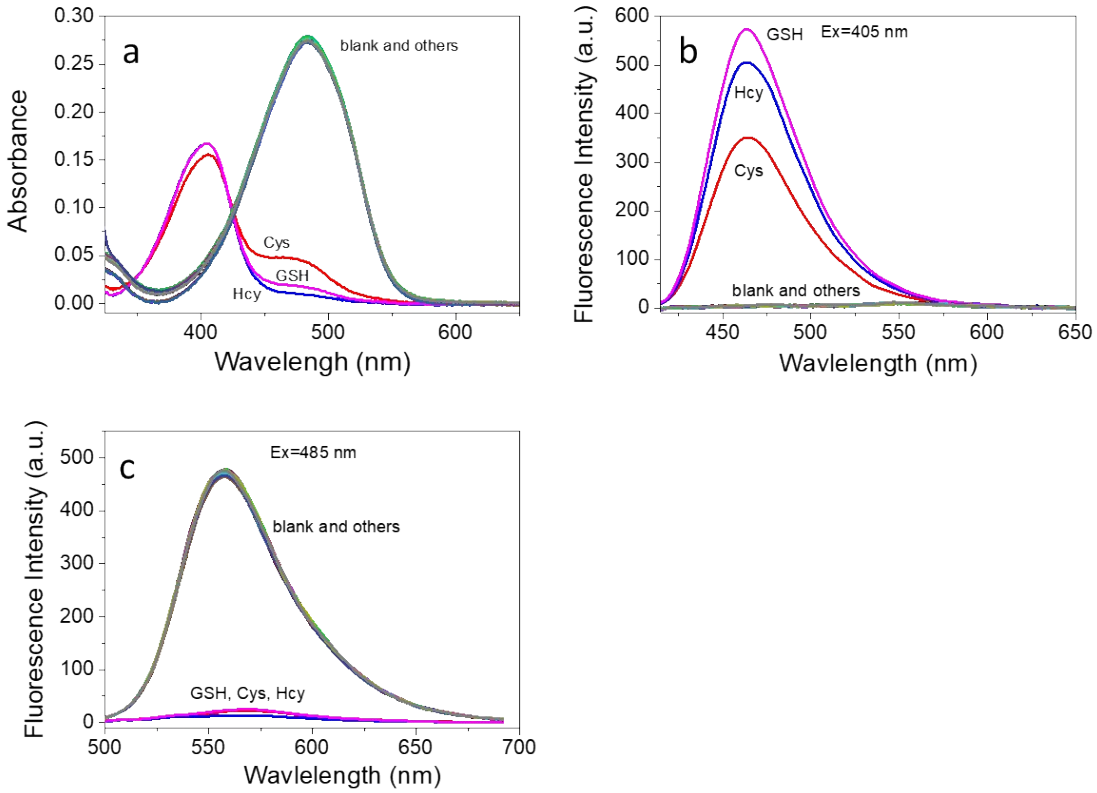



**Figure S6.** UV-vis absorption (a) and fluorescence spectra (b, c) after **rCP-βCD** equilibrated in PBS (pH 7.4, 10 mM) towards different coumpounds (Cys /Hcy /GSH for 0.5 mM, other amino acids for 1 mM, ROS/RNS for 0.1 mM). (b: $\lambda_{ex}$ = 405 nm; slits: 2.5/5 nm; c:□$\lambda_{ex}$ = 485 nm; slits: 5/5 nm)

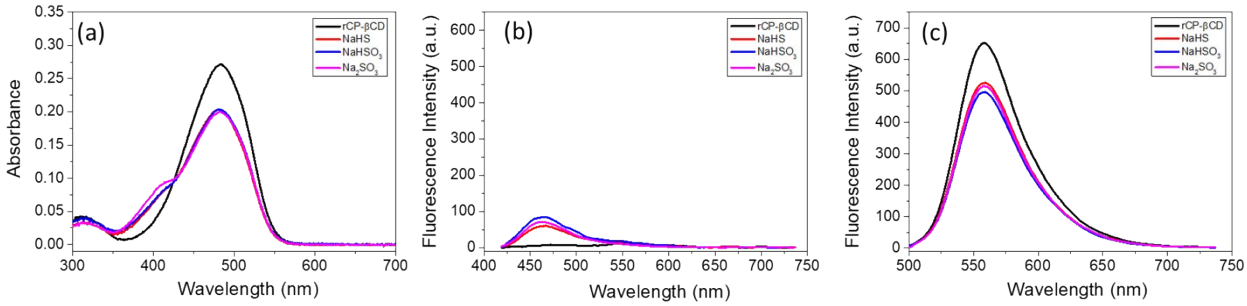



**Figure S7** UV−vis absorption spectrum (a) and fluorescence response (b, c) of **rCP-βCD** towards $Na_2S$, $NaHSO_3$ and $Na_2SO_3$ (0.1 mM) in PBS buffer (pH 7.4, 10 mM). Each spectrum was recorded after 3 min. (b: $\lambda_{ex}$ = 405 nm; slits: 2.5/ 5 nm; c: $\lambda_{ex}$ = 485 nm; slits: 5/ 5 nm).

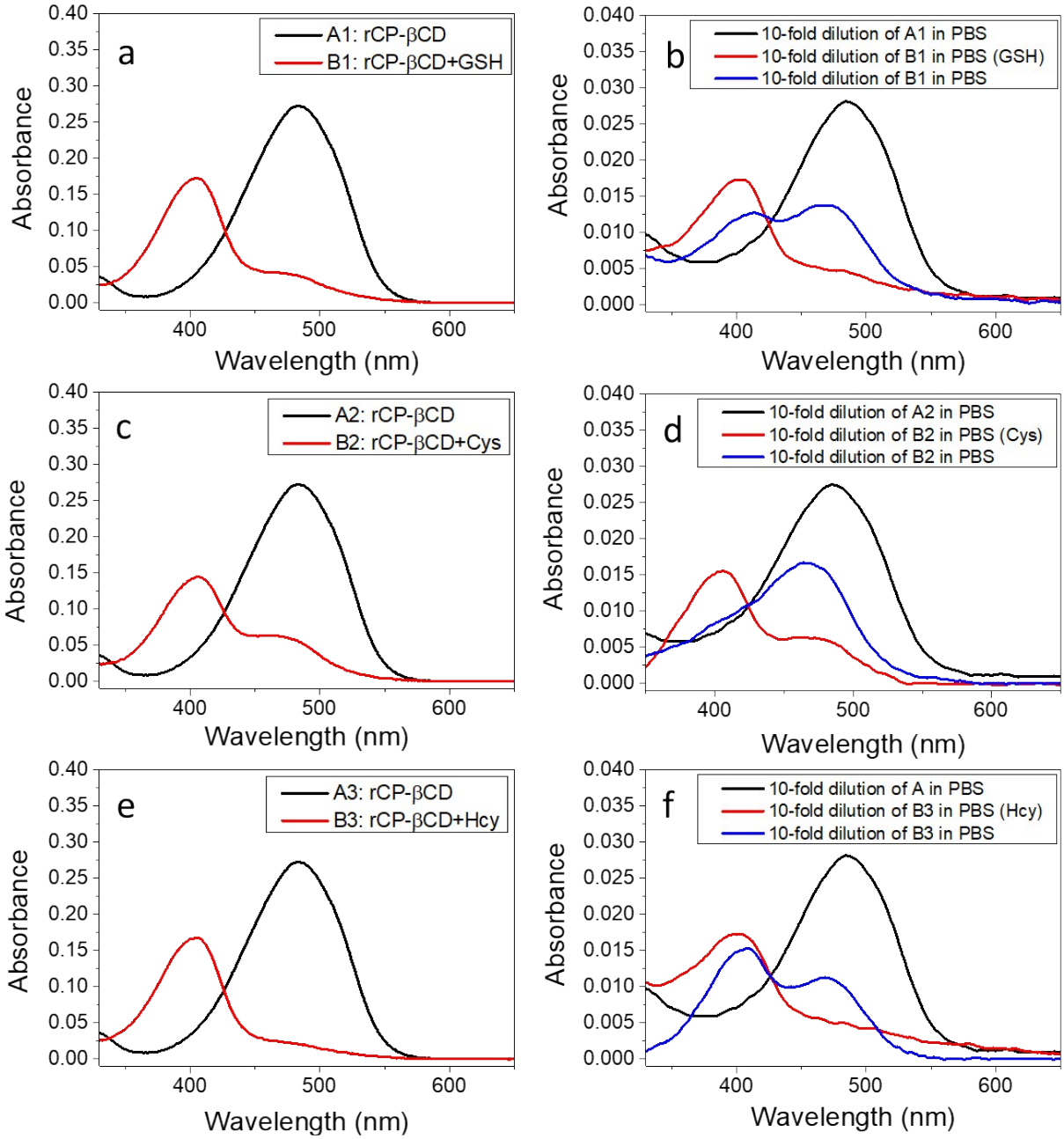



**Figure S8**. Dilution experiments of **rCP-βCD**+biothiols in PBS buffer (pH 7.4, 10 mM). (a, c, e) The absorption of **rCP-βCD** (10 μM) and **rCP-βCD**+biothiols (0.5 mM). (b, d, f) The initial mixture of a, c and e was diluted 10-fold into the buffer containing no (blue) or 0.5 mM biothiols (red), respectively.

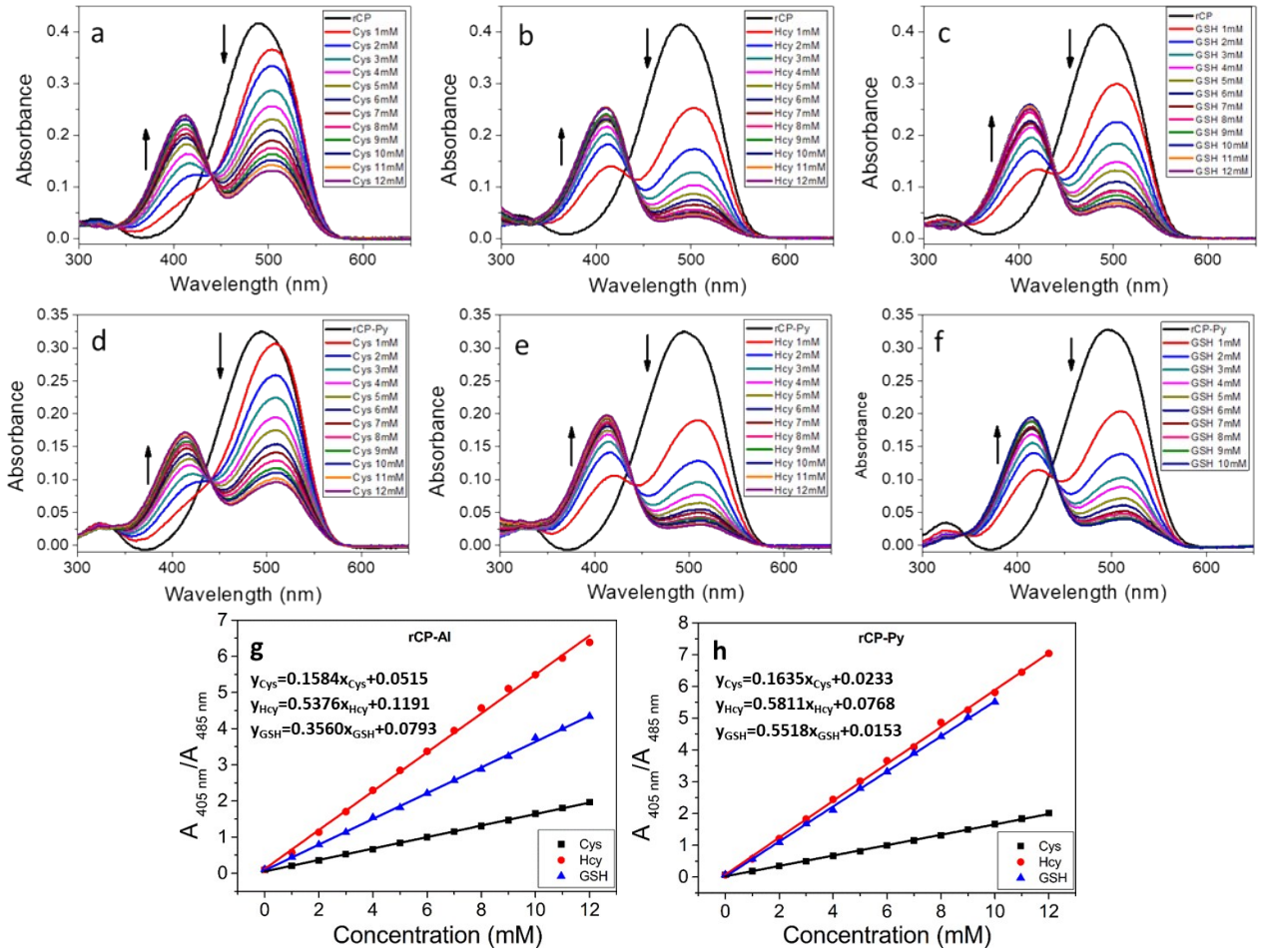



**Figure S9**. (a-f) UV-vis absorption changes of **rCP-Al** and **rCP-Py** (10 μM) upon addition of biothiols (0 - 12 mM). (g,h) Plots of UV−vis absorption peak ratios (A405 nm/A485 nm) for **rCP-Al** and **rCP-Py** as a function of biothiols concentration in PBS. The spectra were recorded 3 min after addition of the biothiols. Solvent: PBS (pH 7.4, 100 mM, containing 15% DMSO for **rCP-Al** and 1% DMSO for **rCP-Py** as a co-solvent).

**Table S1.** $K_d$ values of synthesized compounds towards biothiols (Cys[a], Hcy[b], GSH[c])

| | **rCP-Al** | **rCP-Py** | **rCP-βCD** | **rCP-βCD@ADA** | **rCP-βCD(OMe)** |
|---|---|---|---|---|---|
| $K_d$ (mM) | 6.313[a] | 6.116 [a] | 0.172 [a] | 0.327 [a] | 2.917 [a] |
| | 1.860[b] | 1.721 [b] | 0.027 [b] | 0.092 [b] | 0.631 [b] |
| | 2.809[c] | 1.812 [c] | 0.059 [c] | 0.168 [c] | 1.050 [c] |

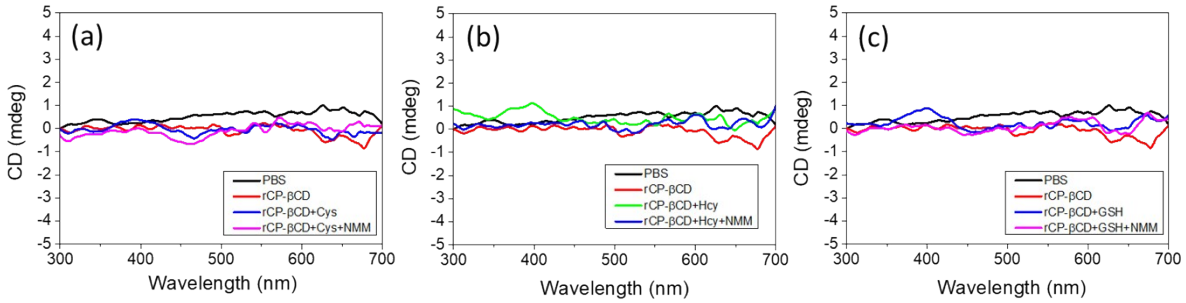



**Figure S10.** Circular dichroism spectra of **rCP-βCD** (10 μM) and **rCP-βCD**+biothiols (0.5 mM) in PBS buffer (pH 7.4, 10 mM).

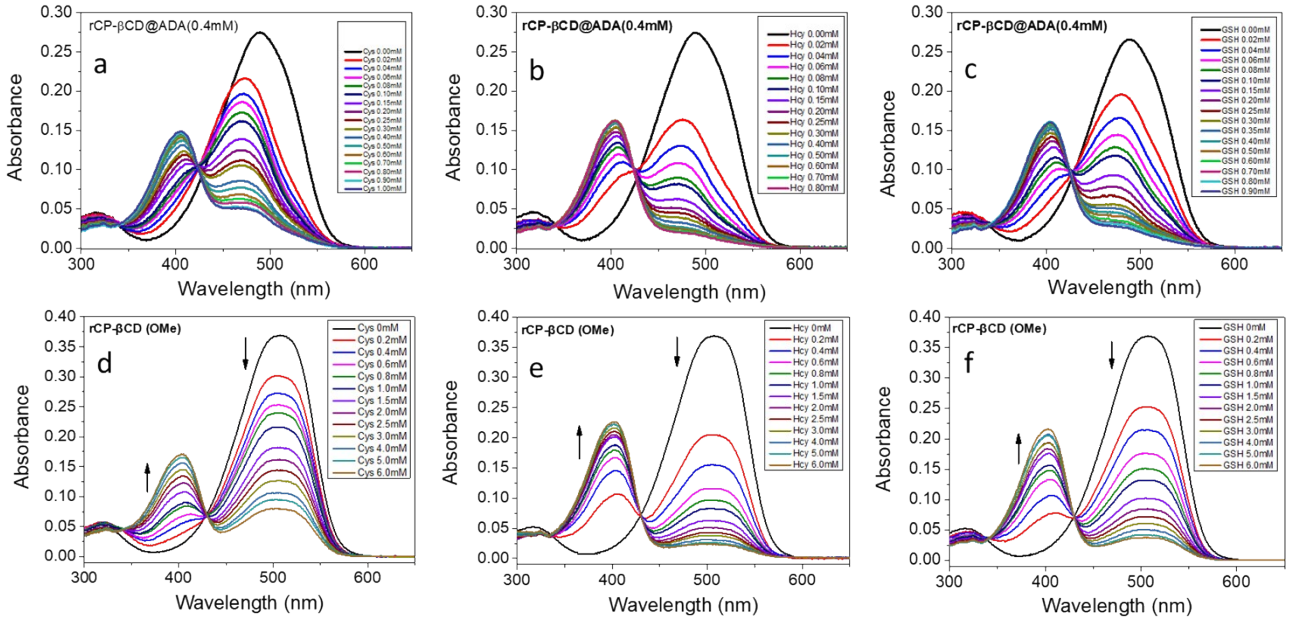



**Figure S11**. UV-vis absorption changes of **rCP-βCD@ADA/ rCP-βCD(OMe)** (10 μM) upon addition of biothiols in PBS buffer. (pH 7.4, 100 mM, containing 1% DMSO for **rCP-βCD(OMe)**); (pH 7.4, 10 mM, pure water solution for **rCP-βCD@ADA**)

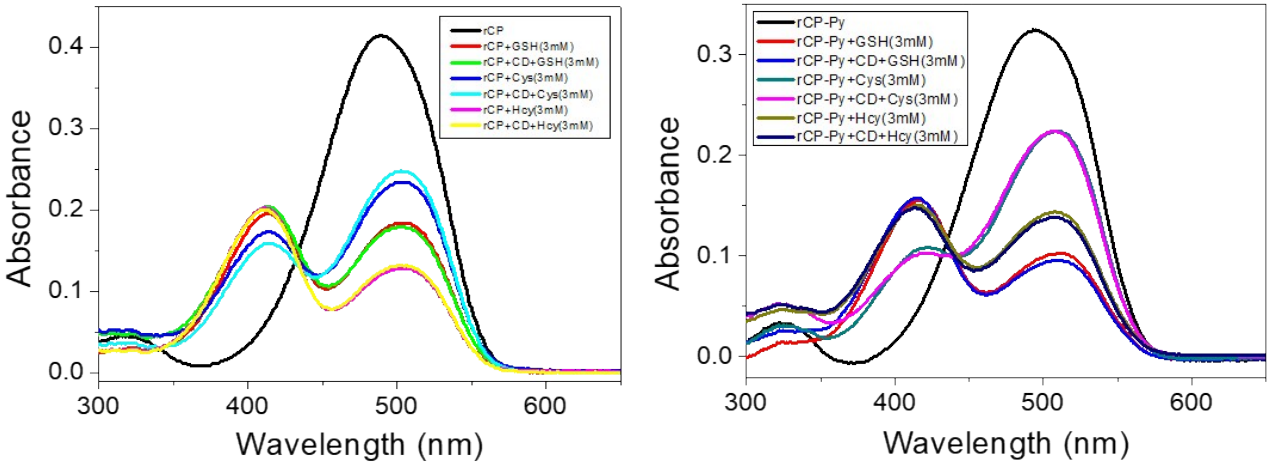



**Figure S12**. UV−vis absorption spectra changes of **rCP-Al/ rCP-Py** (10 μM) in the presence of β-CD (10 μM) upon addition of biothiols (3 mM) in PBS buffer (pH 7.4, 10 mM).

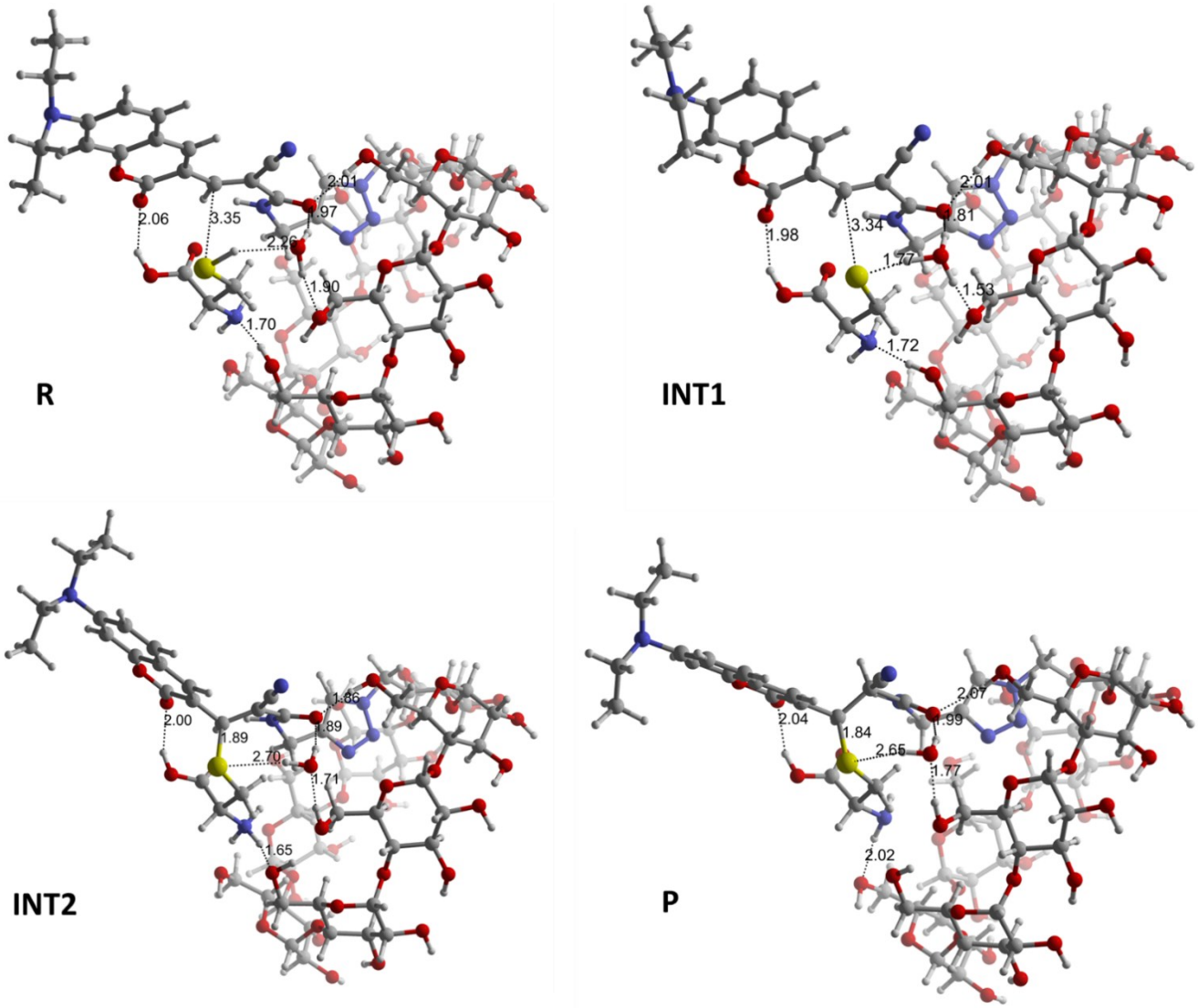



**Figure S13**. Optimized geometries of the stationary points involved in the addition reaction (Distances are given in Å).

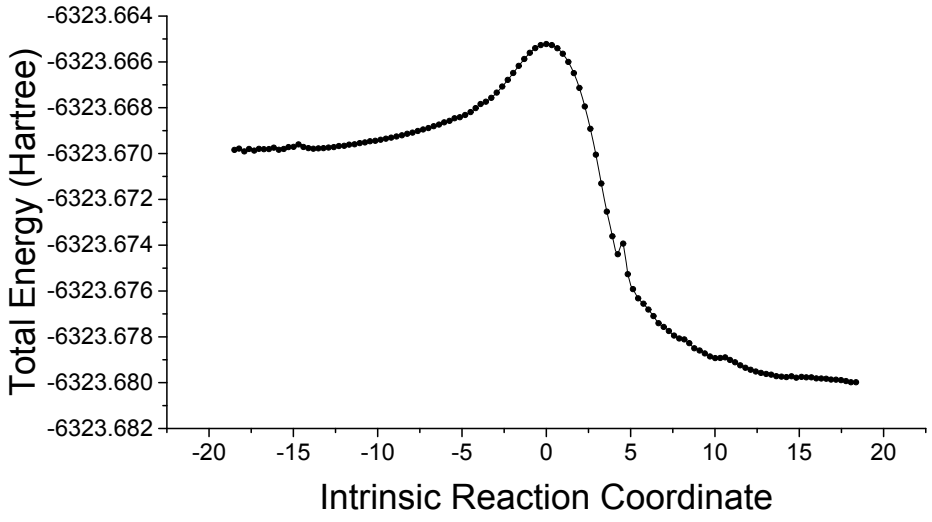



**Figure S14**. IRC points of **TS**.

**Table S2.** The single-point energies (SPE), thermal corrections (δG), Gibbs free energies (G) and imaginary frequency (f) of all optimized structures on the potential energy surface. All energies are in hartree, and frequencies are $cm^{-1}$.

| Structures | SPE[a] | δG[b] | G | f |
|---|---|---|---|---|
| R | -6325.646210 | 1.592502 | -6324.053708 | none |
| INT1 | -6325.627035 | 1.590487 | -6324.036548 | none |
| TS | -6325.620273 | 1.596318 | -6324.023955 | -150.23 |
| INT2 | -6325.653026 | 1.599697 | -6324.053329 | none |
| P | -6325.655807 | 1.592197 | -6324.063610 | none |

a. Calculations at the M06-2X-D3/6-311+G(df,pd)//$SMD_{water}$ level.
b. Calculations at the M06-2X-D3/6-31G(d,p)//$SMD_{water}$ level.

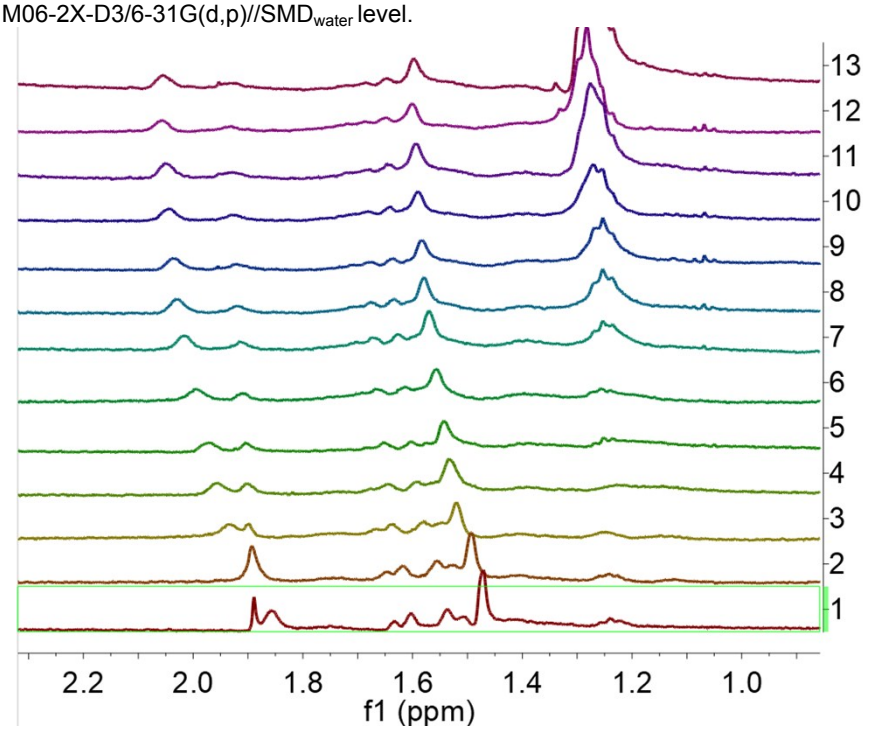



**Figure S15.** $^1H$ NMR spectra of **cRGD-ADA** (0.5 mM) with addition of 0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.75, 1.0, 1.25, 1.5, 2.0, 2.5, 3.0 mM **rCP-βCD** (spectra from 1 to 13) in $D_2O$.

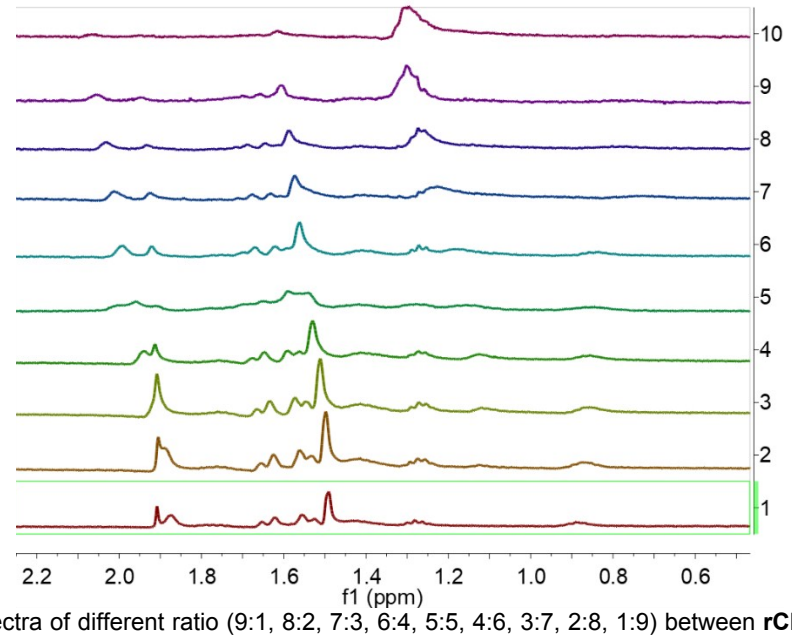



**Figure S16.** $^1H$ NMR spectra of different ratio (9:1, 8:2, 7:3, 6:4, 5:5, 4:6, 3:7, 2:8, 1:9) between **rCP-βCD** (1mM) and **cRGD-ADA** (1mM) (spectra from 2 to 10) and **cRGD-ADA** (spectrum 1) in $D_2O$.

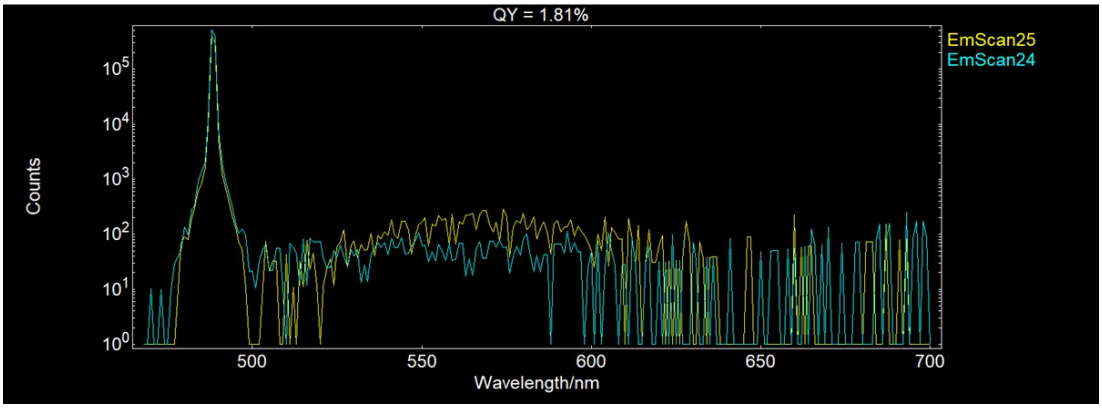



**Figure S17.** Quantum yields for **rCP-βCD@cRGD-ADA** in 560 nm in PBS buffer (pH 7.4, 10 mM).

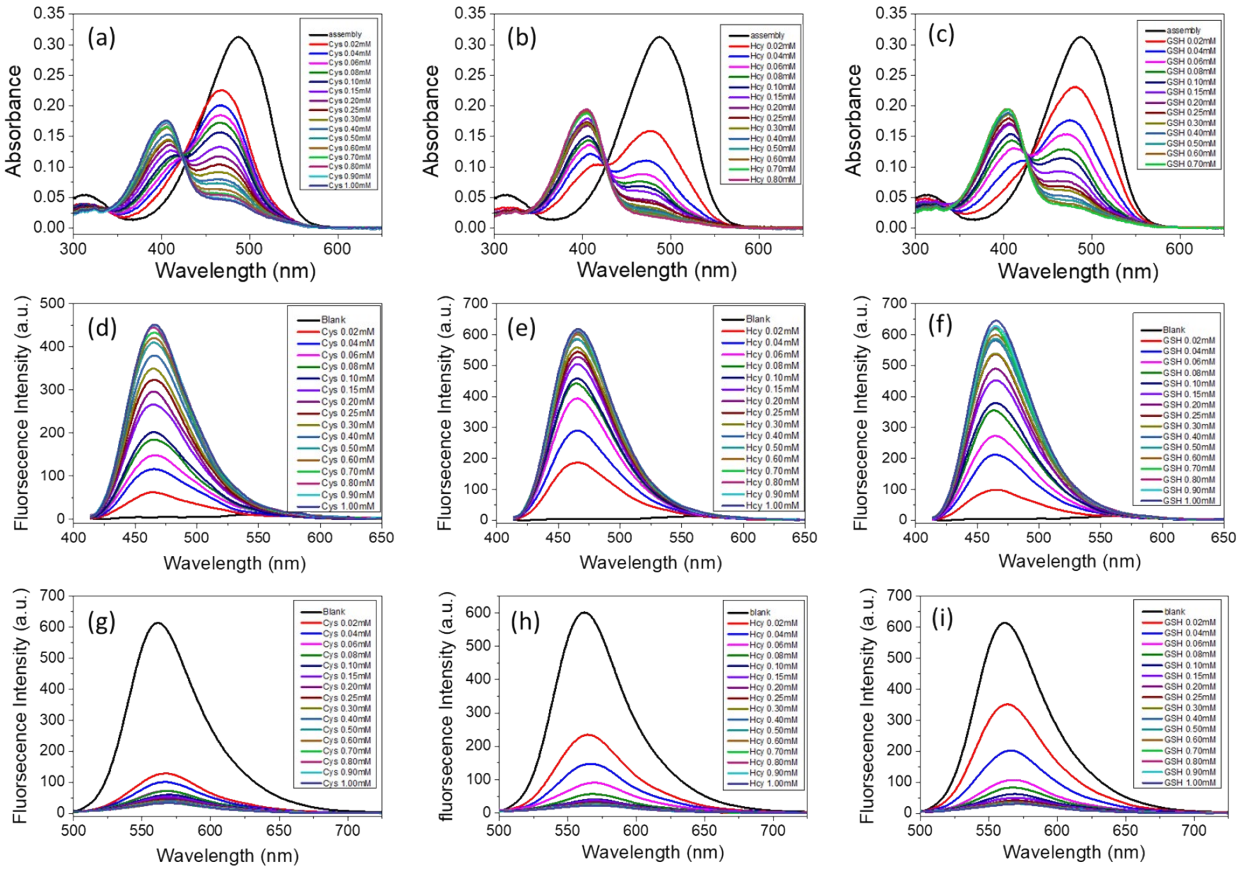



**Figure S18.** (a-c) UV-vis absorption changes of **rCP-βCD@cRGD-ADA** (10 μM) upon addition of biothiols. (d-f) Fluorescence response of **rCP-βCD@cRGD-ADA** upon gradual addition of biothiols (d-e: $\lambda_{ex}$ = 405 nm; slits: 2.5/ 5 nm; g-i: $\lambda_{ex}$ = 485 nm; slits: 5/ 5 nm). Solvent: PBS (pH 7.4, 10 mM).

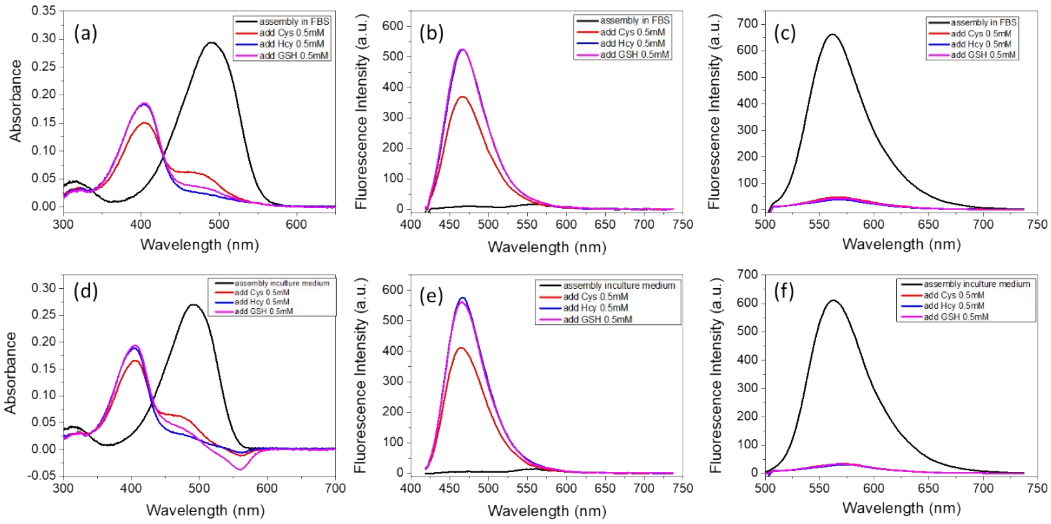



**Figure S19** The detection performance of **rCP-βCD@cRGD-ADA** towards biothiols in FBS and F12 culture medium. UV-vis absorption changes of **rCP-βCD@cRGD-ADA** (10 μM) upon addition of biothiols (0.5 mM) in (a) 10% FBS buffer and (d) culture medium (containing 10% FBS and 1% penicillin-streptomycin). (b, c, e, f) Fluorescence responses of **rCP-βCD@cRGD-ADA** (10 μM) upon addition of biothiols (0.5 mM). (b, e: $\lambda_{ex}$ = 405 nm; slits: 2.5/ 5 nm; c, f: $\lambda_{ex}$ = 485 nm; slits: 5/ 5 nm).

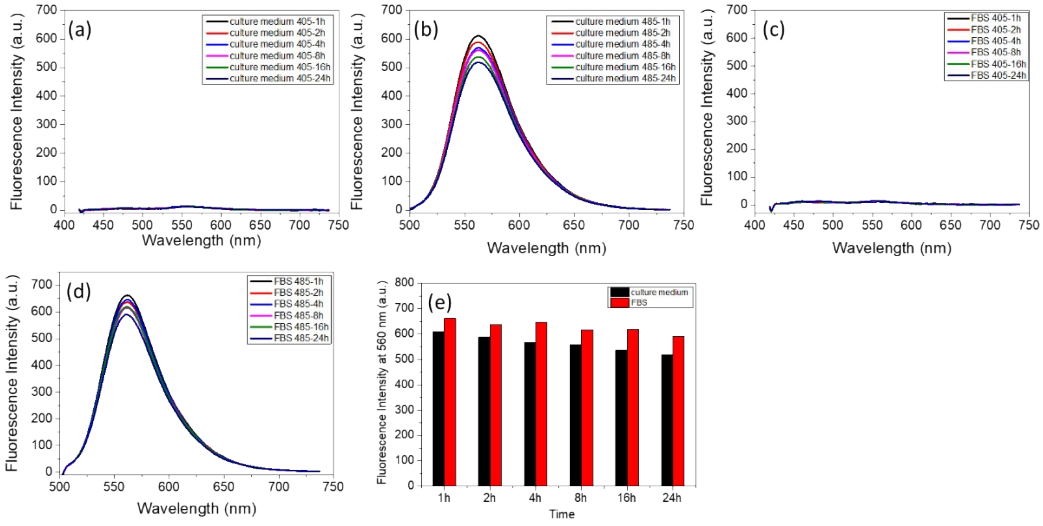



**Figure S20** The stability of the **rCP-βCD@cRGD-ADA** (10 μM) in 10% FBS buffer and F12 culture medium (containing 10% FBS and 1% penicillin-streptomycin). (a-d) Fluorescence spectra of **rCP-βCD@cRGD-ADA** in different time (1h, 2h, 4h, 8h, 16h and 24h) (a, c: $\lambda_{ex}$ = 405 nm; slits: 2.5/ 5 nm; b, d: $\lambda_{ex}$ = 485 nm; slits: 5/ 5 nm). (e) Histogram of related fluorescence spectra.

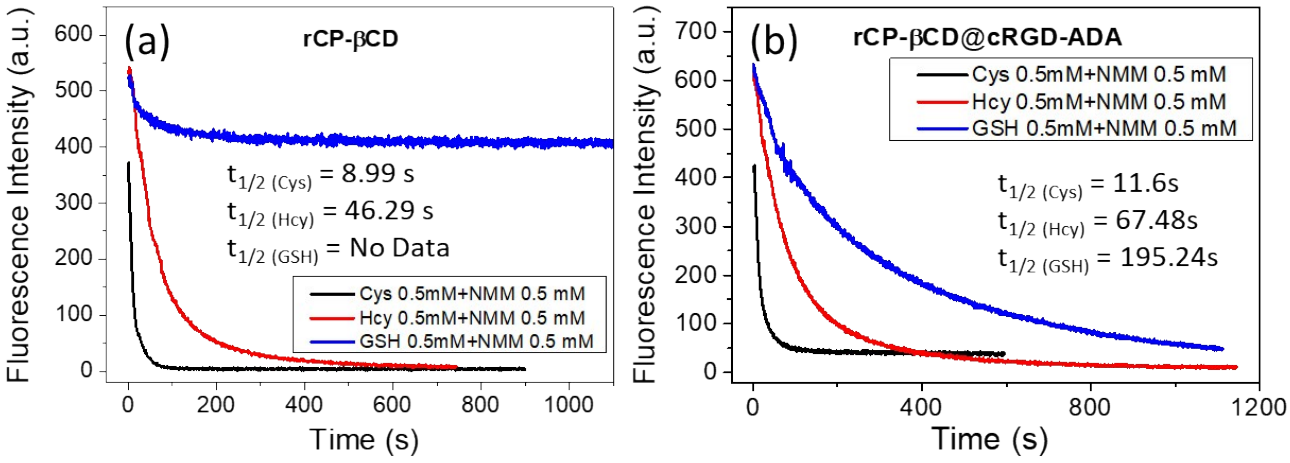



**Figure S21**. Time-dependent fluorescent emission of biothiols adducts for **rCP-βCD** and **rCP-βCD@cRGD-ADA** towards NMM. ($\lambda_{ex}$ = 405 nm; slits: 2.5/ 5 nm; Emission = 463 nm; biothiols = 0.5 mM; NMM = 0.5 mM)

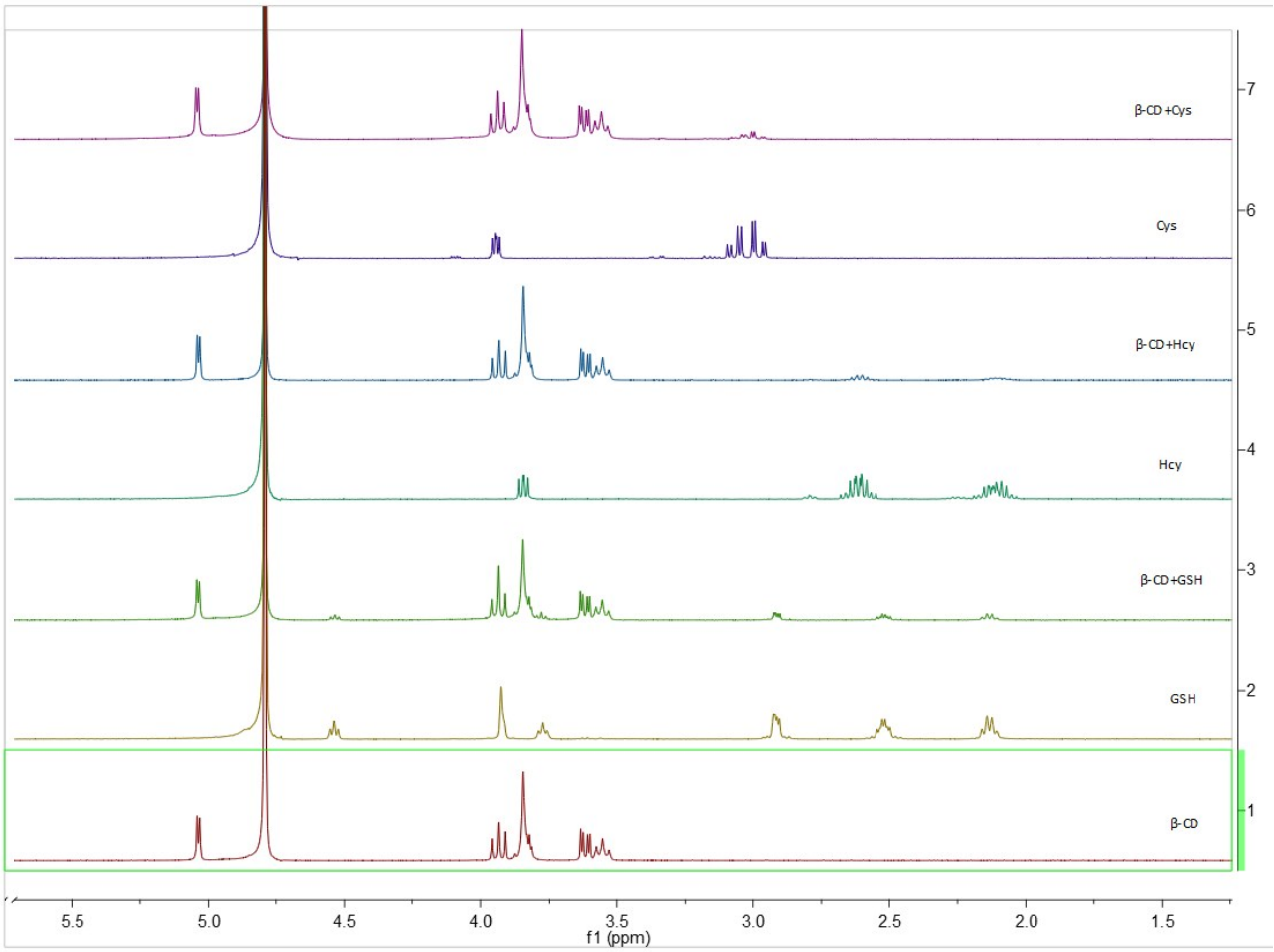



**Figure S22**. $^{1}$H NMR spectra of biothiols (1 mM), β-CD (1 mM) and β-CD@biothiols complex (1 mM) in $D_2O$.

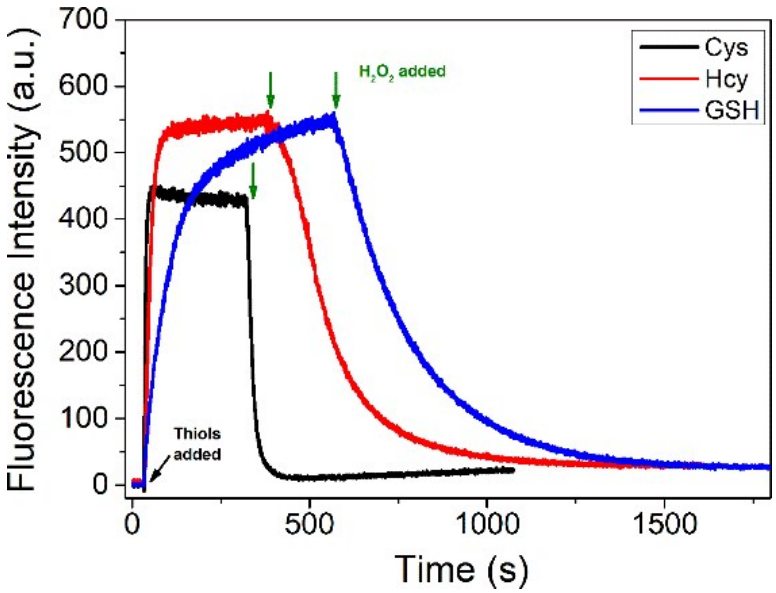



**Figure S23** Time-dependence of the reversible fluorescence emission at 463 nm by **rCP-βCD@cRGD-ADA** in response to biothiols (0.5 mM) and $H_2O_2$ (2 mM) (λex = 405 nm; slits: 2.5/5 nm).

## 3. Cell imaging experiment

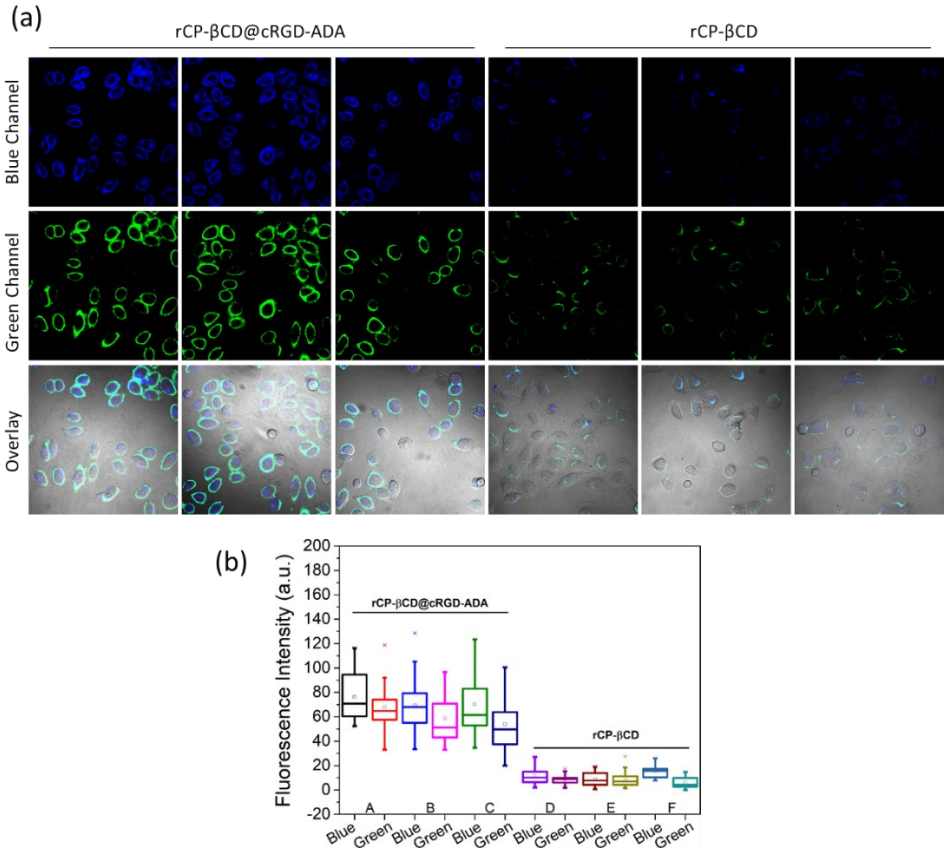



**Figure S24** Cells uptake experiment with **rCP-βCD@cRGD-ADA** and **rCP-βCD**. (a) Confocal and ratiometric images of MCF-7 cells treated with **rCP-βCD** (10 μM) and **rCP-βCD@cRGD-ADA** (10 μM). (b) Box plots of fluorescence intensity in the blue and green channels for **rCP-βCD** and **rCP-βCD@cRGD-ADA** in individual cells (*n* = 20).

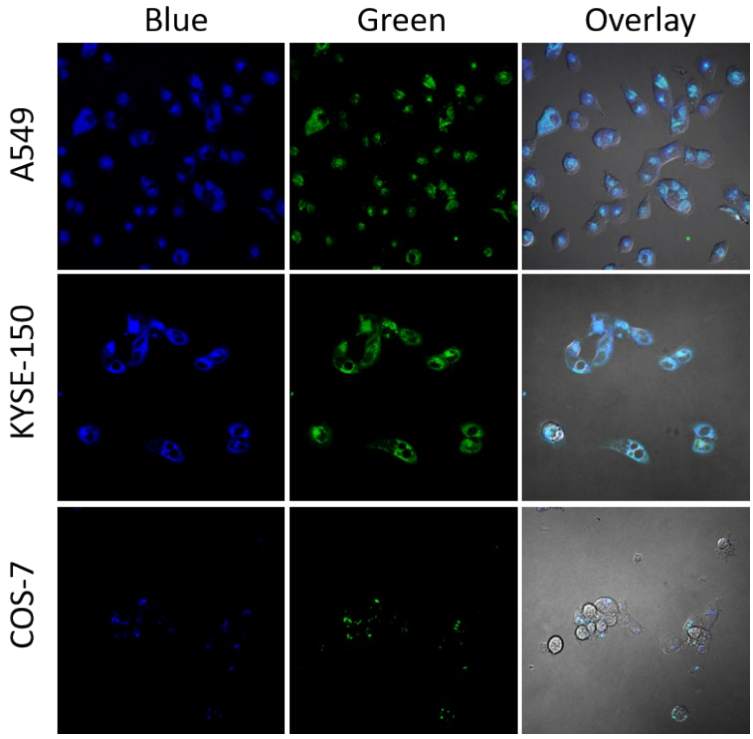



**Figure S25** Cells uptake experiment with **rCP-βCD@cRGD-ADA** (10 μM) in A549, KYSE-150 and COS-7 cells.

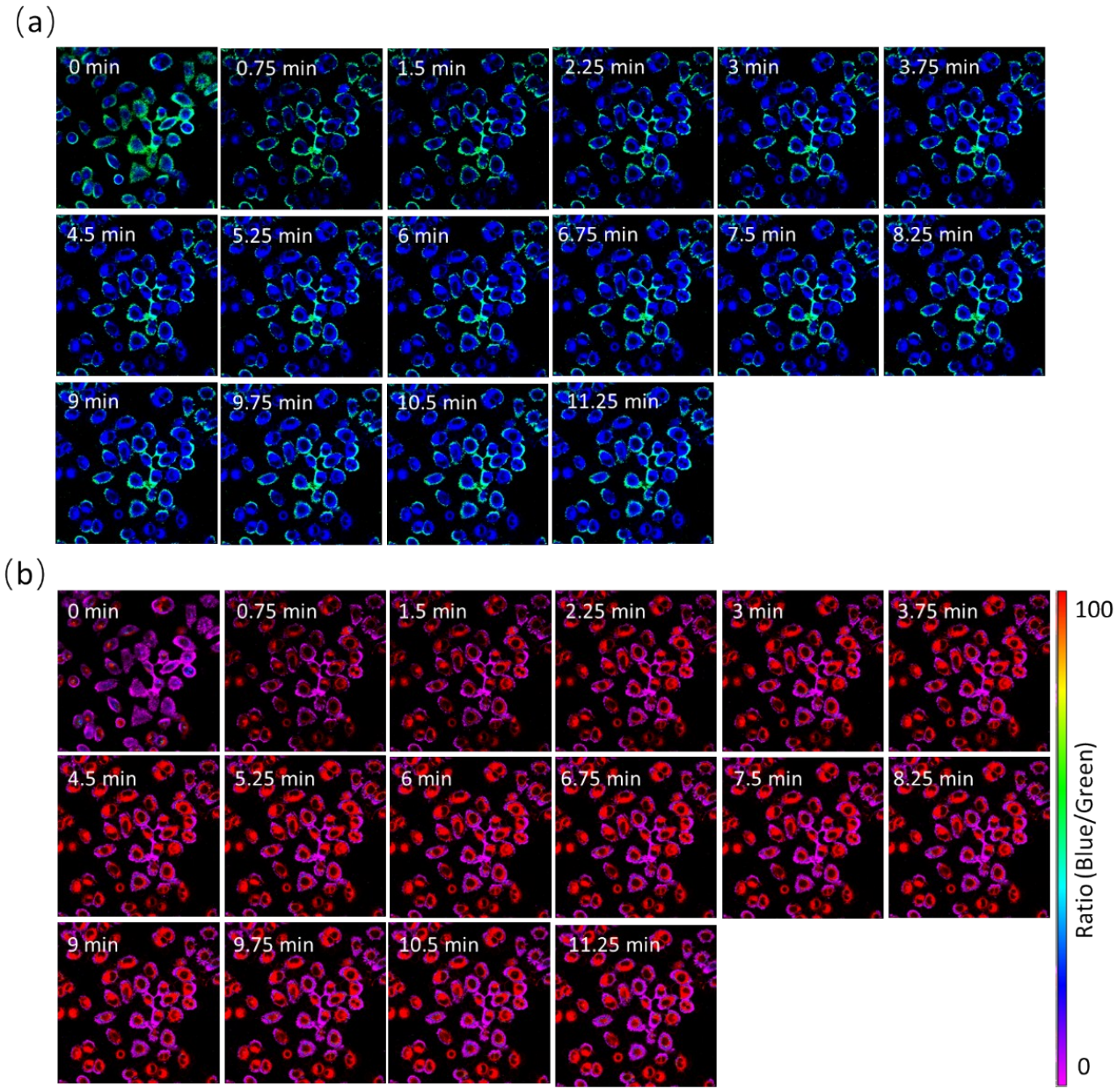



**Figure S26**. (a) Time-dependent imaging with **rCP-βCD@cRGD-ADA** (10 μM) in MCF-7 cells under the condition of cultuer medium upon NMM (0.5 mM) treatment for 11.25 min. (b) Ratio (Blue/Green) imaging of (a).

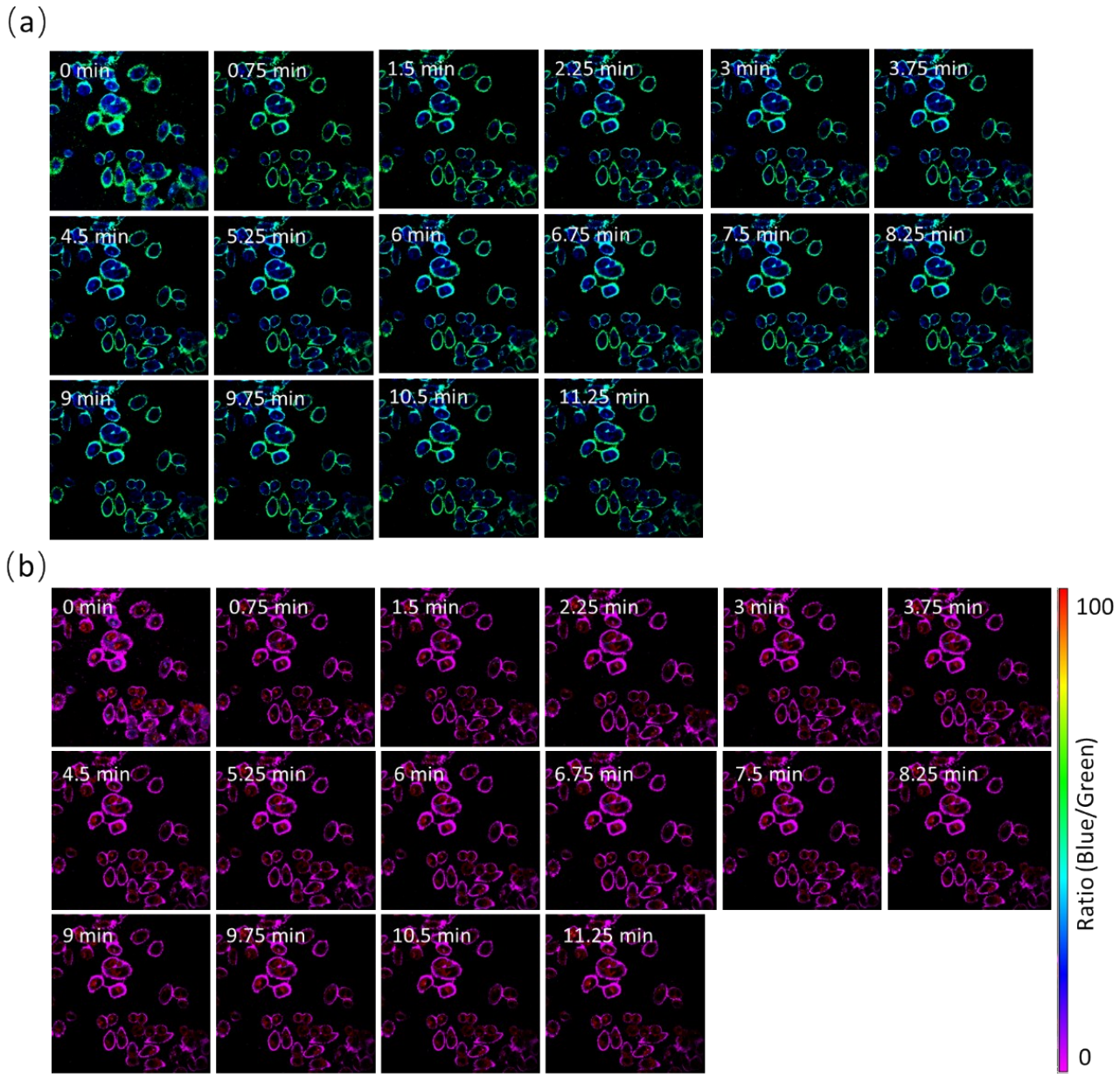



**Figure S27**. (a) Time-dependent imaging with **rCP-βCD@cRGD-ADA** (10 μM) in MCF-7 cells under the condition of PBS upon NMM (0.5 mM) treatment for 11.25 min. (b) Ratio (Blue/Green) imaging of (a).

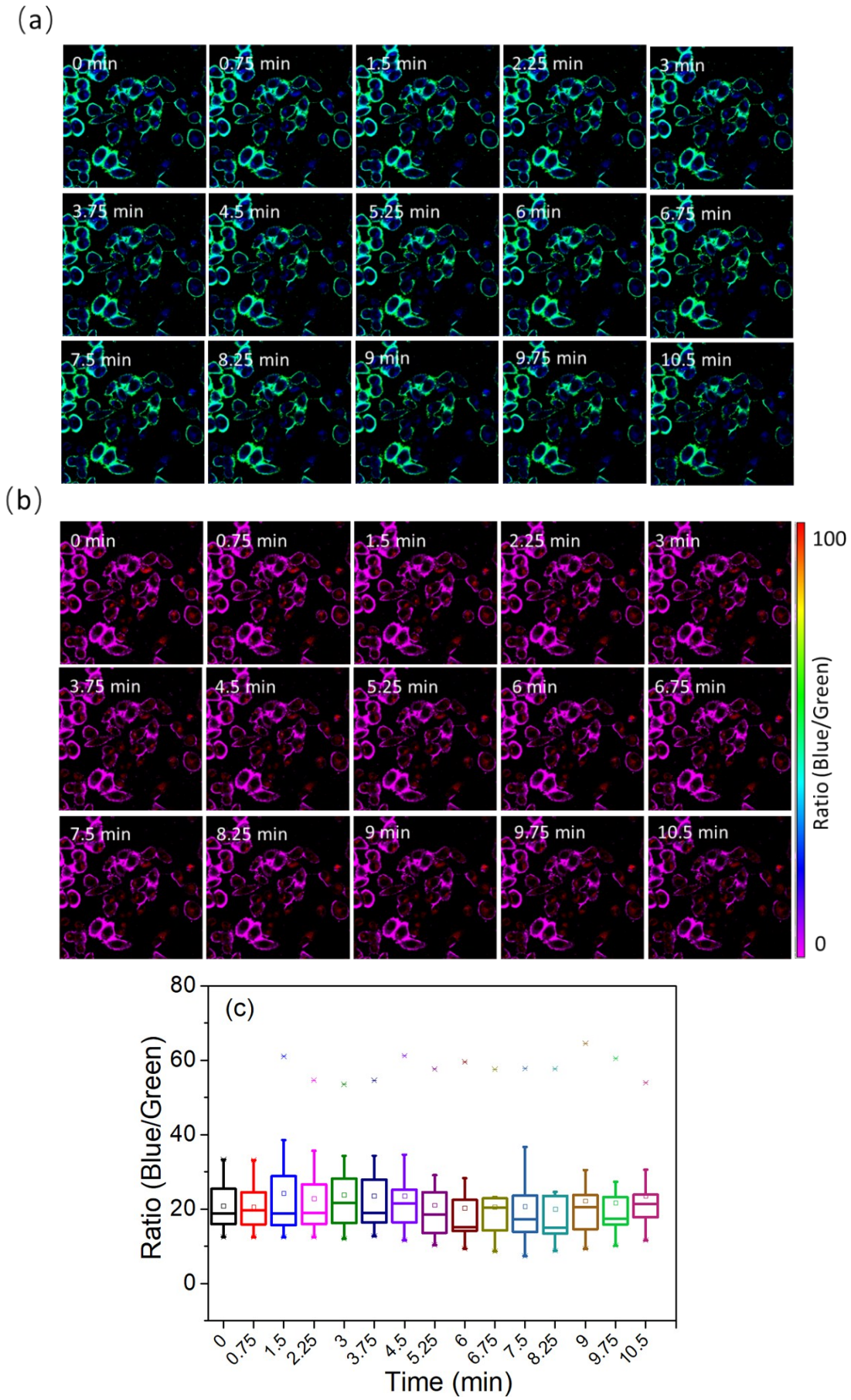



**Figure S28**. (a) Time-dependent imaging with **rCP-βCD@cRGD-ADA** (10 μM) in MCF-7 cells in PBS upon NMM (0.5 mM) treatment for 10.5 min. (b) Ratio (Blue/Green) imaging of (a). (c) Fluorescence quantitative analysis of biothiols change in MCF-7 cells in cell culture medium without NMM in individual cells (n =40) for 10.5 min.

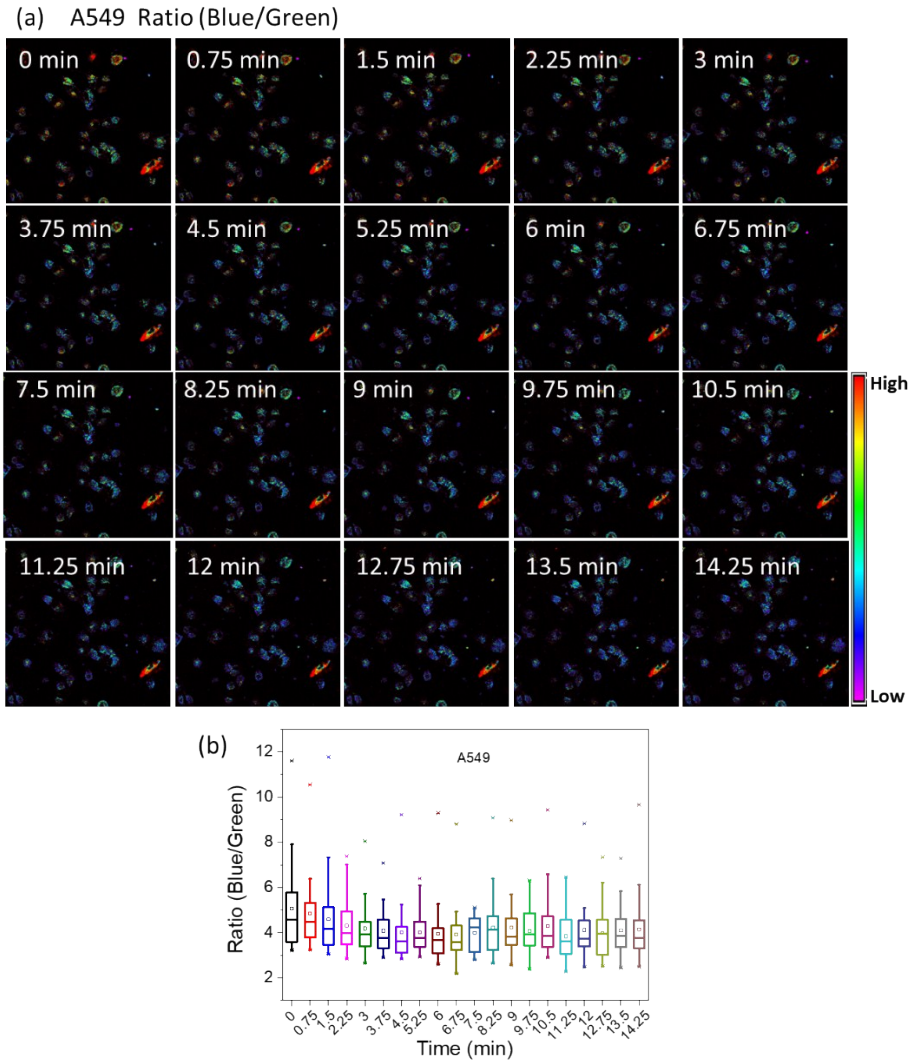



**Figure S29** Real-time biothiols imaging with **rCP-βCD@cRGD-ADA** in A549 cells upon NMM treatment. (a) Real-time blue/green ratio images showing biothiols concentration dynamics in A549 cells treated with **rCP-βCD@cRGD-ADA** (10 μM) and NMM (0.5 mM) in cell culture medium. NMM was added at 0 min. (b) Box plots of fluorescence intensity in the blue and green channels for **rCP-βCD** and **rCP-βCD@cRGD-ADA** in individual cells (*n* = 26).

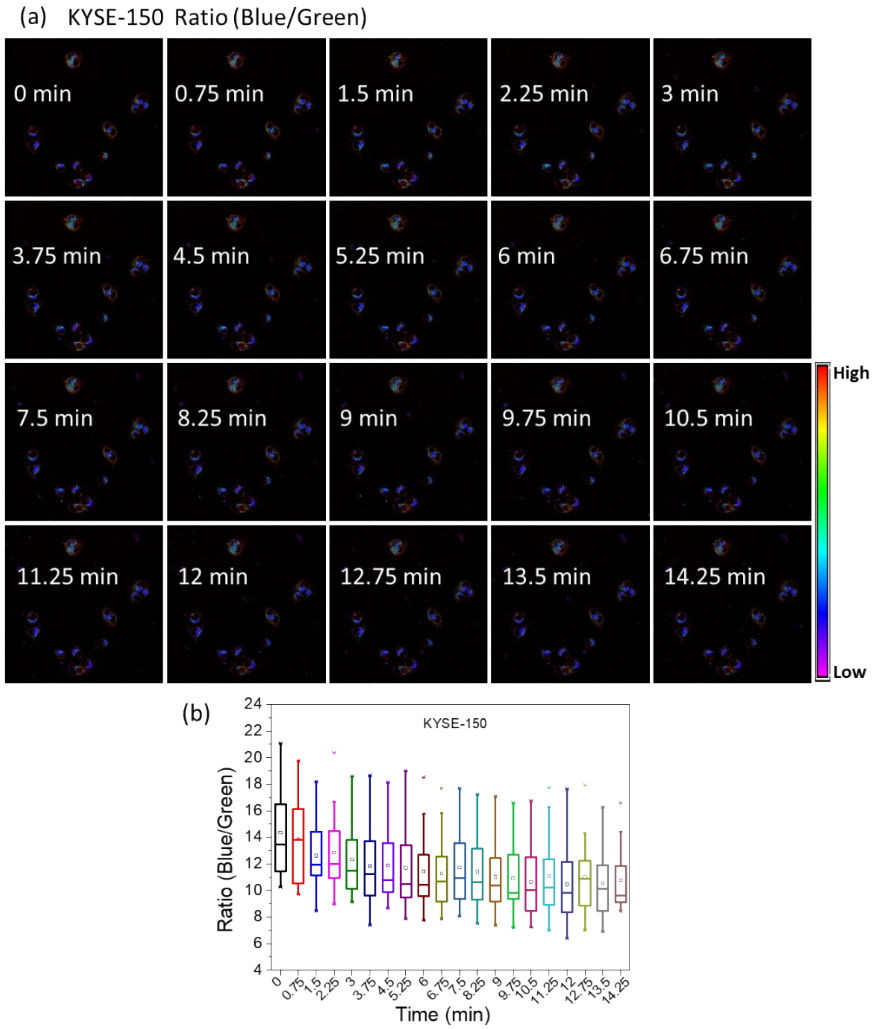



**Figure S30** Real-time biothiols imaging with **rCP-βCD@cRGD-ADA** in KYSE-150 cells upon NMM treatment. (a) Real-time blue/green ratio images showing biothiols concentration dynamics in KYSE-150 cells treated with **rCP-βCD@cRGD-ADA** (10 μM) and NMM (0.5 mM) in cell culture medium. NMM was added at 0 min. (b) Box plots of fluorescence intensity in the blue and green channels for **rCP-βCD** and **rCP-βCD@cRGD-ADA** in individual cells (*n* = 12).

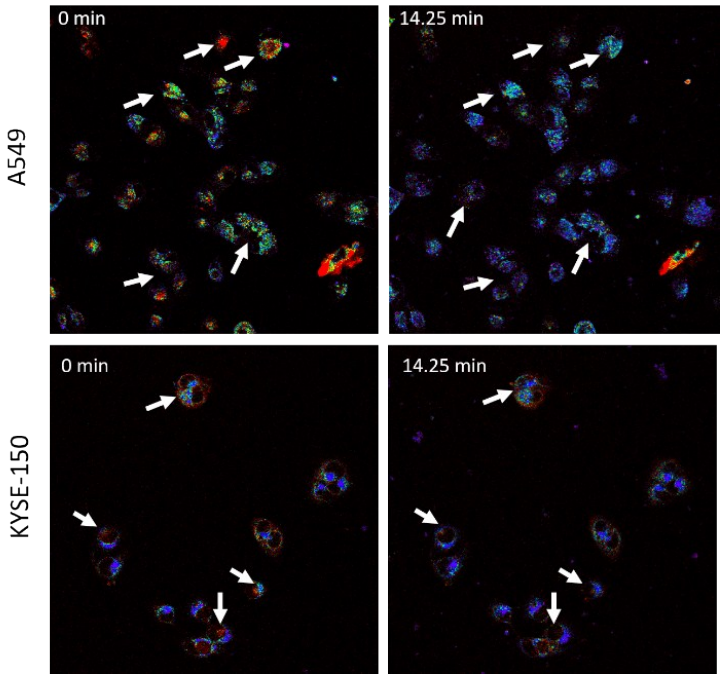



**Figure S31** Representative blue/green ratio images showing biothiols concentration dynamics in A549 and KYSE-150 cells treated with **rCP-βCD@cRGD-ADA** before and after addition of NMM. NMM was added at 0 min.

## 4. Characterization data

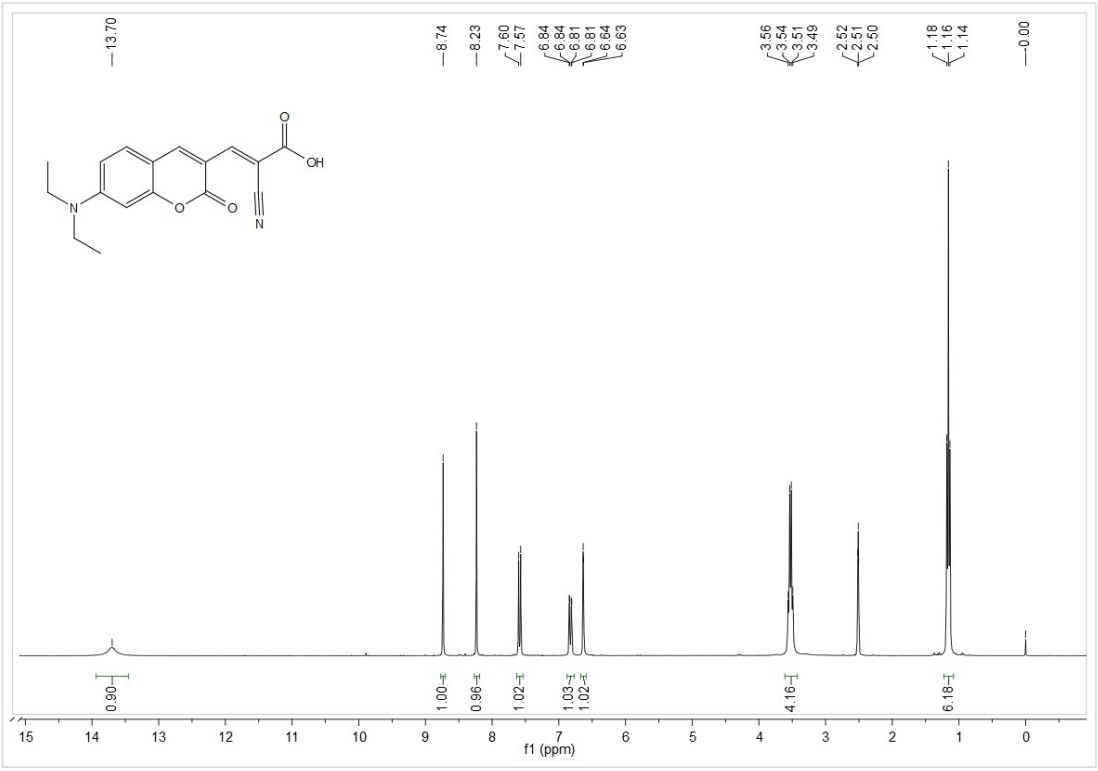



**Figure S32.** $^{1}$H-NMR spectrum of compound **2** (400 MHz, DMSO-$d_6$).

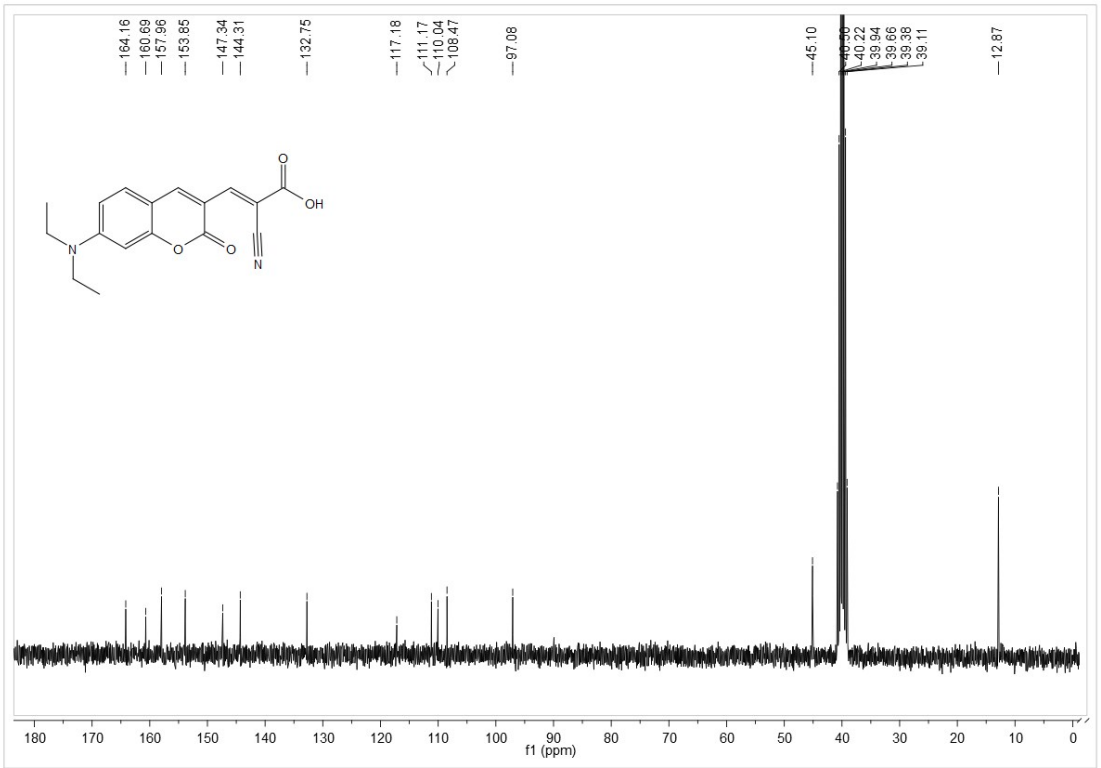



**Figure S33.** $^{13}$C-NMR spectrum of compound **2** (400 MHz, DMSO-$d_6$).

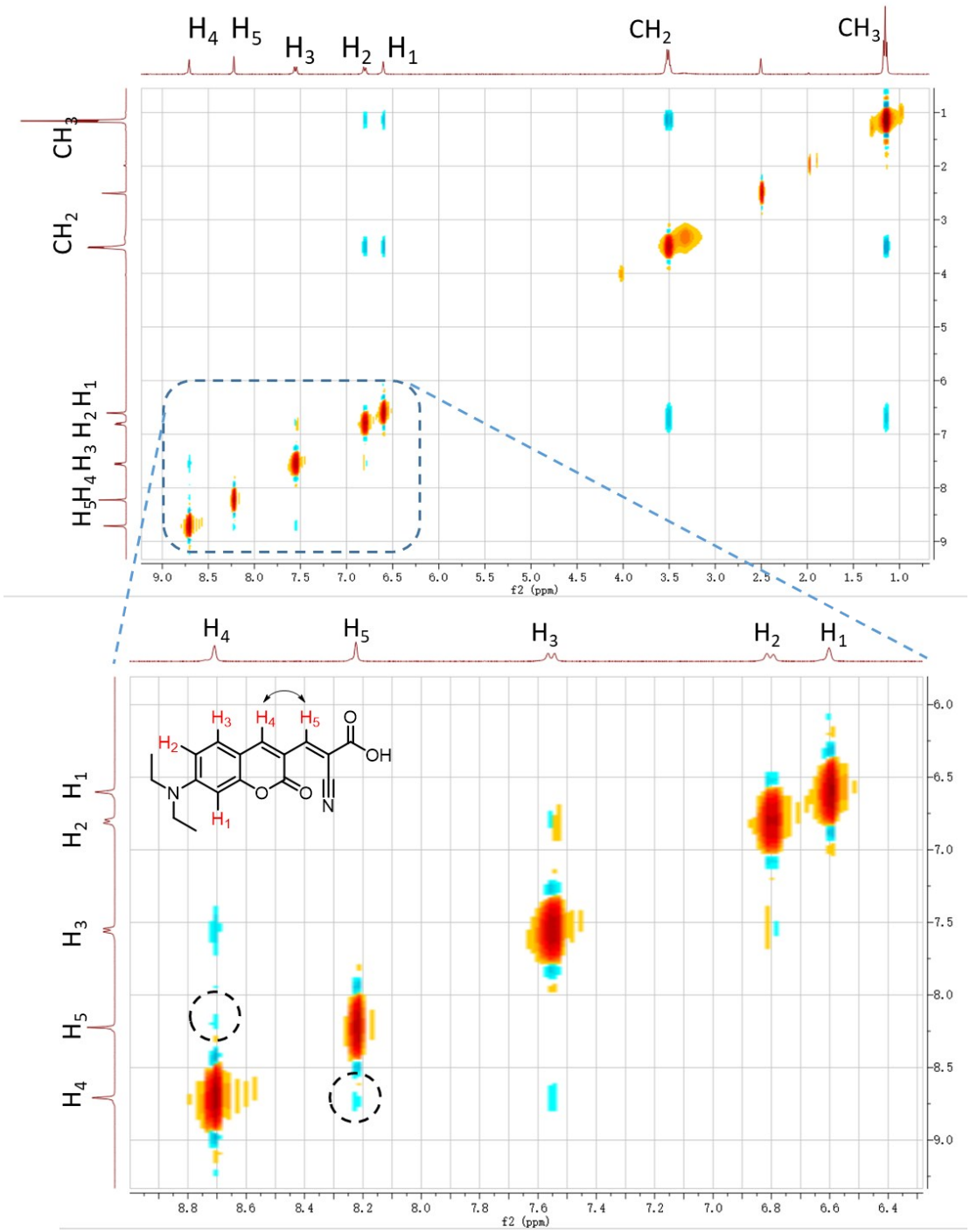



**Figure S34.** 2D NOESY spectrum of compound **2**. Solvent: DMSO-*d6*.

Note: NOE signal was observed between $H_4$ and $H_5$, which confirmed the configuration of compound **2** in DMSO-*d6*

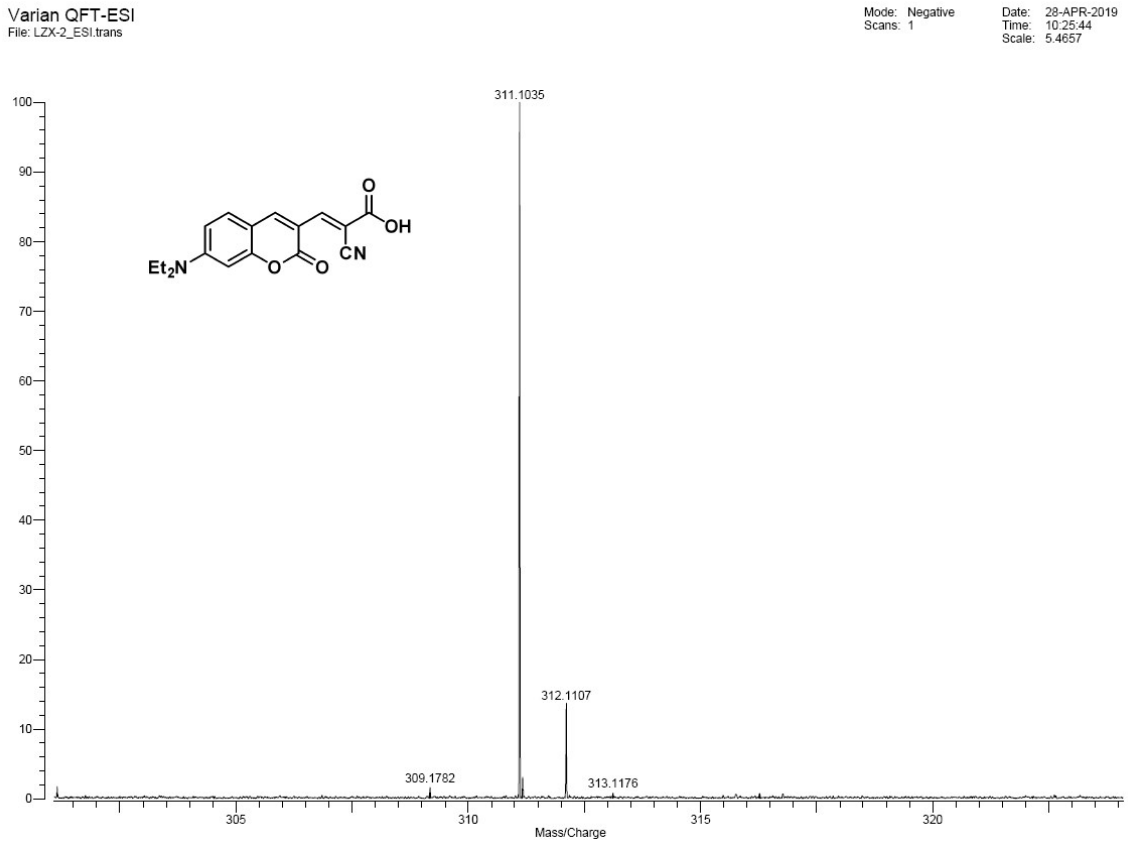



**Figure S35.** HRMS spectrum of compound **2**.

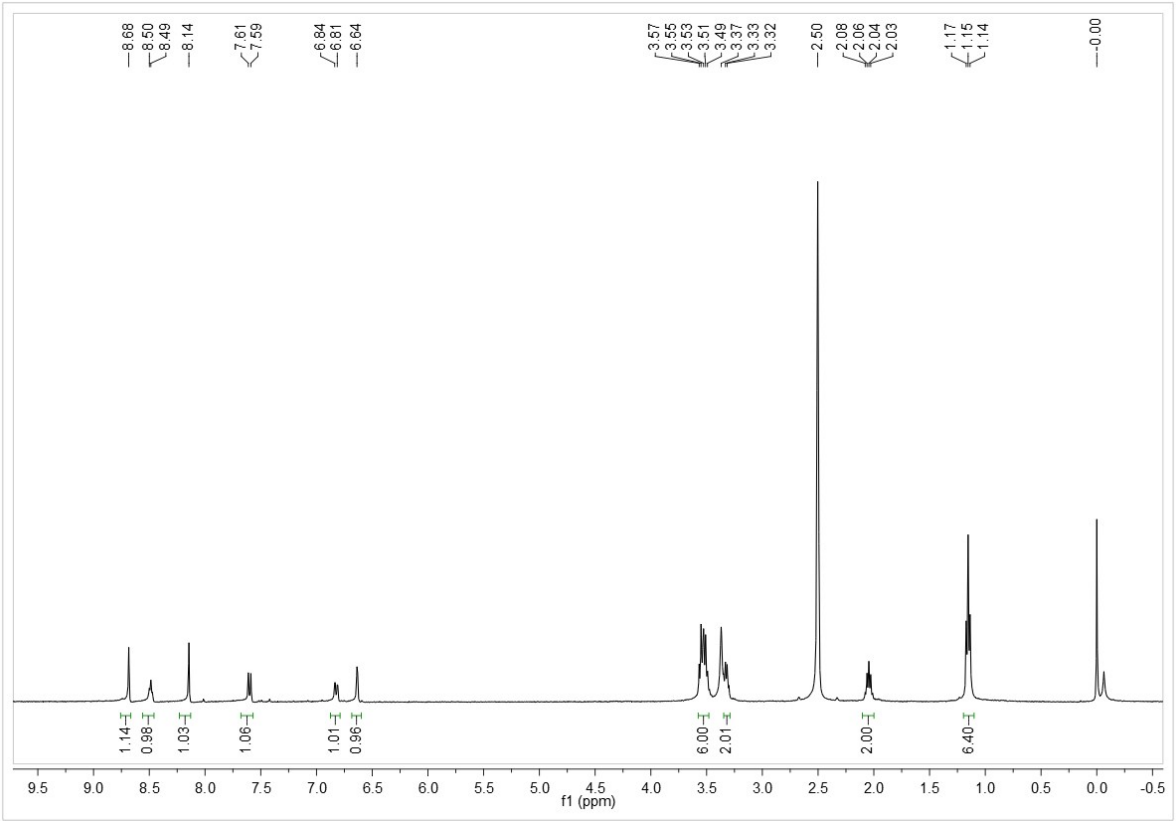



**Figure S36**. $^{1}$H-NMR spectrum of compound **3** (400 MHz, DMSO-$d_6$).

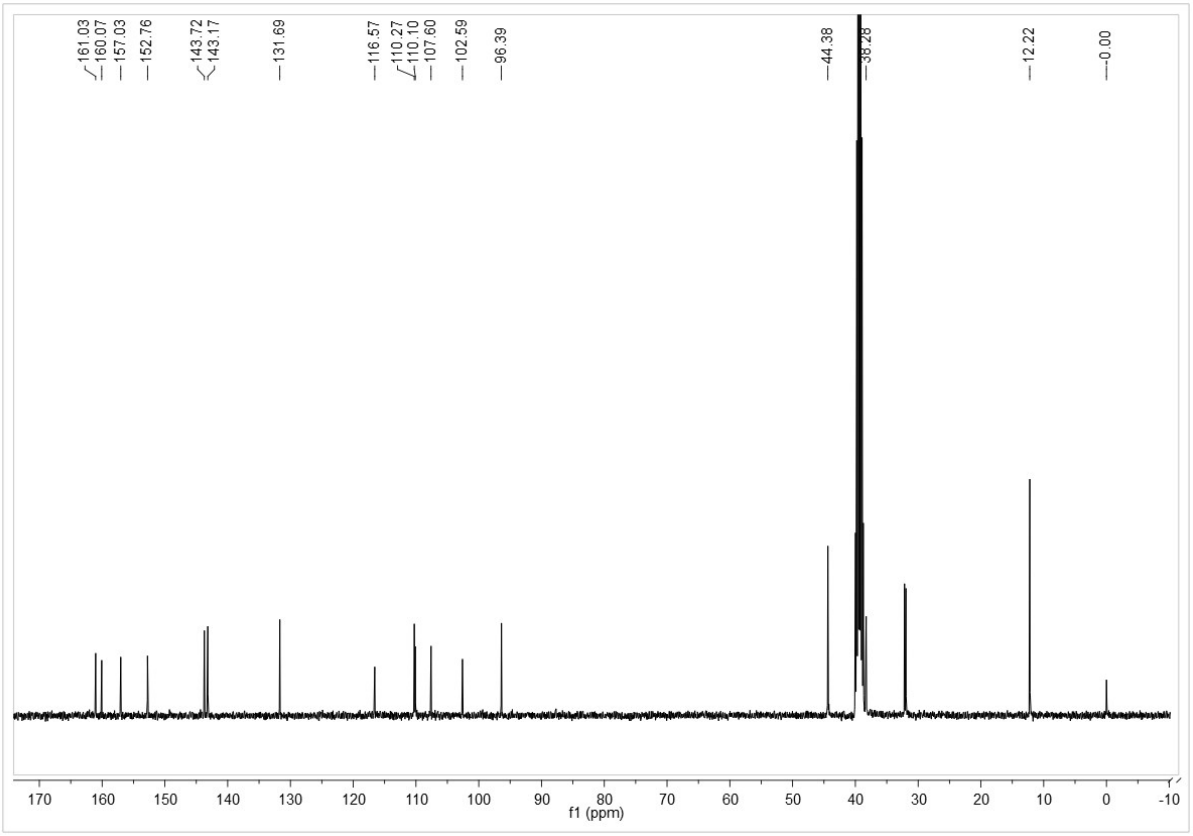



**Figure S37.** $^{13}$C-NMR spectrum of compound **3** (400 MHz, DMSO-$d_6$).

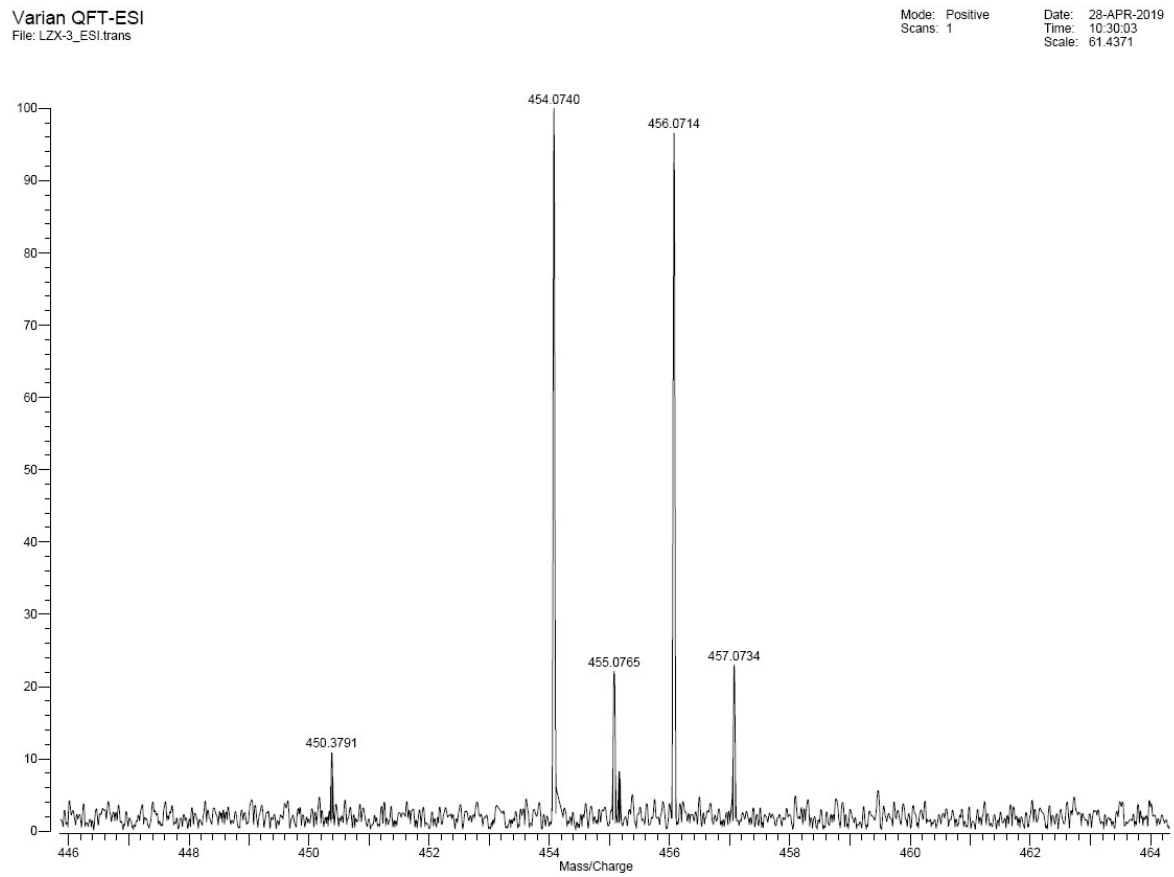



**Figure S38.** HRMS spectrum of compound **3**.

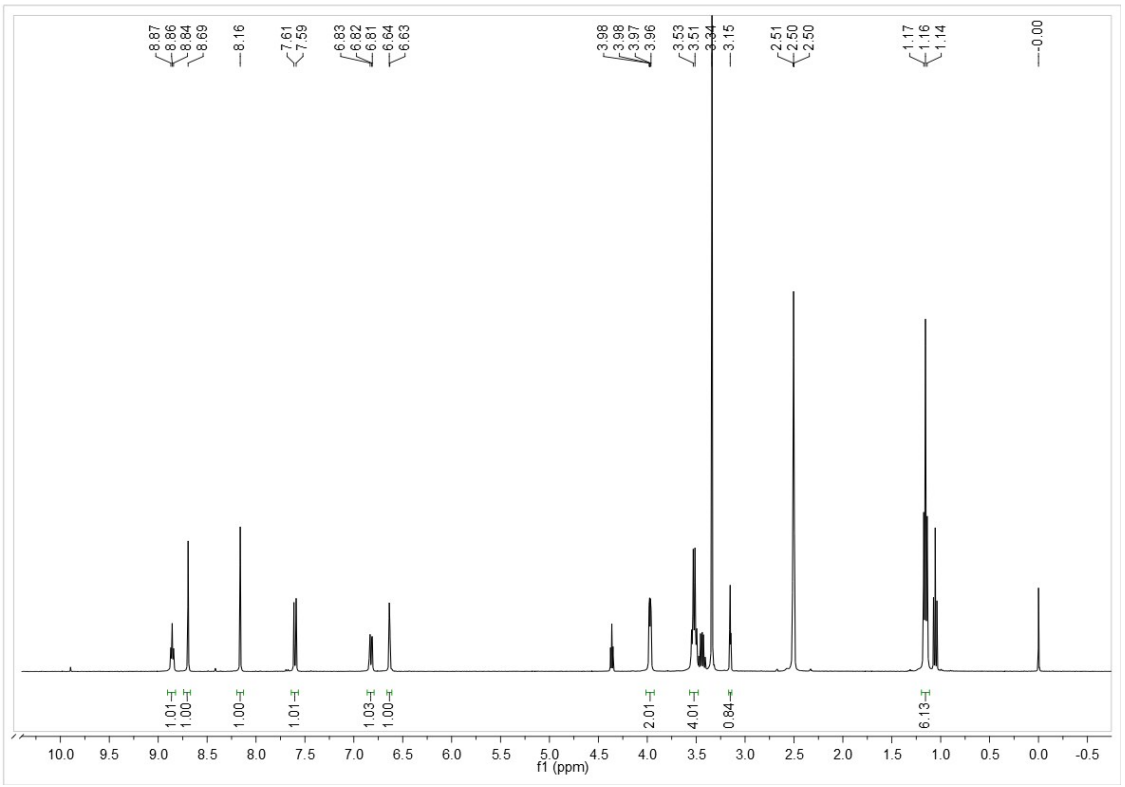



**Figure S39.** $^{1}$H-NMR spectrum of compound **4** (400 MHz, DMSO-$d_6$).

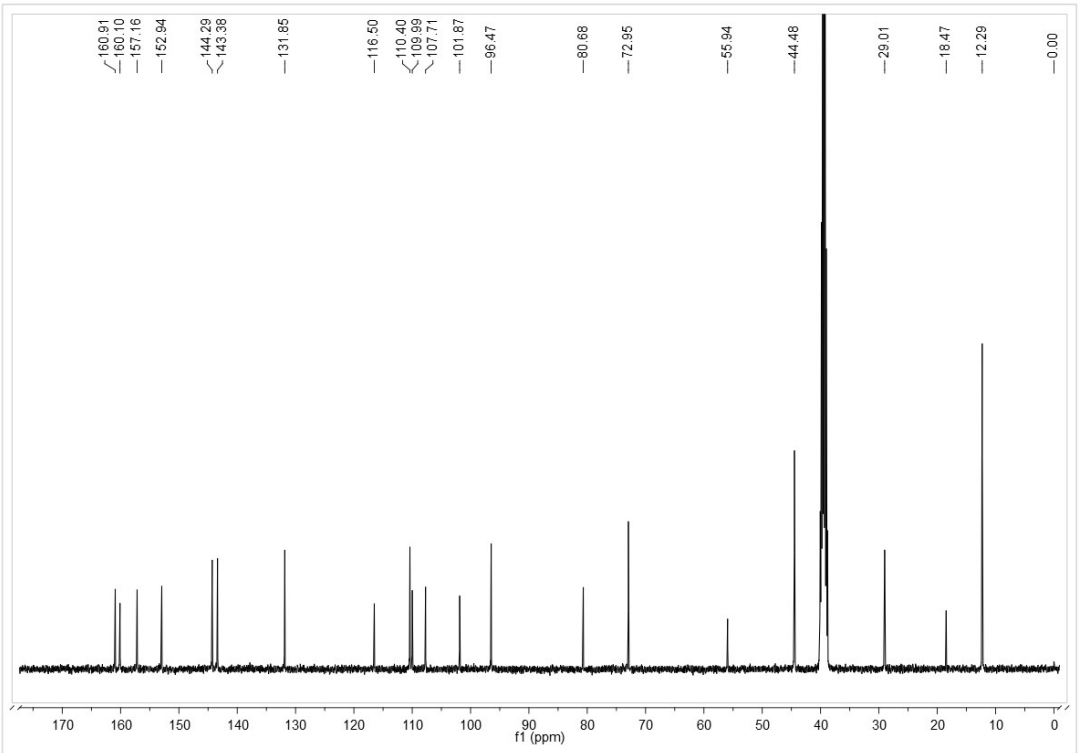



**Figure S40.** $^{13}$C-NMR spectrum of compound **4** (400 MHz, DMSO-$d_6$).

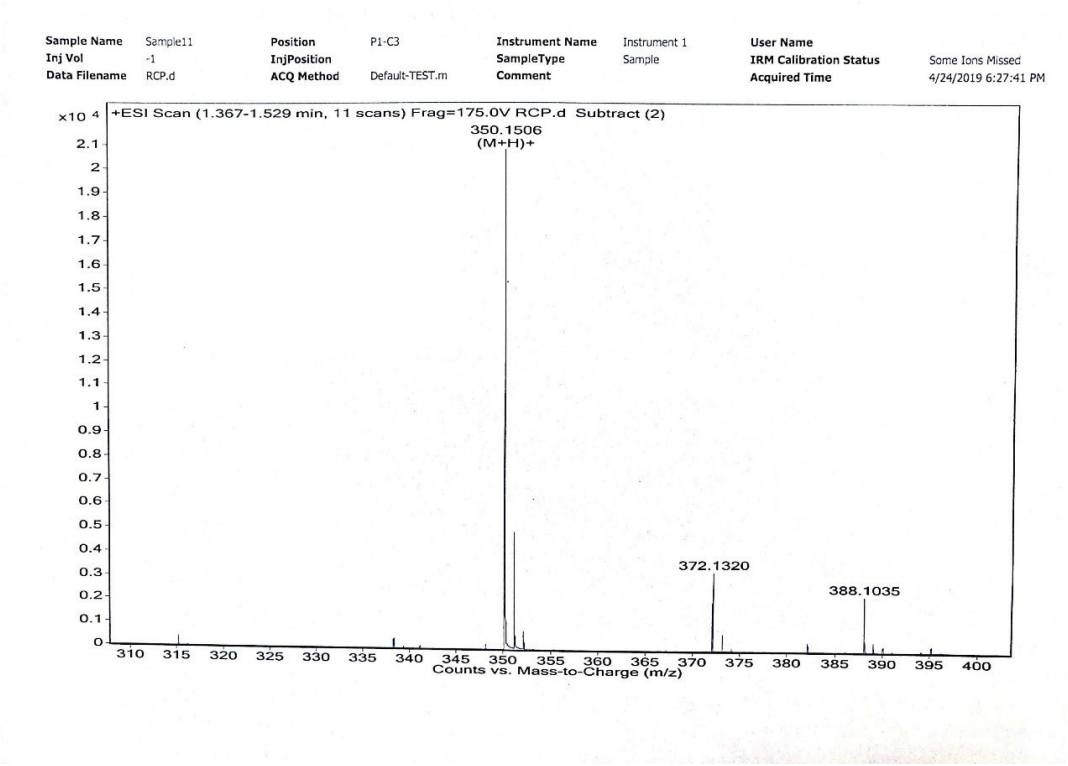



**Figure S41.** HRMS spectrum of compound **4**.

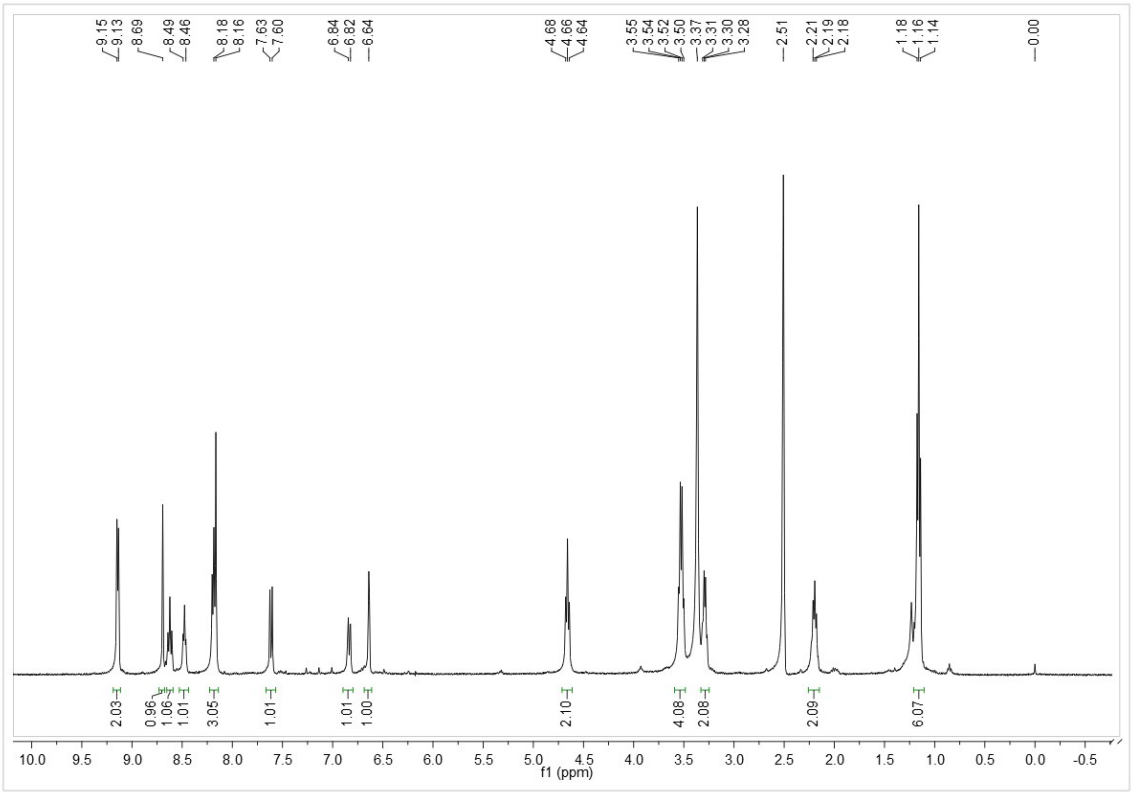



**Figure S42**. $^{1}$H-NMR spectrum of **rCP-Py** (400 MHz, DMSO-$d_6$).

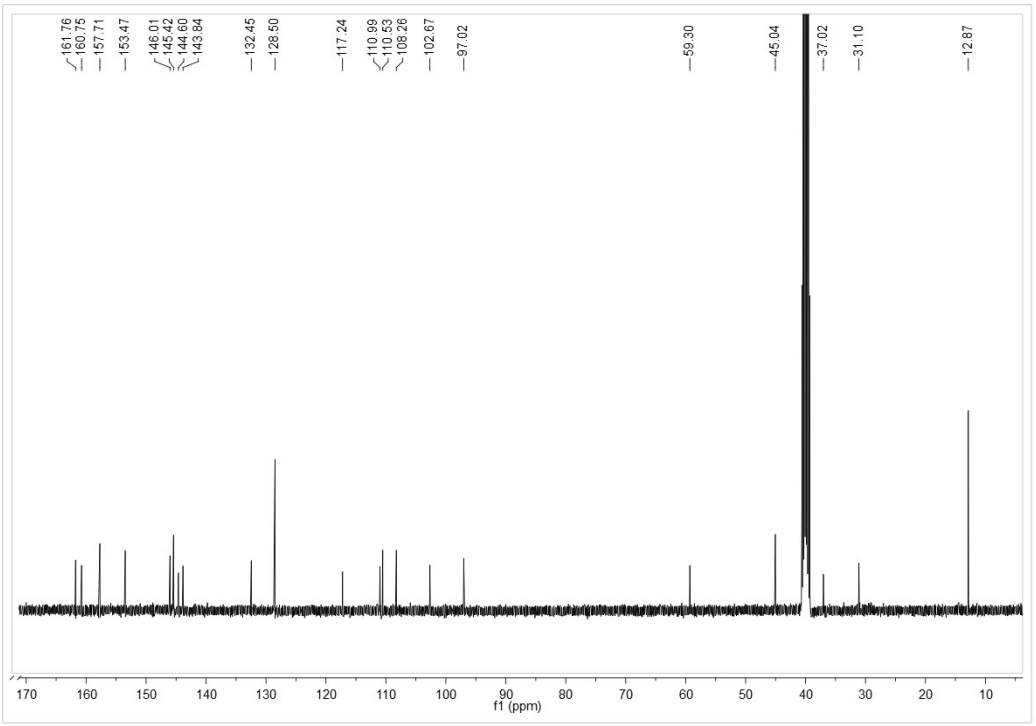



**Figure S43.** $^{13}$C-NMR spectrum of **rCP-Py** (400 MHz, DMSO-$d_6$).

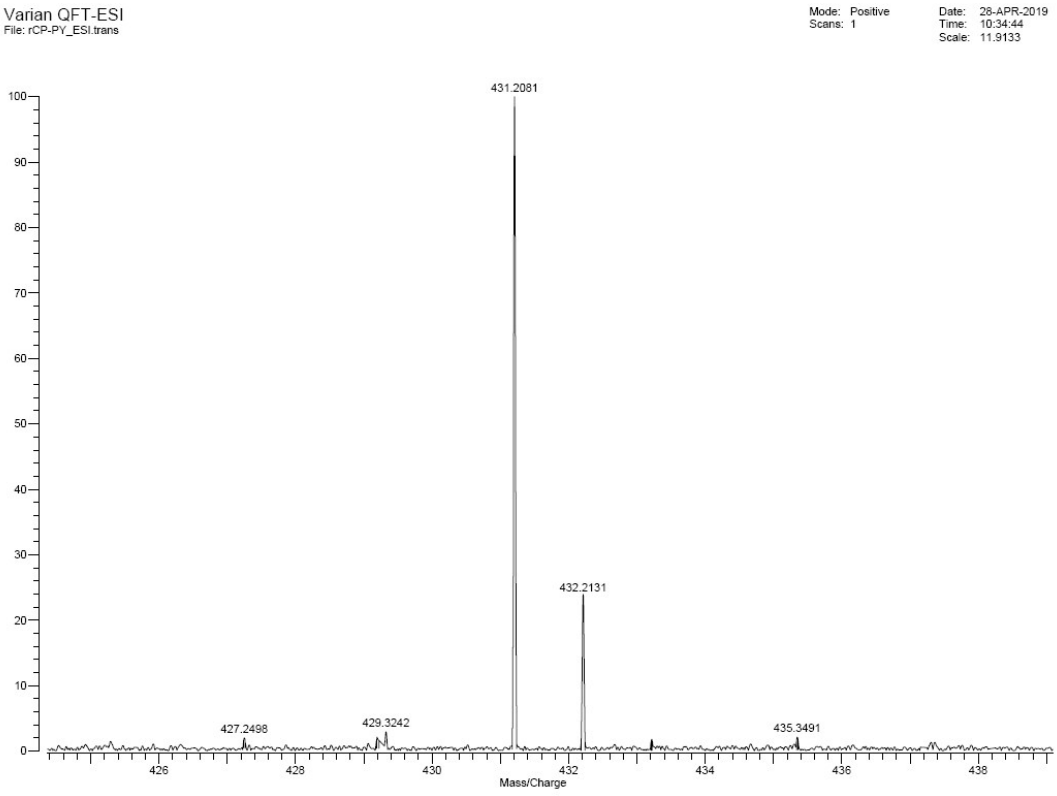



**Figure S44.** HRMS spectrum of **rCP-Py**.

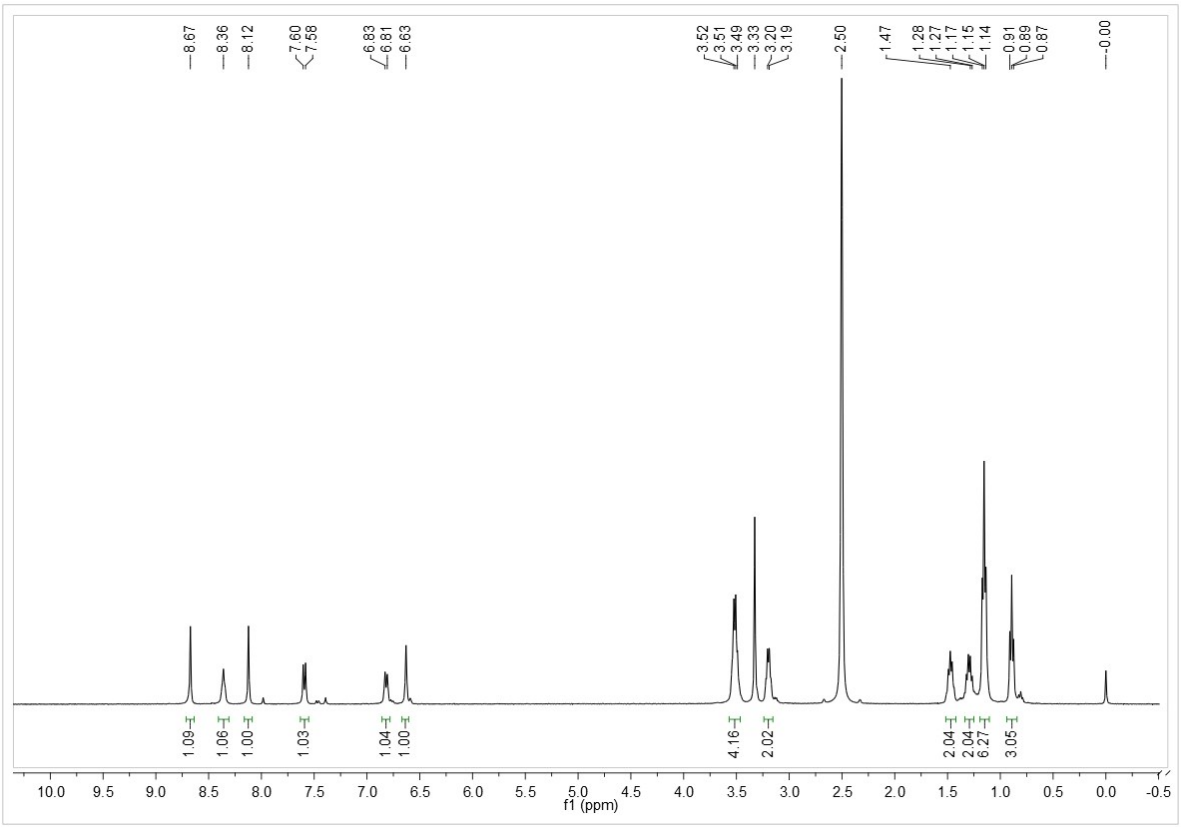



**Figure S45.** $^{1}$H-NMR spectrum of **rCP-AI** (400 MHz, DMSO-$d_6$).

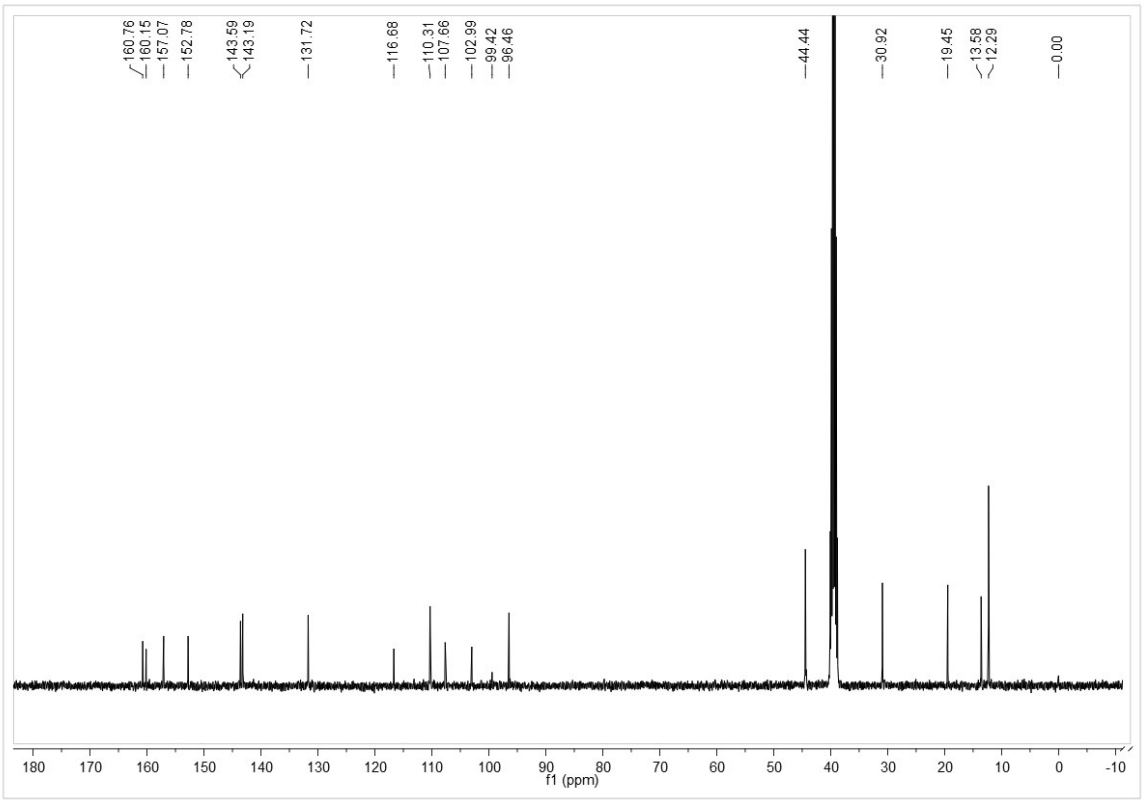



**Figure S46**. $^{13}$C-NMR spectrum of **rCP-AI** (400 MHz, DMSO-$d_6$).

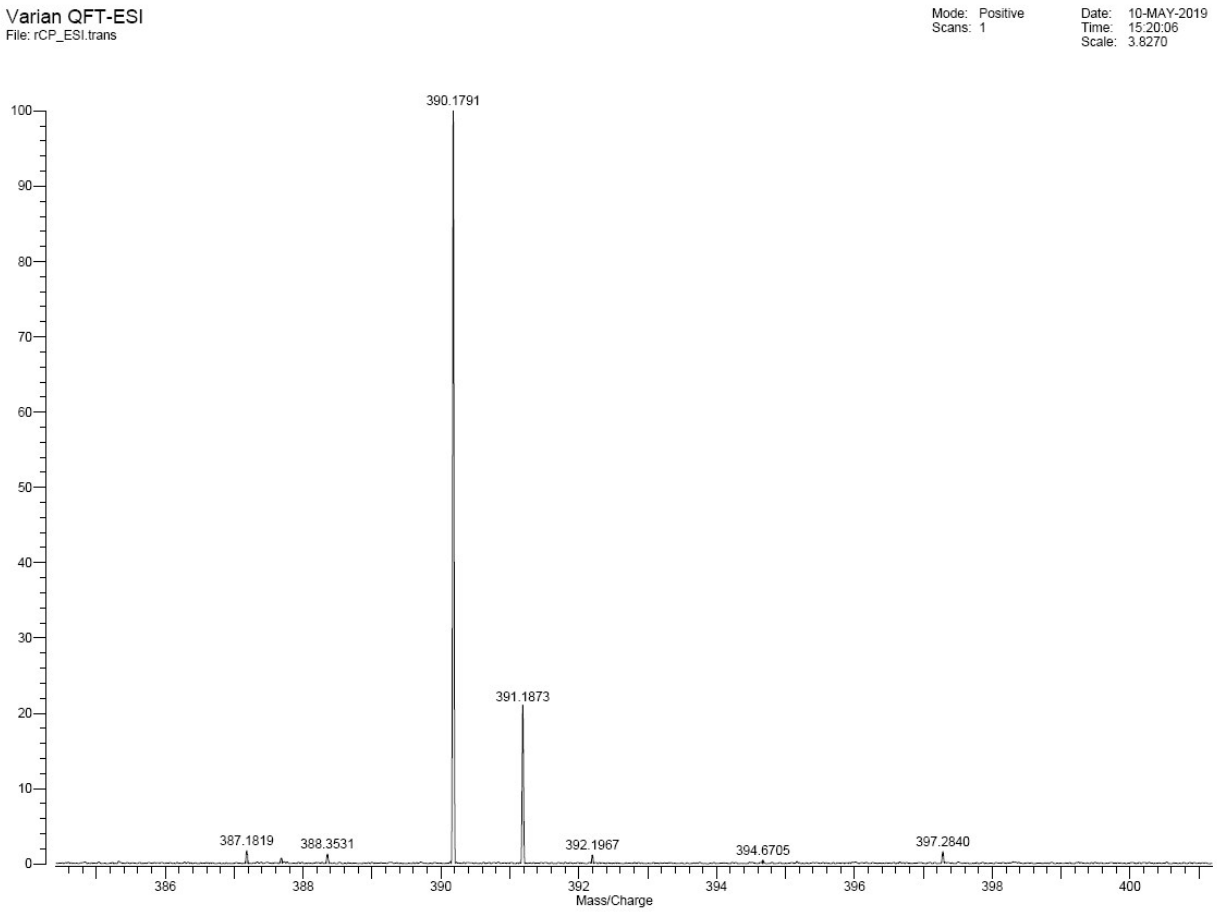



**Figure S47.** HRMS spectrum of **rCP-AI**.

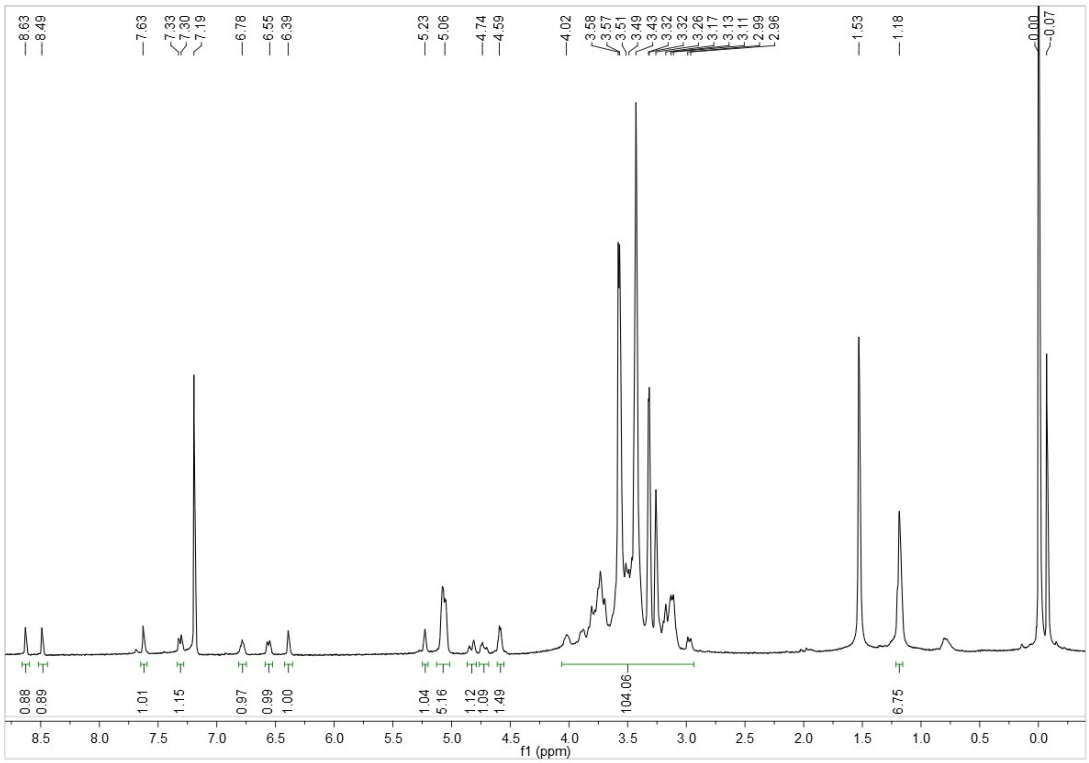



**Figure S48.** $^{1}$H-NMR spectrum of **rCP-βCD (OMe)** (400 MHz, $CDCl_3$).

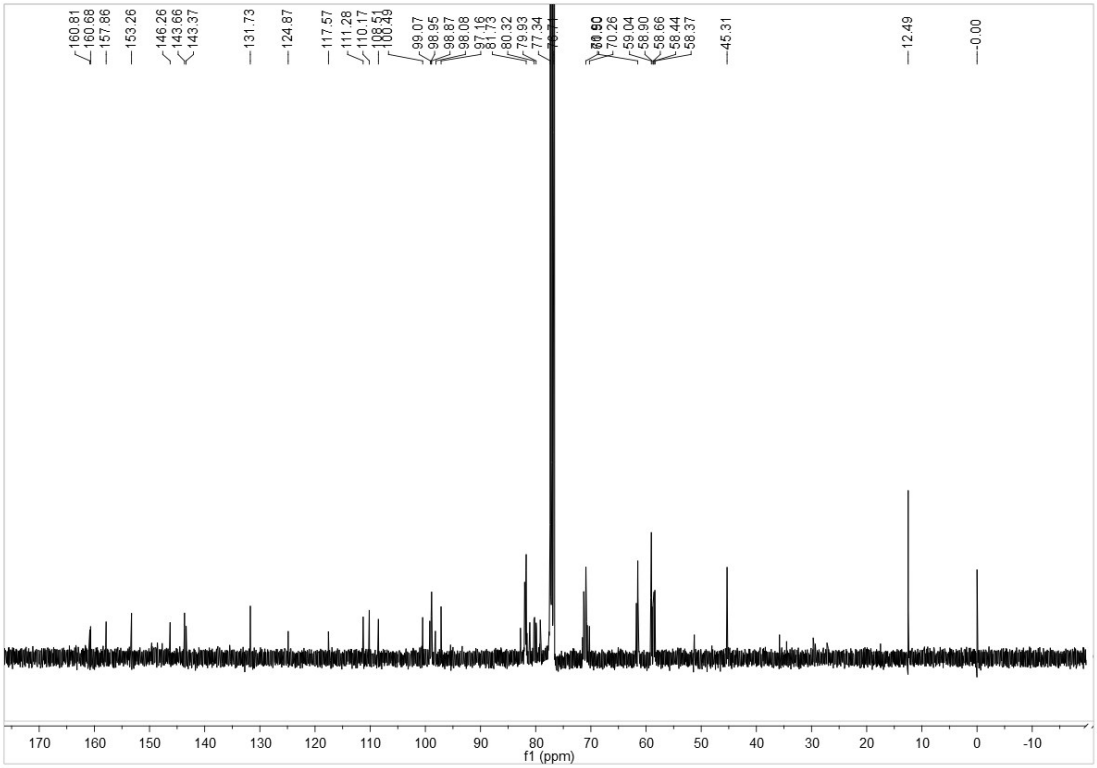



**Figure S49.** $^{13}$C-NMR spectrum of **rCP-βCD (OMe)** (400 MHz, $CDCl_3$).

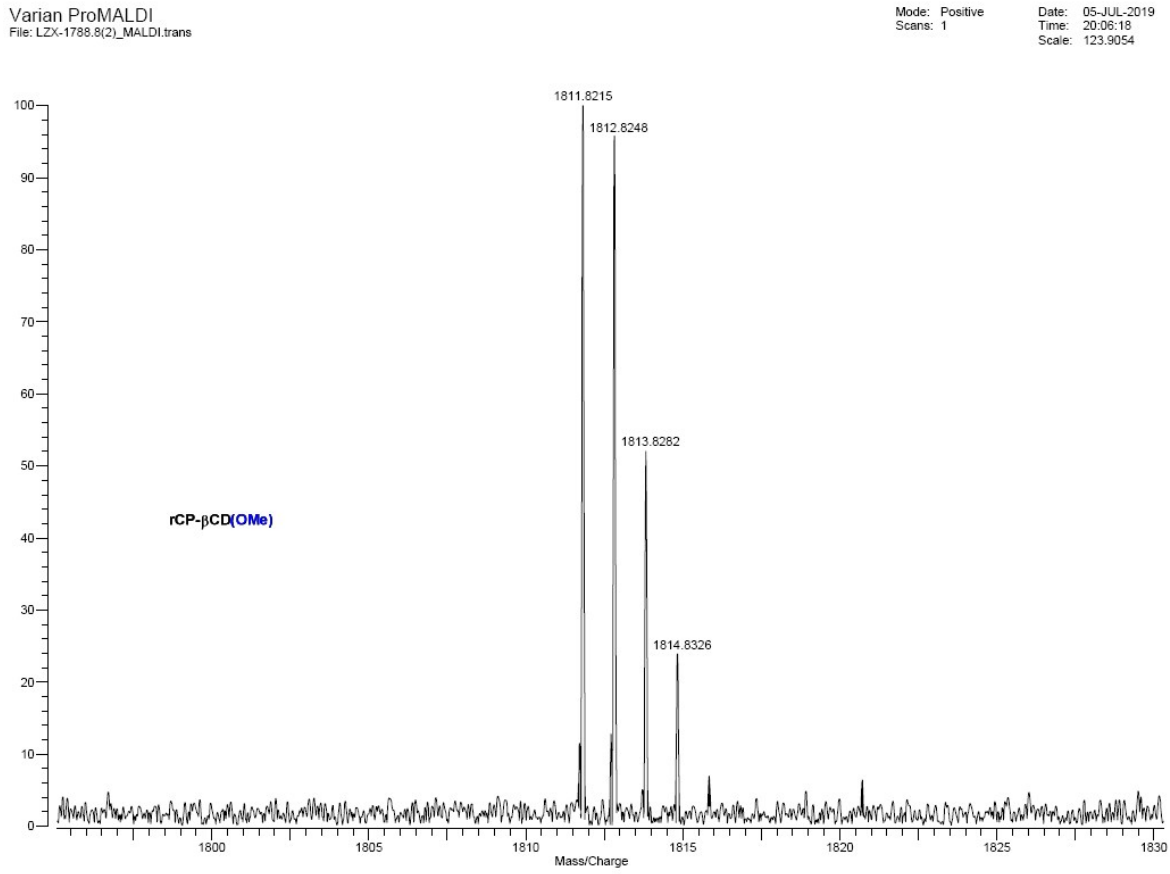



**Figure S50.** HRMS spectrum of **rCP-βCD (OMe)**.

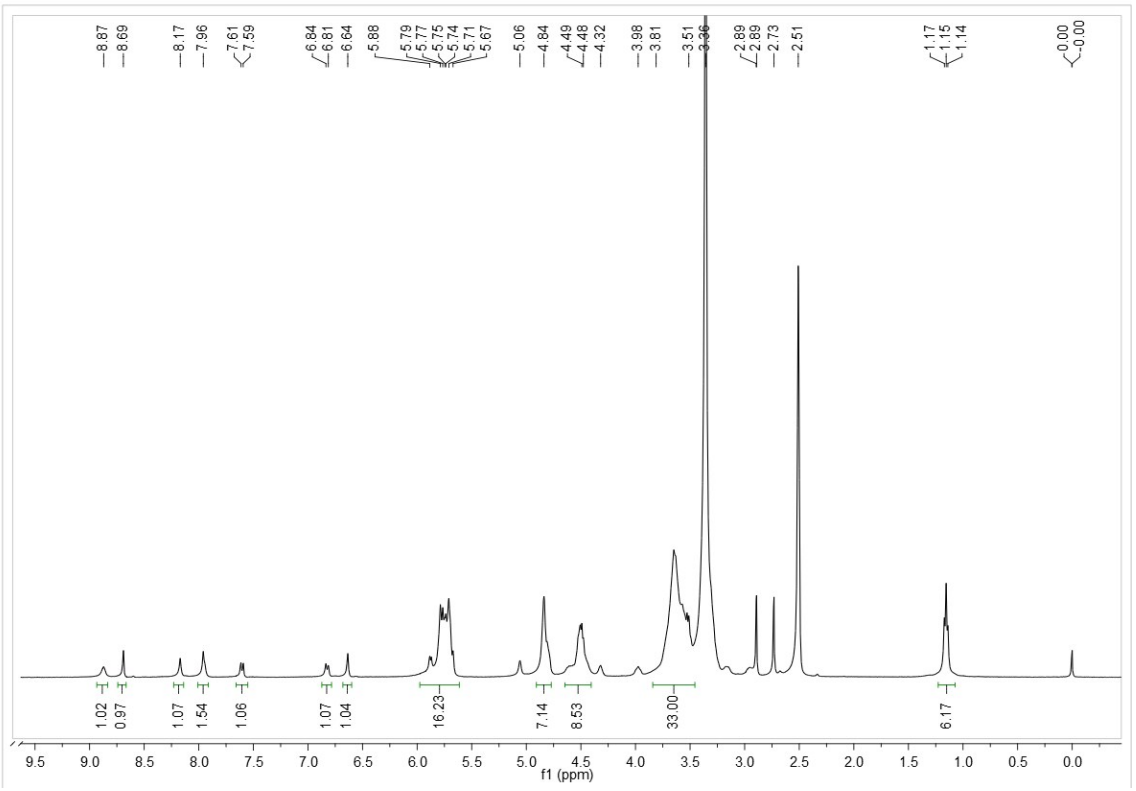



**Figure S51.** $^{1}$H-NMR spectrum of **rCP-βCD** (400 MHz, DMSO-$d_6$).

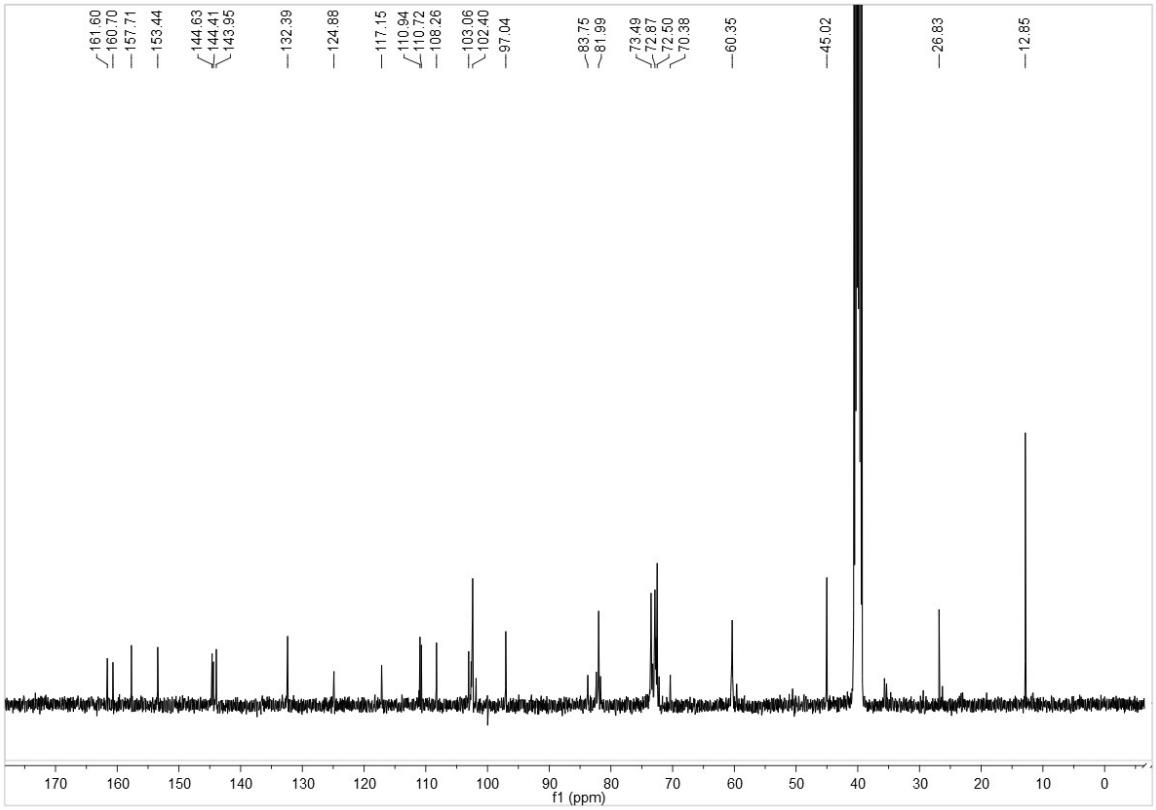



**Figure S52.** $^{13}$C-NMR spectrum of **rCP-βCD** (400 MHz, DMSO-$d_6$).

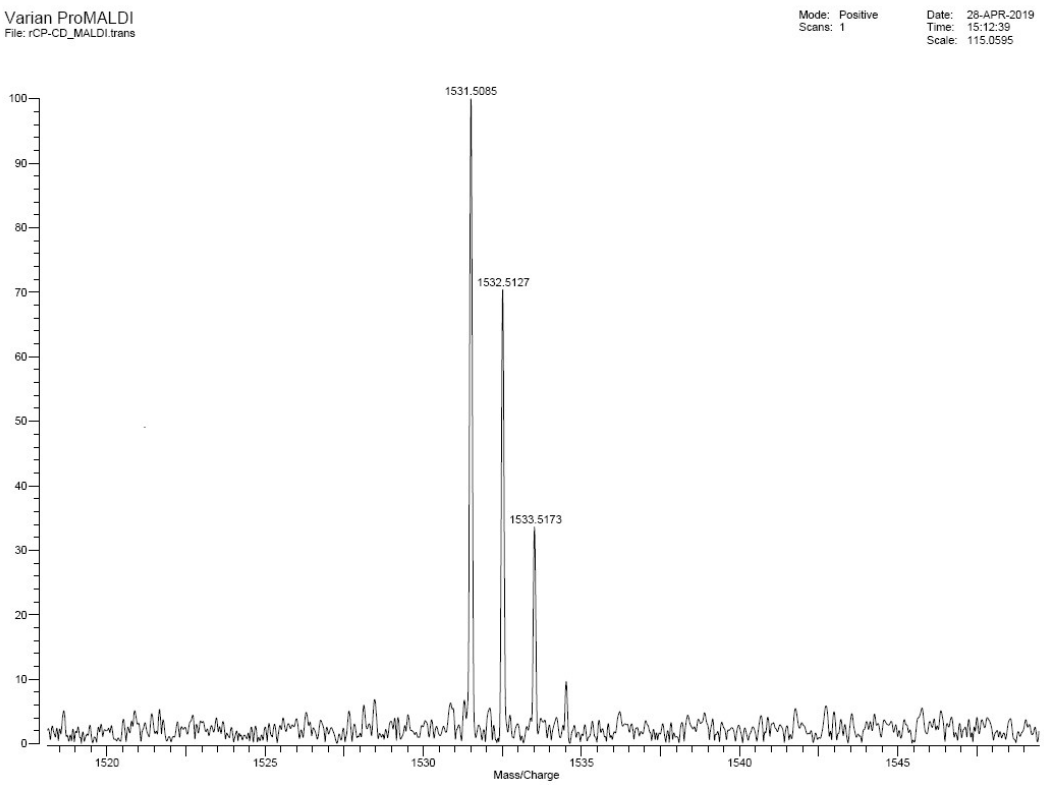



**Figure S53.** HRMS spectrum of **rCP-βCD**.

## 5. References

[1] G. J. Kim, K. Lee, H. Kwon, H. J. Kim, *Org. Lett.* **2011**, *13*, 2799-27801.
[2] H. L. Sun, Y. Chen, X. Han, Y. Liu, *Angew. Chem. Int. Ed.* **2017**, *56*, 7062-7065.
[3] Z. Y. Gu, D. S. Guo, M. Sun, Y. Liu, *J. Org. Chem.* **2010**, *75*, 3600-3607.

## 6. Author contributions

Z. Liu and Prof. Y. Liu conceived and directed the study. Z. Liu performed all experiments. H. Zhang performed the DFT calculations. W. Zhou, J. Li, X. Dai and Y. Liu calculated the bonding constant. Z. Liu wrote the main manuscript and prepared the Figures. Prof. Y. Liu supervised the work and edited the manuscript. All authors analyzed and discussed the results. All authors reviewed the manuscript.

## 7. The Cartesian coordinates of the optimized structures discussed in the text

**R**

| | | | |
|---|---|---|---|
| C | -4.83055200 | -5.02260100 | -2.49774500 |
| C | -5.38963900 | -5.94254900 | -1.40965000 |
| C | -4.74508000 | -5.63705500 | -0.06667500 |
| C | -3.22902100 | -5.64061500 | -0.20423900 |
| C | -2.82560300 | -4.67209600 | -1.31161800 |
| C | -6.58032800 | -0.32446700 | -4.15981100 |
| C | -7.63858900 | -1.25185800 | -3.56828900 |
| C | -7.01193000 | -2.23235600 | -2.59084500 |

| | | | |
|---|---|---|---|
| C | -5.81735700 | -2.92297200 | -3.23668000 |
| C | -4.83333000 | -1.87829500 | -3.75607600 |
| C | -3.58312700 | -2.42991800 | -4.42636600 |
| C | -4.77313400 | 4.43703600 | -2.92009600 |
| C | -6.27284100 | 4.21786500 | -3.13569900 |
| C | -6.63709100 | 2.79047600 | -2.77251100 |
| C | -5.74533500 | 1.83533500 | -3.54829100 |
| C | -4.27181900 | 2.12926600 | -3.27373800 |
| C | -3.30631600 | 1.25378100 | -4.06089800 |
| C | -2.59143700 | 6.14337800 | 1.58460800 |
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| O | -3.42268600 | -5.11549700 | -2.53426300 |
| O | -8.61015600 | -0.42570500 | -2.95415800 |
| O | -7.99256500 | -3.17495200 | -2.20594900 |
| O | -5.23769500 | -3.71238600 | -2.20933500 |
| O | -5.51780300 | -1.06730000 | -4.72208700 |
| O | -2.53896600 | -2.40153600 | -3.46609800 |
| O | -6.96477500 | 5.16172400 | -2.33816800 |
| O | -7.99915600 | 2.57591900 | -3.09094400 |
| O | -6.10993800 | 0.52052300 | -3.14723100 |
| O | -4.03068500 | 3.49396200 | -3.65695900 |
| O | -3.66527800 | 1.09687900 | -5.42327800 |
| O | -4.67419200 | 6.46698300 | 2.68692300 |
| O | -6.04972600 | 5.92197000 | 0.24255000 |
| O | -4.49767500 | 4.31017300 | -1.54751500 |
| O | -1.95594800 | 6.16949600 | 0.32654800 |
| O | -0.23577900 | 5.13618100 | -1.56292700 |
| O | -2.63620100 | 2.42626000 | 6.24148700 |
| C | -4.06564700 | 6.49721800 | 1.40797100 |
| C | -4.71742300 | 5.50423200 | 0.46198700 |
| C | -3.94151300 | 5.41556700 | -0.84574900 |
| C | -2.45052200 | 5.18734700 | -0.59121200 |
| C | -1.61160400 | 5.33529500 | -1.84520200 |
| C | -0.59280700 | 2.70670900 | 5.08203800 |
| C | -1.90253500 | 3.37448800 | 5.48646800 |
| C | -2.66507500 | 3.83505600 | 4.25629600 |
| C | -1.76592300 | 4.66417400 | 3.34451800 |
| C | -0.47827600 | 3.90477700 | 3.03765000 |
| C | 0.52970500 | 4.69467200 | 2.22986800 |
| C | 0.64831000 | -2.33494900 | 4.47296100 |
| C | 0.16994200 | -1.76247500 | 5.80873700 |
| C | -0.73603600 | -0.57016100 | 5.56272900 |
| C | -0.01165100 | 0.42643200 | 4.67257800 |
| C | 0.41893000 | -0.23757400 | 3.36873500 |
| C | 1.17256800 | 0.69587300 | 2.44061800 |
| C | -1.88102900 | -6.09586100 | 1.75914500 |
| C | -2.28147200 | -6.00411300 | 3.22823000 |
| C | -1.99192600 | -4.60990500 | 3.75377300 |
| C | -0.54400800 | -4.22235300 | 3.48141200 |
| C | -0.17386700 | -4.45431800 | 2.01579200 |
| C | 1.30933000 | -4.27697700 | 1.75668800 |
| O | -6.79265100 | -5.75398000 | -1.37281900 |

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| O | -5.18567100 | -6.60419600 | 0.86547700 |
| O | -3.78806000 | 4.58211700 | 4.67836500 |
| O | -2.51944000 | 4.86526400 | 2.15597500 |
| O | 0.16856700 | 3.56476200 | 4.26711400 |
| O | 1.69275700 | 3.91834600 | 1.99559400 |
| O | -0.50358400 | -2.79558500 | 6.50587100 |
| O | -1.06446400 | -0.00045100 | 6.81683800 |
| O | -0.89432600 | 1.50893000 | 4.41495300 |
| O | 1.28350500 | -1.33541600 | 3.70790900 |
| O | 2.16007700 | 1.44099300 | 3.13809200 |
| O | -3.65834400 | -6.32358900 | 3.32086600 |
| O | -2.27696500 | -4.59056500 | 5.13855000 |
| O | -0.46902000 | -2.83308600 | 3.78200500 |
| O | -0.51272800 | -5.79011700 | 1.62061900 |
| O | 1.60220700 | -4.31953600 | 0.36879700 |
| H | -5.18576100 | -5.33207200 | -3.48509200 |
| H | -5.14419900 | -6.97668500 | -1.68761500 |
| H | -5.05086900 | -4.62744300 | 0.24719400 |
| H | -2.87287100 | -6.65038900 | -0.44844100 |
| H | -3.21080800 | -3.67989800 | -1.06406600 |
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| H | -8.07637600 | -1.82229500 | -4.39842800 |
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| H | -4.05623400 | 2.00552000 | -2.20476300 |
| H | -3.21331700 | 0.28243700 | -3.56311200 |
| H | -2.32262100 | 1.73288100 | -4.02765500 |
| H | -2.07856700 | 6.88204900 | 2.20779200 |
| H | -9.31838400 | -0.99435200 | -2.62085800 |
| H | -7.53431500 | -3.90104300 | -1.74264100 |
| H | -1.78024800 | -2.86940400 | -3.83996200 |
| H | -7.90964100 | 4.95714500 | -2.39664000 |
| H | -8.20810500 | 1.65213500 | -2.86535400 |
| H | -4.29786000 | 0.36080700 | -5.46370400 |
| H | -5.63088600 | 6.54336100 | 2.55676700 |
| H | -6.39210500 | 5.43864200 | -0.53410200 |
| H | 0.01759300 | 5.80767600 | -0.91329100 |
| H | -3.41427800 | 2.86790500 | 6.60834200 |
| H | -4.12783100 | 7.50321300 | 0.97256600 |
| H | -4.69357200 | 4.51029100 | 0.93350500 |
| H | -4.08837600 | 6.34527500 | -1.41290800 |
| H | -2.30528200 | 4.18423400 | -0.17004800 |
| H | -1.91201700 | 4.57763600 | -2.57402000 |
| H | -1.78254500 | 6.32941100 | -2.27995800 |
| H | 0.01486000 | 2.50997500 | 5.97006600 |

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| H | -1.65363300 | 4.25279600 | 6.09629400 |
| H | -2.97786100 | 2.94383300 | 3.69026900 |
| H | -1.53750400 | 5.62521900 | 3.82568000 |
| H | -0.74105700 | 2.99084500 | 2.48935000 |
| H | 0.80755100 | 5.59760600 | 2.78808000 |
| H | 0.06903900 | 4.99998900 | 1.28237100 |
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| H | 1.05048400 | -1.42737000 | 6.37333600 |
| H | -1.64384200 | -0.91205500 | 5.04447000 |
| H | 0.88881400 | 0.78541700 | 5.18476900 |
| H | -0.45641200 | -0.61889500 | 2.82833800 |
| H | 0.45482400 | 1.36737700 | 1.95879200 |
| H | 1.63988900 | 0.08608800 | 1.65535100 |
| H | -2.00684500 | -7.11803900 | 1.38968300 |
| H | -1.67594600 | -6.72949300 | 3.78785000 |
| H | -2.63355600 | -3.89676300 | 3.21430600 |
| H | 0.11620800 | -4.79806800 | 4.14525800 |
| H | -0.73464400 | -3.73756300 | 1.40488000 |
| H | 1.85420400 | -5.08816100 | 2.25431200 |
| H | 1.63550700 | -3.32380500 | 2.18836900 |
| H | -7.13077500 | -6.24785900 | -0.61154700 |
| H | -4.78247300 | -6.38682100 | 1.72657200 |
| H | -4.15709800 | 5.03149900 | 3.89404200 |
| H | 1.68342900 | 3.61334600 | 1.04017100 |
| H | -0.91277400 | -2.39133600 | 7.28559100 |
| H | -1.71843700 | 0.70484600 | 6.66213100 |
| H | 2.01683200 | 2.38508000 | 2.91161000 |
| H | -3.94558900 | -6.14549700 | 4.22781600 |
| H | -1.83772600 | -3.80743400 | 5.52271400 |
| H | 1.71494100 | -3.39981200 | 0.08012800 |
| C | -1.31478300 | -4.58721500 | -1.49990200 |
| N | -0.82534600 | -3.22174400 | -1.31845700 |
| H | -1.04529000 | -4.89789600 | -2.51067500 |
| H | -0.78786700 | -5.22202000 | -0.78079900 |
| C | 0.23115800 | -2.64009200 | -1.91956700 |
| N | -1.35803400 | -2.42071100 | -0.40284700 |
| C | 0.32432800 | -1.40829500 | -1.30923700 |
| H | 0.80582700 | -3.13240100 | -2.68947100 |
| N | -0.66454000 | -1.31644500 | -0.38720700 |
| C | 1.29038500 | -0.28823400 | -1.51077000 |
| N | 2.65989000 | -0.74642900 | -1.69395200 |
| H | 1.22914600 | 0.35783400 | -0.62671600 |
| H | 1.03330700 | 0.30619000 | -2.38987500 |
| C | 3.32506800 | -1.30107800 | -0.67418700 |
| H | 3.16194200 | -0.37468100 | -2.48865300 |
| C | 4.81255400 | -1.41533300 | -0.77553700 |
| O | 2.74989300 | -1.70312500 | 0.35235900 |
| C | 5.55163700 | -0.60151900 | -1.56489800 |
| C | 5.36583000 | -2.34284400 | 0.16462400 |
| C | 6.98713500 | -0.48148400 | -1.72166900 |
| H | 5.00700400 | 0.11791300 | -2.17019100 |
| N | 5.79012400 | -3.09829700 | 0.93592900 |

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| C | 7.94542000 | -1.26081000 | -1.13840800 |
| C | 7.39930000 | 0.62326900 | -2.60107100 |
| C | 9.33143400 | -0.99770700 | -1.33913500 |
| H | 7.67968800 | -2.09868900 | -0.50199600 |
| O | 8.73277000 | 0.85601200 | -2.75062500 |
| O | 6.64435600 | 1.34933500 | -3.21879300 |
| C | 9.69444500 | 0.08947600 | -2.14442700 |
| C | 10.36251800 | -1.76039200 | -0.76041800 |
| C | 11.01591500 | 0.42580500 | -2.38314400 |
| C | 11.68471300 | -1.43245200 | -0.97560200 |
| H | 10.09675500 | -2.60396300 | -0.13096100 |
| C | 12.03118700 | -0.32757700 | -1.78676100 |
| H | 11.24922700 | 1.25813100 | -3.03663200 |
| H | 12.46191300 | -2.02728900 | -0.51039400 |
| N | 13.37830600 | 0.05868400 | -2.01887100 |
| C | 13.81334600 | 1.15059800 | -1.11618600 |
| C | 14.35347100 | -1.04021600 | -1.95666100 |
| H | 13.79765500 | 0.79559400 | -0.07266200 |
| H | 14.85801200 | 1.35069300 | -1.36967200 |
| C | 13.02497500 | 2.44407900 | -1.22802300 |
| H | 15.32743300 | -0.58918500 | -2.16676200 |
| H | 14.42626900 | -1.46550200 | -0.94317700 |
| C | 14.08673800 | -2.13164100 | -2.98082400 |
| H | 12.99904700 | 2.80196600 | -2.26103700 |
| H | 11.99876000 | 2.33961300 | -0.86930500 |
| H | 13.51549900 | 3.20495900 | -0.61510400 |
| H | 13.14688700 | -2.65725900 | -2.79480500 |
| H | 14.04876600 | -1.70905200 | -3.98846800 |
| H | 14.89352900 | -2.86803400 | -2.94804200 |
| C | 3.99068700 | 2.82438400 | -1.99460900 |
| N | 1.98229500 | 3.24723100 | -0.59653300 |
| C | 3.44174100 | 3.21156200 | -0.63173200 |
| C | 3.91413700 | 2.15543400 | 0.37415500 |
| S | 5.73982200 | 2.05748600 | 0.46500200 |
| O | 3.50503700 | 1.94615200 | -2.68250600 |
| O | 5.08587700 | 3.50133400 | -2.32523000 |
| H | 3.51601100 | 1.18025100 | 0.07148500 |
| H | 3.52000400 | 2.40302600 | 1.35877500 |
| H | 5.72041200 | 0.95866500 | 1.24315400 |
| H | 1.61983600 | 3.99087600 | -1.19233600 |
| H | 1.61919000 | 2.37297000 | -0.97337700 |
| H | 3.82863900 | 4.19542300 | -0.35561000 |
| H | 5.50458300 | 3.06451500 | -3.09188900 |
| O | 4.27473600 | -0.33223200 | 2.40264300 |
| H | 3.67906500 | 0.37906500 | 2.69960000 |
| H | 3.69825800 | -0.92586600 | 1.89549100 |

**INT1**

| | | | |
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| C | 3.98678900 | 5.47560100 | -2.18614600 |
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| C | 3.89553400 | 5.99080500 | 0.26926800 |
| C | 2.39576600 | 5.75147800 | 0.17764300 |

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| C | 2.11470100 | 4.75291200 | -0.94153200 |
| C | 6.47258300 | 1.28141300 | -4.19702900 |
| C | 7.37340100 | 2.33107900 | -3.55117400 |
| C | 6.61735100 | 3.11690000 | -2.49161500 |
| C | 5.30282000 | 3.63118200 | -3.06493000 |
| C | 4.49898300 | 2.46901700 | -3.64059900 |
| C | 3.14490400 | 2.83358700 | -4.23175300 |
| C | 5.48751300 | -3.78252200 | -3.26948900 |
| C | 6.93620700 | -3.31833000 | -3.43570100 |
| C | 7.05856000 | -1.87210400 | -2.99416000 |
| C | 6.03270200 | -1.02862200 | -3.73389800 |
| C | 4.62355400 | -1.57360400 | -3.51003500 |
| C | 3.53176700 | -0.81991900 | -4.25656000 |
| C | 3.37408300 | -5.97180900 | 1.05942400 |
| O | 1.97354400 | 5.21838600 | 1.42275900 |
| O | 2.58450300 | 5.32348400 | -2.16752800 |
| O | 8.48816900 | 1.63955000 | -3.01963100 |
| O | 7.43336300 | 4.18775200 | -2.06057400 |
| O | 4.62539800 | 4.24399500 | -1.97842700 |
| O | 5.28259500 | 1.87012200 | -4.68306100 |
| O | 2.16630400 | 2.56725100 | -3.23832600 |
| O | 7.75752500 | -4.17854800 | -2.66682700 |
| O | 8.37105200 | -1.42358500 | -3.27479900 |
| O | 6.18251500 | 0.29806700 | -3.24489500 |
| O | 4.61897100 | -2.93123500 | -3.98246000 |
| O | 3.87021300 | -0.50713900 | -5.59672800 |
| O | 5.47224400 | -6.26334500 | 2.13825600 |
| O | 6.80946500 | -5.42559600 | -0.25655100 |
| O | 5.18348400 | -3.76875500 | -1.89942600 |
| O | 2.73596500 | -5.89345300 | -0.19532800 |
| O | 0.95148600 | -4.60380600 | -1.93305100 |
| O | 3.04322000 | -2.78821500 | 6.09762100 |
| C | 4.86782400 | -6.21746900 | 0.85779300 |
| C | 5.45730700 | -5.10809800 | 0.00522500 |
| C | 4.66935200 | -4.94434700 | -1.28808900 |
| C | 3.17672100 | -4.79172200 | -0.99761600 |
| C | 2.32046400 | -4.80465100 | -2.24722100 |
| C | 1.05505600 | -3.13230700 | 4.86442200 |
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| C | 3.24231300 | -3.95396300 | 3.96705300 |
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| C | 1.09108900 | -4.09389000 | 2.69396300 |
| C | 0.18773700 | -4.88404400 | 1.77402300 |
| C | -0.79949800 | 1.75466700 | 4.75386300 |
| C | -0.22639700 | 1.13799800 | 6.03247900 |
| C | 0.81864400 | 0.09181900 | 5.68458300 |
| C | 0.22806700 | -0.90072700 | 4.69434200 |
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| C | -0.85950600 | -1.05375300 | 2.39327000 |
| C | 1.05149900 | 5.95879900 | 2.18045800 |
| C | 1.48673200 | 5.89576600 | 3.64164200 |
| C | 1.42716500 | 4.45965800 | 4.12438400 |

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| C | 0.05801500 | 3.85231200 | 3.85044100 |
| C | -0.37675000 | 4.06326400 | 2.39963300 |
| C | -1.82502700 | 3.67940500 | 2.16239300 |
| O | 5.84683300 | 6.47870300 | -1.09803900 |
| O | 4.20255600 | 6.99094300 | 1.22036500 |
| O | 4.42691600 | -4.63656100 | 4.32650600 |
| O | 3.22851000 | -4.77440000 | 1.77412800 |
| O | 0.39066400 | -3.95148500 | 3.93276700 |
| O | -1.03829100 | -4.19475100 | 1.60658500 |
| O | 0.32252300 | 2.19433400 | 6.80075200 |
| O | 1.22015100 | -0.54990800 | 6.88089700 |
| O | 1.24230400 | -1.83616100 | 4.35810100 |
| O | -1.29042200 | 0.74984100 | 3.89439900 |
| O | -1.82361300 | -1.95142100 | 2.94544800 |
| O | 2.79820100 | 6.42515300 | 3.72059900 |
| O | 1.71802800 | 4.43513900 | 5.50852500 |
| O | 0.22871900 | 2.46734100 | 4.12138700 |
| O | -0.25470000 | 5.44796100 | 2.04734500 |
| O | -2.16150900 | 3.74531700 | 0.78462600 |
| H | 4.23743900 | 5.88147300 | -3.17057300 |
| H | 4.01162700 | 7.42672100 | -1.31144900 |
| H | 4.37375000 | 5.03697600 | 0.53948900 |
| H | 1.87534600 | 6.69492100 | -0.03573100 |
| H | 2.66336100 | 3.82894800 | -0.73758100 |
| H | 6.96959700 | 0.84388300 | -5.06800700 |
| H | 7.68401000 | 3.02847600 | -4.34074400 |
| H | 6.38050900 | 2.44228700 | -1.65426200 |
| H | 5.50724200 | 4.36718600 | -3.85445500 |
| H | 4.32915200 | 1.73654800 | -2.84130300 |
| H | 2.98266600 | 2.20781600 | -5.11946700 |
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| H | 3.26949800 | 0.08290500 | -3.69409200 |
| H | 2.64330900 | -1.45952700 | -4.27604800 |
| H | 2.90616700 | -6.80432200 | 1.59363500 |
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| H | 6.86837800 | 4.80245300 | -1.55575600 |
| H | 1.32828500 | 2.94640300 | -3.53552500 |
| H | 8.65004700 | -3.80256400 | -2.66431300 |
| H | 8.41920500 | -0.48756400 | -3.01076200 |
| H | 4.35982500 | 0.33147300 | -5.57157300 |
| H | 6.43171400 | -6.27379500 | 2.00672300 |
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| H | 0.66354300 | -5.36815700 | -1.41461300 |
| H | 3.85102900 | -3.19485800 | 6.43982200 |
| H | 4.99098500 | -7.17524700 | 0.33502800 |
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| H | 4.84020600 | -5.81896100 | -1.93106000 |

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| H | 3.00840800 | -3.85106300 | -0.45707400 |
| H | 2.63009700 | -3.98481200 | -2.90119600 |
| H | 2.46984700 | -5.75304900 | -2.78072200 |
| H | 0.41901800 | -3.10723600 | 5.75407400 |
| H | 2.25161200 | -4.67339200 | 5.72173900 |
| H | 3.47526700 | -2.98021600 | 3.50880800 |
| H | 2.29156500 | -5.78221800 | 3.33160400 |
| H | 1.27846400 | -3.10638900 | 2.25374400 |
| H | 0.01199700 | -5.87782700 | 2.20994100 |
| H | 0.69428900 | -5.01248400 | 0.81119200 |
| H | -1.64603600 | 2.40923700 | 4.98378700 |
| H | -1.04662800 | 0.64897200 | 6.57509100 |
| H | 1.67566100 | 0.59081400 | 5.20850300 |
| H | -0.62560400 | -1.41528900 | 5.15160700 |
| H | 0.55179300 | 0.40138000 | 2.99569300 |
| H | -0.05816700 | -1.61952200 | 1.91249300 |
| H | -1.33398300 | -0.41783900 | 1.63687700 |
| H | 1.01198200 | 6.99650800 | 1.83585800 |
| H | 0.78520700 | 6.50264500 | 4.22934600 |
| H | 2.16946100 | 3.87550100 | 3.56025700 |
| H | -0.67581200 | 4.29207900 | 4.54070800 |
| H | 0.26993900 | 3.45750900 | 1.75202400 |
| H | -2.46773600 | 4.37833800 | 2.71090200 |
| H | -1.99804700 | 2.66990900 | 2.55148600 |
| H | 6.13125900 | 6.98874100 | -0.32555400 |
| H | 3.86175700 | 6.69102600 | 2.08341600 |
| H | 4.83198300 | -4.97551800 | 3.50556400 |
| H | -1.28575300 | -4.18053000 | 0.63396200 |
| H | 0.77578700 | 1.79353800 | 7.55694800 |
| H | 1.93736300 | -1.16959500 | 6.65700100 |
| H | -1.63565300 | -2.84072800 | 2.56121000 |
| H | 3.13075400 | 6.26906300 | 4.61596200 |
| H | 1.44748800 | 3.56170100 | 5.84965900 |
| H | -2.14012100 | 2.83511500 | 0.45031900 |
| C | 0.63079000 | 4.43473600 | -1.08546300 |
| N | 0.36556700 | 2.99837600 | -1.01352200 |
| H | 0.26722100 | 4.78217000 | -2.05394100 |
| H | 0.04431900 | 4.91451100 | -0.29629000 |
| C | -0.60086200 | 2.31511300 | -1.65604800 |
| N | 1.02033400 | 2.21663900 | -0.16145500 |
| C | -0.50697400 | 1.03878500 | -1.14352700 |
| H | -1.25325500 | 2.77652100 | -2.38209500 |
| N | 0.49633200 | 1.02261100 | -0.23295000 |
| C | -1.34974700 | -0.16392100 | -1.43127900 |
| N | -2.75653600 | 0.19891300 | -1.54369200 |
| H | -1.20680500 | -0.89686400 | -0.62919900 |
| H | -1.06822700 | -0.63573900 | -2.37445400 |
| C | -3.42936300 | 0.68616300 | -0.50510200 |
| H | -3.24422800 | -0.05653400 | -2.39184800 |
| C | -4.89666700 | 0.90755700 | -0.65377400 |
| O | -2.87475300 | 0.96581800 | 0.57940300 |
| C | -5.65409400 | 0.08775900 | -1.41611600 |

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|---|---|---|---|
| C | -5.39659000 | 1.91387100 | 0.23116800 |
| C | -7.09161000 | 0.03718800 | -1.60316800 |
| H | -5.12357900 | -0.68103300 | -1.97067000 |
| N | -5.76453900 | 2.73990300 | 0.95849400 |
| C | -8.01774500 | 0.85240300 | -1.02158000 |
| C | -7.54293300 | -1.02117400 | -2.51878700 |
| C | -9.41369900 | 0.68086000 | -1.26945900 |
| H | -7.72175600 | 1.65202700 | -0.35031900 |
| O | -8.88277000 | -1.16367300 | -2.71671500 |
| O | -6.81611800 | -1.78056100 | -3.12958900 |
| C | -9.81266000 | -0.35162400 | -2.12379900 |
| C | -10.41050200 | 1.48932100 | -0.68945400 |
| C | -11.14990800 | -0.59988800 | -2.40906500 |
| C | -11.74167300 | 1.25659000 | -0.96356900 |
| H | -10.10792700 | 2.29247800 | -0.02481000 |
| C | -12.12017700 | 0.20615500 | -1.82659200 |
| H | -11.42345100 | -1.41065200 | -3.07431600 |
| H | -12.50532500 | 1.88197500 | -0.51230100 |
| N | -13.50072900 | -0.06144900 | -2.12433200 |
| C | -14.24780400 | -0.42150000 | -0.90563400 |
| C | -14.13846700 | 1.09173100 | -2.78470500 |
| H | -14.28240800 | 0.42198600 | -0.19637400 |
| H | -15.27893400 | -0.61296000 | -1.21866300 |
| C | -13.68249300 | -1.65362600 | -0.21922600 |
| H | -15.17566100 | 0.80234400 | -2.98089900 |
| H | -14.17446600 | 1.96603200 | -2.11381800 |
| C | -13.45432200 | 1.46589900 | -4.08878900 |
| H | -13.63017600 | -2.49535600 | -0.91565400 |
| H | -12.67843000 | -1.47124200 | 0.17440100 |
| H | -14.32430200 | -1.93790000 | 0.61830100 |
| H | -12.43760600 | 1.83222800 | -3.92011500 |
| H | -13.40136500 | 0.60360100 | -4.75953600 |
| H | -14.01743000 | 2.25785500 | -4.58866100 |
| C | -4.00788200 | -3.31445200 | -2.04073700 |
| N | -1.90018100 | -4.04360000 | -0.96150800 |
| C | -3.35406900 | -3.91643700 | -0.81234900 |
| C | -3.62665800 | -2.99949600 | 0.38638900 |
| S | -5.36995400 | -2.51360200 | 0.65832500 |
| O | -3.54090900 | -2.36452400 | -2.64499400 |
| O | -5.14996100 | -3.90437100 | -2.37885600 |
| H | -3.00491000 | -2.09985200 | 0.25555800 |
| H | -3.25874300 | -3.52432600 | 1.26933000 |
| H | -4.66271300 | -1.35143500 | 1.78327100 |
| H | -1.67071400 | -4.77406500 | -1.63295900 |
| H | -1.53443900 | -3.17332400 | -1.35057000 |
| H | -3.78572300 | -4.90317200 | -0.63256800 |
| H | -5.60532300 | -3.34842400 | -3.04087100 |
| O | -4.00238100 | -0.72604200 | 2.44496300 |
| H | -3.17635500 | -1.29040200 | 2.68625100 |
| H | -3.66842500 | 0.03127000 | 1.90622600 |

**TS**

| | | | |
|---|---|---|---|
| C | 4.68375300 | 5.02846800 | -2.55085400 |
| C | 5.21724600 | 6.00167200 | -1.49693700 |
| C | 4.59052800 | 5.71594200 | -0.14231300 |
| C | 3.07468300 | 5.67411500 | -0.27148600 |
| C | 2.68774600 | 4.66018000 | -1.34481200 |
| C | 6.65833500 | 0.38771500 | -4.10999800 |
| C | 7.66457000 | 1.36910900 | -3.51483100 |
| C | 6.98257600 | 2.33331400 | -2.55750200 |
| C | 5.76415600 | 2.95636500 | -3.22703100 |
| C | 4.83605500 | 1.85795700 | -3.73756500 |
| C | 3.56354200 | 2.34094300 | -4.41798300 |
| C | 5.04452500 | -4.43149800 | -2.82808700 |
| C | 6.53982100 | -4.15343400 | -2.99943600 |
| C | 6.83033800 | -2.70333600 | -2.65977600 |
| C | 5.92121200 | -1.80392500 | -3.48109600 |
| C | 4.45468700 | -2.15744700 | -3.24495500 |
| C | 3.47356400 | -1.33839700 | -4.07218400 |
| C | 2.71033800 | -6.08870300 | 1.61828000 |
| O | 2.55361200 | 5.26780000 | 0.98465200 |
| O | 3.27378300 | 5.07406100 | -2.58363300 |
| O | 8.66304900 | 0.59335100 | -2.87823900 |
| O | 7.91603700 | 3.32516700 | -2.17958800 |
| O | 5.13466200 | 3.74078500 | -2.22514800 |
| O | 5.56717800 | 1.07338300 | -4.69082300 |
| O | 2.52521800 | 2.30365800 | -3.45107300 |
| O | 7.24313300 | -5.04811900 | -2.15629100 |
| O | 8.19029300 | -2.43545000 | -2.94535300 |
| O | 6.21801100 | -0.46833400 | -3.09382600 |
| O | 4.28795100 | -3.53748100 | -3.61130800 |
| O | 3.86223900 | -1.18378800 | -5.42649500 |
| O | 4.76041700 | -6.42565700 | 2.77891000 |
| O | 6.20800000 | -5.89437400 | 0.37211000 |
| O | 4.72542800 | -4.28682400 | -1.46787600 |
| O | 2.10937600 | -6.10239900 | 0.34302100 |
| O | 0.46030500 | -4.98116700 | -1.58488700 |
| O | 2.56413300 | -2.45745700 | 6.33411900 |
| C | 4.18723800 | -6.45251400 | 1.48375800 |
| C | 4.87319900 | -5.46698200 | 0.55477300 |
| C | 4.13426200 | -5.37750300 | -0.77348100 |
| C | 2.64287600 | -5.12301700 | -0.55597600 |
| C | 1.83275600 | -5.24060400 | -1.83078200 |
| C | 0.58813600 | -2.66351300 | 5.05287500 |
| C | 1.85650500 | -3.37163400 | 5.51552600 |
| C | 2.67768400 | -3.82526500 | 4.32125200 |
| C | 1.81194100 | -4.61061400 | 3.34036900 |
| C | 0.57002400 | -3.80307300 | 2.97279600 |
| C | -0.40498100 | -4.53585400 | 2.07877200 |
| C | -0.66371800 | 2.37144500 | 4.45806700 |
| C | -0.21017000 | 1.80045100 | 5.80422000 |
| C | 0.71835600 | 0.61811500 | 5.58604600 |
| C | 0.05325300 | -0.37728700 | 4.64693300 |
| C | -0.29351200 | 0.31539100 | 3.33406400 |

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|---|---|---|---|
| C | -0.92217700 | -0.58221800 | 2.29607900 |
| C | 1.71336500 | 6.15667900 | 1.67515700 |
| C | 2.11497000 | 6.14028200 | 3.14788700 |
| C | 1.87932800 | 4.75676800 | 3.72172500 |
| C | 0.45239500 | 4.29662000 | 3.45707900 |
| C | 0.07220800 | 4.45671400 | 1.98471000 |
| C | -1.40382000 | 4.21648500 | 1.73208400 |
| O | 6.62617500 | 5.86385500 | -1.46298700 |
| O | 5.00648400 | 6.72164900 | 0.75964600 |
| O | 3.75319800 | -4.61300100 | 4.78998400 |
| O | 2.63151200 | -4.81457100 | 2.19739100 |
| O | -0.14440900 | -3.47595600 | 4.16769000 |
| O | -1.52678600 | -3.70908000 | 1.80395700 |
| O | 0.42879100 | 2.84729800 | 6.51303400 |
| O | 0.99578500 | 0.03401800 | 6.84519800 |
| O | 0.95516700 | -1.45347900 | 4.44203300 |
| O | -1.22634900 | 1.35975600 | 3.65080800 |
| O | -1.98811700 | -1.36025700 | 2.85651100 |
| O | 3.47808400 | 6.51846800 | 3.22476000 |
| O | 2.14585200 | 4.78830900 | 5.11060700 |
| O | 0.45684900 | 2.92185900 | 3.82126800 |
| O | 0.35846100 | 5.79192900 | 1.54561800 |
| O | -1.69543000 | 4.19245600 | 0.34363400 |
| H | 5.02365200 | 5.31806000 | -3.54947500 |
| H | 4.93477500 | 7.01737400 | -1.80582900 |
| H | 4.92672500 | 4.72480900 | 0.19830400 |
| H | 2.69173400 | 6.66594600 | -0.54686400 |
| H | 3.08876400 | 3.68248500 | -1.06379600 |
| H | 7.12335400 | -0.18029800 | -4.92116200 |
| H | 8.08838800 | 1.94951700 | -4.34525100 |
| H | 6.63289900 | 1.76853300 | -1.67931200 |
| H | 6.08474900 | 3.58958100 | -4.06529000 |
| H | 4.54502400 | 1.22773200 | -2.88768300 |
| H | 3.34594400 | 1.66109100 | -5.25252200 |
| H | 3.69317800 | 3.35376600 | -4.82039800 |
| H | 4.79437800 | -5.43713100 | -3.18006100 |
| H | 6.80127200 | -4.32944500 | -4.05149500 |
| H | 6.61867800 | -2.53729200 | -1.59318700 |
| H | 6.13996500 | -1.94487200 | -4.54717400 |
| H | 4.20188900 | -2.02699700 | -2.18493200 |
| H | 3.32352000 | -0.36530500 | -3.59161900 |
| H | 2.51177500 | -1.86113200 | -4.05732800 |
| H | 2.17521000 | -6.82769200 | 2.22206000 |
| H | 9.34509300 | 1.19503100 | -2.54882900 |
| H | 7.42095400 | 4.04606800 | -1.74663300 |
| H | 1.76313200 | 2.77218700 | -3.81731000 |
| H | 8.17918000 | -4.80160900 | -2.18542000 |
| H | 8.34988200 | -1.49631500 | -2.74386800 |
| H | 4.45092400 | -0.41187100 | -5.46149600 |
| H | 5.72056300 | -6.49752600 | 2.67367200 |
| H | 6.58328900 | -5.39038800 | -0.37549700 |
| H | 0.15403800 | -5.65490500 | -0.96093500 |

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|---|---|---|---|
| H | 3.31850800 | -2.92118500 | 6.72270900 |
| H | 4.25369800 | -7.45958000 | 1.05126800 |
| H | 4.84371300 | -4.47139000 | 1.02255000 |
| H | 4.28023300 | -6.31362800 | -1.33011900 |
| H | 2.50671600 | -4.12010100 | -0.13074300 |
| H | 2.18441100 | -4.49743900 | -2.55171400 |
| H | 1.97509600 | -6.24162000 | -2.26006900 |
| H | -0.06736600 | -2.47774800 | 5.90872300 |
| H | 1.55178300 | -4.25711600 | 6.08878500 |
| H | 3.04637800 | -2.93126900 | 3.79454500 |
| H | 1.52442000 | -5.57218900 | 3.78717800 |
| H | 0.89819000 | -2.88498100 | 2.46989800 |
| H | -0.73395800 | -5.45532700 | 2.58088500 |
| H | 0.10217000 | -4.80890000 | 1.14651800 |
| H | -1.44440300 | 3.12507900 | 4.60033000 |
| H | -1.09997500 | 1.45163600 | 6.34565300 |
| H | 1.64553600 | 0.97561200 | 5.11404200 |
| H | -0.87859800 | -0.74368300 | 5.09486600 |
| H | 0.60666000 | 0.75108500 | 2.88268600 |
| H | -0.16807500 | -1.25367000 | 1.88130400 |
| H | -1.31251300 | 0.04516600 | 1.48691600 |
| H | 1.80044300 | 7.16754700 | 1.26564400 |
| H | 1.48021500 | 6.86282900 | 3.67784200 |
| H | 2.55493500 | 4.05333000 | 3.21241100 |
| H | -0.23590100 | 4.86363800 | 4.09980900 |
| H | 0.65949300 | 3.74118700 | 1.39703700 |
| H | -1.97647300 | 5.02672500 | 2.19986400 |
| H | -1.69761700 | 3.27045900 | 2.19904200 |
| H | 6.95050000 | 6.39264600 | -0.71924700 |
| H | 4.60428500 | 6.52436100 | 1.62610300 |
| H | 4.16397200 | -5.04479500 | 4.01660000 |
| H | -1.65990200 | -3.64454500 | 0.80211900 |
| H | 0.80284600 | 2.46042800 | 7.31828900 |
| H | 1.64793500 | -0.67572600 | 6.70544000 |
| H | -1.87139100 | -2.30712900 | 2.53498900 |
| H | 3.77322800 | 6.39161100 | 4.13770400 |
| H | 1.75994600 | 3.98119200 | 5.50067500 |
| H | -1.82189800 | 3.26023600 | 0.10191800 |
| C | 1.17812700 | 4.55059500 | -1.52998800 |
| N | 0.70353900 | 3.17764800 | -1.36625200 |
| H | 0.90069200 | 4.87254800 | -2.53508400 |
| H | 0.64459200 | 5.16772700 | -0.80069900 |
| C | -0.34373400 | 2.59345200 | -1.98012700 |
| N | 1.21974200 | 2.38159000 | -0.43619900 |
| C | -0.44918000 | 1.36396800 | -1.36622300 |
| H | -0.90725800 | 3.08326000 | -2.75972000 |
| N | 0.52668800 | 1.27640600 | -0.42864800 |
| C | -1.42062000 | 0.25131900 | -1.58966900 |
| N | -2.79962800 | 0.71249300 | -1.67228600 |
| H | -1.30866800 | -0.46643800 | -0.76721900 |
| H | -1.20755600 | -0.27307700 | -2.52317100 |
| C | -3.44393500 | 1.17625300 | -0.58927400 |

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|---|---|---|---|
| H | -3.34134300 | 0.37350600 | -2.45605300 |
| C | -4.91313500 | 1.22173700 | -0.61212200 |
| O | -2.81187400 | 1.54886200 | 0.43309100 |
| C | -5.63534900 | 0.21488000 | -1.23229700 |
| C | -5.47319800 | 2.12554500 | 0.33039600 |
| C | -7.08364200 | 0.15266800 | -1.45438600 |
| H | -5.08530000 | -0.40509500 | -1.92889900 |
| N | -5.90751300 | 2.87892700 | 1.10438900 |
| C | -8.04423700 | 0.80904700 | -0.75409000 |
| C | -7.48220600 | -0.74963700 | -2.54558800 |
| C | -9.43548500 | 0.62956000 | -1.05449300 |
| H | -7.78840900 | 1.47208500 | 0.06577100 |
| O | -8.81241800 | -0.91004700 | -2.79002100 |
| O | -6.71701500 | -1.36266100 | -3.26567100 |
| C | -9.78330100 | -0.25241900 | -2.07953300 |
| C | -10.47267600 | 1.27875600 | -0.36005300 |
| C | -11.10604500 | -0.50393800 | -2.42625000 |
| C | -11.79170900 | 1.04216700 | -0.69207300 |
| H | -10.21388900 | 1.96537900 | 0.44006500 |
| C | -12.11742100 | 0.14516100 | -1.72982900 |
| H | -11.33600700 | -1.19688300 | -3.22751000 |
| H | -12.58551600 | 1.54747200 | -0.15084000 |
| N | -13.48301200 | -0.12381100 | -2.09360300 |
| C | -14.22512400 | -0.72675800 | -0.97250400 |
| C | -14.16589900 | 1.09903400 | -2.55072700 |
| H | -14.30545400 | -0.02568500 | -0.12499000 |
| H | -15.24363300 | -0.90396300 | -1.33241200 |
| C | -13.61147800 | -2.03601200 | -0.50535300 |
| H | -15.18763700 | 0.80623700 | -2.81244200 |
| H | -14.24671500 | 1.83871500 | -1.73690100 |
| C | -13.48784000 | 1.72724600 | -3.75670800 |
| H | -13.51262400 | -2.73673100 | -1.33935400 |
| H | -12.62124700 | -1.88330800 | -0.06679300 |
| H | -14.24866000 | -2.49316800 | 0.25575400 |
| H | -12.49029700 | 2.10089500 | -3.50866300 |
| H | -13.38963700 | 1.00033900 | -4.56806400 |
| H | -14.08156800 | 2.57029700 | -4.11864600 |
| C | -4.05979900 | -2.88943000 | -2.15118400 |
| N | -2.07970200 | -3.51806700 | -0.80342100 |
| C | -3.53651100 | -3.35514100 | -0.80653600 |
| C | -3.89677000 | -2.29363800 | 0.23961000 |
| S | -5.65094200 | -1.80247100 | 0.32835800 |
| O | -3.55818300 | -1.97009900 | -2.77436600 |
| O | -5.13505100 | -3.55236500 | -2.56390400 |
| H | -3.26992200 | -1.40884100 | 0.04401500 |
| H | -3.60030100 | -2.68742100 | 1.21432100 |
| H | -4.65788300 | -0.52551700 | 1.78928000 |
| H | -1.79816300 | -4.30903600 | -1.37982600 |
| H | -1.65577700 | -2.69040300 | -1.22392100 |
| H | -4.00615700 | -4.30673500 | -0.55088200 |
| H | -5.51975000 | -3.07731300 | -3.32496200 |
| O | -3.96111000 | -0.05071900 | 2.33581900 |

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|---|---|---|---|
| H | -3.11574900 | -0.73418300 | 2.58584000 |
| H | -3.58534700 | 0.67544500 | 1.77013800 |

**INT2**

| | | | |
|---|---|---|---|
| C | 4.46335000 | 5.25407200 | -2.60558000 |
| C | 5.25009000 | 6.03014800 | -1.54648700 |
| C | 4.82813000 | 5.61231700 | -0.14468000 |
| C | 3.31212800 | 5.66663700 | -0.01263400 |
| C | 2.68742100 | 4.83059300 | -1.12482200 |
| C | 5.43503200 | 0.59897600 | -4.90330400 |
| C | 6.67863100 | 1.37349400 | -4.47433200 |
| C | 6.34843300 | 2.33068400 | -3.34227400 |
| C | 5.13715000 | 3.18097400 | -3.70428800 |
| C | 3.96428100 | 2.28989400 | -4.10539600 |
| C | 2.69654400 | 3.02609200 | -4.52348600 |
| C | 3.50621100 | -4.11211200 | -3.68012100 |
| C | 4.91356200 | -3.95350300 | -4.26050600 |
| C | 5.48809800 | -2.60593500 | -3.86518700 |
| C | 4.51347400 | -1.51614900 | -4.27679800 |
| C | 3.14359600 | -1.75253100 | -3.64581500 |
| C | 2.09931100 | -0.72243500 | -4.05324600 |
| C | 2.56858000 | -6.37259500 | 0.99927800 |
| O | 2.97257500 | 5.11392500 | 1.25083600 |
| O | 3.07652800 | 5.39681600 | -2.38041600 |
| O | 7.64656300 | 0.40995000 | -4.10073500 |
| O | 7.47089900 | 3.15233000 | -3.08809500 |
| O | 4.84982100 | 3.91033300 | -2.52117800 |
| O | 4.37306300 | 1.47606500 | -5.21609200 |
| O | 1.76169300 | 2.89884100 | -3.46435500 |
| O | 5.70323800 | -5.02482900 | -3.77739600 |
| O | 6.73496000 | -2.44533500 | -4.51521900 |
| O | 5.06795700 | -0.27155300 | -3.86761300 |
| O | 2.68522100 | -3.04321200 | -4.08470000 |
| O | 2.11335000 | -0.41477900 | -5.43689500 |
| O | 4.86325100 | -6.67545900 | 1.54542500 |
| O | 5.59727200 | -5.83148500 | -1.07767400 |
| O | 3.58971800 | -4.14184500 | -2.27473600 |
| O | 1.65173100 | -6.34069800 | -0.07328000 |
| O | -0.51217400 | -5.38463900 | -1.45386400 |
| O | 3.62168100 | -3.03329500 | 5.80836900 |
| C | 3.96784400 | -6.62475700 | 0.44855500 |
| C | 4.33978100 | -5.51216500 | -0.51664900 |
| C | 3.27286700 | -5.34992600 | -1.59269900 |
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| C | 1.38950600 | -3.14909200 | 5.04235500 |
| C | 2.71118400 | -3.89947000 | 5.15432300 |
| C | 3.20258400 | -4.30597800 | 3.77613100 |
| C | 2.11182200 | -5.04732700 | 3.00758200 |
| C | 0.81262300 | -4.24705500 | 3.01666900 |
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| C | 0.24590000 | 1.93784700 | 4.94855100 |

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| C | 0.90505700 | 1.25132400 | 6.14727500 |
| C | 1.71937700 | 0.05856300 | 5.67937200 |
| C | 0.83594000 | -0.84290400 | 4.83114400 |
| C | 0.26549200 | -0.06007100 | 3.65404100 |
| C | -0.63822000 | -0.88526500 | 2.75749800 |
| C | 2.29939200 | 5.92506800 | 2.17958200 |
| C | 2.95066200 | 5.71539000 | 3.54390800 |
| C | 2.75751200 | 4.27711500 | 3.98885000 |
| C | 1.28438500 | 3.89725000 | 3.93860600 |
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| C | -0.84024300 | 4.04969900 | 2.57870500 |
| O | 6.62506300 | 5.78015200 | -1.77584600 |
| O | 5.46335700 | 6.47169100 | 0.78080400 |
| O | 4.35324900 | -5.11212400 | 3.92583000 |
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| O | 1.25909400 | 2.48968900 | 4.14766100 |
| O | 0.92780300 | 5.60830800 | 2.25220400 |
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| H | 4.65871200 | 5.65452000 | -3.60497500 |
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| H | 7.01861300 | 1.95671300 | -5.34006500 |
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| H | 5.76348600 | -6.68551500 | 1.18810600 |
| H | 5.70041500 | -5.32102200 | -1.90397500 |
| H | -0.53753400 | -6.10689600 | -0.80816300 |
| H | 4.41781500 | -3.53815900 | 6.02422100 |
| H | 3.95988900 | -7.58114500 | -0.09025300 |
| H | 4.39429700 | -4.56899200 | 0.04679400 |
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| H | 2.53197200 | -4.80357400 | 5.75047100 |
| H | 3.43702000 | -3.39045800 | 3.21158600 |
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| H | 0.98359900 | -3.32556000 | 2.44488600 |
| H | -0.59882200 | -5.85501900 | 3.06081100 |
| H | -0.11317400 | -5.34244500 | 1.42249700 |
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| H | -1.15416200 | -0.19642100 | 2.07550000 |
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| H | 2.45259500 | 6.38092100 | 4.26141800 |
| H | 3.29641900 | 3.62201500 | 3.28777700 |
| H | 0.75158200 | 4.41618600 | 4.74800700 |
| H | 1.11233800 | 3.58564200 | 1.82514800 |
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| H | 7.11881800 | 6.20103200 | -1.05714100 |
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| C | 1.16635700 | 4.77162700 | -1.04515500 |
| N | 0.70085400 | 3.39673900 | -0.87680300 |
| H | 0.72697800 | 5.15642300 | -1.96690000 |
| H | 0.78683000 | 5.35405900 | -0.19997900 |
| C | -0.47125300 | 2.87112300 | -1.28007000 |
| N | 1.40850000 | 2.51530600 | -0.18039400 |
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| H | -1.19411400 | 3.43310400 | -1.85133300 |
| N | 0.71583800 | 1.41032400 | -0.11695200 |
| C | -1.43551300 | 0.47601000 | -0.91343000 |

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| N | -2.82075400 | 0.91955700 | -0.93764200 |
| H | -1.25797200 | -0.21960900 | -0.08216200 |
| H | -1.25818300 | -0.07204800 | -1.84141100 |
| C | -3.43649300 | 1.25775000 | 0.24964000 |
| H | -3.38963700 | 0.42951900 | -1.61511200 |
| C | -4.81122000 | 0.95304100 | 0.42264200 |
| O | -2.74570800 | 1.84279200 | 1.14573900 |
| C | -5.46566300 | -0.23605200 | -0.20283100 |
| C | -5.46509900 | 1.59736800 | 1.48839900 |
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| H | -4.87184600 | -0.56196600 | -1.05150600 |
| N | -6.04133500 | 2.12593000 | 2.35858000 |
| C | -7.93023300 | 0.29518600 | 0.03975000 |
| C | -7.06070900 | -0.32818400 | -2.14682700 |
| C | -9.23794800 | 0.45419900 | -0.53571800 |
| H | -7.81391800 | 0.47474900 | 1.10590600 |
| O | -8.30891700 | -0.16451200 | -2.66400500 |
| O | -6.18987900 | -0.68423700 | -2.92614000 |
| C | -9.38506500 | 0.21866800 | -1.90347200 |
| C | -10.37528500 | 0.83786500 | 0.19597000 |
| C | -10.60743200 | 0.35427900 | -2.55374500 |
| C | -11.59681600 | 0.97709400 | -0.43307200 |
| H | -10.27232700 | 1.02414500 | 1.26056500 |
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| H | -10.68160700 | 0.16298900 | -3.61822000 |
| H | -12.46967900 | 1.27530100 | 0.13940700 |
| N | -12.98026500 | 0.87822800 | -2.49733700 |
| C | -13.98770100 | -0.05212000 | -1.95907700 |
| C | -13.47770100 | 2.26265500 | -2.41515300 |
| H | -14.22434700 | 0.18053400 | -0.90736400 |
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| C | -3.70466000 | -2.60156900 | -1.58355000 |
| N | -1.81859400 | -3.23189700 | -0.17809600 |
| C | -3.29711300 | -3.11660000 | -0.21705300 |
| C | -3.72169900 | -2.14704100 | 0.90628500 |
| S | -5.48651800 | -1.72748600 | 0.96190100 |
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| H | -5.24308600 | -2.43034600 | -2.66731900 |
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**P**

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| C | -7.33709700 | -0.24565500 | -3.70272300 |
| C | -6.92004400 | -1.37077200 | -2.77002400 |
| C | -5.89485200 | -2.26520400 | -3.45519300 |
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| O | -5.10390900 | 6.34217400 | 0.18002000 |
| O | -3.43508300 | 4.67630300 | -1.49724000 |
| O | -1.02714800 | 6.40619900 | 0.66038000 |
| O | 0.82956700 | 5.55394500 | -1.14756100 |
| O | -2.59974800 | 2.57949000 | 6.34758500 |
| C | -3.21423200 | 6.78990800 | 1.53426200 |
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| C | 1.14141100 | 4.44429200 | 2.64440300 |
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| C | 0.09146600 | -0.50447000 | 3.49964100 |
| C | 1.02549700 | 0.31002200 | 2.62732000 |
| C | -2.62961100 | -6.07317100 | 1.52836900 |
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| O | 0.45932200 | 3.25419900 | 4.54565500 |
| O | 2.18136400 | 3.51730100 | 2.38788800 |
| O | -1.37631600 | -2.96201300 | 6.49513700 |
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| H | -5.53017300 | -4.13784100 | -0.03278500 |
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| H | -3.17656000 | 7.80619300 | 1.12086600 |
| H | -3.88420100 | 4.84758200 | 0.94362000 |
| H | -3.00522600 | 6.70273900 | -1.29138800 |
| H | -1.36312700 | 4.46526400 | 0.00658300 |
| H | -0.73951200 | 4.99447700 | -2.31467800 |
| H | -0.68999500 | 6.73412900 | -1.92857400 |
| H | 0.02951400 | 2.18526200 | 6.19028600 |
| H | -1.30518600 | 4.20543800 | 6.29636900 |
| H | -2.70007300 | 3.19335400 | 3.78761000 |
| H | -0.87959400 | 5.61699200 | 4.09515400 |
| H | -0.40030200 | 2.95179000 | 2.67663600 |
| H | 1.49372000 | 5.25929000 | 3.29330300 |
| H | 0.82574000 | 4.87538800 | 1.68763000 |
| H | 0.61021500 | -3.50640000 | 4.75903500 |
| H | 0.36534700 | -1.83489400 | 6.51187100 |
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| H | 0.63970400 | 0.37542000 | 5.36215600 |
| H | -0.80870700 | -0.74223600 | 2.91777000 |
| H | 0.48292300 | 1.16567800 | 2.21710100 |
| H | 1.33910200 | -0.31826600 | 1.78227600 |
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| H | -2.68278800 | -3.92990200 | 5.37862100 |
| H | 1.23653400 | -3.55806700 | 0.10764200 |
| C | -1.81339600 | -4.82479900 | -1.71104600 |
| N | -1.09261200 | -3.55819000 | -1.60767100 |
| H | -1.59049300 | -5.25095100 | -2.69050700 |
| H | -1.42012700 | -5.48809800 | -0.93529200 |
| C | -0.00939000 | -3.14818700 | -2.29387700 |
| N | -1.45497600 | -2.65938000 | -0.69975600 |
| C | 0.28045500 | -1.91452300 | -1.75165300 |

| | | | |
|---|---|---|---|
| H | 0.44015800 | -3.73682900 | -3.07917000 |
| N | -0.62749300 | -1.65822700 | -0.77601200 |
| C | 1.30955900 | -0.89345300 | -2.09573700 |
| N | 2.68652500 | -1.37075100 | -2.02425100 |
| H | 1.16799400 | -0.05889700 | -1.40076100 |
| H | 1.16359300 | -0.51647700 | -3.10870600 |
| C | 3.24496900 | -1.75646900 | -0.87299500 |
| H | 3.29533200 | -1.11702800 | -2.79409800 |
| C | 4.77902400 | -1.79416200 | -0.90643700 |
| O | 2.60344100 | -2.00426300 | 0.15430500 |
| C | 5.35252000 | -0.34531900 | -0.97442700 |
| C | 5.28453000 | -2.54742300 | 0.24020400 |
| C | 6.83074500 | -0.32025500 | -1.25910400 |
| H | 4.85991400 | 0.11697800 | -1.82866800 |
| N | 5.70000000 | -3.13147900 | 1.14805700 |
| C | 7.78711300 | -0.71639100 | -0.38651500 |
| C | 7.21760600 | 0.20848800 | -2.56822100 |
| C | 9.17991000 | -0.64498800 | -0.73004400 |
| H | 7.52467700 | -1.09082500 | 0.60080600 |
| O | 8.54358300 | 0.25697300 | -2.86546500 |
| O | 6.44626100 | 0.61513700 | -3.42202200 |
| C | 9.51881500 | -0.14896700 | -1.99001900 |
| C | 10.21985200 | -1.03910900 | 0.13012100 |
| C | 10.83898200 | -0.03816000 | -2.41335400 |
| C | 11.53604000 | -0.93404100 | -0.27327200 |
| H | 9.96647700 | -1.42494800 | 1.11270800 |
| C | 11.85431500 | -0.43137100 | -1.55155000 |
| H | 11.06317700 | 0.35239700 | -3.39941400 |
| H | 12.33385000 | -1.23884600 | 0.39676300 |
| N | 13.21713800 | -0.30700100 | -1.99490500 |
| C | 13.96863800 | 0.63588100 | -1.14777400 |
| C | 13.89570400 | -1.61443800 | -2.01862800 |
| H | 14.05292800 | 0.26149800 | -0.11383500 |
| H | 14.98501600 | 0.67610300 | -1.55211100 |
| C | 13.36195300 | 2.02900400 | -1.14642600 |
| H | 14.91444600 | -1.43016500 | -2.37417600 |
| H | 13.98611400 | -2.03635600 | -1.00381600 |
| C | 13.20560300 | -2.61097600 | -2.93491300 |
| H | 13.26012900 | 2.40806100 | -2.16734400 |
| H | 12.37402800 | 2.03822500 | -0.67724700 |
| H | 14.00527800 | 2.71263100 | -0.58691500 |
| H | 12.21047900 | -2.87548700 | -2.56605700 |
| H | 13.09953700 | -2.20079100 | -3.94327600 |
| H | 13.79562600 | -3.52878000 | -2.99588300 |
| C | 3.71935000 | 2.20578400 | -1.99878700 |
| N | 1.62634100 | 2.65078600 | -0.76015700 |
| C | 3.06731500 | 2.46819300 | -0.65369600 |
| C | 3.30871300 | 1.25753100 | 0.27176000 |
| S | 5.02096500 | 0.67834500 | 0.51591800 |
| O | 3.17799100 | 1.58508700 | -2.89575200 |
| O | 4.97395700 | 2.64620700 | -2.07696800 |
| H | 2.67785600 | 0.42996200 | -0.05118800 |

| | | | |
|---|---|---|---|
| H | 2.97590500 | 1.53912000 | 1.27286100 |
| H | 4.47715900 | -1.03084400 | 2.46626300 |
| H | 1.41929800 | 3.62552600 | -0.97671400 |
| H | 1.29488900 | 2.09205000 | -1.54464400 |
| H | 3.52830300 | 3.35196800 | -0.20765800 |
| H | 5.39144300 | 2.27025200 | -2.87836100 |
| O | 3.66046600 | -1.40713200 | 2.82747800 |
| H | 2.80667000 | 0.06819200 | 3.31650900 |
| H | 3.19768000 | -1.72712800 | 2.03254400 |
| H | 5.10096300 | -2.31180000 | -1.81838600 |