

## Supporting Information

### Dual-mode biosensor combining transition metal carbonyl-based SERS and colorimetric readout for thiol detection

**Figure S1:** HR ESI-MS for the reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with cysteine (top) with calculated isotopic pattern (bottom), **Figure S2:** HRMS-ESI for the reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with N-(tert-butoxycarbonyl)-L-cysteine methyl ester (top) with calculated isotopic pattern (bottom), **Figure S3:** HRMS-ESI for the reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with N-acetyl-L-cysteine (top) with calculated isotopic pattern (bottom), **Figure S4:** HRMS-ESI for the reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with GSH (top) with calculated isotopic pattern (bottom), **Figure S5:** The reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with 20 amino acids, **Figure S6:** UV-Vis measurements for quantitative thiol detection.

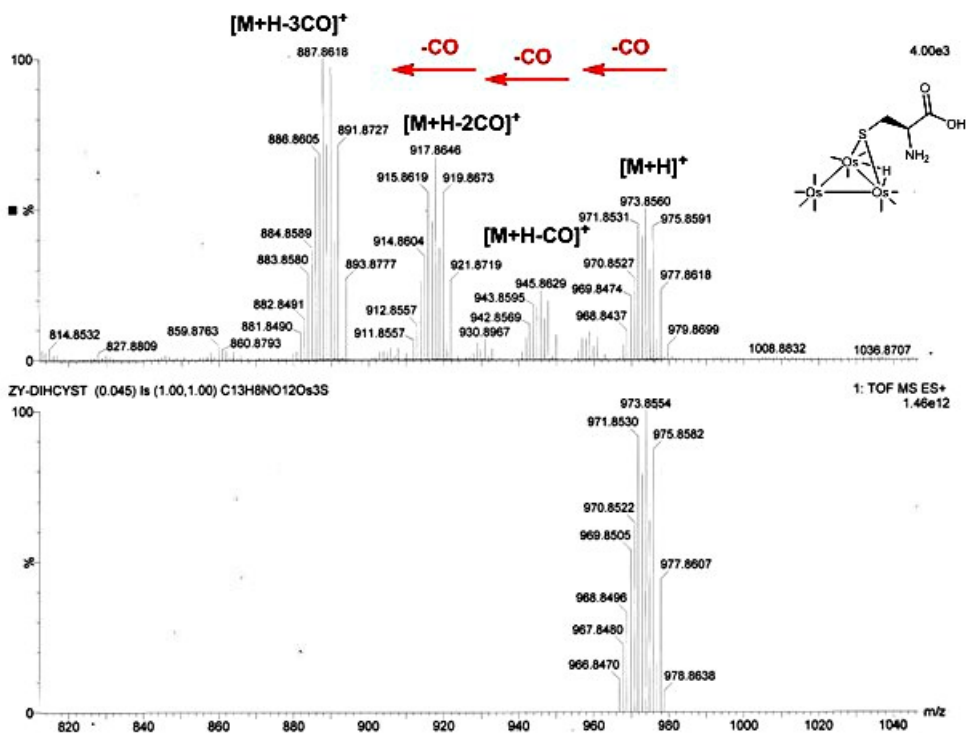


Figure S1. HR ESI-MS for the reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with cysteine (top) with calculated isotopic pattern (bottom).

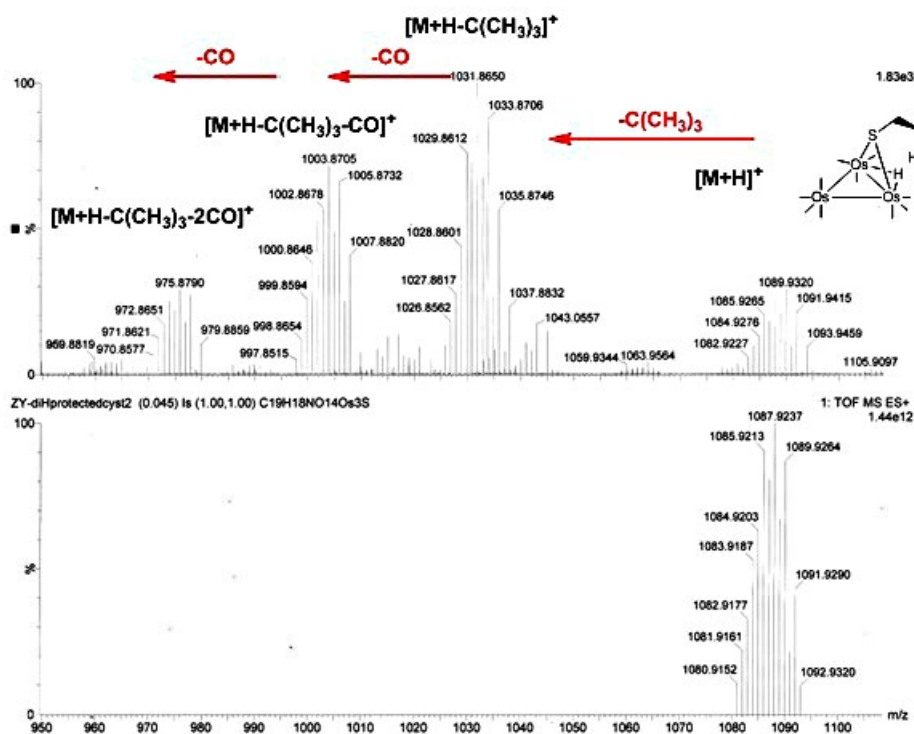
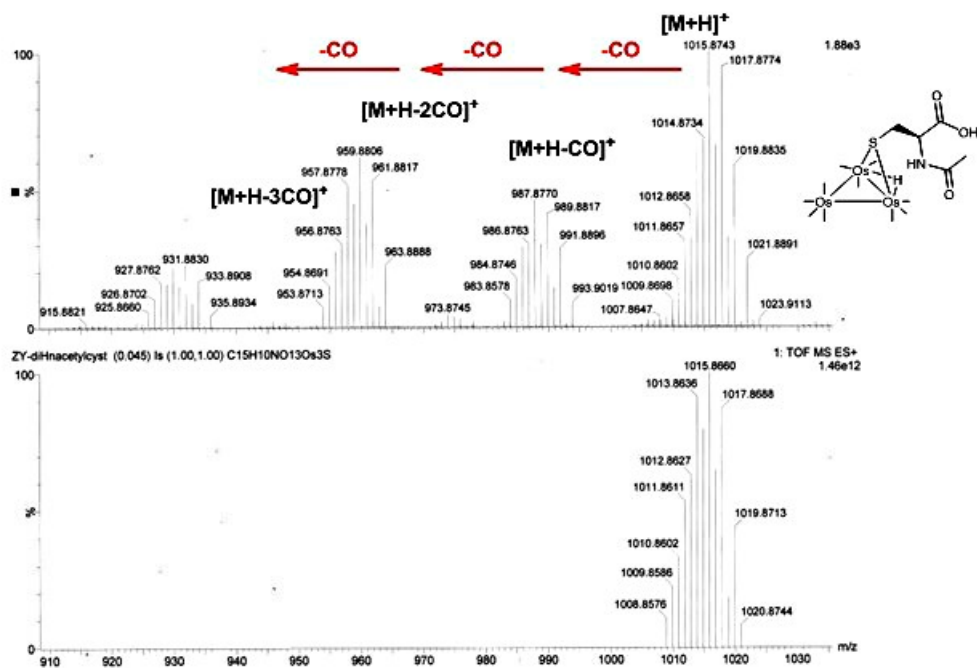
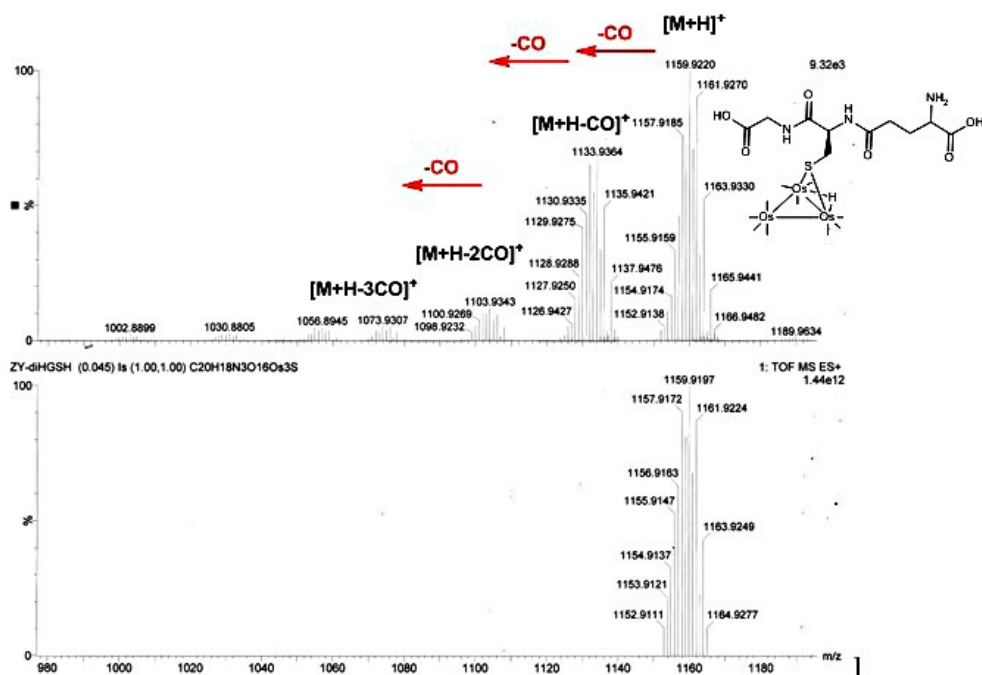


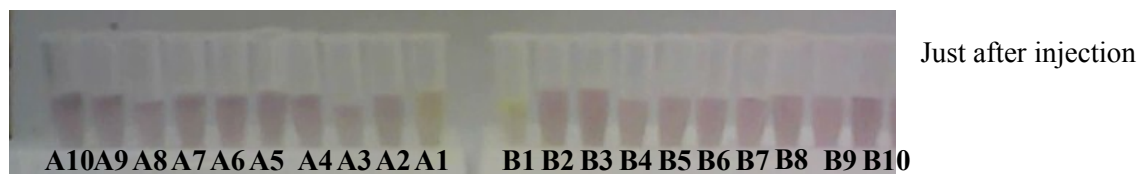
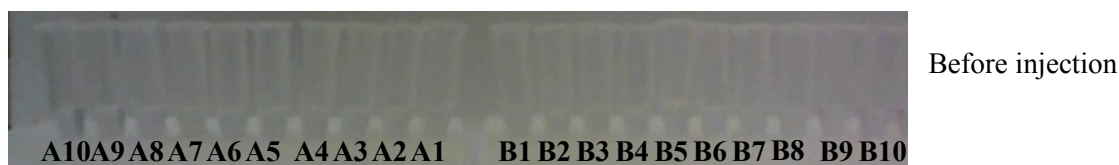
Figure S2. HRMS-ESI for the reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with N-(tert-butoxycarbonyl)-L-cysteine methyl ester (top) with calculated isotopic pattern (bottom).



**Figure S3.** HRMS-ESI for the reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with N-acetyl-L-cysteine (top) with calculated isotopic pattern (bottom).

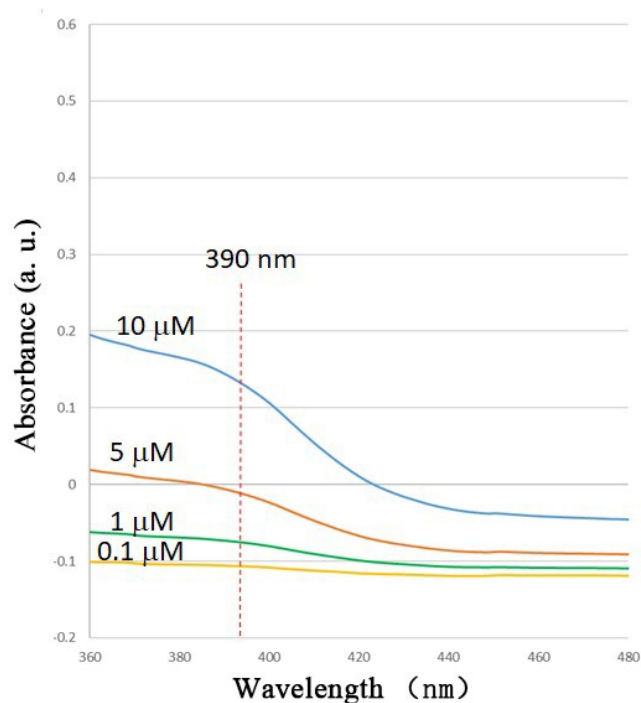


**Figure S4.** HRMS-ESI for the reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with GSH (top) with calculated isotopic pattern (bottom).



- |                    |                  |
|--------------------|------------------|
| A10 = Alanine      | B10 = Tryptophan |
| A9 =               | B9 =             |
| A8 = Aspartic      | B8 =             |
| A7 =               | B7 = Lysine      |
| A6 = Glutamine     | B6 = Histidine   |
| A5 = Glutamic acid | B5 = Leucine     |
| A4 = Glycine       | B4 = Serine      |
| A3 = Isoleucine    | B3 = Proline     |
| A2 = Phenylalanine | B2 = Threonine   |
| A1 = GSH           | B1 = Cysteine    |

**Figure S5.** The reaction of  $\text{Os}_3(\text{CO})_{10}(\mu\text{-H})_2$  with 20 amino acids. (note: a video recording of color change progression of 20 types amino acids for a few seconds is provided).



**Figure S6** UV-Vis measurements for quantitative thiol detection.