

# Ligation motifs in zinc bound sulfonamide drugs assayed by IR ion spectroscopy

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**Figure S1.** Mass spectrum of the isolated deprotonated sulfadiazine ion at  $m/z$  249, recorded a) after irradiation by IR light at  $1500\text{ cm}^{-1}$ ; b) after irradiation at  $1288\text{ cm}^{-1}$ ; and c) without laser.

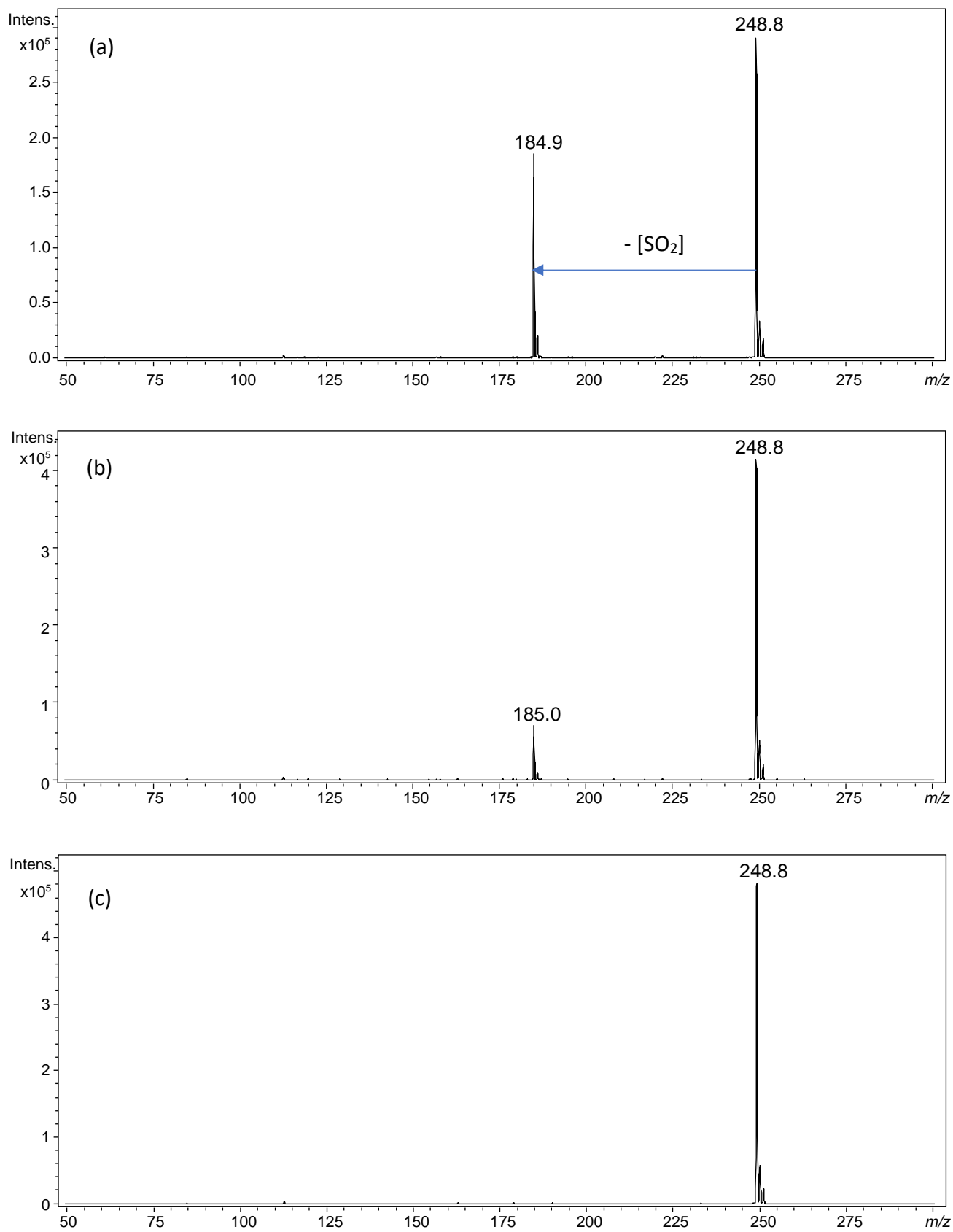
**Figure S2.** Mass spectrum following isolation of  $\text{Zn}(\text{H}_2\text{O}+\text{SDZ-H})^+$  ions at  $m/z$  331, recorded a) after irradiation by IR light at  $1572\text{ cm}^{-1}$ ; b) same wavelength using an attenuator; and c) without laser.

**Figure S3.** Mass spectrum following isolation of  $\text{Zn}(\text{H}_2\text{O}+\text{STZ-H})^+$  ions at  $m/z$  336, recorded a) after irradiation by IR light at  $1640\text{ cm}^{-1}$ ; and b) without laser.

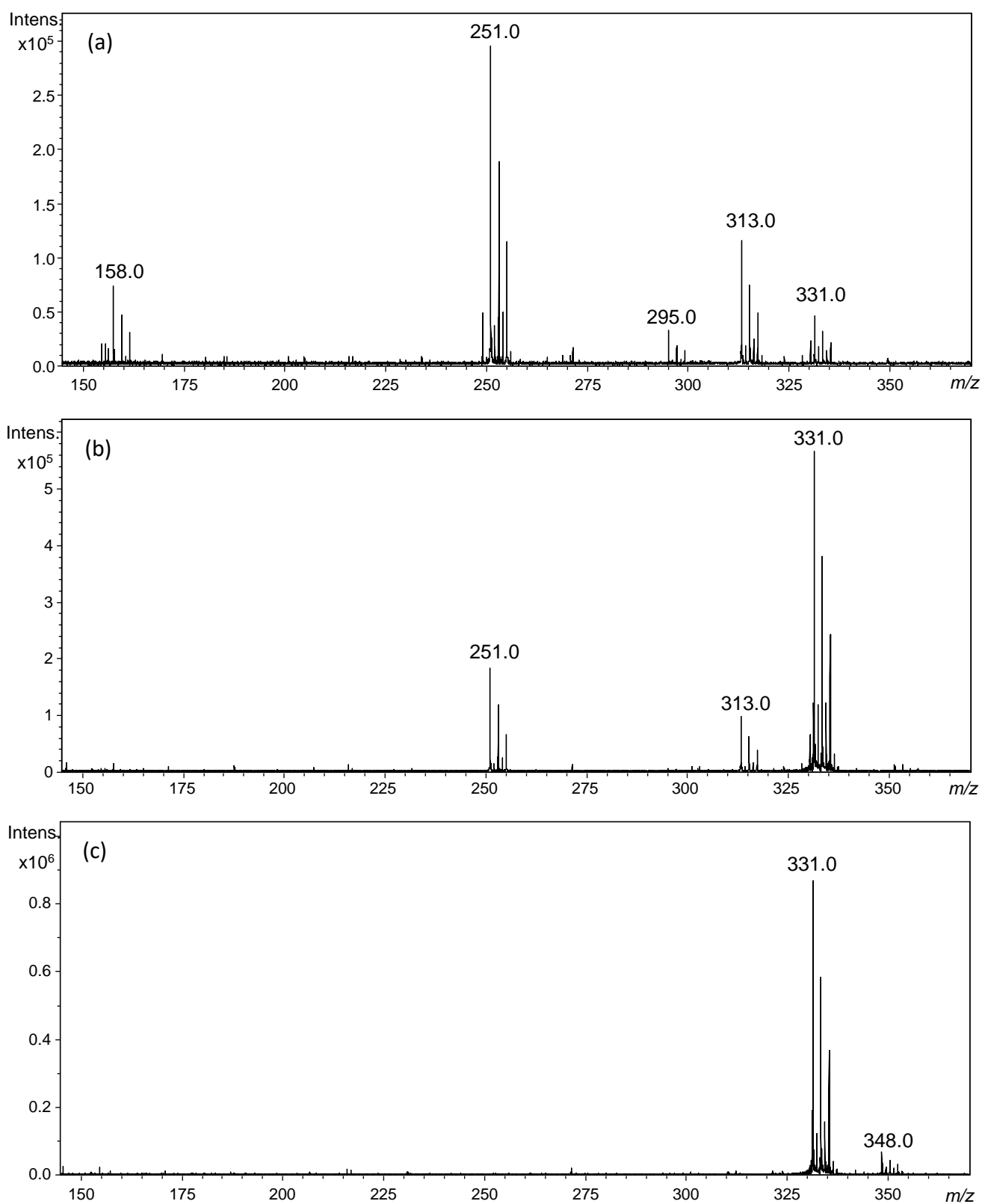
**Figure S4.** IRMPD spectrum of  $(\text{SDZ-H})^-$  (bottom panel) compared with calculated IR spectra of **SDZ-H\_1** and **SDZ-H\_2**, whose optimized structures are reported on the right. Relative free energies (enthalpies) at 298 K are reported in  $\text{kJ mol}^{-1}$ . Calculations are at the B3LYP/6-311+G(d,p) level.

**Figure S5a-b.** IRMPD spectrum of  $\text{Zn}(\text{H}_2\text{O}+\text{SDZ-H})^+$  (bottom panel) compared with calculated IR spectra of isomers whose optimized structures are reported on the right. Relative free energies (enthalpies) at 298 K are reported in  $\text{kJ mol}^{-1}$ . Calculations are at the B3LYP/6-311+G(d,p) level.

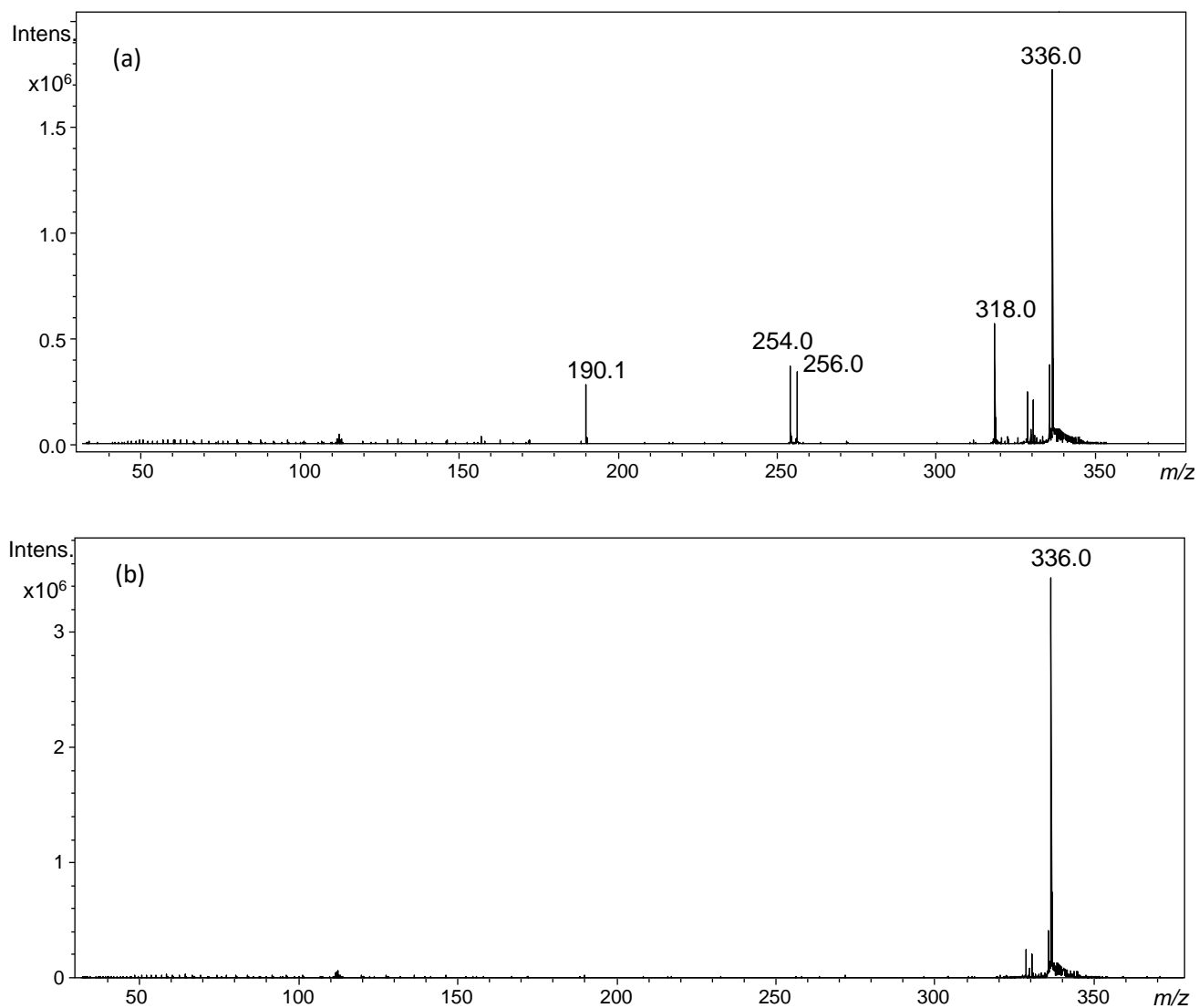
**Figure S6.** IRMPD spectrum of  $\text{Zn}(\text{H}_2\text{O}+\text{STZ-H})^+$  (bottom panel) compared with calculated IR spectra of isomers whose optimized structures are reported on the right. Relative free energies (enthalpies) at 298 K are reported in  $\text{kJ mol}^{-1}$ . Calculations are at the B3LYP/6-311+G(d,p) level.



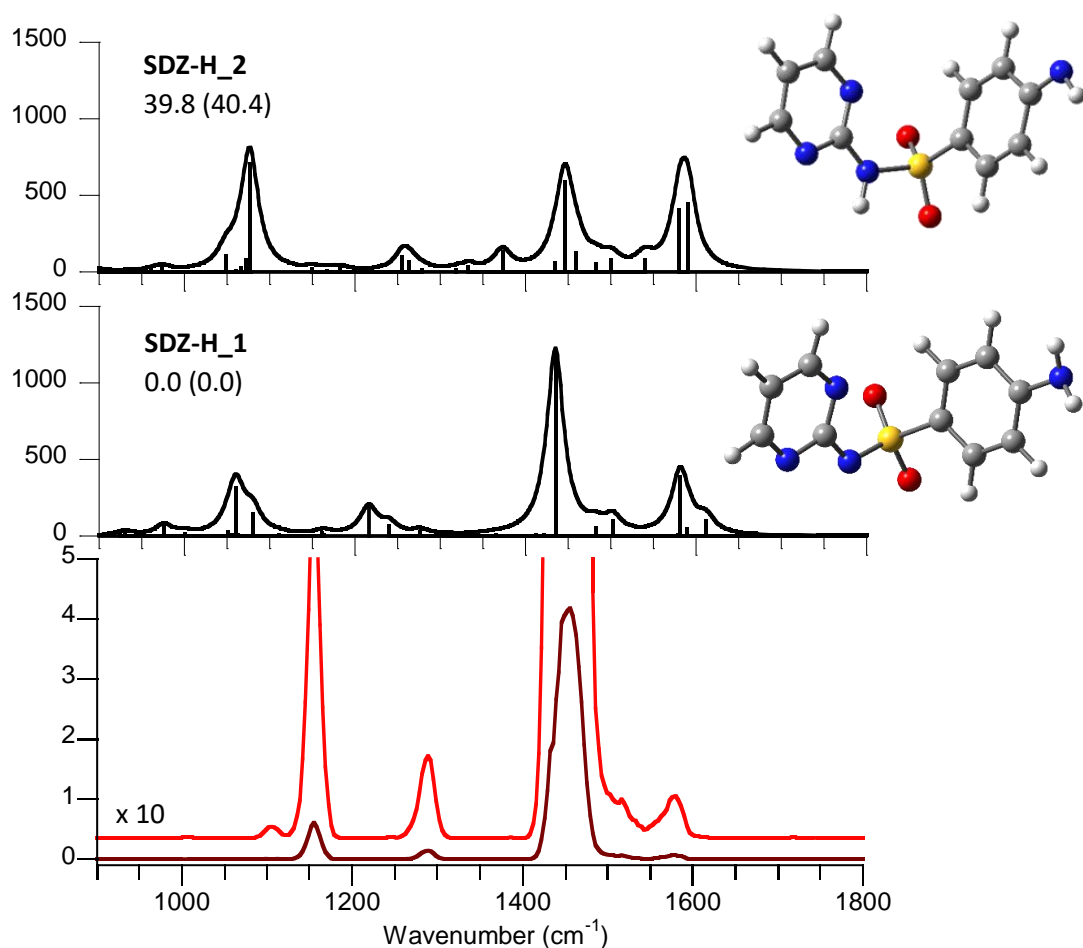
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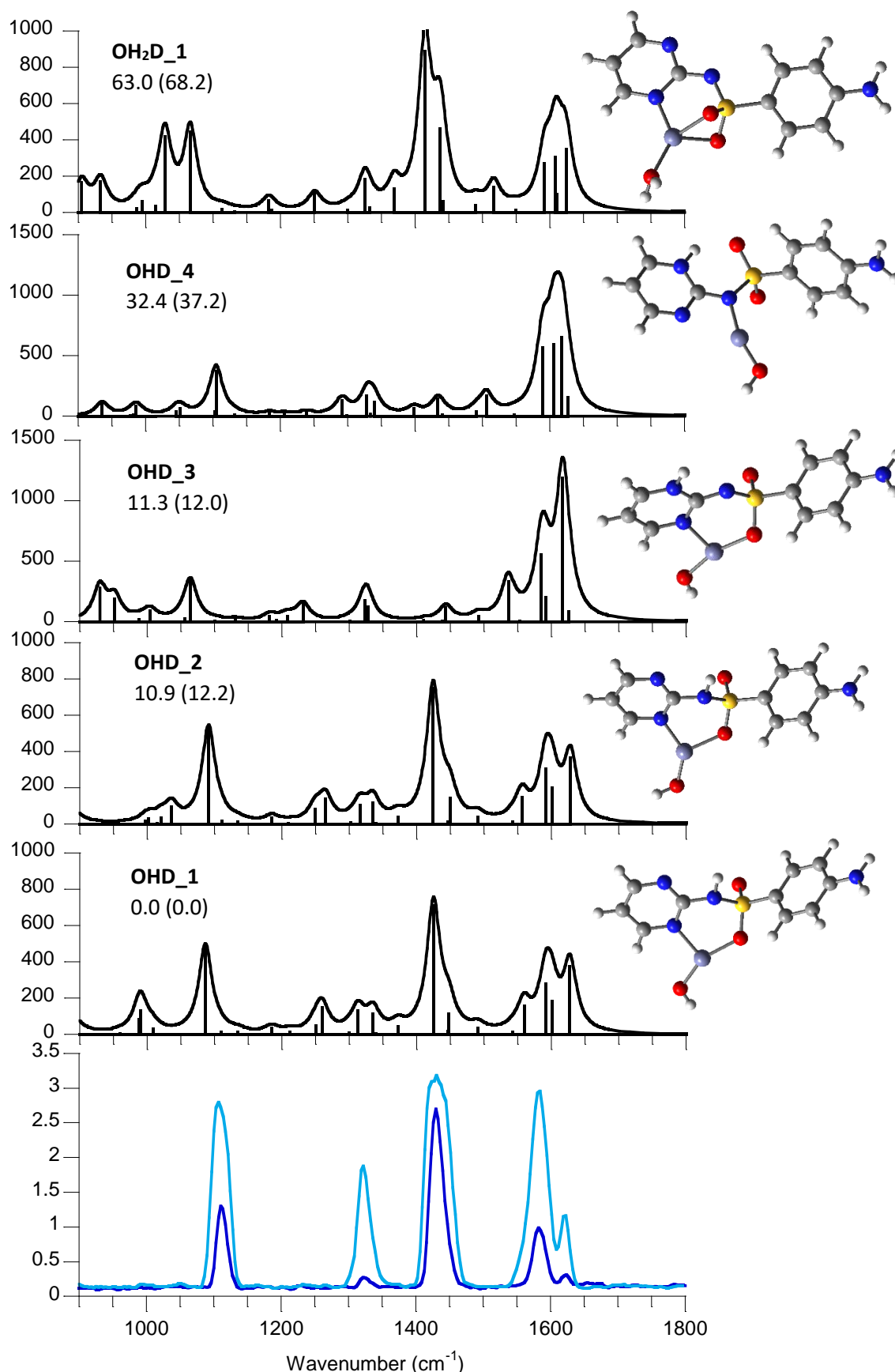
**Figure S2.** Mass spectrum following isolation of  $\text{Zn}(\text{H}_2\text{O}+\text{SDZ-H})^+$  ions at  $m/z$  331, recorded a) after irradiation by IR light at  $1572\text{ cm}^{-1}$ ; b) same wavelength using an attenuator; and c) without laser. The full isotopic cluster is selected and submitted to IR laser radiation.



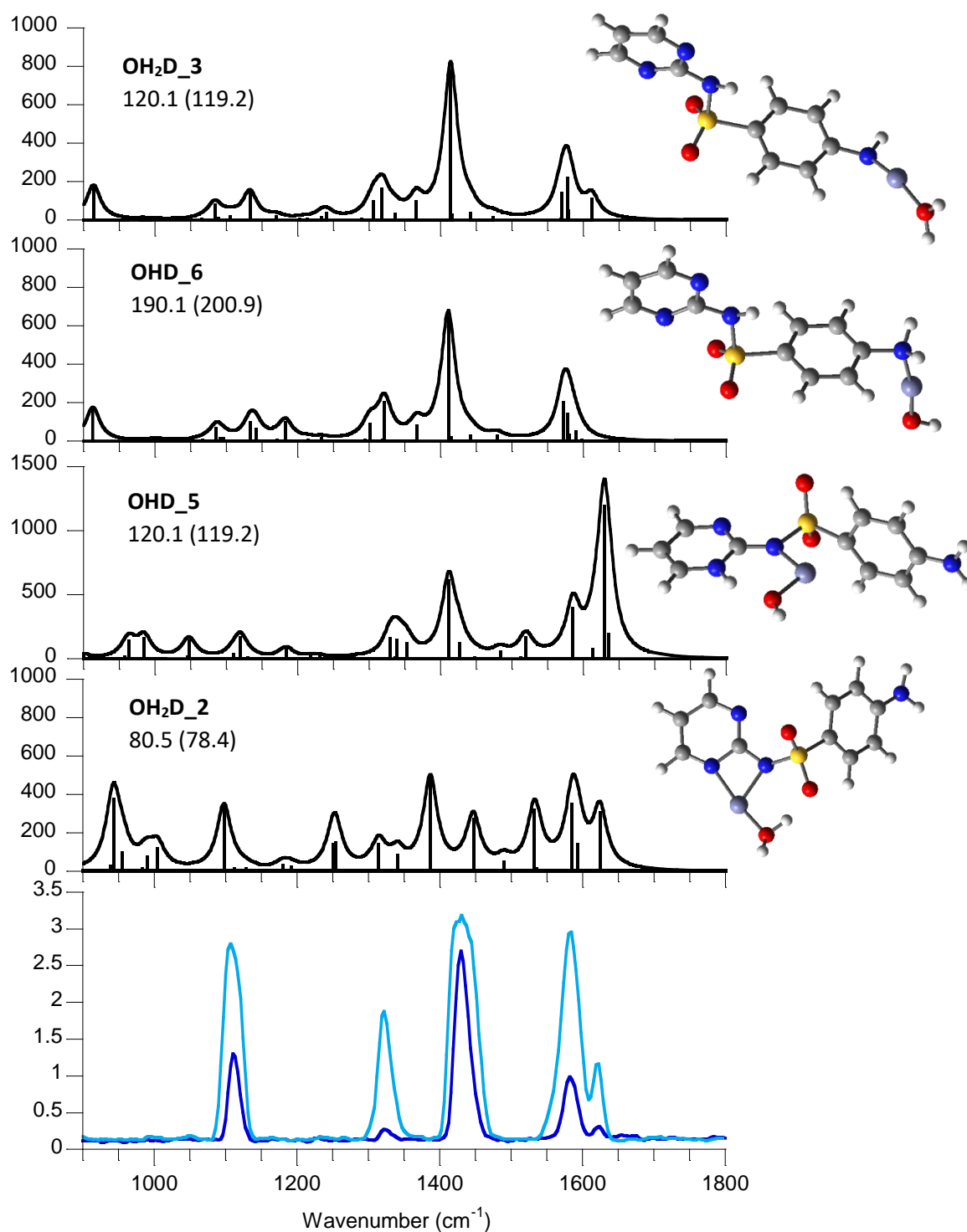
**Figure S3.** Mass spectrum following isolation of  $\text{Zn}(\text{H}_2\text{O}+\text{STZ-H})^+$  ions at  $m/z\ 336$ , recorded a) after irradiation by IR light at  $1640\text{ cm}^{-1}$ ; and b) without laser. The monoisotopic ion ( $^{12}\text{C}_9\text{H}_{10}^{14}\text{N}_3^{16}\text{O}_3^{32}\text{S}_2^{64}\text{Zn}$ ) $^+$  at  $m/z\ 336$  is selected and submitted to IR laser radiation.



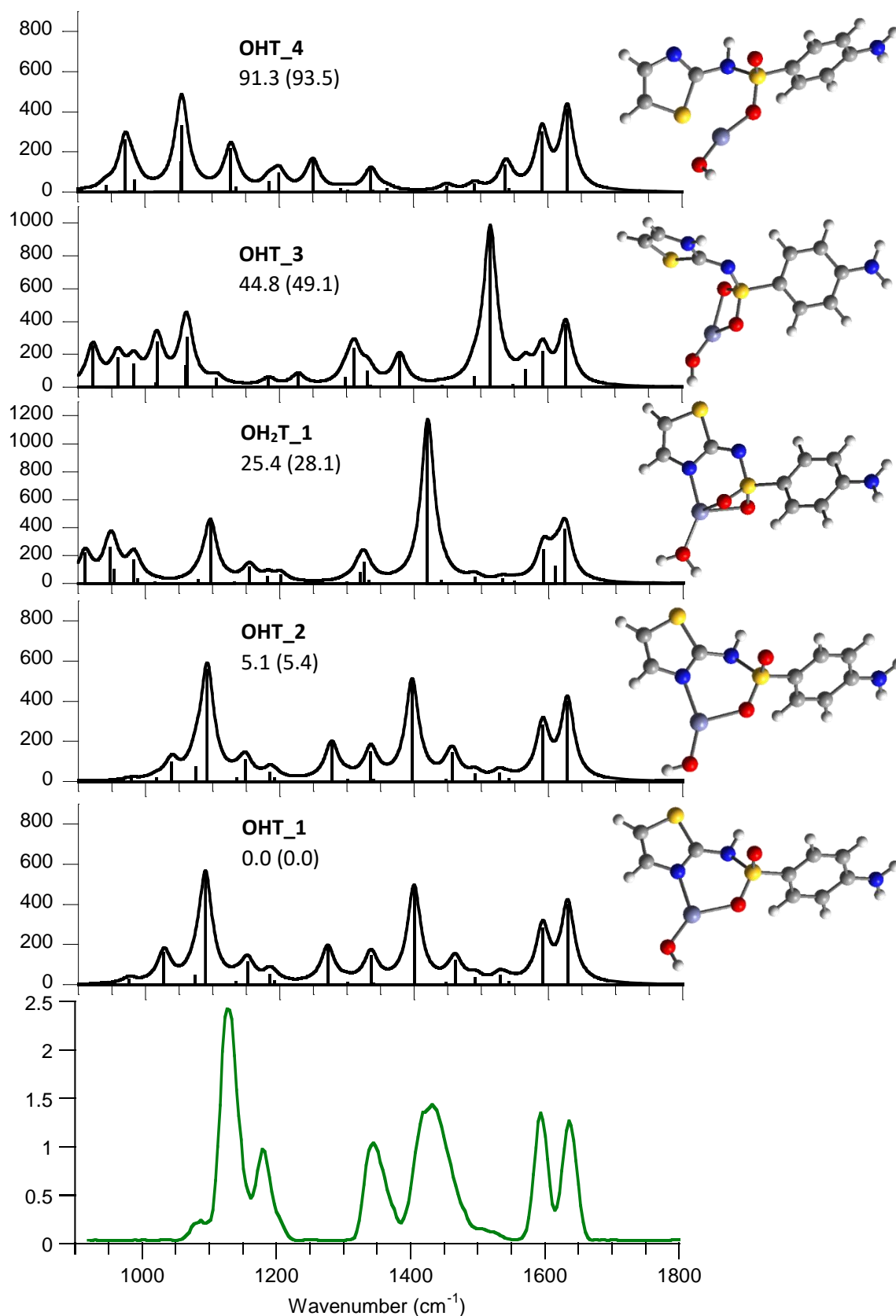
**Figure S4.** IRMPD spectrum of (SDZ-H)<sup>-</sup> (bottom panel) compared with calculated IR spectra of **SDZ-H<sub>1</sub>** and **SDZ-H<sub>2</sub>**, whose optimized structures are reported on the right. Relative free energies (enthalpies) at 298 K are reported in kJ mol<sup>-1</sup>. Calculations are at the B3LYP/6-311+G(d,p) level. Computed harmonic frequencies are scaled by a factor of 0.974 except those regarding S-X stretching modes which are left unscaled.



**Figure S5a.** IRMPD spectrum of  $\text{Zn}(\text{H}_2\text{O}+\text{SDZ-H})^+$  (bottom panel) compared with calculated IR spectra of isomers whose optimized structures are reported on the right. Relative free energies (enthalpies) at 298 K are reported in  $\text{kJ mol}^{-1}$ . Calculations are at the B3LYP/6-311+G(d,p) level. Computed harmonic frequencies are scaled by a factor of 0.974 except those regarding S-X stretching modes which are left unscaled.



**Figure S5b.** IRMPD spectrum of  $\text{Zn}(\text{H}_2\text{O}/\text{SDZ-H})^+$  (bottom panel) compared with calculated IR spectra of isomers whose optimized structures are reported on the right. Relative free energies (enthalpies) at 298 K are reported in  $\text{kJ mol}^{-1}$ . Calculations are at the B3LYP/6-311+G(d,p) level. Computed harmonic frequencies are scaled by a factor of 0.974 except those regarding S-X stretching modes which are left unscaled.



**Figure S6.** IRMPD spectrum of  $\text{Zn}(\text{H}_2\text{O}+\text{STZ-H})^+$  (bottom panel) compared with calculated IR spectra of isomers whose optimized structures are reported on the right. Relative free energies (enthalpies) at 298 K are reported in  $\text{kJ mol}^{-1}$ . Calculations are at the B3LYP/6-311+G(d,p) level. Computed harmonic frequencies are scaled by a factor of 0.974 except those regarding S-X stretching modes which are left unscaled.