

**Direct Dynamics Simulations of Fragmentation of a Zn(II)–2Cys–2His Oligopeptide.  
Comparison with Mass Spectrometry Collision–Induced Dissociation**

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**Figure S1.** MS/MS CID spectrum showing all the observed  $m/z$  values and labelled identified fragments.

**Figure S2.** Mechanisms for dissociation pathways 11-15.

**Figure S3.** Potential energy curves for the C-C bond dissociations of pathways 1 and 2.

**Figure S4.** Procedure employed to calculate the slope and intercept of the weighted regression line and their corresponding uncertainties.

**Table S1.** Mean Absolute Errors (MAEs) in B3LYP and semiempirical methods for Zn-Ligand bond distances for three conformers.

**Table S2.** All the ions ( $m/z$ ) and their observed fragments for conformer *a* at 1600 K.

**Table S3.** All the ions ( $m/z$ ) and their observed fragments for conformer *a* at 1750 K.

**Table S4.** All the ions ( $m/z$ ) and their observed fragments for conformer *a* at 1875 K.

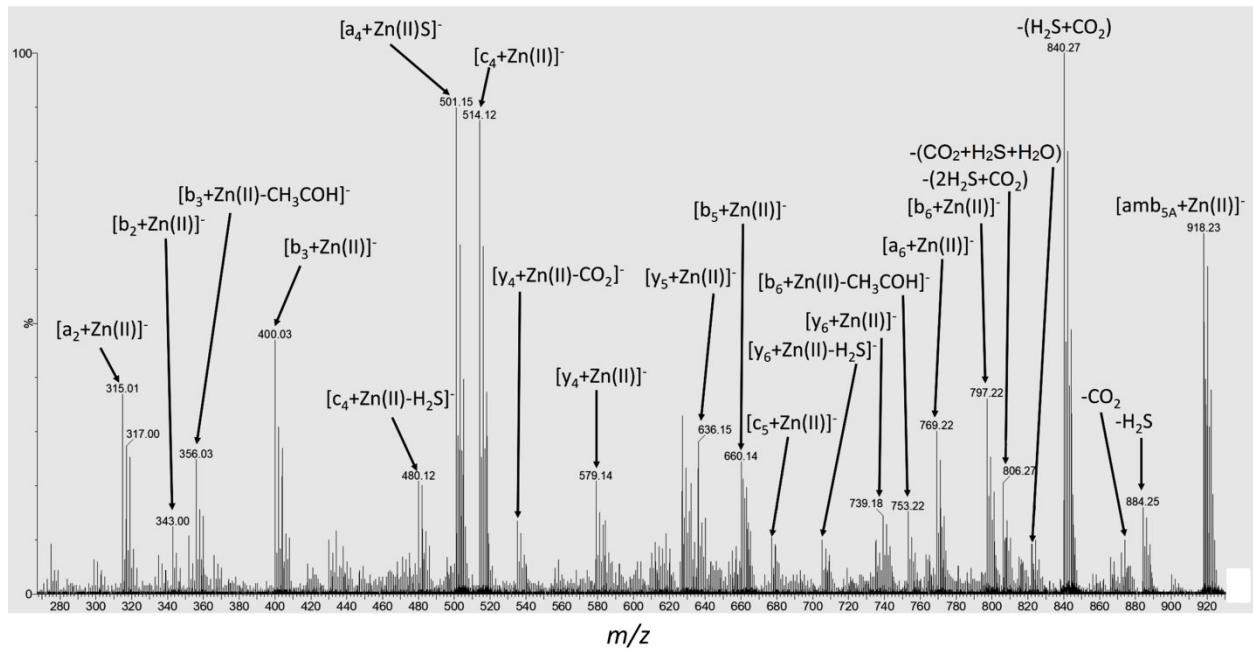
**Table S5.** All the ions ( $m/z$ ) and their observed fragments for conformer *a* at 2000 K.

**Table S6.** All the ions ( $m/z$ ) and their observed fragments for conformer *a* at 2250 K.

**Table S7.** All the ions ( $m/z$ ) and their observed fragments for conformer *b* at 2000 K.

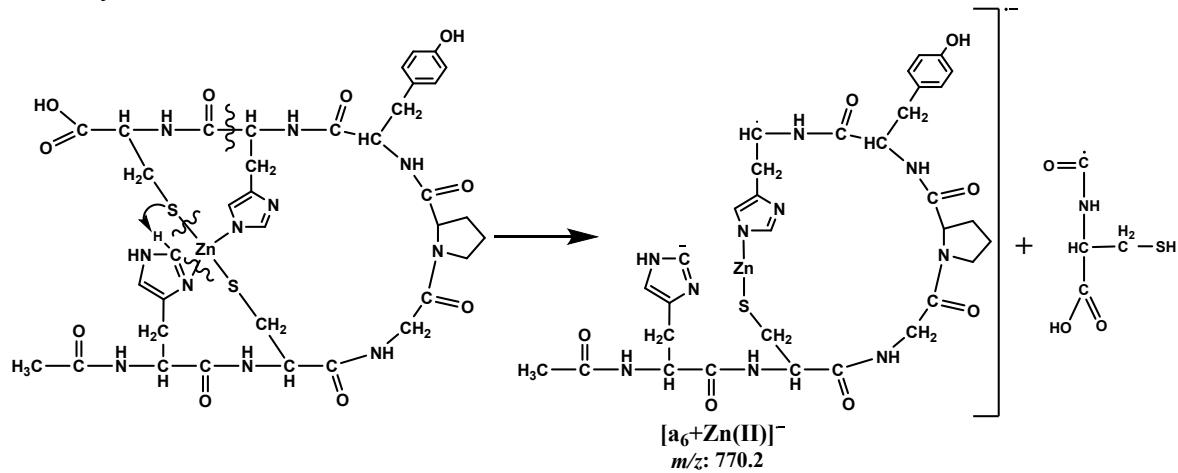
**Table S8.** All the ions ( $m/z$ ) and their observed fragments for conformer *b* at 2250 K.

**Table S9.** All the ions ( $m/z$ ) and their observed fragments for conformer *c* at 2000 K.

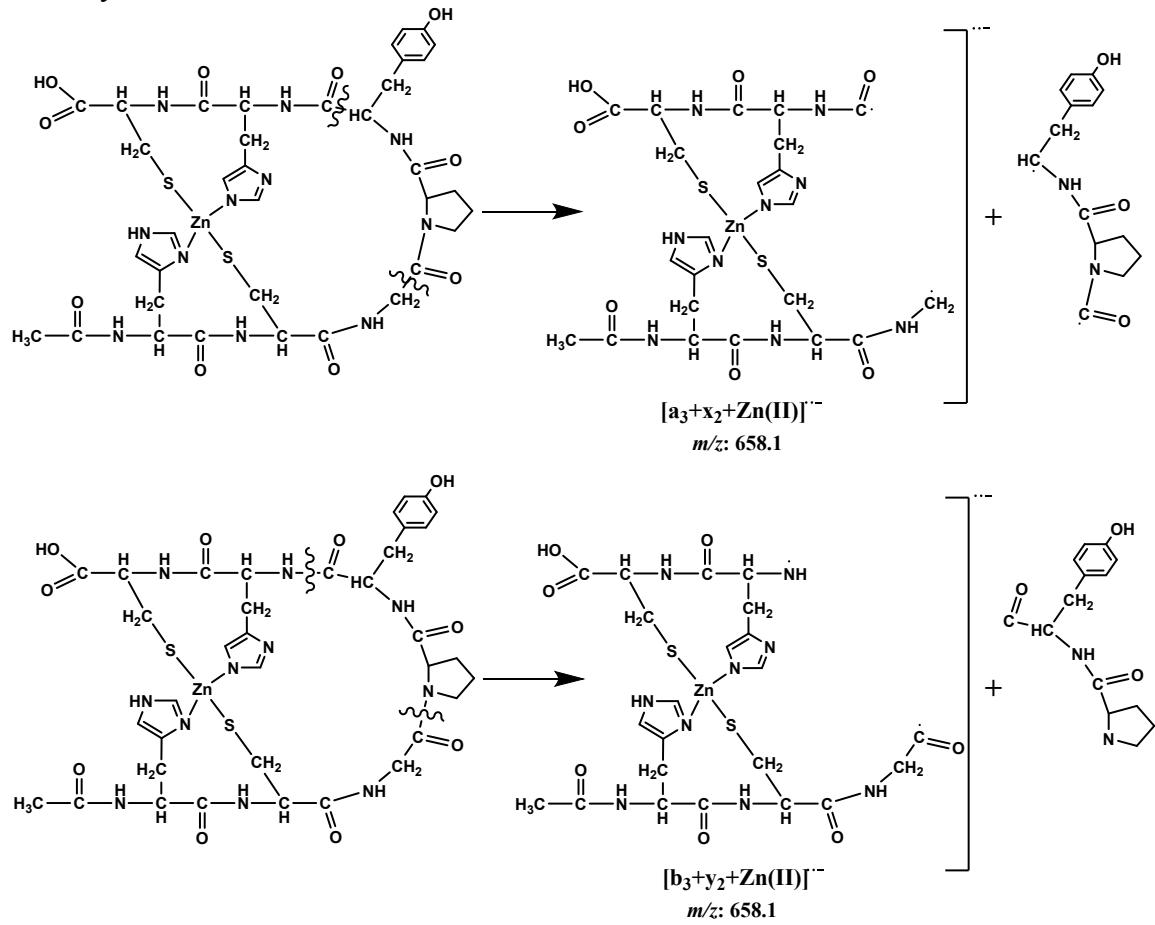


**Figure S1.** MS/MS CID spectrum showing all the observed  $m/z$  values and labelled identified fragments. The channel ( $\text{CO} + \text{H}_2\text{O}$ ) with  $m/z$  872.2 is not labelled.

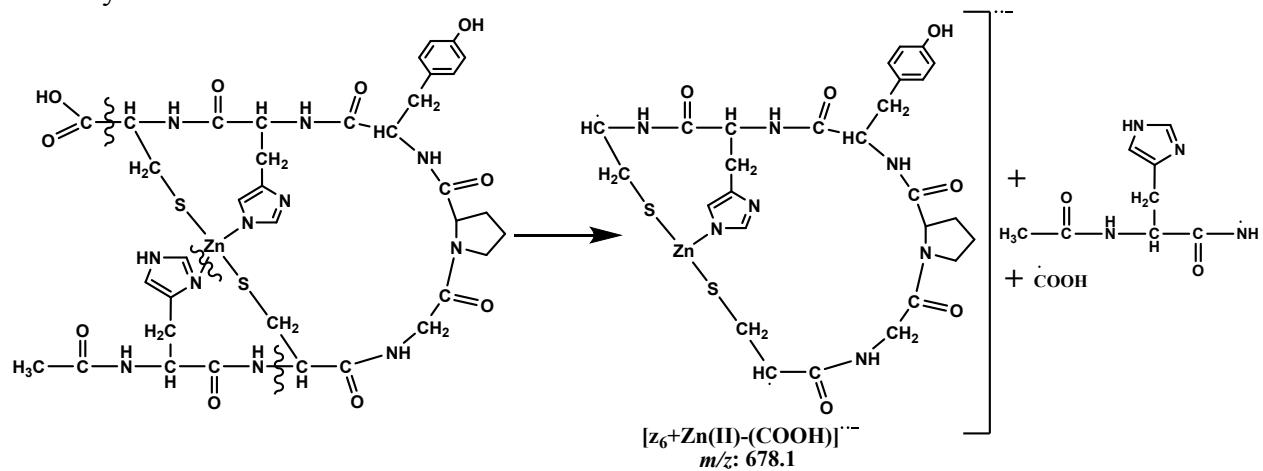
Pathway 11



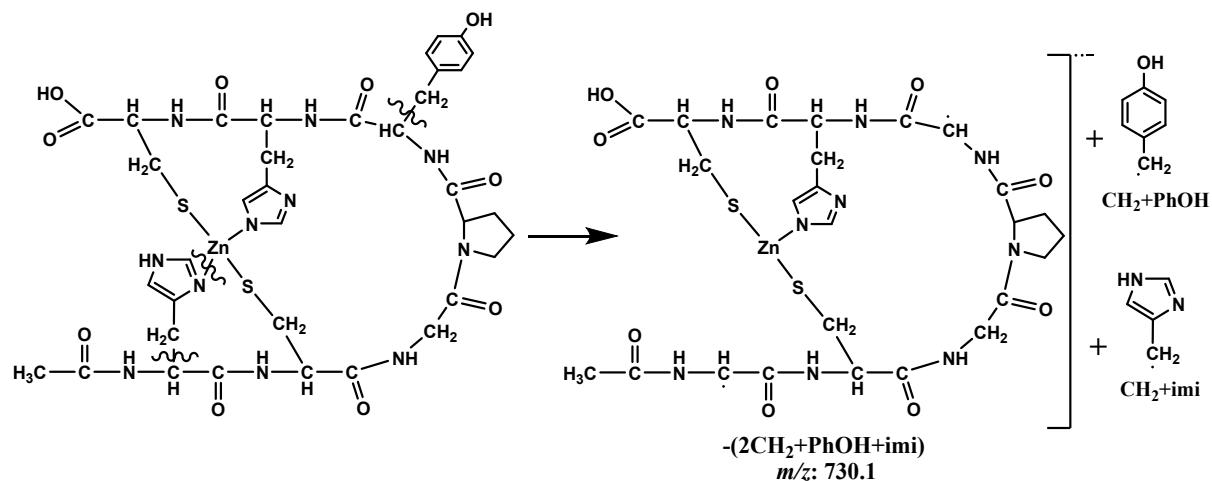
Pathway 12



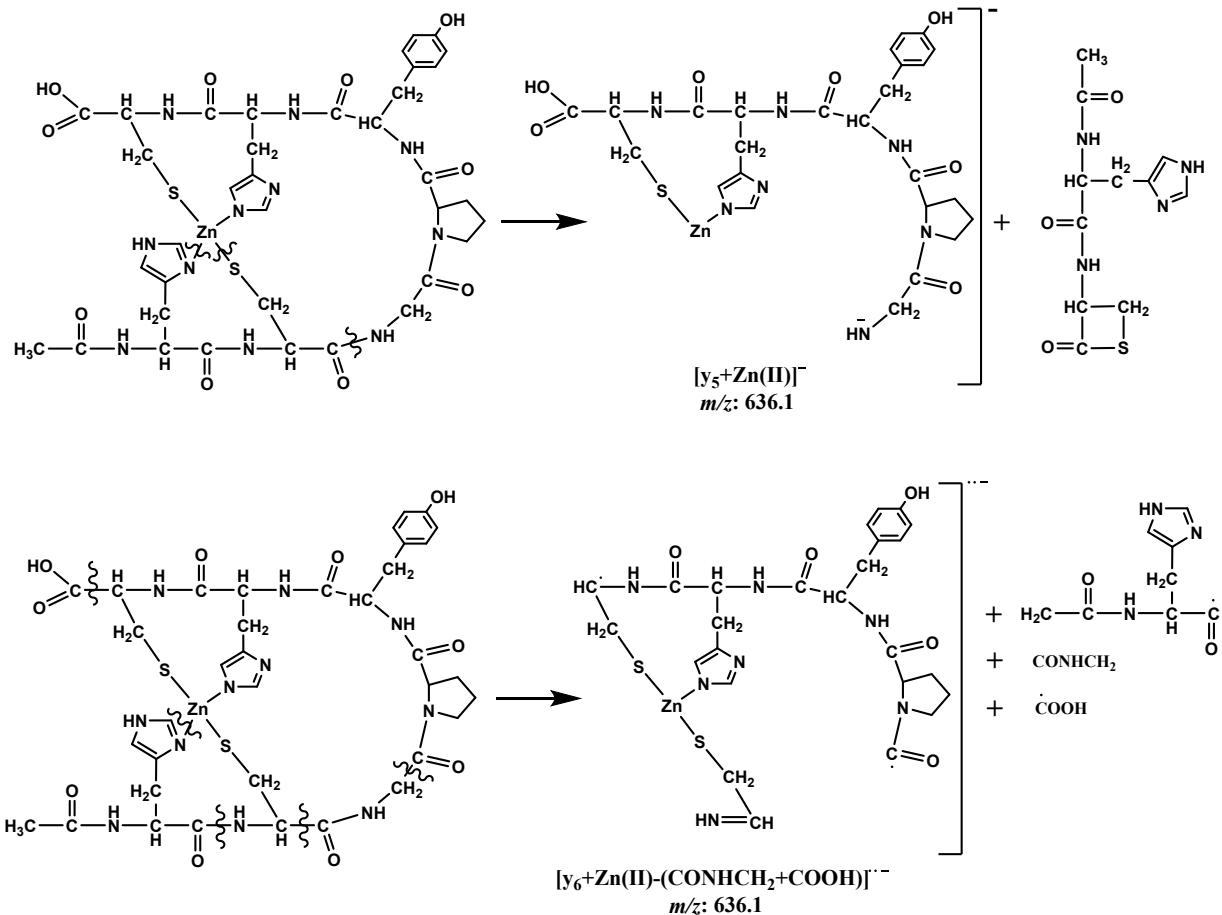
Pathway 13



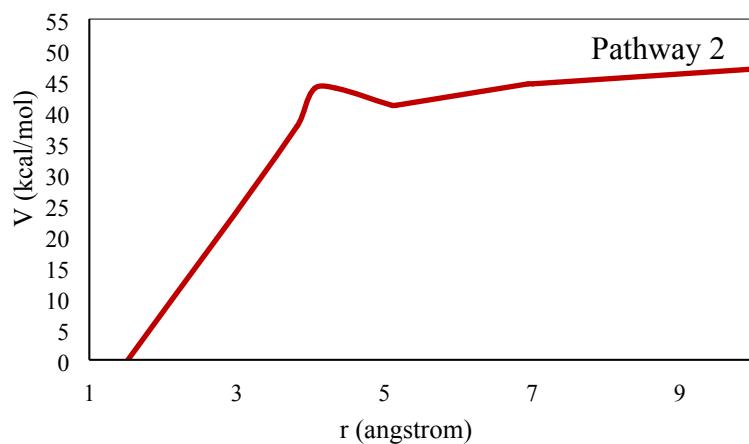
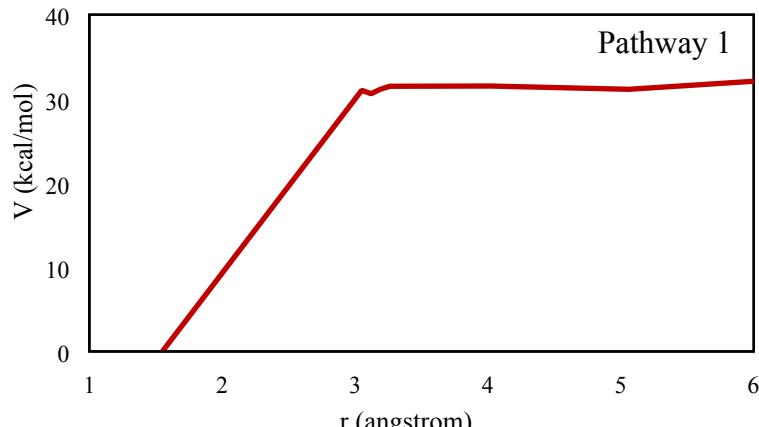
Pathway 14



Pathway 15



**Figure S2.** Mechanisms for dissociation pathways 11-15.



**Figure S3.** Potential energy curves for the C-C bond dissociations of pathways 1 and 2.

Weights are calculated as,

$$w_i = \frac{\Delta y_i^{-2}}{\sum_i \Delta y_i^{-2} / n}$$

$\Delta y_i$  is the standard deviation of a point  $(x_i, y_i)$ .  $n$  is the number of  $x$  values.

Weighted slope of the regression line is given as,

$$m_w = \frac{\sum_i w_i x_i y_i - n \bar{x}_w \bar{y}_w}{\sum_i w_i x_i^2 - n \bar{x}_w^2}$$

Intercept of the weighted regression line is calculated as,

$$b_w = \bar{y}_w - m_w \bar{x}_w$$

whereas,  $\bar{x}_w = \frac{\sum_i w_i x_i}{n}$  and  $\bar{y}_w = \frac{\sum_i w_i y_i}{n}$ .

Standard errors in the slope ( $\sigma_{m_w}$ ) and intercept ( $\sigma_{b_w}$ ) of the weighted regression line are calculated as,

$$\sigma_{m_w} = \sqrt{\frac{\chi^2}{(n-2)S_{xx}}}$$

$$\sigma_{b_w} = \sigma_{m_w} \cdot \sqrt{\frac{S_{xx}}{\sum_i w_i} + \bar{x}_w^2}$$

whereas,

$$\chi^2 = \sum_i w_i (y_i - a_w - b_w x_i)^2$$

and

$$S_{xx} = \sum_i w_i (x_i - \bar{x}_w)^2$$

The propagation of error gives the uncertainty in the slope as  $\sigma_{m_w} \cdot 10^4 \cdot R$  ( $R$  is the gas law constant) and in the intercept as  $A \cdot \sigma_{b_w}$ .

**Figure S4.** Procedure employed to calculate the slope and intercept of the weighted regression line and their corresponding uncertainties. References are provided in the text.

**Table S1.** Mean Absolute Errors (MAEs)<sup>a</sup> in B3LYP and semiempirical methods for Zn-Ligand bond distances for three conformers.

Conformer	MAE (Å)		
	MNDO/d	PM7	B3LYP
<i>a</i>	0.123	0.113	0.075
<i>b</i>	0.052	0.000	0.158
<i>c</i>	0.115	0.100	0.058

<sup>a</sup> Using M05-2X as the benchmark.

**Table S2.** All the ions ( $m/z$ ) and their observed fragments for conformer  $\alpha$  at 1600 K.

m/z	Fragments
890.2	-(CO)
875.2	-(COCH <sub>3</sub> ) or -(CONH)
874.2	-(CO <sub>2</sub> )
873.2	-(COOH)
872.2	-(CO+ H <sub>2</sub> O)
861.2	[a <sub>2</sub> +x <sub>4</sub> +Zn(II)] <sup>-</sup>
766.1	[x <sub>6</sub> +Zn(II)] <sup>-</sup>
764.1	[a <sub>2</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
723.1	[z <sub>6</sub> +Zn(II)] <sup>-</sup>
601.1	[a <sub>2</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>

**Table S3.** All the ions ( $m/z$ ) and their observed fragments for conformer  $\alpha$  at 1750 K.

m/z	Fragments
890.2	-(CO)
875.2	-(CONH)
874.2	-(CO <sub>2</sub> )
873.2	-(COOH)
861.2	[a <sub>2</sub> +x <sub>4</sub> +Zn(II)] <sup>-</sup>
837.2	-(CH <sub>2</sub> +imi)
821.2	[a <sub>3</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
792.2	[b <sub>2</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
766.1	[x <sub>6</sub> +Zn(II)] <sup>-</sup>
727.1	[a <sub>4</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
723.1	[z <sub>6</sub> +Zn(II)] <sup>-</sup>
664.1	[x <sub>5</sub> +Zn(II)] <sup>-</sup>
601.1	[a <sub>2</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
380.0	[x <sub>2</sub> +SH+Zn(II)] <sup>-</sup>

**Table S4.** All the ions ( $m/z$ ) and their observed fragments for conformer  $\alpha$  at 1875 K.

m/z	Fragments
900.2	-(H <sub>2</sub> O)
890.2	-(CO)
875.2	-(CONH)
874.2	-(CO <sub>2</sub> )
873.2	-(COOH)
872.2	-(CO+ H <sub>2</sub> O)
840.2	-(CO <sub>2</sub> +H <sub>2</sub> S)
837.2	-(CH <sub>2</sub> +imi)
821.2	[a <sub>3</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
811.2	-(CH <sub>2</sub> +PhOH)
792.2	[b <sub>2</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
778.1	[a <sub>3</sub> +z <sub>3</sub> +Zn(II)] <sup>-</sup>
766.1	[x <sub>6</sub> +Zn(II)] <sup>-</sup>
764.1	[a <sub>2</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
755.2	[a <sub>4</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
727.1	[a <sub>4</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
723.1	[z <sub>6</sub> +Zn(II)] <sup>-</sup>
712.1	[a <sub>4</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
710.1	[y <sub>6</sub> +Zn(II)-(CO)] <sup>-</sup>
693.1	[y <sub>6</sub> +Zn(II)-(COOH)] <sup>-</sup>
663.1	[x <sub>5</sub> +Zn(II)-H <sup>+</sup> ] <sup>-</sup>
601.1	[a <sub>2</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
573.1	[a <sub>2</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
550.0	[b <sub>3</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>

**Table S5.** All the ions ( $m/z$ ) and their observed fragments for conformer  $\alpha$  at 2000 K.

m/z	Fragments
916.2	–(H <sub>2</sub> )
890.2	–(CO)
875.2	–(CONH) or –(COCH <sub>3</sub> )
874.2	–(CO <sub>2</sub> )
873.2	–(COOH)
872.2	–(CO+H <sub>2</sub> O)
862.2	–(CO+CHNH)
861.2	[a <sub>2</sub> +x <sub>4</sub> +Zn(II)] <sup>-</sup>
847.2	–(CO+CONH)
845.2	–(CO+COOH)
840.2	–(CO <sub>2</sub> +H <sub>2</sub> S)
837.2	–(CH <sub>2</sub> +imi)
830.2	–(COOH+CONH)
828.2	–(SHCH <sub>2</sub> +COCH <sub>3</sub> )
821.2	[a <sub>3</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
811.2	–(CH <sub>2</sub> +PhOH)
796.2	[c <sub>5</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
783.2	–(CO+CH <sub>2</sub> +PhOH)
782.2	[a <sub>5</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
778.1	[a <sub>3</sub> +z <sub>3</sub> +Zn(II)] <sup>-</sup>
771.2	[a <sub>6</sub> +Zn(II)+H <sup>+</sup> ] <sup>-</sup>
770.2	[a <sub>6</sub> +Zn(II)] <sup>-</sup>
767.1	–(CO <sub>2</sub> +CH <sub>2</sub> +PhOH)
766.1	[x <sub>6</sub> +Zn(II)] <sup>-</sup>
764.1	[a <sub>2</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup> or [c <sub>2</sub> +z <sub>3</sub> +Zn(II)] <sup>-</sup>
762.3	–(2CH <sub>2</sub> S+Zn(II))
755.2	[a <sub>4</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
740.1	–(CO+CONH+CH <sub>2</sub> +PhOH)
738.1	[y <sub>6</sub> +Zn(II)] <sup>-</sup> or [x <sub>6</sub> +Zn(II)–(CO)] <sup>-</sup>
730.1	–(2CH <sub>2</sub> +PhOH+imi)
723.1	[z <sub>6</sub> +Zn(II)] <sup>-</sup>
722.1	[x <sub>6</sub> +Zn(II)–(CO <sub>2</sub> )] <sup>-</sup>

721.1	[a <sub>2</sub> +z <sub>3</sub> +Zn(II)] <sup>-</sup>
712.1	[a <sub>4</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
695.1	[z <sub>6</sub> +Zn(II)-(CO)] <sup>-</sup>
693.1	[y <sub>6</sub> +Zn(II)-(COOH)] <sup>-</sup>
682.1	[a <sub>4</sub> +y <sub>2</sub> +Zn(II)-(COOH)] <sup>-</sup>
678.1	[z <sub>6</sub> +Zn(II)-(COOH)] <sup>-</sup> or [c <sub>5</sub> +Zn(II)] <sup>-</sup>
668.1	[y <sub>5</sub> +S+Zn(II)] <sup>-</sup>
664.1	[x <sub>5</sub> +Zn(II)] <sup>-</sup>
658.1	[a <sub>3</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup> or [b <sub>3</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
636.1	[y <sub>5</sub> +Zn(II)] <sup>-</sup> or [y <sub>6</sub> +Zn(II)-(CONHCH <sub>2</sub> +COOH)] <sup>-</sup>
631.1	[y <sub>6</sub> +Zn(II)-(CH <sub>2</sub> +PhOH)] <sup>-</sup>
630.1	[a <sub>3</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
625.1	[y <sub>4</sub> +SCH <sub>2</sub> +Zn(II)] <sup>-</sup>
619.1	[a <sub>4</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
613.1	[a <sub>3</sub> +x <sub>2</sub> +Zn(II)-(COOH)] <sup>-</sup>
601.1	[a <sub>2</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
600.2	[x <sub>5</sub> ] <sup>-</sup>
599.1	[x <sub>5</sub> -H <sup>+</sup> ] <sup>-</sup>
591.1	[a <sub>4</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
576.1	[x <sub>6</sub> +Zn(II)- (CONH+CO+CH <sub>2</sub> +PhOH)] <sup>-</sup>
573.1	[a <sub>2</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
558.1	[a <sub>2</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
550.0	[b <sub>3</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup> or [a <sub>3</sub> +y <sub>2</sub> +Zn(II)- (CH <sub>2</sub> +imi)] <sup>-</sup>
541.1	[z <sub>3</sub> +NHC <sub>2</sub> H <sub>3</sub> S+Zn(II)] <sup>-</sup>
479.0	[a <sub>3</sub> +z <sub>1</sub> +Zn(II)] <sup>-</sup>
467.0	[z <sub>3</sub> +Zn(II)] <sup>-</sup>
421.0	[a <sub>3</sub> +SCH <sub>2</sub> +Zn(II)] <sup>-</sup>
380.0	[x <sub>2</sub> +SH+Zn(II)] <sup>-</sup>
319.0	[y <sub>2</sub> +Zn(II)] <sup>-</sup>
304.0	[z <sub>2</sub> +Zn(II)] <sup>-</sup>
283.1	[x <sub>2</sub> ] <sup>-</sup>

**Table S6.** All the ions ( $m/z$ ) and their observed fragments for conformer  $a$  at 2250 K.

m/z	Fragments
916.2	–(H <sub>2</sub> )
900.2	–(H <sub>2</sub> O)
890.2	–(CO)
875.2	–(CONH) or –(COCH <sub>3</sub> )
874.2	–(CO <sub>2</sub> )
873.2	–(COOH)
872.2	–(CO+H <sub>2</sub> O)
862.2	–(CO+CHNH)
861.2	[a <sub>2</sub> +x <sub>4</sub> +Zn(II)] <sup>-</sup>
849.1	[b <sub>3</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
847.2	–(CO+CONH)
845.2	–(CO+COOH)
840.2	–(CO <sub>2</sub> +H <sub>2</sub> S)
837.2	–(CH <sub>2</sub> +imi)
830.2	–(COOH+CONH)
821.2	[a <sub>3</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
816.2	[a <sub>6</sub> +COOH+Zn(II)] <sup>-</sup>
811.2	–(CH <sub>2</sub> +PhOH)
796.2	[c <sub>5</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
794.1	–(COCH <sub>3</sub> +CH <sub>2</sub> +imi)
792.1	–(COOH+CH <sub>2</sub> +imi)
782.2	[a <sub>5</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
778.1	[a <sub>3</sub> +z <sub>3</sub> +Zn(II)] <sup>-</sup>
770.2	[a <sub>6</sub> +Zn(II)] <sup>-</sup>
766.1	[x <sub>6</sub> +Zn(II)] <sup>-</sup>
764.1	[a <sub>2</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
762.3	–(2CH <sub>2</sub> S+Zn(II))
755.2	[a <sub>4</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
738.1	[y <sub>6</sub> +Zn(II)] <sup>-</sup> or [x <sub>6</sub> +Zn(II)-(CO)] <sup>-</sup>
727.1	[a <sub>4</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
723.1	[z <sub>6</sub> +Zn(II)] <sup>-</sup>

712.1	[a <sub>4</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
707.1	[a <sub>3</sub> +x <sub>3</sub> -x <sub>1</sub> +SH+Zn(II)] <sup>-</sup>
693.1	[y <sub>6</sub> +Zn(II)-(COOH)] <sup>-</sup>
681.1	[y <sub>6</sub> +Zn(II)-(CO+CH <sub>2</sub> NH)] <sup>-</sup>
678.1	[z <sub>6</sub> +Zn(II)-(COOH)] <sup>-</sup> or [c <sub>5</sub> +Zn(II)] <sup>-</sup>
675.3	[a <sub>6</sub> -S] <sup>-</sup>
664.1	[x <sub>5</sub> +Zn(II)] <sup>-</sup>
658.1	[a <sub>3</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
650.1	[z <sub>6</sub> +Zn(II)-(CO+COOH)] <sup>-</sup>
636.1	[y <sub>5</sub> +Zn(II)] <sup>-</sup> or [y <sub>6</sub> +Zn(II)-(CONHCH <sub>2</sub> +COOH)] <sup>-</sup>
619.1	[a <sub>4</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
616.1	[x <sub>6</sub> +Zn(II)-(CONH+CH <sub>2</sub> +PhOH)] <sup>-</sup>
615.1	[a <sub>3</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
614.2	[c <sub>5</sub> ] <sup>-</sup>
607.1	[x <sub>4</sub> +Zn(II)] <sup>-</sup>
601.1	[a <sub>2</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
599.1	[x <sub>5</sub> -H <sup>+</sup> ] <sup>-</sup>
587.1	[a <sub>3</sub> +y <sub>2</sub> +Zn(II)-(CONH)] <sup>-</sup>
573.1	[a <sub>2</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
558.1	[a <sub>2</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
550.0	[b <sub>3</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
549.0	[a <sub>3</sub> +y <sub>2</sub> +Zn(II)-(CH <sub>2</sub> +imi)] <sup>-</sup>
541.1	[z <sub>3</sub> +NHC <sub>2</sub> H <sub>3</sub> S+Zn(II)] <sup>-</sup>
515.2	[y <sub>4</sub> ] <sup>-</sup>
499.0	[z <sub>3</sub> +S+Zn(II)] <sup>-</sup>
449.0	[x <sub>6</sub> -(x <sub>5</sub> -a <sub>5</sub> )+Zn(II)] <sup>-</sup>
421.0	[a <sub>3</sub> +SCH <sub>2</sub> +Zn(II)] <sup>-</sup>
393.1	[y <sub>2</sub> +SCH <sub>2</sub> +Zn(II)] <sup>-</sup>
380.0	[x <sub>2</sub> +SH+Zn(II)] <sup>-</sup>
356.0	[a <sub>2</sub> +y <sub>1</sub> +Zn(II)-(CH <sub>2</sub> +imi)] <sup>-</sup>
347.0	[x <sub>2</sub> +Zn(II)] <sup>-</sup>
319.0	[y <sub>2</sub> +Zn(II)] <sup>-</sup>
237.1	[x <sub>2</sub> -(SCH <sub>2</sub> )] <sup>-</sup>
129.0	[SH+S+Zn(II)] <sup>-</sup>
33.0	[SH] <sup>-</sup>

**Table S7.** All the ions ( $m/z$ ) and their observed fragments for conformer *b* at 2000 K.

m/z	Fragments
916.2	-(H <sub>2</sub> )
892.2	-(C <sub>2</sub> H <sub>4</sub> )
890.2	-(CO)
888.2	-(CO+H <sub>2</sub> )
875.2	-(CONH)
874.2	-(CO <sub>2</sub> )
873.2	-(COOH)
847.2	-(CO+CONH)
837.2	-(CH <sub>2</sub> +imi)
821.2	[a <sub>3</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
811.2	-(CH <sub>2</sub> +PhOH)
809.2	-(CO+CH <sub>2</sub> +imi)
794.1	-(COCH <sub>3</sub> +CH <sub>2</sub> +imi)
793.1	-(CO <sub>2</sub> +CH <sub>2</sub> +imi)
792.1	-(COOH+CH <sub>2</sub> +imi)
791.1	-(CO+H <sub>2</sub> O+CH <sub>2</sub> +imi)
781.1	[a <sub>5</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
768.2	-(CONH+CH <sub>2</sub> +imi)
766.1	[x <sub>6</sub> +Zn(II)] <sup>-</sup>
764.1	[c <sub>2</sub> +z <sub>3</sub> +Zn(II)] <sup>-</sup>
755.2	[a <sub>4</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
753.1	[a <sub>5</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
740.1	[a <sub>3</sub> +x <sub>3</sub> +Zn(II)-(CH <sub>2</sub> +imi)] <sup>-</sup>
738.1	[y <sub>6</sub> +Zn(II)] <sup>-</sup> or [x <sub>6</sub> +Zn(II)-(CO)] <sup>-</sup>
730.1	-(2CH <sub>2</sub> +PhOH+imi)
727.1	[a <sub>4</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
723.1	[z <sub>6</sub> +Zn(II)] <sup>-</sup>
722.1	[x <sub>6</sub> +Zn(II)-(CO <sub>2</sub> )] <sup>-</sup>
721.1	[a <sub>2</sub> +z <sub>3</sub> +Zn(II)] <sup>-</sup>
720.1	[x <sub>6</sub> +Zn(II)-(CO+H <sub>2</sub> O)] <sup>-</sup>
712.1	[a <sub>4</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
710.1	[y <sub>6</sub> +Zn(II)-(CO)] <sup>-</sup>

696.1	[x <sub>5</sub> +Zn(II)] <sup>-</sup>
695.1	[z <sub>6</sub> +Zn(II)-(CO)] <sup>-</sup>
693.1	[y <sub>6</sub> +Zn(II)-(COOH)] <sup>-</sup>
682.1	[a <sub>4</sub> +y <sub>2</sub> +Zn(II)-(COOH)] <sup>-</sup>
681.1	[y <sub>6</sub> +Zn(II)-(CO+CH <sub>2</sub> NH)] <sup>-</sup>
679.1	[z <sub>6</sub> +Zn(II)-(CO <sub>2</sub> )] <sup>-</sup>
678.1	[c <sub>5</sub> +Zn(II)] <sup>-</sup>
668.1	[y <sub>5</sub> +S+Zn(II)] <sup>-</sup>
667.1	[a <sub>5</sub> +S+Zn(II)] <sup>-</sup>
641.1	[x <sub>6</sub> +Zn(II)-(CO <sub>2</sub> +CH <sub>2</sub> +imi)] <sup>-</sup>
613.1	[a <sub>3</sub> +x <sub>2</sub> +Zn(II)-(COOH)] <sup>-</sup>
614.2	[c <sub>5</sub> ] <sup>-</sup>
607.1	[x <sub>4</sub> +Zn(II)] <sup>-</sup>
601.1	[a <sub>2</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
578.1	[x <sub>5</sub> -y <sub>1</sub> +S+Zn(II)] <sup>-</sup>
558.1	[a <sub>2</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
546.1	[a <sub>4</sub> +SC <sub>2</sub> H <sub>3</sub> NH+Zn(II)] <sup>-</sup>
521.0	[a <sub>3</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
515.0	[x <sub>6</sub> -x <sub>2</sub> +S+Zn(II)] <sup>-</sup>
505.1	[a <sub>4</sub> +SH+Zn(II)] <sup>-</sup>
493.0	[a <sub>3</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
467.0	[z <sub>3</sub> +Zn(II)] <sup>-</sup>
464.0	[b <sub>3</sub> +NCH <sub>2</sub> +SH+Zn(II)] <sup>-</sup>
452.0	[c <sub>4</sub> +H <sup>+</sup> +Zn(II)] <sup>-</sup>
421.0	[a <sub>3</sub> +SCH <sub>2</sub> +Zn(II)] <sup>-</sup>
407.0	[a <sub>3</sub> +S+Zn(II)] <sup>-</sup>
393.1	[y <sub>2</sub> +SCH <sub>2</sub> +Zn(II)] <sup>-</sup>
392.0	[a <sub>2</sub> +y <sub>1</sub> +Zn(II)-(CO <sub>2</sub> )] <sup>-</sup>
383.0	[a <sub>2</sub> +x <sub>1</sub> +Zn(II)-(CH <sub>2</sub> +imi)] <sup>-</sup>
378.0	[y <sub>6</sub> -x <sub>5</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
377.0	[a <sub>2</sub> +SC <sub>2</sub> H <sub>3</sub> +Zn(II)] <sup>-</sup>
340.0	[a <sub>2</sub> +z <sub>1</sub> +Zn(II)-(CH <sub>2</sub> +imi)] <sup>-</sup>
284.0	[x <sub>1</sub> +SC <sub>2</sub> H <sub>3</sub> NH+Zn(II)] <sup>-</sup>
283.1	[x <sub>2</sub> ] <sup>-</sup>

**Table S8.** All the ions ( $m/z$ ) and their observed fragments for conformer *b* at 2250 K.

m/z	Fragments
892.2	–(C <sub>2</sub> H <sub>4</sub> )
890.2	–(CO)
875.2	–(CONH)
874.2	–(CO <sub>2</sub> )
873.2	–(COOH)
837.2	–(CH <sub>2</sub> +imi)
821.2	[a <sub>3</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
811.2	–(CH <sub>2</sub> +PhOH)
809.2	–(CO+CH <sub>2</sub> +imi)
794.1	–(COCH <sub>3</sub> +CH <sub>2</sub> +imi)
793.1	–(CO <sub>2</sub> +CH <sub>2</sub> +imi)
792.1	–(COOH+CH <sub>2</sub> +imi)
781.1	[a <sub>5</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
778.1	[a <sub>3</sub> +z <sub>3</sub> +Zn(II)] <sup>-</sup>
767.1	–(CO <sub>2</sub> +CH <sub>2</sub> +PhOH)
766.1	[x <sub>6</sub> +Zn(II)] <sup>-</sup>
764.1	[a <sub>2</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
755.2	[a <sub>4</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
753.1	[a <sub>5</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
738.1	[y <sub>6</sub> +Zn(II)] <sup>-</sup> or [x <sub>6</sub> +Zn(II)–(CO)] <sup>-</sup>
730.1	–(2CH <sub>2</sub> +PhOH+imi)
727.1	[a <sub>4</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
725.1	[b <sub>3</sub> +z <sub>3</sub> +Zn(II)–(CH <sub>2</sub> +imi)] <sup>-</sup>
723.1	[z <sub>6</sub> +Zn(II)] <sup>-</sup>
712.1	[a <sub>4</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
710.1	[y <sub>6</sub> +Zn(II)–(CO)] <sup>-</sup>
696.1	[x <sub>5</sub> +Zn(II)] <sup>-</sup>
695.1	[z <sub>6</sub> +Zn(II)–(CO)] <sup>-</sup>
693.1	[y <sub>6</sub> +Zn(II)–(COOH)] <sup>-</sup>
686.1	[b <sub>3</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
682.1	[a <sub>4</sub> +y <sub>2</sub> +Zn(II)–(COOH)] <sup>-</sup>
681.1	[y <sub>6</sub> +Zn(II)–(CO+CH <sub>2</sub> NH)] <sup>-</sup>

679.1	[z <sub>6</sub> +Zn(II)-(CO <sub>2</sub> )] <sup>-</sup>
678.1	[c <sub>5</sub> +Zn(II)] <sup>-</sup>
676.3	[a <sub>6</sub> -S] <sup>-</sup>
668.1	[y <sub>5</sub> +S+Zn(II)] <sup>-</sup>
667.1	[a <sub>5</sub> +S+Zn(II)] <sup>-</sup>
658.1	[a <sub>3</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
657.1	[a <sub>2</sub> +x <sub>3</sub> +Zn(II)-(CH <sub>2</sub> +PhOH)] <sup>-</sup>
641.1	[x <sub>6</sub> +Zn(II)-(CO <sub>2</sub> +CH <sub>2</sub> +imi)] <sup>-</sup>
620.1	[x <sub>5</sub> +Zn(II)-(CO <sub>2</sub> )] <sup>-</sup>
618.1	[a <sub>4</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
614.2	[c <sub>5</sub> ] <sup>-</sup>
612.0	[x <sub>6</sub> -(x <sub>5</sub> -a <sub>4</sub> )+Zn(II)] <sup>-</sup>
601.1	[a <sub>2</sub> +x <sub>2</sub> +Zn(II)] <sup>-</sup>
599.1	[x <sub>5</sub> -H <sup>+</sup> ] <sup>-</sup>
597.1	[y <sub>4</sub> +SCH <sub>2</sub> +Zn(II)-(CO)] <sup>-</sup>
591.1	[a <sub>4</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
590.1	[a <sub>4</sub> +y <sub>1</sub> +Zn(II)-H <sup>+</sup> ] <sup>-</sup>
575.1	[a <sub>4</sub> +z <sub>1</sub> +Zn(II)] <sup>-</sup>
573.1	[a <sub>2</sub> +y <sub>2</sub> +Zn(II)] <sup>-</sup>
558.1	[a <sub>2</sub> +z <sub>2</sub> +Zn(II)] <sup>-</sup>
550.0	[b <sub>3</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
521.0	[b <sub>3</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
506.0	[a <sub>4</sub> +S+Zn(II)] <sup>-</sup>
505.1	[a <sub>4</sub> +SH+Zn(II)] <sup>-</sup>
464.0	[b <sub>3</sub> +NCH <sub>2</sub> +SH+Zn(II)] <sup>-</sup>
452.0	[c <sub>4</sub> +H <sup>+</sup> +Zn(II)] <sup>-</sup>
449.0	[x <sub>6</sub> -(x <sub>5</sub> -a <sub>5</sub> )+Zn(II)] <sup>-</sup>
438.0	[x <sub>6</sub> -(x <sub>3</sub> -b <sub>6</sub> )+Zn(II)] <sup>-</sup>
436.0	[a <sub>2</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
312.0	[x <sub>6</sub> -(x <sub>5</sub> -a <sub>6</sub> )+Zn(II)] <sup>-</sup>
309.0	[z <sub>6</sub> -x <sub>3</sub> +S+Zn(II)] <sup>-</sup>
292.0	[z <sub>2</sub> +S+Zn(II)-(CO <sub>2</sub> )] <sup>-</sup>
284.0	[x <sub>6</sub> -(x <sub>5</sub> -b <sub>6</sub> )+Zn(II)] <sup>-</sup>
283.1	[x <sub>2</sub> ] <sup>-</sup>
256.0	[x <sub>1</sub> +SCH <sub>2</sub> +Zn(II)] <sup>-</sup>
235.0	[x <sub>2</sub> -SCH <sub>2</sub> ] <sup>-</sup>

228.0 [y<sub>1</sub>+SCH<sub>2</sub>+Zn(II)]<sup>-</sup>  
46.0 [SCH<sub>2</sub>]<sup>-</sup>

**Table S9.** All the ions ( $m/z$ ) and their observed fragments for conformer  $c$  at 2000 K.

m/z	Fragments
890.2	-(CO)
875.2	-(CONH)
874.2	-(CO <sub>2</sub> )
861.2	[a <sub>2</sub> +x <sub>4</sub> +Zn(II)] <sup>-</sup>
846.2	-(CO+CO <sub>2</sub> )
837.2	-(CH <sub>2</sub> +imi)
833.2	[a <sub>2</sub> +y <sub>4</sub> +Zn(II)] <sup>-</sup>
821.2	[a <sub>3</sub> +x <sub>3</sub> +Zn(II)] <sup>-</sup>
811.2	-(CH <sub>2</sub> +PhOH)
766.1	[x <sub>6</sub> +Zn(II)] <sup>-</sup>
753.1	[a <sub>5</sub> +y <sub>1</sub> +Zn(II)] <sup>-</sup>
745.3	-(CO <sub>2</sub> +SHZnS)
723.1	[z <sub>6</sub> +Zn(II)] <sup>-</sup>
693.1	[y <sub>6</sub> +Zn(II)-(COOH)] <sup>-</sup>
618.1	[a <sub>4</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
464.0	[a <sub>2</sub> +x <sub>1</sub> +Zn(II)] <sup>-</sup>
228.0	[y <sub>1</sub> +SCH <sub>2</sub> +Zn(II)] <sup>-</sup>