Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Chemical Dynamics Simulations of Peptide Ion CID. Comparisons between $TIK(H^+)_2$ and $TLK(H^+)_2$ Fragmentation Dynamics, and with Thermal Simulations

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SUPPORTING INFORMATION

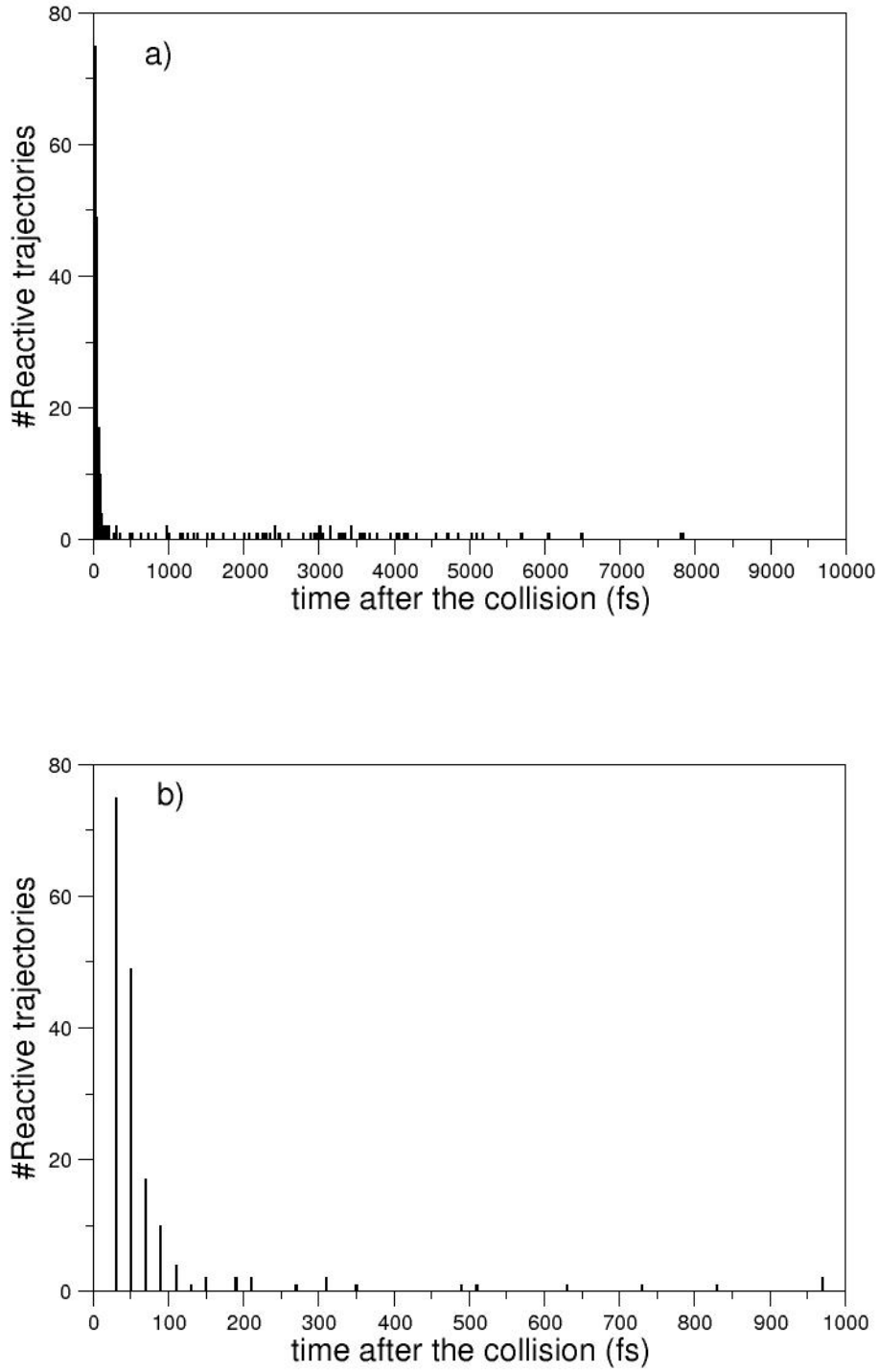
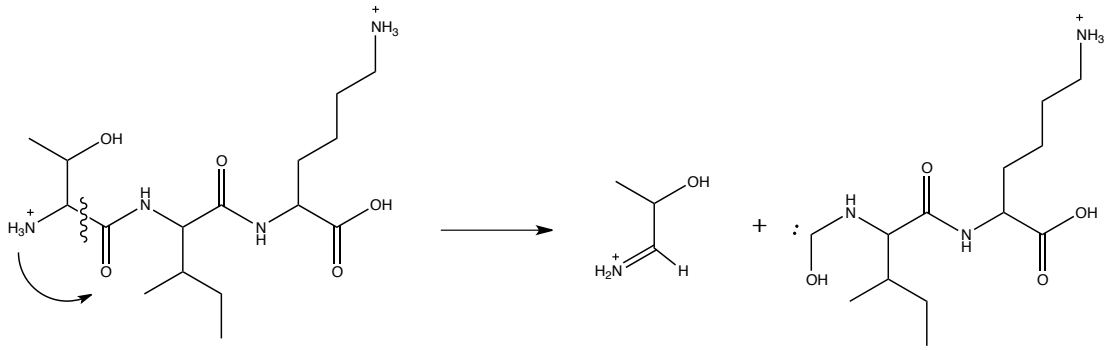


Figure S1. Number of reactive trajectories as a function of time after the collision with N_2 projectile as obtained from TLK$(H^+)_2$ simulation at CE=13 eV. Panel a) shows the counting over the whole simulation time, while panel b) shows a zoom over the first pico-second.

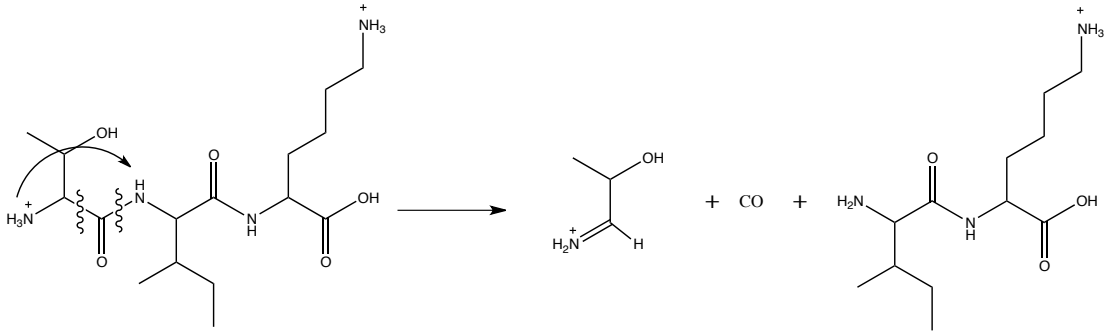
Pathway 1



a_1^+
m/z 74

x_2^+
m/z 288

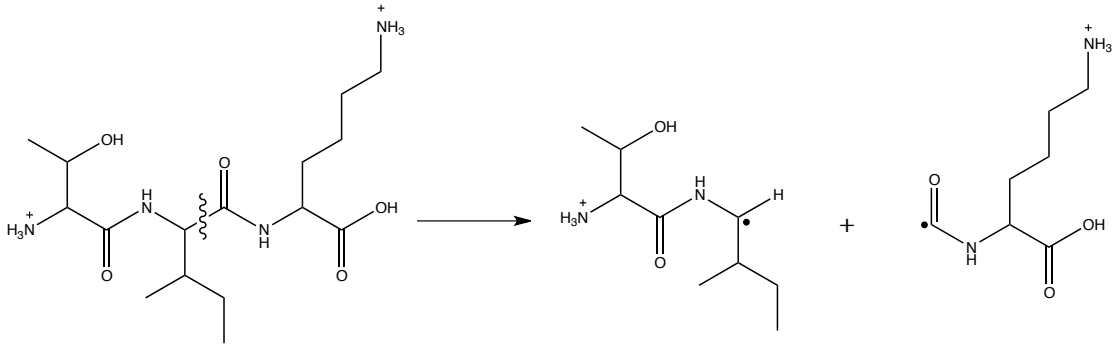
Pathway 2



a_1^+
m/z 74

y_2^+
m/z 260

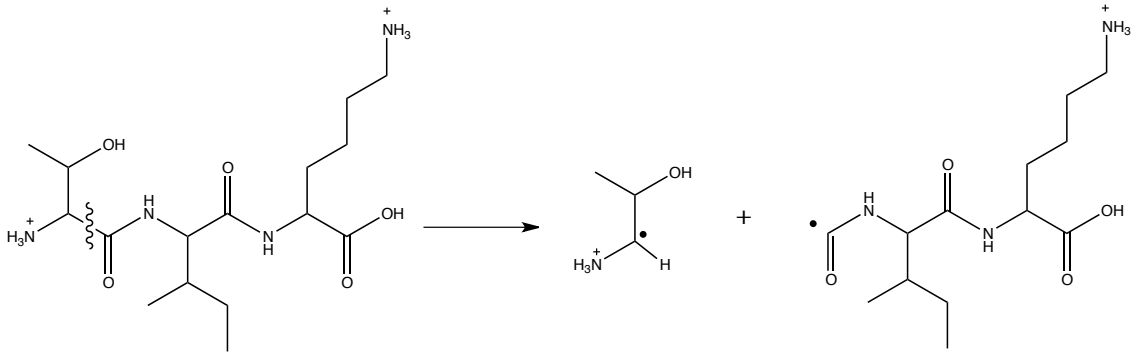
Pathway 3



$a_2^{+\cdot}$
m/z 188

$x_1^{+\cdot}$
m/z 174

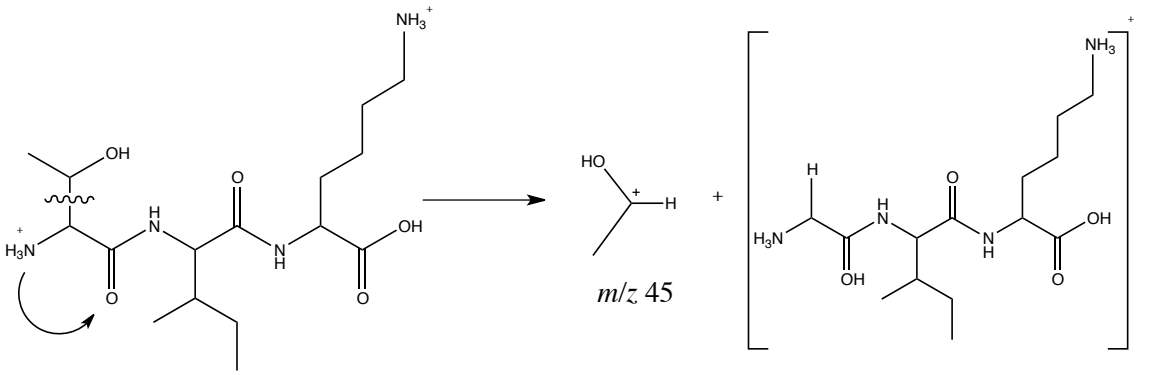
Pathway 4



$a_1^{+\cdot}$
m/z 75

$x_2^{+\cdot}$
m/z 287

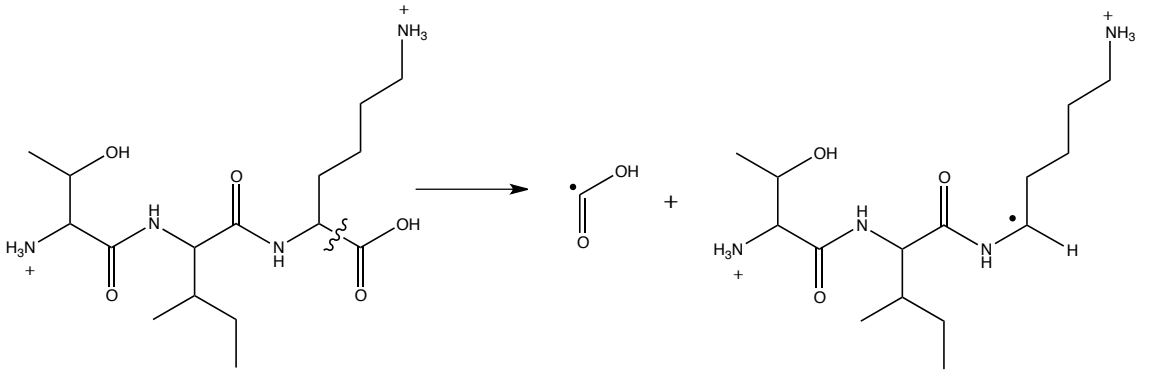
Pathway 5



m/*z* 45

m/*z* 317

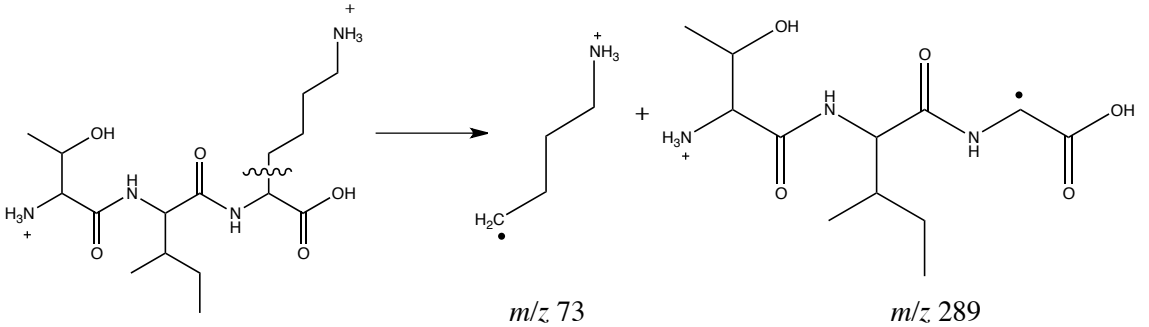
Pathway 6



$a_3^{2+\cdot}$

m/*z* 158.5

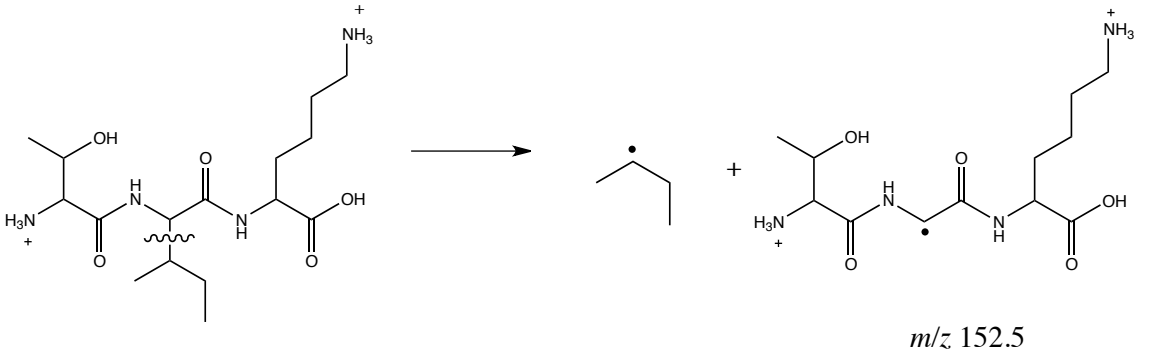
Pathway 7



m/*z* 73

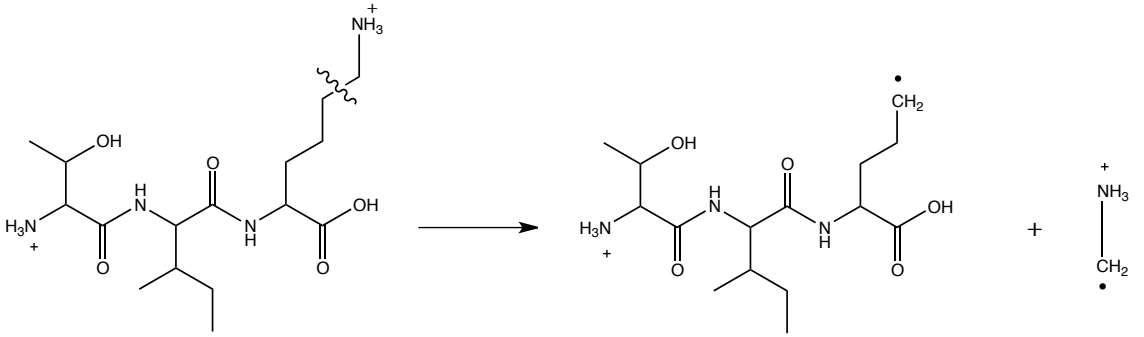
m/*z* 289

Pathway 8



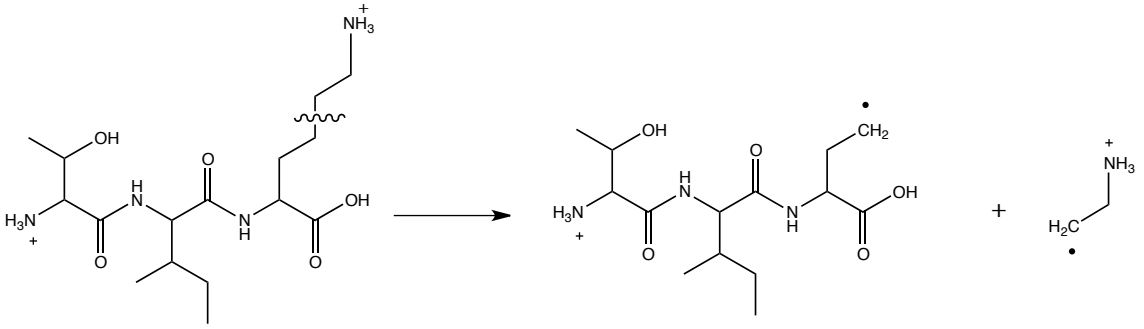
m/*z* 152.5

Pathway 9



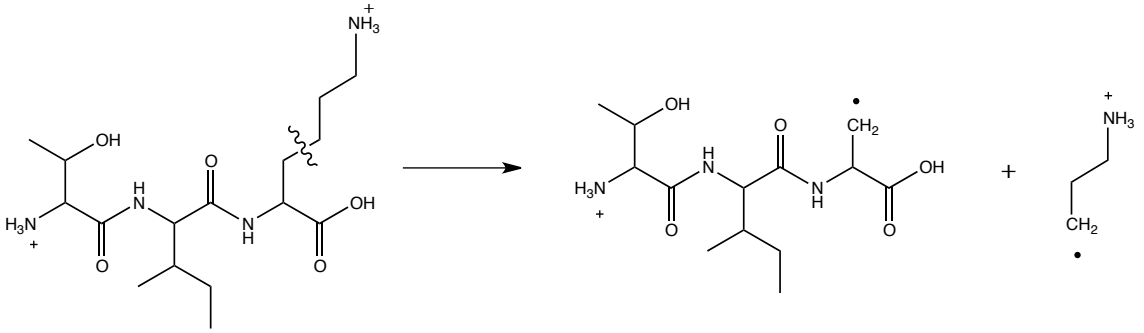
m/*z* 331 *m*/*z* 31

Pathway 10



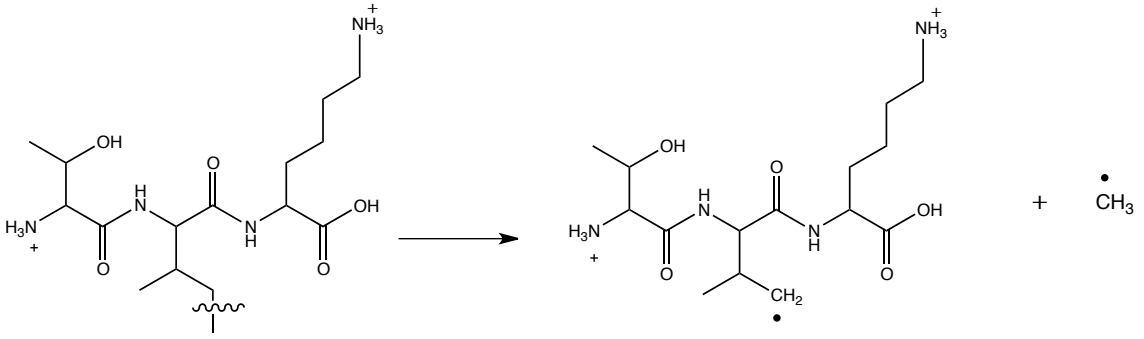
m/*z* 317 *m*/*z* 45

Pathway 11



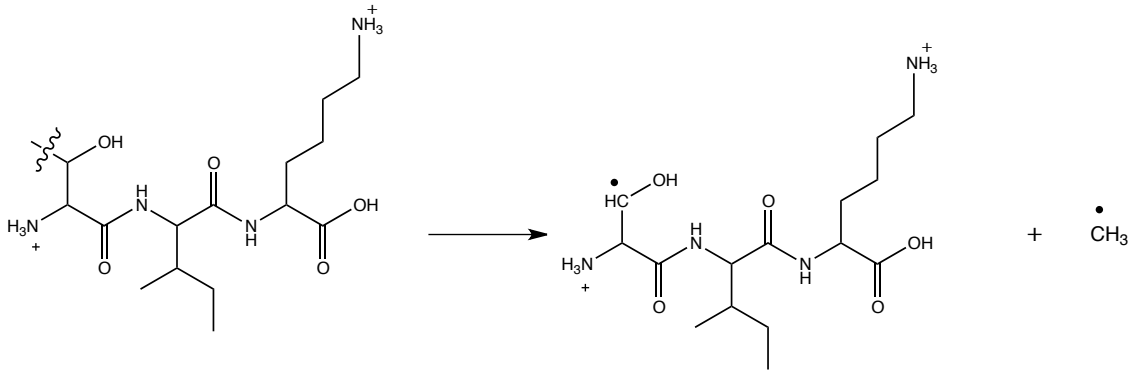
m/*z* 303 *m*/*z* 59

Pathway 12



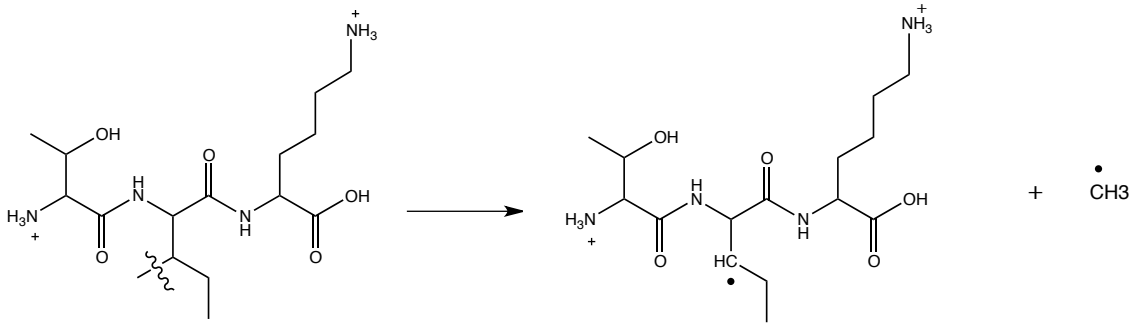
m/*z* 173.5

Pathway 13



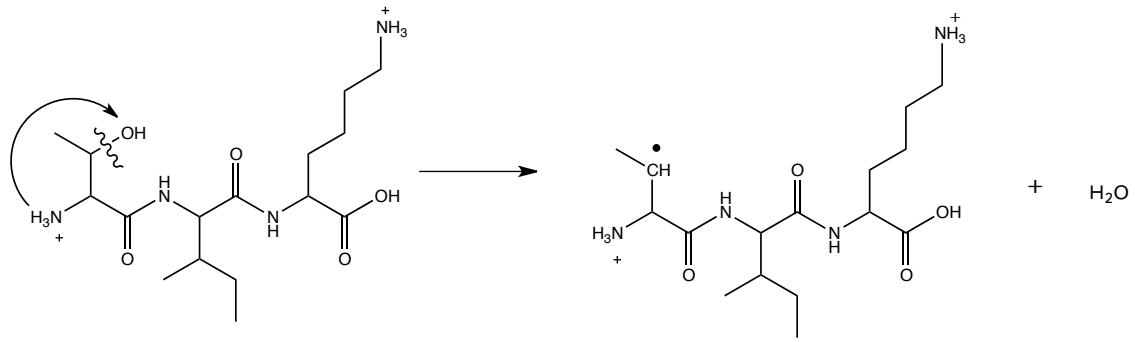
m/*z* 173.5

Pathway 14



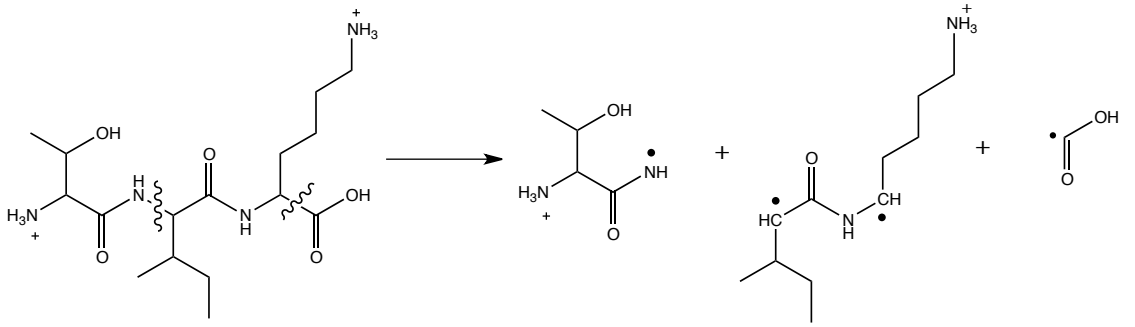
m/*z* 173.5

Pathway 15



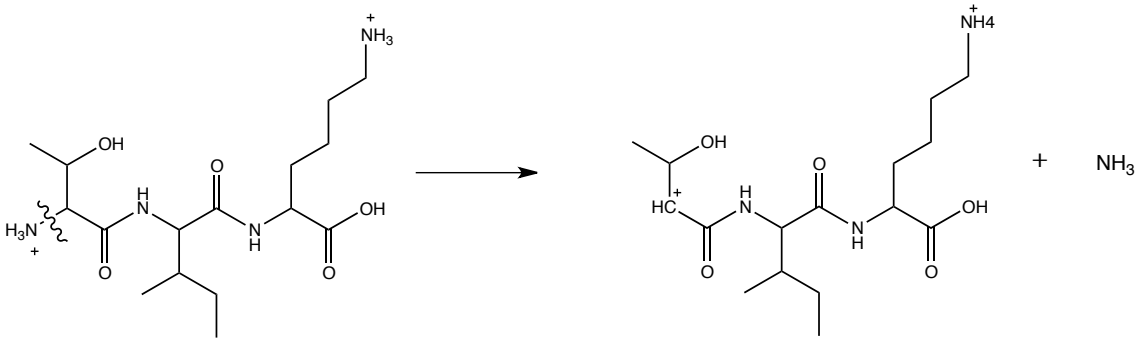
m/*z* 172

Pathway 16



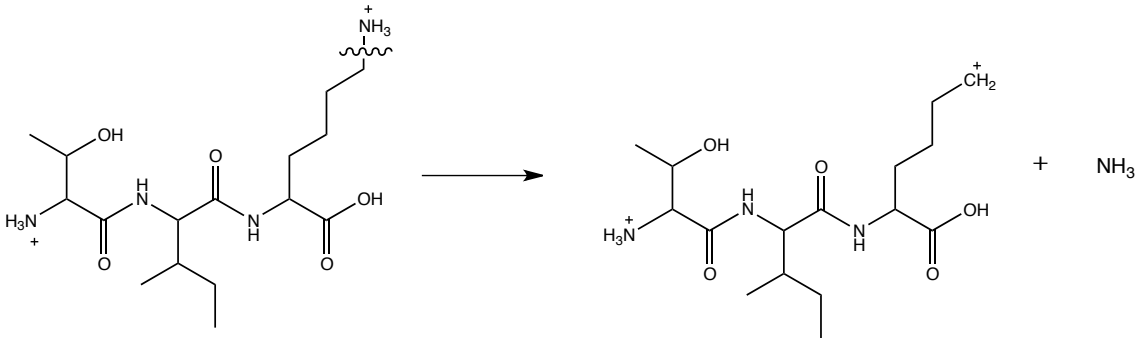
m/*z* 118 *m*/*z* 199

Pathway 17



m/z 172.5

Pathway 18



m/z 172.5

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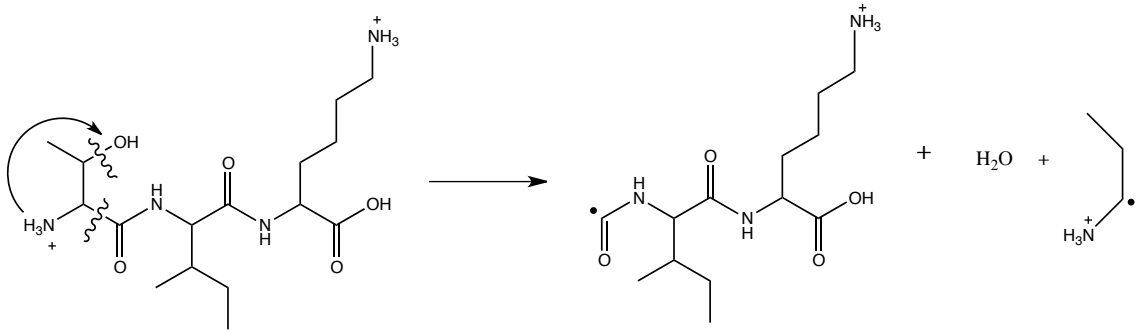

m/z 172.5

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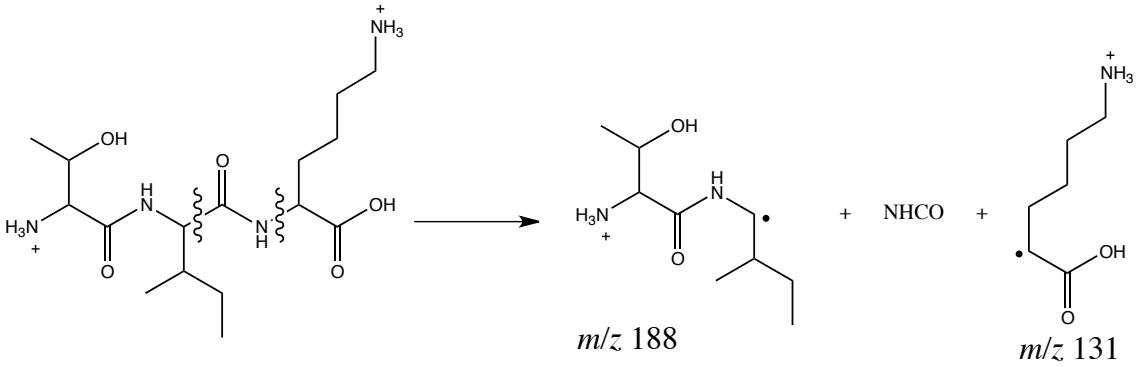
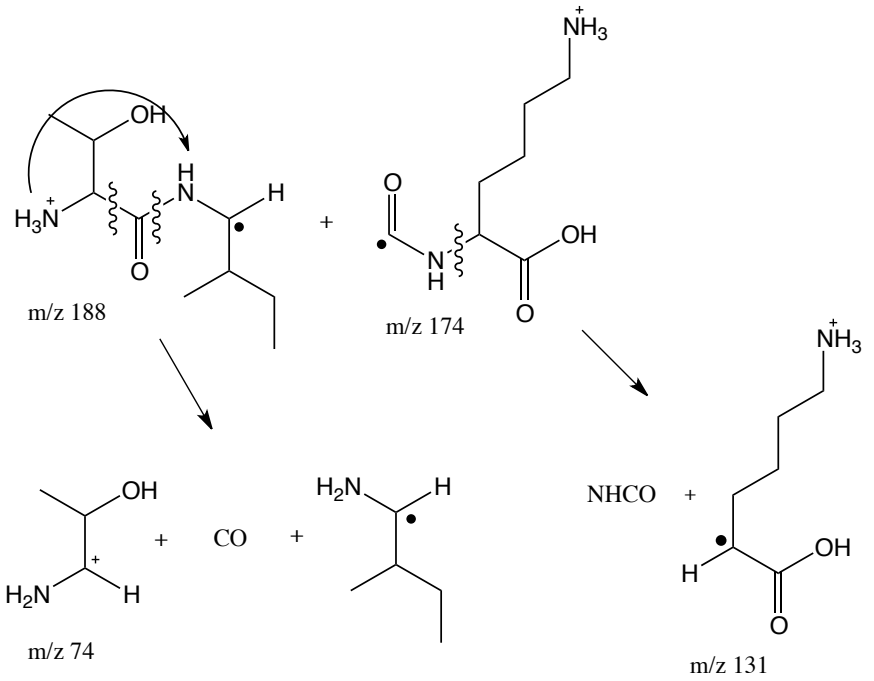


m/z 188

m/z 131

Figure S2. Primary dissociation pathways as from Ref. 29 of the manuscript

Pathway 3



Pathway 4

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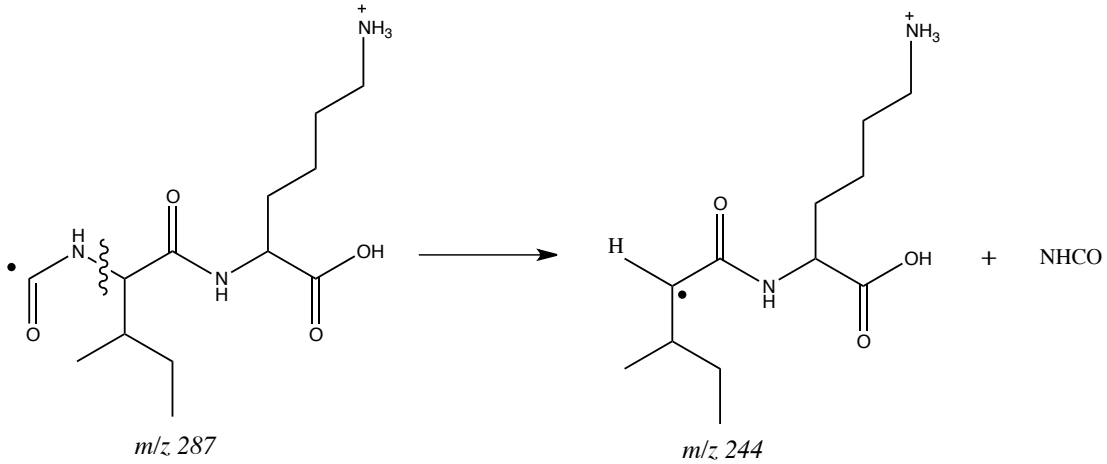
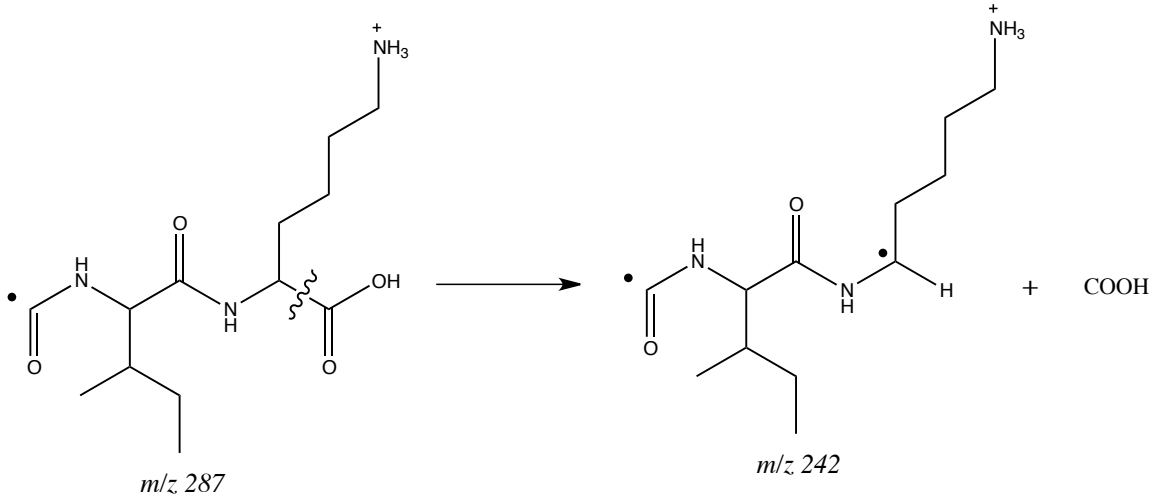


m/z 287 *m/z 244*

2)



m/z 287 *m/z 242*

Pathway 5

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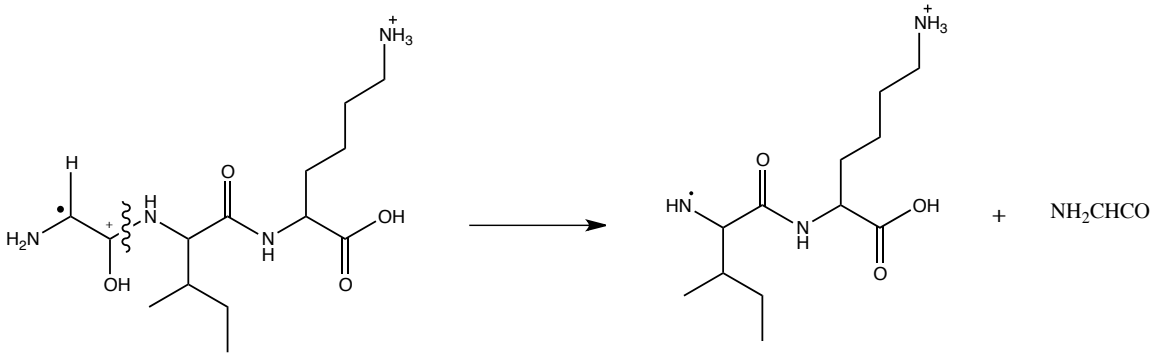
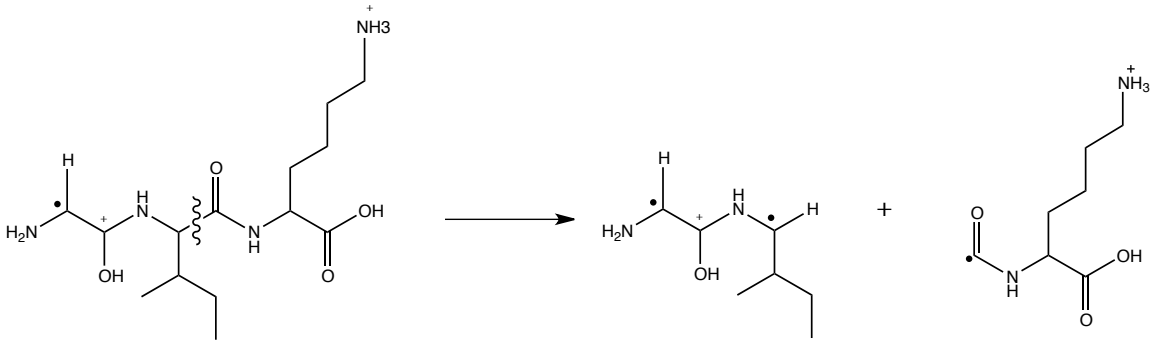


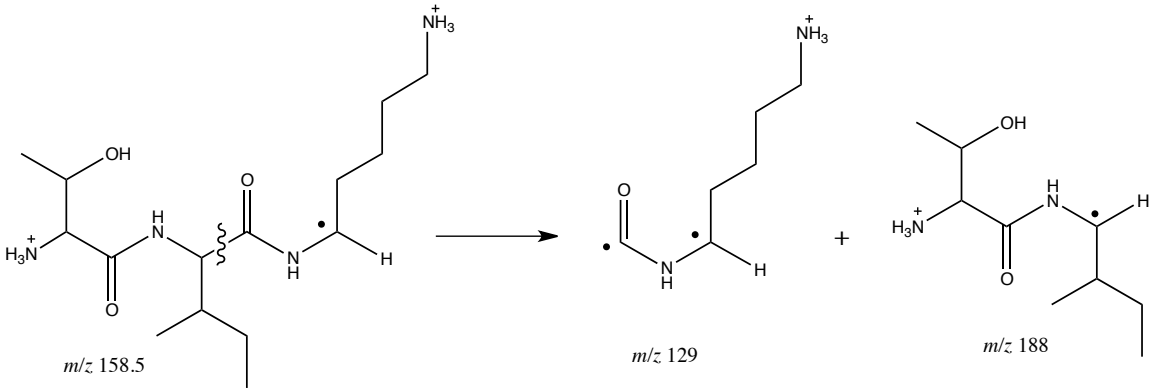
m/z 158.5 *m/z 260* *m/z 57*

2)



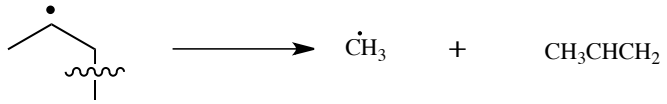
m/z 158.5 *m/z 142* *m/z* 175

Pathway 6

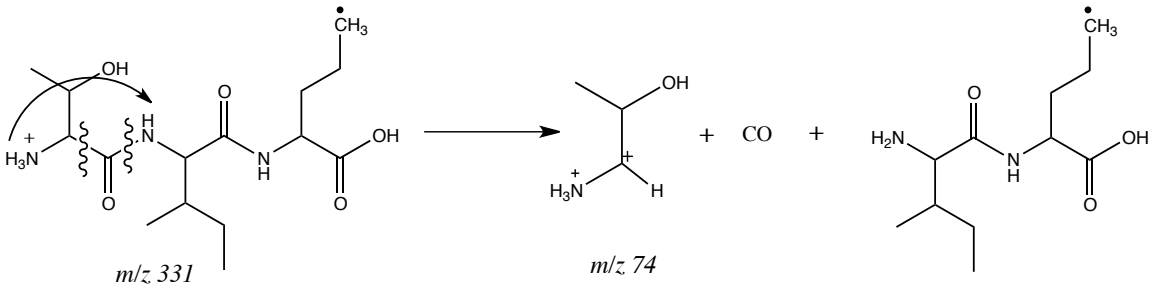


m/z 158.5 *m/z* 129 *m/z* 188

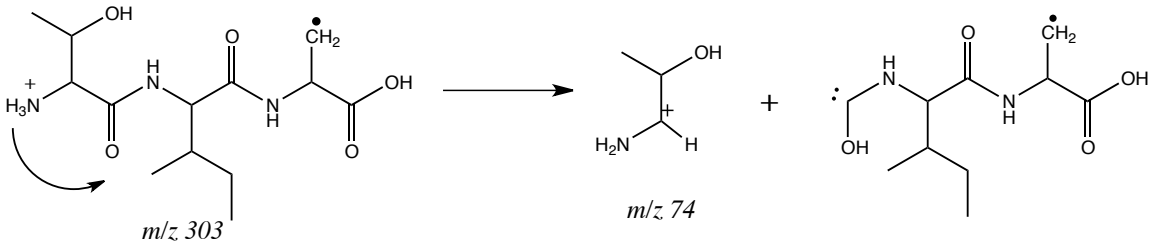
Pathway 8



Pathway 9



Pathway 11



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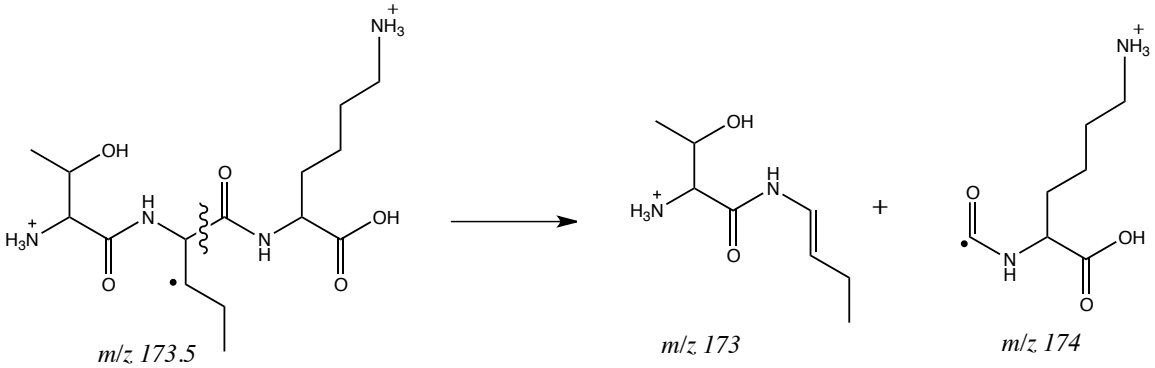
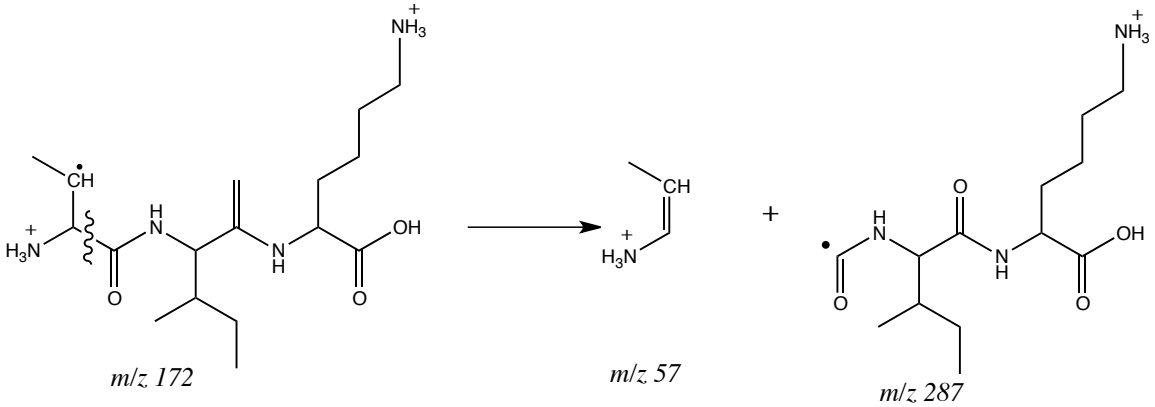


Pathway 15



Pathway 18

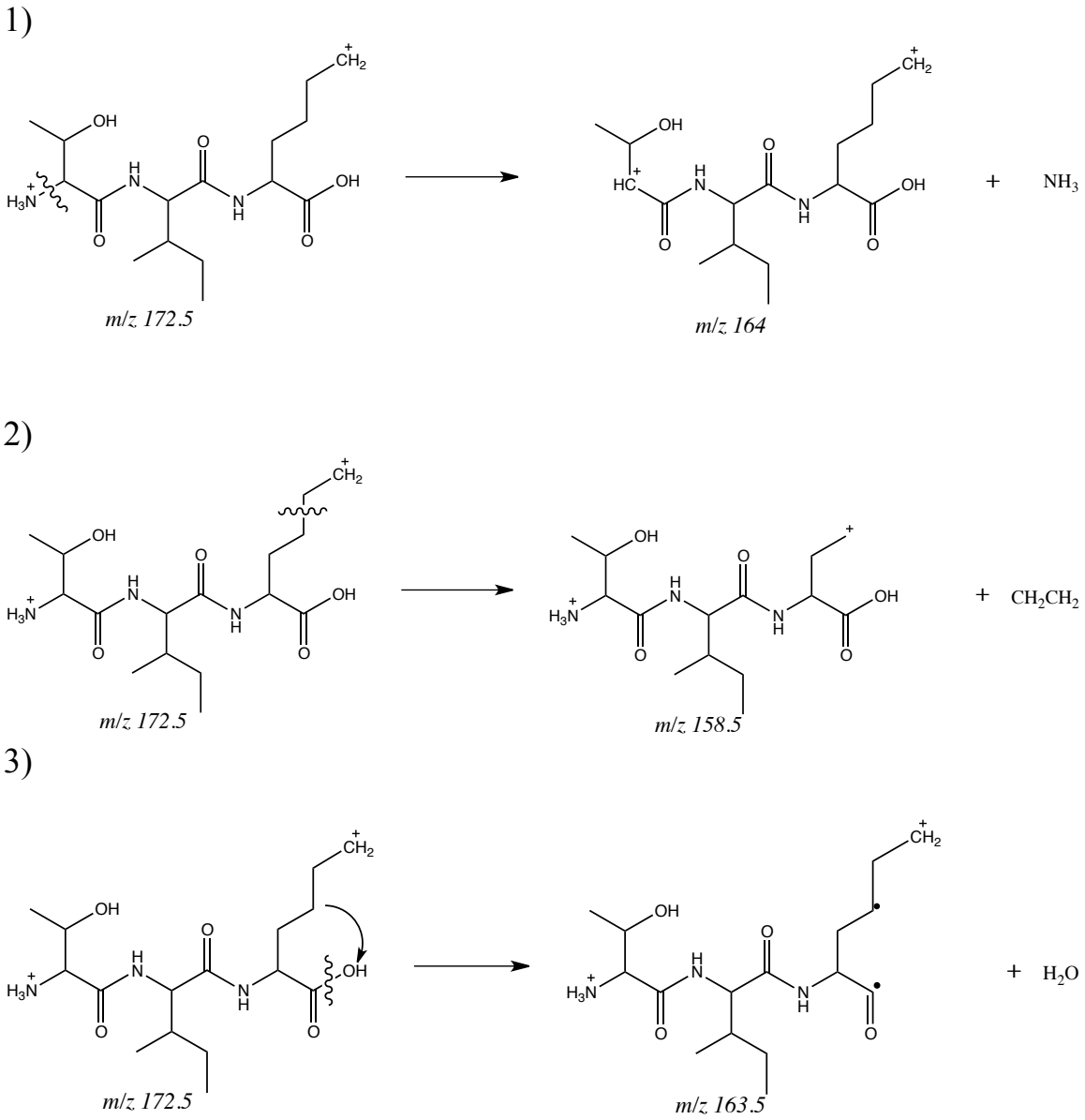
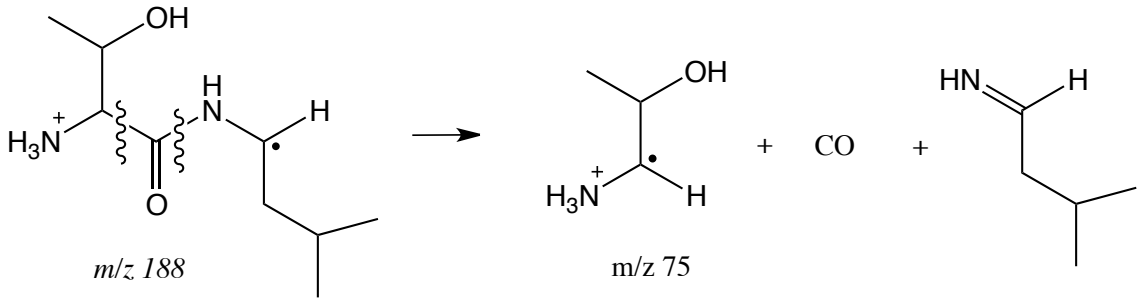


Figure S3. Secondary dissociations for TIK$(H^+)_2$ primary dissociation pathways at E_{rel} = 13.0 eV.

Pathway 3’

1)



m/z 188

m/z 75

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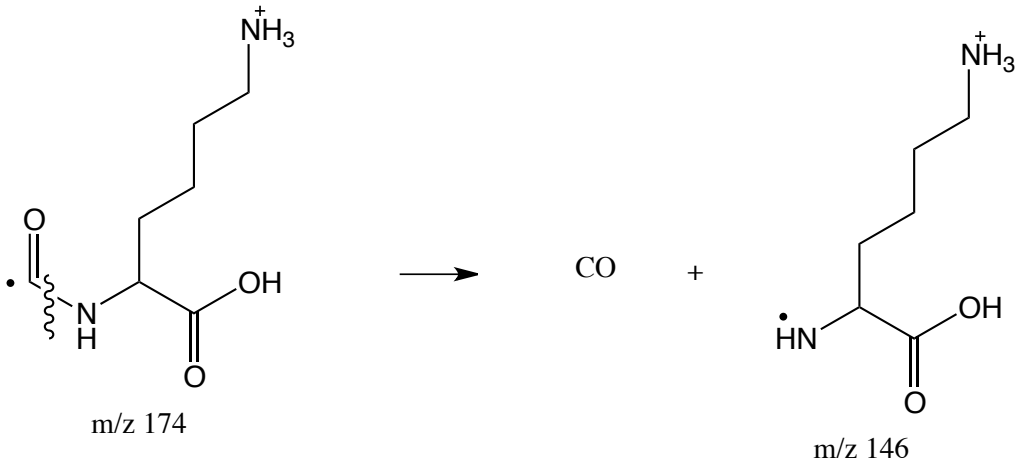

m/z 174

m/z 146

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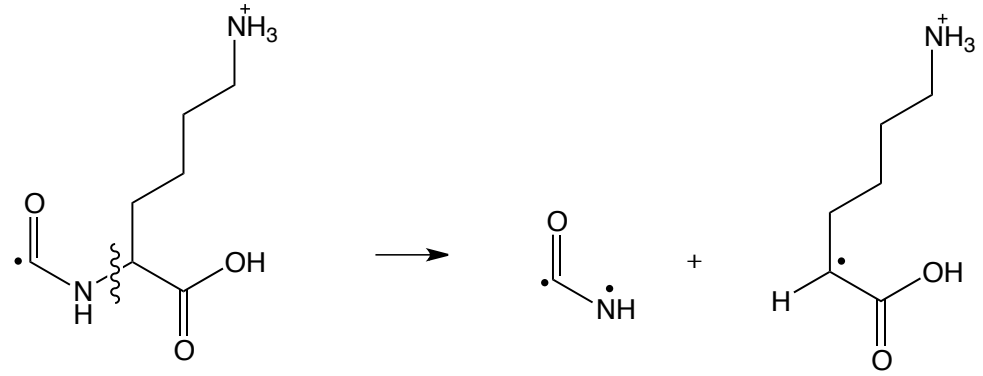

m/z 174

m/z 131

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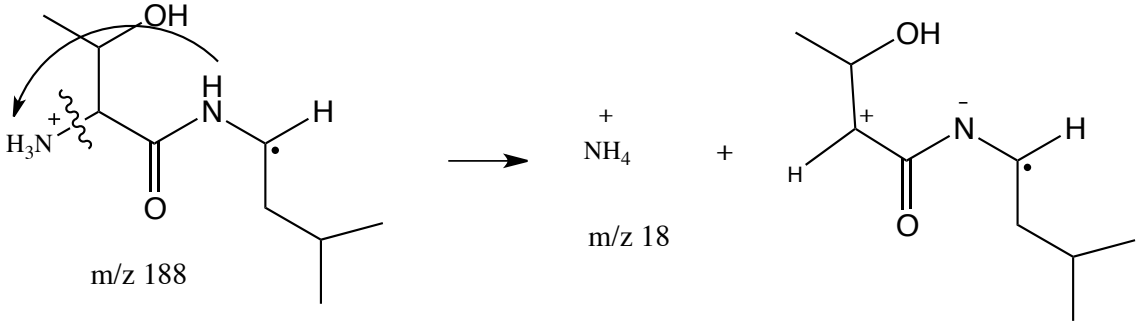

m/z 188

m/z 18

Pathway 4’

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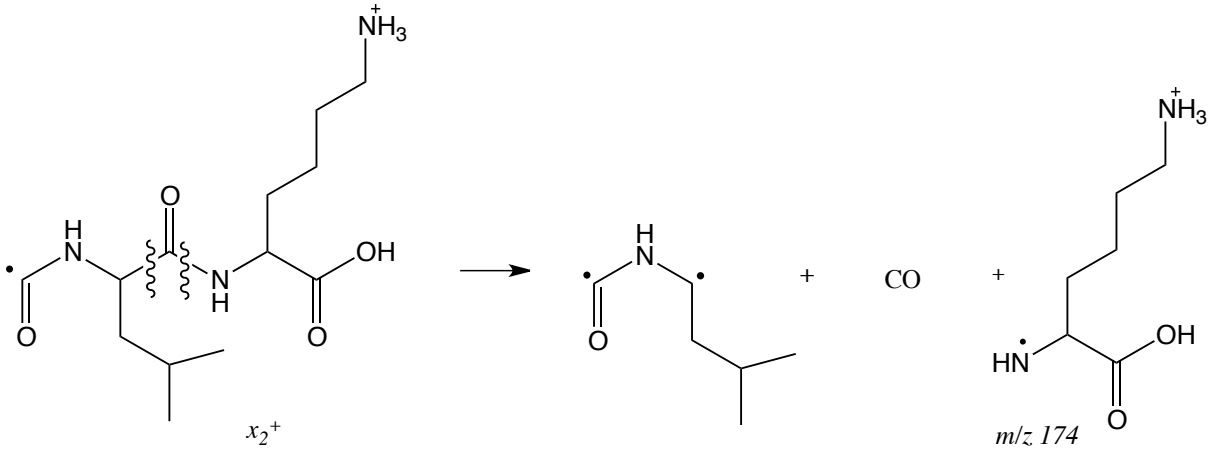

x_2^+
m/z 287

m/z 174

Pathway 5-1’

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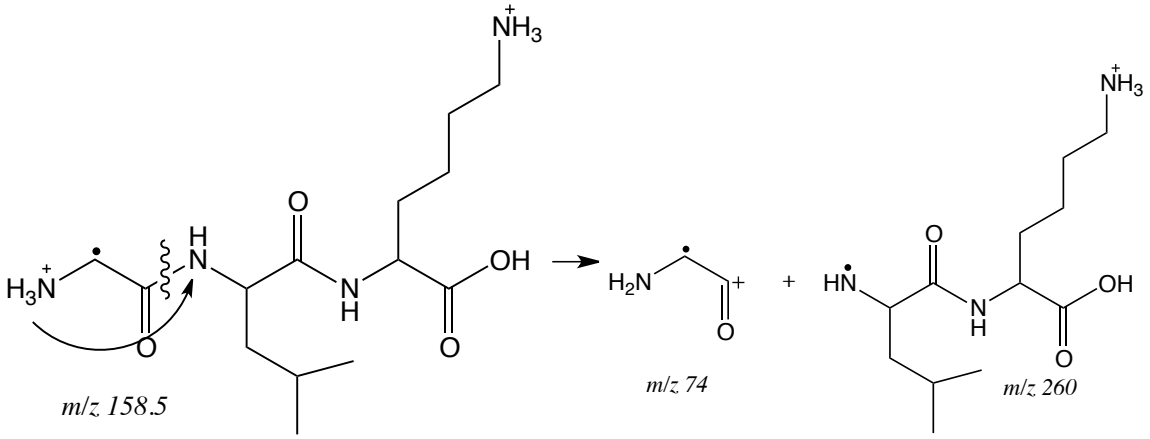

m/z 158.5

m/z 74

m/z 260

Pathway 5-3’

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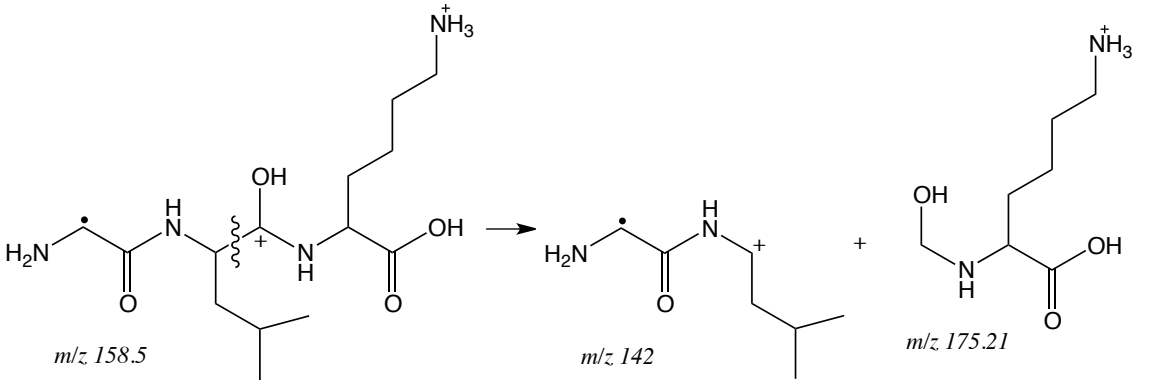


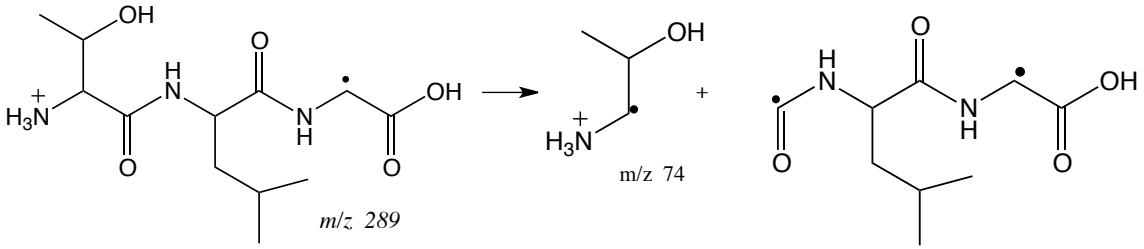
m/z 158.5

m/z 142

m/z 175.21

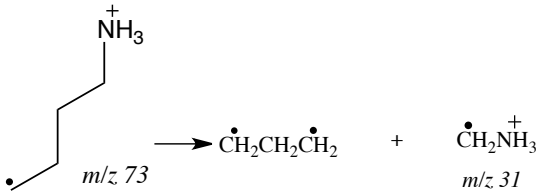
Pathway 7’

1)



m/z 289

2)

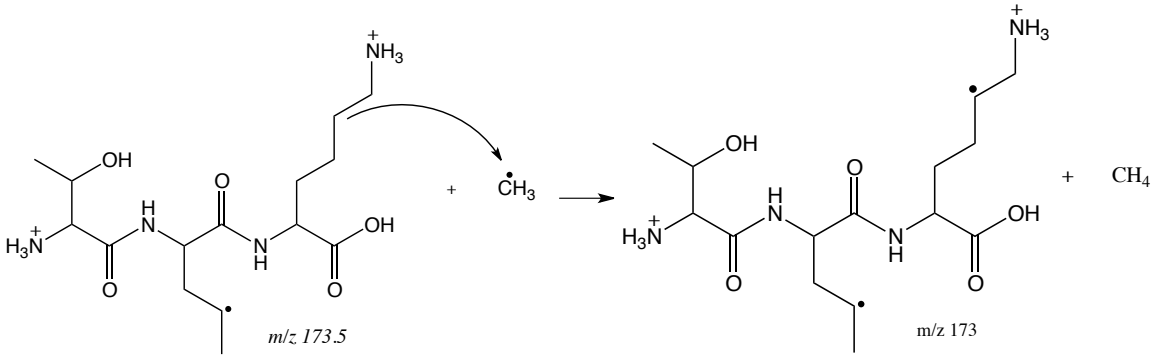


m/z 73

m/z 31

Pathway 12’

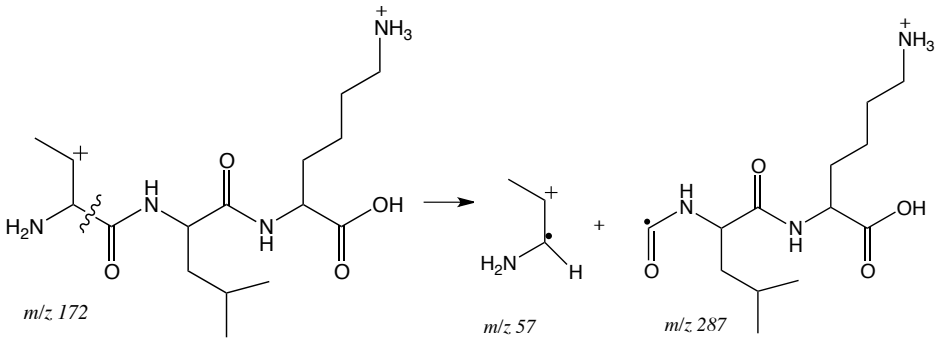
1)



m/z 173.5

Pathway 15’

1)



m/z 172

m/z 57

m/z 287

Pathway 18'

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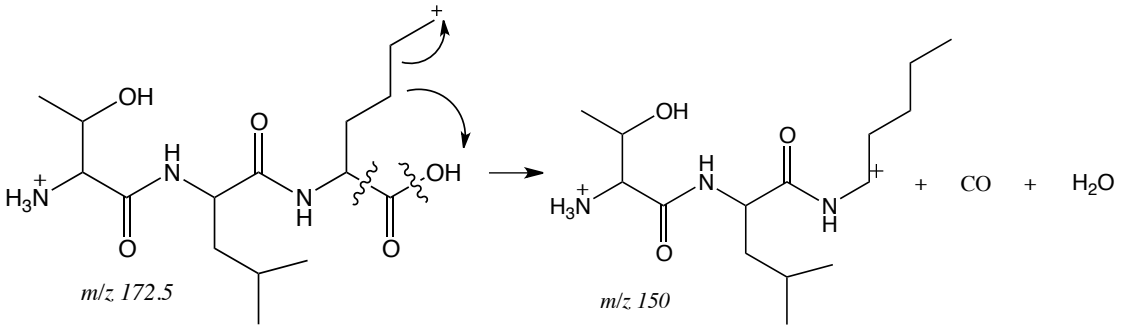

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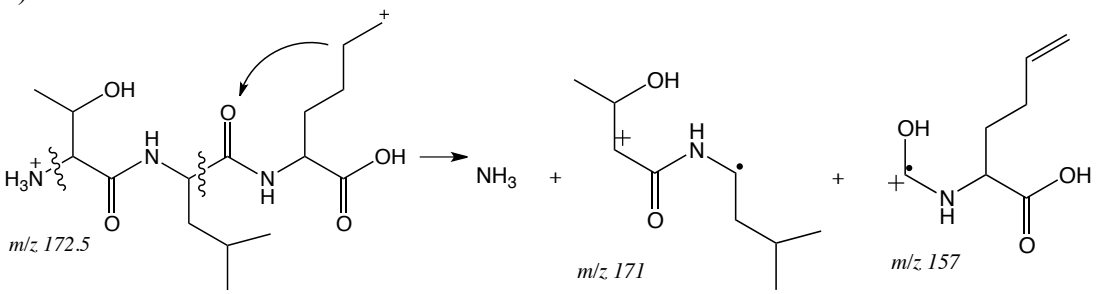

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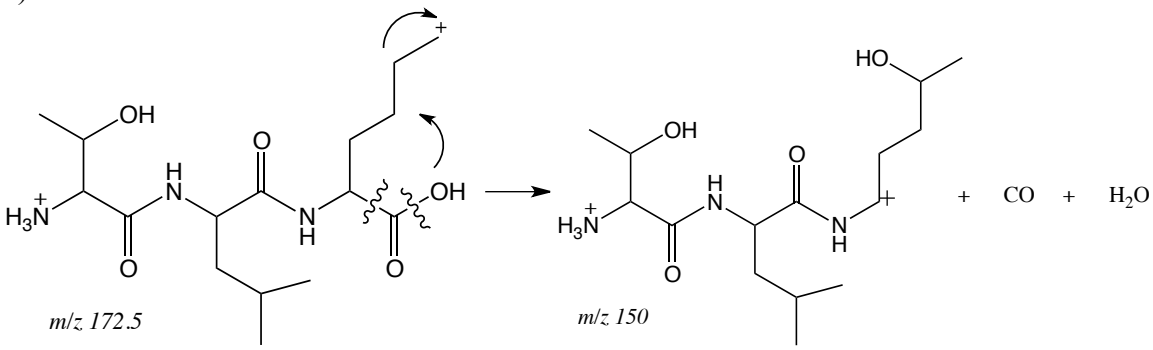

4)

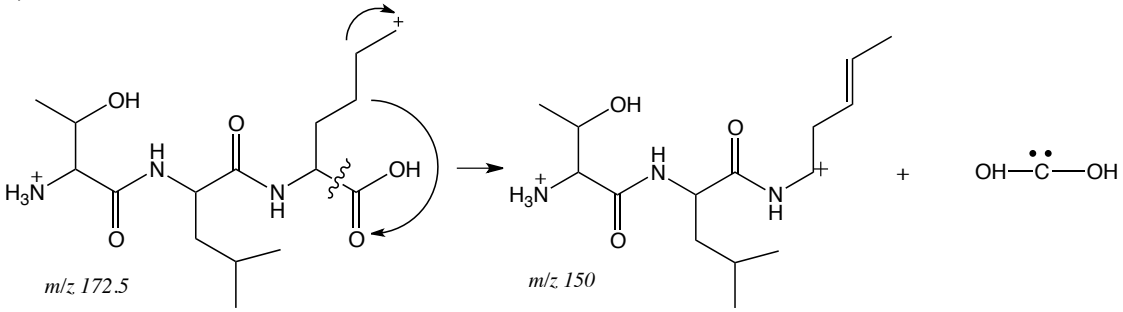

Figure S4. Secondary dissociations for TLK$(H^+)_2$ primary dissociation pathways at E_{rel} = 13.0 eV.

Table S1. Ions occurrence after primary and secondary dissociations.

	$TIK(H^+)_2$		$TLK(H^+)_2$	
E_{rel} (eV)	10.8	13.0	10.8	13.0
# ions (total)	26	66	21	61
# ions with same m/z	26	61	21	55
# ions with intensity > 2%	10	14	11	12