Electronic Supplementary Information for Controlling the diversity of ion-induced fragmentation pathways by *N*-methylation of amino acids

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N–methylglycine (sarcosine)

Geometries of the neutral conformers are shown in Figure S1.



Figure S1. Three-dimensional representation of all selected neutral conformers calculated at a DFT B3LYP/6-311++G(d,p) level of theory.





Figure S2. Graphic representation and tables including the ab initio molecular dynamics statistics of all fragmentation paths for sarcosine conformers.

N,N-dimethylglycine (DMG)

Geometries of the neutral conformers are shown in Figure S3.



Figure S3. Three-dimensional representation of all selected neutral conformers calculated at a DFT B3LYP/6-311++G(d,p) level of theory.

Statistics of the molecular dynamics are given in Figure S4.



Figure S4. Graphic representation and tables including the ab initio molecular dynamics statistics of all fragmentation paths for sarcosine conformers.