Deamidation reactions of asparagine and glutamine containing dipeptides investigated by ion spectroscopy

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Supporting Information

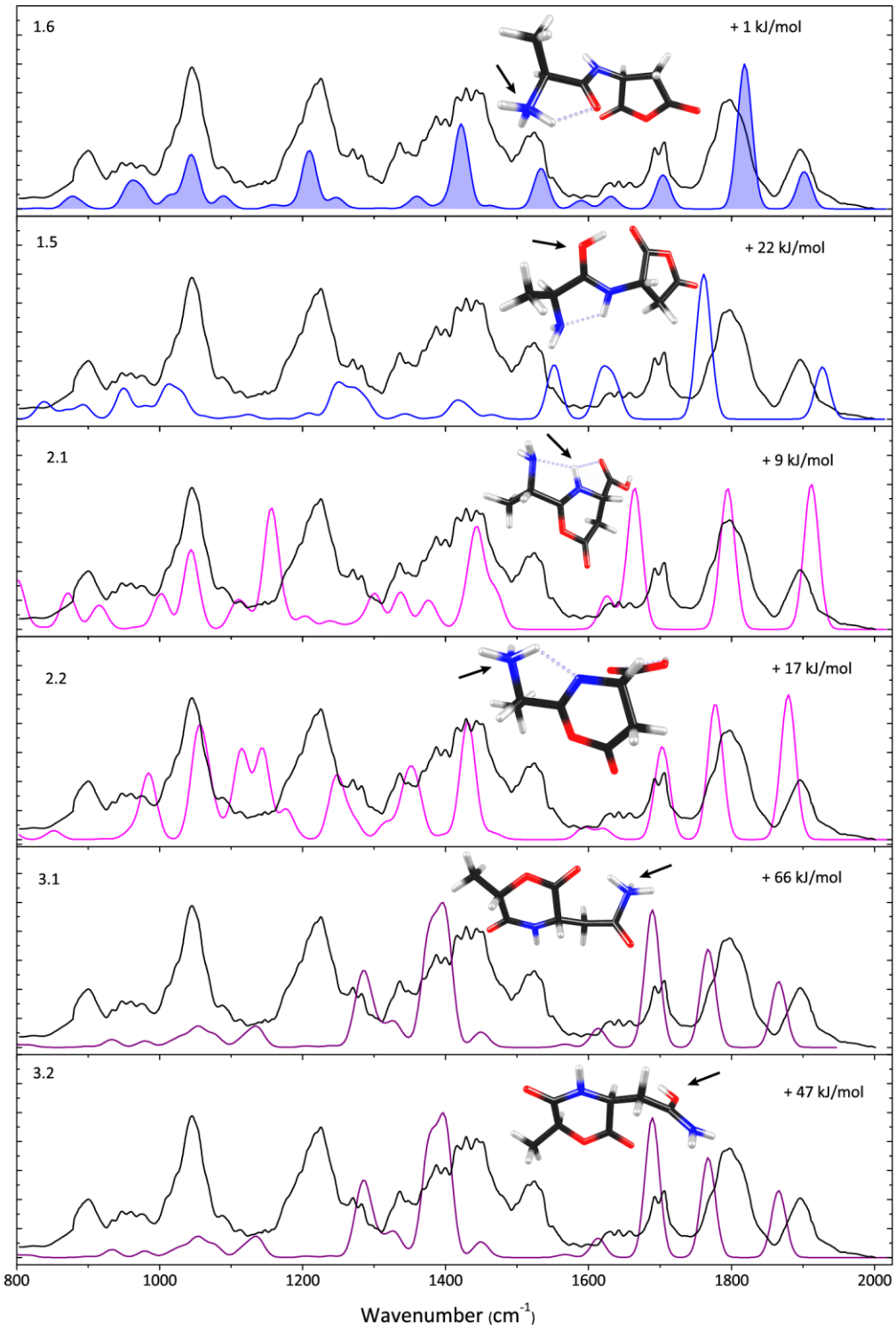


Figure S1. *IRMPD spectrum of AN – 17 compared with the assigned structure calculation (shaded blue spectrum) and alternative structures from Table 1 having relative energies lower than 50 kJ/mol.*

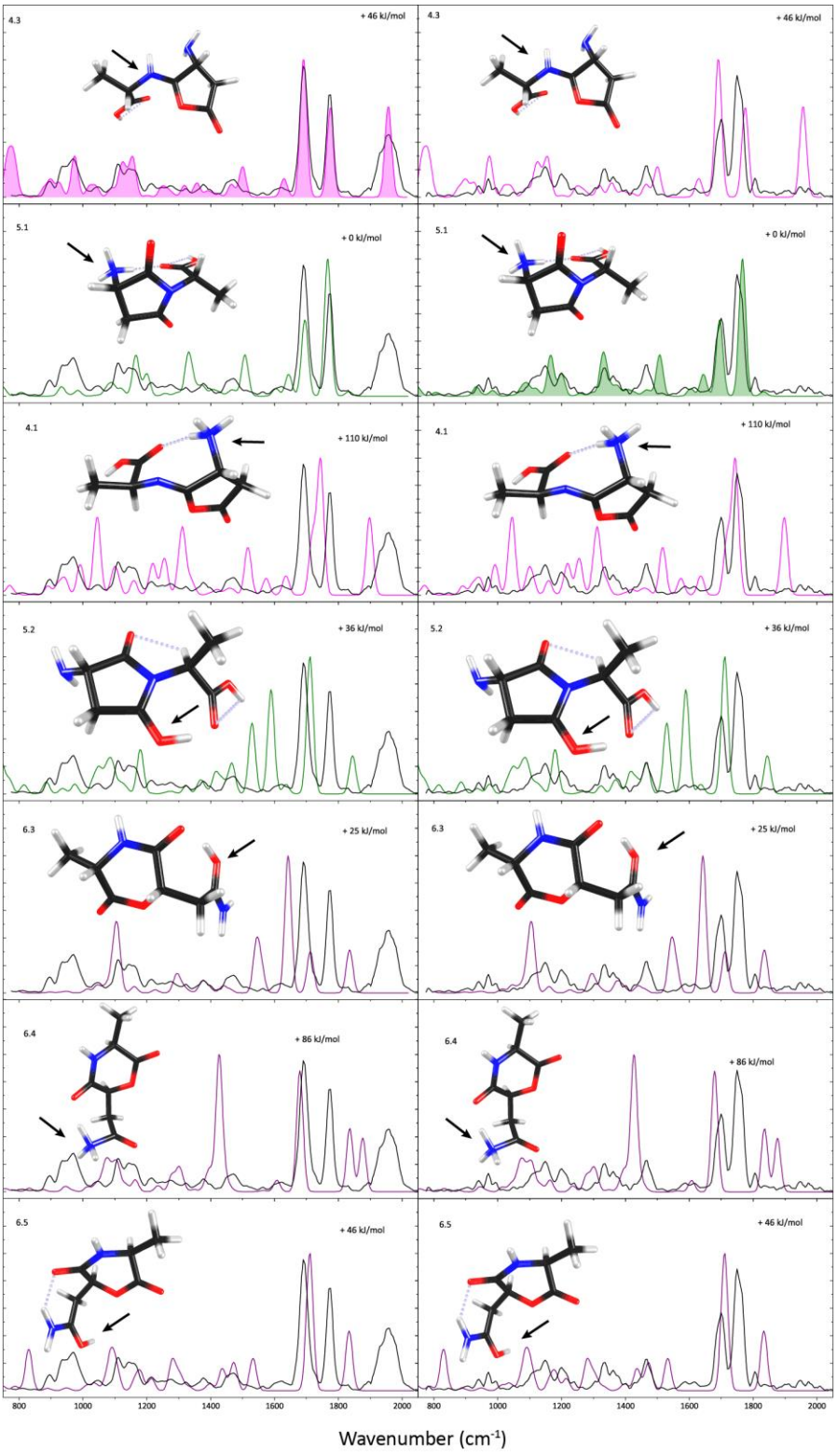


Figure S2. *IRMPD spectra of NA – 17 compared with the computed spectra for alternative structures from Table 2.*

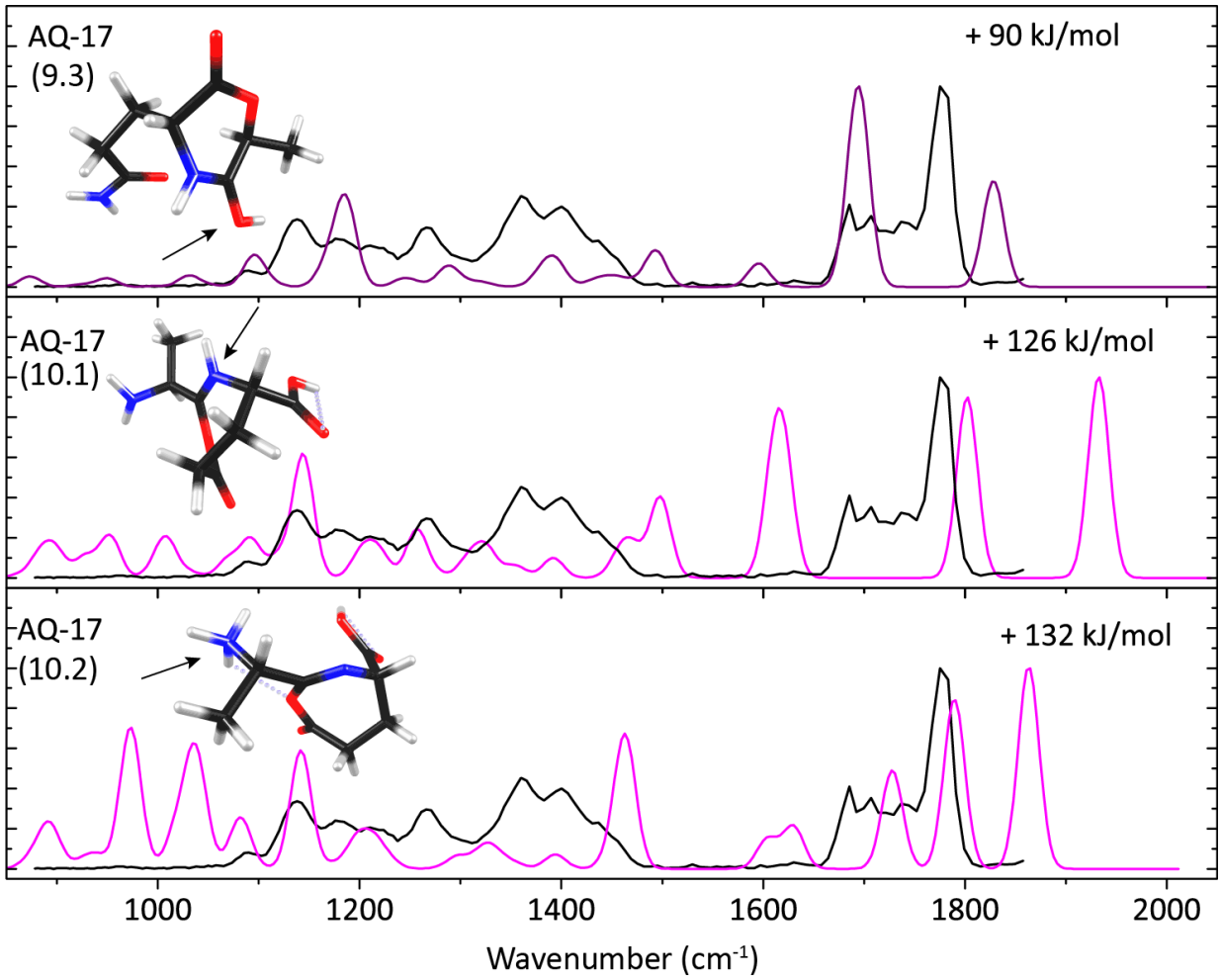


Figure S3. *IRMPD spectrum of AQ – 17 compared with the predicted spectrum of structure* ***9.3*** *(see Table 3) and with those of the previously suggested 7-membered ring structures* ***10.1*** *and* ***10.2****.*

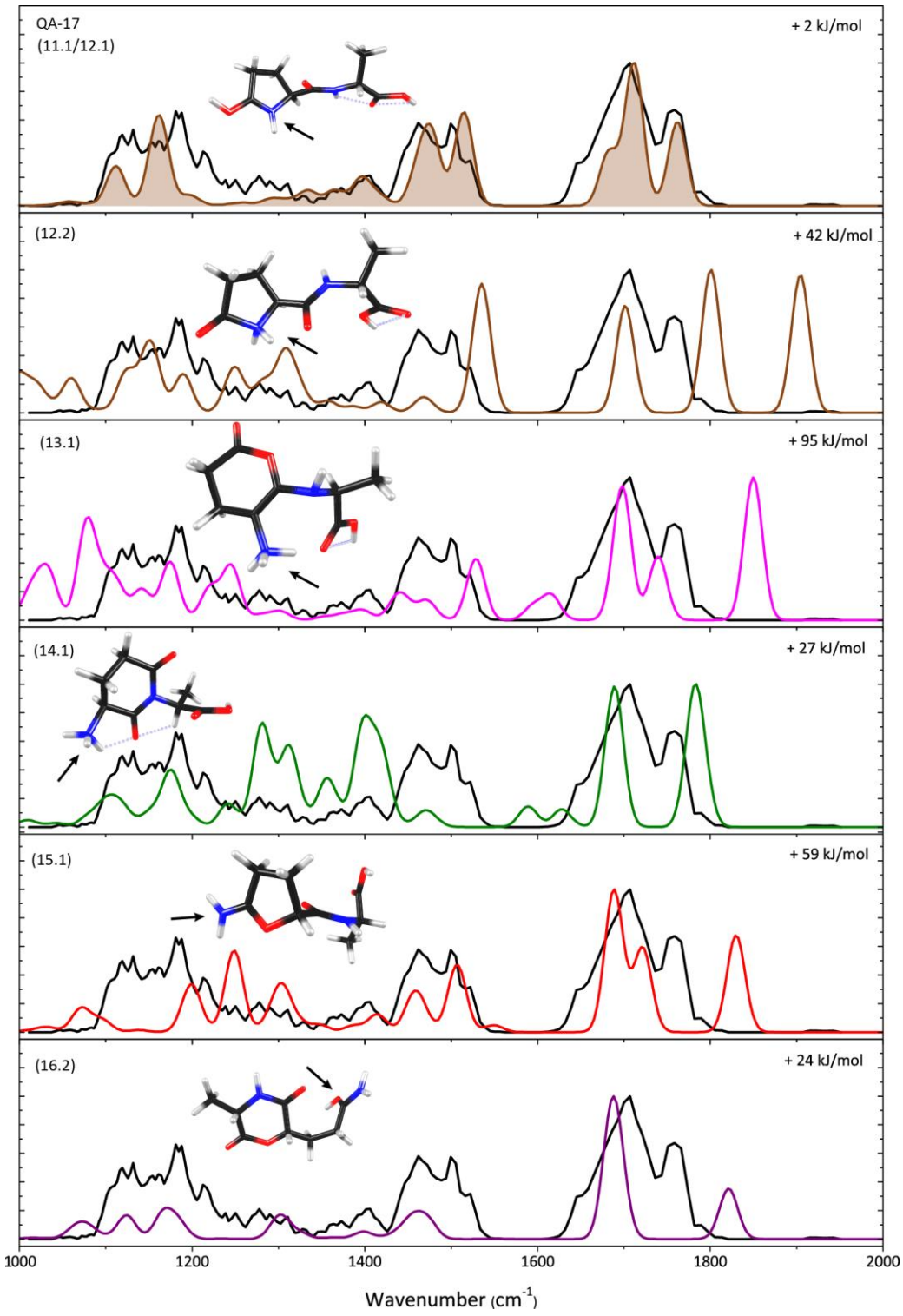
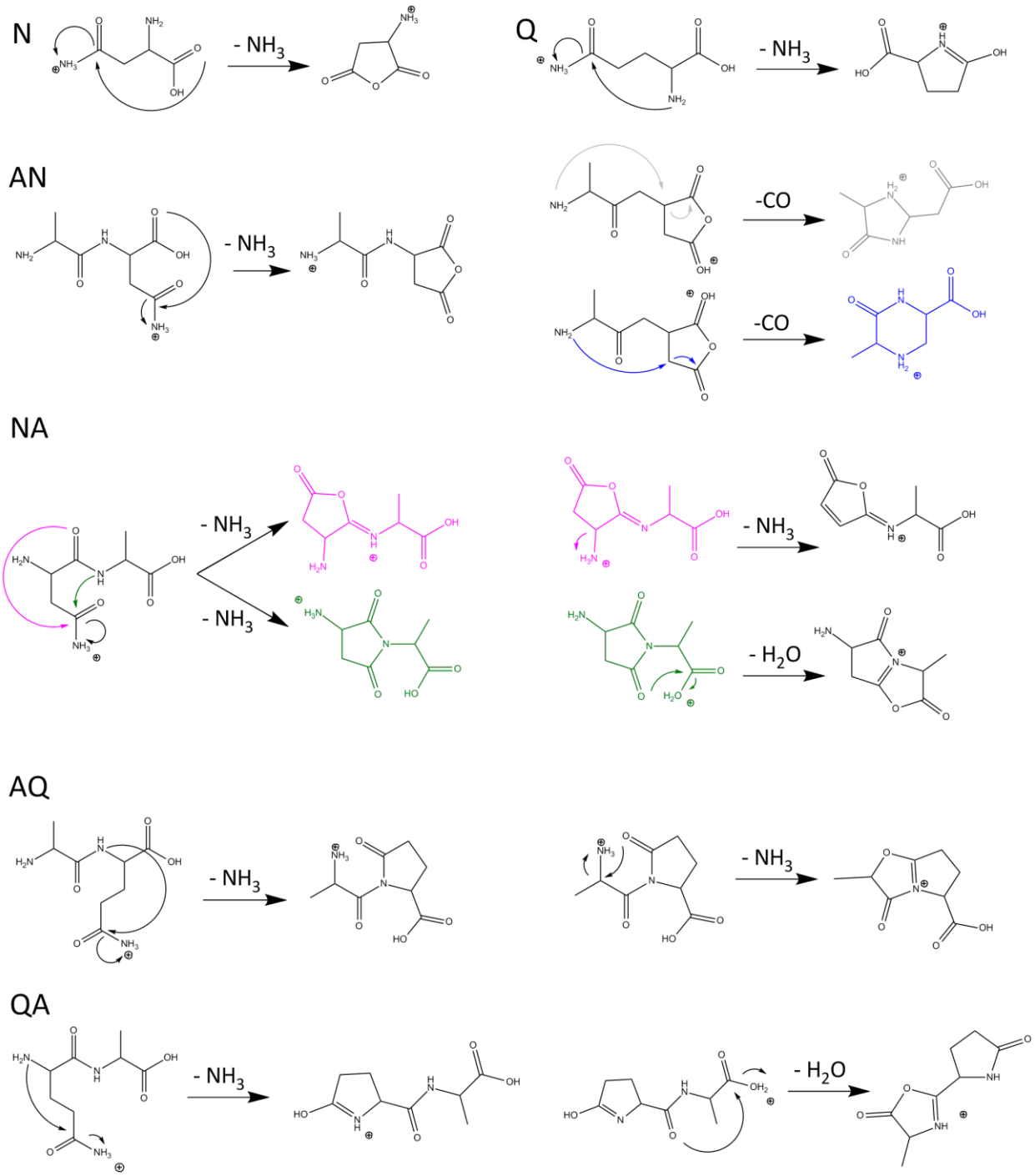


Figure S4. *IRMPD spectrum of QA – 17 compared with the computed spectra for the assigned structure (shaded brown spectrum) and some alternative structures from Table 4.*



Scheme S1: *Overview of identified MS^2 and MS^3 reaction pathways for protonated N and Q compared with those of the dipeptides AN, NA, AQ and QA.*