SUPPORTING INFORMATION

Integration of a Multichannel Pulsed-Valve Inlet System to a Linear Quadrupole Ion Trap Mass Spectrometer for the Rapid Consecutive Introduction of Nine Reagents for Diagnostic Ion/Molecule Reactions

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Figure S8. (a) MS/MS spectrum of isolated protonated benzoic acid (m/z 123) ionized via APCI. (b) Mass chromatogram measured monitoring the ion/molecule reaction product ions of m/z 73, 191, 195, 227, 181, 144, and 155 as (A) MOP, (B) DMDS, (C) DEMB, (D) TMB, (E) TMMS, (F) HSiCl₃, (G) ACE, (H) TDMAB, and (I) DMA were sequentially pulsed into the ion trap in this order and allowed to react with protonated benzoic acid. The identities of the ions and reagents are shown in Table 2. (c) MS/MS spectra measured after isolation and reaction of protonated benzoic

acid with the reagents. Unique reaction product ions specific for the carboxylic acid functionality are highlighted with green circles (\bullet). Part G: The ion of m/z 105 is formed from protonated benzoic acid upon elimination of water. Part I: The ion of m/z 195 is likely due to a trace of TMB remaining in the ion trap. The ion of m/z 155 is a methanol adduct of protonated benzoic acid....S8



Figure S1. (a) Mass chromatogram monitoring the product ion of m/z 139 formed upon reactions of protonated nitrosobenzene with DMDS that was introduced into the ion trap via six pulses, with a 1 s delay between each pulse. (b) MS/MS spectrum measured after reactions of DMDS with protonated nitrosobenzene. The residence time of DMDS was found to be 0.8 s.



Figure S2. (a) Mass chromatogram monitoring the product ion of m/z 185 formed upon reactions of protonated hexanoic acid with DEMB that was introduced into the ion trap via six pulses, with a 1 s delay between each pulse. (b) MS/MS spectrum measured after reactions of DEMB with protonated hexanoic acid. The residence time of DEMB was found to be 0.6 s.



Figure S3. (a) Mass chromatogram monitoring the product ion of m/z 199 formed upon reactions of protonated dimethyl sulfone with TMMS that was introduced into the ion trap via six pulses, with a 1 s delay between each pulse. (b) MS/MS spectrum measured after reactions of TMMS with protonated dimethyl sulfone. The residence time of TMMS was found to be 0.9 s.



Figure S4. (a) Mass chromatogram monitoring the product ion of m/z 173 formed upon reactions of protonated glycylglycine with ACE (DMK) that was introduced into the ion trap via six pulses, with a 1 s delay between each pulse. (b) MS/MS spectrum measured after reactions of ACE with protonated glycylglycine. The residence time of ACE was found to be 0.9 s.



Figure S5. (a) Mass chromatogram monitoring the product ion of m/z 380 formed upon reactions of protonated albendazole sulfoxide with TDMAB that was introduced into the ion trap via six pulses, with a 1 s delay between each pulse. (b) MS/MS spectrum measured after reactions of TDMAB with protonated albendazole sulfoxide. The residence time of TDMAB was found to be 0.6 s.



Figure S6. (a) Mass chromatogram monitoring the product ion of m/z 202 formed upon reactions of protonated 4-hydroxybenzenesulfonamide with DMA that was introduced into the ion trap via six pulses, with a 2 s delay between each pulse. (b) MS/MS spectrum measured after reactions of DMA with protonated 4-hydroxybenzenesulfonamide. The residence time of DMA was found to be 4 s.



Figure S7. (a) Mass chromatogram monitoring the product ion of m/z 643 formed upon reactions of deprotonated carvedilol N^{2} - β -D-glucuronide with HSiCl₃ that was introduced into the ion trap via six pulses, with a 1 s delay between each pulse. (b) MS/MS spectrum measured after reactions of HSiCl₃ with deprotonated carvedilol N^{2} - β -D-glucuronide. The residence time of HSiCl₃ was found to be 0.9 s.



Figure S8. (a) MS/MS spectrum of isolated protonated benzoic acid (m/z 123) ionized via APCI. (b) Mass chromatogram measured monitoring the ion/molecule reaction product ions of m/z 73, 191, 195, 227, 181, 144, and 155 as (A) MOP, (B) DMDS, (C) DEMB, (D) TMB, (E) TMMS, (F) HSiCl₃, (G) ACE, (H) TDMAB, and (I) DMA were sequentially pulsed into the ion trap in this order and allowed to react with protonated benzoic acid. The identities of the ions and reagents are shown in Table 2. (c) MS/MS spectra measured after isolation and reaction of protonated benzoic acid with the reagents. Unique reaction product ions specific for the carboxylic acid functionality are highlighted with green circles (•). Part G: The ion of m/z 105 is formed from protonated benzoic acid upon elimination of water. Part I: The ion of m/z 195 is likely due to a trace of TMB remaining in the ion trap. The ion of m/z 155 is a methanol adduct of protonated benzoic acid.