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Communication

Electrospray Ionization Mass Spectrometric Analysis of Highly Reactive Glycosyl Halides

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Supplementary Information

- Unidentified peaks designated by asterisks * and ** have been used as a kind of internal standards to compare the signal intensities of lithium, sodium, potassium and ammonium adduct ions;
- Identified peaks have labelled in red;
- The desired molecular ion adducts [M+cation]⁺ are shown in blue circles

Spectrum 1. Analyte 2 in acetonitrile without any adduct forming agent.



Spectrum 2. Analyte 2 in acetonitrile with 2% formic acid.



Spectrum 3. Analyte 2 in acetonitrile with LiCl.



Spectrum 4. Analyte 2 in acetonitrile with NaCl.



Spectrum 5. Analyte 2 in acetonitrile with KCI.



Spectrum 6. Analyte **2** in acetonitrile with LiNO₃.



Spectrum 7. Analyte **2** in acetonitrile with NaNO₃.



Spectrum 8. Analyte **2** in acetonitrile with KNO₃.



Spectrum 9. Analyte **2** in acetonitrile with LiClO₄.



Spectrum 10. Analyte **2** in acetonitrile with NaClO₄.



Spectrum 11. Analyte **2** in acetonitrile with KCIO₄.



Spectrum 12. Analyte **2** in acetonitrile with NH₄Cl.



Spectrum 13. Analyte **2** in acetonitrile with NH₄NO₃.



Spectrum 14. Analyte **2** in acetonitrile with NH₄OOCCH₃.



Spectrum 15. Analyte **2** in acetonitrile with NH₄OOCH.



Spectrum 16. Analyte **2** in acetonitrile with NH₄HCO₃.



Spectrum 17. Analyte 2 in acetonitrile with LiBr.



Spectrum 18. Analyte 2 in acetonitrile with Lil.



Spectrum 19. Analyte 2 in acetonitrile with LiF (negative ion mode).



Spectrum 20. Analyte 2 in acetonitrile with LiCI (negative ion mode).



Spectrum 21. Analyte 2 in acetonitrile with LiBr (negative ion mode).



Spectrum 22. Analyte 2 in acetonitrile with LiBr (negative ion mode).



Spectrum 23. Analyte **2** in acetonitrile with NH_4OOCCH_3 (negative ion mode).



Spectrum 24. Accurate mass analysis of analyte **1** in acetonitrile with LiCl.



Table 25. Report of accurate mass analysis of analyte **1** in acetonitrile with LiCl.

Chemical Formula: C₂₁H₂₁ClO₅ Exact Mass: 388.1078 (³⁵Cl)



- Elemental Composition Report
- Single Mass Analysis
- Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
- Element prediction: Off
- Number of isotope peaks used for i-FIT = 3
- Monoisotopic Mass, Even Electron lons
- 65 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
- Elements Used:
- C: 0-500 H: 0-1000 7Li: 1-1 O: 0-20 35Cl: 1-1
- Minimum: -1.5 ٠ Maximum: 5.0 10.0 50.0 ٠ Mass Calc. Mass mDa PPM DBE i-FIT i-FIT ٠ (Norm) Formula 1.8 395.1256 395.1238 4.6 10.5 97.5 0.0 • C21 H21 7Li O5 35Cl

Spectrum 26. CID spectrum of peaks 537/539 of analyte **2** in acetonitrile-LiCl at low collision energy.



Spectrum 27. CID spectrum of peaks 417/419 and 537/539 of analyte2 in acetonitrile-LiCl at high collision energy.

