

Supporting Information

Screening for traces fluorine containing species in complex media made possible by using HPLC coupled parallel to fluorine-specific and molecular specific detection

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HPLC_MAS chromatogram formation.

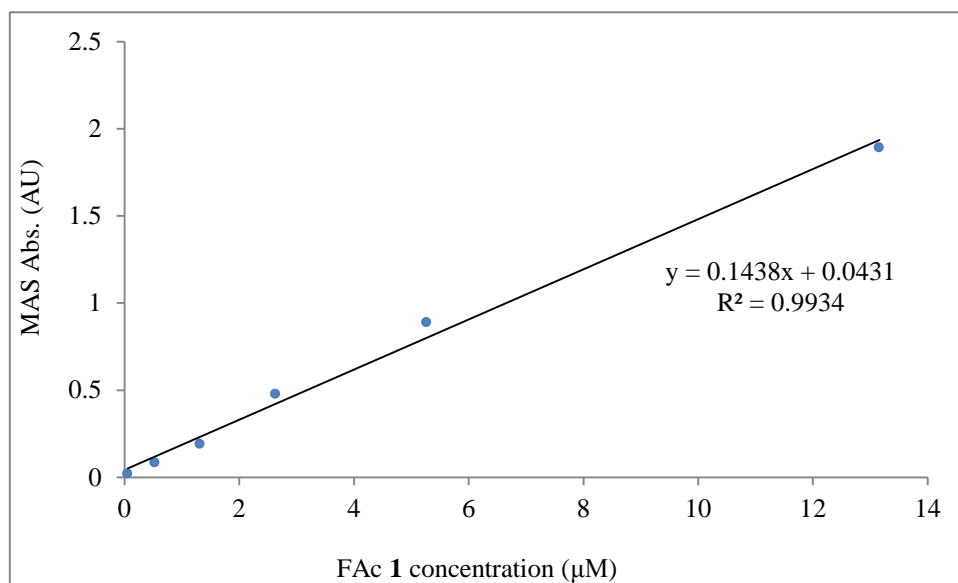
To obtain the RP C8 or Ion Exchange HPLC-MAS chromatogram, fractions eluted by HPLC were collected once per 30s within a certain retention time. Fractions were then placed in the autosampler of the CS-MAS and subsequently measured for fluorine content. Hence the fluoro metabolites separated by HPLC under the particular eluting time could be detected by CS-MAS, the chromatogram could then be established by the CS-MAS absorptions against their retention times.

SI Table 1 Pretreatment and modifier solutions used for the formation of GaF

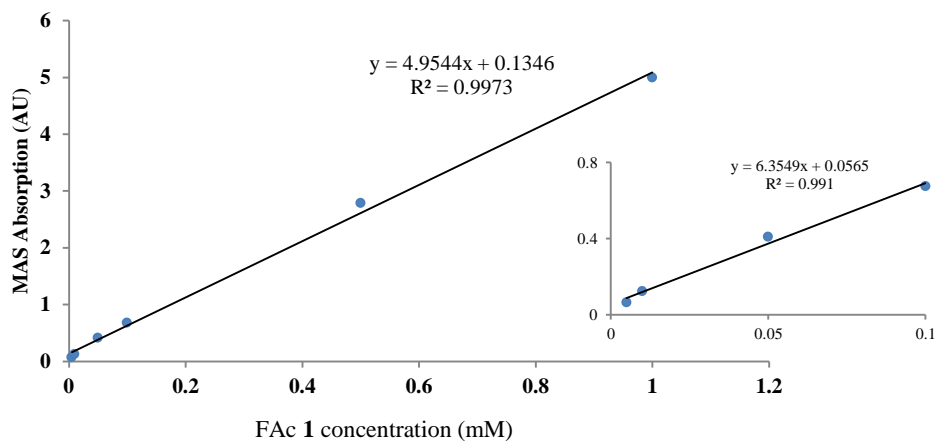
Solution	Concentration	Function
Zr	1 g/L Zr	Graphite tube coating
Ga(NO ₃) ₃	10 g/L Ga	GaF forming agent
NaAc	1 g/L NaAc	Modifier for F stabilization
Zr/Pa(NO ₃) ₂ /Mg(NO ₃) ₂	0.1% m/v Pd, 0.05% m/v Mg and 20 mg/L Zr	Modifiers for gallium stabilization and bonding of the free carbon from graphite tube surface

SI Table 2 Temperature program of graphite furnace for GaF detection

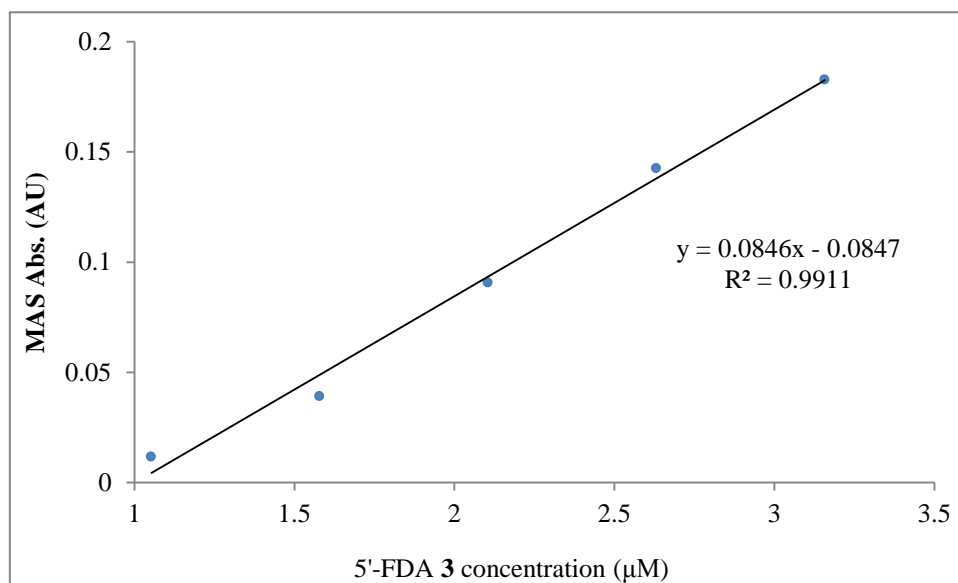
Step	Name	Temperature/°C	Ramp/°Cs ⁻¹	Hold/s
0	Zr Coating	Variable	-	-
1	Drying	75	7	2
2	Drying	85	2	15
3	Drying	95	3	5
4	Drying	350	300	3
5	Pretreatment	1100	500	10
6	Cooling down	85	NP	2
7	Drying	85	0	20
8	Drying	95	3	5
9	Pyrolysis	550	300	10
10	Gas adaption	550	0	5
11	Molecule formation	1150	1000	7
12	Cleaning	2450	500	4



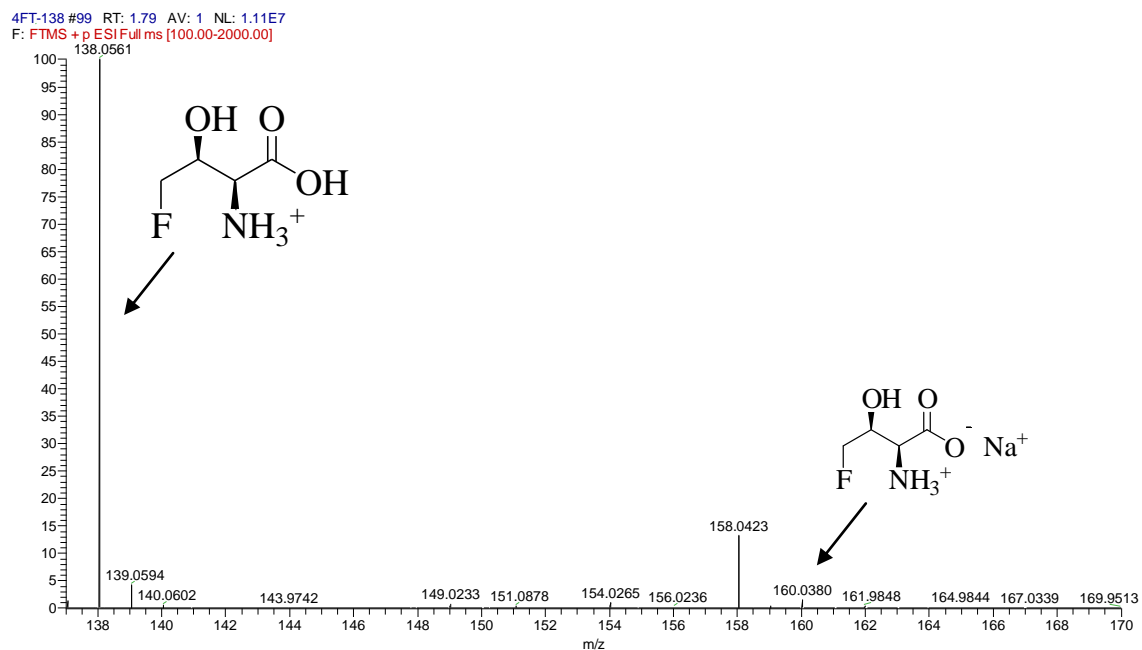
SI Figure S1: Calibration of sodium fluoroacetate. Average standard deviation across all points was 3.2% ($n = 2$).



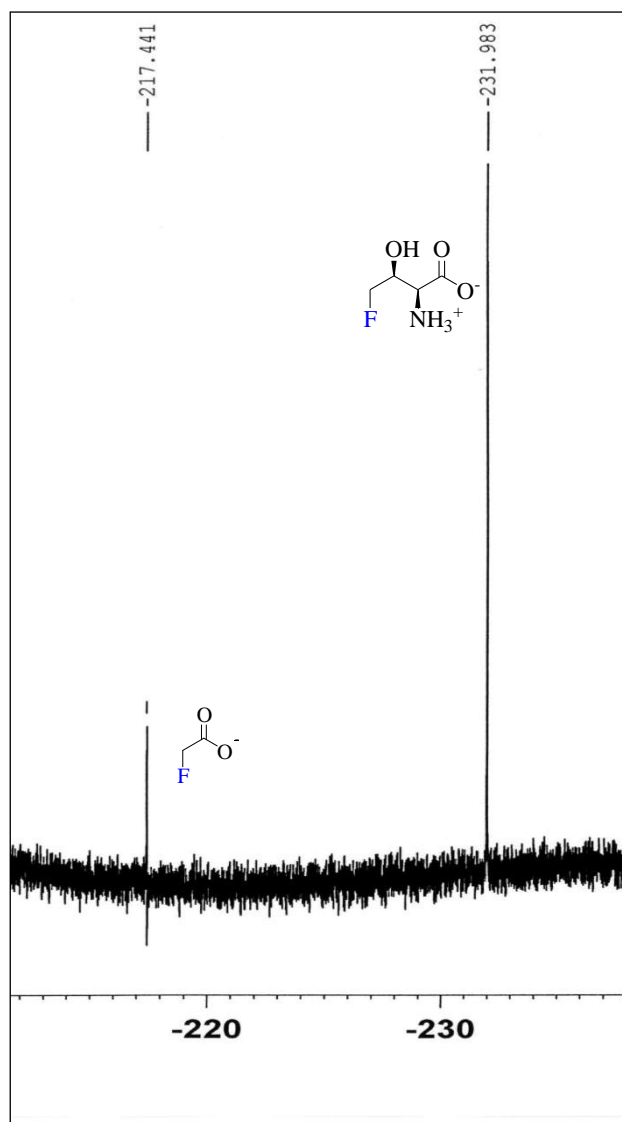
SI Figure S2: Calibration of sodium fluoroacetate after ion exchange chromatography. The blown-up insert indicates the calibration of lower concentrated sodium fluoroacetate after exchange chromatography. Average standard deviation across all points was 1.7% ($n = 2$).



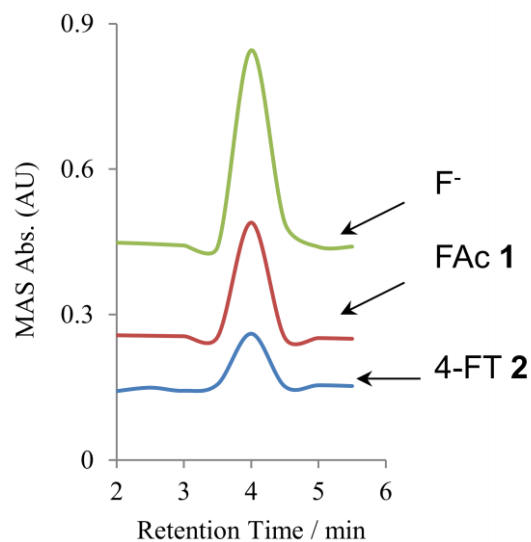
SI Figure S3: Calibration of 5'-FDA after the separation of reverse phase HPLC separation. Average standard deviation across all points was 1.4% ($n = 2$).



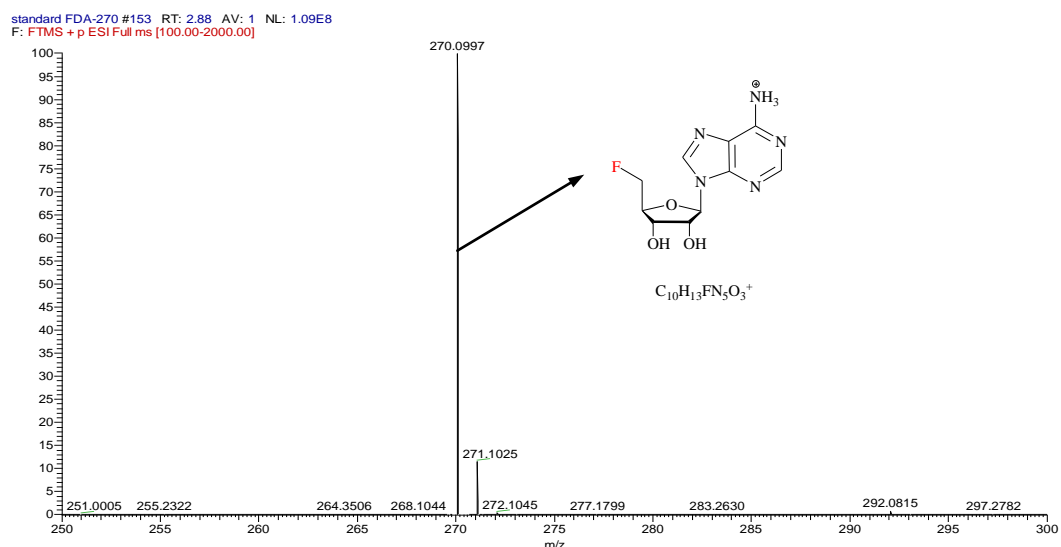
SI Figure S4: High resolution HPLC-ESMS analysis of the synthetic 4-FT 2.



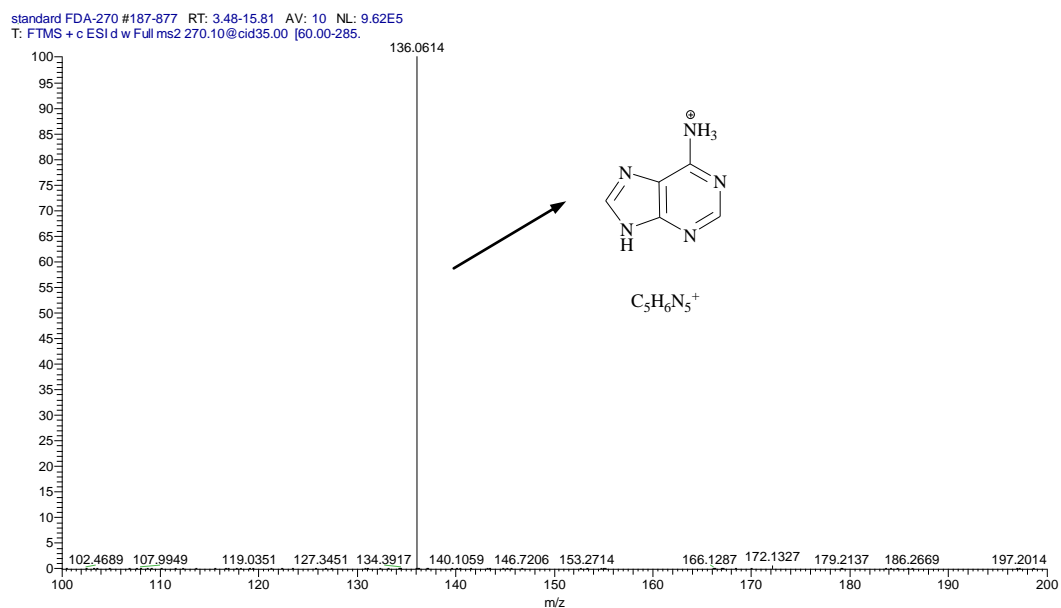
SI Figure S5: ^{19}F NMR of FAc 1 and 4-FT 2



SI Figure S6 CS-MAS identification of individual fluoride, FAc 1 and 4-FT 2 after RP HPLC separation



SI Figure S7: High resolution mass spectra of the synthetic 5'-FDA.



SI Figure S8. MSMS fragmentation analysis of the synthetic 5'-FDA

Reference