

Manuscript supplementary tables

Table S1. Method repeatability.

	Experiment 1		Experiment 2		Experiment 3	
	Conc. (mg/ml)	Rt (min)	Conc. (mg/ml)	Rt (min)	Conc. (mg/ml)	Rt (min)
Derivate 1	2.40	5.99	2.27	5.98	2.49	5.99
Derivate 2	2.50	5.99	2.42	5.98	2.28	5.99
Derivate 3	2.28	5.98	2.08	5.98	2.28	5.99
Derivate 4	2.15	5.98	2.85	5.98	2.07	5.99
Derivate 5	2.29	5.98	2.67	5.99	2.47	5.98
Derivate 6	2.36	5.98	2.74	5.98	1.89	5.99

Table S2. Instrument repeatability.

	Experiment 1		Experiment 2		Experiment 3	
	Conc. (mg/ml)	Rt (min)	Conc. (mg/ml)	Rt (min)	Conc. (mg/ml)	Rt (min)
Run 1	2.38	5.98	2.54	5.98	2.24	5.99
Run 2	2.39	5.98	2.49	5.98	2.23	5.98
Run 3	2.38	5.99	2.49	5.98	2.25	5.99
Run 4	2.45	5.99	2.52	5.98	2.29	5.98
Run 5	2.38	5.99	2.45	5.98	2.19	5.99
Run 6	2.40	5.99	2.51	5.98	2.29	5.98

Table S3. Robustness data.

	Normal	Low	high	Low	High	2 nd
		column	column			
		temp.	temp.	flow rate	flow rate	column
Run1	8.0E+05	8.4E+05	8.0E+05	7.9E+05	7.8E+05	7.0E+05
Run2	8.5E+05	8.1E+05	7.9E+05	8.2E+05	8.0E+05	7.1E+05
Run3	7.8E+05	7.9E+05	7.6E+05	7.7E+05	7.8E+05	7.2E+05
Run4	8.1E+05	8.2E+05	7.7E+05	8.3E+05	7.7E+05	7.7E+05
Run5	8.1E+05	8.3E+05	7.6E+05	8.0E+05	7.7E+05	8.0E+05
Run6	7.8E+05	8.4E+05	8.2E+05	8.1E+05	7.9E+05	7.4E+05

Table S4. System suitability. One representative experiment.

Injection	peak area (counts)	Mean (counts)	%CV ^a	%RE ^b
1	7.14E+05	7.16E+05	1.13	3.05
2	7.19E+05			
3	7.15E+05			
4	7.19E+05			
5	7.01E+05			
6	7.25E+05			
7	6.94E+05			

^a repeatability of peak area results of first six injections

^b peak area difference between a seventh injection at the end of the day and the mean of the first six injections

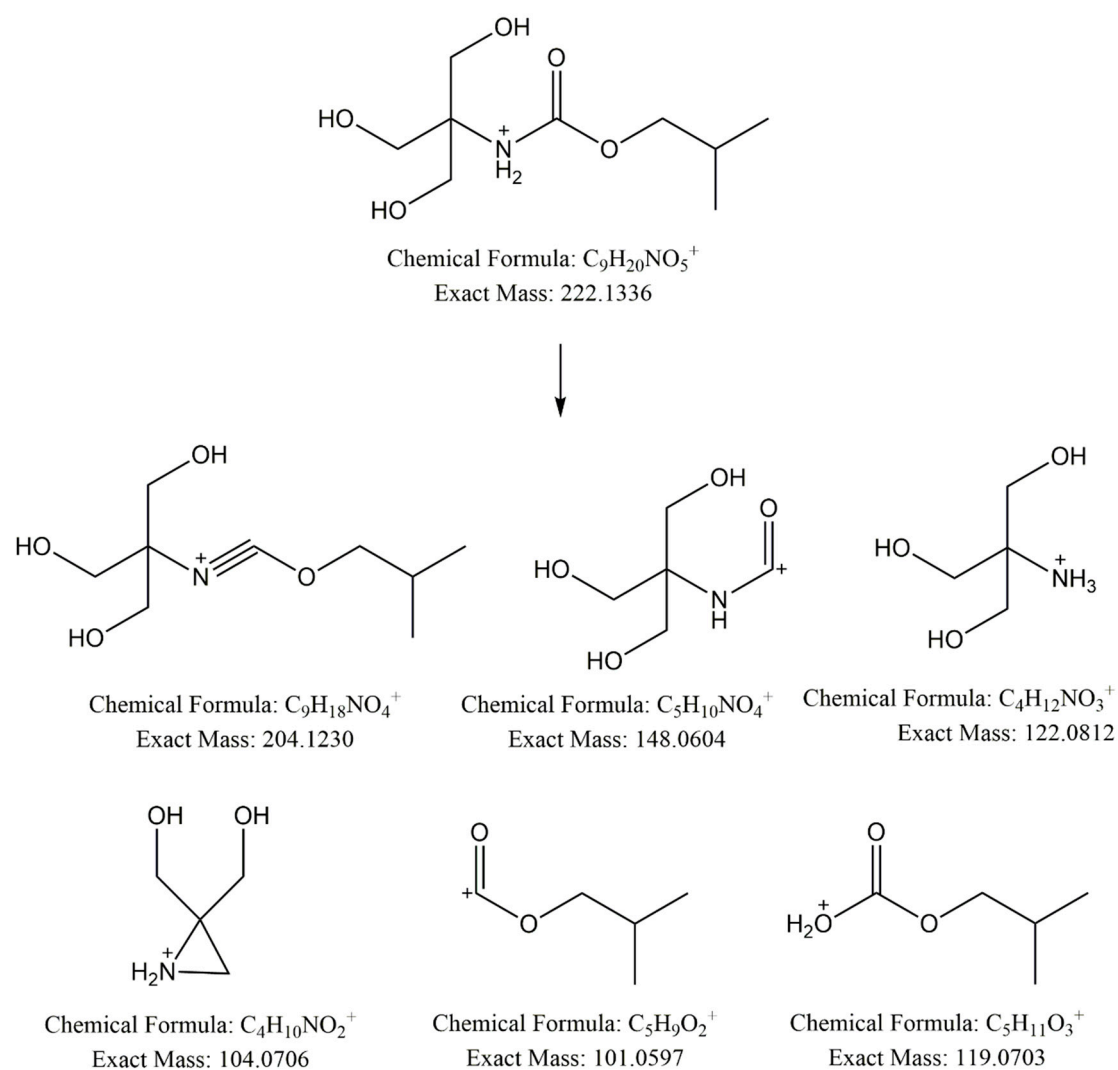


Figure S1. Fragmentation pattern of protonated TRIS-IBCF and plausible ion structures.