

## Targetted MS-parameters:

MS-Q-Trap-5500 Sciex

Ion source: Turbo spray

Curtain gas: 30

CAD Gas: -2

Ion spray Voltage: -4500 V

Temperature: 500°C

Ion source gas 1: 40 psi

Ion source gas 2: 60 psi

**Table 1:** MRM transitions and settings for sulfonate measurements (\* transitions used as quantifiers). DP declustering potential ; CE collision energy. Ionization mode was negative.

Sulfonate	Q1 Mass (Da)	Q3 Mass (Da)	Time (ms)	ID	DP (V)	CE (V)
Cysteate	168.2	151	20	Cysteate_1*	-80	-17
	168.2	86	20	Cysteate_2	-80	-18
	168.2	81	20	Cysteate_3	-80	-27
	168.2	71	20	Cysteate_4	-80	-24
Isethionate	125.3	107	20	Ise_1	-90	-21
	125.3	95	20	Ise_2*	-90	-20
	125.3	80	20	Ise_3	-90	-32
2,3-Dihydroxy-1-propanesulfonate	155	95	20	DHPS_1*	-96	-24
	155	80	20	DHPS_2	-96	-39
Sulfoquinovose	243	123	20	SQ_1*	-110	-31
	243	95	20	SQ_2	-110	-44
	243	153	20	SQ_3	-110	-24
	243	183	20	SQ_4	-110	-23
	243	81	20	SQ_5	-110	-32
Taurine	124	81	20	Taurine_1*	-95	-30
	124	80	20	Taurine_2	-100	-20
	124	65	20	Taurine_3	-100	-19

