Mass Spectrometry

API 4000 Q-TRAP (AB SCIEX)

Get the data

1. Use the “Open Data File” tab to view ion signals and check that values are good, e.g. no aberrant peaks, weird signals at inappropriate times. Switch
2. Plug in flash drive and go to or folder with appropriate project name.
3. Copy data from folder to flash drive. Data files should end in *.wiff.
4. Copy data from flash drive to lab computer for data integration. When the entire project is done, copy and paste all data to the server.

Product ion transitions and Mass spec parameters:
- Q1 is the molecular weight of the mother ion.
- Q3 is the molecular weight of the daughter ion (the part that breaks off).

	Mixture	Compound	F.W.	DP	CE	Q1/Q3
1	IS	**PHAU**	**250.2**	60	25	251.2/114.1
2	IS	**CUDA**	**340.4**	55	25	341/216
3	SSTD	**Choline d9**	148.7	60	31	113/45
4	SSTD	**Betaine d9**	162.7	60	28	127/68
5	SSTD	**Phosphocholine d9**	266.6	60	31	193/95
6	SSTD	**Creatinine d3**	116.1	55	19	117/89
7	SSTD	**Methionine d3**	152.2	55	25	153/56
8	SSTD	**TMAO d9**	84.2	40	31	85/66
9	SSTD	**Carnitine d3**	200.7	60	25	117/89
10	SSTD	**GPC d9**	266.3	60	37	367/125
11	PRM	Choline	139.62	60	31	104/45
12	PRM	Betaine	117.15	60	28	118/59
13	PRM	Phosphocholine	329.73	60	31	184/86
14	PRM	Glycerophosphocholine	257.22	60	37	258/125
15	PRM	Creatinine	113.12	55	19	114/86
16	PRM	Methionine	149.21	55	25	150/56
17	PRM	Dimethylglycine	103.2	40	22	104/58
18	PRM	Carnitine	197.66	60	25	162/60
19	PRM	TMAO	75.11	40	31	76.1/58.1