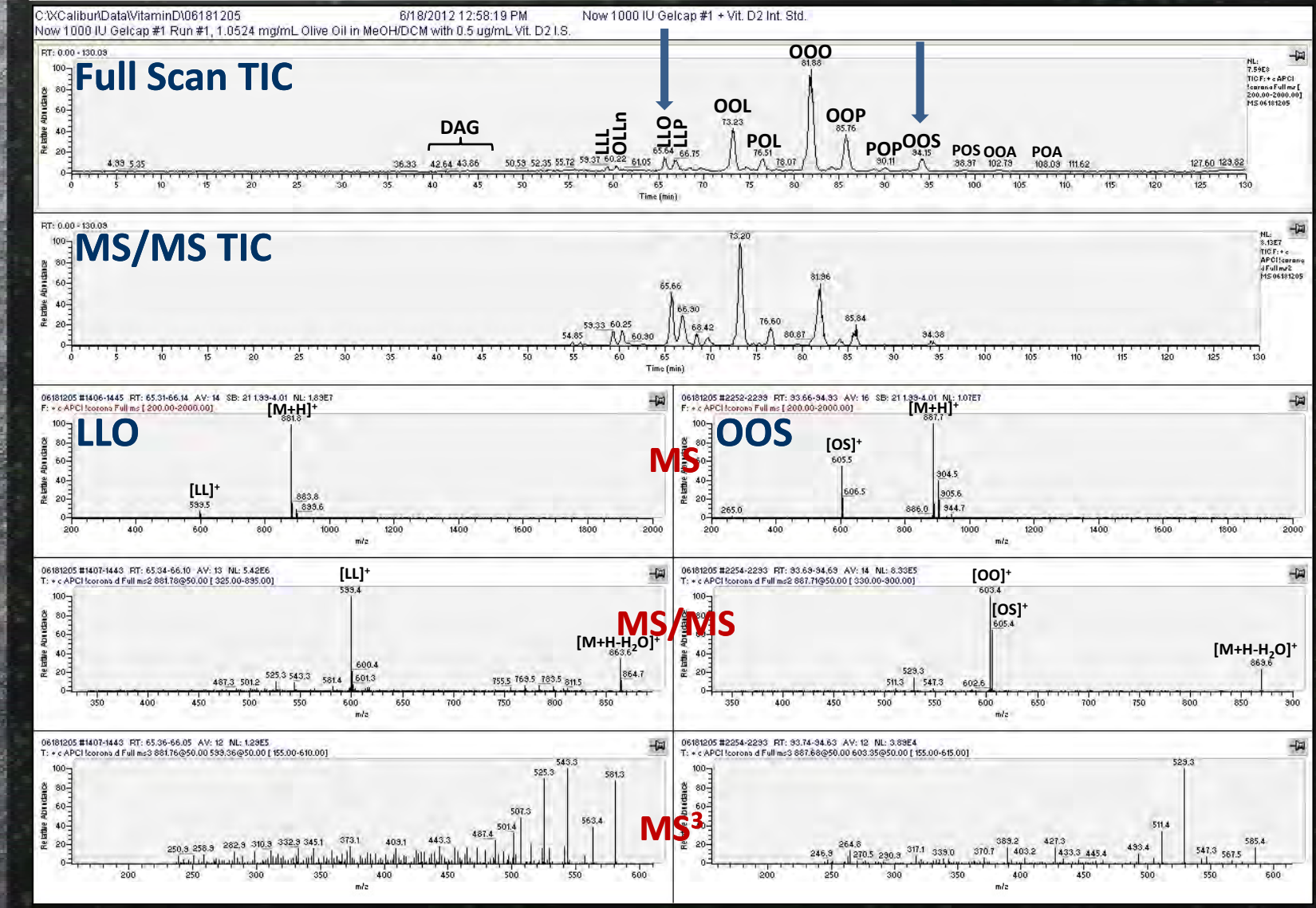
APPI-MS on LCQ Deca XP



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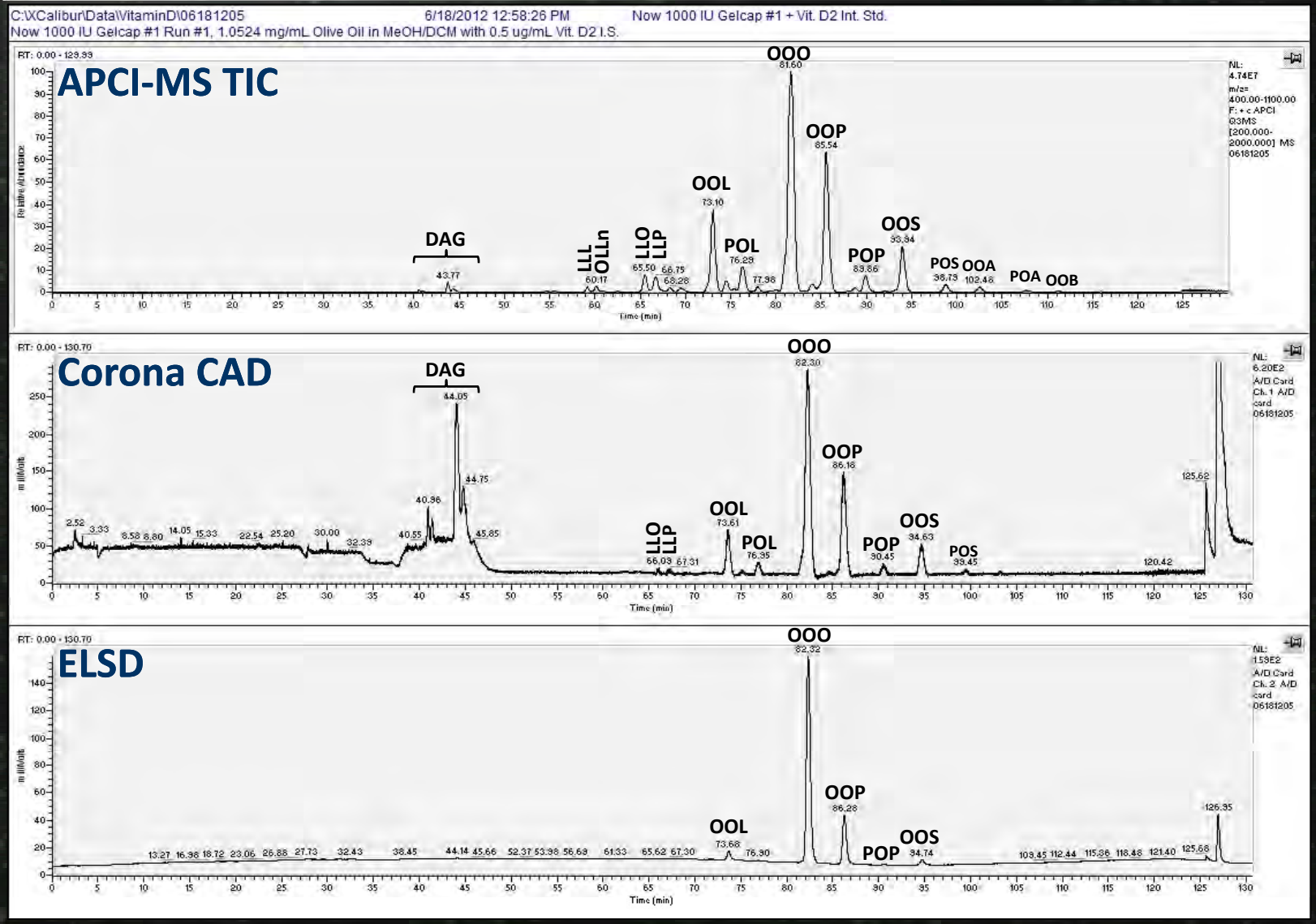
Corona CAD and ELSD



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Quantification of Triacylglycerols

TAG	APCI-MS #1	APCI-MS #2	APPI-MS	ESI-MS	Sat. Adj. ESI-MS	CAD	ELSD
OOO	41.5%	40.4%	40.4%	17.4%	41.0%	49.0%	78.2%
OOP	20.9%	19.9%	13.4%	14.4%	20.4%	23.5%	17.2%
OOL	10.4%	10.4%	15.0%	9.9%	10.4%	9.0%	2.5%
OOS	7.1%	6.4%	4.6%	7.3%	3.5%	7.3%	1.7%
POL	3.5%	3.6%	4.0%	6.7%	3.2%	2.7%	0.2%
POP	2.2%	2.5%	1.0%	5.6%	2.7%	2.5%	0.2%
OOLn1	1.9%	2.2%	3.8%	4.4%	2.1%	1.0%	
LLO	1.9%	2.2%	3.9%	3.9%	1.9%	0.8%	
OOPo	1.3%	1.4%	1.1%	3.7%	1.8%	0.8%	
SLO	1.2%	1.2%	1.6%	2.8%	1.4%	0.6%	
POS	1.2%	1.3%	0.6%	3.2%	1.5%	1.1%	
OOA	0.7%	0.8%	0.6%	1.5%	0.7%	0.5%	
OLLn1	0.6%	0.7%	1.3%	1.6%	0.8%	0.1%	
OOG	0.6%	0.6%	0.6%	1.2%	0.6%	0.2%	
POLn1	0.5%	0.7%	1.1%	2.1%	1.0%	0.1%	
LLP	0.5%	0.6%	0.9%	1.6%	0.8%	0.1%	
LLL	0.4%	0.5%	0.9%	1.1%	0.5%	0.1%	
POPo	0.4%	0.5%	0.3%	1.2%	0.6%	0.2%	
SSO	0.2%	0.3%	0.2%	0.7%	0.3%	0.1%	
DAG/TAG	1.65%	1.67%	0.49%	3.55%	1.72%	21.97%	0.08%

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Comparison of LC-MS Results to GC-FID of FAME

FA	GC-FID *n*=15	APCI-MS #1	APCI-MS #2	APPI-MS	ESI-MS	Sat. Adj. ESI-MS	CAD	ELSD
O	76.2%	75.0%	73.7%	72.5%	58.0%	73.2%	80.1%	92.6%
P	11.0%	10.8%	11.0%	7.8%	15.1%	11.8%	11.0%	5.9%
L	6.8%	7.9%	8.4%	12.5%	13.6%	8.5%	4.8%	0.9%
S	3.2%	3.5%	3.5%	2.7%	5.5%	2.7%	3.1%	0.6%
Ln	1.1%	1.4%	1.7%	2.9%	3.8%	1.8%	0.4%	
Po	0.8%	0.7%	0.8%	0.6%	1.9%	0.9%	0.3%	
A	0.4%	0.3%	0.4%	0.3%	0.8%	0.4%	0.2%	
G	0.3%	0.3%	0.3%	0.4%	0.8%	0.4%	0.1%	
B	0.1%	0.1%	0.1%	0.1%	0.2%	0.1%	0.0%	
Lg	0.0%	0.0%	0.0%	0.0%	0.1%	0.0%		
M	0.0%	0.1%	0.1%	0.1%	0.2%	0.1%	0.0%	
23	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%		
21	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%		
25	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%		
Ce	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%		

1.0%

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Byrdwell et al., J. Agric. Food Chem., 49:446 (2001).

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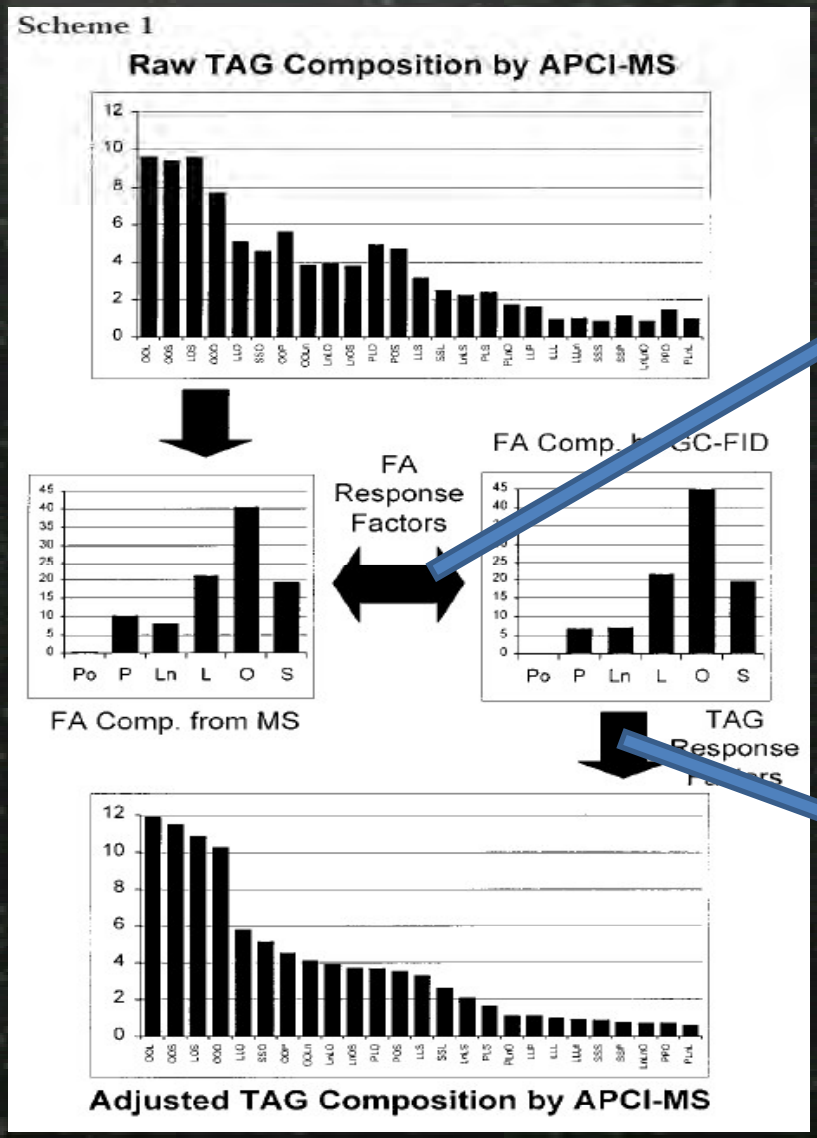

Step 1:

Ratio, r:

$r_{FA} = (FA\%_{GC\text{-}FID}) / (FA\%_{APCI\text{-}MS})$

Step 2:

FA Response Factors:

$RF_{FA} = r_{FA} / r_{min}$

Step 3:

TAG Response Factors:

$R_{TAG} = RF_{FA1} * RF_{FA2} * RF_{FA3}$

Byrdwell et al., J. Agric. Food Chem., 49:446 (2001).

Quantification of Triacylglycerols by Response Factors

TAG	APCI-MS #1	APCI-MS #2	APPI-MS	ESI-MS	Sat. Adj. ESI-MS
OOO	43.6%	44.6%	46.4%	40.8%	46.2%
OOP	22.1%	21.3%	20.7%	18.8%	20.6%
OOL	9.2%	8.9%	8.9%	8.8%	9.0%
OOS	6.8%	6.4%	6.1%	7.7%	4.6%
POL	3.1%	3.0%	3.2%	3.3%	2.5%
POP	2.4%	2.6%	2.0%	4.0%	2.4%
OOLn1	1.6%	1.6%	1.6%	2.3%	1.4%
OOPo	1.5%	1.5%	1.5%	2.6%	1.5%
LLO	1.4%	1.4%	1.2%	1.3%	1.2%
POS	1.1%	1.3%	1.0%	1.9%	1.8%
SLO	1.0%	1.0%	1.1%	1.1%	1.4%
OOA	0.8%	0.8%	0.7%	1.2%	0.7%
OOG	0.6%	0.6%	0.5%	0.9%	0.5%
POPo	0.4%	0.5%	0.5%	0.5%	0.5%
OLLn1	0.4%	0.4%	0.3%	0.3%	0.4%
POLn1	0.4%	0.5%	0.6%	0.6%	0.6%
LLP	0.4%	0.4%	0.4%	0.3%	0.4%
LLL	0.3%	0.2%	0.1%	0.1%	0.3%
OOB	0.2%	0.2%	0.2%	0.4%	0.2%
DAG/TAG	1.34%	1.13%	0.19%	1.51%	1.07%

Byrdwell et al., J. Agric. Food Chem., 49:446 (2001).

RF-Adjusted LC-MS Results vs. GC-FID of FAME

FA	GC-FID	APCI-MS #1	APCI-MS #2	APPI-MS	ESI-MS	Sat. Adj. ESI-MS
O	76.2%	76.4%	76.5%	77.5%	74.8%	76.6%
P	11.0%	11.1%	11.1%	10.6%	11.6%	11.1%
L	6.8%	6.5%	6.4%	6.1%	6.1%	6.4%
S	3.2%	3.2%	3.2%	3.1%	3.9%	3.2%
Ln	1.1%	1.1%	1.1%	1.1%	1.3%	1.0%
Po	0.8%	0.8%	0.8%	0.8%	1.1%	0.8%
A	0.4%	0.4%	0.4%	0.4%	0.5%	0.4%
G	0.3%	0.3%	0.3%	0.3%	0.4%	0.3%
B	0.1%	0.1%	0.1%	0.1%	0.2%	0.1%
Lg	0.0%	0.0%	0.0%	0.0%	0.1%	0.0%
M	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
23	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
21	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
25	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Ce	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%

1.0%

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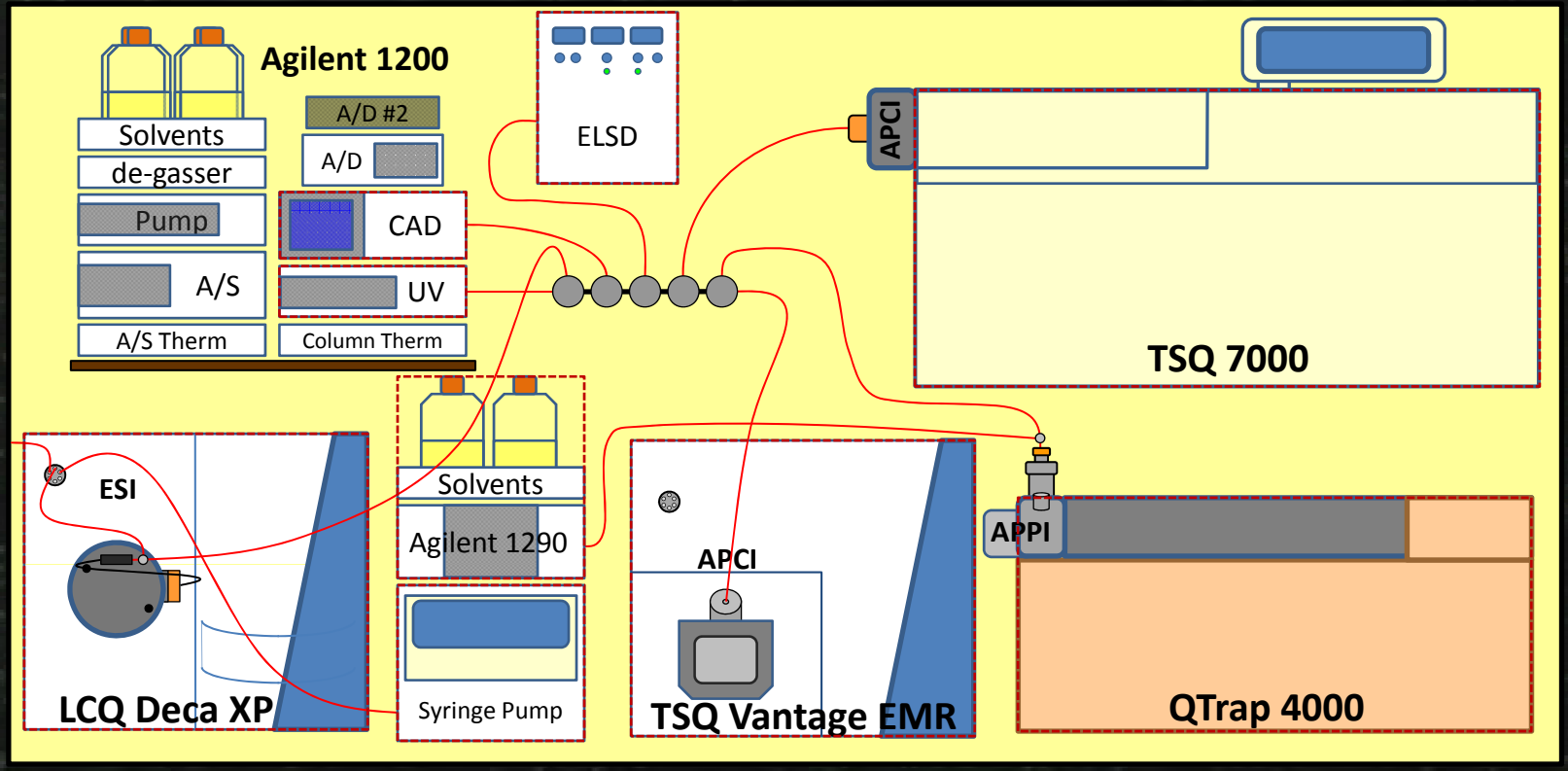
Quadruple Parallel MS Instrumentation



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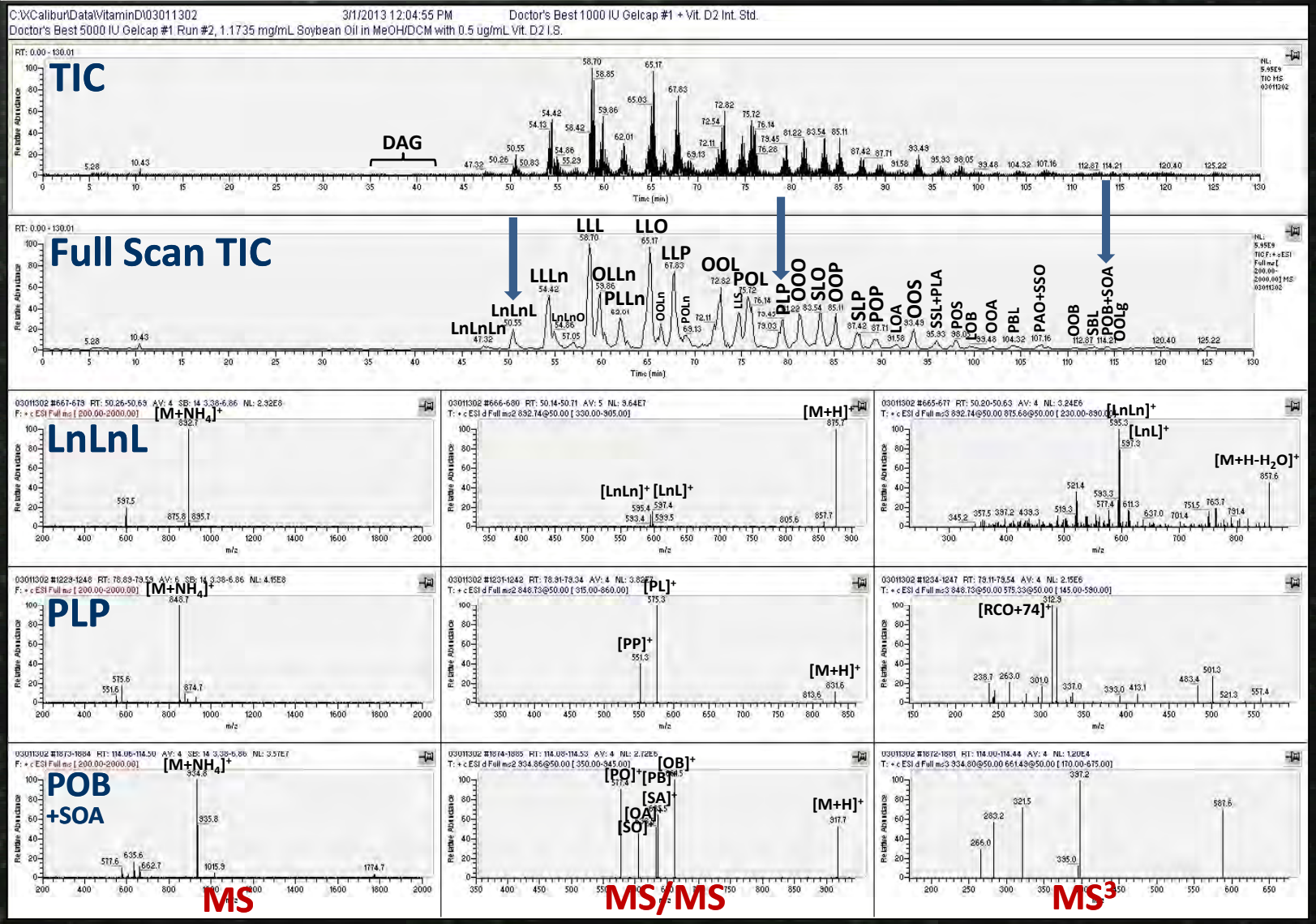
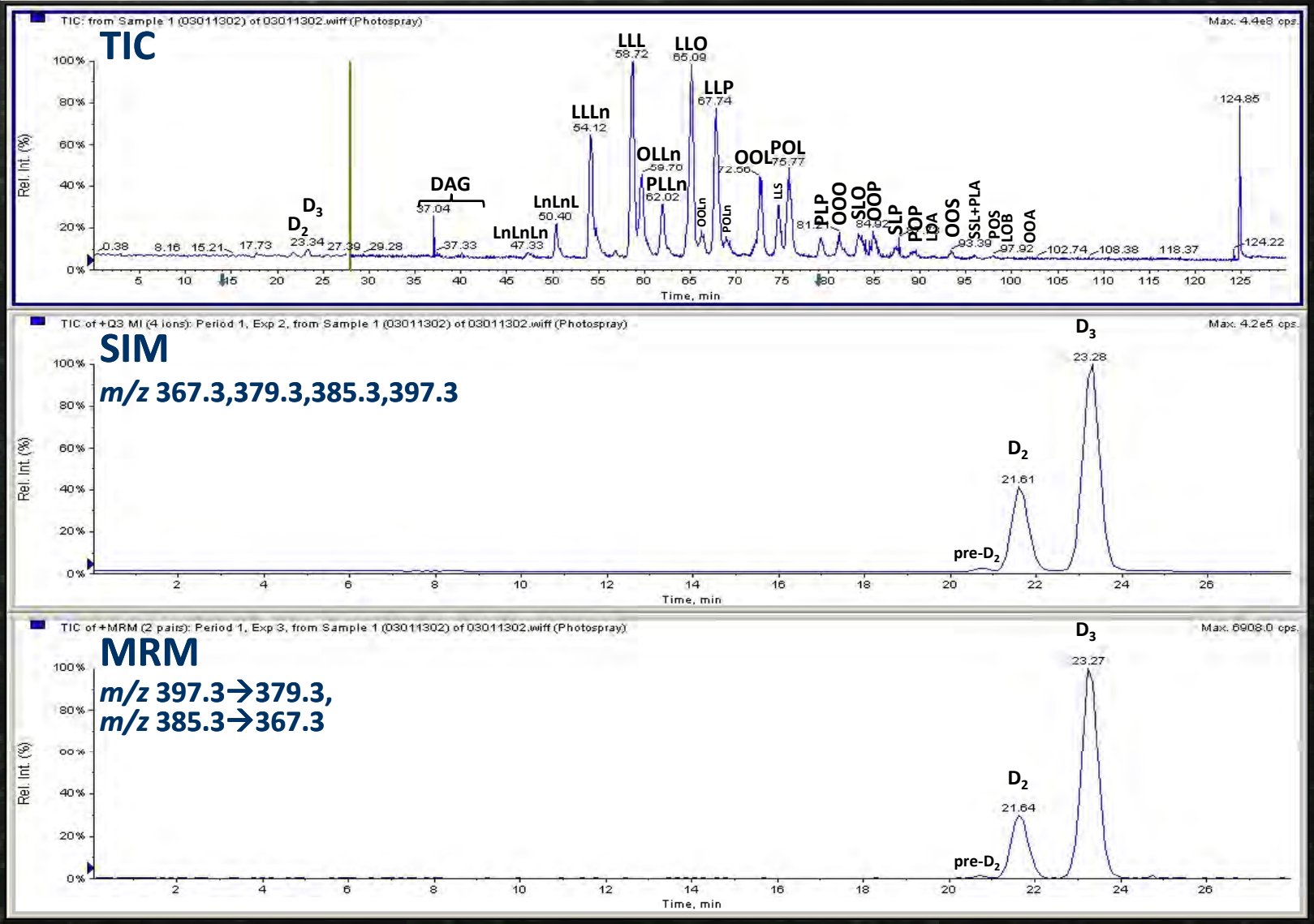
ESI-MS on LCQ Deca XP



B= behenic (22:0); A=arachidic (20:0); Lg=lignoceric (24:0)

APPI-MS on QTrap4000



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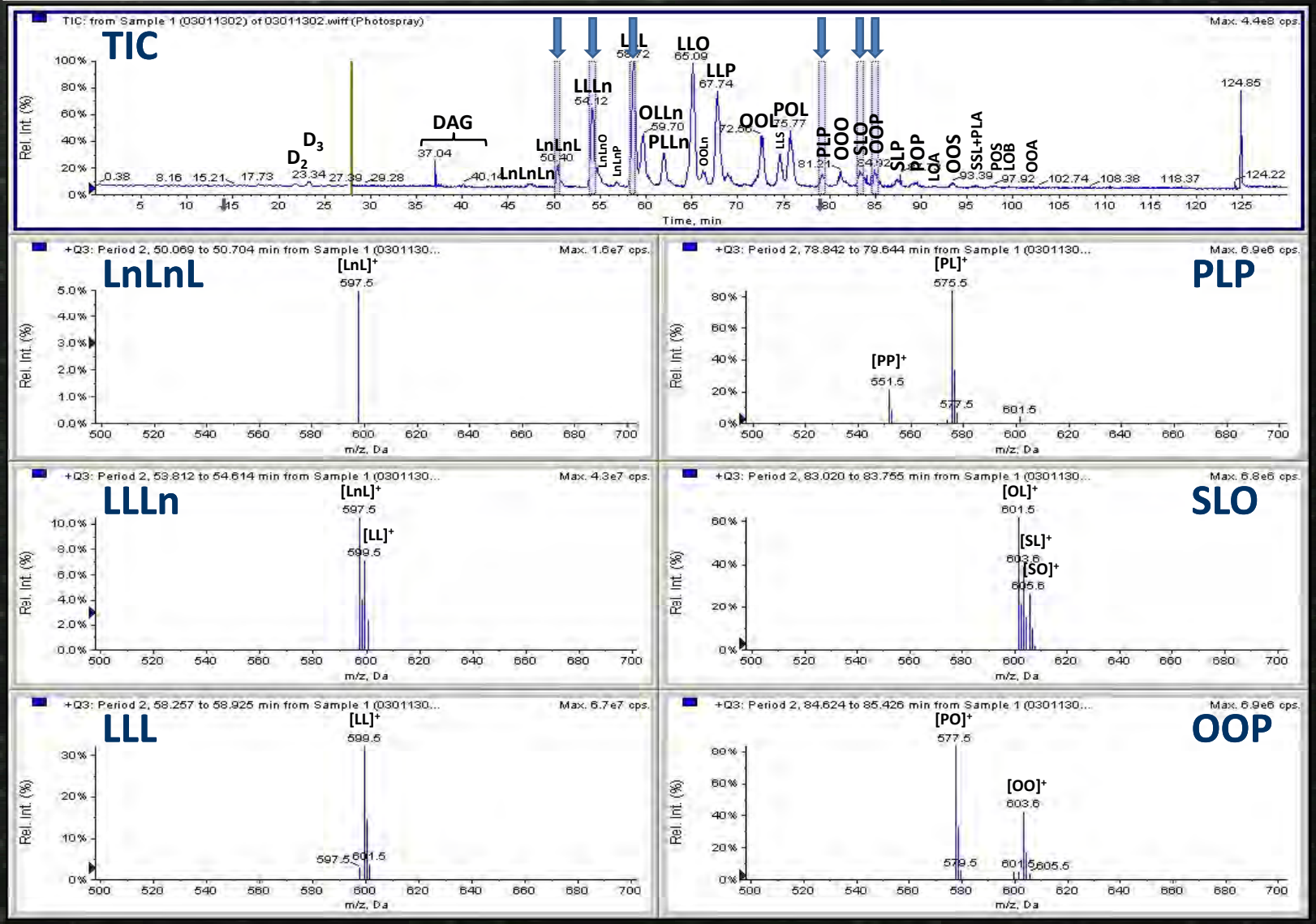
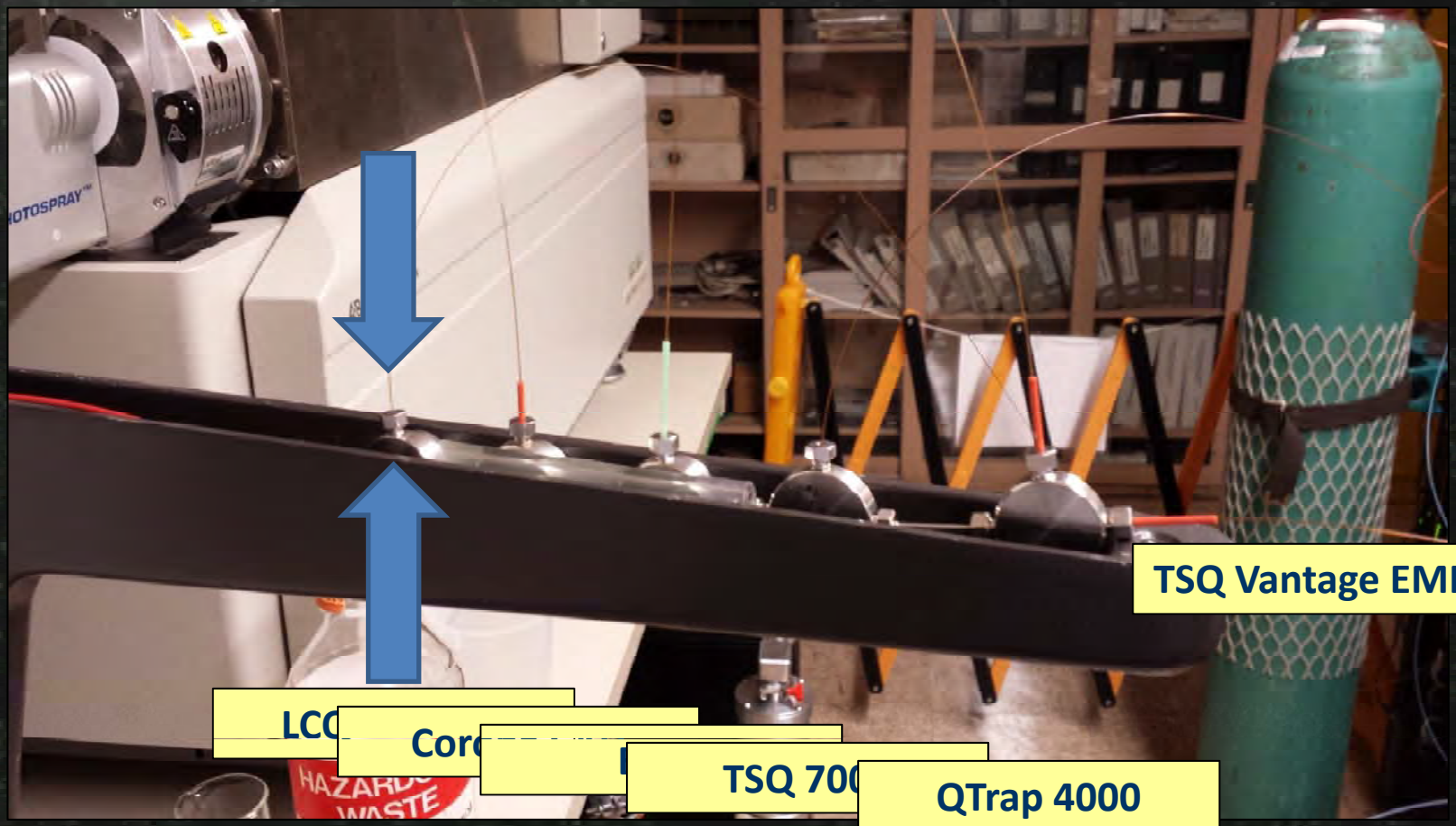
APPI-MS on QTrap4000



Liquid Flow Distribution Manifold



5 x Valco Tees + 6 x Fused Silica Capillary Tubing peices

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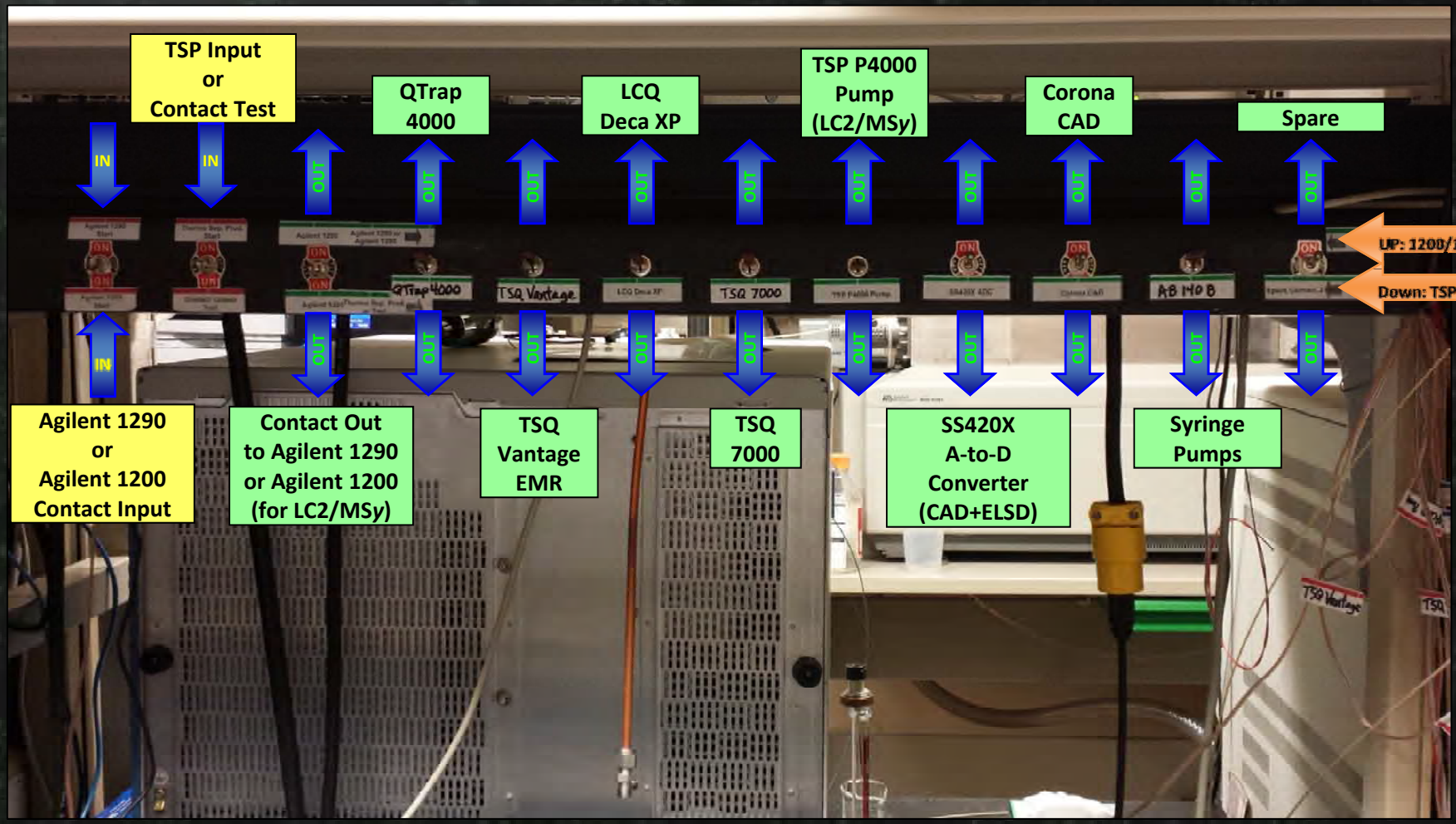
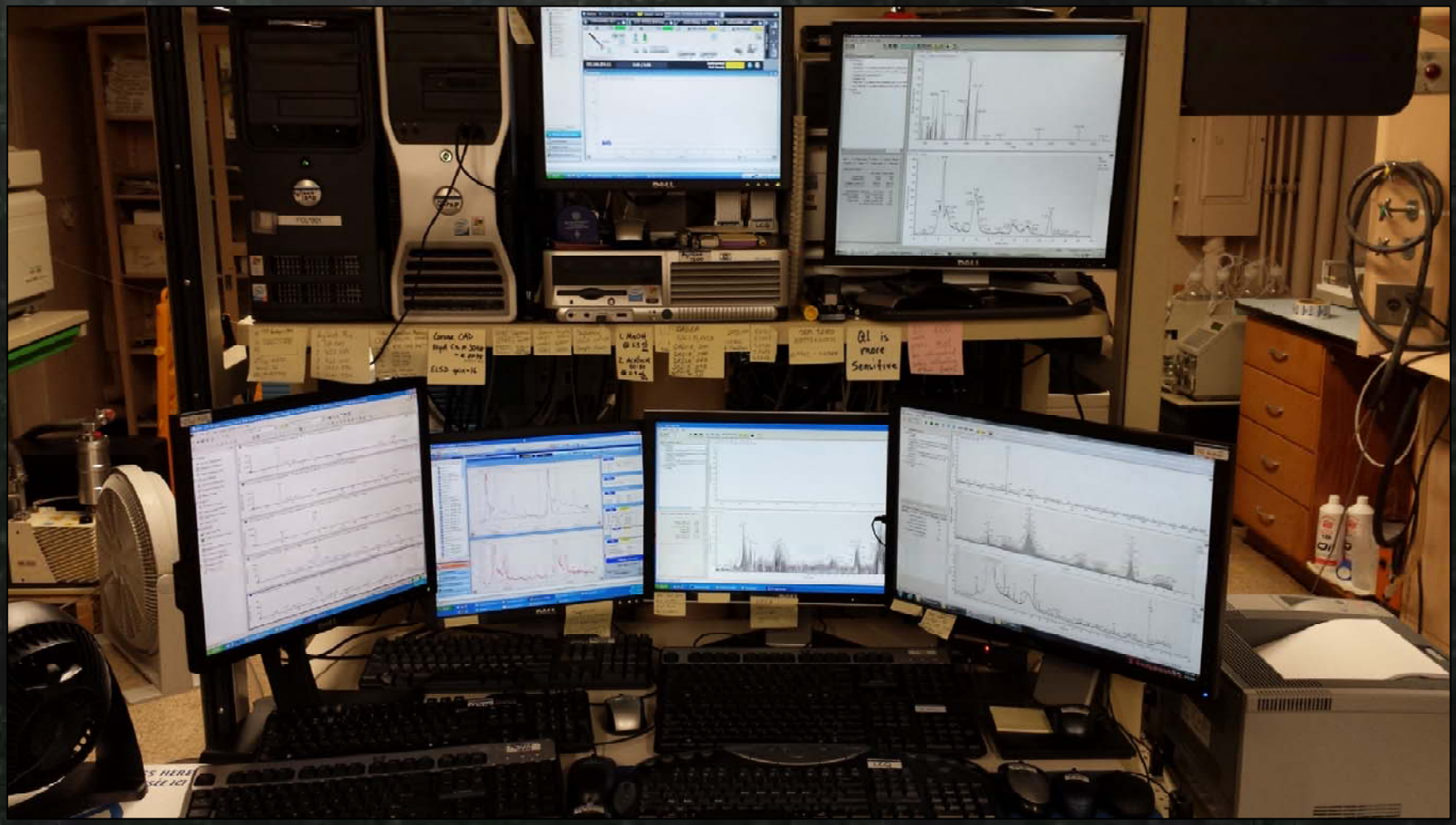
Contact Closure Switching Panel constructed in my lab



3 Autosampler Inputs + Test / 10 Outputs

“Command Central” – HPLC, UHPLC, 4 Mass Spectrometers



6 Computers/monitors/keyboards/mice