

Supplemental Information:

A fast and selective approach for profiling vicinal diols using liquid chromatography-post column derivatization-double precursor ion scanning mass spectrometry

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Table S1. HPLC gradient to separate 1,2-cis-diols

Total Time (min)	Flow Rate ($\mu\text{L}/\text{min}$)	B (%)
0	250	35
0.25	250	35
1	250	45
3	250	55
8.5	250	66
12.5	250	72
15	250	82
16.5	250	95
18	250	95
18.1	250	35
21.5	250	35

Table S2. Optimized mass spectrometric parameters on Q-trap

Parameters	Value
CUR	25 psi
TEM	600 °C
GS1	50 psi
GS2	60 psi
iHe	ON
CAD	Medium
IS	5500
EP	10

Table S3 Optimization of modifiers for post column derivatization

Modifier	Signal intensity (cps)
0.5% Acetic acid, pH 6	265
5% $\text{NH}_3\text{-H}_2\text{O}$, pH 9	930
water	1310

Table S4 Reproducibility of the developed method

Concentration level (ng/mL)	Intra-day Precision	Inter-day Precision
50	13.80%	12.60%
500	3.80%	4.50%
5000	2.50%	7.90%

Note: the data are calculated using the response of 14,15 DiHETrE-BPBA ester to d11-11,12 DiHETrE-BPBA ester.

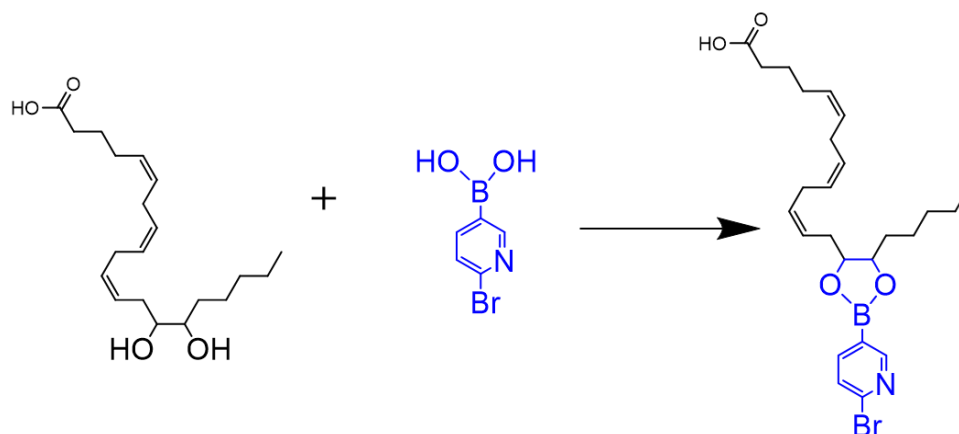


Figure S1: An example (14,15 DiHETrE) of the derivatization of vicinal diols by BPBA.

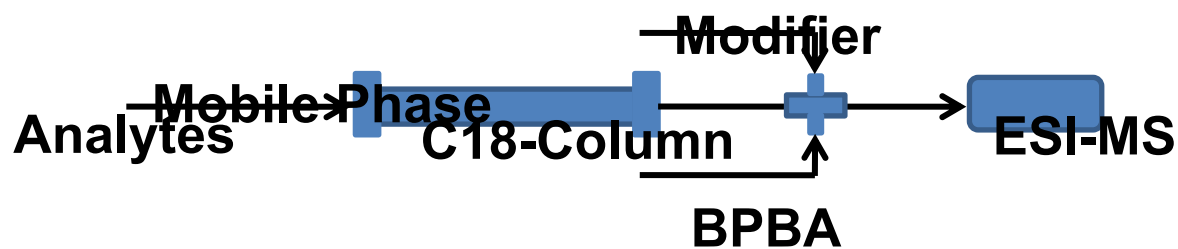


Figure S2: Scheme of the post column derivatization configuration used.

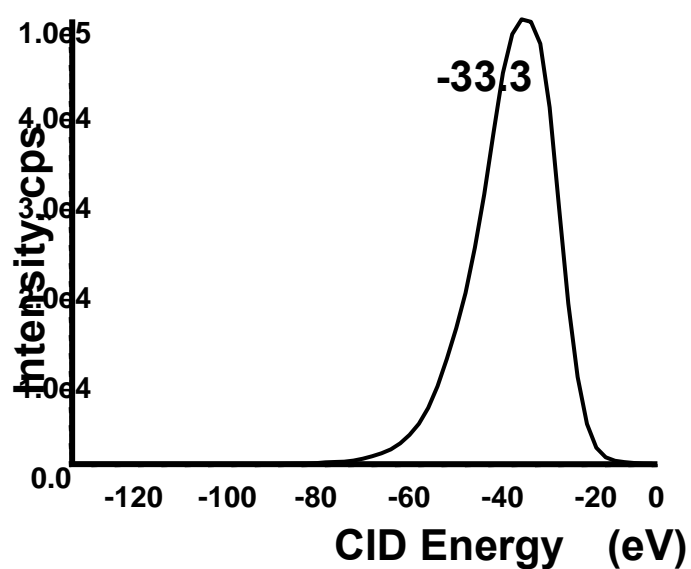


Figure S3: Optimized CID energy for each compound.