SUPPLEMENTARY DATA - JLR/2013/037622

Table 1 – PC species in CSF – To isolate PC species from isobars in CSF, we used the Quan software (Thermo Fisher, San Jose, CA) to extract 0.5 min spectral segments across the PC peak. After exporting the exact mass from each segment to an Excel spreadsheet, peak intensities < 100 were deleted and the data was sorted by increasing m/z. PC peaks that have an equal or higher intensity compared to the odd m/z isobars are shaded with yellow. These data are representative of 70 SF injections.

Table 1 – PC species in SF are highlighted in yellow

Mass	Intensity		Mass	Intensity		Mass	Intensity		Mass	Intensity
690.60	1463		755.77	1282		796.67	58964		838.80	28572
692.63	796		756.84	23404		797.67	32832		839.71	22096
704.68	758		757.65	6503		798.73	11646		840.74	6020
706.74	40708		758.61	449885		799.83	6304		841.70	4920
707.60	14521		759.78	263293		800.74	19412		842.78	2291
710.57	1963		760.87	3486193		801.73	21175		844.62	11046
711.40	898		761.60	1613264		802.60	6067		845.73	7106
716.61	3282		762.67	519846		803.97	11011		846.81	3345
717.38	1239		763.86	173433		804.70	14182		847.65	817
718.70	19638		764.77	92273		805.64	15242		848.73	6095
719.73	13394		765.82	81327		806.82	171919		849.80	6123
720.70	45386		766.93	74509		807.55	75854		850.86	10604
721.79	9048		767.91	23067		808.78	173288		852.52	2894
722.92	5471		768.75	35608		809.84	68610		856.41	2136
726.02	3667		769.93	33043		810.75	392867		859.83	9108
728.50	496		770.74	21048		811.67	192785		860.80	5444
729.53	2603		771.91	9292		812.99	202240		861.75	2272
730.52	8517		772.65	48671		813.69	85888		864.00	1938
731.76	507		773.72	13535		814.61	38297		865.00	1779
732.68	165738		774.65	47560		815.79	25847		866.13	3762
733.70	65488		775.63	27609		816.78	37142		867.64	1738
734.67	554192		776.68	16787		817.69	7482		868.85	134
735.61	222670		777.72	3134		818.96	33352		870.78	1142
736.79	81290		778.70	5634		819.59	15186		871.81	426
737.74	29283		780.76	17311		820.87	16161		872.79	2780
738.53	4697		781.65	10276		821.69	6299		873.70	5436
739.92	7722		782.75	452570		822.75	7448		874.81	14817
740.95	4939		783.67	240658		823.76	4895		876.94	2007
741.93	9327		784.91	222410		824.73	19307		877.92	718
742.61	15599		785.80	127241		825.80	13270		878.69	2125
743.99	9559		786.76	440371		828.68	8741		879.91	1128
744.73	86397		787.83	214830		829.65	1119		883.84	4412
745.76	32469		788.77	382369		830.87	7012		886.90	1138
746.76	111353		789.81	156024		831.70	1407		887.41	751
747.67	36173		790.81	71936		832.76	22167		889.86	1628
748.75	42046		791.79	18542		833.82	5697		896.83	2050
749.76	13365		792.61	46739		834.75	122413		898.57	1952
750.78	4103		793.94	35307		835.93	45957		899.87	1151
752.76	4161		794.90	53117		836.84	22762		900.77	3630
754.66	260		795.78	35504		837.61	7109		901.87	1917

SUPPLEMENTARY DATA

Figure legends

Figure 1 – Spectra of PC showing the appearance of distinct species – To determine whether the clusters of PC are made up of distinct species, we obtained 0.5 min spectral segments across the PC peak. Figure 1 shows spectral segments from 11-13.5 min that differentiates several species within clusters at m/z of ~ 782 and 810. These data are representative of 70 SF injections.

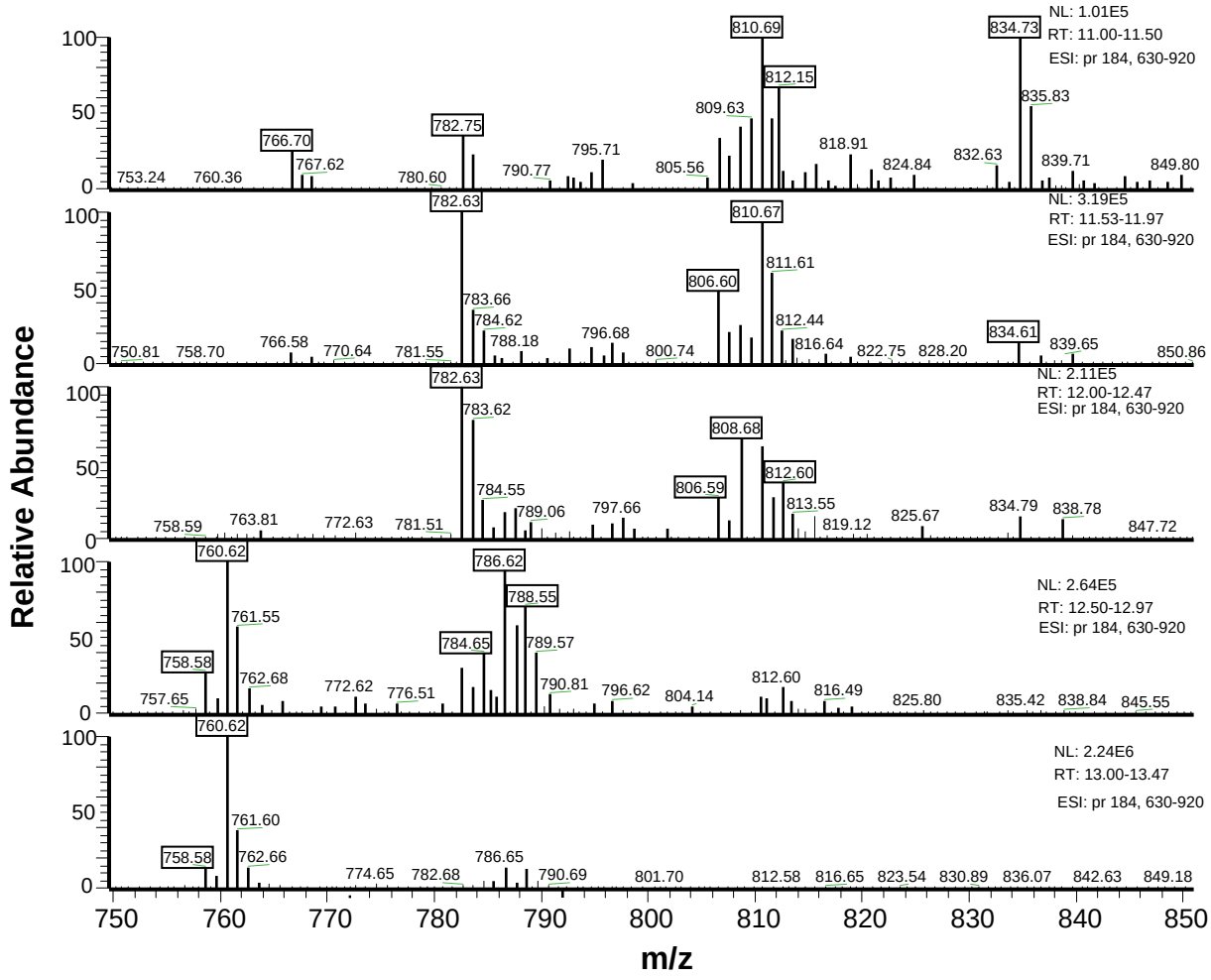
Figure 2 - MRM of PC species in SF and NP - MRM of selected PC species was performed as described in Methods and Supplementary Methods.

Figure 2A is representative of LC-MS/MS analyses from 70 SF injections showing the total ion current, SRM of IS [PC(11:0/11:0), m/z = 594)], and MRM of 42 PC species. The precursor masses used for MS^2 and the relative abundance of each molecular species are shown on each panel. A product m/z of 184 was monitored for each molecular species using MS conditions described in our Supplementary Methods.

Figure 2B is representative of LC-MS/MS analyses from 67 NP injections showing the total ion current, SRM of IS [PC(11:0/11:0), m/z = 594)], and MRM of 60 other PC molecular species. MRM conditions are described in our Methods and in details in Supplementary Methods.

Supplementary Data

Figure 1 – Spectra of PC segments showing appearance of distinct species (boxed *m/z*)



Supplementary Data **Figure 2 –** MRM of selected PC species in SF and NP