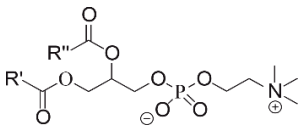


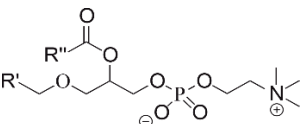
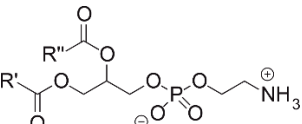
## Supplementary Material to Burk et al., Phospholipid-based MSC phenotyping

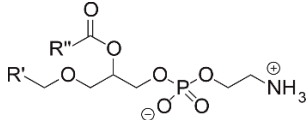
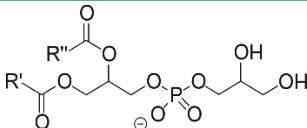
### Supplement 3: Overview and assignment of phospholipids.

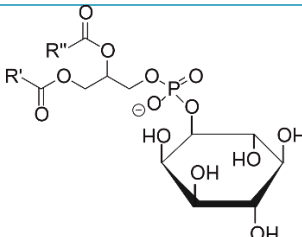
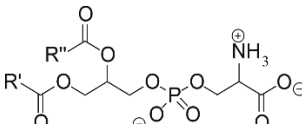
The S3 Supplementary Table displays the assignment of phospholipids in positive and negative ionization mode using reversed-phase liquid chromatography coupled to electrospray ionization mass spectrometry and tandem mass spectrometry (MS/MS) experiments.

| Lipid Species                                 | Accurate<br>m/z value | Adduct                                                                             | Empirical Formula      |
|-----------------------------------------------|-----------------------|------------------------------------------------------------------------------------|------------------------|
| <b>1-Acyl-2-acyl-phosphatidylcholine (PC)</b> |                       |  |                        |
| <b>PC 28:0</b>                                | 678.5068              | $[M+H]^+$                                                                          | $C_{36}H_{73}NO_8P$    |
|                                               | 722.4978              | $[M+HCOO]^-$                                                                       | $C_{37}H_{73}NO_{10}P$ |
| <b>PC 29:0</b>                                | 692.5225              | $[M+H]^+$                                                                          | $C_{37}H_{75}NO_8P$    |
|                                               | 736.5134              | $[M+HCOO]^-$                                                                       | $C_{38}H_{75}NO_{10}P$ |
| <b>PC 30:0</b>                                | 706.5381              | $[M+H]^+$                                                                          | $C_{38}H_{77}NO_8P$    |
|                                               | 750.5291              | $[M+HCOO]^-$                                                                       | $C_{39}H_{77}NO_{10}P$ |
| <b>PC 30:1</b>                                | 704.5225              | $[M+H]^+$                                                                          | $C_{38}H_{75}NO_8P$    |
|                                               | 748.5134              | $[M+HCOO]^-$                                                                       | $C_{39}H_{75}NO_{10}P$ |
| <b>PC 31:0</b>                                | 720.5538              | $[M+H]^+$                                                                          | $C_{39}H_{79}NO_8P$    |
|                                               | 764.5447              | $[M+HCOO]^-$                                                                       | $C_{40}H_{79}NO_{10}P$ |
| <b>PC 31:1</b>                                | 718.5381              | $[M+H]^+$                                                                          | $C_{39}H_{77}NO_8P$    |
|                                               | 762.5291              | $[M+HCOO]^-$                                                                       | $C_{40}H_{77}NO_{10}P$ |
| <b>PC 32:0</b>                                | 734.5694              | $[M+H]^+$                                                                          | $C_{40}H_{81}NO_8P$    |
|                                               | 778.5604              | $[M+HCOO]^-$                                                                       | $C_{41}H_{81}NO_{10}P$ |
| <b>PC 32:1</b>                                | 732.5538              | $[M+H]^+$                                                                          | $C_{40}H_{79}NO_8P$    |
|                                               | 776.5447              | $[M+HCOO]^-$                                                                       | $C_{41}H_{79}NO_{10}P$ |
| <b>PC 32:2</b>                                | 730.5381              | $[M+H]^+$                                                                          | $C_{40}H_{77}NO_8P$    |
|                                               | 774.5291              | $[M+HCOO]^-$                                                                       | $C_{41}H_{77}NO_{10}P$ |
| <b>PC 32:3</b>                                | 728.5225              | $[M+H]^+$                                                                          | $C_{40}H_{75}NO_8P$    |
|                                               | 772.5134              | $[M+HCOO]^-$                                                                       | $C_{41}H_{75}NO_{10}P$ |
| <b>PC 33:1</b>                                | 746.5694              | $[M+H]^+$                                                                          | $C_{41}H_{81}NO_8P$    |
|                                               | 790.5603              | $[M+HCOO]^-$                                                                       | $C_{42}H_{81}NO_{10}P$ |
| <b>PC 33:2</b>                                | 744.5537              | $[M+H]^+$                                                                          | $C_{41}H_{79}NO_8P$    |
|                                               | 788.5447              | $[M+HCOO]^-$                                                                       | $C_{42}H_{79}NO_{10}P$ |
| <b>PC 34:0</b>                                | 762.6007              | $[M+H]^+$                                                                          | $C_{42}H_{85}NO_8P$    |
|                                               | 806.5916              | $[M+HCOO]^-$                                                                       | $C_{43}H_{85}NO_{10}P$ |
| <b>PC 34:1</b>                                | 760.5850              | $[M+H]^+$                                                                          | $C_{42}H_{83}NO_8P$    |
|                                               | 804.5760              | $[M+HCOO]^-$                                                                       | $C_{43}H_{83}NO_{10}P$ |

| Lipid Species | Accurate<br><i>m/z</i> value | Adduct                | Empirical Formula                                  |
|---------------|------------------------------|-----------------------|----------------------------------------------------|
| PC 34:2       | 758.5694                     | [M+H] <sup>+</sup>    | C <sub>42</sub> H <sub>81</sub> NO <sub>8</sub> P  |
|               | 802.5603                     | [M+HCOO] <sup>-</sup> | C <sub>43</sub> H <sub>81</sub> NO <sub>10</sub> P |
| PC 34:3       | 756.5537                     | [M+H] <sup>+</sup>    | C <sub>42</sub> H <sub>79</sub> NO <sub>8</sub> P  |
|               | 800.5447                     | [M+HCOO] <sup>-</sup> | C <sub>43</sub> H <sub>79</sub> NO <sub>10</sub> P |
| PC 35:0       | 776.6163                     | [M+H] <sup>+</sup>    | C <sub>43</sub> H <sub>87</sub> NO <sub>8</sub> P  |
|               | 820.6073                     | [M+HCOO] <sup>-</sup> | C <sub>44</sub> H <sub>87</sub> NO <sub>10</sub> P |
| PC 35:2       | 772.5850                     | [M+H] <sup>+</sup>    | C <sub>43</sub> H <sub>83</sub> NO <sub>8</sub> P  |
|               | 816.5760                     | [M+HCOO] <sup>-</sup> | C <sub>44</sub> H <sub>83</sub> NO <sub>10</sub> P |
| PC 35:3       | 770.5694                     | [M+H] <sup>+</sup>    | C <sub>43</sub> H <sub>81</sub> NO <sub>8</sub> P  |
|               | 814.5603                     | [M+HCOO] <sup>-</sup> | C <sub>44</sub> H <sub>81</sub> NO <sub>10</sub> P |
| PC 35:4       | 768.5537                     | [M+H] <sup>+</sup>    | C <sub>43</sub> H <sub>79</sub> NO <sub>8</sub> P  |
|               | 812.5447                     | [M+HCOO] <sup>-</sup> | C <sub>44</sub> H <sub>79</sub> NO <sub>10</sub> P |
| PC 36:0       | 790.6320                     | [M+H] <sup>+</sup>    | C <sub>44</sub> H <sub>89</sub> NO <sub>8</sub> P  |
|               | 834.6229                     | [M+HCOO] <sup>-</sup> | C <sub>45</sub> H <sub>89</sub> NO <sub>10</sub> P |
| PC 36:1       | 788.6163                     | [M+H] <sup>+</sup>    | C <sub>44</sub> H <sub>87</sub> NO <sub>8</sub> P  |
|               | 832.6073                     | [M+HCOO] <sup>-</sup> | C <sub>45</sub> H <sub>87</sub> NO <sub>10</sub> P |
| PC 36:2       | 786.6007                     | [M+H] <sup>+</sup>    | C <sub>44</sub> H <sub>85</sub> NO <sub>8</sub> P  |
|               | 830.5916                     | [M+HCOO] <sup>-</sup> | C <sub>45</sub> H <sub>85</sub> NO <sub>10</sub> P |
| PC 36:3       | 784.5850                     | [M+H] <sup>+</sup>    | C <sub>44</sub> H <sub>83</sub> NO <sub>8</sub> P  |
|               | 828.5760                     | [M+HCOO] <sup>-</sup> | C <sub>45</sub> H <sub>83</sub> NO <sub>10</sub> P |
| PC 36:4       | 782.5694                     | [M+H] <sup>+</sup>    | C <sub>44</sub> H <sub>81</sub> NO <sub>8</sub> P  |
|               | 826.5603                     | [M+HCOO] <sup>-</sup> | C <sub>45</sub> H <sub>81</sub> NO <sub>10</sub> P |
| PC 36:5       | 780.5537                     | [M+H] <sup>+</sup>    | C <sub>44</sub> H <sub>79</sub> NO <sub>8</sub> P  |
|               | 824.5447                     | [M+HCOO] <sup>-</sup> | C <sub>45</sub> H <sub>79</sub> NO <sub>10</sub> P |
| PC 37:2       | 800.6163                     | [M+H] <sup>+</sup>    | C <sub>45</sub> H <sub>87</sub> NO <sub>8</sub> P  |
|               | 844.6073                     | [M+HCOO] <sup>-</sup> | C <sub>46</sub> H <sub>87</sub> NO <sub>10</sub> P |
| PC 37:4       | 796.5850                     | [M+H] <sup>+</sup>    | C <sub>45</sub> H <sub>83</sub> NO <sub>8</sub> P  |
|               | 840.5760                     | [M+HCOO] <sup>-</sup> | C <sub>46</sub> H <sub>83</sub> NO <sub>10</sub> P |
| PC 37:5       | 794.5694                     | [M+H] <sup>+</sup>    | C <sub>45</sub> H <sub>81</sub> NO <sub>8</sub> P  |
|               | 838.5603                     | [M+HCOO] <sup>-</sup> | C <sub>46</sub> H <sub>81</sub> NO <sub>10</sub> P |
| PC 38:1       | 816.6476                     | [M+H] <sup>+</sup>    | C <sub>46</sub> H <sub>91</sub> NO <sub>8</sub> P  |
|               | 860.6386                     | [M+HCOO] <sup>-</sup> | C <sub>47</sub> H <sub>91</sub> NO <sub>10</sub> P |
| PC 38:2       | 814.6320                     | [M+H] <sup>+</sup>    | C <sub>46</sub> H <sub>89</sub> NO <sub>8</sub> P  |
|               | 858.6229                     | [M+HCOO] <sup>-</sup> | C <sub>47</sub> H <sub>89</sub> NO <sub>10</sub> P |
| PC 38:3       | 812.6163                     | [M+H] <sup>+</sup>    | C <sub>46</sub> H <sub>87</sub> NO <sub>8</sub> P  |
|               | 856.6073                     | [M+HCOO] <sup>-</sup> | C <sub>47</sub> H <sub>87</sub> NO <sub>10</sub> P |
| PC 38:4       | 810.6007                     | [M+H] <sup>+</sup>    | C <sub>46</sub> H <sub>85</sub> NO <sub>8</sub> P  |
|               | 854.5916                     | [M+HCOO] <sup>-</sup> | C <sub>47</sub> H <sub>85</sub> NO <sub>10</sub> P |
| PC 38:5       | 808.5850                     | [M+H] <sup>+</sup>    | C <sub>46</sub> H <sub>83</sub> NO <sub>8</sub> P  |
|               | 852.5760                     | [M+HCOO] <sup>-</sup> | C <sub>47</sub> H <sub>83</sub> NO <sub>10</sub> P |
| PC 38:6       | 806.5694                     | [M+H] <sup>+</sup>    | C <sub>46</sub> H <sub>81</sub> NO <sub>8</sub> P  |
|               | 850.5603                     | [M+HCOO] <sup>-</sup> | C <sub>47</sub> H <sub>81</sub> NO <sub>10</sub> P |

| Lipid Species                                      | Accurate<br><i>m/z</i> value | Adduct                                                                               | Empirical Formula      |
|----------------------------------------------------|------------------------------|--------------------------------------------------------------------------------------|------------------------|
| <b>PC 40:4</b>                                     | 838.6320                     | $[M+H]^+$                                                                            | $C_{48}H_{89}NO_8P$    |
|                                                    | 882.6229                     | $[M+HCOO]^-$                                                                         | $C_{49}H_{89}NO_{10}P$ |
| <b>PC 40:5</b>                                     | 836.6163                     | $[M+H]^+$                                                                            | $C_{48}H_{87}NO_8P$    |
|                                                    | 880.6073                     | $[M+HCOO]^-$                                                                         | $C_{49}H_{87}NO_{10}P$ |
| <b>PC 40:6</b>                                     | 834.6007                     | $[M+H]^+$                                                                            | $C_{48}H_{85}NO_8P$    |
|                                                    | 878.5916                     | $[M+HCOO]^-$                                                                         | $C_{49}H_{85}NO_{10}P$ |
| <b>1-Alkyl-2-acyl-phosphatidylcholine (PC-O)</b>   |                              |    |                        |
| <b>PC O-30:0</b>                                   | 692.5589                     | $[M+H]^+$                                                                            | $C_{38}H_{79}NO_7P$    |
|                                                    | 736.5498                     | $[M+HCOO]^-$                                                                         | $C_{39}H_{79}NO_9P$    |
| <b>PC O-32:0</b>                                   | 720.5902                     | $[M+H]^+$                                                                            | $C_{40}H_{83}NO_7P$    |
|                                                    | 764.5811                     | $[M+HCOO]^-$                                                                         | $C_{41}H_{83}NO_9P$    |
| <b>PC O-34:0</b>                                   | 748.6214                     | $[M+H]^+$                                                                            | $C_{42}H_{87}NO_7P$    |
|                                                    | 792.6123                     | $[M+HCOO]^-$                                                                         | $C_{43}H_{87}NO_9P$    |
| <b>PC O-34:1</b>                                   | 746.6058                     | $[M+H]^+$                                                                            | $C_{42}H_{85}NO_7P$    |
|                                                    | 790.5967                     | $[M+HCOO]^-$                                                                         | $C_{43}H_{85}NO_9P$    |
| <b>PC O-34:2</b>                                   | 744.5901                     | $[M+H]^+$                                                                            | $C_{42}H_{83}NO_7P$    |
|                                                    | 788.5810                     | $[M+HCOO]^-$                                                                         | $C_{43}H_{83}NO_9P$    |
| <b>PC O-36:2</b>                                   | 772.6214                     | $[M+H]^+$                                                                            | $C_{44}H_{87}NO_7P$    |
|                                                    | 816.6123                     | $[M+HCOO]^-$                                                                         | $C_{45}H_{87}NO_9P$    |
| <b>PC O-36:3</b>                                   | 770.6058                     | $[M+H]^+$                                                                            | $C_{44}H_{85}NO_7P$    |
|                                                    | 814.5967                     | $[M+HCOO]^-$                                                                         | $C_{45}H_{85}NO_9P$    |
| <b>PC O-36:4</b>                                   | 768.5901                     | $[M+H]^+$                                                                            | $C_{44}H_{83}NO_7P$    |
|                                                    | 812.5810                     | $[M+HCOO]^-$                                                                         | $C_{45}H_{83}NO_9P$    |
| <b>PC O-38:2</b>                                   | 800.6527                     | $[M+H]^+$                                                                            | $C_{46}H_{91}NO_7P$    |
|                                                    | 844.6436                     | $[M+HCOO]^-$                                                                         | $C_{47}H_{91}NO_9P$    |
| <b>PC O-38:4</b>                                   | 796.6214                     | $[M+H]^+$                                                                            | $C_{46}H_{87}NO_7P$    |
|                                                    | 840.6123                     | $[M+HCOO]^-$                                                                         | $C_{47}H_{87}NO_9P$    |
| <b>PC O-38:5</b>                                   | 794.6058                     | $[M+H]^+$                                                                            | $C_{46}H_{85}NO_7P$    |
|                                                    | 838.5967                     | $[M+HCOO]^-$                                                                         | $C_{47}H_{85}NO_9P$    |
| <b>1-Acyl-2-acyl-phosphatidylethanolamine (PE)</b> |                              |  |                        |
| <b>PE 32:1</b>                                     | 688.4922                     | $[M-H]^-$                                                                            | $C_{37}H_{71}NO_8P$    |
| <b>PE 34:1</b>                                     | 716.5235                     | $[M-H]^-$                                                                            | $C_{39}H_{75}NO_8P$    |
| <b>PE 34:2</b>                                     | 714.5079                     | $[M-H]^-$                                                                            | $C_{39}H_{73}NO_8P$    |
| <b>PE 34:3</b>                                     | 712.4922                     | $[M-H]^-$                                                                            | $C_{39}H_{71}NO_8P$    |
| <b>PE 36:0</b>                                     | 746.5705                     | $[M-H]^-$                                                                            | $C_{41}H_{81}NO_8P$    |
| <b>PE 36:1</b>                                     | 744.5548                     | $[M-H]^-$                                                                            | $C_{41}H_{79}NO_8P$    |

| Lipid Species                                  | Accurate<br><i>m/z</i> value | Adduct             | Empirical Formula                                                                    |
|------------------------------------------------|------------------------------|--------------------|--------------------------------------------------------------------------------------|
| PE 36:2                                        | 742.5392                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>77</sub> NO <sub>8</sub> P                                    |
| PE 36:3                                        | 740.5235                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>75</sub> NO <sub>8</sub> P                                    |
| PE 36:4                                        | 738.5079                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>73</sub> NO <sub>8</sub> P                                    |
| PE 36:5                                        | 736.4922                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>71</sub> NO <sub>8</sub> P                                    |
| PE 38:1                                        | 772.5861                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>83</sub> NO <sub>8</sub> P                                    |
| PE 38:2                                        | 770.5705                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>81</sub> NO <sub>8</sub> P                                    |
| PE 38:3                                        | 768.5548                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>79</sub> NO <sub>8</sub> P                                    |
| PE 38:4                                        | 766.5392                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>77</sub> NO <sub>8</sub> P                                    |
| PE 38:5                                        | 764.5235                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>75</sub> NO <sub>8</sub> P                                    |
| PE 38:6                                        | 762.5079                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>73</sub> NO <sub>8</sub> P                                    |
| PE 40:4                                        | 794.5705                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>81</sub> NO <sub>8</sub> P                                    |
| PE 40:5                                        | 792.5548                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>79</sub> NO <sub>8</sub> P                                    |
| PE 40:6                                        | 790.5392                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>77</sub> NO <sub>8</sub> P                                    |
| 1-Alkyl-2-acyl-phosphatidylethanolamine (PE-O) |                              |                    |  |
| PE O-34:2                                      | 700.5286                     | [M-H] <sup>-</sup> | C <sub>39</sub> H <sub>75</sub> NO <sub>7</sub> P                                    |
| PE O-34:3                                      | 698.5130                     | [M-H] <sup>-</sup> | C <sub>39</sub> H <sub>73</sub> NO <sub>7</sub> P                                    |
| PE O-36:2                                      | 728.5599                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>79</sub> NO <sub>7</sub> P                                    |
| PE O-36:3                                      | 726.5443                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>77</sub> NO <sub>7</sub> P                                    |
| PE O-36:4                                      | 724.5286                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>75</sub> NO <sub>7</sub> P                                    |
| PE O-36:5                                      | 722.5130                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>73</sub> NO <sub>7</sub> P                                    |
| PE O-36:6                                      | 720.4973                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>71</sub> NO <sub>7</sub> P                                    |
| PE O-38:2                                      | 756.5912                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>83</sub> NO <sub>7</sub> P                                    |
| PE O-38:4                                      | 752.5599                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>79</sub> NO <sub>7</sub> P                                    |
| PE O-38:5                                      | 750.5443                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>77</sub> NO <sub>7</sub> P                                    |
| PE O-38:6                                      | 748.5286                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>75</sub> NO <sub>7</sub> P                                    |
| PE O-40:4                                      | 780.5912                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>83</sub> NO <sub>7</sub> P                                    |
| PE O-40:5                                      | 778.5756                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>81</sub> NO <sub>7</sub> P                                    |
| PE O-40:6                                      | 776.5599                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>79</sub> NO <sub>7</sub> P                                    |
| PE O-40:7                                      | 774.5443                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>77</sub> NO <sub>7</sub> P                                    |
| 1-Acyl-2-acyl-phosphatidylglycerol (PG)        |                              |                    |  |
| PG 34:2                                        | 745.5025                     | [M-H] <sup>-</sup> | C <sub>40</sub> H <sub>74</sub> O <sub>10</sub> P                                    |
| PG 36:1                                        | 775.5494                     | [M-H] <sup>-</sup> | C <sub>42</sub> H <sub>80</sub> O <sub>10</sub> P                                    |
| PG 36:2                                        | 773.5338                     | [M-H] <sup>-</sup> | C <sub>42</sub> H <sub>78</sub> O <sub>10</sub> P                                    |
| PG 36:3                                        | 771.5181                     | [M-H] <sup>-</sup> | C <sub>42</sub> H <sub>76</sub> O <sub>10</sub> P                                    |

| Lipid Species                                                                                                                     | Accurate<br><i>m/z</i> value | Adduct             | Empirical Formula                                  |
|-----------------------------------------------------------------------------------------------------------------------------------|------------------------------|--------------------|----------------------------------------------------|
| PG 36:4                                                                                                                           | 769.5025                     | [M-H] <sup>-</sup> | C <sub>42</sub> H <sub>74</sub> O <sub>10</sub> P  |
| PG 38:4                                                                                                                           | 797.5338                     | [M-H] <sup>-</sup> | C <sub>44</sub> H <sub>78</sub> O <sub>10</sub> P  |
| PG 38:5                                                                                                                           | 795.5181                     | [M-H] <sup>-</sup> | C <sub>44</sub> H <sub>76</sub> O <sub>10</sub> P  |
| PG 38:6                                                                                                                           | 793.5025                     | [M-H] <sup>-</sup> | C <sub>44</sub> H <sub>74</sub> O <sub>10</sub> P  |
| PG 40:5                                                                                                                           | 823.5494                     | [M-H] <sup>-</sup> | C <sub>46</sub> H <sub>80</sub> O <sub>10</sub> P  |
| PG 40:6                                                                                                                           | 821.5338                     | [M-H] <sup>-</sup> | C <sub>46</sub> H <sub>78</sub> O <sub>10</sub> P  |
| PG 40:7                                                                                                                           | 819.5181                     | [M-H] <sup>-</sup> | C <sub>46</sub> H <sub>76</sub> O <sub>10</sub> P  |
| PG 40:8                                                                                                                           | 817.5025                     | [M-H] <sup>-</sup> | C <sub>46</sub> H <sub>74</sub> O <sub>10</sub> P  |
| PG 42:8                                                                                                                           | 845.5338                     | [M-H] <sup>-</sup> | C <sub>48</sub> H <sub>78</sub> O <sub>10</sub> P  |
| PG 42:10                                                                                                                          | 841.5025                     | [M-H] <sup>-</sup> | C <sub>48</sub> H <sub>74</sub> O <sub>10</sub> P  |
| <b>1-Acyl-2-acyl-phosphatidylinositol (PI)</b>  |                              |                    |                                                    |
| PI 32:1                                                                                                                           | 807.5029                     | [M-H] <sup>-</sup> | C <sub>41</sub> H <sub>76</sub> O <sub>13</sub> P  |
| PI 34:1                                                                                                                           | 835.5342                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>80</sub> O <sub>13</sub> P  |
| PI 34:2                                                                                                                           | 833.5185                     | [M-H] <sup>-</sup> | C <sub>43</sub> H <sub>78</sub> O <sub>13</sub> P  |
| PI 36:1                                                                                                                           | 863.5655                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>84</sub> O <sub>13</sub> P  |
| PI 36:2                                                                                                                           | 861.5498                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>82</sub> O <sub>13</sub> P  |
| PI 36:3                                                                                                                           | 859.5342                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>80</sub> O <sub>13</sub> P  |
| PI 36:4                                                                                                                           | 857.5185                     | [M-H] <sup>-</sup> | C <sub>45</sub> H <sub>78</sub> O <sub>13</sub> P  |
| PI 38:3                                                                                                                           | 887.5655                     | [M-H] <sup>-</sup> | C <sub>47</sub> H <sub>84</sub> O <sub>13</sub> P  |
| PI 38:4                                                                                                                           | 885.5498                     | [M-H] <sup>-</sup> | C <sub>47</sub> H <sub>82</sub> O <sub>13</sub> P  |
| PI 38:5                                                                                                                           | 883.5342                     | [M-H] <sup>-</sup> | C <sub>47</sub> H <sub>80</sub> O <sub>13</sub> P  |
| PI 40:5                                                                                                                           | 911.5655                     | [M-H] <sup>-</sup> | C <sub>49</sub> H <sub>84</sub> O <sub>13</sub> P  |
| PI 40:6                                                                                                                           | 909.5498                     | [M-H] <sup>-</sup> | C <sub>49</sub> H <sub>82</sub> O <sub>13</sub> P  |
| <b>1-Acyl-2-acyl-phosphatidylserine (PS)</b>  |                              |                    |                                                    |
| PS 32:0                                                                                                                           | 734.4977                     | [M-H] <sup>-</sup> | C <sub>38</sub> H <sub>73</sub> NO <sub>10</sub> P |
| PS 34:0                                                                                                                           | 762.5290                     | [M-H] <sup>-</sup> | C <sub>40</sub> H <sub>77</sub> NO <sub>10</sub> P |
| PS 34:1                                                                                                                           | 760.5134                     | [M-H] <sup>-</sup> | C <sub>40</sub> H <sub>75</sub> NO <sub>10</sub> P |
| PS 36:1                                                                                                                           | 788.5447                     | [M-H] <sup>-</sup> | C <sub>42</sub> H <sub>79</sub> NO <sub>10</sub> P |
| PS 36:2                                                                                                                           | 786.5290                     | [M-H] <sup>-</sup> | C <sub>42</sub> H <sub>77</sub> NO <sub>10</sub> P |
| PS 38:1                                                                                                                           | 816.5760                     | [M-H] <sup>-</sup> | C <sub>44</sub> H <sub>83</sub> NO <sub>10</sub> P |
| PS 38:3                                                                                                                           | 812.5447                     | [M-H] <sup>-</sup> | C <sub>44</sub> H <sub>79</sub> NO <sub>10</sub> P |
| PS 38:4                                                                                                                           | 810.5290                     | [M-H] <sup>-</sup> | C <sub>44</sub> H <sub>77</sub> NO <sub>10</sub> P |

| Lipid Species  | Accurate<br><i>m/z</i> value | Adduct             | Empirical Formula                                  |
|----------------|------------------------------|--------------------|----------------------------------------------------|
| <b>PS 40:1</b> | 844.6073                     | [M-H] <sup>−</sup> | C <sub>46</sub> H <sub>87</sub> NO <sub>10</sub> P |
| <b>PS 40:4</b> | 838.5603                     | [M-H] <sup>−</sup> | C <sub>46</sub> H <sub>81</sub> NO <sub>10</sub> P |
| <b>PS 40:5</b> | 836.5447                     | [M-H] <sup>−</sup> | C <sub>46</sub> H <sub>79</sub> NO <sub>10</sub> P |
| <b>PS 40:6</b> | 834.5290                     | [M-H] <sup>−</sup> | C <sub>46</sub> H <sub>77</sub> NO <sub>10</sub> P |
| <b>PS 42:1</b> | 872.6386                     | [M-H] <sup>−</sup> | C <sub>48</sub> H <sub>91</sub> NO <sub>10</sub> P |
| <b>PS 44:5</b> | 892.6073                     | [M-H] <sup>−</sup> | C <sub>50</sub> H <sub>88</sub> NO <sub>10</sub> P |