List of Lipids

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Annotation of potential isobaric and isomeric lipid species measured with the Absolute*IDQ*® p180 Kit (and p150 Kit)

Introduction

Lipidomics, a branch of metabolomics that aims at elucidating lipid pathways and networks in biological systems, has gained significant attention in the recent years and is considered an essential tool for investigation of many diseases. The Absolute*IDQ*® p180 Kit from Biocrates enables, among other metabolite classes, analysis of phosphatidylcholines (PC), lysophosphatidylcholines (LPC) and sphingomyelins (SM) that are among the most abundant lipid species in human blood samples. The kit has been successfully employed in numerous studies to obtain comprehensive insight into pathways and metabolic signatures of diseases (see selected examples [1-5]).

In order to support on-going efforts of harmonization and standardization of lipid nomenclature and provide a link between the different lipid annotations we have prepared a list with the potential isobars/isomers for all lipid signals measured with Absolute*IDQ*® p180 Kit. Moreover, the presented information can be used to facilitate biological interpretation of the results obtained with the Absolute*IDQ*® p180 Kit.

Lipid analysis and annotation in Absolute*IDQ*® p180 Kit

The lipid measurements in Absolute*IDQ*® p180 Kit are carried out employing flow injection analysis tandem mass spectrometry (FIA-MS/MS), quantified by internal standard. For the FIA-MS/MS analysis, mass spectrometry precursor/product transitions ("MRMs") employs lipid species molecular ions and lipid class specific fragment ions. The employed FIA-MS/MS measurements, therefore, cannot differentiate the fatty acids linked to the glycerol backbone or define their bond type (acyl- or alkyl-). As a consequence the detected MRM signal is a sum of several isobaric/isomeric lipids (Figure 1). For example, according to LIPID MAPS data base (www.lipidmaps.org [6]), the signal of PC aa C36:6 can arise from at least 15 different lipid species that have different fatty acid composition (e.g. PC 16:1/20:5 versus PC 18:4/18:2), various positioning of fatty acids sn-1/sn-2 (e.g. PC 18:4/18:2 versus PC 18:2/18:4) and different double bond positions and stereochemistry in those fatty acid chains (e.g. PC(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z)) versus PC (18:4(9E,11E,13E,15E)/18:2(9Z,12Z))).

The current annotation of the lipids signals in the Absolute*IDQ*® p180 Kit denote representative compounds under individual signals measured. The annotation of measured lipid signal in Absolute*IDQ*® p180 Kit is based on the assumptions that (1) only even number carbon acyl- or alkyl- chains are present and (2) that both ester and ether bonds are present.

- Annotation for phosphatidylcholines

    - "aa" indicates that both moieties at the sn-1 and sn-2 position are fatty acids and bound to the glycerol backbone via ester bonds

    - "ae" denotes that one of the moieties, either in the sn-1 or at sn-2 position is a fatty alcohol and bound via an ether bond.

    - Total number of carbon atoms and double bonds present in both lipid fatty acid chains are denoted as "C x:y", where x is the total carbon number of both chains and y is the total number of double bonds.

- Annotation for sphingomyelins

    - Total number of carbon atoms, the number of double bonds or the presence of hydroxyl group (OH) are indicated only for the fatty acid in the amide bond under assumption that the backbone is formed by sphingosine (d18:1).

    - Total number of carbon atoms and double bonds present in fatty acid chain is denoted as "C x:y", where x is the carbon number and y is the number for double bonds

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Isobars - molecules with the same nominal mass (sum of the masses of the most abundant isotopes) but differing exact masses.

Lipid species	Molecular formula	Nominal mass	Exact mass
PC 34:4	C42H76NO8P	753	753.5309
PC O-35:4	C43H80NO7P	753	753.5670

Isomers - molecules with the same molecular formula but with different chemical structure.
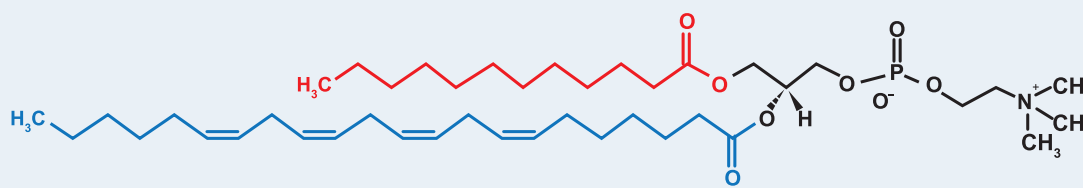
PC(12:0/22:4(7Z,10Z,13Z,16Z))
LIPID MAPS ID: LMGP01011337
Molecular formula: C42H76NO8P
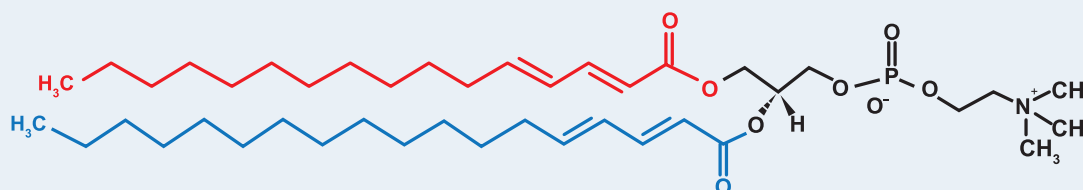
PC(16:2(2E,4E)/18:2(2E,4E))
LIPID MAPS ID: LMGP01010699
Molecular formula: C42H76NO8P

Figure 1. Explanation of isobaric and isomeric molecules

Commonly used lipid annotation

Nowadays most commonly accepted terminology for lipid annotation was defined by LIPID MAPS consortium [7]. The lipid nomenclature used by LIPID MAPS covers full structural information of lipid molecule including fatty acyl/alkyl bond type, specific backbone positions of fatty acids/alcohols and position and stereochemistry of double bonds within the fatty acids/alcohols.

However, the commonly employed MS analysis (including triple quadrupole and high resolution MS) does not automatically provide such structural details without additional analytical steps (e.g. chemical derivatization, complex separation techniques), which are not suitable for high-throughput analysis. In 2013, Liebisch et al. [8] proposed a lipid notation that aimed to add defined levels of information below the LIPID MAPS nomenclature corresponding to the amount of structural information achievable with commonly employed MS analysis, including the Absolute*IDQ*® p180 Kit. This notation reflects the defined levels of lipid structural information identified by a MS analysis. The measurement confidence as well as complexity of employed techniques increases with each level, hence the number of possible lipid molecules contributing to measured signal reduces (Figure 2).

List of Lipids

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Lipid species	Bond type	Fatty acyl/ alkyl composition	Fatty acyl/ alkyl & double bond position
Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C34:3	PC 34:3	PC 14:0_20:3	LMGP01011374; LMGP01011868; LMGP01012127; LMGP01012192
		PC 14:1_20:2	LMGP01011399; LMGP01011838
		PC 16:0_18:3	LMGP01010598; LMGP01010601; LMGP01011646; LMGP01011677
		PC 16:1_18:2	LMGP01010690; LMGP01011620
		PC 17:1_17:2	LMGP01011530; LMGP01011560
	PC O-35:3	PC O-18:1_17:2	LMGP01030056

Figure 2. Example of different confidence levels of lipid measurements

List of Isobaric and isomeric lipid species measured with Absolute*IDQ*® p180 Kit

All potential isobaric and isomeric lipid species (based on LIPID MAPS data base) of particular lipid signals measured with Absolute*IDQ*® p180 Kit are summarized in the annotation list. The list comprises examples of potential isobars and isomers to the best of our current knowledge.

- Potential isobars are given within ±0.5 Da range due to the typical conditions under which triple quadrupole mass spectrometers are operated for the Kit and isobars are reported as sum compositions

- The position of acyl chains (sn-1, sn-2) and double bonds are not indicated for the potential isomers in case of PC and lysoPC

- For each isomer, examples of LIPID MAPS Structure Database (http://www.lipidmaps.org/data/databases.html [6]) entries are listed

- For several lipids the prefix "[13C]" indicates the possible isotope interference from another lipid species having a molecular weight with one mass unit smaller. These interferences have not been removed by the applied isotope correction algorithm due to the limitation of current MS/MS hardware in the maximal number of MRM transitions that can be monitored in parallel.

References

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List of potential isobaric and isomeric lipid species measured with the Absolute*IDQ*® p180 Kit (and p150 Kit)

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C24:0	PC 24:0	PC 12:0_12:0	LMGP01010429
		PC 6:0_18:0	LMGP01011228
PC aa C26:0	PC 26:0	PC 10:0_16:0	LMGP01010388
		PC 12:0_14:0	LMGP01010432; LMGP01010475
		PC 13:0_13:0	LMGP01010456
		PC 17:0_9:0	LMGP01010725
		PC 8:0_18:0	LMGP01011243
	[¹³C] SM 30:0		
PC aa C28:1	PC 28:1	PC 10:0_18:1	LMGP01010392
		PC 12:0_16:1	LMGP01011319; LMGP01011473
		PC 13:0_15:1	LMGP01011341; LMGP01011432
		PC 14:0_14:1	LMGP01011364; LMGP01011381
	PC O-29:1	PC O-16:1_13:0	LMGP01030020
	[¹³C] SM 32:1		
PC aa C30:0	PC 30:0	PC 10:0_20:0	LMGP01010395; LMGP01010995
		PC 11:0_19:0	LMGP01010416; LMGP01010969
		PC 12:0_18:0	LMGP01010438; LMGP01010736
		PC 13:0_17:0	LMGP01010461; LMGP01010702
		PC 14:0_16:0	LMGP01010481; LMGP01010560
		PC 15:0_15:0	LMGP01010530
		PC 9:0_21:0	LMGP01011265
	PC O-31:0	PC O-16:0_15:0	LMGP01020180
		PC O-18:0_13:0	LMGP01020194
	[¹³C] SM 34:0		
PC aa C30:2	PC 30:2	PC 12:0_18:2	LMGP01011323; LMGP01011614
		PC 13:0_17:2	LMGP01011345; LMGP01011552
		PC 14:1_16:1	LMGP01011385; LMGP01011476
		PC 15:1_15:1	LMGP01011436
	PC O-31:2	PC O-16:1_15:1	LMGP01030024

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Absolute*DQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C32:0	PC 32:0	PC 10:0_22:0	LMGP01010397; LMGP01011080
		PC 11:0_21:0	LMGP01010418; LMGP01011062
		PC 12:0_20:0	LMGP01010444; LMGP01010997
		PC 13:0_19:0	LMGP01010463; LMGP01010970
		PC 14:0_18:0	LMGP01010488; LMGP01010739
		PC 15:0_17:0	LMGP01010537; LMGP01010704
		PC 16:0_16:0	LMGP01010564
		PC 9:0_23:0	LMGP01011267
	PC O-33:0	PC O-16:0_17:0	LMGP01020031
		PC O-18:0_15:0	LMGP01020197
		PC O-20:0_13:0	LMGP01020217
	[¹³C] SM 36:0		
PC aa C32:1	PC 32:1	PC 14:0_18:1	LMGP01010490; LMGP01010492; LMGP01010882; LMGP01012145
		PC 16:0_16:1	LMGP01010566; LMGP01011479
		PC 12:0_20:1	LMGP01011329; LMGP01011805
		PC 13:0_19:1	LMGP01011352; LMGP01011757
		PC 14:1_18:0	LMGP01011389; LMGP01011582
		PC 15:0_17:1	LMGP01011413; LMGP01011525
		PC 15:1_17:0	LMGP01011439; LMGP01011500
	PC O-33:1	PC O-16:0_17:1	LMGP01020183
		PC O-18:0_15:1	LMGP01020198
		PC O-16:1_17:0	LMGP01030027
		PC O-18:1_15:0	LMGP01030050
		PC O-20:1_13:0	LMGP01030075
PC aa C32:2	PC 32:2	PC 12:0_20:2	LMGP01011330; LMGP01011835
		PC 14:0_18:2	LMGP01010494; LMGP01010496 LMGP01011616
		PC 14:1_18:1	LMGP01011390; LMGP01011597
		PC 15:0_17:2	LMGP01011414; LMGP01011555
		PC 16:1_16:1	LMGP01010682; LMGP01010684
		PC 15:1_17:1	LMGP01011440; LMGP01011526
	PC O-33:2	PC O-16:0_17:2	LMGP01020184
		PC O-16:1_17:1	LMGP01030028
		PC O-18:1_15:1	LMGP01030051
PC aa C32:3	PC 32:3	PC 14:0_18:3	LMGP01010497; LMGP01011369; LMGP01011642; LMGP01011673
		PC 12:0_20:3	LMGP01011331; LMGP01011866
		PC 14:1_18:2	LMGP01011391; LMGP01011617
		PC 15:1_17:2	LMGP01011441; LMGP01011556
	PC O-33:3	PC O-16:1_17:2	LMGP01030029
	[¹³C] SM 36:3		

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Absolute*DQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C34:1	PC 34:1	PC 12:0_22:1	LMGP01011335; LMGP01012004
		PC 14:0_20:1	LMGP01011372; LMGP01011807
		PC 14:1_20:0	LMGP01011397; LMGP01011787
		PC 15:0_19:1	LMGP01011419; LMGP01011760
		PC 15:1_19:0	LMGP01011448; LMGP01011732
		PC 16:0_18:1	LMGP01010005; LMGP01010575; LMGP01010576; LMGP01010578; LMGP01010581; LMGP01010884; LMGP01012146
		PC 17:0_17:1	LMGP01011503; LMGP01011529
		PC 18:0_16:1	LMGP01010744; LMGP01011483
	PC O-35:1	PC O-17:0_18:1	LMGP01020077
		PC O-16:0_19:1	LMGP01020186
		PC O-18:0_17:1	LMGP01020200
		PC O-20:0_15:1	LMGP01020221
		PC O-16:1_19:0	LMGP01030034
		PC O-18:1_17:0	LMGP01030054
		PC O-20:1_15:0	LMGP01030078
	[^{13}C] SM 38:1		
PC aa C34:2	PC 34:2	PC 12:0_22:2	LMGP01011336; LMGP01012035
		PC 14:0_20:2	LMGP01011373; LMGP01011837
		PC 14:1_20:1	LMGP01011398; LMGP01011808
		PC 15:1_19:1	LMGP01011449; LMGP01011761
		PC 16:0_18:2	LMGP01010585; LMGP01010586; LMGP01010587; LMGP01010588; LMGP01010590; LMGP01010591; LMGP01010592; LMGP01010594; LMGP01010920; LMGP01010926; LMGP01010932
		PC 16:1_18:1	LMGP01010678; LMGP01010687; LMGP01010688; LMGP01010887
		PC 17:0_17:2	LMGP01011504; LMGP01011559
		PC 17:1_17:1	LMGP01010727; LMGP01010728
		PC 18:0_16:2	LMGP01010745
	PC O- 35:2	PC O-18:0_17:2	LMGP01020201
		PC O-16:1_19:1	LMGP01030035
		PC O-18:1_17:1	LMGP01030055
		PC O-20:1_15:1	LMGP01030079
	[^{13}C] SM 38:2		

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C34:3	PC 34:3	PC 14:0_20:3	LMGP01011374; LMGP01011868; LMGP01012127; LMGP01012192
		PC 14:1_20:2	LMGP01011399; LMGP01011838
		PC 16:0_18:3	LMGP01010598; LMGP01010601; LMGP01011646; LMGP01011677
		PC 16:1_18:2	LMGP01010690; LMGP01011620
		PC 17:1_17:2	LMGP01011530; LMGP01011560
	PC O-35:3	PC O-18:1_17:2	LMGP01030056
PC aa C34:4	PC 34:4	PC 12:0_22:4	LMGP01011337; LMGP01012066
		PC 14:0_20:4	LMGP01010506; LMGP01011899; LMGP01012128; LMGP01012209
		PC 14:1_20:3	LMGP01011400; LMGP01011869; LMGP01012132; LMGP01012193
		PC 16:0_18:4	LMGP01010603; LMGP01010604; LMGP01010606; LMGP01010608; LMGP01011706
		PC 16:1_18:3	LMGP01011484; LMGP01011485; LMGP01011647; LMGP01011678
		PC 16:2_18:2	LMGP01010699
		PC 17:2_17:2	LMGP01010731
	PC O-35:4	PC O-15:0_20:4	LMGP01020026
PC aa C36:0	PC 36:0	PC 11:0_25:0	LMGP01010422
		PC 12:0_24:0	LMGP01010449
		PC 13:0_23:0	LMGP01010468
		PC 14:0_22:0	LMGP01010511; LMGP01011085
		PC 15:0_21:0	LMGP01010549; LMGP01011956
		PC 16:0_20:0	LMGP01010616; LMGP01011002
		PC 17:0_19:0	LMGP01011509; LMGP01011735
		PC 18:0_18:0	LMGP01010006
	PC 37:7	PC 15:1_22:6	LMGP01011461; LMGP01012102
		PC 17:2_20:5	LMGP01011574; LMGP01011936
	PC O-37:0	PC O-17:0_20:0	LMGP01020080; LMGP01020223
		PC O-16:0_21:0	LMGP01020189
		PC O-18:0_19:0	LMGP01020207
	PC O-38:7	PC O-16:1_22:6	LMGP01030015
		PC O-18:2_20:5	LMGP01090051; LMGP01090052
	[¹³C] SM 40:0		

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Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C36:1	PC 36:1	PC 14:0_22:1	LMGP01011376; LMGP01012006 LMGP01012129; LMGP01012218
		PC 14:1_22:0	LMGP01011404; LMGP01011980
		PC 15:1_21:0	LMGP01011456; LMGP01011957
		PC 16:0_20:1	LMGP01011468; LMGP01011811
		PC 16:1_20:0	LMGP01011488; LMGP01011790
		PC 17:0_19:1	LMGP01011510; LMGP01011764
		PC 17:1_19:0	LMGP01011537; LMGP01011736
		PC 18:0_18:1	LMGP01010750; LMGP01010751; LMGP01010753; LMGP01010754; LMGP01010758; LMGP01010759; LMGP01010761; LMGP01010840; LMGP01010888
	PC O-37:1	PC O-18:0_19:1	LMGP01020208
		PC O-20:0_17:1	LMGP01020224
		PC O-16:1_21:0	LMGP01030041
		PC O-18:1_19:0	LMGP01030062
		PC O-20:1_17:0	LMGP01030082
	[^{13}C] SM 40:1		
PC aa C36:2	PC 36:2	PC 14:0_22:2	LMGP01011377; LMGP01012037
		PC 14:1_22:1	LMGP01011405; LMGP01012007; LMGP01012219
		PC 16:0_20:2	LMGP01011469; LMGP01011841
		PC 16:1_20:1	LMGP01011489; LMGP01011812
		PC 17:1_19:1	LMGP01011538; LMGP01011765
		PC 17:2_19:0	LMGP01011567; LMGP01011737
		PC 18:0_18:2	LMGP01010764; LMGP01010765; LMGP01010766; LMGP01010768
		PC 18:1_18:1	LMGP01010836; LMGP01010837; LMGP01010841; LMGP01010849; LMGP01010853; LMGP01010855; LMGP01010857; LMGP01010858; LMGP01010860; LMGP01010862; LMGP01010865; LMGP01010866; LMGP01010868; LMGP01010871; LMGP01010873; LMGP01010876; LMGP01010890
	PC O-37:2	PC O-20:0_17:2	LMGP01020225
		PC O-18:1_19:1	LMGP01030063
		PC O-20:1_17:1	LMGP01030083
	[^{13}C] SM 40:2		

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Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C36:3	PC 36:3	PC 14:1_22:2	LMGP01011406; LMGP01012038
		PC 16:0_20:3	LMGP01010622; LMGP01010624; LMGP01010627; LMGP01011872
		PC 16:1_20:2	LMGP01011490; LMGP01011842
		PC 17:2_19:1	LMGP01011568; LMGP01011766
		PC 18:0_18:3	LMGP01011588; LMGP01011589; LMGP01011651; LMGP01011682
		PC 18:1_18:2	LMGP01010893; LMGP01010895; LMGP01011624; LMGP01012149
	PC O-37:3	PC O-20:1_17:2	LMGP01030084
	[^{13}C] SM 40:3		
PC aa C36:4	PC 36:4	PC 14:0_22:4	LMGP01011378; LMGP01012068
		PC 16:0_20:4	LMGP01010007; LMGP01010629 LMGP01011049; LMGP01011056
		PC 16:1_20:3	LMGP01011491; LMGP01011873; LMGP01012138; LMGP01012195
		PC 18:0_18:4	LMGP01010773; LMGP01010774; LMGP01011711
		PC 18:1_18:3	LMGP01010898; LMGP01011603; LMGP01011652; LMGP01012150; LMGP01012174; LMGP01012178
		PC 18:2_18:2	LMGP01010921; LMGP01010924; LMGP01010927; LMGP01010930
	PC O-37:4	PC O-17:0_20:4	LMGP01020081
PC aa C36:5	PC 36:5	PC 14:0_22:5	LMGP01012130; LMGP01012131; LMGP01012232; LMGP01012234
		PC 14:1_22:4	LMGP01011407; LMGP01012069
		PC 16:0_20:5	LMGP01010633; LMGP01011932
		PC 16:1_20:4	LMGP01010695; LMGP01011305; LMGP01011903; LMGP01012139
		PC 18:1_18:4	LMGP01011604; LMGP01011712; LMGP01012152; LMGP01012182
		PC 18:2_18:3	LMGP01011625; LMGP01011626; LMGP01011653; LMGP01011683
PC aa C36:6	PC 36:6	PC 14:0_22:6	LMGP01010512; LMGP01012099
		PC 14:1_22:5	LMGP01012134; LMGP01012135; LMGP01012233; LMGP01012235
		PC 16:1_20:5	LMGP01011492; LMGP01011933
		PC 18:3_18:3	LMGP01010956; LMGP01010954; LMGP01011654; LMGP01011684
		PC 18:4_18:2	LMGP01010960; LMGP01011627; LMGP01011713

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C38:0	PC 38:0	PC 12:0_26:0	LMGP01010452
		PC 13:0_25:0	LMGP01010470
		PC 14:0_24:0	LMGP01010515
		PC 16:0_22:0	LMGP01010636; LMGP01011983
		PC 17:0_21:0	LMGP01011516; LMGP01011960
		PC 17:1_22:6	LMGP01011550; LMGP01012105
		PC 18:0_20:0	LMGP01010781; LMGP01011004
		PC 19:0_19:0	LMGP01010976
	PC O-39:0	PC O-17:0_22:0	LMGP01020083
		PC O-18:0_21:0	LMGP01020212
		PC O-20:0_19:0	LMGP01020232
	PC O-40:7	PC O-18:1_22:6	LMGP01030014
	[¹³C] SM 42:0		
PC aa C38:1	PC 38:1	PC 14:0_24:1	LMGP01010516
		PC 16:0_22:1	LMGP01010638; LMGP01011471; LMGP01012010
		PC 16:1_22:0	LMGP01011494; LMGP01011984
		PC 17:1_21:0	LMGP01011545; LMGP01011961
		PC 18:0_20:1	LMGP01010783; LMGP01010784; LMGP01010785; LMGP01010786; LMGP01011816
		PC 18:1_20:0	LMGP01010879; LMGP01010902; LMGP01011008; LMGP01011009
		PC 19:0_19:1	LMGP01011743; LMGP01011773
	PC 39:8	PC 17:2_22:6	LMGP01011580; LMGP01012106
	PC O-39:1	PC O-20:0_19:1	LMGP01020233
		PC O-18:1_21:0	LMGP01030069
		PC O-20:1_19:0	LMGP01030091
PC aa C38:3	PC 38:3	PC 16:1_22:2	LMGP01011496; LMGP01012042
		PC 18:0_20:3	LMGP01010795; LMGP01010796; LMGP01010798; LMGP01011877; LMGP01012196
		PC 18:1_20:2	LMGP01011608; LMGP01011847; LMGP01012153; LMGP01012190
		PC 18:2_20:1	LMGP01010942; LMGP01011631; LMGP01011818
		PC 18:3_20:0	LMGP01011659; LMGP01011688; LMGP01011794; LMGP01011795
	[¹³C] SM 42:3		

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C38:4	PC 38:4	PC 16:0_22:4	LMGP01010642; LMGP01012072
		PC 18:0_20:4	LMGP01010802; LMGP01010804; LMGP01012144; LMGP01011907
		PC 18:1_20:3	LMGP01010904; LMGP01011609; LMGP01011878; LMGP01012154; LMGP01012155; LMGP01012197; LMGP01012198; LMGP01012206
		PC 18:2_20:2	LMGP01011632; LMGP01011848
		PC 18:3_20:1	LMGP01011660; LMGP01011689; LMGP01011819; LMGP01011820
		PC 18:4_20:0	LMGP01011719; LMGP01011796
PC aa C38:5	PC 38:5	PC 16:0_22:5	LMGP01010645; LMGP01010647
		PC 16:1_22:4	LMGP01011497; LMGP01012073
		PC 18:0_20:5	LMGP01010805; LMGP01010807; LMGP01011937
		PC 18:1_20:4	LMGP01010905; LMGP01011908; LMGP01012156; LMGP01012157; LMGP01012165; LMGP01012208; LMGP01012211
		PC 18:2_20:3	LMGP01011633; LMGP01011879; LMGP01012170; LMGP01012199
		PC 18:3_20:2	LMGP01011661; LMGP01011690; LMGP01011849; LMGP01011850
		PC 18:4_20:1	LMGP01011720; LMGP01011821
PC aa C38:6	PC 38:6	PC 16:0_22:6	LMGP01010650; LMGP01010652; LMGP01011115; LMGP01011116; LMGP01012137
		PC 16:1_22:5	LMGP01012140; LMGP01012141
		PC 18:1_20:5	LMGP01010844; LMGP01010907; LMGP01011057; LMGP01012216
		PC 18:2_20:4	LMGP01010943; LMGP01011909; LMGP01012171; LMGP01012212
		PC 18:3_20:3	LMGP01011662; LMGP01011691; LMGP01011880; LMGP01011881; LMGP01012175; LMGP01012179; LMGP01012200; LMGP01012201
		PC 18:4_20:2	LMGP01011721; LMGP01011851

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Absolute*DQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C40:1	PC 40:1	PC 16:0_24:1	LMGP01010659
		PC 18:0_22:1	LMGP01010811; LMGP01011593; LMGP01012015
		PC 18:1_22:0	LMGP01010839; LMGP01010845; LMGP01010909; LMGP01011089; LMGP01011090; LMGP01011091; LMGP01011092; LMGP01011093; LMGP01011094
		PC 19:1_21:0	LMGP01011781; LMGP01011969
		PC 20:0_20:1	LMGP01011017: LMGP01011018; LMGP01011019; LMGP01011020; LMGP01011824
	PC O-41:1	PC O-20:1_21:0	LMGP01030099
PC aa C40:2	PC 40:2	PC 16:1_24:1	LMGP01012142: LMGP01012239
		PC 18:0_22:2	LMGP01011594; LMGP01012046
		PC 18:1_22:1	LMGP01011611; LMGP01012016; LMGP01012158; LMGP01012166; LMGP01012220; LMGP01012221
		PC 18:2_22:0	LMGP01011636; LMGP01011988
		PC 20:0_20:2	LMGP01011021; LMGP01011854
		PC 20:1_20:1	LMGP01011036; LMGP01011038; LMGP01011042; LMGP01011043
PC aa C40:3	PC 40:3	PC 18:0_22:3	LMGP01010812
		PC 20:0_20:3	LMGP01011022; LMGP01011799; LMGP01011885; LMGP01012185; LMGP01012202
		PC 18:1_22:2	LMGP01011612; LMGP01012047; LMGP01012159; LMGP01012230
		PC 18:2_22:1	LMGP01011637; LMGP01012017; LMGP01012172; LMGP01012222
		PC 18:3_22:0	LMGP01011666; LMGP01011695; LMGP01011989; LMGP01011990
		PC 20:1_20:2	LMGP01011825; LMGP01011855
PC aa C40:4	PC 40:4	PC 18:0_22:4	LMGP01010813; LMGP01012077
		PC 18:2_22:2	LMGP01011638; LMGP01012048
		PC 18:3_22:1	LMGP01011667; LMGP01011696; LMGP01012018; LMGP01012019; LMGP01012180; LMGP01012223; LMGP01012224
		PC 18:4_22:0	LMGP01011726; LMGP01011991
		PC 20:0_20:4	LMGP01011023; LMGP01011915; LMGP01012186; LMGP01012213
		PC 20:1_20:3	LMGP01011826; LMGP01011886; LMGP01012187; LMGP01012203
		PC 20:2_20:2	LMGP01011045; LMGP01011856

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C40:5	PC 40:5	PC 18:0_22:5	LMGP01010816; LMGP01010818
		PC 18:1_22:4	LMGP01011613; LMGP01012078; LMGP01012160; LMGP01012231
		PC 18:3_22:2	LMGP01011668; LMGP01011697; LMGP01012049; LMGP01012050
		PC 18:4_22:1	LMGP01011727; LMGP01012020; LMGP01012183; LMGP01012225
		PC 20:0_20:5	LMGP01011800
		PC 20:1_20:4	LMGP01011827; LMGP01012188; LMGP01012214
		PC 20:2_20:3	LMGP01011857; LMGP01012191; LMGP01012204
PC aa C40:6	PC 40:6	PC 18:0_22:6	LMGP01010821; LMGP01010823; LMGP01012107
		PC 18:1_22:5	LMGP01010846
		PC 18:2_22:4	LMGP01011639; LMGP01012079
		PC 18:4_22:2	LMGP01011728; LMGP01012051
		PC 20:1_20:5	LMGP01011828; LMGP01011945
		PC 20:2_20:4	LMGP01011858; LMGP01011917
		PC 20:3_20:3	LMGP01011888
PC aa C42:0	PC 42:0	PC 16:0_26:0	LMGP01010663
		PC 18:0_24:0	LMGP01010825; LMGP01011150
		PC 20:0_22:0	LMGP01011025; LMGP01011994
		PC 21:0_21:0	LMGP01011072
PC aa C42:1	PC 42:1	PC 18:0_24:1	LMGP01010826; LMGP01012240
		PC 18:1_24:0	LMGP01010915; LMGP01012236; LMGP01011151; LMGP01011152
		PC 20:0_22:1	LMGP01011026; LMGP01012023; LMGP01012226
		PC 20:1_22:0	LMGP01011830; LMGP01011040; LMGP01011041; LMGP01011097
PC aa C42:2	PC 42:2	PC 16:0_26:2	LMGP01010665; LMGP01011203
		PC 18:1_24:1	LMGP01012162; LMGP01012167; LMGP01012241; LMGP01012242
		PC 18:2_24:0	LMGP01012173; LMGP01012237
		PC 20:0_22:2	LMGP01011803; LMGP01012054
		PC 20:1_22:1	LMGP01011831; LMGP01012189 LMGP01012024; LMGP01012227
		PC 20:2_22:0	LMGP01011861; LMGP01011995

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC aa C42:4	PC 42:4	PC 18:3_24:1	LMGP01012177; LMGP01012181; LMGP01012243; LMGP01012244
		PC 18:4_24:0	LMGP01012184; LMGP01012238
		PC 20:0_22:4	LMGP01011804; LMGP01012085
		PC 20:2_22:2	LMGP01011863; LMGP01012056
		PC 20:3_22:1	LMGP01011893; LMGP01012205; LMGP01012207; LMGP01012026; LMGP01012228; LMGP01012229
		PC 20:4_22:0	LMGP01011921; LMGP01012215; LMGP01011997; LMGP01012217
PC aa C42:5	PC 42:5	PC 20:0_22:5	LMGP01011027
		PC 20:1_22:4	LMGP01011833; LMGP01012086
		PC 20:3_22:2	LMGP01011894; LMGP01012057
		PC 20:4_22:1	LMGP01011922; LMGP01012027
		PC 20:5_22:0	LMGP01011951; LMGP01011998
PC aa C42:6	PC 42:6	PC 20:0_22:6	LMGP01011028; LMGP01012115
		PC 20:2_22:4	LMGP01011864; LMGP01012087
		PC 20:4_22:2	LMGP01011923; LMGP01012058
		PC 20:5_22:1	LMGP01011952; LMGP01012028
PC ae C30:0	PC O-30:0	PC O-14:0_16:0	LMGP01020012; LMGP01020178
		PC O-18:0_12:0	LMGP01020193
	PC 29:0	PC 10:0_19:0	LMGP01010394; LMGP01010968
		PC 12:0_17:0	LMGP01011320; LMGP01011498
		PC 13:0_16:0	LMGP01011342; LMGP01011462
		PC 14:0_15:0	LMGP01010479; LMGP01011410
		PC 20:0_9:0	LMGP01011035; LMGP01011264
		PC 8:0_21:0	LMGP01011246
	[¹³C] SM 33:0		
PC ae C30:1	PC O-30:1	PC O-14:0_16:1	LMGP01020014; LMGP01030021
		PC O-16:0_14:1	LMGP01020179
		PC O-18:1_12:0	LMGP01030046
	PC 29:1	PC 12:0_17:1	LMGP01011321; LMGP01011521
		PC 13:0_16:1	LMGP01011343; LMGP01011474
		PC 14:0_15:1	LMGP01011365; LMGP01011433
		PC 14:1_15:0	LMGP01011382; LMGP01011411
		PC 18:0_11:1	LMGP01010735
PC ae C30:2	PC O-30:2	PC O-16:1_14:1	LMGP01030022
	PC 29:2	PC 12:0_17:2	LMGP01011322; LMGP01011551
		PC 14:1_15:1	LMGP01011383; LMGP01011434
	[¹³C] SM 33:2		

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Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C32:1	PC O-32:1	PC O-14:0_18:1	LMGP01020016; LMGP01030048; LMGP01090001
		PC O-16:0_16:1	LMGP01020182; LMGP01030025
		PC O-18:0_14:1	LMGP01020196
		PC O-20:1_12:0	LMGP01030074
	PC 31:1	PC 12:0_19:1	LMGP01011328; LMGP01011756
		PC 13:0_18:1	LMGP01011347; LMGP01011596
		PC 14:0_17:1	LMGP01011367; LMGP01011523
		PC 15:0_16:1	LMGP01010535; LMGP01011477
		PC 16:0_15:1	LMGP01010002; LMGP01011437; LMGP01011464
		PC 17:0_14:1	LMGP01010008
PC ae C32:2	PC O-32:2	PC O-14:0_18:2	LMGP01020017; LMGP01090002; LMGP01090003, LMGP01030133
		PC O-14:1_18:1	LMGP01030004; LMGP01090004; LMGP01030049
		PC O-16:1_16:1	LMGP01030026; LMGP01090020
	PC 31:2	PC 13:0_18:2	LMGP01011348; LMGP01011615
		PC 14:0_17:2	LMGP01011368; LMGP01011553
		PC 14:1_17:1	LMGP01011387; LMGP01011524
		PC 15:1_16:1	LMGP01011438; LMGP01011478
PC ae C34:0	PC O-34:0	PC O-16:0_18:0	LMGP01020033; LMGP01020086; LMGP01080024
		PC O-17:0_17:0	LMGP01020076
		PC O-20:0_14:0	LMGP01020218
	PC 33:0	PC 10:0_23:0	LMGP01010399
		PC 11:0_22:0	LMGP01010419
		PC 13:0_20:0	LMGP01010465
		PC 15:0_18:0	LMGP01010539; LMGP01011583
		PC 16:0_17:0	LMGP01010569; LMGP01011501
		PC 19:0_14:0	LMGP01010971
		PC 21:0_12:0	LMGP01011063

Absolute*DQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C34:1	PC O-34:1	PC O-16:0_18:1	LMGP01020003; LMGP01020261; LMGP01020152; LMGP01030052
		PC O-18:0_16:1	LMGP01020089; LMGP01020256; LMGP01030030
		PC O-20:0_14:1	LMGP01020219
		PC O-20:1_14:0	LMGP01030076
	PC 33:1	PC 13:0_20:1	LMGP01011353; LMGP01011806
		PC 14:0_19:1	LMGP01011371; LMGP01011758
		PC 14:1_19:0	LMGP01011395; LMGP01011731
		PC 15:0_18:1	LMGP01010541; LMGP01011415; LMGP01011598
		PC 15:1_18:0	LMGP01011442; LMGP01011584
		PC 16:0_17:1	LMGP01010571; LMGP01011527
		PC 16:1_17:0	LMGP01011480; LMGP01011502
	[¹³C] SM 37:1		
PC ae C34:2	PC O-34:2	PC O-16:0_18:2	LMGP01020039; LMGP01030134; LMGP01090006; LMGP01090007
		PC O-16:1_18:1	LMGP01030006; LMGP01030053; LMGP01090009
		PC O-20:1_14:1	LMGP01030077
	PC 33:2	PC 13:0_20:2	LMGP01011354
		PC 14:1_19:1	LMGP01011396
		PC 15:0_18:2	LMGP01010543
		PC 15:1_18:1	LMGP01011443
		PC 16:0_17:2	LMGP01011465; LMGP01011557
		PC 16:1_17:1	LMGP01011481; LMGP01011528
PC ae C34:3	PC O-34:3	PC O-16:0_18:3	LMGP01020041; LMGP01020042
		PC O-16:1_18:2	LMGP01020257; LMGP01030008; LMGP01090010; LMGP01030135; LMGP01090011; LMGP01030145
	PC 33:3	PC 13:0_20:3	LMGP01011355; LMGP01011867
		PC 15:0_18:3	LMGP01011416; LMGP01011417; LMGP01011644; LMGP01011675
		PC 15:1_18:2	LMGP01011444; LMGP01011619
		PC 16:1_17:2	LMGP01011482; LMGP01011558

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C36:0	PC O-36:0	PC O-14:0_22:0	LMGP01020023
		PC O-16:0_20:0	LMGP01020051; LMGP01020122
		PC O-18:0_18:0	LMGP01020091
	PC 35:0	PC 10:0_25:0	LMGP01010401
		PC 11:0_24:0	LMGP01010421
		PC 12:0_23:0	LMGP01010448
		PC 15:0_20:0	LMGP01011420; LMGP01011788
		PC 16:0_19:0	LMGP01011466; LMGP01011733
		PC 17:0_18:0	LMGP01010709; LMGP01011585
		PC 21:0_14:0	LMGP01011065; LMGP01011375
		PC 22:0_13:0	LMGP01011084; LMGP01011358
	PC 36:7	PC 14:1_22:6	LMGP01011408; LMGP01012100
		PC 18:3_18:4	LMGP01011656; LMGP01011685; LMGP01011714; LMGP01011715
PC ae C36:1	PC O-36:1	PC O-16:0_20:1	LMGP01020052; LMGP01030080; LMGP01020187
		PC O-18:0_18:1	LMGP01020202; LMGP01030057
		PC O-20:0_16:1	LMGP01020222
		PC O-16:1_20:0	LMGP01020258; LMGP01030036
	PC 35:1	PC 13:0_22:1	LMGP01011359; LMGP01012005
		PC 14:1_21:0	LMGP01011403; LMGP01011955
		PC 15:0_20:1	LMGP01011421; LMGP01011809
		PC 15:1_20:0	LMGP01011450; LMGP01011789
		PC 16:0_19:1	LMGP01011467; LMGP01011762
		PC 16:1_19:0	LMGP01011486; LMGP01011734
		PC 17:0_18:1	LMGP01010711; LMGP01011600
		PC 17:1_18:0	LMGP01011531; LMGP01011586
	PC 36:8	PC 18:4_18:4	LMGP01010961; LMGP01011716; LMGP01010964
	[¹³C] SM 39:1		

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Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C36:2	PC O-36:2	PC O-16:0_20:2	LMGP01020188
		PC O-18:0_18:2	LMGP01020203; LMGP01030136; LMGP01030146
		PC O-18:1_18:1	LMGP01020263; LMGP01030013; LMGP01030130; LMGP01090013
		PC O-16:1_20:1	LMGP01030037; LMGP01090036; LMGP01030081
	PC 35:2	PC 13:0_22:2	LMGP01011360; LMGP01012036
		PC 15:0_20:2	LMGP01011422; LMGP01011839
		PC 15:1_20:1	LMGP01011451; LMGP01011810
		PC 16:1_19:1	LMGP01011487; LMGP01011763
		PC 17:0_18:2	LMGP01011505; LMGP01011621
		PC 17:1_18:1	LMGP01011532; LMGP01011601
		PC 17:2_18:0	LMGP01011561; LMGP01011587
	[^{13}C] SM 39:2		
PC ae C36:3	PC O-36:3	PC O-16:0_20:3	LMGP01020053
		PC O-18:0_18:3	LMGP01020204; LMGP01020205
		PC O-18:1_18:2	LMGP01020262; LMGP01090014; LMGP01090015; LMGP01090017; LMGP01090016; LMGP01030137; LMGP01020264; LMGP01030058
		PC O-16:1_20:2	LMGP01030038; LMGP01090037
	PC 35:3	PC 15:0_20:3	LMGP01011423; LMGP01011870
		PC 15:1_20:2	LMGP01011452; LMGP01011840
		PC 17:0_18:3	LMGP01011506; LMGP01011507; LMGP01011648; LMGP01011679
		PC 17:1_18:2	LMGP01011533; LMGP01011622
		PC 17:2_18:1	LMGP01011562; LMGP01011602

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Absolute*DQ®* p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C36:4	PC O-36:4	PC O-16:0_20:4	LMGP01020054; LMGP01020056; LMGP01020245
		PC O-16:1_20:3	LMGP01030039; LMGP01090040; LMGP01090044; LMGP01030129
		PC O-18:0_18:4	LMGP01020206
		PC O-18:1_18:3	LMGP01030059; LMGP01090026; LMGP01090028; LMGP01030060
		PC O-18:2_18:2	LMGP01020270; LMGP01090022; LMGP01090023
	PC 35:4	PC 13:0_22:4	LMGP01011361; LMGP01012067
		PC 15:0_20:4	LMGP01011424; LMGP01011901
		PC 15:1_20:3	LMGP01011453; LMGP01011871
		PC 17:0_18:4	LMGP01011508; LMGP01011708
		PC 17:1_18:3	LMGP01011534; LMGP01011535; LMGP01011649; LMGP01011680
		PC 17:2_18:2	LMGP01011563; LMGP01010931; LMGP01011623
PC ae C36:5	PC O-36:5	PC O-16:0_20:5	LMGP01020058
		PC O-16:1_20:4	LMGP01020259; LMGP01030010
		PC O-18:1_18:4	LMGP01030061; LMGP01090032
		PC O-18:2_18:3	LMGP01090024; LMGP01090025; LMGP01090030; LMGP01090031
	PC 35:5	PC 15:0_20:5	LMGP01011425; LMGP01011930
		PC 15:1_20:4	LMGP01011454; LMGP01011902
		PC 17:1_18:4	LMGP01011536; LMGP01011709
		PC 17:2_18:3	LMGP01011564; LMGP01011565; LMGP01011650; LMGP01011681
PC ae C38:0	PC O-38:0	PC O-16:0_22:0	LMGP01020060
		PC O-18:0_20:0	LMGP01020097; LMGP01020226
	PC 37:0	PC 15:0_22:0	LMGP01011426; LMGP01011981
		PC 16:0_21:0	LMGP01011470; LMGP01011958
		PC 17:0_20:0	LMGP01011511; LMGP01011791
		PC 18:0_19:0	LMGP01011590; LMGP01010975
	PC 38:7	PC 16:1_22:6	LMGP01010696; LMGP01011306; LMGP01012103
		PC 18:2_20:5	LMGP01011634; LMGP01011938
		PC 18:3_20:4	LMGP01011663; LMGP01011692; LMGP01011910; LMGP01011911
		PC 18:4_20:3	LMGP01011722; LMGP01011882

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Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C38:1	PC O-38:1	PC O-16:0_22:1	LMGP01020190
		PC O-16:1_22:0	LMGP01020260; LMGP01030042
		PC O-18:0_20:1	LMGP01020099; LMGP01020209; LMGP01030085
		PC O-18:1_20:0	LMGP01020265; LMGP01030064; LMGP01020227
	PC 37:1	PC 15:0_22:1	LMGP01011427; LMGP01012008
		PC 15:1_22:0	LMGP01011457; LMGP01011982
		PC 16:1_21:0	LMGP01011493; LMGP01011959
		PC 17:0_20:1	LMGP01011512; LMGP01011813
		PC 17:1_20:0	LMGP01011539; LMGP01011792
		PC 18:0_19:1	LMGP01011591; LMGP01011767
		PC 18:1_19:0	LMGP01011605; LMGP01011738
	PC 38:8	PC 18:3_20:5	LMGP01011664; LMGP01011693; LMGP01011939; LMGP01011940
		PC 18:4_20:4	LMGP01011723; LMGP01011912
PC ae C38:2	PC O-38:2	PC O-16:0_22:2	LMGP01020191
		PC O-18:0_20:2	LMGP01020210
		PC O-18:1_20:1	LMGP01020266; LMGP01030065; LMGP01030086
		PC O-18:2_20:0	LMGP01020271; LMGP01020228
		PC O-16:1_22:1	LMGP01030043
	PC 37:2	PC 15:0_22:2	LMGP01011428; LMGP01012039
		PC 15:1_22:1	LMGP01011458; LMGP01012009
		PC 17:0_20:2	LMGP01011513; LMGP01011843
		PC 17:1_20:1	LMGP01011540; LMGP01011814
		PC 17:2_20:0	LMGP01011569; LMGP01011793
		PC 18:1_19:1	LMGP01011606; LMGP01011768
		PC 18:2_19:0	LMGP01011628; LMGP01011739
	PC 38:9	PC 18:4_20:5	LMGP01011724; LMGP01011941
PC ae C38:3	PC O-38:3	PC O-18:0_20:3	LMGP01020211
		PC O-16:1_22:2	LMGP01030044
		PC O-18:1_20:2	LMGP01030066
		PC O-18:2_20:1	LMGP01030087
		P O-18:3_20:0	LMGP01020229; LMGP01020230
	PC 37:3	PC 15:1_22:2	LMGP01011459; LMGP01012040
		PC 17:0_20:3	LMGP01011514; LMGP01011874
		PC 17:1_20:2	LMGP01011541; LMGP01011844
		PC 17:2_20:1	LMGP01011570; LMGP01011815
		PC 18:2_19:1	LMGP01011629; LMGP01011769
		PC 18:3_19:0	LMGP01011657; LMGP01011686; LMGP01011740; LMGP01011741

List of Lipids

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C38:4	PC O-38:4	PC O-16:0_22:4	LMGP01020192
		PC O-18:0_20:4	LMGP01020100; LMGP01020102; LMGP01020247
		PC O-20:0_18:4	LMGP01020231
		PC O-18:1_20:3	LMGP01030067; LMGP01090041; LMGP01090045; LMGP01030131
		PC O-18:2_20:2	LMGP01030138; LMGP01090038; LMGP01090039
		PC O-20:1_18:3	LMGP01030088; LMGP01030089
	PC 37:4	PC 15:0_22:4	LMGP01011429; LMGP01012070
		PC 17:0_20:4	LMGP01010003; LMGP01011904
		PC 17:1_20:3	LMGP01011542; LMGP01011875
		PC 17:2_20:2	LMGP01011571; LMGP01011845
		PC 18:3_19:1	LMGP01011658; LMGP01011770; LMGP01011771
		PC 18:4_19:0	LMGP01011717 LMGP01011742
PC ae C38:5	PC O-38:5	PC O-16:0_22:5	LMGP01020066
		PC O-16:1_22:4	LMGP01030045
		PC O-18:0_20:5	LMGP01020104
		PC O-18:1_20:4	LMGP01020157; LMGP01020267; LMGP01030012
		PC O-18:2_20:3	LMGP01090042; LMGP01090043; LMGP01090046; LMGP01090047
		PC O-18:4_20:1	LMGP01030090
	PC 37:5	PC 15:1_22:4	LMGP01011460; LMGP01012071
		PC 17:0_20:5	LMGP01011515; LMGP01011934
		PC 17:1_20:4	LMGP01011543; LMGP01011905
		PC 17:2_20:3	LMGP01011572; LMGP01011876
		PC 18:4_19:1	LMGP01011718; LMGP01011772
PC ae C38:6	PC O-38:6	PC O-16:0_22:6	LMGP01020064
		PC O-18:1_20:5	LMGP01030068
		PC O-18:2_20:5	LMGP01090048; LMGP01090049
	PC 37:6	PC 15:0_22:6	LMGP01011430; LMGP01012101
		PC 17:1_20:5	LMGP01011544; LMGP01011935
		PC 17:2_20:4	LMGP01011573; LMGP01011906

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Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C40:1	PC O-40:1	PC O-18:0_22:1	LMGP01020213
		PC O-18:1_22:0	LMGP01020268; LMGP01030070
		PC O-20:0_20:1	LMGP01020235; LMGP01030093
	PC 39:1	PC 17:0_22:1	LMGP01011518; LMGP01012012
		PC 17:1_22:0	LMGP01011546; LMGP01011986
		PC 18:1_21:0	LMGP01011610; LMGP01011963
		PC 19:0_20:1	LMGP01011745; LMGP01011822
		PC 19:1_20:0	LMGP01011775; LMGP01011798
	PC 40:8	PC 18:2_22:6	LMGP01010947; LMGP01012109
		PC 18:4_22:4	LMGP01011729; LMGP01012082
		PC 20:3_20:5	LMGP01011890; LMGP01011947
		PC 20:4_20:4	LMGP01011047; LMGP01011052
PC ae C40:2	PC O-40:2	PC O-18:0_22:2	LMGP01020214
		PC O-18:1_22:1	LMGP01030071
		PC O-18:2_22:0	LMGP01020272
		PC O-20:0_20:2	LMGP01020236
		PC O-20:1_20:1	LMGP01030094
	PC 39:2	PC 17:0_22:2	LMGP01011519; LMGP01012043
		PC 17:1_22:1	LMGP01011547; LMGP01012013
		PC 17:2_22:0	LMGP01011576; LMGP01011987
		PC 18:2_21:0	LMGP01011635; LMGP01011964
		PC 19:0_20:2	LMGP01011746; LMGP01011852
		PC 19:1_20:1	LMGP01011776; LMGP01011823
	PC 40:9	PC 18:3_22:6	LMGP01011670; LMGP01011699; LMGP01012110; LMGP01012111
		PC 20:4_20:5	LMGP01011919; LMGP01011948
	[13C] SM 43:2		
PC ae C40:3	PC O-40:3	PC O-18:1_22:2	LMGP01030072; LMGP01090055
		PC O-18:2_22:1	LMGP01030139; LMGP01090053; LMGP01090054; LMGP01030147
		PC O-20:0_20:3	LMGP01020237
		PC O-20:1_20:2	LMGP01030095
		PC O-22:0_18:3	LMGP01020249
	PC 39:3	PC 17:1_22:2	LMGP01011548; LMGP01012044
		PC 17:2_22:1	LMGP01011577; LMGP01012014
		PC 18:3_21:0	LMGP01011665; LMGP01011694; LMGP01011965; LMGP01011966
		PC 19:0_20:3	LMGP01011747; LMGP01011883
		PC 19:1_20:2	LMGP01011777; LMGP01011853
	PC 40:10	PC 18:4_22:6	LMGP01011730; LMGP01012112
		PC 20:5_20:5	LMGP01011949

List of Lipids

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Version: 1-2018

Absolute*DQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C40:4	PC O-40:4	PC O-18:0_22:4	LMGP01020215
		PC O-18:2_22:2	LMGP01030140; LMGP01090056; LMGP01090057; LMGP01030148
		PC O-20:0_20:4	LMGP01020238; LMGP01020248
		PC O-20:1_20:3	LMGP01030096
	PC 39:4	PC 17:0_22:4	LMGP01011520; LMGP01012074
		PC 17:2_22:2	LMGP01011578; LMGP01012045
		PC 18:4_21:0	LMGP01011725; LMGP01011967
		PC 19:0_20:4	LMGP01011748; LMGP01011913
		PC 19:1_20:3	LMGP01011778; LMGP01011884
PC ae C40:5	PC O-40:5	PC O-18:0_22:5	LMGP01020107; LMGP01020109
		PC O-18:1_22:4	LMGP01030073; LMGP01090058
		PC O-20:0_20:5	LMGP01020239
		PC O-20:1_20:4	LMGP01020274; LMGP01030097
	PC 39:5	PC 16:0_23:5	LMGP01010656
		PC 17:0_22:5	LMGP01010719
		PC 17:1_22:4	LMGP01011549; LMGP01012075
		PC 19:0_20:5	LMGP01011749; LMGP01011942
		PC 19:1_20:4	LMGP01011779; LMGP01011914
PC ae C40:6	PC O-40:6	PC O-18:0_22:6	LMGP01020110
		PC O-18:2_22:4	LMGP01090059
		PC O-20:1_20:5	LMGP01030098
	PC 39:6	PC 17:0_22:6	LMGP01010720; LMGP01012104
		PC 17:2_22:4	LMGP01011579; LMGP01012076
		PC 19:1_20:5	LMGP01011780; LMGP01011943
PC ae C42:0	PC O-42:0	PC O-20:0_22:0	LMGP01020125
	PC 41:0	PC 19:0_22:0	LMGP01011751; LMGP01011992
		PC 20:0_21:0	LMGP01011801; LMGP01011970
		PC 23:0_18:0	LMGP01011130
	PC 42:7	PC 20:1_22:6	LMGP01011834; LMGP01012116
		PC 20:3_22:4	LMGP01011895; LMGP01012088
		PC 20:5_22:2	LMGP01011953; LMGP01012059
PC ae C42:1	PC O-42:1	PC O-20:0_22:1	LMGP01020241
		PC O-18:1_24:0	LMGP01020269
		PC O-20:1_22:0	LMGP01030100; LMGP01020250
	PC 40:1	PC 19:0_22:1	LMGP01011752; LMGP01012021
		PC 19:1_22:0	LMGP01011782; LMGP01011993
		PC 20:1_21:0	LMGP01011829; LMGP01011971
	PC 42:8	PC 20:2_22:6	LMGP01011865; LMGP01012117
		PC 20:4_22:4	LMGP01011924; LMGP01012089

Absolute*IDQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
PC ae C42:2	PC O-42:2	PC O-20:0_22:2	LMGP01020242
		PC O-18:2_24:0	LMGP01020273; LMGP01030141; LMGP01030149; LMGP01090060; LMGP01090061
		PC O-20:1_22:1	LMGP01030101
		PC O-18:1_24:1	LMGP01030132; LMGP01090062
	PC 41:2	PC 19:0_22:2	LMGP01011753; LMGP01012052
		PC 19:1_22:1	LMGP01011783; LMGP01012022
		PC 20:2_21:0	LMGP01011860; LMGP01011972
	PC 42:9	PC 20:3_22:6	LMGP01011896; LMGP01012118
		PC 20:5_22:4	LMGP01011954; LMGP01012090
PC ae C42:3	PC O-42:3	PC O-24:0_18:3	LMGP01020252; LMGP01020253
		PC O-20:1_22:2	LMGP01030102
		PC O- 18:2_24:1	LMGP01030142; LMGP01030150; LMGP01090063; LMGP01090064
	PC 41:3	PC 21:0_20:3	LMGP01011973; LMGP01011891
		PC 19:1_22:2	LMGP01011784; LMGP01012053
		PC 20:3_21:0	LMGP01011891; LMGP01011973
	PC 42:10	PC 20:5_22:5	LMGP01011058
		PC 20:4_22:6	LMGP01011925; LMGP01012119
PC ae C42:4	PC O-42:4	PC O-20:0_22:4	LMGP01020243
	PC 41:4	PC 19:0_22:4	LMGP01011754; LMGP01012083
		PC 20:4_21:0	LMGP01011920; LMGP01011974
	PC 42:11	PC 20:5_22:6	LMGP01011059; LMGP01012120
PC ae C42:5	PC O-42:5	PC O-20:1_22:4	LMGP01030103
	PC 41:5	PC 19:1_22:4	LMGP01011785; LMGP01012084
		PC 20:5_21:0	LMGP01011950; LMGP01011975
PC ae C44:3	PC O-44:3	PC O-22:0_22:3	LMGP01020251
		PC O-22:1_22:2	LMGP01020275
	PC 44:10	PC 22:4_22:6	LMGP01012096; LMGP01012125
PC ae C44:4	PC O-44:4	PC O-24:0_20:4	LMGP01020254
		PC O-22:1_22:3	LMGP01020276
		PC O-22:2_22:2	LMGP01020277
	PC 43:4	PC 21:0_22:4	LMGP01011979; LMGP01012091
PC ae C44:5	PC O-44:5	PC O-22:2_22:3	LMGP01020278
	PC 44:12	PC 22:6_22:6	LMGP01011119
PC ae C44:6	PC O-44:6	PC O-22:2_22:4	
	PC 43:6	PC 21:0_22:6	LMGP01010004; LMGP01012121
lysoPC a C14:0	LPC 14:0	PC 14:0_0:0	LMGP01050012, LMGP01050073
	PC O-14:0	PC O-12:0_2:0	LMGP01020009
	LPC O-15:0	PC O-15:0_0:0	LMGP01060009

Absolute*DQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
lysoPC a C16:0	LPC 16:0	PC 16:0_0:0	LMGP01050018; LMGP01050074
	PC O-16:0	PC O-14:0_2:0	LMGP01020019
	LPC O-17:0	PC O-17:0_0:0	LMGP01060013
lysoPC a C16:1	LPC 16:1	PC 16:1_0:0	LMGP01050021; LMGP01050022
	PC O-17:1	PC O-17:1_0:0	LMGP01070007
lysoPC a C17:0	LPC 17:0	PC 17:0_0:0	LMGP01050024
	PC O-17:0	PC O-1:0_16:0	LMGP01020004; LMGP01020028; LMGP01080021
		PC O-15:0_2:0	LMGP01020024
	LPC O-18:0	PC O-18:0_0:0	LMGP01060014
	PC 16:0	PC 14:0_2:0	LMGP01010504
		PC 8:0_8:0	LMGP01011251
lysoPC a C18:0	LPC 18:0	PC 18:0_0:0	LMGP01050026; LMGP01050076
	PC O-18:0	PC O-16:0_2:0	LMGP01020046
	LPC O-19:0	PC O-19:0_0:0	LMGP01060017
lysoPC a C18:1	LPC 18:1	PC 18:1_0:0	LMGP01050029; LMGP01050030; LMGP01050032; LMGP01050079; LMGP01050082; LMGP01050138
	PC O-18:1	PC O-16:1_2:0	LMGP01020147; LMGP01030009
lysoPC a C18:2	LPC 18:2	PC 18:2_0:0	LMGP01050034; LMGP01050035
	PC O-19:2	PC O-19:2_0:0	LMGP01070010
lysoPC a C20:3	LPC 20:3	PC 20:3_0:0	LMGP01050133; LMGP01050139
lysoPC a C20:4	LPC 20:4	PC 20:4_0:0	LMGP01050048; LMGP01050121; LMGP01050140
lysoPC a C24:0	LPC 24:0	PC 24:0_0:0	LMGP01050057
lysoPC a C26:0	LPC 26:0	PC 26:0_0:0	
	PC 25:0	PC 12:0_13:0	LMGP01010001; LMGP01011338
		PC 16:0_9:0	LMGP01010677
lysoPC a C26:1	LPC 26:1	PC 26:1_0:0	
	PC 25:1	PC 16:1_9:0	
lysoPC a C28:0	LPC 28:0	PC 28:0_0:0	
	PC 27:0	PC 17:0_10:0	LMGP01010700
		PC 8:0_19:0	LMGP01011244
		PC 9:0_18:0	LMGP01011262
		PC 12:0_15:0	LMGP01011317; LMGP01011409
		PC 13:0_14:0	LMGP01011339; LMGP01011363
	PC O-28:0	PC O-16:0_12:0	LMGP01020176
	[13C] SM 31:0		

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List of Lipids

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Absolute*DQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
lysoPC a C28:1	LPC 28:1	PC 28:1_0:0	
	PC 27:1	PC 12:0_15:1	LMGP01011318; LMGP01011431
		PC 13:0_14:1	LMGP01011340; LMGP01011380
	PC O-28:1	PC O-16:1_12:0	LMGP01030019
SM C16:0	SM 34:1	SM d16:1/18:0	LMSP03010042
		SM d17:1/17:0	LMSP03010043
		SM d18:1/16:0	LMSP03010003
SM C16:1	SM 34:2	SM d16:1/18:1	LMSP03010040
		SM d18:1/16:1	LMSP03010041
		SM d18:2/16:0	LMSP03010090
SM C18:0	SM 36:1	SM d16:1/20:0	LMSP03010052
		SM d18:0/18:1	LMSP03010031
		SM d18:1/18:0	LMSP03010001
	[¹³C] PC 32:2		
SM C18:1	SM 36:2	SM d16:1/20:1	LMSP03010048
		SM d18:0/18:2	LMSP03010049
		SM d18:1/18:1	LMSP03010029
		SM d18:2/18:0	LMSP03010050
		SM d19:1/17:1	LMSP03010051
SM C20:2	SM 38:3	SM d18:1/20:2	
		SM d18:2/20:1	LMSP03010057
SM C22:3	SM 40:4	SM d18:1/22:3	
		SM d18:2/22:2	
SM C24:0	SM 42:1	SM d18:0/24:1	LMSP03010023
		SM d18:1/24:0	LMSP03010008
	[¹³C] PC 38:2		
SM C24:1	SM 42:2	SM d18:1/24:1	LMSP03010007
		SM d18:2/24:0	LMSP03010081
SM C26:0	SM 44:1	SM d18:1/26:0	LMSP03010010
		SM d18:0/26:1	LMSP03010025
		SM d20:0/24:1	LMSP03010088
SM C26:1	SM 44:2	SM d18:1/26:1	LMSP03010009
SM (OH) C14:1	SM OH-32:2	SM d18:1/HO-14:1	
	SM 33:1	SM d16:1/17:0	LMSP03010037
		SM d18:1/15:0	LMSP03010038
SM (OH) C16:1	SM OH-34:2	SM d18:1/HO-16:1	
	SM 35:1	SM d18:1/17:0	LMSP03010044
		SM d19:1/16:0	LMSP03010045

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Absolute*DQ*® p180 Kit lipid annotation	Potential isobars within ± 0.5 Da	Potential isomers	LIPID MAPS data base entries
SM (OH) C22:1	SM OH-40:2	SM d18:1/HO-22:1	
	SM 41:1	SM d16:1/25:0	LMSP03010076
		SM d17:1/24:0	LMSP03010077
		SM d18:1/23:0	LMSP03010078
	[¹³C] PC 37:2		
SM (OH) C22:2	SM OH-40:3	SM d18:1/HO-22:2	
	SM 41:2	SM d17:1/24:1	LMSP03010074
		SM d18:2/23:0	LMSP03010075
SM (OH) C24:1	SM OH-42:2	SM d18:1/HO-24:1	
	SM 43:1	SM d18:1/25:0	LMSP03010027
		SM d19:0/24:1	LMSP03010085
		SM d19:1/24:0	LMSP03010086
		SM d20:1/23:0	LMSP03010087
	[¹³C] PC 39:2		

Abbreviations and separators used in the table:

PC – Phosphatidylcholines

SM – Sphingomyelins

LPC – Lysophosphatidylcholines

O – O-alkyl-bond

_ – separator for lipid fatty acids if sn-position is not known

/ – separator for lipid fatty acids if sn-position is proven (order sn-1/sn-2)

[¹³C] – Indicates possible isotope interference from another lipid species having a molecular weight with a mass unit smaller. This interference has not been corrected due to technical limitation.