#### **Supplemental Material**

## liputils - a Python module to manage individual fatty acid moieties from complex lipids

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## **Supplementary Figure S1**

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Calibri								
A1 $\checkmark$ $f_{x} \Sigma^{*} =$								
	A	В	С	D	E	F	0	
1		Group	Plpp3_WT	Plpp3_WT	Plpp3_KO	Plpp3_WT	Plpp3	
2		Diet	western	western	western	western	west	
3	Lipid class	Lipid name	16-1	16-11	16-12	16-2	16	
4	CE	CE 14:0	337.62167	487.77843	457.52704	358.94604	488.6	
5	CE	CE 15:0	201.57888	284.39835	244.04901	185.30819	285.5	
6	CE	CE 16:0	6063.54769	8875.01807	7159.75140	5527.55985	9049.6	
7	CE	CE 16:1	2128.69699	4389.60990	3579.84433	3010.09907	<b>3</b> 493.8	
8	CE	CE 17:0	838.04332	1066.96406	885.65583	757.92779	1052.	
9	CE	CE 17:1	358.28467	512.73542	478.67850	407.68995	<b>47</b> 5.7	
10	CE	CE 18:0	1535.53361	1859.99044	1598.96027	1178.68799	1807.1	
11	CE	CE 18:1	8720.33776	11175.62366	9223.33774	9949.22209	<b>129</b> 83.	
12	CE	CE 18:2	1479.38418	2299.69718	2088.33231	1875.98259	2071.8	
13	CE	CE 18:3	215.65419	354.54567	317.47278	256.70301	313.6	
14	CE	CE 19:0	51.32035	100.10614	76.29747	46.02304	81.70	
15	CE	CE 19:1	79.71011	104.21516	93.38671	78.67111	119.0	
16	CE	CF 19-2	9 31680	15 70018	12 /0222	16 71022		

	16-4	16-3	16-2	16-12	16-11	16-1	
500	<b>394.195</b> 228	517.263376	391.997333	489.623404	519.080276	366.207151	14:0
256	203.610721	285.598587	185.308187	244.049011	284.398350	201.578879	15:0
<b>105</b> 44	8722.796188	12123.860802	8855.969034	NaN	12477.578985	8719.581657	16:0
<b>3</b> 463	<b>2995.19</b> 4100	3638.123680	3188.963147	3825.726416	4661.111102	2263.292995	16:1
<b>10</b> 14	789.159200	1052.758402	757.927793	885.655828	1066.964064	838.043317	17:0
501	<b>372.042</b> 406	475.720716	407.689948	478.678504	512.735415	358.284673	17:1
3041	2440.301592	3282.076417	2632.689125	2657.698155	3012.836369	2777.439159	18:0
<b>1</b> 4531	12791.730402	15512.540700	13083.144031	11941.622887	14282.296976	10997.217033	18:1
<b>30</b> 48	2428.383267	NaN	NaN	NaN	NaN	2398.447524	18:2
293	218.063460	314.452189	257.375889	318.100907	NaN	216.516554	18:3
64	52.746490	81.708145	46.023043	76.297469	100.106145	51.320348	19:0
109	80.840988	119.009738	78.671108	93.386714	104.215156	79.710113	19:1
	14.385706	25.750033	16.710221	13.403230	15.700177	9.316802	19:2
	35.475635	39.205712	NaN	NaN	59.859201	32.585812	20:0

**Graphical visualization of tabular data**. For a quick tutorial of how to use liputils to extract residue information from lipidomics data, the following table is used (**A**). Data is arranged with samples in column, with analytes in row. To be processed directly with liputils make\_residues\_table() function, a table needs to avoid column multi-indexing, and have lipids as row index. This table needs to be loaded in pandas by specifying to skip the first two rows and to index the second column, or needs prior editing and all unwanted columns and row removed.

In **B**, all lipid residues have ben counted per sample. NaN stands for "not a number", and it is the way Numpy has to represent blank/missing values. When saved to a csv or Excel file, these values will result in empty cells. Missing values derive from residues that are present in the data, but are not represented in that particular sample.

## **Supplementary Figure S2**



**Fatty acid moieties extracted from stock media**. Residues extracted from lipidomic data of HepG2, human hepatocyte-like cells (HLCs) and human primary hepatocytes (HPPs) culture media are shown (**A**-**B**) (n=1 per sample). HLCs and PHHs media were chemically defined, while HepG2 medium included 10% FBS comprised of complex lipid molecules. Units were unchanged during the extraction and are the same as the input data (pmol/µg protein).

# **Supplementary Figure S3**

## A

### Download results as tab-delimited text

Input name	RefMet name	Formula	Mass	MW structure
PE(P-40:6)/PE(O-40:7)	PE(P-40:6)/PE(O-40:7)	C45H78NO7P	775.5516	

# В

# RefMet Compounds with Formula C45H78NO7P

Name	Formula	Mass
PC(P-37:6)/PC(O-37:7)	C45H78NO7P	775.551592
PE(P-16:0/24:6)/PE(O-16:1/24:6)	C45H78NO7P	775.551592
PE(P-18:0/22:6)/PE(O-18:1/22:6)	C45H78NO7P	775.5516
PE(P-18:1/22:5)/PE(O-18:2/22:5)	C45H78NO7P	775.5516
PE(P-20:1/20:5)/PE(O-20:2/20:5)	C45H78NO7P	775.551592
PE(P-40:6)/PE(O-40:7)	C45H78NO7P	775.5516

**Graphical output of the online RefMet translator**. The RefMet compound name translator, available at the following address:

(https://www.metabolomicsworkbench.org/databases/refmet/name\_to\_ref met\_form.php) attempts at translating non-RefMet compliant strings into official RefMet compounds (A). For low-resolution mass isomers, a list of possible molecular lipids that can be the parent compound is given (B).

#### Supplementary Table 1

14:0         HepG2-HLC-3         4.504313941         0.930846547         8.077781336         0.008694647           14:0         HepG2-HLC-4         4.765475723         1.136602429         8.394349017         0.005990598           14:0         HepG2-PHH         8.171247305         3.794661441         12.54783317         0.000106378           14:0         HLC-3-PHH         8.16693336         0.093465969         7.240400759         0.042326626           14:0         HLC-4-PHH         3.4056731582         0.22310171         7.034644876         0.073199923           14:0         HLC-4-PHH         3.0257731582         0.123107059         1.243256.09           14:1         HepG2-HLC-4         0.25600038         0.19505552         0.318744425         8.0487E-11           14:1         HepG2-HLC-4         0.25600038         0.19505552         0.318744425         8.0487E-10           14:1         HepG2-HLC-4         0.25600055         0.0407743         0.131577707         0.01736879           15:2         HepG2-HLC-4         0.155224912         0.10657215         0.209792609         1.303957           15:2         HepG2-HLC-4         0.155224912         0.10672515         0.209792609         1.303957           15:2         HepG2-HLC-	Residue	Comparison	Difference	Lower	Upper	Adjusted p-value
14:0         HepG2-HLC-4         4.765475723         1.136602429         8.394349017         0.005990598           14:0         HepG2-PHL<5	14:0	HepG2-HLC-3	4.504313941	0.930846547	8.077781336	0.008694647
14:0         HepG2-HLC-5         5.895734412         2.105499871         9.685968952         0.001038805           14:0         HepG2-PHH         8.171247305         3.794661441         12.54783317         0.001016378           14:0         HLC-3-PHH         3.666733364         0.93465969         7.240400759         0.042326626           14:0         HLC-5-PHH         2.775512894         -1.51472165         6.065747434         0.413794388           14:1         HepG2-HLC-4         0.25690038         0.19505552         0.318744425         8.0487E-11           14:1         HepG2-HLC-5         0.224820162         0.184225806         0.31414517         3.7936679           14:1         HepG2-HLC-4         0.25690038         0.083570279         0.131577707         0.01736879           15:2         HepG2-HLC-4         0.155224912         0.100677143         0.131577707         0.01736879           15:2         HepG2-HLC-4         0.159215569         0.10400445         0.23562668         7.2534E-07           15:2         HepG2-HLC-4         0.1597353         0.1618325         0.02810973         1.43257E-07           15:2         HepG2-HLC-4         0.1597359         0.12827351         1.43257E-07           15:1         HepG2-HLC-4	14:0	HepG2-HLC-4	4.765475723	1.136602429	8.394349017	0.005990598
14:0       HepG2-PHH       8.171247305       3.794661441       12.54783317       0.000106378         14:0       HLC3-PHH       3.666933364       0.09346596       7.240400759       0.042326626         14:0       HLC3-PHH       3.06571582       0.2231017       7.04464476       0.07319923         14:1       HepG2-HLC-3       0.220805953       0.15990581       0.281706095       1.28435E-09         14:1       HepG2-HLC-4       0.25600038       0.199055552       0.318744425       8.0447F-11         14:1       HepG2-HLC-5       0.248820162       0.184225806       0.31874425       8.0447F-11         14:1       HepG2-HLC-5       0.248820162       0.184225806       0.31874425       8.0447F-11         14:1       HepG2-HLC-5       0.137304833       0.08570279       0.191039387       8.57222F-07         15:2       HepG2-HLC-6       0.161825569       0.10400445       0.235626688       7.2534F-07         15:2       HepG2-HLC-4       0.169815569       0.10400445       0.235626688       7.2534F-07         15:1       HepG2-HLC-4       0.499752905       2.0997292       0.510581085       1.831         18:1       HepG2-HLC-4       2.490752905       2.029920535       0.002810973 <tr< td=""><td>14:0</td><td>HepG2-HLC-5</td><td>5.895734412</td><td>2.105499871</td><td>9.685968952</td><td>0.001038805</td></tr<>	14:0	HepG2-HLC-5	5.895734412	2.105499871	9.685968952	0.001038805
14:0         H.C-3-PHH         3.666933364         0.093465969         7.240400759         0.042326626           14:0         HLC-4-PHH         3.405771582         -0.22310171         7.034644876         0.073199923           14:0         HLC-5-PHH         2.27551284         -1.51472165         0.665747343         0.41379488           14:1         Hep62-HLC-3         0.220805953         0.15905552         0.318744425         8.0487F-11           14:1         Hep62-HLC-4         0.25500028         0.138225806         0.318414517         3.79588E-100           14:1         Hep62-HLC-4         0.070677555         0.009777423         0.131741777         0.01736879           15:2         Hep62-HLC-5         0.16128325         0.10057215         0.209792609         1.30395E-07           15:2         Hep62-HLC-5         0.16128325         0.104280149         0.218277551         1.43257E-07           15:2         Hep62-HLC-4         2.40752905         -0.0952291         7.072028722         0.510881085           18:1         Hep62-HLC-4         2.40752905         -0.0952291         7.072028722         0.510881085           18:1         Hep62-HLC-4         2.40752933         7.66673716         9.9220535         0.0066871231 <t< td=""><td>14:0</td><td>HepG2-PHH</td><td>8.171247305</td><td>3.794661441</td><td>12.54783317</td><td>0.000106378</td></t<>	14:0	HepG2-PHH	8.171247305	3.794661441	12.54783317	0.000106378
14:0         HLC-4-PHH         3.405771582         -0.22310171         7.034644876         0.073199923           14:0         HLC-5-PHH         2.275512894         -1.51472165         6.065747434         0.413794388           14:1         HepG2-HLC-4         0.25690038         0.195055652         0.318744425         8.0487E-11           14:1         HepG2-HLC-5         0.248820162         0.184225806         0.313414517         3.79583E-10           14:1         HepG2-HLC-5         0.24883518         0.216896381         0.366070655         2.83046E-10           14:1         HLC-3-PHH         0.070677565         0.009777423         0.131577707         0.01736879           15:2         HepG2-HLC-4         0.15229122         0.100657215         0.209792609         1.30395E-07           15:2         HepG2-HLC-4         0.16128325         0.10428149         0.218277351         1.43257E-07           15:2         HepG2-HLC-4         24.90752905         2.03052291         70.7028722         0.510581085           18:1         HLC-3-PHH         83.87080932         13.2575365         103.484095         0.006871231           18:1         HLC-4-PHH         53.47929533         7.6653716         99.2920535         0.00657215           18	14:0	HLC-3-PHH	3.666933364	0.093465969	7.240400759	0.042326626
14:0         HLC-S-PHH         2.275512894         -1.51472165         6.065747434         0.413794388           14:1         HepG2-HLC-3         0.220805955         0.15990581         0.281706095         1.28435E-09           14:1         HepG2-HLC-4         0.25690038         0.15905555         0.318744425         8.0487E-11           14:1         HepG2-HLC-4         0.25690038         0.316070655         2.83046E-10           14:1         HLC3-PHH         0.070677565         0.009777423         0.13157770         0.01736879           15:2         HepG2-HLC-3         0.137304833         0.083570279         0.191039387         8.57222E-07           15:2         HepG2-HLC-4         0.155224912         0.100607215         0.209792609         1.30395E-07           15:2         HepG2-HLC-4         0.49752905         -20.9052291         70.7028722         0.510581085           18:1         HepG2-PHH         78.38682438         23.13455912         13.36390896         0.006871231           18:1         HLC4-PHH         53.47929533         7.66653716         99.2920535         0.016581797           18:1         HLC5-PHH         43.4783345         -4.37132989         91.32840078         0.0087584786           18:2         PHH-HC3<	14:0	HLC-4-PHH	3.405771582	-0.22310171	7.034644876	0.073199923
14:1         HepG2-HLC-3         0.220805953         0.15990581         0.281706095         1.28435E-09           14:1         HepG2-HLC-4         0.25690038         0.195055652         0.313414517         3.7953E-10           14:1         HepG2-HLC-4         0.248820162         0.184225806         0.313414517         3.7953E-10           14:1         HepG2-HLC-3         0.13704833         0.083570279         0.131597707         0.01736879           15:2         HepG2-HLC-4         0.155224912         0.100657215         0.209792609         1.30395E-07           15:2         HepG2-HLC-4         0.155224912         0.100657215         0.209792609         1.30395E-07           15:2         HepG2-PHH         0.16128325         0.10400445         0.235626688         7.2534E-07           15:1         HepG2-PHH         0.169815569         0.10400445         0.235626688         7.2534E-07           18:1         HepG2-PHH         7.8362433         2.313455912         133.6300895         0.002810973           18:1         HepG2-PHH         7.8362633         2.313455912         13.3630856         0.002810973           18:1         HLC-3-PHH         53.472653716         99.2920535         0.016871231           18:2         PHH-HEC3 </td <td>14:0</td> <td>HLC-5-PHH</td> <td>2.275512894</td> <td>-1.51472165</td> <td>6.065747434</td> <td>0.413794388</td>	14:0	HLC-5-PHH	2.275512894	-1.51472165	6.065747434	0.413794388
14:1         HepG2-HLC-4         0.256900038         0.195055652         0.318724425         8.0487E-11           14:1         HepG2-HLC-5         0.24820160         0.18422806         0.318414517         3.79583E-100           14:1         HepG2-HLC-3         0.137304833         0.021689581         0.366070655         2.83046E-10           14:1         HLC-3-PHH         0.070677565         0.009777423         0.131577707         0.01736879           15:2         HepG2-HLC-4         0.155224912         0.10657215         0.209792609         1.30395E-07           15:2         HepG2-HLC-4         0.16128325         0.10400445         0.235626688         7.2534E-07           15:2         HepG2-HLC-4         24.90752905         -20.9052291         70.7028772         0.510581085           18:1         HepG2-HLC-4         24.90752905         -20.9052795         10.3484095         0.006871231           18:1         HLC-4-PHH         58.37080932         13.25752365         10.3484095         0.0087584786           18:2         PHH-HEG2         26.67016662         21.63910102         31.70123622         4.61E-13           18:2         PHH-HEG2         27.06354373         22.95593424         31.70123622         4.61E-14           18	14:1	HepG2-HLC-3	0.220805953	0.15990581	0.281706095	1.28435E-09
14:1         HepG2-HLC-5         0.248820162         0.184225806         0.313414517         3.79583E-10           14:1         HEpG2-HH         0.2016896381         0.366070655         2.83046E-10           14:1         HLC-3-PHH         0.070677565         0.009777423         0.13157770         0.01736879           15:2         HepG2-HLC-4         0.155224912         0.100657215         0.209792609         1.30395E-07           15:2         HepG2-HLC-4         0.155224912         0.1040289149         0.218277351         1.43257E-07           15:2         HepG2-HLC-4         24.90752905         -20.9052291         70.72028722         0.510581085           18:1         HepG2-PHH         78.38682438         23.13455912         133.6390896         0.002810973           18:1         HLC-3-PHH         58.37080932         13.25752365         103.484095         0.006871231           18:1         HLC-5-PHH         43.47853545         -4.37132989         91.32840078         0.087584786           18:2         PHH-HepG2         26.67016862         21.63910102         31.70123622         4.61E-13           18:2         PHH-HC-4         28.73763907         24.56609819         22.905594         31.17139323         2.4E-14           18:	14:1	HepG2-HLC-4	0.256900038	0.195055652	0.318744425	8.0487E-11
14:1         HepG2-PHH         0.291483518         0.216896381         0.366070655         2.83046E-10           14:1         HLC-3-PHH         0.070677565         0.009777423         0.131577707         0.01736879           15:2         HepG2-HLC-4         0.155224912         0.100657215         0.209792609         1.30395E-07           15:2         HepG2-HLC-4         0.155224912         0.100657215         0.20792609         1.30395E-07           15:2         HepG2-HHL         0.16128325         0.104289149         0.218277351         1.43257E-07           15:2         HepG2-HHL         0.169815569         0.10400445         0.235626688         7.2534E-07           18:1         HepG2-PHH         78.38682438         23.13455912         133.6390896         0.002810973           18:1         HeC4-PHH         53.37080932         13.25752365         103.484095         0.006871231           18:1         HLC-4-PHH         53.47929533         7.66653716         99.2920535         0.015581797           18:1         HLC-5-PHH         43.47853545         -4.37132989         91.32840078         0.087584786           18:2         PHH-HC-3         27.06354373         22.95569424         31.17139323         2.4E-14           18:2	14:1	HepG2-HLC-5	0.248820162	0.184225806	0.313414517	3.79583E-10
14:1         HLC-3-PHH         0.070677565         0.009777423         0.13157707         0.01736879           15:2         HepG2-HLC-3         0.137304833         0.083570279         0.191039387         8.57222F-07           15:2         HepG2-HLC-4         0.155224912         0.100657215         0.209792609         1.30395E-07           15:2         HepG2-HLC-5         0.16128325         0.104289149         0.218277351         1.43257E-07           15:2         HepG2-HLC-4         24.9075205         -20.9052291         70.72028722         0.510581085           18:1         HepG2-PHH         78.38682438         23.13455912         133.6390896         0.002810973           18:1         HLC-4-PHH         53.47929533         7.66653716         99.2920535         0.016581797           18:1         HLC-5-PHH         43.4785345         -4.37132989         91.32840078         0.087584786           18:2         PHH-HLC-3         27.06354373         22.95569424         31.17139323         2.4E-14           18:2         PHH-HLC-5         28.21689171         23.8598936         32.573246         0.6E-14           19:1         HepG2-HLC-4         0.16054723         0.028781198         0.257786128         0.009269628           19:1 <td>14:1</td> <td>HepG2-PHH</td> <td>0.291483518</td> <td>0.216896381</td> <td>0.366070655</td> <td>2.83046E-10</td>	14:1	HepG2-PHH	0.291483518	0.216896381	0.366070655	2.83046E-10
15:2       HepG2-HLC-3       0.137304833       0.083570279       0.191039387       8.57222E-07         15:2       HepG2-HLC-4       0.155224912       0.100657215       0.209792609       1.30395E-07         15:2       HepG2-HLC-5       0.16128325       0.104289149       0.218277351       1.43257E-07         15:2       HepG2-HH       0.169815560       0.10400445       0.235626688       7.2534E-07         18:1       HepG2-HH       7.83682438       23.13455912       133.6390896       0.002810973         18:1       HLC-3-PHH       53.4792953       7.6653716       99.220535       0.016581797         18:1       HLC-5-PHH       43.47853545       -4.37132989       91.32840078       0.087584786         18:2       PHH-HC-3       27.06354373       22.95569424       31.17139323       2.4E-14         18:2       PHH-HLC-3       28.21689171       23.85985936       32.57392406       2.6E-14         19:1       HepG2-HLC-4       0.140283663       0.028781198       0.257786128       0.009269628         19:1       HepG2-HLC-5       0.14823663       0.028781198       0.257786128       0.009269628         19:1       HepG2-HLC-4       0.160547234       0.044627425       0.28952833       0.00072	14:1	HLC-3-PHH	0.070677565	0.009777423	0.131577707	0.01736879
15:2         HepG2-HLC-4         0.155224912         0.100657215         0.209792609         1.30395E-07           15:2         HepG2-HLC-5         0.16128325         0.104289149         0.218277351         1.43257E-07           15:2         HepG2-PHH         0.169815569         0.10400445         0.235626688         7.2534E-07           18:1         HepG2-PHH         78.38682438         23.13455912         133.6390896         0.002810973           18:1         HuC-3-PHH         58.37080932         13.25752365         103.484095         0.006871231           18:1         HuC-4-PHH         53.47929533         7.66653716         99.2920535         0.016581797           18:1         HuC-5-PHH         43.47853545         -4.37132989         91.32840078         0.087584786           18:2         PHH-HuC3         26.67016862         21.63910102         31.70123622         4.61E-13           18:2         PHH-HLC-4         28.73763907         24.56609819         32.90917995         2.2E-14           18:2         PHH-HLC-5         28.21689171         23.85985936         32.57392406         2.6E-14           19:1         HepG2-HLC-4         0.160547234         0.24762432         0.276825037         0.003666694           19:1	15:2	HepG2-HLC-3	0.137304833	0.083570279	0.191039387	8.57222E-07
15:2         HepG2-HLC-5         0.16128325         0.104289149         0.218277351         1.43257E-07           15:2         HepG2-PHH         0.169815569         0.10400445         0.235626688         7.2534E-07           18:1         HepG2-HLC-4         24.90752905         -20.9052291         70.72028722         0.510581085           18:1         HecG2-PHH         78.8682438         23.13455912         133.639086         0.002810973           18:1         HLC-3-PHH         58.37080932         13.25752365         103.484095         0.006871231           18:1         HLC-4-PHH         53.47929533         7.66653716         99.2920535         0.016581797           18:1         HLC-5-PHH         43.4783545         -4.37132989         91.32840078         0.087584786           18:2         PHH-HLC-3         27.06354373         22.95569424         31.71739323         2.4E-14           18:2         PHH-HLC-3         27.06354373         2.290917995         2.2E-14           18:2         PHH-HLC-3         28.21689171         23.8598596         32.57392406         2.6E-14           19:1         HepG2-HLC-4         0.160547234         0.04627425         0.2852383         0.00072411           19:1         HepG2-HLC-4         <	15:2	HepG2-HLC-4	0.155224912	0.100657215	0.209792609	1.30395E-07
15:2       HepG2-PHH       0.169815569       0.10400445       0.235626688       7.2534E-07         18:1       HepG2-HLC-4       24.90752905       -20.9052291       70.72028722       0.510581085         18:1       HepG2-PHH       78.38682438       23.13455912       133.6390896       0.002810973         18:1       HLC-3-PHH       58.37080932       13.2575265       103.484095       0.006871231         18:1       HLC-4-PHH       53.47929533       7.66653716       99.2920535       0.016581797         18:1       HLC-5-PHH       43.47853545       -4.37132989       91.32840078       0.087584786         18:2       PHH-HLC3       27.06354373       2.95569424       31.17139323       2.4E-14         18:2       PHH-HLC4       28.73763007       24.56609819       32.90917995       2.2E-14         18:2       PHH-HLC5       0.143283663       0.028781198       0.257786128       0.0009269628         19:1       HepG2-HLC4       0.160547234       0.044269432       0.276825037       0.003696694         19:1       HepG2-HLC4       0.160547254       0.28952383       0.00072411         20:1       HepG2-HLC4       0.1605871514       0.8816969       0.365289583       0.00072411	15:2	HepG2-HLC-5	0.16128325	0.104289149	0.218277351	1.43257E-07
18:1         HepG2-HLC-4         24.90752905         -20.9052291         70.72028722         0.510581085           18:1         HepG2-PHH         78.38682438         23.13455912         133.6390896         0.002810973           18:1         HLC-3-PHH         58.37080932         13.25752365         103.484095         0.006871231           18:1         HLC-4-PHH         53.47929533         7.66653716         99.2920535         0.016581797           18:1         HLC-5-PHH         43.47853545         -4.37132989         91.32840078         0.087584786           18:2         PHH-HepG2         26.67016862         21.63910102         31.70123622         4.61E-13           18:2         PHH-HLC-3         27.06354373         22.95569424         31.17139323         2.4E-14           18:2         PHH-HLC-5         28.21689171         23.85985936         32.507392406         2.6E-14           19:1         HepG2-HLC-4         0.143283663         0.028781198         0.257786128         0.009269628           19:1         HepG2-HLC-4         0.16057529         0.046627425         0.28952383         0.00072411           20:1         HepG2-HLC-4         1.605891514         0.882698667         2.255993072         1.32953E-05           20:1 <td>15:2</td> <td>HepG2-PHH</td> <td>0.169815569</td> <td>0.10400445</td> <td>0.235626688</td> <td>7.2534E-07</td>	15:2	HepG2-PHH	0.169815569	0.10400445	0.235626688	7.2534E-07
18:1         HepG2-PHH         78.38682438         23.13455912         133.6390896         0.002810973           18:1         HLC-3-PHH         58.37080932         13.25752365         103.484095         0.006871231           18:1         HLC-4-PHH         53.47929533         7.66653716         99.2920355         0.016581797           18:1         HLC-5-PHH         43.47853545         -4.37132989         91.32840078         0.087584786           18:2         PHH-HepG2         26.67016862         21.63910102         31.70123622         4.61E-13           18:2         PHH-HLC-3         27.06354373         22.95569424         31.17139323         2.4E-14           18:2         PHH-HLC-5         28.21689171         23.85985936         32.57392406         2.6E-14           19:1         HepG2-HLC-3         0.143283663         0.028781198         0.257786128         0.009269628           19:1         HepG2-HLC-4         0.166075629         0.046627425         0.28952383         0.00072411           20:1         HepG2-HLC-5         1.54129587         0.826598667         2.25593072         1.32953E-05           20:1         HepG2-HLC-4         1.605891514         0.880113074         2.331669954         8.95599E-06           20:1	18:1	HepG2-HLC-4	24.90752905	-20.9052291	70.72028722	0.510581085
18:1         HLC-3-PHH         58.37080932         13.25752365         103.484095         0.006871231           18:1         HLC-4-PHH         53.47929533         7.66653716         99.2920535         0.016581797           18:1         HLC-5-PHH         43.47853545         -4.37132989         91.32840078         0.087584786           18:2         PHH-HepG2         26.67016862         21.63910102         31.70123622         4.61E-13           18:2         PHH-HLC-3         27.06354373         22.95569424         31.17139323         2.4E-14           18:2         PHH-HLC-4         28.73763907         24.56609819         32.90917995         2.2E-14           18:2         PHH-HLC-5         28.21689171         23.8598596         32.57392406         2.6E-14           19:1         HepG2-HLC-3         0.143283663         0.028781198         0.257786128         0.009269628           19:1         HepG2-HLC-4         0.160547234         0.04627425         0.289523833         0.003612389           19:1         HepG2-HLC-3         1.54129587         0.826598667         2.25993072         1.32953E-05           20:1         HepG2-HLC-4         1.605891514         0.880113074         2.331669954         8.95599E-06           20:1	18:1	HepG2-PHH	78.38682438	23.13455912	133.6390896	0.002810973
18:1         HLC-4-PHH         53.47929533         7.66653716         99.2920535         0.016581797           18:1         HLC-5-PHH         43.47853545         -4.37132989         91.32840078         0.087584786           18:2         PHH-HepG2         26.67016862         21.63910102         31.70123622         4.61E-13           18:2         PHH-HLC-3         27.06354373         22.95569424         31.7139323         2.4E-14           18:2         PHH-HLC-4         28.73763907         24.5609819         32.90917995         2.2E-14           18:2         PHH-HLC-5         28.21689171         23.85985936         2.57392406         2.6E-14           19:1         HepG2-HLC-4         0.160547234         0.044269432         0.276825037         0.003696694           19:1         HepG2-HLC-5         0.168075629         0.046627425         0.289523833         0.00072411           20:1         HepG2-HLC-3         1.54129587         0.826598667         2.255999072         1.32953E-05           20:1         HepG2-HLC-5         1.684624653         1.086573796         2.602675511         1.94759E-06           20:1         HepG2-HLC-4         1.06567378         3.149775806         17.7930318         8.53755E-07           20:4	18:1	HLC-3-PHH	58.37080932	13.25752365	103.484095	0.006871231
18:1HLC-5-PHH43.47853545-4.3713298991.328400780.08758478618:2PHH-HepG226.6701686221.6391010231.701236224.61E-1318:2PHH-HLC-327.0635437322.9556942431.171393232.4E-1418:2PHH-HLC-428.7376390724.5660981932.909179952.2E-1418:2PHH-HLC-528.2168917123.8598593632.573924062.6E-1419:1HepG2-HLC-30.1432836630.0287811980.277861280.00926962819:1HepG2-HLC-40.1605472340.0442694320.2768250370.00369669419:1HepG2-HLC-50.1680756290.0484169690.3652895830.0007241120:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:4PHH-HepG211.81818195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.1973571754.31178E-0720:4PHH-HLC-413.061673788.14977580617.797571754.31178E-0720:4PHH-HLC-50.237277950.076864990.343587690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-05 <tr< td=""><td>18:1</td><td>HLC-4-PHH</td><td>53.47929533</td><td>7.66653716</td><td>99.2920535</td><td>0.016581797</td></tr<>	18:1	HLC-4-PHH	53.47929533	7.66653716	99.2920535	0.016581797
18:2       PHH-HepG2       26.67016862       21.63910102       31.70123622       4.61E-13         18:2       PHH-HLC-3       27.06354373       22.95569424       31.17139323       2.4E-14         18:2       PHH-HLC-4       28.73763907       24.56609819       32.90917995       2.2E-14         18:2       PHH-HLC-5       28.21689171       23.85985936       32.57392406       2.6E-14         19:1       HepG2-HLC-3       0.143283663       0.028781198       0.257786128       0.009269628         19:1       HepG2-HLC-4       0.160547234       0.044269432       0.276825037       0.00366694         19:1       HepG2-HLC-5       0.168075629       0.046627425       0.28952383       0.00072411         20:1       HepG2-HLC-5       0.168075629       0.046627425       0.28952383       0.00072411         20:1       HepG2-HLC-5       0.168075629       0.04821598667       2.25593072       1.32953E-05         20:1       HepG2-HLC-5       1.54129587       0.826598667       2.255993072       1.32953E-05         20:1       HepG2-HLC-5       1.844624653       1.086573796       2.602675511       1.94759E-06         20:1       HepG2-HLC-5       1.844624653       1.086573798       3.080608619       1	18:1	HLC-5-PHH	43.47853545	-4.37132989	91.32840078	0.087584786
18:2PHH-HLC-327.0635437322.9556942431.171393232.4E-1418:2PHH-HLC-428.7376390724.5660981932.909179952.2E-1418:2PHH-HLC-528.2168917123.8598593632.573924062.6E-1419:1HepG2-HLC-30.1432836630.0287811980.2577861280.00926962819:1HepG2-HLC-50.1680756290.046274250.2895238330.00361238919:1HepG2-HH0.2250532760.0848169690.3652895830.0007241120:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-HHLC-51.8446246531.08651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.2132E-0520:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-40.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-10 <tr< td=""><td>18:2</td><td>PHH-HepG2</td><td>26.67016862</td><td>21.63910102</td><td>31.70123622</td><td>4.61E-13</td></tr<>	18:2	PHH-HepG2	26.67016862	21.63910102	31.70123622	4.61E-13
18:2PHH-HLC-428.7376390724.5660981932.909179952.2E-1418:2PHH-HLC-528.2168917123.8598593632.573924062.6E-1419:1HepG2-HLC-30.1432836630.0287811980.2577861280.00926962819:1HepG2-HLC-40.1605472340.0442694320.2768250370.00369669419:1HepG2-HLC-50.1680756290.0466274250.2895238330.0007241120:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-31.541295870.8265737962.6026755111.94759E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-HLC-51.8446246531.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0524:5HepG2-HLC-30.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-60.3384110940.1451108810.4717713069.10419E-0524:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-	18:2	PHH-HLC-3	27.06354373	22.95569424	31.17139323	2.4E-14
18:2PHH-HLC-528.2168917123.8598593632.573924062.6E-1419:1HepG2-HLC-30.1432836630.0287811980.2577861280.00926962819:1HepG2-HLC-40.1605472340.0442694320.2768250370.00369669419:1HepG2-HLC-50.1680756290.0466274250.2895238330.00361238919:1HepG2-PHH0.2250532760.0848169690.3652895830.0007241120:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-PHH2.2052868861.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-50.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-60.45544570.3677459110.6414030039.15416E-1024:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0	18:2	PHH-HLC-4	28.73763907	24.56609819	32.90917995	2.2E-14
19:1HepG2-HLC-30.1432836630.0287811980.2577861280.00926962819:1HepG2-HLC-40.1605472340.0442694320.2768250370.00369669419:1HepG2-HLC-50.1680756290.0466274250.2895238330.00361238919:1HepG2-PHH0.2250532760.0848169690.3652895830.0007241120:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-PHH2.2052868861.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0524:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-30.454415770.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.33229900220.6181403039.	18:2	PHH-HLC-5	28.21689171	23.85985936	32.57392406	2.6E-14
19:1HepG2-HLC-40.1605472340.0442694320.2768250370.00369669419:1HepG2-HLC-50.1680756290.0466274250.2895238330.00361238919:1HepG2-HH0.2250532760.0848169690.3652895830.0007241120:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HH2.205286861.3299651533.0806086191.08941E-0620:1HepG2-HH2.205286861.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-310.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0524:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-30.454415770.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322900020.6181245137.02772E-09 <td>19:1</td> <td>HepG2-HLC-3</td> <td>0.143283663</td> <td>0.028781198</td> <td>0.257786128</td> <td>0.009269628</td>	19:1	HepG2-HLC-3	0.143283663	0.028781198	0.257786128	0.009269628
19:1HepG2-HLC-50.1680756290.0466274250.2895238330.00361238919:1HepG2-PHH0.2250532760.0848169690.3652895830.0007241120:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-HLC<5	19:1	HepG2-HLC-4	0.160547234	0.044269432	0.276825037	0.003696694
19:1HepG2-PHH0.2250532760.0848169690.3652895830.0007241120:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-PHH2.2052868861.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-40.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-30.2102272090.0788686490.3435857690.00089153324:5HepG2-HLC-40.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-50.237277350.396763320.5891552085.34231E-0924:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-0924:6HepG2-HLC-50.4752117580.3322990020.6181245137.0277	19:1	HepG2-HLC-5	0.168075629	0.046627425	0.289523833	0.003612389
20:1HepG2-HLC-31.541295870.8265986672.2559930721.32953E-0520:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-PHH2.2052868861.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-50.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-0924:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	19:1	HepG2-PHH	0.225053276	0.084816969	0.365289583	0.00072411
20:1HepG2-HLC-41.6058915140.8801130742.3316699548.95599E-0620:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-PHH2.2052868861.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-50.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-30.2102272090.0768686490.3435857690.00042513424:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-40.3084410940.1451108810.4717713069.10419E-0524:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-0924:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	20:1	HepG2-HLC-3	1.54129587	0.826598667	2.255993072	1.32953E-05
20:1HepG2-HLC-51.8446246531.0865737962.6026755111.94759E-0620:1HepG2-PHH2.2052868861.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-50.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	20:1	HepG2-HLC-4	1.605891514	0.880113074	2.331669954	8.95599E-06
20:1HepG2-PHH2.2052868861.3299651533.0806086191.08941E-0620:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0520:4PHH-HLC-50.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-PHH0.3084410940.1451108810.4717713069.10419E-0524:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-0924:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	20:1	HepG2-HLC-5	1.844624653	1.086573796	2.602675511	1.94759E-06
20:4PHH-HepG211.818168195.89419633917.742140034.21323E-0520:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0524:5HepG2-HLC-30.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-PHH0.3084410940.1451108810.4717713069.10419E-0524:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	20:1	HepG2-PHH	2.205286886	1.329965153	3.080608619	1.08941E-06
20:4PHH-HLC-312.362400427.52549766117.199303188.53755E-0720:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0524:5HepG2-HLC-30.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-PHH0.3084410940.1451108810.4717713069.10419E-0524:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	20:4	PHH-HepG2	11.81816819	5.894196339	17.74214003	4.21323E-05
20:4PHH-HLC-413.061673788.14977580617.973571754.31178E-0720:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0524:5HepG2-HLC-30.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	20:4	PHH-HLC-3	12.36240042	7.525497661	17.19930318	8.53755E-07
20:4PHH-HLC-510.595958325.4656482115.726268432.54284E-0524:5HepG2-HLC-30.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-PHH0.3084410940.1451108810.4717713069.10419E-0524:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	20:4	PHH-HLC-4	13.06167378	8.149775806	17.97357175	4.31178E-07
24:5HepG2-HLC-30.2102272090.0768686490.3435857690.00089153324:5HepG2-HLC-40.2739727690.1385465120.4093990273.44339E-0524:5HepG2-HLC-50.237277350.0958292370.3787254630.00042513424:5HepG2-PHH0.3084410940.1451108810.4717713069.10419E-0524:6HepG2-HLC-30.454415770.3196763320.5891552085.34231E-0924:6HepG2-HLC-40.5045744570.3677459110.6414030039.15416E-1024:6HepG2-HLC-50.4752117580.3322990020.6181245137.02772E-09	20:4	PHH-HLC-5	10.59595832	5.46564821	15.72626843	2.54284E-05
24:5       HepG2-HLC-4       0.273972769       0.138546512       0.409399027       3.44339E-05         24:5       HepG2-HLC-5       0.23727735       0.095829237       0.378725463       0.000425134         24:5       HepG2-PHH       0.308441094       0.145110881       0.471771306       9.10419E-05         24:6       HepG2-HLC-3       0.45441577       0.319676332       0.589155208       5.34231E-09         24:6       HepG2-HLC-4       0.504574457       0.367745911       0.641403003       9.15416E-10         24:6       HepG2-HLC-5       0.475211758       0.332299002       0.618124513       7.02772E-09	24:5	HepG2-HLC-3	0.210227209	0.076868649	0.343585769	0.000891533
24:5       HepG2-HLC-5       0.23727735       0.095829237       0.378725463       0.000425134         24:5       HepG2-PHH       0.308441094       0.145110881       0.471771306       9.10419E-05         24:6       HepG2-HLC-3       0.45441577       0.319676332       0.589155208       5.34231E-09         24:6       HepG2-HLC-4       0.504574457       0.367745911       0.641403003       9.15416E-10         24:6       HepG2-HLC-5       0.475211758       0.332299002       0.618124513       7.02772E-09	24:5	HepG2-HLC-4	0.273972769	0.138546512	0.409399027	3.44339E-05
24:5       HepG2-PHH       0.308441094       0.145110881       0.471771306       9.10419E-05         24:6       HepG2-HLC-3       0.45441577       0.319676332       0.589155208       5.34231E-09         24:6       HepG2-HLC-4       0.504574457       0.367745911       0.641403003       9.15416E-10         24:6       HepG2-HLC-5       0.475211758       0.332299002       0.618124513       7.02772E-09         24.6       HepG2-BLU-4       0.544402625       0.27026725       0.702420121       0.125725	24:5	HepG2-HLC-5	0.23727735	0.095829237	0.378725463	0.000425134
24:6       HepG2-HLC-3       0.45441577       0.319676332       0.589155208       5.34231E-09         24:6       HepG2-HLC-4       0.504574457       0.367745911       0.641403003       9.15416E-10         24:6       HepG2-HLC-5       0.475211758       0.332299002       0.618124513       7.02772E-09         24.6       HepG2-BLU-4       0.544402685       0.27020205       0.2702120121       0.125725	24:5	HepG2-PHH	0.308441094	0.145110881	0.471771306	9.10419E-05
24:6         HepG2-HLC-4         0.504574457         0.367745911         0.641403003         9.15416E-10           24:6         HepG2-HLC-5         0.475211758         0.332299002         0.618124513         7.02772E-09           24:6         HepG2-BLU-5         0.544409685         0.370207325         0.70212121         0.125725	24:6	HepG2-HLC-3	0.45441577	0.319676332	0.589155208	5.34231E-09
24:6         HepG2-HLC-5         0.475211758         0.332299002         0.618124513         7.02772E-09           24:6         HepG2-BLUE         0.544400605         0.37000772E         0.700100101         0.100772E-09	24:6	HepG2-HLC-4	0.504574457	0.367745911	0.641403003	9.15416E-10
	24:6	HepG2-HLC-5	0.475211758	0.332299002	0.618124513	7.02772E-09
24:6 HEPG2-PHH 0.544408685 0.37938725 0.709430121 8.18578E-09	24:6	HepG2-PHH	0.544408685	0.37938725	0.709430121	8.18578E-09

**Detailed statistically significant differences for each comparison, per residue**. Statistically significant differences were determined with ANOVA followed by Tukey's post-hoc test (n=9 HLC-3, n=8 HLC-4, n=6 HLC-5, n=3 PHH and HepG2 samples).

#### Supplementary Table 2

Residue	Comparison	Difference	Lower	Upper	Adjusted p-value
18:3	Overfeeding-Saturated fats	83.0989348	32.55919384	133.6386758	0.001497514
20:1	Saturated fats-Overfeeding	69.95086247	21.33220413	118.5695208	0.004720554
20:1	Unsaturated fats-Overfeeding	79.98050715	31.36184881	128.5991655	0.001490594
20:2	Saturated fats-Overfeeding	37.06273322	1.541102354	72.58436408	0.040064848
20:2	Unsaturated fats-Overfeeding	37.24209302	1.720462156	72.76372389	0.039035724
20:3	Overfeeding-Saturated fats	46.92097803	1.782919941	92.05903611	0.040873888
20:3	Overfeeding-Unsaturated fats	46.96134996	1.82329187	92.09940804	0.040686328
20:4	Saturated fats-Overfeeding	23.63496846	3.364934857	43.90500207	0.02103841
20:4	Unsaturated fats-Overfeeding	31.10317186	10.83313825	51.37320547	0.002767359
20:5	Overfeeding-Saturated fats	22.77345043	0.33089319	45.21600767	0.046393858
20:5	Overfeeding-Unsaturated fats	26.9670954	4.524538156	49.40965264	0.017378353
22:2	Unsaturated fats-Overfeeding	66.11189494	10.99301677	121.2307731	0.01758215
22:3	Saturated fats-Overfeeding	60.9218937	2.183451685	119.6603357	0.041365586
22:4	<b>Overfeeding-Saturated fats</b>	56.98806747	4.495712921	109.480422	0.032177736
22:6	Saturated fats-Overfeeding	29.37200864	11.42672197	47.31729532	0.001561442
22:6	Unsaturated fats-Overfeeding	22.6405984	4.695311727	40.58588508	0.012548342
24:1	Saturated fats-Overfeeding	39.81046071	12.01919479	67.60172662	0.004888639
24:1	Unsaturated fats-Overfeeding	66.73494923	38.94368331	94.52621514	2.47704E-05
26:0	Saturated fats-Unsaturated fats	384.6559913	60.23615386	709.0758288	0.018933907
30:1	Saturated fats-Unsaturated fats	92.89024137	8.0615839	177.7188988	0.030635146

**Detailed statistically significant differences for each comparison, per residue.** Statistically significant differences were determined with ANOVA followed by Tukey's post-hoc test (n=7 subjects per group).

#### **Supplemental Materials and Methods**

**General description**. We have developed liputils as a lightweight Python library focused on text-based recognition of lipid identifiers that can be seamlessly integrated in a Pythonbased data analysis pipeline. Its primary function is to provide fatty acid moieties information from any RefMet-compliant lipid annotation.

An in-depth, Python-based analysis of a dataset is available as Supplemental analysis protocol online in PDF form, or in its native Jupyter notebook file format at the <u>following address</u>.

In the main text, the User is presented with a basic protocol that automatically processes lipidomics data in tabular format in order to extract residue information and package the results into a new, easily readable data table. In here, we will be discussing some useful functions and methods of the library that can be exploited by the more advanced User and suited to personalized analysis pipelines.

**Functionality of the Lipid class**. In liputils, every lipid identifier (a text string) is managed through the Lipid class. Then, lipid properties can be accessed through each object's methods. An example:

>>> from liputils import Lipid
>>> lip = Lipid("Cer(d20:0/22:0)")
>>> lip.name
'Cer(d20:0/22:0)'
>>> lip.refmet\_class()
'Cer'

Lipid.name is produced by the class constructor. The vast majority of other methods are callable, in order to save time when initializing each new Lipid object. In this case, Lipid.refmet\_class() is a method that computes the lipid class, given as abbreviation, upon call. If needed, the amount parameter can be used to define the amount of the lipid being processed (it defaults to picomoles), and to calculate the number of molecules:

>>> lip = Lipid("Cer(d20:0/22:0)", amount=0.12512)

>>> lip.molecules
75349026402.78401

Other units can be specified:

```
>>> lip = Lipid("Cer(d20:0/22:0)", amount=0.12512, unit="attomoles")
>>> lip.molecules
75349.02640278402
```

**Fatty moieties identification**. The backbone of the Lipid class functionality is the ability of decoding from lipid identifiers their carbon chains composition. liputils accepts a generic lipid format in the form of CLASS N:N/M:M/../. or CLASS(N:N/M:M/../.)(other mass isobars), or <u>fully RefMet-compliant residue naming</u>. If unsure about your data format, you can try and batch-translate your lipid IDs with RefMet's online translator. By adhering to RefMet's nomenclature, any compliant lipid name will be properly managed by liputils's method Lipid.refmet\_residues().

```
>>> lip1 = Lipid("octadecatrienoic acid")
>>> lip2 = Lipid("linolenic acid")
>>> lip3 = Lipid("FA(18:3)")
>>> lip4 = Lipid("linoleyl palmitate")
>>> lip1.refmet_residues()
(['18:3'], 1)
>>> lip2.refmet_residues()
(['18:3'], 1)
>>> lip3.refmet_residues()
(['18:3'], 1)
>>> lip4.refmet_residues()
(['18:1', '16:0'], 1)
```

The method returns a list of residues that were found in the lipid identifier, and an integer index that refers to the *ambiguities* found within the lipid identifiers. This feature was introduced to let the User choose what to do in the presence of unresolved mass isobars.

For example, in the case of this non-RefMet compliant lipid identifier taken from a commercial lipidomic analysis:

```
>>> lip = Lipid("TAG 48:2 total (14:0/16:0/18:2)(14:0/16:1/18:1)(16:0/16:1/16:1)")
>>> lip.refmet_residues()
(['48:2', '14:0', '16:0', '18:2', '14:0', '16:1', '18:1', '16:0', '16:1', '16:1'],
3)
```

In this case, liputils reports each residue in the list it returns, but it also returns 3 as ambiguity index, to reflect the fact that the molecular lipid was not fully resolved, and there were three different but equivalent mass isobars.

When using non-Refmet compliant lipids, Users are encouraged to use Lipid.lipid\_class() and Lipid.residues() methods instead:

```
>>> lip.refmet_class() # not appropriate
'TAG 48:2 total'
>>> lip.lipid_class() # appropriate
'TAG'
>>> lip.residues() # same result, in this case
(['14:0', '16:0', '18:2', '14:0', '16:1', '18:1', '16:0', '16:1', '16:1'],
3)
```

If desired, it can be useful to suppress all unresolved mass isobars by setting the drop ambiguous parameter to True (it defaults to False):

>>> lip.residues(drop\_ambiguous=True)
([], 0)

In this case, an empty list is returned together with 0 ambiguity index.

Helper functions. liputils contains some functions that complement the Lipid class functionality. In the manuscript (Materials and Methods  $\rightarrow$  Procedure), the basic use case of make\_residues\_table() is presented. There are parameters that can be set to alter the function's default behavior:

drop\_ambiguous: defaults to False. As in the case mentioned above, this produces a residues table that does not take into account unresolved mass isobars.

- name: as make\_residues\_table() returns a nameless pandas.DataFrame object, this parameters sets a string attribute within the object, under pandas.DataFrame.name, that can be useful when a string identifier for exporting the table to a .csv file (or for otherwise any other use), especially when working with multiple objects simultaneously. Defaults to "residues\_table".
- replace\_nan: this replaces any missing value (empty cells) in the input table with the desired value. It defaults to 0.
- cleanup: this parameter is used to avoid processing some lipids that may be found in the data but are not meaningful to process. These may include, for example, identifiers with "total" (like "total cholesterol"), or abbreviations thereof (like "TC" for total cholesterol, or "FC" for free cholesterol). The list of unwanted terms is read from another parameter, unwanted (see below). It defaults to True.
- unwanted: this parameter defaults to a list of unwanted identifiers, that are altogether skipped in the processing if cleanup is True (the default behavior). This parameter can be replaced by a User-defined list of choice. It defaults to ["total", "fc", "tc"].
- absolute\_amount: this switches the function from counting the actual residues amount, in the same unit as in the input table, to counting in the actual number of residues. For example, if the input table is in picomoles/µg tissue, by default the table produced by make\_residues\_table() will be in picomoles/µg tissue. Otherwise, if absolute\_amount is set to True, then the actual number of residues will be counted. The default unit is "picomoles", but this can be set otherwise by passing another unit as keyword argument. It defaults to False.

In addition to the use case presented in the manuscript, an additional example can be found in the Supplemental analysis protocol at page 5.

Two other functions come handy when processing residues subsets. To focus on particular residues, it is possible to mix saturated() and max\_carbon() to dictate which residues to keep and which to discard. Specifically:

saturated(): its intended use is with string residue identifiers (in the form of \d:\d). It
returns True if the residue contains unsaturations, False otherwise.

max\_carbon(): its intended use is with string residue identifiers (in the form of \d:\d). An integer number of desired carbon atoms must also be specified when calling the function. If

the number of carbon atoms in the residue is lower or equal to the specified maximum allowed value, the function returns True, False otherwise.

Some examples:

```
>>> from liputils import saturated, max_carbon
>>> saturated("12:0")
True
>>> saturated("12:1")
False
>>> max_carbon("12:1", 11)
False
>>> max_carbon("12:1", 12)
True
>>> max_carbon("12:1", 13)
True
```

These functions come handy in *list comprehensions* (especially useful when the result is then used to exclude/include elements in an index):

```
>>> my_residues = ["12:0", "17:1", "24:0", "24:1", "24:2", "26:3"]
```

```
>>> [not saturated(x) and max_carbon(x, 24) for x in my_lipids]
[False, True, False, True, True, False]
```

Conveniently, saturated() can be negated via the not operator if the residue is required to having exactly zero unsaturations.

Example use of these functions can be found in the Supplemental analysis protocol, starting from page 16, when they are used to restrict the plots to specific residues.

**Online Documentation**. As liputils is in active development, the online documentation reflects the latest changes and updates to the library. It can be accessed at <u>liputil's pip</u> package manager page, or in <u>liputil's GitHub repository</u>.