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<http://metlin.scripps.edu> → **CLICK METLIN β Version**

## SIMPLE SEARCH

Mass: 524.405 Tolerance (s): 10 ppm: Neutral Positive Negative M

Charge: Neutral Positive Negative M-NH4 M-NH4 M-H-2H2O M-H-H2O M-K M-ACN+H M-ACN+Na M+2Na-H

Select: all | none

Find Metabolites Reset

Total: 1 Metabolite

METLIN ID	MASS	Appm	NAME	MS/MS	STRUCTURE
4316	[M+H] <sup>+</sup> 524.4074 M 524.4002	4	1-O-octadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine Formula: C27H50NO4P CAS: 77286-66-9	YES	

**Simple Search (New METLIN Feature).** Simple Search allows users to select different adduct(s) as targets for the database search. Also it provides users to select tolerance between Dalton (Da) and parts per million (ppm). The result list will be ordered by Appm.

## BATCH SEARCH

Masses: 162.1124, 246.1699, 288.2173, 232.1546, 257.2478, 283.2834, 281.2472, 285.2793, 229.2164, 496.3373, 522.3542, 524.3720

Charge: Neutral Positive Negative M-NH4 M-H M-H-2H2O M-H-H2O M-K M-ACN+H M-ACN+Na M+2Na-H

Accuracy (ppm): 10

Display Structure:  Remove peptides from search:

Select: all | none

Download result as CSV file

162.1124 m/z  
[161.1020 - 161.1020 daltons]: 1 Metabolite [M+H]<sup>+</sup>  
Metabolite Mass Appm Name Formula CAS MS/MS  
52 161.1020 0 Carnitine C7H13NO3 541-15-1 YES

246.1699 m/z  
[245.1602 - 246.1691 daltons]: 2 Metabolites [M+H]<sup>+</sup>  
Metabolite Mass Appm Name Formula CAS MS/MS  
937 246.1627 0 2-Methylbutylamine C10H21NO4 ND ND  
1941 246.1840 5 Prnacetyl C13H19NS 65660-33-0 YES

288.2173 m/z  
[287.2071 - 287.2129 daltons]: 2 Metabolites [M+H]<sup>+</sup>  
Metabolite Mass Appm Name Formula CAS MS/MS  
3665 287.2056 1 Octadecyl-β-carbitaine C18H35NO4 ND ND  
960 287.2097 1 L-Octadecylamine C18H37NO4 25243-95-2 ND

**Batch Search (New METLIN Feature).** New Batch Search offers users to search features for different adduct(s) as targets for the database search with multiple masses. From the result list, users can download the data in CSV format for easy import to Excel to re-sort data as users need to identify and classify the known and unknown metabolites.

## FRAGMENT SEARCH

Fragment m/z: 104.1072 Tolerance (s): 0.01 Da Mode: Positive IS Fragments with Structure Only

104.1072 m/z [104.0972 - 104.1172 daltons]: 26 Fragments

METLIN ID	Name	Reg. No.	Appm	Element	CE	Predicted Ion Type	Predicted Fragment Structure	Compound Structure
4316	1-O-octadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine	194.979 523.4002	0	40.0	10, 20, 40	[M+H] <sup>+</sup>		
270	Octanephosphocholine	194.1071 291.1028	0	100.0	10, 20, 40	[M+H] <sup>+</sup>		
4316	1-O-octadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine	194.1071 523.3704	0	1.0	40	[M+H] <sup>+</sup>		
4316	1-O-octadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine	194.1071 523.3608	0	2.3	40	[M+H] <sup>+</sup>		
3400	Octadecylphosphocholine	194.1072 301.2028	0	3.7	40	[M+H] <sup>+</sup>		

**Fragment Search (New METLIN Feature).** Users are able to use the newly introduced Fragment/Neutral Loss Search, where users can manually search the MS/MS library by specific MS/MS fragment masses. Fragment structures are predicted using in-silico fragmentation<sup>3</sup>. This permits characterization of chemical functional groups for unknown metabolites (i.e., metabolites currently not in the METLIN database).

## METABOLITE INFORMATION

MID: 43416  
Mass: 524.4002  
Name: 1-Octadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine NOTE: Please click the name  
Formula: C<sub>27</sub>H<sub>50</sub>NO<sub>4</sub>P  
CAS: 77286-66-9  
KEGG: S-Synthetic PAF C-18 Edaphone ET-18-C04  
Notes: [Click here for ISI Web of Knowledge!](#)  
Updated: 0000-00-00 00:00:00  
Created: 0000-00-00 00:00:00  
Drug

Structure

Spectrum

1-O-octadecyl-2-O-methyl-sn-glyceryl-3-phosphorylcholine  
MD: 43416

Mode: (+) Collision Energy: 40 V  
m/z: 104.1072 Intensity: 41.1%

Predicted Fragment Structure [M+H]<sup>+</sup>

## SPECTRUM SEARCH

Preselected m/z: 104.1072, 116.0762, 128.0452, 140.0142, 152.0832, 164.0522, 176.0212, 188.0902, 200.0592, 212.0282, 224.0972, 236.0662, 248.0352, 260.0042, 272.0732, 284.0422, 296.0112, 308.0802, 320.0492, 332.0182, 344.0872, 356.0562, 368.0252, 380.0942, 392.0632, 404.0322, 416.0012, 428.0702, 440.0392, 452.0082, 464.0772, 476.0462, 488.0152, 500.0842, 512.0532, 524.0222, 536.0912, 548.0602, 560.0292, 572.0982, 584.0672, 596.0362, 608.0052, 620.0742, 632.0432, 644.0122, 656.0812, 668.0502, 680.0192, 692.0882, 704.0572, 716.0262, 728.0952, 740.0642, 752.0332, 764.0022, 776.0712, 788.0402, 800.0092, 812.0782, 824.0472, 836.0162, 848.0852, 860.0542, 872.0232, 884.0922, 896.0612, 908.0302, 920.0992, 932.0682, 944.0372, 956.0062, 968.0752, 980.0442, 992.0132, 1004.0822, 1016.0512, 1028.0202, 1040.0892, 1052.0582, 1064.0272, 1076.0962, 1088.0652, 1100.0342, 1112.0032, 1124.0722, 1136.0412, 1148.0102, 1160.0792, 1172.0482, 1184.0172, 1196.0862, 1208.0552, 1220.0242, 1232.0932, 1244.0622, 1256.0312, 1268.0002, 1280.0692, 1292.0382, 1304.0072, 1316.0762, 1328.0452, 1340.0142, 1352.0832, 1364.0522, 1376.0212, 1388.0902, 1400.0592, 1412.0282, 1424.0972, 1436.0662, 1448.0352, 1460.0042, 1472.0732, 1484.0422, 1496.0112, 1508.0802, 1520.0492, 1532.0182, 1544.0872, 1556.0562, 1568.0252, 1580.0942, 1592.0632, 1604.0322, 1616.0012, 1628.0702, 1640.0392, 1652.0082, 1664.0772, 1676.0462, 1688.0152, 1700.0842, 1712.0532, 1724.0222, 1736.0912, 1748.0602, 1760.0292, 1772.0982, 1784.0672, 1796.0362, 1808.0052, 1820.0742, 1832.0432, 1844.0122, 1856.0812, 1868.0502, 1880.0192, 1892.0882, 1904.0572, 1916.0262, 1928.0952, 1940.0642, 1952.0332, 1964.0022, 1976.0712, 1988.0402, 2000.0092, 2012.0782, 2024.0472, 2036.0162, 2048.0852, 2060.0542, 2072.0232, 2084.0922, 2096.0612, 2108.0302, 2120.0992, 2132.0682, 2144.0372, 2156.0062, 2168.0752, 2180.0442, 2192.0132, 2204.0822, 2216.0512, 2228.0202, 2240.0892, 2252.0582, 2264.0272, 2276.0962, 2288.0652, 2300.0342, 2312.0032, 2324.0722, 2336.0412, 2348.0102, 2360.0792, 2372.0482, 2384.0172, 2396.0862, 2408.0552, 2420.0242, 2432.0932, 2444.0622, 2456.0312, 2468.0002, 2480.0692, 2492.0382, 2504.0072, 2516.0762, 2528.0452, 2540.0142, 2552.0832, 2564.0522, 2576.0212, 2588.0902, 2600.0592, 2612.0282, 2624.0972, 2636.0662, 2648.0352, 2660.0042, 2672.0732, 2684.0422, 2696.0112, 2708.0802, 2720.0492, 2732.0182, 2744.0872, 2756.0562, 2768.0252, 2780.0942, 2792.0632, 2804.0322, 2816.0012, 2828.0702, 2840.0392, 2852.0082, 2864.0772, 2876.0462, 2888.0152, 2900.0842, 2912.0532, 2924.0222, 2936.0912, 2948.0602, 2960.0292, 2972.0982, 2984.0672, 2996.0362, 3008.0052, 3020.0742, 3032.0432, 3044.0122, 3056.0812, 3068.0502, 3080.0192, 3092.0882, 3104.0572, 3116.0262, 3128.0952, 3140.0642, 3152.0332, 3164.0022, 3176.0712, 3188.0402, 3200.0092, 3212.0782, 3224.0472, 3236.0162, 3248.0852, 3260.0542, 3272.0232, 3284.0922, 3296.0612, 3308.0302, 3320.0992, 3332.0682, 3344.0372, 3356.0062, 3368.0752, 3380.0442, 3392.0132, 3404.0822, 3416.0512, 3428.0202, 3440.0892, 3452.0582, 3464.0272, 3476.0962, 3488.0652, 3500.0342, 3512.0032, 3524.0722, 3536.0412, 3548.0102, 3560.0792, 3572.0482, 3584.0172, 3596.0862, 3608.0552, 3620.0242, 3632.0932, 3644.0622, 3656.0312, 3668.0002, 3680.0692, 3692.0382, 3704.0072, 3716.0762, 3728.0452, 3740.0142, 3752.0832, 3764.0522, 3776.0212, 3788.0902, 3800.0592, 3812.0282, 3824.0972, 3836.0662, 3848.0352, 3860.0042, 3872.0732, 3884.0422, 3896.0112, 3908.0802, 3920.0492, 3932.0182, 3944.0872, 3956.0562, 3968.0252, 3980.0942, 3992.0632, 4004.0322, 4016.0012, 4028.0702, 4040.0392, 4052.0082, 4064.0772, 4076.0462, 4088.0152, 4100.0842, 4112.0532, 4124.0222, 4136.0912, 4148.0602, 4160.0292, 4172.0982, 4184.0672, 4196.0362, 4208.0052, 4220.0742, 4232.0432, 4244.0122, 4256.0812, 4268.0502, 4280.0192, 4292.0882, 4304.0572, 4316.0262, 4328.0952, 4340.0642, 4352.0332, 4364.0022, 4376.0712, 4388.0402, 4400.0092, 4412.0782, 4424.0472, 4436.0162, 4448.0852, 4460.0542, 4472.0232, 4484.0922, 4496.0612, 4508.0302, 4520.0992, 4532.0682, 4544.0372, 4556.0062, 4568.0752, 4580.0442, 4592.0132, 4604.0822, 4616.0512, 4628.0202, 4640.0892, 4652.0582, 4664.0272, 4676.0962, 4688.0652, 4700.0342, 4712.0032, 4724.0722, 4736.0412, 4748.0102, 4760.0792, 4772.0482, 4784.0172, 4796.0862, 4808.0552, 4820.0242, 4832.0932, 4844.0622, 4856.0312, 4868.0002, 4880.0692, 4892.0382, 4904.0072, 4916.0762, 4928.0452, 4940.0142, 4952.0832, 4964.0522, 4976.0212, 4988.0902, 5000.0592, 5012.0282, 5024.0972, 5036.0662, 5048.0352, 5060.0042, 5072.0732, 5084.0422, 5096.0112, 5108.0802, 5120.0492, 5132.0182, 5144.0872, 5156.0562, 5168.0252, 5180.0942, 5192.0632, 5204.0322, 5216.0012, 5228.0702, 5240.0392, 5252.0082, 5264.0772, 5276.0462, 5288.0152, 5300.0842, 5312.0532, 5324.0222, 5336.0912, 5348.0602, 5360.0292, 5372.0982, 5384.0672, 5396.0362, 5408.0052, 5420.0742, 5432.0432, 5444.0122, 5456.0812, 5468.0502, 5480.0192, 5492.0882, 5504.0572, 5516.0262, 5528.0952, 5540.0642, 5552.0332, 5564.0022, 5576.0712, 5588.0402, 5600.0092, 5612.0782, 5624.0472, 5636.0162, 5648.0852, 5660.0542, 5672.0232, 5684.0922, 5696.0612, 5708.0302, 5720.0992, 5732.0682, 5744.0372, 5756.0062, 5768.0752, 5780.0442, 5792.0132, 5804.0822, 5816.0512, 5828.0202, 5840.0892, 5852.0582, 5864.0272, 5876.0962, 5888.0652, 5900.0342, 5912.0032, 5924.0722, 5936.0412, 5948.0102, 5960.0792, 5972.0482, 5984.0172, 5996.0862, 6008.0552, 6020.0242, 6032.0932, 6044.0622, 6056.0312, 6068.0002, 6080.0692, 6092.0382, 6104.0072, 6116.0762, 6128.0452, 6140.0142, 6152.0832, 6164.0522, 6176.0212, 6188.0902, 6200.0592, 6212.0282, 6224.0972, 6236.0662, 6248.0352, 6260.0042, 6272.0732, 6284.0422, 6296.0112, 6308.0802, 6320.0492, 6332.0182, 6344.0872, 6356.0562, 6368.0252, 6380.0942, 6392.0632, 6404.0322, 6416.0012, 6428.0702, 6440.0392, 6452.0082, 6464.0772, 6476.0462, 6488.0152, 6500.0842, 6512.0532, 6524.0222, 6536.0912, 6548.0602, 6560.0292, 6572.0982, 6584.0672, 6596.0362, 6608.0052, 6620.0742, 6632.0432, 6644.0122, 6656.0812, 6668.0502, 6680.0192, 6692.0882, 6704.0572, 6716.0262, 6728.0952, 6740.0642, 6752.0332, 6764.0022, 6776.0712, 6788.0402, 6800.0092, 6812.0782, 6824.0472, 6836.0162, 6848.0852, 6860.0542, 6872.0232, 6884.0922, 6896.0612, 6908.0302, 6920.0992, 6932.0682, 6944.0372, 6956.0062, 6968.0752, 6980.0442, 6992.0132, 7004.0822, 7016.0512, 7028.0202, 7040.0892, 7052.0582, 7064.0272, 7076.0962, 7088.0652, 7100.0342, 7112.0032, 7124.0722, 7136.0412, 7148.0102, 7160.0792, 7172.0482, 7184.0172, 7196.0862, 7208.0552, 7220.0242, 7232.0932, 7244.0622, 7256.0312, 7268.0002, 7280.0692, 7292.0382, 7304.0072, 7316.0762, 7328.0452, 7340.0142, 7352.0832, 7364.0522, 7376.0212, 7388.0902, 7400.0592, 7412.0282, 7424.0972, 7436.0662, 7448.0352, 7460.0042, 7472.0732, 7484.0422, 7496.0112, 7508.0802, 7520.0492, 7532.0182, 7544.0872, 7556.0562, 7568.0252, 7580.0942, 7592.0632, 7604.0322, 7616.0012, 7628.0702, 7640.0392, 7652.0082, 7664.0772, 7676.0462, 7688.0152, 7700.0842, 7712.0532, 7724.0222, 7736.0912, 7748.0602, 7760.0292, 7772.0982, 7784.0672, 7796.0362, 7808.0052, 7820.0742, 7832.0432, 7844.0122, 7856.0812, 7868.0502, 7880.0192, 7892.0882, 7904.0572, 7916.0262, 7928.0952, 7940.0642, 7952.0332, 7964.0022, 7976.0712, 7988.0402, 8000.0092, 8012.0782, 8024.0472, 8036.0162, 8048.0852, 8060.0542, 8072.0232, 8084.0922, 8096.0612, 8108.0302, 8120.0992, 8132.0682, 8144.0372, 8156.0062, 8168.0752, 8180.0442, 8192.0132, 8204.0822, 8216.0512, 8228.0202, 8240.0892, 8252.0582, 8264.0272, 8276.0962, 8288.0652, 8300.0342, 8312.0032, 8324.0722, 8336.0412, 8348.0102, 8360.0792, 8372.0482, 8384.0172, 8396.0862, 8408.0552, 8420.0242, 8432.0932, 8444.0622, 8456.0312, 8468.0002, 8480.0692, 8492.0382, 8504.0072, 8516.0762, 8528.0452, 8540.0142, 8552.0832, 8564.0522, 8576.0212, 8588.0902, 8600.0592, 8612.0282, 8624.0972, 8636.0662, 8648.0352, 8660.0042, 8672.0732, 8684.0422, 8696.0112, 8708.0802, 8720.0492, 8732.0182, 8744.0872, 8756.0562, 8768.0252, 8780.0942, 8792.0632, 8804.0322, 8816.0012, 8828.0702, 8840.0392, 8852.0082, 8864.0772, 8876.0462, 8888.0152, 8900.0842, 8912.0532, 8924.0222, 8936.0912, 8948.0602, 8960.0292, 8972.0982, 8984.0672, 8996.0362, 9008.0052, 9020.0742, 9032.0432, 9044.0122, 9056.0812, 9068.0502, 9080.0192, 9092.0882, 9104.0572, 9116.0262, 9128.0952, 9140.0642, 9152.0332, 9164.0022, 9176.0712, 9188.0402, 9200.0092, 9212.0782, 9224.0472, 9236.0162, 9248.0852, 9260.0542, 9272.0232, 9284.0922, 9296.0612, 9308.0302, 9320.0992, 9332.0682, 9344.0372, 9356.0062, 9368.0752, 9380.0442, 9392.0132, 9404.0822, 9416.0512, 9428.0202, 9440.0892, 9452.0582, 9464.0272, 9476.0962, 9488.0652, 9500.0342, 9512.0032, 9524.0722, 9536.0412, 9548.0102, 9560.0792, 9572.0482, 9584.0172, 9596.0862, 9608.0552, 9620.0242, 9632.0932, 9644.0622, 9656.0312, 9668.0002, 9680.0692, 9692.0382, 9704.0072, 9716.0762, 9728.0452, 9740.0142, 9752.0832, 9764.0522, 9776.0212, 9788.0902, 9800.0592, 9812.0282, 9824.0972, 9836.0662, 9848.0352, 9860.0042, 9872.0732, 9884.0422, 9896.0112, 9908.0802, 9920.0492, 9932.0182, 9944.0872, 9956.0562, 9968.0252, 9980.0942, 9992.0632, 10004.0322, 10016.0012, 10028.0702, 10040.0392,