0.08	metabolite = r_0652 0.08 0.06 0.04 0.02 0.00 -0.02		metabolite = r_1355 0.08 0.06 0.04 0.02 0.00 0.00 0.00 0.00 0.00	metabolite = r_1356  0.08  0.06  0.04  0.02  0.00  -0.02	metabolite = r_1164  0.08  0.06  0.04  0.02  0.00  -0.02	metabolite = r_1163
-0.04 - -0.06 - -0. 0.3 - 0.2 - 0.1 - 0.0 -	-0.04 -0.06 15-0.10-0.05 0.00 0.05 0.10 0.15 0.20 metabolite = r_0111 0.15 0.10	-0.15 -0.10 -0.05 0.00 0.05 0.10 0.15 0.20  metabolite = r_0232	0.4	metabolite = r_0726 0.20 - 0.15 - 0.10 - 0.05 -	metabolite = r 1091	0.10 -0.05 0.00 0.05 0.10 0.15 0.20 metabolite = r_0536
0.0 - -0.1 - -0.2 - -0 0.15 - 0.10 -	0.00 -0.05 -0.10 .8 -0.6 -0.4 -0.2 0.0 0.2 0.4 metabolite = r_0527 0.15	-0.15 -0.10 -0.05 0.00 0.05 0.10 0.15 0.20  metabolite = r_0528	-0.05 -0.2 -0.3 -0.10	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	-0.05 -0.10 -0.15 0.3 -0.2 -0.1 0.0 0.1 0.2 - metabolite = r_1301 0.25 0.20	0.250.200.150.100.050.000.050.100.150.20 metabolite = r_0235
0.05 – 0.00 – 0.05 – 0.10 – 0.15 – 0.05	0.05 0.00 -0.05 -0.10 -0.15 25-0.20-0.15-0.10-0.050.00 0.05 0.10 0.15 0.20 metabolite = r_0190		$0.05 - 0.00 - 0.00 - 0.05$ $0.05 - 0.00 - 0.05$ $0.10 - 0.15 - 0.15$ $-0.250.200.150.100.050.000.050.100.150.20$ metabolite = $r_0725$			0.15 -0.10 -0.05 0.00 0.05 0.10 0.15 0.20 metabolite = r_0525
0.20 - 0.15 - 0.10 - 0.05 - 0.05 - 0.05 - 0.10 - 0.15 - 0.20 - 0.25	0.15 0.10 0.05 0.00 -0.05		0.15 0.10 0.05 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.06 - 0.04 - 0.02 - 0.02 - 0.04 - 0.06 - 0.	0.06 0.04 0.02 0.00 -0.02 -0.04 -0.06	Thetabolite = 1_0323
-0.25 - -0 0.08 - 0.06 - 0.04 - 0.02 - 0.00 - 0.02 -	-0.10 .5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 metabolite = r_1036 0.08 0.06 0.04 0.02 0.00 -0.02	-0.15 -0.10 -0.05 0.00 0.05 0.10  metabolite = r_1041	0.20	metabolite = $r_1505$ 0.06	metabolite = r 0239	
-0.04 - -0.06 - -0.08 - -0. 0.20 - 0.15 - 0.10 -	metabolite = r 1387	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0.15 -0.15	-0.04 -0.08-0.06-0.04-0.02 0.00 0.02 0.04 0.06 0.08 -0.08-0.08-0.08-0.08-0.08-0.08-0.0	metabolite = r_0691 0.20 0.15 0.10	
0.05 – 0.00 – 0.05 – 0.10 – 0.15 – 0.3 –	0.05 0.00 -0.05 -0.10 10-0.05 0.00 0.05 0.10 0.15 0.20 0.25 metabolite = r_1325 0.3	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.05 - 0.00 - 0.05 0.00 -0.05 - 0.10 -0.15 - 0.15 -	metabolite = r 1035	metabolite = r 0898	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
0.2 - 0.1 - 0.0 - 0.10.10.20.3 -	0.2 0.1 0.0 -0.1 -0.2 -0.3 .2 -0.1 0.0 0.1 0.2 0.3 0.4		0.10 - 0.05 - 0.05 - 0.00 - 0.05 - 0.10 - 0.15 - 0.20 - 0.15 - 0.10 - 0.05 0.00 - 0.05 - 0.10 - 0.15	0.2 - 0.1 - 0.0 - 0.1 - 0.2 - 0.3 - 0.4 - 0.5 -	0.25 0.20 0.15 0.10 0.05 0.00 -0.05 0.8 -0.6 -0.4 -0.2 0.0 0.2 0.4	
0.6 - 0.4 - 0.2 - 0.0 - 0.4 -	metabolite = r_1769  0.15  0.10  0.05  0.00  -0.05  -0.10	metabolite = r_0817	metabolite = r_0493  0.20  0.15  0.10  0.05  0.00  0.05  0.00  -0.05  0.10  -0.10	metabolite = r_0648	metabolite = r_1057	metabolite = r_1058
0.4 - -0.6 - -1 0.25 - 0.20 - 0.15 - 0.10 - 0.05 - 0.00 -	metabolita = r. 1524	metabolite = r_0866	0.7	metabolite = r_1372	metabolite = r 1373	-0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5  metabolite = r_0580
-0.10 - -0.15 - -0.20 -	-0.10 -0.15 -0.20	metabolite = r_0915	0.3 - 0.1 0.1 - 0.2 0.0 - 0.2 0.4 0.6 - 0.3 -0.2 0.0 0.2 0.4 0.6 - 0.15 0.15 0.10 - 0.15	-0.10.20.30.10-0.050.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35  metabolite = r_1391  0.8 - 0.6 -	-0.1 -0.2 -0.3 0.100.050.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 metabolite = r_1517 0.4 0.3	0.100.050.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35  metabolite = r_0897
0.3 - 0.2 - 0.1 - 0.0 - -0.1 - -0.2 - -0	0.05 0.00 -0.05 -0.10 -0.15 -0.20 -0.25 .8 -0.6 -0.4 -0.2 0.0 0.2	-0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8 1.0		0.4 - 0.2 - 0.0 -0.2 - 0.4 -0.2 0.0 0.2 0.4 0.6 0.8 1.0 - 0.4 - 0.2 0.0 0.2 0.4 0.8 0.8 1.0 - 0.4 - 0.2 0.0 0.2 0.4 0.8 0.8 1.0 - 0.4 - 0.2 0.0 0.2 0.4 0.8 0.8 1.0 - 0.4 - 0.2 0.0 0.2 0.4 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8 0.8		-0.6 -0.4 -0.2 0.0 0.2
0.06 - 0.04 - 0.02 - 0.02 - 0.04 - 0.04 0.06 0.08 0.10 - 0.1	metabolite = r_1370  0.6  0.4  0.2  0.0  -0.2		metabolite = r_0221  0.4  0.05  0.00  0.05  0.10  -0.2  0.10  -0.4  -0.6  0.15  -0.8  -1.0  0.25	metabolite = r_0791  0.4  0.2  0.0  -0.2  -0.4  -0.6  -0.8  -1.0  -1.2	metabolite = r_0731	
	metabolite = r_0398 0.7 0.6 0.5 0.4 0.3 0.2 0.1	-1.0-0.8-0.6-0.4-0.2 0.0 0.2 0.4 0.6 0.8  metabolite = r_1518		-1.5 -1.0 -0.5 0.0 0.5 1.0 -  metabolite = r_0513  0.06	metabolite = $r$ 0510	
-0.15 - -0.20 - -0 0.06 - 0.04 - 0.02 -	metabolite = r_0515 0.06 0.04 0.02 0.00	-0.8 -0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8  metabolite = r_0551	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	-0.08 -0.01 -0.01 -0.10	-0.08 -0.10 0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 -	-0.3 -0.2 -0.1 0.0 0.1 0.2 0.3  metabolite = r_0061
0.00 - 0.02 - 0.04 - 0.06 - 0.08 - 0.10 - 0.3 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.2 - 0.3 - 0.2 - 0.2 - 0.3 - 0.2 - 0.2 - 0.3 - 0.2 - 0.2 - 0.3 - 0.2 - 0.2 - 0.3 - 0.2 - 0.2 - 0.3 - 0.2 -	-0.02 -0.04 -0.06 -0.08 -0.10 .3 -0.2 -0.1 0.0 0.1 0.2 0.3 metabolite = r_0578	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	metabolite = $r = 0.575$	metabolite = $r = 1504$	-0.6 -0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2  metabolite = r 1763
0.2 - 0.1 - 0.0 - 0.1 - -0.2 - -0.3 -	0.4 0.2 0.0 -0.2 -0.1 0.0 0.1 0.2 0.3	2	0.02 - 0.00 - 0.01 0.0 0.1 0.2 0.3 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3	0.08 · 0.06 · 0.04 · 0.02 · 0.00 · 0.00 · 0.02 · 0.	0.2 0.0 -0.2 -0.4 -0.6 -0.8	-4 -3 -2 -1 0 1 2 3 4 5
0.15 - 0.10 - 0.05 0.05 0.10 - 0.10 -	metabolite = r_0350 0.06 0.04 0.02 0.00 -0.02 -0.04		0.06   metabolite = r_0549   0.06   0.04   0.02   0.00   0.00   0.00   0.00   0.00   0.00   0.004   0.	metabolite = r_1021	metabolite = r_0539 0.06 0.04 0.02 0.00 -0.02 -0.04	
-0.15 - -0.06 - 0.04 - 0.02 - 0.00 -	-0.06 15 -0.10 -0.05 0.00 0.05 0.10 0.15 metabolite = r_1302 0.06 0.04 0.02 0.00 -0.02	-0.04 -0.02 0.00 0.02 0.04 0.06 0.08 0.10  metabolite = r_1303	metabolite = $r_0268$ 0.6  0.4  0.2  0.0  -0.2	metabolite = r_0132	metabolite = $r$ 0277	
-0.04 - -0.06 - -0. 0.6 - 0.4 - 0.2 -	metabolite = r_0710 0.4 0.2 0.0	metabolite = r_0130	0.5 $0.4 - 0.05$ 0.00 metabolite = r_0262 0.10 0.05	metabolite = r_0646 0.10 - 0.05 - 0.00 -	-0.10 -0.15 0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 -	0.15 -0.10 -0.05 0.00 0.05 0.10 0.15  metabolite = r_1182  FDR < 5%  FDR >= 5%
-0.4 - -0.6 - -0.8 -	-0.2 -0.4 -0.6 -0.8 -0.8 -1.0 .0 -0.8 -0.6 -0.4 -0.2 0.0 0.2 0.4 metabolite = r_1442 0.10 0.05	-1.5 -1.0 -0.5 0.0 0.5 1.0  metabolite = r_0697	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	-0.150.200.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 -  metabolite = r 1291	metabolite = r_1186	-0.4 -0.2 0.0 0.2 0.4 0.6 metabolite = r_0890
0.05 –  page 0.00 –  0.05 –  -0.05 –  -0.10 –	0.00 -0.05 -0.10 -0.15 -0.20 -0.25	0 -	0.00 - 0.05 0.05 - 0.10 - 0.15 0.15 - 0.20 - 0.25	0.04 · 0.02 · 0.00 · 0.	0.3 0.2 0.1 0.0 -0.1 -0.2 0.6 -0.4 -0.2 0.0 0.2 0.4 0.6	
0.20 - 0.15 - 0.10 - 0.00 - 0.05 0.10 -	metabolite = r_0352		metabolite = r_0651  0.15  0.10  0.05  0.00  0.05  0.10  0.05  0.10  0.15  0.10  0.15  0.20  0.15		metabolite = r_0588  0.1  0.0  -0.1  -0.2	
-0.15 - 0.10 - 0.05 - 0	-0.08 15 -0.10 -0.05 0.00 0.05 0.10 0.15 metabolite = r_0174 0.06 0.04 0.02 0.00 -0.02 -0.04	-0.15 -0.10 -0.05 0.00 0.05 0.10  metabolite = r_1368	0.06   metabolite = r_0234	metabolita = r 0303	metabolite = r_1369 0.10 0.05 0.00 -0.05 -0.10	_
-0.10 - -0.15 - -0. 0.5 - 0.4 -	-0.06 -0.08 -0.10 06 -0.04 -0.02 0.00 0.02 0.04 0.06 metabolite = r_0048 0.06 0.04 0.02 0.00	-0.20-0.15-0.10-0.050.00 0.05 0.10 0.15 0.20  metabolite = r_0229	-0.15 -0.20 -0.06	metabolita = r. 0671	metabolite = $r$ 0173	0.30-0.25-0.20-0.15-0.10-0.05 0.00 0.05 0.10  metabolite = r_0885
0.3 - 0.2 - 0.1 - 0.0 - 0.1 - 0.0 - 0.1 - 0.0 - 0.1 - 0.0 -	-0.02 -0.04 -0.06 -0.08 -0.10 -0.12 .5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 metabolite = r_0606 0.10	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0.2 ${7}$ metabolite = r_1027	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	metabolite = r_0226 0.30	-0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8
0.4 -  0.2 -  0.0 -  0.4 -  0.6 -  -0.6 -  -0.6 -	0.05 0.00 -0.05 -0.10 -0.15 -0.20 .6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8		0.1 - 0.6 0.0 - 0.1 - 0.2 -0.2 - 0.30.4 -0.4 - 0.6 -0.5 - 0.7 - 0.6 - 0.5 - 0.4 - 0.3 - 0.2 - 0.1 0.0 0.1	0.04 : 0.02 : 0.00 : 0.00 : -0.02 : -0.04 : -0.06 : -0.06 : -0.08 : -0.06 -0.5 -0.4 -0.3 -0.2 -0.1 0.0 0.1 -0.0	0.15 0.10 0.05 0.00 -0.05 -0.10	
0.15 7 0.10 - 0.05 - 0.00 - 0.05 - -0.10 -	metabolite = r_0424 0.15 0.10 0.05 0.00 -0.05 -0.10	metabolite = r_0440	metabolite = $r_0494$ 1.5  1.0  0.5  -0.5  -1.0  -0.5	metabolite = r_1033	metabolite = r_0524  0.15  0.10  0.05  0.00  -0.05  -0.10  -0.15	metabolite = r 0662
0.12 - 0.10 - 0.08 - 0.06 - 0.04 -	metabolite = r_0787 0.12 0.10 0.08 0.06 0.04	-0.250.200.150.100.050.000.050.100.150.20  metabolite = r_1010	-0.2 0.0 0.2 0.4 0.6 0.8 1.0 1.2  metabolite = r_0633  0.12  0.10  0.08  0.06  0.04	metabolite = r_1004	-0.20 0.2 0.0 0.2 0.4 0.6 0.8 1.0 1.2	-1.0 -0.5 0.0 0.5 1.0 1.5 2.0  metabolite = r_1764
0.02 - 0.00 - -0.02 - -0. 0.8 - 0.6 - 0.4 -	metabolite = r_0297 0.20 0.15 0.10	metabolite = r_0090	0.25 0.20 - 0.15 0.10 - 0.15	0.02 - 0.00 - 0.	metabolite = $r \cdot 0.155$	-0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 metabolite = r_1056
0.0 - 0.2 0.4 0.6 0.8 0.2 - 0.2	0.05 0.00 -0.05 -0.10 -0.15	65 - C C C C C C C C C C C C C C C C C C	0.10 0.05 0.00 0.05 0.10	-0.050.100.150.200.250.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 - metabolite = r_0619  0.15 -	0.0 -0.2 -0.4 -0.6 -0.8 0.2 0.0 0.2 0.4 0.6 0.8 1.0 1.2 metabolite = r_1439	-0.2 -0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 metabolite = r_1332
0.1 -  0.0 -  0.0 -  0.1 -  0.1 -  0.2 -  -0.3 -  -0.4 -	0.1 0.0 -0.1 -0.2 -0.3 -0.4 -0.4 -0.2 0.0 0.2 0.4		0.1 - 0.00 - 0.15 0.00 - 0.05 -0.1 - 0.00 -0.2 - 0.3 - 0.15 -0.4 - 0.2 0.0 0.2 0.4 - 0.25	0.10 - 0.05 - 0.00 - 0.010 - 0.10 - 0.15 - 0	0.1 0.0 -0.1 -0.2 -0.3 0.25-0.20-0.15-0.10-0.050.00 0.05 0.10 0.15 0.20	
0.1 – 0.0 – 0.1 – -0.2 –	metabolite = r_0925	metabolite = r_0331	0.3 metabolite = r_0609  0.3	metabolite = r. 1185	metabolite = $r$ 1184	metabolite = r_1181
-0.3 - -0 0.20 - 0.15 - 0.10 - 0.05 - 0.00 -	metabolite = r_0453 0.3 0.2 0.1 0.0	-0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4  metabolite = r_0734	1.5   metabolite = r_0062   0.5   0.4   0.3   0.5   0.1   0.0   0.0	metabolite = r_0069 0.15 0.10 0.05 0.00 -0.05	metabolite = r_0661	_
-0.10 - -0.15 - -0.20 - -0. 0.5 - 0.4 - 0.3 -	-0.1 -0.2 -0.3 25-0.200.15-0.100.050.0000.050.100.150.20 metabolite = r_0487 0.10 0.05 0.00	-0.30-0.25-0.20-0.15-0.10-0.050.00 0.05 0.10  metabolite = r_0790	-0.50.1 -0.2 -0.3 -1.50.4	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	-0.05 -0.10 -0.15 -0.20 0.4 -0.2 0.0 0.2 0.4 0.6 0.8 1.0 -  metabolite = r_0792  0.3  0.2  0.1	-0.4 -0.3 -0.2 -0.1 0.0 0.1 0.2 0.3 0.4  metabolite = r_0224
90.2 - 0.1 - 0.1 - 0.1 - 0.2 - 0.3 - 0.10	-0.05 -0.10 -0.15 -0.20 08-0.06-0.04-0.02 0.00 0.02 0.04 0.06 0.08 metabolite = r_0233 0.20	-0.1 0.0 0.1 0.2 0.3 0.4 0.5  metabolite = r_0195	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	metabolite = r_1329 0.20	-0.1 0.0 0.1 0.2 0.3 0.4 0.5  metabolite = r 1330
0.05 -  p 0.00 -  0.05 -  -0.05 -  -0.10 -  -0.15 -	0.15 0.10 0.05 0.00 -0.05 -0.10 -0.15 -0.20 -0.25		1.5 - 0.15 1.0 - 0.05 0.0 - 0.05 -0.05 - 0.10 -0.05 -0.10 - 0.15 -0.10 - 0.20 -0.25	0.15 - 0.10 - 0.05 - 0.00 - 0.15 - 0.10 - 0.15 - 0.20 - 0.25 - 0.25	0.15 0.10 0.05 0.00 -0.05 -0.10 -0.15 -0.20 -0.25	
0.3 - 0.2 - 0.1 - 0.0 - -0.1 - -0.2 -	metabolite = r_0026  0.5  0.4  0.3  0.2  0.1  0.0  -0.1	4 - 3 - 2 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1	0.6	metabolite = $r = 0.066$	metabolite = r 1073	
-0.3 - -0.4 - -0.5 - 0.25 - 0.20 - 0.15 - 0.10 - 0.05 - 0.00 -	-0.2 -0.3 15 -0.10 -0.05 0.00 0.05 0.10 metabolite = r_0065		-0.80.15 -1.00.20	-0.3	-0.3	0.15 -0.10 -0.05 0.00 0.05 0.10 measured
-0.10 - -0.15 - -0.20 -	20 -0.15 -0.10 -0.05 0.00 0.05 0.10 measured					