# **Supplemental Information**

## Supplemental Table S1 Demographic details from Dupuytren and Carpal

Tunnel cases.

Patient No.	Patient Group	Technique	Patient ID	Age	Gender	Ethnic Background	Anatomical Tissue Location
1			DD8	77	Male	White	Nodule, Cord, Fascia
2			DD9	58	Male	White	Nodule, Cord, Fascia, Fat, SON
3	Cohort A	Metabolic Fingerprint	DD10	76	Male	White	Nodule, Cord, Fascia
4			DD11	67	Male	White	Nodule, Cord, Fascia, Fat, SON
5			DD12	52	Male	White	Nodule, Cord, Fascia, Fat, SON
6			DD13	74	Female	White	Nodule, Cord, Fascia, Fat, SON
7		Analysis with FT-IR	DD2	71	Male	White	Nodule, Cord, Fascia, Fat, SON
8		Experiment 1	DD17	67	Male	White	Cord, Fascia
9			DD18	68	Male	White	Nodule, Cord
10	Cohort B		CT5	78	Male	White	Fascia
11			CT6	62	Female	White	Fascia
12			CT7	50	Female	White	Fascia
13			CT8	28	Male	White	Fascia
14	Cohort C	Metabolic Identification with GC-MS Experiment 2	DD44	64	Male	White	Nodule, Cord, Fascia
15			DD60	67	Male	White	Nodule, Cord, Fascia
16			DD61	77	Male	White	Nodule, Cord, Fascia

**Supplemental Table S2** List of categories and the sample set chosen for chemometric analyses of FT-IR and GC-MS data.

Experiment	<b>Patient Cohort</b>	Sample set
1.1 Metabolic Fingerprinting	A,B	DD N,C, <b>F</b>
1.2 Metabolic Fingerprinting	В	DD N,C, <b>F</b> & CT F*
1.3 Metabolic Fingerprinting	A,B	DD N,C, <b>F</b> ,T,S
1.4 Metabolic Fingerprinting	A,B	DD N,C, <b>F</b> ,T,S (Passage 0-6)
1.5 Metabolic Footprinting	А	DD N,C, <b>F</b>
2 Metabolic Profiling	С	DD N,C, <b>F</b>

\*external control, N=Nodule, C=Cord, **F**=Fascia (internal control), T=Fat, S=Skin overlying nodule

### **Supplemental Table S3**

Table S3 List of 69 known detected metabolite features (peaks) and their involvement in corresponding pathways. 'Yes' to Definitive ID = the metabolite in the sample has matched (by retention index and mass spectrum) to an authentic chemical standard present in MMD's EI-MS mass spectral library. 'No' = the mass spectrum only matches to a metabolite in other mass spectral libraries (i.e. not the Manchester library). Definitive ID = Due to the nature of the analysis, not all metabolites detected can be accurately identified and some have similar chemical structure and were assigned by best possible match score. Γ

Immethylamice-Noxide       no         2       HMABR032       cystine       yes         3       HMABR032       cystine       yes         4       HMABR032       cystine       yes         5       HMABR032       leucine       yes         5       HMABR032       leucine       yes         8       HMABR032       givene       yes         9       HMABR032       givene       yes         11       HMABR0332       givene       yes         12       HMABR0332       givene       yes         13       HMABR0332       givene       yes         14       HMABR034       cystsine       yes         15       HMABR0353       givene       yes         16       HMABR0354       cystsine       yes         17       HMABR0355       givene       yes         18       HMABR0353       givene       yes         19       HMABR0353       givene       yes         21       HMABR0353       givene       yes         22       HMABR0353       givene	Metabolite No	HMDB Accession ID	Metabolite Identification	Definitive	Pathway
2   HM080083   value   yes     3   HM080022   cyston   yes     4   HM080022   trystophan   yes     6   HM0800005   adenosine   yes     7   HM0800002   iscurine   yes     8   HM0800002   iscurine   yes     9   HM0800002   givene   yes     10   HM0800002   givene   yes     11   HM0800001   atrine   yes     12   HM0800001   atrine   yes     13   HM0800001   atrine   yes     14   HM0800001   atrine   yes     15   HM0800005   methonine   yes     16   HM0800005   methonine   yes     17   HM080005   givene   yes     18   HM080005   givene   yes     19   HM080005   givene   yes     21   HM080005   givene   yes     22   HM080005   givene   yes     23   HM080013   givene   yes     24   HM080013   givene   yes     25   HM080013   givene   yes     26   HM080013	1		trimethylamine-N-oxide	no	
3   HM080032   cystine   yes     4   HM0800587   Leucine   yes     5   HM0800587   leucine   yes     6   HM080057   lsoleucine   yes     7   HM080057   lsoleucine   yes     9   HM080052   proline   yes     9   HM080052   proline   yes     11   HM080052   proline   yes     13   HM080053   alarine   yes     14   HM080057   thereinice   yes     15   HM080057   cysteine   yes     16   HM080057   cysteine   yes     17   HM080057   cysteine   yes     18   HM080057   cysteine   yes     19   HM080057   cysteine   yes     21   HM080057   cysteine   yes     23   HM080057   gyranicadd   yes     24   HM080057   gyranicadd   yes     25   HM080057   gyranicadd   yes     26   HM080057   gyranicadd   yes     27   HM080057   gyranicadd   yes     28   HM080057   gyranicadd   yes <td< td=""><td>2</td><td>HMDB00883</td><td>valine</td><td>yes</td><td></td></td<>	2	HMDB00883	valine	yes	
4   HM0800373   Invotophan   yes     5   HM0800037   leucine   yes     6   HM0800037   adenosine   yes     7   HM0800037   leucine   yes     8   HM0800037   leucine   yes     9   HM0800123   givine   yes     10   HM0800137   serine   yes     11   HM0800137   asparticaid   yes     12   HM0800131   asparticaid   yes     13   HM0800056   methionine   yes     14   HM080057   chysteine   yes     15   HM080056   methionine   yes     16   HM080059   phenylalarine   yes     20   HM080059   phenylalarine   yes     21   HM0800132   givine   yes     22   HM0800132   givine   yes     23   HM0800132   givine   yes     24   HM0800132   givine   yes     25   HM0800133   givyine   yes     26   HM0800134   givyine   yes     27   HM0800135   troosine   yes     28   HM0800133   givyine   yes	3	HMDB00192	cystine	yes	
MADB00057       leucine       yes         6       HANDB00057       isoleucine       yes         7       HANDB00057       lsoleucine       yes         9       HANDB00057       lsoleucine       yes         91       HANDB00052       proline       yes         91       HANDB00057       science       yes         91       HANDB00057       science       yes         91       HANDB00057       science       yes         91       HANDB00057       science       yes         91       HANDB00057       scynticaid       yes         91       HANDB00057       cysteine       yes         92       HANDB00057       cysteine       yes         93       HANDB00057       cysteine       yes         94       HANDB00057       cysteine       yes         94       HANDB00052       phenylalanine       yes         95       HANDB00058       tyronine       yes         95       HANDB00059       tyronine       yes         95       HANDB00059       tyronine       yes    9	4	HMDB00929	tryptophan	yes	
6   HMDB0002   adenosine   yes     7   HMDB0002   leucine   yes     8   HMDB00023   glycine   yes     10   HMDB00023   glycine   yes     11   HMDB00124   glycine   yes     12   HMDB00125   asrine   yes     13   HMDB00167   threonine   yes     14   HMDB00172   aspartic add   yes     15   HMDB00172   cysteine   yes     16   HMDB00266   methionine   yes     17   HMDB00273   cysteine   yes     18   HMDB00266   methionine   yes     19   HMDB00273   glycine   yes     20   HMDB00123   glycine   yes     21   HMDB00123   glycine   yes     22   HMDB00123   glycine   yes     23   HMDB00138   tyrosine   yes     24   HMDB00158   tyrosine   yes     25   HMDB00158   tyrosine   yes     26   HMDB00159   asgar   no     27   HMDB00159   glycrol   yes     28   HMDB00157   threanine   yes  2	5	HMDB00687	leucine	yes	
/       HMD80087       isofeurine       yes         9       HMD800872       isofeurine       yes         9       HMD800172       isofeurine       yes         11       HMD800123       givine       yes         12       HMD800162       proline       yes         13       HMD800161       alanine       yes         14       HMD800172       asparticadd       yes         15       HMD800191       asparticadd       yes         16       HMD800172       crysteine       yes         17       HMD800574       crysteine       yes         18       HMD800159       phenylaanine       yes         21       HMD800159       phenylaanine       yes         22       HMD800159       phenylaanine       yes         23       HMD800132       lysine       yes         24       HMD800132       lysine       yes         25       HMD800133       giycrine       yes         26       HMD800133       giycrine       yes         27       HMD800133       giycrine       yes </td <td>6</td> <td>HMDB00050</td> <td>adenosine</td> <td>yes</td> <td></td>	6	HMDB00050	adenosine	yes	
8       HMD00072       isoleucine       yes         9       HMD000723       glycine       yes         10       HMD000723       glycine       yes         12       HMD000167       serine       yes         13       HMD000167       threonine       yes         14       HMD000167       threonine       yes         15       HMD000172       opstricaid       yes         16       HMD000172       opstricaid       yes         17       HMD00074       opstricaid       yes         18       HMD00075       plenwislanine       yes         19       HMD00075       plenwislanine       yes         20       HMD00072       glycine       yes         21       HMD00072       glycine       yes         22       HMD00073       glycine       yes         23       HMD0073       glycine       yes         24       HMD0073       glycine       yes         25       HMD0073       glycine       yes         26       HMD0073       glycine       yes         <	7	HMDB00172	isoleucine	yes	
9       HMDB00122       isoleuone       yes         10       HMDB00122       proine       yes         11       HMDB00162       proine       yes         13       HMDB00173       serine       yes         13       HMDB00171       abaine       yes         14       HMDB00171       aspartcadid       yes         15       HMDB00171       aspartcadid       yes         16       HMDB00174       crysteine       yes         17       HMDB00174       crysteine       yes         18       HMDB00174       crysteine       yes         19       HMDB00174       crysteine       yes         21       HMDB00159       phenylalanine       yes         22       HMDB00182       lysine       yes         23       HMDB00182       lysine       yes         24       HMDB00183       tyrosine       yes         25       HMDB00183       tyrosine       yes         26       HMDB00134       glycarce       yes         27       HMDB00133       glycarce       yes <tr< td=""><td>8</td><td>HMDB00687</td><td>leucine</td><td>yes</td><td></td></tr<>	8	HMDB00687	leucine	yes	
International model       International model       International model       International model         11       HMD800125       gronine       yes         12       HMD800126       atainine       yes         13       HMD800127       threanine       yes         14       HMD800131       asparticaid       yes         15       HMD800123       asparticaid       yes         16       HMD800124       cysteine       yes         17       HMD800737       cysteine       yes         18       HMD800737       cysteine       yes         20       HMD800739       phenylaanine       yes         21       HMD800739       phenylaanine       yes         22       HMD800732       glycine       yes         23       HMD800732       lysine       yes         24       HMD800732       lysine       yes         25       HMD800735       tyrosine       yes         26       HMD800735       tyrosine       yes         27       HMD800735       tyrosine       yes         28       mobasugar	9	HMDB00172	isoleucine	yes	
11       HMDB00161       promine       Ves         12       HMDB00151       alonine       Ves         13       HMDB00151       alonine       Ves         14       HMDB00151       aspartic acid       Ves         15       HMDB00574       cysteine       Ves         16       HMDB00574       cysteine       Ves         17       HMDB00574       cysteine       Ves         20       HMDB00574       cysteine       Ves         21       HMDB00159       phenylainine       Ves         221       HMDB00152       lysine       Ves         23       HMDB00152       lysine       Ves         24       HMDB00152       lysine       Ves         25       HMDB00152       lysine       Ves         26       HMDB00152       lysine       Ves         27       HMDB00153       supartic acid       Ves         28       HMDB00154       gapartic acid       Ves         31       HMDB00157       threonine       Ves         32       HMDB00158       tyrosine       Ves	10	HMDB00123	giycine	yes	
L2       HNUB200167       serme       Yes         13       HNUB200167       threenine       Yes         14       HNUB200167       threenine       Yes         15       HNUB200191       aspartic acid       Yes         16       HNUB200191       aspartic acid       Yes         17       HNUB200266       methionine       Yes         20       HNUB200266       methionine       Yes         21       HNUB200259       phenylaanne       Yes         22       HNUB200123       glychine       Yes         23       HNUB200123       glychine       Yes         24       HNUB200123       glychine       Yes         25       HNUB200123       glychine       Yes         26       HNUB200126       tyrosine       Yes         27       HNUB200128       tyrosine       Yes         28       HNUB200147       threenine       Yes         29       HNUB200147       threenine       Yes         31       HNUB200147       sugar       no         32       HNUB200147       sugar	11	HIVIDB00162	proline	yes	
13   Moundoil   atamine   yes     14   HMDB00151   aspartic acid   yes     15   HMDB00151   aspartic acid   yes     16   HMDB00574   cysteline   yes     17   HMDB00574   cysteline   yes     18   HMDB00566   methionine   yes     20   HMDB00566   methionine   yes     21   HMDB00573   phenylalanine   yes     22   HMDB00159   phenylalanine   yes     23   HMDB00159   phenylalanine   yes     24   HMDB00122   lysine   yes     25   HMDB00123   glycnie   yes     26   HMDB00125   tyrosine   yes     27   HMDB00158   tyrosine   yes     30   HMDB00157   threonine   yes     31   HMDB00157   threonine   yes     33   HMDB00158   tyrosine   yes     34   HMDB00159   asyspart   no     35   sugar   no   carbohydrate Metabolism     36   sugar   no   sugar   no     37   sugar   no   carbohydrate Metabolism     36   sugar	12	HIVIDB00187	serine	yes	
in   molecular   unservice and separtic acid   yes     in   HM0B00151   aspartic acid   yes     in   HM0B00574   cysteline   yes     in   HM0B00566   methionine   yes     in   HM0B00566   methionine   yes     in   HM0B00566   methionine   yes     in   HM0B0059   phenylalanine   yes     in   HM0B00132   itysine   yes     in   HM0B00157   threenine   yes     in   HM0B00157   threenine   yes     in   HM0B00157   threenine   yes     in   sugar   no   sugar   no     in   <	13		aldillie	yes	
15       HM080031       aspartic add       yes         17       HM080031       cysteline       yes         18       HM0800574       cysteline       yes         19       HM0800574       cysteline       yes         20       HM080059       phenylalanine       yes         21       HM0800159       phenylalanine       yes         22       HM0800152       lysine       yes         23       HM0800152       lysine       yes         24       HM0800152       lysine       yes         25       HM0800152       lysine       yes         26       HM0800152       lysine       yes         27       HM0800153       tyrosine       yes         28       HM0800154       tyrosine       yes         30       HM0800158       tyrosine       yes         31       HM0800143       galaticse       yes         32       HM0800143       galatricaid       yes         33       HM0800143       galatricaid       yes         34       HM0800013       glycerol-sphosphate       yes <td>14</td> <td></td> <td>threonine</td> <td>yes</td> <td></td>	14		threonine	yes	
10   IMM0500574   Gysteline   yes   Amino Acid Metabolism     18   HM0500566   methionine   yes   Amino Acid Metabolism     19   HM0500574   Gysteline   yes     20   HM0500595   phenylalanine   yes     21   HM0500595   phenylalanine   yes     22   HM0500159   phenylalanine   yes     23   HM0500159   phenylalanine   yes     24   HM0500132   lysine   yes     25   HM0500133   tyrsine   yes     26   HM0500133   tyrsine   yes     27   HM0500133   tyrsine   yes     28   HM0500133   tyrsine   yes     29   HM0500134   galactose   yes     31   HM0500167   threonine   yes     33   HM0500167   threonine   yes     34   HM0500167   sugar   no     35   sugar   no   sugar   no     36   sugar   no   sugar   no     37   sugar   no   sugar   no     38   HM0500131   glycerol   yes     41   HM0500220   hecadecanoic acid<	15		aspartic acid	yes voc	
1       Investigation       yes       Participation         18       HMDB00056       cysteline       yes         19       HMDB00574       cysteline       yes         20       HMDB00559       phenylalanine       yes         21       HMDB00159       phenylalanine       yes         22       HMDB00123       glycine       yes         23       HMDB00123       glycine       yes         24       HMDB00132       lysine       yes         25       HMDB00132       lysine       yes         26       HMDB00159       phenylalanine       yes         27       HMDB00132       lysine       yes         28       HMDB00133       glycrighycine       no         31       HMDB00167       threenine       yes         33       HMDB00167       threenine       yes         34       HMDB00143       glycrelidatose       yes         35       sugar       no       sugar       no         36       sugar       no       sugar       no         37       octadecanolc add	10		asparticació	yes voc	Amino Acid Metabolism
19   HMDB00272   Opsteine   yes     20   HMDB00259   phenylalanine   yes     21   HMDB00159   phenylalanine   yes     22   HMDB00159   phenylalanine   yes     23   HMDB00123   glychine   yes     24   HMDB00123   glychine   yes     25   HMDB00132   lysine   yes     26   HMDB00132   lysine   yes     27   HMDB00138   lyrosine   yes     28   HMDB00138   lyrosine   yes     29   HMDB00157   thronine   yes     31   HMDB00167   thronine   yes     33   HMDB00167   thronine   yes     34   HMDB00167   thronine   yes     35   sugar   no   sugar   no     36   Sugar   no   sugar   no     36   Sugar   no   sugar   no     36   Sugar   no   sugar   no     37   Sugar   no   sugar   no     38   Carbohydrate Metabolism   glycerol   yes     40   HMDB0026   glycerol-phosphate   yes     41	18	HMDB00696	methionine	ves	
20   HMD800056   methionine   yes     21   HMD800159   phenylalanine   yes     22   HMD800159   phenylalanine   yes     23   HMD800159   phenylalanine   yes     24   HMD800122   glyvine   yes     25   HMD800132   lysine   yes     26   HMD800132   lysine   yes     27   HMD800132   lysine   yes     28   HMD800133   glyvine   yes     29   HMD800153   lyrosine   yes     30   HMD800153   lyrosine   yes     31   HMD800157   threonine   yes     33   HMD800157   threonine   yes     34   HMD800157   sugar   no     35   sugar   no   sugar   no     36   sugar   no   sugar   no     37   sugar   no   sugar   no     38   HMD80022   octadecanoic acid   yes     41   HMD80023   glycerol   yes     42   sugar   no   Glyceroligid Metabolism     43   HMD80023   glycerol   yes     44   HMD80023	10	HMDB000574	cysteine	ves	
21   HMD800159   phenylalanine   yes     22   HMD800159   phenylalanine   yes     23   HMD800123   glycine   yes     24   HMD800123   glycine   yes     25   HMD800182   lysine   yes     26   HMD800182   lysine   yes     27   HMD800182   lysine   yes     28   HMD800158   tyrosine   yes     30   HMD800158   tyrosine   yes     31   HMD800157   threonine   yes     32   HMD800131   galactose   yes     33   HMD800131   galactose   yes     34   HMD800133   sugar   no     35   usgar   no   sugar     36   usugar   no   sugar     37   usugar   no   sugar     38   usugar   no   sugar     40   sugar   no   sugar     41   HMD800827   octadecanolc acid   yes     42   HMD80031   glycerol-   yes     43   HMD800320   hexadecanoic acid   yes     44   HMD800256   glucose-6-phosphate   yes <tr< td=""><td>20</td><td>HMDB00696</td><td>methionine</td><td>ves</td><td></td></tr<>	20	HMDB00696	methionine	ves	
22       HMD800159       phenylalanine       yes         23       HMD800159       phenylalanine       yes         24       HMD800152       glycine       yes         25       HMD800182       lysine       yes         26       HMD800182       lysine       yes         27       HMD800182       lysine       yes         28       HMD801173       glycylgycine       no         29       HMD800158       tyrosine       yes         31       HMD800167       threenine       yes         32       HMD800167       threenine       yes         33       HMD800167       threenine       yes         34       HMD80017       asparticaid       no         35       sugar       no       sugar       no         36       usugar       no       sugar       no         38       sugar       no       sugar       no         39       sugar       no       sugar       no         41       HMD800827       cholesterol       yes       Fatty Acid Metabolism         4	21	HMDB00159	nbenylalanine	ves	
23   HMD800159   phenylalanine   yes     24   HMD800123   Blyvine   yes     25   HMD800182   lysine   yes     26   HMD800182   lysine   yes     27   HMD800182   lysine   yes     28   HMD80158   tyrosine   yes     29   HMD800158   tyrosine   yes     30   HMD800167   threnne   yes     31   HMD800174   gapartic acid   yes     33   HMD800191   aspartic acid   yes     34   HMD800174   gapartic acid   yes     35   sugar   no   or     36   asugar   no   or     37   sugar   no   or     38   sugar   no   or     39   sugar   no   or     31   HMD800827   cholesterol   yes     41   sugar   no   or     42   sugar   no   sugar     43   HMD80031   glycerol   yes     44   HMD800328   octanoic acid   yes     45   HMD80031   glycerol   yes     46   HMD80026   g	22	HMDB00159	phenylalanine	ves	
24   HMD800123   glycine   yes     25   HMD800182   lysine   yes     26   HMD800182   lysine   yes     27   HMD800182   lysine   yes     28   HMD80173   Blycylgvine   no     29   HMD80158   tyrosine   yes     30   HMD80167   threenine   yes     31   HMD80083   valine   yes     32   HMD801167   threenine   yes     33   HMD800143   galactose   yes     34   HMD800143   sugar   no     35   sugar   no   sugar   no     36   usugar   no   sugar   no     38   sugar   no   sugar   no     39   sugar   no   sugar   no     41   HMD800827   octadecanoic acid   yes     43   HMD80082   octanoic acid   yes     44   HMD80082   octanoic acid   yes     45   HMD80031   glycerol   yes     46   HMD80032   glycerol   yes     50   HMD80014   glucose-6-phosphate   yes     51   HMD800210	23	HMDB00159	phenylalanine	ves	
25HMDB00182Usineyes26HMDB00182lysineyes27HMDB00182lysineyes28HMDB1733glycylglycineno29HMDB00158tyrosineyes30HMDB00158tyrosineyes31HMDB00157threennineyes33HMDB00191asparticatidyes34HMDB00191asparticatidyes35HMDB00191asparticatidyes36inositolnono37sugarno38sugarno39sugarno40sugarno41sugarno42sugarno43HMDB00827cholesterol44HMDB00882cholesterol45HMDB0082hexadecanoicatid46HMDB00820hexadecanoicatid47HMDB00821glycerol-3-phosphate48HMDB00820nicotinamide49sugarno50HMDB00210glucose-6-phosphate51HMDB00210glucose-6-phosphate52HMDB00211glucose-6-phosphate53HMDB00230nicotinamide54HMDB00241glutamine55HMDB00241glutamine56HMDB00241glutamine57HMDB00241glutamine58HMDB00241glutamine59HMDB00241glutamine66HMDB0	24	HMDB00123	glycine	ves	
26HMD800132lysineyes27HMD80132lysineyes28HMD81733glycylglycineno29HMD800158tyrosineyes30HMD800158tyrosineyes31HMD800167threenineyes32HMD80113galactoseyes33HMD800131galactoseyes36inositolno37sugarno38sugarno39sugarno34HMD800827octadecanoic acidyes35sugarno36sugarno37sugarno38sugarno39sugarno40sugarno41sugarno42octadecanoic acidyes43HMD800827octadecanoic acidyes44HMD80082hexadecanoic acidyes45HMD80082hexadecanoic acidyes46HMD80031glycerolyes47HMD80042glycerolyes53HMD80041glucose-6-phosphateyes54HMD80041glutamineyes55HMD80041glutamineyes56HMD80030uracilyes57HMD80030glutamineyes58HMD80030uracilyes59HMD80030uracilyes61succinic acidy	25	HMDB00182	lysine	ves	
27HMD800382lysineyes28HMD81733glycylglycineno29HMD80058tyrosineyes30HMD80058tyrosineyes31HMD80083valineyes32HMD800191asparticaddyes33HMD800191asparticaddyes34HMD800143galactoseyes35inositolnono36sugarnono37sugarnono38sugarnono40sugarnono41sugarnono42sugarno43HMD800827octanoicaddyes44HMD80031glycerolyes45HMD80031glycerolyes46HMD80031glycerolyes47HMD80031glycerolyes50HMD800131glycerolyes51HMD80131glycerolyes52HMD802641glucose-6-phosphateyes53HMD800210uracid and/or beta-alanineyes54HMD800300uracilyes55HMD800301glutamineyes56HMD800300uracilyes57HMD80041glutamineyes58HMD800300uracilyes59HMD800301glutamineyes60HMD800300uracilyes58HMD	26	HMDB00182	lysine	ves	
28HMDB11733glycylglycineno29HMDB00158tyrosineyes30HMDB00158tyrosineyes31HMDB00883valineyes32HMDB00167threonineyes33HMDB00143galactoseyes34HMDB00143galactoseyes35sugarno36sugarno37sugarno38sugarno39sugarno40sugarno41sugarno42sugarno43HMDB00827ottadecanoic acidyes44HMDB00827ottadecanoic acidyes44HMDB008266cholesterolyes45HMDB00826glycerol-s-phosphateyes46HMDB0031glycerol-s-phosphateyes47HMDB0031glycerol-s-phosphateyes48HMDB0031glycerol-s-phosphateyes50HMDB00401glucose-s-phosphateyes51HMDB00401glutamineyes52HMDB0041glutamineyes53HMDB00200uracilyes54HMDB00241glutamineyes55Ssucroseno66HMDB00244gurcroic acidyes56HMDB002454sucroseno66HMDB002454sucroseno66HMDB00245glutamineyes <td>27</td> <td>HMDB00182</td> <td>lysine</td> <td>ves</td> <td></td>	27	HMDB00182	lysine	ves	
29HMDB00158tyrosineyes30HMDB00158tyrosineyes31HMDB00167threonineyes32HMDB00191aspartic acidyes33HMDB00191aspartic acidyes34HMDB00143galactoseyes35sugarno36sugarno37sugarno38sugarno39sugarno40sugarno41sugarno42sugarno43HMDB00827octatecanic acid44HMDB00136glycerol45HMDB00131glycerol46HMDB00126glycerol47HMDB00131glycerol48HMDB00126glycerol49sucose-6phosphate50HMDB0012651HMDB0027044HMDB0013155sucrose56HMDB00264157HMDB0030058HMDB0030059HMDB0030161sucrose56HMDB0030161sucrose56HMDB0030061sucrose56HMDB0030161sucrose56HMDB0030161sucrose56HMDB0030161sucrose56HMDB0030161sucrose56HMDB0030161sucrose62sucr	28	HMDB11733	glycylglycine	no	
30HMDB00158tyrosineyes31HMDB00883valineyes32HMDB00157aspartic acidyes33HMDB0011aspartic acidyes34HMDB00131aspartic acidyes35IMDB00143galactoseyes36inositolno37sugarno38sugarno39sugarno40sugarno41sugarno42sugarno43HMDB00827octadecanoic acid44HMDB00827octadecanoic acid45HMDB00482octanoic acid46HMDB00482octanoic acid47HMDB00482octanoic acid48HMDB00311glycerol99yesGlycerolipid Metabolism50HMDB001401glucose-6-phosphate51HMDB001401glucose-6-phosphate52HMDB00411glutamine53HMDB00401glutamine54HMDB00300uracil55sureidopropionic acid and/or beta-alanineno56HMDB00300uracil57HMDB00300uracil61suroseno56HMDB00300uracil57HMDB00300uracil63HMDB0030064HMDB0030065HMDB0030066surose67HMDB003468thioureano <t< td=""><td>29</td><td>HMDB00158</td><td>tyrosine</td><td>yes</td><td></td></t<>	29	HMDB00158	tyrosine	yes	
31HMDB00883 HMDB00167 HMDB00161valine threonine aspartic acidyes yes33HMDB00167 HMDB00131galactose 	30	HMDB00158	tyrosine	yes	
32HMDB00167 aspartic acidthreenine aspartic acidyes yes yes33HMDB00191 aspartic acidaspartic acidyes yes34HMDB00143galactose sugarno no no sugarno no sugar36Sugarno sugarno o sugarno no sugar38Sugarno sugarno sugar40Sugarno sugarno sugar41Sugarno sugarno sugar42Octadecanoic acidyes thexadecanoic acidyes yes43HMDB00827octadecanoic acid glycerolyes yes44HMDB00311 glycerolglycerol yesyes yes45HMDB00131 glycerol-s-phosphate glucose-6-phosphateyes yes50HMDB001401 glucose-6-phosphate glucose-6-phosphate yesGlycolysis pathway51HMDB00210 glucose-6-phosphate glucose-6-phosphate yesMetabolism of Cofactors and Vitamins55SSucrose sucroseno sucrose56HMDB00300 glutamineyes yesStarch and sucrose metabolism56HMDB00300 glutamineyes yesStarch and sucrose metabolism56HMDB00304 glutamineyes yesStarch and sucrose metabolism56HMDB00304 glutamineyes yesStarch and sucrose metabolism56HMDB00304 glutamineyes yesStarch and sucrose metabolism56HMDB00304 glutamineyes y	31	HMDB00883	valine	yes	
33HMDB00191 MDB00143aspartic acid galactose yes sugaryes yes no no no sugaryes yes no no no sugar36Sugar sugarno sugarno no sugarno no sugarno no sugar38Sugar sugarno sugarno no sugarno no sugarCarbohydrate Metabolism40Sugar sugarno sugarno sugarCarbohydrate Metabolism41Sugar sugarno sugarno sugarCarbohydrate Metabolism42Sugar sugarno sugarno sugarno sugar43HMDB00827octanoic acid glycerolyes yesFatty Acid Metabolism44HMDB00311 glycerolglycerol glycerol-sphosphate yesyes glycerol-sphosphate yesGlycerolipid Metabolism55HMDB00420 glycerol-sphosphate gl duccose-6-phosphate gl duccose-6-phosphate yesyes yesGlycolysis pathway55HMDB00411 glutamine glutamine sglutamine yes yesMetabolism of Cofactors and Vitamins56HMDB00641 HMDB00300 Gl Glycerolsidyes yesStarch and sucrose metabolism56HMDB00541 HMDB00304 Gl Gl Gl Gl Glyes yesStarch and sucrose metabolism56HMDB00541 HMDB00304 Gl Gl Gl Gl Gl Gl HMDB00304glutamine yes yesyes yes61Sucrose HMDB0034 Gl Gl Gl Gl HMDB0034glutamine yes yesSt	32	HMDB00167	threonine	yes	
34HMDB00143galactose sugaryes no no sugaryes no no no36Sugarno sugarno no sugarno no no no sugarno no no sugarno no no sugarCarbohydrate Metabolism40Sugarno sugarno sugarCarbohydrate Metabolism41Sugarno sugarno sugarCarbohydrate Metabolism42Sugarno sugarno sugarFatty Acid Metabolism43HMDB00827octaolc acid glycerolyes yesFatty Acid Metabolism44HMDB00131 glycerolglycerol yesyes glycerol-laphosphate yesGlycerolipid Metabolism45HMDB00126 glycerol-3-phosphate glucose-6-phosphate gl staryes yesGlycolysis pathway55MMDB0210 glucose-6-phosphate glucase-6-phosphate glucase-6-phosphate glucase-6-phosphate yesMetabolism of Cofactors and Vitamins56HMDB00210 glucase-6-phosphate glucaseMetabolism of Cofactors and Vitamins56HMDB00210 glucaseglucase glucaseglucase glucasemo glucase<	33	HMDB00191	aspartic acid	yes	
35Sugarno36inositolno37Sugarno38Sugarno39Sugarno40Sugarno41Sugarno42Sugarno43HMD800827octadecanoic acidyes44HMD800827octadecanoic acidyes44HMD800482octanoic acidyes45HMD800482octanoic acidyes46HMD800482octanoic acidyes47HMD800131glycerolyes48HMD800131glycerolyes50HMD80131glycerol-3-phosphateyes51HMD80120glycerol-3-phosphateyes53HMD80120Pantothenic acidyes54HMD800210Pantothenic acid and/or beta-alanineno55J-ureidopropionic acid and/or beta-alanineno56HMD800300uracilyes57HMD800301glutamineyes58HMD800301uracilyes59HMD800300uracilyes61SucrosenoStarch and sucrose metabolism62HMD80024Sucroseno63HMD80024Sucroseno64HMD80030uracilyes55HMD80030uracilyes66HMD80024Sucroseno67HMD80024Sucroseno68HMD80030 <td< td=""><td>34</td><td>HMDB00143</td><td>galactose</td><td>yes</td><td></td></td<>	34	HMDB00143	galactose	yes	
36inositolno37Sugarno38Sugarno39Sugarno40Sugarno41Sugarno42Sugarno43HMD800827octadecanoic acidyes44HMD80138cotadecanoic acidyes45HMD800482octanoic acidyes46HMD800131glycerolyes47HMD800131glycerolyes48HMD80131glycerolyes50HMD801401glucose-6-phosphateyes51HMD801401glucose-6-phosphateyes52HMD801401glucase-6-phosphateyes53HMD80210Pantothenic acidyes54HMD80641glutamineyes55Sucroseno56HMD80641glutamineyes57HMD80641glutamineyes58HMD80641glutamineyes60HMD80030uracilyes61Sucroseno62Sucroseno63HMD80024Sucroseno64HMD80024Sucroseno65HMD80024Sucroseno66HMD80024Sucroseno66HMD80024Sucroseno66HMD80024Sucroseno66HMD80024Sucroseno66HMD80024Pah-Galactopyranosiduronic acid<	35		sugar	no	
37sugarnoCarbohydrate Metabolism38Sugarno039Sugarno040Sugarno41Sugarno42Sugarno43HMD800827Octadecanoic acidYes44HMD800282Octadecanoic acidYes45HMD80020hexadecanoic acidYes46HMD80020hexadecanoic acidYes47HMD800131glycerolYes48HMD800131glycerolYes48HMD800131glycerolYes50HMD800126glycerol-3-phosphateYes51HMD801401glucose-6-phosphateYes52HMD801401glucose-6-phosphateYes53HMD80210Pantothenic acid and/or beta-alanineyes54HMD80041glutamineYes55Sureidopropionic acid and/or beta-alanineyes56HMD800300uracilYes60HMD800300uracilYes61SucrosenoStarch and sucrose metabolism62SucrosenoStarch and sucrose metabolism63HMD800244Sucroseno64HMD800243Pyruvic acid65HMD800244Sucroseno66HMD800244Sucroseno66HMD800244Sucroseno67AD-Galactopyranosiduronic acidno68Holourean	36		inositol	no	
38sugarnoCarbohydrate Metabolism39sugarnono40sugarno41sugarno42sugarno43HMD800827octadecanoic acidyes44HMD80328cholesterolyes45HMD800482octanoic acidyes46HMD800220hexadecanoic acidyes47HMD800131glycerolyes48HMD800126glycerol-3-phosphateyes50HMD801012glucose-6-phosphateyes51HMD801401glucose-6-phosphateyes52HMD80120Pantothenic acidyes53HMD80210glutamineyes54HMD800210glutamineyes553-ureidopropionic acid and/or beta-alanineno56HMD800641glutamineyes57HMD800641glutamineyes58HMD800300uracilyes60HMD800300uracilyes61sucroseno62sucroseno63HMD800254succinic acidyes64HMD800244pruvic acidyes65HMD800244glucanic acidyes66HMD800254succinic acidyes66HMD800244pruvic acidyes66HMD800244brucic acidyes66HMD800244brucic acidyes67brucic ac	37		sugar	no	
39sugarnoConstruction of the construction o	38		sugar	no	Carbohydrate Metabolism
40sugarno41sugarno42sugarno43HMD80827Octadecanoic acidyes43HMDB0368cholesterolyes44HMDB00482octanoic acidyes45HMD800131glycerolyes46HMDB00131glycerolyes47HMDB00131glycerolyes50HMDB00146glycerolyes51HMDB0126glycerolyes52HMDB01270nicotinamideyes53HMDB0270Pantothenic acidyes54HMDB0041glucose-6-phosphateyes553-ureidopropionic acid and/or beta-alanineyes56HMDB00641glutamineyes57HMDB00641glutamineyes58HMDB00300uracilyes60HMDB00300uracilyes61sucroseno62sucroseno63HMDB0034fitric acidyes64HMDB00243pyruvic acidyes65HMDB00243pyruvic acidyes66thioureanoUrea cycle67idthioureano68idthioureano69id-D-Galactopyranosiduronic acidnoUronic acid pathway	39		sugar	no	carbonyurate metabonam
41sugarno42sugarno43HMD800827octadecanoic acidyes44HMD80368cholesterolyes45HMD80020hexadecanoic acidyes46HMD80020hexadecanoic acidyes47HMD800131glycerolyes48HMD80131glycerolyes50HMD801401glycose-6-phosphateyes51HMD801401glucose-6-phosphateyes52HMD801401glucose-6-phosphateyes53HMD801401glutamineyes54HMD806411glutamineyes553-ureidopropionic acid and/or beta-alanineno56HMD800641glutamineyes57HMD800641glutamineyes58HMD800300uracilyes61sucroseno62sucroseno63HMD800244sucrose64HMD800244pyruvic acid65HMD80024466thioureano67idid <id td="" yes<="">68id-ordalyes69id-ordalactopyranosiduronic acidno69id-ordalactopyranosiduronic acidno</id>	40		sugar	no	
42sugarno49sugarno43HMD800827octadecanoic acidyes44HMDB1368cholesterolyes45HMD800482octanoic acidyes46HMD800131glycerolyes47HMD800131glycerolyes48HMD80126glycerol-3-phosphateyes50HMD801401glucose-6-phosphateyes51HMD801401glucose-6-phosphateyes52HMD801401glucose-6-phosphateyes53HMD801401glucose-6-phosphateyes54HMD800210Pantothenic acidyes55Jureidopropionic acid and/or beta-alanineno56HMD800641glutamineyes57HMD800641glutamineyes58HMD800300uracilyes61Sucroseno62Sucroseno63HMD800243pyruvic acidyes64HMD800243pyruvic acidyes66HMD800243pyruvic acidyes66thioureanoUrea cycle68ithioureanoUrea cycle	41		sugar	no	
49sugarno43HMDB00827octadecanoic acidyes44HMDB10368cholesterolyes45HMDB00482octanoic acidyes46HMDB00131glycerolyes47HMDB00131glycerolyes48HMDB00131glycerolyes50HMDB00126glycerol-3-phosphateyes51HMDB01401glucose-6-phosphateyes52HMDB01401glucose-6-phosphateyes53HMDB02730nicotinamideyes54HMDB00411glutamineyes553-ureidopropionic acid and/or beta-alanineno56HMDB00641glutamineyes57HMDB00641glutamineyes59HMDB00300uracilyes60HMDB00300uracilyes61Sucroseno62Sucroseno63HMDB00243pyruvic acid64HMDB00243pyruvic acid65HMDB00243pyruvic acid66MDB00243pyruvic acid69à-D-Galactopyranosiduronic acidno69i-D-Galactopyranosiduronic acidno69i-D-Galactopyranosiduronic acidno69i-D-Galactopyranosiduronic acidno	42		sugar	no	
43HMD800827octadecanoic acidyes44HMD810368cholesterolyes45HMD800482octanoic acidyes46HMD800200hexadecanoic acidyes47HMD800131glycerolyes48HMD800131glycerol-sphosphateyes50HMD801401glycerol-sphosphateyes51HMD801401glucose-6-phosphateyes52HMD801401glucose-6-phosphateyes53HMD802100Pantothenic acidyes54HMD800210Pantothenic acidyes553-ureidopropionic acid and/or beta-alanineno56HMD800641glutamineyes57HMD800641glutamineyes60HMD800300uracilyes61Sucroseno62Sucroseno63HMD800254Succinic acidyes64HMD800243pyruvic acidyes65HMD800244succinic acidyes66thioureanoUracid cycle67thioureanoUrac cycle68idthioureano69id-D-Galactopyranosiduronic acidnoUronic acid pathway	49		sugar	no	
44HMDB10368cholesterolyesFatty Acid Metabolism45HMDB00482octanoic acidyesFatty Acid Metabolism46HMDB0020hexadecanoic acidyesGlycerolipid Metabolism47HMDB00131glycerolyesGlycerolipid Metabolism48HMDB00126glycerol-3-phosphateyesGlycolysis pathway50HMDB01401glucose-6-phosphateyesGlycolysis pathway51HMDB0126glycerol-3-phosphateyesMetabolism of Cofactors and Vitamins53HMDB02730niciotinamideyesMetabolism of Cofactors and Vitamins54HMDB00411glutamineyesMetabolism of Other Amino Acids553-ureidopropionic acid and/or beta-alaninenoMetabolism of Other Amino Acids57HMDB00641glutamineyesMetabolism of Other Amino Acids58HMDB0300uracilyesMetabolism of Other Amino Acids60HMDB00300uracilyesStarch and sucrose metabolism61sucrosenoStarch and sucrose metabolism62sucroisenoUracid cycle63HMDB00254succinic acidyes64HMDB00243pyruvic acidyes65HMDB00243pyruvic acidyes66thioureanoUrea cycle68ibioureanoUronic acid pathway	43	HMDB00827	octadecanoic acid	yes	
45HMDB00482octanoic acidyes46HMDB0020hexadecanoic acidyes47HMDB00131glycerolyes48HMDB00126glycerol-3-phosphateyes50HMDB0126glycerol-3-phosphateyes51HMDB01401glucose-6-phosphateyes52HMDB01401glucose-6-phosphateyes53HMDB02730nicotinamideyes54HMDB0210Pantothenic acidyes553-ureidopropionic acid and/or beta-alanineno56HMDB00641glutamineyes57HMDB00641glutamineyes58HMDB00641glutamineyes60HMDB00300uracilyes61Sucroseno62sucroseno63HMDB0094citric acidyes64HMDB0094citric acidyes65HMDB0094citric acidyes66thioureanoUrea cycle67a-b-Galactopyranosiduronic acidnoUrea cycle68à-D-Galactopyranosiduronic acidnoUronic acid pathway	44	HMDB10368	cholesterol	yes	Fatty Acid Metabolism
46HMDB00220hexadecanoic acidyes47HMDB00131glycerolyes48HMDB00131glycerolyes50HMDB00126glycerol-3-phosphateyes51HMDB01401glucose-6-phosphateyes52HMDB02730nicotinamideyes53HMDB00210Pantothenic acidyes54HMDB00210glutamineyes553-ureidopropionic acid and/or beta-alanineyes56HMDB00641glutamineyes57HMDB00641glutamineyes58HMDB00300uracilyes60HMDB00300uracilyes61sucroseno62sucroseno63HMDB00254succinic acidyes64HMDB00243pyruvic acidyes65HMDB00243pyruvic acidyes66thioureanoUrea cycle67aabout and ano	45	HMDB00482	octanoic acid	yes	
47HMDB00131glycerolyesGlycerolipid Metabolism48HMDB00131glycerolyesGlycerolipid Metabolism50HMDB00126glycerol-3-phosphateyesGlycolysis pathway51HMDB01401glucose-6-phosphateyesGlycolysis pathway52HMDB01401glucose-6-phosphateyesMetabolism of Cofactors and Vitamins53HMDB02730nicotinamideyesMetabolism of Cofactors and Vitamins54HMDB00641glutamineyesMetabolism of Other Amino Acids56HMDB00641glutamineyesMetabolism of Other Amino Acids58HMDB00641glutamineyesMetabolism of Other Amino Acids59HMDB00300uracilyesStarch and sucrose metabolism60HMDB00254SuccosenoStarch and sucrose metabolism63HMDB00243pyruvic acidyesTricarboxylic acid cycle64HMDB00243pyruvic acidyesTricarboxylic acid cycle66thioureanoUrea cycle68ithioureanoUrea cycle69ii-D-Galactopyranosiduronic acidnoUronic acid pathway	46	HMDB00220	hexadecanoic acid	yes	
48HMDB00131glycerolyes50HMDB0126glycerol-3-phosphateyes51HMDB01401glucose-6-phosphateyes52HMDB01401glucose-6-phosphateyes53HMDB02730nicotinamideyes54HMDB00210Pantothenic acidyes553-ureidopropionic acid and/or beta-alanineno56HMDB00641glutamineyes57HMDB00641glutamineyes58HMDB00641glutamineyes59HMDB00300uracilyes60HMDB00300uracilyes61Sucroseno62Sucroseno63HMDB00254Succinic acid64HMDB00243pyruvic acid65HMDB00243pyruvic acid66thioureano67thioureano68à-D-Galactopyranosiduronic acidno69à-D-Galactopyranosiduronic acidno0Uronic acid pathway	47	HMDB00131	glycerol	yes	Glycerolipid Metabolism
50HMDB0012bglycerol-3-phosphateyesyes51HMDB01401glucose-6-phosphateyesGlycolysis pathway52HMDB01401glucose-6-phosphateyesMetabolism of Cofactors and Vitamins53HMDB02730NicotinamideyesMetabolism of Cofactors and Vitamins54HMDB00210Pantothenic acidyesMetabolism of Cofactors and Vitamins553-ureidopropionic acid and/or beta-alaninenoyes56HMDB00641glutamineyesMetabolism of Other Amino Acids58HMDB00641glutamineyesMetabolism of Other Amino Acids59HMDB00300uracilyesMetabolism of Other Amino Acids60HMDB00300uracilyesStarch and sucrose metabolism61SucrosenoStarch and sucrose metabolism62SucrosenoStarch and sucrose metabolism63HMDB00254Succinic acidyes64HMDB00243pyruvic acidyes65HMDB00243pyruvic acidyes66thioureanoUrea cycle67thioureanoUrea cycle68thioureanoUronic acid pathway	48	HMDB00131	glycerol	yes	
S1HNDB01401glucose-o-phosphateyes52HMDB01401glucose-o-phosphateyes53HMDB02730nicotinamideyes54HMDB00210Pantothenic acidyes553-ureidopropionic acid and/or beta-alanineyes56HMDB00641glutamineyes57HMDB00641glutamineyes58HMDB00641glutamineyes59HMDB00300uracilyes60HMDB00300uracilyes61sucroseno62sucroseno63HMDB00254succinic acid64HMDB00254yes65HMDB00243pyruvic acid66thioureano67thioureano68à-D-Galactopyranosiduronic acidno69à-D-Galactopyranosiduronic acidnoUronic acid pathway	50	HMDB00126	glycerol-3-phosphate	yes	Glycolysis pathway
32HMDB01411grucose-opinospirateyes53HMDB02730nicotinamideyes54HMDB00210Pantothenic acidyes553-ureidopropionic acid and/or beta-alanineyesMetabolism of Cofactors and Vitamins56HMDB00641glutamineyes57HMDB00641glutamineyes58HMDB00641glutamineyes59HMDB00300uracilyes60HMDB00300uracilyes61sucroseno62sucroseno63HMDB00254succinic acid64HMDB0094citric acid65HMDB00243pyruvic acid66thioureano67thioureano68à-D-Galactopyranosiduronic acidno69à-D-Galactopyranosiduronic acidno0Uronic acid pathway	51		glucose 6 phosphate	yes	
33HMDB02730IntrollatingyesMetabolism of Cofactors and Vitamins54HMDB00210Pantothenic acidyesMetabolism of Cofactors and Vitamins553-ureidopropionic acid and/or beta-alaninenono56HMDB00641glutamineyesMetabolism of Other Amino Acids57HMDB00641glutamineyesMetabolism of Other Amino Acids58HMDB00300uracilyesMetabolism of Other Amino Acids60HMDB00300uracilyesMetabolism of Other Amino Acids61SucrosenoStarch and sucrose metabolism62Succinic acidyesTricarboxylic acid cycle63HMDB00254Succinic acidyes64HMDB0094citric acidyes65HMDB00243pyruvic acidyes66thioureanoUrea cycle67thioureanoUrea cycle68à-D-Galactopyranosiduronic acidnoUronic acid pathway	52		giucose-o-priospirate	yes	
34HindboozioParticultarite actualyes553-ureidopropionic acid and/or beta-alanineno56HMDB00641glutamineyes57HMDB00641glutamineyes58HMDB00641glutamineyes59HMDB00300uracilyes60HMDB00300uracilyes61sucroseno62sucroseno63HMDB00254sucroseno64HMDB0094citric acidyes65HMDB00243pyruvic acidyes66thioureanoUrea cycle67thioureanoUronic acid pathway69à-D-Galactopyranosiduronic acidnoUronic acid pathway	55		Pantothonic acid	yes	Metabolism of Cofactors and Vitamins
55HMDB00641glutamineyes57HMDB00641glutamineyes58HMDB00641glutamineyes59HMDB00300uracilyes60HMDB00300uracilyes61sucroseno62sucroseno63HMDB00254sucroseno64HMDB0094citric acidyes65HMDB00243pyruvic acidyes66thioureano67thioureano68thioureano69à-D-Galactopyranosiduronic acidno0thioureano0Uronic acid pathway	55	TIVIDBOOZIO	3-ureidopronionic acid and/or beta-alanine	yes no	
57HMDB00641glutamineyesMetabolism of Other Amino Acids58HMDB00641glutamineyesMetabolism of Other Amino Acids59HMDB00300uracilyesMetabolism of Other Amino Acids60HMDB00300uracilyesMetabolism of Other Amino Acids61sucrosenoStarch and sucrose metabolism62sucrosenoStarch and sucrose metabolism63HMDB00254sucroic acidyes64HMDB0094citric acidyes65HMDB00243pyruvic acidyes66thioureanoUrea cycle67thioureanoUrea cycle68à-D-Galactopyranosiduronic acidnoUronic acid pathway	56	HMDB00641	glutamine	ves	
SiHMDB000641glutamineyesMetabolism of Other Amino Acids58HMDB00300uracilyes60HMDB00300uracilyes61sucroseno62sucroseno63HMDB00254sucroic acid64HMDB0094citric acid65HMDB00243pyruvic acid66thioureano67thioureano68thioureano69à-D-Galactopyranosiduronic acidno0uracid pathway	57	HMDB00641	glutamine	ves	
SSHMDB00300uracilyes59HMDB00300uracilyes60HMDB00300uracilyes61sucroseno62sucroseno63HMDB00254succinic acidyes64HMDB0094citric acidyes65HMDB00243pyruvic acidyes66thioureano67thioureano68thioureano69à-D-Galactopyranosiduronic acidno0Uronic acid pathway	58	HMDB00641	glutamine	ves	Metabolism of Other Amino Acids
60HMDB00300uracilyes61sucroseno62sucroseno63HMDB00254succinic acidyes64HMDB0094citric acidyes65HMDB00243pyruvic acidyes66thioureanoUrea cycle67thioureanoUrea cycle68bthioureano69bb-D-Galactopyranosiduronic acidno69bb-D-Galactopyranosiduronic acidno	59	HMDB00300	uracil	ves	
61sucroseno62sucroseno63HMDB00254sucrose64HMDB0094citric acidyes65HMDB00243pyruvic acidyes66thioureano67thioureano68thioureano69à-D-Galactopyranosiduronic acidno09b-D-Galactopyranosiduronic acidno	60	HMDB00300	uracil	ves	
62sucrosenoStarch and sucrose metabolism63HMDB00254succinic acidyes64HMDB00094citric acidyes65HMDB00243pyruvic acidyes66thioureano67thioureano68thioureano69à-D-Galactopyranosiduronic acidno	61		sucrose	no	Charach and the state of the state
63HMDB00254succinic acidyes64HMDB00094citric acidyesTricarboxylic acid cycle65HMDB00243pyruvic acidyes66thioureanoUrea cycle67thioureanoUrea cycle68thioureano69à-D-Galactopyranosiduronic acidnoUronic acid pathway	62		sucrose	no	starch and sucrose metabolism
64HMDB00094citric acidyesTricarboxylic acid cycle65HMDB00243pyruvic acidyes66thioureano67thioureano68thioureano69à-D-Galactopyranosiduronic acidno	63	HMDB00254	succinic acid	yes	
65HMDB00243pyruvic acidyes66thioureano67thioureano68thioureano69à-D-Galactopyranosiduronic acidno	64	HMDB00094	citric acid	yes	Tricarboxylic acid cycle
66thioureano67thioureano68thioureano69à-D-Galactopyranosiduronic acidnoUronic acid pathwayUronic acid pathway	65	HMDB00243	pyruvic acid	yes	
67thioureanoUrea cycle68thioureano69à-D-Galactopyranosiduronic acidnoUronic acid pathway	66		thiourea	no	
68   thiourea   no     69   à-D-Galactopyranosiduronic acid   no   Uronic acid pathway	67		thiourea	no	Urea cycle
69 à-D-Galactopyranosiduronic acid no Uronic acid pathway	68		thiourea	no	
	69		à-D-Galactopyranosiduronic acid	no	Uronic acid pathway

#### **Figure Legends**

Supplemental Figure S1A The five sites from the diseased hand. The Dupuytren's disease-associated tissues that are subjected to analysis in this study. Five different Dupuytren's disease-associated tissues in each patient's hand are collected, the normal fascia (unaffected transverse fascia), palmar nodule and cord, skin overlying nodule, and fat. Supplemental Figure S1B The palm of an unaffected individual used as control. The palm of the hand of a control subject, where the overlying skin has been removed to demonstrate the position of the palmar fascia harvested. Skin, palmar fascia (transverse carpal ligament) and fat were obtained from control subjects, individuals undergoing carpal tunnel

release.



Supplemental Figure S2 Hematoxylin and eosin slides displaying cross sections

from disease and control tissues.



Fibroblasts in fat cushioning nodule

Fibroblasts in skin overlying the nodule



**Supplemental Figure S3** A workflow representing the procedure implemented to analyse the samples from Dupuytren's disease and control fibroblast cell cultures.

WORK	EX	
<b>Meta Data</b> Patient No. Age, Gender, Health	Sample collection & Preparation	oerimental Design
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**Supplemental Figure S4** Flowchart of metabolomics experiment – from experimental design through to data analysis.



## Supplemental Figure S5 Mass spectrometry spectra of metabolites features

reported in Figures 8A-F.

8 a) L-Leucine MW 131.173

Reference Spectrum - Reference "Samrina May10", Analyte "Samrina May10 16"

