

## Supporting Information

### **<sup>1</sup>H NMR metabolomics identifies underlying inflammatory pathology in osteoarthritis and rheumatoid arthritis synovial joints**

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Supplementary Table S1. List of 50 metabolites detected in OA and RA SF by <sup>1</sup>H NMR spectroscopy, assignment levels according to the Metabolomics Society Initiative(24).

Class	Metabolite name	HMDB	Assignment levels	Chemomx annotation (y/n)	Confirmed by in-house 1H (n = no standard available; y = present)	Observed in in-house 2D HSQC (n1 = no standard available; n2 = below level of detection; y = present)
<b><i>Amino Acids</i></b>	2-Aminobutyrate	HMDB00650	2	y	n	n1
	5-Aminolevulinate	HMDB01149	2	y	n	n1
	Alanine	HMDB00161	1	y	y	y
	Asparagine	HMDB00168	2	y	n	n2
	Creatine	HMDB00064	1	y	y	y
	Creatinine	HMDB00562	1	y	y	n2
	Glutamine	HMDB00641	1	y	y	y
	Glycine	HMDB00123	1	y	y	y
	Guanidoacetate	HMDB00128	2	y	n	n1
	Histidine	HMDB00177	1	y	y	n2
	Isoleucine	HMDB00172	1	y	y	y
	Leucine	HMDB00687	1	y	y	y
	Lysine	HMDB00182	1	y	y	y
	Methionine	HMDB00696	1	y	y	n2
	n-acetylaminoacid	-	3	y	n	n1
	Ornithine	HMDB00214	1	y	y	n2
	Phenylalanine	HMDB00159	1	y	y	y
	Proline	HMDB00162	1	y	y	n2
	Sarcosine	HMDB00271	2	y	n	n2
	Threonine	HMDB00167	1	y	y	y
Tyrosine	HMDB00158	1	y	y	n2	
Valine	HMDB00883	1	y	y	y	
<b><i>Fatty and Organic Acids</i></b>	2-Hydroxybutyrate	HMDB00729	2	y	n	n1
	3-Hydroxybutyrate	HMDB00357	2	y	n	n1

	3-Hydroxyisovalerate	HMDB00754	2	y	n	n1
	Acetate	HMDB00042	1	y	y	y
	Acetoacetate	HMDB00060	2	y	n	n1
	Carnitine	HMDB00062	2	y	n	n1
	Citrate	HMDB00094	1	y	y	n2
	Formate	HMDB00142	2	y	n	n1
	Lactate	HMDB00190	1	y	y	y
	Malonate	HMDB00691	2	y	n	n2
	Pyruvate	HMDB00243	1	y	y	n2
	Taurine	HMDB00251	1	y	y	n2
<b>Sugars</b>	Acetylated-saccharide	-	3	y	y	y
	Glucose	HMDB00122	1	y	y	y
	Glycerol	HMDB00131	1	y	y	y
	Mannose	HMDB00169	1	y	y	y
	Myoinositol	HMDB00211	1	y	y	n2
<b>Other</b>	Acetylcholine	HMDB00895	2	y	n	n1
	Adenosine	HMDB00050	2	y	n	n1
	Choline	HMDB00097	1	y	y	y
	Dimethylamine	HMDB00087	1	y	y	y
	Ethanol	HMDB00108	1	y	y	y
	Isopropanol	HMDB00863	2	y	n	n1
	Mobile-lipid	-	3	y	n	n1
	o-Phosphocholine	HMDB01565	2	y	n	n2
	Oxypurinol	HMDB00086	2	y	n	n1
	sn-Glycero-3-phosphocholine	HMDB00086	2	y	n	n1
	Xanthine	HMDB00292	2	y	n	n2

Abbreviation: HSQC = Heteronuclear Single Quantum Coherence