Supporting Information

A Microdialysis Workflow for Metabotyping Superficial Pathologies: Application to Burn Injury

Dominic Friston[1], Helen Laycock[1], Istvan Nagy[1], Elizabeth J. Want[2*]

[1]Nociception Group, Section of Anaesthetic, Pain Medicine and Intensive Care, Department of Surgery and Cancer, Imperial College London, London UK

[2]Integrative Systems Medicine and Digestive Diseases; Department of Surgery and Cancer, Imperial College London, London UK

*corresponding author: e.want@imperial.ac.uk

Table of Contents

Table S1. A description of the different sample groups, together with the number of samples collected and analysed during the study.

Sample Group	Number of samples/animal	Number of animals	Total	Description
Burn	6	4	24	*Microdialysate fractions collected from the BURN site AFTER the burn induction.*
Control	6	4	24	*Microdialysate fractions collected from the CONTROL site AFTER the burn induction.*
Pre-burn Flush	2	4	8	*The single "flush" microdialysate fractions collected from BOTH microdialysis sites BEFORE the burn induction.*
Quality Control			1	*Mixtures of all microdialysates injected throughout the run for monitoring UPLC-MS stability.*

Table S2. The top 30 metabolite features as ranked by VIP value from PLS-DA analysis in positive and negative mode respectively. *RT = retention time in seconds*.

Positive Mode	Feature (m/z/RT)	VIP value	Negative Mode	Feature (m/z/RT)	VIP value
	1029.1/331	4.32004		281/188	3.74991
	1028.8/332	4.28977		736.9/86	3.68634
	1029.8/332	4.28663		926.9/86	3.57676
	591.2/221	4.26254		296.1/186	3.55986
	938.9/334	4.23014		1051/86	3.54795
	1022.1/331	4.21074		378.1/208	3.48508
	598.6/274	4.18326		926.3/333	3.43265
	605.6/273	4.17587		827.4/627	3.40225
	580.2/221	4.16793		737.9/86	3.39798
	479.1/265	4.16299		826.4/627	3.39054
	241.1/36	4.14028		281.1/265	3.37713
	1152.8/323	4.1053		343/60	3.34414
	584.6/299	4.07239		281.1/253	3.3383
	1160.8/323	4.06432		540.9/86	3.32827
	1153.8/323	4.0474		319.2/503	3.27589
	967.4/339	4.03355		337/41	3.26099
	1028.9/381	4.01782		351/177	3.26068
	939.9/334	3.98913		925.8/333	3.25349
	760.4/284	3.98441		365/60	3.24528
	1021.8/357	3.97549		225.1/36	3.23956
	939.4/335	3.96471		547/86	3.23445
	1028.8/356	3.9451		927.9/86	3.23045
	939.4/334	3.94004		1116.9/86	3.22414
	1055.8/352	3.92358		920.9/86	3.21574
	396.7/181	3.91901		548/86	3.17935
	1029.2/381	3.91443		284/177	3.17277
	479.1/252	3.90525		1116.9/86	3.16146
	585/299	3.90098		320.2/503	3.15953
	631.2/265	3.88911		920.9/86	3.1566
	570.3/195	3.87106		715/86	3.15085
	1029.1/331	4.32004		281/188	3.74991