全谱绝对定量代谢组学研究

池逸 Ph.D.

ychi@metaboprofile.com

香港浸会大学 贾伟教授课题组

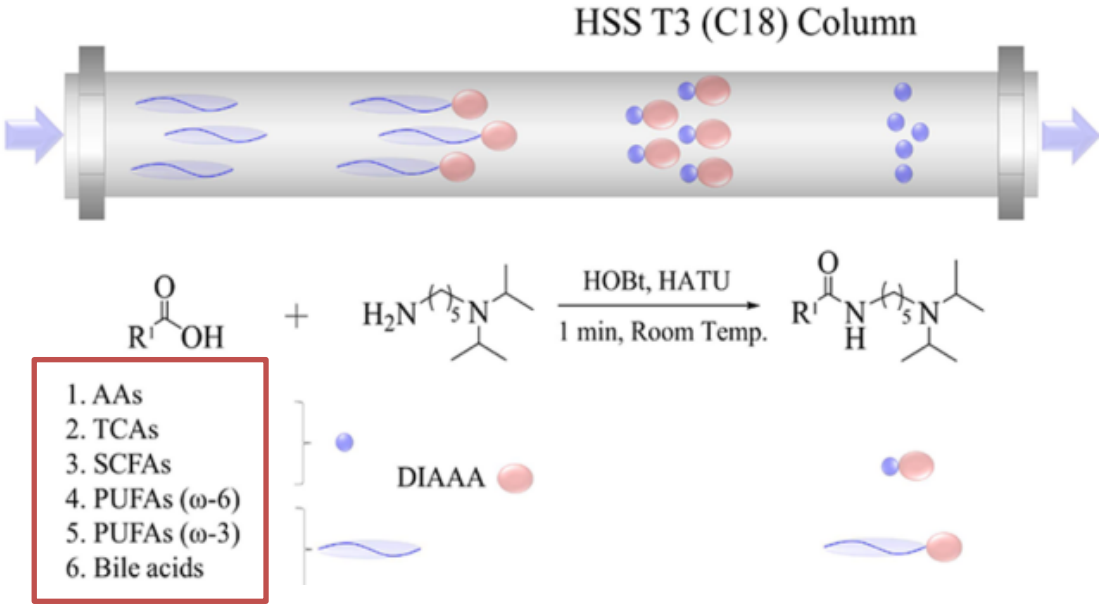
专注代谢组学服务

全谱绝对定量代谢组学方法

analytical chemistry

Polarity-Tuning Derivatization-LC-MS Approach for Probing Global Carboxyl-Containing Metabolites in Colorectal Cancer

Xiqing Bian,[†] Na Li,[*,†] Binbin Tan,[‡] Baoqing Sun,[§] Ming-Quan Guo,[∥] Guoxin Huang,[†] Li Fu,[‡] W. L. Wendy Hsiao,[†] Liang Liu,[*,†] and Jian-Lin Wu[*,†]

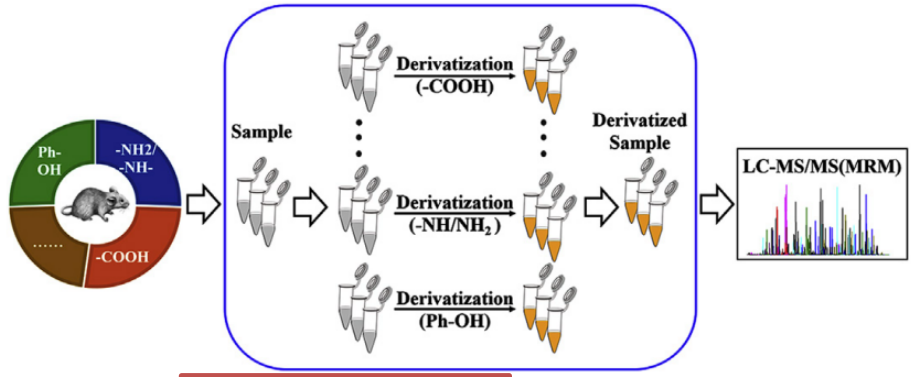


1. AAs
2. TCAs
3. SCFAs
4. PUFAs (ω-6)
5. PUFAs (ω-3)
6. Bile acids

68种代谢物

An extendable all-in-one injection twin derivatization LC-MS/MS strategy for the absolute quantification of multiple chemical-group-based submetabolomes

Yezhen Huang [a, 1], Yu Jiao [a, b, 1], Yiqiao Gao [a], Pei Zhang [a, c, d], Wanqiu Huang [a], Yong Liu [a, b], Yin Huang [a], Yuan Tian [a], Jian-Bo Wan [e], Zunjian Zhang [a], Kun Hao [a, f, **], Fengguo Xu [a, *]



1. Polyamines
2. AAs
3. Indole
4. Bile acids
5. FFA

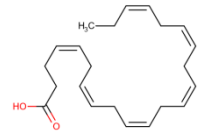
80种代谢物

麦特绽谱 Metabo-Profile

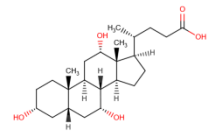
Q300™全谱绝对定量代谢组学

总代谢物数	306
氨基酸类	60
脂肪酸类	55
有机酸类	41
胆汁酸类	39
碳水化合物	25
苯环型	21
肉碱类	21
短链脂肪酸	10
吲哚类	9
苯丙酸类	9
其他	16

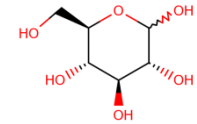
UPLC-MS/MS



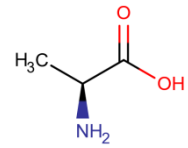
中长链脂肪酸



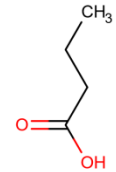
胆汁酸



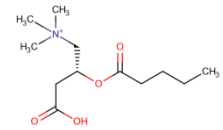
还原糖



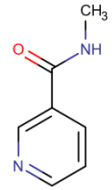
氨基酸



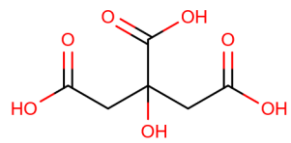
短链脂肪酸



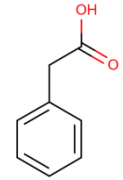
肉碱



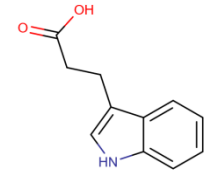
吡啶衍生物



有机酸



苯环型化合物



吲哚衍生物


证书号第3911262号

发明专利证书

发明名称：生物样品中多种代谢物定量检测方法及代谢芯片

发明人：贾伟;谢国祥;王鹭

- ✓ 覆盖范围广
- ✓ 绝对定量，同位素内标矫正
- ✓ 兼容各种生物样本

麦特绘谱 Metabo-Profile

Q300全谱绝对定量代谢组学

样本类型：

血清/血浆：20uL

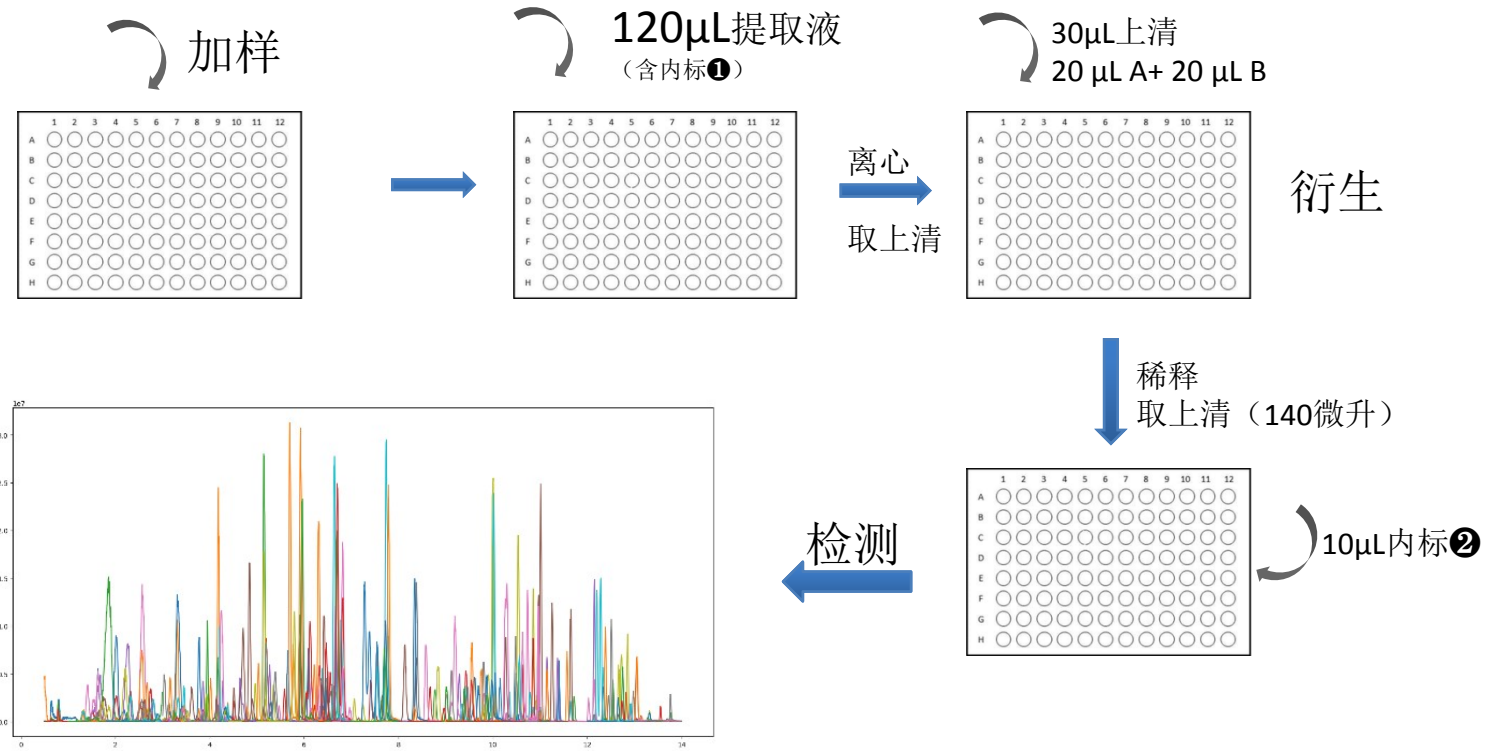
血片：3个

尿液：20uL

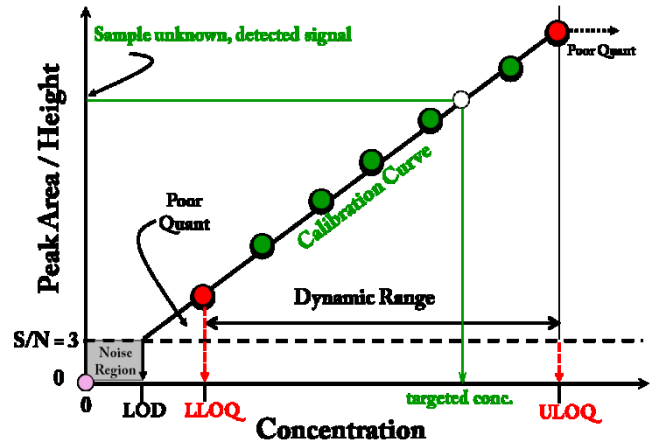
冻干粪便：5mg

组织：10mg

细胞：10^6



For FTN &FL: 96 well plate (Waters 700 uL round well, Mfr#: 186005837; 7 mm round plug cap-mat, pre-slit, Mfr#: 186006332)												
	1	2	3	4	5	6	7	8	9	10	11	12
A 01	S01	S02	S03	S04	S05	S06	S07	S08	S09	S10	S11	S12
B 13	S13	S14	S15	S16	S17	S18	S19	S20	S21	S22	S23	S24
C 25	S25	S26	S27	S28	S29	S30	S31	S32	S33	S34	S35	S36
D 37	S37	S38	S39	S40	S41	S42	S43	S44	S45	S46	S47	S48
E 49	S49	S50	S51	S52	S53	S54	S55	S56	S57	S58	S59	S60
F 61	S61	S62	S63	S64	S65	S66	S67	S68	S69	S70	S71	S72
G 73	S73	S74	S75	S76	S77	S78	S79	S80	S81	S82	S83	S84
H	CAL0	CAL1	CAL2	CAL3	CAL4	CAL5	CAL6	CAL7	QC1	QC2	QC3	QC4
	85	86	87	88	89	90	91	92	93	94	95	96



代表物质回收率

类别	代谢物	回收率%	CV%	类别	代谢物	回收率%	CV%
氨基酸类	甘氨酸	106	13.3	胆汁酸	胆酸	98	3.3
	丙氨酸	89	2.6		脱氧胆酸	93	3.1
	瓜氨酸	92	2.7		牛磺胆酸	110	9.8
	酪氨酸	103	0.6		牛磺脱氧胆酸	103	4.7
	色氨酸	108	2.3		甘氨胆酸	87	2.6
	亮氨酸	102	0.5		甘氨脱氧胆酸	92	7.6
脂肪酸类	DHA	93	5.7	还原糖	葡萄糖	84	6.2
	EPA	110	2.8		果糖	80	4.5
	ARA	102	1.2	肉碱类	乙酰肉碱	114	0.8
	油酸	98	4.6		丙酰肉碱	106	0.4
	肉豆蔻酸	116	12.8		戊二酰肉碱	96	1.2
有机酸	柠檬酸	82	1.2	SCFA	丙酸	83	2.2
	琥珀酸	99	0.6		丁酸	87	1.4
	延胡索酸	98	4.5	苯环型化合物	苯乙酸	97	0.6
	2-羟基戊二酸	91	2.2	吲哚类	吲哚乙酸	98	0.9

批量定量软件

靶向代谢物组批量定量系统（TMBQ）

登录

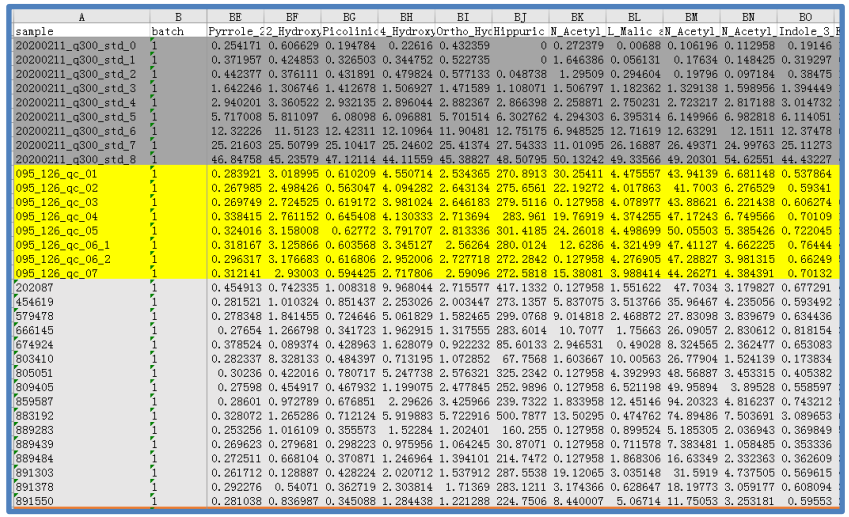
用户名

密码

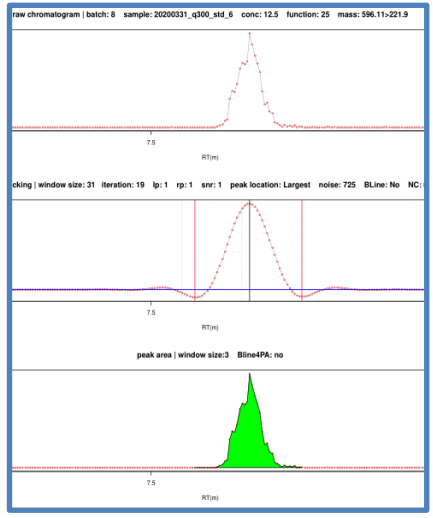
登录

专利申请号：
CN201910170381.0

物质信息配置表　样本列表　原始数据

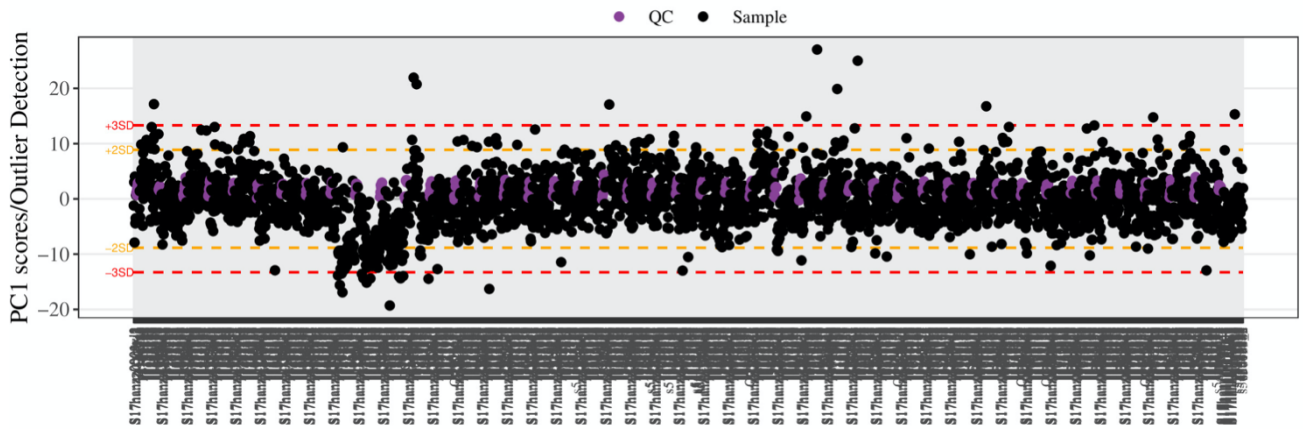


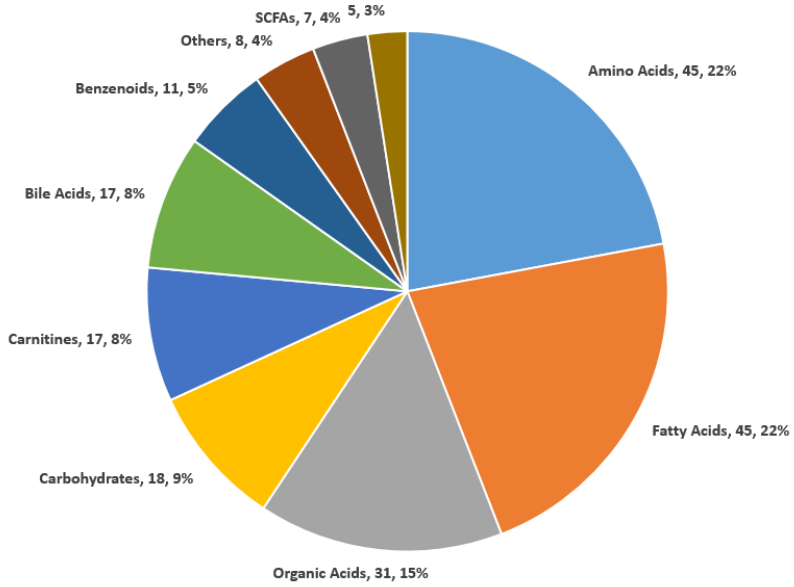
A	B	BE	BF	BG	BH	BI	BJ	BK	BL	BM	BN	BO
sample	batch	Pyrrole_2_HydroxyPicolinic	4_HydroxyOrtho_Hyc	Hippuric	N_Acetyl_L_Malic a	N_Acetyl_N_Acetyl_	Indole_3_F					
20200211_q300_std_0	1	0.254171	0.606629	0.194784	0.22616	0.432359	0	0.272379	0.00688	0.106196	0.112958	0.19146
20200211_q300_std_1	1	0.371957	0.424853	0.326503	0.344752	0.522735	0	1.646386	0.056131	0.17634	0.148425	0.319297
20200211_q300_std_2	1	0.442377	0.376111	0.431891	0.479824	0.577133	0.048738	1.29509	0.294604	0.19796	0.097184	0.38475
20200211_q300_std_3	1	1.642246	1.306746	1.412678	1.506927	1.471589	1.108071	1.506797	1.182362	1.329138	1.598956	1.394449
20200211_q300_std_4	1	2.940201	3.360522	2.932135	2.896044	2.882367	2.866398	2.258871	2.750231	2.723217	2.817188	3.014732
20200211_q300_std_5	1	5.717008	5.811097	6.08098	6.096881	5.701514	6.302762	4.294303	6.395314	6.149966	6.982818	6.114051
20200211_q300_std_6	1	12.32226	11.5123	12.42311	12.10964	11.90481	12.75175	6.948525	12.71619	12.63291	12.1511	12.37478
20200211_q300_std_7	1	25.21603	25.50799	25.10417	25.24602	25.41374	27.54333	11.01095	26.16887	26.49371	24.99763	25.11273
20200211_q300_std_8	1	46.84758	45.23579	47.12114	44.11559	45.38827	48.50795	50.13242	49.33566	49.20301	54.62551	44.43227
095_126_qc_01	1	0.283921	3.018995	0.610209	4.550714	2.534365	270.8913	30.25411	4.475557	43.94139	6.681148	0.537864
095_126_qc_02	1	0.267985	2.498426	0.563047	4.094282	2.643134	275.6561	22.19272	4.017863	41.7003	6.276529	0.59341
095_126_qc_03	1	0.269749	2.724525	0.619172	3.981024	2.646183	279.5116	0.127958	4.078977	43.88621	6.221438	0.606274
095_126_qc_04	1	0.338415	2.761152	0.645408	4.130333	2.713694	283.961	19.76919	4.374255	47.17243	6.749566	0.70109
095_126_qc_05	1	0.324016	3.158008	0.62772	3.791707	2.813336	301.4185	24.26018	4.498699	50.05503	5.385426	0.722045
095_126_qc_06_1	1	0.318167	3.125866	0.603568	3.345127	2.56264	280.0124	12.6286	4.321499	47.41127	4.662225	0.76444
095_126_qc_06_2	1	0.296317	3.176683	0.616806	2.952006	2.727718	272.2842	0.127958	4.276905	47.28827	3.981315	0.66249
095_126_qc_07	1	0.312141	2.93003	0.594425	2.717806	2.59096	272.5818	15.38081	3.988414	44.26271	4.384391	0.70132
202087	1	0.454913	0.742335	1.008318	9.968044	2.715577	417.1332	0.127958	1.551622	47.7034	3.179827	0.677291
454619	1	0.281521	1.010324	0.851437	2.253026	2.003447	273.1357	5.837075	3.513766	35.96467	4.235056	0.593492
579478	1	0.278348	1.841455	0.724646	5.061829	1.582465	299.0768	9.014818	2.468872	27.83098	3.839679	0.634436
666145	1	0.27654	1.266798	0.341723	1.962915	1.317555	283.6014	10.7077	1.75663	26.09057	2.830612	0.818154
674924	1	0.378524	0.089374	0.428963	1.628079	0.922232	85.60133	2.946531	0.49028	8.324565	2.362477	0.653083
803410	1	0.282337	8.328133	0.484397	0.713195	1.072852	67.7568	1.603667	10.00563	26.77904	1.524139	0.173834
805051	1	0.30236	0.422016	0.780717	5.247738	2.576321	325.2342	0.127958	4.392993	48.56887	3.453315	0.405382
809405	1	0.27598	0.454917	0.467932	1.199075	2.477845	252.9896	0.127958	6.521198	49.95894	3.89528	0.558597
859587	1	0.28601	0.972789	0.676851	2.29626	3.425966	239.7322	1.833958	12.45146	94.20323	4.816237	0.743212
883192	1	0.328072	1.265286	0.712124	5.919883	5.722916	500.7877	13.50295	0.474762	74.89486	7.503691	3.089653
889283	1	0.253256	1.016109	0.355573	1.52284	1.202401	160.255	0.127958	0.899524	5.185305	2.036943	0.369849
889439	1	0.269623	0.279681	0.298223	0.975956	1.064245	30.87071	0.127958	0.711578	7.383481	1.058485	0.353336
889484	1	0.272511	0.668104	0.370871	1.246964	1.394101	214.7472	0.127958	1.868306	16.63349	2.332363	0.362609
891303	1	0.261712	0.128887	0.428224	2.020712	1.537912	287.5538	19.12065	3.035148	31.5919	4.737505	0.569615
891378	1	0.292276	0.54071	0.362719	2.303814	1.71369	283.1211	3.174366	0.628647	18.19773	3.059177	0.608094
891550	1	0.281038	0.836987	0.345088	1.284438	1.221288	224.7506	8.440007	5.06714	11.75053	3.253181	0.59553

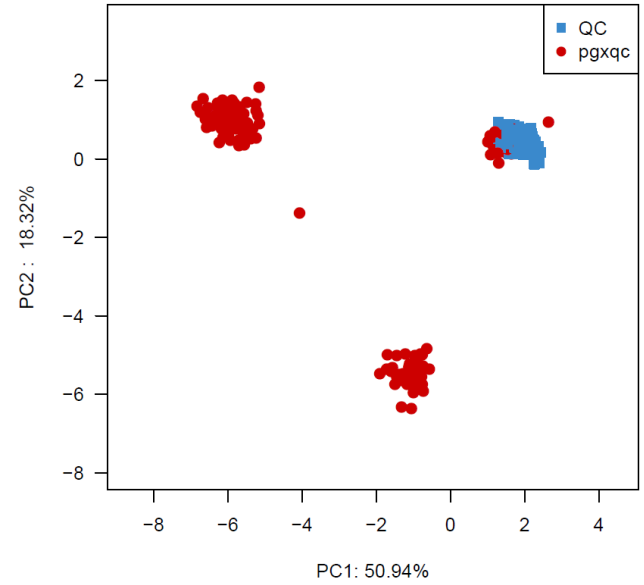


Q300检测案例

图1　多变量质控图

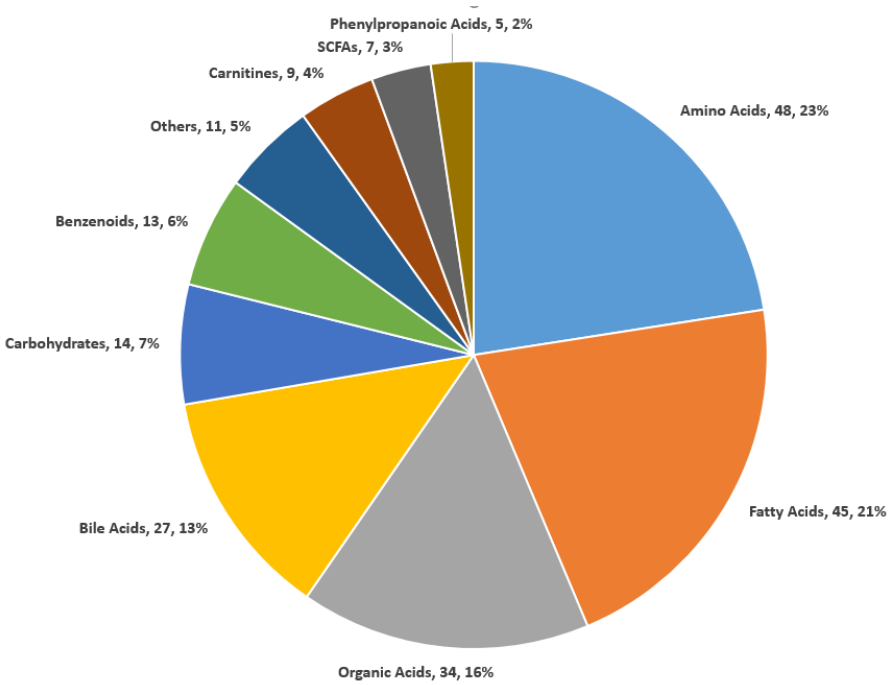


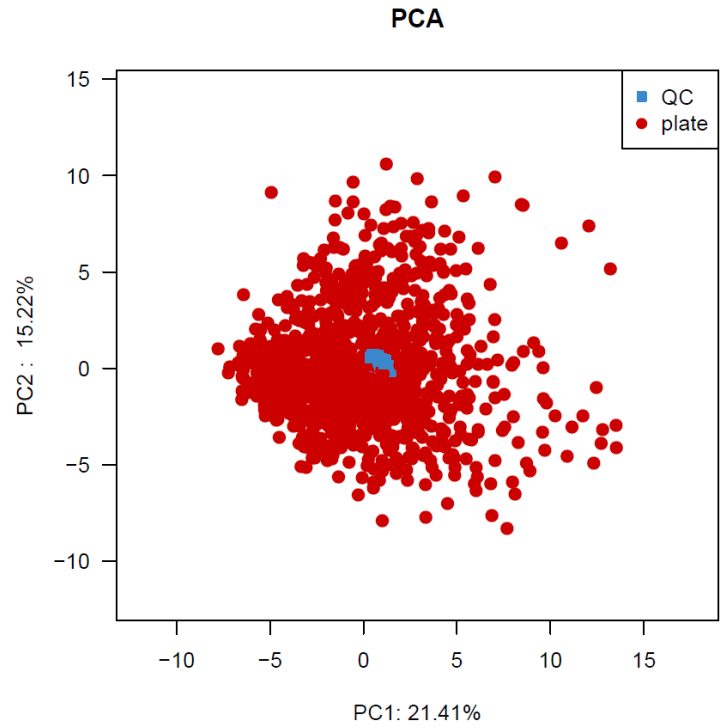




✓　3000+例血浆队列样本

Q300检测案例





✓ 1000+例粪便队列样本

Q300检测案例

类别	血清/血浆	粪便	尿液	组织	干血斑
氨基酸	44	42	46	45	35
有机酸	27	32	32	32	29
脂肪酸	45	34	24	46	35
胆汁酸	17	32	18	20	5
碳水化合物	20	17	17	16	17
苯环类	17	13	16	10	8
肉碱	21	13	13	18	19
苯丙酸类	4	8	6	/	/
短链脂肪酸	8	8	5	5	6
吲哚类	3	2	4	/	/
其他	3	4	19	15	11
总代谢物	209	205	200	207	165

Q300™ kit

检测 → 定量 → 分析

云平台iMAP

- 多维统计
- 单维统计
- 通路分析
- 诊断分析
- 关联分析

Waters THE SCIENCE OF WHAT'S POSSIBLE.™

AB SCIEX

ThermoFisher SCIENTIFIC

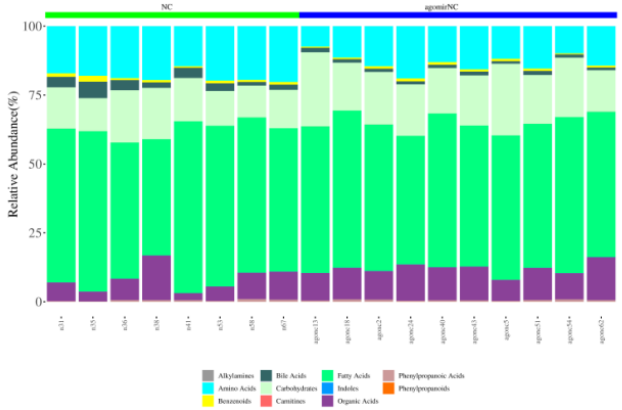
Agilent Technologies

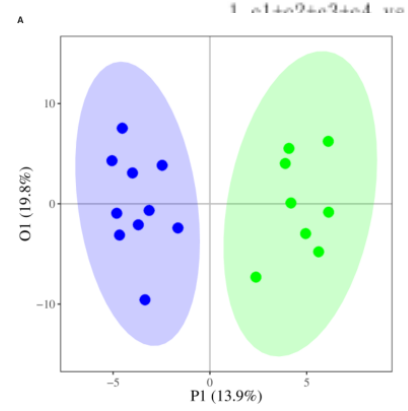
岛津 SHIMADZU

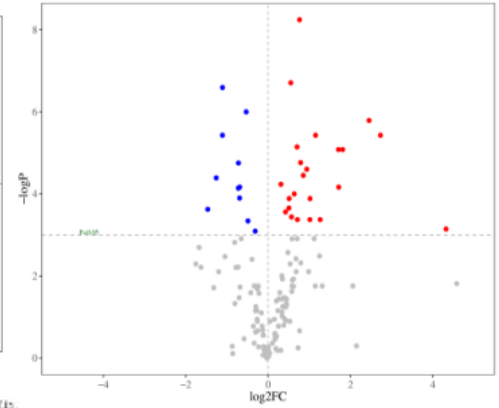
BRUKER

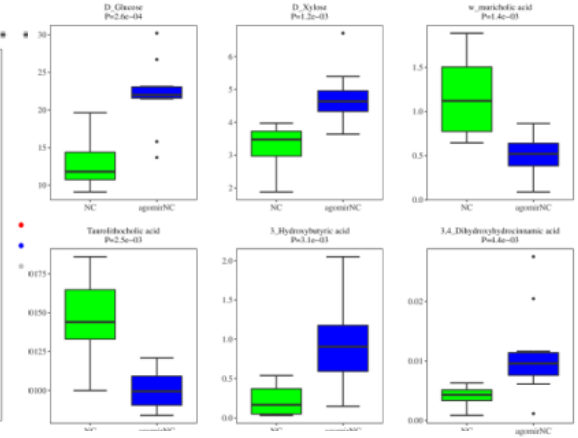
麦特绽谱 Metabo-Profile

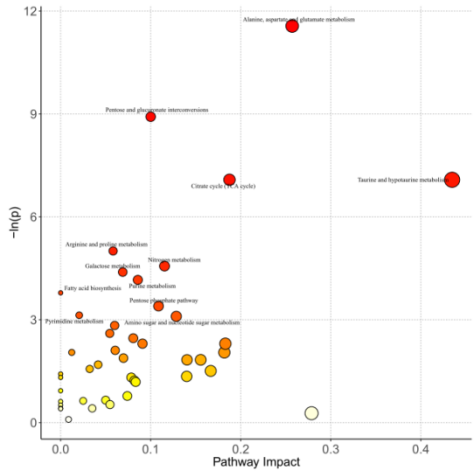
目录

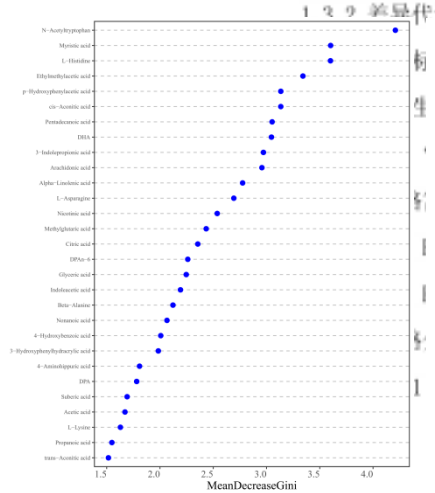


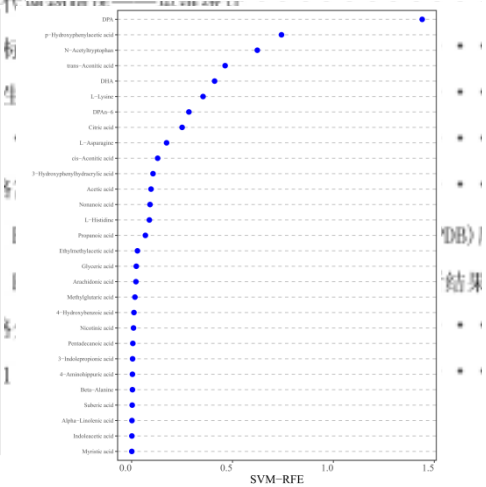


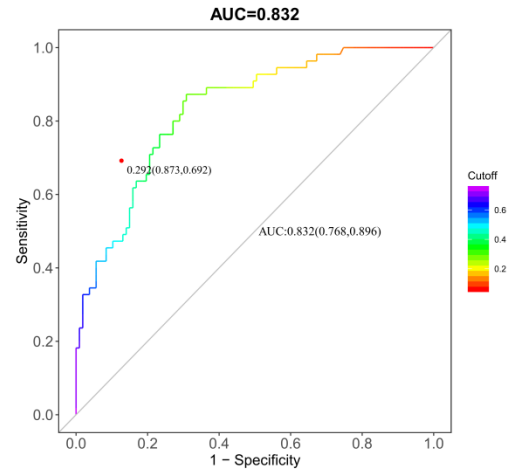




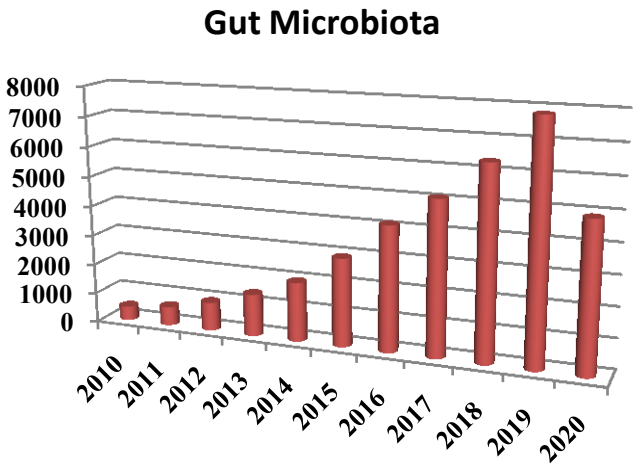


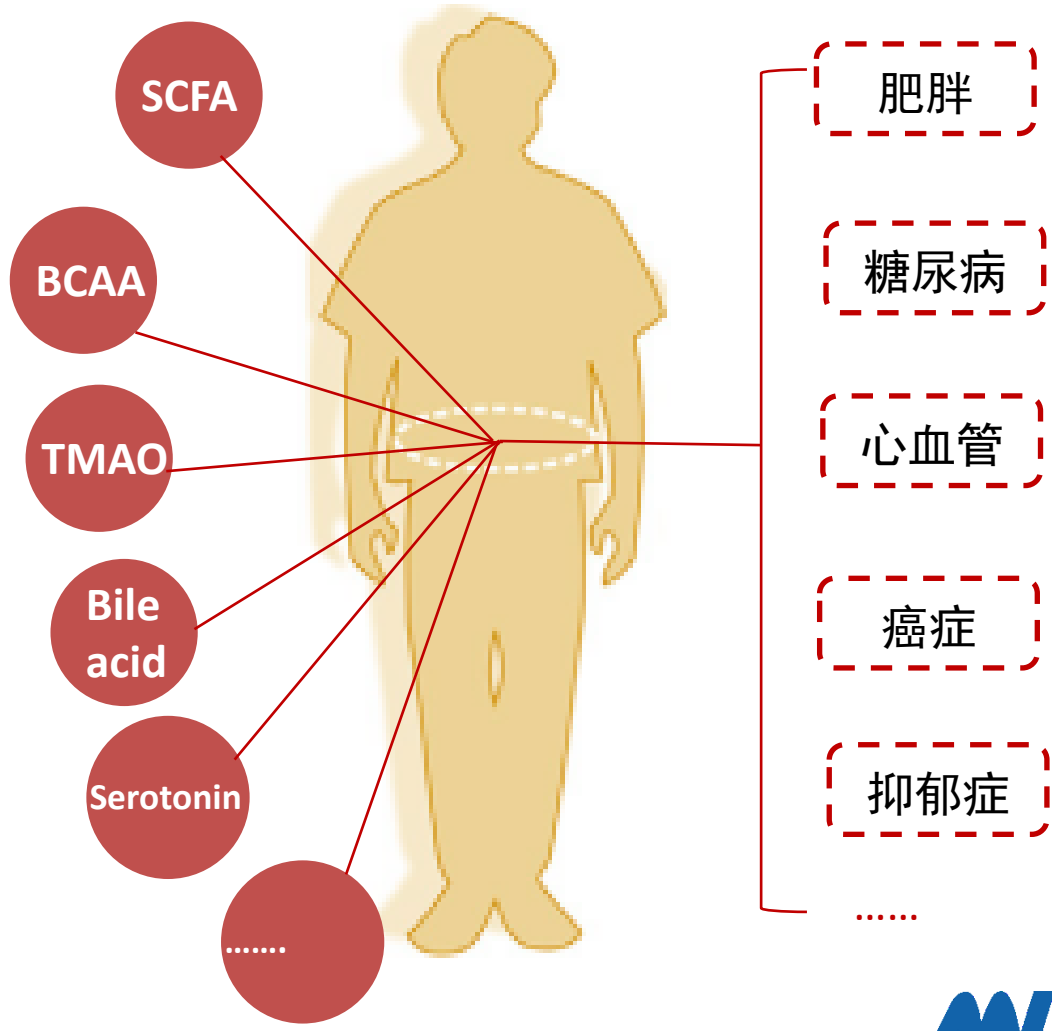






肠道菌群是生命科学研究热点





麦特绘谱 Metabo-Profile

Q200™ kit介绍

analytical chemistry

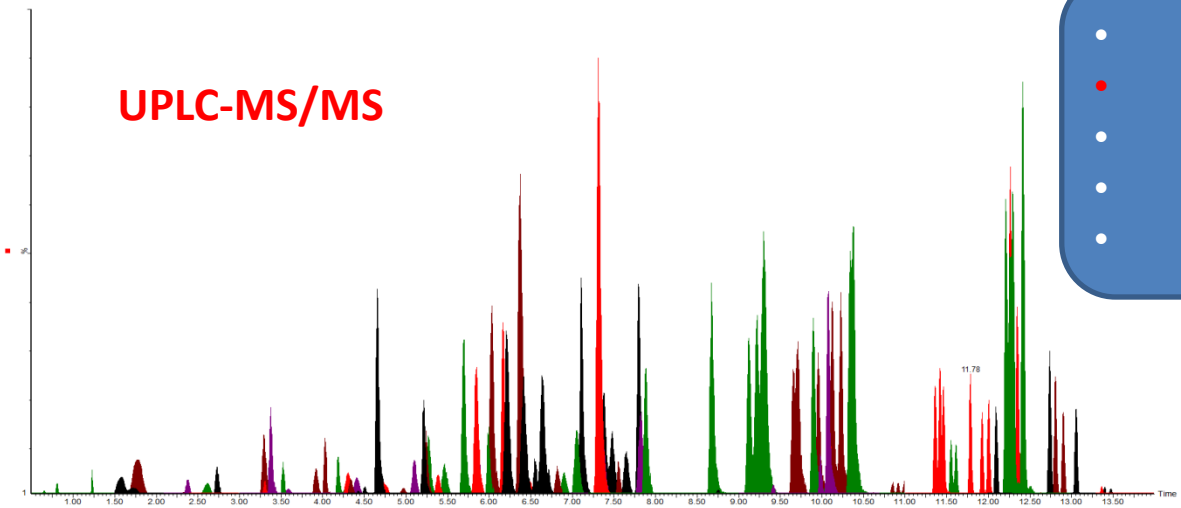
Article

pubs.acs.org/ac

2017年首次建立基于GC-TOFMS的自动化全定量肠道菌群代谢物分析方法

High Throughput and Quantitative Measurement of Microbial Metabolome by Gas Chromatography/Mass Spectrometry Using Automated Alkyl Chloroformate Derivatization

Linjing Zhao,[†,‡,#] Yan Ni,[†,§,#] Mingming Su,[†,§,#] Hongsen Li,[‡] Fangcong Dong,[§] Wenlian Chen,[§] Runmin Wei,[§] Lulu Zhang,[§] Seu Ping Guiraud,[∥] Francois-Pierre Martin,[∥] Cynthia Rajani,[§] Guoxiang Xie,[§] and Wei Jia[*,†,§]



- 短链脂肪酸（12）
- 胆汁酸（40+）
- 苯类（20+）
- 吲哚类（10+）
- 苯丙酸类（7）
- 氨基酸（40+）
- 中长链脂肪酸（40+）
- 碳水化合物（10+）
- 有机酸（30+）
- 其他（5）

麦特绘谱 Metabo-Profile

胆汁酸新功能

nature medicine

LETTERS

https://doi.org/10.1038/s41591-019-0509-0

Gut microbiota-bile acid-interleukin-22 axis orchestrates polycystic ovary syndrome

Xinyu Qi[1,11], Chuyu Yun[1,2,11], Lulu Sun[1,2], Jialin Xia[1,2], Qing Wu[1,2], Ying Wang[1,3,4], Lina Wang[1,3,4], Yangming Zhang[1,2], Xianyi Liang[1,2], Liying Wang[1,3,4], Frank J. Gonzalez[5], Andrew D. Patterson[6], Huiying Liu[1,2], Liangshan Mu[1,3], Zehong Zhou[1,3], Yue Zhao[1,3,7], Rong Li[1,3,4,7], Ping Liu[1,3,4,7], Chao Zhong[8], Yanli Pang[1,3,7*], Changtao Jiang[1,2*] and Jie Qiao[1,3,4,7,9,10*]

GDCA通过激活肠道3型固有淋巴细胞（ILC3）的GATA3通路刺激IL-22分泌，进一步促进白色脂肪棕色化以及抑制卵巢局部炎症，进而改善PCOS样表型。

Ma *et al.*, *Science* **360**, eaan5931 (2018)

Gut microbiome-mediated bile acid metabolism regulates liver cancer via NKT cells

Chi Ma, Miaojun Han, Bernd Heinrich, Qiong Fu, Qianfei Zhang, Milan Sandhu, David Agdashian, Masaki Terabe, Jay A. Berzofsky, Valerie Fako, Thomas Ritz, Thomas Longerich, Casey M. Theriot, John A. McCulloch, Soumen Roy, Wuxing Yuan, Vishal Thovarai, Shurjo K. Sen, Mathuros Ruchirawat, Firouzeh Korangy, Xin Wei Wang, Giorgio Trinchieri, Tim F. Greten*

初级胆酸可激活CXL蛋白，进而激活NKT细胞，抑制肿瘤，而次级胆汁酸有相反的作用。

Nature, 2019, doi:10.1038/s41586-019-1785-z

Article

Bile acid metabolites control T_H17 and T_{reg} cell differentiation

3-oxo-LCA可抑制Th17细胞的分化，而isoalloLCA可增强Treg胞的分化。

胆汁酸新功能

Alzheimer's & Dementia

Alzheimer's & Dementia 15 (2019) 76-92

Alzheimer's & Dementia ■ (2018) 1-13

Altered bile acid profile in mild cognitive impairment and Alzheimer's disease: Relationship to neuroimaging and CSF biomarkers

Kwangsik Nho[a,1], Alexandra Kueider-Paisley[b,a], Siamak MahmoudianDehkordi[b,a], Matthias Arnold[b,c], Shannon L. Risacher[a], Gregory Louie[b], Colette Blach[d], Rebecca Baillie[e], Xianlin Han[f], Gabi Kastenmüller[c,g], Wei Jia[h], Guoxiang Xie[h], Shahzad Ahmad[i], Thomas Hankemeier[j], Cornelia M. van Duijn[i], John Q. Trojanowski[k], Leslie M. Shaw[k], Michael W. Weiner[l], P. Murali Doraiswamy[b,m,n], Andrew J. Saykin[a,**], Rima Kaddurah-Daouk[b,m,n,*], for the Alzheimer's Disease Neuroimaging Initiative and the Alzheimer Disease Metabolomics Consortium[2]

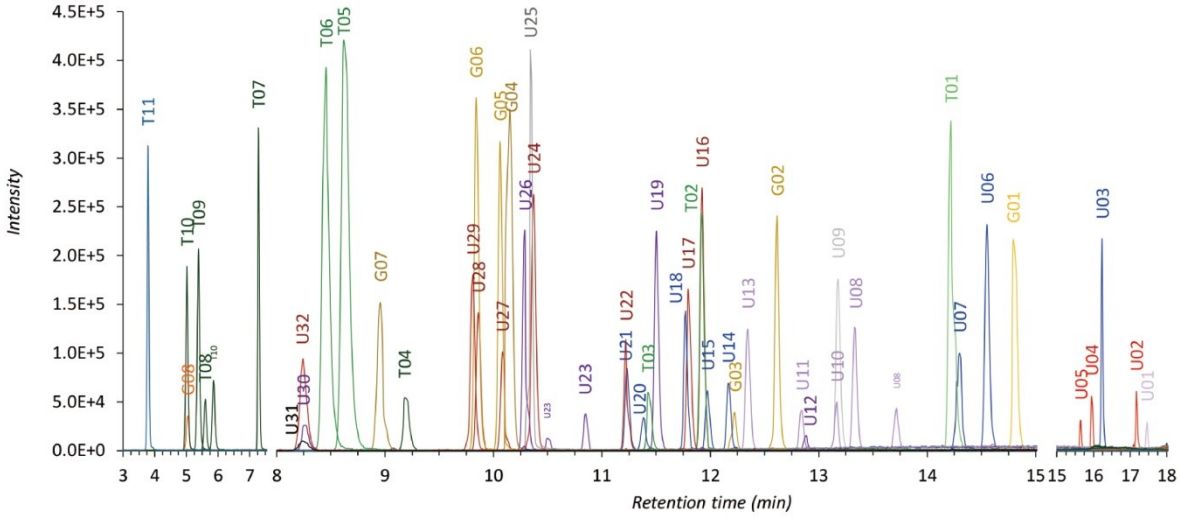
Altered bile acid profile associates with cognitive impairment in Alzheimer's disease—An emerging role for gut microbiome

Siamak MahmoudianDehkordi[a,1], Matthias Arnold[a,b,1], Kwangsik Nho[c,1], Shahzad Ahmad[d], Wei Jia[e,f], Guoxiang Xie[e], Gregory Louie[a], Alexandra Kueider-Paisley[a], M. Arthur Moseley[g], J. Will Thompson[g], Lisa St John Williams[g], Jessica D. Tenenbaum[h], Colette Blach[i], Rebecca Baillie[j], Xianlin Han[k], Sudeepa Bhattacharyya[l], Jon B. Toledo[m], Simon Schafferer[n], Sebastian Klein[n], Therese Koal[n], Shannon L. Risacher[c], Mitchel Allan Kling[o], Alison Motsinger-Reif[p], Daniel M. Rotroff[p], John Jack[p], Thomas Hankemeier[q], David A. Bennett[r], Philip L. De Jager[s], John Q. Trojanowski[t], Leslie M. Shaw[t], Michael W. Weiner[u], P. Murali Doraiswamy[a,v,w], Cornelia M. van Duijn[d], Andrew J. Saykin[c,**], Gabi Kastenmüller[b,x,*], Rima Kaddurah-Daouk[a,v,w,***], for the Alzheimer's Disease Neuroimaging Initiative and the Alzheimer Disease Metabolomics Consortium

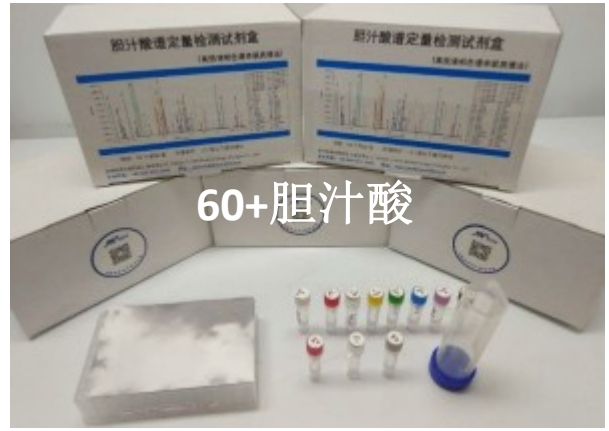
胆汁酸可能通过肠-肝-脑轴影响AD的进展。

麦特绥谱 Metabo-Profile

BAP™ kit (Bile Acid Profiling)介绍



m/z 375	m/z 482	m/z 389			
m/z 391	m/z 498	m/z 405			
m/z 407	m/z 514	m/z 403			
m/z 432	m/z 508	m/z 377			
m/z 448	m/z 458	m/z 393			
m/z 464	m/z 373	m/z 401			
U01	dehydroLCA	U14	HDCA	G05	GHDCA
U02	LCA	U15	UDCA	U28	βCA
U03	isoDCA	U16	CA	G06	GUDCA
U04	isoLCA	T02	TDCA	U29	ωMCA
U05	alloLCA	U17	ACA	T04	TCA
G01	GLCA	U18	βHDCA	G07	GHCA
U06	DCA	U19	3-DHCA	T05	THDCA
U07	CDCA	T03	TCDCA	T06	TUDCA
T01	TLCA	U20	βUDCA	U30	7,12-diketoLCA
U08	apoCA	U21	muroCA	U31	DHCA
U09	NorDCA	U22	HCA	U32	UCA
U10	12-ketoLCA	U23	12-DHCA	T07	THCA
U11	7-ketoLCA	U24	βMCA	T08	TβMCA
U12	6,7-diketoLCA	U25	NorCA	T09	TαMCA
G02	GDCA	U26	7-ketoDCA	G08	GDHCA
U13	6-ketoLCA	G04	GCA	T10	TωMCA
G03	GCDCA	U27	αMCA	T11	TDHCA



Anal Chem, 2016, 88(14): 7041-7048
Anal Bioanal Chem, 2017, 409(23):5533-45
Anal Bioanal Chem, 2018, 410(21):5287-300
Nat Commun. 2019. 10:4971
Alzheimer's & Dementia, 2019, 15： 76-92
Nat Rev Gastroenterol Hepatol, 2018, 15(2):111-28
Alzheimer's & Dementia, 2018, doi:10.1016/j.jalz.2018.08.012
EBioMedicine, 2018, doi:10.1016/j.ebiom.2018.10.030
BMC Biology , 2017,15:120 -34
International Journal of Cancer, 2016, 139(8):1764-75

麦特绘谱 Metabo-Profile

麦特绘谱代谢组学及肠道菌群产品及服务

麦特绘谱 Metabo-Profile

非靶向及定量代谢组学

- Q300全定量代谢组
- 宏代谢组
- 胆汁酸
- 氨基酸
- 有机酸
- 短链脂肪酸
- 中长链脂肪酸
- 氧化三甲胺（TMAO）
- 核苷酸
- 辅酶
- 糖代谢
- 激素
- 脂质
- 维生素
- 还原糖
- 神经递质

微生物组

- 16S rDNA测序
- 宏基因组

同位素代谢流分析

- 代谢流分析
- 同位素示踪分析

定量方法检测试剂盒

- Q300全定量代谢芯片
- Q200宏代谢
- 胆汁酸
- 脂肪酸

https://www.metaboprofile.com/

麦特绘谱部分合作客户/文章

Cell Metabolism,2020,31,1-15 (IF=22.41)

Immunity, 2019, 50,1-16 (**IF=19.73**)

Gut, 2019, doi:10.1136/gutjnl-2018-317609 (**IF=17.02**)

Hepatology, 2020, doi:10.1002/hep.31280 (**IF=14.97**)

Signal Transduction and Targeted Therapy, 2020,5: 177-90 (**IF=13.49**)

Microbiome, 2020, 8: 74 (**IF=11.61**)

Microbiome, 2020, 8: 133 (**IF=11.61**)

The EMBO Journal,2020, 39:e103304 (IF=**9.89**)

Arthritis Rheumatol, 2020, doi:10.1002/art.41419 (**IF=9.59**)

Chemical Science, 2020, 11: 6111 ((**IF=9.35**)

Theranostics ,2019; 9(3): 900-919 (**IF=8.71**)

Theranostics 2019; 9(10): 2999-3013 (**IF=8.71**)

Clin Gastroenterol Hepatol, doi:10.1016/j.cgh.2020.06.067 (**IF=8.55**)

Carbohydrate Polymers, 2020,248,116780-92 (**IF=7.18**)

Oncogene. 2020,39,2358-76 (**IF=6.64**)

麦特绘谱 Metabo-Profile

麦特绘谱
Metabo-Profile

优质服务

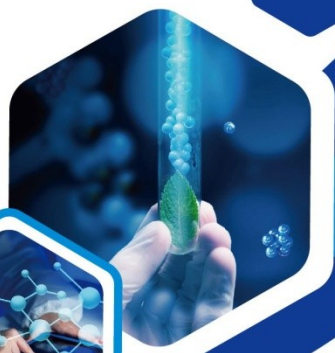
不断超越客户期望
建立长期合作关系

专业化人才队伍
不断创新,追求新高度

精益求精

科学管理

全方位科学管理
为客户提供专业产品



Thank you