Supplementary Table 1: Annotated differentially enriched metabolites between the newly diagnosed T2DM and IGR groups

Supplementary Table 2: Annotated differentially enriched metabolites between the newly diagnosed T2DM and NGT groups

Supplementary Table 3: Annotated differentially enriched metabolites between the IGR and NGT groups

Supplementary Figure 1: Box plot of COG function classification. Microbial sequences mapped by Greengenes database, the functional gene contents of the gut microbiota were predicted by PICRUSt and were mapped on COG.

Supplementary Figure 2: Correlation heatmap of differentially enriched metabolites and gut microbiota phylum between the newly diagnosed T2DM and IGR group (a); Correlation heatmap of differentially enriched metabolites and gut microbiota phylum between the newly diagnosed IGR and NGT group (b)

Note: Each column in the graph represents a metabolite, each row represents a microbiota phylum, the colour in the graph indicates the Pearson coefficient between the bacterial phylum and the metabolite, and the red colour indicates positive correlation. The green colour is representative negative correlation. The darker colour indicate the greater the correlation. * is represents a significant correlation (P < 0.05).

Supplementary Figure 3: Correlation heatmap of differentially enriched metabolites and gut microbiota genus between the newly diagnosed T2DM and IGR group (a); Correlation heatmap of differentially enriched metabolites and gut microbiota genus between the newly diagnosed IGR and NGT group (b).

Note: Each column in the graph represents a metabolite, each row represents a microbiota genus, the colour in the graph indicates the Pearson coefficient between the bacterial genus and the metabolite, and the red colour indicates positive correlation. The green colour is representative negative correlation. The darker colour indicate the greater the correlation. * is represents a significant correlation (P < 0.05).

Supplementary Figure 4: Correlation heatmap of differentially enriched metabolites and gut microbiota phylum level between the newly diagnosed T2DM and NGT group (a), Correlation heatmap of differentially enriched metabolites and gut microbiota genus level between the newly diagnosed T2DM and NGT group (b).



Supplementary Figure 1: Box plot of COG function classification. Microbial sequences mapped by Greengenes database, the functional gene contents of the gut microbiota were predicted by PICRUSt and were mapped on COG.



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Correlation heatmap of differentially enriched metabolites and gut microbiota genus level between the newly diagnosed T2DM and NGT group (b).

	Supplement	ntary I a	die 1: Annotated	a differentially	ennen	ed meta	bontes bet	ween the newly di	agnosed 12DW a	nd IOR groups	
Metabolites	m/z	RT (min)	Compound ID	Formula	VIP value	p value	FC (T2DM/ IGR)	Pathways	superclass	class	subclass
L-Tyrosine	180.07	1.14	HMDB00158	C9H11NO3	1.36	0.00	1.64	Phenylalanine, tyrosine and tryptophan biosynthesis	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
Epothilone A	476.25	5.84	LMPK0400004 0	C26H39NO6 S	4.02	0.03	0.79	Type I polyketide structures	Lipids and lipid- like molecules	Polyketides	Macrolides and lactone polyketides
Anhydrorhodovibrin	565.44	6.68	LMPR0107013 5	C41H58O	1.86	0.01	3.27	Metabolic pathways,Caroteno id biosynthesis	Lipids and lipid- like molecules	Prenol lipids	Isoprenoids
Protorifamycin I	657.34	11.13	LMPK0500000 7	C35H45NO1 0	1.71	0.00	0.78	Biosynthesis of ansamycins,Biosyn thesis of antibiotics	Phenylpropanoids and polyketides	Coumarins and derivatives	Furanocoumarins
Pimelic acid	159.07	1.16	LMFA0117005 1	C7H12O4	1.04	0.05	0.15	Metabolic pathways Glycerophospholip	Lipids and lipid- like molecules	Fatty acyls	Fatty acids and conjugates
LysoPC(15:0)	480.31	6.26	HMDB10381	C23H48NO7 P	5.44	0.05	0.36	id metabolism,Cholin e metabolism in cancer	Lipids and lipid- like molecules	Glycerophospholipi ds	Glycerophosphocholin es
Matricin	613.30	2.35	LMPR0103410 003	C17H22O5	3.11	0.02	0.64	Unknown	Organoheterocycl ic compounds	Lactones	Gamma butyrolactones
bacteriohopane-32,33,34,35- tetrol	564.50	7.83	LMPR0400000 4	C35H62O4	1.80	0.05	2.06	Unknown	Lipids and lipid- like molecules	Prenol lipids	Hopanoids
5alpha,6beta- dihydroxycholestanol	443.35	5.23	LMST0101005 2	C27H48O3	1.41	0.02	1.33	Unknown	Lipids and lipid- like molecules	Sterol lipids	Sterols
Cytochalasin A	460.25	2.12	LMPK1100000 1	C29H35NO5	1.24	0.02	1.26	Unknown	Lipids and lipid- like molecules	Polyketides	Cytochalasins
(6S)-dehydrovomifoliol	221.12	3.27	LMPR0103050 009	C13H18O3	1.08	0.00	0.74	Unknown	Lipids and lipid- like molecules	Prenol lipids	Isoprenoids

Supplementary Table 1: Annotated differentially enriched metabolites between the newly diagnosed T2DM and IGR groups

	Supp	lement	ary Table 2: An	notated differe	entially	enriched	metabolites between the new	ly diagnosed T2E	M and NGT group	S
Metabolites	m/z	RT (min)	Compound ID	Formula	VIP value	p value	Pathways	superclass	class	subclass
Cristacarpin	355.15	3.25	LMPK1207011 4	C21H22O5	3.85	0.03	Unknown	Phenylpropanoi ds and polyketides	Isoflavonoids	Furanoisoflavonoids
Piceid	373.13	2.35	LMPK1309001 2	C20H22O8	3.49	0.01	Unknown	Phenylpropanoi ds and polyketides	Stilbenes	Stilbene glycosides
7-dehydro-desmosterol	383.33	4.95	LMST0101012 1	C27H42O	2.63	0.00	Steroid biosynthesis,Metabolic pathways	Lipids and lipid- like molecules	Sterol lipids	Sterols
PE(14:0/20:3)	712.49	9.32	HMDB08836	C39H72NO8 P	1.78	0.02	Unknown	Lipids and lipid- like molecules	Glycerophospholipi ds	Glycerophosphoethanolamin es
Gamma- Glutamylglutamine	274.10	0.64	HMDB11738	C10H17N3O 6	1.19	0.03	Unknown	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues

		Suppler	mentary Table 3	: Annotated d	lifferent	ially en	riched m	etabolites between the I	GR and NGT gro	oups	
Metabolites	m/z	RT (min)	Compound ID	Formula	VIP value	p value	FC (IGR/ NGT)	Pathways	superclass	class	subclass
Dodecanedioic acid	229.14	3.27	HMDB00623	C12H22O4	4.60	0.01	2.43	Biosynthesis of secondary metabolites,alpha- Linolenic acid metabolism	Lipids and lipid- like molecules	Fatty acyls	Fatty acids and conjugates
Matricin	613.30	2.35	LMPR0103410 003	C17H22O5	3.05	0.01	1.68	unknown	Organoheterocyc lic compounds	Lactones	Gamma butyrolactones
L-Tyrosine	180.07	1.14	HMDB00158	C9H11NO3	2.67	0.00	0.47		Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
LysoPC(14:1)	464.28	6.06	HMDB10380	C22H44NO7 P	2.59	0.01	2.92	Choline metabolism in cancer,Glycerophospholi pid metabolism	Lipids and lipid- like molecules	Glycerophospholipi ds	Glycerophosphocholi nes
7-dehydro-desmosterol	383.33	4.95	LMST0101012 1	C27H42O	2.23	0.01	0.58	Steroid biosynthesis,metabolic pathways	Lipids and lipid- like molecules	Sterol lipids	Sterols
5alpha,6beta- dihydroxycholestanol	443.35	5.23	LMST0101005 2	C27H48O3	2.15	0.01	0.66	unknown	Lipids and lipid- like molecules	Sterol lipids	Sterols
Epothilone A	476.25	5.84	LMPK0400004 0	C26H39NO6 S	1.96	0.04	1.24	Type I polyketide structures	Lipids and lipid- like molecules	Polyketides	Macrolides and lactone polyketides
Protorifamycin I	657.34	11.13	LMPK0500000 7	C35H45NO1 0	1.90	0.00	1.29	Biosynthesis of ansamycins,Biosynthesis of antibiotics	Phenylpropanoid s and polyketides	Coumarins and derivatives	Furanocoumarins
(+)-cucurbic acid	211.13	3.27	LMFA0202001 3	C12H20O3	1.62	0.00	1.91	unknown	Lipids and lipid- like molecules	Sterol lipids	Sterols
Teasterone	447.35	5.63	LMST0103012 1	C28H48O4	1.61	0.01	0.37	Biosynthesis of secondary metabolites,Brassinoster oid biosynthesis,Metabolic pathways	Lipids and lipid- like molecules	Fatty acyls	Octadecanoids
Manoalide	415.25	3.85	LMPR0105020 001	C25H36O5	1.59	0.01	0.40	unknown	Lipids and lipid- like molecules	Sterol lipids	Sterols
Gamma-Glutamylglutamine	274.10	0.64	HMDB11738	C10H17N3O 6	1.50	0.00	0.43	unknown	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
(6S)-dehydrovomifoliol	221.12	3.27	LMPR0103050 009	C13H18O3	1.25	0.01	1.35	unknown	Lipids and lipid- like molecules	Prenol lipids	Isoprenoids
Estrone 3-glucuronide	445.19	1.40	LMST0501001 1	C24H30O8	1.22	0.00	0.09	Steroid hormone biosynthesis	Lipids and lipid- like molecules	Steroids and steroid derivatives	Steroidal glycosides
Anhydrorhodovibrin	565.44	6.68	LMPR0107013 5	C41H58O	1.17	0.02	0.37	Carotenoid biosynthesis, Metabolic	Lipids and lipid- like molecules	Prenol lipids	Isoprenoids

Quassin	389.2	2.68	LMPR01061100	C22H28O6	1.11	0.02	0.71	unknown	Lipids and lipid- like molecules	Prenol lipids	Terpene lactones
Scillaren A	715.3 3	2.30	LMST01130005	C36H52O13	1.03	0.04	0.74	unknown	Lipids and lipid- like molecules	Sterol lipids	Sterols
2-Hydroxyadipic acid	161.0 5	0.64	LMFA01170049	C6H10O5	1.01	0.04	1.97	unknown	Lipids and lipid- like molecules	Fatty acyls	Fatty acids and conjugates
L-Lysine	145.1 0	0.55	HMDB00182	C6H14N2O2	1.01	0.00	0.46		Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues

pathways