

Supplementary table 1 220 differentially expressed metabolites in model group and sham group.

Metabolite Formula	Fold Change	VIP	<i>P</i> Value
C32H60NO10P	2.62	2.28	0.00
C40H64O	3.91	1.59	0.03
C20H34O6	0.61	1.71	0.02
C30H47O4P	0.63	1.67	0.02
C13H26N2	0.09	2.25	0.00
C22H43NO2	1.78	1.99	0.00
C30H52O	1.49	1.81	0.01
C30H50O	1.48	1.72	0.02
C27H46O6	2.24	2.01	0.00
C23H41NO5	0.40	1.93	0.01
C22H43NO5	0.28	1.84	0.01
C20H22O3	0.36	1.64	0.01
C19H28O4	0.46	1.81	0.01
C17H31NO5	5.55	1.69	0.02
C13H12O4	0.08	1.92	0.00
C24H36O5	0.55	1.49	0.04
C22H41NO5	0.23	2.09	0.00
C22H36O2	0.23	1.85	0.01
C22H36O5	0.48	2.23	0.00
C17H37NO2	1.20	1.45	0.05
C47H76O2	6.40	1.82	0.01
C32H61NO4	2.98	2.10	0.00
C35H71NO4	2.88	1.75	0.02
C42H81NO3	0.26	1.69	0.03
C34H69NO4	3.58	1.73	0.02
C13H12O8	0.33	1.76	0.01
C43H74O5	6.79	1.97	0.00
C32H67NO2	4.28	1.59	0.03
C44H78O4	2.27	1.67	0.04
C8H17NO2	1.76	1.87	0.01
C16H32O2	0.61	1.53	0.04
C36H70O2	3.54	1.63	0.03
C21H44O5P	0.28	1.93	0.00
C34H66O4	4.20	1.58	0.04
C34H64O4	3.59	1.50	0.05
C66H121NO23	0.10	1.86	0.01
C11H20N2O5	2.79	1.81	0.01
C62H114N2O23	0.35	1.60	0.03
C11H14NO4P	0.08	1.97	0.00
C14H26O10	0.62	1.66	0.02
C9H17NO4	5.32	1.72	0.01

C30H45N3O9S	0.31	1.66	0.03
C24H50NO7P	1.51	1.65	0.02
C26H54NO7P	1.54	1.51	0.05
C26H52NO7P	1.35	1.51	0.05
C23H31NO2	0.28	1.97	0.00
C19H36O3	1.64	1.93	0.01
C27H54O4	2.05	1.61	0.03
C19H28N2O5S	0.33	1.51	0.05
C23H33NO4	0.14	2.24	0.00
C32H46N2O3	0.49	1.54	0.04
C26H39N3O3	1.72	1.71	0.02
C14H16N2O4	2.56	1.70	0.02
C22H45NO5	0.28	1.79	0.01
C26H53NO3	1.47	1.72	0.02
C32H65NO7	3.20	1.50	0.05
C30H44N2O6	0.48	1.67	0.03
C22H40O4	0.64	1.63	0.04
C47H85O8P	0.06	2.00	0.00
C46H79O8P	0.07	1.99	0.00
C20H39NO3S	0.27	1.75	0.02
C32H62NO8P	0.31	1.85	0.01
C39H72NO8P	0.49	2.19	0.00
C47H78NO8P	0.23	1.73	0.02
C49H76NO8P	0.26	1.98	0.00
C40H73O10P	1.97	1.82	0.01
C26H53O9P	1.62	1.53	0.04
C43H85O10P	0.18	1.78	0.01
C37H73O9P	0.50	2.16	0.00
C42H80O13P2	0.09	1.81	0.01
C42H76O13P2	0.07	2.04	0.00
C48H78O13P2	0.39	2.01	0.00
C43H81O13P	0.27	2.00	0.00
C43H79O13P	0.12	1.96	0.00
C41H76O16P2	0.59	1.71	0.01
C10H19NO4	5.68	1.57	0.03
C44H80NO10P	0.10	1.91	0.01
C46H78NO10P	0.30	2.11	0.00
C48H74NO10P	0.09	1.85	0.01
C26H38O7	0.42	1.93	0.00
C50H94O6	1.96	2.02	0.00
C55H96O5	0.32	1.72	0.02
C12H27O3P	9.32	1.74	0.01
C12H24NO4	1.39	2.05	0.00
C21H32O5	8.70	1.69	0.03

C19H30O4	0.53	1.69	0.03
C11H16O6S	1.52	1.67	0.04
C21H43NO4	0.43	1.73	0.02
C15H14O8S	0.27	1.83	0.02
C7H9NO5	1.46	1.81	0.03
C8H10N4O3	0.54	1.99	0.00
C25H36O4	0.57	1.90	0.01
C29H50O3	0.56	1.88	0.01
C20H38O3	3.66	1.99	0.01
C23H34O4	0.27	2.53	0.00
C24H40O6	2.17	1.92	0.01
C9H10O5	0.57	1.84	0.02
C11H15NO4S	0.67	1.73	0.04
C28H53NO5	1.46	1.69	0.03
C30H47O4P	0.53	1.91	0.01
C3H4O3	0.79	1.87	0.02
C6H10O3	0.47	1.84	0.02
C9H13N3O4S	0.65	1.81	0.03
C17H18N2O8	0.64	1.66	0.04
C10H10O4	0.36	1.86	0.02
C23H38O3	0.66	1.61	0.04
C9H12N2O4	0.65	2.12	0.00
C15H24O3	0.09	2.59	0.00
C8H12O6	1.99	1.89	0.01
C15H10O5	0.31	2.09	0.01
C17H24N2O4	0.39	2.25	0.00
C15H10O4	0.10	2.07	0.01
C27H48O2	0.47	1.93	0.01
C24H40O5	0.24	1.90	0.02
C33H50O4	4.08	2.06	0.01
C22H29NO2	3.47	1.54	0.05
C20H24N8O6	0.42	1.60	0.05
C19H19N3O3	0.11	2.53	0.00
C22H39O6	0.31	1.90	0.01
C14H26O3	0.52	2.35	0.00
C30H46O4	0.35	1.83	0.02
C11H8O3	1.51	1.74	0.03
C24H38O5	0.32	1.93	0.01
C25H38O4	0.24	2.02	0.01
C27H44O5	0.42	2.13	0.00
C12H10N4O3	0.69	1.75	0.03
C16H22O4	0.61	1.92	0.01
C5H8O3	0.51	1.98	0.01
C24H42O7	5.19	1.85	0.02

C10H19N3O4	0.62	1.71	0.03
C7H6O2	0.73	1.70	0.04
C45H76O2	5.85	1.91	0.01
C42H85NO3	4.66	1.63	0.04
C38H71NO3	5.09	1.63	0.03
C61H110O17P2	0.32	1.65	0.05
C24H49NO7	5.81	1.99	0.01
C44H86O5	0.36	1.97	0.01
C21H43O6P	1.38	1.71	0.04
C15H20O4	0.70	1.81	0.02
C36H38N4O4	2.05	1.95	0.01
C20H44NO5P	0.24	1.90	0.02
C8H14N2O5S	1.28	1.74	0.03
C30H46O8	1.32	1.77	0.02
C16H30O4	1.75	1.55	0.05
C13H18O4	0.69	1.60	0.05
C5H4N4O	1.64	1.64	0.04
C11H14NO4P	0.11	2.11	0.00
C27H30O15	0.47	1.78	0.02
C69H124N2O31	0.06	1.78	0.03
C12H18N2O4	0.50	1.97	0.01
C12H23O14P	0.54	2.27	0.00
C25H48NO7P	1.69	1.72	0.03
C34H38N4O4	1.58	1.93	0.01
C18H41N2O5P	0.65	1.59	0.04
C27H41NO4	4.33	2.08	0.00
C17H18N6O5	0.40	2.07	0.01
C20H22N2O7	1.21	1.65	0.05
C12H18NO5P	1.23	1.80	0.02
C11H16N2O8	1.24	1.63	0.05
C11H11NO5	2.35	2.03	0.01
C13H23N3O2	0.09	2.59	0.00
C23H37NO5	0.33	1.92	0.01
C27H43NO3	0.65	1.88	0.01
C19H37NO3	3.36	1.96	0.01
C10H18N4O6	0.52	1.91	0.02
C11H15N3O6	0.67	1.68	0.04
C9H17NO8	0.63	1.67	0.04
C10H18N2O6	0.68	1.69	0.03
C5H6O5	0.59	1.95	0.01
C13H16O7	0.54	1.85	0.02
C7H8O4S	0.20	1.61	0.04
C45H83O8P	1.93	1.87	0.01
C45H69O8P	0.23	1.66	0.05

C46H83O8P	1.83	1.96	0.01
C41H77O7P	4.49	1.68	0.04
C33H63O7P	0.67	2.12	0.00
C45H82NO8P	1.84	2.13	0.00
C27H50NO7P	1.31	1.67	0.03
C48H90NO7P	2.16	1.69	0.04
C52H84NO8P	0.29	1.64	0.04
C44H90NO7P	2.18	1.70	0.03
C20H44NO6P	1.45	1.65	0.04
C44H80NO8P	2.07	2.13	0.00
C46H92NO8P	0.54	1.71	0.04
C23H47O9P	1.71	1.93	0.01
C45H81O10P	0.11	2.00	0.01
C45H83O10P	0.21	1.94	0.01
C26H55O8P	1.70	1.70	0.03
C24H49O8P	3.29	1.68	0.05
C42H71O13P	0.36	2.22	0.00
C43H81O13P	0.45	1.78	0.03
C53H97O13P	3.39	1.73	0.02
C25H51O11P	1.28	1.64	0.04
C49H85O12P	1.97	1.75	0.03
C25H49O11P	2.56	2.25	0.00
C44H82NO10P	0.22	1.92	0.01
C44H78NO10P	0.55	1.60	0.05
C44H80NO10P	0.15	1.90	0.01
C46H80NO10P	0.46	1.77	0.03
C25H48NO9P	3.92	1.78	0.03
C50H92NO10P	1.98	1.66	0.03
C45H76NO12P	0.34	2.06	0.01
C41H82NO9P	1.73	1.87	0.01
C17H20N4O6	0.61	1.73	0.03
C14H21N3O10S	0.42	2.08	0.00
C4H9NO2Se	1.35	1.85	0.02
C46H94N2O6P	2.49	1.74	0.02
C18H40NO5P	7.84	1.66	0.03
C26H45NO10S2	0.03	1.62	0.05
C49H98O4	3.37	1.78	0.02
C50H92O6	2.19	1.60	0.04
C54H92O6	1.98	1.60	0.05
C53H98O5	2.51	2.05	0.00
C53H96O5	3.55	1.81	0.02
C58H92O6	3.74	2.02	0.01
C56H104O5	6.06	2.22	0.00
C30H56O7	3.03	1.74	0.03

C6H6N2O2	0.56	1.66	0.04
C6H9NO3	0.50	1.57	0.05
C11H6O4	0.13	2.20	0.00

Supplementary table 2 276 differentially expressed metabolites in prebiotics group and model group.

Metabolite Formula	Fold Change	VIP	P Value
C15H12O4	3.53	2.10	0.00
C9H12O5	0.54	1.70	0.02
C11H16O6S	0.87	1.80	0.02
C16H29N3O2	1.62	1.66	0.04
C19H41O6P	0.57	1.98	0.00
C6H8N2O2	0.39	1.74	0.02
C24H40O5S	1.47	1.61	0.03
C9H10O5	2.22	2.15	0.00
C11H19N4O4	0.48	1.66	0.03
C23H44O3	2.34	1.95	0.01
C7H9N3O2	0.67	1.59	0.03
C8H11NO6	0.52	1.72	0.02
C28H53NO5	0.53	1.68	0.02
C12H9NO5	0.80	1.53	0.05
C30H47O4P	1.68	1.65	0.03
C26H52O3	2.69	1.64	0.03
C21H43NO3	2.36	2.00	0.00
C24H44O3	2.56	1.70	0.02
C7H12O5	0.44	1.92	0.01
C6H10O3	2.62	2.24	0.00
C16H16O11	0.47	1.71	0.02
C10H12O5	0.57	1.65	0.03
C7H6O4	0.73	1.66	0.03
C22H44O3	2.42	2.03	0.00
C22H37NO5S	3.29	1.89	0.01
C24H48O3	1.73	1.91	0.01
C9H10O3	0.66	1.56	0.04
C11H14O4	0.86	1.72	0.02
C17H18N2O8	1.75	1.67	0.03
C10H10O4	2.30	1.76	0.02
C13H12O3	1.46	1.54	0.05
C25H48O3	1.90	2.00	0.00
C13H16O3	0.77	1.72	0.02
C6H12O3	0.50	1.65	0.03
C20H40O3	1.79	1.64	0.03
C19H38O3	2.05	1.58	0.04
C4H6O4	0.55	1.81	0.01
C15H24O3	7.45	1.52	0.04
C24H46O3	2.36	2.03	0.00
C15H10O4	3.48	2.21	0.00
C24H40O5	3.27	2.09	0.00

C12H15NO3	0.54	1.73	0.02
C14H20O4	0.74	1.62	0.04
C28H46O3	0.54	1.67	0.02
C21H20O8	0.40	1.88	0.01
C6H13O7PS	0.60	1.57	0.04
C10H15N2O8P	5.90	1.94	0.01
C18H16O8	0.69	1.55	0.05
C10H11N5O4	0.58	2.10	0.00
C27H48O4	0.11	2.04	0.00
C22H39O6	4.04	2.27	0.00
C20H20O10	1.45	1.85	0.01
C8H13N3OS	1.43	1.56	0.04
C14H26O3	2.20	1.85	0.01
C18H32O2	5.51	1.94	0.01
C18H14O4	0.54	1.56	0.04
C24H38O5	2.50	2.16	0.00
C22H42O3	2.44	1.80	0.02
C3H4O	0.62	1.61	0.04
C5H8N5O4P	0.52	1.75	0.02
C5H8O3	2.35	2.12	0.00
C23H39NO3	0.63	1.82	0.01
C9H16O4	0.81	1.60	0.04
C7H6O2	1.65	2.00	0.01
C2H5N3O3	0.57	1.79	0.02
C41H75N3O15P2	2.38	1.82	0.01
C34H69NO5	0.62	1.76	0.02
C38H75NO3	0.49	1.54	0.04
C67H122O17P2	2.79	2.21	0.00
C9H14N3O8P	5.55	1.96	0.00
C10H16N3O7P	0.63	1.76	0.02
C42H70O7	0.60	1.75	0.02
C42H74O5	0.69	1.55	0.04
C42H72O5	0.69	1.54	0.05
C47H84O5	0.60	1.53	0.05
C44H80O5	0.39	1.75	0.02
C42H82O5	2.79	1.70	0.03
C24H31NO4	0.59	1.87	0.01
C20H18O8	0.52	1.99	0.01
C9H15NO5	0.47	1.86	0.01
C20H44NO5P	3.22	2.09	0.00
C18H39O3P	0.51	1.76	0.02
C27H33N9O15P2	0.45	1.61	0.03
C40H62O4	0.53	1.61	0.04
C54H101NO13	0.04	2.06	0.00

C38H71NO9	0.67	1.77	0.02
C60H113N2O23P	1.51	1.82	0.01
C6H13NO8S	0.57	1.57	0.04
C3H7N3O2	2.71	2.15	0.00
C30H41NO6	0.69	1.78	0.02
C29H48O5	1.47	1.51	0.05
C10H18N2O4S	0.54	1.67	0.03
C11H14NO4P	3.43	2.21	0.00
C11H9NO3	1.92	1.62	0.04
C10H13N4O8P	3.83	1.64	0.03
C22H22O10	1.62	1.80	0.01
C10H15N3O7	0.72	1.57	0.04
C3H6O3	0.69	1.64	0.03
C12H23NO10	0.36	2.21	0.00
C19H39O6P	0.49	1.73	0.02
C25H49O12P	0.62	1.69	0.02
C6H12O4	0.49	2.10	0.00
C25H48O4	3.01	1.96	0.00
C21H42O3	2.19	1.83	0.01
C16H31NO3	3.27	2.51	0.00
C16H35N3O2	1.74	1.82	0.01
C18H17NO5	1.25	1.58	0.04
C17H18N6O5	2.21	1.72	0.02
C16H18N2O3	0.46	1.60	0.03
C16H34N2O2	0.68	1.63	0.03
C30H43NO5	1.79	1.56	0.04
C12H18NO5P	0.78	1.82	0.01
C11H13NO3	0.63	1.74	0.02
C7H12N2O4S	0.69	2.04	0.00
C11H16N2O8	0.78	1.72	0.02
C12H14N2O2	0.47	2.15	0.00
C11H11NO5	0.55	1.58	0.03
C7H13NO4	0.61	1.81	0.01
C15H27N3O2	2.22	1.69	0.02
C8H15NO4	0.53	1.56	0.04
C23H37NO5	2.45	2.16	0.00
C12H13N3O2	0.66	1.69	0.03
C27H45NO3	0.53	1.74	0.02
C23H45NO3	2.42	2.10	0.00
C18H33NO3	0.47	1.87	0.01
C17H28O3S	0.85	1.66	0.03
C31H48N2O3	0.26	1.73	0.02
C8H13NO5	0.54	1.78	0.02
C21H35N5O2	0.72	1.72	0.02

C17H33NO4	0.56	2.04	0.00
C5H6O5	1.88	1.79	0.02
C9H17NO5	0.79	1.57	0.04
C45H82NO8P	0.72	1.62	0.04
C48H96NO8P	0.75	1.62	0.03
C20H40NO8P	0.73	1.56	0.04
C18H38NO6P	0.52	1.98	0.00
C44H90NO7P	0.45	1.70	0.02
C44H80NO8P	0.62	2.03	0.00
C48H80NO8P	0.53	1.59	0.04
C45H80NO8P	3.30	1.74	0.02
C41H74NO7P	1.88	1.49	0.05
C23H47O9P	0.63	2.27	0.00
C45H81O10P	5.31	2.11	0.00
C45H83O10P	3.42	2.16	0.00
C40H77O9P	0.59	1.91	0.01
C43H87O9P	0.47	1.94	0.01
C22H45O8P	0.48	1.80	0.02
C43H81O9P	0.74	1.58	0.04
C48H78O13P2	2.32	2.35	0.00
C6H6O	3.05	1.57	0.04
C43H81O13P	1.92	2.15	0.00
C3H6O2	0.59	1.71	0.02
C20H38NO9P	1.43	1.52	0.05
C44H82NO10P	3.31	2.15	0.00
C44H80NO10P	4.02	2.21	0.00
C46H80NO10P	1.95	2.16	0.00
C48H86NO10P	2.99	1.72	0.02
C28H52NO9P	0.63	1.71	0.02
C45H76NO12P	2.61	2.29	0.00
C41H82NO9P	0.74	1.61	0.04
C42H78NO9P	0.60	1.81	0.01
C17H24N8O7S	0.58	1.59	0.03
C46H94N2O6P	0.48	1.59	0.04
C48H78O19	2.12	1.60	0.04
C4H4O3	0.56	1.80	0.02
C59H90O6	1.67	1.61	0.04
C60H112O6	2.48	1.70	0.02
C64H118O6	3.25	2.03	0.00
C61H114O5	2.03	1.58	0.04
C55H92O6	2.12	1.77	0.02
C68H124O6	1.76	1.81	0.01
C65H96O6	0.23	1.63	0.04
C73H136O6	14.77	1.80	0.02

C6H6N2O2	1.89	1.61	0.04
C10H12N4O6	0.67	1.59	0.04
C18H39O4P	5.28	2.02	0.00
C17H16O7S	1.91	1.60	0.04
C7H9N3O	0.83	1.88	0.01
C33H51NO2	0.25	1.83	0.01
C40H64O	0.15	1.73	0.02
C16H32O3	1.58	1.64	0.04
C30H54O7	0.67	1.70	0.03
C8H8O7S	0.66	1.72	0.01
C13H26N2	4.45	1.58	0.04
C22H43NO2	0.68	1.83	0.01
C30H52O	0.80	1.66	0.03
C30H50O	0.79	1.72	0.02
C21H37O4	0.93	1.57	0.04
C22H43NO5	3.18	2.17	0.00
C9H12O7S	0.67	1.50	0.05
C20H22O3	2.53	1.58	0.02
C11H14O6	0.29	2.02	0.00
C7H16N2	0.56	1.59	0.03
C7H15NO2	0.62	1.62	0.03
C7H10N4O3	0.77	1.54	0.03
C24H41NO	0.57	1.64	0.02
C16H34N2O	0.51	1.49	0.03
C33H54O4	0.63	1.42	0.04
C13H12O4	3.67	2.19	0.00
C6H6N4O	1.49	1.53	0.05
C24H36O5	1.64	1.52	0.05
C11H9NO4	0.77	1.53	0.03
C22H41NO5	2.59	1.71	0.02
C22H36O2	3.28	2.08	0.00
C12H22O11	0.35	1.55	0.03
C10H13NO2	0.59	1.54	0.04
C9H14N2O7	2.18	1.52	0.04
C51H91N3O15P2	1.49	1.46	0.04
C42H81NO3	9.30	2.31	0.00
C46H93NO3	0.44	2.15	0.00
C34H69NO4	0.12	2.27	0.00
C27H46O	0.69	1.59	0.03
C13H12O8	2.34	1.48	0.04
C19H21N7O6	0.49	1.47	0.04
C9H15NO5	0.47	1.82	0.01
C32H67NO2	0.14	1.71	0.02
C41H80O16P2	0.49	1.54	0.04

C16H32O2	1.48	1.77	0.02
C8H11NO2	0.37	1.98	0.00
C36H70O2	0.11	2.26	0.00
C20H41NO3	1.84	1.71	0.02
C21H44O5P	2.62	1.93	0.00
C34H66O4	0.15	1.70	0.02
C68H125NO23	0.44	2.07	0.00
C62H114N2O23	2.51	2.06	0.00
C50H97NO8	0.30	2.43	0.00
C2H6N4O	0.76	1.66	0.02
C11H14NO4P	4.07	2.16	0.00
C30H45N3O9S	1.97	1.63	0.04
C23H31NO2	2.94	2.20	0.00
C11H11NO4	1.72	1.46	0.05
C19H36O3	1.32	1.88	0.01
C21H42O4	0.58	1.60	0.03
C14H16N2O4	0.14	2.15	0.00
C26H45NO	0.66	1.62	0.02
C22H45NO5	3.25	2.03	0.00
C26H53NO3	0.79	1.68	0.03
C32H65NO7	0.26	1.53	0.04
C9H21N3O	0.52	1.64	0.03
C47H85O8P	9.35	1.92	0.01
C46H79O8P	7.82	2.25	0.00
C25H49O8P	1.75	1.55	0.05
C19H39NO3	2.10	1.72	0.02
C20H39NO3S	2.95	2.03	0.00
C38H76NO7P	1.63	1.93	0.01
C39H72NO8P	1.42	1.95	0.00
C47H78NO8P	2.78	2.07	0.00
C43H76NO7P	1.25	1.89	0.01
C49H76NO8P	2.61	1.99	0.00
C37H74NO7P	1.42	1.71	0.02
C21H21O10	0.25	2.01	0.00
C43H85O10P	3.47	2.10	0.00
C42H80O13P2	6.63	2.01	0.00
C42H76O13P2	9.03	2.16	0.00
C34H68NO13P	0.37	1.52	0.04
C37H67O13P	0.35	1.55	0.04
C43H81O13P	2.42	1.97	0.00
C43H79O13P	6.06	2.23	0.00
C48H83O13P	4.40	1.64	0.02
C51H87O13P	0.51	1.74	0.02
C37H73O12P	0.26	2.15	0.00

C41H76O16P2	0.42	2.17	0.00
C42H72NO10P	1.26	1.61	0.03
C44H80NO10P	5.53	2.14	0.00
C46H78NO10P	1.60	1.53	0.05
C46H76NO10P	7.05	2.12	0.00
C48H74NO10P	6.98	2.03	0.00
C52H98NO10P	0.03	1.77	0.02
C40H70NO9P	0.31	2.06	0.00
C6H10OS	0.65	1.54	0.05
C7H19N3	0.55	1.67	0.02
C50H94O6	0.41	2.43	0.00
C61H98O6	0.06	1.72	0.03
C5H6N2O2	0.55	1.48	0.04
C12H24NO4	0.85	1.62	0.03
C10H12N4O6	0.69	1.62	0.03

Supplementary table 3 81 metabolites beneficially regulated in prebiotics group vs. sham group.

Metabolite	Model vs. Sham FC	Prebiotics vs. Model FC	Trends in prebiotic
1,2-Epoxy-1,2,7,7',8,8',11',12'-octahydro-psi	3.9078	0.15305	↓
2-Nonyl-1,4,5,6-tetrahydropyrimidine	0.089258	4.4472	↑
22-Hydroxydocos-13-enamide	1.7805	0.68089	↓
24-ethyl-24-methyl-cholesterol	1.4944	0.80435	↓
24-Isopropyl-22E-dehydrocholesterol	1.4828	0.7858	↓
3-hydroxypentadecanoyl carnitine	0.27607	3.1802	↑
3-methyl-4-oxo-1,2-diphenylbutan-2-yl propanoate	0.36056	2.5328	↑
7-hydroxy-6-(3-oxobutyl)-2H-chromen-2-one	0.082544	3.67	↑
7a,12a-Dihydroxy-3-oxo-4-cholenoic acid	0.55097	1.6395	↑
Acetyl carboxymethyl stearyl glycine	0.22832	2.5856	↑
Adrenic acid	0.23077	3.2835	↑
Cer(d18:1/24:1(15Z))	0.26214	9.3041	↑
Cer(t18:0/16:0)	3.5836	0.11636	↓
cis-Coutaric acid	0.32937	2.336	↑
Dimethylaurylamine isostearate	4.275	0.14303	↓
Dodecyl butyrate	0.61125	1.4835	↑
Dotriacontyl methacrylate	3.5373	0.10832	↓
Ethyl 3-(hexadecyloxy)propyl phosphate	0.27539	2.6196	↑
FAHFA(16:0/9-O-18:0)	4.2018	0.14828	↓
Ganglioside GA1 (d18:1/18:0)	0.35147	2.5148	↑
Indolepropanol phosphate	0.084962	4.0726	↑
Leukotriene C5	0.31485	1.9694	↑
Methadyl Acetate	0.27641	2.9402	↑
N-lactoyl-Tryptophan	2.5601	0.13641	↓

N,N-Bis(2-hydroxyethyl)palmitamide acetate	0.27551	3.2497	↑
N,N-Bis(4-hydroxybutyl)octadecanamide	1.4713	0.79197	↓
N,N-Bis{2-[3-(decyloxy)-2-hydroxypropoxy]ethyl}acetamide	3.2047	0.25671	↓
PA(20:3(8Z,11Z,14Z)/24:1(15Z))	0.05859	9.3535	↑
PA(21:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	0.073742	7.8211	↑
Palmitoylhomocysteine	0.26723	2.9455	↑
PE(14:0/20:3(8Z,11Z,14Z))	0.49298	1.4193	↑
PE(20:2(11Z,14Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	0.23206	2.7755	↑
PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:5(7Z,10Z,13Z,16Z,19Z))	0.26226	2.6064	↑
PG(a-13:0/i-24:0)	0.1794	3.4706	↑
PGP(18:1(11Z)/18:1(11Z))	0.090461	6.6282	↑
PGP(20:4(5Z,8Z,11Z,14Z)/16:0)	0.07341	9.0326	↑
PI(16:0/18:1(11Z))	0.2742	2.4151	↑
PI(16:0/18:2(9Z,12Z))	0.11904	6.0647	↑
PIP(16:1(9Z)/16:1(9Z))	0.59132	0.42408	↓
PS(18:0/20:3(8Z,11Z,14Z))	0.1021	5.525	↑
PS(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))	0.29935	1.5993	↑
PS(20:4(8Z,11Z,14Z,17Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	0.085305	6.9847	↑
TG(14:0/15:0/18:1(11Z))	1.9624	0.40722	↓
Valerylcarnitine	1.3927	0.8485	↓
[4-(3-hydroxybutyl)-2-methoxyphenyl]oxidanesulfonic acid	1.5236	0.86716	↓
2-(2,4,5-trihydroxyphenyl)propanoic acid	0.566	2.2238	↑
2-[(2-dodecanoyloxyacetyl)amino]ethyl dodecanoate	1.4616	0.52634	↓
2-Heptylundecyl diphenyl phosphate	0.52721	1.6805	↑
2-Methyl-3-ketovaleric acid	0.46679	2.616	↑
3-(4-Methoxybenzoyl)uridine	0.6422	1.7494	↑

3-(4-methoxyphenyl)-2-oxopropanoic acid	0.35872	2.2987	↑
3-Methyl-5-pentyl-2-furanpentanoic acid	0.090747	7.4476	↑
3,7-dihydroxy-2-phenyl-4H-chromen-4-one	0.10253	3.4775	↑
3a,7a,12b-Trihydroxy-5b-cholanoic acid	0.23943	3.2668	↑
6-(Acetyloxy)-2-(7-ethoxy-7-oxoheptyl)undecanoate	0.312	4.0423	↑
6-Ketomyristic acid	0.51895	2.1984	↑
7-Ketodeoxycholic acid	0.31766	2.5019	↑
alpha-Ketoisovaleric acid	0.51469	2.3501	↑
Benzoic acid	0.7306	1.6451	↑
dioctyl bis(2-hydroxyethyl)phosphoramidate	0.24105	3.2164	↑
Indolepropanol phosphate	0.10812	3.4331	↑
N-(Phenylcarbamoyl)adenosine	0.40181	2.2076	↑
N-[Ethoxy(phenyl)phosphoryl]-L-threonine	1.229	0.77759	↓
N-Acetylaspartylglutamic acid	1.2385	0.78141	↓
N-Benzoylaspartic acid	2.3537	0.54695	↓
N-Octadeca-9,12,15-trienoyl-L-glutamic acid	0.32752	2.454	↑
Oxoglutaric acid	0.59198	1.882	↑
PC(15:0/22:4(7Z,10Z,13Z,16Z))	1.8433	0.72486	↓
PC(O-16:0/20:0)	2.1828	0.45322	↓
PE-NMe(16:0/22:4(7Z,10Z,13Z,16Z))	2.0705	0.6225	↓
PG(17:0/0:0)	1.7119	0.62871	↓
PG(17:0/22:4(7Z,10Z,13Z,16Z))	0.11138	5.3118	↑
PG(17:1(9Z)/22:2(13Z,16Z))	0.21354	3.4216	↑
PI(16:0/18:1(11Z))	0.45369	1.9245	↑
PS(14:1(9Z)/24:1(15Z))	0.2199	3.3054	↑
PS(18:0/20:3(8Z,11Z,14Z))	0.14608	4.0165	↑

PS(18:0/22:5(7Z,10Z,13Z,16Z,19Z))	0.45645	1.9455	↑
PS(DiMe(11,3)/MonoMe(11,3))	0.33656	2.6147	↑
PS(O-18:0/17:0)	1.726	0.74269	↓
SM(d17:1/24:0)	2.4898	0.48485	↓
Urocanic acid	0.56225	1.8869	↑
