

Supplementary Table S1 – Plasma metabolomic signatures associated with long-term breast cancer risk in the SU.VI.MAX prospective cohort.

Supplementary Table S1 Ions associated with breast cancer risk from multivariable conditional logistic regression^a (FDR≤0.2)

Name (mass_retention time for unknown)	Mode	Cases/ Controls	Mean	SD	OR [95% CI]	P-trend	Corrected P-trend ^b
M98.919T2.24	ESI +	211/211	2627	339	1.63 [1.28-2.09]	0.0001	0.06
M96.9218T2.24	ESI +	211/211	6326	751	1.63 [1.28-2.08]	0.0001	0.06
M415.2078T22.4	ESI -	203/203	3432	639	0.61 [0.47-0.80]	0.0003	0.1
M80.9474T2.25	ESI +	211/211	50550	4469	1.49 [1.20-1.87]	0.0004	0.1
M201.149T18.18	ESI -	203/203	1449	918	1.51 [1.19-1.91]	0.0006	0.1
M265.3932T3.1	ESI +	211/211	829	1038	1.87 [1.31-2.69]	0.0006	0.1
M548.8294T2.17	ESI +	211/211	1937	183	0.66 [0.53-0.84]	0.0007	0.1
M424.8961T2.05	ESI +	211/211	1727	305	1.47 [1.17-1.85]	0.001	0.1
M153.0162T1.93	ESI +	211/211	2824	438	1.46 [1.16-1.84]	0.001	0.1
M160.9894T1.9	ESI +	211/211	2683	383	1.45 [1.16-1.81]	0.001	0.1
M114.9883T1.9	ESI +	211/211	10204	1454	1.43 [1.15-1.77]	0.001	0.1
M483.1958T22.45	ESI -	203/203	1400	444	0.66 [0.52-0.86]	0.002	0.1
M474.7265T2.04	ESI -	203/203	3160	354	0.68 [0.54-0.86]	0.002	0.1
L-Phenylalanine M166.0869T10.11	ESI +	211/211	227718	42535	1.43 [1.14-1.78]	0.002	0.1
M556.3244T16.85	ESI -	203/203	3113	847	1.46 [1.15-1.86]	0.002	0.1
M320.068T2.31	ESI +	211/211	2292	1195	1.47 [1.16-1.88]	0.002	0.1
M332.8363T2.21	ESI +	211/211	3017	380	1.44 [1.14-1.81]	0.002	0.1
L-valine/norvaline M72.0803T3.08	ESI +	211/211	115033	24435	1.45 [1.15-1.83]	0.002	0.1
5-aminovaleric acid M140.0686T2.29	ESI +	211/211	10219	5139	1.46 [1.14-1.86]	0.003	0.2
M485.2107T23.95	ESI -	203/203	1268	330	0.70 [0.55-0.88]	0.003	0.2
M629.6992T2.23	ESI +	211/211	926	1028	1.71 [1.20-2.43]	0.003	0.2
M152.0367T1.91	ESI +	211/211	3377	525	1.40 [1.12-1.74]	0.003	0.2
M476.8958T2.06	ESI +	211/211	1697	245	1.39 [1.12-1.74]	0.003	0.2
M74.528T1.89	ESI +	211/211	17127	2227	1.39 [1.12-1.73]	0.003	0.2
O-succinyl-L-homoserine M240.0464T2.86	ESI -	203/203	919	400	0.70 [0.55-0.89]	0.004	0.2
M131.0476T10.12	ESI +	211/211	1353	277	1.43 [1.12-1.81]	0.004	0.2
M488.8728T2.15	ESI +	211/211	6003	409	0.72 [0.58-0.90]	0.004	0.2
M634.8771T2.08	ESI +	211/211	6580	528	0.72 [0.58-0.90]	0.004	0.2
M430.9143T2.09	ESI +	211/211	24103	1302	0.73 [0.58-0.90]	0.004	0.2
M222.8676T2.21	ESI +	211/211	1376	189	1.42 [1.11-1.80]	0.005	0.2
M518.7449T2.21	ESI +	211/211	1579	258	1.38 [1.10-1.72]	0.005	0.2
M111.0109T1.91	ESI +	211/211	4464	681	1.38 [1.10-1.72]	0.005	0.2

M190.0186T2.77	ESI -	203/203	1074	887	1.41 [1.11-1.80]	0.005	0.2
ATBC (acetyl tributyl citrate) M425.2172T19.31	ESI +	211/211	2198	964	1.40 [1.10-1.79]	0.006	0.2
M544.8888T2.06	ESI +	211/211	1398	203	1.36 [1.09-1.68]	0.006	0.2
M586.6522T2.02	ESI -	203/203	1427	199	0.72 [0.57-0.91]	0.006	0.2
M121.0844T10.12	ESI +	211/211	3317	634	1.36 [1.09-1.69]	0.006	0.2
M208.8913T2.22	ESI +	211/211	5336	576	1.34 [1.09-1.66]	0.006	0.2
M68.0197T1.9	ESI +	211/211	7421	1019	1.35 [1.09-1.68]	0.006	0.2
M359.0438T3.08	ESI +	211/211	1782	575	1.43 [1.11-1.86]	0.007	0.2
L-tryptophan M227.0784T11.09	ESI +	211/211	799	180	1.40 [1.10-1.79]	0.007	0.2
M294.9383T2.1	ESI +	211/211	12723	681	0.73 [0.59-0.92]	0.007	0.2
M90.9764T2.13	ESI +	211/211	126879	3773	0.73 [0.58-0.92]	0.007	0.2
M285.2066T19.04	ESI -	203/203	948	1114	1.41 [1.10-1.82]	0.007	0.2
M391.2072T23.51	ESI -	203/203	3549	950	0.72 [0.56-0.91]	0.007	0.2
M192.0305T3.01	ESI +	211/211	1705	1224	1.37 [1.09-1.73]	0.007	0.2
M169.0362T3.1	ESI +	211/211	41324	9207	1.41 [1.10-1.83]	0.008	0.2
M88.0579T1.94	ESI +	211/211	975	754	1.37 [1.08-1.72]	0.008	0.2
L-γ-glutamyl-L-threonine M231.1436T2.52	ESI +	211/211	1054	601	1.39 [1.09-1.78]	0.008	0.2
M609.3187T19.97	ESI -	203/203	2815	419	0.75 [0.60-0.93]	0.009	0.2
M410.8577T2.18	ESI +	211/211	5805	350	0.73 [0.58-0.93]	0.009	0.2
M458.7861T2.2	ESI +	211/211	2052	254	1.33 [1.07-1.65]	0.009	0.2
L-glutamine / L-isoglutamine M90.0547T2.32	ESI +	211/211	13187	2982	1.33 [1.07-1.66]	0.009	0.2
M363.9292T2.09	ESI +	211/211	1431	140	0.75 [0.61-0.93]	0.009	0.2
M82.9449T2.24	ESI +	211/211	18486	4576	1.38 [1.08-1.77]	0.009	0.2
M276.888T2.21	ESI +	211/211	3901	345	1.32 [1.07-1.63]	0.009	0.2
M53.0185T1.89	ESI +	211/211	5522	837	1.34 [1.07-1.68]	0.01	0.2
pregnene-triol sulfate M413.2002T16.11	ESI -	203/203	2441	1254	1.38 [1.08-1.77]	0.01	0.2
M286.143T16.48	ESI +	211/211	1931	2491	0.71 [0.55-0.92]	0.01	0.2
M166.0387T2.4	ESI -	203/203	1697	703	0.73 [0.57-0.93]	0.01	0.2
M201.8018T2.34	ESI -	203/203	2321	598	1.38 [1.08-1.77]	0.01	0.2
M588.3285T19.13	ESI -	203/203	38789	12941	1.37 [1.07-1.75]	0.01	0.2
M204.9569T2.03	ESI +	211/211	2579	364	1.31 [1.06-1.61]	0.01	0.2
M112.0076T1.91	ESI +	211/211	3917	627	1.32 [1.06-1.64]	0.01	0.2
M590.3434T19.69	ESI -	203/203	11805	5362	1.38 [1.07-1.77]	0.01	0.2
M540.3295T19.89	ESI -	203/203	168053	32521	1.38 [1.07-1.78]	0.01	0.2
M73.5317T1.89	ESI +	211/211	108235	14722	1.31 [1.06-1.62]	0.01	0.2
M412.8538T2.18	ESI +	211/211	3853	277	0.74 [0.58-0.94]	0.01	0.2
M412.8055T2.02	ESI -	203/203	3495	361	1.34 [1.06-1.68]	0.01	0.2
M185.1292T10.52	ESI +	211/211	1379	433	1.32 [1.06-1.65]	0.01	0.2
M558.9914T2.38	ESI +	211/211	1347	243	1.33 [1.06-1.67]	0.01	0.2
M794.4134T2.12	ESI -	203/203	1887	210	0.74 [0.58-0.94]	0.01	0.2
M112.0389T2.78	ESI -	203/203	822	635	1.32 [1.06-1.65]	0.01	0.2

^a Multivariable models were adjusted for age (continuous), BMI (continuous), smoking status (current smokers, former smokers and non-smokers), season of blood draw (a priori-defined periods: October-November/December-January-February/March-April-May), height (continuous), alcohol intake (continuous), physical activity (irregular/< 1h/d walking equivalent/ \geq 1h/d walking equivalent), education level (primary/secondary/superior), family history of breast cancer (yes/no), number of children (continuous), and use of hormone replacement therapy for menopause (yes/no) (reference model). Tests for linear trend were performed using continuous variables. ORs were presented for an increment of 1 SD for each metabolite.

^b P-trend after Benjamini Hochberg correction for multiple testing

SD, Standard Deviation