

Metabolomics and cheminformatics bioprospection of corn silk against key enzymes implicated in type 2 diabetes mellitus and its complications

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SUPPLEMENTARY MATERIALS

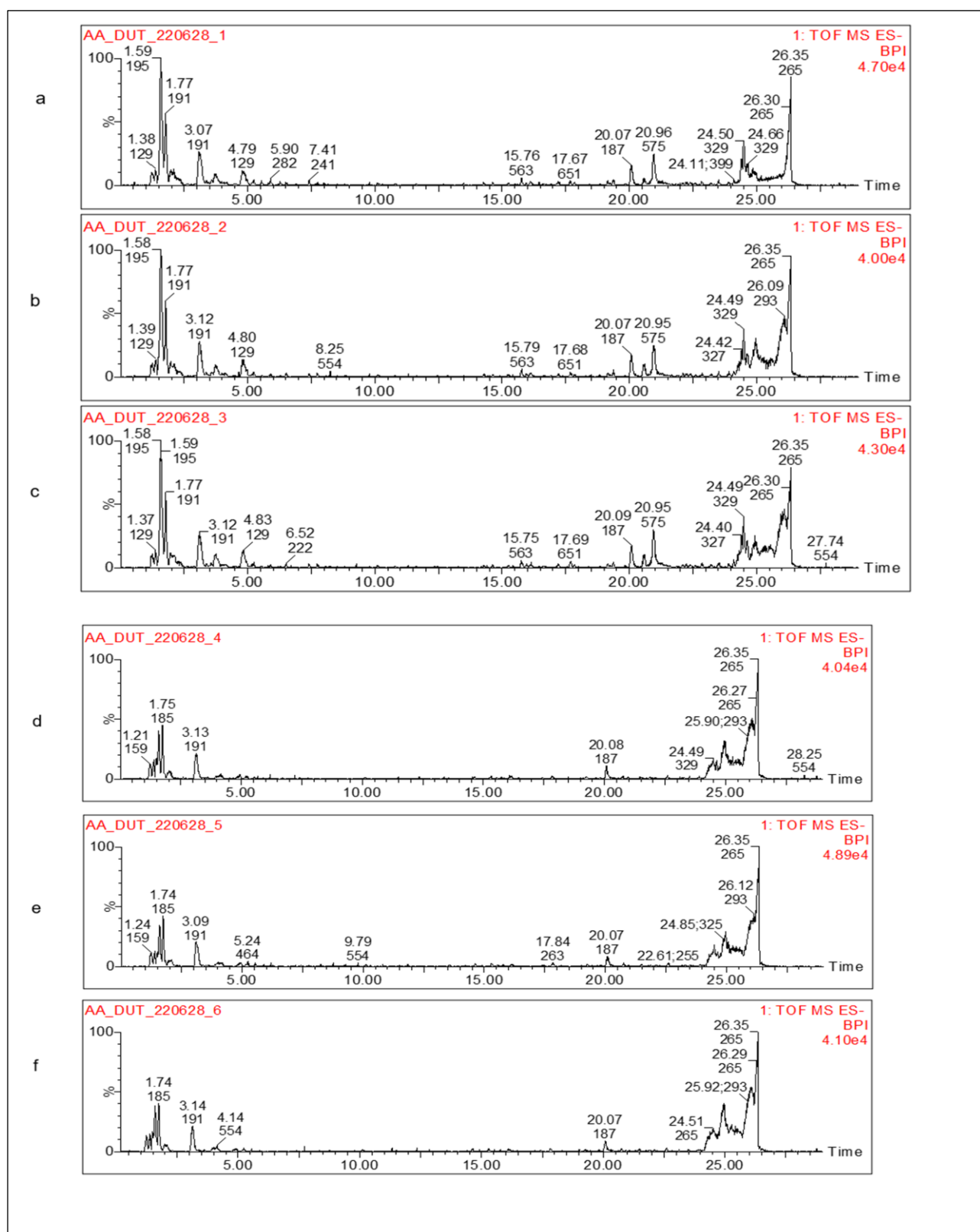


Figure S1: Chromatograms produced showing mass-to-charge ratio and retention times of a CS metabolites found in replicates of raw CS: a) raw premature CS 1, b) raw premature CS 2, c) raw premature CS 3, d) raw mature CS 1, e) raw mature CS 2 and f) raw mature CS 3

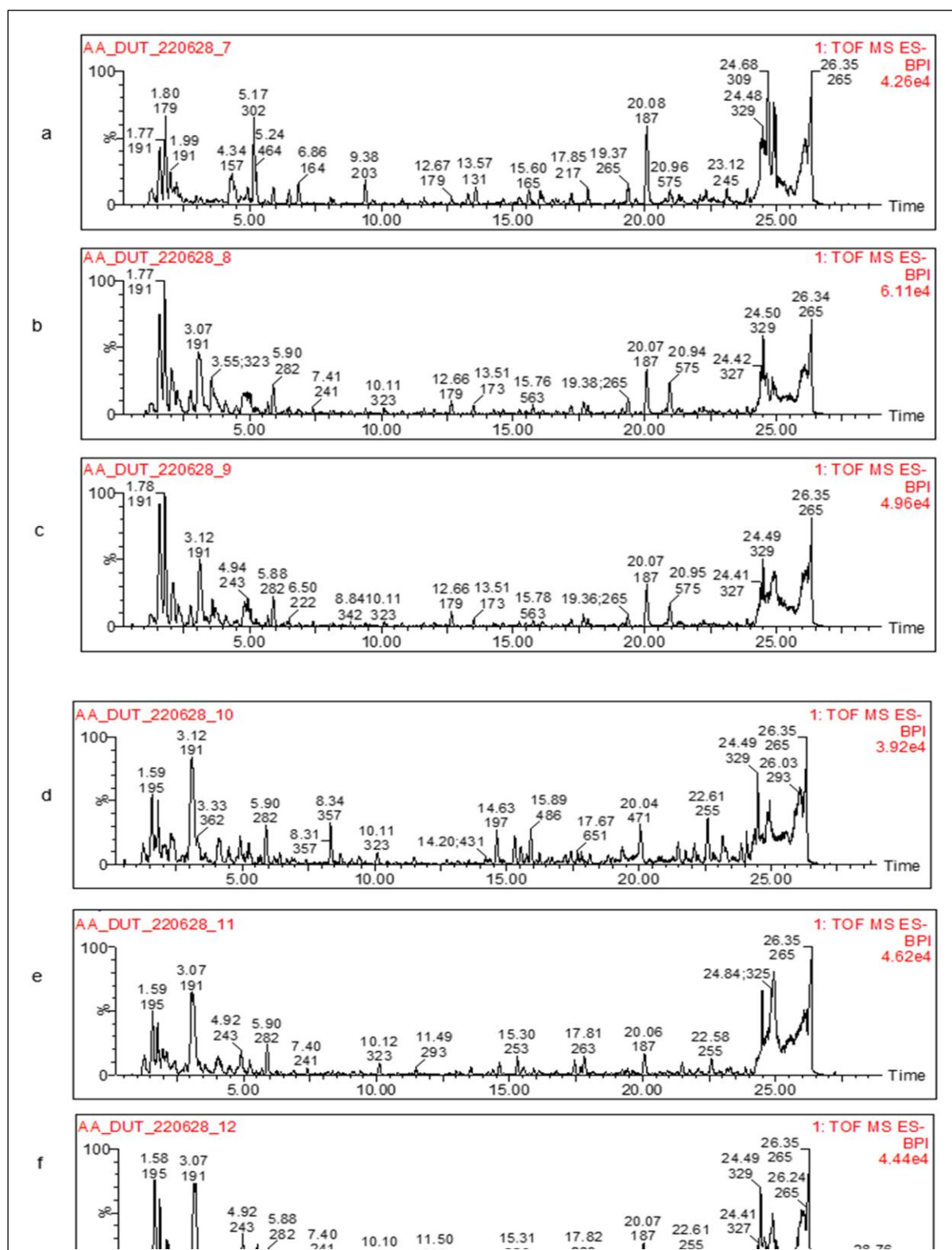


Figure S2: Chromatograms produced showing mass-to-charge ratio and retention times of a CS metabolites found in replicates of aqueous extracts of CS: a) aqueous extract of premature CS 1, b) aqueous extract of premature CS 2. C) aqueous extract of premature CS 3, d) aqueous extract of mature CS 1, e) aqueous extract of mature CS 2 and f) aqueous extract of mature CS 3.

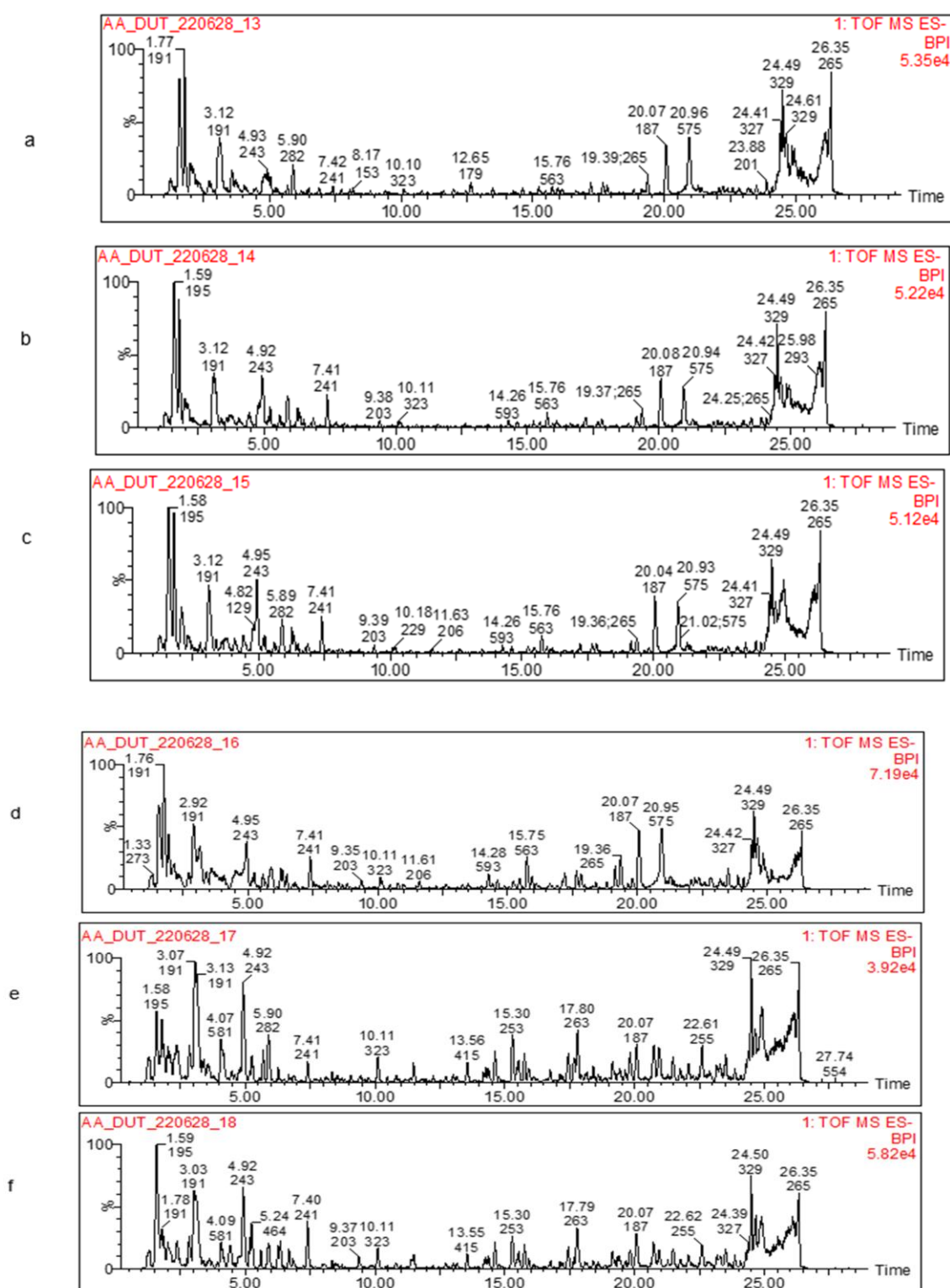


Figure S3: Chromatograms produced showing mass-to-charge ratio and retention times of a CS metabolites found in replicates of hydro-ethanolic extracts of extract of CS: a) hydro-ethanolic extract of premature CS 1, b) hydro-ethanolic extract of premature CS 2, c) hydro-ethanolic extract of premature CS, d) hydro-ethanolic extract of mature CS 1, e) hydro-ethanolic extract of mature CS 2 and f) hydro-ethanolic extract of mature CS.

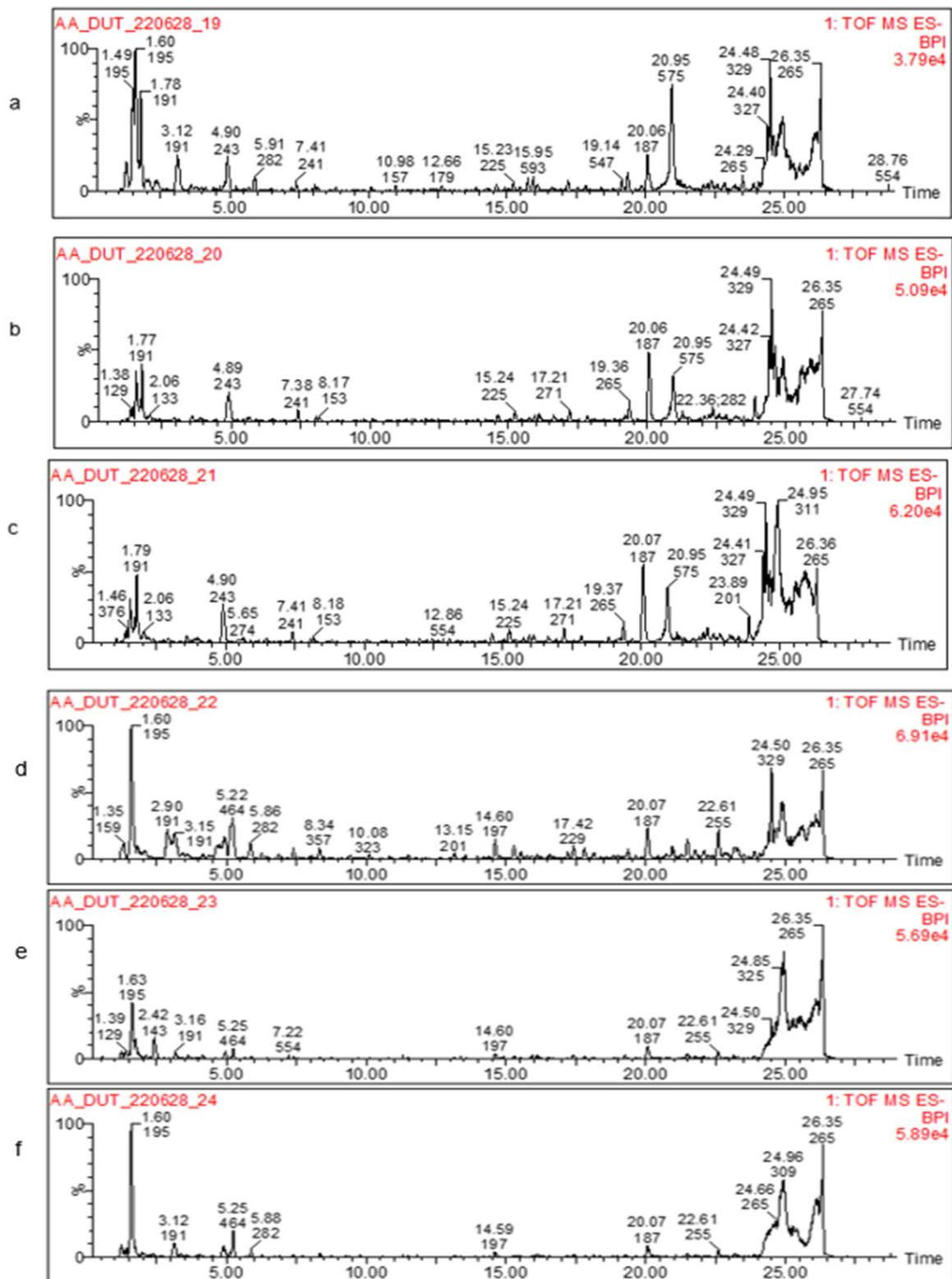


Figure S4: Chromatograms produced showing mass-to-charge ratio and retention times of a CS metabolites found in replicates of ethanolic extracts of CS: a) ethanolic extracts of premature CS 1, b) ethanolic extracts of premature CS 2. C) ethanolic extracts of premature CS 3, d) ethanolic extracts of mature CS 1, e) ethanolic extracts of mature CS 2 and f) ethanolic extracts of mature CS

Table S1: Secondary metabolites identified in various extracts corn silk through ultra-performance liquid chromatography-mass spectrometry analysis showing average retention times and mass-to-charge (m/z) ratio.

Compound number	Identity	Average retention time (minute)	m/z [M - H]-
C1	(7'R)-(+)-Lyoniresinol 9'-glucoside	4.07	581.22
C2	Estriol-16-Glucuronide	4.15	509.20
C3	Ascorbic acid	4.31	175.02
C4	Methylisocitric acid	4.39	205.03
C5	Citraconic acid	4.52	129.02
C6	Oxalosuccinic acid	4.98	189.01
C7	Pinocembrin 7-apiosyl-(1->5)-apiosyl-(1->2)-glucoside; 5,7-Dihydroxyflavanone 7-apiosyl-(1->5)-apiosyl-(1->2)-glucoside	4.99	681.21
C8	Mevalonic acid	5.09	147.07
C9	D-2-Hydroxyglutaric acid	5.18	147.03
C10	(2R,3S)-2,3-dimethylmalic acid	5.24	161.04
C11	UNPD109129	6.35	251.08
C12	Glutaric acid	6.15	131.03
C13	Cinnamic acid	6.85	147.04
C14	(6E)-1-(4-hydroxyphenyl)-7-phenylhepta-4,6-dien-3-one	8.45	277.13
C15	Vanillic acid	8.55	167.03
C16	1-O-vanilloyl-beta-D-glucose	8.55	329.09
C17	Isorhamnetin 3-(6"-malonylglucoside)	8.64	563.10
C18	Saccharumoside C	9.08	461.13
C19	7-hydroxy-4-{3-oxo-3H-benzo[f]chromen-2-yl}-2H-chromen-2-one	9.14	355.06
C20	Sarmentose	9.45	161.08
C21	CNP0447999	9.57	353.08
C22	1-O-Caffeoylglucose	9.75	341.09
C23	1-O-Galloylglycerol	10.05	243.05
C24	C00051555	10.11	323.13
C25	3-Isopropylmalate	10.79	175.06
C26	Diaportinic acid	10.82	279.05
C27	Benzyl beta-D-glucopyranoside; (-)-Benzyl-O-beta-D-glucopyranoside	11.15	269.10
C28	Domesticoside	11.35	343.10
C29	Dihydrophaseic acid 4'-O-beta-D-glucopyranoside	11.37	443.19
C30	Ketoleucine	11.47	129.05
C31	Aesculin	11.47	339.07
C32	Chlorogenic acid	12.00	353.09
C33	Quinic acid	12.00	191.06

C34	Cudraphenone A	12.23	363.16
C35	Pimelic acid	12.26	159.07
C36	(-)-6-((2S,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-methoxytetrahydro-2H-pyran-2-ylloxy)-8-hydroxy-3-methyl-1H-isochromen-1-one	12.46	367.10
C37	(-)-11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucoside	12.52	389.18
C38	Caffeic acid	12.65	179.03
C39	5-Carboxyvanillic acid	12.73	211.02
C40	Phellodendric acid A;(+) -Phellodendric acid A	12.75	203.09
C41	(-)-Epigallocatechin	13.27	305.07
C42	D-Leucic acid	13.29	131.07
C43	cis-Aconitic acid	13.50	173.01
C44	MINEs-320976	14.20	431.19
C45	Loganic acid	14.25	375.13
C46	Astragalin 7-rhamnoside	14.27	593.15
C47	Quing hau sau; quinghaosu; artemisinin	14.35	281.14
C48	3-Hydroxy-4-butanolide	14.43	263.08
C49	Annularin A;(+) -Annularin A	14.62	197.08
C50	Traumatic acid	14.78	227.13
C51	Methyl geranate	14.87	181.12
C52	3-Hydroxytetradecanedioic acid	14.87	273.17
C53	Dihydrophaseic acid	14.94	281.14
C54	Tuberonic acid	15.24	225.11
C55	Daldiniapyrone	15.29	253.11
C56	4-Hydroxycinnamic acid	15.48	163.04
C57	Monascusone A	15.54	253.11
C58	Acetovanillone; Apocynin	15.60	165.05
C59	Apiin	15.76	563.14
C60	Quercitrin	15.95	447.09
C61	2-Hydroxydecanedioic acid	16.18	217.11
C62	UNPD221406	16.24	241.11
C63	Cichorioside M;(+) -Cichorioside M	16.62	427.19
C64	Austricin; 8-Deacetylmatricarin; Desacetylmatricarin	16.71	261.12
C65	trans-Ferulic acid	17.09	193.05
C66	UNPD19396	17.12	577.15
C67	UNPD77208	17.21	271.15
C68	Nepetaside	17.24	345.16
C69	Dodecanedioic acid	17.42	229.14
C70	Kaempferitrin	17.55	577.15
C71	Chrysoeriol 4',7-diglucuronide	17.68	651.12
C72	Erythronolide B	17.73	401.25
C73	UNPD230015	17.82	263.06

C74	3-Hydroxysebacic acid	17.84	217.11
C75	Tricin 7-diglucuronoside	17.96	681.13
C76	Esculetin	18.08	177.02
C77	ethyl 5-[(2,5-dimethylphenyl) methoxy]-2-phenyl-1-benzofuran-3-carboxylate	18.09	399.16
C78	xi-2,2,6-Trimethyl-1,4-cyclohexanedione	18.25	153.09
C79	Quercetin 3-(2",3",4"-triacetylgalactoside)	18.31	589.12
C80	[4]-Gingerol	18.84	265.14
C81	Phaseic acid	18.56	279.12
C82	Diaportinol	18.60	265.07
C83	Herbacetin 7-(6"-quinoylglucoside)	18.68	637.14
C84	12-deoxyerythronolide A	19.05	401.25
C85	UNPD156113	19.09	605.12
C86	Mirificin	19.15	547.14
C87	Phaseolic acid	19.24	261.13
C88	Curvularol	19.37	265.14
C89	(+)-(S)-Carvone	19.65	149.10
C90	Kaempferol 3-rhamnoside 7-galacturonide	19.87	607.13
C91	Azelaic acid	20.07	187.10
C92	(3R,4S,6S)-3,4,5-trihydroxy-6-[5-hydroxy-2-(4-hydroxyphenyl)-4-oxo-3-[(2S,3S,5R)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxychromen-7-yl]oxyoxane-2-carboxylic acid	20.29	607.13
C93	Stagonolide F;(-)-Stagonolide F	20.68	183.10
C94	Isowertin 2"-rhamnoside	20.73	1183.34
C95	UNPD223815	20.86	255.16
C96	9-hydroxynonanoic acid	20.89	173.12
C97	Maysin	20.94	1151.29
C98	5,7,4'-Trihydroxy-3'-methoxyflavone	21.01	475.09
C99	Quercetin 3-O-(6"-acetyl-glucoside)	21.14	505.10
C100	Blennin D	21.15	265.14
C101	10-Deoxygeniposidic acid	21.27	357.12
C102	Gallicynoic acid F;(-)-Gallicynoic acid F	21.41	343.21
C103	Pandangolide 1a;(-)-Pandangolide 1a	21.46	243.12
C104	4-Hydroxynonenal	21.57	155.11
C105	Tetradecanedioic acid	21.76	257.17
C106	(R)-7-butyl-6,8-dihydroxy-3-[(3E)-pent-3-en-1-yl]-3,4-dihydroisochromen-1-one	21.82	303.16
C107	Genistin	21.82	431.10

C108	p-Coumaroyl malic acid	20.85	282.11
C109	Kaempferol 3-[2'''-acetyl-alpha-L-arabinopyranosyl-(1->6)-galactoside]	21.94	621.14
C110	Cyperine	22.09	259.10
C111	(+)-Cnicin; Cnicin	22.11	377.16
C112	(S)-Absciscic acid	22.20	263.13
C113	Sydnic acid; Sydonic acid	22.23	265.14
C114	Gallicynoic acid A;(+)-Gallicynoic acid A	22.81	253.14
C115	Apigenin 7-O-(6''-O-acetylglucoside)	22.85	473.11
C116	UNPD127537	23.18	255.16
C117	Olivetol	23.21	179.11
C118	Ginsenoyn E	23.29	303.16
C119	Caffeoyl tartaric acid	23.33	312.12
C120	Luteolin 3'-methyl ether 7-glucuronide	23.48	265.14
C121	UNPD205010	23.48	343.17
C122	Maysin 3'-methyl ether	23.51	589.15
C123	Artemin	23.66	265.15
C124	Gallicynoic acid B	23.69	267.16
C125	Aspergillide A	23.80	253.14
C126	(S)-Oleuropeic acid	23.89	183.10
C127	Sebacic acid	23.89	201.11
C128	7-Acetoxy-5,6-dimethoxycoumarin	17.82	263.06

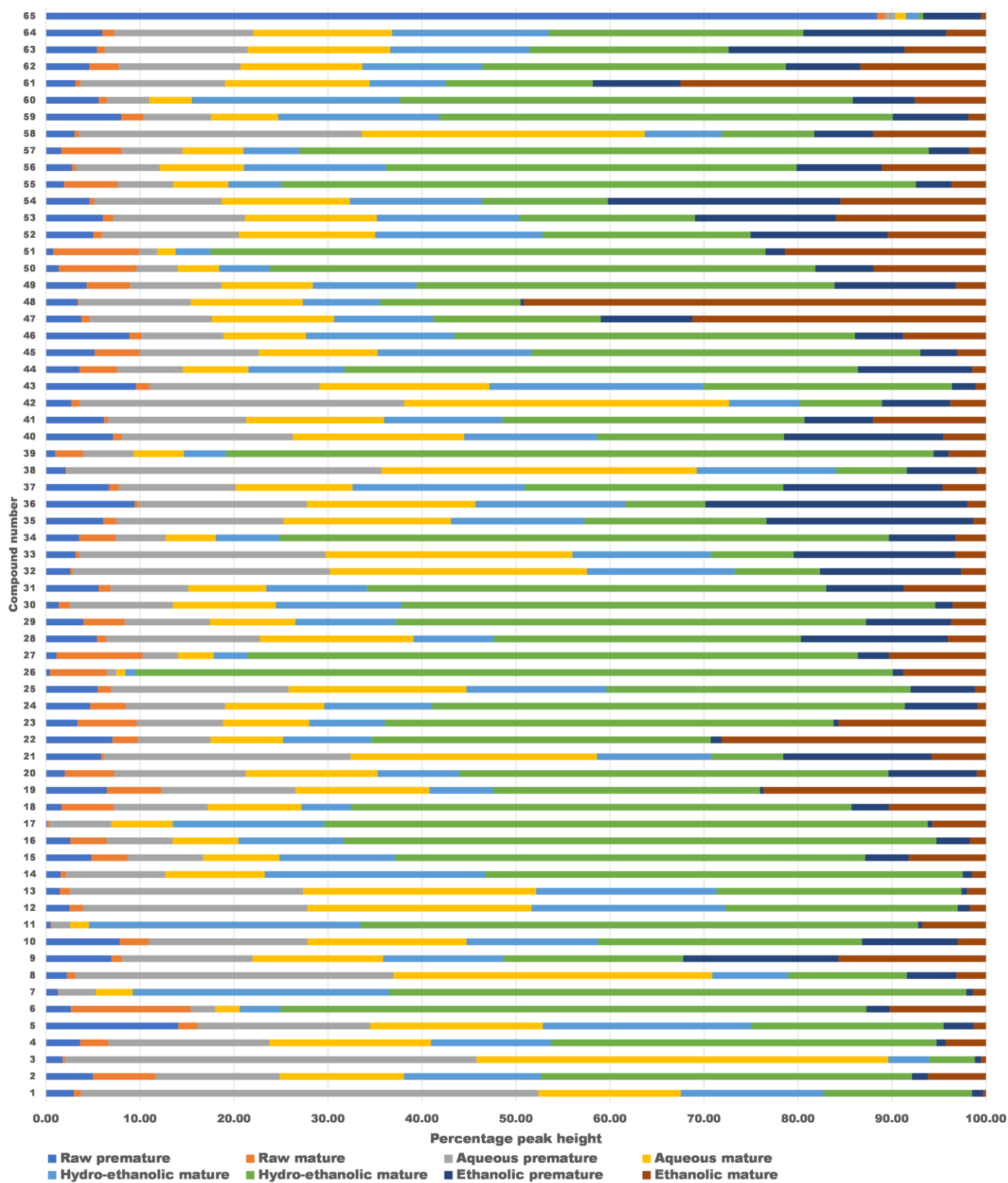


Figure S5: Stacked bar chart showing relative abundance of CS metabolites 1-65 in different extracts of CS



Figure S6: Stacked bar chart showing relative abundance of CS metabolites 66-128 in different extracts of CS.

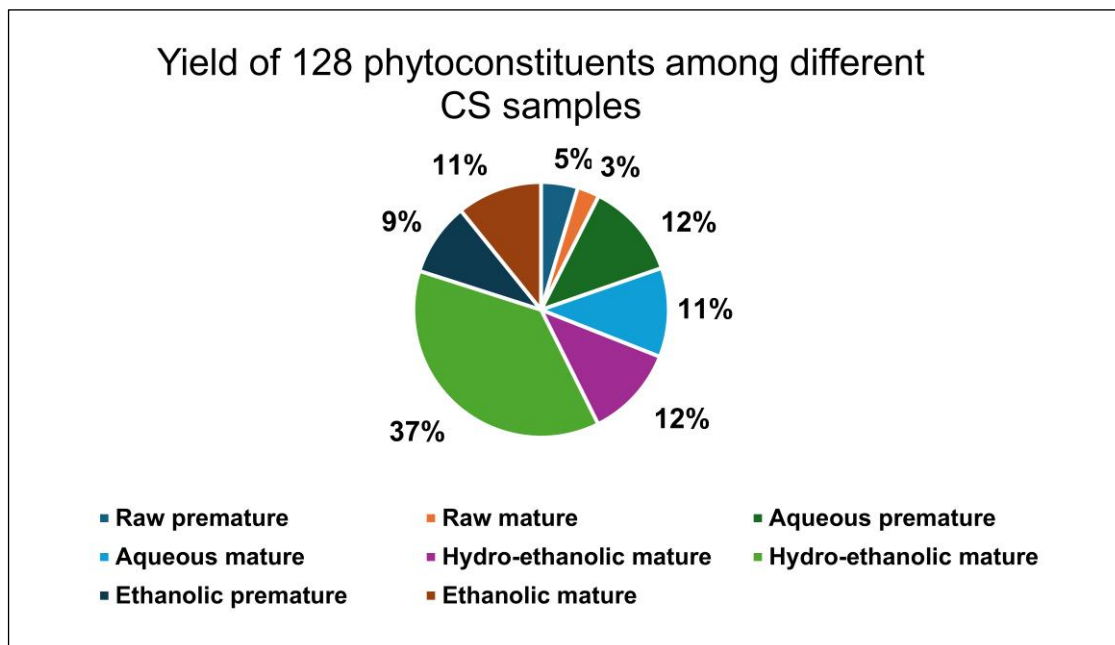


Figure S7: Yield (%) of the 128 metabolites identified in corn silk among the different extracts (aqueous, hydro-ethanolic and ethanollic) at two different developmental growth stages (premature and mature)

Table S2: Percentage relative abundance of CS metabolites identified in different samples of CS based on peak height percentage

Compound number	Raw premature CS	Raw mature CS	Aqueous extract of premature CS	Aqueous extract of mature CS	Hydro-ethanolic extract of premature CS	Hydro-ethanolic extract of mature CS	Ethanolic extract of premature CS	Ethanolic extract of mature CS
C1	2.96	0.77	48.65	15.15	15.15	15.83	1.16	0.32
C2	5.00	6.65	13.21	13.21	14.58	39.47	1.71	6.16
C3	1.78	0.25	43.79	43.79	4.40	4.83	0.66	0.51
C4	3.64	2.98	17.17	17.17	12.75	41.02	0.99	4.27
C5	14.08	2.08	18.34	18.34	22.16	20.49	3.20	1.31
C6	2.65	12.75	2.61	2.61	4.35	62.32	2.44	10.27
C7	1.28	0.07	3.94	3.94	27.29	61.39	0.71	1.38
C8	2.23	0.85	33.90	33.90	8.11	12.59	5.28	3.13
C9	6.95	1.14	13.89	13.89	12.83	19.10	16.52	15.68
C10	7.85	3.11	16.88	16.88	13.98	28.12	10.18	2.99
C11	0.49	0.10	1.99	1.99	28.93	59.28	0.44	6.78
C12	2.50	1.46	23.85	23.85	20.67	24.67	1.31	1.70
C13	1.47	1.06	24.81	24.81	19.20	26.04	0.60	2.01
C14	1.56	0.57	10.57	10.57	23.46	50.79	1.00	1.47
C15	4.83	3.81	8.09	8.09	12.38	49.95	4.66	8.19
C16	2.60	3.89	7.00	7.00	11.15	63.10	3.56	1.70
C17	0.14	0.25	6.56	6.56	16.07	64.23	0.49	5.70
C18	1.65	5.58	9.98	9.98	5.25	53.26	4.00	10.31
C19	6.48	5.78	14.27	14.27	6.78	28.35	0.42	23.64
C20	2.00	5.27	14.01	14.01	8.71	45.62	9.40	0.98
C21	5.87	0.35	26.21	26.21	12.14	7.67	15.78	5.78
C22	7.08	2.72	7.71	7.71	9.40	36.10	1.16	28.12
C23	3.36	6.29	9.17	9.17	8.06	47.74	0.52	15.69
C24	4.70	3.81	10.54	10.54	11.47	50.32	7.73	0.89
C25	5.50	1.41	18.91	18.91	14.88	32.37	6.84	1.17
C26	0.39	6.10	0.97	0.97	1.15	80.51	1.08	8.83
C27	1.10	9.18	3.78	3.78	3.56	64.97	3.31	10.32
C28	5.44	0.98	16.35	16.35	8.53	32.68	15.65	4.03
C29	3.98	4.40	9.08	9.08	10.69	50.01	9.06	3.70
C30	1.35	1.20	10.95	10.95	13.39	56.77	1.84	3.55
C31	5.62	1.26	8.29	8.29	10.72	48.83	8.25	8.76
C32	2.59	0.25	27.35	27.35	15.72	9.08	15.04	2.62
C33	3.15	0.36	26.25	26.25	14.73	8.80	17.20	3.27
C34	3.53	3.90	5.31	5.31	6.85	64.79	7.09	3.23
C35	6.09	1.41	17.80	17.80	14.19	19.37	22.03	1.32
C36	9.43	0.42	17.91	17.91	15.98	8.50	27.88	1.97
C37	6.72	1.02	12.44	12.44	18.33	27.49	16.96	4.61
C38	2.08	0.11	33.52	33.52	14.81	7.55	7.45	0.96
C39	1.00	2.98	5.34	5.34	4.48	75.28	1.61	3.96
C40	7.14	0.92	18.22	18.22	14.12	19.92	16.94	4.53
C41	6.18	0.45	14.66	14.66	12.62	32.12	7.32	11.98

C42	2.71	0.87	34.54	34.54	7.52	8.76	7.27	3.79
C43	9.58	1.44	18.08	18.08	22.77	26.44	2.53	1.09
C44	3.58	3.99	6.99	6.99	10.19	54.64	12.15	1.47
C45	5.19	4.81	12.64	12.64	16.39	41.34	3.92	3.07
C46	8.89	1.25	8.76	8.76	15.82	42.59	5.10	8.82
C47	3.77	0.88	13.00	13.00	10.53	17.86	9.73	31.24
C48	3.37	0.10	11.92	11.92	8.21	14.95	0.36	49.17
C49	4.33	4.65	9.71	9.71	11.03	44.46	12.92	3.19
C50	1.35	8.32	4.37	4.37	5.41	58.03	6.20	11.94
C51	0.78	9.13	1.94	1.94	3.74	59.03	2.05	21.40
C52	5.03	0.94	14.53	14.53	17.80	22.13	14.61	10.43
C53	6.06	1.08	14.04	14.04	15.22	18.62	15.01	15.94
C54	4.63	0.50	13.60	13.60	14.06	13.38	24.74	15.49
C55	1.92	5.72	5.88	5.88	5.63	67.53	3.78	3.67
C56	2.77	0.38	8.95	8.95	15.14	43.68	9.06	11.07
C57	1.62	6.44	6.47	6.47	6.00	66.93	4.26	1.81
C58	3.05	0.48	30.08	30.08	8.23	9.81	6.26	12.00
C59	8.01	2.38	7.16	7.16	17.15	48.22	8.04	1.87
C60	5.62	0.83	4.54	4.54	22.12	48.19	6.59	7.57
C61	3.13	0.54	15.38	15.38	8.14	15.62	9.31	32.51
C62	4.63	3.11	12.96	12.96	12.78	32.26	7.94	13.35
C63	5.43	0.85	15.18	15.18	14.81	21.17	18.73	8.66
C64	5.98	1.30	14.77	14.77	16.67	27.09	15.18	4.24
C65	88.42	0.85	1.11	1.11	1.31	0.52	6.16	0.52
C66	4.93	1.18	5.89	5.89	11.10	42.56	3.78	24.67
C67	5.57	0.87	15.60	15.60	15.21	21.75	19.24	6.17
C68	0.93	4.50	1.74	1.74	3.21	75.17	2.41	10.31
C69	0.28	11.69	1.53	1.53	3.08	76.14	4.13	1.63
C70	7.14	0.82	2.60	2.60	11.05	10.05	36.51	29.23
C71	6.77	0.71	16.03	16.03	13.86	37.08	0.50	9.03
C72	1.05	5.56	2.82	2.82	2.79	53.76	2.46	28.74
C73	0.15	7.97	0.60	0.60	0.99	86.16	1.22	2.30
C74	1.75	8.60	3.22	3.22	6.90	58.83	9.06	8.42
C75	5.34	1.82	13.93	13.93	12.50	47.47	0.06	4.95
C76	1.56	1.07	1.07	1.07	4.07	9.68	10.32	71.16
C77	2.94	3.77	3.30	3.30	7.34	72.28	5.11	1.97
C78	7.55	0.57	17.44	17.44	17.39	19.83	18.11	1.67
C79	4.67	1.05	6.30	6.30	23.67	48.72	3.92	5.37
C80	6.08	4.81	9.47	9.47	11.16	39.58	11.08	8.36
C81	7.10	0.73	15.99	15.99	15.84	17.84	16.19	10.32
C82	0.25	3.67	0.70	0.70	0.49	41.50	0.74	51.95
C83	5.31	2.44	3.85	3.85	13.17	48.57	1.37	21.43
C84	1.13	6.00	3.05	3.05	3.01	58.08	2.66	23.02
C85	3.31	0.65	12.39	12.39	13.11	34.03	21.93	2.20
C86	6.00	1.15	7.24	7.24	14.34	43.11	7.35	13.56
C87	8.57	7.61	10.82	10.82	15.27	19.28	19.96	7.68
C88	5.15	1.03	12.54	12.54	12.94	17.72	12.95	25.13
C89	1.33	3.08	3.01	3.01	3.22	27.08	2.03	57.24

C90	4.40	0.48	29.80	13.91	9.66	26.16	13.91	1.68
C91	6.31	3.32	17.69	17.69	15.91	18.50	20.41	0.17
C92	4.46	2.13	66.92	5.12	10.37	5.12	3.50	2.38
C93	2.09	8.59	5.59	5.59	6.86	58.39	9.81	3.07
C94	1.74	7.76	1.06	1.06	4.94	79.57	3.63	0.25
C95	2.98	3.76	8.78	8.78	6.33	37.31	11.71	20.36
C96	4.93	0.58	16.56	16.56	16.51	13.09	29.35	2.42
C97	4.62	0.77	4.78	4.78	10.32	31.68	16.10	26.94
C98	7.24	1.99	5.00	5.00	19.91	57.90	1.10	1.85
C99	1.65	1.06	1.88	1.88	7.01	34.43	0.86	51.23
C100	6.30	1.47	22.41	14.85	17.41	14.85	13.75	8.96
C101	0.83	8.06	1.39	1.39	3.22	60.96	2.07	22.08
C102	4.88	0.96	26.27	16.52	14.55	16.52	14.25	6.05
C103	2.41	0.18	5.88	5.88	7.12	8.08	7.23	63.21
C104	3.06	0.48	10.43	10.43	11.56	42.47	15.26	6.32
C105	1.12	0.87	42.09	44.02	2.14	2.14	4.00	3.62
C106	0.31	4.00	1.27	1.27	1.88	34.17	1.09	56.01
C107	5.74	1.03	3.80	3.80	18.14	60.99	4.46	2.02
C108	7.99	0.85	1.19	1.19	17.93	27.59	39.28	3.99
C109	1.81	1.40	4.82	4.82	16.74	60.50	4.92	4.98
C110	5.64	3.99	13.78	13.78	12.99	34.76	11.97	3.10
C111	0.45	4.75	1.94	1.94	2.56	58.84	0.97	28.56
C112	5.91	2.01	15.02	15.02	14.75	27.09	18.12	2.06
C113	6.14	1.58	14.94	14.94	14.02	20.85	16.54	10.99
C114	4.03	3.08	11.28	11.28	12.36	32.08	16.33	9.56
C115	2.56	0.42	3.59	3.59	22.80	34.66	28.94	3.44
C116	2.86	2.98	9.59	9.59	10.81	40.67	15.13	8.35
C117	4.25	0.40	15.47	15.47	17.19	19.03	16.53	11.66
C118	0.93	5.25	2.51	2.51	2.79	67.69	1.35	16.98
C119	6.02	1.11	1.62	1.62	17.52	41.33	25.31	5.47
C120	7.24	1.99	5.00	5.00	19.91	57.90	1.10	1.85
C121	1.30	8.24	3.37	3.37	2.72	68.18	3.13	9.70
C122	6.61	2.25	4.92	4.92	15.46	48.27	13.13	4.44
C123	3.52	5.01	8.92	14.71	9.95	31.56	9.93	16.41
C124	0.91	1.78	40.34	41.84	4.00	2.80	4.77	3.58
C125	5.46	1.41	12.95	12.95	14.61	21.28	21.68	9.66
C126	4.04	2.69	13.93	13.93	12.80	16.31	27.95	8.35
C127	5.14	2.66	14.50	15.86	15.52	17.14	28.93	0.25
C128	0.14	7.78	0.59	0.73	0.96	84.09	1.19	4.51

Table S3: ADME and drug-likeness predictions of corn silk metabolites

C#	Formula	MW (g/mol)	HA	HD	iLOG P	TPS A	GIA	BB P	P S	CY P1A 2-I	CYP 2C19 -I	CY P2C 9-I	C YP 2D 6-I	CY P3A 4-I	LV	GV	VV	E V	M V	BS
C1	C ₂₈ H ₃₈ O ₁₃	582.59	13	7	4.71	196.99	L	N	Y	N	N	N	N	N	3	3	1	1	3	0.17
C2	C ₂₄ H ₃₂ O ₉	464.51	9	6	1.67	156.91	L	N	Y	N	N	N	N	N	1	0	1	1	2	0.11
C3	C ₆ H ₈ O ₆	176.12	6	4	0.39	107.22	H	N	N	N	N	N	N	N	0	2	0	0	1	0.56
C4	C ₇ H ₁₀ O ₇	206.15	7	4	-0.94	132.13	H	N	N	N	N	N	N	N	0	1	0	1	0	0.56
C5	C ₅ H ₆ O ₄	130.10	4	2	0.46	74.6	H	N	N	N	N	N	N	N	0	3	0	0	1	0.85
C6	C ₆ H ₆ O ₇	190.11	7	3	-0.71	128.97	H	N	N	N	N	N	N	N	0	3	0	0	1	0.56
C7	C ₃₁ H ₃₈ O ₁₇	682.62	17	9	2.27	263.75	L	N	Y	N	N	N	N	N	3	4	1	1	4	0.17
C8	C ₆ H ₁₂ O ₄	148.16	4	3	0.39	77.76	H	N	N	N	N	N	N	N	0	3	0	0	1	0.56
C9	C ₅ H ₈ O ₅	148.11	5	3	0.18	94.83	H	N	N	N	N	N	N	N	0	4	0	0	1	0.56
C10	C ₆ H ₁₀ O ₅	162.14	5	3	0.34	94.83	H	N	N	N	N	N	N	N	0	2	0	0	1	0.56
C11	C ₉ H ₁₆ O ₈	252.22	8	5	0.37	136.68	L	N	Y	N	N	N	N	N	0	1	0	1	1	0.56
C12	C ₅ H ₈ O ₄	132.11	4	2	0.45	74.6	H	N	N	N	N	N	N	N	0	3	0	0	1	0.85
C13	C ₉ H ₈ O ₂	148.16	2	1	1.55	37.3	H	Y	N	N	N	N	N	N	0	2	0	0	1	0.85
C14	C ₁₉ H ₁₈ O ₂	278.35	2	1	2.79	37.3	H	Y	N	Y	Y	Y	Y	Y	0	0	0	0	0	0.55
C15	C ₈ H ₈ O ₄	168.15	4	2	1.40	66.76	H	N	N	N	N	N	N	N	0	0	0	0	1	0.85
C16	C ₁₄ H ₁₈ O ₉	330.29	9	5	1.88	145.91	L	N	N	N	N	N	N	N	0	1	1	1	0	0.55
C17	C ₂₅ H ₂₄ O ₁₅	564.45	15	7	1.77	242.88	L	N	Y	N	N	N	N	N	3	2	1	1	3	0.11
C18	C ₁₉ H ₂₆ O ₁₃	462.40	13	7	1.35	204.83	L	N	N	N	N	N	N	N	2	1	1	1	3	0.17
C19	C ₂₂ H ₁₂ O ₅	356.33	5	1	2.52	80.65	H	N	N	Y	Y	N	N	N	0	0	0	0	0	0.55
C20	C ₇ H ₁₄ O ₄	162.18	4	2	0.94	66.76	H	N	N	N	N	N	N	N	0	2	0	0	1	0.55
C21	C ₂₃ H ₁₄ O ₄	354.35	4	1	2.41	71.44	H	Y	N	Y	N	Y	N	N	0	0	0	0	0	0.85
C22	C ₁₅ H ₁₈ O ₉	342.30	9	6	0.23	156.91	L	N	N	N	N	N	N	N	1	1	1	1	2	0.55
C23	C ₁₀ H ₁₂ O ₇	244.20	7	5	0.63	127.45	H	N	N	N	N	N	N	N	0	1	0	0	0	0.55
C24	C ₁₃ H ₂₄ O ₉	324.32	9	5	1.95	138.07	L	N	Y	N	N	N	N	N	0	1	0	1	1	0.55
C25	C ₇ H ₁₂ O ₅	176.17	5	3	0.24	94.83	H	N	N	N	N	N	N	N	0	0	0	0	1	0.56
C26	C ₁₃ H ₁₂ O ₇	280.23	7	3	1.54	117.2	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C27	C ₁₃ H ₁₈ O ₆	270.28	6	4	1.60	99.38	H	N	N	N	N	N	N	N	0	1	0	0	0	0.55
C28	C ₁₅ H ₂₀ O ₉	344.31	9	5	2.05	145.91	L	N	N	N	N	N	N	N	0	1	1	1	0	0.55
C29	C ₂₁ H ₃₂ O ₁₀	444.47	10	6	1.89	166.14	L	N	N	N	N	N	N	N	1	1	1	1	2	0.11
C30	C ₆ H ₁₀ O ₃	130.14	3	1	1.06	54.37	H	Y	N	N	N	N	N	N	0	3	0	0	1	0.85
C31	C ₁₅ H ₁₆ O ₉	340.28	9	5	1.04	149.82	L	N	N	N	N	N	N	N	0	1	1	1	0	0.55
C32	C ₁₆ H ₁₈ O ₉	354.31	9	6	0.96	164.	L	N	N	N	N	N	N	N	1	1	1	1	2	0.11

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C33	C ₇ H ₁₂ O ₆	192.17	6	5	-0.12	118.22	L	N	Y	N	N	N	N	N	0	1	0	0	2	0.56
C34	C ₂₃ H ₂₄ O ₄	364.43	4	2	3.70	66.76	H	Y	N	Y	Y	Y	N	Y	0	0	0	0	1	0.55
C35	C ₇ H ₁₂ O ₄	160.17	4	2	0.94	74.6	H	N	N	N	N	N	N	N	0	1	0	0	1	0.85
C36	C ₁₇ H ₂₀ O ₉	368.34	9	4	2.54	138.82	L	N	N	N	N	N	N	N	0	0	0	1	0	0.55
C37	C ₁₈ H ₃₀ O ₉	390.43	9	5	2.35	153.75	L	N	Y	N	N	N	N	N	0	1	1	1	1	0.11
C38	C ₉ H ₈ O ₄	180.16	4	3	0.97	77.76	H	N	N	N	N	N	N	N	0	0	0	0	1	0.56
C39	C ₉ H ₈ O ₆	212.16	6	3	0.24	104.06	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C40	C ₉ H ₁₆ O ₅	204.22	5	2	1.55	83.83	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C41	C ₁₅ H ₁₄ O ₇	306.27	7	6	0.98	130.61	H	N	N	N	N	N	N	N	1	0	0	0	1	0.55
C42	C ₆ H ₁₂ O ₃	132.16	3	2	1.17	57.53	H	N	N	N	N	N	N	N	0	2	0	0	1	0.85
C43	C ₆ H ₆ O ₆	174.11	6	3	-0.13	111.9	H	N	N	N	N	N	N	N	0	3	0	0	1	0.56
C44	C ₂₀ H ₃₂ O ₁₀	432.46	10	6	1.57	173.98	L	N	Y	N	N	N	N	N	1	1	1	1	2	0.11
C45	C ₁₆ H ₂₄ O ₁₀	376.36	10	6	1.26	166.14	L	N	Y	N	N	N	N	N	1	1	1	1	2	0.11
C46	C ₂₇ H ₃₀ O ₁₅	594.52	15	9	1.80	249.2	L	N	Y	N	N	N	N	N	3	4	1	1	3	0.17
C47	C ₁₅ H ₂₂ O ₅	282.33	5	0	2.75	53.99	H	Y	N	Y	N	N	N	N	0	0	0	0	0	0.55
C48	C ₁₀ H ₁₆ O ₈	264.23	8	4	0.97	125.68	L	N	Y	N	N	N	N	N	0	1	0	0	1	0.55
C49	C ₁₀ H ₁₄ O ₄	198.22	4	1	2.32	59.67	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.55
C50	C ₁₂ H ₂₀ O ₄	228.28	4	2	2.04	74.6	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.85
C51	C ₁₁ H ₁₈ O ₂	182.26	2	0	3.05	26.3	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.55
C52	C ₁₄ H ₂₆ O ₅	274.35	5	3	2.34	94.83	H	N	N	N	N	N	N	N	0	0	1	0	0	0.56
C53	C ₁₅ H ₂₂ O ₅	282.33	5	3	2.09	86.99	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C54	C ₁₂ H ₁₈ O ₄	226.27	4	2	1.46	74.6	H	N	N	N	N	N	N	N	0	0	0	0	0	0.85
C55	C ₁₃ H ₁₈ O ₅	254.28	5	0	3.07	65.74	H	Y	N	Y	Y	N	N	N	0	0	0	0	0	0.55
C56	C ₉ H ₈ O ₃	164.16	3	2	0.95	57.53	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.85
C57	C ₁₃ H ₁₈ O ₅	254.28	5	3	1.82	86.99	H	N	N	N	N	N	N	N	0	0	0	0	0	0.55
C58	C ₉ H ₁₀ O ₃	166.17	3	1	1.77	46.53	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.55
C59	C ₂₆ H ₂₈ O ₁₄	564.49	14	8	2.11	228.97	L	N	Y	N	N	N	N	N	3	3	1	1	3	0.17
C60	C ₂₁ H ₂₀ O ₁₁	448.38	11	7	1.27	190.28	L	N	N	N	N	N	N	N	2	0	1	1	3	0.17
C61	C ₁₀ H ₁₈ O ₅	218.25	5	3	0.96	94.83	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C62	C ₁₂ H ₁₈ O ₅	242.27	5	2	1.81	79.29	H	N	N	N	N	N	N	N	0	0	0	0	0	0.55
C63	C ₂₁ H ₃₂ O ₉	428.47	9	5	1.97	145.91	L	N	Y	N	N	N	N	N	0	1	1	1	0	0.55
C64	C ₁₅ H ₁₈ O ₄	262.30	4	1	2.03	63.6	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.55
C65	C ₁₀ H ₁₀ O ₄	194.18	4	2	1.62	66.76	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.85
C66	C ₃₄ H ₂₆ O ₉	578.56	9	6	3.45	160.82	L	N	N	N	N	Y	N	N	2	3	1	2	3	0.17
C67	C ₁₄ H ₂₄ O ₅	272.34	5	1	2.71	64.9	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.55

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C68	C ₁₆ H ₂₆ O ₈	346.37	8	4	2.06	125.68	H	N	Y	N	N	N	N	N	0	1	0	0	0	0.55
C69	C ₁₂ H ₂₂ O ₄	230.30	4	2	1.83	74.6	H	Y	N	N	N	N	N	N	0	0	1	0	0	0.85
C70	C ₂₇ H ₃₀ O ₁₄	578.52	14	8	1.89	228.97	L	N	Y	N	N	N	N	N	3	4	1	1	3	0.17
C71	C ₂₈ H ₂₈ O ₁₈	652.51	18	9	0.94	292.57	L	N	Y	N	N	N	N	N	3	4	1	1	4	0.11
C72	C ₂₁ H ₃₈ O ₇	402.52	7	4	2.83	124.29	H	N	Y	N	N	N	N	Y	0	0	0	0	0	0.55
C73	C ₁₃ H ₁₂ O ₆	264.23	6	3	1.70	100.13	H	N	N	N	N	N	N	N	0	0	0	0	0	0.55
C74	C ₁₀ H ₁₈ O ₅	218.25	5	3	1.32	94.83	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C75	C ₂₉ H ₃₀ O ₁₉	682.54	19	9	1.95	301.8	L	N	Y	N	N	N	N	N	3	4	1	1	4	0.11
C76	C ₉ H ₆ O ₄	178.14	4	2	1.25	70.67	H	N	N	Y	N	N	N	N	0	1	0	0	1	0.55
C77	C ₂₆ H ₂₄ O ₄	400.47	4	0	4.45	48.67	H	N	Y	Y	Y	Y	N	Y	1	1	0	1	1	0.55
C78	C ₉ H ₁₄ O ₂	154.21	2	0	1.63	34.14	H	Y	N	N	N	N	N	N	0	1	0	0	1	0.55
C79	C ₂₇ H ₂₆ O ₁₅	590.49	15	5	1.94	228.72	L	N	Y	N	N	N	N	N	2	2	1	1	2	0.17
C80	C ₁₅ H ₂₂ O ₄	266.33	4	2	2.38	66.76	H	Y	N	N	N	N	Y	N	0	0	0	0	0	0.55
C81	C ₁₅ H ₂₀ O ₅	280.32	5	2	1.76	83.83	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C82	C ₁₃ H ₁₄ O ₆	266.25	6	3	2.33	100.13	H	N	N	N	N	N	N	N	0	0	0	0	0	0.55
C83	C ₂₈ H ₃₀ O ₁₇	638.53	17	11	1.81	297.5	L	N	Y	N	N	N	N	N	3	4	1	1	4	0.17
C84	C ₂₁ H ₃₈ O ₇	402.52	7	4	2.83	124.29	H	N	Y	N	N	N	N	Y	0	0	0	0	0	0.55
C85	C ₂₇ H ₂₆ O ₁₆	606.49	16	9	2.59	262.36	L	N	Y	N	N	N	N	N	3	2	1	1	4	0.17
C86	C ₂₆ H ₂₈ O ₁₃	548.49	13	8	0.66	219.74	L	N	N	N	N	N	N	N	3	3	1	1	3	0.17
C87	C ₁₂ H ₂₂ O ₆	262.30	6	4	1.32	115.06	H	N	N	N	N	N	N	N	0	0	1	0	0	0.56
C88	C ₁₅ H ₂₂ O ₄	266.33	4	2	2.35	62.22	H	Y	Y	N	N	N	N	N	0	0	0	0	0	0.55
C89	C ₁₀ H ₁₄ O	150.22	1	0	2.27	17.07	H	Y	N	N	N	N	N	N	0	1	0	0	2	0.55
C90	C ₂₇ H ₂₈ O ₁₆	608.50	16	9	1.66	266.27	L	N	Y	N	N	N	N	N	3	4	1	1	4	0.11
C91	C ₉ H ₁₆ O ₄	188.22	4	2	1.44	74.6	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.85
C92	C ₂₇ H ₂₈ O ₁₆	608.50	16	9	1.66	266.27	L	N	Y	N	N	N	N	N	3	4	1	1	4	0.11
C93	C ₁₀ H ₁₆ O ₃	184.23	3	1	2.03	46.53	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.55
C94	C ₂₈ H ₃₂ O ₁₄	592.55	14	8	0.80	228.97	L	N	Y	N	N	N	N	N	3	4	1	1	3	0.17
C95	C ₁₄ H ₂₄ O ₄	256.34	4	1	3.26	55.76	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.85
C96	C ₉ H ₁₈ O ₃	174.24	3	2	1.83	57.53	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.85
C97	C ₂₇ H ₂₈ O ₁₄	576.50	14	8	1.95	236.81	L	N	Y	N	N	N	N	N	3	3	1	1	3	0.17
C98	C ₂₂ H ₂₀ O ₁₂	476.39	12	6	2.02	196.35	L	N	Y	N	N	N	N	N	2	0	1	1	3	0.11
C99	C ₂₃ H ₂₂ O ₁₃	506.41	13	7	1.61	216.58	L	N	Y	N	N	N	N	N	3	1	1	1	3	0.17
C100	C ₁₅ H ₂₂ O ₄	266.33	4	2	2.46	66.76	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.55

C101	C ₁₆ H ₂₂ O ₉	358.34	9	5	1.24	145.91	L	N	Y	N	N	N	N	N	0	1	1	1	0	0.56
C102	C ₁₈ H ₃₂ O ₆	344.44	6	5	2.95	118.22	H	N	Y	N	N	N	N	N	0	0	1	0	0	0.56
C103	C ₁₂ H ₂₀ O ₅	244.28	5	2	1.91	83.83	H	N	N	N	N	N	N	N	0	0	0	0	0	0.55
C104	C ₉ H ₁₆ O ₂	156.22	2	1	2.15	37.3	H	Y	N	N	N	N	N	N	0	1	0	0	1	0.55
C105	C ₁₄ H ₂₆ O ₄	258.35	4	2	2.49	74.6	H	Y	N	N	N	N	N	N	0	0	1	0	0	0.85
C106	C ₁₈ H ₂₄ O ₄	304.38	4	2	3.45	66.76	H	Y	N	Y	N	Y	N	N	0	0	0	0	1	0.55
C107	C ₂₁ H ₂₀ O ₁₀	432.38	10	6	2.11	170.05	L	N	N	N	N	N	N	N	1	0	1	1	2	0.55
C108	C ₁₃ H ₁₂ O ₇	280.23	7	3	0.62	121.13	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C109	C ₂₈ H ₃₀ O ₁₆	622.53	16	8	1.81	255.27	L	N	Y	N	N	N	N	N	3	4	1	1	4	0.17
C110	C ₁₅ H ₁₆ O ₄	260.29	4	2	2.73	58.92	H	Y	N	Y	Y	Y	Y	Y	0	0	0	0	0	0.55
C111	C ₂₀ H ₂₆ O ₇	378.42	7	3	1.97	113.29	H	N	N	N	N	N	N	N	0	0	0	0	0	0.55
C112	C ₁₅ H ₂₀ O ₄	264.32	4	2	1.97	74.6	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.85
C113	C ₁₅ H ₂₂ O ₄	266.33	4	3	2.59	77.76	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.56
C114	C ₁₄ H ₂₂ O ₄	254.32	4	3	2.19	77.76	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C115	C ₂₃ H ₂₂ O ₁₁	474.41	11	5	2.31	176.12	L	N	Y	N	N	N	N	N	1	0	1	1	2	0.55
C116	C ₁₄ H ₂₄ O ₄	256.34	4	2	2.66	66.76	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.55
C117	C ₁₁ H ₁₆ O ₂	180.24	2	2	2.04	40.46	H	Y	N	Y	N	N	Y	N	0	0	0	0	1	0.55
C118	C ₁₇ H ₂₂ O ₂	258.36	2	0	4.10	29.6	H	Y	N	N	Y	Y	N	N	0	0	0	0	0	0.55
C119	C ₁₃ H ₁₂ O ₉	312.23	9	5	0.55	161.59	L	N	N	N	N	N	N	N	0	1	1	1	1	0.11
C120	C ₂₈ H ₃₀ O ₁₆	622.50	4	3	2.59	77.76	H	Y	N	N	N	N	N	N	1	0	0	0	0	0.56
C121	C ₁₇ H ₂₈ O ₇	344.40	7	2	2.59	102.29	H	N	Y	N	N	N	N	N	0	0	0	0	0	0.55
C122	C ₂₈ H ₃₀ O ₁₄	590.53	14	7	1.76	225.81	L	N	Y	N	N	N	N	N	3	3	1	1	3	0.17
C123	C ₁₅ H ₂₂ O ₄	266.33	4	2	2.19	66.76	H	Y	Y	N	N	N	N	N	0	0	0	0	0	0.55
C124	C ₁₅ H ₂₄ O ₄	268.35	4	3	2.87	77.76	H	N	N	N	N	N	N	N	0	0	0	0	0	0.56
C125	C ₁₄ H ₂₂ O ₄	254.32	4	1	2.59	55.76	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.55
C126	C ₁₀ H ₁₆ O ₃	184.23	3	2	1.65	57.53	H	Y	N	N	N	N	N	N	0	0	0	0	1	0.85
C127	C ₁₀ H ₁₈ O ₄	202.25	4	2	1.77	74.6	H	Y	N	N	N	N	N	N	0	0	0	0	0	0.85
C128	C ₁₃ H ₁₂ O ₆	264.23	6	3	1.70	100.13	H	N	N	N	N	N	N	N	1	0	0	0	0	0.55

C#-Compound number, MW-Molecular weight, HA-Hydrogen acceptor number, HD-Hydrogen donor number, TPAS-Topological Polar Surface Area, iLOGP-octanol/ water partition coefficient, GIA-Gastrointestinal absorption, BBP-Blood-brain barrier permeant, PS-Phosphoglycoprotein substrate, I-Inhibitor, Y-Yes, N-No, L-Low, H-High, LV-Lipinski's violations number, GV-Ghose violations number, VV-Veber violations number, EV-Egan violations number, MV-Muegge violations number, BS-Bioavailability Score

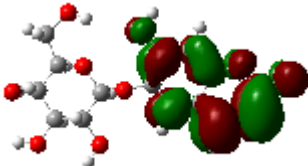
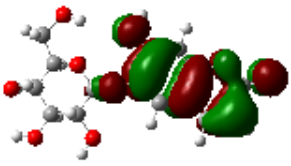
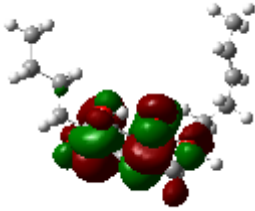
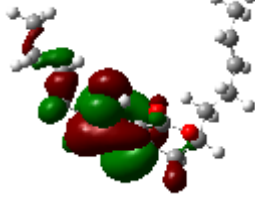
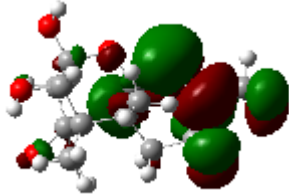
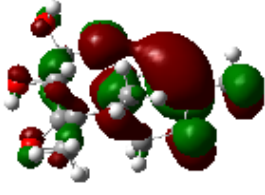
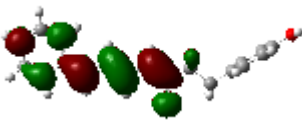
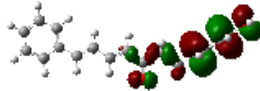
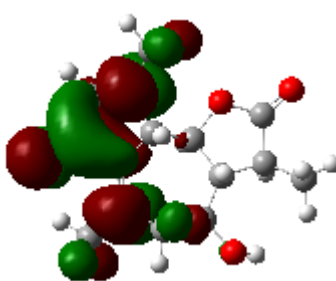
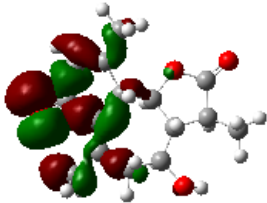
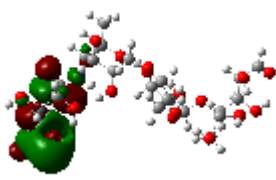
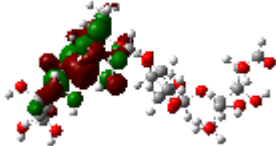
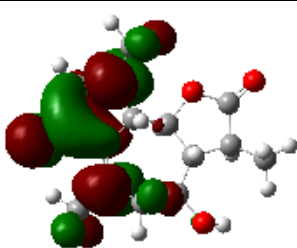
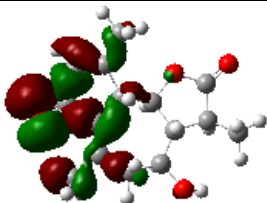
Table S4: Molecular docking analysis of corn silk metabolites against enzyme targets

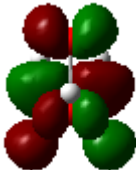
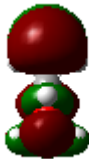
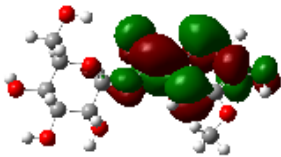
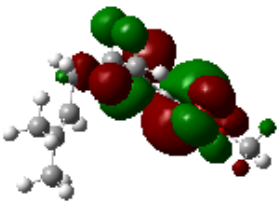
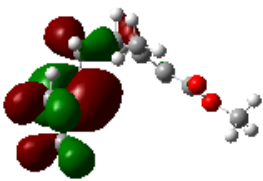
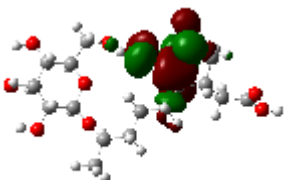
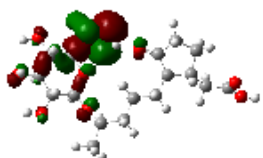
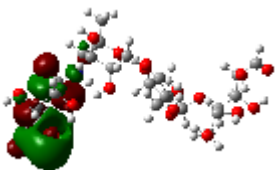
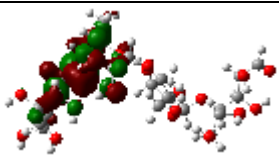
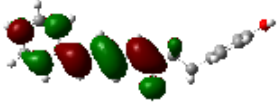
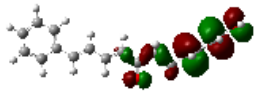
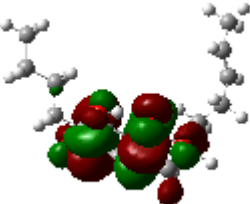
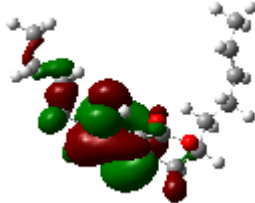
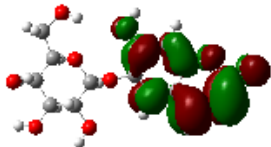
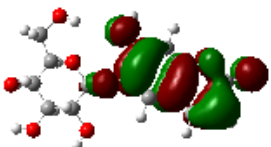
Compound number	Identity	AA	AG	AR	DPP-4	PTP1B	SDH
2	Estriol-16-Glucuronide	-6.8	-6.7	-7.2	-6.2	-4.8	-7.5
3	Ascorbic acid	-6.1	-5.6	-6.8	-7.2	-4.5	-6.3
4	Methylisocitric acid	-6.9	-5.8	-7.8	-6.8	-5.2	-7.1
5	Citraconic acid	-5.7	-7.2	-5.6	-6.4	-4.9	-5.9
6	Oxalosuccinic acid	-6.2	-6.3	-7.1	-6.7	-4.7	-6.8
8	Mevalonic acid	-7.2	-5.4	-6.3	-7.4	-4.4	-7.3
9	D-2-Hydroxyglutaric acid	-5.8	-6.1	-7.5	-6.1	-4.8	-5.7
10	(2R,3S)-2,3-dimethylmalic acid	-6.5	-7.1	-6.9	-5.7	-4.5	-6.1
11	UNPD109129	-6.7	-6.9	-7.3	-6.9	-4.6	-6.9
12	Glutaric acid	-6.3	-7.7	-6	-6	-4.9	-6.5
13	Cinnamic acid	-5.3	-5.3	-5.4	-7	-4.7	-7.7
14	(6E)-1-(4-hydroxyphenyl)-7-phenylhepta-4,6-dien-3-one	-7.8	-7.0	-9.9	-5.8	-4.4	-7
15	Vanillic acid	-5.6	-6.2	-8	-6.3	-4.8	-5.4
16	1-O-vanilloyl-beta-D-glucose	-6.4	-7.5	-5.8	-5.9	-4.5	-6.2
18	Saccharumside C	-6.0	-7	-6.5	-7.3	-4.6	-8
19	7-hydroxy-4-{3-oxo-3H-benzo[f]chromen-2-yl}-2H-chromen-2-one	-6.9	-5.9	-7.4	-6.6	-4.9	-7.8
20	Sarmentose	-7.1	-6.6	-6.2	-6.5	-4.7	-6.6
21	CNP0447999	-5.9	-6.4	-7	-5.6	-4.4	-5.2
22	1-O-Caffeoylglucose	-6.8	-5.7	-5.2	-7.5	-4.8	-6.4
23	1-O-Galloylglycerol	-6.2	-7.3	-7.9	-5.3	-4.5	-7.4
24	C00051555	-5.4	-6.8	-6.6	-7.1	-4.6	-6.7
25	3-Isopropylmalate	-6.7	-5.2	-7.7	-7.6	-4.9	-5.5
26	Diaportinic acid	-6.5	-6.7	-5.9	-6.2	-4.7	-7.2
27	Benzyl beta-D-glucopyranoside;(-)-Benzyl-O-beta-D-glucopyranoside	-5.7	-5.6	-6.1	-6.8	-4.4	-6
28	Domesticoside	-6.3	-6.1	-8.1	-6.4	-4.8	-7.9
29	Dihydrophaseic acid 4'-O-beta-D-glucopyranoside	-5.5	-7.4	-5.3	-7.4	-4.5	-6.3
30	Ketoleucine	-6.0	-6.3	-7.6	-6.7	-4.6	-5.9
31	Aesculin	-8.1	-5.4	-8.5	-5.7	-4.9	-7
32	Chlorogenic acid	-5.2	-6.9	-7.2	-7.2	-4.7	-6.8
33	Quinic acid	-6.4	-6	-5.7	-6.1	-4.4	-5.6
34	Cudraphenone A	-5.6	-5.3	-6.3	-5.9	-4.8	-8.1
35	Pimelic acid	-6.1	-6.5	-8.2	-6.9	-4.5	-6.5
36	(-)-6-((2S,3R,4R,5S,6R)-3,4-dihydroxy-6-(hydroxymethyl)-5-methoxytetrahydro-2H-pyran-2-yloxy)-8-hydroxy-3-methyl-1H-isochromen-1-one	-7.0	-5.8	-5.5	-6	-4.6	-7.3
37	(-)-11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucoside	-6.6	-7.4	-8.5	-8.6	-4.9	-8.4
38	Caffeic acid	-5.8	-6.2	-6.8	-5.8	-4.7	-5.8

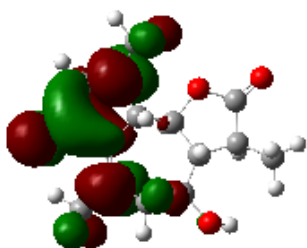
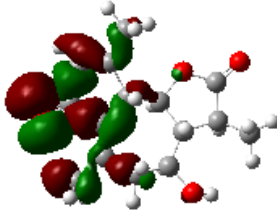
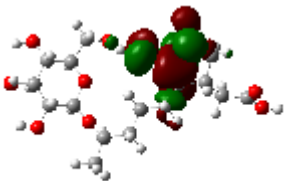
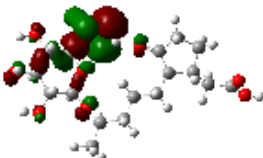
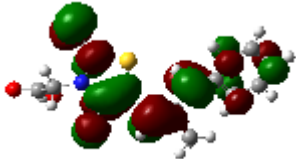
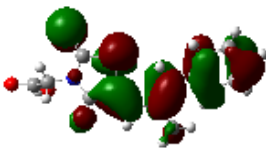
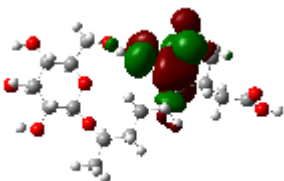
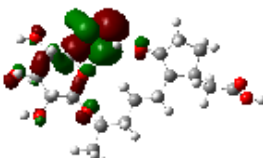
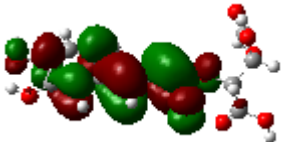
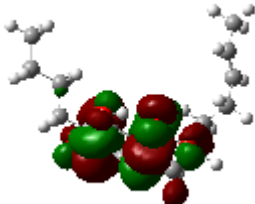
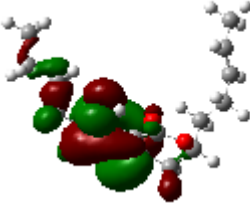
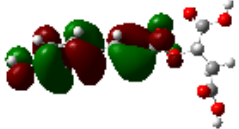
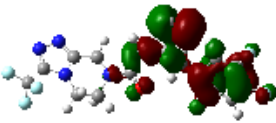
39	5-Carboxyvanillic acid	-6.9	-5.5	-5	-6.3	-4.4	-7.6
40	Phellodendric acid A;(+) -Phellodendric acid A	-5.3	-7.1	-7	-7.3	-4.8	-6.1
41	(-) -Epigallocatechin	-6.2	-6.6	-6.6	-6.6	-4.5	-7.7
42	D-Leucic acid	-6.8	-5.7	-8.3	-6.5	-4.6	-6.4
43	cis-Aconitic acid	-5.4	-6.4	-5.2	-5.6	-4.9	-5.2
44	MINEs-320976	-6.5	-6.8	-6.9	-7.5	-4.7	-6.9
45	Loganic acid	-6.7	-5.9	-7.1	-5.3	-4.4	-6.6
47	Quing hau sau; quinghaosu; artemisinin	-5.9	-7	-5.4	-7.1	-4.8	-8.2
48	3-Hydroxy-4-butanolide	-6.3	-6.1	-6.5	-7.6	-4.5	-5.4
49	Annularin A;(+) -Annularin A	-7.2	-5.2	-7.4	-6.2	-4.6	-7.1
50	Traumatic acid	-5.7	-6.7	-6.2	-6.8	-4.9	-5.7
51	Methyl geranate	-6.4	-7.4	-7.8	-6.4	-4.7	-6.3
52	3-Hydroxytetradecanedioic acid	-5.5	-6.3	-5.6	-7.4	-4.4	-8
53	Dihydrophaseic acid	-6.0	-7.4	-7.5	-6.7	-4.8	-7.8
54	Tuberonic acid	-6.6	-5.4	-6	-5.7	-4.5	-6
55	Daldiniapyrone	-7.1	-6.5	-6.3	-7.2	-4.6	-5.6
56	4-Hydroxycinnamic acid	-5.2	-6	-8	-6.1	-4.9	-6.8
57	Monascusone A	-6.9	-5.3	-5.8	-5.9	-4.7	-7.5
58	Acetovanillone; Apocynin	-5.3	-7.3	-6.7	-6.9	-4.4	-6.2
60	Quercitrin	-6.1	-6.2	-7.2	-6	-4.8	-7.4
61	2-Hydroxydecanedioic acid	-6.8	-5.5	-5.9	-7	-5.4	-5.5
62	UNPD221406	-5.4	-6.9	-7.9	-5.8	-4.6	-7.2
63	Cichorioside M;(+) -Cichorioside M	-6.2	-6.4	-6.4	-6.3	-4.9	-6.7
64	Austriecin; 8-Deacetylmatricarin; Desacetylmatricarin	-7.7	-7.8	-8.5	-7.3	-4.7	-5.9
65	trans-Ferulic acid	-6.7	-7.2	-5.3	-6.6	-4.4	-6.4
66	UNPD19396	-6.5	-6.8	-8.1	-6.5	-4.8	-8.1
67	UNPD77208	-5.7	-5.2	-6.1	-5.6	-4.5	-6.6
68	Nepetaside	-6.3	-6.7	-7.6	-7.5	-4.6	-5.2
69	Dodecanedioic acid	-7.0	-5.6	-5.5	-5.3	-5.2	-7.9
72	Erythronolide B	-5.9	-6.1	-6.2	-7.1	-4.7	-9.2
73	UNPD230015	-6.0	-7.4	-8.2	-7.6	-4.4	-7
74	3-Hydroxysebacic acid	-6.4	-6.3	-5.7	-6.2	-4.8	-5.8
76	Esculetin	-7.2	-5.4	-7.3	-6.8	-4.5	-7.3
77	ethyl 5-[(2,5-dimethylphenyl)methoxy]-2-phenyl-1-benzofuran-3-carboxylate	-6.6	-6.9	-6.8	-6.4	-4.6	-6.1
78	xi-2,2,6-Trimethyl-1,4-cyclohexanedione	-5.5	-6	-5	-7.4	-4.9	-7.7
79	Quercetin 3-(2'',3'',4''-triacylgalactoside)	-6.8	-5.3	-7	-6.7	-4.7	-6.5
80	[4]-Gingerol	-5.8	-6.5	-6.6	-5.7	-4.4	-5.4
81	Phaseic acid	-6.1	-5.8	-8.3	-7.8	-6	-6.2
82	Diaportinol	-7.1	-7.1	-5.2	-6.1	-4.5	-8.2
84	12-deoxyerythronolide A	-5.3	-6.2	-6.9	-5.9	-4.6	-7.1
87	Phaseolic acid	-6.9	-5.5	-7.1	-6.9	-4.9	-5.7
88	Curvularol	-7.9	-7	-5.4	-6	-4.7	-6.9

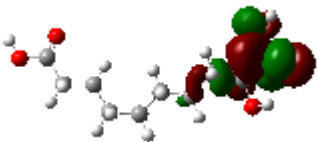
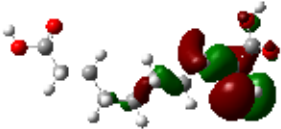
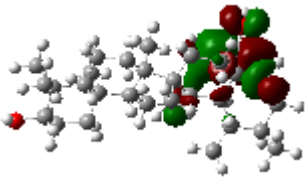
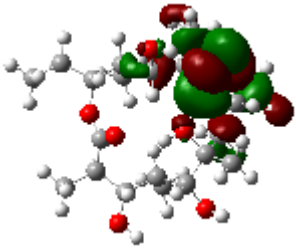
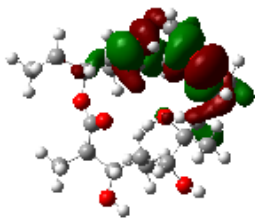
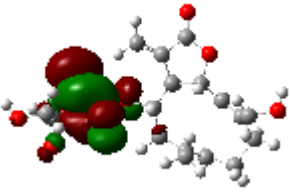
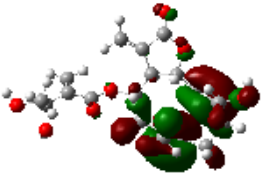
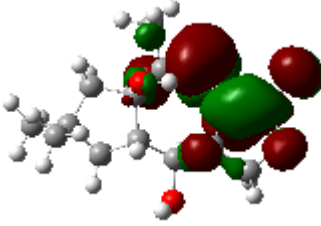
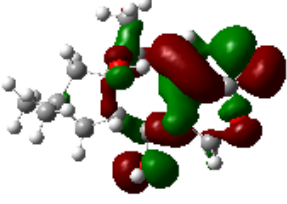
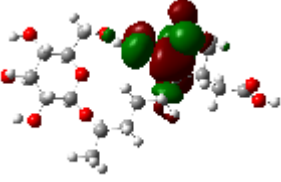
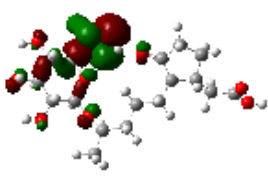
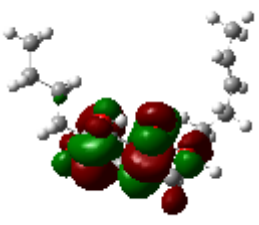
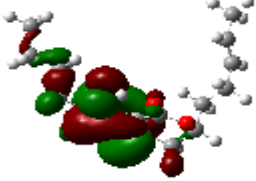
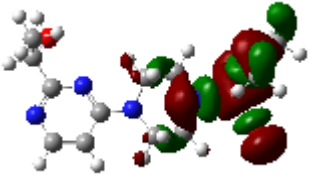
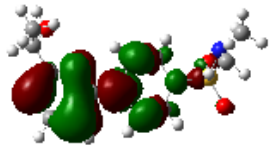
89	(+)-(S)-Carvone	-5.4	-6.6	-6.5	-7	-4.4	-6
91	Azelaic acid	-6.7	-5.7	-7.4	-5.8	-4.8	-7.8
93	Stagonolide F;(-)-Stagonolide F	-6.5	-6.4	-6.2	-6.3	-4.5	-6.4
95	UNPD223815	-5.7	-6.8	-7.8	-7.3	-4.6	-5.6
96	9-hydroxynonanoic acid	-6.3	-5.9	-5.6	-6.6	-4.9	-7.5
98	5,7,4'-Trihydroxy-3'-methoxyflavone	-6.0	-7.2	-7.5	-6.5	-4.7	-6.2
100	Blennin D	-7.3	-6.1	-6	-5.6	-4.4	-8.5
101	10-Deoxygeniposidic acid	-5.6	-5.2	-6.3	-7.5	-4.8	-5.5
102	Gallicynoic acid F;(-)-Gallicynoic acid F	-6.4	-6.7	-8	-5.3	-4.5	-7.2
103	Pandangolide 1a;(-)-Pandangolide 1a	-6.6	-5.6	-5.8	-7.1	-4.6	-6.7
104	4-Hydroxynonenal	-5.9	-6.3	-6.7	-7.6	-4.9	-5.9
105	Tetradecanedioic acid	-6.8	-7.4	-7.2	-6.2	-5.8	-6.3
106	(R)-7-butyl-6,8-dihydroxy-3-[(3E)-pent-3-en-1-yl]-3,4-dihydroisochromen-1-one	-8.0	-5.4	-8.6	-7.8	-4.4	-8.3
107	Genistin	-5.5	-6.5	-7.9	-6.4	-4.8	-7.6
108	p-Coumaroyl malic acid	-6.2	-6	-6.4	-7.7	-4.5	-6.1
110	Cyperine	-5.8	-5.3	-7.7	-6.7	-4.6	-7.9
111	(+)-Cnicin; Cnicin	-6.1	-7.3	-5.3	-5.7	-4.9	-8.7
112	(S)-Absciscic acid	-6.9	-6.2	-8.1	-7.2	-4.7	-5.2
113	Sydnic acid; Sydonic acid	-5.3	-5.5	-6.1	-6.1	-4.4	-7.3
114	Gallicynoic acid A;(+)Gallicynoic acid A	-6.7	-6.9	-7.6	-5.9	-4.8	-6.8
115	Apigenin 7-O-(6"-O-acetylglucoside)	-6.5	-6.4	-5.5	-6.9	-4.5	-5.4
116	UNPD127537	-5.7	-5.7	-6.2	-6	-4.6	-6.5
117	Olivetol	-6.3	-7.2	-8.2	-7	-4.9	-7
118	Ginsenoyn E	-6.0	-6.8	-5.7	-5.8	-4.7	-5.8
119	Caffeoyl tartaric acid	-7.2	-5.2	-7.3	-8	-4.4	-7.1
120	Luteolin 3'-methyl ether 7-glucuronide	-5.6	-6.7	-6.8	-7.3	-4.8	-6.2
121	UNPD205010	-6.4	-5.6	-5	-6.6	-4.5	-8.1
123	Artemin	-6.8	-6.1	-7	-6.5	-4.6	-6.4
124	Gallicynoic acid B	-5.9	-7.4	-6.6	-5.6	-4.9	-5.6
125	Aspergillide A	-6.6	-6.3	-8.3	-7.5	-4.7	-7.7
126	(S)-Oleuropeic acid	-7.1	-5.4	-5.2	-5.3	-4.4	-6.3
127	Sebacic acid	-5.2	-6.9	-6.9	-7.1	-4.8	-5.9
128	7-Acetoxy-5,6-dimethoxycoumarin	-6.1	-6	-7.1	-7.6	-4.5	-6

Table S5: Frontier molecular orbitals of the top-ranked compounds against enzymes implicated in T2DM

Compound	LUMO	HOMO	Energy gap (eV)
AA			
Aesculin			4.35
(R)-7-butyl-6,8-dihydroxy-3-[(3e)-pent-3-en-1-yl]-3,4-dihydroisochromen-1-one			4.86
Curvularol			6.01
(4E,6E)-1-(4-hydroxyphenyl)-7-phenylhepta-4,6-dien-3-one			3.61
Austricin			4.70
Acarbose			5.22
AG			
Austricin			4.70

Glutaric acid			7.29
1-O-vanilloyl-beta-D-glucose			4.71
Methyl geranate			5.24
(-)-11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucoside			5.29
Acarbose			5.22
AR			
(4E,6E)-1-(4-hydroxyphenyl)-7-phenylhepta-4,6-dien-3-one			3.61
(R)-7-butyl-6,8-dihydroxy-3-[(3E)-pent-3-en-1-yl]-3,4-dihydroisochromen-1-one			4.86
Aesculin			4.35

Austricin			4.70
(-)-11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucoside			5.29
Epalrestat			3.21
DPP-4			
(-)-11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucoside			5.29
caffeoyl tartaric acid			4.06
(R)-7-butyl-6,8-dihydroxy-3-[(3E)-pent-3-en-1-yl]-3,4-dihydroisochromen-1-one			4.86
p-coumaroyl malic acid			4.26
sitagliptin			5.30
PTP1B			

2-hydroxydecanedioic acid			6.66
Ursolic acid			5.85
SDH			
Erythronolide B			5.85
Cnicin			4.46
(+)-blennin D			5.72
(-)-11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucoside			5.29
(R)-7-butyl-6,8-dihydroxy-3-[(3E)-pent-3-en-1-yl]-3,4-dihydroisochromen-1-one			4.86
4-[2-(1R-hydroxy-ethyl)-pyrimidin-4-yl]piperazine-1-sulfonic acid dimethylamide			4.39

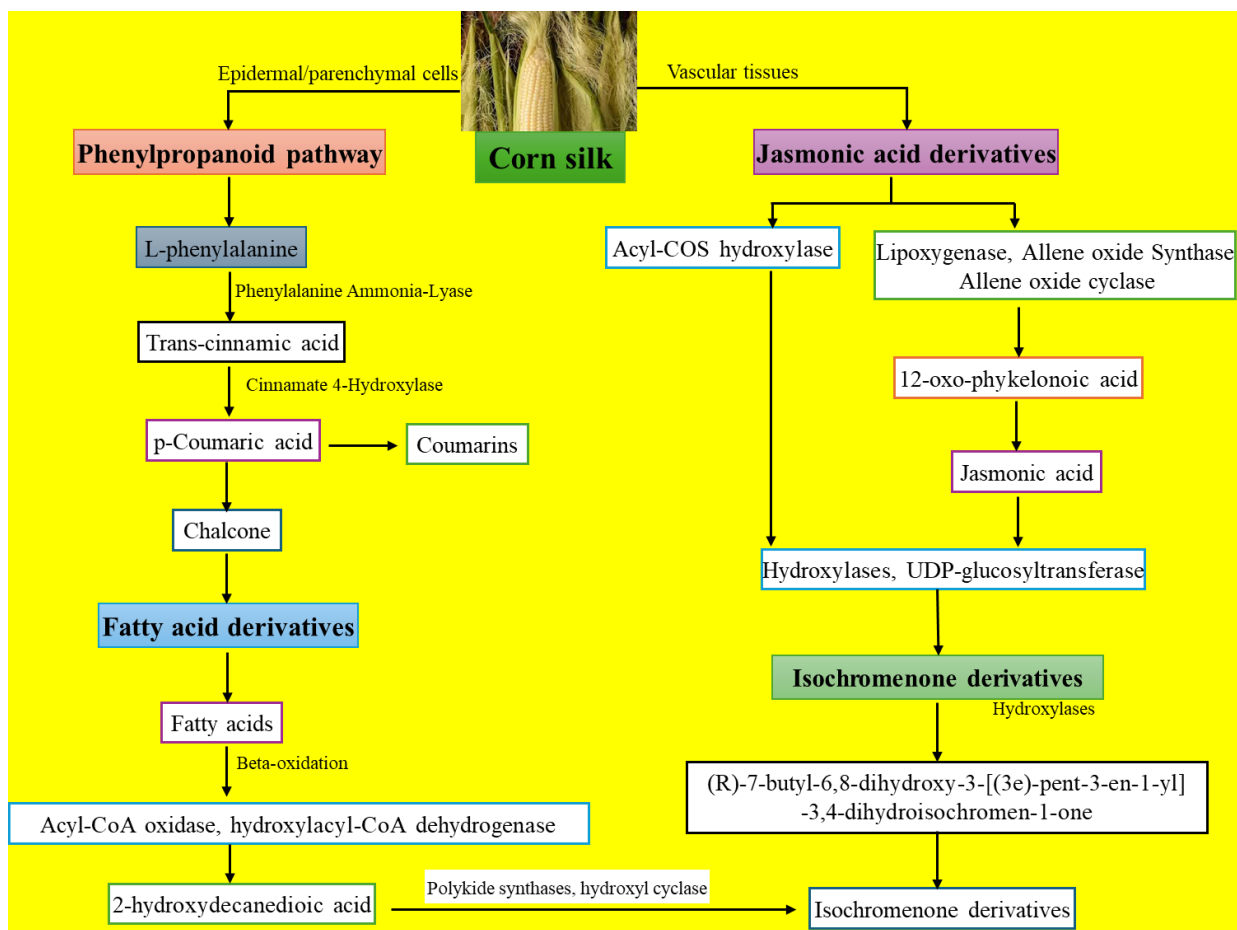


Figure S8: Proposed biosynthetic pathway of some metabolites identified in corn silk