Hyphenated Mass Spectrometry Methods for Enlarged Capacity Data Storage Systems based on Chemical Mixtures

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Table S1. Storage capacity per mixture (bits), defined as $C = \log_2 L$,[1] (C = capacity, M library size and L is the discrete concentration levels distinguishable for each species) for the most commonly used encoding / decoding methods.

Encoding / decoding analytical tool[a]	Storage capacity per mixture (bits); $C = M \log_2 L$	Ref.
LDI-MS	30-40	[2,3]
SAMDI-MS	30-40	[4]
DESI-MS	20	[5]
GC-FID	24	[6]
fluorescence	7	[7]
Raman	24[b]	[8]
NMR	8	[6]
NMR	70[c]	[9]
NMR	16	[10]
Cascade enzymatic reaction	5	[11]
FIA-MS	10^2	This work
LC-MS	10^3-10^4	This work

[a] Abbreviations LDI-MS, Laser Desorption Ionization MS; SAMDI-MS, Self-Assembled Monolayer Desorption and Ionization MS; GC-FID, Gas Chromatography Flame Ionization Detector; NMR, Nuclear Magnetic Resonance; FIA-MS, Flow Injection Analysis; LC-MS, Liquid Chromatography MS; [b] 8 (M) compounds at 8 (L) concentration levels; [c] 22 (M) compounds at 10 (L) concentration levels.

Materials and methods

SI_1.1. Chemicals

All flavonoids were purchased from TargetMol. Plant hormones as well as dicarboxylic acids were purchased from Sigma Aldrich. Deuterated plant hormones were prepared following literature procedures.[12] Formic acid, acetonitrile and methanol were all LC/MS grade and purchased from Scharlab. Deionized water was obtained from a Milli-Q system from Millipore (Bedford, MA, USA). A list of the 200 metabolites (full names, molecular formula, compound class as well as the monoisotopic m/z value of each [M – H]- ion) is provided in Table S2.

Table S2. List of the 200 metabolites (full names, molecular formula, compound class as well as the monoisotopic m/z value of each [M – H]- ion)

	compound	formula	[M-H]- ion	compound type
1	1-Aminocyclopropanecarboxylic acid	C4H7NO2	100,0399	***R-CO2H***
2	malonic acid	C3H3O4	101,9953	***R-CO2H***
3	serine	C3H7NO3	104,0348	***R-CO2H***
4	fumaric acid	C4H4O4	115,0031	***R-CO2H***
5	maleic acid	C4O4H4	115,0031	***R-CO2H***
6	succinic acid	C6H4O6	117,0188	***R-CO2H***
7	cysteine	C3H7NO2S	120,0119	***R-CO2H***
8	taurine	C2H7NO3S	124,0068	***R-CO2H***
9	2-pyrrolidone-5-carboxylic acid	C5H7NO3	128,0348	***R-CO2H***
10	pipecolic acid	C6H11NO2	128,0712	***R-CO2H***
11	aminolevulinic acid	C5H9NO3	130,0504	***R-CO2H***
12	aspartic acid	C4H7NO4	132,0297	***R-CO2H***
13	malic acid	C4H6O5	133,137	***R-CO2H***
14	homocysteine	C4H9NO2S	134,0276	***R-CO2H***
15	phenylalanine	C9H11NO2	134,0712	***R-CO2H***
16	4-aminobenzoic acid	C7H7NO2	136,0399	***R-CO2H***
17	ketoglutaric acid	C5H6O5	145,01	***R-CO2H***
18	adipic acid	C6H10O4	145,0501	***R-CO2H***
19	glutamic acid	C5H9NO4	146,0453	***R-CO2H***
20	methionine	C5H11NO2S	148,0432	***R-CO2H***
21	tartaric acid	C4H6O6	149,0086	***R-CO2H***
22	salicylhydroxamic acid	C7H7NO3	152,0348	***R-CO2H***
23	orotic acid	C5H4N2O4	155,0093	***R-CO2H***
24	2-aminoadipic acid	C6H11NO4	160,061	***R-CO2H***
25	3-dehidroshikimic acid	C7H8O5	171,0372	***R-CO2H***
26	shikimic acid	C7H10O5	173,045	***R-CO2H***
27	N-acetyl-L-aspartic acid	C6H9NO5	174,0402	***R-CO2H***
28	hippuric acid	C9H9NO3	178,0504	***R-CO2H***
29	galacturonic acid	C6H10O7	193,034	***R-CO2H***
30	gluconic acid	C6H12O7	195,0505	***R-CO2H***

31	Indole-3-butyric acid	C12H13NO2	202,0868	***R-CO2H***
32	Indole-3-pyruvic acid	C11H9NO3	202,0504	***R-CO2H***
33	dihydrojasmonic acid	C12H20O3	223,0606	***R-CO2H***
34	traumatic acid	C12H20O4	227,1283	***R-CO2H***
35	stearidonic acid	C18H28O2	275,2011	***R-CO2H***
36	linolenic acid	C18H30O2	277,2168	***R-CO2H***
37	linoleic acid	C18H32O2	279,2324	***R-CO2H***
38	sinapic acid	C11H12O5	223,0606	***R-CO2H***
39	gibbellerin A7	C19H22O5	329,1389	***R-CO2H***
40	gibellerin A4	C19H24O5	331,1545	***R-CO2H***
41	gibberellic acid	C19H22O6	345,1338	***R-CO2H***
42	folic acid	C19H19N7O6	440,1319	***R-PO3H***
43	adenosine-monophosphate (AMP)	C10H14N5O7P	346,0553	***R-PO3H***
44	adenosine-diphosphate (ADP)	C10H15N5O10P2	426,0216	***R-PO3H***
45	adenosine-triphosphate (ATP)	C10H16N5O13P3	505,9879	***R-PO3H***
46	nicotinamide adenine dinucleotide (NADH)	C21H28N7O14P2	663,1091	***R-PO3H***
47	flavin adenine dinucleotide (FAD)	C27H33N9O15P2	784,1493	***plant hormones***
48	salicylic acid	C7H6O3	137,0240	***plant hormones***
49	salicylic acid-d5	C7HD5O3	142,0547	***plant hormones***
50	cinnamic acid	C9H7O2	147,0450	***plant hormones***
51	indole acetic acid	C10H9NO2	174,0550	***plant hormones***
52	caffeic Acid	C9H8O4	179,0344	***plant hormones***
53	ferulic Acid	C10H10O4	193,0500	***plant hormones***
54	jasmonic Acid	C12H18O3	209,1178	***plant hormones***
55	abscisic Acid	C15H20O4	263,1280	***plant hormones***
56	abscisic acid-d6	C15H14O4D6	269,1654	***plant hormones***
57	12-oxo-phytodienoic acid (OPDA)	C18H28O3	291,196	***plant hormones***
58	glucosyl salicylate	C13H16O8	299,0767	***plant hormones***
59	salicylic glucosyl ester	C13H16O8	299,0767	***plant hormones***
60	jasmonate-isoleucine	C18H29NO4	322,2018	***plant hormones***
61	chlorogenic acid	C16H18O9	353,087	***plant hormones***
62	abscisic acid D-glucopyranosyl ester	C21H30O9	425,181	***flavonoids***
63	vanilin	C8H8O3	151,0395	***flavonoids***
64	5,7-dihydroxychromone	C9H6O4	177,0188	***flavonoids***
65	scopoletin	C10H8O4	191,0344	***flavonoids***
66	4-hydroxychalcone	C15H12O2	223,0759	***flavonoids***
67	3-hydroxyflavone	C15H10O3	237,0552	***flavonoids***
68	6-hydroxyflavone	C15H10O3	237,0552	***flavonoids***
69	chrysin	C15H10O4	253,0501	***flavonoids***
70	7,8-dihydroxyflavone	C15H10O4	253,0501	***flavonoids***
71	daidzein	C15H10O4	253,0501	***flavonoids***
72	liquiritigenin	C15H12O4	255,0657	***flavonoids***
73	pinocembrin	C15H12O4	255,0657	***flavonoids***
74	formononetin	C16H12O4	267,0657	***flavonoids***
75	Tectochrysin	C16H12O4	267,0657	***flavonoids***

76	galangin	C15H10O5	269,045	***flavonoids***
77	genistein	C15H10O5	269,045	***flavonoids***
78	baicalein	C15H10O5	269,045	***flavonoids***
79	Apigenin	C15H10O5	269,045	***flavonoids***
80	alpinetin	C16H14O4	269,0814	***flavonoids***
81	naringenin	C15H12O5	271,0606	***flavonoids***
82	4',7-dimethoxyisoflavone	C17H14O4	281,0814	***flavonoids***
83	5,7-dimethoxiflavone	C17H14O4	281,0814	***flavonoids***
84	biochanin A	C16H12O5	283,0606	***flavonoids***
85	calycosin	C16H12O5	283,0606	***flavonoids***
86	oroxylin A	C16H12O5	283,0606	***flavonoids***
87	genkwanin	C16H12O5	283,0606	***flavonoids***
88	galangin-3-methylether	C16H12O5	284,0685	***flavonoids***
89	kaempferol	C15H10O6	285,0399	***flavonoids***
90	scutellarein	C15H10O6	285,0399	***flavonoids***
91	Isosakuranetin	C16H14O5	285,0763	***flavonoids***
92	brazilin	C16H14O5	285,0763	***flavonoids***
93	eriodictyol	C15H12O6	287,0556	***flavonoids***
94	epicatechin	C15H14O6	289,0712	***flavonoids***
95	5-hydroxy-7,8-dimethoxyflavone	C17H14O5	297,0763	***flavonoids***
96	mosloflavone	C17H14O5	297,0763	***flavonoids***
97	tectorigenin	C16H12O6	299,0556	***flavonoids***
98	diosmetin	C16H12O6	299,0556	***flavonoids***
99	farrerol	C17H16O5	299,0919	***flavonoids***
100	quercetin	C15H10O7	301,0348	***flavonoids***
101	tricetin	C15H10O7	301,0348	***flavonoids***
102	herbacetin	C15H10O7	301,0712	***flavonoids***
103	hesperetin	C16H14O6	301,0712	***flavonoids***
104	taxifolin	C15H12O7	303,0505	***flavonoids***
105	capsaicin	C18H27NO3	304,1913	***flavonoids***
106	(+)-gallocatechin	C15H14O7	305,0661	***flavonoids***
107	cimifugin	C16H18O6	305,1025	***flavonoids***
108	Isorhamnetin	C16H12O7	315,0505	***flavonoids***
109	myricetin	C15H10O8	317,0297	***flavonoids***
110	ampelopsin	C15H12O8	319,0454	***flavonoids***
111	dihydromyricetin	C15H12O8	319,0454	***flavonoids***
112	neobavaisoflavone	C20H18O4	321,1127	***flavonoids***
113	glabridin	C20H20O4	323,1283	***flavonoids***
114	bavachin	C20H20O5	323,1283	***flavonoids***
115	isobavachin	C20H20O4	323,1283	***flavonoids***
116	jaceosidin	C17H14O7	329,0661	***flavonoids***
117	bavachinin	C21H22O4	337,144	***flavonoids***
118	eupatilin	C18H16O7	343,0818	***flavonoids***
119	lysionotin	C18H16O7	343,0818	***flavonoids***
120	isoxanthohumol	C21H22O5	353,1389	***flavonoids***

121	irigenin	C18H16O8	359,0767	***flavonoids***
122	Icaritin	C21H20O6	367,1182	***flavonoids***
123	isosinensetin	C20H20O7	371,1131	***flavonoids***
124	tangeretin	C20H20O7	371,1131	***flavonoids***
125	Vitexicarpin	C19H18O8	373,0923	***flavonoids***
126	chrysosptertin B	C19H18O8	373,0923	***flavonoids***
127	briboflavin	C17H20N4O6	375,01305	***flavonoids***
128	Irisflorentin	C20H18O8	385,0923	***flavonoids***
129	medroxyprogesterone acetate	C24H34O4	385,2379	***flavonoids***
130	5-demethylnobiletin	C20H20O8	387,108	***flavonoids***
131	corylifol A	C25H26O4	389,1753	***flavonoids***
132	morusin	C25H24O6	419,1495	***flavonoids***
133	ononin	C22H22O9	429,1186	***flavonoids***
134	isovitexin	C21H20O10	431,0978	***flavonoids***
135	oroxin A	C21H20O10	431,0978	***flavonoids***
136	vitexin	C21H20O10	431,0978	***flavonoids***
137	Avicularin	C20H18O11	433,0771	***flavonoids***
138	guaijaverin	C20H18O11	433,0771	***flavonoids***
139	engeletin	C21H22O10	433,1135	***flavonoids***
140	casanthranol	C21H22O10	433,1135	***flavonoids***
141	Sec-O-Glucosylhamaudol	C21H26O10	437,1448	***flavonoids***
142	(-)-epicatechin gallate	C22H18O10	441,0822	***flavonoids***
143	apigenin-7-glucuronide	C21H18O11	445,0771	***flavonoids***
144	baicalin	C21H18O11	445,0771	***flavonoids***
145	calycosin-7-O-beta-D-glucoside	C22H22O10	445,1135	***flavonoids***
146	Orientin	C21H20O11	447,0927	***flavonoids***
147	Isoorientin	C21H20O11	447,0927	***flavonoids***
148	astragalin	C21H20O11	447,0927	***flavonoids***
149	astilbin	C21H22O11	449,1084	***flavonoids***
150	gallocatechin gallate	C22H18O11	457,0771	***flavonoids***
151	Oroxylin A 7-O-beta-D-glucuronide	C22H20O11	459,0927	***flavonoids***
152	wogonoside	C22H20O11	459,0927	***flavonoids***
153	homoplantaginin	C22H22O11	461,1084	***flavonoids***
154	tectoridin	C22H22O11	461,1084	***flavonoids***
155	Diosmetin-7-O-beta-D-glucopyranoside	C22H22O11	461,1084	***flavonoids***
156	Luteolin-7-glucuronide	C21H18O12	461,072	***flavonoids***
157	isoquercitrin	C21H20O12	463,0877	***flavonoids***
158	7,2'-dihydroxy-3',4'-dimethoxyisoflavane-7-O-glucoside	C23H28O10	463,1604	***flavonoids***
159	plantagoside	C21H22O12	465,1033	***flavonoids***
160	nepitrin	C22H22O12	477,1033	***flavonoids***
161	silibin	C25H22O10	481,1135	***flavonoids***
162	sylimarin	C25H22O10	481,1135	***flavonoids***
163	baohuoside I	C27H30O10	513,1761	***flavonoids***
164	amentoflavone	C30H18O10	537,0822	***flavonoids***

165	mirificin	C26H28O13	547,1452	***flavonoids***
166	puerarin 6-O-xyloside	C26H28O13	547,1452	***flavonoids***
167	schaftoside	C26H28O14	563,1401	***flavonoids***
168	Procyanidin B2	C30H26O12	577,1346	***flavonoids***
169	kaempferitrin	C27H30O14	577,1557	***flavonoids***
170	rhoifolin	C27H30O14	577,1557	***flavonoids***
171	Vitexin-2''-O-rhamnoside	C27H30O14	577,1557	***flavonoids***
172	leucoside	C26H28O15	579,135	***flavonoids***
173	naringin	C27H32O14	579,1714	***flavonoids***
174	narirutin	C27H32O14	579,1714	***flavonoids***
175	linarin	C28H32O14	591,1714	***flavonoids***
176	Tiliroside	C30H26O13	593,1295	***flavonoids***
177	kaempferol 3-glucorhamnoside	C27H30O15	593,1506	***flavonoids***
178	Oroxin B	C27H30O15	593,1506	***flavonoids***
179	nicotiflorin	C27H30O15	593,1506	***flavonoids***
180	didymin	C28H34O14	593,187	***flavonoids***
181	eriocitrin	C27H32O15	595,1663	***flavonoids***
182	spinosin	C28H32O15	607,1663	***flavonoids***
183	rutin	C27H30O16	609,1456	***flavonoids***
184	glucosylvitexin	C27H30O16	609,1456	***flavonoids***
185	neohesperidin	C28H34O15	609,1819	***flavonoids***
186	neohesperidin dihydrochalcone	C28H36O15	611,1976	***flavonoids***
187	2-O-galloylhyperin	C28H24O16	615,0986	***flavonoids***
188	Isorhamnetin 3-O-neohesperidin	C28H32O16	623,1612	***flavonoids***
189	narcissoside	C28H32O16	623,1612	***flavonoids***
190	quercetin-3-O-sophoroside	C27H30O17	625,1405	***flavonoids***
191	Icariin	C33H40O15	675,2289	***flavonoids***
192	kuwanon G	C40H36O11	691,2179	***flavonoids***
193	theaflavin-3'-gallate	C36H28O16	715,1299	***flavonoids***
194	ligustroflavone	C33H40O18	723,2136	***flavonoids***
195	vaccarin	C32H38O19	725,1929	***flavonoids***
196	Troxerutin	C33H42O19	741,2242	***flavonoids***
197	typhaneoside	C34H42O20	769,2191	***flavonoids***
198	epimedin B	C38H48O19	807,2712	***flavonoids***
199	epimedin C	C39H50O19	821,2868	***flavonoids***
200	epimedin A	C39H50O20	837,2817	***flavonoids***

SI_1.2. Standard solutions

Stock solutions of flavonoids, plant hormones and carboxylic acids were prepared by dissolving them in methanol to afford stock solutions at concentrations of 500 μg/mL (ppm, parts-per-million). These solutions were stored refrigerated at -80 ºC and in the absence of moisture or antioxidants due to the well-known thermal instability of flavonoids.[13,14] We also avoid the presence of oxygen that may reduce the long term

stability of nucleotides and some of the carboxylic acids. Under these conditions, these 500 ppm solutions are stable for more than two years.

SI_1.2.1 Binary encoding: if a metabolite is meant to be included, we manually transfer a 5 μL aliquot from the stock solution (at 500 μg/mL) to the vial. If it is meant to be excluded, no transfer is performed. Each chemical mixture was prepared at 2.5 μg/mL (total volume 1 mL) and it was further brought to the concentration compatible (50-500 ng / mL) with FIA-MS and LC-MS methods by simple dilution. Such initial 2.5 ppm solutions were stored refrigerated and in the absence of moisture, antioxidants and the presence of oxygen. During the normal course of our experiments, such 2.5 ppm intermediate solutions were used satisfactorily over 9 months to prepare our encoding chemical mixtures in the 50-500 ng / mL (ppb) range.

SI_1.2.2. Quaternary and octal encoding: for this purpose, calibration curves were built covering two orders of magnitudes from 10 to 1250 ng/mL from successive dilution from the 500 μg/mL stock solution. Of the 25 encoding flavonoids. Hence, aliquots of the 25 flavonoids were combined into a single high-concentration standard mixture (1250 ppb), from which a series of dilution points were prepared (10 - 1250 ng/mL). For quaternary encoding, analyte concentrations (**quaternary code**) were 100 (**1**), 500 (**2**) and 1250 (**3**) (ng/ mL; ppb). For octal encoding, denser analyte concentrations (**octal code**) were used 50 (**1**), 125 (**2**), 250 (**3**), 500 (**4**), 750 (**5**), 1000 (**6**) and 1500 (**7**) (ng/ mL; ppb). These values can be user-customized depending on the relative ionization efficiencies of the analytes of interest as well as the inherent sensitivity of the hyphenated MS platform. As shown in the section *¨SI_1.6 Calibration details using quaternary and octal encoding schemes and ion suppression considerations¨* LC-MS analysis showed no significant ion suppression effect when quantifying a reduced set of 25 flavonoids. Decoding of data encoded in quaternary and octal formats was deemed satisfactory. However, while ion suppression was observed in FIA-MS analysis, the quaternary encoding scheme itself helped mitigate this issue by employing concentration values that were spaced half an order of magnitude apart (for example, codes 1 and 2 corresponded to 100 and 500 ppb, respectively).

SI_1.3. Flow injection analysis and Ultra high-performance liquid chromatography coupled to ESI-MS

A Waters Acquity I-Class UPLC system (Waters Corp., Milford, MA, USA) coupled to a Synapt HDMS mass spectrometer using an Electrospray Ionization (ESI) interface was used in both FIA-MS and LC-MS methods. The TOF was operated in the V resolution mode (resolution was ca. 25000 FWHM (*m/z* 554)) in the negative ionization mode. The ESI capillary voltage was 1.5 kV, using a cone voltage of 25 V. The source temperature was set to 120 °C, and the desolvation temperature at 650 °C. Nitrogen was used as the desolvation gas at 1200 L/h and cone gas at 250 L/h. Calibration was performed using the sodium formate solutions using the Waters Intelllistart routine according to the manufacturer's

recommendations. Leucine enkephalin (200 µg/L in water: acetonitrile 1:1 containing 0.01% formic acid) was used for continuous mass correction during all FIA or LC chromatographic runs. A full scan function was acquired in each injection in the range of *m/z* 50 - 1000 with a scan time of 0.2 s.

L*iquid chromatography coupled to Mass Spectrometry (LC-MS):* Chromatographic separations were performed at 40 °C on a reverse phase analytical column Acquity BEH C18 1.7 µm, 2.1×50 mm (Waters, Milford, MA). Ultra-performance liquid chromatography (UPLC) uses small-diameter particles (typically 1.7µm) in the stationary phase and short columns, which lead to narrower LC peaks (5-10 s wide) and improved chromatographic separations, with short analysis times. The mobile phase consisted of acetonitrile (B) and 0.1 % formic acid in water (A) delivered at a flow rate of 0.3 mL/min and changing as follows: 10% B at 0 min; 95% B at 0 minutes linearly increased until 8 minutes; then the system was set to its initial conditions in 0.1 min and was conditioned until 8.5 minutes before the next injection. *Flow Injection Analysis coupled to Mass Spectrometry (FIA-MS):* FIA-MS methods employ the same instrumental hardware to that described for LC-MS and simply use autosamplers and injectors to introduce samples into the mass spectrometer. The analyte peak shape in a FIA-MS is affected by the specific system configuration such as transfer tubing dimensions as well as injection volume and flow rate. Moreover, metabolite peaks must be defined by enough data points the for accurate quantitation, and this may not be achievable if the peak widths are too small.[15] Optimal parameters should balance analyte sensitivity while maintaining adequate peak width for data collection. The analysis was carried at a flow rate of 0.3 mL/min and 1 µL of the sample was injected into the system, transferred through a medium-size peek tube of 0.13 mm of diameter. Scan time acquisitions were 0.2 seconds. The total run time of the analysis was 35 seconds / injection and peak widths were *ca.* 5 seconds which gave satisfactory quali- and quantitation identification of our chemical mixtures. For Ion mobility experiments, the Synapt HDMS mass spectrometer was used. Nitrogen was used as the drift gas, with an IMS wave velocity of 1050 m/s and wave height of 30 V. For complementary experiments using a FIA-MS and LC-MS coupled to a low resolution ESI mass spectrometry (triple quadrupole), an Acquity liquid chromatography system (Waters Corp., Milford, MA, USA) interfaced to a triple quadrupole mass spectrometer Xevo TQS equipped with an orthogonal Z-Spray electrospray ionization interface (ESI) (Waters Corp, Manchester, UK) was used for sample analysis. The same FIA-MS method as well a as UPLC separation was performed using the same inlet methods and chromatographic column and maintained at 40 ◦C. The ESI capillary voltage was 1.5 kV, using a cone voltage of 25 V. The source temperature was set to 120 °C, and the desolvation temperature at 650 °C. Nitrogen was used as the desolvation gas at 1200 L/h and cone gas at 250 L/h. Calibration was performed using the sodium iodide solutions using the Waters Intelllistart routine according to the manufacturer's recommendations. A full scan function was acquired in each injection in the range of *m/z* 50-1000 with a scan time of 0.5 s.

SI_1.4. Data processing

Several data processing strategies were used for data visualization or retrieval of the encoded message: *Chrotool*: Chrotool is an application embedded in Masslynx 4.2 intended for automatic chromatogram display. In the present work, it was used to group of 8 metabolites (byte) according to the encoding scheme of each message where the extracted ion chromatograms (XICs´) of each byte can be visualized with a single "one-click" operation. *TargetLynx*: Target screening was performed by filtering data based on observed retention time, accurate-mass matching experimental data with the previously created empirical mass spectra library of the 200 metabolites. Data were processed using MassLynx 4.2 software and evaluated both quali- or quantitatively with the TargetLynx application (Waters Corp, Manchester, UK). A schematic workflow combining Targetlynx is shown in Figure S1. To read the information stored in the vials, different python scripts for automatic data processing were written. These scripts search for the peak areas of all of the metabolites used for encoding in the report output file exported from Targetlynx. If the particular m/z value is found with user-defined threshold area, it is designated by “1”, or if not, by “0” bit and all bites that are then concatenated and the ASCII code retrieved. Another python scripts were used for decoding messages encoded in quaternary or octal code, respectively where the threshold ranges for assigning the 0-3 or 0-7 values were also user-defined.

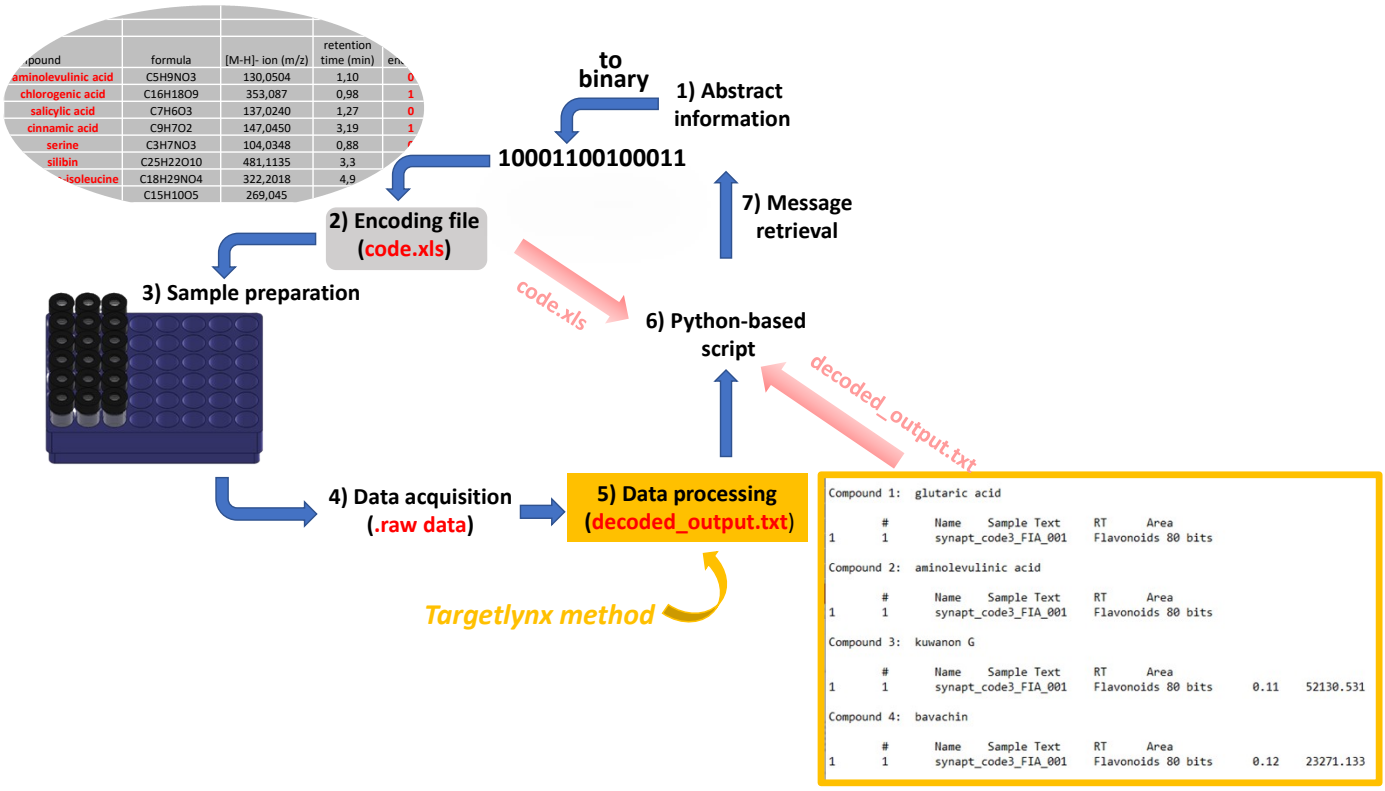

Figure S1. Schematic workflow for automatic data processing

1) **Encoding the Information:** The abstract information is first converted into a binary (or quaternary/octal) sequence.
2) **Creation of the Encoding File:** An Excel file (**code.xls**) is generated by selecting metabolites from a pre-established, home-built database comprising a 200-metabolite library. This file contains a structured list of metabolites representing the encoded message, where each analyte corresponds to a specific bit in a predefined order. The format of this file, shown as an inset, includes columns detailing compound names, molecular formulas, *m/z* values, and their assigned binary (0 or 1) codes.
3) **Sample Preparation:** Aliquots of the selected analytes are transferred to individual vials or multiple vials if spatial ordering is applied.
4) **Data Acquisition:** The samples are analysed using LC-MS or FIA-MS in full-scan mode, generating *raw* data files containing LC or FIA chromatograms.
5) **Data Processing:** The *raw* data files are processed using TargetLynx, where user-defined parameters can be adjusted to optimize integration, calibration, and quantification. TargetLynx produces an output file (**decoded_output.txt**), which contains qualitative information on the presence or absence of analytes based on their integrated peak areas. A sample of this file format, highlighted in orange, is shown as an inset, displaying compound names, sample names, retention times, and peak areas. For quantitative purposes, calibration curves are generated using a mixture of all target analytes at high concentrations,

followed by serial dilutions. After peak area Integration of each analyte, TargetLynx constructs calibration curves for sample components, using linear regression to establish a relationship between concentration and response. Unknown samples are then quantified using the fitted calibration curves. The final summary output is provided as a (**decoded_output.txt**) file, which serves as input for the Python-based retrieval of the original encoded message.

6) **Automated Information Extraction and Decoding:** A Python-based script is employed to extract encoded information. The script reads the compound names from **code.xls** and searches for their corresponding peak areas in **decoded_output.txt**. If the analyte is present (determined by its area value exceeding a predefined threshold), it is assigned a binary value of 1; if absent, it is assigned a binary value of 0. The resulting concatenated binary sequence is then used to reconstruct the original message.

SI_1.5 Schematic representation of sample reconstitution from filter paper

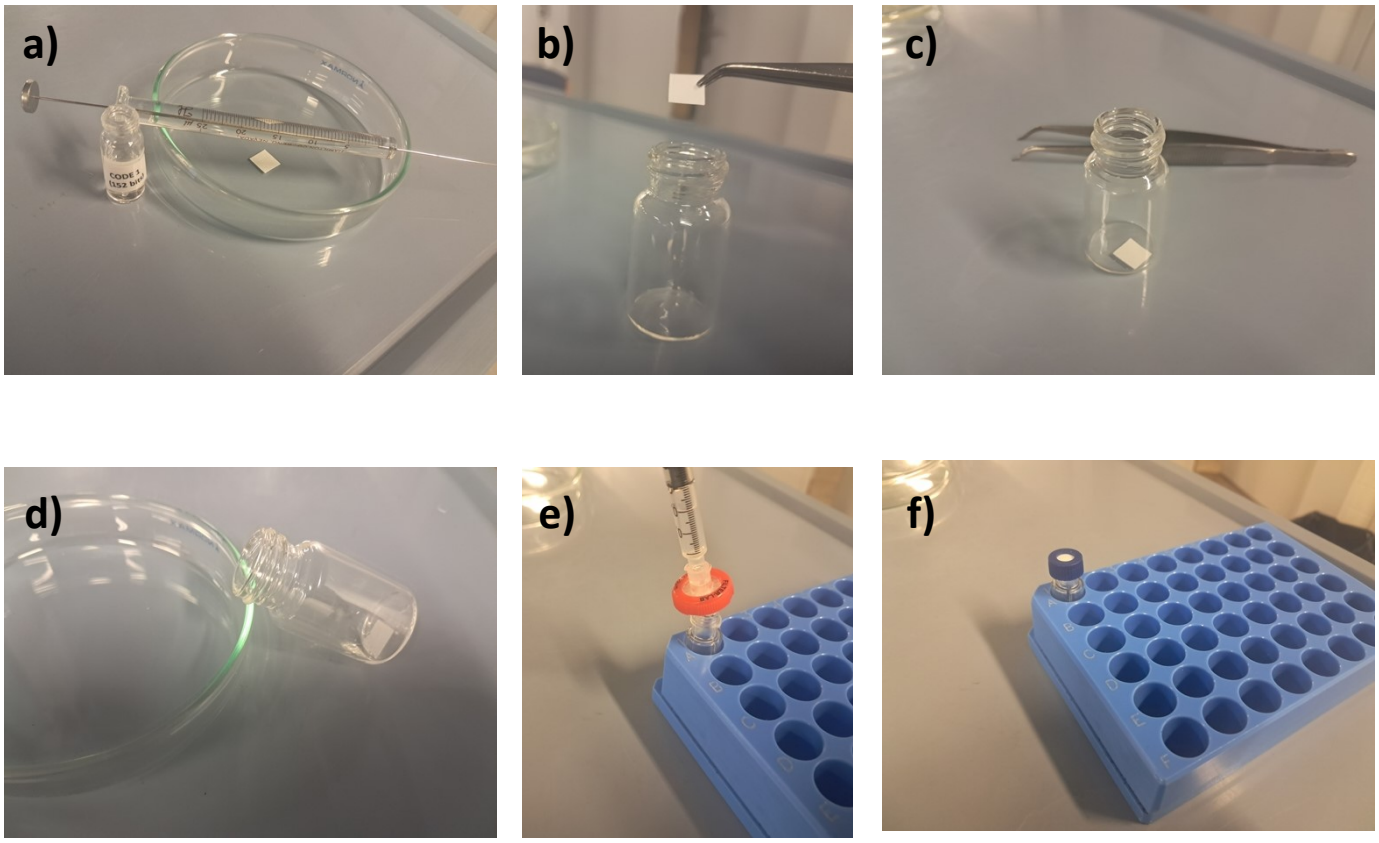

Figure S2. Workflow for reconstituting messages encoded in chemical mixtures adsorbed on filter paper; **a)** a 2.5 ppm solution of a chemical mixture encoding 152 bits (*CODE1_LCMS*) was prepared, and 5 µL of this solution was deposited onto a small section of filter paper (*ca.* 10 mm^2); **b) and c)** Images of the filter paper after the application of the 5 µL chemical mixture, left to dry in an open vial; **d)** the dried filter paper was subsequently suspended in 200 µL of methanol within the same vial to facilitate analyte extraction; **e)** the resulting solution was filtered using a 0.22 µm PTFE filter and transferred into a final vial for analysis; **f)** the final vial was placed on the sample plate, prepared for injection and decoding via LC-MS.

SI_1.6 Calibration details using quaternary and octal encoding schemes and ion suppression considerations

The consequences of matrix effects in ESI mass spectrometry analysis are a major issue of concern especially for quantitative purposes. We have mentioned along the text that ion suppression is present during qualitative FIA-MS analysis (used to decode binary-encoded information) due to the coelution of all encoding analytes; this indeed limited the use of large data sets to 80-100 analytes. Our quantitative method relied on the quantitation of each component of a mixture of 25 flavonoids to yield the associated quaternary or octal representation. Accuracy must be sufficient for distinguishing up to four or eight concentration levels which span over two orders of magnitude. Explanations and additional experiments aimed at identifying and quantifying ion suppression as well as accuracy of our quantitative method are given below.

As ion suppression varies by compound family, we examined its impact on three representative analytes: myricetin (flavone family), didymin (conjugated flavonoid family), and abscisic acid (plant hormone family). Comparison of matrix and solvent calibrations is a simple, yet effective technique for quantifying the effect of ion suppression in a MS method.[16] Calibration curves for each of the three analytes were constructed both in neat solvent and in a matrix comprising 25 flavonoids, mimicking real sample composition, at concentrations of 75 and 750 ppb. In LC-MS analysis, the presence of this flavonoid matrix yielded calibration curves that closely overlapped with those obtained in solvent, indicating negligible ion suppression effects. In contrast, FIA-MS exhibited a higher potential for ion suppression due to the simultaneous analysis of multiple flavonoids and the use of short, non-resolving chromatographic runs. This matrix effect was evident in the reduced slopes of calibration curves in the presence of the flavonoid matrix compared to those in neat solvent (see Figure S3 for myricetin).

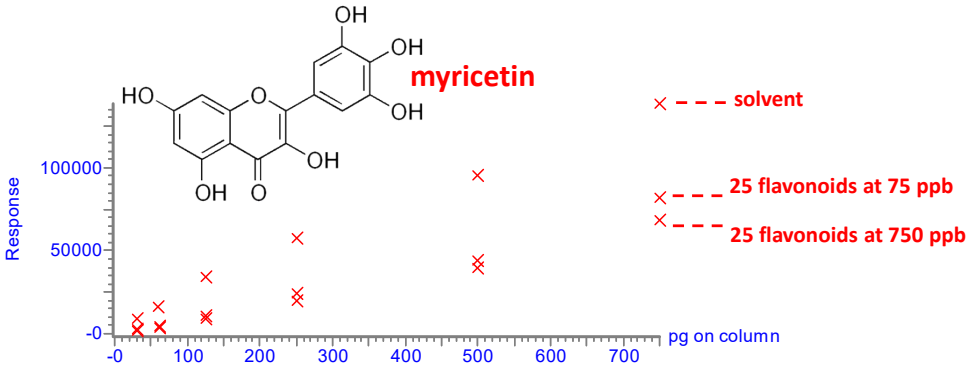

Figure S3. Calibration curves of myricetin in neat (H_2O:CH_3CN 9:1) solvent (upper trace) and in the presence of matrix at 75 ppb (medium trace) and 750 ppb (lower trace). The slope ratio between the calibration curves at 75 to 750 ppb is 15 %.

Similarly, didymin calibration curves (see figure S4) showed slope flattening when transitioning from neat solvent to matrix at both low and high concentrations.

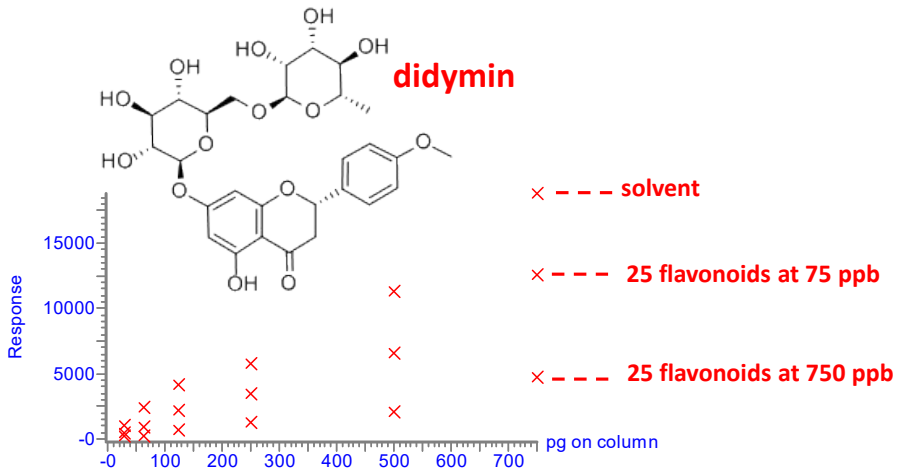

Figure S4. Calibration curves of didymin in a neat solvent (H_2O:CH_3CN 9:1) shown in the upper trace, and in the presence of matrix at concentrations of 75 ppb (medium trace) and 750 ppb (lower trace). The slope ratio between the calibration curves at 75 ppb and 750 ppb is 45%.

Once ion suppression was identified in FIA-MS decoding, we explored mitigation strategies. Firstly, we considered matrix-matched calibration, which requires calibration curves on each separated flavonoid in a matrix resembling real samples. However, due to variations in flavonoid composition and concentration across samples, achieving an appropriate blank matrix is not trivial and preparing such a large number of calibration curves is impractical. While matrix effects can differ across sample types, variations within similar matrices, (such as blood or urine from different test subjects), tend to be minor. In our case, this variation was estimated from Figures 1 and 2, showing response differences for myricetin and didymin of 15 - 45% across matrices ranging from 75 to 750 ppb. This suggests that accuracy and precision are not highly sensitive to matrix differences across calibration and unknown samples. Hence, we adopted a simplified calibration approach by combining aliquots of the 25 flavonoids into a single high-concentration standard mixture (1250 ppb), from which a series of dilution points were prepared (15 - 1250 ng/mL). This avoided extensive matrix-matched calibration on separated flavonoids while still accounting for interfering flavonoid components to identify any matrix effect. By using this approach, higher concentration calibration points of some flavonoids displayed suppressed signals whereas dilution to prepare the lower concentration calibration points presented improved ionization efficiency by reducing competing analytes.

Despite ion suppression was evident, the quaternary encoding scheme itself mitigated ion suppression by using concentration values separated by half an order of magnitude (e.g., codes 1 and 2 correspond to 100 and 500 ppb, respectively). Hence, method validation was successful, as quaternary-encoded messages were

accurately quantified and decoded. However, repeated attempts to distinguish eight concentration levels by FIA-MS-based quantitation showed an increase in classification errors, thus reducing the overall readout accuracy. Therefore, decoding of octal encoding schemes was restricted to LC-MS as decoding method.

Secondly, another method aimed at achieving greater accuracy and precision involved the use of an internal standard. This approach relies on maintaining a consistent response ratio between the analyte of interest and its corresponding internal standard, despite potential variations in absolute analyte responses due to matrix effects. In the context of this study, employing internal standards could significantly expand the range of distinguishable quantitation levels, particularly beneficial for higher (decimal, hexadecimal) encoding schemes. Specifically concerning flavonoids, the availability of isotopically labelled derivatives for use as internal standards is limited. Nevertheless, experiments were conducted using d^6-abscisic acid as an internal standard for its non-deuterated counterpart. The effectiveness of ion suppression compensation using an internal standard was evaluated by comparing calibration curves of the analyte in solvent versus in matrix, both in the presence of a fixed amount of internal standard. This evaluation is illustrated in figures S5 a), b), and c), which depict calibration curves of abscisic acid under solvent conditions (a), in a mixture of 25 flavonoids at 75 ppb (b), and at 750 ppb (c), and a matrix mixture at 750 ppb in the presence of a fixed (250 ppb) amount of d^6-abscisic acid.

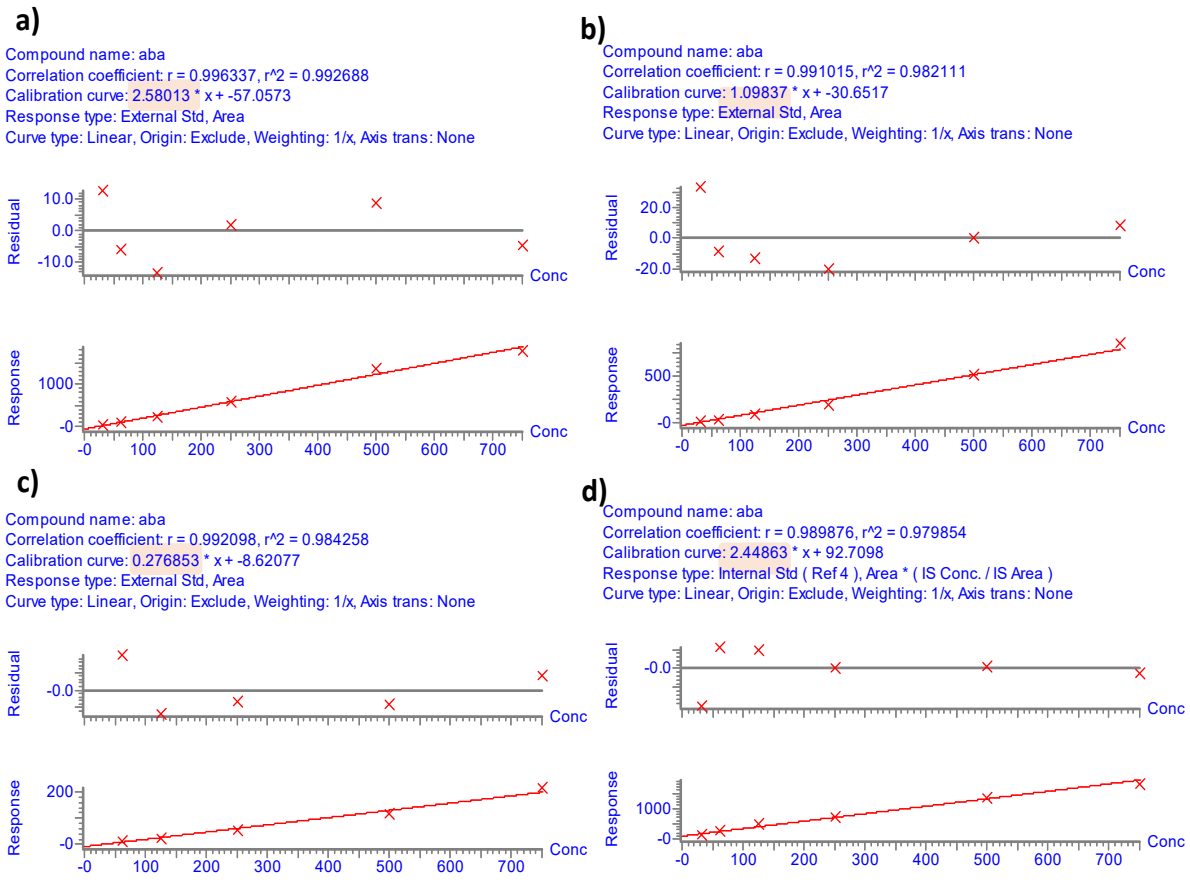

Figure S5. Calibration curves of abscisic acid in neat (H_2O:CH_3CN 9:1) solvent (a) and in the presence of matrix at 75 ppb (b), 750 ppb (c) and this later in the presence of d6-absisic acid as internal standard (d).

Figures S5 a) and S5 d) show significant overlap in calibration curve slopes, indicating that internal standard correction effectively minimizes ion suppression. Furthermore, we have conducted a preliminary investigation into the feasibility of extending the number of distinguishable quantitation levels by utilizing five plant hormones for which isotopically labelled standards are available: abscisic acid, salicylic acid, jasmonic acid, cinnamic acid, and ferulic acid. Given the three-order dynamic range of modern MS instruments, preliminary results indicated that both LC-MS and FIA-MS combined with internal standards enabled the accurate distinction of up to 32 levels. This preliminary finding is currently being further explored in our laboratory within the framework of high-order encoding schemes.

***Encoded message and decoded method*:** quaternary encoding scheme of an image (logo UJI) using FIA-MS or LC-MS as decoding methods. The list of metabolites used to encode this message is given in Table S3. Analyte concentrations were 100, 500 and 1250 ppb to depict the 1, 2 and 3 states.

Table S3

Text
image_UJI

Set of 25 metabolites used for text encoding

	Compound	formula	[M-H]- ion (m/z)	vial1	vial2	vial3	vial4	vial5	vial6	vial7	vial8	vial9	vial10
1	6-hydroxyflavone	C15H10O3	237,0552	0	0	0	0	0	0	0	0	0	0
2	guaijaverin	C20H18O11	433,0771	0	0	0	0	0	0	0	0	0	0
3	wogonoside	C22H20O11	459,0927	0	0	0	0	0	0	0	0	0	0
4	Orientin	C21H20O11	447,0927	0	0	0	0	0	0	0	1	1	0
5	5,7-dihydroxychromone	C9H6O4	177,0188	0	0	1	1	1	1	1	1	1	0
6	4-hydroxychalcone	C15H12O2	223,0759	0	0	1	1	1	1	1	1	1	0
7	corylifol A	C25H26O4	389,1753	0	0	1	1	1	1	1	1	1	0
8	formononetin	C16H12O4	267,0657	0	0	0	0	0	0	0	1	1	0
9	baicalein	C15H10O5	269,0450	0	0	0	0	0	0	0	1	1	0
10	naringenin	C15H12O5	271,0606	0	0	1	1	1	1	1	1	1	0
11	acacetin	C16H12O5	283,0606	0	0	1	1	1	1	1	1	1	0
12	scutellarein	C15H10O6	285,0399	0	0	1	1	1	1	1	1	1	0
13	morusin	C25H24O6	418,1432	0	0	0	0	0	0	0	0	0	0
14	eriodictyol	C15H12O6	287,0556	0	0	0	0	0	0	0	2	2	0
15	epicatechin	C15H14O6	289,0712	0	0	0	0	0	0	0	2	2	0
16	tectorigenin	C16H12O6	299,0556	0	0	0	0	0	0	0	2	2	0
17	eupatilin	C18H16O7	343,0818	0	0	2	2	2	2	2	2	2	0
18	taxifolin	C15H12O7	303,0505	0	0	2	2	2	2	2	2	2	0
19	neobavaisoflavone	C20H18O4	321,1127	0	0	2	2	2	2	2	2	2	0
20	bavachin	C21H22O12	465,1033	0	0	0	0	0	0	0	0	0	0
21	mirificin	C26H28O13	547,1452	0	0	3	3	3	3	3	3	3	0
22	amentoflavone	C30H18O10	537,0822	0	0	3	3	3	3	3	3	3	0
23	silibinin	C25H22O10	481,1135	0	0	3	3	3	3	3	3	3	0
24	jaceosidin	C21H22O4	337,1440	0	0	0	0	0	0	0	0	0	0
25	rhoifolin	C27H30O14	577,1557	0	0	0	0	0	0	0	0	0	0

Quantify compound summary report for the image (logo UJI) using a quaternary encoding scheme and LC-MS as decoding method

Quantify Compound Summary Report

Compound 1: 6-hydroxiflavone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2	4.03	92.613	15.000	12.76
3	3	synapt_cvb_quat_LCMS_003	mix_3	4.03	239.778	31.000	25.50
4	4	synapt_cvb_quat_LCMS_004	mix_4	4.03	552.067	62.000	52.54
5	5	synapt_cvb_quat_LCMS_005	mix_5	4.02	1367.667	125.000	123.17
6	6	synapt_cvb_quat_LCMS_006	mix_6	4.03	3074.708	250.000	270.99
7	7	synapt_cvb_quat_LCMS_007	mix_7	4.03	5682.255	500.000	496.80
8	8	synapt_cvb_quat_LCMS_008	mix_8	4.05	8565.732	750.000	746.50
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary				
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary				
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

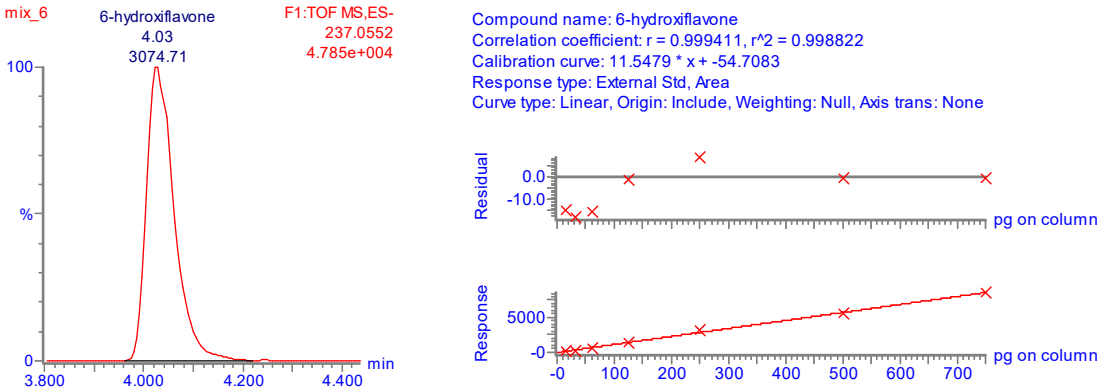

Figure S6. Compound summary report, illustrative trace and calibration curve and residuals of 6-hydroxiflavone.

Quantify Compound Summary Report

Compound 2: guayjaverin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	1.97	48.024	31.000	40.84
4	4	synapt_cvb_quat_LCMS_004	mix_4	1.98	182.019	62.000	56.01
5	5	synapt_cvb_quat_LCMS_005	mix_5	1.98	555.197	125.000	98.27
6	6	synapt_cvb_quat_LCMS_006	mix_6	1.98	1684.148	250.000	226.12
7	7	synapt_cvb_quat_LCMS_007	mix_7	1.98	4072.199	500.000	496.55
8	8	synapt_cvb_quat_LCMS_008	mix_8	2.00	6441.045	750.000	764.80
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary				
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary				
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

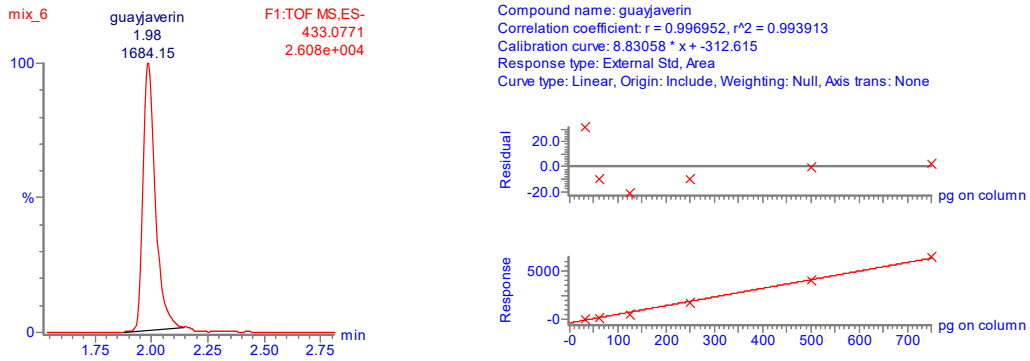

Figure S7. Compound summary report, illustrative trace and calibration curve and residuals of guayjaverin.

Quantify Compound Summary Report

Compound 3: wogonoside

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	3.10	45.353	31.000	45.16
4	4	synapt_cvb_quat_LCMS_004	mix_4	3.11	115.336	62.000	57.58
5	5	synapt_cvb_quat_LCMS_005	mix_5	3.10	333.446	125.000	96.29
6	6	synapt_cvb_quat_LCMS_006	mix_6	3.10	1082.496	250.000	229.24
7	7	synapt_cvb_quat_LCMS_007	mix_7	3.10	2458.072	500.000	473.37
8	8	synapt_cvb_quat_LCMS_008	mix_8	3.12	4181.436	750.000	779.24
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary				
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary				
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

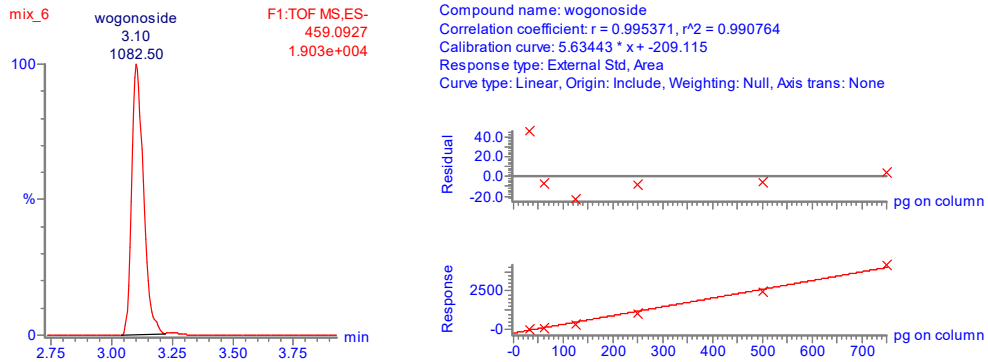

Figure S8. Compound summary report, illustrative trace and calibration curve and residuals of wogonoside.

Quantify Compound Summary Report

Compound 4: orientin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	1.54	47.154	31.000	39.54
4	4	synapt_cvb_quat_LCMS_004	mix_4	1.55	128.990	62.000	54.53
5	5	synapt_cvb_quat_LCMS_005	mix_5	1.55	388.985	125.000	102.16
6	6	synapt_cvb_quat_LCMS_006	mix_6	1.55	1100.225	250.000	232.46
7	7	synapt_cvb_quat_LCMS_007	mix_7	1.55	2535.738	500.000	495.45
8	8	synapt_cvb_quat_LCMS_008	mix_8	1.56	3995.865	750.000	762.95
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary				
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary				
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

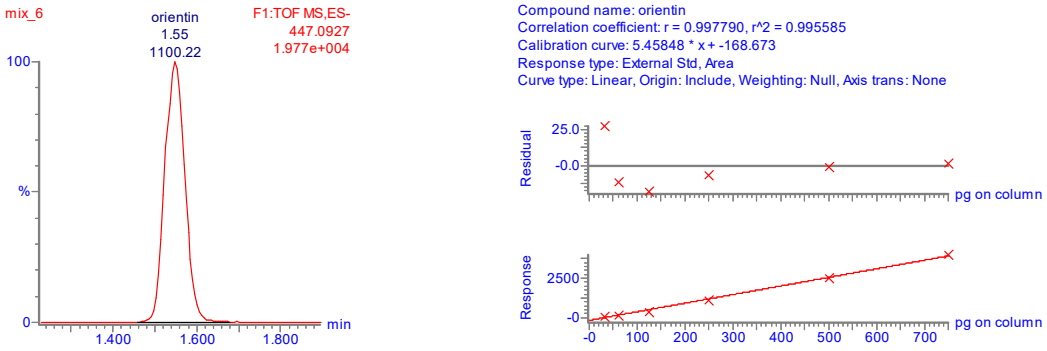

Figure S9. Compound summary report, illustrative trace and calibration curve and residuals of orientin.

Quantify Compound Summary Report

Compound 5: 5,7 dihydroxichromone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on colum
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2	2.10	82.375	15.000	18.57
3	3	synapt_cvb_quat_LCMS_003	mix_3	2.09	195.078	31.000	29.10
4	4	synapt_cvb_quat_LCMS_004	mix_4	2.09	484.522	62.000	56.14
5	5	synapt_cvb_quat_LCMS_005	mix_5	2.09	1157.071	125.000	118.98
6	6	synapt_cvb_quat_LCMS_006	mix_6	2.09	2653.580	250.000	258.80
7	7	synapt_cvb_quat_LCMS_007	mix_7	2.09	4976.996	500.000	475.88
8	8	synapt_cvb_quat_LCMS_008	mix_8	2.12	8067.516	750.000	764.64
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	2.09	987.468		103.14
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	2.08	995.014		103.84
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	2.08	943.146		98.99
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	2.09	909.803		95.88
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	2.09	875.133		92.64
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	2.09	1275.722		130.07
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	2.09	1223.173		125.16
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

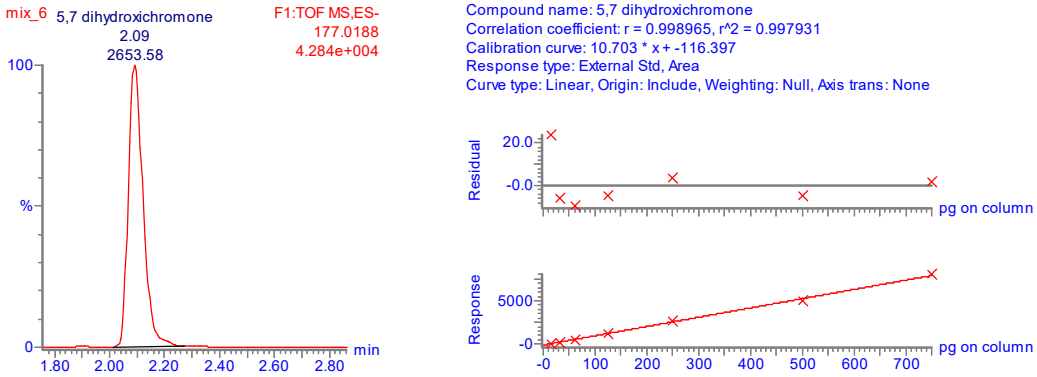

Figure S10. Compound summary report, illustrative trace and calibration curve and residuals of 5,7-dihydroxichromone.

Quantify Compound Summary Report

Compound 6: 4-hydroxychalcone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	4.51	1657.705	31.000	21.67
4	4	synapt_cvb_quat_LCMS_004	mix_4	4.51	3359.665	62.000	62.32
5	5	synapt_cvb_quat_LCMS_005	mix_5	4.51	6488.589	125.000	137.05
6	6	synapt_cvb_quat_LCMS_006	mix_6	4.51	12458.951	250.000	279.66
7	7	synapt_cvb_quat_LCMS_007	mix_7	4.51	21278.107	500.000	490.30
8	8	synapt_cvb_quat_LCMS_008	mix_8	4.53	31938.641	750.000	744.93
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	4.51	5234.669		107.10
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	4.51	5148.387		105.04
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	4.51	4991.214		101.29
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	4.51	4810.939		96.98
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	4.50	4731.058		95.07
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	4.51	6488.026		137.04
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	4.51	6374.303		134.32
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

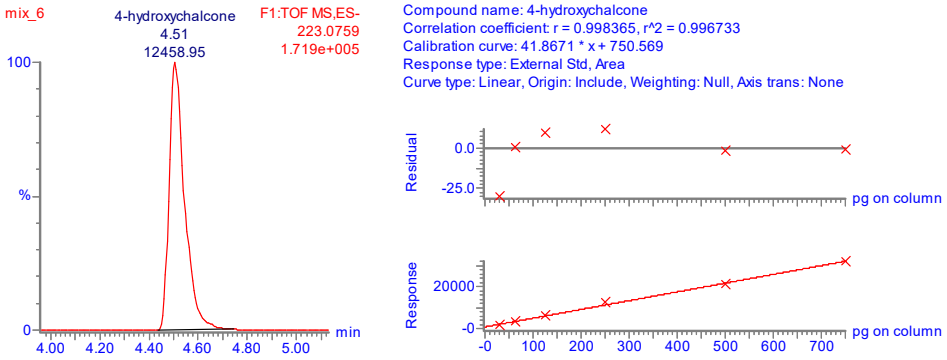

Figure S11. Compound summary report, illustrative trace and calibration curve and residuals of 4-hydroxichalcone.

Quantify Compound Summary Report

Compound 7: corylifol A

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1	6.59	375.428	10.000	6.60
2	2	synapt_cvb_quat_LCMS_002	mix_2	6.59	850.097	19.000	21.38
3	3	synapt_cvb_quat_LCMS_003	mix_3	6.59	1750.404	38.000	49.41
4	4	synapt_cvb_quat_LCMS_004	mix_4	6.59	3295.943	78.000	97.54
5	5	synapt_cvb_quat_LCMS_005	mix_5	6.59	6329.921	156.000	192.01
6	6	synapt_cvb_quat_LCMS_006	mix_6	6.59	11135.169	312.000	341.63
7	7	synapt_cvb_quat_LCMS_007	mix_7	6.59	17166.771	625.000	529.44
8	8	synapt_cvb_quat_LCMS_008	mix_8			940.000	
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	6.59	1854.331		52.65
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	6.59	1840.330		52.21
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	6.59	1734.610		48.92
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	6.59	1716.368		48.35
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	6.59	1655.649		46.46
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	6.59	2618.469		76.44
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	6.59	2582.919		75.34
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

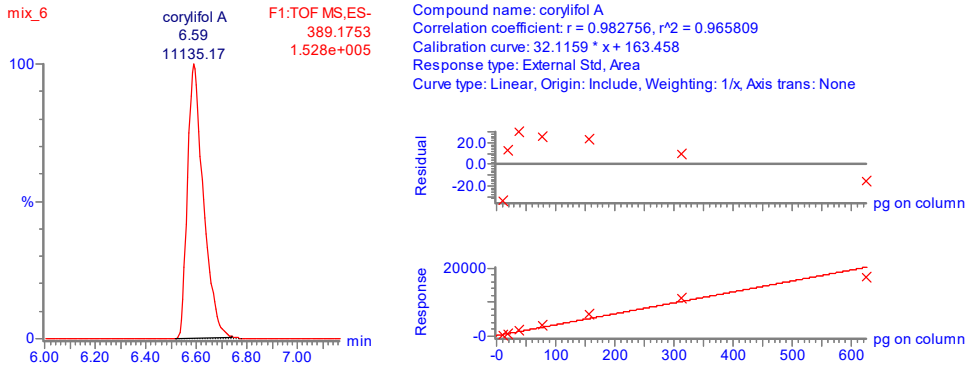

Figure S12. Compound summary report, illustrative trace and calibration curve and residuals of corylifol A

Quantify Compound Summary Report

Compound 8: formononetin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2	3.99	285.810	15.000	6.39
3	3	synapt_cvb_quat_LCMS_003	mix_3	3.99	747.531	31.000	24.75
4	4	synapt_cvb_quat_LCMS_004	mix_4	3.98	1592.396	62.000	58.34
5	5	synapt_cvb_quat_LCMS_005	mix_5	3.98	3562.618	125.000	136.67
6	6	synapt_cvb_quat_LCMS_006	mix_6	3.98	7080.589	250.000	276.55
7	7	synapt_cvb_quat_LCMS_007	mix_7	3.98	12348.684	500.000	486.01
8	8	synapt_cvb_quat_LCMS_008	mix_8	4.00	18969.920	750.000	749.27
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	3.99	102.334		
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	3.98	106.393		
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	3.98	106.762		
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	3.98	107.988		
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	3.98	88.698		
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	3.98	3236.911		123.72
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	3.98	2988.003		113.83
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

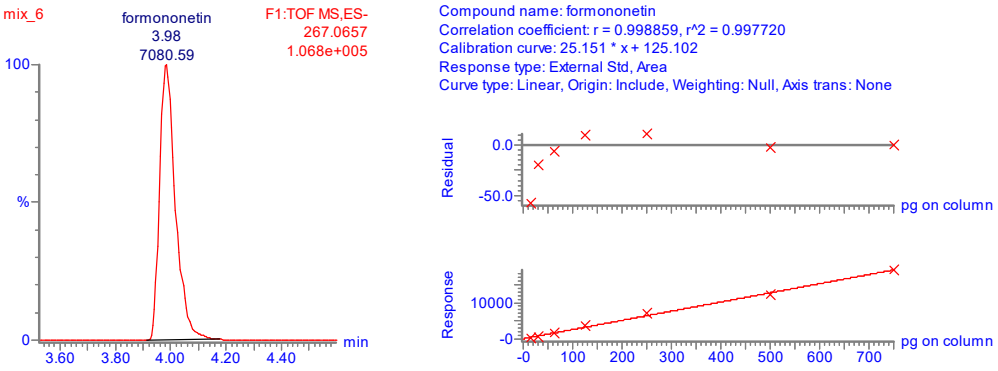

Figure S13. Compound summary report, illustrative trace and calibration curve and residuals of formononetin.

Quantify Compound Summary Report

Compound 9: baicalein

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	3.74	12.928	31.000	38.65
4	4	synapt_cvb_quat_LCMS_004	mix_4	3.76	32.792	62.000	50.85
5	5	synapt_cvb_quat_LCMS_005	mix_5	3.76	114.066	125.000	100.76
6	6	synapt_cvb_quat_LCMS_006	mix_6	3.75	310.957	250.000	221.69
7	7	synapt_cvb_quat_LCMS_007	mix_7	3.75	819.128	500.000	533.80
8	8	synapt_cvb_quat_LCMS_008	mix_8	3.77	1157.393	750.000	741.55
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	3.75	111.127		98.96
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	3.75	105.704		95.63
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

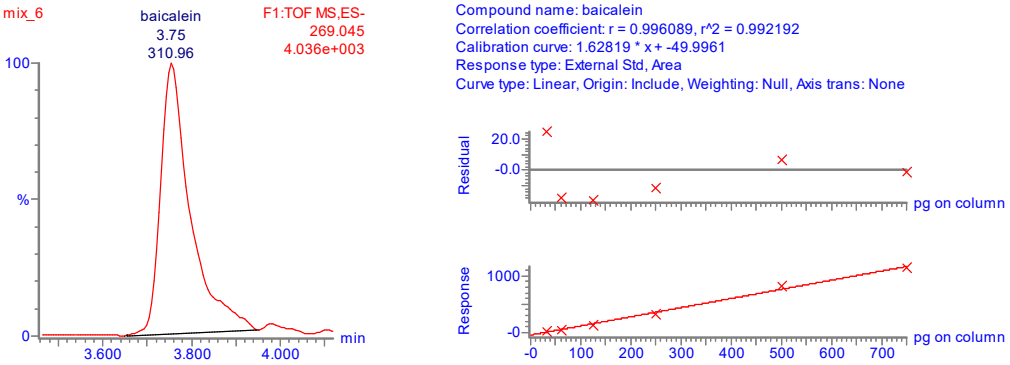

Figure S14. Compound summary report, illustrative trace and calibration curve and residuals of baicalein.

Quantify Compound Summary Report

Compound 10: naringenin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1	3.34	69.371	7.000	6.30
2	2	synapt_cvb_quat_LCMS_002	mix_2	3.34	135.825	15.000	10.31
3	3	synapt_cvb_quat_LCMS_003	mix_3	3.33	395.137	31.000	25.96
4	4	synapt_cvb_quat_LCMS_004	mix_4	3.33	947.532	62.000	59.29
5	5	synapt_cvb_quat_LCMS_005	mix_5	3.33	2182.328	125.000	133.79
6	6	synapt_cvb_quat_LCMS_006	mix_6	3.33	4377.479	250.000	266.23
7	7	synapt_cvb_quat_LCMS_007	mix_7	3.33	7871.505	500.000	477.04
8	8	synapt_cvb_quat_LCMS_008	mix_8	3.37	12544.406	750.000	758.97
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	3.34	1962.739		120.54
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	3.33	1887.804		116.02
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	3.33	1817.901		111.80
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	3.33	1774.789		109.20
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	3.33	1681.999		103.60
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	3.33	1906.629		117.15
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	3.33	1789.749		110.10
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

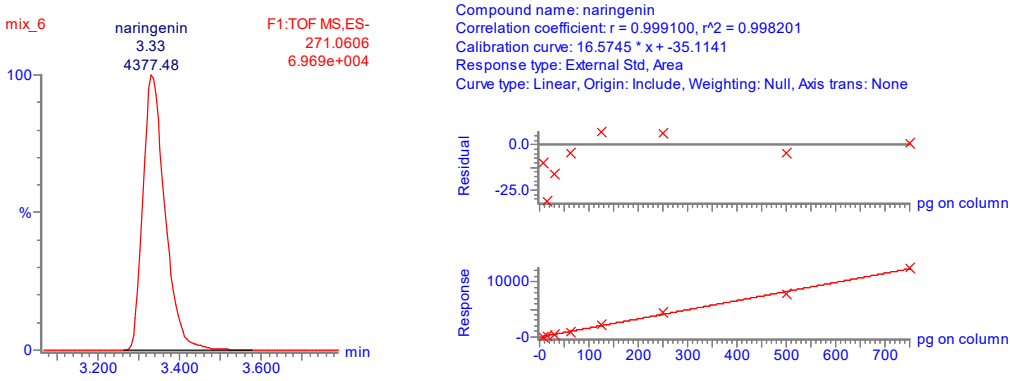

Figure S15. Compound summary report, illustrative trace and calibration curve and residuals of naringenin

Quantify Compound Summary Report

Compound 11: acacetin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1	4.62	103.268	7.000	7.60
2	2	synapt_cvb_quat_LCMS_002	mix_2	4.61	209.768	15.000	11.70
3	3	synapt_cvb_quat_LCMS_003	mix_3	4.61	502.278	31.000	22.97
4	4	synapt_cvb_quat_LCMS_004	mix_4	4.62	1306.623	62.000	53.95
5	5	synapt_cvb_quat_LCMS_005	mix_5	4.61	3043.683	125.000	120.86
6	6	synapt_cvb_quat_LCMS_006	mix_6	4.61	7109.161	250.000	277.47
7	7	synapt_cvb_quat_LCMS_007	mix_7	4.61	12826.779	500.000	497.72
8	8	synapt_cvb_quat_LCMS_008	mix_8	4.63	19223.135	750.000	744.11
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary	4.62	160.151		9.79
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary	4.61	331.932		16.41
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	4.61	2533.611		101.22
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	4.61	2491.546		99.60
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	4.61	2488.738		99.49
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	4.61	2234.043		89.68
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	4.61	2203.919		88.52
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	4.61	3219.114		127.62
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	4.61	3100.247		123.04
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary	4.61	168.266		10.10

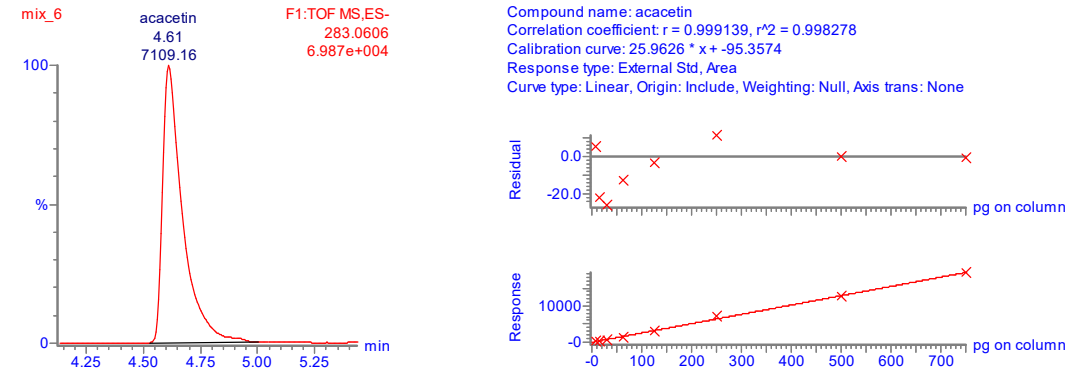

Figure S16. Compound summary report, illustrative trace and calibration curve and residuals of acacetin.

Quantify Compound Summary Report

Compound 12: scutellarein

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3			31.000	
4	4	synapt_cvb_quat_LCMS_004	mix_4	2.55	6.693	62.000	67.58
5	5	synapt_cvb_quat_LCMS_005	mix_5	2.52	10.269	125.000	83.84
6	6	synapt_cvb_quat_LCMS_006	mix_6	2.50	42.458	250.000	230.17
7	7	synapt_cvb_quat_LCMS_007	mix_7	2.51	105.274	500.000	515.72
8	8	synapt_cvb_quat_LCMS_008	mix_8	2.53	157.368	750.000	752.53
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	2.49	12.198		92.61
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	2.50	11.316		88.60
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	2.51	10.629		85.48
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	2.51	14.668		103.84
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	2.51	17.299		115.80
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	2.50	22.404		139.00
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	2.50	15.505		107.64
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

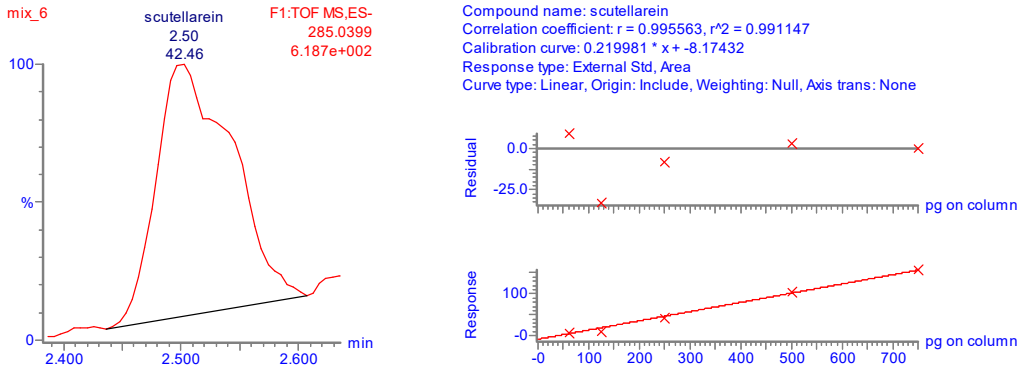

Figure S17. Compound summary report, illustrative trace and calibration curve and residuals of scutellarein.

Compound 13: morusin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	7.04	1763.410	31.000	4.38
4	4	synapt_cvb_quat_LCMS_004	mix_4	7.04	3084.157	62.000	71.92
5	5	synapt_cvb_quat_LCMS_005	mix_5	7.04	5626.239	125.000	201.92
6	6	synapt_cvb_quat_LCMS_006	mix_6	7.04	8302.094	250.000	338.75
7	7	synapt_cvb_quat_LCMS_007	mix_7	7.04	10219.681	500.000	436.81
8	8	synapt_cvb_quat_LCMS_008	mix_8			750.000	
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary				
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary				
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

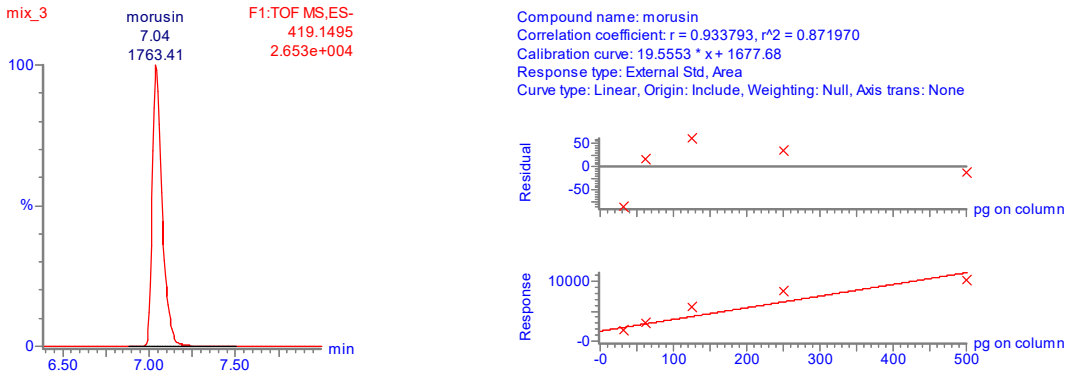

Figure S18. Compound summary report, illustrative trace and calibration curve and residuals of morusin.

Quantify Compound Summary Report

Compound 14: eriodictyol

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	2.82	34.514	31.000	46.08
4	4	synapt_cvb_quat_LCMS_004	mix_4	2.82	98.291	62.000	60.93
5	5	synapt_cvb_quat_LCMS_005	mix_5	2.82	260.578	125.000	98.72
6	6	synapt_cvb_quat_LCMS_006	mix_6	2.82	747.771	250.000	212.16
7	7	synapt_cvb_quat_LCMS_007	mix_7	2.82	1927.498	500.000	486.86
8	8	synapt_cvb_quat_LCMS_008	mix_8	2.85	3165.893	750.000	775.22
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	2.82	2841.507		699.69
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	2.82	2716.554		670.59
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

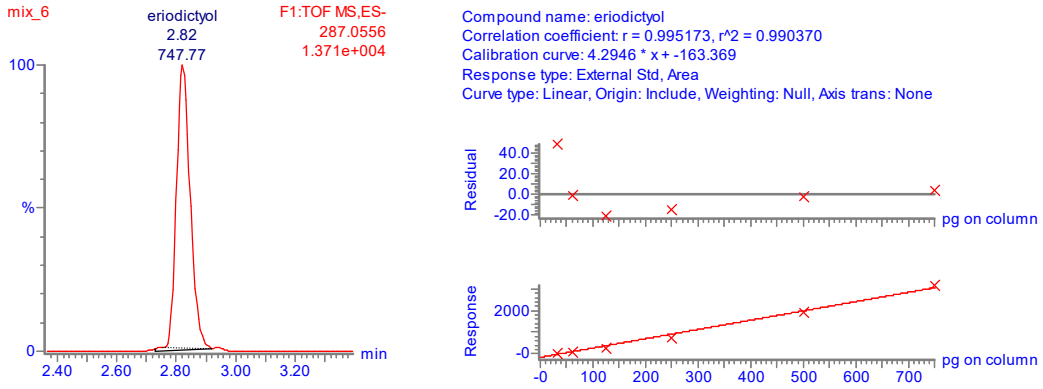

Figure S19. Compound summary report, illustrative trace and calibration curve and residuals of eriodictyol.

Quantify Compound Summary Report

Compound 15: epicatechin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	1.26	26.725	31.000	46.19
4	4	synapt_cvb_quat_LCMS_004	mix_4	1.26	71.308	62.000	57.55
5	5	synapt_cvb_quat_LCMS_005	mix_5	1.26	237.578	125.000	99.92
6	6	synapt_cvb_quat_LCMS_006	mix_6	1.26	652.300	250.000	205.59
7	7	synapt_cvb_quat_LCMS_007	mix_7	1.27	1815.355	500.000	501.95
8	8	synapt_cvb_quat_LCMS_008	mix_8	1.29	2857.187	750.000	767.42
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	1.27	2094.771		573.15
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	1.27	2087.782		571.37
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

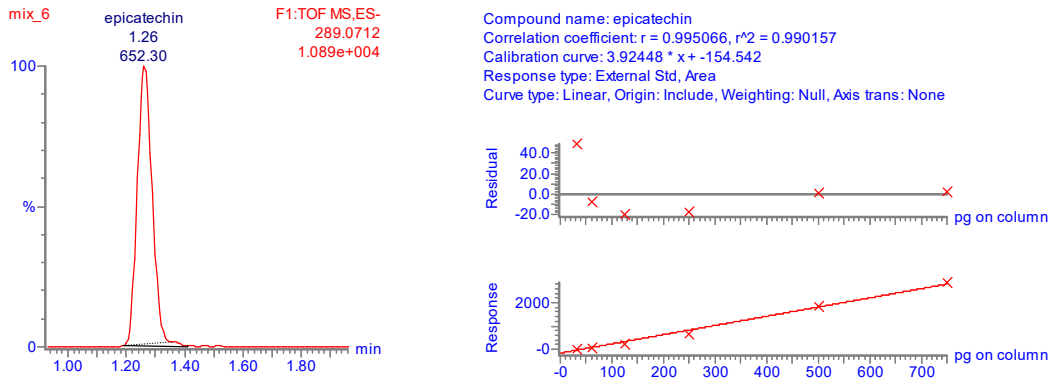

Figure S20. Compound summary report, illustrative trace and calibration curve and residuals of epicatechin.

Quantify Compound Summary Report

Compound 16: tectorigenin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1	3.39	42.272	7.000	7.81
2	2	synapt_cvb_quat_LCMS_002	mix_2	3.40	115.578	15.000	13.29
3	3	synapt_cvb_quat_LCMS_003	mix_3	3.40	295.455	31.000	26.71
4	4	synapt_cvb_quat_LCMS_004	mix_4	3.40	669.102	62.000	54.61
5	5	synapt_cvb_quat_LCMS_005	mix_5	3.40	1623.659	125.000	125.87
6	6	synapt_cvb_quat_LCMS_006	mix_6	3.40	3548.895	250.000	269.59
7	7	synapt_cvb_quat_LCMS_007	mix_7	3.40	6367.261	500.000	479.98
8	8	synapt_cvb_quat_LCMS_008	mix_8	3.42	10084.717	750.000	757.49
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	3.39	8504.422		639.52
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	3.39	7940.888		597.45
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

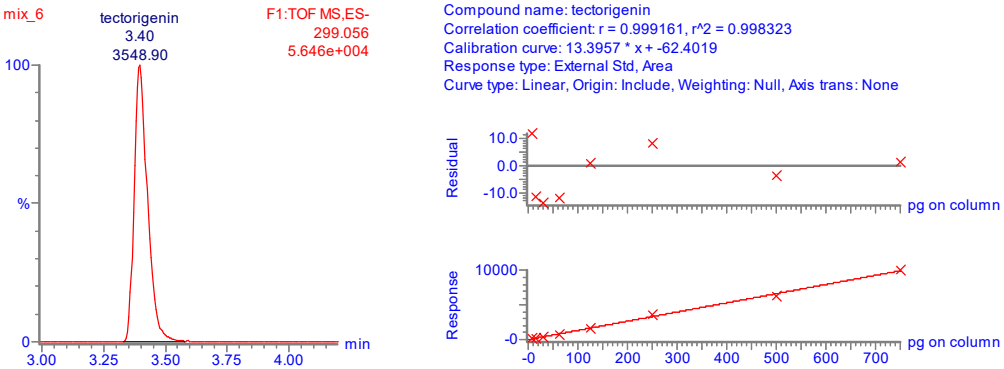

Figure S21. Compound summary report, illustrative trace and calibration curve and residuals of tectoginerin

Quantify Compound Summary Report

Compound 17: eupatilin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2	4.25	105.912	15.000	15.08
3	3	synapt_cvb_quat_LCMS_003	mix_3	4.24	349.558	31.000	26.60
4	4	synapt_cvb_quat_LCMS_004	mix_4	4.24	791.741	62.000	47.50
5	5	synapt_cvb_quat_LCMS_005	mix_5	4.24	2323.057	125.000	119.88
6	6	synapt_cvb_quat_LCMS_006	mix_6	4.24	5428.829	250.000	266.69
7	7	synapt_cvb_quat_LCMS_007	mix_7	4.24	10396.618	500.000	501.51
8	8	synapt_cvb_quat_LCMS_008	mix_8	4.26	15561.802	750.000	745.66
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	4.24	10852.617		523.06
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	4.24	10624.841		512.30
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	4.24	10146.751		489.70
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	4.24	9686.595		467.95
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	4.24	9493.704		458.83
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	4.24	13600.556		652.96
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	4.24	12952.957		622.35
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

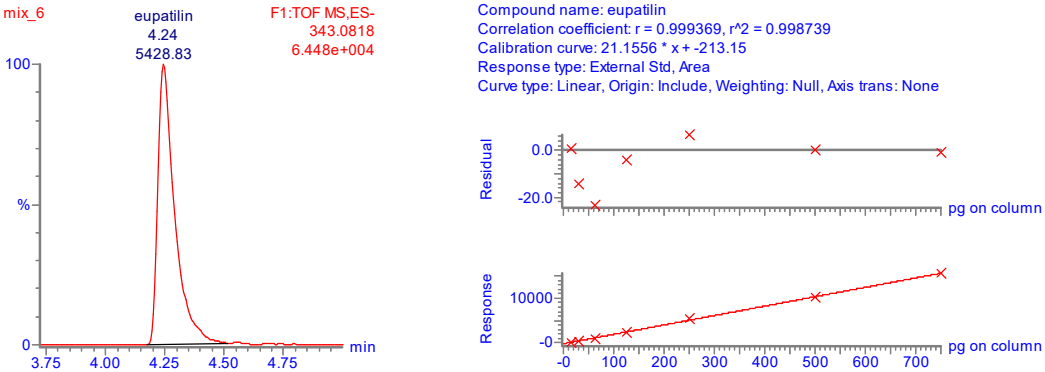

Figure S22. Compound summary report, illustrative trace and calibration curve and residuals of eupatilin.

Quantify Compound Summary Report

Compound 18: taxifolin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3			31.000	
4	4	synapt_cvb_quat_LCMS_004	mix_4	1.90	54.419	62.000	68.31
5	5	synapt_cvb_quat_LCMS_005	mix_5	1.90	150.453	125.000	103.02
6	6	synapt_cvb_quat_LCMS_006	mix_6	1.90	448.651	250.000	210.81
7	7	synapt_cvb_quat_LCMS_007	mix_7	1.90	1165.840	500.000	470.05
8	8	synapt_cvb_quat_LCMS_008	mix_8	1.93	2040.369	750.000	786.17
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	1.90	1429.953		565.52
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	1.90	1457.228		575.38
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	1.90	1365.535		542.24
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	1.90	1244.388		498.45
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	1.90	1239.002		496.50
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	1.90	2183.665		837.97
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	1.90	2146.742		824.62
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

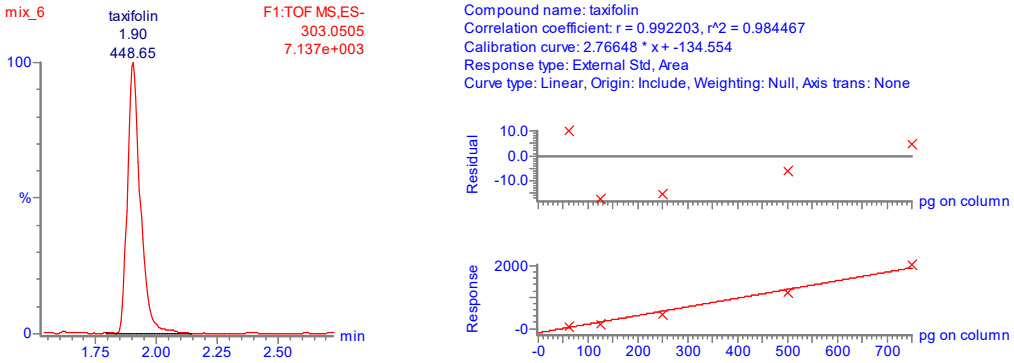

Figure S23. Compound summary report, illustrative trace and calibration curve and residuals of taxifolin.

Quantify Compound Summary Report

Compound 19: neobavaisoflavone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	4.88	1126.746	31.000	22.05
4	4	synapt_cvb_quat_LCMS_004	mix_4	4.87	2407.341	62.000	60.57
5	5	synapt_cvb_quat_LCMS_005	mix_5	4.87	4803.700	125.000	132.66
6	6	synapt_cvb_quat_LCMS_006	mix_6	4.87	9492.488	250.000	273.71
7	7	synapt_cvb_quat_LCMS_007	mix_7	4.88	16970.033	500.000	498.64
8	8	synapt_cvb_quat_LCMS_008	mix_8	4.89	25066.918	750.000	742.21
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	4.88	18487.422		544.29
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	4.88	17974.318		528.85
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	4.87	17373.080		510.77
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	4.88	16514.631		484.94
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	4.88	16182.600		474.96
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	4.87	21821.988		644.60
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	4.88	21272.105		628.06
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

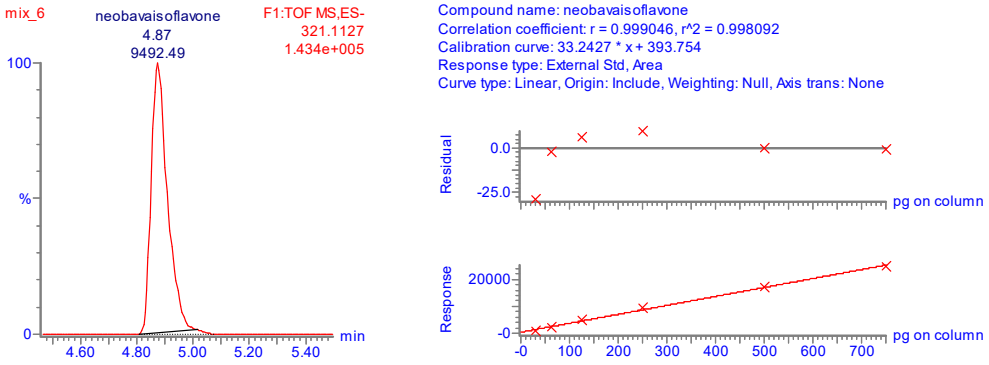

Figure S24. Compound summary report, illustrative trace and calibration curve and residuals of neobavaisoflavone.

Quantify Compound Summary Report

Compound 20: bavachin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2	5.08	797.293	15.000	4.40
3	3	synapt_cvb_quat_LCMS_003	mix_3	5.08	1722.675	31.000	25.33
4	4	synapt_cvb_quat_LCMS_004	mix_4	5.08	3571.226	62.000	67.13
5	5	synapt_cvb_quat_LCMS_005	mix_5	5.08	6820.748	125.000	140.61
6	6	synapt_cvb_quat_LCMS_006	mix_6	5.08	12811.328	250.000	276.07
7	7	synapt_cvb_quat_LCMS_007	mix_7	5.08	21966.197	500.000	483.09
8	8	synapt_cvb_quat_LCMS_008	mix_8			750.000	
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary				
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary				
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

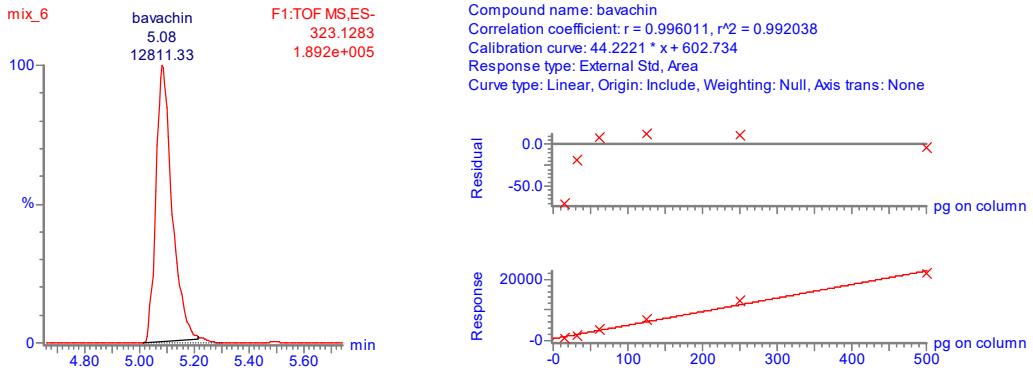

Figure S25. Compound summary report, illustrative trace and calibration curve and residuals of bavachin.

Quantify Compound Summary Report

Compound 21: mirificin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2	1.23	19.553	15.000	16.56
3	3	synapt_cvb_quat_LCMS_003	mix_3	1.22	88.930	31.000	29.36
4	4	synapt_cvb_quat_LCMS_004	mix_4	1.22	199.570	62.000	49.78
5	5	synapt_cvb_quat_LCMS_005	mix_5	1.22	539.110	125.000	112.43
6	6	synapt_cvb_quat_LCMS_006	mix_6	1.22	1341.825	250.000	260.56
7	7	synapt_cvb_quat_LCMS_007	mix_7	1.23	2667.809	500.000	505.24
8	8	synapt_cvb_quat_LCMS_008	mix_8	1.23	3973.219	750.000	746.13
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	1.22	8801.052		1637.01
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	1.22	8369.158		1557.31
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	1.23	8106.898		1508.92
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	1.22	7325.313		1364.69
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	1.22	5697.541		1064.32
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	1.22	10088.987		1874.67
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	1.22	9815.266		1824.16
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

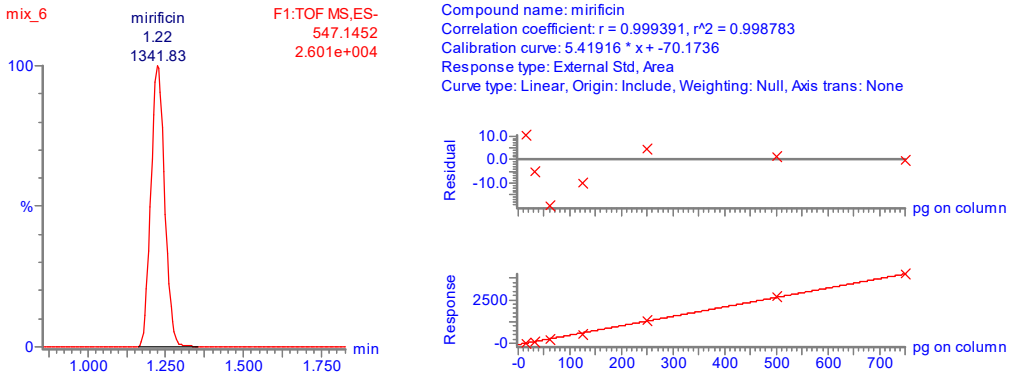

Figure S26. Compound summary report, illustrative trace and calibration curve and residuals of mirificin.

Quantify Compound Summary Report

Compound 22: amentoflavone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	3.89	76.785	31.000	34.40
4	4	synapt_cvb_quat_LCMS_004	mix_4	3.89	248.328	62.000	49.47
5	5	synapt_cvb_quat_LCMS_005	mix_5	3.90	717.625	125.000	90.70
6	6	synapt_cvb_quat_LCMS_006	mix_6	3.89	2454.092	250.000	243.24
7	7	synapt_cvb_quat_LCMS_007	mix_7	3.89	5843.641	500.000	540.99
8	8	synapt_cvb_quat_LCMS_008	mix_8	3.91	8012.726	750.000	731.54
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	3.89	16397.947		1468.14
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	3.89	15194.006		1362.38
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	3.89	16274.637		1457.31
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	3.88	15602.785		1398.29
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	3.88	15849.326		1419.94
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	3.89	21357.898		1903.85
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	3.88	21151.867		1885.75
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

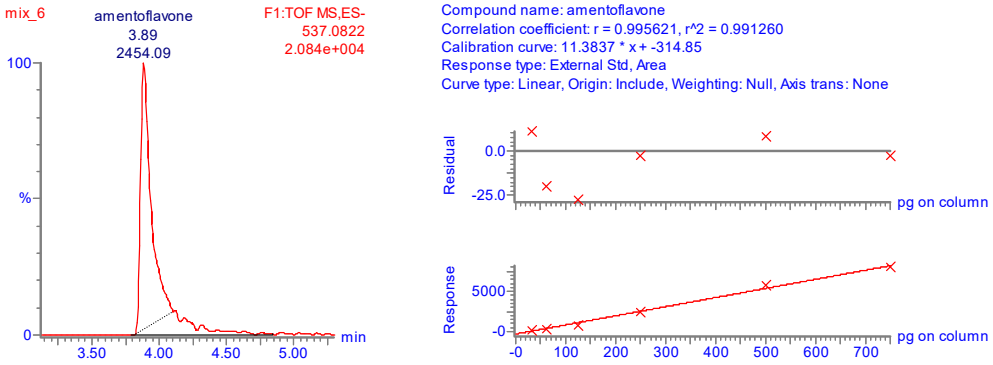

Figure S27. Compound summary report, illustrative trace and calibration curve and residuals of amentoflavone.

Quantify Compound Summary Report

Compound 23: silibinin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			10.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			19.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	3.28	1725.765	38.000	21.81
4	4	synapt_cvb_quat_LCMS_004	mix_4	3.28	3572.831	78.000	75.34
5	5	synapt_cvb_quat_LCMS_005	mix_5	3.28	7198.317	156.000	180.41
6	6	synapt_cvb_quat_LCMS_006	mix_6	3.28	13122.800	312.000	352.09
7	7	synapt_cvb_quat_LCMS_007	mix_7	3.28	22439.619	625.000	622.09
8	8	synapt_cvb_quat_LCMS_008	mix_8	3.30	32907.699	940.000	925.45
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary	3.28	44913.605		1273.38
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary	3.28	43063.973		1219.77
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary	3.28	42131.922		1192.76
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary	3.28	40121.707		1134.51
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary	3.28	38882.977		1098.61
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary	3.28	58937.867		1679.79
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary	3.28	56205.832		1600.62
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

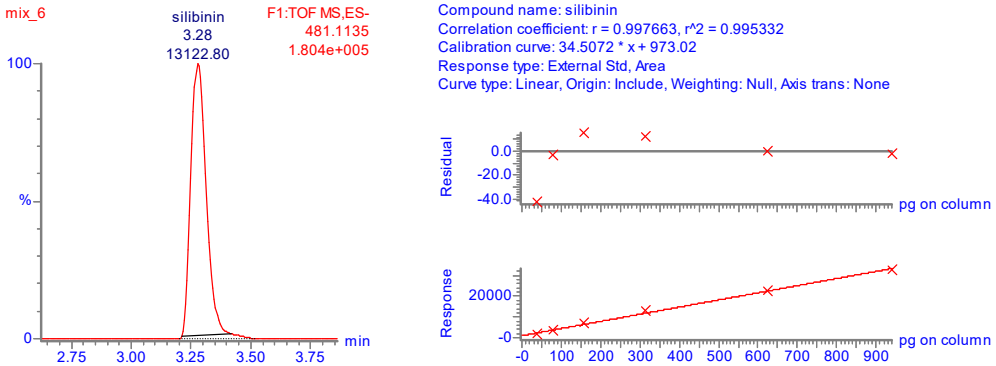

Figure S28. Compound summary report, illustrative trace and calibration curve and residuals of silibinin.

Quantify Compound Summary Report

Compound 24: jaceosidin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2	1.54	6.538	15.000	21.33
3	3	synapt_cvb_quat_LCMS_003	mix_3	1.52	11.955	31.000	24.28
4	4	synapt_cvb_quat_LCMS_004	mix_4	1.55	75.401	62.000	58.84
5	5	synapt_cvb_quat_LCMS_005	mix_5	1.55	182.385	125.000	117.12
6	6	synapt_cvb_quat_LCMS_006	mix_6	1.55	375.770	250.000	222.46
7	7	synapt_cvb_quat_LCMS_007	mix_7	1.55	941.951	500.000	530.87
8	8	synapt_cvb_quat_LCMS_008	mix_8	1.56	1326.479	750.000	740.33
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary				
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary				
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

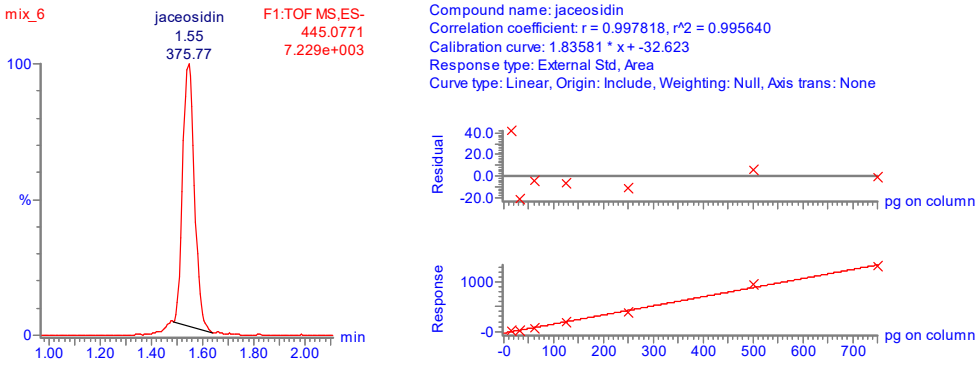

Figure S29. Compound summary report, illustrative trace and calibration curve and residuals of jaceosidin.

Quantify Compound Summary Report

Compound 25: rhoifolin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_LCMS_001	mix_1			7.000	
2	2	synapt_cvb_quat_LCMS_002	mix_2			15.000	
3	3	synapt_cvb_quat_LCMS_003	mix_3	2.15	96.707	31.000	37.36
4	4	synapt_cvb_quat_LCMS_004	mix_4	2.15	269.326	62.000	58.56
5	5	synapt_cvb_quat_LCMS_005	mix_5	2.15	669.256	125.000	107.66
6	6	synapt_cvb_quat_LCMS_006	mix_6	2.15	1675.713	250.000	231.23
7	7	synapt_cvb_quat_LCMS_007	mix_7	2.15	3828.907	500.000	495.59
8	8	synapt_cvb_quat_LCMS_008	mix_8	2.16	5999.641	750.000	762.11
9	9	synapt_cvb_quat_LCMS_009	vial 1 quaternary				
10	10	synapt_cvb_quat_LCMS_010	vial 2 quaternary				
11	11	synapt_cvb_quat_LCMS_011	vial 3 quaternary				
12	12	synapt_cvb_quat_LCMS_012	vial 4 quaternary				
13	13	synapt_cvb_quat_LCMS_013	vial 5 quaternary				
14	14	synapt_cvb_quat_LCMS_014	vial 6 quaternary				
15	15	synapt_cvb_quat_LCMS_015	vial 7 quaternary				
16	16	synapt_cvb_quat_LCMS_016	vial 8 quaternary				
17	17	synapt_cvb_quat_LCMS_017	vial 9 quaternary				
18	18	synapt_cvb_quat_LCMS_018	vial 10 quaternary				

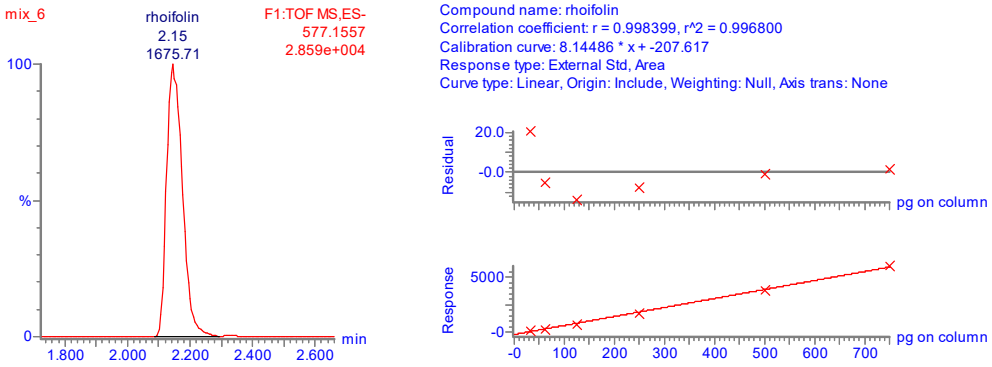

Figure S30. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Quantify compound summary report for the image (logo UJI) using a quaternary encoding scheme and FIA-MS as decoding method

Quantify Compound Summary Report

Compound 1: 6-hydroxiflavone

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	49.576	30.000	33.17
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard			62.000	
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	80.600	125.000	111.18
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	142.767	250.000	267.49
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	207.104	500.000	429.27
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	349.617	750.000	787.61
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	444.536	1000.000	1026.28
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte				
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte				
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

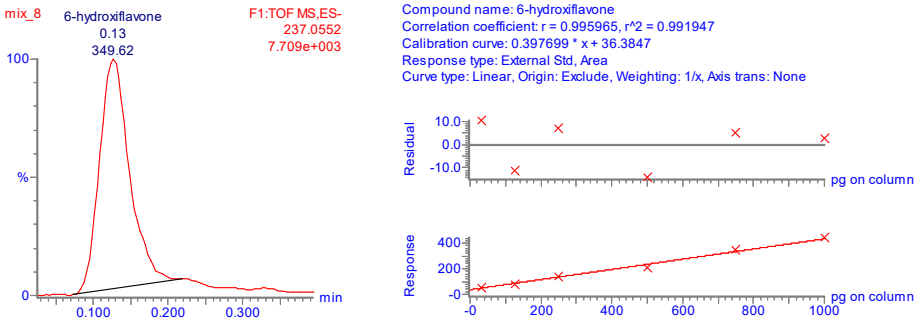

Figure S31. Compound summary report, illustrative trace and calibration curve and residuals of 6-hydroxiflavone.

Quantify Compound Summary Report

Compound 2: guayjaverin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	37.561	30.000	18.19
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.12	65.418	62.000	55.67
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	149.561	125.000	168.87
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	243.610	250.000	295.40
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	425.618	500.000	540.26
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	568.082	750.000	731.92
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	698.002	1000.000	906.70
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte				
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte				
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

>

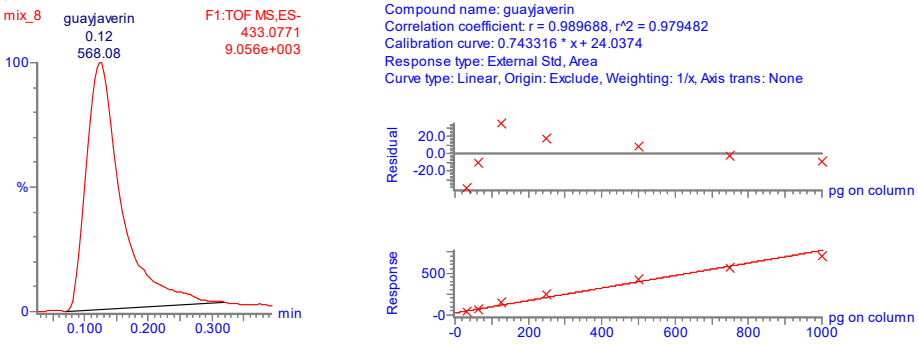

Figure S32. Compound summary report, illustrative trace and calibration curve and residuals of guayjaverin.

Quantify Compound Summary Report

Compound 3: wogonoside

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard			30.000	
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	21.042	62.000	74.55
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.14	32.126	125.000	131.56
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	45.996	250.000	202.90
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.12	81.978	500.000	387.97
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	162.663	750.000	802.96
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.12	217.900	1000.000	1087.07
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte				
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte				
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

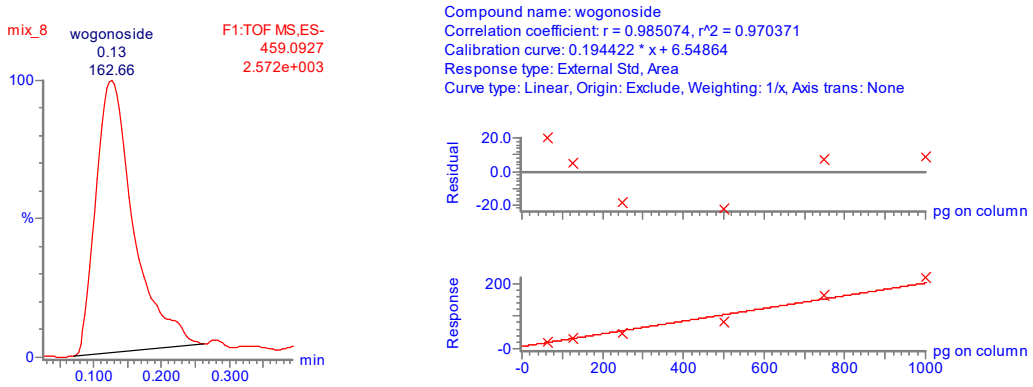

Figure S33. Compound summary report, illustrative trace and calibration curve and residuals of wogonoside.

Quantify Compound Summary Report

Compound 4: orientin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.12	29.186	30.000	30.77
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	42.794	62.000	53.65
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	88.670	125.000	130.80
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	165.354	250.000	259.76
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.12	308.521	500.000	500.53
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	512.025	750.000	842.76
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.12	545.293	1000.000	898.71
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte				
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte				
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

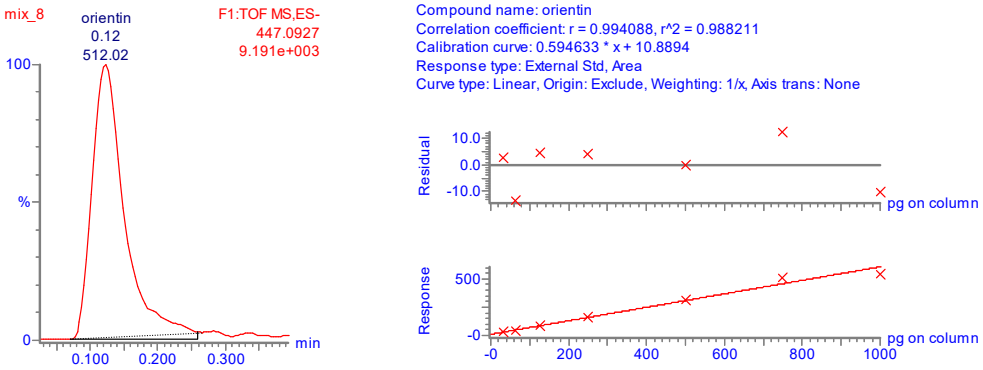

Figure S34. Compound summary report, illustrative trace and calibration curve and residuals of orientin.

Quantify Compound Summary Report

Compound 5: 5,7 dihydroxichromone

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.12	23.711	30.000	39.46
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	54.624	62.000	63.19
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	125.097	125.000	117.27
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	234.328	250.000	201.09
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	449.170	500.000	365.96
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	992.256	750.000	782.71
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	1467.380	1000.000	1147.32
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.12	112.574		107.66
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.12	135.387		125.16
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	123.820		116.29
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.13	138.100		127.25
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.12	130.424		121.36
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	172.825		153.89
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	180.961		160.14
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

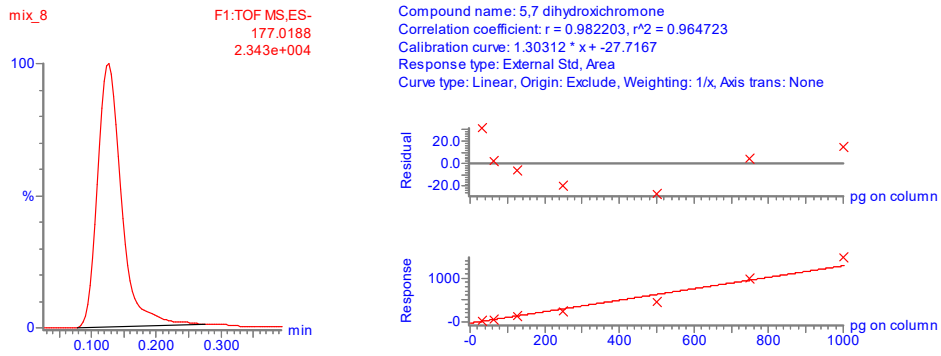

Figure S35. Compound summary report, illustrative trace and calibration curve and residuals of 5,7-dihydroxichromone.

Quantify Compound Summary Report

Compound 6: 4-hydroxychalcone

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.12	29.796	30.000	29.17
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	156.161	62.000	74.45
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	316.584	125.000	131.94
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	536.235	250.000	210.65
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	1072.955	500.000	402.97
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	2081.970	750.000	764.54
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	3027.261	1000.000	1103.27
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.12	174.596		81.06
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.13	197.798		89.37
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.12	199.075		89.83
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.12	220.435		97.49
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.12	187.905		85.83
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	300.257		126.09
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	316.765		132.00
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

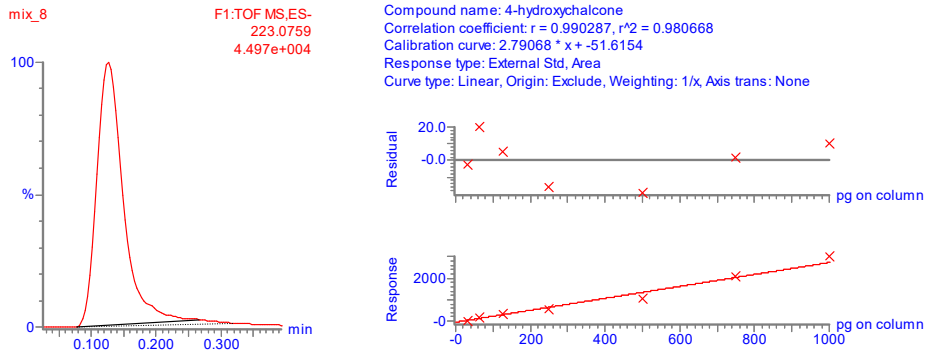

Figure S36. Compound summary report, illustrative trace and calibration curve and residuals of 4-hydroxichalcone.

Quantify Compound Summary Report

Compound 7: corylifol A

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	80.700	41.000	32.16
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	150.528	81.000	95.18
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	250.472	161.000	185.39
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	383.626	312.000	305.58
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	656.930	625.000	552.27
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	1029.876	940.000	888.90
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	1541.299	1250.000	1350.52
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.12	110.268		58.84
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.13	105.154		54.23
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	106.005		55.00
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.12	111.234		59.72
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.13	111.455		59.92
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	125.601		72.68
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	125.061		72.20
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

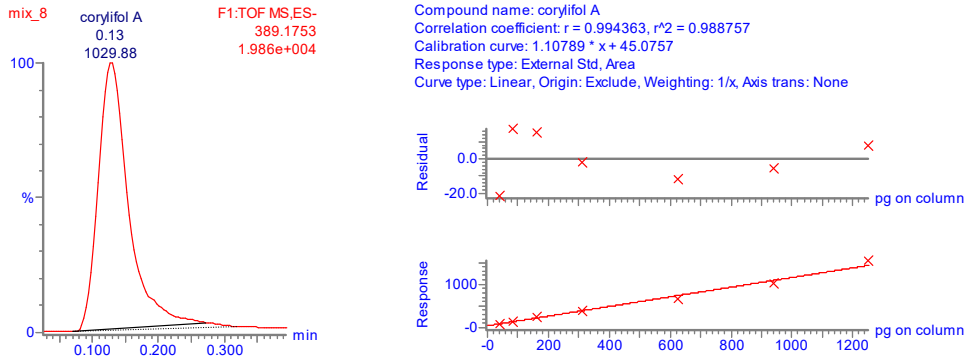

Figure S37. Compound summary report, illustrative trace and calibration curve and residuals of corylifol A

Quantify Compound Summary Report

Compound 8: formononetin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard			30.000	
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.12	96.214	62.000	62.68
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	243.970	125.000	141.68
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	424.337	250.000	238.12
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	747.486	500.000	410.89
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	1369.286	750.000	743.36
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	2018.138	1000.000	1090.28
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.12	161.730		97.71
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	165.761		99.86
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

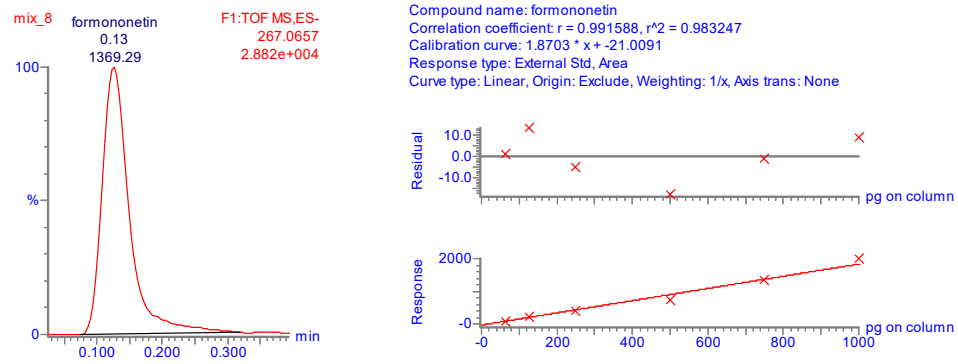

Figure S38. Compound summary report, illustrative trace and calibration curve and residuals of formononetin.

Quantify Compound Summary Report

Compound 9: baicalein

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.12	59.476	30.000	44.96
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	64.117	62.000	53.23
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.12	95.453	125.000	109.09
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	138.803	250.000	186.36
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	268.603	500.000	417.75
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	511.692	750.000	851.08
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	625.828	1000.000	1054.54
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.12	50.498		28.95
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.12	50.041		28.14
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	50.513		28.98
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.12	50.078		28.20
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.13	48.557		25.49
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	105.584		127.15
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	104.420		125.07
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

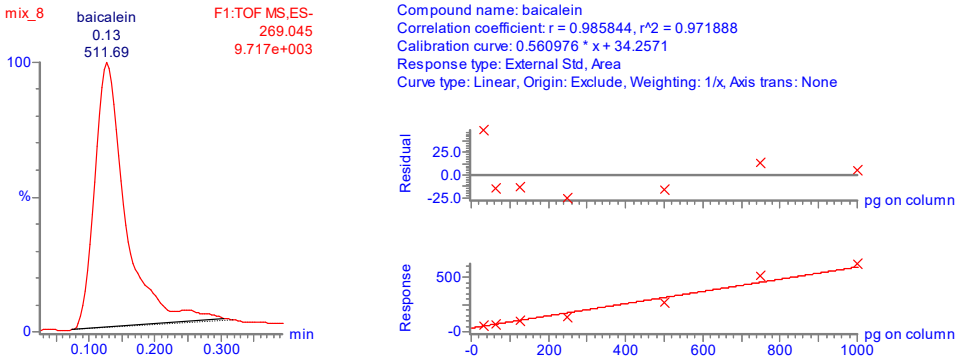

Figure S39. Compound summary report, illustrative trace and calibration curve and residuals of baicalein.

Quantify Compound Summary Report

Compound 10: naringenin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard			30.000	
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	44.588	62.000	65.06
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.12	108.033	125.000	138.64
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.12	187.404	250.000	230.69
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	358.752	500.000	429.42
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	600.956	750.000	710.33
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	948.016	1000.000	1112.85
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.13	72.137		97.01
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.12	60.749		83.80
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	74.142		99.33
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.13	67.861		92.05
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.13	62.368		85.68
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	56.725		79.13
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.12	81.610		107.99
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

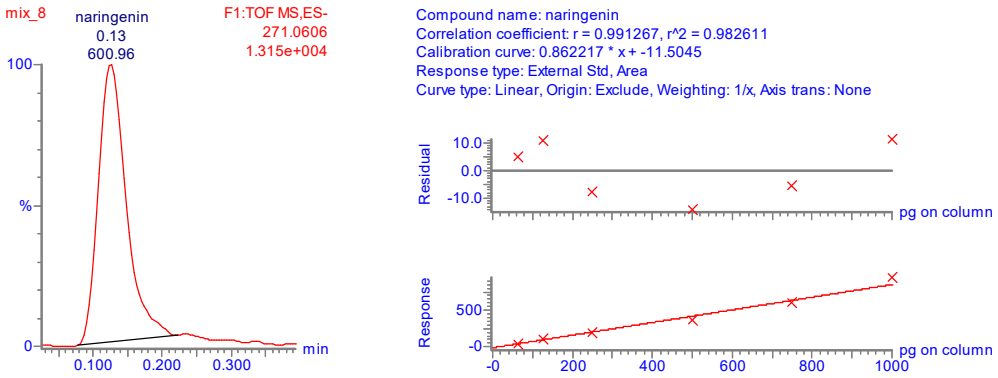

Figure S40. Compound summary report, illustrative trace and calibration curve and residuals of naringenin

Quantify Compound Summary Report

Compound 11: acacetin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	45.954	30.000	32.94
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	92.181	62.000	65.71
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	186.762	125.000	132.77
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	294.791	250.000	209.36
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	572.239	500.000	406.06
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	1100.522	750.000	780.59
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	1536.338	1000.000	1089.57
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.13	138.884		98.83
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.12	121.456		86.47
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	140.831		100.21
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.13	130.657		92.99
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.13	153.461		109.16
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	138.089		98.26
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	147.879		105.20
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

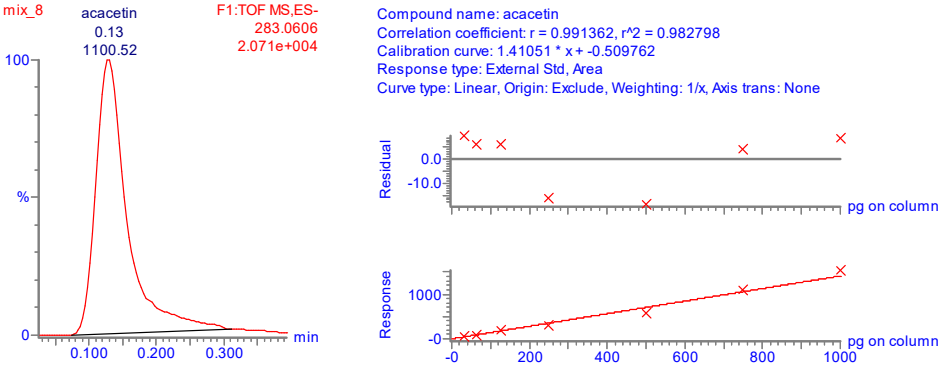

Figure S41. Compound summary report, illustrative trace and calibration curve and residuals of acacetin.

Quantify Compound Summary Report

Compound 12: scutellarein

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.12	15.370	30.000	42.34
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	23.678	62.000	58.65
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.12	47.691	125.000	105.82
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	97.698	250.000	204.03
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	208.593	500.000	421.84
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	378.870	750.000	756.27
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	568.167	1000.000	1128.06
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.12	88.770		186.50
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.13	75.423		160.28
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	86.306		181.66
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.12	95.564		199.84
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.13	88.794		186.54
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.12	92.890		194.59
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	92.659		194.14
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

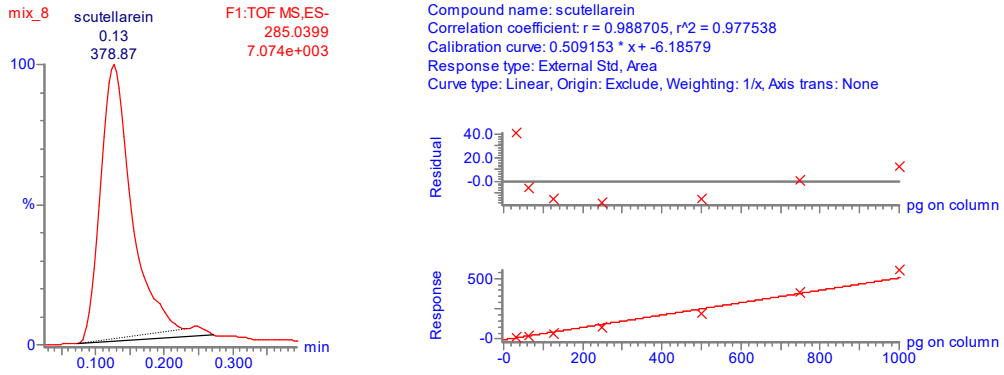

Figure S42. Compound summary report, illustrative trace and calibration curve and residuals of scutellarein.

Quantify Compound Summary Report

Compound 13: morusin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard			30.000	
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	85.999	62.000	44.75
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	182.421	125.000	134.56
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	366.051	250.000	305.60
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	636.289	500.000	557.32
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	746.387	750.000	659.87
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	1095.345	1000.000	984.90
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte				
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte				
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

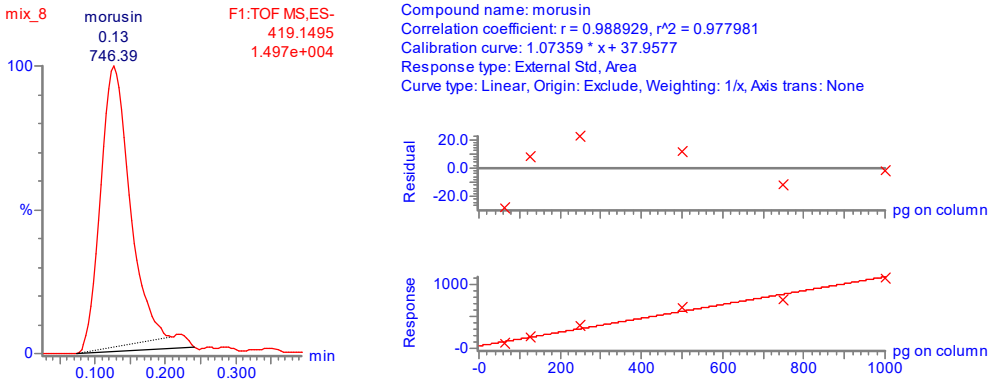

Figure S43. Compound summary report, illustrative trace and calibration curve and residuals of morusin.

Quantify Compound Summary Report

Compound 14: eriodictyol

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	26.435	30.000	31.20
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	32.180	62.000	49.88
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.12	62.886	125.000	149.73
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.12	91.767	250.000	243.64
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.12	169.328	500.000	495.84
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	242.431	750.000	733.55
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	328.416	1000.000	1013.15
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.12	140.827		403.17
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	141.797		406.32
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

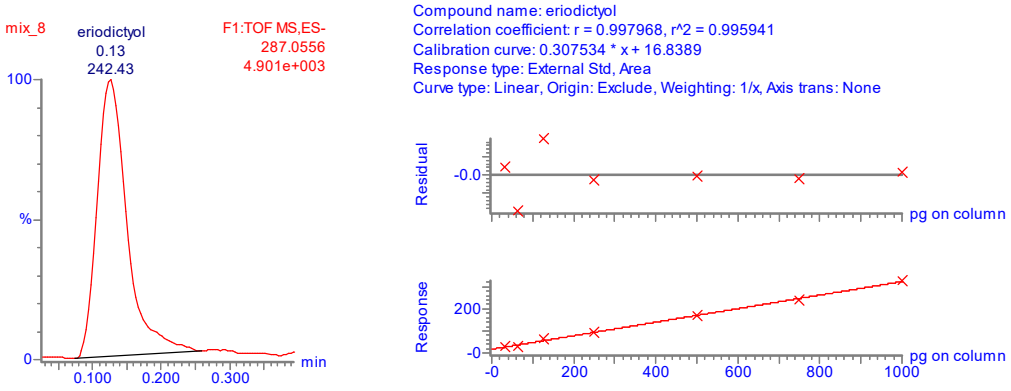

Figure S44. Compound summary report, illustrative trace and calibration curve and residuals of eriodictyol.

Quantify Compound Summary Report

Compound 15: epicatechin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	29.763	30.000	27.14
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	37.093	62.000	52.36
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.12	71.023	125.000	169.14
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.12	89.351	250.000	232.21
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.12	163.726	500.000	488.18
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	235.059	750.000	733.67
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.12	316.601	1000.000	1014.30
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.12	144.369		421.56
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	143.453		418.41
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

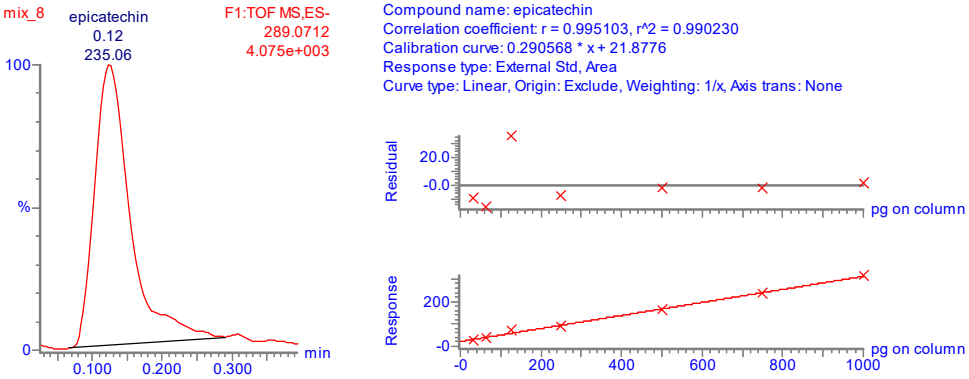

Figure S45. Compound summary report, illustrative trace and calibration curve and residuals of epicatechin.

Quantify Compound Summary Report

Compound 16: tectorigenin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	23.089	30.000	40.37
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	44.182	62.000	62.68
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	97.741	125.000	119.34
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	173.096	250.000	199.04
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	308.872	500.000	342.66
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	705.528	750.000	762.22
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	1110.599	1000.000	1190.68
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	593.886		644.13
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.12	595.400		645.73
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

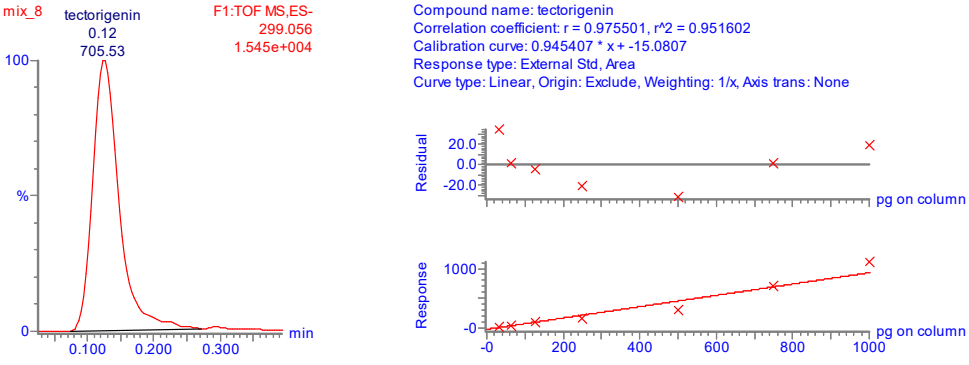

Figure S46. Compound summary report, illustrative trace and calibration curve and residuals of tectoginerin

Quantify Compound Summary Report

Compound 17: eupatilin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	36.215	30.000	31.13
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	53.468	62.000	64.85
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	85.583	125.000	127.62
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.12	142.856	250.000	239.57
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	241.706	500.000	432.78
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	404.963	750.000	751.87
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	567.308	1000.000	1069.19
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.13	241.763		432.89
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.13	245.402		440.00
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	243.786		436.84
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.13	246.389		441.93
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.13	253.583		455.99
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	285.252		517.89
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	292.570		532.19
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

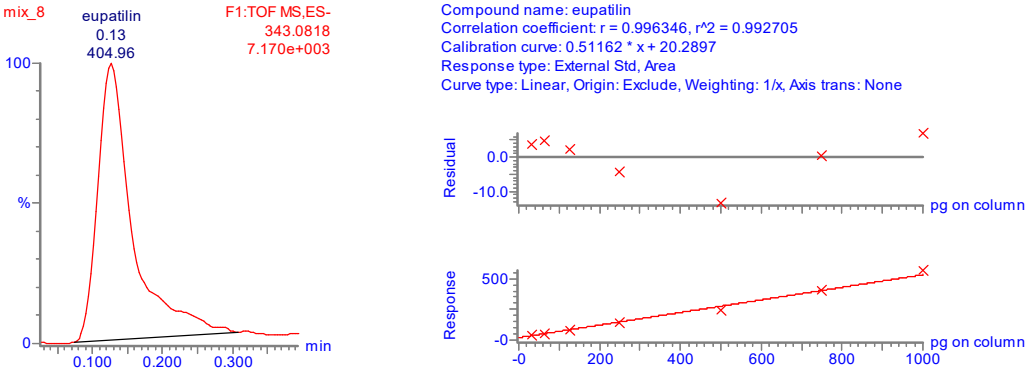

Figure S47. Compound summary report, illustrative trace and calibration curve and residuals of eupatilin.

Quantify Compound Summary Report

Compound 18: taxifolin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard			30.000	
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	37.051	62.000	52.58
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	58.210	125.000	141.38
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.12	88.169	250.000	267.12
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	137.350	500.000	473.52
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	205.374	750.000	759.01
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	261.219	1000.000	993.39
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.13	169.071		606.65
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.13	177.832		643.42
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	172.481		620.96
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.12	182.685		663.79
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.13	180.775		655.77
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	164.016		585.44
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	172.009		618.98
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

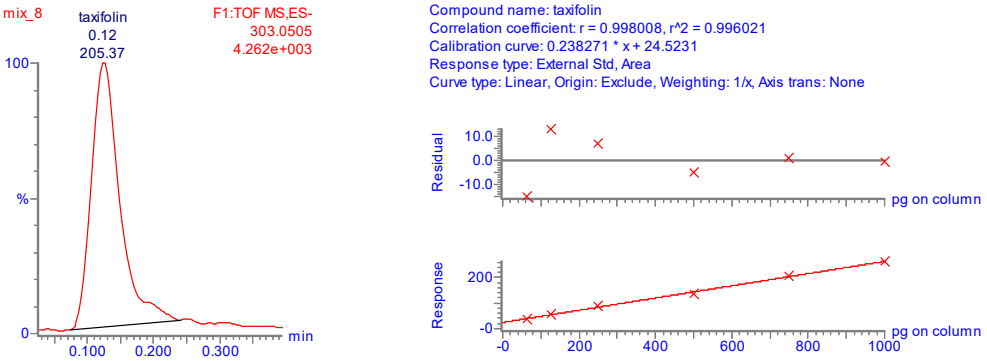

Figure S48. Compound summary report, illustrative trace and calibration curve and residuals of taxifolin.

Quantify Compound Summary Report

Compound 19: neobavaisoflavone

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	71.476	30.000	23.86
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	131.955	62.000	69.05
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	241.082	125.000	150.58
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	372.789	250.000	248.97
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	608.072	500.000	424.75
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	1007.374	750.000	723.07
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	1480.723	1000.000	1076.71
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.13	716.491		505.75
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.13	695.363		489.97
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	727.976		514.33
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.13	734.066		518.88
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.12	714.504		504.27
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	790.997		561.42
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	784.497		556.56
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte	0.13	54.521		11.20

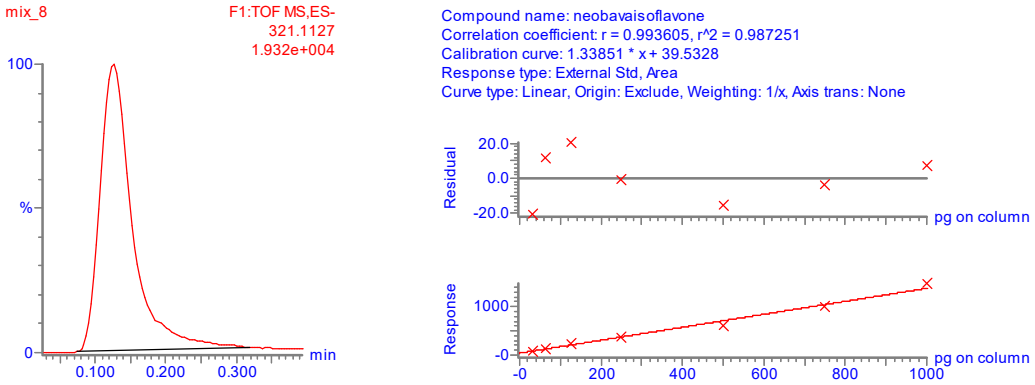

Figure S49. Compound summary report, illustrative trace and calibration curve and residuals of neobavaisoflavone.

Quantify Compound Summary Report

Compound 20: bavachin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.15	26.738	30.000	40.72
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.14	40.354	62.000	50.22
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.12	116.739	125.000	103.51
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	314.902	250.000	241.75
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.13	677.876	500.000	494.98
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	1094.790	750.000	785.83
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard			1000.000	
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte				
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte				
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

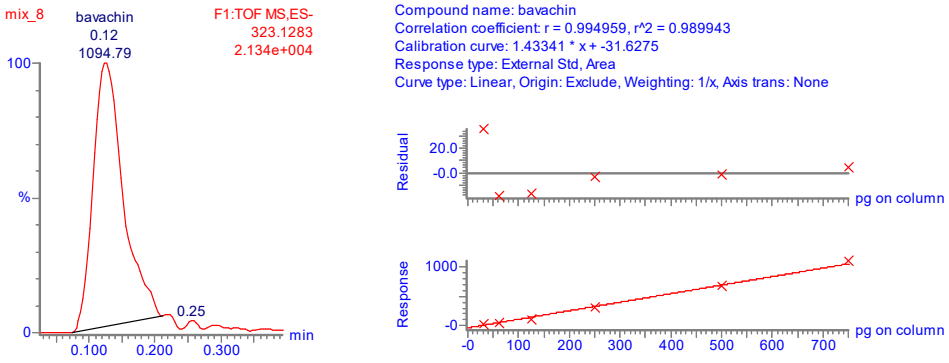

Figure S50. Compound summary report, illustrative trace and calibration curve and residuals of bavachin.

Quantify Compound Summary Report

Compound 21: mirificin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.13	15.342	30.000	27.93
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.12	34.338	62.000	64.21
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	66.900	125.000	126.41
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.12	133.191	250.000	253.03
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.12	270.804	500.000	515.89
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	391.107	750.000	745.68
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	515.790	1000.000	983.84
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.12	557.745		1063.98
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.12	555.772		1060.21
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.12	555.293		1059.29
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.12	579.982		1106.45
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.12	581.932		1110.18
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	551.650		1052.34
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.12	557.308		1063.14
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

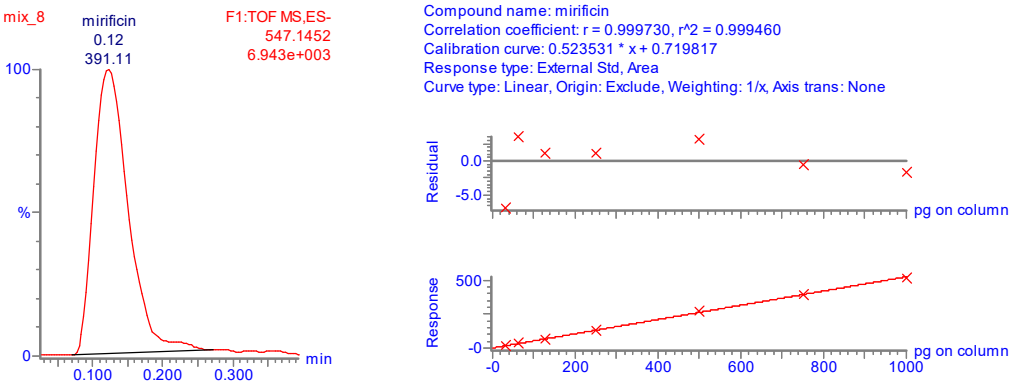

Figure S51 Compound summary report, illustrative trace and calibration curve and residuals of mirificin.

Quantify Compound Summary Report

Compound 22: amentoflavone

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard			30.000	
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.14	50.204	62.000	47.10
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	124.574	125.000	139.96
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.13	236.332	250.000	279.50
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.14	453.327	500.000	550.43
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.13	569.544	750.000	695.54
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	792.946	1000.000	974.48
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.13	899.198		1107.14
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.13	942.571		1161.30
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.13	957.291		1179.68
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.13	958.714		1181.45
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.13	981.280		1209.63
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	1140.533		1408.47
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	1059.169		1306.88
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

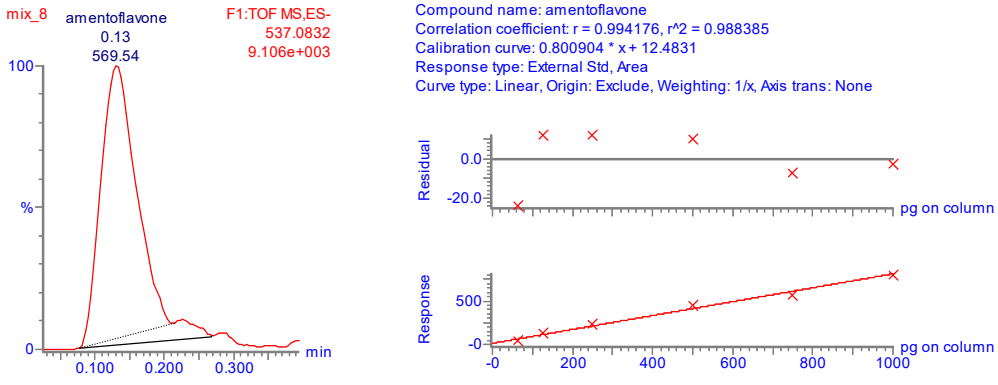

Figure S52. Compound summary report, illustrative trace and calibration curve and residuals of amentoflavone.

Quantify Compound Summary Report

Compound 23: silibinin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.12	82.636	41.000	22.92
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.12	196.115	81.000	86.84
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.12	400.603	161.000	202.02
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.12	693.649	312.000	367.09
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.12	1203.328	625.000	654.18
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	1584.023	940.000	868.61
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.13	2187.152	1250.000	1208.34
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte	0.12	71.875		16.86
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte	0.12	63.463		12.12
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte	0.12	2085.604		1151.14
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte	0.13	2126.746		1174.31
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte	0.12	2188.967		1209.36
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte	0.12	2089.611		1153.39
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte	0.12	2018.057		1113.09
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte	0.13	2105.498		1162.34
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte	0.13	2050.471		1131.35
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte	0.13	90.392		27.29

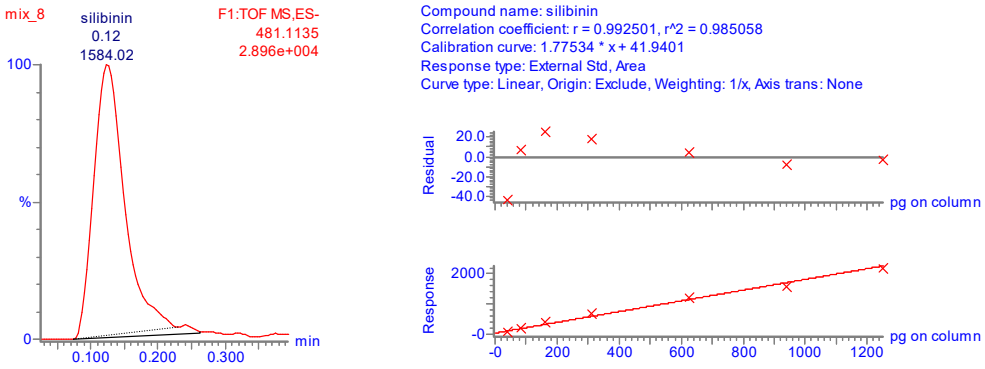

Figure S53. Compound summary report, illustrative trace and calibration curve and residuals of silibinin.

Quantify Compound Summary Report

Compound 24: jaceosidin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3			30.000	
2	2	synapt_cvb_quat_FIA_002	mix_4			62.000	
3	3	synapt_cvb_quat_FIA_003	mix_5			125.000	
4	4	synapt_cvb_quat_FIA_004	mix_6			250.000	
5	5	synapt_cvb_quat_FIA_005	mix_7	0.13	9.511	500.000	520.58
6	6	synapt_cvb_quat_FIA_006	mix_8	0.13	10.930	750.000	688.27
7	7	synapt_cvb_quat_FIA_007	mix_9	0.17	13.916	1000.000	1041.15
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary				
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary				
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary				

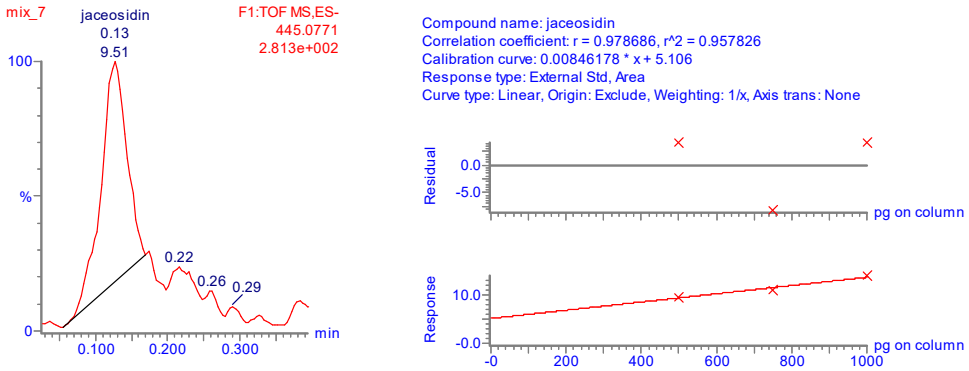

Figure S54. Compound summary report, illustrative trace and calibration curve and residuals of jaceosidin.

Quantify Compound Summary Report

Compound 25: rhoifolin

	#	Name	Sample Text	Type	RT	Area	Std. Conc	pg on column
1	1	synapt_cvb_quat_FIA_001	mix_3	Standard	0.14	10.667	30.000	28.40
2	2	synapt_cvb_quat_FIA_002	mix_4	Standard	0.13	14.670	62.000	62.12
3	3	synapt_cvb_quat_FIA_003	mix_5	Standard	0.13	23.788	125.000	138.92
4	4	synapt_cvb_quat_FIA_004	mix_6	Standard	0.12	34.971	250.000	233.11
5	5	synapt_cvb_quat_FIA_005	mix_7	Standard	0.14	66.021	500.000	494.65
6	6	synapt_cvb_quat_FIA_006	mix_8	Standard	0.12	99.339	750.000	775.28
7	7	synapt_cvb_quat_FIA_007	mix_9	Standard	0.12	124.179	1000.000	984.51
8	8	synapt_cvb_quat_FIA_008	vial 1 quaternary	Analyte				
9	9	synapt_cvb_quat_FIA_009	vial 2 quaternary	Analyte				
10	10	synapt_cvb_quat_FIA_010	vial 3 quaternary	Analyte				
11	11	synapt_cvb_quat_FIA_011	vial 4 quaternary	Analyte				
12	12	synapt_cvb_quat_FIA_012	vial 5 quaternary	Analyte				
13	13	synapt_cvb_quat_FIA_013	vial 6 quaternary	Analyte				
14	14	synapt_cvb_quat_FIA_014	vial 7 quaternary	Analyte				
15	15	synapt_cvb_quat_FIA_015	vial 8 quaternary	Analyte				
16	16	synapt_cvb_quat_FIA_016	vial 9 quaternary	Analyte				
17	17	synapt_cvb_quat_FIA_017	vial 10 quaternary	Analyte				

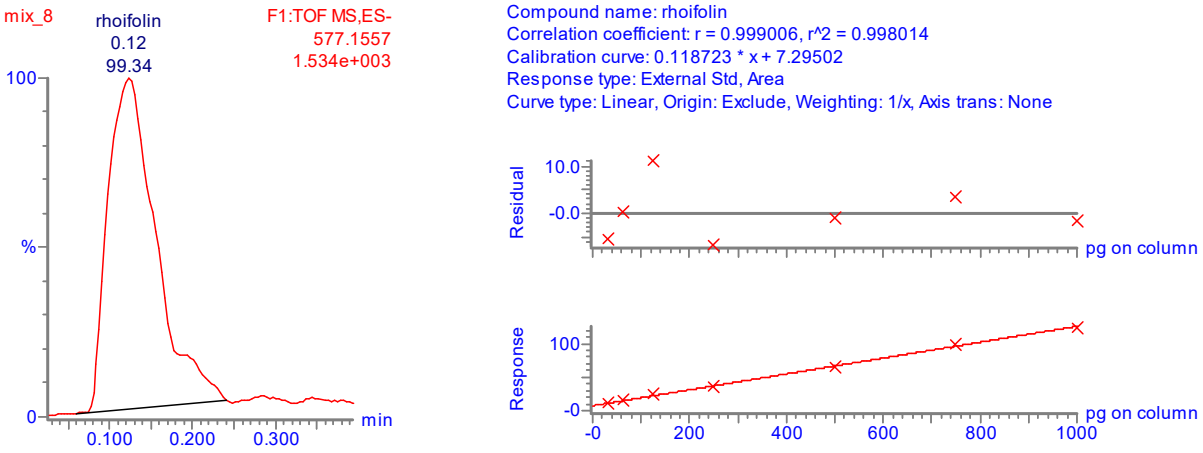

Figure S55. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

***Encoded message and decoded method*:** octal encoding scheme of the Flavonoids word using LC-MS as decoding method. The list of metabolites used to encode this message is given in Table S4. Analyte concentrations ranged from 50 to 1500 ppb to depict the 1 to 7 states.

Table S4

Text
Flavonoids

Set of 27 metabolites used for text encoding

				octal encoding
	Compound	**formula**	**[M-H]- ion (m/z)**	**vial1**
1	5,7 dihydroxichromone	C9H6O4	177,0188	1
2	wogonoside	C22H20O11	459,0927	0
3	4-hydroxychalcone	C15H12O2	223,0759	6
4	silibinin	C25H22O10	237,0552	3
5	formononetin	C16H12O4	267,0657	3
6	rhoifolin	C27H30O14	577,1557	0
7	baicalein	C15H10O5	269,045	6
8	bavachin	C30H18O10	323,1283	0
9	naringenin	C15H12O5	271,0606	5
10	acacetin	C16H12O5	283,0606	6
11	scutellarein	C15H10O6	285,0399	6
12	eriodictyol	C15H12O6	287,0556	3
13	epicatechin	C15H14O6	289,0712	3
14	tectorigenin	C16H12O6	299,0556	6
15	herbacetin	C15H10O7	301,0348	6
16	taxifolin	C15H12O7	303,0505	7
17	6-hydroxiflavone	C15H10O3	317,0297	1
18	neobavaisoflavone	C20H18O4	321,1127	5
19	amentoflavone	C20H20O4	323,1283	7
20	orientin	C21H20O11	447,0927	3
21	eupatilin	C18H16O7	343,0818	2
22	guayjaverin	C21H22O5	353,1389	2
23	morusin	C21H20O6	367,1182	6
24	colyfoil A	C19H18O8	373,0923	2
25	isoquercetin	C21H20O12	463,088	1
26	isoxanthohumol	C21H22O5	353,1389	6
27	baicalin	C21H18O11	445,0771	3

Quantify compound summary report for the word Flavonoids using an octal encoding scheme and LC-MS as decoding method

Quantify Compound Summary Report

Compound 1: 5,7 dihydroxichromone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1	2.12	59.103	15.000	14.29
2	2	scic_synapt_cvb_code_370	mix_2	2.12	151.615	31.000	28.70
3	3	scic_synapt_cvb_code_371	mix_3	2.11	322.803	62.000	55.36
4	4	scic_synapt_cvb_code_372	mix_4	2.11	703.505	125.000	114.66
5	5	scic_synapt_cvb_code_373	mix_5	2.11	1532.625	250.000	243.80
6	6	scic_synapt_cvb_code_374	mix_6	2.11	3405.593	500.000	535.52
7	7	scic_synapt_cvb_code_375	mix_7	2.12	6295.130	1000.000	985.58
8	8	scic_synapt_cvb_code_386	octal_UPLC	2.11	261.545		45.82

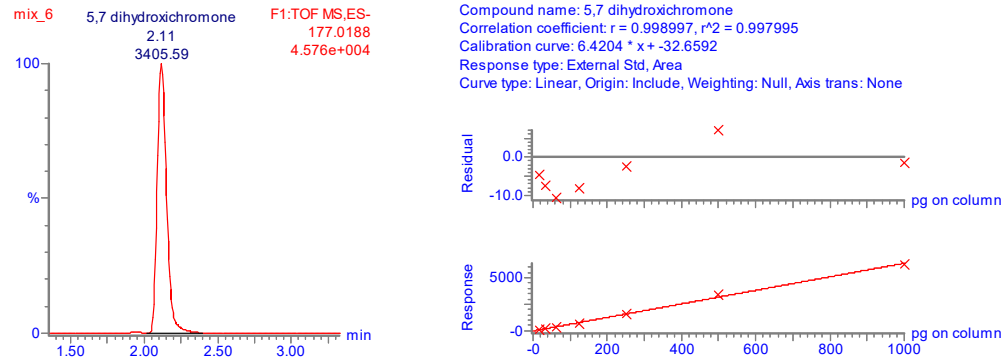

Figure S56. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 2: wogonoside

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	3.12	43.160	31.000	43.01
3	3	scic_synapt_cvb_code_371	mix_3	3.13	102.878	62.000	59.08
4	4	scic_synapt_cvb_code_372	mix_4	3.13	286.617	125.000	108.50
5	5	scic_synapt_cvb_code_373	mix_5	3.13	683.070	250.000	215.13
6	6	scic_synapt_cvb_code_374	mix_6	3.13	1744.272	500.000	500.57
7	7	scic_synapt_cvb_code_375	mix_7	3.13	3639.333	1000.000	1010.30
8	8	scic_synapt_cvb_code_386	octal_UPLC				

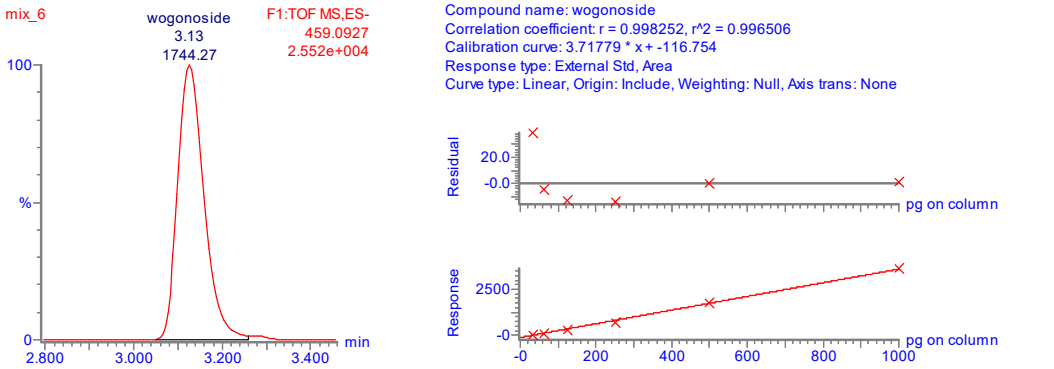

Figure S57. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 3: 4-hydroxychalcone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	4.53	878.672	31.000	12.09
3	3	scic_synapt_cvb_code_371	mix_3	4.53	1953.209	62.000	54.72
4	4	scic_synapt_cvb_code_372	mix_4	4.54	3880.825	125.000	131.20
5	5	scic_synapt_cvb_code_373	mix_5	4.53	7449.261	250.000	272.78
6	6	scic_synapt_cvb_code_374	mix_6	4.53	14457.224	500.000	550.81
7	7	scic_synapt_cvb_code_375	mix_7	4.54	25001.736	1000.000	969.16
8	8	scic_synapt_cvb_code_386	octal_UPLC	4.53	24776.693		960.23

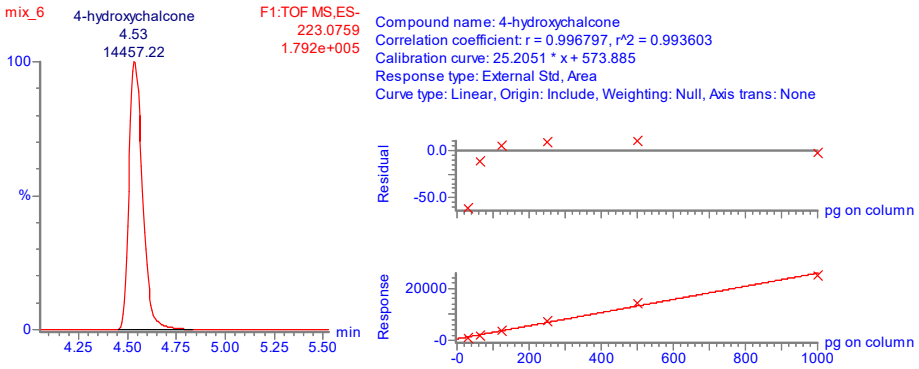

Figure S58. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 4: silibinin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			19.000	
2	2	scic_synapt_cvb_code_370	mix_2	3.30	858.473	39.000	14.00
3	3	scic_synapt_cvb_code_371	mix_3	3.30	2047.982	78.000	69.51
4	4	scic_synapt_cvb_code_372	mix_4	3.30	4056.903	156.000	163.26
5	5	scic_synapt_cvb_code_373	mix_5	3.30	7779.555	312.000	336.99
6	6	scic_synapt_cvb_code_374	mix_6	3.31	15371.694	625.000	691.29
7	7	scic_synapt_cvb_code_375	mix_7	3.31	26508.715	1250.000	1211.02
8	8	scic_synapt_cvb_code_386	octal_UPLC	3.30	5253.510		219.10

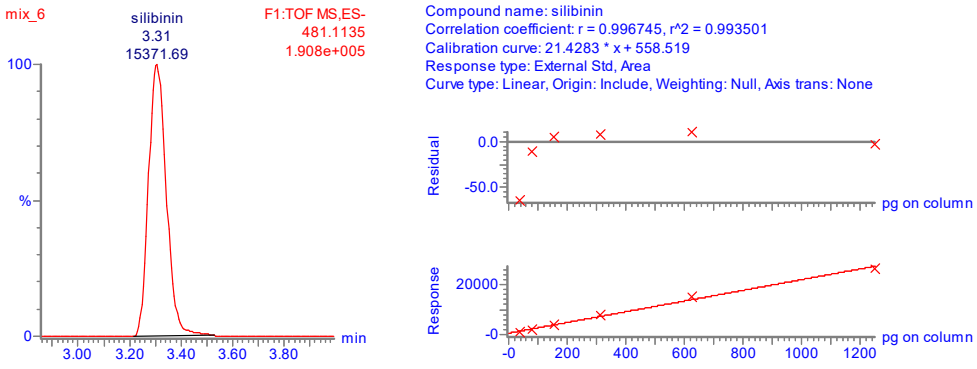

Figure S59. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 5: formononetin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	4.01	417.994	31.000	17.49
3	3	scic_synapt_cvb_code_371	mix_3	4.01	927.586	62.000	51.52
4	4	scic_synapt_cvb_code_372	mix_4	4.01	2059.845	125.000	127.14
5	5	scic_synapt_cvb_code_373	mix_5	4.01	4055.389	250.000	260.41
6	6	scic_synapt_cvb_code_374	mix_6	4.01	8352.141	500.000	547.36
7	7	scic_synapt_cvb_code_375	mix_7	4.01	14748.335	1000.000	974.52
8	8	scic_synapt_cvb_code_386	octal_UPLC	4.00	4042.777		259.56

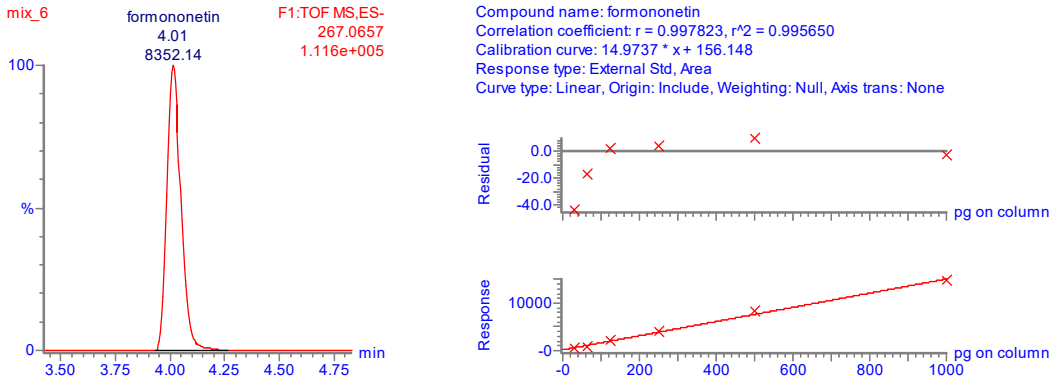

Figure S60. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 6: rhofolin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1	2.18	23.807	15.000	21.37
2	2	scic_synapt_cvb_code_370	mix_2	2.17	76.036	31.000	33.53
3	3	scic_synapt_cvb_code_371	mix_3	2.16	177.487	62.000	57.15
4	4	scic_synapt_cvb_code_372	mix_4	2.17	380.722	125.000	104.47
5	5	scic_synapt_cvb_code_373	mix_5	2.17	922.688	250.000	230.64
6	6	scic_synapt_cvb_code_374	mix_6	2.17	2186.892	500.000	524.95
7	7	scic_synapt_cvb_code_375	mix_7	2.17	4206.244	1000.000	995.06
8	8	scic_synapt_cvb_code_386	octal_UPLC				

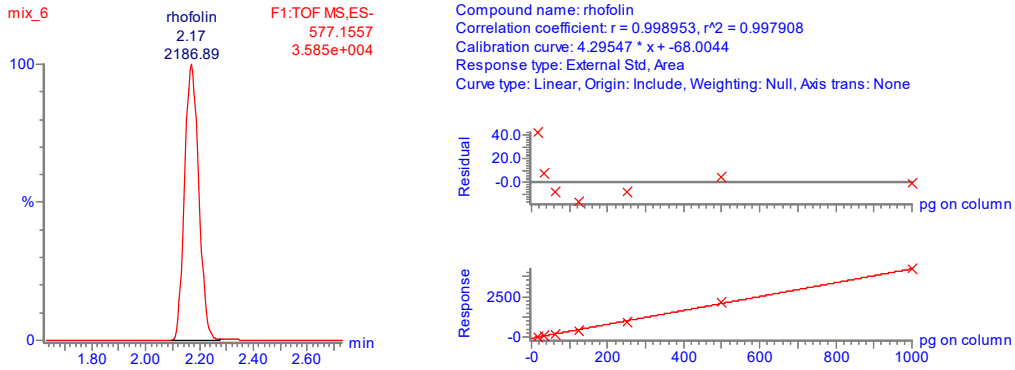

Figure S61. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 7: baicalein

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2			31.000	
3	3	scic_synapt_cvb_code_371	mix_3	3.78	74.274	62.000	73.86
4	4	scic_synapt_cvb_code_372	mix_4	3.78	171.970	125.000	100.77
5	5	scic_synapt_cvb_code_373	mix_5	3.78	511.854	250.000	194.40
6	6	scic_synapt_cvb_code_374	mix_6	3.79	1609.438	500.000	496.76
7	7	scic_synapt_cvb_code_375	mix_7	3.79	3500.905	1000.000	1017.81
8	8	scic_synapt_cvb_code_386	octal_UPLC	3.78	3784.695		1095.99

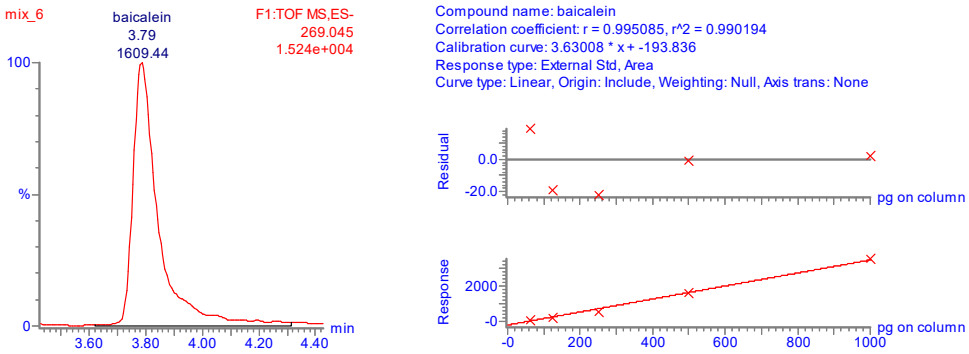

Figure S62. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 8: bavachin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	5.11	902.596	31.000	9.06
3	3	scic_synapt_cvb_code_371	mix_3	5.11	1899.630	62.000	52.68
4	4	scic_synapt_cvb_code_372	mix_4	5.11	3742.976	125.000	133.34
5	5	scic_synapt_cvb_code_373	mix_5	5.11	6906.056	250.000	271.76
6	6	scic_synapt_cvb_code_374	mix_6	5.12	13805.264	500.000	573.65
7	7	scic_synapt_cvb_code_375	mix_7	5.12	22587.588	1000.000	957.95
8	8	scic_synapt_cvb_code_386	octal_UPLC	5.12	4.437		

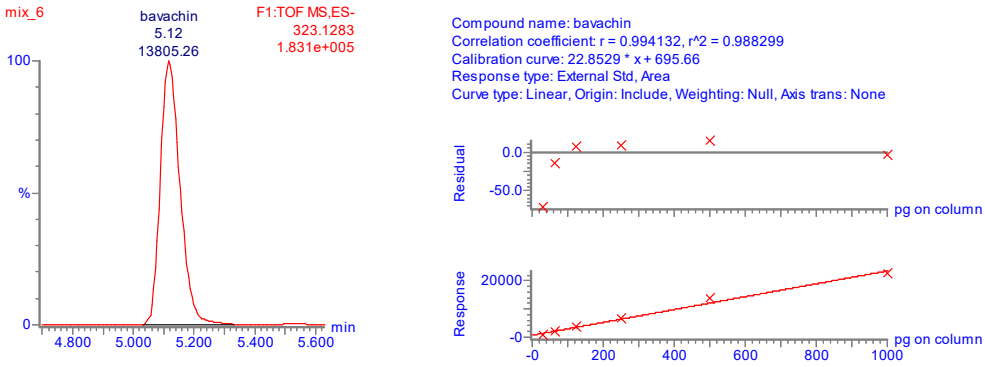

Figure S63. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 9: naringenin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	3.37	210.008	31.000	17.31
3	3	scic_synapt_cvb_code_371	mix_3	3.36	529.600	62.000	51.96
4	4	scic_synapt_cvb_code_372	mix_4	3.36	1185.222	125.000	123.03
5	5	scic_synapt_cvb_code_373	mix_5	3.36	2423.286	250.000	257.25
6	6	scic_synapt_cvb_code_374	mix_6	3.36	5113.041	500.000	548.85
7	7	scic_synapt_cvb_code_375	mix_7	3.37	9044.392	1000.000	975.05
8	8	scic_synapt_cvb_code_386	octal_UPLC	3.36	6179.295		664.45

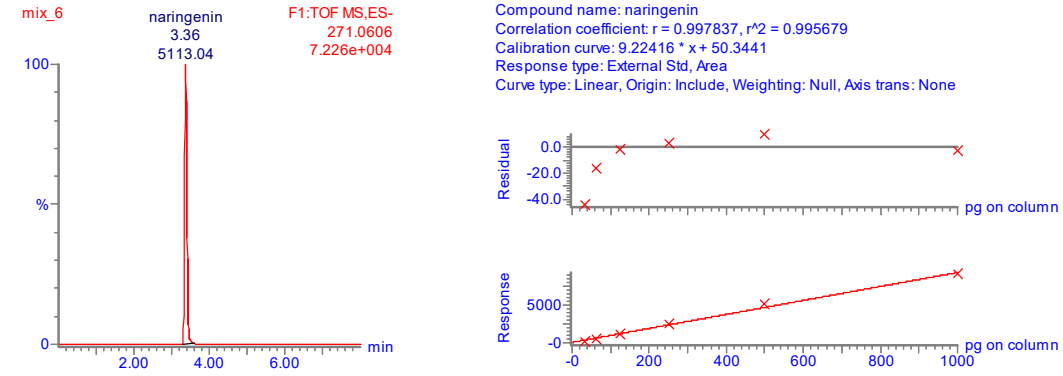

Figure S64. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 10: acacetin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	4.63	305.161	31.000	19.52
3	3	scic_synapt_cvb_code_371	mix_3	4.64	806.182	62.000	52.20
4	4	scic_synapt_cvb_code_372	mix_4	4.64	1823.192	125.000	118.54
5	5	scic_synapt_cvb_code_373	mix_5	4.64	3865.518	250.000	251.76
6	6	scic_synapt_cvb_code_374	mix_6	4.64	8438.804	500.000	550.08
7	7	scic_synapt_cvb_code_375	mix_7	4.64	14972.639	1000.000	976.29
8	8	scic_synapt_cvb_code_386	octal_UPLC	4.63	15238.568		993.64

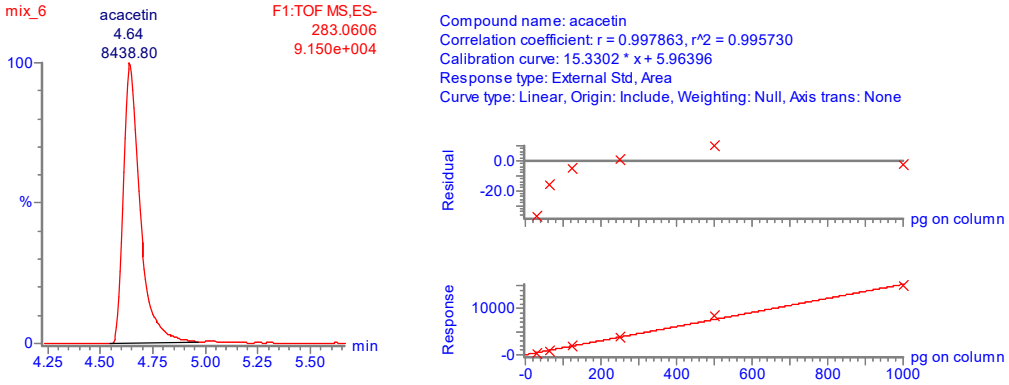

Figure S65. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 11: scutellarein

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2			31.000	
3	3	scic_synapt_cvb_code_371	mix_3	2.85	28.348	62.000	88.96
4	4	scic_synapt_cvb_code_372	mix_4	2.85	64.918	125.000	126.39
5	5	scic_synapt_cvb_code_373	mix_5	2.85	153.791	250.000	217.37
6	6	scic_synapt_cvb_code_374	mix_6	2.86	308.817	500.000	376.07
7	7	scic_synapt_cvb_code_375	mix_7	2.54	985.020	1000.000	1068.28
8	8	scic_synapt_cvb_code_386	octal_UPLC	2.53	913.212		994.77

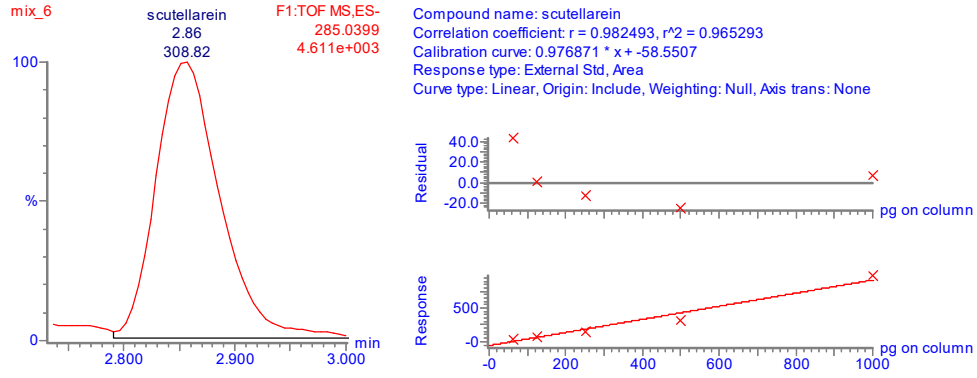

Figure S66. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 12: eriodictyol

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	2.85	27.551	31.000	38.84
3	3	scic_synapt_cvb_code_371	mix_3	2.84	103.617	62.000	66.37
4	4	scic_synapt_cvb_code_372	mix_4	2.85	221.306	125.000	108.98
5	5	scic_synapt_cvb_code_373	mix_5	2.84	512.299	250.000	214.31
6	6	scic_synapt_cvb_code_374	mix_6	2.85	1302.762	500.000	500.45
7	7	scic_synapt_cvb_code_375	mix_7	2.86	2710.902	1000.000	1010.19
8	8	scic_synapt_cvb_code_386	octal_UPLC	2.84	517.859		216.32

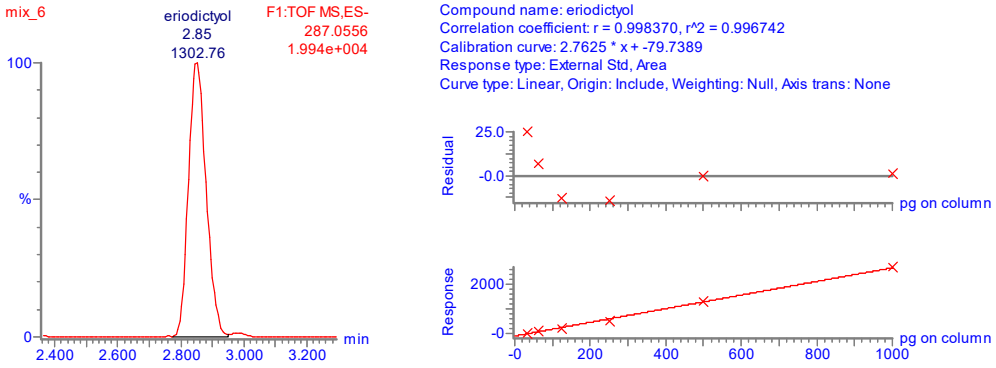

Figure S67. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 13: epicatechin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column	
1	1	scic_synapt_cvb_code_369		mix_1			15.000	
2	2	scic_synapt_cvb_code_370		mix_2	1.29	45.139	31.000	40.02
3	3	scic_synapt_cvb_code_371		mix_3	1.29	121.176	62.000	64.61
4	4	scic_synapt_cvb_code_372		mix_4	1.28	256.175	125.000	108.28
5	5	scic_synapt_cvb_code_373		mix_5	1.28	575.222	250.000	211.46
6	6	scic_synapt_cvb_code_374		mix_6	1.29	1510.141	500.000	513.85
7	7	scic_synapt_cvb_code_375		mix_7	1.29	3026.739	1000.000	1004.36
8	8	scic_synapt_cvb_code_386		octal_UPLC	1.28	501.891		187.75

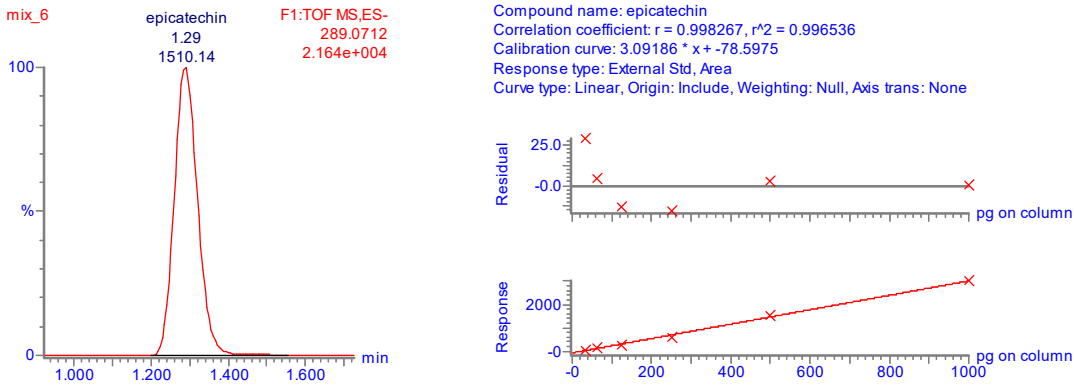

Figure S68. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 14: tectorigenin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1	3.42	68.822	15.000	12.84
2	2	scic_synapt_cvb_code_370	mix_2	3.42	146.357	31.000	23.08
3	3	scic_synapt_cvb_code_371	mix_3	3.42	369.041	62.000	52.51
4	4	scic_synapt_cvb_code_372	mix_4	3.42	863.054	125.000	117.78
5	5	scic_synapt_cvb_code_373	mix_5	3.42	1885.165	250.000	252.82
6	6	scic_synapt_cvb_code_374	mix_6	3.42	4046.002	500.000	538.32
7	7	scic_synapt_cvb_code_375	mix_7	3.43	7403.305	1000.000	981.90
8	8	scic_synapt_cvb_code_386	octal_UPLC	3.42	8043.519		1066.49

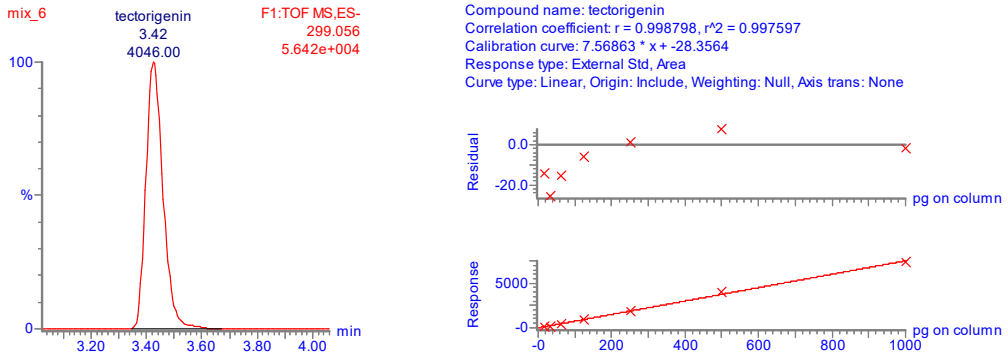

Figure S69. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 15: herbacetin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2			31.000	
3	3	scic_synapt_cvb_code_371	mix_3	2.71	3.148	62.000	74.71
4	4	scic_synapt_cvb_code_372	mix_4	2.71	12.832	125.000	108.44
5	5	scic_synapt_cvb_code_373	mix_5	2.72	41.434	250.000	208.09
6	6	scic_synapt_cvb_code_374	mix_6	2.72	108.146	500.000	440.52
7	7	scic_synapt_cvb_code_375	mix_7	2.73	280.641	1000.000	1041.50
8	8	scic_synapt_cvb_code_386	octal_UPLC	2.72	309.612		1142.43

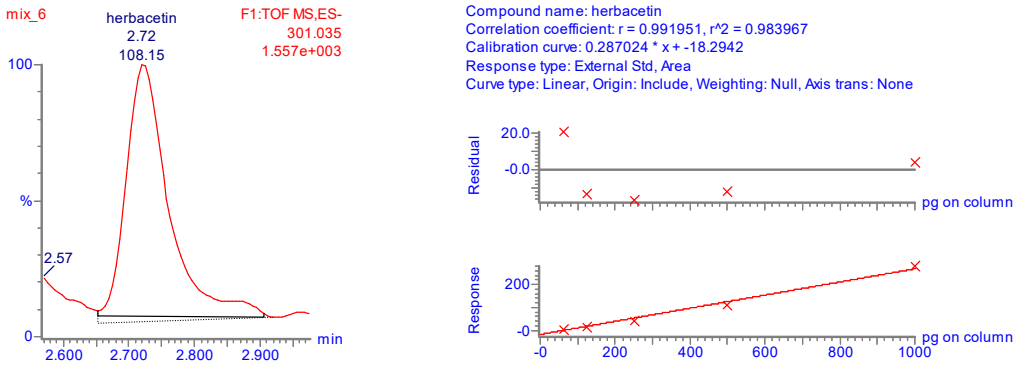

Figure S70. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 16: taxifolin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	1.92	29.726	31.000	47.37
3	3	scic_synapt_cvb_code_371	mix_3	1.93	78.459	62.000	75.61
4	4	scic_synapt_cvb_code_372	mix_4	1.93	148.876	125.000	116.42
5	5	scic_synapt_cvb_code_373	mix_5	1.93	294.425	250.000	200.77
6	6	scic_synapt_cvb_code_374	mix_6	1.93	761.322	500.000	471.34
7	7	scic_synapt_cvb_code_375	mix_7	1.93	1719.030	1000.000	1026.36
8	8	scic_synapt_cvb_code_386	octal_UPLC	1.93	2980.249		1757.26

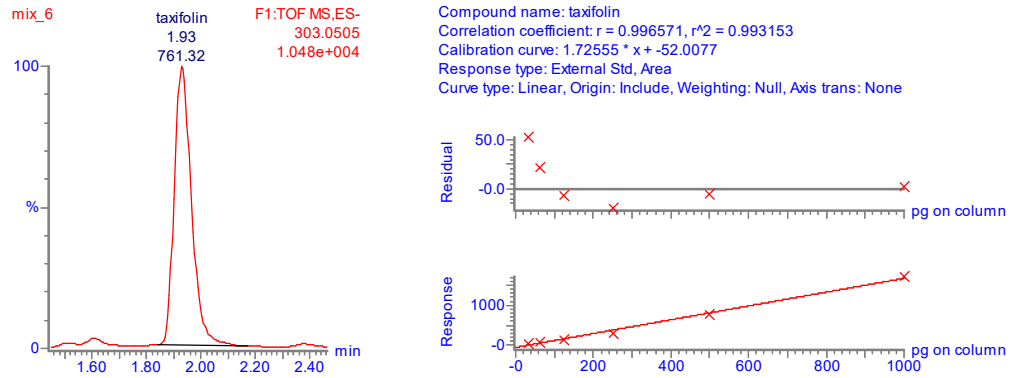

Figure S71. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 17: 6-hydroxiflavone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1	4.05	46.786	15.000	13.57
2	2	scic_synapt_cvb_code_370	mix_2	4.05	137.452	31.000	27.73
3	3	scic_synapt_cvb_code_371	mix_3	4.05	293.756	62.000	52.15
4	4	scic_synapt_cvb_code_372	mix_4	4.06	679.890	125.000	112.46
5	5	scic_synapt_cvb_code_373	mix_5	4.06	1524.147	250.000	244.34
6	6	scic_synapt_cvb_code_374	mix_6	4.06	3452.583	500.000	545.57
7	7	scic_synapt_cvb_code_375	mix_7	4.06	6239.774	1000.000	980.93
8	8	scic_synapt_cvb_code_386	octal_UPLC	4.05	210.903		39.20

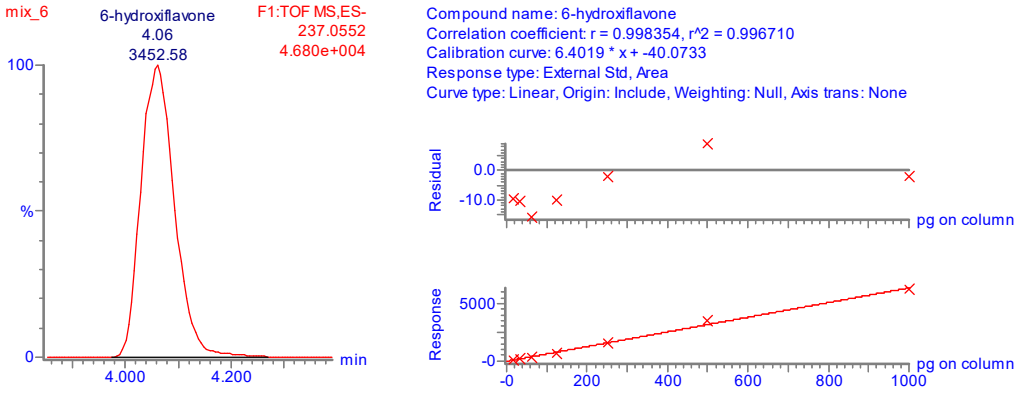

Figure S72. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 18: neobavaisoflavone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	4.90	680.627	31.000	19.10
3	3	scic_synapt_cvb_code_371	mix_3	4.90	1346.400	62.000	53.60
4	4	scic_synapt_cvb_code_372	mix_4	4.91	2775.128	125.000	127.63
5	5	scic_synapt_cvb_code_373	mix_5	4.91	5432.916	250.000	265.34
6	6	scic_synapt_cvb_code_374	mix_6	4.91	10802.563	500.000	543.56
7	7	scic_synapt_cvb_code_375	mix_7	4.91	19128.072	1000.000	974.95
8	8	scic_synapt_cvb_code_386	octal_UPLC	4.90	14001.161		709.30

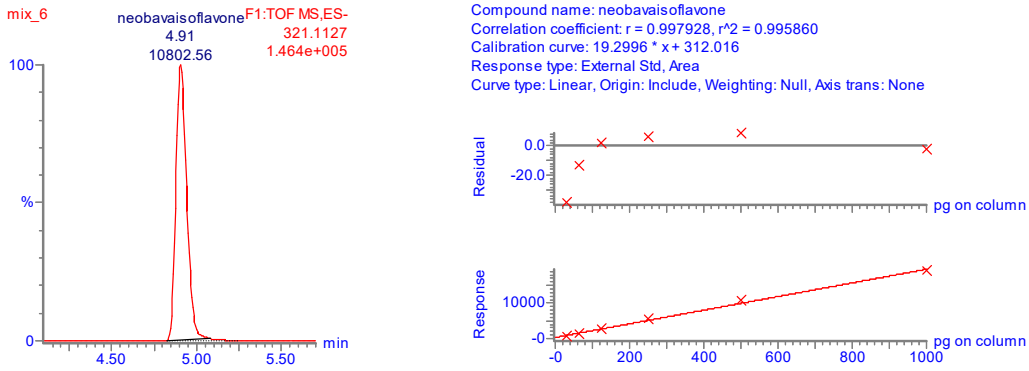

Figure S73. Compound summary report, illustrative trace and calibration curve and residuals of rhoifolin.

Compound 19: amentoflavone

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1	3.91	78.705	15.000	16.71
2	2	scic_synapt_cvb_code_370	mix_2	3.91	157.512	31.000	26.85
3	3	scic_synapt_cvb_code_371	mix_3	3.91	348.710	62.000	51.46
4	4	scic_synapt_cvb_code_372	mix_4	3.91	822.110	125.000	112.39
5	5	scic_synapt_cvb_code_373	mix_5	3.91	1837.055	250.000	243.03
6	6	scic_synapt_cvb_code_374	mix_6	3.91	4173.924	500.000	543.81
7	7	scic_synapt_cvb_code_375	mix_7	3.92	7579.639	1000.000	982.17
8	8	scic_synapt_cvb_code_386	octal_UPLC	3.91	11539.968		1491.91

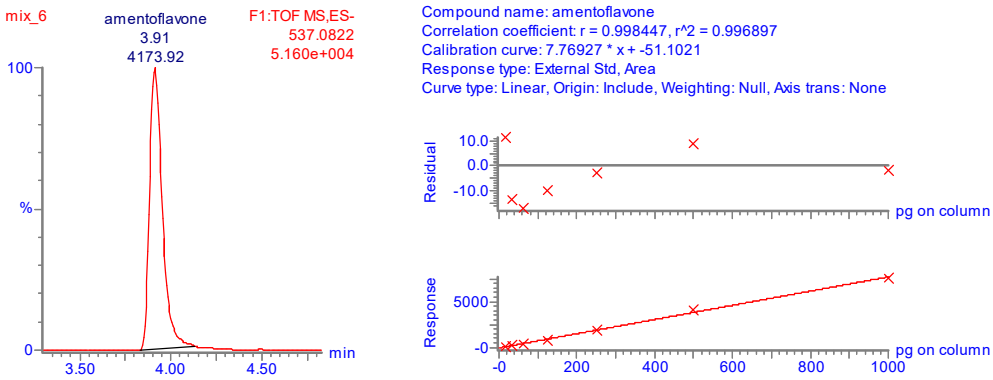

Figure S74. Compound summary report, illustrative trace and calibration curve and residuals of amentoflavone.

Compound 20: orientin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	1.56	43.695	31.000	42.32
3	3	scic_synapt_cvb_code_371	mix_3	1.56	106.842	62.000	59.58
4	4	scic_synapt_cvb_code_372	mix_4	1.56	283.617	125.000	107.89
5	5	scic_synapt_cvb_code_373	mix_5	1.56	678.754	250.000	215.88
6	6	scic_synapt_cvb_code_374	mix_6	1.57	1729.200	500.000	502.97
7	7	scic_synapt_cvb_code_375	mix_7	1.57	3580.664	1000.000	1008.98
8	8	scic_synapt_cvb_code_386	octal_UPLC	1.56	690.415		219.07

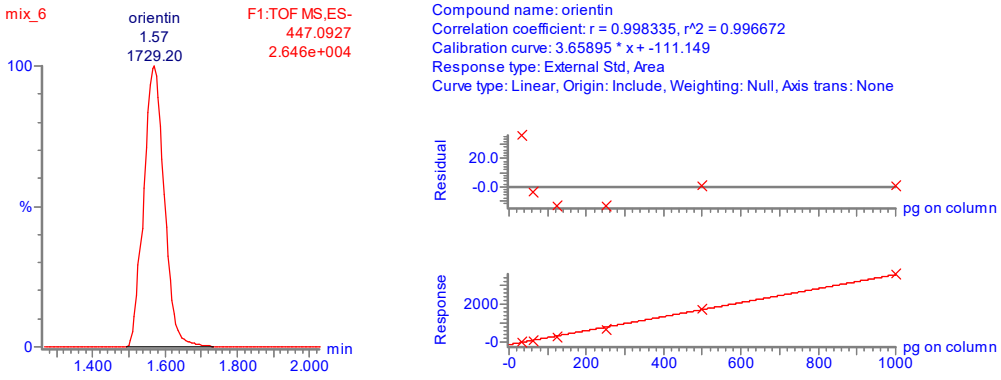

Figure S75. Compound summary report, illustrative trace and calibration curve and residuals of orientin.

Compound 21: eupatilin

column	#	Name	Sample Text	RT	Area	Std. Conc	pg on
1	1	scic_synapt_cvb_code_369	mix_1	4.26	99.221	15.000	10.64
2	2	scic_synapt_cvb_code_370	mix_2	4.26	228.406	31.000	21.89
3	3	scic_synapt_cvb_code_371	mix_3	4.26	567.127	62.000	51.40
4	4	scic_synapt_cvb_code_372	mix_4	4.27	1367.583	125.000	121.13
5	5	scic_synapt_cvb_code_373	mix_5	4.27	2917.689	250.000	256.16
6	6	scic_synapt_cvb_code_374	mix_6	4.27	6172.097	500.000	539.66
7	7	scic_synapt_cvb_code_375	mix_7	4.27	11228.264	1000.000	980.12
8	8	scic_synapt_cvb_code_386	octal_UPLC	4.26	1419.353		125.64

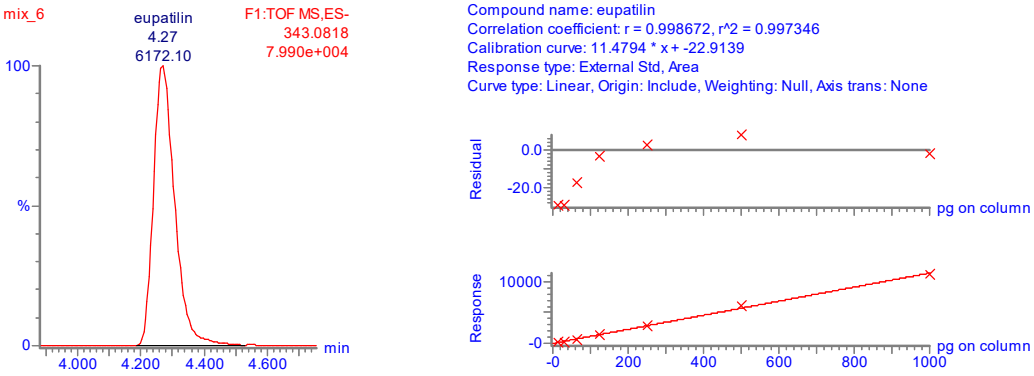

Figure S76. Compound summary report, illustrative trace and calibration curve and residuals of eupatilin.

Compound 22: guayjaverin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2	2.01	33.316	31.000	31.47
3	3	scic_synapt_cvb_code_371	mix_3	2.00	200.336	62.000	60.05
4	4	scic_synapt_cvb_code_372	mix_4	2.00	448.897	125.000	102.59
5	5	scic_synapt_cvb_code_373	mix_5	2.00	1191.257	250.000	229.62
6	6	scic_synapt_cvb_code_374	mix_6	2.00	2894.061	500.000	521.00
7	7	scic_synapt_cvb_code_375	mix_7	2.01	5678.770	1000.000	997.51
8	8	scic_synapt_cvb_code_386	octal_UPLC	2.00	480.635		108.02

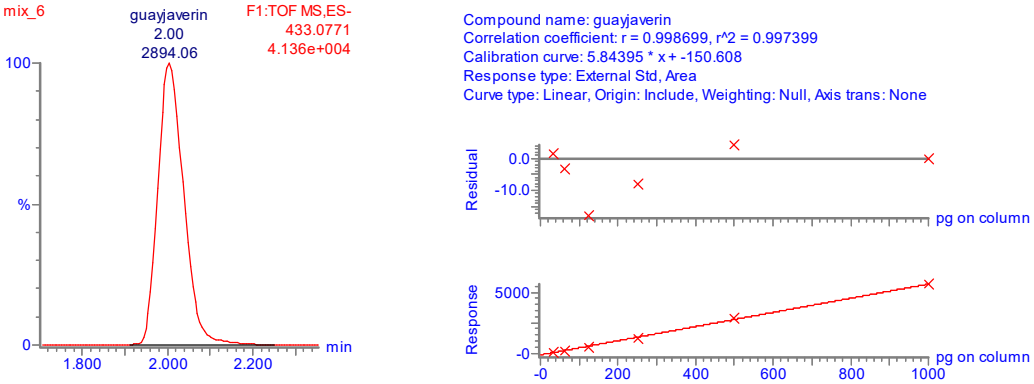

Figure S77 Compound summary report, illustrative trace and calibration curve and residuals of guayjaverin.

Compound 23: morusin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2			31.000	
3	3	scic_synapt_cvb_code_371	mix_3	7.08	1470.552	62.000	28.15
4	4	scic_synapt_cvb_code_372	mix_4	7.08	2696.771	125.000	151.43
5	5	scic_synapt_cvb_code_373	mix_5	7.08	4441.953	250.000	326.89
6	6	scic_synapt_cvb_code_374	mix_6	7.08	7569.297	500.000	641.30
7	7	scic_synapt_cvb_code_375	mix_7	7.08	10231.231	1000.000	908.92
8	8	scic_synapt_cvb_code_386	octal_UPLC	7.07	12611.355		1148.21

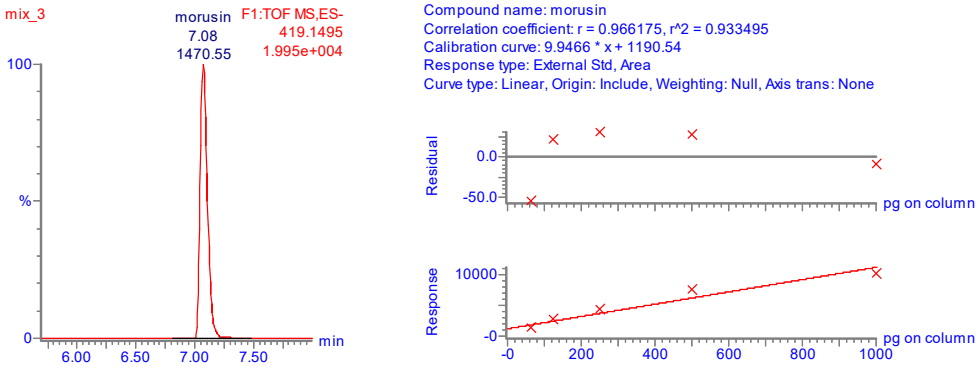

Figure S78. Compound summary report, illustrative trace and calibration curve and residuals of morusin.

Compound 24: corylifol A

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			19.000	
2	2	scic_synapt_cvb_code_370	mix_2			39.000	
3	3	scic_synapt_cvb_code_371	mix_3	6.62	1958.593	78.000	50.57
4	4	scic_synapt_cvb_code_372	mix_4	6.62	3717.063	156.000	169.98
5	5	scic_synapt_cvb_code_373	mix_5	6.62	6574.436	312.000	364.01
6	6	scic_synapt_cvb_code_374	mix_6	6.62	12093.059	625.000	738.75
7	7	scic_synapt_cvb_code_375	mix_7	6.63	18592.596	1250.000	1180.11
8	8	scic_synapt_cvb_code_386	octal_UPLC	6.62	3000.299		121.31

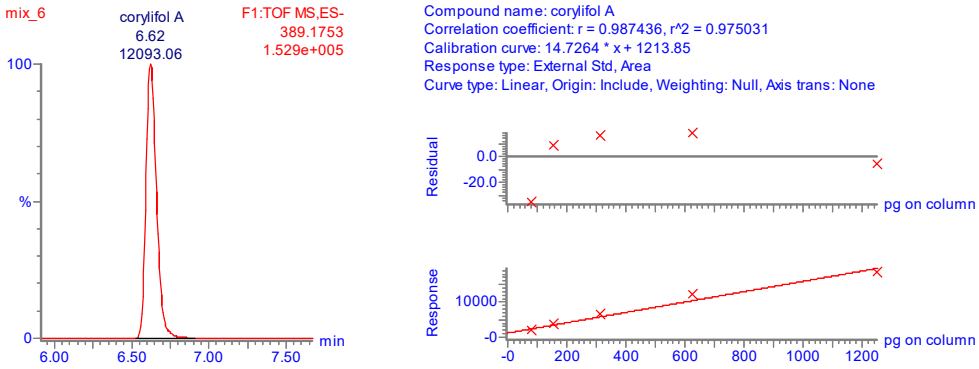

Figure S79. Compound summary report, illustrative trace and calibration curve and residuals of corylifol A.

Compound 25: isoquercetin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2			31.000	
3	3	scic_synapt_cvb_code_371	mix_3	3.30	4.717	62.000	61.52
4	4	scic_synapt_cvb_code_372	mix_4	3.31	10.367	125.000	167.64
5	5	scic_synapt_cvb_code_373	mix_5	3.30	14.016	250.000	236.18
6	6	scic_synapt_cvb_code_374	mix_6	3.31	28.124	500.000	501.16
7	7	scic_synapt_cvb_code_375	mix_7	3.31	54.554	1000.000	997.58
8	8	scic_synapt_cvb_code_386	octal_UPLC	3.30	5.118		69.05

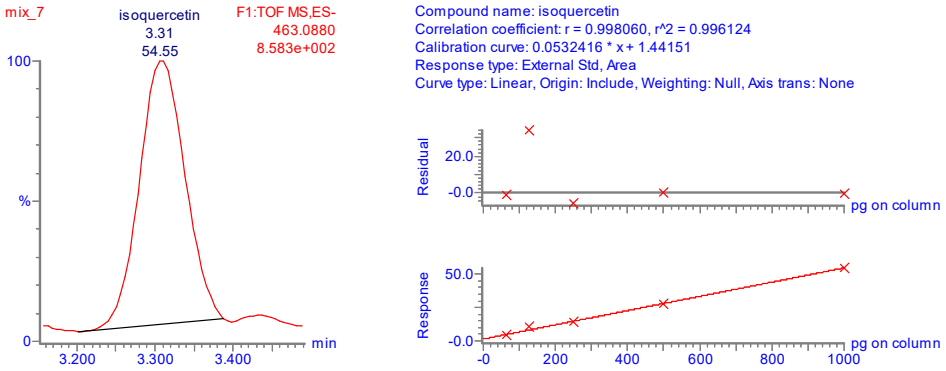

Figure S80. Compound summary report, illustrative trace and calibration curve and residuals of isoquercetin.

Compound 26: isoxanthohumol

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1			15.000	
2	2	scic_synapt_cvb_code_370	mix_2			31.000	
3	3	scic_synapt_cvb_code_371	mix_3			62.000	
4	4	scic_synapt_cvb_code_372	mix_4	1.17	4.241	125.000	137.16
5	5	scic_synapt_cvb_code_373	mix_5	1.17	6.437	250.000	231.80
6	6	scic_synapt_cvb_code_374	mix_6	1.18	14.917	500.000	597.24
7	7	scic_synapt_cvb_code_375	mix_7	1.18	23.205	1000.000	954.41
8	8	scic_synapt_cvb_code_386	octal_UPLC	1.18	21.408		876.97

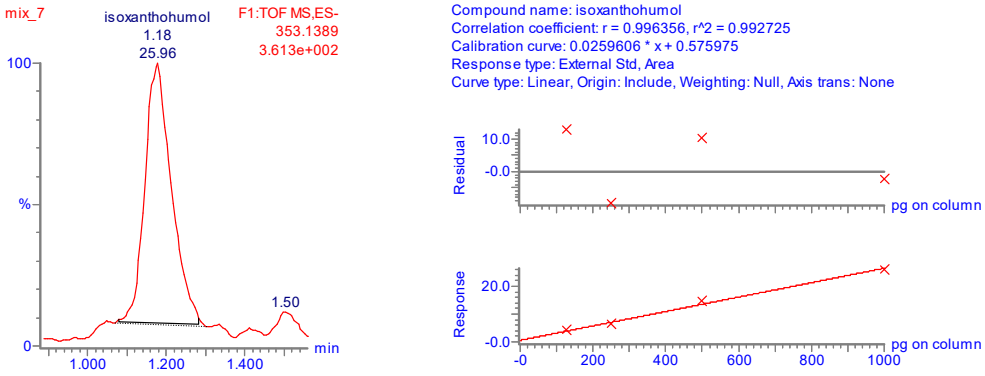

Figure S81. Compound summary report, illustrative trace and calibration curve and residuals of isoxanthohumol.

Compound 27: baicalin

	#	Name	Sample Text	RT	Area	Std. Conc	pg on column
1	1	scic_synapt_cvb_code_369	mix_1	1.58	8.631	15.000	15.51
2	2	scic_synapt_cvb_code_370	mix_2	1.57	20.224	31.000	29.15
3	3	scic_synapt_cvb_code_371	mix_3	1.56	44.693	62.000	57.94
4	4	scic_synapt_cvb_code_372	mix_4	1.56	103.311	125.000	126.92
5	5	scic_synapt_cvb_code_373	mix_5	1.56	200.865	250.000	241.71
6	6	scic_synapt_cvb_code_374	mix_6	1.57	427.646	500.000	508.55
7	7	scic_synapt_cvb_code_375	mix_7	1.57	843.482	1000.000	997.86
8	8	scic_synapt_cvb_code_386	octal_UPLC	1.56	157.125		190.24

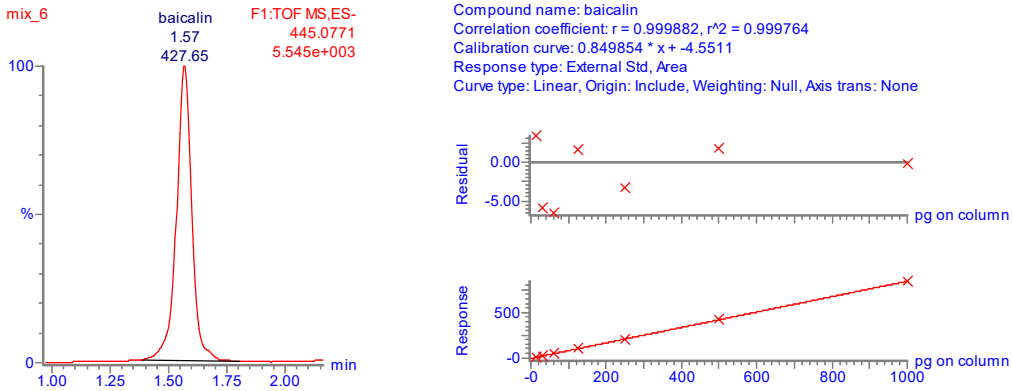

Figure S82. Compound summary report, illustrative trace and calibration curve and residuals of baicalin.

SI_1.7 Python scripts and MATLAB procedure for message retrieval

Python scripts for retrieval of binary-encoded abstract information

This Python script processes chemical mixture data to extract and binary-encode peak area information associated with specific compounds. It begins by reading an Excel file without predefined headers, dynamically identifying the location of the keyword "Compound", and subsequently extracting the list of compound names located beneath this label. It then parses a structured text file—generated as an output from automated TargetLynx processing—to locate and isolate blocks of data corresponding to each compound.

Within each block, only lines containing the term "vial" are considered, from which numeric peak area values are extracted. The script ensures a uniform vector of five values per compound, padding with zeros where necessary. These peak areas are then binarized according to a predefined threshold (values > 50 are encoded as "1", otherwise "0").

The resulting binary vectors are compiled into an output table and subsequently used to generate ASCII characters via 8-bit binary-to-character conversion. This is performed column-wise (per vial), and the resulting substrings are concatenated to construct a final decoded message, representing the presence or absence of compounds in a binary-encoded form.

File paths for both input and output files are fully customizable, rendering the script adaptable to a variety of experimental datasets.

The script employs the following Python libraries:

- pandas: For data manipulation and Excel file handling.
- openpyxl: Backend engine for reading .xlsx files using pandas.
- re: For regular expression-based pattern matching and text extraction.

Python scripts for retrieval of quaternary-encoded abstract information

This Python script processes quaternary-encoded data in chemical mixtures by classifying compound concentrations into discrete levels and generating corresponding visual representations. It begins by parsing an Excel file lacking predefined headers, in which it dynamically locates the cell containing the keyword "Compound" and extracts the list of compound names found beneath it.

Subsequently, the script reads a text file generated after automated processing and quantitation using TargetLynx, from which it isolates compound-specific data blocks. Within each block, only entries labeled as Analyte are selected, and their associated numeric values—corresponding to vial-specific concentration levels—are extracted. The script ensures that each compound is represented by a consistent set of ten vial values, padding with zeros when necessary.

Each concentration value is then classified into one of four predefined intensity categories (quaternary encoding: 0 to 3), based on empirically determined thresholds. These categorized values are stored in a

structured output table and used to construct a color-coded heatmap, which visually summarizes the quaternary-encoded dataset.

Two heatmap images are generated: one that preserves the raw matrix orientation and another that is rotated and flipped for improved visual interpretation. This dual-output format facilitates the inspection of encoded chemical mixture profiles and enhances compatibility with various hyphenated mass spectrometry platforms operating under different quantitation regimes. All file paths are user-configurable, allowing straightforward adaptation of the script to alternative experimental datasets.

The script employs the following Python libraries:

- pandas: For structured data handling and Excel file processing.
- openpyxl: Required by pandas to interface with .xlsx file formats.
- re: For compound-specific block identification via regular expressions.
- numpy: For numerical array manipulation and image matrix construction.
- PIL (Python Imaging Library): For image creation and export of heatmaps.

Python scripts for retrieval of octal-encoded abstract information

This Python script processes chemical mixture data to retrieve octal-encoded information mapped to specific compounds. It begins by reading an Excel file without predefined headers and dynamically locating the column containing the keyword "Compound", from which the list of compound names is extracted. Subsequently, a text file—generated following automated processing and quantitation via TargetLynx—is parsed to isolate data blocks corresponding to each compound.

Within each block, the script searches for lines labeled as octal_UPLC, from which it extracts a single vial-specific concentration value per compound. These values are then categorized into eight predefined intensity levels (0 to 7), according to empirically determined thresholds. The resulting classification is stored in a structured output table, providing an octal-encoded fingerprint for each compound.

Finally, the script converts the octal values into a binary bitstream (each category represented as 3 bits), trims or aligns the bitstream as needed (e.g., reducing 81 bits to 80), and groups the bits into bytes. These bytes are then decoded into ASCII characters to reconstruct a hidden textual message encoded in the concentration data.

All file paths are customizable, allowing the script to be easily adapted for various datasets and analytical contexts.

The script uses the following Python libraries:

- pandas: For structured data manipulation and Excel handling.
- openpyxl: Backend engine for reading .xlsx files using pandas.
- re: For identifying and extracting compound-specific text blocks.
- numpy: For array manipulation and bit-level operations.

All Python decoding scripts and supplementary examples are available in the following GitHub repository: https://github.com/catm542-ai/ChemDataProcessor

Procedure of MATLAB for image encoding, storage, retrieval, and reconstitution:

```
%% multicoloured image encoding
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% An image in the .png format is imported; the RGB image is the official logo of our
% institution, namely UJI. Each image component has the 0 value for the background and
% 255 for each letter, the latter obtained via normalization of each component to the values
% 1,2 o 3, respectively. A matrix with coefficients ranging from 0 to 3 is obtained where
% each coefficient corresponds to the RGB components; 0, black (background), 1, red (U),
%2, green (J) and 3, blue (I). The matrix is scaled to 30 x 10
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

clearvars; % remove all image variables
close all; %
I = imread('UJIim.png'); % read the RGB image
R = I(:,:,1); % R component of the RGB image
G = I(:,:,2); % G component of the RGB image
B = I(:,:,3); % B component of the RGB image
S = R/255+2*(G/255)+3*(B/255); % Matrix with variable 0, black (background), 1, red (U), % 2, green (J) and 3, blue (I).
S2 = imresize(S,1/8,'nearest'); % matrix scaling
xlswrite('UJI.xls',S2); % matrix output in the .xls format

%% image reconstitution
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% an RGB image is reconstructed to a .png format from a .xls file that contains a matrix
% with the 0, 1, 2, 3 values previously decoded both from FIA-MS or LC-MS methods
clearvars;
close all;
M = xlsread('UJI.xls'); % data reading
I(:,:,1) = 255*(M==1); % R component of the RGB image
I(:,:,2) = 255*(M==2); % G component of the RGB image
I(:,:,3) = 255*(M==3); % B component of the RGB image
Ir = imresize(I,8,'nearest'); % matrix scaling
imwrite(Ir, 'UJIrec.png')
```

References

1 J. K. Rosenstein, C. Rose, S. Reda, P. M. Weber, E. Kim, J. Sello, J. Geiser, E. Kennedy, C. Arcadia, A. Dombroski, K. Oakley, S. L. Chen, H. Tann and B. M. Rubenstein, *IEEE Trans. Nanobioscience*, 2020, **19**, 378–384.

2 E. Kennedy, C. E. Arcadia, J. Geiser, P. M. Weber, C. Rose, B. M. Rubenstein and J. K. Rosenstein, *PLoS One*, 2019, **14**, 1–12.

3 C. E. Arcadia, E. Kennedy, J. Geiser, A. Dombroski, K. Oakley, S. L. Chen, L. Sprague, M. Ozmen, J. Sello, P. M. Weber, S. Reda, C. Rose, E. Kim, B. M. Rubenstein and J. K. Rosenstein, *Nat. Commun.*, , DOI:10.1038/s41467-020-14455-1.

4 B. J. Cafferty, A. S. Ten, M. J. Fink, S. Morey, D. J. Preston, M. Mrksich and G. M. Whitesides, *ACS Cent. Sci.*, 2019, **5**, 911–916.

5 V. Pardi-Tóth, Á. Kuki, M. Á. Kordován, G. Róth, L. Nagy, M. Zsuga, T. Nagy and S. Kéki, *Sci. Rep.*, 2023, **13**, 1–7.

6 P. Bohn, M. P. Weisel, J. Wolfs and M. A. R. Meier, *Sci. Rep.*, 2022, **12**, 1–8.

7 A. A. Nagarkar, S. E. Root, M. J. Fink, A. S. Ten, B. J. Cafferty, D. S. Richardson, M. Mrksich and G. M. Whitesides, *ACS Cent. Sci.*, 2021, **7**, 1728–1735.

8 Y. Tang, C. He, X. Zheng, X. Chen and T. Gao, *Chem. Sci.*, 2020, **11**, 3096–3103.

9 T. Ratner, O. Reany and E. Keinan, *ChemPhysChem*, 2009, **10**, 3303–3309.

10 J. M. Lee, H. Jang, S. W. Lee and K. T. Kim, *JACS Au*, 2022, **2**, 2108–2118.

11 Z. Tong, S. Hou, Z. Zhang, Z. Liu and Y. Zhang, *Sensors Actuators B Chem.*, 2025, **422**, 136618.

12 A. Durgbanshi, V. Arbona, O. Pozo, O. Miersch, J. V Sancho and A. Gómez-Cadenas, *J. Agric. Food Chem.*, 2005, **53**, 8437–8442.

13 H. Chaaban, I. Ioannou, L. Chebil, M. Slimane, C. Gérardin, C. Paris, C. Charbonnel, L. Chekir and M. Ghoul, *J. Food Process. Preserv.*, 2017, **41**, e13203.

14 A. Castañeda-Ovando, M. de L. Pacheco-Hernández, M. E. Páez-Hernández, J. A. Rodríguez and C. A. Galán-Vidal, *Food Chem.*, 2009, **113**, 859–871.

15 S. C. Nanita and L. G. Kaldon, *Anal. Bioanal. Chem.*, 2016, **408**, 23–33.

16 A. Furey, M. Moriarty, V. Bane, B. Kinsella and M. Lehane, *Talanta*, 2013, **115**, 104–122.