

## 「ワイドターゲットメタボローム分析」支援について

理化学研究所  
代謝システム研究チーム

本研究支援では、あらかじめ決めてある約 500 種類の一次、二次代謝産物を対象に、LC-MS による分析を行います。本研究支援は共同研究として実施させていただきます。以下の注意点をよくお読みいただいたうえで担当者までお問い合わせください。

### 対象代謝産物

一次および二次代謝産物 約 500 種類 (別表 1)

### 研究支援の流れ

#### ①事前連絡 (メール、貴研究室→当チーム)

目的、対象、サンプル数など

#### ②事前打ち合わせ

必要情報、納期の確認など

#### ③申請書提出 (メール、貴研究室→当研究チームおよび事務局)

#### ④メタボローム分析依頼票・サンプルリスト・植物サンプルの授受における確認書の提出、サンプル送付日の連絡 (メール、貴研究室→当チーム)

※ 形質転換植物の種子の場合は別途、遺伝子組換え生物搬出入の手続きが必要です。

#### ⑤サンプル送付 (貴研究室→当チーム)

・受け取りは平日のみ (午後 3 時までには到着するよう時間指定) でお願います。

#### ⑥ワイドターゲットメタボローム分析

#### ⑦測定結果の送付 (当チーム→貴研究室)

#### ⑧結果の解釈のフィードバック (貴研究室→当チーム)

論文化の相談など

#### ⑨データ公開 (貴研究室、当チーム)

### ワイドターゲットメタボローム分析の流れ

#### ①サンプルの準備 (貴研究室)

※ 詳細は別サイト「サンプルについて」

<https://masspec-phytohormone.riken.jp/sample/>

#### ②サンプルの凍結乾燥・破碎・秤量 (貴研究室または当チーム)

#### ③代謝産物の抽出、調製 (当チーム)

#### ④UPLC-タンデム四重極質量分析機を用いたターゲット分析 (当チーム)

⑤データ精査、エクセルファイル形式にまとめ（貴研究室と当チーム）

費用負担

- ・サンプリングチューブとサンプル破碎用のビーズをご購入くださいますようお願いいたします。
- ・サンプル数に応じて溶媒等の購入をお願いすることがあります。
- ・別途高額な試薬等が必要な場合はご相談させていただきます。

納期

- ・納期は機器の使用状況によって異なりますので、余裕を持った実験計画でお願いします。
- ・大幅に遅れる場合は事前にご連絡します。

共著のお願い

解析結果を用いた発表をする場合（学会発表、論文投稿）は共著者としていただきますようお願いいたします。事前にご連絡ください。

連絡先

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別表1

in-house ID	Annotation
X00004	1-Amino-1-cyclopentanecarboxylic acid
X00006	4-Hydroxy-3-methoxycinnamaldehyde
X00010	Citric acid,Anhydrous
X00013	N-6-(delta-2-Isopentenyl)adenosinehemihydrate
X00015	(-)-Shikimic acid
X00020	(R)-(-)-Phenylephrine hydrochloride
X00022	1,1-Dimethylbiguanide hydrochloride
X00025	1-Aminocyclopropane-1-carboxylic acid
X00034	Serotonin hydrochloride
X00035	5-Methylcytosine hydrochloride
X00037	6-(gamma,gamma-Dimethylallylamino)purine
X00039	Adenine
X00040	Adenosine
X00041	Allantoic acid
X00042	Anthranilic acid
X00045	Caffeine,Anhydrous
X00046	cis-Aconitic Acid
X00049	Glycine
X00051	L-Histidine
X00053	L-Methionine
X00054	L-(-)-Phenylalanine
X00055	L-Tryptophane
X00056	L-Tyrosine
X00060	Sucrose
X00061	Uracil
X00066	L-Kynurenine
X00069	3-(2-Aminoethyl)indole Hydrochloride
X00073	D(+)-Galacturonic acid monohydrate
X00080	2-Hydroxypyridine
X00093	Mesaconic acid
X00095	Methylmalonic acid
X00099	Pyridoxamine dihydrochloride
X00106	3-Methyladenine
X00107	4-Aminobenzoic acid
X00114	Agmatine sulfate salt
X00119	D-Glucosamine-6-phosphate sodium salt
X00125	Harmaline hydrochloride dihydrate
X00127	L-Carnosine
X00128	Leupeptin hemisulfate salt
X00132	Pterine
X00138	1-Methylhistamine dihydrochloride
X00139	2-Aminoethylphosphonic acid
X00140	2'-Deoxyadenosine monohydrate
X00144	2'-Deoxycytidine
X00146	2'-Deoxyguanosine monohydrate
X00147	2'-Deoxyinosine
X00155	3,4-Dihydroxy-L-phenylalanine
X00157	3-Amino-1,2,4-triazole
X00165	Adenosine-3',5'-cyclic monophosphate
X00168	Adonitol
X00169	Allantoin
X00170	Amantadine hydrochloride
X00173	Argininosuccinic acid disodium salt
X00174	Benzamidine hydrochloride hydrate
X00175	Benzocaine solution
X00177	Caffeic acid
X00184	Creatine,anhydrous
X00185	Creatinine,anhydrous
X00187	Cystathionine
X00188	Cytidine,cell culture tested
X00189	Cytidine-3',5'-cyclic monophosphate
X00210	Diethanolamine
X00212	DL-2,3-Diaminopropionic acid monohydrochloride
X00218	DL-threo-beta-Methylaspartic acid
X00220	DL-beta-Hydroxybutyric acid
X00223	D-Ribose-5-phosphate disodium salt hydrate
X00231	Fumaric acid
X00232	Fusaric acid
X00233	Gibberellin A4
X00235	Glutathione (oxidized form)
X00237	Gly-Gly
X00240	Guanine
X00241	Guanosine
X00242	Guanosine-3',5'-cyclic monophosphate
X00251	Hypotaurine
X00252	Hypoxanthine
X00255	3-Indoleacetic acid
X00256	Inosine
X00258	Inosine-5'-monophosphate
X00261	Isoguvacine hydrochloride
X00267	L-Asparagine
X00268	L-Aspartic acid
X00270	L-Cystine
X00271	Leucylleucyltyrosine

X00272	L-Glutamic acid
X00273	L-Glutamine
X00274	L-Glutathione (reduced form)
X00275	L-Histidinol dihydrochloride
X00276	L-Homocarnosine
X00277	L-Homocystine
X00282	L-Methionine sulfone
X00285	L-Ornithine monohydrochloride
X00286	L-Proline
X00287	L-Pyroglutamic acid
X00288	L-Serine
X00295	Maltotriose
X00296	Mecamylamine hydrochloride
X00299	1-Methylguanidine hydrochloride
X00306	3-Ureidopropionic acid
X00307	N-Formyl-L-methionine
X00309	Nicotinic acid mono nucleotide
X00314	2-Hydroxycinnamic acid, predominantly trans
X00317	Orotic acid ,Anhydrous
X00322	Piperacillin sodium salt
X00325	4-Nitrophenol
X00328	3,4-Dihydroxybenzoic acid
X00332	Pyridoxine
X00333	Quisqualic acid
X00336	S-Adenosyl-L-homocysteine
X00338	S-Carboxymethyl-L-cysteine
X00339	Sebacic acid
X00342	Spermine
X00344	Succinic acid
X00355	Thymidine
X00356	Thymidine-3',5'-cyclic monophosphate
X00361	Thymine
X00363	trans-Zeatin-ribose
X00364	Tyramine
X00365	Uridine
X00372	Uridine-5'-monophosphate
X00373	Xanthine
X00379	alpha-Lactose monohydrate
X00383	3-Guanidinopropionic acid
X00386	beta-Nicotinamide adenine dinucleotide hydrate
X00387	beta-Nicotinamide mononucleotide
X00388	Sodium phenylpyruvate
X00389	gamma-Amino-n-butyric acid
X00391	delta-Aminolevulinic acid hydrochloride
X00392	6-Aminohexanoic acid
X00394	Catechol
X00398	Eriodictyol
X00400	Genistein
X00407	Naringenin
X00408	Pelargonin chloride
X00413	Apigenin-7-O-glucoside
X00414	Rhoifolin
X00416	Keracyanin Chloride
X00419	Isorhamnetin-3-O-glucoside
X00421	Robinin
X00422	Kaempferol-3-O-glucoside
X00425	Homoorientin
X00428	Naringenin-7-O-glucoside
X00430	Puerarin
X00431	Peltatoside
X00432	Hyperoside
X00434	Quercetin-3-O-glucose-6"-acetate
X00441	Capsaicin
X00442	Dihydrocapsaicin
X00443	Nordihydrocapsaicin
X00451	4-Coumaric acid
X00452	Rosmarinic acid
X00461	Kaempferol-7-O-alpha-L-rhamnoside
X00469	3-Cyanopyridine
X00473	Urocanic acid
X00474	N-Acetylneuraminic acid,Type IV-S,Synthetic
X00476	N-Acetyl-D-mannosamine
X00477	O-Acetyl-L-serine hydrochloride
X00485	4-Methylumbelliferyl acetate
X00491	Pyridoxal-5'-phosphate hydrate
X00492	Pyridoxal hydrochloride
X00499	N-Acetyl putrescine hydrochloride
X00502	L-Saccharopine
X00534	D-(+)-Arabitol
X00542	D-Glucoheptose
X00544	Dulcitol
X00573	3-Hydroxyanthranilic acid
X00574	(+)-Jasmonic acid
X00584	Abcsicic acid
X00617	L-beta-homovaline-HCl
X00629	D-(-)-Quinic acid

X00630	Dihydro-L- <i>orotic Acid</i>
X00633	(+)-2'- <i>Deoxyuridine</i>
X00636	<i>Chlorogenic acid Hemihydrate</i>
X00639	6- <i>Hydroxynicotinic Acid</i>
X00640	O- <i>Succinyl-L-homoserine</i>
X00644	<i>Gibberelin A3</i>
X00646	<i>cis,cis-Muconic acid</i>
X00647	<i>Pimelic acid</i>
X00652	4- <i>Methyl-5-thiazoleethanol</i>
X00655	<i>Syringic Acid</i>
X00659	O- <i>Acetyl-L-homoserine hydrochloride</i>
X00664	D- <i>Ala-D-Ala</i>
X00666	<i>Carbamoyl-DL-aspartic acid</i>
X00668	<i>Sodium Cholate Hydrate</i>
X00675	5'- <i>Deoxy-5'-Methylthioadenosine</i>
X00677	DL- <i>Dihydrozeatin</i>
X00682	2- <i>Isopropylmalic acid</i>
X00686	3- <i>Methyl-2-oxobutyric acid sodium salt</i>
X00693	<i>Scoulerin</i>
X00695	L- <i>allo-threonine</i>
X00696	(+)- <i>Taxifolin</i>
X00698	<i>Lignoceric Acid</i>
X00701	<i>Methyl Jasmonate</i>
X00735	<i>Vanillin</i>
X00741	4- <i>Hydroxypyridine</i>
X00748	<i>gamma-Glu-Cys</i>
X00750	D- <i>erythro-Dihydrosphingosine</i>
X00751	<i>Zeatin-9-glucoside</i>
X00752	<i>Syringaldehyde</i>
X00754	<i>Citraconic Acid</i>
X00755	5- <i>Aminovaleric acid</i>
X00760	3,4- <i>Dimethoxycinnamic acid</i>
X00761	3,5- <i>Dimethoxycinnamic acid (predominantly trans)</i>
X00763	<i>m-Hydroxycinnamic acid</i>
X00764	3- <i>Hydroxypyridine</i>
X00766	4- <i>Methoxycinnamic acid</i>
X00780	<i>Hesperetin</i>
X00781	<i>Itaconic acid</i>
X00787	N- <i>Acetylglycine</i>
X00791	<i>trans-3,5-Dimethoxy-4-hydroxycinnamaldehyde</i>
X00792	D- <i>Sorbitol-6-phosphate barium salt</i>
X00794	<i>Suberic acid</i>
X00797	L- <i>Threonine acid hemicalcium salt</i>
X00799	2,2',2''- <i>Nitrilotriethanol</i>
X00813	<i>Phosphocholine,1-Lauroyl-2-Hydroxy-sn-Glycero-3-</i>
X00814	<i>Phosphocholine,1-Decanoyl-2-Hydroxy-sn-Glycero-3-</i>
X00820	D- <i>Glucosyl-beta1-1'-D-erythro-Sphingosine</i>
X00838	<i>Malvin chloride</i>
X00843	4- <i>deoxyphloridzin</i>
X00844	2',6'- <i>Dihydroxy-4-Methoxychalcone-4'-O-Neohesperidoside</i>
X00846	<i>Flavanomarein</i>
X00849	<i>Hesperidin</i>
X00853	<i>Luteolin-3',7-di-O-glucoside</i>
X00854	<i>Luteolin-4'-O-glucoside</i>
X00859	<i>Neohiocitrin</i>
X00860	<i>Neohesperidin</i>
X00861	<i>Neohesperidin dihydrochalcone</i>
X00862	<i>Ononin</i>
X00863	<i>Orientin</i>
X00864	<i>Phloridzin</i>
X00865	<i>Poncirin</i>
X00867	<i>Saponarin</i>
X00868	<i>Sissotrin</i>
X00873	<i>Solasodine</i>
X00874	<i>Vitexin</i>
X00890	<i>Methyl Dihydrojasmonate</i>
X00900	N- <i>Acetyl-DL-serine</i>
X00906	<i>Cysteinylglycine</i>
X00907	DL- <i>Homocysteine</i>
X00909	S-(5'- <i>Adenosyl</i> )-L- <i>methionine chloride</i>
X00921	<i>Kaempferol-3-Rhamnoside-4''-Rhamnoside,-7-Rhamnoside</i>
X00922	<i>Kaempferol-3-O-alpha-L-arabinoside</i>
X00924	<i>Kaempferol-3-Glucuronide</i>
X00928	<i>Myricetin-3-Galactoside</i>
X00930	<i>Myricetin-3-Xyloside</i>
X00931	7- <i>O-Methylquercetin-3-Galactoside-6''-Rhamnoside-3'''-Rhamnoside</i>
X00933	<i>Quercetin-3-Glucuronide</i>
X00943	<i>alpha-Methyl-DL-histidine dihydrochloride</i>
X00945	3- <i>Hydroxy-3-methylglutarate</i>
X00946	3- <i>Indoxylsulfate potassium salt</i>
X00952	2,5- <i>dihydroxy benzoic acid</i>
X00953	<i>Hippuric Acid</i>
X00959	<i>Salicylic Acid</i>
X00961	<i>Trimethylamine N-oxide dihydrate</i>
X00967	3- <i>Methyl-L-histidine</i>
X00968	5- <i>Hydroxyindole-3-acetate (5-HIAA)</i>

X00971	DL-5-Hydroxylysine hydrochloride
X00973	DL-p-Hydroxyphenyllactic acid
X00983	2-Hydroxyisocaproic acid
X00986	L-Anserine
X00987	DL-3-Phenyllactic acid
X00988	Homovanillic acid
X00989	DL-4-Hydroxy-3-methoxymandelic acid
X00991	S-Sulfocysteine
X00995	2-Hydroxyphenylacetic acid
X00997	N-Acetyl-DL-aspartic acid
X00998	O-Acetyl-L-carnitine hydrochloride
X01000	Glycyl-L-proline
X01002	N-Tigloylglycine
X01004	(-)-Riboflavin
X01010	Oxypurinol
X01011	trans-Aconitic acid
X01012	3-hydroxy-3-methylbutanoic acid
X01014	N-Isovaleroylglycine
X01016	Choline chloride
X01020	Kynurenic acid
X01023	Acetaminophen
X01025	Glycocyanine
X01026	Trigonelline hydrochloride
X01028	Phenaceturic acid
X01029	1,3-Dimethylurate
X01031	3-Methylxanthine
X01035	3-Hydroxymandelic acid
X01038	4-Hydroxy-3-methoxybenzoic acid
X01041	4-Pyridoxate
X01042	5-Methoxysalicylic acid
X01046	N-Acetyl-DL-glutamic acid
X01054	3,5-Dibromo-L-tyrosine
X01061	1-Isothiocyanato-7-(methylsulfinyl)-heptane
X01062	1-Isothiocyanato-6-(methylsulfinyl)-hexane
X01063	1-Isothiocyanato-9-(methylsulfinyl)-nonane
X01064	1-Isothiocyanato-8-(methylsulfinyl)-octane
X01066	1-Isothiocyanato-6-(methylsulfonyl)-hexane
X01069	S-Sulforaphane
X01070	But-3-enylglucosinolate
X01076	4-(Methylsulfinyl)but-3-enylglucosinolate
X01078	Benzylglucosinolate
X01079	Gluconasturtiin
X01081	p-Hydroxybenzylglucosinolate
X01082	(2R)-2-Hydroxy-2-phenethylglucosinolate
X01091	Indole-3-carboxylic acid
X01097	DL-Pipecolinic acid
X01098	Maleic acid
X01099	D-(+)-Raffinose pentahydrate
X01128	Cyanidin-3-O-rhamnoside chloride
X01131	Zearalenone
X01139	DL-Sulforaphane
X01144	S-Methyl-L-cysteine
X01147	D-Glucuronic acid
X01152	Betaine
X01158	Nonasaccharide, Glc4Xyl3Gal2
X01159	Heptasaccharide, Glc4Xyl3
X01174	Quercetin-3-O-alpha-L-rhamnopyranosyl(1->2)-beta-D-glucopyranoside-7-O-alpha-L-rhamnopyranoside
X01179	Sinapoyl malate
X01181	1-O-beta-D-Glucopyranosyl sinapate
X01184	DL-Glyceric Acid calcium Salt
X01206	Folic acid, approx
X01207	Procyanidin C1
X01209	D-Glucurono-6,3-lactone
X01210	Prostaglandin E1
X01214	Cyanidin-3-O-alpha-arabinopyranoside
X01216	Peonidin-3-O-alpha-arabinopyranoside
X01218	Petunidin-3-O-beta-glucopyranoside
X01219	Quercetin-3,4'-O-di-beta-glucopyranoside
X01220	Cyanidin-3-O-(2''-O-beta-xylopyranosyl-beta-glucopyranoside)
X01222	Peonidin-3,5-O-di-beta-glucopyranoside
X01223	Delphinidin-3-O-(6''-O-alpha-rhamnopyranosyl-beta-glucopyranoside)
X01224	Delphinidin-3-O-(2''-O-beta-xylopyranosyl-beta-glucopyranoside)
X01225	Cyanidin-3-O-(2''-O-beta-xylopyranosyl-beta-glucopyranoside)-5-O-beta-glucopyranoside
X01226	Cyanidin-3-O-[6''-O-(E-p-coum)-2''-O-(beta-xylopyranosyl)-beta-glucopyranoside]-5-O-beta-glucopyranoside
X01227	Petunidin-3-O-(6''-O-(4''-O-E-coum)-alpha-rhamnopyranosyl-beta-glucopyranosyl)-5-O-beta-glucopyranoside
X01228	E-3,4,5'-trihydroxy-3'-glucopyranosylstilbene
X01229	E-4,5'-dihydroxy-3-methoxy-3'-glucopyranosylstilbene
X01237	L-Ethionine
X01238	o-Anisic Acid
X01239	Sodium Deoxycholate
X01248	Daphnetin
X01249	6,7-Dihydroxycoumarin
X01250	Esculin sesquihydrate
X01261	Stachyose n-Hydrate
X01262	Melatonin
X01263	L-Canavanine

X100001	Lidocain
X100002	10-Camphorsulfonic acid
X100003	Sinigrin
X100004	3-Methylsulfinyl-n-propyl-glucosinolate
X100005	4-Methylsulfinyl-n-butyl-glucosinolate
X100006	5-Methylsulfinyl-n-pentyl-glucosinolate
X100007	6-Methylsulfinyl-n-hexyl-glucosinolate
X100008	7-Methylsulfinyl-n-heptyl-glucosinolate
X100009	8-Methylsulfinyl-n-octyl-glucosinolate
X100010	3-Methylthio-n-propyl-glucosinolate
X100011	4-Methylthio-n-butyl-glucosinolate
X100012	5-Methylthio-n-pentyl-glucosinolate
X100013	6-Methylthio-n-hexyl-glucosinolate
X100014	7-Methylthio-n-heptyl-glucosinolate
X100015	8-Methylthio-n-octyl-glucosinolate
X100016	3-Hydroxy-n-propyl-glucosinolate
X100017	4-Hydroxy-n-butyl-glucosinolate
X100018	3-Benzoyloxy-n-propyl-glucosinolate
X100019	4-Benzoyloxy-n-butyl-glucosinolate
X100020	Indol-3-ylmethyl-glucosinolate
X100021	1-Methoxyindole-glucosinolate
X100022	4-Methoxyindole-glucosinolate
X100023	Camalexin
X100024	L-Leucine, (Cell Culture Reagent, Crystalline)
X100025	L-Isoleucine
X100026	S-Methylmethionine
X100027	Methionine sulfoxide
X100029	L-Homomethionine
X100030	Octanoylcarnitine
X100031	Decanoylcarnitine
X100032	Lauroylcarnitine
X100033	Myristoylcarnitine
X100034	Palmitoylcarnitine
X100036	Stearoylcarnitine
X100038	beta-Alanine
X100039	Luteolin 7-O-glucuronide
X100040	Apigenin 7-O-glucuronide
X100041	Hispidol
X100042	Aureusidin
X100043	2i Leu Ile
X100044	2i Gln Lys
X200001	2i Kaempferol-3-O-alpha-L-rhamnopyranosyl(1->2)-beta-D-glucopyranoside-7-O-alpha-L-rhamnopyranoside_Kaempferol-3-Glucoside-2"-Rhamnoside,-7-Rhamnoside
X200004	3i Isorhamnetin-3-O-rutinoside_Isorhamnetin-3-Glucoside-6"-Rhamnoside_Isorhamnetin-3-Galactoside-6"-Rhamnoside
X200005	7i Kaempferol-3-O-rutinoside_Datiscin_Kaempferol-3-O-beta-D-glucoside-7-O-alpha-L-rhamnoside_Kaempferol-3-O-beta-D-galactoside-7-O-alpha-L-rhamnoside_Kaempferol-3-O-b-glucopyranosyl-7-O-a-rhamnopyranoside_kaempferol-7-O-neohesperidoside_Kaempferol-3-Gluc
X200006	2i Fortunellin_Linarin
X200007	2i Cyanidin-3,5-di-O-glucoside chloride_Cyanidin-3-O-(2"-O-beta-glucopyranosyl)-beta-glucopyranoside)
X200009	4i Kaempferol-3-Rhamnoside-7-Rhamnoside_vitexin-2"-O-rhamnoside_Kaempferol-3,7-O-bis-alpha-L-rhamnoside_Kaempferol-3,7-O-di-rhamnopyranoside
X200010	2i Kaempferol-3-O-alpha-L-rhamnoside_Kaempferol-3-Rhamnoside
X200011	2i Ideain chloride_Cyanidin-3-glucoside chloride
X200012	2i Maritimein_luteolin-7-O-glucoside
X200013	2i Eriodictyol-7-O-glucoside_Marein
X200014	2i Quercetin-3-Arabinoside_Quercetin-3-D-xyloside
X200015	2i Quercetin-3-Rhamnoside_Quercetin-3-O-alpha-L-rhamnopyranoside
X200016	2i Malvidin-3-galactoside chloride_Oenin
X200017	2i Syringetin-3-O-glucoside_Syringetin-3-O-galactoside
X200019	2i Myricitrin_Myricetin-3-Rhamnoside
X200020	2i Peonidin-3-o-beta-d-glucopyranoside_Peonidin-3-O-beta-galactopyranoside
X200023	Cytidine-5'-diphosphocholine sodium salt dihydrate
X200026	3i (+)-Catechin hydrate_(+)-Epicatechin
X200028	3i Sodium pantothenate_D-Pantothenic acid hemicalcium salt_Calcium (+)-pantothenate
X200029	2i alpha-D-Glucose-1-phosphate dipotassium salt dihydrate_alpha-D-Galactose-1-phosphate dipotassium salt pentahydrate
X200030	2i D-Mannose-6-phosphate barium salt hydrate_D-Mannose 6-phosphate mono sodium salt
X200031	4i D-Fructose-6-phosphate disodium salt hydrate_D-Glucose-6-phosphate sodium salt_alpha-D-(+)-mannose-1-phosphate sodium salt hydrate_alpha-D-(+)-Mannose 1-phosphate bis(cyclohexylammonium) salt
X200034	2i D-(+)-Galactosamine hydrochloride_D-(+)-Glucosamine hydrochloride
X200035	2 or 3-Methoxycinnamic acid
X200036	2i 4-Methylumbelliferone_7-Hydroxy-4-methylcoumarin
X200037	2i Theophylline,anhydrous_1,7-Dimethylxanthine
X200038	cis or trans-Zeatin
X200039	2i alpha-Lipoamide_DL-Thioctamide
X200040	cis or trans-4-Hydroxy-3-methoxycinnamic acid_Ferulic acid
X200041	Guanosine-5'-monophosphate disodium salt hydrate
X200042	2i D-(+)-Cellobiose_Lactulose
X200043	6i Melibiose hydrate_D-(+)-Turanose_Isomaltose_Gentiobiose_MelibiosePalatinose Monohydrate
X200046	3i L-Iditol_D-Sorbitol_D-(-)-Mannitol
X200047	4i L-(+)-Arginine HCl_N-alpha-Acetyl-L-ornithine_L-Citrulline
X200049	3i rac-Glycerol 3-phosphoate disodium salt hexahydrate_Disodium Glycerophosphate 5,5-Hydrate_L-Glycerol-2-phosphate Disodium Salt
X200053	2i Histamine_Cytosine
X200054	DL-Cysteine
X200055	2i Nicotinamide_Niacinamide
X200056	3i Glycolaldehyde dimer,mixture of stereoisomers_D-Erythrose_D-(-)-Threose
X200057	2i L-Alanine_Sarcosine

X200058	2i 1,3-Diaminopropane dihydrochloride 1,3-Propanediamine
X200060	2i L-Norvaline L-Valine
X200061	3i L-Threonine alpha-Methyl-DL-serine L-Homoserine
X200062	2i 2-Hydroxyisobutyric acid DL-alpha-Hydroxybutyric acid barium salt
X200063	3i L-2-Aminobutyric acid N,N-Dimethylglycine hydrochloride N-Methyl-DL-Alanine
X200064	2i D-alpha-Hydroxyisovaleric acid DL-2-Hydroxyvaleric acid sodium salt hydrate
X200065	2i (S)-(+)-1-Aminoethylphosphonic acid Taurine
X200067	2i Indole-3-carboxyaldehyde Indole-3-aldehyde
X200068	DL-Malic acid
X200070	2i alpha-Ketoglutaric acid disodium salt 2-Oxoglutaric Acid
X200071	DL-Mandelic acid
X200072	L-CarnitineHCl
X200073	DL-2-Amino adipic Acid
X200076	2i Adipic acid 2-Methylglutaric Acid
X200077	(-)-Citramalic acid
X200079	4-Hydroxybenzoate
X200080	3i Ethylmalonic acid Glutaric acid Methylsuccinic acid
X200082	L-Lysine HCl
X200084	2i Nicotinic Acid Isonicotinic acid
X200085	2i L-Norleucine D-Alloisoleucine
X200086	2i Quercitrin Quercetin-7-O-rhamnoside
X200087	2i Rutin Quercetin-3-O-b-glucopyranosyl-7-O-a-rhamnopyranoside
X200088	2i (2R) (2S)-2-Hydroxybut-3-enylglucosinolate
X200089	2i D-(+)-Melezitose monohydrate 1-Kestose
X210001	Apigeninidin
X210002	Luteolinidin
X210003	Apigenin
X210004	Luteolin
X210005	Diosmetin
X210008	Apiferol
X210009	Pelargonidin
X210010	Cyanidin
X210012	Cyanidin 3-(6"-malonylglucoside)
X210013	Cyanidin 3-(3",6"-dimalonylglucoside)
X250001	Quercetin 3-Glucoside <Isoquercitrin>
X250005	Soyasaponin I (Bb)
X250006	Soyasaponin V (Ba)
X250007	Soyasaponin II
X250008	Licochalcone A
X250009	Glabridin
X250010	Liquiritin
X250012	Schaftoside
X250013	Isoliquiritin
X250014	Liquiritin apioside
X250015	Isoliquiritin apioside
X260001	gamma-Glu-PRENCs
X260002	gamma-Glu-PRENCsO
X260003	2-CPGTH
X260004	Cycloalliin
X260005	PRENCsO
X260006	MCSO
X260007	Alliin
X260008	Allicin
X260009	Alliospiroside A
X260010	Alliospiroside B
X400001	Formononetin
X400003	Glycitin
X400005	Genistin
X400008	Daidzein
X400009	Daidzin
X400023	6"-O-Malonyldaidzin
X400024	6"-O-Malonylgenistin
X500001	Acetyl-soyasaponin A1
X500002	Acetyl-soyasaponin A4
X500003	Soyasaponin Bd
X500004	Soyasaponin Be
X500005	Glycitein
X500006	Genistein
X500009	(+)-Synephrine
X500010	6',-7'-Dihydroxybergamottin
X500011	Citrinin
X500014	Matairesinol
X500016	Rhein
X500017	(-)-Crucumol
X500018	(-)-Epigallocatechin
X500019	(-)-Gallocatechin
X500024	Aloin
X500033	Chelidonic acid
X500038	5-Methoxy psoralen
X500039	Arbutin
X500040	Harmine
X500044	(+)-Nootkatone
X500048	11-Keto-beta-boswellic acid
X500052	6,7-Dimethoxycoumarin
X500053	7-Methoxycoumarin
X500054	Berberamine dihydrochloride



X500056	Cytisine
X500059	Gallic acid
X500060	Hexahydrocurcumin
X500061	cis-Jasmone
X500062	Methyl 2-aminobenzoate
X500063	Purine
X500064	R-(+)-Citronellie acid
X500065	S-(-)-Citronellie acid
X500066	Secoisolariciresinol
X500067	Tangeretin
X500068	Tetrahydrocurcumin
X500071	Coumestrol
X500072	Prunetin
X500073	(+)-Equol
X500074	Ginkgolide A
X500075	Deacylgymnemic acid
X500076	Verbascoside <Acteoside>
X500077	Tectorigenin
X500078	Tectorigenin 7-o-Xylosylglucoside
X500080	Quercetin 4'-glucoside
X500081	Quercetin 3, 4'-Diglucoside
X500083	3,5,7-Trimethoxyflavone
X500084	SoyasapogenolA
X500085	Ginkgolide B
X500086	Geniposide
X500089	Chicoric acid
X500092	6"-O-Malonylglycitin
X500093	6"-O-Acetyldaidzin
X500094	6"-O-Acetylglycitin
X500095	6"-O-Acetylgenistin
X500096	Malvidin 3-Glucoside Chloride
X500097	Delphinidin 3-Rutinoside Chloride
X500098	Delphinidin 3-Galactoside Chloride
X500099	Cyanidin 3-Galactoside Chloride
X500101	Petunidin 3-Glucoside Chloride
X500102	Petunidin 3-Galactoside Chloride
X500103	Peonidin 3-Galactoside Chloride
X500104	Malvidin 3-Galactoside Chloride
X500105	Petunidin 3-Arabinoside Chloride
X500106	Peonidin 3-Arabinoside Chloride
X500107	(-)-Epigallocatechin 3-(3"-O-methyl)gallate
X500108	Biochanin A
X500109	Glyceollin I
X500110	Glyceollin mixture (I, II, III)
X500111	Glyceollin IV
X500112	Glyceollin V
X500113	2'-Hydroxydaidzein
X500114	7,2',4'-Trihydroxyisoflavanone
X500115	3'-Prenyldaidzein
X500116	3,9-Dihydroxypterocarpan
X500118	Apiin
X500120	Echinatin
X500121	(-)-Sativan
X500122	Licoflavonol
X500123	Garbanzol
X500124	Licoricidin
X500126	Pratensein
X500127	3'-Methoxydaidzein
X500128	Demethylvestitol
X500129	Lupiwighteone
X500130	Afromosine
X500131	Vicenin -1
X500132	Vicenin -2
X500133	Vicenin -3
X500134	Orobol
X500135	Phaseollidin
X500136	3'-O-Methylorobol
X500137	Vestitol
X500138	Medicarpin
X500140	Phaseollin
X500141	6-Hydroxydaidzein
X500143	Liquiritigenin