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Leveraging metabolic similarity in a ^{1}H NMR database of medicinal plants to advance pharmacognostic insights

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Natural products remain a central resource for drug discovery, and increasing evidence suggests that therapeutic effects often arise from the combined action of multiple constituents rather than single compounds. In this context, metabolomic profiling is essential for comparing complex plant chemical phenotypes, and ^{1}H NMR provides robust whole-profile fingerprints that support cross-species metabolic barcoding and systematic comparison. In this study, we establish and apply a standardized large-scale ^{1}H NMR database to enable macroscopic metabolomic similarity profiling of medicinal plants. Specifically, using ^{1}H NMR profiles from 656 traditional medicinal herbs, we demonstrate how this standardized large-scale metabolomic framework can be applied to key challenges in medicinal plant research, including quality control across different locations and time periods, identification of metabolically similar alternative species, and compositional analysis of multi-herb formulations. Our findings demonstrate the utility of this NMR-based strategy as a scalable approach for standardization, authentication, and holistic characterization of medicinal plants, advancing the field beyond reductionist paradigms. This study establishes a standardized large-scale ^{1}H NMR database of medicinal plants and introduces a macroscopic framework for large-scale metabolomic similarity profiling that enables chemotaxonomic contextualization, quality surveillance, and identification of metabolically similar candidate substitutes.

Keywords Metabolic profiling, Medicinal plants, NMR, Metabolic similarities, Macroscopic approach, Quality control, Multi-herbal drugs

Natural products have long been vital for human health, providing amongst other things, herbal medicines with centuries of empirical knowledge as a proof of their efficacy. With the advancement of modern science, it has become essential to scientifically explain and validate these traditional remedies. The discovery of active compounds such as strychnine[1], emetine[2], quinine[3], and various terpenoids[4] has provided a scientific foundation for the efficacy of these natural products. Notable examples of natural product-based medicines include aspirin, derived from salicylic acid in willow bark[5,6], and artemisinin, an antimalarial drug extracted from *Artemisia annua*[7]. These cases underscore the significant role that natural bioactive substances play in pharmaceutical innovation. As research progresses, natural products will continue to be a crucial resource for the development of new drugs and treating diseases through their diverse biological actions.

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The diversity of chemical compounds in natural products is a unique opportunity for drug discovery and development. However, paradoxically, this chemical diversity has proved to be the major challenge to the possibility of taking full advantage of its potential as the identification and isolation of specific bioactive compounds from among the numerous chemical substances present in natural products, is often considerably time and resource consuming. Thus, in order to tackle this issue, natural product research demands the use of sophisticated analytical techniques and methods to evaluate their bioactivity, requiring a multifaceted approach.

Chemical profiling for these active compounds is currently a critical step in modern drug development, highlighting the significant role that natural bioactive substances can play in pharmaceutical innovation. Metabolomics and untargeted chemical profiling methods allow for the detection of numerous metabolites in biological systems without the time-consuming steps of compound isolation, facilitating both the qualitative and quantitative analysis of bioactive compounds. In this study, we establish and apply a standardized large-scale ^{1}H NMR database to enable macroscopic metabolomic similarity profiling of medicinal plants, providing an integrated framework for chemotaxonomic contextualization, quality surveillance, and the evaluation of multi-herb formulations. Throughout this study, metabolomic fingerprinting refers to whole spectrum of ^{1}H NMR profiles used as reproducible chemical fingerprints, while metabolic barcoding denotes their use for authentication and identification in a chemotaxonomic context. We use the term macroscopic to describe database-driven comparisons of overall chemical relatedness across many samples through large-scale metabolomic similarity profiling.

Analytical platforms used in chemical profiling must possess key features: reproducibility, high sensitivity, and high resolution. Reproducibility is critical for robust fingerprinting, as it ensures consistent results under identical experimental conditions - an essential factor for the reliability of research findings. High sensitivity and resolution are necessary for the accurate identification of target compounds, enabling precise structural characterization and the detection of subtle differences among analytes. Among the various analytical techniques available, mass spectrometry (MS)[8,9] and nuclear magnetic resonance (NMR)[10,11] have received considerable attention for meeting these requirements. Each method has its own advantages and limitations. Notably, NMR is a non-destructive technique that provides highly reproducible spectra, allowing for consistent results across replicates and even from long-term stored samples. Furthermore, NMR gives unique spectra that help establish the metabolic fingerprints of plants to characterise them. This long-term reproducibility of NMR-generated data results in NMR-based metabolomics databases that are frontrunners in terms of relevance if compared to those based on other analytical techniques. Along with its suitability for databases, NMR-based metabolomics has been successfully employed in the discovery of various bioactive substances due to its powerful identification capabilities[12,13]. The number of published studies using NMR-based metabolomics attest to its standing as a highly efficient tool for the discovery of new drugs from natural products, highlighting its potential in the systematic analysis of complex chemical compositions and the identification of promising drug candidates[14–16].

Recently, there has been a shift in the approach for therapeutical solutions, from single drugs to complex mixtures of compounds. Given the growing importance of natural products in drug development, the complex interactions between the multiple components of natural products cannot be ignored when searching for the mechanisms behind their activity[17]. A possible explanation for the activity of these complex mixtures versus isolated compounds sourced from natural products, may be that they are involved in synergistic effects, providing more effective alternatives for the treatment of various diseases. This underscores the close connection between natural product research and complex drug development, indicating that natural products will continue to be a vital source for new pharmaceutical discoveries.

In agreement with this idea, the efficacy of traditional herbal medicines has not been typically attributed to a single component or a common set of components but rather to the interactions among an entire array of active constituents[18,19]. This, which is in itself complex, is further complicated when considering that these metabolites are produced through unique biosynthetic pathways specific to each species, which can result in variations in component profiles and compositions based on origin, cultivation conditions, and other factors. Additionally, the therapeutic effects of one same medicinal herb can vary depending on factors such as the formulation, dosage, and preparation methods. This complexity has historically led to a reliance on empirical evidence for assessing the efficacy of herbal medicines, an approach which does not provide the necessary information on which to base their standardization from a modern pharmacological perspective. In this context, revisiting NMR profiling holds significant value for herbal medicine research as it has proved to be a powerful tool for the precise analysis of complex herbal components, helping to understand interactions among all constituents and discover new pharmacologically active substances[20]. This approach can play a crucial role in advancing the study and use of herbal medicines.

The foundation of this investigation was to identify metabolic similarities among different plant species. NMR analysis proved particularly well-suited for this purpose, as it allows for the detection of functional group-specific signals across a broad spectrum of molecules, thereby facilitating the recognition of shared metabolic features among species. Importantly, NMR enables the quantitative comparison of metabolite profiles, offering a promising approach for exploring similarities in traditional herbal medicines. Many traditional herbs have well-documented therapeutic efficacy, which often arises from the synergistic action of multiple compounds rather than a single active metabolite.

Despite the unique advantages of NMR, its application in metabolomics-based natural products research has often been underestimated in previous studies. It has frequently been treated as interchangeable with other analytical techniques, particularly mass spectrometry (MS)-based approaches, without full recognition of its distinct strengths. To address this gap, we conducted a systematic comparison of metabolic similarities among over 656 established traditional herbal medicines (Table 1) using NMR analysis. This approach aims to identify shared chemical components and investigate their potential associations with specific therapeutic effects. The detected similarities were further explored for their implications in quality control, domestic substitution,

No.	Sample code	Family	Genus	Species	Used part
1	NPL-KHU-001	*Fabaceae*	*Pueraria*	*lobata*	Root
2	NPL-KHU-002	*Zingiberaceae*	*Curcuma*	*longa*	Root
3	NPL-KHU-003	*Zingiberaceae*	*Zingiber*	*officinale*	Root
4	NPL-KHU-004	*Anacardiaceae*	*Rhus*	*verniciflua*	Rind
5	NPL-KHU-005	*Nymphaeaceae*	*Euryale*	*ferox*	Seed
6	NPL-KHU-006	*Lauraceae*	*Cinnamomum*	*cassia*	Rind
7	NPL-KHU-007	*Lauraceae*	*Cinnamomum*	*cassia*	Rind
8	NPL-KHU-008	*Zingiberaceae*	*Alpinia*	*officinarum*	Root
9	NPL-KHU-009	*Fabaceae*	*Sophora*	*flavescens*	Root
10	NPL-KHU-010	*Viscaceae*	*Viscum*	*coloratum*	Whole plant
11	NPL-KHU-011	*Poaceae*	*Oryza*	*sativa*	Seed
12	NPL-KHU-012	*Laminariaceae*	*Laminaria*	*japonica*	Whole plant
13	NPL-KHU-013	*Lamiaceae*	*Agastache*	*rugosa*	Whole plant
14	NPL-KHU-014	*Fabaceae*	*Sophora*	*japonica*	Flower and seed
15	NPL-KHU-015	*Celastraceae*	*Euonymus*	*alatus*	Rind
16	NPL-KHU-016	*Rosaceae*	*Rosa*	*laevigata*	Fruit
17	NPL-KHU-017	*Balsaminaceae*	*Impatiens*	*balsamina*	Whole plant
18	NPL-KHU-018	*Poaceae*	*Oryza*	*sativa*	Seed
19	NPL-KHU-019	*Fabaceae*	*Vigna*	*radiatus*	Seed
20	NPL-KHU-020	*Lamiaceae*	*Salvia*	*miltiorrhiza*	Root
21	NPL-KHU-021	*Poaceae*	*Lophatherum*	*gracile*	Whole plant
22	NPL-KHU-022	*Apiaceae*	*Angelica*	*gigas*	Root
23	NPL-KHU-023	*Polygonaceae*	*Rheum*	*palmatum*	Root
24	NPL-KHU-024	*Cucurbitaceae*	*Benincasa*	*cerifera*	Fruit
25	NPL-KHU-025	*Fabaceae*	*Glycine*	*max*	Seed
26	NPL-KHU-026	*Rosaceae*	*Rosa*	*rugosa*	Fruit
27	NPL-KHU-027	*Malvaceae*	*Hibiscus*	*syriacus*	Flower
28	NPL-KHU-028	*Paeoniaceae*	*Paeonia*	*suffruticosa*	Root
29	NPL-KHU-029	*Cucurbitaceae*	*Momordica*	*cochinchinensis*	Fruit
30	NPL-KHU-030	*Actinidiaceae*	*Actinidia*	*polygama*	Fruit
31	NPL-KHU-031	*Lamiaceae*	*Mentha*	*arvensis*	Leaf
32	NPL-KHU-032	*Lamiaceae*	*Scutellaria*	*barbata*	Whole plant
33	NPL-KHU-033	*Araceae*	*Pinellia*	*ternata*	Root
34	NPL-KHU-034	*Menispermaceae*	*Sinomenium*	*acutum*	Root
35	NPL-KHU-035	*Ginkgoaceae*	*Ginkgo*	*biloba*	Leaf
36	NPL-KHU-036	*Cupressaceae*	*Platycladus*	*orientalis*	Seed and leaf
37	NPL-KHU-037	*Paeoniaceae*	*Paeonia*	*japonica*	Root
38	NPL-KHU-038	*Rubiaceae*	*Oldenlandia*	*herbacea*	Whole plant
39	NPL-KHU-039	*Poaceae*	*Triticum*	*aestivum*	Seed
40	NPL-KHU-040	*Lemnaceae*	*Spirodela*	*polyrhiza*	Whole plant
41	NPL-KHU-041	*Dioscoreaceae*	*Dioscorea*	*tokoro*	Root
42	NPL-KHU-042	*Arecaceae*	*Areca*	*catechu*	Seed
43	NPL-KHU-043	*Cucurbitaceae*	*Cucumis*	*melo*	Fruit
44	NPL-KHU-044	*Combretaceae*	*Quisqualis*	*indica*	Flower
45	NPL-KHU-045	*Apiaceae*	*Aegopodium*	*podagraria*	Whole plant
46	NPL-KHU-046	*Cornaceae*	*Cornus*	*officinalis*	Fruit
47	NPL-KHU-047	*Lythraceae*	*Punica*	*granatum*	Fruit
48	NPL-KHU-048	*Zingiberaceae*	*Elettaria*	*cardamomum*	Seed
49	NPL-KHU-049	*Apiaceae*	*Anethum*	*graveolens*	Whole plant
50	NPL-KHU-050	*Ebenaceae*	*Diospyros*	*kaki*	Fruit
51	NPL-KHU-051	*Apiaceae*	*Bupleurum*	*falcatum*	Root
52	NPL-KHU-052	*Polygonaceae*	*Rumex*	*japonicus*	Whole plant
53	NPL-KHU-053	*Primulaceae*	*Lysimachia*	*foenum-graecum*	Whole plant
54	NPL-KHU-054	*Lardizabalaceae*	*Akebia*	*quinata*	Fruit and stem
55	NPL-KHU-055	*Crassulaceae*	*Orostachys*	*japonica*	Whole plant
56	NPL-KHU-056	*Caryophyllaceae*	*Silene*	*firma*	Whole plant

Continued

No.	Sample code	Family	Genus	Species	Used part
57	NPL-KHU-057	*Solanaceae*	*Solanum*	*nigrum*	Whole plant
58	NPL-KHU-058	*Asteraceae*	*Arctium*	*lappa*	Root
59	NPL-KHU-059	*Brassicaceae*	*Brassica*	*napus*	Seed
60	NPL-KHU-060	*Asteraceae*	*Artemisia*	*anomala*	Leaf
61	NPL-KHU-061	*Ulmaceae*	*Ulmus*	*macrocarpa*	Rind
62	NPL-KHU-062	*Burseraceae*	*Boswellia*	*carteri*	Resin
63	NPL-KHU-063	*Lauraceae*	*Cinnamomum*	*cassia*	Rind
64	NPL-KHU-064	*Orobanchaceae*	*Cistanche*	*deserticola*	Whole plant
65	NPL-KHU-065	*Asteraceae*	*Artemisia*	*capillaris*	Leaf
66	NPL-KHU-066	*Apiaceae*	*Angelica*	*acutiloba*	Root
67	NPL-KHU-067	*Fabaceae*	*Pterocarpus*	*santalinus*	Wood
68	NPL-KHU-068	*Lamiaceae*	*Perilla*	*frutescens*	Leaf
69	NPL-KHU-069	*Lauraceae*	*Cinnamomum*	*camphora*	Leaf and rind
70	NPL-KHU-070	*Polyporaceae*	*Polyporus*	*umbellatus*	Mushroom
71	NPL-KHU-071	*Urticaceae*	*Boehmeria*	*nivea*	Stem
72	NPL-KHU-072	*Adoxaceae*	*Sambucus*	*williamsii*	Fruit
73	NPL-KHU-073	*Tamaricaceae*	*Tamarix*	*chinensis*	Whole plant
74	NPL-KHU-074	*Myrtaceae*	*Syzygium*	*aromaticum*	Flower bud
75	NPL-KHU-075	*Campanulaceae*	*Adenophora*	*remotiflora*	Root
76	NPL-KHU-076	*Rhamnaceae*	*Hovenia*	*dulcis*	Fruit
77	NPL-KHU-077	*Amaranthaceae*	*Kochia*	*scoparia*	Whole plant
78	NPL-KHU-078	*Rutaceae*	*Poncirus*	*trifoliata*	Fruit
79	NPL-KHU-079	*Plantaginaceae*	*Plantago*	*asiatica*	Seed and leaf
80	NPL-KHU-080	*Apiaceae*	*Cnidium*	*officinale*	Root
81	NPL-KHU-081	*Apiaceae*	*Ligusticum*	*chuanxiong*	Root
82	NPL-KHU-082	*Amaranthaceae*	*Celosia*	*argentea*	Whole plant
83	NPL-KHU-083	*Malvaceae*	*Alcea*	*rosea*	Flower
84	NPL-KHU-084	*Amaryllidaceae*	*Allium*	*fistulosum*	Whole plant
85	NPL-KHU-085	*Lamiaceae*	*Leonurus*	*japonicus*	Whole plant
86	NPL-KHU-086	*Cupressaceae*	*Platycladus*	*orientalis*	Rind
87	NPL-KHU-087	*Rubiaceae*	*Gardenia*	*jasminoides*	Fruit
88	NPL-KHU-088	*Thymelaeaceae*	*Aquilaria*	*agallocha*	Resin
89	NPL-KHU-089	*Apiaceae*	*Carum*	*carvi*	Seed
90	NPL-KHU-090	*Apiaceae*	*Cuminum*	*cyminum*	Seed
91	NPL-KHU-091	*Schisandraceae*	*Illicium*	*verum*	Seed
92	NPL-KHU-092	*Euphorbiaceae*	*Ricinus*	*communis*	Seed
93	NPL-KHU-093	*Nelumbonaceae*	*Nelumbo*	*nucifera*	Flower, seed and root
94	NPL-KHU-094	*Asteraceae*	*Carpesium*	*abrotanoides*	Whole plant
95	NPL-KHU-095	*Asteraceae*	*Eclipta*	*prostrata*	Whole plant
96	NPL-KHU-096	*Lamiaceae*	*Phlomis*	*umbrosa*	Whole plant
97	NPL-KHU-097	*Asteraceae*	*Artemisia*	*gmelinii*	Leaf
98	NPL-KHU-098	*Lygodiaceae*	*Lygodium*	*japonicum*	Whole plant
99	NPL-KHU-099	*Apiaceae*	*Glehnia*	*littoralis*	Root
100	NPL-KHU-100	*Pinaceae*	*Pinus*	*koraiensis*	Seed
101	NPL-KHU-101	*Lamiaceae*	*Elsholtzia*	*ciliata*	Whole plant
102	NPL-KHU-102	*Geraniaceae*	*Geranium*	*thunbergii*	Root
103	NPL-KHU-103	*Lamiaceae*	*Nepeta*	*tenuifolia*	Whole plant
104	NPL-KHU-104	*Juglandaceae*	*Juglans*	*regia*	Seed and rind
105	NPL-KHU-105	*Asteraceae*	*Carthamus*	*tinctorius*	Flower
106	NPL-KHU-106	*Lamiaceae*	*Scutellaria*	*baicalensis*	Root
107	NPL-KHU-107	*Lauraceae*	*Lindera*	*obtusiloba*	Whole plant
108	NPL-KHU-108	*Apiaceae*	*Foeniculum*	*vulgare*	Seed
109	NPL-KHU-109	*Fabaceae*	*Glycine*	*max*	Seed
110	NPL-KHU-110	*Pedaliaceae*	*Sesamum*	*indicum*	Seed
111	NPL-KIOM-001	*Fabaceae*	*Pueraria*	*lobata*	Root
112	NPL-KIOM-002	*Asteraceae*	*Chrysanthemum*	*indicum*	Flower

Continued

No.	Sample code	Family	Genus	Species	Used part
113	NPL-KIOM-003	*Fabaceae*	*Glycyrrhiza*	*glabra*	Root
114	NPL-KIOM-004	*Fabaceae*	*Glycyrrhiza*	*inflata*	Root
115	NPL-KIOM-005	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
116	NPL-KIOM-006	*Apiaceae*	*Notopterygium*	*forbesii*	Root
117	NPL-KIOM-007	*Apiaceae*	*Notopterygium*	*incisum*	Root
118	NPL-KIOM-008	*Apiaceae*	*Ostericum*	*koreanum*	Root
119	NPL-KIOM-009	*Zingiberaceae*	*Curcuma*	*longa*	Root
120	NPL-KIOM-010	*Brassicaceae*	*Brassica*	*juncea*	Seed and leaf
121	NPL-KIOM-011	*Zingiberaceae*	*Zingiber*	*officinale*	Root
122	NPL-KIOM-012	*Fagaceae*	*Castanea*	*crenata*	Fruit
123	NPL-KIOM-013	*Nymphaeaceae*	*Euryale*	*ferox*	Seed
124	NPL-KIOM-014	*Fabaceae*	*Cassia*	*obtusifolia*	Seed
125	NPL-KIOM-015	*Fabaceae*	*Cassia*	*tora*	Seed
126	NPL-KIOM-016	*Lauraceae*	*Cinnamomum*	*cassia*	Rind
127	NPL-KIOM-017	*Zingiberaceae*	*Alpinia*	*officinarum*	Root
128	NPL-KIOM-018	*Apiaceae*	*Ligusticum*	*sinense*	Root
129	NPL-KIOM-019	*Apiaceae*	*Ligusticum*	*tenuissima*	Root
130	NPL-KIOM-020	*Santalaceae*	*Viscum*	*album*	Whole plant
131	NPL-KIOM-021	*Fabaceae*	*Caragana*	*sinica*	Root
132	NPL-KIOM-022	*Polypodiaceae*	*Drynaria*	*fortunei*	Root
133	NPL-KIOM-023	*Lamiaceae*	*Agastache*	*rugosa*	Whole plant
134	NPL-KIOM-024	*Cucurbitaceae*	*Trichosanthes*	*kirilowii*	Root
135	NPL-KIOM-025	*Cucurbitaceae*	*Trichosanthes*	*rosthornii*	Root
136	NPL-KIOM-026	*Cucurbitaceae*	*Trichosanthes*	*kirilowii*	Root
137	NPL-KIOM-027	*Cucurbitaceae*	*Trichosanthes*	*rosthornii*	Root
138	NPL-KIOM-028	*Lamiaceae*	*Pogostemon*	*cablin*	Whole plant
139	NPL-KIOM-029	*Solanaceae*	*Lycium*	*barbarum*	Fruit
140	NPL-KIOM-030	*Solanaceae*	*Lycium*	*chinense*	Fruit
141	NPL-KIOM-031	*Asteraceae*	*Chrysanthemum*	*zawadskii*	Flower
142	NPL-KIOM-032	*Asteraceae*	*Chrysanthemum*	*zawadskii*	Flower
143	NPL-KIOM-033	*Dicksoniaceae*	*Cibotium*	*barometz*	Root
144	NPL-KIOM-034	*Asteraceae*	*Chrysanthemum*	*morifolium*	Flower
145	NPL-KIOM-035	*Caprifoliaceae*	*Lonicera*	*japonica*	Flower and leaf
146	NPL-KIOM-036	*Primulaceae*	*Lysimachia*	*christinae*	Root
147	NPL-KIOM-037	*Campanulaceae*	*Platycodon*	*grandiflorum*	Root
148	NPL-KIOM-038	*Brassicaceae*	*Raphanus*	*sativus*	Root
149	NPL-KIOM-039	*Poaceae*	*Phragmites*	*communis*	Whole plant
150	NPL-KIOM-040	*Lamiaceae*	*Salvia*	*miltiorrhiza*	Root
151	NPL-KIOM-041	*Apiaceae*	*Angelica*	*gigas*	Root
152	NPL-KIOM-042	*Campanulaceae*	*Codonopsis*	*pilosula*	Root
153	NPL-KIOM-043	*Campanulaceae*	*Codonopsis*	*tangshen*	Root
154	NPL-KIOM-044	*Campanulaceae*	*Codonopsis*	*pilosula*	Root
155	NPL-KIOM-045	*Arecaceae*	*Areca*	*catechu*	Seed
156	NPL-KIOM-046	*Rhamnaceae*	*Zizyphus*	*jujuba*	Fruit
157	NPL-KIOM-047	*Rhamnaceae*	*Zizyphus*	*jujuba*	Fruit
158	NPL-KIOM-048	*Rosaceae*	*Prunus*	*davidiana*	Seed
159	NPL-KIOM-049	*Rosaceae*	*Prunus*	*persica*	Fruit
160	NPL-KIOM-050	*Araliaceae*	*Aralia*	*continentalis*	Root
161	NPL-KIOM-051	*Eucommiaceae*	*Eucommia*	*ulmoides*	Rind
162	NPL-KIOM-052	*Eucommiaceae*	*Eucommia*	*ulmoides*	Rind
163	NPL-KIOM-053	*Cannabaceae*	*Cannabis*	*sativa*	Whole plant
164	NPL-KIOM-054	*Portulacaceae*	*Portulaca*	*oleracea*	Whole plant
165	NPL-KIOM-055	*Ephedraceae*	*Ephedra*	*sinica*	Whole plant
166	NPL-KIOM-056	*Ephedraceae*	*Ephedra*	*intermedia*	Whole plant
167	NPL-KIOM-057	*Ephedraceae*	*Ephedra*	*equisetina*	Whole plant
168	NPL-KIOM-058	*Ephedraceae*	*Ephedra*	*intermedia*	Whole plant
Continued					

No.	Sample code	Family	Genus	Species	Used part
169	NPL-KIOM-059	*Ephedraceae*	*Ephedra*	*equisetina*	Whole plant
170	NPL-KIOM-060	*Verbenaceae*	*Vitex*	*rotundifolia*	Seed
171	NPL-KIOM-061	*Verbenaceae*	*Vitex*	*trifolia*	Seed
172	NPL-KIOM-062	*Asparagaceae*	*Liriope*	*platyphylla*	Root
173	NPL-KIOM-063	*Asparagaceae*	*Ophiopogon*	*japonicus*	Root
174	NPL-KIOM-064	*Poaceae*	*Hordeum*	*vulgare*	Whole plant
175	NPL-KIOM-065	*Rosaceae*	*Chaenomeles*	*sinensis*	Fruit
176	NPL-KIOM-066	*Rosaceae*	*Chaenomeles*	*speciosa*	Fruit
177	NPL-KIOM-067	*Paeoniaceae*	*Paeonia*	*suffruticosa*	Root
178	NPL-KIOM-068	*Equisetaceae*	*Equisetum*	*hyemale*	Whole plant
179	NPL-KIOM-069	*Lardizabalaceae*	*Akebia*	*quinata*	Fruit
180	NPL-KIOM-070	*Asteraceae*	*Aucklandia*	*lappa*	Root
181	NPL-KIOM-071	*Lamiaceae*	*Mentha*	*arvensis*	Whole plant
182	NPL-KIOM-072	*Araceae*	*Pinellia*	*ternata*	Root
183	NPL-KIOM-073	*Menispermaceae*	*Sinomenium*	*acutum*	Root
184	NPL-KIOM-074	*Apiaceae*	*Saposhnikovia*	*divaricata*	Root
185	NPL-KIOM-075	*Ginkgoaceae*	*Ginkgo*	*biloba*	Leaf
186	NPL-KIOM-076	*Papaveraceae*	*Chelidonium*	*majus*	Whole plant
187	NPL-KIOM-077	*Zingiberaceae*	*Amomum*	*kravanh*	Seed
188	NPL-KIOM-078	*Zingiberaceae*	*Amomum*	*compactum*	Seed
189	NPL-KIOM-079	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
190	NPL-KIOM-080	*Apiaceae*	*Angelica*	*dahurica*	Root
191	NPL-KIOM-081	*Apiaceae*	*Angelica*	*dahurica*	Root
192	NPL-KIOM-082	*Asteraceae*	*Atractylodes*	*japonica*	Root
193	NPL-KIOM-083	*Asteraceae*	*Atractylodes*	*macrocephala*	Root
194	NPL-KIOM-084	*Fabaceae*	*Dolichos*	*lablab*	Fruit
195	NPL-KIOM-085	*Rubiaceae*	*Hedyotis*	*diffusa*	Whole plant
196	NPL-KIOM-086	*Fabaceae*	*Psoralea*	*corylifolia*	Seed
197	NPL-KIOM-087	*Polyporaceae*	*Poria*	*cocos*	Mycelium
198	NPL-KIOM-088	*Rosaceae*	*Rubus*	*coreanus*	Fruit
199	NPL-KIOM-089	*Ranunculaceae*	*Aconitum*	*carmichaeli*	Root
200	NPL-KIOM-090	*Ranunculaceae*	*Aconitum*	*carmichaeli*	Root
201	NPL-KIOM-091	*Arecaceae*	*Areca*	*catechu*	Seed
202	NPL-KIOM-092	*Campanulaceae*	*Adenophora*	*triphylla*	Root
203	NPL-KIOM-093	*Apiaceae*	*Cnidium*	*monieri*	Seed
204	NPL-KIOM-094	*Apiaceae*	*Torilis*	*japonica*	Seed
205	NPL-KIOM-095	*Zingiberaceae*	*Amomum*	*villosum*	Seed
206	NPL-KIOM-096	*Zingiberaceae*	*Amomum*	*villosum*	Seed
207	NPL-KIOM-097	*Rosaceae*	*Crataegus*	*pinnatifida*	Fruit
208	NPL-KIOM-098	*Cornaceae*	*Cornus*	*officinalis*	Fruit
209	NPL-KIOM-099	*Dioscoreaceae*	*Dioscorea*	*batatas*	Root
210	NPL-KIOM-100	*Dioscoreaceae*	*Dioscorea*	*japonica*	Root
211	NPL-KIOM-101	*Rhamnaceae*	*Zizyphus*	*jujuba*	Fruit and root
212	NPL-KIOM-102	*Rhamnaceae*	*Zizyphus*	*jujuba*	Fruit and root
213	NPL-KIOM-103	*Rutaceae*	*Zanthoxylum*	*piperitum*	Rind and seed
214	NPL-KIOM-104	*Rutaceae*	*Zanthoxylum*	*schinifolium*	Rind and seed
215	NPL-KIOM-105	*Rutaceae*	*Zanthoxylum*	*bungeanum*	Rind and seed
216	NPL-KIOM-106	*Sparganiaceae*	*Sparganium*	*stoloniferum*	Root
217	NPL-KIOM-107	*Moraceae*	*Morus*	*alba*	Leaf and fruit
218	NPL-KIOM-108	*Moraceae*	*Morus*	*alba*	Leaf and fruit
219	NPL-KIOM-109	*Moraceae*	*Morus*	*bombycis*	Leaf and root
220	NPL-KIOM-110	*Moraceae*	*Morus*	*alba*	Leaf and fruit
221	NPL-KIOM-111	*Orchidaceae*	*Dendrobium*	*fimbriatum*	Whole plant
222	NPL-KIOM-112	*Orchidaceae*	*Dendrobium*	*candidum*	Whole plant
223	NPL-KIOM-113	*Acoraceae*	-	*Acorus*	gramineus
224	NPL-KIOM-114	*Hypoxidaceae*	*Curculigo*	*orchioides*	Root
Continued					

No.	Sample code	Family	Genus	Species	Used part
225	NPL-KIOM-115	*Aristolochiaceae*	*Asiasarum*	*heterotropoides*	Root
226	NPL-KIOM-116	*Aristolochiaceae*	*Asiasarum*	*sieboldii*	Root
227	NPL-KIOM-117	*Fabaceae*	*Cassia*	*angustifolia*	Leaf and seed
228	NPL-KIOM-118	*Fabaceae*	*Caesalpinia*	*sappan*	Seed and rind
229	NPL-KIOM-119	*Dipsacaceae*	*Dipsacus*	*asperoides*	Root
230	NPL-KIOM-120	*Ranunculaceae*	*Cimicifuga*	*heracleifolia*	Root
231	NPL-KIOM-121	*Ranunculaceae*	*Cimicifuga*	*dahurica*	Root
232	NPL-KIOM-122	*Apiaceae*	*Anethum*	*graveolens*	Whole plant
233	NPL-KIOM-123	*Ebenaceae*	*Diospyros*	*kaki*	Fruit
234	NPL-KIOM-124	*Apiaceae*	*Bupleurum*	*falcatum*	Root
235	NPL-KIOM-125	*Apiaceae*	*Bupleurum*	*scorzonerifolium*	Root
236	NPL-KIOM-126	*Apiaceae*	*Peucedanum*	*japonicum*	Root
237	NPL-KIOM-127	*Lycopodiaceae*	*Lycopodium*	*clavatum*	Whole plant
238	NPL-KIOM-128	*Zingiberaceae*	*Curcuma*	*kwangsiensis*	Root
239	NPL-KIOM-129	*Zingiberaceae*	*Curcuma*	*phaeocaulis*	Root
240	NPL-KIOM-130	*Zingiberaceae*	*Curcuma*	*wenyujin*	Root
241	NPL-KIOM-131	*Asteraceae*	*Artemisia*	*argyi*	Leaf
242	NPL-KIOM-132	*Asteraceae*	*Artemisia*	*princeps*	Leaf
243	NPL-KIOM-133	*Asteraceae*	*Artemisia*	*montana*	Leaf
244	NPL-KIOM-134	*Saururaceae*	*Houttuynia*	*cordata*	Whole plant
245	NPL-KIOM-135	*Oleaceae*	*Ligustrum*	*lucidum*	Fruit and leaf
246	NPL-KIOM-136	*Oleaceae*	*Ligustrum*	*japoricum*	Fruit and leaf
247	NPL-KIOM-137	*Oleaceae*	*Forsythia*	*viridissima*	Fruit and leaf
248	NPL-KIOM-138	*Oleaceae*	*Forsythia*	*suspensa*	Fruit and leaf
249	NPL-KIOM-139	*Nelumbonaceae*	*Nelumbo*	*nucifera*	Seed and root
250	NPL-KIOM-140	*Araliaceae*	*Acanthopanax*	*sessiliflorum*	Root
251	NPL-KIOM-141	*Scolopendridae*	*Scolopendra*	*subspinipes*	Whole plant
252	NPL-KIOM-142	*Schisandraceae*	*Schisandra*	*chinensis*	Fruit
253	NPL-KIOM-143	*Rutaceae*	*Evodia*	*rutaecarpa*	Fruit and seed
254	NPL-KIOM-144	*Lauraceae*	*Lindera*	*strichnifolia*	Whole plant
255	NPL-KIOM-145	*Convallariaceae*	*Polygonatum*	*odoratum*	Root
256	NPL-KIOM-146	*Gentianaceae*	*Gentiana*	*manshurica*	Root
257	NPL-KIOM-147	*Gentianaceae*	*Gentiana*	*scabra*	Root
258	NPL-KIOM-148	*Sapindaceae*	*Dimocarpus*	*longan*	Fruit
259	NPL-KIOM-149	*Asteraceae*	*Arctium*	*lappa*	Root
260	NPL-KIOM-150	*Amaranthaceae*	*Achyranthes*	*japonica*	Root
261	NPL-KIOM-151	*Zingiberaceae*	*Curcuma*	*wenyujin*	Root
262	NPL-KIOM-152	*Polygalaceae*	*Polygala*	*tenuifolia*	Root
263	NPL-KIOM-153	*Ranunculaceae*	*Clematis*	*manshurica*	Root
264	NPL-KIOM-154	*Ranunculaceae*	*Clematis*	*chinensis*	Root
265	NPL-KIOM-155	*Ulmaceae*	*Ulmus*	*macrocarpa*	Rind
266	NPL-KIOM-156	*Lauraceae*	*Cinnamomum*	*cassia*	Rind
267	NPL-KIOM-157	*Orobanchaceae*	*Cistanche*	*deserticola*	Whole plant
268	NPL-KIOM-158	*Ginkgoaceae*	*Ginkgo*	*biloba*	Leaf
269	NPL-KIOM-159	*Berberidaceae*	*Epimedium*	*koreanum*	Whole plant
270	NPL-KIOM-160	*Berberidaceae*	*Epimedium*	*sagittatum*	Whole plant
271	NPL-KIOM-161	*Berberidaceae*	*Epimedium*	*brevicornum*	Whole plant
272	NPL-KIOM-162	*Poaceae*	*Coix*	*lacryma-jovi*	Seed
273	NPL-KIOM-163	*Lamiaceae*	*Leonurus*	*japonicus*	Whole plant
274	NPL-KIOM-164	*Zingiberaceae*	*Alpinia*	*oxyphylla*	Root
275	NPL-KIOM-165	*Caprifoliaceae*	*Lonicera*	*japonica*	Flower and leaf
276	NPL-KIOM-166	*Araliaceae*	*Panax*	*ginseng*	Root
277	NPL-KIOM-167	*Asteraceae*	*Artemisia*	*capillaris*	Leaf
278	NPL-KIOM-168	*Apiaceae*	*Angelica*	*acutiloba*	Root
279	NPL-KIOM-169	*Apiaceae*	*Angelica*	*acutiloba*	Root
280	NPL-KIOM-170	*Boraginaceae*	*Lithospermum*	*erythrorhizon*	Root

Continued

No.	Sample code	Family	Genus	Species	Used part
281	NPL-KIOM-171	*Boraginaceae*	*Arnebia*	*euchroma*	Root
282	NPL-KIOM-172	*Boraginaceae*	*Arnebia*	*guttata*	Root
283	NPL-KIOM-173	*Lamiaceae*	*Perilla*	*frutescens*	Leaf
284	NPL-KIOM-174	*Lamiaceae*	*Perilla*	*frutescens*	Leaf
285	NPL-KIOM-175	*Lamiaceae*	*Perilla*	*frutescens*	Leaf
286	NPL-KIOM-176	*Lamiaceae*	*Perilla*	*frutescens*	Leaf
287	NPL-KIOM-177	*Asteraceae*	*Aster*	*tataricus*	Whole plant
288	NPL-KIOM-178	*Paeoniaceae*	*Paeonia*	*lactiflora*	Root
289	NPL-KIOM-179	*Polyporaceae*	*Polyporus*	*umbellatus*	Mycelium
290	NPL-KIOM-180	*Apiaceae*	*Angelica*	*decursiva*	Root
291	NPL-KIOM-181	*Apiaceae*	*Peucedanum*	*praeruptorum*	Root
292	NPL-KIOM-182	*Liliaceae*	*Fritillaria*	*thunbergii*	Bulb
293	NPL-KIOM-183	*Ranunculaceae*	*Aconitum*	*carmichaeli*	Root
294	NPL-KIOM-184	*Fabaceae*	*Gleditsia*	*sinensis*	Seed and rind
295	NPL-KIOM-185	*Polygonaceae*	*Rheum*	*undulatum*	Root
296	NPL-KIOM-186	*Poaceae*	*Phyllostachys*	*nigra*	Stem
297	NPL-KIOM-187	*Poaceae*	*Phyllostachys*	*bambusoides*	Stem
298	NPL-KIOM-188	*Rutaceae*	*Citrus*	*aurantium*	Rind and fruit
299	NPL-KIOM-189	*Rutaceae*	*Citrus*	*natsudaidai*	Rind and fruit
300	NPL-KIOM-190	*Solanaceae*	*Lycium*	*chinense*	Fruit
301	NPL-KIOM-191	*Solanaceae*	*Lycium*	*barbarum*	Fruit
302	NPL-KIOM-192	*Rhamnaceae*	*Hovenia*	*dulcis*	Fruit
303	NPL-KIOM-193	*Asparagaceae*	*Anemarrhena*	*asphodeloides*	Root
304	NPL-KIOM-194	*Amaranthaceae*	*Kochia*	*scoparia*	Whole plant
305	NPL-KIOM-195	*Rutaceae*	*Poncirus*	*trifoliata*	Fruit and rind
306	NPL-KIOM-196	*Rosaceae*	*Sanguisorba*	*officinalis*	Root
307	NPL-KIOM-197	*Rosaceae*	*Sanguisorba*	*officinalis*	Root
308	NPL-KIOM-198	*Orobanchaceae*	*Rehmannia*	*glutinosa*	Root
309	NPL-KIOM-199	*Gentianaceae*	*Gentiana*	*dahurica*	Root
310	NPL-KIOM-200	*Rutaceae*	*Citrus*	*reticulata*	Rind and fruit
311	NPL-KIOM-201	*Rutaceae*	*Citrus*	*unshiu*	Rind and fruit
312	NPL-KIOM-202	*Zygophyllaceae*	*Tribulus*	*terrestris*	Fruit
313	NPL-KIOM-203	*Plantaginaceae*	*Plantago*	*asiatica*	Seed and whole plant
314	NPL-KIOM-204	*Plantaginaceae*	*Plantago*	*depressa*	Seed and whole plant
315	NPL-KIOM-205	*Asteraceae*	*Atractylodes*	*chinensis*	Root
316	NPL-KIOM-206	*Asteraceae*	*Atractylodes*	*lancea*	Root
317	NPL-KIOM-207	*Apiaceae*	*Cnidium*	*officinale*	Root
318	NPL-KIOM-208	*Apiaceae*	*Ligusticum*	*chuanxiong*	Root
319	NPL-KIOM-209	*Araceae*	*Arisaema*	*amurense*	Root
320	NPL-KIOM-210	*Orchidaceae*	*Gastrodia*	*elata*	Bulb
321	NPL-KIOM-211	*Asparagaceae*	*Asparagus*	*cochinchinensis*	Root
322	NPL-KIOM-212	*Rutaceae*	*Citrus*	*reticulata*	Rind and fruit
323	NPL-KIOM-213	*Rutaceae*	*Citrus*	*unshiu*	Rind and fruit
324	NPL-KIOM-214	*Zingiberaceae*	*Amomum*	*tsao-ko*	Seed
325	NPL-KIOM-215	*Zingiberaceae*	*Alpinia*	*katsumadai*	Seed and root
326	NPL-KIOM-216	*Rubiaceae*	*Gardenia*	*jasminoides*	Fruit
327	NPL-KIOM-217	*Anacardiaceae*	*Rhus*	*verniciflua*	Rind
328	NPL-KIOM-218	*Lamiaceae*	*Lycopus*	*lucidus*	Whole plant
329	NPL-KIOM-219	*Alismataceae*	*Alisma*	*orientale*	Root
330	NPL-KIOM-220	*Asteraceae*	*Inula*	*helenium*	Root
331	NPL-KIOM-221	*Smilacaceae*	*Smilax*	*china*	Root
332	NPL-KIOM-222	*Convolvulaceae*	*Cuscuta*	*chinensis*	Whole plant
333	NPL-KIOM-223	*Rubiaceae*	*Morinda*	*officinalis*	Root
334	NPL-KIOM-224	*Asteraceae*	*Eupatorium*	*fortunei*	Whole plant
335	NPL-KIOM-225	*Asteraceae*	*Taraxacum*	*coreanum*	Whole plant
336	NPL-KIOM-226	*Asteraceae*	*Taraxacum*	*mongolicum*	Whole plant

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No.	Sample code	Family	Genus	Species	Used part
337	NPL-KIOM-227	*Asteraceae*	*Taraxacum*	*officinale*	Whole plant
338	NPL-KIOM-228	*Piperaceae*	*Piper*	*longum*	Fruit
339	NPL-KIOM-229	*Polygonaceae*	*Polygonum*	*multiflorum*	Root
340	NPL-KIOM-230	*Asteraceae*	*Eclipta*	*prostrata*	Whole plant
341	NPL-KIOM-231	*Asteraceae*	*Artemisia*	*iwayomogi*	Leaf
342	NPL-KIOM-232	*Fabaceae*	*Albizzia*	*julibrissin*	Flower and fruit
343	NPL-KIOM-233	*Araliaceae*	*Kalopanax*	*pictus*	Rind
344	NPL-KIOM-234	*Apiaceae*	*Glehnia*	*littoralis*	Root
345	NPL-KIOM-235	*Rosaceae*	*Prunus*	*armeniaca*	Fruit
346	NPL-KIOM-236	*Rosaceae*	*Prunus*	*mandshurica*	Fruit
347	NPL-KIOM-237	*Cyperaceae*	*Cyperus*	*rotundus*	Root
348	NPL-KIOM-238	*Lamiaceae*	*Elsholtzia*	*ciliata*	Whole plant
349	NPL-KIOM-239	*Scrophulariaceae*	*Scrophularia*	*buergeriana*	Whole plant
350	NPL-KIOM-240	*Scrophulariaceae*	*Scrophularia*	*ningpoensis*	Whole plant
351	NPL-KIOM-241	*Geraniaceae*	*Geranium*	*thunbergii*	Whole plant
352	NPL-KIOM-242	*Papaveraceae*	*Corydalis*	*ternata*	Root
353	NPL-KIOM-243	*Papaveraceae*	*Corydalis*	*yanhusuo*	Root
354	NPL-KIOM-244	*Lamiaceae*	*Schizonepeta*	*tenuifolia*	Whole plant
355	NPL-KIOM-245	*Fabaceae*	*Trigonella*	*foenum-graecum*	Seed
356	NPL-KIOM-246	*Polygonaceae*	*Polygonum*	*cuspidatum*	Root
357	NPL-KIOM-247	*Asteraceae*	*Carthamus*	*tinctorius*	Flower and seed
358	NPL-KIOM-248	*Asteraceae*	*Carthamus*	*tinctorius*	Flower and seed
359	NPL-KIOM-249	*Lamiaceae*	*Scutellaria*	*baicalensis*	Root
360	NPL-KIOM-250	*Fabaceae*	*Astragalus*	*membranaceus*	Root
361	NPL-KIOM-251	*Fabaceae*	*Astragalus*	*membranaceus*	Root
362	NPL-KIOM-252	*Ranunculaceae*	*Coptis*	*chinensis*	Root
363	NPL-KIOM-253	*Ranunculaceae*	*Coptis*	*deltoidea*	Root
364	NPL-KIOM-254	*Ranunculaceae*	*Coptis*	*japonica*	Root
365	NPL-KIOM-255	*Ranunculaceae*	*Coptis*	*teeta*	Root
366	NPL-KIOM-256	*Rutaceae*	*Phellodendron*	*amurense*	Rind
367	NPL-KIOM-257	*Rutaceae*	*Phellodendron*	*chinense*	Rind
368	NPL-KIOM-258	*Asparagaceae*	*Polygonatum*	*sibiricum*	Root
369	NPL-KIOM-259	*Asparagaceae*	*Polygonatum*	*cyrtonema*	Root
370	NPL-KIOM-260	*Asparagaceae*	*Polygonatum*	*falcatum*	Root
371	NPL-KIOM-261	*Asparagaceae*	*Polygonatum*	*kingianum*	Root
372	NPL-KIOM-262	*Apiaceae*	*Foeniculum*	*vulgare*	Seed
373	NPL-KIOM-263	*Magnoliaceae*	*Magnolia*	*officinalis*	Rind
374	NPL-KIOM-264	*Magnoliaceae*	*Magnolia*	*obovata*	Rind
375	NPL-KIOM-265	*Pedaliaceae*	*Sesamum*	*indicum*	Seed
376	NPL-NET-001	*Ericaceae*	*Vaccinium*	*bracteatum*	Leaves
377	NPL-NET-002	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
378	NPL-NET-003	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
379	NPL-NET-004	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
380	NPL-NET-005	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
381	NPL-NET-006	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
382	NPL-NET-007	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
383	NPL-NET-008	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
384	NPL-NET-009	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
385	NPL-NET-010	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
386	NPL-NET-011	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
387	NPL-NET-012	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
388	NPL-NET-013	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
389	NPL-NET-014	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
390	NPL-NET-015	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
391	NPL-NET-016	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
392	NPL-NET-032	*Apiaceae*	*Ostericum*	*koreanum*	Root
Continued					

No.	Sample code	Family	Genus	Species	Used part
393	NPL-NET-033	*Araliaceae*	*Aralia*	*cordata*	Root
394	NPL-NET-034	*Apiaceae*	*Angelica*	*dahurica*	Root
395	NPL-NET-035	*Apiaceae*	*Anthriscus*	*sylvestris*	Root
396	NPL-NET-036	*Apiaceae*	*Angelica*	*gigas*	Root
397	NPL-NET-037	*Apiaceae*	*Angelica*	*acutiloba*	Root
398	NPL-NET-038	*Apiaceae*	*Angelica*	*sinensis*	Root
399	NPL-NET-039	*Apiaceae*	*Levisticum*	*officinale*	Root
400	NPL-NET-040	*Apiaceae*	*Angelica*	*gigas*	Root
401	NPL-NET-041	*Apiaceae*	*Angelica*	*gigas*	Root
402	NPL-NET-042	*Asteraceae*	*Chrysanthemum*	*cinerariifolium*	Flower
403	NPL-NET-043	*Loganiaceae*	*Strychnos*	-	Seed
404	NPL-NET-044	*Caprifoliaceae*	*Valeriana*	*officinalis*	Root
405	NPL-NPL-001	*Ginkgoaceae*	*Ginkgo*	*biloba*	Leaves
406	NPL-NPL-002	*Fabaceae*	*Sophora*	*japonica*	Flowers
407	NPL-NPL-003	*Asteraceae*	*Senecio*	*jacobaea*	-
408	NPL-NPL-004	*Ranunculaceae*	*Aconitum*	*carmichaelii*	Root
409	NPL-NPL-005	*Ranunculaceae*	*Aconitum*	*carmichaelii*	Root
410	NPL-NPL-006	*Ephedraceae*	*Ephedra*	*sinica*	Aerial parts
411	NPL-NPL-007	*Rutaceae*	*Phellodendron*	*amurense*	Bark
412	NPL-NPL-008	*Rutaceae*	*Phellodendron*	*amurense*	Bark
413	NPL-NPL-009	*Ranunculaceae*	*Coptis*	*japonica*	Root
414	NPL-NPL-010	*Ulmaceae*	*Ulmus*	*davidiana*	Bark
415	NPL-NPL-011	*Araliaceae*	*Acanthopanax*	*sessiliflorum*	Root and stem
416	NPL-NPL-012	*Paeoniaceae*	*Paeonia*	*suffriticosa*	Root
417	NPL-NPL-013	*Paeoniaceae*	*Paeonia*	*suffriticosa*	Root
418	NPL-NPL-014	*Fabaceae*	*Glycyrrhiza*	*glabra*	Root
419	NPL-NPL-015	*Fabaceae*	*Glycyrrhiza*	*glabra*	Root
420	NPL-NPL-016	*Lamiaceae*	*Scutellaria*	*baicalensis*	Root
421	NPL-NPL-017	*Rubiaceae*	*Uncaria*	*rhynchophylla*	Stem and hooks
422	NPL-NPL-018	*Rubiaceae*	*Uncaria*	*tomentosa*	Stem and hooks
423	NPL-NPL-019	*Taxaceae*	*Taxus*	*chinensis*	-
424	NPL-NPL-020	*Fabaceae*	*Genista*	*monspesulana*	Leaves
425	NPL-NPL-021	*Fabaceae*	*Astragalus*	*membranaceus*	Root
426	NPL-NPL-022	*Solanaceae*	*Lycium*	*chinensis*	Fruit
427	NPL-NPL-023	*Amaranthaceae*	*Achyranthes*	*bidentata*	Root
428	NPL-NPL-024	*Amaranthaceae*	*Achyranthes*	*japonica*	Root
429	NPL-NPL-025	*Amaranthaceae*	*Cyathula*	*officinalis*	Root
430	NPL-NPL-026	*Aquifoliaceae*	*Ilex*	*aquifolium*	Leaves
431	NPL-NPL-027	*Malvaceae*	*Adansonia*	*digitata*	Fruit and leaves
432	NPL-NPL-028	*Campanulaceae*	*Codonopsis*	*pilosula*	Root
433	NPL-NPL-029	*Apocynaceae*	*Catharanthus*	*roseus*	Leaves
434	NPL-NPL-031	*Poaceae*	*Zea*	*mays*	Seed
435	NPL-NPL-032	*Asteraceae*	*Calendula*	*arvensis*	Flower
436	NPL-NPL-033	*Moraceae*	*Morus*	*alba*	Leaves
437	NPL-NPL-034	*Moraceae*	*Morus*	*alba*	Leaves
438	NPL-NPL-037	*Boraginaceae*	*Arnebia*	*euchroma*	Root
439	NPL-NPL-038	*Asteraceae*	*Synurus*	*deltoides*	Leaves
440	NPL-NPL-039	*Fabaceae*	*Millettia*	*saptholobi*	Stem
441	NPL-NPL-040	*Apocynaceae*	*Hoodia*	*gordonii*	Stem
442	NPL-NPL-041	*Lamiaceae*	*Orthosiphon*	*stamineus*	Leaves
443	NPL-NPL-042	*Polygalaceae*	*Polygala*	*tenuifolia*	Root
444	NPL-NPL-043	*Polygalaceae*	*Polygala*	*tenuifolia*	Root
445	NPL-NPL-044	*Apiaceae*	*Angelica*	*acutiloba*	Root
446	NPL-NPL-045	*Schisandraceae*	*Schisandra*	*chinensis*	Fruit
447	NPL-NPL-046	*Asteraceae*	*Chrysanthemum*	*indicum*	Flower
448	NPL-NPL-047	*Rhamnaceae*	*Zizyphus*	*jujuba*	Fruit

Continued

No.	Sample code	Family	Genus	Species	Used part
449	NPL-NPL-048	*Apiaceae*	*Ligusticum*	*striatum*	Root
450	NPL-RDA-001	*Araliaceae*	*Panax*	*ginseng*	Root
451	NPL-RDA-002	*Zingiberaceae*	*Zingiber*	*officinale*	Root
452	NPL-RDA-003	*Schisandraceae*	*Schisandra*	*chinensis*	Fruit
453	NPL-RDA-004	*Paeoniaceae*	*Paeonia*	*lactiflora*	Root
454	NPL-RDA-005	*Asteraceae*	*Atractylodes*	*macrocephala*	Root
455	NPL-RDA-006	*Asteraceae*	*Artemisia*	*iwayomogi*	Leaves
456	NPL-RDA-007	*Campanulaceae*	*Codonopsis*	*lanceolata*	Root
457	NPL-RDA-008	*Apiaceae*	*Angelica*	*gigas*	Root
458	NPL-RDA-009	*Apiaceae*	*Cnidium*	*officinale*	Root
459	NPL-RDA-010	*Asteraceae*	*Artemisia*	*argyi*	Leaves
460	NPL-RDA-011	*Araliaceae*	*Acanthopanax*	*senticosus*	Root and stem
461	NPL-RDA-012	*Amaranthaceae*	*Achyranthes*	*japonica*	Root
462	NPL-RDA-013	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
463	NPL-RDA-014	*Cornaceae*	*Cornus*	*officinalis*	Fruit
464	NPL-RDA-015	*Zingiberaceae*	*Curcuma*	*longa*	Rhizome
465	NPL-RDA-016	*Fabaceae*	*Astragalus*	*membranaceus*	Root
466	NPL-RDA-017	*Asteraceae*	*Ixeris*	*strigosa*	Leaves
467	NPL-RDA-018	*Lamiaceae*	*Scutellaria*	*baicalensis*	Root
468	NPL-RDA-019	*Rosaceae*	*Rubus*	*coreanus*	Fruit
469	NPL-RDA-020	*Araliaceae*	*Aralia*	*continentalis*	Root
470	NPL-RDA-021	*Poaceae*	*Coix*	*lacryma-jobi*	Seed
471	NPL-RDA-022	*Campanulaceae*	*Platycodon*	*grandiflorum*	Root
472	NPL-RDA-023	*Orobanchaceae*	*Rehmannia*	*glutinosa*	Root
473	NPL-RDA-024	*Asteraceae*	*Carthamus*	*tinctorius*	Flower
474	NPL-RDA-025	*Asparagaceae*	*Liriope*	*platyphylla*	Root
475	NPL-RDA-026	*Polygonaceae*	*Polygonum*	*multiflorum*	Root
476	NPL-RDA-027	*Asparagaceae*	*Polygonatum*	*sibiricum*	Root
477	NPL-RDA-028	*Apocynaceae*	*Cynanchum*	*wilfordii*	Root
478	NPL-SUB-001	*Apiaceae*	*Notopterygium*	-	Root
479	NPL-SUB-002	*Apiaceae*	*Glehnia*	*littoralis*	Root
480	NPL-SUB-003	*Apiaceae*	*Glehnia*	*littoralis*	Root
481	NPL-SUB-004	*Zingiberaceae*	*Zingiber*	-	Root
482	NPL-SUB-005	*Zingiberaceae*	*Alpinia*	*officinarum*	Root
483	NPL-SUB-006	*Apiaceae*	*Ligusticum*	*chuanxiong*	Root
484	NPL-SUB-007	*Polypodiaceae*	*Drynaria*	*fortunei*	Root
485	NPL-SUB-008	*Cibotiaceae*	*Cibotium*	*barometz*	Root
486	NPL-SUB-009	*Polygonaceae*	*Fagopyrum*	*dibotryis*	Root
487	NPL-SUB-010	*Campanulaceae*	*Platycodon*	*grandiflorus*	Root
488	NPL-SUB-011	*Lamiaceae*	*Salvia*	*miltiorrhiza*	Root
489	NPL-SUB-012	*Lamiaceae*	*Salvia*	*miltiorrhiza*	Root
490	NPL-SUB-013	*Lamiaceae*	*Salvia*	*miltiorrhiza*	Root
491	NPL-SUB-014	*Lamiaceae*	*Salvia*	*miltiorrhiza*	Root
492	NPL-SUB-015	*Apiaceae*	*Angelica*	*sinensis*	Root
493	NPL-SUB-016	*Campanulaceae*	*Adenophora*	*remotiflora*	Root
494	NPL-SUB-017	*Euphorbiaceae*	*Euphorbia*	*pekinensis*	Root
495	NPL-SUB-018	*Polygonaceae*	*Rheum*	*palmatum*	Root
496	NPL-SUB-019	*Apiaceae*	*Cnidium*	*officinale*	Root
497	NPL-SUB-020	*Apiaceae*	*Angelica*	*pubescens*	Root
498	NPL-SUB-021	*Araliaceae*	*Aralia*	*cordata*	Root
499	NPL-SUB-022	*Eucommiaceae*	*Eucommia*	*ulmoides*	Rind
500	NPL-SUB-023	*Dioscoreaceae*	*Dioscorea*	*oposita*	Root
501	NPL-SUB-024	*Poaceae*	*Imperata*	*cylindrica*	Root
502	NPL-SUB-025	*Urticaceae*	*Boehmeria*	*nivea*	Root
503	NPL-SUB-026	*Asteraceae*	*Aucklandia*	*lappa*	Root
504	NPL-SUB-027	*Asteraceae*	*Saussurea*	*costus*	Root
Continued					

No.	Sample code	Family	Genus	Species	Used part
505	NPL-SUB-028	*Menispermaceae*	*Stephania*	*tetrandra*	Root
506	NPL-SUB-029	*Asparagaceae*	*Ledebouria*	*seseloides*	Root
507	NPL-SUB-030	*Ranunculaceae*	*Pulsatilla*	*chinensis*	Root
508	NPL-SUB-031	*Vitaceae*	*Ampelopsis*	*radix*	Root
509	NPL-SUB-032	*Stemonaceae*	*Stemona*	*japonica*	Root
510	NPL-SUB-033	*Paeoniaceae*	*Paeonia*	*lactiflora*	Root
511	NPL-SUB-034	*Asclepiadaceae*	*Cynanchum*	*stauntonii*	Root
512	NPL-SUB-035	*Apiaceae*	*Angelica*	*dahurica*	Root
513	NPL-SUB-036	*Asteraceae*	*Atractylodes*	*macrocephala*	Root
514	NPL-SUB-037	*Asteraceae*	*Rhaponticum*	*uniflorum*	Root
515	NPL-SUB-038	*Zingiberaceae*	*Kaempferia*	*galanga*	Root
516	NPL-SUB-039	*Dipsacaceae*	*Dipsacus*	*asper*	Root
517	NPL-SUB-040	*Araliaceae*	*Panax*	*notoginseng*	Root
518	NPL-SUB-041	*Araliaceae*	*Panax*	*notoginseng*	Root
519	NPL-SUB-042	*Araliaceae*	*Panax*	*notoginseng*	Root
520	NPL-SUB-043	*Phytolaccaceae*	*Phytolacca*	*acinosa*	Root
521	NPL-SUB-044	*Polygonaceae*	*Polygonum*	*multiflorum*	Root
522	NPL-SUB-045	*Acoraceae*	*Acorus*	*tatarinowii*	Root
523	NPL-SUB-046	*Liliaceae*	*Ophiopogon*	*japonicus*	Root
524	NPL-SUB-047	*Dipsacaceae*	*Dipsacus*	*asper*	Root
525	NPL-SUB-048	*Apiaceae*	*Bupleurum*	*chinense*	Root
526	NPL-SUB-049	*Ranunculaceae*	*Anemone*	*raddeana*	Root
527	NPL-SUB-050	*Schisandraceae*	*Schisandra*	*chinensis*	Fruit
528	NPL-SUB-051	*Zingiberaceae*	*Curcuma*	*longa*	Root
529	NPL-SUB-052	*Asparagaceae*	*Polygonatum*	*sibiricum*	Root
530	NPL-SUB-053	*Amaranthaceae*	*Achyranthes*	*bidentata*	Root
531	NPL-SUB-054	*Amaranthaceae*	*Achyranthes*	*bidentata*	Root
532	NPL-SUB-055	*Amaranthaceae*	*Achyranthes*	*bidentata*	Root
533	NPL-SUB-056	*Polygalaceae*	*Polygala*	*tenuifolia*	Root
534	NPL-SUB-057	*Ranunculaceae*	*Clematis*	*chinensis*	Root
535	NPL-SUB-058	*Caryophyllaceae*	*Stellaria*	*media*	Root
536	NPL-SUB-059	*Araliaceae*	*Panax*	*ginseng*	Root
537	NPL-SUB-060	*Araliaceae*	*Panax*	*ginseng*	Root
538	NPL-SUB-061	*Araliaceae*	*Panax*	*ginseng*	Root
539	NPL-SUB-062	*Araliaceae*	*Panax*	*ginseng*	Root
540	NPL-SUB-063	*Asteraceae*	*Aster*	*tataricus*	Root
541	NPL-SUB-064	*Boraginaceae*	*Arnebia*	*euchroma*	Root
542	NPL-SUB-065	*Paeoniaceae*	*Paeonia*	*lactiflora*	Root
543	NPL-SUB-066	*Apiaceae*	*Anthriscus*	*sylvestris*	Root
544	NPL-SUB-067	*Asparagaceae*	*Anemarrhena*	*asphodeloides*	Root
545	NPL-SUB-068	*Asparagaceae*	*Anemarrhena*	*asphodeloides*	Root
546	NPL-SUB-069	*Asparagaceae*	*Anemarrhena*	*asphodeloides*	Root
547	NPL-SUB-070	*Asparagaceae*	*Anemarrhena*	*asphodeloides*	Root
548	NPL-SUB-071	*Rosaceae*	*Sanguisorba*	*officinalis*	Root
549	NPL-SUB-072	*Boraginaceae*	*Arnebia*	*euchroma*	Root
550	NPL-SUB-073	*Asteraceae*	*Atractylodes*	*macrocephala*	Root
551	NPL-SUB-074	*Apiaceae*	*Ligusticum*	*chuanxiong*	Root
552	NPL-SUB-075	*Apiaceae*	*Ligusticum*	*chuanxiong*	Root
553	NPL-SUB-076	*Apiaceae*	*Ligusticum*	*chuanxiong*	Root
554	NPL-SUB-077	*Ranunculaceae*	*Semiaquilegia*	*adoxoides*	Root
555	NPL-SUB-078	*Asparagaceae*	*Asparagus*	*cochinchinensis*	Root
556	NPL-SUB-079	*Orchidaceae*	*Gastrodia*	*elata*	Root
557	NPL-SUB-080	*Orchidaceae*	*Gastrodia*	*elata*	Root
558	NPL-SUB-081	*Smilacaceae*	*Smilax*	*china*	Root
559	NPL-SUB-082	*Smilacaceae*	*Smilax*	*china*	Root
560	NPL-SUB-083	*Caryophyllaceae*	*Pseudostellaria*	*heterophylla*	Root

Continued

No.	Sample code	Family	Genus	Species	Used part
561	NPL-SUB-084	*Caryophyllaceae*	*Pseudostellaria*	*heterophylla*	Root
562	NPL-SUB-085	*Smilacaceae*	*Smilax*	*china*	Root
563	NPL-SUB-086	*Cruciferae*	*Isatis*	*tinctoria*	Root
564	NPL-SUB-087	*Zingiberaceae*	*Zingiber*	-	Root
565	NPL-SUB-088	*Cyperaceae*	*Cyperus*	*rotundus*	Root
566	NPL-SUB-089	*Scrophulariaceae*	*Scrophularia*	*ningpoensis*	Root
567	NPL-SUB-090	*Poaceae*	*Phragmites*	*communis*	Root
568	NPL-SUB-091	*Polygonaceae*	*Polygonum*	*cuspidatum*	Root
569	NPL-SUB-092	*Scrophulariaceae*	*Picrorhiza*	*kurroa*	Root
570	NPL-SUB-093	*Fabaceae*	*Hedysarum*	*polybotrys*	Root
571	NPL-SUB-094	*Araliaceae*	*Panax*	*ginseng*	Root
572	NPL-SUB-095	*Araliaceae*	*Panax*	*ginseng*	Root
573	NPL-SUB-096	*Lamiaceae*	*Scutellaria*	*baicalensis*	Root
574	NPL-SUB-097	*Fabaceae*	*Astragalus*	*membranaceus*	Root
575	NPL-SUB-098	*Fabaceae*	*Astragalus*	*membranaceus*	Root
576	NPL-SUB-099	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
577	NPL-SUB-100	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
578	NPL-SUB-101	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
579	NPL-SUB-102	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
580	NPL-SUB-103	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
581	NPL-SUB-104	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
582	NPL-SUB-105	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
583	NPL-SUB-106	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
584	NPL-SUB-107	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
585	NPL-SUB-108	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
586	NPL-SUB-109	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
587	NPL-SUB-110	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
588	NPL-SUB-111	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
589	NPL-SUB-112	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
590	NPL-SUB-113	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
591	NPL-SUB-114	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
592	NPL-SUB-115	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
593	NPL-SUB-116	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
594	NPL-SUB-117	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
595	NPL-SUB-118	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
596	NPL-SUB-119	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
597	NPL-SUB-120	*Fabaceae*	*Astragalus*	*membranaceus*	Root
598	NPL-SUB-121	*Fabaceae*	*Astragalus*	*membranaceus*	Root
599	NPL-SUB-122	*Fabaceae*	*Astragalus*	*membranaceus*	Root
600	NPL-SUB-123	*Fabaceae*	*Astragalus*	*membranaceus*	Root
601	NPL-SUB-124	*Fabaceae*	*Astragalus*	*membranaceus*	Root
602	NPL-SUB-125	*Fabaceae*	*Astragalus*	*membranaceus*	Root
603	NPL-SUB-126	*Fabaceae*	*Astragalus*	*membranaceus*	Root
604	NPL-SUB-127	*Fabaceae*	*Astragalus*	*membranaceus*	Root
605	NPL-SUB-128	*Fabaceae*	*Astragalus*	*membranaceus*	Root
606	NPL-SUB-129	*Fabaceae*	*Astragalus*	*membranaceus*	Root
607	NPL-SUB-130	*Fabaceae*	*Astragalus*	*membranaceus*	Root
608	NPL-SUB-131	*Fabaceae*	*Astragalus*	*membranaceus*	Root
609	NPL-SUB-132	*Fabaceae*	*Astragalus*	*membranaceus*	Root
610	NPL-SUB-133	*Fabaceae*	*Astragalus*	*membranaceus*	Root
611	NPL-SUB-134	*Fabaceae*	*Astragalus*	*membranaceus*	Root
612	NPL-SUB-135	*Fabaceae*	*Astragalus*	*membranaceus*	Root
613	NPL-SUB-136	*Fabaceae*	*Astragalus*	*membranaceus*	Root
614	NPL-SUB-137	*Fabaceae*	*Astragalus*	*membranaceus*	Root
615	NPL-SUB-138	*Fabaceae*	*Astragalus*	*membranaceus*	Root
616	NPL-SUB-139	*Fabaceae*	*Astragalus*	*membranaceus*	Root
Continued					

No.	Sample code	Family	Genus	Species	Used part
617	NPL-SUB-140	*Fabaceae*	*Astragalus*	*membranaceus*	Root
618	NPL-SUB-141	*Fabaceae*	*Astragalus*	*membranaceus*	Root
619	NPL-SUB-142	*Fabaceae*	*Astragalus*	*membranaceus*	Root
620	NPL-SUB-143	*Fabaceae*	*Astragalus*	*membranaceus*	Root
621	NPL-SUB-144	*Zingiberaceae*	*Zingiber*	*officinale*	Root
622	NPL-SUB-145	*Acoraceae*	*Acorus*	*tatarinowii*	Root
623	NPL-SUB-146	*Polygonaceae*	*Rheum*	*palmatum*	Root
624	NPL-SUB-147	*Ranunculaceae*	*Cimicifuga*	*foetida*	Root
625	NPL-SUB-148	*Lauraceae*	*Cinnamomum*	*cassia*	Branch
626	NPL-SUB-149	*Fabaceae*	*Glycyrrhiza*	*uralensis*	Root
627	NPL-SUB-150	*Rosaceae*	*Prunus*	*persica*	Seed
628	NPL-SUB-151	*Zingiberaceae*	*Alpinia*	*officinarum*	Root
629	NPL-SUB-152	*Acoraceae*	*Acorus*	*calamus*	Root
630	NPL-SUB-153	*Zingiberaceae*	*Curcuma*	*longa*	Root
631	NPL-SUB-154	*Zingiberaceae*	*Curcuma*	*aromatica*	Root
632	NPL-SUB-155	*Zingiberaceae*	*Zingiber*	*officinale*	Root
633	NPL-SUB-156	*Zingiberaceae*	*Alpinia*	*officinarum*	Root
634	NPL-SUB-157	*Acoraceae*	*Acorus*	*calamus*	Root
635	NPL-SUB-158	*Zingiberaceae*	*Curcuma*	*longa*	Root
636	NPL-SUB-159	*Zingiberaceae*	*Curcuma*	*aromatica*	Root
637	NPL-SUB-160	*Zingiberaceae*	*Zingiber*	*officinale*	Root
638	NPL-SUB-161	*Zingiberaceae*	*Alpinia*	*officinarum*	Root
639	NPL-SUB-162	*Acoraceae*	*Acorus*	*calamus*	Root
640	NPL-SUB-163	*Zingiberaceae*	*Curcuma*	*longa*	Root
641	NPL-SUB-164	*Zingiberaceae*	*Curcuma*	*aromatica*	Root
642	NPL-SUB-165	*Zingiberaceae*	*Zingiber*	*officinale*	Root
643	NPL-SUB-166	*Zingiberaceae*	*Alpinia*	*officinarum*	Root
644	NPL-SUB-167	*Acoraceae*	*Acorus*	*calamus*	Root
645	NPL-SUB-168	*Zingiberaceae*	*Curcuma*	*longa*	Root
646	NPL-SUB-169	*Zingiberaceae*	*Curcuma*	*aromatica*	Root
647	NPL-SUB-170	*Zingiberaceae*	*Zingiber*	*officinale*	Root
648	NPL-SUB-171	*Zingiberaceae*	*Alpinia*	*officinarum*	Root
649	NPL-SUB-172	*Acoraceae*	*Acorus*	*calamus*	Root
650	NPL-SUB-173	*Zingiberaceae*	*Curcuma*	*longa*	Root
651	NPL-SUB-174	*Zingiberaceae*	*Curcuma*	*aromatica*	Root
652	NPL-SUB-175	*Zingiberaceae*	*Zingiber*	*officinale*	Root
653	NPL-HBD-332	*Apiaceae*	*Angelica*	*gigas*	Root
654	NPL-HBD-334	*Apiaceae*	*Angelica*	*gigas*	Root
655	NPL-HBD-336	*Apiaceae*	*Angelica*	*gigas*	Stems and leaves
656	NPL-HBD-338	*Apiaceae*	*Angelica*	*gigas*	Stems and leaves

Table 1. Medicinal plant samples analyzed by ^{1}H NMR, including the information of sample codes, scientific names (family, genus, and species), and used parts.

and the chemical characterization of multi-herbal formulations. By elucidating the metabolic similarities and differences among these herbs, our findings contribute to a deeper understanding of how specific combinations of compounds in complex herbal mixtures may enhance therapeutic efficacy. Ultimately, this research seeks to reassess the value of traditional medicines through a modern scientific lens and to support the development of new drugs based on natural products.

Results and discussion

Selection of extraction solvents for ^{1}H NMR measurements

The selection of extraction solvents was done with the aim of the study in mind, i.e., building a database of the metabolic profile of medicinal plants for various applications. This required the detection of as many metabolites as possible on one hand and the robustness of all the variables, ^{1}H resonances in this case. For this, all protons involved in hydrogen bonding, such as -OH need to be removed due to their great susceptibility to temperature, concentration or pH, that results in large variations This is achieved by using deuterated methanol, water or their mixtures. However, 100% deuterated water is not recommended due to signal broadening caused by large

molecules (proteins and polysaccharides) that can be extracted and the low solubility of secondary metabolites in aqueous medium. Thus, the ^{1}H NMR analysis was conducted on samples treated with two solvents: CH_3OH-d_4 and CH_3OH-d_4-KH_2PO_4 buffer (1:1, v/v). with the expectation of detecting a broader range of metabolites.

This is exemplified in Fig. 1 that shows a very distinct metabolome of samples of the roots of *Astragalus membranaceus* according to the solvent. Using CH_3OH-d_4-KH_2PO_4 buffer (1:1, v/v), higher levels of isoflavonoids were detected, while flavonoids were more abundant in the CH_3OH-d_4 extracts (Fig. 1A). In the case of sugars, the level of sucrose and glucose, as well as saponins vary in the extracts (Fig. 1B and C). Thus, both extracts provided different chemical profiles and ^{1}H NMR data obtained from both extracts were combined to get a wider range of metabolites. This study establishes a standardized ^{1}H NMR database of medicinal plants and introduces a framework for large-scale metabolomic similarity profiling that enables chemotaxonomic context, quality surveillance, and identification of metabolically similar candidates.

Classification or quality control of medicinal plants based on their chemotaxonomy (examples of *Angelica*, *Glycyrrhiza*, and *Schisandra* genera)

The NMR-based metabolomic database constructed in this study comprises 656 herbal samples, representing 113 plant families, 243 genera, and 299 species (Table 1). To evaluate the feasibility of chemotaxonomic classification using NMR profiling, we selected representative genera for detailed analysis based on medicinal relevance and intra-genus diversity. Among them, *Angelica* and *Glycyrrhiza* were chosen as model cases to examine whether metabolomic clustering reflects genus-level classification. NMR-based metabolomics has become a valuable tool in chemotaxonomy for chemotype-based classification and quality control. For instance, chemical profiling of *Euphorbia* species using NMR has been employed to investigate phylogenetic relationships, demonstrating its utility in identifying biomarkers associated with specific genetic or ecological traits[21]. However, despite its advantages, previous applications of NMR-based chemical profiling in chemotaxonomy have predominantly focused on limited single species or closely related genera. This narrow scope has limited its broader applicability across diverse plant taxa and left interspecies variability largely unexplored. Current NMR studies have primarily succeeded at the species level due to the presence of distinct metabolic markers. To determine whether NMR-based chemical profiling could be effectively applied at higher taxonomic levels, such as the genus, it is essential to account for the inherent variability among species. Expanding the scope to the genus level may require the integration of more advanced multivariate models and a broader dataset encompassing multiple species. This approach could help identify shared, stable markers while addressing environmental and genetic variability, which often obscure or hide genus-level distinctions. In this study, two representative genera, *Angelica* and *Glycyrrhiza*, were investigated to test the feasibility of this approach by determining whether they were classified closely in the clustering. For this application, the ^{1}H NMR data obtained after processing with bucketing (every 0.04 ppm) of data from both CH_3OH-d_4 and CH_3OH-d_4-KH_2PO_4 buffer (1:1, v/v) extracts, was analysed by a soft independent modelling cluster analogy (SIMCA) analysis, for which *Angelica* and *Glycyrrhiza* were classified separately and the distance of each sample to the cluster was then measured.

The global PCA model showed R2X(cum) = 0.859 and Q2(cum) = 0.474. The genus *Angelica* represents one of the most diverse groups of medicinal plants. Notably, the herbal medicine commonly known as *Angelica* refers to different species depending on the region: *A. sinensis* in China, *A. acutiloba* in Japan, and *A. gigas* in Korea. Figure 2 displays the clustering of *Angelica* samples based on numerical similarity. Similarity was evaluated using the SIMCA class model in PCA-class (R2X(cum) = 0.691 and Q2(cum) = 0.549), and the Distance to the Model in X-space (DModX) was calculated as a diagnostic measure of each sample's distance from the class model. Samples with DModX values below the critical threshold of 1.27235 ($p < 0.05$) were considered to fit closely within the *Angelica* cluster. These samples are listed in (Table 2).

Interestingly, among the analysed samples, *Ostericum koreanum* - represented by NPL-NET-032 and NPL-KIOM-008 - exhibited DModXPS[2] values of 0.77189 and 0.55494, respectively. Both values fall below the critical threshold of 1.27235, indicating strong alignment with the *Angelica* cluster based on M2 component analysis. This numerical similarity suggests that, despite being classified separately, these samples share substantial metabolomic features with *Angelica*. This finding aligns with recent literature that has reclassified *Ostericum koreanum* as *Angelica reflex*[22], highlighting the potential of this clustering approach to distinguish or associate plant species at the genus level based on numerical metabolomic similarity.

The results of the Glycyrrhiza species were different. The clustering result of the SIMCA class model (R2X(cum) = 0.933 and Q2(cum) = 0.763) showed that non-*Glycyrrhiza uralensis* samples generally exhibited higher DModX values, clearly distinguishing them from *Glycyrrhiza uralensis* in the DModX plot (Fig. 3). The corresponding values are provided in Table 3. These results support the utility of a genus-level SIMCA model as a practical screening tool for detecting samples that deviate from a reference class, thereby contributing to within-genus quality control, although this observation requires validation using a larger set of non-*G. uralensis* samples.

To complement the visual interpretation of the global PCA, we quantified local neighborhood agreement in the PCA score space (t[1]–t[2]) for the two case-study genera. For each sample, we identified its k nearest neighbors (k = 1 or 10) and calculated the percentage of samples whose nearest-neighbor set contained at least one sample sharing the same genus label. Within Angelica ($n = 23$), the 1-NN and 10-NN agreements were 34.8% and 69.6%, whereas within Glycyrrhiza ($n = 27$) they were 81.5% and 96.3%, respectively.

To further explore the chemotaxonomic capabilities of NMR-based metabolomics, *Schisandra chinensis* was analyzed to investigate how geographical origins impacted clustering and chemical profiles. This study incorporated five *Schisandra* samples collected from different locations: Korea (NPL-NPL-045, NPL-RDA-003, NPL-KIOM-042), China (NPL-SUB-050), and the Netherlands (a market sample). As illustrated in Fig. 4, the clustering results revealed that samples from Korea and China clustered closely together, exhibiting strong chemical similarity. The *Schisandra* sample obtained from the Netherlands formed a cluster far from the Korean

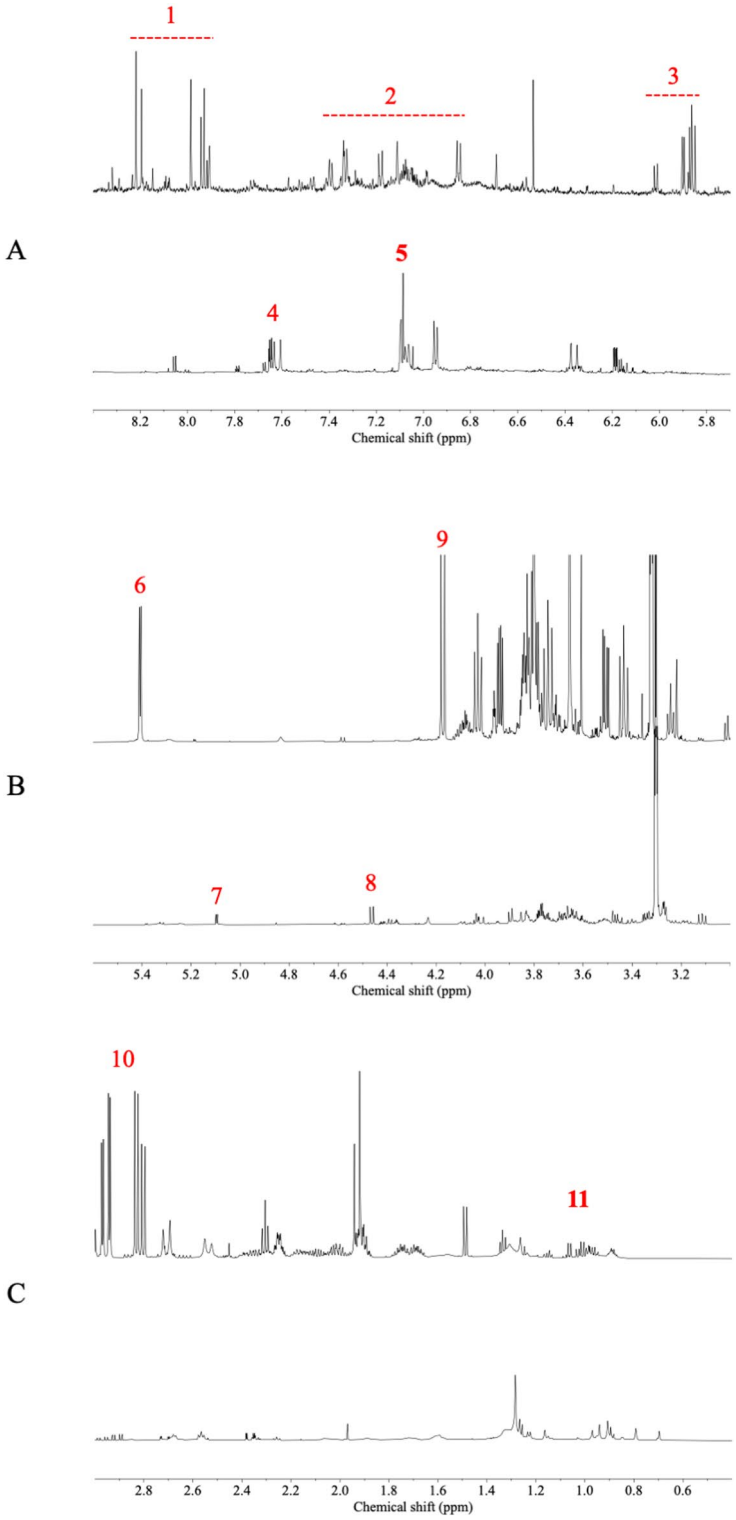

Fig. 1. ^{1}H NMR spectra of *Astragalus membranaceus* radix in the range of δ 8.3–5.7 (**A**), δ 5.6–3.0 (**B**), δ 3.0–0.5 (**C**) measured in CH_3OH-d_4-KH_2PO_4 buffer in D_2O (pH 6.0) (spectra on the top) and CH_3OH-d_4 (spectra on the bottom). 1: H-2 of isoflavonoids, 2: B-ring of flavonoids and isoflavonoids, 3: A-ring of flavonoids and isoflavonoids, 4: H-2' and H-6' of kaempferol analogues, 5: H-3' and H-5' of kaempferol analogues, 6: H-1 of sucrose, 7: H-1 of α-glucose, 8: H-1 of β-glucose, 9: H-2' of sucrose, 10: aspartic acid and asparagine, 11: methyls of saponins.

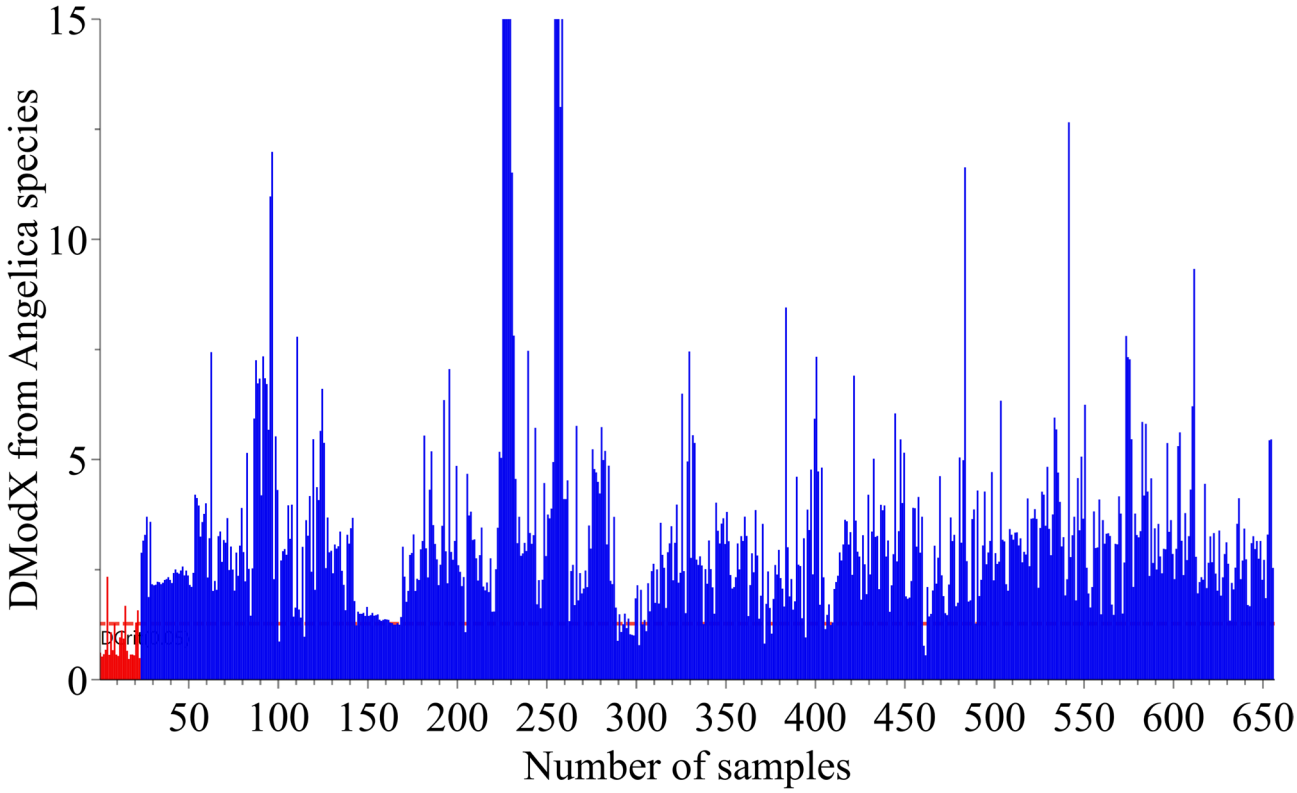

Fig. 2. Distance to the model (DModX) values from the cluster of *Angelica* species to other samples. *Angelica* species are in red marked by *. The SIMCA class model yielded R2X(cum) = 0.691 and Q2(cum) = 0.549. Samples with DModX of each sample less than 1.0 are listed in (Table 2).

and Chinese samples. This finding emphasizes the proposed potential of the clustering method to trace medicinal plants' geographical origins. Even within the same species, differences in the origin can lead to distinct chemical profiles, a pattern that was also evident in the standardized ^{1}H NMR spectra, Fig. 5 provides a representative visualization of these origin-dependent spectral differences observed at the ^{1}H NMR level. Importantly, the samples from Korea and China exhibited only minor variability and remained grouped within the same primary cluster, further supporting the consistency within their shared origin. Conversely, the Netherlands sample deviated significantly, reflecting its different cultivation environment or processing methods.

Such chemical variability underscores the importance of evaluating therapeutic consistency and quality reliability, as differences in cultivation or harvesting environments can influence the chemical profile and potentially affect therapeutic activity and overall bioactivity. Taken together, these findings demonstrate that NMR-based metabolomics is effective not only for discriminating medicinal plants across taxonomic levels but also for detecting environmentally driven chemical variation within species. The consistent clustering of samples by geographical origin further supports the utility of this approach for origin tracking and quality assessment, providing a robust analytical basis for the scientific modernization of traditional medicines.

Comparison between domestic and imported medicinal plants and searching for domestic alternatives to replace imported products

While medicinal plants may share their name or traditional usage, their chemical compositions can vary significantly depending on their geographic origin, genetic variation, and environmental factors as discussed previously. This discrepancy poses challenges for the quality control and functional consistency in herbal medicine. Therefore, rather than relying solely on taxonomic identity or traditional nomenclature, metabolomic profiling might offer a robust solution for characterizing and comparing actual chemical profiles, enabling a more accurate substitution and standardization of medicinal resources. For example, while *Taxus chinensis* is primarily known for diterpenoid alkaloids such as taxane derivates, recent studies have demonstrated that its leaves contain a variety of other bioactive metabolites[23]. This highlights the limitations of relying solely on known marker compounds and reinforces the need for a more holistic metabolomic approach. By profiling and clustering species based on their full metabolite profiles, this study provides a more robust framework for identifying functionally similar and potentially substitutable medicinal plants. In this context, ^{1}H NMR-based metabolomics is particularly advantageous, as it enables holistic and untargeted profiling of the entire metabolic landscape of a plant, providing a macroscopic view of species-specific chemical variation. Building on the robustness of NMR-based metabolomics for chemotaxonomy and quality control, this study further explores its potential for identifying alternative medicinal plants. The ability to compare and classify plants based on

No.	Sample code	Genus	Species	M2. DModX [2] (Norm), Weighted residuals
1	NPL-KHU-022	*Angelica*	*gigas*	0.572366
2	NPL-KHU-066	*Angelica*	*acutiloba*	0.615103
3	NPL-KIOM-041	*Angelica*	*gigas*	0.571566
4	NPL-KIOM-080	*Angelica*	*dahurica*	1.07631
5	NPL-KIOM-081	*Angelica*	*dahurica*	0.670917
6	NPL-KIOM-168	*Angelica*	*acutiloba*	0.525833
7	NPL-KIOM-169	*Angelica*	*acutiloba*	0.68044
8	NPL-KIOM-180	*Angelica*	*decursiva*	1.28192
9	NPL-NET-034	*Angelica*	*dahurica*	0.565141
10	NPL-NET-036	*Angelica*	*gigas*	0.540228
11	NPL-NET-037	*Angelica*	*acutiloba*	0.579614
12	NPL-NET-038	*Angelica*	*sinensis*	0.552658
13	NPL-NET-040	*Angelica*	*gigas*	0.656834
14	NPL-NET-041	*Angelica*	*gigas*	0.472327
15	NPL-NPL-044	*Angelica*	*acutiloba*	2.33752
16	NPL-RDA-008	*Angelica*	*gigas*	0.570281
17	NPL-SUB-015	*Angelica*	*sinensis*	0.491321
18	NPL-SUB-020	*Angelica*	*pubescens*	1.57637
19	NPL-SUB-035	*Angelica*	*dahurica*	1.29916
20	NPL-HBD-332	*Angelica*	*gigas*	0.935537
21	NPL-HBD-334	*Angelica*	*gigas*	0.961212
22	NPL-HBD-336	*Angelica*	*gigas*	1.67758
23	NPL-HBD-338	*Angelica*	*gigas*	1.11894

Table 2. Distance to the model (DModX) values of *Angelica* species in the model of soft independent model of class analogy (SIMCA) for the *Angelica* class and the distance of non-*Angelica* samples having DModX < 1.27235 (Dcrit = 0.05). Outliers are marked and defined as samples with DModX values exceeding the 95% confidence threshold (Dcrit = 0.05) based on SIMCA analysis (DModX > 1.27235).

their chemical profiles provides a strong foundation for discovering substitutes for existing medicinal resources, especially in cases where sustainability, cost, or availability is a concern.

With this in mind, we compared *Taxus* and *Viscum*, two widely used but taxonomically distant medicinal plants, that are found to be metabolically close in ^{1}H NMR analysis. As illustrated in Fig. 6, the ^{1}H NMR spectra of *Taxus chinensis* leaves (NPL-NPL-019) and *Viscum album* stems (NPL-KIOM-020) revealed distinct yet overlapping chemical profiles. To assess whether this approach could be generalized across medicinal species, we extended the analysis to additional taxa. The analysis of *Uncaria tomentosa* stem barks (NPL-NPL-018), *Uncaria rhynchophylla* hooks (NPL-NPL-017), and *Vaccinium bracteatum* stems (NPL-NET-001) further demonstrated the utility of NMR profiling in the discovery of alternatives to existing medicinal plants, as shown in Fig. 7. The results highlight the value of NMR-based metabolomics in this context. By uncovering both shared and unique chemical features, this approach supports the rational selection of alternative resources based on functional and therapeutic equivalence, although further validation is needed to confirm this. Importantly, the metabolic patterns identified in this study provide a directional framework for future research on medicinal plants.

To compare the value of NMR-based studies with other available analytical techniques, we conducted a molecular networking analysis using UHPLC-DAD-QToF-MS data via the GNPS platform to investigate structural similarities between *Taxus chinensis* and *Viscum album*. To improve annotation accuracy, ion-identity molecular networking (IIMN) was applied, integrating both precursor ion masses and MS/MS fragmentation data. This enabled the construction of a detailed molecular network (Fig. 8), that allowed the direct comparison and visualization of shared and unique chemical features of both species, consistent with previously reported strategies for comparative chemotaxonomic analysis that used GNPS-based MN platforms[24] .

Several structurally annotated compounds with known or predicted bioactivities were detected among the shared nodes. Putative annotations included taccalonolide B[25,26], a microtubule-stabilizing agent structurally related to paclitaxel[27]; atractylenolide III[28], known for its anti-inflammatory and gastrointestinal modulatory effects; and pterosin B[29], a phenolic compound with reported enzyme inhibition properties. Additionally, shared clusters contained nodes presumably corresponding to micheliolide[30], further suggesting overlapping metabolite families between the two species.

Notably, both *Taxus chinensis* and *Viscum album* have been independently reported to exhibit anticancer and immunomodulatory effects, albeit through different mechanisms. While paclitaxel from *Taxus* is a well-known chemotherapeutic agent targeting microtubule dynamics, *Viscum album* extracts - particularly mistletoe lectins and viscotoxins- are used in complementary cancer therapies for their immune-modulating and cytotoxic activities. The identification of network features putatively matching taccalonolide B[31] and tricin[32], both of which have documented anticancer properties, supports the hypothesis of functional similarity. This

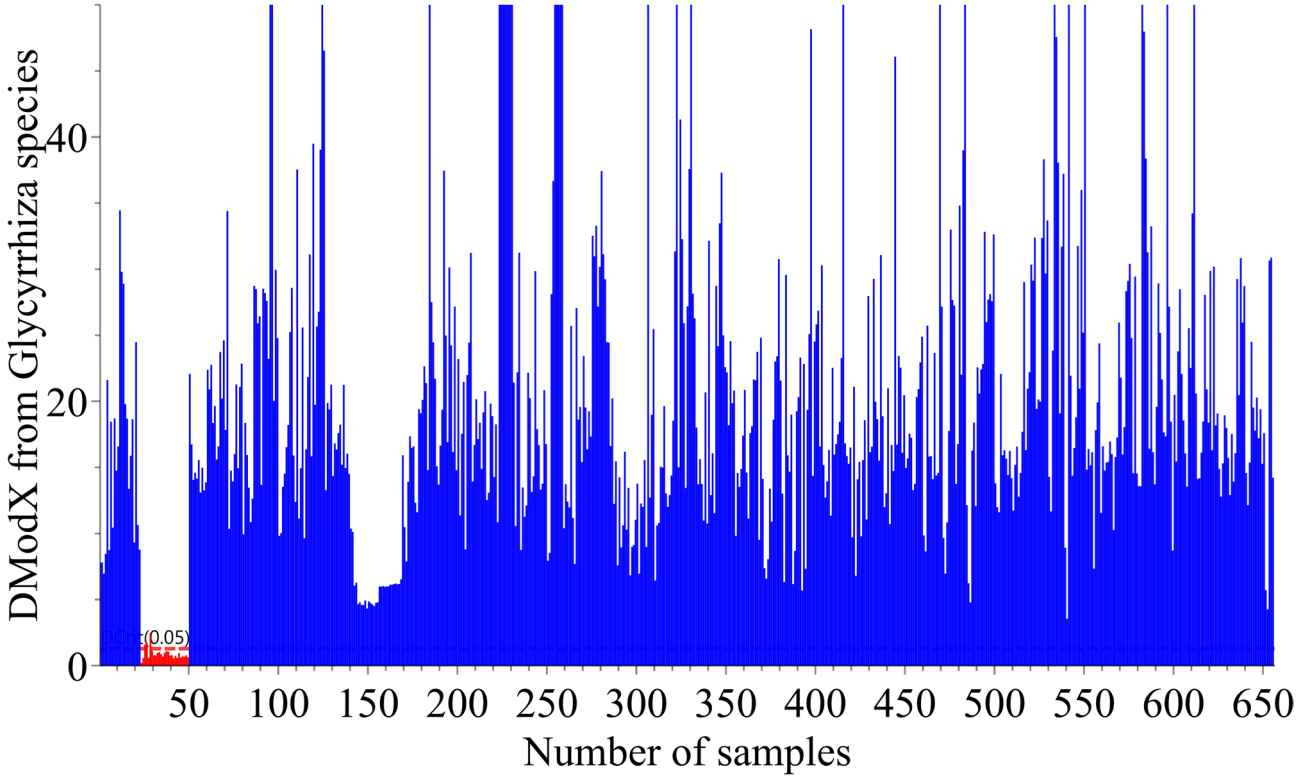

Fig. 3. Distance to the model (DModX) values from the cluster of *Glycyrrhiza* species to other samples. *Glycyrrhiza* species are in red marked by *. The SIMCA class model yielded R2X(cum) = 0.933 and Q2(cum) = 0.763. Samples with DModX of each sample less than 1.0 are listed in (Table 3).

biochemical convergence not only reflects a structural overlap but also suggests a potential pharmacological parallel worthy of further investigation. While some of the shared compounds are well-characterized, others remain structurally significant yet functionally unverified. Therefore, although pharmacological validation was beyond the scope of this study, the observed metabolomic overlap offers a rational basis for future research into functional substitutability and therapeutic equivalence.

A second molecular networking analysis was performed on *Uncaria tomentosa*, *Uncaria rhynchophylla*, and *Vaccinium bracteatum* (Fig. 9). Despite notable differences in their taxonomic classification and traditional medicinal applications, these three medicinal plants exhibited a considerable overlap in their secondary metabolite profiles. *Uncaria tomentosa*, traditionally used in South American ethnomedicine for its immunomodulatory and anti-inflammatory effects, has been shown to exhibit corresponding pharmacological activities, largely attributed to oxindole alkaloids[33]. Neutroprotective and anti-inflammatory properties have also been reported in modern studies for *Uncaria rhynchophylla*, long utilized in East Asian medicine for treating hypertension and neurological disorders[34]. *Vaccinium bracteatum*, widely applied in East Asian practices for hepatoprotection and detoxification, has similarly been reported to possess antioxidant and liver-protective effects[35]. These overlapping pharmacological profiles further support the rationale for exploring functional substitution among these botanically distinct species.

Molecular networking revealed shared clusters containing features allegedly corresponding to key alkaloids, such as uncarine C[36], alongside polyphenolic glycosides structurally distributed across all three species. Among the shared features, uncarine C has demonstrated neuroprotective potential through antioxidant and calcium-channel modulating effects[37], while several glycosides structurally analogous to tricin are known to exert anticancer and anti-inflammatory activity[38–40]. These observations suggest a degree of biosynthetic convergence, particularly in the production of indole alkaloids and phenolic derivatives. Additionally, *Vaccinium bracteatum* shared chemical features with *Uncaria* species, reinforcing the notion of a chemically interconnected profile despite botanical divergence. Taken together, these findings highlight the potential for functional substitution or therapeutic complementation among these species, based on shared metabolite structures and overlapping pharmacological potential. Further validation through bioactivity-guided assays may clarify the extent of their functional equivalence. All molecular-network nodes are linked to their feature IDs and corresponding precursor *m/z*, RT, library match information, and MSI confidence level, and the sample metadata used in GNPS are provided in Supplementary Table S2-S3.

These findings further support the utility of molecular networking in screening functionally relevant alternatives across traditionally distinct medicinal species. This comparative analysis illustrates how metabolomic fingerprints can support evidence-based selection of candidate substitutes, offering practical solutions for sustainability and compliance with international resource-sharing protocols. All considered, the molecular

No.	Primary ID	Genus	Species	M3. DModX [5] (Norm), Weighted residuals
1	NPL-KIOM-003	*Glycyrrhiza*	*glabra*	1.60065
2	NPL-KIOM-004	*Glycyrrhiza*	*inflata*	1.72332
3	NPL-KIOM-005	*Glycyrrhiza*	*uralensis*	2.47028
4	NPL-NPL-014	*Glycyrrhiza*	*glabra*	0.209195
5	NPL-NPL-015	*Glycyrrhiza*	*glabra*	0.583945
6	NPL-RDA-013	*Glycyrrhiza*	*uralensis*	0.582314
7	NPL-SUB-099	*Glycyrrhiza*	*uralensis*	1.12873
8	NPL-SUB-100	*Glycyrrhiza*	*uralensis*	0.77614
9	NPL-SUB-101	*Glycyrrhiza*	*uralensis*	0.781782
10	NPL-SUB-102	*Glycyrrhiza*	*uralensis*	0.967299
11	NPL-SUB-103	*Glycyrrhiza*	*uralensis*	1.02192
12	NPL-SUB-104	*Glycyrrhiza*	*uralensis*	0.870343
13	NPL-SUB-105	*Glycyrrhiza*	*uralensis*	0.695624
14	NPL-SUB-106	*Glycyrrhiza*	*uralensis*	0.980659
15	NPL-SUB-107	*Glycyrrhiza*	*uralensis*	1.10028
16	NPL-SUB-108	*Glycyrrhiza*	*uralensis*	1.05198
17	NPL-SUB-109	*Glycyrrhiza*	*uralensis*	0.764558
18	NPL-SUB-110	*Glycyrrhiza*	*uralensis*	0.786217
19	NPL-SUB-111	*Glycyrrhiza*	*uralensis*	0.553723
20	NPL-SUB-112	*Glycyrrhiza*	*uralensis*	0.747157
21	NPL-SUB-113	*Glycyrrhiza*	*uralensis*	0.582447
22	NPL-SUB-114	*Glycyrrhiza*	*uralensis*	0.954206
23	NPL-SUB-115	*Glycyrrhiza*	*uralensis*	0.611436
24	NPL-SUB-116	*Glycyrrhiza*	*uralensis*	0.710566
25	NPL-SUB-117	*Glycyrrhiza*	*uralensis*	0.680215
26	NPL-SUB-118	*Glycyrrhiza*	*uralensis*	0.779586
27	NPL-SUB-119	*Glycyrrhiza*	*uralensis*	0.622515

Table 3. Distance to the model (DModX) values of *Glycyrrhiza* species in the model of soft independent model of class analogy (SIMCA) for the *Angelica* class and the distance of non-*Glycyrrhiza* samples having DModX < 1.28031 (Dcrit = 0.05). Outliers are marked and defined as samples with DModX values exceeding the 95% confidence threshold (Dcrit = 0.05), based on SIMCA analysis (DModX < 1.28031).

networks derived from UHPLC-DAD-QToF-MS data demonstrate that functionally relevant metabolite clusters are not strictly confined by taxonomy. This supports the macroscopic metabolic approach and suggests practical frameworks for identifying alternative sources of bioactive compounds with equivalent therapeutic potential.

Applications of ^{1}H NMR in multi-herbal mixture profiling

To gain a comprehensive understanding of plant metabolites, it is essential to adopt a broad analytical perspective. NMR spectroscopy offers such a perspective, enabling detailed insights into plant metabolomics. Notably, NMR can also be effectively applied to complex mixtures of medicinal herbs - an approach particularly relevant in traditional medicine, where multi-herbal formulations are commonly used as therapeutic solutions.

This study addresses a key question: can the emergent properties of these mixtures - often cited in traditional medicine - be analysed to elucidate the mechanisms underlying their synergistic effects? Furthermore, if one or more components exhibit significant chemical variability due to environmental or geographical factors, how might this influence the overall therapeutic efficacy of the mixture?

These questions form the basis of this investigation into the application of NMR-based metabolomics for understanding, characterizing, and potentially optimizing multi-herbal formulations.

Multi-herbal medicines have long been a cornerstone of traditional medical systems, often demonstrating synergistic effects that cannot be replicated by single components alone. In this study, we focus on *Huanglian Jiedu Decoction* (HJD), a classical prescription in East Asian medicine, known for its potent anti-inflammatory, antimicrobial, and detoxifying properties being prescribed traditionally for heat-related syndromes, infections, and inflammatory conditions. HJD comprises four primary herbs: *Coptis chinensis*, *Phellodendron amurense*, *Scutellaria baicalensis*, and *Gardenia jasminoides*. A broad spectrum of bioactive compounds, including alkaloids (e.g., berberine, palmatine) and flavonoids (e.g., baicalin, geniposide), which contribute to its therapeutic efficacy have been identified in HJD previously.

Despite its clinical relevance, the precise chemical interactions among the components of HJD remain poorly understood. Recent trends in drug development have emphasized the integration of traditional medicinal knowledge with modern analytical techniques. Multi-herbal formulations like HJD are increasingly viewed as templates for novel drug discovery, owing to their multitarget therapeutic potential. While most current

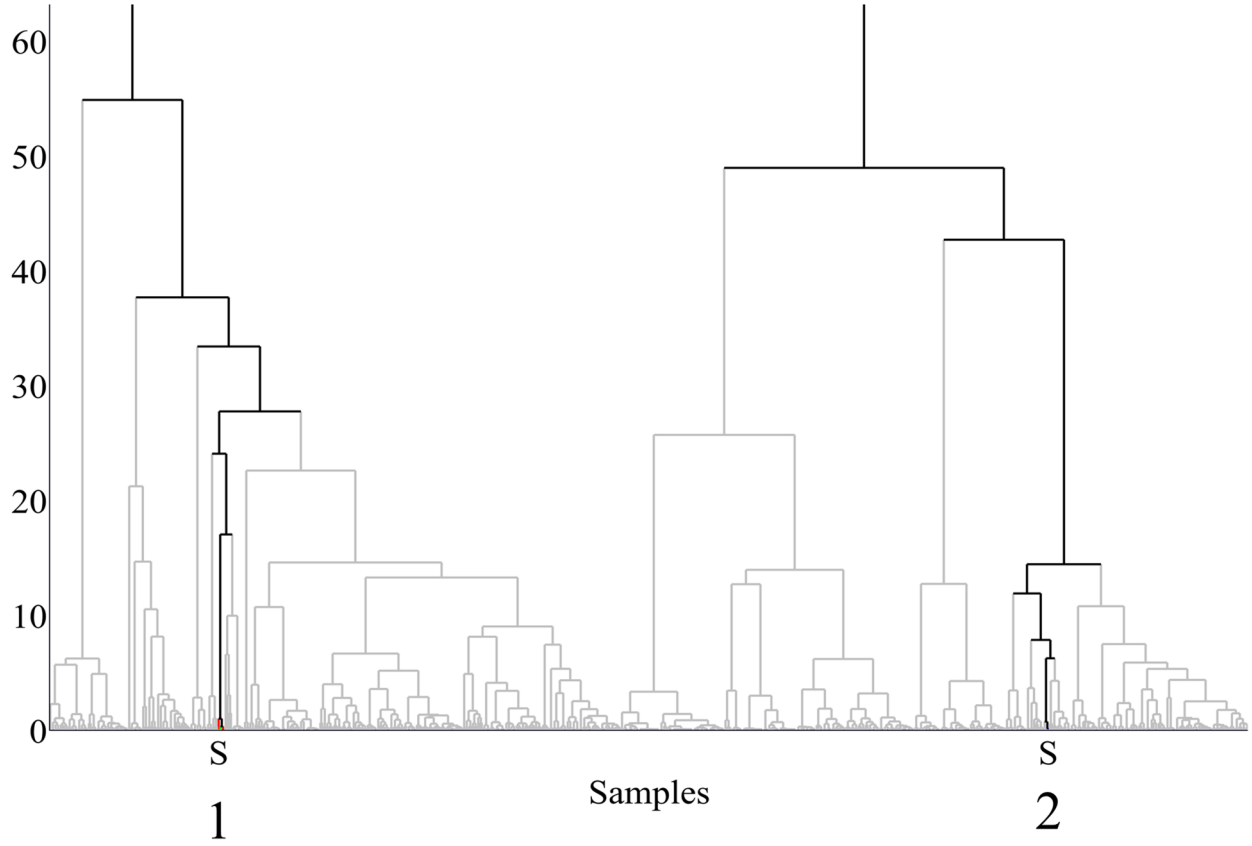

Fig. 4. Dendrogram of 45 principal components of 656 samples employed in the study. Branch colors indicate sample origin: Korea (red), China (green), and the Netherlands (blue). 1: *Schisandra chinensis* fruits collected from Korea (NPL-NPL-045, NPL-RDA-003, and NPL-KIOM-042) in red and China (NPL-SUB-050) in green, 2: *Schisandra chinensis* fruits collected from a market in the Netherlands in blue.

studies focus on efficacy evaluation, there is a growing need to apply advanced methodologies to investigate the underlying mechanisms and discover new clinical applications.

In this context, the present study employs NMR-based metabolomics to unravel the chemical complexity of HJD. Using ^{1}H NMR fingerprints and PCA, we compared individual herbs and mixtures to evaluate mixture positioning in score space.

For this approach, ^{1}H NMR spectra were acquired for each individual herb and their combinations. Principal component analysis (PCA) was used to visualize the chemical relationships among samples. Figure 10 shows the PCA score plot of ^{1}H NMR data from *Scutellaria baicalensis* (S), *Phellodendron amurense* (P), *Coptis japonica* (C), *Gardenia jasminoides* (G), and their mixtures. Distinct clustering of individual plant extracts (black symbols) was observed, while the mixtures showed different clustering patterns. Blue symbols represent co-extracted mixtures, and red symbols represent mixtures prepared from individually extracted components. Interestingly, both preparation methods yielded similar results, suggesting that the chemical profile of the mixture remains consistent regardless of the extraction method.

This study demonstrated the efficacy of NMR-based metabolomics in distinguishing component herbs, assessing chemical interactions, and identifying potential synergistic effects in complex herbal mixtures. Furthermore, the ability to model and predict the behaviour of herbal formulations can be extended by comparing experimental mixtures with multivariate expectations derived from the constituent extracts, enabling a systematic assessment of mixture positioning in score space.

In addition to enabling the monitoring of changes in chemical profiles, NMR analysis yielded another noteworthy result through HJD analysis. Specifically, the NMR spectra of the individual medicinal plants revealed significant chemical similarities between *Phellodendron amurense* (P) and *Coptis japonica* (C). As shown in Fig. 11, both species contain benzylisoquinoline alkaloids, such as berberine, as a major component. Despite these similarities, the presence of additional, distinct compounds served to differentiate the two, highlighting the sensitivity of NMR in detecting subtle but meaningful variations in chemical composition. These results underscore that, even among chemically similar herbs, each plant contributes uniquely to traditional formulations through its characteristic metabolite profile. This distinction plays a critical role in optimizing the overall therapeutic effect of the prescription and highlights the importance of carefully considering the individual contributions of each component when interpreting or modifying traditional herbal formulas. Although their general chemical profiles may appear alike, variations such as the presence or concentration of

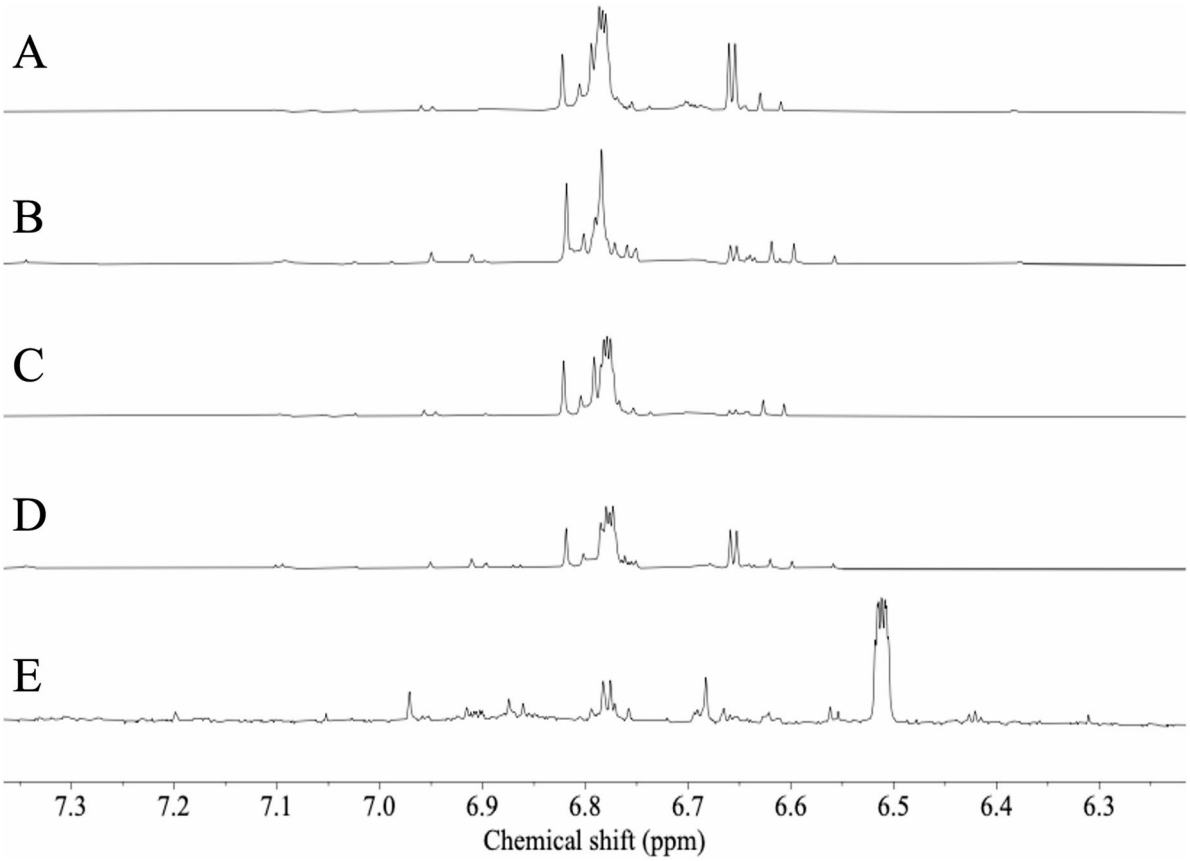

Fig. 5. ^{1}H NMR spectra (600 MHz, CH_3OH-d_4-KH_2PO_4 buffer (1:1, v/v, pH 6.0) of *Schisandra chinensis* fruits collected from Korea (A: NPL-KIOM-042, B: NPL-RDA-003, and C: NPL-NPL-045), from China (D: NPL-SUB-050), and from a market of the Netherlands (E).

specific bioactive compounds like berberine suggest that substitutions between herbs should be approached with caution to preserve the formulation's intended efficacy. By capturing both the individual and emergent metabolic profiles of herbal mixtures, NMR-based analysis supports a deeper mechanistic understanding of synergy in traditional formulations and provides a scalable approach for evaluating multi-component therapeutics.

The implications of this research extend beyond HJD. Applying this approach to other widely used traditional formulations may reveal common chemical markers or synergistic patterns that contribute to the development of generalized quality control methods. Ultimately, insights from this study contribute to the rational design of multi-component therapeutics.

Ultimately, to assess how the insights from this study may contribute to the rational design of multi-component therapeutics, we examined whether the multivariate profile of mixed extracts could be approximated from the ^{1}H NMR spectra of the individual component herbs (Fig. 12). A key question emerging from these results is whether the multivariate profile of mixed extracts can be reasonably approximated from the ^{1}H NMR spectra of the individual plant extracts. To evaluate this at the multivariate level, we performed PCA using the ^{1}H NMR spectra of the individual extracts and the corresponding mixed extracts. Figure 12 addresses this by comparing the PCA positioning of the mixed extract relative to the individual extracts based on their ^{1}H NMR profiles. The high degree of similarity observed in the PCA score space suggests that the mixture profile can be approximated from the constituent extracts under the tested conditions. This finding holds significant potential for streamlining the analysis of complex herbal formulations, reducing the need for exhaustive experimental testing while enabling more efficient prediction of mixture properties.

However, the advantage of achieving a reliable chemical characterization of herbal mixtures extends further to practical applications within global regulatory frameworks, such as the Nagoya Protocol. This international agreement requires equitable benefit-sharing in the use of biological resources, increasing the pressure to identify and use domestically sourced medicinal plants. However, formulating effective substitutes is challenging when traditional remedies rely on complex combinations of herbs, where therapeutic efficacy arises not from a single component but from synergistic interactions.

In this study, NMR-based metabolomic profiling was applied to analyse multi-herb mixtures and compare their chemical signatures at the formulation level. This approach enabled the identification of candidate substitutes whose combined metabolic fingerprints align with those of established mixtures. For example, clustering analysis of *Angelica* and *Glycyrrhiza* species illustrated how multivariate methods can reveal interspecies

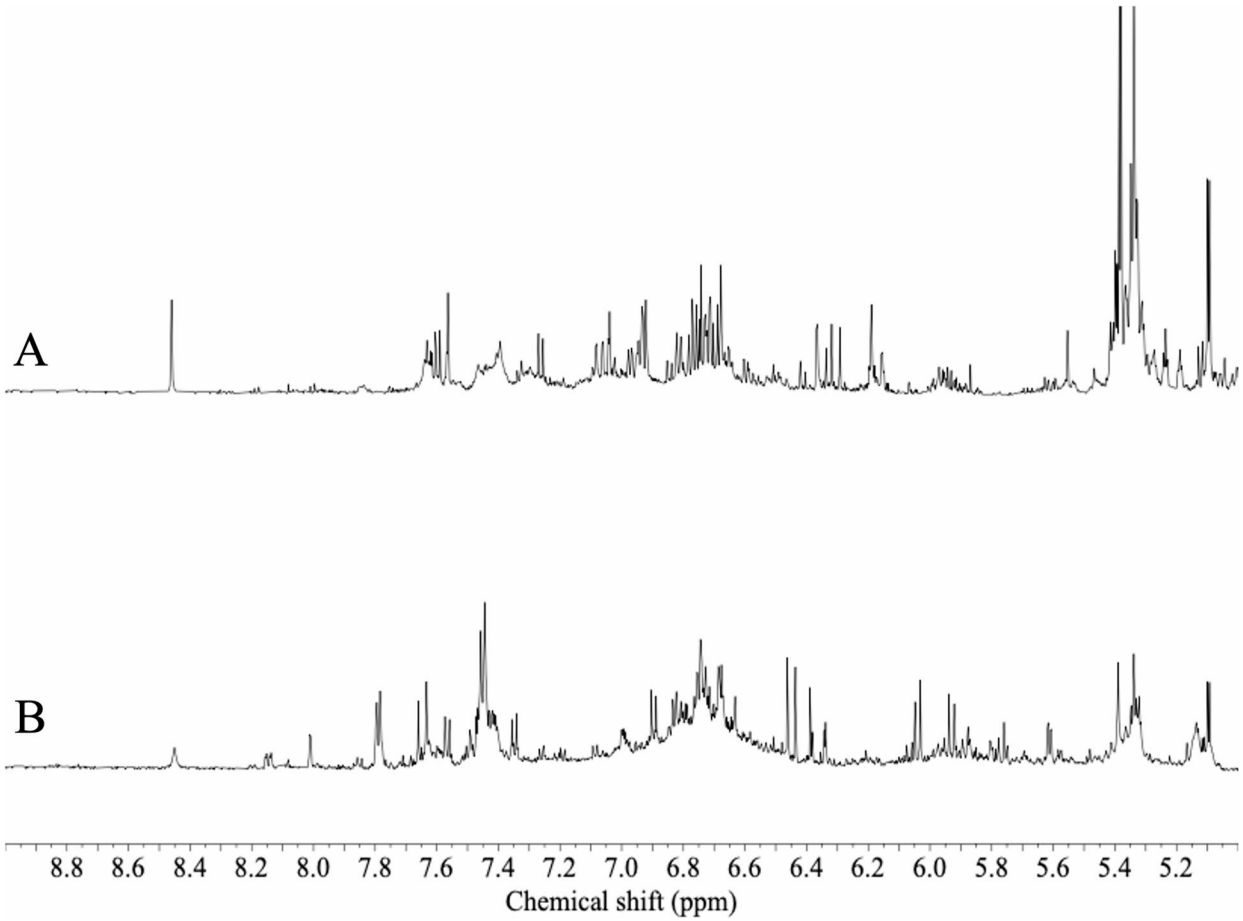

Fig. 6. Comparison of ^{1}H NMR spectra (600 MHz, CH_3OH-d_4) *Taxus chinensis* leaves (NPL-NPL-019, **A**) and *Viscum album* stems (NPL-KIOM-020, **B**).

chemical similarity allowing informed domestic substitution decisions. By evaluating both structural overlap and functional potential, mixture-level analysis supports more precise and evidence-based substitution without compromising therapeutic consistency.

This strategy not only addresses scientific and therapeutic considerations but also aligns with regulatory demands for sustainable sourcing. It provides a path forward for reducing dependence on imports, conserving biodiversity, and strengthening compliance with international protocols. Future research should refine this framework by characterizing inter-compound interactions and validating the clinical relevance of identified substitutes. Collectively, these findings support the development of sustainable, regulation-compliant herbal therapeutics and highlight the value of a macroscopic, database-driven approach to medicinal plant analysis.

However, the formulation-level comparisons presented here primarily support substitution-oriented prioritization rather than definitive equivalence testing. Because ^{1}H NMR fingerprints emphasize relatively abundant metabolites, low abundant bioactives and trace markers may be under-represented. In addition, neighborhood similarity and clustering outcomes are contingent on the current database composition and may not fully capture within-species variability associated with origin, season, processing, and chemotype. Finally, the "candidate substitutes" identified in this study reflect chemical similarity at the mixture level and require follow-up confirmation using orthogonal analytical approaches, including targeted assays and verification with authentic standards where needed, and ultimately pharmacological or clinical validation to substantiate therapeutic interchangeability.

Methods

Medicinal plant samples

A total of 656 herbal samples were obtained from Korea, China and the Netherlands, being generously provided by Kyung Hee University (Seoul, Korea), Korea Institute of Oriental Medicine (Daejeon, Korea), National Institute of Horticultural and Herbal Science (Eumseong, Chungcheongbuk-do, Korea), and SU BioMedicine (Leiden, The Netherlands). All the samples were identified by authors (Young Pyo Jang, Jeeyeoun Jung, Dae Young Lee, and Mei Wang). A detailed description of the samples is given in Table 1.

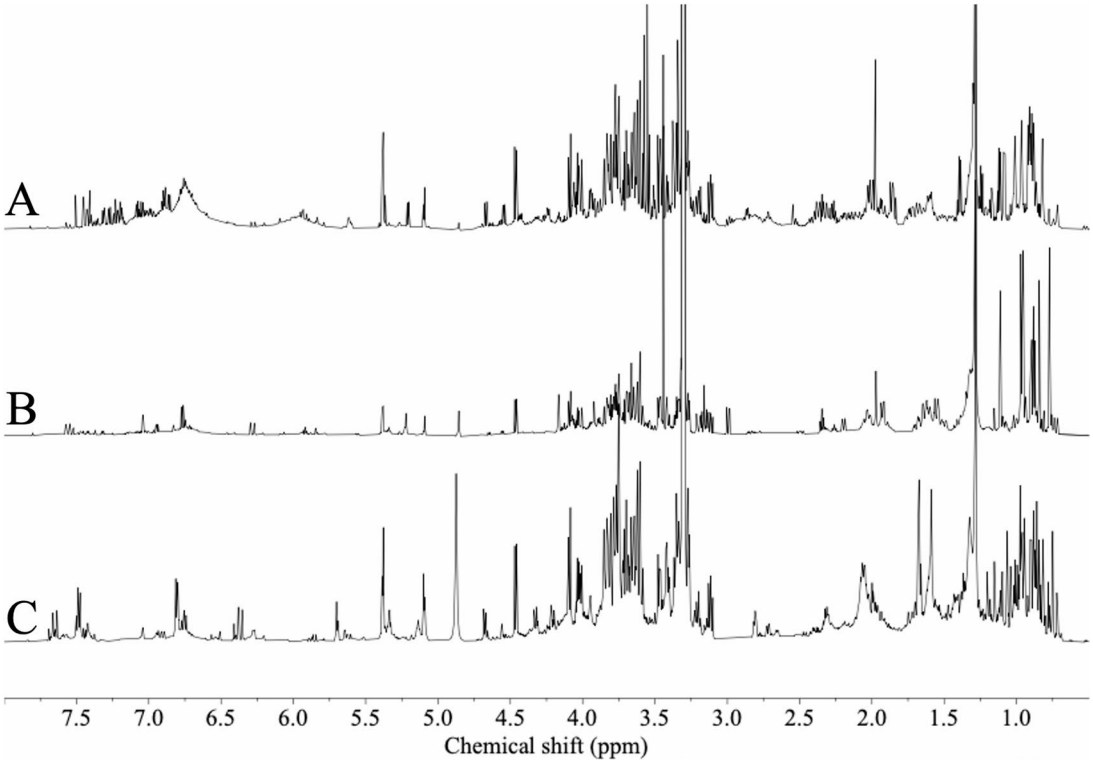

Fig. 7. Comparison of ^{1}H NMR spectra (600 MHz, CH_3OH-d_4) *Uncaria tomentosa* stem barks (NPL-NPL-018, **A**), *Uncaria rhynchophylla* hooks (NPL-NPL-017, **B**), and *Vaccinium bracteatum* stems (NPL-NET-001, **C**).

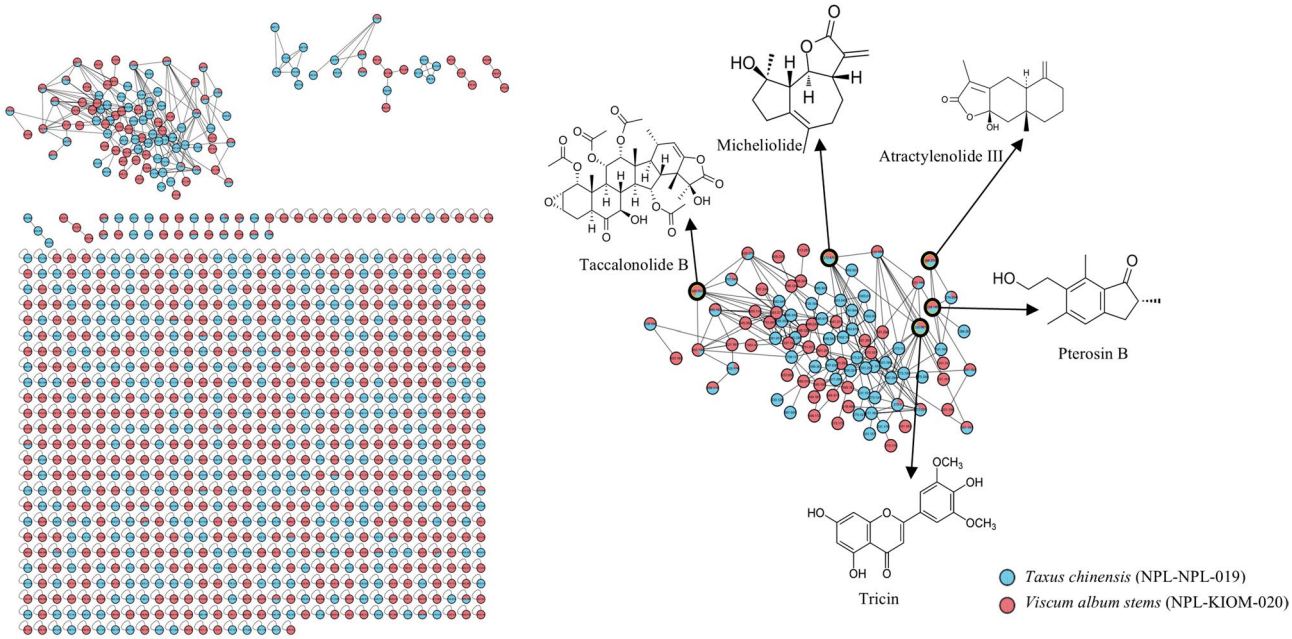

Fig. 8. Feature-based molecular networking (FBMN) of taxonomically distinct medicinal plants highlighting metabolite overlaps and functional similarity. The network generated from UHPLC-DAD-QToF-MS data of the *Taxus chinensis* and *Viscum album* using ion identity molecular networking (IIMN) shows shared molecular families, including a lactone-related cluster, observed across both species. Node labels correspond to feature IDs, and the corresponding precursor *m/z*, RT, library match information, and MSI confidence levels are provided in Supplementaray Table S2.

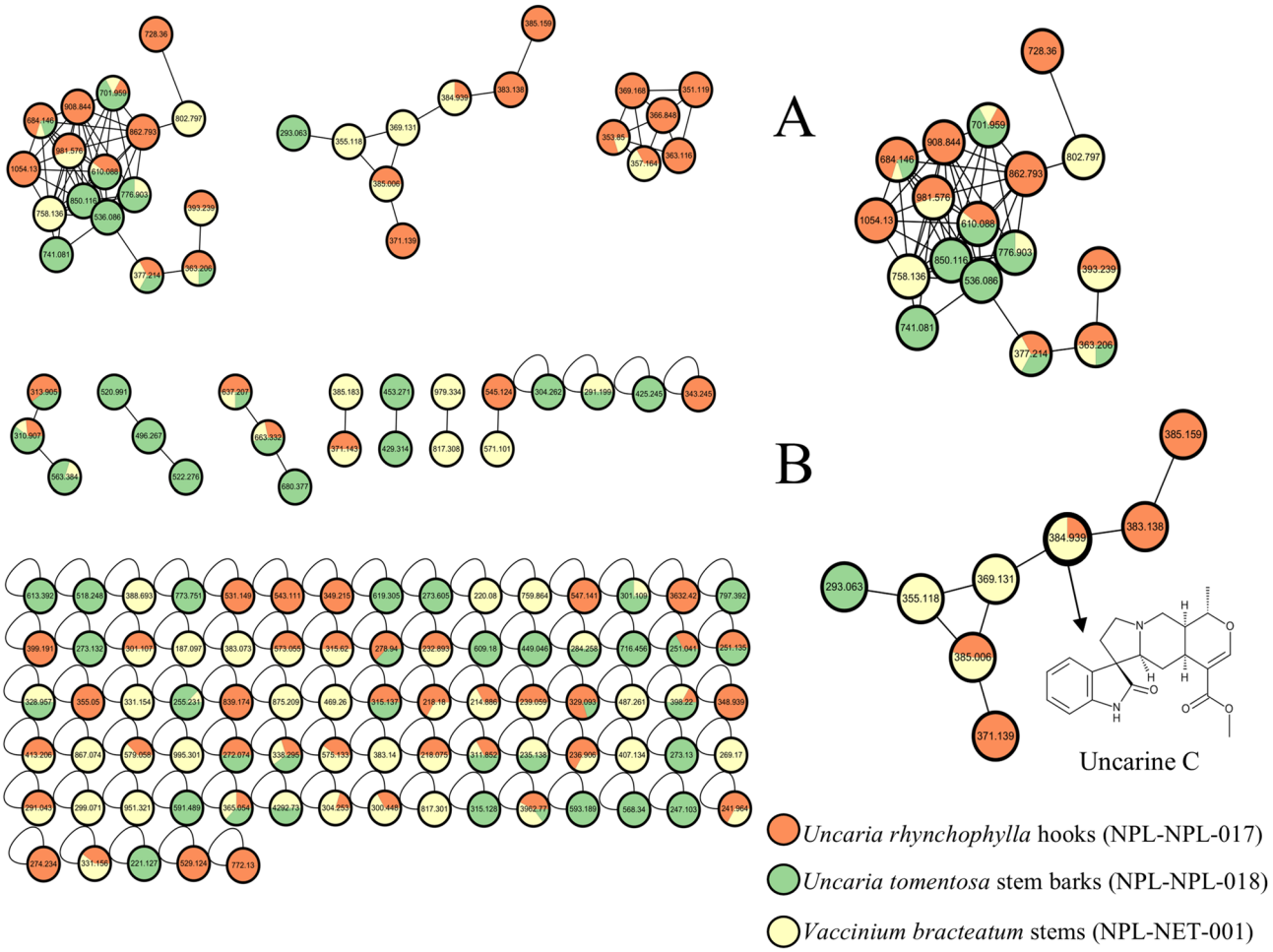

Fig. 9. Comparative FBMN analysis of *Uncaria tomentosa*, *Uncaria rhynchophylla*, and *Vaccinium bracteatum*, highlighting shared alkaloid and polyphenol clusters. (A) Molecular networking revealed clusters in alkaloid and polyphenol features. (B) Enlarged view of a representative cluster showing features putatively annotated as uncarine C and structurally related polyphenolic glycosides detected across all three species. Highlighted nodes are traceable to their feature IDs and corresponding annotation details, including precursor *m/z*, RT, library match information, and MSI confidence levels, provided in Supplementaray Table S3.

Sample preparation for ^{1}H NMR analysis using two solvent systems (CH_3OH-d_4-KH_2PO_4 buffer and CH_3OH-d_4)

For the ^{1}H NMR analysis, two solvent systems were prepared: (1) CH_3OH-d_4-KH_2PO_4 buffer (1:1, v/v) and (2) CH_3OH-d_4. The CH_3OH-d_4-KH_2PO_4 buffer (1:1, v/v), a 90 mM phosphate buffer solution containing 0.58 mM TMSP (internal standard), was prepared by dissolving 1.232 g of KH_2PO_4 in 100 ml of water and adjusting the pH of the buffer to 6.0 using 1.0 M NaOD. For CH_3OH-d_4, hexamethyldisiloxane (HMDSO) was added to CH_3OH-d_4 (0.418 mM) as an internal standard. For the ground-dried plant samples, 30 mg of ground sample were transferred into 2 mL microtubes using a spatula and 1 mL of either CH_3OH-d_4-KH_2PO_4 buffer (1:1, v/v) or CH_3OH-d_4 were added to each tube, and vortexed for 1 min at room temperature. The microtubes were then ultrasonicated for 20 min at room temperature to facilitate extraction and centrifuged at 17,000 g at room temperature for 20 min (to obtain a clear supernatant). An aliquot of 300 µL of the supernatant were then transferred to a 3 mm NMR tube. The HJD mixture was prepared by combining the four constituent plants in an equal mass ratio (7.5 mg each; total 30 mg). Additionally, all subset combinations of the four components were prepared using equal mass ratios while maintaining a total mass of 30 mg. All samples were extracted in 1 mL of solvent (30 mg/mL) under the same vortexing, ultrasonication, and centrifugation conditions before ^{1}H NMR analysis.

^{1}H NMR analysis

NMR measurements were performed on a Bruker Avance-III 600 MHz standard bore liquid-state NMR spectrometer with a 14.1 Tesla magnetic field. In this field, ^{1}H resonates at 600.13 MHz. A type of TCI H&F/C/N-D cryoprobe with Z gradient was used. 3 mm NMR tubes (Z112272) were purchased from Cortecnet and used for the experiments. The temperature was kept constant at 298 K. For internal locking, CH_3OH-d_4 was used. For each proton experiment, a 30-degree pulse of 2.64 msec at 5.5 W power with a fid resolution of 0.36 Hz,

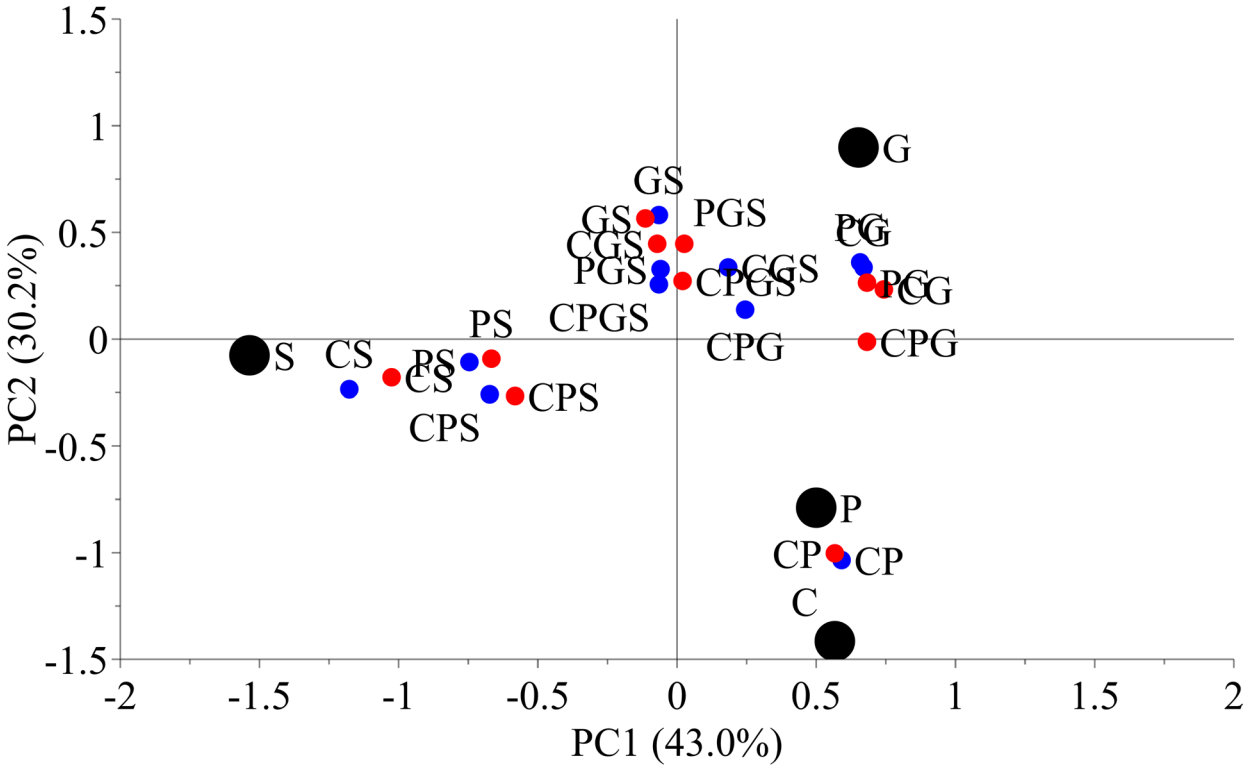

Fig. 10. Score plot of principal component analysis based on ^{1}H NMR data of *Coptis japonica* (C), *Phellodendron amurense* (P), *Gardenia jasminoides* (G), *Scutellaria baicalensis* (S), and their mixtures. Symbols in black are single plants, blue ones are co-extracted, and red ones are mixture of individually extracted ones.

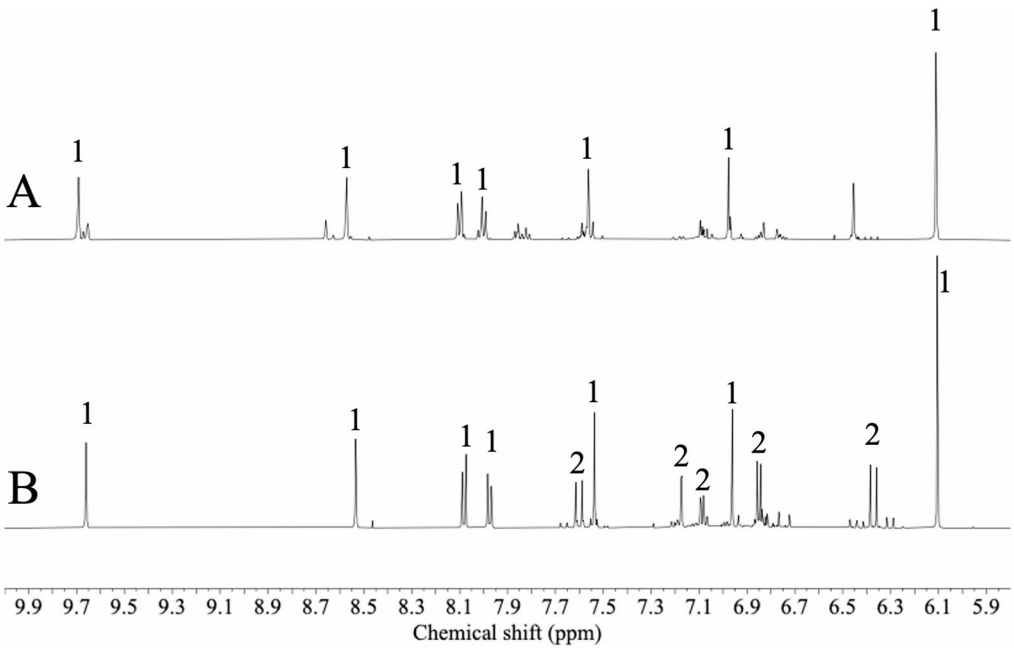

Fig. 11. Comparison between ^{1}H NMR spectra of *Coptis japonica* (**A**) and *Phellodendron amurense* (**B**). 1: ^{1}H resonances of berberine. 2: ^{1}H resonances of chlorogenic acid.

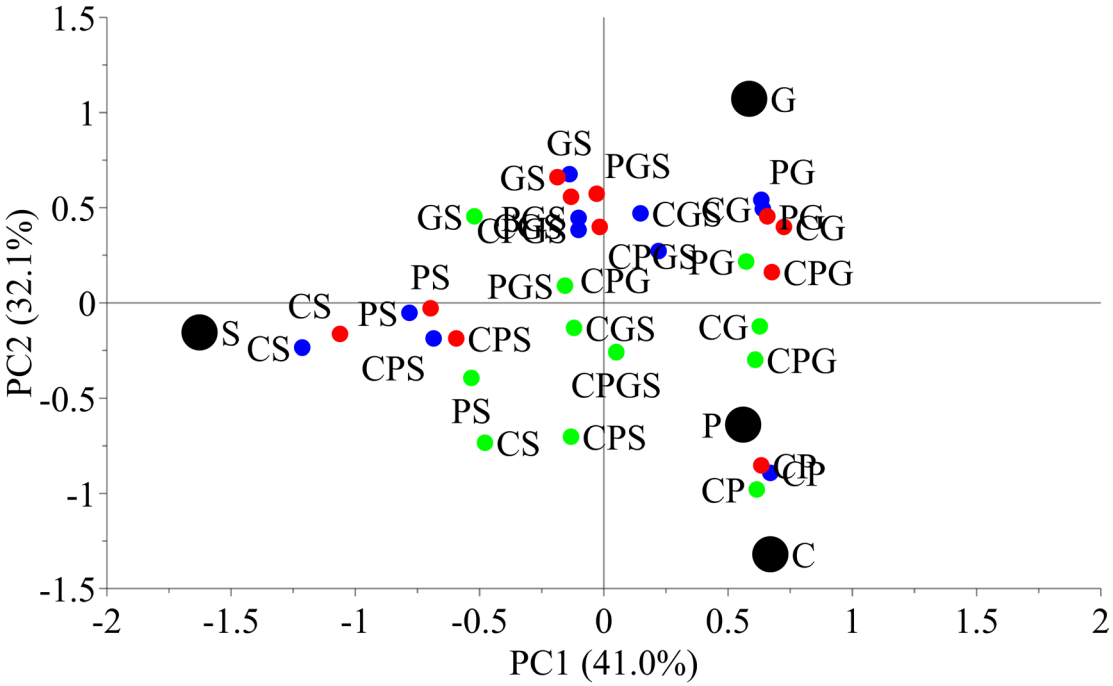

Fig. 12. PCA score plot based on ^{1}H NMR data of *Coptis japonica* (C), *Phellodendron amurense* (P), *Gardenia jasminoides* (G), *Scutellaria baicalensis* (S), and their mixtures. Black symbols represent single-herb extracts; blue symbols, co-extracted mixtures; red symbols, mixtures prepared by combining individually extracted components; and green symbols, computed average profiles calculated from the constituent single-herb spectra.

64 scans with a relaxation delay of 1.5 s, and acquisition time of 2.7 s was used taking a total time of 5 min to complete the experiment. The water signal was suppressed using a pre-saturation method and low-power selective irradiation at 0.3 Hz H_2O at 4.87 ppm. Time domain data was transformed to the frequency domain by Fourier transformation with a window function of exponential function and a line broadening parameter set to 0.3 Hz for smoothing. The generated spectrums were manually phased, baseline corrected and calibrated to TMSP-d_4 at 0.0 ppm or HMDSO at 0.06 ppm.

^{1}H NMR data processing for multivariate data analysis

Bucketing using NMR data processing software facilitates the normalization of ^{1}H NMR spectra obtained from plant extracts prepared with two solvent systems -CH_3OH-d_4 and a mixture of CH_3OH-d_4 with KH_2PO_4 buffer (pH 6.0, 1:1, v/v). In this study, TopSpin software (version 3.7, Bruker BioSpin GmbH) was used for spectral processing. To enable comparison of the relative concentrations of extracted metabolites, total intensity normalization was applied to the spectral region from δ 10.0 to δ 0.3, using a bucket width of 0.04 ppm. Regions corresponding to residual solvent peaks - δ 3.28–3.24 for CH_3OH-d_4 and δ 5.0–4.7 for HDO - were excluded from analysis. The resulting bucketed data from each solvent (243 variables in total) were combined into a single data matrix for each sample (486 variables in total). The complete data matrix for all 656 samples is provided in the Supplementary Table S1.

Multivariate-and statistical analysis

Multivariate and statistical analyses were performed using SIMCA-P software (version 18.0.1, Sartorius) based on matrices derived from ^{1}H NMR data. The bucketed dataset was analysed by principal component analysis (PCA) and hierarchical clustering analysis (HCA) using PCA-reduced components. Model quality and robustness were evaluated using the cumulative fraction of explained variance (R2X(cum)) and the predictive ability (Q2(cum)) based on seven-fold internal cross-validation. To investigate genus- and species-related metabolic variation, soft independent modeling of class analogy (SIMCA) was applied by defining plant genus or geographical origin as PCA classes, depending on the specific analysis. In SIMCA, separate local PCA models are constructed for each predefined class, and the distance of each sample to its corresponding class model is calculated as the distance to the model (DModX). For species-level effects, DModX values were calculated by setting each plant genus as a PCA class. DModX values were log-transformed and used to screen potential outliers; however, no samples were excluded solely based on outlier diagnostics. All data were scaled using unit variance (UV) scaling.

UHPLC-DAD-QToF analysis

Selected samples were further analyzed using a UHPLC-DAD-QToF system (Ultimate 3000, Thermo Scientific) coupled with a QTOF-II mass spectrometer (Bruker) operating in positive ESI mode. Samples were extracted

in 70% methanol, filtered, and diluted tenfold prior to injection. Chromatographic separation was achieved on a 2.1 × 150 mm Kinetex C_{18} column (2.6 µm) with a 0.3 mL/min gradient flow. The gradient program was set using 0.1% formic acid in water (A) and 0.1% formic acid in acetonitrile (B). The gradient elution profile was as follows: 5% B to 95% B (16 min), 95% B (2 min), and 5% B (2 min) and the total run time was 20 min. The oven temperature was set at 40 °C. The sample injection volume was 1 µL. MS parameters included a capillary voltage of 4000 V, a drying gas temperature of 350 °C with a flow rate of 6 L/min, and a nebulizer gas pressure of 2.0 bar. Sodium formate was used for mass calibration. Spectra were recorded in positive ESI full-scan mode over an *m/z* range of 100–1650. No pooled QC samples or internal standards were included, as the LC–HRMS analysis was conducted for qualitative and comparative molecular networking purposes.

Molecular networking analysis

A molecular network was constructed using the molecular networking (MN) workflow available on the GNPS platform (https://gnps.ucsd.edu). Specifically, Feature-Based Molecular Networking (FBMN) was applied. Raw LC–HRMS data were converted to the .mzML format using the MSConvert tool within the ProteoWizard software suite and subsequently uploaded to GNPS for feature deconvolution and molecular networking analysis. Sample group information was incorporated during post-network analysis to support comparative interpretation of molecular clusters. The precursor ion mass tolerance was defined as 0.02 Da, and the fragment ion tolerance in MS/MS was also set at 0.02 Da. Molecular networks were established by filtering edges to retain only those with a cosine similarity score greater than 0.5 and at least four matched peaks. Additionally, connections between nodes were preserved in the network only if each node was within the top 10 most similar nodes of the other. The maximum allowable size for each molecular family was limited to 100 nodes, and edges with lower scores were progressively removed until each molecular family complied with this maximum size. Spectral matches within the network were compared against GNPS public spectral libraries. Library spectra underwent the same filtering procedures as the experimental input data. Matches between experimental spectra and library spectra were accepted only if they achieved a cosine score higher than 0.7 and had a minimum of four matched peaks. Finally, the molecular network was visualized using Cytoscape software (version 3.9.1), a widely adopted bioinformatics tool for network analysis.

Data availability

Data sets generated during the current study are available from the corresponding author on reasonable request.

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Author contributions

YHC conceptualized the study and designed the experiments. YHC and HKK developed the analytical methods. SS, ÖE, and HKK and conducted the experimental work. YHC and SS performed data analysis. HGJVM contributed to the refinement of statistical and multivariate analysis methods. JJ, YPJ, and DYL selected the Korean medicinal plants and verified their identification. MW selected and verified the identification of the Chinese medicinal plants. SS and YHC drafted the manuscript. HS and HSB reviewed and revised the analytical data. All authors contributed to writing and provided feedback on the manuscript. All authors have read and approved the final version.

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Declarations

Competing interests

The authors declare no competing interests.

Additional information

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