

**Supplementary File**

**Computational workflow to study the diversity of  
secondary metabolites in fourteen different *Isatis* species**

## Sample preparation and GC-MS analysis

**Table S2.** The information of the source of the seeds (14 species).

**Figure S1.** The phenotypes of 14 *Isatis* species.

**Figure S2.** Structural information of metabolites for li-1~66.

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**Table S3.** The detailed information of 74 reference standards.

**Table S4.** An in-house library covers 269 metabolites from phytochemical research (up to 2020) in the whole *Isatis* L. genus.

**Table S7.** Validation results of detection of 73 reference standards by application of feature-rating rule.

**Figure S7.** Investigation of different chromatographic columns for achieving better separation and peak capacity (*Ind* as an example).

**Figure S8.** Investigation of different mobile phase additives for achieving better ionization (*Ind* as an example).

**Figure S9.** A standard mixture contains 12 purity compounds with different chemical classifications for the demonstration of mass features and adducts types before the large-scale acquisition.

**Figure S10.** The operation of detailed manual annotation of each feature in each cluster.

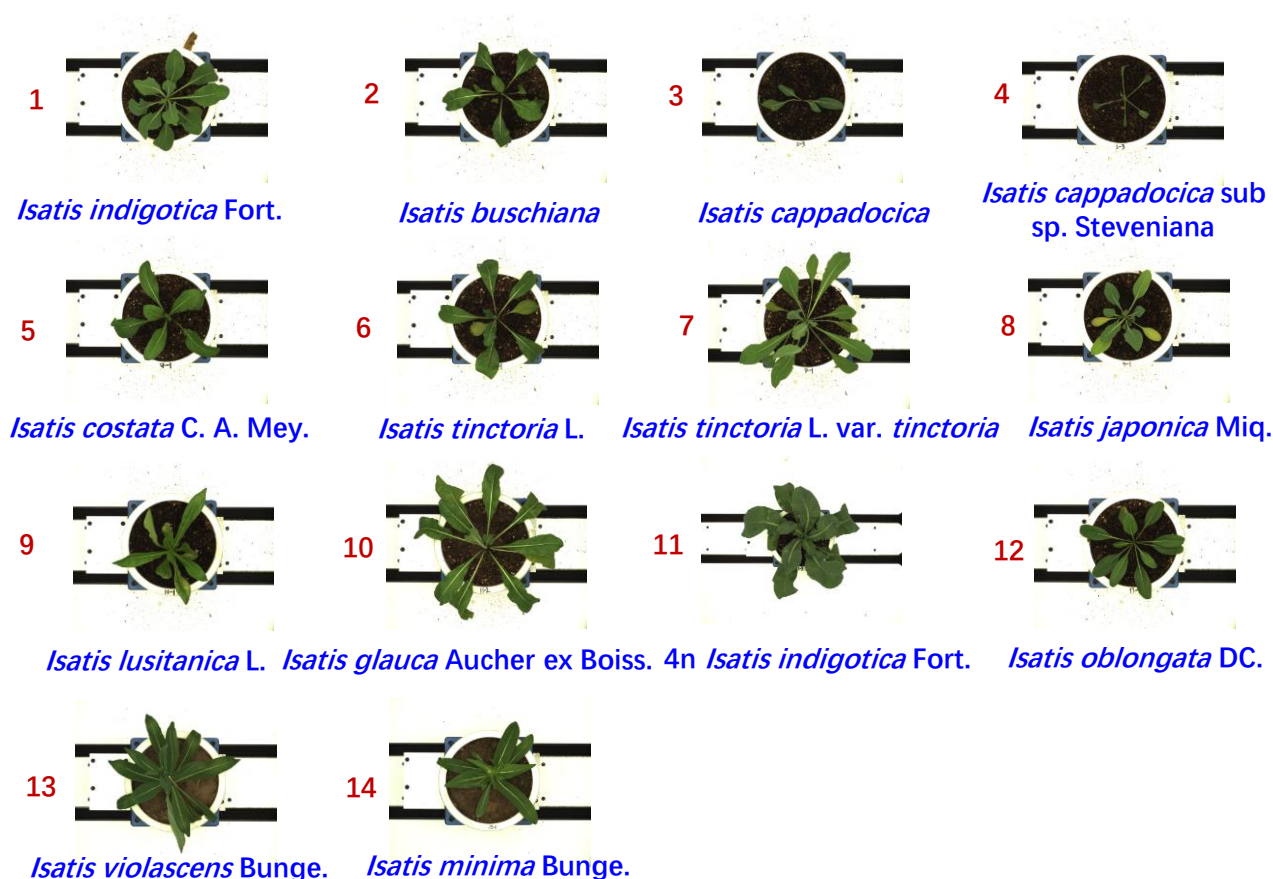
**Figure S11.** The relative content of indole compound by applying GC-MS among 12 species.

### **Sample preparation and GC-MS analysis**

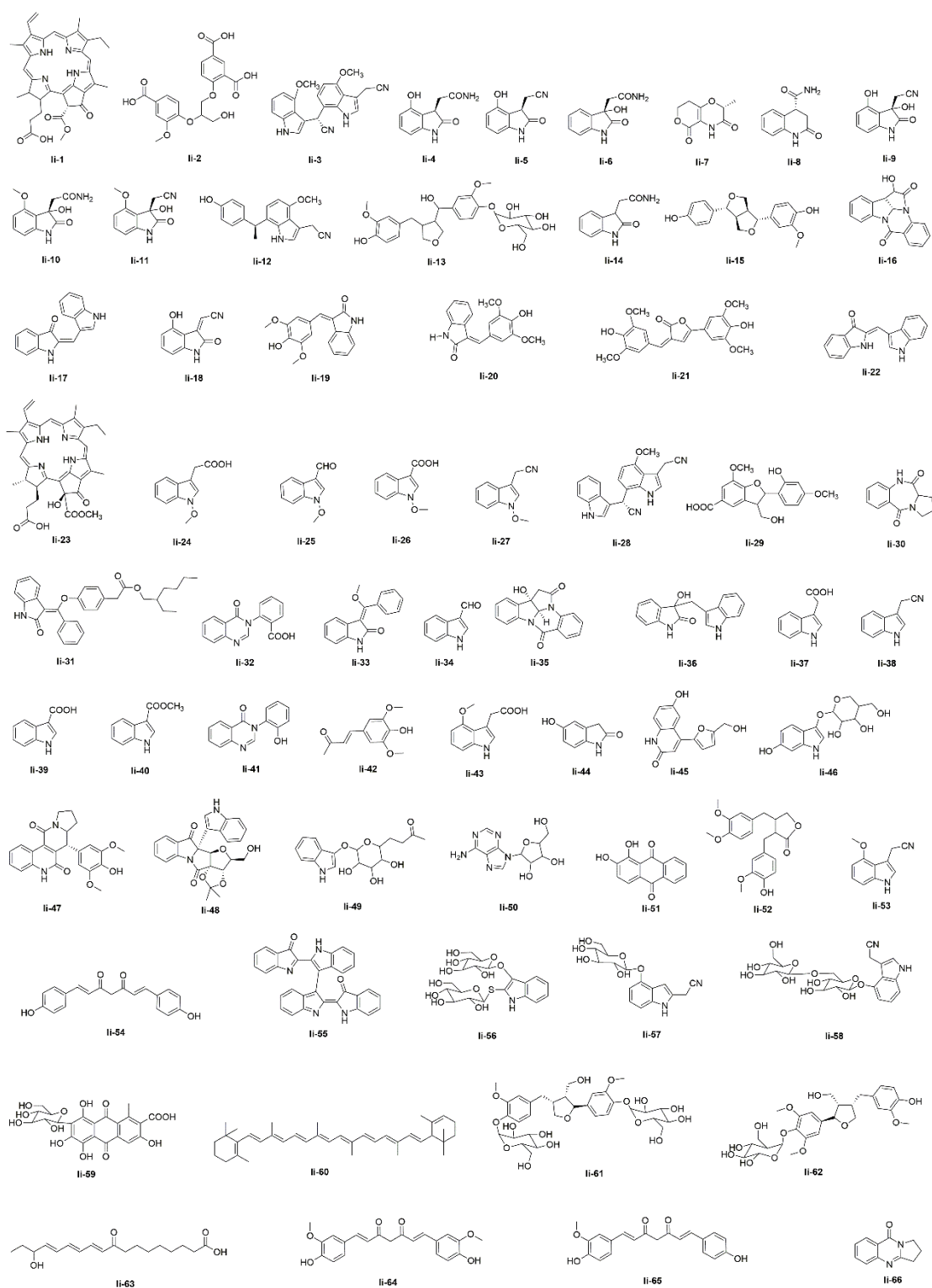
An amount of 10 mg of fresh samples was prepared using ultrasound extraction in 4 mL MeOH for 30 min. Then, the supernatant was dried under nitrogen-blow, which was redissolved in 1 mL cyclohexane, and kept in sealed vials at 4 °C until GC-MS analysis. GC-MS analysis was performed on Clarus 580 Gas Chromatograph (Perkin-Elmer, USA) equipped with an Elite-5 MS capillary column (30 m length, 0.25 mm internal diameter and 0.25 µm film thickness) and coupled with a SQ-8 MS detector. 0.1 µl volume of essential oil was injected. The oven temperature was programmed at 60 °C then increased to 220 °C at a rate of 3 °C per min and the final temperature was kept for 7 min at 220 °C. Helium at a flow rate of 1 ml/min was used as a carrier gas. The injector and transfer interface temperature was kept at 250 °C. Mass spectra were recorded at 70 electron volt. The source temperature was kept at 250 °C.

**Table S2** The information of the source of the seeds (14 species).

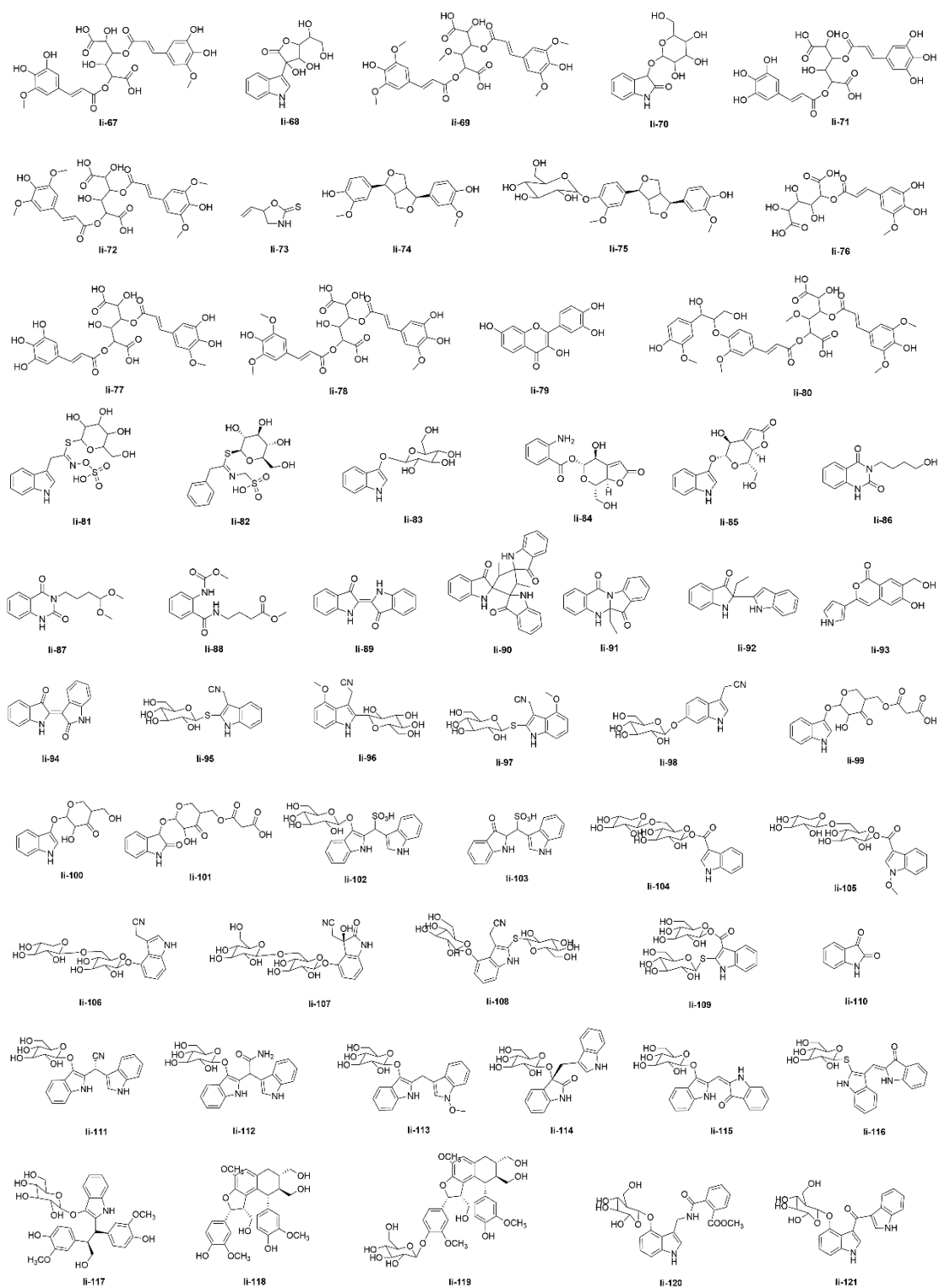
Species Name	Collection location
<i>Isatis indigotica</i> Fort. ( <i>ind</i> )	Shanghai, China
<i>Isatis buschiana</i> ( <i>bus</i> )	North Korea
<i>Isatis cappadocica</i> ( <i>cap</i> )	Turkey
<i>Isatis cappadocica</i> subsp. <i>Steveniana</i> ( <i>capS</i> )	Iran
<i>Isatis costata</i> C. A. Mey. ( <i>cosC</i> )	Xinjiang, China
<i>Isatis tinctoria</i> L. ( <i>tin</i> )	Germany
<i>Isatis tinctoria</i> L. var. <i>tinctoria</i> ( <i>tinV</i> )	Xinjiang, China
<i>Isatis japonica</i> Miq. ( <i>jap</i> )	Pyongyang, North Korea
<i>Isatis lusitanica</i> L. ( <i>lus</i> )	Israel
<i>Isatis glauca</i> Aucherex Boiss. ( <i>glaA</i> )	Israel
Tetraploid <i>Isatis indigotica</i> Fort. ( $4n=28$ ), ( <i>4ind</i> )	Shanghai, China
<i>Isatis oblongata</i> DC. ( <i>obl</i> )	Xinjiang, China
<i>Isatis violascens</i> Bunge. ( <i>vio</i> )	Xinjiang, China
<i>Isatis minima</i> Bunge. ( <i>min</i> )	Xinjiang, China



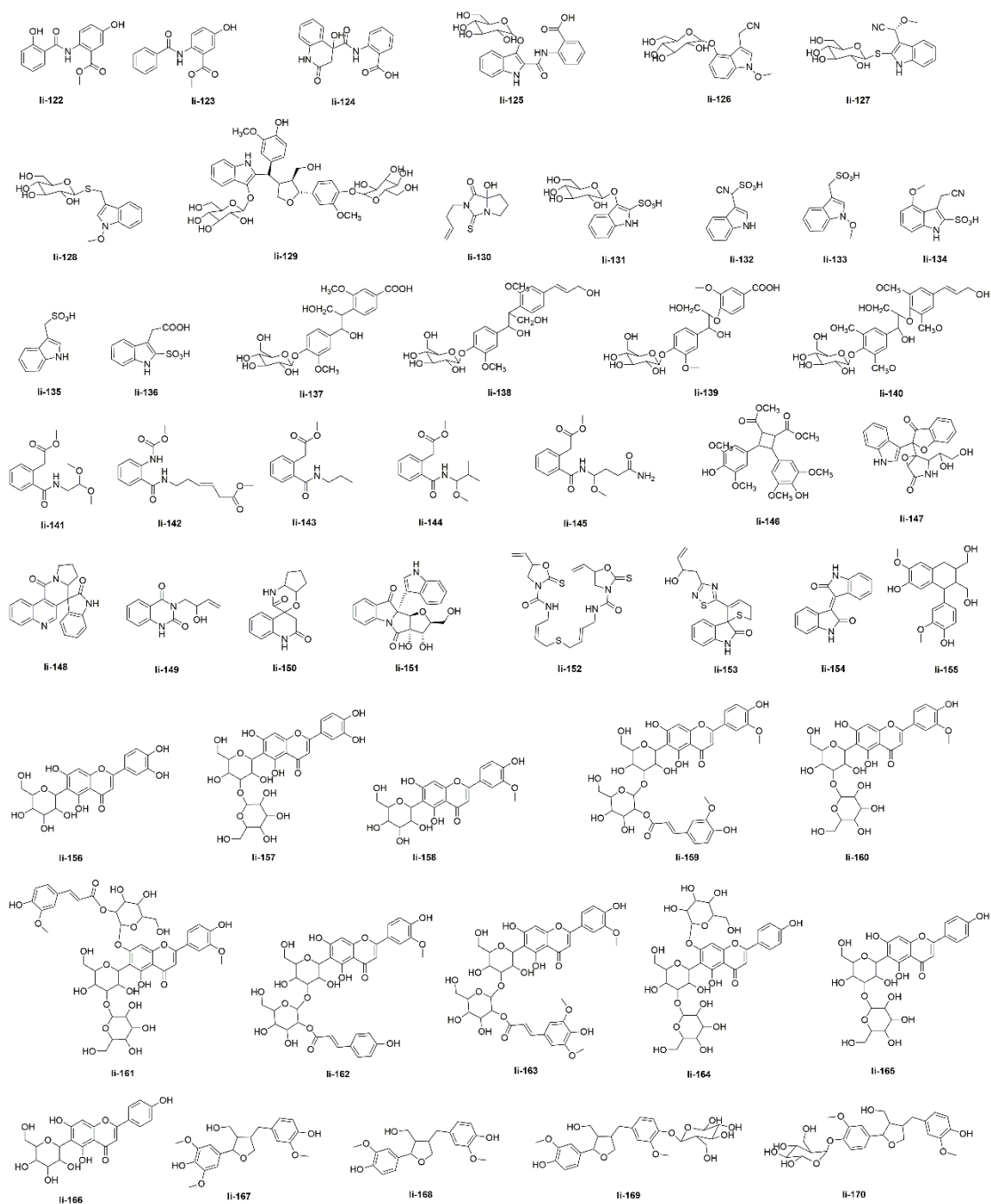
**FigureS1.** The phenotypes of 14 *Isatis* species.



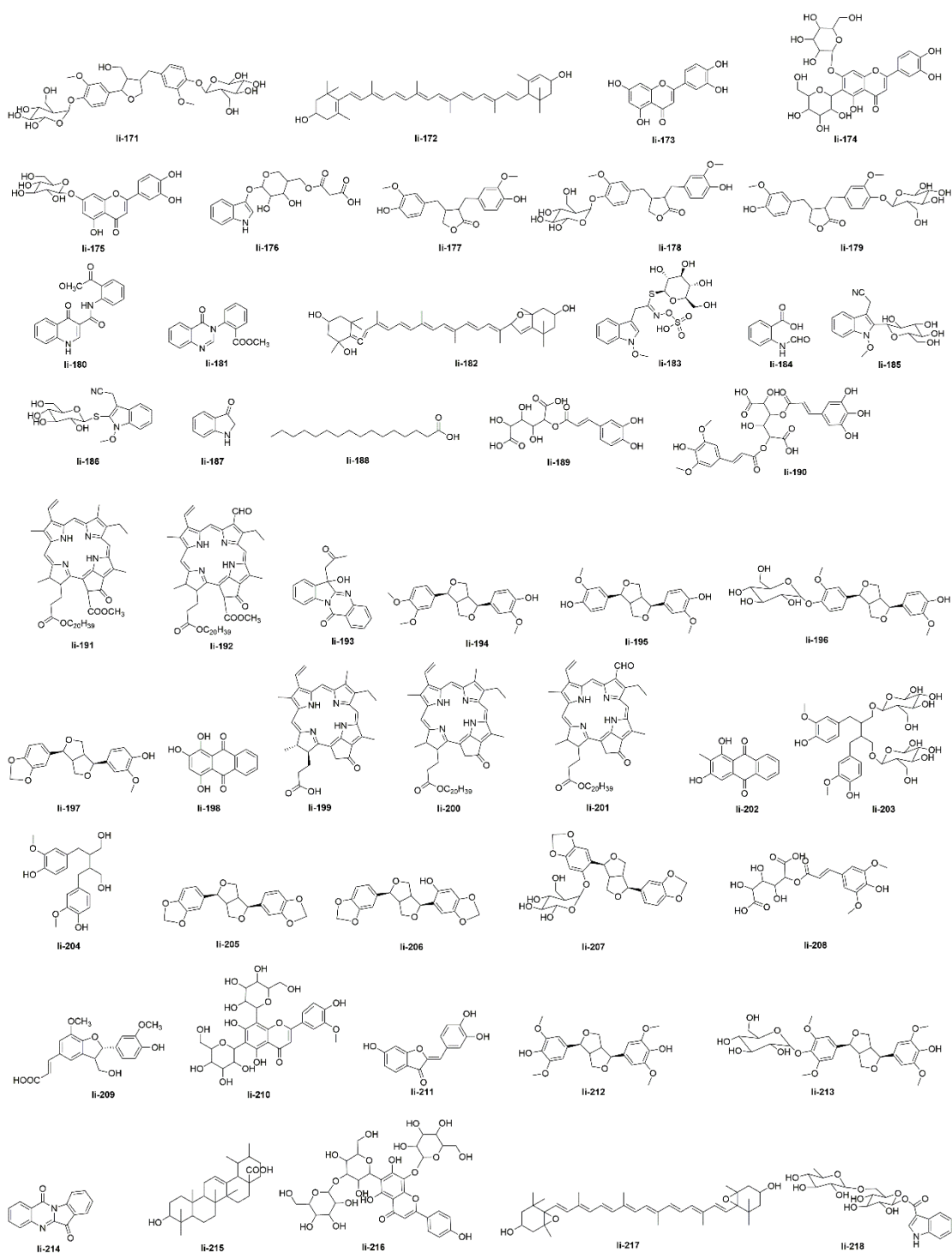
**Figure S2.** Structural information of metabolites for li-1~66.



**Figure S3.** Structural information of metabolites for li-67~121.

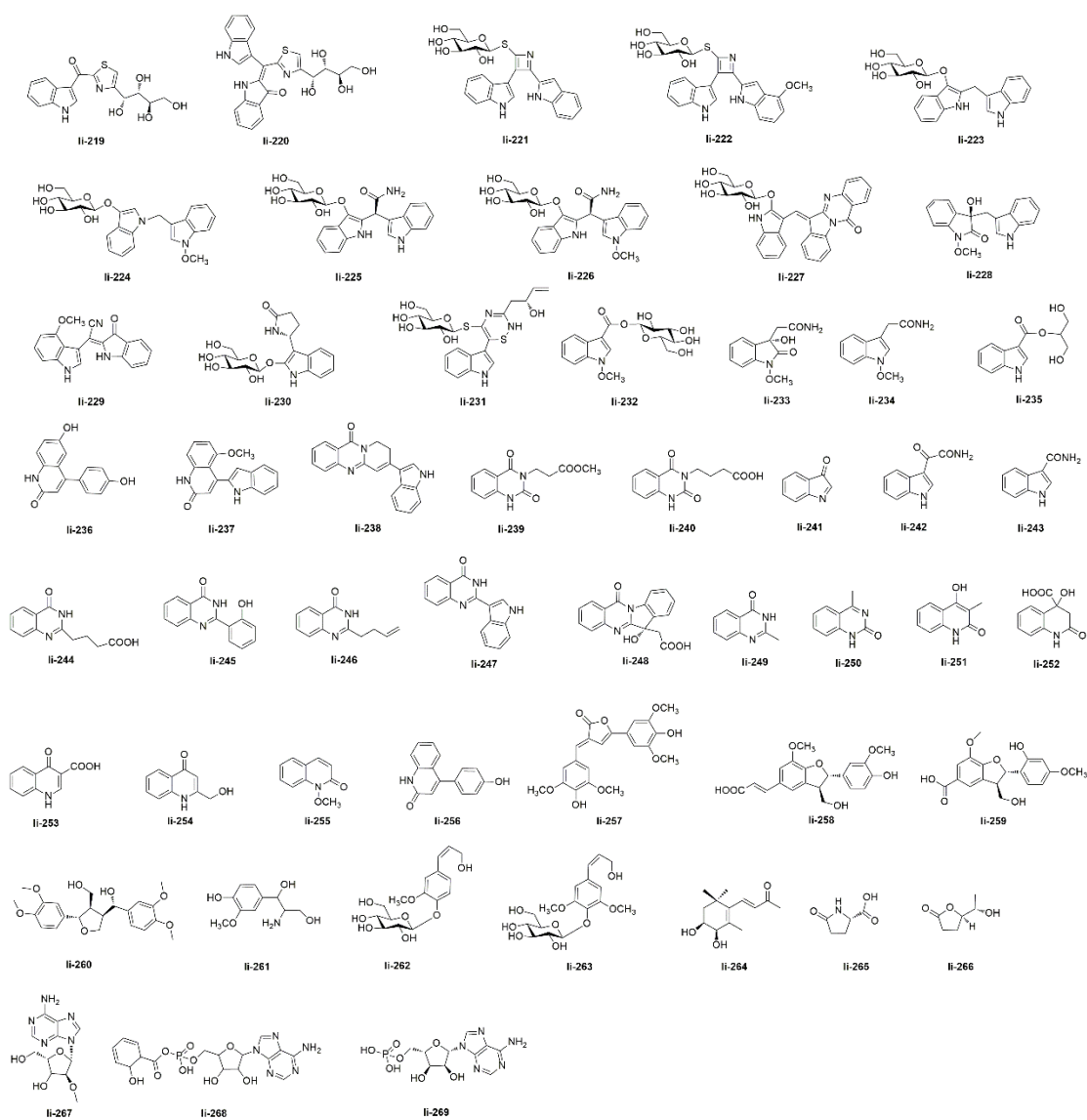


**Figure S4.** Structural information of metabolites for li-122~170.



**Figure S5.** Structural information of metabolites for li-171~218.





**Figure S6.** Structural information of metabolites for li-219~269.

**Table S3** The detailed information of 74 reference standards.

No.	Name	Formula	CAS
1	Benzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	65-85-0
2	Vanillin	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	121-33-5
3	3,4-Dihydroxybenzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>	99-50-3
4	Benzoyleneurea	C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub>	86-96-4
5	L-Phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	63-91-2
6	Gallic acid	C <sub>7</sub> H <sub>6</sub> O <sub>5</sub>	149-91-7
7	L(+)-Arginine	C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>	74-79-3
8	Caffeic acid	C <sub>9</sub> H <sub>8</sub> O <sub>4</sub>	331-39-5
9	D-Mannose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	3458-28-4
10	Scopoletin	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	92-61-5
11	Ferulic Acid	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	1135-24-6
12	3-Hydroxy-4-methoxycinnamic acid	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	537-73-5
13	Wogonin	C <sub>16</sub> H <sub>12</sub> O	632-85-9
14	L-Tryptophan	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	73-22-3
15	Isofraxidin	C <sub>11</sub> H <sub>10</sub> O <sub>5</sub>	486-21-5
16	Sulbactam	C <sub>8</sub> H <sub>11</sub> NO <sub>5</sub> S	68373-14-8
17	Gemcitabine	C <sub>9</sub> H <sub>11</sub> F <sub>2</sub> N <sub>3</sub> O <sub>4</sub>	95058-81-4
18	Aloe emodin	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	481-72-1
19	Naringenin	C <sub>15</sub> H <sub>12</sub> O <sub>5</sub>	480-41-1
20	Acacetin	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	480-44-4
21	Fludarabine	C <sub>10</sub> H <sub>12</sub> FN <sub>5</sub> O <sub>4</sub>	21679-14-1
22	3-Indoxyl-beta-D-glucopyranoside	C <sub>14</sub> H <sub>17</sub> NO <sub>6</sub>	487-60-5
23	Hispidulin	C <sub>16</sub> H <sub>12</sub> O <sub>6</sub>	1447-88-7
24	Salidroside	C <sub>14</sub> H <sub>20</sub> O <sub>7</sub>	10338-51-9
25	Mycophenolic acid	C <sub>17</sub> H <sub>20</sub> O <sub>6</sub>	24280-93-1
26	Gliclazide	C <sub>15</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> S	21187-98-4
27	Tricin	C <sub>17</sub> H <sub>14</sub> O <sub>7</sub>	520-32-1
28	Neochlorogenic acid	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	906-33-2
29	Cryptochlorogenic acid	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	905-99-7
30	Chlorogenic acid	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	327-97-9
31	Pinoresinol	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>	487-36-5
32	Prednisolone	C <sub>21</sub> H <sub>28</sub> O <sub>5</sub>	50-24-8
33	Loganin	C <sub>17</sub> H <sub>26</sub> O <sub>10</sub>	18524-94-2
34	Icotinib	C <sub>22</sub> H <sub>21</sub> N <sub>3</sub> O <sub>4</sub>	610798-31-7
35	4,11-Diethyl-4,9-dihydroxy-1H-pyrano[3',4':6,7]indolizino[1,2-b]quinoline-3,14(4H,12H)-dione	C <sub>22</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>	130144-34-2
36	Erlotinib	C <sub>22</sub> H <sub>23</sub> N <sub>3</sub> O <sub>4</sub>	183321-74-6
37	3β,5,14-Trihydroxy-5β-bufa-20,22-dienolide	C <sub>24</sub> H <sub>34</sub> O <sub>5</sub>	472-26-4
38	2,3,5,4' -Tetrahydroxy stilbene-2-O-β-D-glucoside	C <sub>20</sub> H <sub>22</sub> O <sub>9</sub>	82373-94-2
39	Liquiritin	C <sub>21</sub> H <sub>22</sub> O <sub>9</sub>	551-15-5
40	Sec-O-glucosylhamaudol	C <sub>21</sub> H <sub>26</sub> O <sub>10</sub>	80681-44-3
41	Cynaroside	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	5373-11-5

42	Astragalin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	480-10-4
43	Oleanic acid	C <sub>30</sub> H <sub>48</sub> O <sub>3</sub>	508-02-1
44	Oxytetracycline	C <sub>22</sub> H <sub>24</sub> N <sub>2</sub> O <sub>9</sub>	79-57-2
45	Hyperoside	C <sub>21</sub> H <sub>20</sub> O <sub>12</sub>	482-36-0
46	Maslinic acid	C <sub>30</sub> H <sub>48</sub> O <sub>4</sub>	4373-41-5
47	Corosolic acid	C <sub>30</sub> H <sub>48</sub> O <sub>4</sub>	4547-24-4
48	Paeoniflorin	C <sub>23</sub> H <sub>28</sub> O <sub>11</sub>	23180-57-6
49	Asiatic acid	C <sub>30</sub> H <sub>48</sub> O <sub>5</sub>	464-92-6
50	Caudatin	C <sub>28</sub> H <sub>42</sub> O <sub>7</sub>	<u>38395-02-7</u>
51	Baohuoside I	C <sub>27</sub> H <sub>30</sub> O <sub>10</sub>	113558-15-9
52	Isochlorogenic acid C	C <sub>25</sub> H <sub>24</sub> O <sub>12</sub>	57378-72-0
53	Ganoderic acid C2	C <sub>30</sub> H <sub>46</sub> O <sub>7</sub>	98296-48-1
54	Forsythin	C <sub>27</sub> H <sub>34</sub> O <sub>11</sub>	487-41-2
55	Arctiin	C <sub>27</sub> H <sub>34</sub> O <sub>11</sub>	7770-78-7
56	Epirubicin	C <sub>27</sub> H <sub>29</sub> NO <sub>11</sub>	56420-45-2
57	Ceritinib (LDK378)	C <sub>28</sub> H <sub>36</sub> ClN <sub>5</sub> O <sub>3</sub> s	1032900-25-6
58	Polygalaxanthone III	C <sub>25</sub> H <sub>28</sub> O <sub>15</sub>	162857-78-5
59	Procyanidin B3	C <sub>30</sub> H <sub>26</sub> O <sub>12</sub>	23567-23-9
60	Etoposide	C <sub>29</sub> H <sub>32</sub> O <sub>13</sub>	33419-42-0
61	Vicenin	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	23666-13-9
62	Saponarin	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	20310-89-8
63	Rutin	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	153-18-4
64	Hesperidin	C <sub>28</sub> H <sub>34</sub> O <sub>15</sub>	520-26-3
65	Ritonavir	C <sub>37</sub> H <sub>48</sub> N <sub>6</sub> O <sub>5</sub> S <sub>2</sub>	155213-67-5
66	Timosaponin A-III	C <sub>39</sub> H <sub>64</sub> O <sub>13</sub>	41059-79-4
67	Heterophyllin B	C <sub>40</sub> H <sub>58</sub> N <sub>8</sub> O <sub>8</sub>	145459-19-4
68	Saikosaponin A	C <sub>42</sub> H <sub>68</sub> O <sub>13</sub>	20736-09-8
69	Epmedin C	C <sub>39</sub> H <sub>50</sub> O <sub>19</sub>	110642-44-9
70	3-[(6-Deoxy-3-O-beta-D-glucopyranosyl-alpha-L-mannopyranosyl)oxy]-7-(beta-D-glucopyranosyloxy)-5-hydroxy-2-(4-methoxyphenyl)-8-(3-methyl-2-buten-1-yl)-4H-1-benzopyran-4-one	C <sub>39</sub> H <sub>50</sub> O <sub>20</sub>	140147-77-9
71	Paclitaxel	C <sub>47</sub> H <sub>51</sub> NO <sub>14</sub>	33069-62-4
72	Timosaponin BII	C <sub>45</sub> H <sub>76</sub> O <sub>19</sub>	136656-07-0
73	Asiaticoside	C <sub>48</sub> H <sub>78</sub> O <sub>19</sub>	16830-15-2
74	p-Hydroxybenzaldehyde	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	123-08-0

**Table S4.** An in-house library covers 269 metabolites from phytochemical research (up to 2020) in the whole *Isatis* L. genus.

Code	Name	Formula
Ii-1	pheophorbide a	C <sub>35</sub> H <sub>36</sub> N <sub>4</sub> O <sub>5</sub>
Ii-2	(-)-(R)- and(+)-(S)-isatindigotriolic acid	C <sub>19</sub> H <sub>18</sub> O <sub>10</sub>
Ii-3	(-)-(R)-2-(3-cyanomethyl-4-methoxy-1H-indol-7-yl)-2-(4-methoxy-1H-indol-3-yl) acetonitrile	C <sub>22</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>

Ii-4	(-)-(R)-2-(4-hydroxy-2-oxoindolin-3-yl) acetamide	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Ii-5	(-)-(R)-2-(4-hydroxy-2-oxoindolin-3-yl)-acetonitrile	C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
Ii-6	(-)-(S)-2-(3-hydroxy-2-oxoindolin-3-yl) acetamide	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Ii-7	(+)-(R)-2-methyl-7,8-dihydropyrano [4,3-b]-[1,4]oxazine-3,5(2H,4H)-dione	C <sub>8</sub> H <sub>9</sub> NO <sub>4</sub>
Ii-8	(+)-(R)-2-oxo-1,2,3,4-tetrahydroquino-line-4-carboxamide	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Ii-9	(+)-(S)-2-(3,4-dihydroxy-2-oxoindolin-3-yl) acetonitrile	C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>
Ii-10	(+)-(S)-2-(3-hydroxy-4-methoxy-2-oxoindolin-3-yl) acetamide	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>
Ii-11	(+)-(S)-2-(3-hydroxy-4-methoxy-2-oxoindolin-3-yl) acetonitrile	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Ii-12	(+)-(S)-2-{7-[1-(4-hydroxyphenyl)-ethyl]-4-methoxy-1H-indol-3-yl} acetonitrile	C <sub>19</sub> H <sub>18</sub> N <sub>2</sub> O <sub>2</sub>
Ii-3	(+)-larch rosin-4-O-B-D-glucoside	C <sub>26</sub> H <sub>34</sub> O <sub>11</sub>
Ii-14	(±)-2-(2-oxoindolin-3-yl) acetamide	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Ii-15	(1S,2R,5S,6R)-2-(4-hydroxyphenyl)-6-(3-methoxy-4-hydroxyphenyl)-3,7-dioxabicyclo[3.3.0]octane	C <sub>19</sub> H <sub>20</sub> O <sub>5</sub>
Ii-16	(2R,3R)-3-hydroxy-2Hpyrrolo[2,3-b]indolo[5,5a,6-b,a]quinazoline-9(8H),7'-dione	C <sub>17</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Ii-17	(2E)-2-(1H-indol-3-ylmethylidene)-1,2-dihydro-3H-indol-3-one	C <sub>17</sub> H <sub>12</sub> N <sub>2</sub> O
Ii-18	(E)-2-(4-hydroxy-2-oxoindolin-3-ylidene) acetonitrile	C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub>
Ii-19	(E)-3-(3',5'-dimethoxy-4'-hydroxybenzylidene)-2-indolinone.	C <sub>17</sub> H <sub>15</sub> NO <sub>4</sub>
Ii-20	(E)-3-(30,50-dimethoxy-40-hydroxy-benzylidene)-2-indolinone	C <sub>17</sub> H <sub>15</sub> NO <sub>4</sub>
Ii-21	(E)-5-(4-hydroxy-3,5-dimethoxyphenyl)-3-[(4-hydroxy-3,5-dimethoxyphenyl)-methylethylene]-2(3H)-furanone	C <sub>21</sub> H <sub>20</sub> O <sub>8</sub>
Ii-22	(Z)-2-(1H-indol-3-ylmethylidene)-1,2-dihydro-3H-indol-3-one	C <sub>17</sub> H <sub>12</sub> N <sub>2</sub> O
Ii-23	10-Hydroxy phaeophorbide	C <sub>35</sub> H <sub>36</sub> N <sub>4</sub> O <sub>6</sub>
Ii-24	1-methoxy-3-indoleacetic acid	C <sub>11</sub> H <sub>11</sub> NO <sub>3</sub>
Ii-25	1-methoxy-3-indolecarbaldehyde	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>
Ii-26	1-methoxy-3-indoleformic acid	C <sub>10</sub> H <sub>9</sub> NO <sub>3</sub>
Ii-27	1-methoxy-indole-3-acetonitrile	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O
Ii-28	2-(3-cyanomethyl-4-methoxy-1H-indol-7-yl)-2--(1H-indol-3-yl)acetonitrile	C <sub>21</sub> H <sub>16</sub> N <sub>4</sub> O
Ii-29	2-(3-hydroxy-5-methoxyphenyl)-3-hydroxymethyl-7-methoxy-2,3-dihydrobenzofuran-5-carboxylic acid	C <sub>18</sub> H <sub>18</sub> O <sub>7</sub>
Ii-30	2,3-dihydro-1 H-pyrrolo[2,1 -Cl[1 ,4]benzodiazepine-5,1 1(1 OH,1 I aH)-dione	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Ii-31	2-ethylhexyl 2-{4-[2-oxo-1, 2-dihydro-3H-indol-3-ylidene) (phenyl) methoxy] phenyl} acetate	C <sub>31</sub> H <sub>33</sub> NO <sub>4</sub>
Ii-32	3-(2'-carboxyphenyl)-4(3H)-quinazolinone	C <sub>15</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>
Ii-33	3-[(E)-methoxy (phenyl) methylidene]-1,3-dihydro-2H-indol-2-one	C <sub>16</sub> H <sub>13</sub> NO <sub>2</sub>
Ii-34	3-aldehyde indole	C <sub>9</sub> H <sub>7</sub> NO
Ii-35	3-hydroxy-2H-pyrrolo[2,3-b]indolo[5,5a,6-b,a]quinazoline-9(8H),7'-dione	C <sub>17</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Ii-36	3-hydroxy-2-ox-3,3'-diindolylmethane	C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Ii-37	3-indoleacetic acid	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>
Ii-38	3-indoleacetonitrile	C <sub>10</sub> H <sub>8</sub> N <sub>2</sub>
Ii-39	3-indoleformic acid	C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub>

Ii-40	3-indoleformic acid methyl ester	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>
Ii-41	4-(3H)-quinazolinone	C <sub>14</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Ii-42	4-(4'-hydroxy-3',5'-dimethoxyphenyl)-3-buten-2-one	C <sub>12</sub> H <sub>14</sub> O <sub>4</sub>
Ii-43	4-methoxy-3-indoleacetic acid	C <sub>11</sub> H <sub>11</sub> NO <sub>3</sub>
Ii-44	5-Hydroxyoxindole	C <sub>8</sub> H <sub>7</sub> NO <sub>2</sub>
Ii-45	6-hydroxy-4-(5-hydroxymethylfuran-2-yl)quinolin-2(1H)-one	C <sub>14</sub> H <sub>11</sub> NO <sub>4</sub>
Ii-46	6-OH-ICOOGlc	C <sub>14</sub> H <sub>17</sub> NO <sub>6</sub>
Ii-47	7-(3',5'-dimethoxy-4'-hydroxyphenyl)-7a,8,9,10-tetrahydroindolizino[7,6-c]quinoline-6,12(5H,7H)-dione	C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub>
Ii-48	9a,13a-Dihydroxylisopropylidenylisatisine A	C <sub>25</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub>
Ii-49	acetylindican	C <sub>17</sub> H <sub>21</sub> NO <sub>6</sub>
Ii-50	adenosine	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>
Ii-51	alizarin	C <sub>14</sub> H <sub>8</sub> O <sub>4</sub>
Ii-52	arctigentin	C <sub>21</sub> H <sub>24</sub> O <sub>6</sub>
Ii-53	arvelexin	C <sub>111</sub> H <sub>10</sub> N <sub>2</sub> O
Ii-54	bisdemethoxycurcumin	C <sub>19</sub> H <sub>16</sub> O <sub>4</sub>
Ii-55	bisindigotin	C <sub>32</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub>
Ii-56	calanthoside	C <sub>20</sub> H <sub>27</sub> NO <sub>11</sub> S
Ii-57	cappariloside A	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub>
Ii-58	cappariloside B	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>11</sub>
Ii-59	carminic acid	C <sub>22</sub> H <sub>20</sub> O <sub>13</sub>
Ii-60	carotene	C <sub>38</sub> H <sub>54</sub>
Ii-61	clemastain B	C <sub>32</sub> H <sub>44</sub> O <sub>16</sub>
Ii-62	conicaoside	C <sub>27</sub> H <sub>36</sub> O <sub>12</sub>
Ii-63	corchorifatty acid B	C <sub>18</sub> H <sub>28</sub> O <sub>4</sub>
Ii-64	curcumin	C <sub>21</sub> H <sub>20</sub> O <sub>6</sub>
Ii-65	demethoxycurcumin	C <sub>20</sub> H <sub>18</sub> O <sub>5</sub>
Ii-66	deoxyvasicinone	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O
Ii-67	diferuloylglucaric acid	C <sub>26</sub> H <sub>26</sub> O <sub>16</sub>
Ii-68	dihydroascorbigen	C <sub>14</sub> H <sub>15</sub> NO <sub>6</sub>
Ii-69	dinsinapoylmethoxyglucaric acid	C <sub>29</sub> H <sub>32</sub> O <sub>16</sub>
Ii-70	dioxindoleglucoside	C <sub>14</sub> H <sub>17</sub> NO <sub>7</sub>
Ii-71	di-p-coumaroylglucaric acid	C <sub>24</sub> H <sub>22</sub> O <sub>16</sub>
Ii-72	disinapoylglucaric acid	C <sub>28</sub> H <sub>30</sub> O <sub>16</sub>
Ii-73	epigoitrin	C <sub>5</sub> H <sub>7</sub> NOS
Ii-74	epipinoresinol	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>
Ii-75	epipinoresinol-4-O-D-glucoside	C <sub>26</sub> H <sub>32</sub> O <sub>11</sub>
Ii-76	feruloylglucaric acid	C <sub>16</sub> H <sub>18</sub> O <sub>12</sub>
Ii-77	feruloyl p-coumaroylglucaric acid	C <sub>25</sub> H <sub>24</sub> O <sub>16</sub>
Ii-78	feruloylsinapoylglucaric acid	C <sub>27</sub> H <sub>28</sub> O <sub>16</sub>

Ii-79	fisetin	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>
Ii-80	G(8-O-4)feruloylsinapolylgulcaric acid	C <sub>38</sub> H <sub>42</sub> O <sub>19</sub>
Ii-81	glucobrassicin	C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>9</sub> S <sub>2</sub>
Ii-82	glucotropaeolin	C <sub>15</sub> H <sub>21</sub> NO <sub>8</sub> S <sub>2</sub>
Ii-83	indican	C <sub>14</sub> H <sub>17</sub> NO <sub>6</sub>
Ii-84	indiforine A	C <sub>15</sub> H <sub>15</sub> NO <sub>7</sub>
Ii-85	indiforine B	C <sub>16</sub> H <sub>15</sub> NO <sub>6</sub>
Ii-86	indiforine C	C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Ii-87	indiforine D	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>4</sub>
Ii-88	indiforine F	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>
Ii-89	indigo	C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Ii-90	indigodole A	C <sub>28</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub>
Ii-91	indigodole B	C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Ii-92	indigodole C	C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O
Ii-93	indigotiisocoumarinA	C <sub>14</sub> H <sub>11</sub> NO <sub>4</sub>
Ii-94	indirubin	C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Ii-95	indole-3-acetonitrile-2-S-β-d-glucopyranoside	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> S
Ii-96	indole-3-acetonitrile-4-methoxy-2-C-β-D-glucopyranoside	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub>
Ii-97	indole-3-acetonitrile-4-methoxy-2-S-β-d-glucopyranoside	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub> S
Ii-98	indole-3-acetonitrile-6-O-β-D-glucopyranoside	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub>
Ii-99	isatan A	C <sub>17</sub> H <sub>17</sub> NO <sub>8</sub>
Ii-100	isatan B	C <sub>14</sub> N <sub>15</sub> NO <sub>5</sub>
Ii-101	isatan C	C <sub>17</sub> H <sub>17</sub> NO <sub>9</sub>
Ii-102	isatibisindosulfonic acid A 3-O-β-D-glucopyranoside	C <sub>23</sub> H <sub>24</sub> N <sub>3</sub> O <sub>9</sub> S
Ii-103	isatibisindosulfonic acid B	C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> S
Ii-104	isatigotindoledioside A	C <sub>20</sub> H <sub>25</sub> NO <sub>11</sub>
Ii-105	isatigotindoledioside B	C <sub>21</sub> H <sub>27</sub> NO <sub>12</sub>
Ii-106	isatigotindoledioside C	C <sub>21</sub> H <sub>26</sub> N <sub>2</sub> O <sub>10</sub>
Ii-107	isatigotindoledioside D	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>13</sub>
Ii-108	isatigotindoledioside E	C <sub>22</sub> H <sub>28</sub> N <sub>2</sub> O <sub>11</sub> S
Ii-109	isatigotindoledioside F	C <sub>21</sub> H <sub>27</sub> NO <sub>12</sub> S
Ii-110	isatin	C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub>
Ii-111	isatindigobisindoloside A	C <sub>24</sub> H <sub>23</sub> N <sub>3</sub> O <sub>6</sub>
Ii-112	isatindigobisindoloside C	C <sub>24</sub> H <sub>25</sub> N <sub>3</sub> O <sub>7</sub>
Ii-113	isatindigobisindoloside D	C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>7</sub>
Ii-114	isatindigobisindoloside E	C <sub>23</sub> H <sub>24</sub> N <sub>2</sub> O <sub>7</sub>
Ii-115	isatindigobisindoloside F	C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> O <sub>7</sub>
Ii-116	isatindigobisindoloside G	C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> O <sub>6</sub> S
Ii-117	isatindigodiphindoside	C <sub>31</sub> H <sub>35</sub> NO <sub>11</sub>
Ii-118	isatindigosquilignan A	C <sub>30</sub> H <sub>34</sub> O <sub>9</sub>

Ii-119	isatindigosquillignan B	C <sub>36</sub> H <sub>44</sub> O <sub>14</sub>
Ii-120	isatindigoside A	C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>9</sub>
Ii-121	isatindigoside B	C <sub>23</sub> H <sub>22</sub> N <sub>2</sub> O <sub>7</sub>
Ii-122	isatindigoticamide A	C <sub>15</sub> H <sub>13</sub> NO <sub>5</sub>
Ii-123	isatindigoticamide B	C <sub>15</sub> H <sub>13</sub> NO <sub>4</sub>
Ii-124	isatindigoticoic acid A and epiisatindigoticoic acid A	C <sub>17</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub>
Ii-125	isatindigotindoloside A	C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> O <sub>9</sub>
Ii-126	isatindigotindoloside B	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>7</sub>
Ii-127	isatindigotindoloside C&D	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub> S
Ii-128	isatindigotindoloside E	C <sub>16</sub> H <sub>21</sub> NO <sub>6</sub> S
Ii-129	isatindolignanoside A	C <sub>40</sub> H <sub>49</sub> NO <sub>17</sub>
Ii-130	isatindopyrromizol A and epiisatindopyrromizol A	C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S
Ii-131	isatindosulfonic acid A 3-O-β-D-glucopyranoside	C <sub>14</sub> H <sub>17</sub> NO <sub>9</sub> S
Ii-132	isatindosulfonic acid B	C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> S
Ii-133	isatindosulfonic acid C	C <sub>10</sub> H <sub>11</sub> NO <sub>4</sub> S
Ii-134	isatindosulfonic acid D	C <sub>11</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> S
Ii-135	isatindosulfonic acid E	C <sub>9</sub> H <sub>9</sub> NO <sub>3</sub> S
Ii-136	isatindosulfonic acid F	C <sub>19</sub> H <sub>9</sub> NO <sub>5</sub> S
Ii-137	isatioxyneolignoside A	C <sub>24</sub> H <sub>30</sub> O <sub>12</sub>
Ii-138	isatioxyneolignosideE	C <sub>26</sub> H <sub>34</sub> O <sub>11</sub>
Ii-139	isatioxyneolignosideB	C <sub>24</sub> H <sub>30</sub> O <sub>13</sub>
Ii-140	isatioxyneolignoside X	C <sub>28</sub> H <sub>34</sub> O <sub>14</sub>
Ii-141	isatisaloids A	C <sub>14</sub> H <sub>19</sub> NO <sub>5</sub>
Ii-142	isatisaloids B	C <sub>16</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>
Ii-143	isatisaloids C	C <sub>13</sub> H <sub>17</sub> NO <sub>3</sub>
Ii-144	isatisaloids D	C <sub>15</sub> H <sub>21</sub> NO <sub>4</sub>
Ii-145	isatisaloids E	C <sub>15</sub> H <sub>20</sub> N <sub>2</sub> O <sub>5</sub>
Ii-146	isatisycloneolignan A	C <sub>24</sub> H <sub>28</sub> O <sub>10</sub>
Ii-147	isatisindigoticanine A	C <sub>22</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub>
Ii-148	isatisindigoticanine B	C <sub>22</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub>
Ii-149	isatisindigoticanine C	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Ii-150	isatisindigoticanine D	C <sub>15</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Ii-151	isatisine A	C <sub>22</sub> H <sub>18</sub> N <sub>2</sub> O <sub>6</sub>
Ii-152	isatithioetherin A	C <sub>20</sub> H <sub>26</sub> N <sub>4</sub> O <sub>4</sub> S <sub>3</sub>
Ii-153	isatithiopyrin B	C <sub>18</sub> H <sub>17</sub> N <sub>3</sub> O <sub>2</sub> S <sub>2</sub>
Ii-154	isoindigo	C <sub>16</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Ii-155	Isolariciresinol	C <sub>20</sub> H <sub>24</sub> O <sub>6</sub>
Ii-156	isoorientin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>
Ii-157	isoorientin-3"-O-glucoside	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>
Ii-158	isoscoparin	C <sub>22</sub> H <sub>22</sub> O <sub>11</sub>

Ii-159	isoscoparin-3"-O-feruloylglucoside	C <sub>38</sub> H <sub>40</sub> O <sub>19</sub>
Ii-160	isoscoparin-3"-O-glucoside	C <sub>28</sub> H <sub>32</sub> O <sub>16</sub>
Ii-161	isoscoparin-3"-O-glucoside-7-O-glucoside	C <sub>44</sub> H <sub>50</sub> O <sub>21</sub>
Ii-162	isoscoparin-3"-O-p-coumaroylglucoside	C <sub>37</sub> H <sub>38</sub> O <sub>18</sub>
Ii-163	isoscoparin-3"-O-sinapoylglucoside	C <sub>39</sub> H <sub>42</sub> O <sub>20</sub>
Ii-164	isovitexin-3"-O-glucoside-7-O-glucoside	C <sub>33</sub> H <sub>40</sub> O <sub>20</sub>
Ii-165	isovitexin-3"-O-glucoside	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>
Ii-166	isovitexin	C <sub>21</sub> H <sub>20</sub> O <sub>10</sub>
Ii-167	justiciresinol	C <sub>21</sub> H <sub>26</sub> O <sub>7</sub>
Ii-168	lariciresinol	C <sub>20</sub> H <sub>24</sub> O <sub>6</sub>
Ii-169	lariciresinol-4'-O-D-glucopyranoside	C <sub>26</sub> H <sub>34</sub> O <sub>11</sub>
Ii-170	lariciresinol-4-O-D-glucopyranoside	C <sub>26</sub> H <sub>34</sub> O <sub>11</sub>
Ii-171	lariciresinol-diglucoside	C <sub>32</sub> H <sub>44</sub> O <sub>16</sub>
Ii-172	lutein	C <sub>38</sub> H <sub>54</sub> O <sub>2</sub>
Ii-173	luteolin	C <sub>15</sub> H <sub>10</sub> O <sub>6</sub>
Ii-174	luteolin-6-C-glicoside-7-O-giucoside	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>
Ii-175	luteolin-7-O-glucoside	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>
Ii-176	malonylindican	C <sub>17</sub> H <sub>19</sub> NO <sub>8</sub>
Ii-177	matairesinol	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>
Ii-178	matairesinol-4'-O-D-glucopyranoside	C <sub>26</sub> H <sub>32</sub> O <sub>11</sub>
Ii-179	matairesinol-4-O-D-glucopyranoside	C <sub>26</sub> H <sub>32</sub> O <sub>11</sub>
Ii-180	methyl 2-(4-oxo-1,4-dihydroquinoline-3-carboxamido)-benzoate	C <sub>18</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub>
Ii-181	methyl 2-(4-oxoquinazolin-3(4H)-yl)benzoate	C <sub>16</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Ii-182	neochrome	C <sub>38</sub> H <sub>54</sub> O <sub>4</sub>
Ii-183	neoglucobrassicin	C <sub>17</sub> H <sub>22</sub> N <sub>2</sub> O <sub>10</sub> S <sub>2</sub>
Ii-184	N-formylanthranilic acid	C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub>
Ii-185	N-methoxy-indole-3-acetonitrile-2-C-β-D-glucopyranoside	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub>
Ii-186	N-methoxy-indole-3-acetonitrile-2-S-β-D-glucopyranoside	C <sub>17</sub> H <sub>20</sub> N <sub>2</sub> O <sub>6</sub> S
Ii-187	indoxyl	C <sub>8</sub> H <sub>7</sub> NO
Ii-188	palmitic acid	C <sub>16</sub> H <sub>32</sub> O <sub>2</sub>
Ii-189	p-coumaroylglucaric acid	C <sub>15</sub> H <sub>16</sub> O <sub>11</sub>
Ii-190	p-coumaroylsinapoylglucaric acid	C <sub>26</sub> H <sub>26</sub> O <sub>16</sub>
Ii-191	phaeophytin a	C <sub>55</sub> H <sub>74</sub> N <sub>4</sub> O <sub>5</sub>
Ii-192	phaeophytin b	C <sub>55</sub> H <sub>72</sub> N <sub>4</sub> O <sub>6</sub>
Ii-193	phaitanthrin A and epiphaitanthrin A	C <sub>18</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>
Ii-194	phillygenin	C <sub>21</sub> H <sub>24</sub> O <sub>6</sub>
Ii-195	pinoresinol	C <sub>20</sub> H <sub>22</sub> O <sub>6</sub>
Ii-196	pinoresinol 4-O-D-glucopyranoside	C <sub>26</sub> H <sub>32</sub> O <sub>11</sub>
Ii-197	piperitol	C <sub>20</sub> H <sub>20</sub> O <sub>6</sub>
Ii-198	purpurin	C <sub>14</sub> H <sub>8</sub> O <sub>5</sub>



Ii-199	pyrophaeophorbide a	C <sub>33</sub> H <sub>34</sub> N <sub>4</sub> O <sub>3</sub>
Ii-200	pyrophaeophytin a	C <sub>53</sub> H <sub>72</sub> N <sub>4</sub> O <sub>3</sub>
Ii-201	pyrophaeophytin b	C <sub>53</sub> H <sub>70</sub> N <sub>4</sub> O <sub>4</sub>
Ii-202	rubiadin	C <sub>15</sub> H <sub>10</sub> O <sub>4</sub>
Ii-203	secoisolariciresinol	C <sub>20</sub> H <sub>26</sub> O <sub>6</sub>
Ii-204	secoisolariciresinoldiglucoside	C <sub>32</sub> H <sub>46</sub> O <sub>16</sub>
Ii-205	sesamin	C <sub>20</sub> H <sub>18</sub> O <sub>6</sub>
Ii-206	sesaminol	C <sub>20</sub> H <sub>18</sub> O <sub>7</sub>
Ii-207	sesaminol-2'-O-D-glucose	C <sub>26</sub> H <sub>28</sub> O <sub>12</sub>
Ii-208	sinapoylglucaric acid	C <sub>17</sub> H <sub>20</sub> O <sub>12</sub>
Ii-209	spicatlignan B	C <sub>20</sub> H <sub>20</sub> O <sub>7</sub>
Ii-210	stellarin-2	C <sub>28</sub> H <sub>32</sub> O <sub>16</sub>
Ii-211	sulfuretin	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>
Ii-212	syringaresinol	C <sub>22</sub> H <sub>26</sub> O <sub>8</sub>
Ii-213	syringaresinol-4-O-D-glucoside	C <sub>28</sub> H <sub>36</sub> O <sub>13</sub>
Ii-214	tryptanthrin	C <sub>15</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
Ii-215	ursolic acid	C <sub>30</sub> H <sub>48</sub> O <sub>3</sub>
Ii-216	vicenin-2	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>
Ii-217	violaxanthin	C <sub>38</sub> H <sub>54</sub> O <sub>4</sub>
Ii-218	$\alpha$ -L-rhamnopyranosyl-(1 $\rightarrow$ 6)- $\beta$ -D-glucopyranosyl 3-indolecarbonate	C <sub>21</sub> H <sub>27</sub> NO <sub>11</sub>
Ii-219	isatisindigoticanine H	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> S
Ii-220	isatisindigoticanine I	C <sub>24</sub> H <sub>21</sub> N <sub>3</sub> O <sub>5</sub> S
Ii-221	isatindigoside F	C <sub>25</sub> H <sub>23</sub> N <sub>3</sub> O <sub>5</sub> S
Ii-222	isatindigoside G	C <sub>26</sub> H <sub>25</sub> N <sub>3</sub> O <sub>6</sub> S
Ii-223	isatindigoside H	C <sub>23</sub> H <sub>24</sub> N <sub>2</sub> O <sub>6</sub>
Ii-224	isatindigoside I	C <sub>24</sub> H <sub>26</sub> N <sub>2</sub> O <sub>7</sub>
Ii-225	isatindigoside D	C <sub>24</sub> H <sub>25</sub> N <sub>3</sub> O <sub>7</sub>
Ii-226	isatindigoside J	C <sub>25</sub> H <sub>27</sub> N <sub>3</sub> O <sub>8</sub>
Ii-227	isatindigoside E	C <sub>30</sub> H <sub>25</sub> N <sub>3</sub> O <sub>7</sub>
Ii-228	isatisindigoticanine J	C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>
Ii-229	isatisindigoticanine K	C <sub>19</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>
Ii-230	isatindigoside K	C <sub>18</sub> H <sub>22</sub> N <sub>2</sub> O <sub>7</sub>
Ii-231	isatindigoside L	C <sub>21</sub> H <sub>25</sub> N <sub>3</sub> O <sub>6</sub> S <sub>2</sub>
Ii-232	isatindigoside M	C <sub>16</sub> H <sub>19</sub> NO <sub>8</sub>
Ii-233	isatisindigoticanine L	C <sub>11</sub> H <sub>12</sub> N <sub>4</sub> O <sub>4</sub>
Ii-234	isatisindigoticanine M	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>
Ii-235	isatisindigoticanine N	C <sub>12</sub> H <sub>13</sub> NO <sub>4</sub>
Ii-236	isatisindigoticanine E	C <sub>15</sub> H <sub>11</sub> NO <sub>3</sub>
Ii-237	isatisindigoticanine F	C <sub>18</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>
Ii-238	isatisindigoticanine G	C <sub>20</sub> H <sub>15</sub> N <sub>3</sub> O

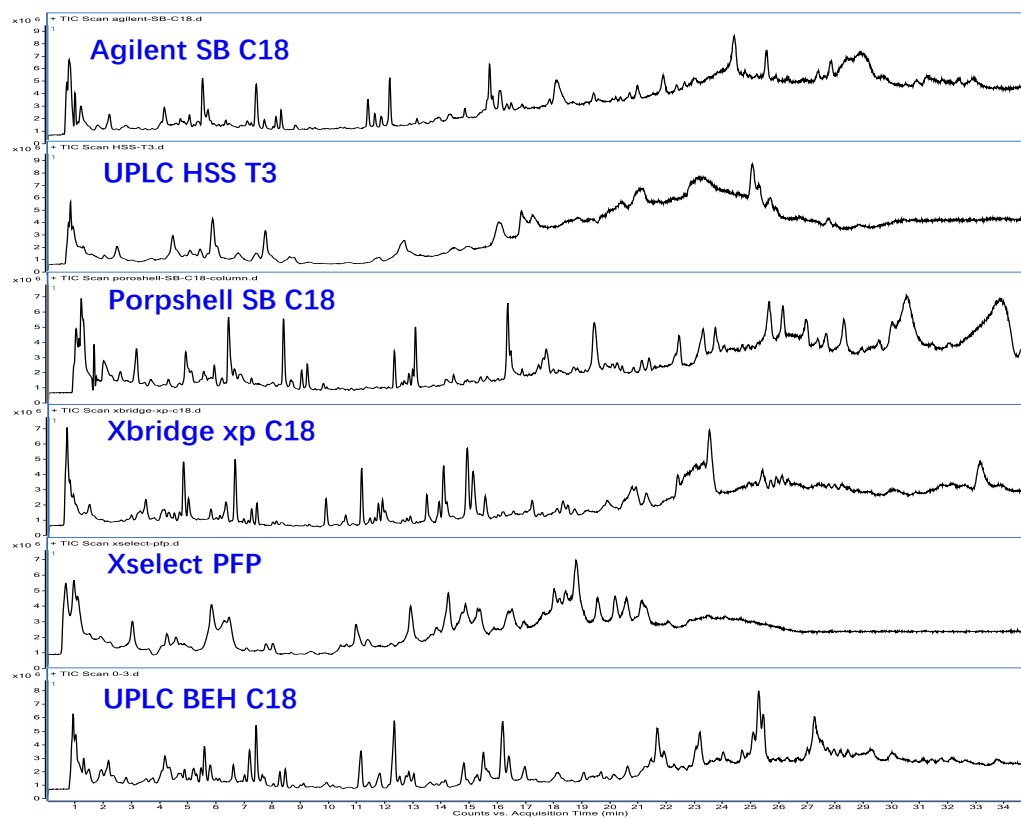
Ii-239	methyl 3-(2,4-dioxo-1,2-dihydroquinazolin-3(4H)-yl)propanoate	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>
Ii-240	4-(2,4-dioxo-1,2-dihydroquinazolin-3(4H)-yl)butanoic acid	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>
Ii-241	3H-indol-3-one	C <sub>8</sub> H <sub>5</sub> NO
Ii-242	(1H-Indol-3-yl)oxoacetamide	C <sub>10</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>
Ii-243	1H-indole-3-carboxamide	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O
Ii-244	4-(4-oxo-3,4-dihydroquinazolin-2-yl)butanoic acid	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub>
Ii-245	2-(2-hydroxyphenyl)-4(3H)-quinazolinone	C <sub>14</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub>
Ii-246	2-(but-3-en-1-yl)-4(3H)-quinazolinone	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O
Ii-247	2-(1H-indol-2-yl)-4(3H)-quinolinone	C <sub>16</sub> H <sub>11</sub> N <sub>3</sub> O
Ii-248	cephalanthrin A	C <sub>17</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub>
Ii-249	2-methyl-4(3H)-quinazolinone	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O
Ii-250	4-methyl-1,2-dihydro-2-oxoquinazoline	C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O
Ii-251	4-hydroxy-3-methyl-2(1H)-quinolone	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>
Ii-252	1,2,3,4-tetrahydro-4-hydroxy-quinolinecarboxylic acid	C <sub>10</sub> H <sub>9</sub> NO <sub>4</sub>
Ii-253	4(1H)-quinolone-3-carboxylic acid	C <sub>10</sub> H <sub>7</sub> NO <sub>3</sub>
Ii-254	2-(Hydroxymethyl)-4(1H)-quinolinone	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>
Ii-255	1-methoxy-2(1H)-quinolinone	C <sub>10</sub> H <sub>9</sub> NO <sub>2</sub>
Ii-256	4-p-hydroxyphenyl-2(1H)-quinolinone	C <sub>15</sub> H <sub>11</sub> NO <sub>2</sub>
Ii-257	(E)-5-(4-hydroxy-3,5-dimethoxyphenyl)-3-[(4-hydroxy-3,5-dimethoxyphenyl)-methylene]-2(3H)-furan one	C <sub>21</sub> H <sub>20</sub> O <sub>8</sub>
Ii-258	spicatolignan B	C <sub>20</sub> H <sub>20</sub> O <sub>7</sub>
Ii-259	2-(3'-hydroxy-5'-methoxyphenyl)-3-hydroxymethyl-7-methoxy-2,3-dihydrobenzofuran-5-carboxylic acid	C <sub>18</sub> H <sub>18</sub> O <sub>7</sub>
Ii-260	(7S,8R,7'S,8'R)-3,4,3',4'-tetramethoxy-9,7-dihydroxy-8.8',7.O.9'-lignan	C <sub>22</sub> H <sub>28</sub> O <sub>7</sub>
Ii-261	2-amino-1-(4-hydroxy-3-methoxyphenyl)propane-1,3-diol	C <sub>10</sub> H <sub>15</sub> NO <sub>4</sub>
Ii-262	cis-coniferin	C <sub>16</sub> H <sub>22</sub> O <sub>8</sub>
Ii-263	cis-syringin	C <sub>17</sub> H <sub>22</sub> O <sub>10</sub>
Ii-264	(E)-4-((3R,4S)-3,4-dihydroxy-2,6,6-trimethylcyclohex-1-en-1-yl)but-3-en-2-one	C <sub>13</sub> H <sub>20</sub> O <sub>3</sub>
Ii-265	L-pyroglutamate	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>
Ii-266	(4R,5S)-5-hydroxyhexan-4-olide	C <sub>6</sub> H <sub>10</sub> O <sub>3</sub>
Ii-267	2'-O-methyladenosine	C <sub>11</sub> H <sub>15</sub> N <sub>5</sub> O <sub>4</sub>
Ii-268	adenosine monophosphatederivatives	C <sub>17</sub> H <sub>20</sub> N <sub>5</sub> O <sub>9</sub> P
Ii-269	adenosine monophosphate	C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>7</sub> P

**Table S7.** Validation results of detection of 73 reference standards by application of feature-rating rule.

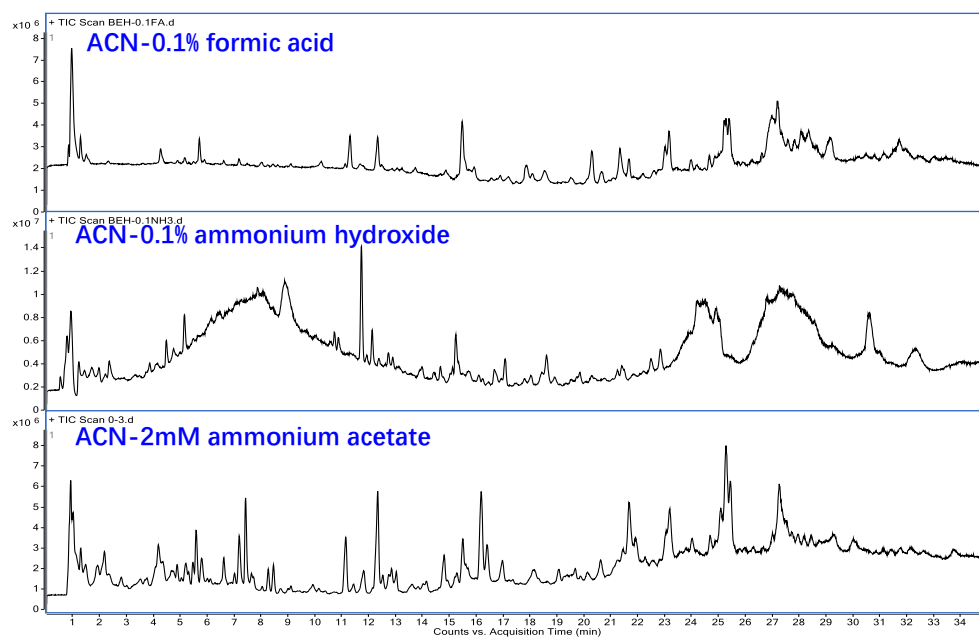
No.	RT (min)	m/z	Identification	Adduct types	Most intense
1	0.869	173.1046	L(+)-Arginine	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
2	0.921	215.0337	D-Mannose	[M+Cl] <sup>-</sup>	[M+Cl] <sup>-</sup>
3	0.95	298.0422	Gemcitabine	[M+Cl] <sup>-</sup> , [M+NO <sub>3</sub> -H] <sup>-</sup> , [M+COOH] <sup>-</sup>	[M+Cl] <sup>-</sup>
4	1.55	169.0149	Gallic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
5	2.104	164.0721	L-Phenylalanine	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
6	2.2	320.0567	Fludarabine	[M+Cl] <sup>-</sup>	[M+Cl] <sup>-</sup>
7	2.469	153.0202	3,4-Dihydroxybenzoic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
8	2.59	353.0879	Neochlorogenic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
9	2.838	345.1194	Salidroside	[M+COOH] <sup>-</sup>	[M+COOH] <sup>-</sup>
10	2.934	203.083	L-Tryptophan	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
11	3.031	577.135	Procyanidin B3	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
12	3.255	353.0883	Cryptochlorogenic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
13	3.261	407.1123	Eleutheroside B	[M+Cl] <sup>-</sup> , [M+K-2H] <sup>-</sup> , [M+COOH] <sup>-</sup>	[M+Cl] <sup>-</sup>
14	3.408	353.0884	Chlorogenic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
15	3.512	161.0371	Benzoyleneurea	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
16	3.555	330.0754	3-Indoxyl-beta-D-glucopyranoside	[M+Cl] <sup>-</sup> , [M+COOH] <sup>-</sup>	[M+Cl] <sup>-</sup>
17	3.715	179.0352	Caffeic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
18	3.825	593.1509	Vicenin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
19	3.922	435.1514	Loganin	[M+COOH] <sup>-</sup>	[M+COOH] <sup>-</sup>
20	4.188	593.1506	Saponarin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
21	4.255	459.1401	Oxytetracycline	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
22	4.409	441.0944	2,3,5,4'-Tetrahydroxy stilbene-2-O-β-D-glucoside	[M+Cl] <sup>-</sup> , [M-H] <sup>-</sup>	[M+Cl] <sup>-</sup>
23	4.525	525.1608	Paeoniflorin	[M+COOH] <sup>-</sup>	[M+COOH] <sup>-</sup>
24	4.593	567.1343	Polygalaxanthone III	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
25	4.672	151.0403	Vanillin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
26	4.798	609.1458	Rutin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
27	4.942	463.0889	Hyperoside	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
28	5.021	191.0355	Scopoletin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
29	5.045	441.0954	2,3,5,4'-Tetrahydroxy stilbene-2-O-β-D-glucoside	[M+Cl] <sup>-</sup>	[M+Cl] <sup>-</sup>
30	5.045	453.0964	Liquiritin	[M+Cl] <sup>-</sup> , [M+NO <sub>3</sub> -H] <sup>-</sup>	[M+Cl] <sup>-</sup>
31	5.088	193.051	Ferulic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
32	5.106	483.0685	Cynaroside	[M+Cl] <sup>-</sup>	[M+Cl] <sup>-</sup>
33	5.231	221.046	Isofraxidin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
34	5.335	193.051	3-Hydroxy-4-methoxycinnamic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
35	5.536	447.0931	Astragalin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
36	5.857	515.1192	Isochlorogenic acid C	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
37	5.891	645.158	Hesperidin	[M+Cl] <sup>-</sup>	[M+Cl] <sup>-</sup>

38	6.032	121.0296	Benzoic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
39	6.644	919.4899	Timosaponin BII	[M+Cl] <sup>-</sup> , [M-H] <sup>-</sup>	[M-H] <sup>-</sup>
40	6.644	426.1231	Icotinib	[M+Cl] <sup>-</sup> , [M+K-2H] <sup>-</sup>	[M+Cl] <sup>-</sup>
41	6.884	329.0663	Tricin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
42	6.982	579.2072	Forsythin	[M+COOH] <sup>-</sup>	[M+COOH] <sup>-</sup>
43	7.01	391.1303	4,11-Diethyl-4,9-dihydroxy-1H-pyrano[3',4':6,7]indol izino[1,2-b]quinoline-3,14(4H,12H)-dione	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
44	7.03	873.2579	3-[(6-Deoxy-3-O-beta-D-glucopyranosyl-alpha-L-ma nnopyranosyl)oxy]-7-(beta-D-glucopyranosyloxy)-5- hydroxy-2-(4-methoxyphenyl)-8-(3-methyl-2-buten-1 -yl)-4H-1-benzopyran-4-one	[M+Cl] <sup>-</sup> , [M+NO <sub>3</sub> -H] <sup>-</sup>	[M+Cl] <sup>-</sup>
45	7.082	578.1428	Epirubicin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
46	7.093	579.2067	Arctiin	[M+COOH] <sup>-</sup>	[M+COOH] <sup>-</sup>
47	7.272	993.4821	Asiaticoside	[M+Cl] <sup>-</sup>	[M+Cl] <sup>-</sup>
48	7.351	473.1222	Sec-O-glucosylhamaudol	[M+Cl] <sup>-</sup> , [M+COOH] <sup>-</sup>	[M+Cl] <sup>-</sup>
49	7.408	395.1638	Prednisolone	[M+Cl] <sup>-</sup> , [M+K-2H] <sup>-</sup>	[M+Cl] <sup>-</sup>
50	7.426	884.2804	Epmedin C	[M+NO <sub>3</sub> -H] <sup>-</sup>	[M+NO <sub>3</sub> -H] <sup>-</sup>
51	7.432	623.1536	Etoposide	[M+Cl] <sup>-</sup>	[M+Cl] <sup>-</sup>
52	7.66	428.1384	Erlotinib	[M+Cl] <sup>-</sup> , [M+K-2H] <sup>-</sup>	[M+Cl] <sup>-</sup>
53	8.118	271.0619	Naringenin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
54	8.241	553.2932	Ganoderic acid C2 (SH)	[M+Cl] <sup>-</sup> , [M+K-2H] <sup>-</sup> , [M+NO <sub>3</sub> -H] <sup>-</sup>	[M+Cl] <sup>-</sup>
55	8.245	299.0564	Hispidulin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
56	8.575	813.4068	Heterophyllin B	[M+Cl] <sup>-</sup> , [M+NO <sub>3</sub> -H] <sup>-</sup>	[M+Cl] <sup>-</sup>
57	8.652	447.2381	3β,5,14-Trihydroxy-5β-bufa-20,22-dienolide	[M+COOH] <sup>-</sup>	[M+COOH] <sup>-</sup>
58	9.828	341.1006	Mycophenolic acid	[M-Na-2H] <sup>-</sup>	[M-Na-2H] <sup>-</sup>
59	9.9	269.0483	Aloe emodin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
60	10.409	283.061	Acacetin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
61	10.529	815.4357	Saikosaponin A	[M+Cl] <sup>-</sup> , [M+COOH] <sup>-</sup> , [M+NO <sub>3</sub> -H] <sup>-</sup>	[M+Cl] <sup>-</sup>
62	10.581	283.0608	Wogonin	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
63	10.893	322.1231	Gliclazide	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
64	10.971	513.1757	Baohuoside I	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
65	11.243	556.2142	Ceritinib	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
66	11.527	523.3182	Asiatic acid	[M+Cl] <sup>-</sup> , [M+K-2H] <sup>-</sup>	[M+Cl] <sup>-</sup>
67	11.951	527.2603	Caudatin	[M-H] <sup>-</sup> , [M+Cl] <sup>-</sup> , [M+K-2H] <sup>-</sup>	[M+Cl] <sup>-</sup>
68	12.286	915.3181	Paclitaxel	[M+NO <sub>3</sub> -H] <sup>-</sup>	[M+NO <sub>3</sub> -H] <sup>-</sup>
69	12.796	765.3094	Ritonavir	[M+COOH] <sup>-</sup> , [M+NO <sub>3</sub> -H] <sup>-</sup>	[M+COOH] <sup>-</sup>
70	13.075	775.4041	Timosaponin A-III	[M+Cl] <sup>-</sup> , [M+NO <sub>3</sub> -H] <sup>-</sup>	[M+Cl] <sup>-</sup>
71	14.737	471.3481	Maslinic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
72	14.917	471.3475	Corosolic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>

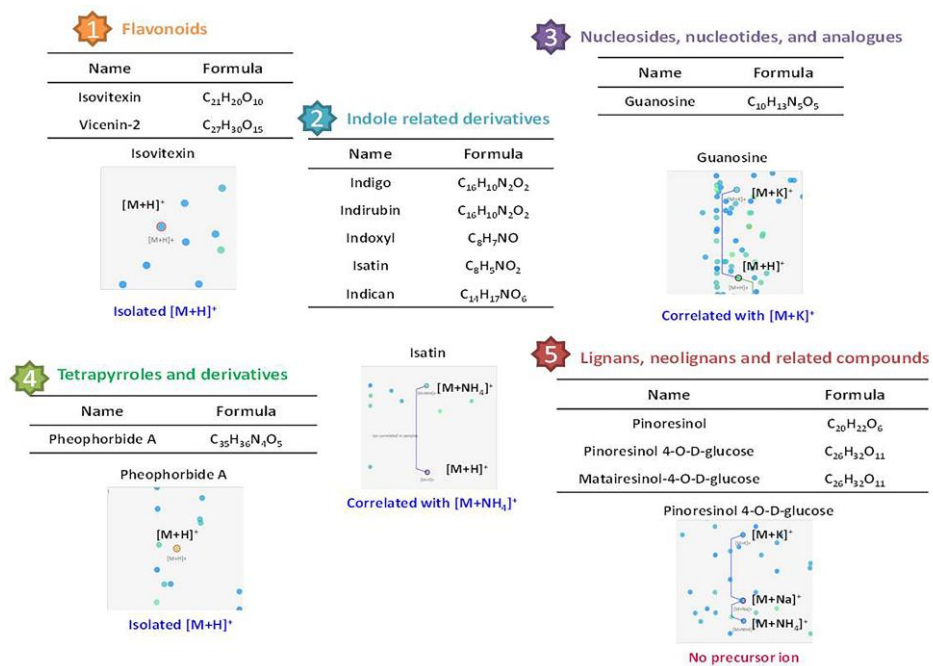
73	17.888	455.352	Oleanic acid	[M-H] <sup>-</sup>	[M-H] <sup>-</sup>
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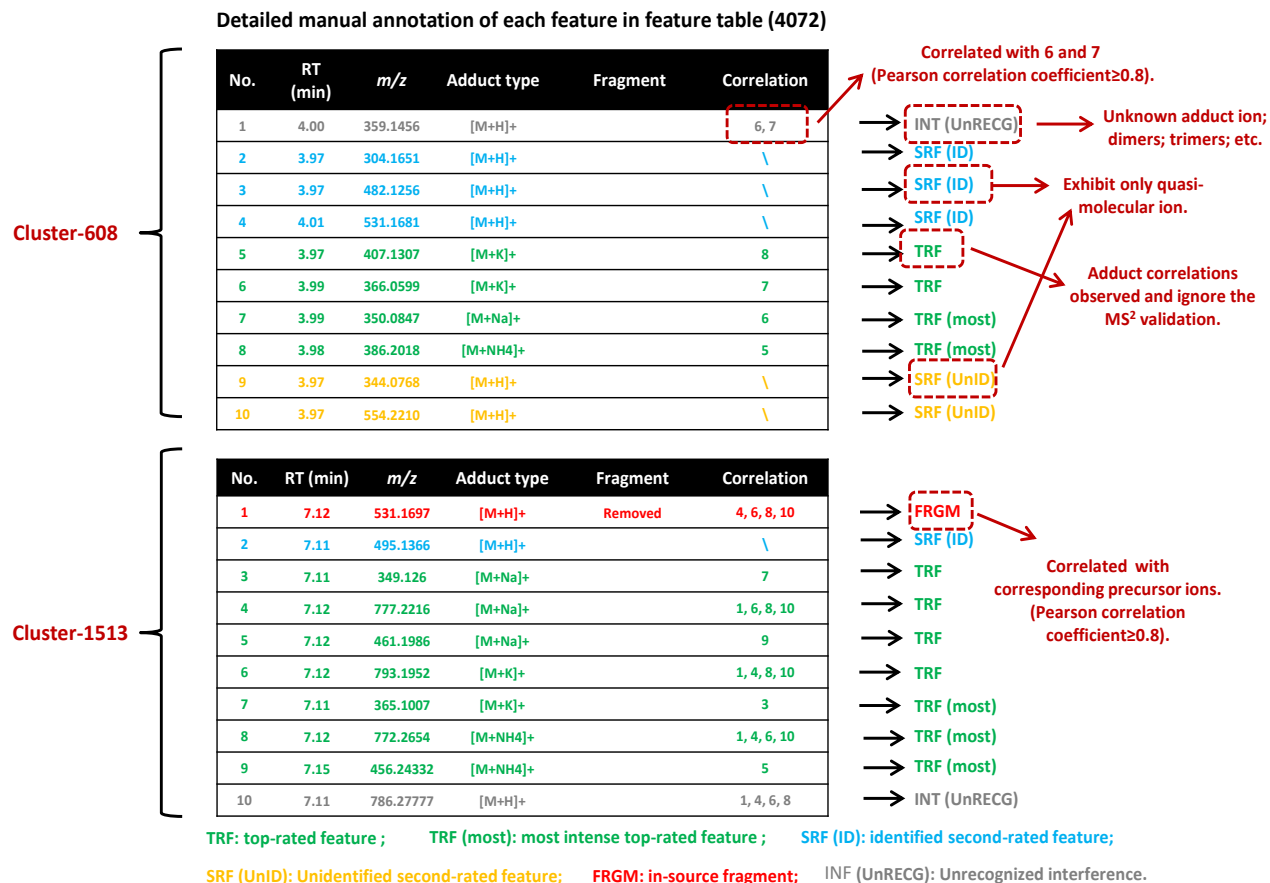
**Figure S7.** Investigation of different chromatographic columns for achieving better separation and peak capacity (*Ind* as an example).



**Figure S8.** Investigation of different mobile phase additives for achieving better ionization (*Ind* as an example).

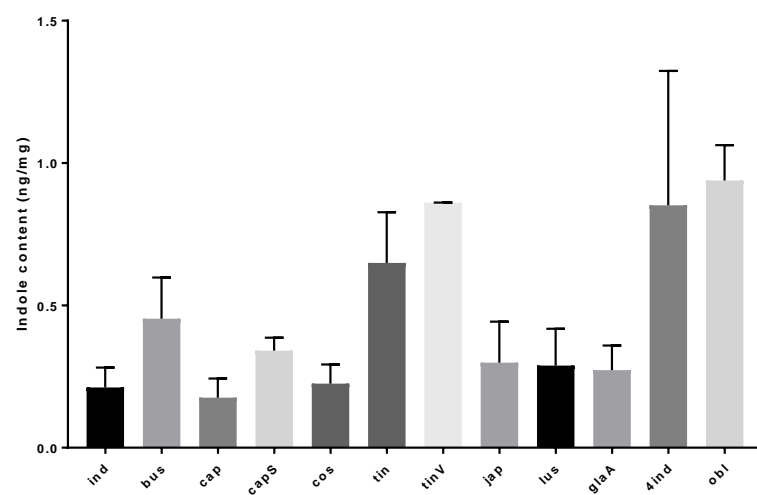


**Figure S9.** A standard mixture contains 12 purity compounds with different chemical classifications for the demonstration of  $m/z$  and adducts types before the large-scale acquisition.



**Figure S10.** The operation of detailed manual annotation of each feature in each cluster.





**Figure S11.** The relative content of indole compound by applying GC-MS among 12 species.