

### Research Article

## Uncovering the Anticancer Mechanism of Compound Sophorae Decoction against Ulcerative Colitis-Related Colorectal Cancer in Mice

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Received 30 May 2019; Accepted 4 August 2019; Published 20 October 2019

Academic Editor: Barbara Romano

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Compound sophorae decoction (CSD), a traditional Chinese medicine (TCM) formula, has been voluminously used in China to deal with ulcerative colitis and gained significant therapeutic effect. Tremendous explorations have unraveled a contributory role of inflammatory bowel disease (IBD) like ulcerative colitis (UC) and Crohn's disease (CD) at the onset of colorectal cancer, scilicet, and colitis-related cancer (CRC). In light of the anti-inflammatory properties of CSD in UC, we appraised its chemoprevention capacity and underlying mechanism in ulcerative colitis-related colorectal cancer (UCRCC), employing a model of azoxymethane (AOM) plus dextran sulfate sodium- (DSS-) induced colorectal cancer (CRC) in C57BL/6 mice. Rapturously, our results illuminated the ameliorative effect of CSD against UCRCC in mice portrayed by lesser polyps or adenomas, attenuated colonic xenograft tumor growth in company with the preferable well-being of mice in contrast to the Model Group. We examined significant downregulation of proinflammatory cytokines such as TNF-α, NF-κB, IL-6, STAT3, and IL-17 after exposure to CSD, with the concomitant repression of inflammation-associated proteins, including COX-2 and iNOS. Independent of this, treatment with CSD declined the proportion of T helper 17 cells (Th17) and protein level of matrix metallopeptidase 9 (MMP-9). Moreover, transmission electron microscopy (TEM) detected observably suppressed mitophagy in mice administered with CSD and that was paralleled by the pro-apoptotic effect as indicated by upregulating caspase-3 together with caspase-9 and deregulating B-cell lymphoma 2 (Bcl-2). In closing, these findings suggest CSD executes the UCRCC-inhibitory activity through counteracting inflammatory responses and rescuing detuning of apoptosis as well as neutralizing overactive mitophagy, concurring to build up an oncosuppressive microenvironment.

#### 1. Introduction

Ulcerative colitis (UC) is a long-lasting and relapsing inflammatory intestinal disturbance, whose etiology and pathogenesis is still elusive, with a growing body of compelling evidence defining its promoting role in the initiation of colorectal cancer [1–3]. It has been well-acknowledged that long-standing proinflammatory cytokines comprising tumor necrosis factor (TNF- $\alpha$ ), interleukin- (IL-) 17, and NF- $\kappa$ B/IL-6/STAT3 cascade in colon harbor a close relationship between UC and colon cancer and simultaneously behave as pivotal mediators in the onset and deterioration of UC and colorectal cancer [4–9]. Accordingly, these data underscore a crucial role of proinflammatory responses in the context of UCRCC and confer the urgency to address the related concrete mechanism.

Mitochondria are cardinal double membrane-bound organelles and cellular stress sensors involved in multifaceted cellular activities containing energy production, senescence, apoptosis, oxidative stress regulation, and metabolism in addition to signaling. Hence, these cellular properties of mitochondria denote a highly-associated link connecting cellular dysfunction in the context of cancer or noncancer and abnormalities in mitochondrial status along with activity and meanwhile, authenticate the magnitude of the timely elimination of damaged and aged mitochondria which is called mitophagy for maintaining the cellular integrity [10–17]. To our knowledge, cancer is a disturbance in the homeostatic balance between cell growth and cell death, which is featured by metabolic reprogramming, uncontrolled cellular proliferation, and enhanced resistance to apoptosis of tumor cell. Massive reports [10-12, 16, 17] have identified that mitophagy is activated under conditions of stimuli such as nutrient depletion, hypoxia, and activated oncogenes, imparting considerable flexibility for tumor cell growth and survival. In addition, mitochondria-targeted drugs and targeting apoptosis pathways open up the opportunity for the development of novel therapeutic strategies for cancer abrogation [10, 11]. Therefore, it is anticipated that a broad understanding of mitophagy and apoptosis in UCRCC may shed light on investigating the tumor-promoting mechanisms to the next level.

Compound sophorae decoction (CSD) is a classical traditional Chinese medicine (TCM) preparation developed from qingre zaoshi liangxue fang (QRZSLXF) [18] has been widely applied in China to medicate UC patients and is clinically efficient [19, 20]. Kushen, videlicet, *Sophora flavescens* Ait., is the sovereign drug of CSD and is used extensively to treat fibrosis, asthma, inflammatory disorders, ulcers, and solid tumor [19–26]. However, definitive mechanisms that demonstrate the role of CSD in UCRCC are still obscure. Thereby, further studies analyzing the contribution of CSD to the amelioration of UCRCC and identifying its active ingredients via mass spectrometry (MS) appear warranted.

Taken together, we hypothesize that inflammatory responses along with uncontrollable homeostasis between mitophagy and cellular apoptosis synergistically facilitate the formation of ambience in favor of UCRCC, and CSD overturns the tumourigenesis effect (Figure 1(a)). This study may provide novel insights into the carcinogenesis of UCRCC and open a promising therapeutic approach to UCRCC.

#### 2. Materials and Methods

2.1. Animals and Mouse Model of UCRCC. Male C57BL/6J mice (6–8 weeks old) were lodged under specific pathogenfree (SPF) conditions with free access to autoclaved food and water in the experimental animal center of Huazhong University of Science and Technology (HUST, Wuhan, China). They were stochastically grouped into Model Group (AOM/DSS), CSD Group (AOM/DSS + CSD), and Normal Group. UCRCC model was conducted based on a typical protocol [27, 28], that is, the administration of a single intraperitoneal injection of AOM (12 mg/kg, Sigma) in conjunction with three rounds of 2.5% DSS (36–50 kDa; MP Biochemicals) application (Figure 1(b)). All animal care and experimental processes were performed in accordance with guidelines of the Animal Research Institute Committee of HUST and National Institutes of Health guidelines and regulations.

2.2. Composition and Preparation of CSD. CSD is a Chinese herbal mixture composed of Sophora flavescens Ait. (15 gram), Radix Sanguisorbae (15 gram), Indigo Naturalis (3 gram), Bletilla striata (Thund.) Reichb. f. (10 gram), Panax notoginseng (Burk.) F. H. Chen (3 gram), and Glycyrrhiza uralensis Fisch. (10 gram). All the raw herbal medicines were purchased from Hubei Provincial Hospital of Traditional Chinese Medicine (Wuhan, China) and then mixed according to the weight ratio before soaking for 1 h. Eventually, the mixture was condensed into a concentration of 1.076 g/ml as CSD and stored at 4°C after undergoing initial hard boil and being simmered for 1 h and incurring succedent filter. 150  $\mu$ l CSD was administrated by gavage daily, synchronizing the procedure of DSS induction.

2.3. Behavioral and Physiological Assessment. Body weight, stool consistency, and hemafecia ratio in addition to intake of food and water were recorded daily throughout the whole span of the experiment. After figuring out weight and length of colons, the number and diameter of tumors were calculated.

2.4. Western Blot Analysis. Proteins of each colon were extracted in RIPA buffer supplemented with phosphatase and protease inhibitors. 40  $\mu$ g proteins were utilized for the investigation of inflammatory responses in the colon as described previously [29]. Antibodies recognizing the proteins were as follows: anti-IL-6 (1:500, Bioss, Beijing, China), anti- TNF- $\alpha$  (1:1000, Abcam, Cambridge, UK), anti-NF- $\kappa$ B (1:2000, Cell Signaling Technology, USA), and anti-IL-17 (1:1000, Abcam, Cambridge, UK).

2.5. Histological Evaluation and Immunohistochemistry. Fresh colon sections were embedded in paraffin after being fixed in 4% paraformaldehyde and then were cut into 4  $\mu$ m slides that would be stained with haematoxylin-eosin (H&E) hereafter. An expert pathologist carried out histopathological examinations blindly. For immunohistochemical assessment, the paraffin-embedded colonic slides were subjected to immunohistochemical staining and incubated with primary antibodies for cyclooxygenase-2 (COX-2; 1: 100, Cell Signaling Technology, USA), inducible nitric oxide synthase (iNOS; 1:100, Boster, Wuhan, China), matrix metallopeptidase 9 (MMP-9; 1:100, Ruiying Biological, Suzhou, China), TNF- $\alpha$  (1:50, Santa, Dallas, TX, USA), B-cell lymphoma 2 (Bcl-21:100, Boster, Wuhan, China), caspase-3 (1:100; PTG, Wuhan, China), and caspase-9

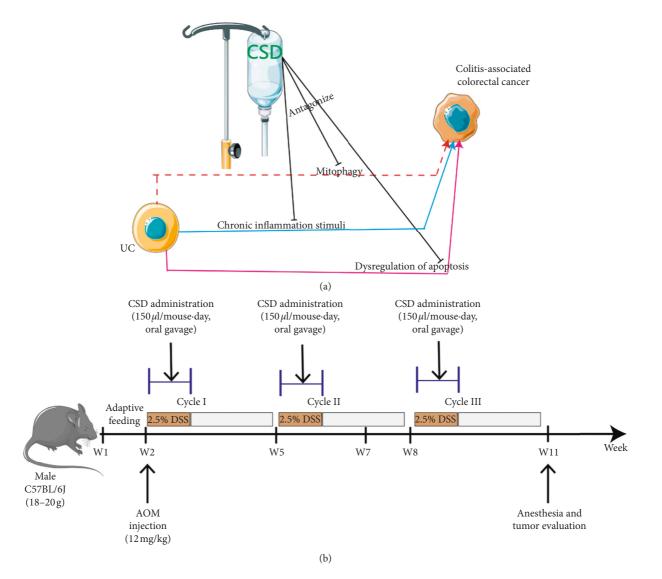


FIGURE 1: A schematic diagram of the workflow of CSD in UCRCC (a) and experimental protocol for UCRCC model and validation for investigation of the mechanisms of CSD (b).

(1:100; Boster, Wuhan, China) complying with the manufactures' protocols.

2.6. Transmission Electron Microscopy Observation. For the transmission electron microscopic (TEM) analysis of mitochondria, pretreated colon tissues underwent a series of procedures reported as previously [10] and the stained ultrathin colonic sections (60–80 nm) were detected using a Hitachi-HT7700 electron microscope (Tokyo, Japan).

2.7. Flow Cytometry. After being stimulated with phorbol myristate acetate (PMA; Abcam, Cambridge, UK), ionomycin, and GolgiPlug protein transport inhibition (BD Biosciences, San Diego, USA) in a humidified  $37^{\circ}$ C and 5% CO<sub>2</sub> incubator for 7 h, single-cell suspension of splenocytes and mesenteric lymph nodes (MLNs) were stained with FITC-labeled antimouse CD4 and PE-labeled antimouse IL-17A antibodies (BD Biosciences, MD, USA). Isotype antibody was adopted as the negative control. Thenceforward, the stained cells were washed and analyzed by using a FACSCalibur flow cytometer (BD Biosciences, San Diego, CA).

2.8. High-Resolution Metabolomics.  $100 \,\mu$ l CSD liquid samples underwent methanol extraction by adding  $900 \,\mu$ l methanol or pure water extraction by adding  $900 \,\mu$ l pure water, following the procedures listed as follows: vortexing for 1 min; centrifuging for 10 min, 12000 r/min, 4°C; filtering the supernatant through a  $2 \,\mu$ m filter; and analyzing the filtrate on the machine. Untargeted metabolic profiling of CSD was performed employing high-resolution mass spectrometry (HRMS; Q-Exactive High-Resolution Mass Spectrometer, Thermo Fisher Scientific). Analyte separation was accomplished with the aid of liquid chromatography (Ulti-Mate 3000 RS, Thermo Fisher Scientific) fitted with chromatographic column (Thermo Hypersil GOLD  $100 \times 2.1 \,\text{mm}$ , 1.9  $\mu$ m) manoeuvred at 0.3 mL/min with aqueous phase (0.1% aqueous formic acid) and organic phase (0.1% formic acid acetonitrile). The operating gradient came as follows: 0–2 min (aqueous phase: 95% —> 80%, organic phase: 5% —> 20%); 2–6 min (aqueous phase: 80% —> 25%, organic phase: 20% —> 75%); 6–8.5 min (aqueous phase: 25% —> 5%, organic phase: 75% —> 95%); 8.5–12.5 min (aqueous phase: 5% —> 95%, organic phase: 95% —> 5%); and 13–16 min (aqueous phase: 5%).

The electrospray ionization source was performed in positive ion mode with a spray voltage of 3.8 kV, capillary temperature of 300°C, sheath gas (nitrogen, purity  $\geq$ 99.999%) flow of 40 arbitrary units (Arb), and auxiliary gas (nitrogen, purity  $\geq$ 99.999%) temperature of 350°C. The resolution was set to 70000 (full mass), 17500 (dd-MS2), and the scan range was 70–1000 *m/z*. Data acquisition time was 16 min.

Mass spectral features represented by accurate mass m/z, retention time, and intensity were detected by high-resolution FTMS and sorted using CD2.1 software (Thermo Fisher) and then identified, aligned, and quantified according to databases such as Mzcloud, MzVault, and ChemSpider with the value of mzCloud Best Match  $\geq$ 80%.

2.9. Statistical Analysis. All experimental data obtained from this study were presented as mean  $\pm$  standard deviation (SD). Statistical significance between the data from different groups was calculated by one-way analysis of variance (ANOVA) or Student's *t*-test using SPSS software (version 19.0). A *p* value <0.05 was deemed as statistically significant.

#### 3. Results

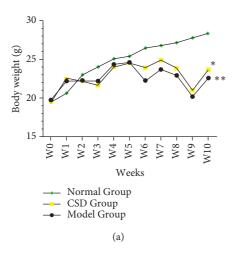
3.1. CSD Upgrades Clinical Symptoms in Mice Treated with AOM/DSS and Allays AOM/DSS-Induced Malignancy. As shown in Figure 2(a), significant body weight loss during the experimental period in mice from Model Group compared with Normal Group was alleviated by CSD administration, particularly after the third DSS cycle. In agreement with this, CSD treatment posed a decrement in the incidence ratio of hematochezia accompanied by postponed occurrence of diarrhea and blood in feces, as evaluated (Figure 2(b)). The shortening of colons, signifying the aggravation of colonic damage, was observed in mice exposed to AOM/DSS in comparison with mice in the CSD Group (p < 0.05) (Figures 2(c) and 2(d)). Furthermore, our data manifested higher polyp/adenoma multiplicity escorted by higher grade of epithelial dysplasia in the Model Group (Figures 2(e) and 2(f)).

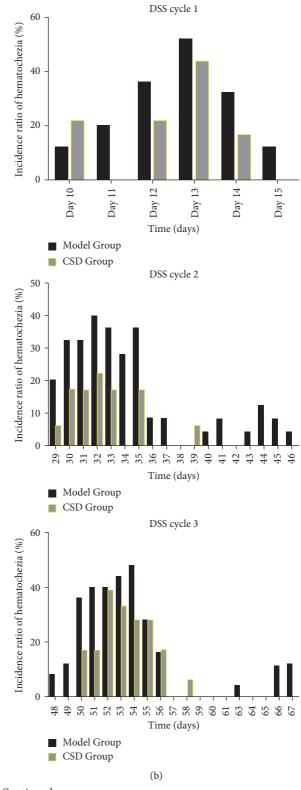
3.2. CSD Moderates the Malignant Inflammatory Features in AOM/DSS-Induced UCRCC. Incremental expression of proinflammatory cytokines such as NF- $\kappa$ B and TNF- $\alpha$  and overactivation of IL-6/STAT3 passage have been well determined to exercise definitive implication in the pathogenesis of UC and colon cancer. In line with this, mice received AOM/DSS exhibited a rise in intestinal production

of these parameters and IL-17 concentration in comparison with Normal Group, whereas intake of CSD significantly reversed the reaction expectably as illustrated by western blot and immunohistochemistry (Figures 3(a)–3(c)). Given the traditional role of Th17 cells in binding UC and UCRCC together, we explored the disparities in the proportion of Th17 cells isolated from spleens and MLNs of mice via flow cytometry (Figure 3(d)). Not surprisingly, the analysis revealed that Th17 cells may prompt the incipience of UCRCC and can be partially overthrown by CSD (Figure 3(e)). Regarding intestinal iNOS and COX-2 expression profiles, they were incremental in colon tissues from mice treated with AOM/DSS compared with the untreated mice, being diminished by treatment with CSD (Figure 3(f)).

3.3. CSD Modulates Ultrastructural Changes and Apoptosis in AOM/DSS-Induced Mice. Apoptosis and mitophagy are two representative procedures that act in synergy to regulate cell survival and death in numerous types of cancer. To gain further insight into the pattern of CSD on apoptosis and mitophagy, we determined the changes in the levels of apoptosis regulatory proteins and mitochondrial morphology in the colons with the aid of immunohistochemical staining and TEM, respectively. The data came out with significant up-regulation of mitochondrial cleaved-caspase-3, caspase-9 and down-regulation of Bcl-2 in colons after implementing CSD therapy, evincing the apoptosis-encouraging efficacy of CSD (Figure 4(a)). We extended our attempts to probe mitochondrial structure from TEM images (Figure 4(b)), as demonstrated by the phenomenon that there was a pronounced increase in vacuolization (black asterisk panels), massive mitochondrial fission and loss of cristae as well as highly electron-condensation (arrowheads), and even lysosomes engulfing damaged mitochondria (arrows) in Model Group. To the contrary, the conspicuous mitochondrial morphological alternations brought on by AOM/DSS were perceptibly absent following CSD administration (Figure 4(b)), establishing mitophagy as an etiological factor in UCRCC tumorigenesis. The expression profile of MMP-9, whose well-appreciated pathologies is the relationship to cancer owing to its role in extracellular matrix remodeling and angiogenesis, was depicted to experience a slight diminution inflicted by CSD (Figure 3(f)).

3.4. Identification of Chemical Ingredients in CSD by Mass Spectrographic Analysis. We attempted to identify the active constituents in CSD using high-resolution mass spectrometry (HRMS) and part of a summary of the various abundant constituents detected and identified by the channel of methanol extraction (Figure 5(a)) and pure water extraction (Figure 5(b)) was given, respectively. HRMS confirmed oxymatrine as the most abundant ingredient in the CSD liquid (Figures 5(a) and 5(b)). The active compounds from CSD extraction through methanol extraction were as follows: oxymatrine, isoliquiritigenin, (–)-maackiain, DL-stachydrine, cytisine, indirubin,  $18-\beta$ -glycyrrhetinic acid, ginsenoside Rg3, licochalcone A,







(c)



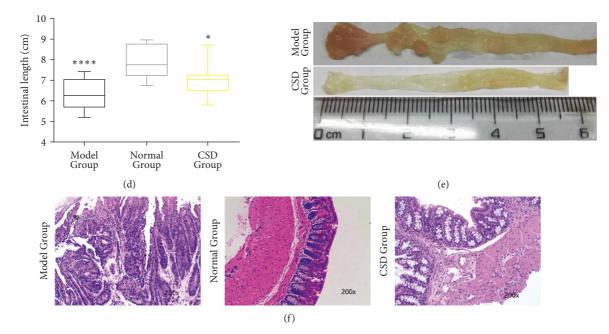
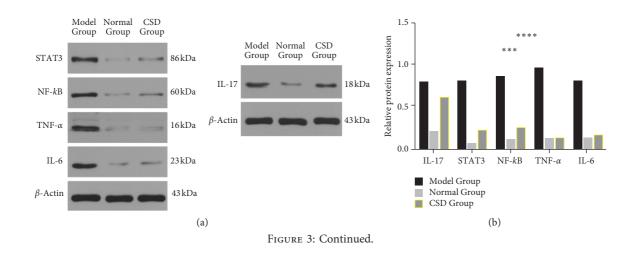


FIGURE 2: CSD overcomes AOM/DSS-induced malignancy of colon. (a) Body weight per mouse measured per day during all the experiment. \*p < 0.05, \*\*p < 0.01, significantly different from the Normal Group. (b) Effect of CSD on the incidence ratio of hematochezia. \*p < 0.05 vs. Model Group. (c) Colonic length of mice from the three groups. (d) Comparison of colon length among the three groups, \*p < 0.05, \*\*p < 0.01 vs. Normal Group. (e) Effect of CSD on multiplicity of polyp/adenoma on colons. (f) Colon sections stained with H&E (×200) from each group.



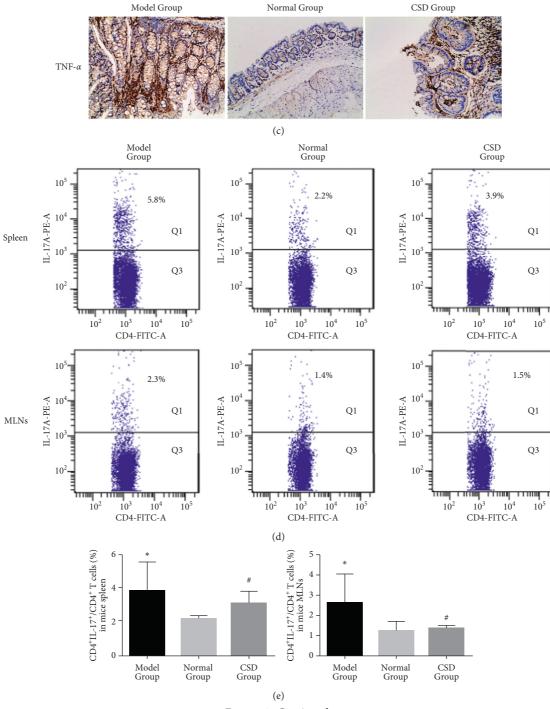


FIGURE 3: Continued.

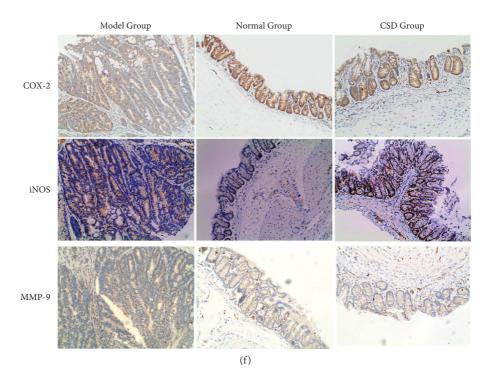


FIGURE 3: AOM/DSS-induced inflammatory response is impeded by CSD. (a) Western blot analysis of classical inflammatory proteins expression profiles in colon. (b) Representative histogram of densitometry analysis of the data derived from western blot, \*\* p < 0.01, significantly different from the Model Group. (c) Immunohistochemical staining analysis of TNF- $\alpha$  expression in colons. (d) Representative flow cytometry dot plot of the percentages of CD4<sup>+</sup>IL-17<sup>+</sup>Th17 cells in CD4+ cells in the spleen and MLNs of each group. (e) Trends of Th17 cells in mice, \* p < 0.05, # p > 0.05 vs. Model Group. (f) Effect of CSD on COX-2, iNOS, and MMP-9 expression in colon tissues in C57BL/6 mice.

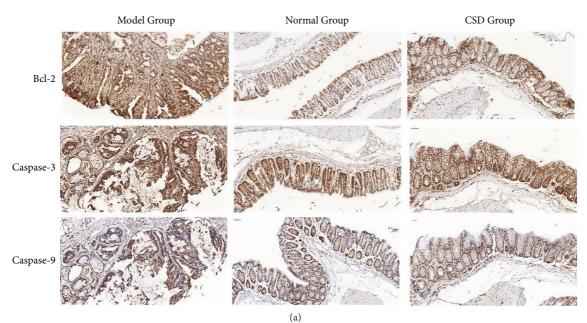


FIGURE 4: Continued.

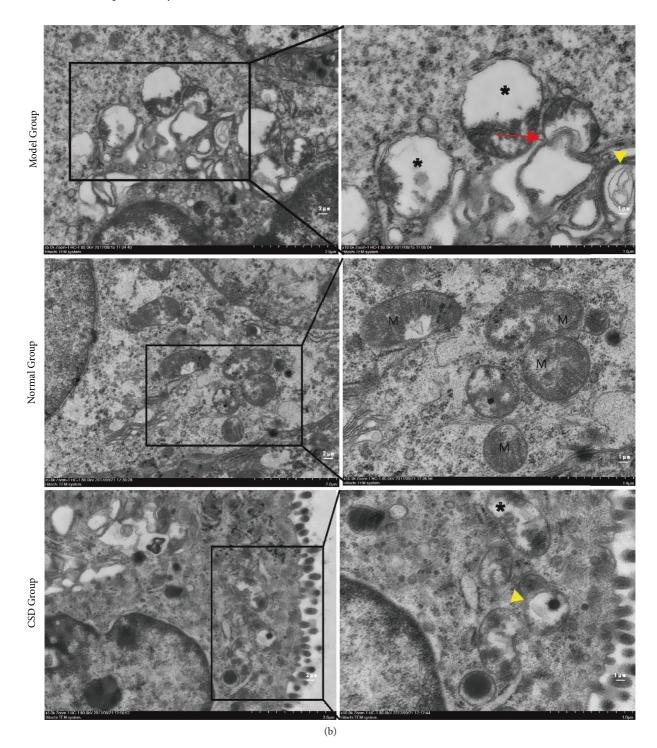


FIGURE 4: (a) CSD attunes apoptosis-related proteins expression language illustrated by immunohistochemistry. (b) Electron micrographs of mitochondrial morphology colonic tissues in mice. Arrowheads indicate the disrupted mitochondria undergoing mitochondrial fission, absence of cristae or electron-condensation; Arrows symbolize lysosomes engulfing damaged mitochondria. M means mitochondrion.

Name	Formula	Annotation Source: Predicted Compositions	Annotation Source: mzCloud Search	Annotation Source: ChemSpider Search	Annotation Source: MassList Match	FISh Coverage	Molecular Weight	RT [min]	Area (Max.)	# ChemSpid er Results	# mzCloud Results	# mzVault Results	mzCloud Best Match	Group Area: F2
Oxymatrine	C15 H24 N2 O2	Full match	Full match	Partial match	Full match	16.07	264.1833	2.316	515109927	2	6	0	95.7	515109927.3
Proline	C5 H9 N O2	Full match	Full match	Full match	Full match		115.0635	0.961	131425796	50	- 4	0	85.8	131425795.9
	C16 H22 O4	Full match	Full match	Full match	Full match		278.1515	8.352	48424764.8	21	9	0	95.2	48424764.81
Isoliquiritigenin	C15 H12 O4	Full match	Full match	Full match	Full match	54.55	256.0731	4.506	48376399.4	34	6	0	97.3	48376399.37
DL-Arginine	C6 H14 N4 O2	Full match	Full match	Full match	Full match		174.1116	0.799	44987026.2	7	4	0	93.2	44987026.15
Bis(4-ethylbenzylidene)sorbitol	C24 H30 O6	Full match	Full match	Partial match	Full match		414.2037	7.155	40586940.1	8	- 4	0	94.9	40586940.07
Hexamethylenetetramine	C6 H12 N4	Full match	Full match	Full match	No results	17.65	140.106	14.473	38328386.8	3	2	0	97.4	38328386.75
Erucamide	C22 H43 N O	No match	Invalid mass	No match	No results	45.07	320.3071	11.739	35366872.9	1	2	0	95.7	35366872.87
D-(+)-Maltose	C12 H22 O11	No match	Invalid mass	No match	No results		364.0978	0.944	28665838.1	2	4	0	89.8	28665838.11
Choline	C5 H13 N O	Full match	Full match	Partial match	Full match		103.1001	0.808	25933085.1	12	2	0	85.2	25933085.13
(-)-Maackiain	C16 H12 O5	Full match	Full match	Partial match	Full match		284.0681	5.404	24623436.9	42	16	0	88.5	24623436.89
Asparagine	C4 H8 N2 O3	Full match	Full match	Partial match	Full match		132.0536	0.966	21140114.9	27	6	0	86.8	21140114.93
L-Norleucine	C6 H13 N O2	Full match	Full match	Not the top hit	Full match		131.0947	1.35	19032179.1	56	10	0	86	19032179.1
	C7 H13 N O2	Full match	Full match	Partial match	Full match		143.0946	0.933	12954247.6	52	2	0	86.2	12954247.61
Trigonelline	C7 H7 N O2	Full match	Full match	Not the top hit	Full match		137.0476	0.982	12927754.5	47	18	0	91.8	12927754.52
	C11 H14 N2 O	Full match	Full match	Not the top hit	Full match		190.1106	0.876	12783681.3	32	2	0	89.6	12783681.35
	C9 H11 N O2	Full match	Full match	Full match	Full match	34.78	165.079	1.931	11606902	95	4	0	95.4	11606902.02
	C11 H12 N2 O2	No match	Invalid mass	No match	No match	63.04	187.0636	3.067	11467917.6	33	6	0	96.9	11467917.59
5-Hydroxymethyl-2-furaldehyde		Full match	Full match	Partial match	Full match		126.0318	1.946	10120207	26	18	0	88.2	10120207.04
	C16 H12 O4	Full match	Full match	Full match	Full match	47.17	268.0732	6.188	7676456.6	34	4	0	96.5	7676456.596
	C6 H7 NO	Full match	Full match	Not the top hit	Full match	47.47	109.0531	0.907	7058284.23	36	15	0	86.4	7058284.229
	C12 H22 O11	No match	Invalid mass	No match	No results		359.1424		6851306.67	2	2	0	87.8	6851306.672
	C6 H6 O3	Full match	Full match	Partial match	Full match		126.0318	2.749	6495269.32	26	12	0	88.4	6495269.32
	C22 H22 O9	Poil match	Foil match	Not the top hit	Full match		430.1261	5.161	6324440.85	20	2	0	91	6324440.854
	C18 H35 N O	Pull match	Full match			36.51	264.2451		5130179.81	5	2	0	91	5130179.81
		No match	Invalid mass	No match	No results	30.51		9.847		0		0		
	C16 H10 N2 O2	Full match	Full match	Full match	No results		262.0739	6.761	5005072.7		10		90	5005072.7
	C18 H37 N O	Full match	Full match	Full match	Full match	-	283.287	10.645	4477466.55	4	3	0	94.2	4477466.549
Anthranilic acid	C7 H7 N O2	Full match	Full match	Partial match	Full match		137.0476	4.242	4072977.66	47	18	0	92.7	4072977.662
											2	0	83.5	3488495.572
	C30 H50 O2	Full match	Full match	Partial match	Full match	-	442.3806	5.596	3488495.57	42	-			
	C30 H50 O2 C30 H46 O4	Full match Full match	Full match Full match	Partial match Partial match	Full match Full match	14.91	442.3806 470.3392	6.089	3457136.7	23	2	0	96.9	3457136.704
		Full match Annotation Source: Predicted	Full match Annotation Source: mzCloud			14.91 FISh Coverage				23	-			
18-β-Glycyrrhetinic acid	C30 H46 O4	Full match Annotation Source:	Full match Annotation	Partial match Annotation Source:	Full match Annotation Source: MassList	FISh	470.3392 Molecular Weight	6.089 RT	3457136.7	23 # ChemSpid	2 # mzCloud	0 # mzVault	96.9 mzCloud	3457136.704
18-β-Glycyrrhetinic acid Name	C30 H46 O4 Formula	Full match Annotation Source: Predicted Compositions	Full match Annotation Source: mzCloud Search	Partial match Annotation Source: ChemSpider Search	Full match Annotation Source: MassList Match	FISh Coverage	470.3392 Molecular Weight	6.089 RT [min]	3457136.7 " Area (Max.)	23 # ChemSpid er Results	2 # mzCloud Results	0 # mzVault Results	96.9 mzCloud Best Match	3457136.704 Group Area: F2 3457136.704
18-β-Glycyrrhetinic acid Name 18-β-Glycyrrhetinic acid	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2	Full match Annotation Source: Predicted Compositions Full match	Full match Annotation Source: mzCloud Search Full match	Partial match Annotation Source: ChemSpider Search Partial match	Full match Annotation Source: MassList Match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392	6.089 RT [min] 6.089	3457136.7 Area (Max.) 3457136.7	23 # ChemSpid er Results 23	2 # mzCloud Results 2	0 # mzVault Results 0	96.9 mzCloud Best Match 96.9	3457136.704 Group Area: F2
18-β-Glycyrrhetinic acid Name 18-β-Glycyrrhetinic acid α-Eleostearic acid	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 (C11 H20 O4	Full match Annotation Source: Predicted Compositions Full match Full match	Full match Annotation Source: mzCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No match	Full match Annotation Source: MassList Match Full match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245	6.089 RT [min] 6.089 7.936	3457136.7 " Area (Max.) 3457136.7 3189018.09	23 # ChemSpid er Results 23 19	# mzCloud Results 2 3	0 # mzVault Results 0 0	96.9 mzCloud Best Match 96.9 92.2	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784
18-β-Glycyrrhetinic acid Name 18-β-Glycyrrhetinic acid α-Eleostearic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 (C11 H20 O4 C6 H9 N3 O2	Full match Annotation Source: Predicted Compositions Full match Full match No match Full match	Full match Annotation Source: m2Cloud Search Full match Full match Invalid mass Full match	Partial match Annotation Source: ChemSpider Search Partial match Portial match No match Full match	Full match Annotation Source: MassList Match Full match Full match Full match Full match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255	6.089 RT [min] 6.089 7.936 6.84	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78	23 # ChemSpid er Results 23 19 4	2 # mzCloud Results 2 3 2	0 # mzVault Results 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Eleostenic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecaamide	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O	Full match Annotation Source: Predicted Compositions Full match Full match No match	Full match Annotation Source: mzCloud Search Full match Full match Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match No match Full match Full match	Full match Annotation Source: MassList Match Full match Full match Full match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256	6.089 RT [min] 6.089 7.936 6.84 0.828 9.729	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98	23 # ChemSpid er Results 23 19 4 18 4	2 # mzCloud Results 2 3 2 3 2 3 2	# mzVault Results 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978
18-β-Glycyrrhetinic acid Name 18-β-Glycyrrhetinic acid α-Elcostearic acid (35,4R)-3-(1-yydroxyheyl)-4- L-Histidine Hexadecanamide 3-[2-(3-Hydroxyheyl)ethyl]-!	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 (C11 H20 O4 C6 H9 N3 O2 C16 H33 N O SC15 H16 O3	Full match Annotation Source: Predicted Compositions Full match	Full match Annotation Source: m2Cloud Search Full match Invalid mass Full match Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Portial match No match Full match	Full match Annotation Source: MassList Match Full match Full match Full match Full match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097	6.089 RT [min] 6.089 7.936 6.84 0.828 9.729 6.2	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03	23 # ChemSpid er Results 23 19 4 18 4 36	2 # mzCloud Results 2 3 2 3 2 6	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcosteric acid (35,48)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide 3-[2-13-Hydroxyhenyl)ethyl]-5 Bic(2-ethythexyl) phthalate	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O SC15 H16 O3 C24 H38 O4	Full match Annotation Source: Predicted Connositions Full match Full match Full match Full match Full match Full match Not the top hit	Full match Annotation Source: m2Cloud Search Full match Invalid mass Full match Full match Full match Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match Full match Full match Partial match Full match	Full match Annotation Source: MassList Match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38	23 # ChemSpid er Results 23 19 4 4 18 4 36 26	2 # mzCloud Results 2 3 2 3 2 6 10	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.97 2567369.032 2420907.381
18-B-Glycyrrhetinic acid Name 18-B-Glycyrhetinic acid a-Elcotlearic acid (35,4R)-3-(1-hydroxyhetyl)-4- 1-Histidine Hexade-canamide 3-[2-(3-Hydroxyhetyl)phthalate 2-Hydroxyhetylalanise	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 (C11 H20 O4 C6 H9 N3 O2 C16 H33 N O 5C15 H16 O3 C24 H38 O4 C9 H11 N O3	Full match Annotation Source: Predicted Compositions Full match Full match Full match Full match Not the top hit No match	Full match Annotation Source: mzCloud Search Full match Invalid mass	Partial match Annotation Source: ChemSpider Search Partial match Partial match Full match Full match Full match Full match No match	Full match Annotation Source: MassList Match Full match Full match Full match Full match No results Full match No results No match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2420907.38 2309984.25	23 # ChemSpid er Results 23 19 4 18 4 36 26 41	2 # mzCloud Results 2 3 2 3 2 6 10 5	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032 2420907.381 2309984.246
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcosteric acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine L-Histidine 2-(2-d)-Hydroxyhexyl-hyll-f Bls(2-ethylHexyl) phthalate 2-Hydroxyphenylalanine Adenosine	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O C15 H16 O3 C24 H38 O4 C9 H11 N O3 C10 H13 N5 O4	Full match Annotation Source: Predicted Compositions Full match No match Full match Full match Full match Not the top hit No match Full match Full match	Full match Annotation Source: mzCloud Sarch Full match Invalid mass Full match Invalid mass Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match Full match Full match Full match Full match No match No match No the top hit	Full match Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match No results Full match No match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965	6.089 RT [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.3 2309984.25 2270151.36	23 # ChemSpid er Results 23 19 4 18 4 36 26 41 34	2 # mzCloud Results 2 3 2 3 2 6 6 10 5 1	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 94.8 8.1 80.9	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032 2420907381 200998.246 2270151.362
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcotteric acid (55,4R)-3-(1-hydroxyhexyl)-4- L-Hittidine Hexade-anamide 3-[2-(3-Hydroxyhenyl)ethyl]-5 Bit(2-ethylhexyl)phrhalate 2-Hydroxyherylalanine Adenosine 9-One-10(E),12(E)-octadecadi	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O C15 H16 O3 C24 H38 O4 C9 H11 N O3 C10 H13 N5 O4 C18 H30 O3	Full match Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Full match Not the top hit No match Full match Full match Full match Full match	Full match Annotation Source: mcCloud Search Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match Full match Full match Full match Full match No match Not match phit Not the top hit	Full match Amotation Source: MassList Match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194	6.089 RT [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2270151.36 2180416.19	23 # ChemSpid er Results 23 19 4 18 4 36 26 41 34 34 24	2 # mzCloud Results 2 3 2 3 2 6 10 5 1 2	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94. 88.1 80.9 95	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907381 2309984.246 2270151362 2180416.19
18-B-Glycyrthetinic acid Name 18-B-Glycyrthetinic acid a-Elcostenic acid (38,4R)-3-(1-hydroxythetyl)-4 - LHistidine Hexafecanamide 3-(2-3-Hydroxythetyl)-pithalate 2-Hydroxythenyltalanine Adenosine 9-Oxo-10(E),12(E)-octadecadii Glycitin	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H38 N0 5C15 H16 O3 C24 H38 O4 C19 H11 N5 O4 C18 H30 O3 C10 H13 N5 O4 C18 H30 O3 C22 H22 O10	Full match Annotation Source: Predicted Convections Full match	Full match Annotation Source: mcCloud Search Full match Full match Full match Full match Full match Full match Full match Full match Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match No match Partial match Partial match Partial match Partial match No match No match No the top hit Partial match	Full match Amotation Source: MassList Match Full match Full match Full match Full match Full match No results Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2270151.36 2180416.19 2099593.48	23 # ChemSpid er Results 23 19 4 18 4 36 26 41 34	2 # mzCloud Results 2 3 2 2 3 2 2 6 10 5 1 1 2 2 2	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 87.7	3457136.704 Group Area: F2 3457136.704 3184560.784 3181520.407 3032768.978 2567369.032 2420907381 2309984.246 2270151.362 2180416.19 2099593.479
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Eleostearic acid (3-4,R)-3(1-yhdrox)nexy[)-4- L-Hutidine Herzadocanamide 3-[2-(3-Hydroxypheny])ethalate 2-Hydroxyphenylalanine Adenosine 9-0xo-10(2),12(E)-octadecadi Glycitin Ginsenoside Rg3	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C18 H30 O2 C16 H33 N O C16 H33 N O C16 H33 N O C14 H38 O4 C9 H11 N O3 C14 H30 O3 C16 H30 O3 C17 H	Full match Anotation Source: Predicted Compositions Full match Not the top hit No match	Full match Annotation Source: mcCloud Search Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match Full match Full match Full match Full match Full match No match No match Not the top hit Not the top hit Partial match Not Match	Fail match Amotation Source: MassList Match Fail match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3131520.41 3032768.98 2567369.03 242090738 2309984.25 2270151.36 2180416.19 2099593.48 2096363.33	23 # ChemSpid er Results 23 19 4 4 18 4 36 226 41 34 24 11 1 1	2 # mzCloud Results 2 3 2 2 6 10 5 1 2 2 2 4	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 87.7 82.7	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2309984.246 2270151.362 2180416.19 2099593.479 2099593.479
18-B-Glycyrthetinic acid Name 15-B-Glycyrthetinic acid a-Elcostearic acid (38, 4R)-3-(1-hydroxyhetyr)-4- L-Histidine Hexafecanamide 3-(2-3-Hydroxyhenyl)ethyl]-5 Bis(2-ethylhexyl) phthalate 2-Hydroxyhenylalanine Adenosine 9-Ono-10(E),12(E)-octadecadii Glyctiin Ginsenoside Rg3 D-(-)-Glutamine	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 (C11 H20 O4 C6 H9 N3 O2 C16 H33 N O C16 H33 N O C16 H33 N O C24 H38 O4 C9 H11 N O3 C10 H13 N5 O4 C7 H11 N O3 C10 H13 N5 O4 C21 H22 O10 C42 H72 O13 C42 H72 O13 C45 H10 N2 O3	Full match Anotation Source: Predicted Constitutions Full match	Full match Annotation Source: mcCloud Source: mcCloud Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match Partial match Fall match Fall match Fall match Not the top hit Not the top hit Not the top hit Not the top hit No match Hall match Not the top hit Partial match	Full match Amotation Source: MassList Match Full match	FISh Coverage	470.3392 Molecular Weight 470.3392 278.2245 198.1255 195.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0691	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2200151.36 2180416.19 2096363.33 1867381	23 # ChemSpid er Results 23 199 4 4 36 26 41 34 24 11 1 31	2 # mzCloud Results 2 3 2 3 3 2 6 10 5 5 1 1 2 2 4 4 6	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 87.7 82.7 82.7 84.6	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032 2567369.032 236974.242 2369416.19 2099593.479 2096363.325 1867381
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcostearic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Hittidine L-Hittidine 2-(3-Hydroxyhenyl)phfnalate 2-Hydroxyhenylphfnalate 3-(2-3-Hydroxyhenylphfnalate) 3-(2-3-Hydroxyhenylphfnalate	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C18 H30 O2 C16 H33 N O C16 H33 N O C15 H16 O3 C24 H38 O4 C9 H11 N O3 C16 H1 N O3 C16 H1 N O3 C16 H1 N O3 C17 H18 O3 C22 H22 O10 C42 H72 O13 C5 H10 N2 O3 C5 H10 H10 H10 C5	Full match Anotation Source: Predicted Compositions Full match Not the top hit No match	Full match Annolation Source: mcCloud Rearch Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match No match Fail match Fail match Fail match No match No match Not the top hit Not the top hit Not the top hit Not match No match Fail match No match No match Fail match No match Fail match No match Fail match No match	Fail match Amotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 195.0695 245.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0691 339.3495	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 242090738 2309984.25 2270151.36 2309984.25 2270151.36 2180416.19 2099593.48 2096563.33 1867381 1574239.28	23 # ChemSpid er Results 23 19 4 4 18 4 36 26 41 34 24 11 1 1 31 0 0	2 # mzCloud Results 2 3 2 2 6 6 10 5 1 1 2 2 4 4 6 2 2	0 # m2Vault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	969 mrCloud Best Match 969 922 838 901 919 923 94 881 809 95 5 87.7 82.7 84.6 932	3457136.704 Group Area: F2 3457136.704 3189018.093 318450.784 3131520.407 3032768.978 2420907.381 2309984.246 2270151.362 2180416.19 209959.479 2096363.325 1867381 1574239.278
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcostearic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Hhtidine Hexafe-anamide 3-[2-(3-Hydroxyhenyl)ethyl]-5 Bia(2-ethythexyl) phthalate 2-Hydroxyhenylalanine Adenosine 9-Ono-10(E),12(E)-octafecadii Glysetiin Ginsenoside Rg3 D-(-)-Glutamine Docosanamide Licochalcone A	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C18 H30 O2 C16 H33 N O C24 H38 O4 C24 H38 O4 C19 H11 N O3 C10 H13 N5 O4 C18 H30 O3 C22 H22 O10 C42 H72 O13 C22 H42 O13 C22 H42 N O C21 H42 O4	Full match Anotation Source: Predicted Connouitions Full match	Full match Annotation Source-mcCloud Source-mcCloud Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match Pail match Pail match Pail match Pail match Pail match Not the top hit Partial match Not the top hit Partial match Not the top hit Partial match Not match Pail match No match Pail Pail Pail Pail Pail Pail Pail Pail Pail	Fail match Amotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 195.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0691 339.3495 338.1515	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084 6.997	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2309984.25 22070151.36 2180416.19 2096363.33 1867381 1574239.28 1574239.28	23 # ChemSpid er Results 23 19 4 18 4 4 36 26 41 1 34 24 11 1 1 1 31 0 0 15	2 # mzCloud Results 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 2 3 3 2 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 2 3 3 3 2 3 3 3 3 3 2 3 3 3 3 3 2 3 3 3 3 3 2 3 3 3 2 3 3 3 3 2 3 3 3 2 3 3 3 3 3 2 3 3 3 3 3 2 3 3 3 3 3 3 2 3 3 3 3 2 3 3 3 3 3 3 2 3 3 3 3 3 3 2 3	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 83.8 90.1 91.9 94 88.1 80.9 95 87.7 82.7 82.7 84.6 93.2 89.8	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2209984.246 22100416.19 2099583.479 2180416.19 2099583.4325 1867381 15771849.911
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcostearic acid a-Elcostearic acid (35,4R)-3-(1-hydroxyhexy)-4- L-Histidine L-Histidine 3-(2-3-Hydroxyhexy) ahrhalate 2-Hydroxypherylalanine Adenosine 9-Ox-10(E),12(E)-octadecadis Glycitin Ginsenoside Rg3 D-(-)-Glutamine Docosanamide Licochalcone A EfG n10	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 (C11 H20 O4 C6 H9 N3 O2 C16 H33 N O C24 H38 O4 C9 H11 N O3 C24 H38 O4 C9 H11 N O3 C10 H13 N5 O4 C18 H30 O3 C22 H22 O10 C42 H72 O13 C22 H45 N O C21 H42 O4 C20 H42 O11	Full match Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Not the top hit Full match	Full match Annolation Source: mcCloud Carch Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match No match Fall match Fall match Fall match Fall match Not the top hit Not the top hit No match Fall match Partial match Fall match	Fail match Amoriation Source: MassList Mutch Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 198.1255 198.1255 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0691 339.3495 338.1515	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084 6.997 4.159	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2267768.98 2267768.98 2267768.98 22090513.36 22090514.36 220905348 2096363.33 1867381 1571243.92.8 1571849.91 1477574.46	23 ChemSpid er Results 23 19 4 4 18 4 4 6 26 41 34 24 11 1 1 31 0 15 1	2 # mzCloud Results 2 3 2 3 2 6 6 10 5 5 1 1 2 2 4 4 6 6 2 2 4 4 6 2 2 4 4 6 2 2 2 4 4 6 2 2 2 2	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcClond Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 95 87.7 84.6 6 93.2 89.8 87.9 84.8 87.9 82.8	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2427097381 2209954.242 2180416.19 2099593.479 2099563.375 2099563.479 2099563.375 1571849.911 1477574.46
18-B-Glycyrrhetinic acid Name 18-B-Glycyrhetinic acid a-Elcostearic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Hhtidia Hexade-anamide 3-[2-(3-Hydroxyhemyl)ethyl]-5 Bis(2-ethythexyl) phthalate 2-Hydroxyhemyllaanine Adenosine 9-Oxo-10(E),12(E)-octadecadii Glycitin Ginsenoside Rg3 D-(-)-Glutamine Dacosanamide Licochalcone A PEG n10 Xamthohumol	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C16 H33 N O C16 H33 N O C24 H38 O4 C25 H16 O3 C24 H38 O4 C18 H30 O3 C2 H22 O10 C2 H12 NO C2 H10 N2 O3 C2 H10 N2 O3 C3 H10 N2 N2 N3 C3 H10 N2 N3 C	Full match  Anotation Source: Predicted Compositions Full match	Full match Annotation Source-mcCloud Source-mcCloud Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match Pail match Pail match Pail match Pail match Pail match Not the top hit Partial match Partial match Partial match Partial match Partial match Fail match	Fail match Amotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0691 339.3495 338.1515 458.2729 354.1463	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.888 8.157 4.432 5.594 0.948 13.084 6.997 4.159 6.238	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 2032768.98 2032768.98 2032768.98 2032768.98 2030958.24 2009593.48 2096363.33 1867381 157439.9 1577184.9 1477574.46	23 # ChemSpid er Results 23 19 4 4 36 266 41 34 24 4 11 1 31 0 15 1 25	2 # mzCloud Results 2 3 2 2 3 2 2 6 6 10 0 5 1 1 2 2 4 4 6 6 2 2 4 4 2 8 8	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 84.6 88.1 80.9 95 87.7 82.7 82.7 84.6 93.2 89.8 87.9 90.8	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 24209973.81 24209973.81 24209973.81 24209973.81 24209973.81 24209973.81 299593.479 2095959.479 2095959.479 209595.479 209595.479 209595.299 200595.299 200595.299 2005955.299 200595.299 2005955.299 2005955.299 2005955.299 2005955.299 2005955.299 200555.299 200555.299 200555.299 200555.299 200555.299 200555.299 200555.299 200555.299 200555.2
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcostearic acid (35,4R)-3-(1-hydroxyhetyl)-4- L-Hittidine Hexafecanamide 3-(2-a-Hydroxyhetyl)-4hyl-3 Bis(2-ethylbexyl) phthalate 2-Hydroxyphenylalanine Adenosine 9-0x-1-0(E),12(E)-octadecadi Glycitin Ginsenoside Rg3 D-()-Glutamine Decosnamide Licochalcone A PEG n10 Xantholumol 7.8-Dihydroxy-4-methylcouma	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C16 H33 N O C16 H33 N O C16 H38 O4 C18 H36 O4 C18 H36 O4 C18 H36 O4 C18 H36 O4 C24 H38 O4 C44 H72 O13 C24 H45 N O C22 H42 O10 C24 H45 N O C24 H45 N O C34 H45 N O C44 H72 O13 C44 H50 O C44 H72 O13 C44 H50 O C44 H72 O13 C44 H50 O C44 H22 O4 C41 H22 O5 C10 H46 O4 C10 H47 O4 C10 H	Full match Annotation Source: Predicted Convocations Full match Full match Full match Full match Full match Full match Not match Full match	Full match Annolation Source: mcCloud Cource: mcCloud Cource: mcCloud Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match No match Fall match Fall match Fall match Not the top hit Not the top hit No match Fall match Not match Fall match	Fail match Annotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.9065 294.2194 446.1211 766.4856 146.0691 339.3495 338.1515 458.2729 354.1463 192.0425	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084 6.997 4.132 8.153 4.323 3.723	34571367 Area (Max.) 34571367 31859018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2270151.36 2270151.36 2280416.19 209953.48 2096363.33 1857381 2096363.33 1857381 25718499.11 5718499.11 15718499.11 477574.46 1432077.92	23 Chemespid or Respid or Respid 23 19 4 4 18 4 18 4 18 4 16 26 41 34 4 24 11 1 31 0 15 15 15 15 15 15 15 15 15 15	# mzCloud Results 2 3 3 2 2 3 3 2 6 6 10 5 1 1 2 2 4 4 6 6 2 2 4 4 8 8 8	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 919 92.3 94 88.1 80.9 955 87.7 84.6 93.2 87.9 84.8 87.9 90.8 87.9 90.8	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2267369.032 2420907.381 2270151.362 2180416.19 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099574.461 1477574.46 1448182.689 1432077.925
18-β-Glycyrrhetinic acid Name 18-β-Glycyrrhetinic acid a-Eloostearic acid (35,4R)-3-(1-hydroxyhexy)-4- L-Hintidine Herade-anamide J-(2-3-HydroxyhenyDethyl]-1 Bi4(2-ehythexy1) phrhalate 2-Hydroxyhenyl-Hyllaaine Adenosine 9-Onc-10(E),12(E)-octadecadii Glycitin Ginsenoside Rg3 D-(-)-Glutamine Docosanamide Licochalcone A PEG n10 Xunthohumol 7,8-Dihydroxy-4-methylcouma	C30 H46 O4 Formula C30 H46 O4 C13 H30 O2 C11 H20 O4 C6 H39 N3 O2 C16 H33 N O C24 H38 O4 C315 H16 O3 C24 H38 O4 C315 H16 O3 C24 H22 O10 C18 H30 O3 C22 H22 O10 C31 H20 O3 C21 H22 O4 C21 H42 O11 C21 H42 O1 C21 H42 O1 C21 H42 O1 C21 H42 O1 C315 H10 O4	Full match  Anotation Source: Predicted Compositions Full match	Full match Amotation Source-mcCloud Source-mcCloud Full match Full match	Partial match Amotation Source: Chemöpider Search Partial match Partial match Partial match Patil match Patil match Patil match Patil match Not match Patil match Not the top hit Patil match Not the top hit Patil match Patil Pati	Fail match Amotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0691 339.3495 338.1515 458.2729 354.1463 192.0425 254.0577	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084 6.997 4.159 6.233 3.723 5.231	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2270151.36 2180416.19 2099593.48 2099593.48 1571849.91 1477574.46 1445182.69 1432077.92 1268752.83	23 # Chemspid er Results 23 19 4 4 36 26 411 34 24 11 1 31 0 0 15 1 1 25 38 44	2 # mzCloud Results 2 3 3 2 2 3 3 2 2 3 3 2 2 3 3 2 2 4 4 6 6 6 2 2 4 4 6 2 2 4 8 8 8 8 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.9 85.9 87.7 82.7 84.6 93.2 89.8 87.9 90.8 87.9 90.8	3457136.704 Group Area: F2 3457136.704 3189018.009 3184569.784 3131520.407 3032768.978 420907.381 2309984.246 22180416.19 2099593.479 2099593.479 2099593.479 2099593.479 21571849.911 1477574.48 1571849.911 1477574.48 1571849.911
18-B-Glycyrthetinic acid Name 18-B-Glycyrthetinic acid a-Elcostearic acid (35,4R)-3-(1-hydroxythexyt)-4- L-Histidine Hexafecanamide 12-(3-Hydroxythenyt)ethyl]- Bia(2-ethythexyt) pathalate 2-Hydroxythenytalanine Adenosine 9-Oxo-10(E),12(E)-octadecadi Glyctin Ginsenoside Rg3 D-(-)-Glutamine Dacosanamide Licochalcone A PEG n10 Xanthohumol 7.a-Dihydroxy-4-methylcouma Daideein	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C16 H33 N O C10 H13 N5 O4 C18 H30 O3 C10 H13 N5 O4 C18 H30 O3 C22 H42 O10 C42 H72 O13 C22 H42 O10 C42 H72 O13 C21 H22 O4 C20 H42 O11 C21 H22 O5 C10 H80 O4 C15 H10 O4 C16 H10	Full match Annotation Source: Predicted Convocations Full match Full match Full match Full match Full match Full match Not match Full match	Full match Source mCloud Source mCloud Source Source Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match No match Fall match Fall match Fall match Not the top hit Not the top hit Not the top hit Partial match Fall match	Fail match Annotation Source: MassList Mark Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 255.256 254.20761 164.0475 294.2194 446.1211 766.4856 146.0691 339.1495 338.1515 458.2729 354.1463 192.0425 254.0577 238.1418	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.24 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084 4.432 5.594 0.948 13.084 5.594 0.288 5.291 2.86	34571367 Area (Max.) 34571367 31315021 3131520.41 3032768.98 2567369.03 242090738 2309984.25 2270151.36 2309984.25 2270151.36 2309984.25 2270151.36 2096363.33 1867381 1574239.28 1574239.28 1577429.28 1577426 1448182.69 1448182.69 1448182.69 1426275.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 126875.28 1166294.07 1166294.07 1166294.07 1166294.07 1166294.07 1166294.07 1167294.07 1167294.07 1167294.07 1167294.07 1167294.07 1167294.07 1167294.07 117294.07 1167294.07 117294.07 1167294.07 1175744.07 1167294.07 1175744.07 1167294.07 117574.07 1167294.07 117574.07 1167294.07 117574.07 117574.07 117574.07 117574.07 117574.07 117574.07 117574.07 117574.07 117574.07 117574.07 117574.07 117574.07 117574.07	23 # ChemSpid er Results 23 19 4 18 4 18 4 4 36 26 41 1 34 24 11 1 31 0 15 1 25 38 4 4 4 4 4 15 15 15 15 15 15 15 15 15 15	# mzCloud Results 2 3 3 2 2 3 3 2 6 6 10 5 1 1 2 2 4 4 6 6 2 2 4 4 8 8 8	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 85.1 80.9 95 87.7 84.6 93.2 87.9 90.8 87.9 90.8 87.9 90.8 87.9 90.6 8.7 9.9 8.7 9.9 8.8 8.7 9.9 9.0 8.8 8.7 9.9 9.0 8.8 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9.0	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 240907381 2209954.246 2270151.362 2180416.19 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 209552.828 1571849.911 1477574.68 144312.689 1432077.925 21268752.828 1146224.075
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcotteric acid (35,4R)-3-(1-hydroxyhery)-4- 1-Hittidine Hexade-camanide 1-2(3-Hydroxyhery)Dethyl]-5 Bia(2-ehythoxyt)Dethyl]-5 Bia(2-ehythoxyt)Dethyl]-5 Bia(2-ehythoxyt)Dethyl Bi	C30 H46 O4 Formula C30 H46 O4 C13 H30 O2 C14 H20 O4 C6 H9 N3 O2 C16 H33 N O C24 H38 O4 C315 H16 O3 C24 H38 O4 C315 H16 O3 C24 H22 O10 C21 H22 O10 C21 H22 O10 C21 H22 O4 C21 H22 O4 C21 H22 O4 C21 H22 O4 C21 H22 O4 C21 H22 O5 C10 H10 O4 C10 H22 O5 C10 H10 O4 C10 H22 O5 C10 H10 V2 V2 V10 V2 V10 C10 H10 V2 V1	Full match  Full match  Compositions  Full match  Full	Full match Amotation Source-mcCloud Source-mcCloud Full match Full match	Partial match Annotation Source: Chemöpider Search Partial match Not match Fall match Fall match Fall match Not the top hit Not the top hit Partial match Fall match	Fail match Amotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 198.1255 198.1255 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0891 339.1495 338.1515 254.0577 238.1418 224.1887	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 5.094 8.157 4.432 5.094 8.157 4.432 5.094 8.157 4.159 6.238 3.723 5.231 2.86 6.574	34571367 Area (Max.) 3457136.7 3189018.09 3184569.78 3184569.78 3131520.41 3032768.98 2309984.25 2270151.36 2180416.19 2099593.48 2096563.33 1571849.91 1574239.23 1571849.91 1477574.46 143207792 1268752.83 1146294.07 1070298.05	23 # Chemspid er Results 23 19 4 4 18 36 26 41 34 24 4 11 1 31 1 0 15 1 5 38 44 41 1 6 15 15 15 15 15 15 15 15 15 15	2 # mzCloud Results 2 3 3 2 2 3 3 2 2 3 3 2 2 3 3 2 2 4 4 6 6 6 2 2 4 4 6 2 2 4 8 8 8 8 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.8 81.1 80.9 95 87.7 82.7 82.7 82.7 82.7 82.8 87.9 9.9 9.0 8 87.9 9.9 0.8 87.9 9.9 0.8 87.9 9.9 0.8 87.9 9.9 0.8 87.9 9.9 0.8 87.9 9.9 0.8 87.9 9.9 0.8 87.9 9.9 0.8 87.8 87.8 87.8 87.8 87.8 87.8 87.8	3457136.704 Group Area: F2 3457136.704 3189018.009 3184569.784 3131520.407 3032768.978 420907381 2309984.246 22180416.19 209953.479 2180416.19 209953.479 21840941.1 1477574.46 1571849.911 1477574.812.689 1433182.689 1433182.689 1433182.689 1433182.689
18-B-Glycyrthetinic acid Name 18-B-Glycyrthetinic acid a-Elcostearic acid (38,4R)-3-(1-hydroxythetyrt)-4- L-Hhitdine Hexafecanamide 1-(2-3-Hydroxythenyt)-ethyl]-5 Bia(2-ethythexyt) phthalate 2-Hydroxythenythalanine Adenosine 9-0xo-10(E),12(E)-octadecadii Glycitin Ginsenoside Rg3 D-(-)-Glutamine Docosanamide Licochalcone A PEG n10 Xamtholumol 7,8-Dihydroxy-4-methylcouma Daidzein PEG n5	C30 H46 O4 Formula C30 H46 O4 C18 H50 O2 C11 H20 O4 C18 H50 O2 C16 H33 N O C26 H33 N O C26 H38 O4 C18 H60 O3 C29 H11 N O3 C10 H13 N5 O4 C18 H30 O3 C22 H22 O10 C42 H72 O13 C22 H42 O11 C20 H42 O11 C21 H22 O4 C20 H42 O11 C11 H20 O4 C15 H10 O4 C15 H12 O4 C15 H10 O4 C15 H12 O4 C1	Full match  Anotation Source: Predicted Compositions Full match	Full match Anotation Source mcCloud Source mcCloud Source mcCloud Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match No match Fall match Fall match Fall match Not the top hit Not the top hit Not the top hit Partial match Fall match	Fail match Annotation Source: MassList Mark Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0665 294.2194 446.1211 766.4856 146.0691 339.3495 458.2729 338.1515 458.2729 354.1463 192.4425 254.0577 238.1418 224.1887 502.299	6.089 RT [min] 6.089 7.936 6.88 9.729 6.2 11.144 0.828 8.157 0.88 8.157 0.88 8.157 4.159 6.238 6.397 4.159 6.239 5.231 2.86 6.574 4.283	34571367 Area (Max.) 3457136,7 3189018,09 3184569,78 3184569,78 3131520,41 3032768,58 22070151,36 2180416,19 2099493,48 2096363,33 1867381 15718499,11 477574,46 1448182,69 14207792,12 1268752,83 1146294,07 1070298,03 1053909,78	23 ChemSpid er Result 23 19 4 4 18 4 4 36 266 411 34 24 11 1 31 0 0 15 1 25 38 44 4 1 6 0 0 0 0 15 1 1 0 0 0 0 0 0 0 0 0 0 0 0 0	# mzCloud Results 2 3 2 2 6 6 10 5 5 1 1 2 2 2 4 4 6 6 2 2 2 8 8 8 8 8 4 4 4 2 2 8	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 87.7 82.7 84.6 93.2 89.8 87.9 90.8 87.9 90.6 81.2 93.2 89.8 87.9 90.6 8.3 87.9 90.6 8.3 87.9 90.6 8.3 8.3 8.3 8.3 8.3 8.3 8.3 8.3 8.3 8.3	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2209984.246 2270151.362 2180416.19 2099539.479 2099636.332 1867381 1577849.911 1477574.66 1438182.689 1432077.925 186752.828 1146294.075 1070298.034
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Elcotteric acid (55 4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexade-anamide 3-[2-(3-Hydroxyhenyl)ethyl]-5 Bia(2-ethythexyl) phrhalate 2-Hydroxyhenyl-Hyl]-5 Bia(2-ethythexyl) phrhalate 2-Hydroxyhenyl-Hyl]-5 Bia(2-ethythexyl) phrhalate 2-Hydroxyhenyl-Hyl]-5 Bia(2-ethythexyl) phrhalate 2-Hydroxyhenyl-Hyl]-5 Bia(2-ethythexyl) phrhalate 2-Hydroxyhenyl-Hyll D-(3-Clutamine D-(3-Clutamine) D-(3-C	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O C16 H33 N O C24 H38 O4 C315 H16 O3 C2 H418 O4 C18 H30 O3 C2 H22 O10 C2 H22 O10 C2 H22 O10 C2 H42 N O C2 H22 O4 C2 H42 N O C2 H22 O4 C16 H10 N2 O3 C2 H22 O4 C10 H10 N2 O3 C15 H10 O4 C15 H10 O4 C15 H10 O4 C15 H10 O4 C15 H10 O4 C15 H10 O5 C15 H10 O5 C15 H10 O5 C15 H10 O4 C15 H10 O5 C15 H10	Full match  Pull match  Compositions  Full match  Full	Full match Amotation Source-mcCloud Source-mcCloud Source-mcCloud Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Not match Fall match Fall match Fall match Fall match Not the top hit Partial match Fall match	Fail match Annotation Annotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 195.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 6146.0691 339.1495 338.1515 458.2729 354.166 192.0425 254.0577 238.1418 224.1887 502.299 272.0683	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084 6.354 4.459 6.238 3.723 2.86 6.574 4.283 4.447	34571367 Area (Max.) 3189018.09 3184569.78 3184569.78 3134520.42 230984.25 2209151.36 2180416.19 2099593.48 2096563.33 1571849.91 1477574.46 1477574.46 1477574.46 1477574.46 1477574.87 1432077.92 1268752.83 1145294.07 1070298.03 1073090.78 975615.82	23 # ChemSpid er Results 23 19 4 4 18 4 4 36 26 41 34 24 34 24 11 1 1 31 0 15 1 1 34 25 34 26 4 11 1 1 1 1 1 1 1 1 1 1 1 1	# mcCload Results 2 3 3 2 2 6 6 10 5 1 1 2 2 4 4 6 2 2 4 4 6 8 8 8 8 8 8 8 8 4 4 2 2 2 1 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 3 3 2 2 2 3 3 3 3 3 2 2 2 2 3 3 3 3 3 2 2 2 2 4 4 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.4 88.1 80.9 95.5 87.7 84.6 93.2 89.8 87.9 90.5 87.9 90.5 81.2 93.5 81.2 93.5 81.2 83.5 87.5 81.2 93.5 81.2 83.5 83.5 83.5 83.5 83.5 83.5 83.5 83.5	3457136.704 Group Area: F2 3457136.704 3189018.005 3184569.784 3131520.407 3032768.978 2420907381 2309984.246 221051362 2180416.19 2099533.479 2099533.479 2099533.479 2099533.479 2099533.479 21845911 1477574.46 1448182.689 1432077.925 1268752.828 1144294.075 1268752.828 1146294.075 1268752.828
18-B-Glycyrrhetinic acid Name 18-B-Glycyrrhetinic acid a-Eloostearic acid (35 4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexade-camanide 3-[2-(3-Hydroxyhenyl)ethyl]-5 Bit(2-ethythexyl)phthalate 2-Hydroxyhenyl-Hyl]-1 Bit(2-ethythexyl)phthalate 2-Hydroxyhenyl-Hyl[2- Ginsenoside Rg3 D-()-Glutamine Decosanamide Licochalcone A PEG n10 Xambolumol	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C16 H33 N O C24 H38 O4 C25 H16 O3 C24 H38 O4 C26 H3 N O3 C26 H38 O4 C27 H11 N O3 C29 H11 N O3 C29 H11 N O3 C22 H22 O10 C42 H72 O13 C22 H42 O11 C20 H42 O11 C20 H42 O11 C21 H22 O5 c10 H8 O4 C10 H22 O5 c10 H8 O4 C10 H22 O5 C13 H10 O4 C10 H22 O5 C13 H10 V3 C15 H10 V4 C10 H22 O5 C15 H10 V4 C15 H10 V5 C15	Full match  Full match  Compositions  Full match  Full	Full match Anotation Source-mcCloud Source-mcCloud Source-mcCloud Full match	Partial match Annotation Source: Chemöpider Search Partial match Not match Fall match Fall match Fall match Not the top hit Not the top hit Partial match Fall match	Fail match Amotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 198.1255 155.0695 254.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0691 339.1495 339.1495 339.1495 339.1418 192.425 254.0577 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 272.0683 164.0475 272.0685 164.0475	6.089 RT [min] 6.089 7.936 6.88 9.729 6.2 11.144 0.828 8.157 0.88 8.157 0.88 8.157 4.159 6.238 6.397 4.159 6.239 5.231 2.86 6.574 4.283	34571367 Area (Max.) 3457136,7 3189018,09 3184569,78 3184569,78 3181450,78 3131520,41 3032768,58 2270151,36 22009583,48 2009583,48 20095959,48 20095959,48 20095959,48 20095959,48 20095959,48 20095959,48 20095959,48 20095	23 ChemSpid or Results 23 19 4 4 34 4 34 4 24 11 31 31 0 15 38 44 4 1 1 25 38 44 1 0 15 34 4 19 19 19 19 19 19 19 19 19 19	# mcCload Results 2 3 2 2 3 2 2 3 2 2 6 6 10 0 5 1 1 2 2 4 4 6 2 2 4 4 2 8 8 8 4 4 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 4 4 5 5 3 2 2 3 3 3 2 2 2 4 4 4 4 4 2 2 2 3 3 3 2 2 2 4 4 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 83.8 80.9 95 87.7 84.6 93.2 87.9 90.8 87.9 90.6 81.2 93.2 87.9 90.6 81.2 83.8 83.1 87.9 90.0 84.6 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 87.9 90.0 87.9 90.0 87.9 90.0 87.9 90.0 87.9 90.0 87.9 90.0 87.0 87.0 87.0 87.0 87.0 87.0 87.0 8	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 240907.381 2209984.246 22150416.19 2099593.479 2090363.325 2180416.19 2099593.479 2090363.325 1857381 1577849.911 1477574.65 1571849.911 1477574.85 1146294.075 1070298.034 1146294.075 1070298.034 1146294.075 1070298.034 2126575.2828
18-β-Glycyrthetinic acid     Name     18-β-Glycyrthetinic acid     o-Elcostearic acid     (23,4,R)-3-(1-hydroxyhexyl)-4-     L-Hittidine     Hexade-anamide     12-(3-Hydroxyhenyl)ethyl]-2     Bi4(2-athythexyl)phthalate     2-Hydroxyphenyllanine     Adenosine     9-Oxo-10(E),12(E)-octadecadi     Glycitin     Ginsenoside Rg3     D-(-)-Glutamine     Docosanamide     Licochalcone A     PEG n10     Xamtholumol     7,3-Dihydroxy-4-methylcouma     Diddeelin     PEG n5     NN-Dicyclohexylurea     PEG n1     Naringenin     2-Hydroxyphenylanine	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O C16 H33 N O C24 H38 O4 C315 H16 O3 C2 H418 O4 C18 H30 O3 C2 H22 O10 C2 H22 O10 C2 H22 O10 C2 H42 N O C2 H22 O4 C2 H42 N O C2 H22 O4 C16 H10 N2 O3 C2 H22 O4 C10 H10 N2 O3 C15 H10 O4 C15 H10 O4 C15 H10 O4 C15 H10 O4 C15 H10 O4 C15 H10 O5 C15 H10 O5 C15 H10 O5 C15 H10 O4 C15 H10 O5 C15 H10	Full match  Pull match  Compositions  Full match  Full	Full match Amotation Source-mcCloud Source-mcCloud Source-mcCloud Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Not match Fall match Fall match Fall match Fall match Not the top hit Partial match Fall match	Fail match Amotation Source: MassList Match Fail match Fail match Fail match Fail match Fail match No resuls Fail match F	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 195.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 6146.0691 339.1495 338.1515 458.2729 354.166 192.0425 254.0577 238.1418 224.1887 502.299 272.0683	6.089 <b>RT</b> [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084 6.354 4.459 6.238 3.723 2.86 6.574 4.283 4.447	34571367 Area (Max.) 3189018.09 3184569.78 3184569.78 3134520.42 230984.25 2209151.36 2180416.19 2099593.48 2096563.33 1571849.91 1477574.46 1477574.46 1477574.46 1477574.46 1477574.87 1432077.92 1268752.83 1145294.07 1070298.03 1073090.78 975615.82	23 # ChemSpid er Results 23 19 4 4 18 4 4 36 26 41 34 24 34 24 11 1 1 31 0 15 1 1 34 25 34 26 4 11 1 1 1 1 1 1 1 1 1 1 1 1	# mcCload Results 2 3 3 2 2 6 6 10 5 1 1 2 2 4 4 6 2 2 4 4 6 8 8 8 8 8 8 8 8 4 4 2 2 2 1 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 1 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 3 3 2 2 2 3 3 3 3 3 2 2 2 2 3 3 3 3 3 2 2 2 2 4 4 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9           mcCloud           Best Match           96.9           92.2           83.8           901           91.9           92.3           94           88.1           901           92.2           83.8           90.1           91.9           92.3           88.0           91.9           92.2           87.9           90.8           87.9           90.6           81.2           93           90.6           81.2           93           80.3           80.3	3457136.704 Group Area: F2 3457136.704 3189018.005 3184569.784 3131520.407 3032768.978 2420907381 2309984.246 221051362 2180416.19 2099533.479 2099533.479 2099533.479 2099533.479 2099533.479 21845911 1477574.46 1448182.689 1432077.925 1268752.828 1144294.075 1268752.828 1146294.075 1268752.828
18-β-Glycyrrhetinic acid Name 18-β-Glycyrrhetinic acid a-Eloostearic acid (35,4R)-3-(1-yrhotroyhexyl)-4- L-Hittidine Hexadecanamide 3-[2-(3-Hydroxyphenyl)ethyl]-5 Bit(2-dnylhexyl) phrhalate 2-HydroxyphenylJalanine Adenosine 9-Ono-10(E),12(E)-octadecadi Glycitin Ginsenoside Rg3 D-(>-Glutamine Docosanamide Licochalcone A PEG n10 Xamfohumol 7.4-Dihydroxy-4-methylcouma Diddein DEG n5 N-Dicyclohexylurea PEG n5 N-Dicyclohexylurea	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C16 H33 N O C24 H38 O4 C25 H16 O3 C24 H38 O4 C26 H3 N 30 C27 H11 N 03 C29 H11 N 03 C29 H11 N 03 C22 H22 O10 C42 H72 O13 C22 H42 O11 C20 H42 O11 C20 H42 O11 C21 H22 O5 c10 H8 O4 C10 H22 O5 c10 H8 O4 C13 H20 O2 C15 H10 O4 C13 H20 O2 C15 H10 O4 C13 H20 O5 C13 H24 N O C13 H24 N O C13 H20 N C15 H10	Full match  Anotation Source: Predicted Connomitions Full match Fu	Full match Source mcCloud Source mcCloud Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match Partial match Pail match Pail match Pail match Pail match Not the top hit Partial match Not the top hit Partial match Not the top hit Partial match Pail match Pail match Fail match	Fail match Amotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 198.1255 155.0695 254.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 146.0691 339.1495 339.1495 339.1495 339.1418 192.425 254.0577 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 238.1418 254.0827 272.0683 164.0475 272.0685 164.0475	6.089 RT [min] 6.089 7.936 6.84 9.729 6.2 9.729 6.2 9.729 6.2 9.729 6.2 9.729 6.2 9.729 6.2 9.858 8.157 8.157 6.858 9.739 6.238 3.723 5.334 6.238 3.723 5.236 6.238 3.723 5.236 6.238 3.723 5.236 6.238 3.723 5.236 6.238 3.723 5.236 6.238 3.723 5.236 6.238 3.723 5.236 6.238 3.723 5.236 6.238 7.296 6.238 7.296 7.297 7.29	34571367 Area (Max.) 3457136,7 3189018,09 3184569,78 3184569,78 3181450,78 3131520,41 3032768,58 2270151,36 22009583,48 2009583,48 20095959,48 20095959,48 20095959,48 20095959,48 20095959,48 20095959,48 20095959,48 20095	23 ChemSpid or Results 23 19 4 4 34 4 34 4 24 11 31 31 0 15 38 44 4 1 1 25 38 44 1 0 15 34 4 19 19 19 19 19 19 19 19 19 19	# mcCload Results 2 3 2 2 3 2 2 3 2 2 6 6 10 0 5 1 1 2 2 4 4 6 2 2 4 4 2 8 8 8 4 4 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 4 4 5 5 3 2 2 3 3 3 2 2 2 4 4 4 4 4 2 2 2 3 3 3 2 2 2 4 4 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 83.8 80.9 95 87.7 84.6 93.2 87.9 90.8 87.9 90.6 81.2 93.2 87.9 90.6 81.2 83.8 83.1 87.9 90.0 84.6 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 85.2 87.9 90.0 87.9 90.0 87.9 90.0 87.9 90.0 87.9 90.0 87.9 90.0 87.9 90.0 87.0 87.0 87.0 87.0 87.0 87.0 87.0 8	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 240907.381 2209984.246 22150416.19 2099593.479 2090363.325 2180416.19 2099593.479 2090363.325 1867381 1577849.911 1477574.46 1448182.689 143207.925 1285752.828 1146294.075 1070298.034 1146294.075 1070298.034 216572.828 2165752.828
18-β-Glycyrrhetinic acid Name 18-β-Glycyrrhetinic acid a-Elcostearic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexade-anamide 3-[2-(3-Hydroxyhenyl)ethyl]-5 Bis(2-ethylhexyl)phthalate 2-Hydroxyhenyllaanine Adenosine 9-Oxo-10(E),12(E)-octadecadii Glycitin Ginsenovide Rg 3 D-(-)-Glutamine Docosanamide Licochalcone A PEG n10 Xaenthohumol 7,8-Dihydroxy-4-methylcoumat Daidaein PEG n5 Nx-Dicyclohexylurea PEG n11 Naringenin 2-Hydroxyhenylalanine Sakuranetin 1-Linolocyl glycerol	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 02 C16 H33 N0 C16 H33 N0 C16 H33 N0 C16 H33 N0 C16 H33 N0 C16 H33 N0 C16 H33 N0 C18 H30 O3 C22 H22 O10 C18 H30 O3 C22 H22 O10 C21 H22 O4 C21 H22 O4 C18 H30 O3 C21 H22 O4 C18 H30 O3 C21 H22 O4 C18 H30 O3 C21 H22 O4 C19 H11 N0 C10 H22 O5 C10 H26 O4 C13 H24 N0 C13 H22 O6 C13 H24 N2 C15 H12 O5 C9 H11 N03 C16 H14 O5 C9 H11 N03 C21 H22 O5 C15 H12 O5 C9 H11 N03 C19 H20 C16 H14 O5 C16 H15 O5 C16 H14 O	Full match  Anotation Source: Predicted Compositions Full match	Full match Amotation Source-mcClood Source-mcClood Full match	Partial match Annotation Source: Chem5pider Search Partial match Not match Fall match Fall match Fall match Fall match Not the top hit Not the top hit Partial match Fall match	Fail match Amotation Source: MassList Match Fail match Fail match Fail match Fail match Fail match No resuls Fail match F	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 178.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4856 1446.0971 338.1515 254.0577 258.1418 192.0425 254.0577 238.1418 224.1887 502.299 272.0683 164.0475 286.0841	6.089 RT [min] 6.089 7.936 6.84 9.729 6.2 11.144 0.828 8.157 0.88 8.157 0.88 8.157 0.88 8.157 0.88 8.157 0.88 8.157 0.88 8.157 0.88 8.157 0.88 8.157 0.88 8.157 0.432 5.594 0.948 6.997 4.432 5.594 0.948 6.6997 4.432 5.524 6.574 4.432 5.526 1.285 6.574 4.858 5.526 1.285 6.574 4.858 5.526 1.285 6.574 1.285 1	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3022768.89 22507369.03 2420907.38 2309984.25 2270151.36 2230984.25 22005181.33 1867381 1571289.93 1571289.93 1070298.03 1070298.	23 ChemSpile er Results er Results 23 19 4 4 36 26 26 26 26 26 26 26 26 26 2	# mcCload Results 2 3 2 2 3 3 2 2 6 6 10 5 1 1 2 2 2 4 4 6 6 2 4 4 2 2 4 4 2 2 4 4 2 2 3 3 7 2 5 10 10 5 5 110 10 5 5 110 10 10 5 5 10 10 10 10 10 10 10 10 10 10 10 10 10	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9           mcCloud           Best Match           96.9           92.2           83.8           901           91.9           92.3           94           88.1           901           92.2           83.8           90.1           91.9           92.3           88.0           91.9           92.2           87.9           90.8           87.9           90.6           81.2           93           90.6           81.2           93           80.3           80.3	3457136.704 Group Area: F2 3457136.704 31835018.005 3184569.784 3131520.407 3032768.978 2420907381 2309984.246 22180416.19 2099593.479 2098593.479 2098593.479 2098593.479 2098593.479 2098593.479 2098593.479 2098593.479 2098593.479 2098593.479 2098593.479 2098593.479 2098593.479 200859.479 200859 200859.479 200859.479 200859
Be-B-Glycyrrhetinic acid           Name           18-B-Glycyrrhetinic acid           a-Eloostearic acid           (S4,R4)-3-(1-hydroxyheyf)-4-           L-Hittidine           Hexadecaamide           3-[2-(3-Hydroxyheyf)-thyl]-5           Dis(2-6hyfhayf)           Dis(2-6hyfhayf)           Dis(2-6hyfhayf)           Dis(2-6hyfhayf)           Dis(2-6hyfhayf)           Dis(2-6hyfhayf)           Dis(2-6hyfhayf)           Dis(2-6hyfhayfhaine           Adenosine           D-Co-Clutamine           Daccoanamide           Licochalcone A           PEG n10           Xanthohumol           Assingenin           Dickyclohexylurea           PEG n11           Nx-Dicyclohexylurea           PEG n11           Nxringenin           2-Hydroxyphenylalanie           2-Hydroxyphenylalanie           Stydroxyphenylalanie	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C16 H33 N O C26 H33 N O C27 H11 N O3 C10 H13 N5 O4 C18 H30 O3 C22 H22 O10 C25 H10 N2 O3 C22 H40 N O C20 H22 O1 C20 H22 O5 C15 H10 O4 C10 H22 O6 C13 H20 N2 C25 H40 O12 C15 H10 O4 C16 H22 O6 C22 H46 O12 C15 H10 O4 C16 H12 O5 C22 H46 O12 C15 H10 O4 C16 H12 O5 C22 H46 O12 C15 H10 O4 C16 H12 O5 C22 H46 O12 C15 H10 O4 C16 H14 O5 C16 H14 O5 C16 H14 O5 C12 H38 O4	Full match  Anotation Source: Predicted Corresortions Full match	Full match Source-mcCloud Source-mcCloud Full match Full match	Partial match Amotation Source: ChemSpider Search Partial match Partial match Partial match Pail match Pail match Pail match Pail match Not the top hit Not the top hit Partial match Not the top hit Partial match Partial match Partial match Partial match Pail match No match Pail match No match Pail match Pai	Fail match Amotation Amotation Source: MassList Match Fail match F	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 198.1255 195.0695 244.1097 390.2761 164.0475 267.0965 204.2194 446.1211 766.4856 458.02761 338.1515 458.2729 354.1463 192.4425 254.0877 238.1418 224.1887 502.299 272.0683 164.0475 286.0841 354.2766	6089 RT [min] 6089 7.936 6082 9.739 60.828 9.729 11.144 1.195 0.828 9.729 11.144 1.195 0.828 8.157 4.432 5.594 4.432 6.973 1.286 6.574 4.423 4.423 4.447 0.886 5.263 9.33 9.33	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 318450.78 3131320.41 3032768.98 2270151.36 2270151.36 2209584.25 2200584.25 20096363.33 11571849.91 1571849.91 157714.64 1448182.69 1448182.69 1070296.05 1053099.78 975615.82 85740.277.2 85740.277.2 85740.277.25 1070286.05 1073289.05 10728	23 (ChernSpid er Results 23 19 4 4 36 26 41 34 24 24 11 1 1 31 0 15 1 25 38 44 41 1 1 31 0 15 34 26 4 19 34 34 26 4 19 34 34 26 4 19 34 34 26 4 19 34 34 26 26 34 19 34 26 26 34 19 34 26 26 34 19 34 26 36 36 26 38 38 41 11 1 25 38 38 44 41 1 1 25 38 44 41 1 1 25 38 38 44 44 4 38 44 4 4 4 4 4 4 4 4 4 4 4 4	# mcCloud Results 2 3 2 2 3 2 2 3 2 2 3 2 2 4 4 6 6 2 2 2 4 4 6 4 2 2 2 4 4 6 8 8 8 4 4 2 2 3 7 7 2 3 7 2 7 2 3 3 2 2 3 3 3 2 2 3 3 2 2 3 3 3 2 2 3 3 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 3 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 3 2 2 3 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 4 4 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9 mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 83.8 9.9 9.9 87.7 82.7 82.7 82.7 84.6 9.3 2 89.8 87.9 90.8 87.9 90.6 81.2 93.3 87.7 83.8 8.7 9.9 0.6 81.2 8.9 8.8 8.7 9.9 9.0 8.8 8.7 9.9 9.0 8.8 8.8 8.7 9.9 9.0 8.8 8.8 8.8 8.7 9.9 9.0 8.8 8.8 8.8 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9.0	3457136.704 Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2420997381 2420997381 2420997381 2420997381 2420997381 2420997381 242099738 21807381 1577849.911 1477574.46 21867381 1577849.911 1477574.45 21867381 1577849.911 1477574.45 21867381 218752.828 1146294.075 218578.2888 218578.288788 21857878.28878 218578.28878 218578.2887878 21
18-B-Glycyrthetinic acid Name 18-B-Glycyrthetinic acid a-Elcostearic acid (38,4R)-3-(1-hydroxythetyrt)-4- L-Hhitdine Hexafecanamide 1-(2-3-Hydroxythenyt)-ethyl]-5 Bia(2-ethythexyt) phthalate 2-Hydroxythenythalanine Adenosine 9-0xo-10(E),12(E)-octadecadii Glycitin Ginsenoside Rg3 D-(-)-Glutamine Docosanamide Licochalcone A PEG n10 Xamtholumol 7,8-Dihydroxy-4-methylcouma Daidzein PEG n5	C30 H46 O4 Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 02 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C18 H30 O3 C19 H11 N 0 C18 H30 O3 C22 H22 O10 C22 H22 O10 C22 H22 O10 C21 H22 O4 C21 H22 O4 C19 H12 N 0 C19 H12 O5 C21 H22 O4 C19 H12 O5 C10 H22 O6 C13 H22 O6 C13 H22 O6 C13 H22 O5 C22 H46 012 C15 H10 O4 C15 H10 O5 C21 H8 O4 C15 H10 O5 C11 H20 N2 O3 C11 H20 N2 O5 C11	Full match  Full m	Full match Amotation Source-mcClood Source-mcClood Full match Full	Partial match Annotation Source: Chem5pider Search Partial match Not match Fail match Fail match Fail match Fail match Not the top hit Partial match Not the top hit Partial match Fail mat	Fail match Amotation Source: MassList Match Fail match	FISh Coverage 14.91 	470.3392 Molecular Weight 470.3392 278.2245 198.1255 195.0695 255.256 244.1097 390.2761 164.0475 294.2194 446.1211 766.4856 146.0891 338.1515 458.2729 354.1463 192.0425 254.0577 238.1418 228.1475 502.299 272.0683 164.0475 354.266 284.1765 228.1475 285.0815 164.0475	6 0.89 RT [min] 6 0.89 7.936 6.84 0.828 9.729 6.24 11.144 1.195 0.88 8.157 4.432 0.948 4.437 5.594 0.948 4.159 6.238 5.231 2.865 4.423 5.231 2.8657 4.423 5.231 2.8657 4.423 5.231 2.8657 4.423 2.8657 4.423 2.8657 4.423 2.8657 4.423 2.8657 4.423 2.8657 4.423 2.8657 4.432 2.8657 4.432 2.8657 4.432 2.8657 4.432 2.8657 4.432 2.8657 4.432 2.8657 4.432 2.8657 4.432 2.8657 4.432 2.8657 4.432 2.8657 4.435 2.8657 4.432 2.8657 4.437 2.8657 4.437 2.8657 4.437 2.8657 4.447 2.833 2.833 2.833 2.833 2.833 2.833 2.833 2.833 2.835 2.833 2.835 2.833 2.8355 2.8355 2.8355 2.8355 2.8355 2.8355 2.8	3457136.7 Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3131520.41 302276.86 2420907.38 230984.25 2270151.36 2230984.25 2200518.33 1867381 15713849.91 1472574.46 143207792 1268752.83 11632909.78 975615.82 5738959.076 1073298.03 105309.78 975615.82 5738959.076 773889.514 7734846.835 14482.57 14482.57 107289.51 105309.78 10	23 ChemSpile r R-sults r R-sults r R-sults 23 19 4 4 36 41 11 31 0 15 15 15 15 16 44 41 1 1 31 0 15 16 4 4 4 4 4 5 6 6 4 4 4 4 5 6 6 6 6 6 6 6 6 6 6 6 6 6	# mcCload Results 2 3 2 2 3 3 2 2 6 6 10 5 1 1 2 2 2 4 4 6 6 2 2 4 4 2 2 8 8 8 4 4 2 2 2 4 10 5 10 10 5 10 10 5 10 10 10 2 2 2 3 3 2 2 2 2 3 3 2 2 2 2 3 3 2 2 2 2 3 3 3 2 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 3 3 3 2 2 2 3 3 3 3 2 2 2 2 3 3 3 3 2 2 2 2 2 2 3 3 3 3 2	# mzVanlt Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	96.9           mcCloud           Best Match           96.9           92.2           83.8           90.1           91.9           92.3           94           80.9           95.8           87.7           84.6           93.2           89.8           87.9           90.8           87.9           90.8           87.9           90.8           87.9           90.8           87.9           90.8           87.9           90.8           87.9           90.8           87.9           90.8           87.9           90.8           87.9           90.8           81.2           92.8           81.5	3457136.704 Group Area: F2 3457136.704 31859018.003 3184569784 3131520.407 3032768.978 2567369.032 2420907381 2569369.032 2420907381 2569369.032 2180416.19 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2186738 157429.278 15774.46 1445182.689 1432077.925 2186752.825 1146294.075 1070298.014 114727514.62 1146294.075 1070298.014 1070298.014 1070298.014 1070298.014 107399.0777 275959.0762 275959.0762

(a)

FIGURE 5: Continued.

Name	Formula	Annotation Source: Predicted Compositions	Annotation Source: mzCloud Search	Annotation Source: ChemSpider Search	Annotation Source: MassList Match	FISh Coverage	Molecular Weight	RT [min]	Area (Max.)	# ChemSpi der	# mzCloud Results	# mzVault Results	mzCloud Best Match	Group Area: F8
Oxymatrine	C15 H24 N2 O2	Full match	Full match	Partial match	Full match	14.55	264.18303	2.356	579229024.8	2	6	0	95.7	579229025
Proline	C5 H9 N O2	Full match	Full match	Full match	Full match	-	115.06352	0.865	128291737.3	50	4	0	83.2	128291737
Dibutyl phthalate	C16 H22 O4	Full match	Full match	Full match	Full match	47.83	278.15139		43509917.34	21	6	0	95.1	43509917.3
Isoliquiritigenin	C15 H12 O4	Full match	Full match	Full match	Full match	45.1	256.0732		43149066.46	34	6	0	97.5	43149066.5
Hexamethylenetetrami	C6 H12 N4 C5 H7 N O3	Full match Full match	Full match Full match	Full match	No results	23.53	140.10596 129.04274	14.469	36810028.01 31014849.17	3	2	0	97.5 81.7	36810028 31014849.2
L-Pyroglutamic acid Choline	C5 H13 N O	Full match	Full match	Not the top hit Partial match	Full match Full match	-	129.04274	0.816	28680713.24	12	4	0	81.7	28680713.2
DL-Stachydrine	C7 H13 N O2	Full match	Full match	Partial match	Full match		143.09467	1.062	23521925.51	52	4	0	85.2	23521925.5
DL-Arginine	C6 H14 N4 O2	No match	Invalid mass	No match	No results		157.08506		22767400.18	5	2	0	93.5	22767400.2
L-Norleucine	C6 H13 N O2	Full match	Full match	Not the top hit	Full match	-	131.09474		21421231.76	56	10	0	89	21421231.8
Pipecolic acid	C6 H11 N O2	Full match	Full match	Not the top hit	Full match	-	129.0791		20770655.33	68	8	0	82.8	20770655.3
Cytisine	C11 H14 N2 O	Full match	Full match	Not the top hit	Full match	33.33	190.11061		20174721.62	32	4	0	95.6	20174721.6
Asparagine	C4 H8 N2 O3	No match	Invalid mass	No match	No match	-	115.02698	0.844	17236595.01	11	4	0	86.4	17236595
D-(+)-Maltose	C12 H22 O11	No match	Invalid mass	No match	No results	-	364.0978	0.828	16746970.51	2	4	0	90.9	16746970.5
Trigonelline	C7 H7 N O2	Full match	Full match	Not the top hit	Full match	-	137.04758	0.867	14037685.87	47	18	0	93.7	14037685.9
(+)-Maackiain	C16 H12 O5	Full match	Full match	Partial match	Full match	-	284.06816	5.404	13303900.11	42	24	0	93.4	13303900.1
L-Phenylalanine	C9 H11 N O2	No match	Invalid mass	No match	No match	39.13	148.05249	1.985	12962993.12	33	4	0	96.9	12962993.1
DL-Tryptophan	C11 H12 N2 O2	No match	Invalid mass	No match	No match	-	187.06349	3.094	10793994.04	33	6	0	94.9	10793994
3-Hydroxy-2-methylp		Full match	Full match	Not the top hit	Full match	-	109.05311	0.862	8755620.954	36	10	0	86.5	8755620.95
Ononin	C22 H22 O9	Not the top hit	Full match	Not the top hit	Full match	-	430.12602	5.17	6128388.745	5	2	0	90.1	6128388.74
L-Tyrosine	C9 H11 N O3	No match	Invalid mass	No match	No match	-	164.04753	1.166	5143034.87	41	6	0	85.8	5143034.87
5-Hydroxymethyl-2-fa		Full match	Full match	Partial match	Full match	-	126.03195		4956561.398	26	12	0	89.1	4956561.4
Erucamide	C22 H43 N O	Full match	Full match	Partial match	Full match	39.13	337.33367		4661529.045	3	3	0	95.9	4661529.04
18-β-Glycyrrhetinic ac		Not the top hit	Full match	Partial match	Full match	15.88	470.3391	6.089	4402208.806	23	2	0	96.7	4402208.81
Anthranilic acid	C7 H7 N O2	Full match	Full match	Partial match	Full match	-	137.04758		3986402.448	47	12	0	93.5	3986402.45
a-Lactose	C12 H22 O11	Full match	Full match	Not the top hit	Full match	-	342.11555		3745394.204	17	2	0	86.9	3745394.2
Adenosine	C10 H13 N5 O4	Full match	Full match	Not the top hit	Full match	-	267.0967		3565462.707	34	2	0	89.8	3565462.71
	C5 H10 N2 O3	No match	Invalid mass	No match	No match	-	129.04262		3447711.429	24	3	0	86.3	3447711.43
L-Glutamine								6.861	3107090.822	4	3	0	83.7	
L-Glutamine (3S,4R)-3-(1-hydroxyl Betulin		No match Full match Annotation Source:	Invalid mass Full match	No match Partial match	No results Full match		198.12547 442.38046		2850840.167	42	2	0	83.7	3107090.82 2850840.17
(3S,4R)-3-(1-hydroxy Betulin Name	C11 H20 O4 C30 H50 O2 Formula	No match Full match Annotation Source: Predicted Compositions	Full match Annotation Source: mzCloud Search	Partial match Annotation Source: ChemSpider Search	Full match Annotation Source: MassList Match	FISh Coverage	442.38046 Molecular Weight	5.59 RT [min]	2850840.167 Area (Max.)	42 # ChemSpi der	# mzCloud Results	0 # mzVault Results	83.7 mzCloud Best Match	2850840.17 Group Area: F8
(3S,4R)-3-(1-hydroxy Betulin Name Betulin	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2	Full match Annotation Source: Predicted Compositions Full match	Full match Annotation Source: mzCloud Search Full match	Partial match Annotation Source:	Full match Annotation Source: MassList Match Full match		442.38046 Molecular Weight 442.38046	5.59 RT [min] 5.59	2850840.167 Area (Max.) 2850840.167	42 #	# mzCloud	0 # mzVault Results 0	83.7 mzCloud Best Match 83.7	2850840.17 Group Area: F8 2850840.17
(3S,4R)-3-(1-hydroxy) Betulin Name Betulin PEG n10	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11	Full match Annotation Source: Predicted	Full match Annotation Source: mzCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Full match	Full match Annotation Source: MassList Match Full match Full match		442.38046 Molecular Weight 442.38046 458.27269	5.59 RT [min] 5.59 4.161	2850840.167 Area (Max.) 2850840.167 2782623.267	42 # ChemSpi der 42 1	# mzCloud Results 2 2	0 # mzVault Results 0 0	83.7 mzCloud Best Match 83.7 88.1	2850840.17 Group Area: F8 2850840.17 2782623.27
(3S,4R)-3-(1-hydroxy) Betulin Name Betulin PEG n10 Maltol	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H50 O2 C20 H42 O11 C6 H6 O3	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match	Full match Annotation Source: mzCloud Search Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Full match Partial match	Full match Annotation Source: MassList Match Full match Full match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195	5.59 RT [min] 5.59 4.161 2.799	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77	42 # ChemSpi der 42 1 26	# mzCloud Results 2 12	0 # mzVault Results 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77
(35,4R)-3-(1-hydroxyl Betulin Betulin PEG n10 PEG n11	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit	Full match Annotation Source: mzCloud Search Full match Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No results	Full match Annotation Source: MassList Match Full match Full match Full match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909	5.59 RT [min] 5.59 4.161 2.799 4.284	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253	42 # ChemSpi der 42 1	# mzCloud Results 2 12 2 2	# mzVault Results 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2 88.5	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25
(35,4R)-3-(1-hydroxyl Betulin Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13	Full match Annotation Source: Predicted Compositions Full match Not the top hit Not the top hit Not match	Full match Annotation Source: mzCloud Search Full match Full match Full match Invalid mass	Partial match Annotation Source: ChemSpider Search Partial match Full match Full match No results No match	Full match Annotation Source: MassList Match Full match Full match Full match No results		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447	42 # ChemSpi der 42 1 26 0 1	# mzCloud Results 2 12	0 # mzVault Results 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2 88.5 83.2	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45
(3S,4R)-3-(1-hydroxyl Betulin Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C22 H22 O10	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit	Full match Annotation Source: mzCloud Search Full match Full match Full match Invalid mass Full match	Partial match Annotation Source: ChemSpider Search Partial match Full match No results No match Partial match	Full match Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822	42 # ChemSpi der 42 1 26 0 1 11	# mzCloud Results 2 2 2 12 2 4 2 4 2	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82
(3S.4R)-3-(1-hydroxyl Betulin PEG n10 Maltol PEG n10 Giusenoside Rg3 Glyeitin L-Giutamie acid	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C22 H20 O10 C5 H9 N O4	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit Not the top hit Full match	Full match Annotation Source: mzCloud Search Full match Full match Full match Full match Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No results No results No match Partial match	Full match Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852	2850840.167 Area (Max.) 2850840.167 2782623.267 2098519.253 1792976.447 1783088.822 1748442.833	42 # ChemSpi der 42 1 26 0 1 11 31	# mzCloud Results 2 2 12 2 2 4 2 5	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 88.5 83.2 86.7 82.7	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1792976.45 1783088.82 1748442.83
(3S.4R)-3-(1-hydroxyl Betulin PEG n10 Maltol PEG n10 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylhexyl) phth	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C22 H22 O10 C5 H9 N O4 C24 H38 O4	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit No match Not the top hit Full match Not the top hit Full match Not the top hit Full match	Full match Annotation Source: mzCloud Search Full match Full match Full match Invalid mass Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Full match Full match	Full match Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 706.48533 446.12103 147.05307 390.2762	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007	42 # ChemSpi der 42 1 26 0 1 11 31 26	# mzCloud Results 2 2 2 2 2 2 4 2 2 5 10	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 83.2 86.7 82.7 94.2	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1782442.83 1545042.01
(35,4R)-3-(1-hydroxyl Betulin PEG n10 Maltol PEG n10 Ginsenoside Rg3 Glycitin L-Ghatamic acid Bis(2-ethylfacyl) phth 7,8-Dhyldycory-4-mett	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C42 H72 O13 C42 H72 O10 C5 H9 N O4 C24 H38 O4 C10 H8 O4	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match	Full match Annotation Source: mzCloud Search Full match Full match Full match Full match Full match Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Full match Partial match No results No match Partial match Full match Full match Full match	Full match Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match Full match Full match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 147.05307 390.2762 192.04254	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919	42 # ChemSpi der 42 1 26 0 1 11 11 31 26 38	# mzCloud Results 2 2 12 2 2 4 2 5	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 82.7 94.2 88.1	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82 1748442.83 1545042.01 1545042.01 1252325.92
(3S.4R)-3-(1-hydroxyl Betulin PEG n10 Maltol PEG n10 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylhexyl) phth	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C42 H72 O13 C42 H72 O10 C5 H9 N O4 C24 H38 O4 C10 H8 O4	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit Full match Not the top hit Full match Full match Full match	Full match Annotation Source: mzCloud Search Full match Full match Full match Invalid mass Full match Full match Full match Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Full match Full match	Full match Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match Full match Full match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 706.48533 446.12103 147.05307 390.2762	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007	42 # ChemSpi der 42 1 26 0 1 11 31 26	# mzCloud Results 2 2 2 2 2 2 4 2 2 5 10	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 83.2 86.7 82.7 94.2	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1782442.83 1545042.01
(35.4R)-3-(1-hydroxy) Betulin Detulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Ghttamie acid Bis(2-ethylhexyl) phth 7.8-Dihydroxy-4-meth N.N-Dicyclohexylure PEG n5	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C24 H32 O10 C5 H9 N O4 C24 H38 O4 C10 H8 O4 C13 H24 N2 O	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match Full match Full match Full match Full match Full match	Full match Annotation Source: mzCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Full match Full match Full match Full match	Full match Annotation Source: MassList Match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852	5.59 <b>RT [min]</b> 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.47 1792976.47 1792305.41 1792305.41 1545042.007 1252325.919 1171308.019	42 # ChemSpi der 42 1 26 0 1 1 11 311 26 38 6	# mzCloud Results 2 2 2 12 2 4 4 2 5 10 0 8 1	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 82.7 94.2 88.1 91.5 86.4	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792076.45 1793088.82 1748442.83 1545042.01 1252325.92 1171308.02 1165243.83
(IS.4R)-3-(1-hydroxyl Betulin PEG n10 PEG n10 PEG n11 Ginsenoside Rg3 Glyciin L-Ghtamis acid Bis(2-ethyfhexyl) pHi 7.8-Dihydroxy-4-mett N-N-Dicyclohexylure PEG n5 9-Oxo-10(E),12(E)-oc	C11 H20 04 C30 H50 02 Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C42 H72 013 C42 H72 013 C42 H38 04 C24 H38 04 C10 H20 04 C10 H20 05 C18 H30 03	Full match Amoution Source: Predicted Compositions Foll match Not the top hit Full match Not the top hit Not the top hit Not the top hit Not the top hit Full match Full match Full match Full match Full match Full match	Full match Annotation Source: mcCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Full match Partial match No results No match Partial match Full match Full match Full match	Full match Annotation Source: MaseList Match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29009 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.232	2850840.167 Area (Max.) 2850840.167 2782623.267 2999740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1171308.019 1165243.832 1003683.429	42 # ChemSpi der 42 1 26 0 0 1 1 11 31 26 38 6 6 1	# mzCloud Results 2 2 2 12 2 4 4 2 5 10 8 1 4 4 4 2 5 10 8 1 4 4	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.1 85.2 88.5 83.2 86.7 82.7 94.2 88.1 91.5 86.4 91.1	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82 1748442.83 1545042.01 1252325.92 1165243.83 1003683.43
(35.4R)-3-(1-hydroxyl Betulin Detulin Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycifin L-Ghttamic acid Bis(2-ethylhexyl) phth 7.8-Dihydroxy-4-meti NN-Dicyclohexylure PEG n5 9-0xo-10(E),12(E)-oc Naringenin	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C24 H32 O10 C5 H9 N O4 C24 H38 O4 C10 H8 O4 C13 H24 N2 O	Full match Annotation Source: Predicted Compositions Full match Not the top hit Full match Full match Full match Full match Full match Full match	Full match Annotation Source: mzCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Full match Full match Full match Full match	Full match Annotation Source: MassList Match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29009 766.48533 766.48533 147.05307 390.2762 192.04254 124.18852 238.14166	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.232 4.445	2850840.167 Area (Max.) 2850840.167 2782623.267 2999740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1171308.019 1165243.832 1003683.429	42 # ChemSpi der 42 1 26 0 1 111 31 26 38 6 1 1 24	# mzCloud Results 2 2 2 2 2 2 2 4 2 5 5 10 8 1 4 2 2 2 2 4 2 2 2 2 2 2 2 2 2 2 2 2 2	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 83.1 83.2 88.5 83.2 86.7 82.7 94.2 88.1 91.5 86.4 91.1	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1793088.82 1748442.83 1545042.01 1252325.92 1171308.02 1165243.83
(35.4R)-3-(1-hydroxyl Betulin Detulin Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycifin L-Ghttamic acid Bis(2-ethylhexyl) phth 7.8-Dihydroxy-4-meti NN-Dicyclohexylure PEG n5 9-0xo-10(E),12(E)-oc Naringenin	C11 H20 O4 C30 H50 O2 C20 H50 O2 C20 H42 O11 C42 H42 O11 C42 H72 O13 C42 H46 O12 C42 H72 O13 C42 H72 O10 C5 H9 N O4 C10 H8 O4 C10 H8 O4 C10 H22 O6 C18 H30 O3 C15 H12 O5	Full match Aunotation Source: Predicted Compositions Fall match Not the top hit Fall match Not the top hit Fall match Not the top hit Fall match	Full match Annotation Source: mcCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match Partial match No results No match Partial match Full match Full match Full match Full match Full match Full match Not the top hit Full match Not the top hit Full match	Full match Annotation Source: MaskList Match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48333 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935 272.06832	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.232 4.445	2850840.167 Area (Max.) 2850840.167 278263.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1165243.832 1003683.429 948756.3665	42 # ChemSpi der 42 266 0 0 1 11 311 266 38 6 1 244 46	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 2 4 2 5 10 8 8 1 4 4 2 10 10	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 83.7 83.2 86.7 83.2 86.7 94.2 88.1 91.5 86.4 91.1 87.1	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792076.45 1792076.45 1792076.45 1792076.45 1783088.82 1748442.83 1545042.01 1252325.92 171308.02 1165243.83 1003683.43 948756.367
(35.4R)-3-(1-hydroxyl Betulin PEG II 10 Maltol PEG II 10 Ginsenoside Rg3 Glyciin L-Ghtamie acid Bisi(2-ethylhexyl) phil N-R-Dipylohexylure PEG II 5 9-Chor-10(E),12(E)-oc Naringenin Glucose 1-phoophate	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C24 H72 O13 C24 H22 O10 C24 H38 O4 C10 H38 O4 C10 H38 O4 C10 H24 N2 O C10 H20 O3 C15 H12 O5 C18 H30 O3 C15 H12 O5 C18 H30 O3 C15 H12 O5	Full match Amoution Source: Predicted Compositions Full match Not the top hit Full match Not the top hit Full match Not the top hit Full match Full match Full match Full match Full match Full match Full match Full match	Full match Annotation Source: mcCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match Partial match No results No match Partial match Full match Full match Full match Full match Full match Full match Not the top hit Full match Not the top hit Full match	Full match MassList Match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29009 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935 272.068322 260.02962	5.59 RT [min] 5.59 4.161 2.799 4.284 5.439 0.852 11.155 3.746 6.584 2.895 7.232 4.439 0.852 0.901	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792076.447 1783088.822 1748442.833 1792076.447 1783088.822 1748442.833 17454052.007 1252325.919 1173308.019 1165243.832 948756.3665 941408.0067	42 # ChemSpi der 42 1 26 0 1 111 31 31 26 38 6 6 1 1 24 46 6 39	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 2 4 2 5 10 8 8 1 4 4 2 10 10	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzCloud Best Match 83.7 88.5 83.2 88.5 83.2 88.7 94.2 88.1 91.5 86.4 91.1 87.1 87.1 87.1	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82 1784842.83 1545042.01 1253232.92 1171308.02 1165243.83 1003083.43 948756.367 911408.607
(IS.4R)-3-(1-hydroxyl Betulin Betulin PEG n10 Maltol PEG n10 Ginsenoside Rg3 Glycitin L-Glutamie acid Bis(2-ethylhexyl) phth 7.8-Dilydroxy-4-meti NN-Dicyelohexylure PEG n5 9-Orae-10(E),12(E)-oc Naringenin Glucose 1-phosphate Stearamide	C11 H20 04 C30 H50 02 C20 H50 02 C20 H42 011 C26 H6 03 C22 H46 012 C42 H72 013 C42 H72 013 C42 H72 013 C22 H22 010 C5 H9 N 04 C10 H8 04 C10 H8 04 C13 H24 N2 0 C19 H22 06 C18 H30 03 C15 H12 05 C6 H13 09 P C18 H37 N 0	Full match Aunotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit Full match Not the top hit Full match	Full match mcCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Partial match Partial match Full match Partial match Partial match Partial match	Full match Annotation Source: Massatist Match Full match		442.38046 Molecular Weight 442.38046 4458.27269 126.03195 502.29909 766.48533 446.12103 147.0307 390.2762 192.04254 224.18852 224.18852 224.18852 224.18852 224.18852 226.002962 260.02962 263.28703	5.59 <b>RT [min]</b> 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.232 4.285 7.232 4.658 0.901 10.658 0.876 0.876	2850840.167 Area (Max.) 2850840.167 2782623.267 2599740.77 2008519.253 1792976.447 178308.822 1748442.833 1545042.007 1252325.91 117308.019 1165243.832 100363.429 914876.3605 911408.6067	42 # ChemSpi der 42 1 26 0 1 1 11 31 26 38 6 1 24 46 6 39 4 4 6 39 4 20 6	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 2 4 2 5 10 8 8 1 4 4 2 10 10	0 # mzVauk Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mtCload Best Match \$3.7 \$8.1 \$9.2 \$8.5 \$3.2 \$6.7 \$2.7 \$4.2 \$8.1 91.5 \$6.4 91.1 \$7.1 \$7.1 \$8.9 \$1.5 \$6.4 \$9.1 \$1.5 \$1.5 \$6.4 \$1.5 \$1.5 \$1.5 \$1.5 \$1.5 \$1.5 \$1.5 \$1.5	2850840.17 Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1793088.26 1745442.83 1545042.01 1253235.92 1175208.83 115523.83 948755.367 911408.607 885834.119
(35.4R)-3-(1-hydroxyl Betulin PEG n10 Małtol PEG n10 Glusenoside Rg3 Glyciin L-Ghtamie acid Bis(2-ethylhexyl) phł N-N-Dicyclohexyhure PEG n5 9-Oxo-10(E),12(E)-oc Naringenin Glucose 1-phosphate Stearamide Guanine	C11 H20 O4 C30 H50 O2 Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C24 H72 O13 C24 H72 O13 C24 H72 O13 C24 H27 O13 C24 H22 O10 C10 H38 O4 C13 H24 N2 O C10 H24 N2 O C10 H22 O6 C15 H37 N O C15 H37 N O C15 H37 N O C15 H37 N O C11 H12 O N2 O3 C11 H12 N2 O3 C14 H30 N3 O1 C14 H20 N2 O3 C14 H20 N2 O4 C14 H37 N O	Full match Amoution Source: Predictor Compositions Pall match Not the top hit Full match Not the top hit Full match Not the top hit Full match	Full match Annotation Source: mr2Cloud Search Foil match Foil match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Full match	Full match MaskList Match Full match		442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48333 446.12103 446.12103 446.12103 192.04254 224.18852 224.18852 224.18852 224.18852 224.18852 224.18852 224.2835 272.06832 200.02962 283.28703 151.04936	5.59 <b>RT [min]</b> 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.232 4.445 0.901 10.658 0.901 10.658 0.858	2850840.167 Area (Max.) 2850840.167 2599740.77 2098519.233 1792976.447 1783088.822 1748442.833 1748442.833 1748442.833 1748442.833 1748442.833 174854.855 911408.8425 911408.8425 911408.8405	42 # ChemSpi der 42 1 26 0 0 1 1 11 31 26 0 0 1 1 31 26 0 0 1 1 11 31 26 0 0 1 1 11 26 0 0 0 1 1 11 26 0 0 0 1 1 11 26 0 0 0 1 1 12 0 0 0 0 1 1 12 0 0 0 0 1 1 1 1	# mzCloud Results 2 2 2 2 2 4 4 2 5 5 10 8 11 4 4 2 10 0 2 2 1 1	0 # mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mtCload Best Match \$3.7 \$8.1 \$9.2 \$8.5 \$3.2 \$6.7 \$2.7 \$4.2 \$8.1 91.5 \$6.4 91.1 \$7.1 \$7.1 \$8.9 \$1.5 \$6.4 \$9.1 \$1.5 \$1.5 \$6.4 \$1.5 \$1.5 \$1.5 \$1.5 \$1.5 \$1.5 \$1.5 \$1.5	2850840.17 Group Area: F8 2850840.17 27599740.77 20599740.77 2059519.25 1748442.83 1748442.83 1748442.83 1545042.00 1165243.83 1003083.43 948756.367 911408.607 885834.119 840032.158
(IS.4R)-3-(1-hydroxyl Betulin PEG n10 Maltol PEG n10 Maltol PEG n11 Giusenoside Rg3 Glycinin L-Ghatamie acid Bis(2-ethyfhexyl) phth 7.8-Dilydroxy-4-meti Bis(2-ethyfhexyl) phth 7.8-Dilydroxy-4-meti Bis(2-ethyfhexyl) phth 7.8-Dilydroxy-4-meti Bis(2-ethyfhexyl) phth 7.8-Dilydroxy-4-meti Bis(2-ethyfhexyl) phth 7.8-Dilydroxy-4-meti Bis(2-ethyfhexyl) phth 8-Cox-10 (DE),12(E)-oc Naringenin Glucose 1-phosphate Stearamide Guanine Leusylprofine	C11 H20 04 C30 H50 02 C30 H50 02 C20 H42 011 C20 H42 011 C2 H46 012 C42 H72 013 C42 H72 013 C42 H72 013 C42 H72 013 C42 H72 013 C14 H38 04 C10 H8 04 C10 H8 04 C13 H24 N2 04 C16 H13 03 C15 H12 05 C18 H50 03 C15 H12 05 C1 H20 N2 03 C5 H5 N5 0 C1 H20 N2 03 C26 H54 014 C16 H30 N2 02 C26 H54 014 C16 H30 N2 02 C26 H54 014 C26 H30 N2 02 C26 H54 014 C26 H30 N2 02 C26 H54 014 C26 H30 N2 02 C36 H54 014 C36 H30 N2 02 C36 H54 014 C36 H30 N2 02 C36 H50 N2 02	Full match Amototion Source: Predicted Compositions Full match Not the top hit Full match Not the top hit Not match Not the top hit Full match	Full match Annotation Source: mcCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Full match Partial match No metch Partial match Full match Full match Full match Full match Full match Full match Full match Full match Partial match Partial match Partial match Partial match	Full match Annotation Source: Mascilat Match Full match	Coverage	442.38046 Molecular Weight 442.38046 445.27269 126.03195 502.29099 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 224.18852 224.18852 224.18852 224.18852 224.18852 224.18852 224.1852 224.1852 224.1852 260.02962 283.28703 151.04936 228.1476 590.35113 112.02789	5.59 <b>RT [min]</b> 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.232 4.285 7.232 4.658 0.901 10.658 0.876 0.876	2850840.167 Area (Max.) 2850840.167 2890840.167 2890740.77 2899740.77 2098519.233 1792976.447 1783088.822 1784842.833 17454042.007 1165243.832 1165243.832 1165243.832 1160368.422 914876.636 91408.6605 84032.4178 84032.1577	42 # ChemSpi der 42 1 266 0 1 111 311 266 388 6 6 1 1 244 406 399 4 420 6 0 0 288	# mzCloud Results 2 2 2 2 2 4 4 2 5 5 10 8 11 4 4 2 10 0 2 2 1 1	* mzVauk Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzClood Best Match 83.7 83.7 83.7 83.7 83.7 91.2 83.1 91.5 86.4 91.1 81.9 91.5 86.4 91.1 81.9 85.9 81.6 87.3 83.4 83.3 83.4	2850840.17 Group Area: F8 2850840.17 2782623.27 2589740.77 2098519.25 1792976.45 1792976.45 17450442.83 17450442.83 1545042.01 1252325.92 1171308.02 1155243.83 1003683.43 948756.367 911408.637 885834.119 8840032.158 840032.158
(35.4R)-3-(1-hydroxyl Betulin PEG n10 Maltol PEG n10 Maltol PEG n11 Glycriin L-Ghtamie acid Bis(2-ethylhexyl) phth 7.8-Dhydroxy-4-mett N.N-Dicyclohexylure PEG n5 9-0xo-10(E),12(E)-ec Naringenin Glucoxe 1-phosphate Stearmnide Guanine Leuxylproline PEG n13 Uracil Monobutyl phthalate	C11 H20 04 C30 H50 02 Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C24 H22 010 C24 H27 013 C24 H27 013 C24 H27 013 C24 H22 010 C10 H28 04 C13 H24 N2 0 C10 H24 N2 0 C15 H30 09 P C15 H30 09 C15 H30 09 C1	Full match Amototion Source: Predicted Compositions Full match Not the top hit Full match Not the top hit Full match Not the top hit Full match	Full match Annotation Source: mcCloud Search Foll match Foll match	Partial match Annotation Source: ChemSpider Search Partial match Partial match No match Partial match Partial match Full match Full match Full match Full match Partial ma	Full match Annotation Source: Massatist Match Full match	Coverage	442.38046 Molecular Weight 442.38046 445.27269 126.03195 502.29909 766.48333 446.12103 147.05307 390.2762 192.04254 224.18852 272.06832 204.21935 272.06832 260.02962 228.1876 590.35113 112.02769 222.0889	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 7.232 4.445 0.807 7.232 4.445 0.807 7.232 4.445 0.807 7.232 4.445 0.807 7.232 4.445 0.807 7.232 4.469 1.094 6.327 4.69 1.094 1.054 1.055 1.057 1	2850840.167 Area (Max.) 2850840.167 278260840.167 278260840.167 278260840.2008519.253 2008519.253 2008519.253 2008519.253 2008519.253 2008519.253 21784842.833 1792076.447 1783088.822 1784842.833 1165243.855 911408.6067 858384.1188 840032.1577 804307.6478 879721.2017 672279.754 662943.6763	42 # ChemSpi der 42 1 266 0 0 1 1 11 31 266 388 6 1 24 46 399 4 24 46 399 4 228 45 24 45 26 28 45 28	# mzCloud Results 2 2 2 2 2 4 4 2 5 5 10 8 11 4 4 2 10 0 2 2 1 1	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzClood Best Match \$3.7 \$3.1 \$9.2 \$3.5 \$3.2 \$3.2 \$3.5 \$3.2 \$3.2 \$3.2 \$3.5 \$3.2 \$3.2 \$3.5 \$3.2 \$3.7 \$3.7 \$3.7 \$3.7 \$3.7 \$3.7 \$3.7 \$3.7	2850840.17 Group Ares: F8 2850840.17 2850840.12 2599740.77 2098519.25 1792076.45 1792076.45 1792076.45 1783088.82 1745442.83 1745442.83 1030683.43 948756.367 911408.607 885834.119 440302.158 804307.648 804307.648 662943.376 662943.376 662943.376
(IS.4R)-3-(1-hydroxyl Betulin PEG n10 Maltol PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Ghtamis acid Bis(2-ethyfhexyl) phft N-Dicyclochexylure PEG n5 9-Oxo-10(E),12(E)-oc Naringenin Ghucose 1-phosphate Stearamide Guanine Leucylproline PEG n13 Urracil Monobutyl phthalate L-Histidine	C11 H20 04 C30 H50 02 C30 H50 02 C20 H42 011 C20 H42 011 C21 H46 012 C42 H72 013 C42 H72 013 C42 H72 013 C42 H72 013 C24 H72 013 C24 H72 013 C24 H38 04 C10 H38 04 C10 H38 04 C10 H20 05 C18 H30 03 C15 H12 05 C18 H30 03 C15 H12 05 C18 H37 N 0 C18 H37 N 0 C26 H37 N 0 C26 H37 N 0 C11 H20 N2 03 C36 H37 N 0 C11 H20 N2 03 C11 H20 N2 03 C11 H20 N3 03 C11 H20 N3 02 C11 H20 N3 03 C11 H20 N3 03 C13 H21 H20 N3 03 C13 H20 N3 03 C14 H30 N3 03 C14 H	Full match Annotation Source: Predicted Compositions Fall match Not the top hit Fall match Not the top hit Fall match Not the top hit Fall match	Full match Annotation Source: mcCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Putl match Putl match No results No match Partial match Full match Ful	Full match Annotation Source: MascList March Full match	Coverage	442.38046 Molecular Weight 442.38046 442.38046 442.38046 442.38046 442.38046 126.03195 502.2900 766.48533 446.12103 446.12103 192.04254 224.18852 228.14166 244.21935 272.06832 228.1426 290.238147 590.35113 112.02769 222.0889 125.06849 222.0889 155.06949 255.08490 222.0889 255.08590 222.0889 255.08590 222.0889 255.08590 222.0889 255.08590 255.08590 222.0889 255.085900 255.085900 255.085900 255.085900 255.085	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.852 1.055 7.232 4.445 0.901 10.658 0.876 2.987 4.469 1.094 6.327 0.832	2850840.167 Area (Max.) 2850840.167 25978623.267 2599740.77 2599740.77 2098519.253 1792976.447 1783088.822 1748442.831 1745442.807 11753088.422 1030583.429 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3655	42 # ChemSpi der 42 1 266 0 0 1 111 311 266 388 6 1 1 44 46 338 6 1 244 46 339 4 20 6 6 0 0 28 5 45 1 28 5 1 28 5 1 28 5 1 28 5 1 20 1 20 1 20 1 20 1 20 1 20 1 20 1	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 4 4 2 5 5 00 8 8 1 1 4 2 2 2 2 1 2 2 4 3 4 4 2 2 2 4 4 3 4 4 2 2 2 2 2 2	* mzVauk Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mzClood Best Match 83.7 83.7 83.5 83.5 83.5 83.2 83.7 94.2 83.1 91.5 86.4 91.1 87.1 81.9 91.1 81.9 91.1 81.9 91.3 81.6 83.4 83.4 83.4 83.4 83.4 83.4 88.5 9.8 88.5 83.4 83.4 83.4 83.5 83.5 83.5 83.5 83.5 83.5 83.5 83.5	2850840.17 Group Area: F8 2850840.17 2759263.23 27592740.77 2599740.77 2098519.25 1783088.82 1783088.82 1783088.82 1783088.82 1783088.83 1545042.01 1253225.92 1173308.02 115524.33 1003683.43 948756.367 911408.637 911408.637 911408.037 645943.475 6659854.489
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(SS.4R)-3-(1-hydroxyl Betulin PEG n10 PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glyciin L-Ghtamie acid Bisi(2-ethylhexyl) phth Glycoin acid NN-Dicyclohexylure PEG n5 9-Oxo-10(E),12(E)-oc Naringenin Glucose 1-phosphate Stearamide Guanine Leucylproline PEG n13 Uracil Monobutyl phthalate L-Histidine 2-Hydroxycinnamic as Cyclo(Eucsylprolyl)	C11 H20 04 C30 H50 02 C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C24 H72 013 C24 H72 013 C24 H72 013 C24 H22 010 C10 H50 04 C10 H50 04 C10 H50 04 C10 H50 03 C16 H12 05 C11 H20 N2 03 C15 H37 N0 C11 H20 N2 03 C26 H3 01 C26 H3 01 C26 H3 03 C11 H120 N2 03 C12 H14 04 C12 H160 N2 C12 H160 N2 C11 H180 N2 C	Full match  Amoution Source: Prediction Compositions Pall match Not the top hit Full match Full	Full match Annotation Source: mcCloud Search Full match Full match	Partial match Annotation Source: ChemSpider Search Putl match Putl match No results No match Putl match Full match Putl Putl Putl Putl Putl Putl Putl Putl	Full match Annotation Source: Masalist Match Full match	Coverage	442.38046 Molecular Weight 442.38046 442.38046 442.38046 442.38046 445.2726 50.29909 766.48533 446.12103 147.05307 390.2762 192.0424 224.18852 228.1476 590.35113 151.04936 228.3476 590.35113 112.02769 222.0889 155.06949 154.04749 210.13866	5.59 RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.435 0.901 10.658 0.876 2.987 4.469 1.094 6.327 0.833 3.412 4.22	2850840.167 Area (Max.) 2850840.167 2782031.267 2989740.77 2098519.253 1792976.447 1793085.822 1748442.833 1793097.444 171308.019 1165243.832 171454042.007 885884.41188 840032.1577 804307.6478 759721.2017 672297.374 662943.6763 6629854.4199 612912.9287 571451.973	42 # ChemSpi der 42 1 26 0 1 1 11 31 3 1 24 4 6 6 3 9 4 4 5 6 0 0 2 8 8 6 0 1 2 4 4 5 6 8 9 4 2 0 0 1 1 1 3 1 2 6 9 9 9 4 2 1 2 6 9 9 1 2 6 9 9 1 2 6 9 9 1 2 6 9 9 1 2 6 9 9 1 1 1 1 3 1 2 6 9 9 1 2 6 9 9 1 1 1 1 1 1 2 6 9 9 1 1 1 1 1 1 2 6 9 9 1 1 1 1 1 2 6 9 9 1 1 1 1 1 2 6 9 9 1 1 1 1 1 2 6 9 9 1 1 1 1 1 2 6 9 9 1 1 1 1 1 2 6 9 9 1 1 1 1 2 6 9 9 1 1 1 1 1 1 1 1 2 6 9 9 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 4 4 2 5 5 00 8 8 1 1 4 2 2 2 2 1 2 2 4 3 4 4 2 2 2 4 4 3 4 4 2 2 2 2 2 2	* mzVauk Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mrCloud Best Match 83.7 88.1 83.2 86.7 82.7 94.2 88.1 91.5 86.4 91.1 87.1 81 92.1 87.1 81.6 87.3 83.4 83.6 87.3 83.8 85.8 83.4 83.8 83.8 83.8 83.8 83.8 83.8 83	2850840.17 Group Area: F8 285084.01 285084.01 285084.01 2559740.77 2088519.25 1792976.42 1783088.52 1783088.52 1784842.83 1783088.52 1783088.52 1783088.52 1783088.52 1783088.52 178308.52 1783
(IS.4R)-3-(1-hydroxyl Betulin PEG n10 Maltol PEG n10 Maltol PEG n11 Giusenoside Rg3 Glycitin L-Ghttamie acid Bis(2-ethylhexyl) phth 7.8-Dihydroxy-4-meti Bis(2-ethylhexyl) phth 7.8-Dihydroxy-4-meti Bis(2-ethylhexyl) phth 7.8-Dihydroxy-4-meti Disylochoexylare PEG n5 9-Oxo-10(E),12(E)-oc Naringenin Glucose 1-phosphate Stearamide Guanise Leusylproline PEG n13 Urracil Monobutyl phthalate L-Histidine 2-Hydroxycinnamic as Cyclo(leusylprolyl)	C11 H20 04 C30 H50 02 C20 H50 02 C20 H42 011 C2 H42 011 C2 H46 012 C2 H46 012 C2 H22 010 C5 H9 N 04 C10 H8 04 C11 H20 N2 05 C18 H30 N3 C2 H37 N 0 C5 H9 N 50 C11 H20 N2 03 C2 H437 N 0 C5 H9 N5 0 C11 H20 N2 03 C2 H437 N 0 C5 H9 N5 0 C11 H20 N2 03 C2 H43 N3 02 C12 H14 04 C6 H9 N3 02 C9 H8 03 C11 H18 N2 02 C2 H43 N 0	Full match Aunotation Source: Predicter Predicter Source: Predicter Source: Predicter Not the top hit Pail match Not the top hit Not the top hit Full match Not the top hit Full match Full	Full match  Annotation Source: mrCloud Search  Full match Full mat	Partial match Annotation Source: ChemSpider Search Full match Full	Full match Annotation Source: Maski at Match Full match	Coverage	442.38046 Molecular Weight 442.38046 458.27269 126.03195 502.29090 766.48533 147.05307 390.2762 192.04254 294.21035 294.21035 294.21035 294.21035 294.21035 294.21035 151.04936 228.1476 590.35113 151.04936 228.1476 590.35113 151.04936 228.1476 590.35113 151.04936 228.1476 590.35113 151.04936 228.1476 590.35113 152.06949 155.06949 155.06949 155.06949 210.13686 339.34957 210.13686 339.34957 210.13686 339.34957 210.13686 200.14686	5.59 <b>RT [min]</b> 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.232 4.445 0.901 10.658 0.861 2.987 4.469 1.094 4.6327 0.833 3.412 4.27 1.033 3.412 4.27 1.3101	2850840.167 Area (Max.) 2850840.167 2782623.267 2589740.77 2008519.253 2008519.253 2008519.253 2008519.253 2008519.253 2008519.253 2008519.253 2008519.253 2008519.253 21748442.833 1792976.447 178308.822 1748442.833 1792976.447 171308.019 1165243.832 1171308.019 218528.445 210327.57 2174544.833 1003683.429 21454.452 216528.452 217577577 21757574 21297574 21297575 21297574 21297575 21297574 21297575 21297574 2129757575 2129757575 212975757575 212975757575 2129757575757575 212975757575757575757575757575757575757575	42 # ChemSpi der 42 1 1 26 0 0 1 1 11 31 26 38 6 6 1 1 11 26 38 6 6 1 24 4 6 39 4 4 20 0 6 9 28 45 18 8 45 8 9 45 24 24 24 24 26 0 10 10 10 10 10 10 10 10 10 10 10 10 1	# mzCloud Results 2 2 2 2 2 2 2 2 4 4 2 2 5 5 10 8 11 4 4 2 2 2 2 11 2 4 4 2 5 5 10 8 11 2 2 5 10 2 2 4 4 2 2 5 10 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	# mzVauk Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	83.7 mrCloud Best Match 83.1 89.2 88.5 85.7 82.7 94.2 88.5 86.4 91.1 87.1 81 92.1 83.9 81.6 87.3 83.4 82.9 81.6 83.4 83.4 83.4 83.5 83.6 85.3 83.6 88.6 88.6 88.6 88.6 88.6 88.6 88	2850840.17 Group Area: F8 F8 2850840.12 2550940.77 2088519.25 1792976.45 1792976.45 1792976.45 1783088.82 1748442.83 1545042.01 1252325.92 1748442.83 1030883.43 948756.367 911408.607 885834.119 84032.158 85834.119 84032.158 859854.459 612912.92 672297.954 659854.459 612912.92 571451.973 446503.359
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(b)

FIGURE 5: Detection of CSD by high-resolution FTMS analysis. Illustration of part of a summary of the various abundant constituents detected and identified in CSD by channel of (a) methanol extraction and (b) pure water extraction.

xanthohumol, 7,8-dihydroxy-4-methylcoumarin, and naringenin. Meanwhile, quantitative monitoring of part of the components was illustrated in Figures 6 and 7. Simultaneously, the active ingredients by pure water extraction were as follows: oxymatrine, isoliquiritigenin, DL-stachydrine, cytisine, (+)-maackiain,  $18-\beta$ -glycyrrhetinic acid, ginsenoside Rg3, 7,8-dihydroxy-4-methylcoumarin, and naringenin. Quantitative monitoring of part of the components was delineated in Figure 8.

#### 4. Discussion

UCRCC is a malignant colonic disease and a multistep process with high mortality for which the accurate pathogenesis is inconclusive and well-appreciated effective therapy is limited. Recent advances have subscribed to the belief that continual inflammatory excitation structures a favourable background for UCRCC formation, providing proof that pivotal inflammatory mediators encompassing IL-6, TNF- $\alpha$ , NF- $\kappa$ B, and IL-17 (also called IL-17A) coupled with Th17 cells are enriched in UC and colorectal cancer [8, 30–34]. Given its remarkable therapeutic capacity of CSD in UC [19, 20], the concept has fueled our hypothesis that CSD may mitigate the progression of UCRCC to a certain degree. Delightedly, in our study, CSD demonstrates an inhibitory effect on the release of these inflammation-related cytokines and secretion of Th17 cells coinciding with reduced occurrence of polyp/tumor and preferable well-being. Thereupon, the outcomes may help to develop a mind map for the investigation of mechanism and therapy with respect to UCRCC.

Apoptosis conducted in the intrinsic pathway, mainly by the mitochondrial apoptosis-induced channel, is an essential practice of programmed cell death characterized by cellular morphological changes and death [35, 36]. Bcl-2 is localized to the outer membrane of mitochondria, where it exerts a significant role in promoting cellular survival and opposing the actions of pro-apoptotic proteins such as mitochondriacleaved caspase-3 and caspase-9. Mitophagy is the selective degradation of malfunctioning or damaged mitochondria

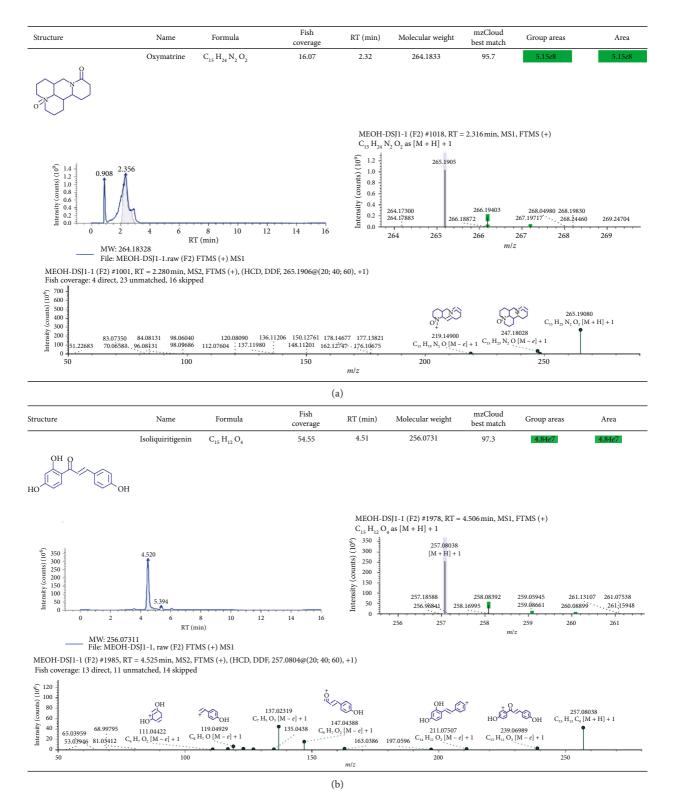


FIGURE 6: Positive-ion mode FTMS spectrum of the partial active ingredients from CSD extraction via methanol extraction. The active ingredients listed were oxymatrine (a) and isoliquiritigenin (b).

via autophagy to retain the mitochondrial quality, thus making cells adapted to various types of stress. Accumulating evidence has delineated a fundamental role of mitochondrial energy production and apoptotic mechanism in the tumor initiation [12, 16, 37]. The lipid composition of mitochondrial membrane has been reckoned capable of regulating mitochondrial membrane permeability and thence, cell death [11, 12, 38]. Considering the multifaceted

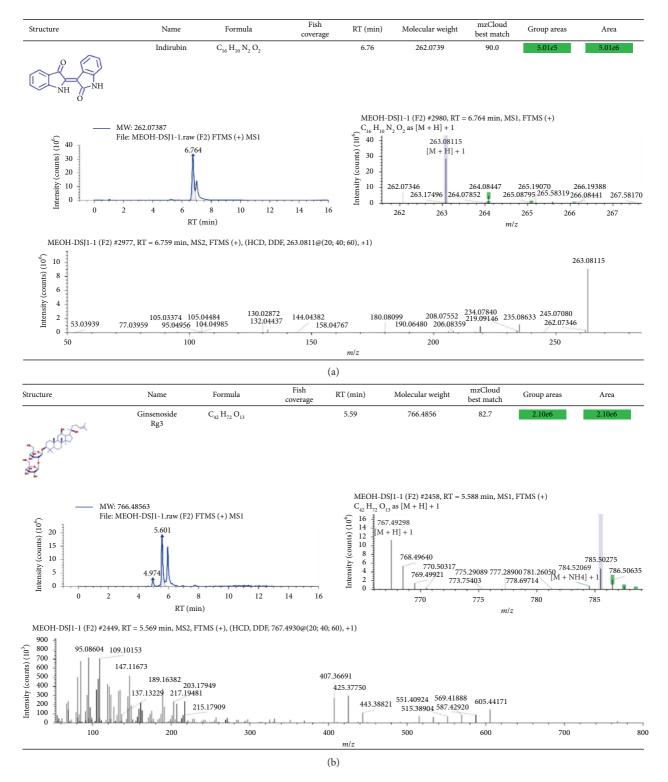
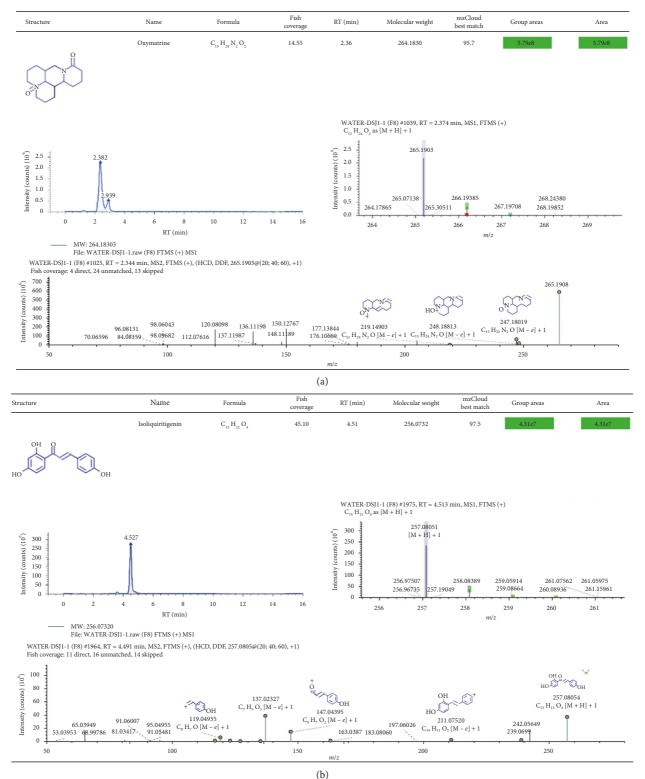


FIGURE 7: Positive-ion mode FTMS spectrum of the partial active ingredients from CSD extraction via methanol extraction. The active ingredients listed were indirubin (a) and ginsenoside Rg3 (b).



(b) FIGURE 8: Continued.

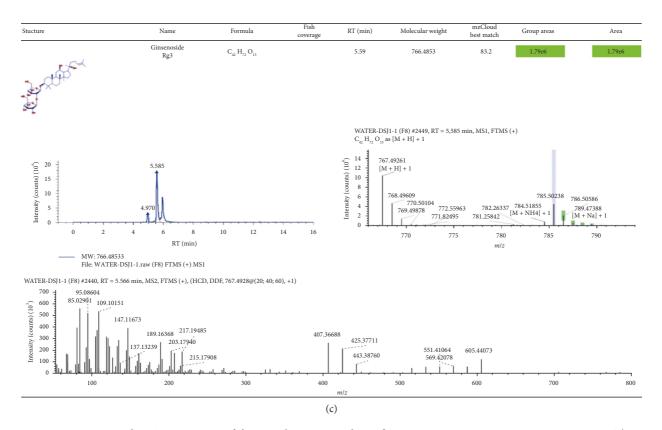


FIGURE 8: Positive-ion mode FTMS spectrum of the partial active ingredients from CSD extraction via pure water extraction. The active ingredients listed were oxymatrine (a), isoliquiritigenin (b), and ginsenoside Rg3 (c).

roles of mitochondria and intricate functions of mitophagy in tumorigenesis, care is exercised in the present study to decipher the role of the network comprising apoptosis, mitophagy, and inflammation responses in UCRCC and then to highlight innovative curative perception about UCRCC in support of the possibility that CSD can fine-tune the network.

Ultimately, our result that mitophagy and inflammation are positively joined to tumor progression in contrary to the fashion of apoptosis and CSD capsizes the trend remarkably may develop a new roadmap for the development of antitumor drugs for UCRCC.

#### **Data Availability**

The data used to support the findings of this study are available from the corresponding author upon request.

#### **Conflicts of Interest**

The authors declare that they have no conflicts of interest regarding the publication of this paper.

#### **Authors' Contributions**

Shuangjiao Deng, Qing Tang, and Xueyun Duan contributed equally to this work.

#### Acknowledgments

This work was supported by the National Natural Science Foundation of China (Nos. 81503433 and 81573784).

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