### Research Article

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

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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 × 2.1 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.



(a) 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.

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Name	Formula	Annotation Source: Predicted	Annotation Source: mzCloud	Annotation Source:	Annotation Source: MassList	FISh	Molecular	RT	Area (Max.)	# ChemSpid	# mzCloud Results	# mzVault Results	mzCloud Best Match	Group Area: F2
		Compositions	Search	chemopider search	Match	coverage	weight	(uuu)		er Results	Results	Acount	Dest Maten	
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
Dibutyl phthalate	C16 H22 O4	Full match	Full match	Full match	Full match		278.1515	8 3 5 2	48424764.8	21	9	0	95.2	48424764.81
Isoliouiritigenin	C15 H12 O4	Full match	Full match	Full match	Full match	54.55	256.0731	4 506	48376399.4	34	6	0	973	48376399 37
DI Arainina	C6 H14 N4 02	Full match	Full match	Full match	Full match	54.55	174 1116	0.700	44987026.2	7	4	0	02.2	44987026.15
Dis(4 athelian milder a) achitel	CO HI41402	Full match	Full match	Portial match	Full match	-	414 2027	7.166	44987020.2	0		0	93.4	49586040.07
Bis(4-ethyloenzylidene)sorollol	C24 H30 00	Puil match	Full match	Partial match	Pull match		414.2037	7.155	40580940.1	0	4	0	94.9	40380940.07
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
DI Stachadrina	C7 H12 N O2	Full match	Full match	Dartial match	Full match		143.0046	0.022	12054247.6	52	2	0	86.2	12054247.61
Prisonallian	C7 HIS NO2	Full match	Full match	Partial match	Full match		107.0476	0.933	12007764.6	12		0	01.6	120022264.62
Irigonelline	C/H/NO2	Full match	Full match	Not the top hit	Full match		137.0476	0.982	12927754.5	47	18	0	91.8	12927754.52
Cytisine	C11 H14 N2 O	Full match	Full match	Not the top hit	Full match	-	190.1106	0.876	12/83681.3	32	2	0	89.6	12/83681.35
L-Phenylalanine	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
DL-Tryptophan	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	C6 H6 O3	Full match	Full match	Partial match	Full match	-	126.0318	1.946	10120207	26	18	0	88.2	10120207.04
Formononetin	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
3-Hydroxy-2-methylpyridine	C6 H7 NO	Full match	Full match	Not the top hit	Full match	-	109.0531	0.907	7058284.23	36	15	0	86.4	7058284,229
g-Lactose	C12 H22 O11	No match	Invalid mass	No match	No results		359 1424	1 3 4 3	6851306.67	2	2	0	87.8	6851306.672
Maltal	C6 H6 O2	Full match	Full match	Destial match	Full match		126.0218	2 740	6406260.32	26	12	0	01.0	6405260 32
Station Operation	C0 H0 U3	Full match	Foll match	Partial match	Foll match	-	120.0318	6.149	6493209.32	20	12	0	00.4	6224440.954
Ononin	C22 H22 U9	Full match	Full match	Not the top hit	Full match	-	430.1201	5.101	0324440.85	5	4	0	91	0324440.834
Oleamide	C18 H35 N O	No match	Invalid mass	No match	No results	36.51	264.2451	9.847	5130179.81	5	2	0	97.2	5130179.81
Indirubin	C16 H10 N2 O2	Full match	Full match	Full match	No results	-	262.0739	6.761	5005072.7	9	10	0	90	5005072.7
Stearamide	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
Betulin	C30 H50 O2	Full match	Full match	Partial match	Full match	-	442.3806	5.596	3488495.57	42	2	0	83.5	3488495.572
18-B-Glycyrrhetinic acid	C30 H46 O4	Full match	Full match	Partial match	Full match	14.91	470 3392	6.089	3457136.7	23	2	0	96.9	3457136.704
	-	Annotation Source:	Annotation	-	Annotation						-			
Name	Formula	Annotation Source:	Annotation Source: m2Cloud	Annotation Source:	Annotation Source: MassI ist	FISh	Molecular	RT	Area (Max.)	# ChamSnid	# mzCloud	# mzVault	mzCloud	Group Area: F2
Name	Formula	Annotation Source: Predicted	Annotation Source: mzCloud	Annotation Source: ChemSpider Search	Annotation Source: MassList	FISh Coverage	Molecular Weight	RT [min]	" Area (Max.)	# ChemSpid	# mzCloud Results	# mzVault Results	mzCloud Best Match	Group Area: F2
Name	Formula	Annotation Source: Predicted Compositions	Annotation Source: mzCloud Search	Annotation Source: ChemSpider Search Partial match	Annotation Source: MassList Match	FISh Coverage	Molecular Weight	RT [min]	Area (Max.)	# ChemSpid er Results 23	# mzCloud Results 2	# mzVault Results	mzCloud Best Match	Group Area: F2
Name 18-β-Glycyrrhetinic acid	Formula C30 H46 O4 C18 H30 O2	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mzCloud Search Full match	Annotation Source: ChemSpider Search Partial match Partial match	Annotation Source: MassList Match Full match	FISh Coverage 14.91	Molecular Weight 470.3392 278 2245	RT [min] 6.089	Area (Max.) 3457136.7 3189018.09	# ChemSpid er Results 23	# mzCloud Results 2	# mzVault Results 0	mzCloud Best Match 96.9	Group Area: F2 3457136.704 3159015.093
Name 18-β-Glycyrrhetinic acid α-Eleostearic acid (24 (R)) 2 (L) bulgerschard) 4	Formula C30 H46 O4 C18 H30 O2	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mzCloud Search Full match Full match	Annotation Source: ChemSpider Search Partial match Partial match	Annotation Source: MassList Match Full match Full match	FISh Coverage 14.91	Molecular Weight 470.3392 278.2245	RT [min] 6.089 7.936	Area (Max.) 3457136.7 3189018.09	# ChemSpid er Results 23 19	# mzCloud Results 2 3	# mzVault Results 0 0	mzCloud Best Match 96.9 92.2	Group Area: F2 3457136.704 3189018.093
Name 18-β-Glycyrrhetinic acid α-Eleostearic acid (38,48)-3-(1-hydroxyhexyl)-4-	Formula C30 H46 O4 C18 H30 O2 (C11 H20 O4	Annotation Source: Predicted Compositions Full match Full match No match	Annotation Source: mzCloud Search Full match Full match Invalid mass	Annotation Source: ChemSpider Search Partial match Partial match No match	Annotation Source: MassList Match Full match Full match No results	FISh Coverage 14.91	Molecular Weight 470.3392 278.2245 198.1255	RT [min] 6.089 7.936 6.84	Area (Max.) 3457136.7 3189018.09 3184569.78	# ChemSpid er Results 23 19 4	# mzCloud Results 2 3 2	# mzVault Results 0 0 0	mzCloud Best Match 96.9 92.2 83.8	Group Area: F2 3457136.704 3189018.093 3184569.784
Name 18-β-Glycyrrhetinic acid o-Eleostearic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine	Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2	Annotation Source: Predicted Compositions Full match Full match Full match	Annotation Source: mzCloud Search Full match Full match Invalid mass Full match	Annotation Source: ChemSpider Search Partial match Partial match No match Full match	Annotation Source: MassList Match Full match Full match Full match Full match	FISh Coverage 14.91	Molecular Weight 470.3392 278.2245 198.1255 155.0695	RT [min] 6.089 7.936 6.84 0.828	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41	# ChemSpid er Results 23 19 4 18	# mzCloud Results 2 3 2 3	# mzVault Results 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407
Name 18-β-Glycyrthetinic acid α-Eleostearic acid (38,48)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide	Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O	Annotation Source: Predicted Compositions Full match Full match Full match Full match	Annotation Source: mzCloud Search Full match Full match Invalid mass Full match Full match	Annotation Source: ChemSpider Search Partial match Partial match No match Full match Full match	Annotation Source: MassList Match Full match Full match Full match Full match Full match	FISh Coverage 14.91	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256	RT [min] 6.089 7.936 6.84 0.828 9.729	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98	# ChemSpid er Results 23 19 4 18 4	# mzCloud Results 2 3 2 3 2 3 2	# mzVault Results 0 0 0 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1 91.9	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978
Name 18-β-Glycyrrhetinic acid o-Eleostearic acid (58,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide 3-[2-(3-Hydroxyphenyl)ethyl]-	Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O SC15 H16 O3	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match	Annotation Source: mzCloud Search Full match Invalid mass Full match Full match Full match	Annotation Source: ChemSpider Search Partial match Partial match No match Full match Full match Partial match	Annotation Source: MassList Match Full match Full match Full match Full match Full match No results	FISh Coverage 14.91 - - -	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097	RT [min] 6.089 7.936 6.84 0.828 9.729 6.2	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03	# ChemSpid er Results 23 19 4 18 4 36	# mzCloud Results 2 3 2 3 2 3 2 6	# mzVault Results 0 0 0 0 0 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032
Name 18-6-Glycyrrhetinic acid o-Elcostearic acid (35,4R)-3-(1-hydroxyhety)-4- L-Histidine Hexadecanamide 3-{2-(3-Hydroxyheny)hethyllethyl]-5 Bis(2-ethylhexy) phthalate	Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O C15 H16 O3 C15 H16 O3 C15 H36 O4	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Full match Not the top hit	Amotation Source: mzCloud Search Full match Invalid mass Full match Full match Full match Full match	Annotation Source: ChemSpider Search Partial match Partial match Full match Full match Partial match	Annotation Source: MassList Match Full match Full match Full match No results Full match Full match	FISh Coverage 14.91	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761	RT [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38	# ChemSpid er Results 23 19 4 18 4 36 26	# mzCloud Results 2 3 2 3 2 3 2 6 10	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032 2420907.381
Name 18-β-Glycyrrhetinic acid α-Elcottaric acid (S3,4R)-3-(1-hydroxyheyt)-4- L-Histidine Hercadocanamide 3-[2-(3-Hydroxyheny1)ethyl]-5 Bis(2-ethylhexy1) pithalate 2-Hydroxyheny1alanine	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	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Full match Not the top hit No match	Annotation Source: m2Cloud Search Full match Invalid mass Full match Full match Full match Full match Invalid mass	Annotation Source: ChemSpider Search Partial match Partial match Full match Full match Full match Full match Full match No match	Annotation Source: MassList Match Full match Full match Full match Full match No results Full match No match	FISh Coverage 14.91 - - - - -	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475	RT [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25	# ChemSpid er Results 23 19 4 18 4 36 26 41	# mzCloud Results 2 3 2 3 2 6 10 5	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032 2420907.381 2309984.246
Name 18-f-Olycyrthetinic acid o-Eleostenic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexade-caamide 3-[2-4]-Hydroxyherylpethyl]-f Bis(2-ettyl)Hexylpathalae 2-Hydroxyherylpathalae Adenosine	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	Amotation 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 Full match Full match Full match Full match Full match Invalid mass Full match	Annotation Source: ChemSpider Search Partial match No match Full match Full match Full match Full match No match No match No the top hit	Amotation Source: MassList Match Full match Full match Full match Full match No results Full match No match Full match	FISh Coverage 14.91 - - - - -	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965	RT [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2309984.25 2270151.36	# ChemSpid er Results 23 19 4 18 4 36 26 41 34	# mzCloud Results 2 3 2 3 2 6 10 5 1	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032 2420907.381 230998.246 2270151.362
Name 18-β-Glycyrrhetinic acid α-Ecostearic acid (Ss,4R)-3-(1-ydroxyhexyl)-4- L-Histidine Hexadoceanamide 3-[2-(3-Hydroxyphenyl)ethyl]-1 Bis(2-ethylhexyl) phrhalate 2-Hydroxyphenylalanine Adenosine 9-Oxo-10E1 [2/E)-octadecadi	Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O SC15 H16 O3 C24 H38 O4 C9 H11 N O3 C10 H13 N5 O4 C18 H30 O3	Amotation Source: Predicted Compositions Full match Full match Full match Full match Full match Full match Full match Full match Full match	Annotation Source: m2Cloud Search Full match Full match Full match Full match Full match Invalid mass Full match Full match	Annotation Source: ChemSpider Search Partial match Partial match Full match Full match Full match Full match No match Not match Not the top hit Not the top hit	Annotation Source: MassList Match Full match Full match Full match Full match Full match No match Full match Full match Full match	FISh Coverage 14.91 	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194	RT [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2270151.36 2180416.19	# ChemSpid er Results 23 19 4 18 4 36 26 41 34 24	# mzCloud Results 2 3 2 2 6 10 5 1 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 24507907.381 2309984.246 2270151.362 2180416.19
Name 18-f-Olycyrthetinic acid a-Eleostenic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexade-azamide 3-[2-(3-Hydroxyheryl)ethyl]-1 Bic3-ethylhexyl) phthalate Bic3-ethylhexyl) phthalate	Formula C30 H46 O4 C18 H30 O2 (C11 H20 O4 C6 H9 N3 O2 C16 H16 O3 C24 H38 O4 C9 H11 N O3 C10 H13 N5 O4 C18 H30 O3 C22 H22 O10	Annotation Source: Predicted Compositions Full match No match Full match Full match Not the top hit No match Full match Full match Full match Full match Full match Full match	Annotation Source: mzCloud Full match Invalid mass Full match Full match Full match Full match Full match Full match Full match Full match	Amotation Source: ChemSpider Search Partial match No match Full match Full match Full match Full match No match No the top hit Not the top hit Partial match	Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match Full match Full match Full match	FISh Coverage 14.91 - - - - - - - - - - - - - - - - - - -	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446 1211	RT [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 0.88 8.157 4.432	Area (Max.) 3457136.7 3189018.09 31894569.78 3131520.41 3032768.98 2567369.03 2420907.38 2420907.38 2420907.38 2420907.38 2420907.38 2420907.38	ChemSpid er Results 23 19 4 18 4 36 26 41 34 24	# mzCloud Results 2 3 2 3 2 6 10 5 1 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 87.7	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032 2420907381 2309984.246 2270151.362 2180416.19 2009058.479
Name 18-f-Olycyrthetinic acid a-Eleostearic acid (Ss,RP, 3-(1-hydroxyhexyl)-4- L-Histidine Hexadacaamide 3-[2-(3-Hydroxyhenyl)phthalate 2-Hydroxyhenylbathilate 2-Hydroxyhenylbathilate 2-Hydroxyhenylbathilate Adenosine 9-0xo-10(E),12(E)-octadecadii Glycitiin Giysenoside Re3	Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C16 H33 N O SC15 H16 O3 C24 H38 O4 C9 H11 N O3 C10 H13 N5 O4 C18 H30 O3 C22 H22 O10 C42 H22 O13	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Full match Full match Full match Full match Not the top hit Not the top hit Not match	Annotation Source: mrCloud Search Full match Full match	Annotation Source: ChemSpider Search Partial match No match Full match Partial match Full match Full match Full match Not the top hit Not the top hit Partial match Not the top hit Partial match	Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match Full match Full match Full match Full match	FISh Coverage 14.91 - - - - - - - - - - - - - - - - - - -	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	RT [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	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2270151.36 2180416.19 2099593.48 2096343.33	ChemSpid er Results 23 19 4 18 366 26 41 34 24 11	# mzCloud Results 2 3 2 3 2 6 10 5 1 2 2 2 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	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	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2309984.246 221051362 2180416.19 2099593.479 209559.453
Name 18-f-Olycyrrhetinic acid a-Eleostenic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Herado-azamide 3-[2-(3-Hydroxyheryl)ethyl]-1 Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl Bic	Formula C30 H46 O4 C18 H30 O2 C16 H33 O2 C16 H33 N O C16 H33 N O C16 H33 N O C15 H16 O3 C24 H38 O4 C18 H30 O3 C10 H13 N5 O4 C18 H30 O3 C12 H12 O13 C42 H72 O13 C	Annotation Source: Predicted Compositions Full match Full match Full match Full match No match Full match No the top hit No the top hit	Annotation Source mcCloud Search Full match Invalid mass Full match Full match Full match Full match Full match Full match Full match Full match Invalid mass Full match Invalid mass	Annotation Source: ChemSpider Search Partial match No match Full match Full match Full match Full match Not match Not the top hit Not the top hit Not match No match	Annotation Source: MassList Match Full match No results Full match No results Full match Full match Full match Full match Full match No results Full match No results	FISh Coverage 14-91 - - - - - - - - - - - - - - - - - -	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	RT [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 0.945	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2270151.36 2180416.19 2099593.48 2096363.33 1867722	" ChemSpid er Results 23 19 4 18 4 36 26 41 34 24 11 1 1	# mzCloud Results 2 3 2 3 2 6 6 10 5 1 10 5 2 2 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	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	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2467369.032 240907.381 2309984.246 2270151.362 2180416.19 2099593.479 2099563.325
Name 18-f-Glycyrthetinic acid a-Eleostearic acid (Ss,R)-3-(1-hydroxyhexyl)-4- Hexadacanamide 3-[2-(3-Hydroxyhexyl-pathalate 2-Hydroxyhemylalanine Adenosine 9-0xo-10(E),12(E)-octadecadi Glycitin Ginsenoside Rg3 D-(-)-Glutamine D-(-)-Glutamine	Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C15 H16 O3 C15 H16 O3 C24 H38 O4 C9 H11 N O3 C10 H13 N5 O4 C18 H30 O3 C22 H22 O10 C22 H22 O10 C24 H27 O13 C5 H10 N2 O3	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Not the top hit Not match Full match Full match Full match Full match Full match Full match Full match Full match Full match	Annotation Source: mcCloud Sarch Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Fall match Fall match Partial match Partial match No match Not the top hit Not the top hit Partial match Fall match Fall match Fall match	Amodation Source: MassList Match Full match Full match	FISh Coverage 14.91 - - - - - - - - - - - - - - - - - - -	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	RT [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	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 242090738 2309984.25 2270151.36 2180416.19 2099593.48 2096563.33 1867381	# ChemSpid er Results 19 4 4 18 4 36 6 26 41 34 34 24 11 1 1 31	# mzCloud Results 2 3 2 2 3 3 2 2 6 10 0 5 5 1 1 2 2 4 4 6	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	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 92.5	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 2099593.479
Name 18-f-Olycyrthetinic acid a-Eleostearic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexade-azamide 3-[2-(3-Hydroxyheryl)ethyl]-1 Bic3-ethylhexyl) phthalate Bic3-ethylhexyl) phthalate	Formula C30 H46 O4 C18 H30 O2 C16 H30 O2 C16 H33 NO C16 H33 NO C15 H16 O3 C24 H38 O4 C18 H38 O4 C18 H30 O3 C10 H13 N5 O4 C18 H30 O3 C12 H22 O10 C42 H72 O13 C42	Annotation Source: Predicted Compositions Full match Full match Full match Full match Not the top hit No that top hit Not the top hit Not the top hit Not match Full match Full match Full match Full match Full match	Annotation Source: mcCloud Suarch Full match Invalid mass Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match No match Fall match Partial match Partial match No match Not the top hit Not the top hit Not the top hit Not match No match No match No match No match No match	Annotation Source: MassList Match Full match No results Full match No results Full match Full match Full match Full match Full match Full match Full match Full match Full match	FISh Coverage 14.91 	Molecular Weight 470.3392 278.2245 198.1255 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0965 294.2194 446.1211 766.4859 1349.3495	RT [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	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 2309984.25 2270151.36 2180416.19 2099593.48 2096503.33 1867381 1574239.28	" ChemSpid er Results 23 19 4 18 4 36 26 411 34 24 11 1 31 0 0	# mzCloud Results 2 3 2 2 6 6 10 5 5 2 2 2 2 4 4 6 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 94 88.1 80.9 95 87.7 82.7 84.6 93.2	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2402097381 2209984.246 2270151362 2180416.19 2099593.479 2099533.479 20996363.325 1867381 1574239.278
Name 18-f-Olycyrrhetinic acid c-Ecostenic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexafocanamide 3-2(-3-Hydroxyherylethyl)- Bis(2-ethylhexyt) phthalate 2-Hydroxyherylethyllanine Adenoisine 9-0xo-10(E),12(E)-octadecadis Glycitin Ginsenoiside Rg3 Dc(-)-Glutamine Dccosnamide Licochalcone A	Formula C30 H46 O4 C18 H30 O2 C11 H20 O4 C6 H9 N3 O2 C15 H16 O3 C24 H38 O4 C9 H11 N O3 C12 H10 N3 O4 C18 H30 O3 C12 H22 O10 C12 H10 N2 O3 C2 H10 N2 O3 C2 H10 N2 O3 C2 H10 N2 O3 C21 H22 O4	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mcCloud Sarch Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match No match Fall match Fall match Fall match Not match Not match Not the top hit Partial match Not match Fall match Not match Fall match Not match Partial match	Amodation Source: MassList Match Full match Full match	FISh Coverage 14.91 	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.096 294.2194 294.2194 446.1211 766.4856 146.0691 339.3495 338.1515	RT [min] 6.089 7.936 6.84 0.828 9.729 7.22 11.144 1.195 0.88 8.157 4.432 5.594 0.948 13.084 6.997	Area (Max.) 3457136.7 3189018.09 3184569.78 313152041 3032768.98 2567369.03 2420907.38 23099842.5 2100151.36 2180416.19 2099593.48 2099593.48 2099593.48 2099593.48 2099593.48 2099593.48 2095959.48 2005959.48 2	# ChemSpid er Results 199 4 4 18 36 26 41 34 24 4 11 34 24 11 1 1 31 0 0 15	# mzCloud Results 2 3 3 2 2 6 6 10 5 1 1 2 2 4 4 6 6 2 4 4 4 6 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCloud Best Match 9669 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 87.7 82.7 84.6 93.2 83.8 80.9	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032765.978 2420907381 2309984.246 2270151362 2180416.19 2099593.479 2099593.479 2099553.479 21867381 15771849.911
Name 18-f-Olycyrthetinic acid a-Eleostearic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexado-azamide 3-12-(3-Hydroxyheryl)ethyl]-5 Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl) phthalate Bic3-ethylHexyl phthalate Bic3-ethyl	Formula C30 H46 04 C18 H30 02 C11 H20 04 C6 H9 N3 02 C15 H16 03 C24 H38 04 C9 H11 N 03 C1 H11 N 03 C1 H11 N 03 C1 H13 N 504 C18 H30 03 C22 H42 V17 C18 H30 03 C5 H10 N2 03 C5 H10 N2 03 C21 H22 04 C21 H22 04 C21 H22 04 C19 H11 C19 C19 C19 C19 C19 C19 C19 C19 C19 C	Annotation Source: Predicted Compositions Full match Full match Full match Full match No match Full match	Annotation Source: mcCloud Sarche Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Partial match Pall match Pall match Pall match No match Not the top hit Not the top hit Not the top hit Partial match Fall match Partial match Partial match Partial match Pall match	Annotation Source: MassList Match Full match Full match	Fish Coverage 14-91 	Molecular Weight 470,3392 278,2245 198,1255 198,1255 255,256 244,1097 390,2761 164,0475 267,0965 294,2194 446,1211 766,4856 146,0691 339,3495 338,15115	RT [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	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 22567369.03 2420907.38 2309884.25 2270151.36 2270151.36 2290953.48 2096363.33 1867381 15774239.28 15771849.91 1477574.46	# ChemSpid er Results 23 3 19 4 4 18 4 4 18 4 4 13 6 411 34 24 4 11 1 1 31 0 0 15 1	# mzCloud Results 2 3 2 2 3 2 2 6 10 5 11 2 2 2 4 6 6 2 2 4 4 2 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mrCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.8 88.1 80.9 95 87.7 84.6 93.2 87.9 84.8 87.9 84.8 87.9	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2309984.246 2270151.362 22100416.19 2099593.479 2096365.325 1867381 1574239.278 1571849.911 1477574.46
Name 18-f-Olycyrrhetinic acid c-Ecostenic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide 3-2(-3-Hydroxyhenylahyl)- Bis(2-ethylhexyl) plrthalate 2-Hydroxyhenylahaine Adenoisia 9-0xo-10(E),12(E)-octadecadi Giystiin Ginsenoside Rg3 Dc(-)-Giutamine Dccosnamide Licochalcone A PEG n10 Xanthohumol	Formula C30 H46 04 C18 H30 02 C18 H30 02 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C24 H38 04 C19 H11 N 03 C19 H11 N 03 C19 H11 N 03 C18 H30 03 C22 H22 010 C42 H72 013 C22 H22 010 C42 H72 013 C22 H45 N 0 C21 H22 04 C20 H42 011 C20 H42 011 C20 H42 015	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mcCloud Search Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match No match Fell match Fell match Fell match Not match Not the top hit Not the top hit Not the top hit Not the top hit Not the top hit Partial match So results Partial match Fell match Fell match Fell match Fell match	Amortation Source: MassList Match Full match Full match	FISh Coverage 14-91 	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 338.1515	RT [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 6.238	Area (Max.) 3457136.7 3189018.09 3131520.41 3032768.98 22567369.03 2420907.38 2200151.36 2180416.19 2099593.48 2096363.33 1867381 1574239.28 1571849.91 1477574.46 1448182.69	# ChemSpid or Results 23 199 4 4 18 4 36 26 26 41 34 4 34 24 11 1 1 31 1 0 0 15 1 2 5	* mzCloud Results 2 3 3 2 2 3 3 2 2 6 10 15 1 1 2 2 2 4 4 6 6 2 2 4 8 8	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0	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 84.6 93.2 89.8 87.9 90.8	Group Area: F2 3457136 704 3189018.093 3184569.784 3131520.407 3032768.978 2567369.032 2420907.381 2309984.246 2210014.6.19 2099593.479 2099593.479 2099593.479 2099593.479 21867381 15771849.911 1477574.46 1448182.689
Name 18-f-Olycyrrhetinic acid a-Eleostenic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Bi(2-ettylhezyl) phthalate Bi(2-ettylhezyl) ph	Formula C30 H46 04 C18 H30 02 C11 H10 04 C6 H9 N3 02 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C16 H16 03 C24 H38 04 C9 H11 N 03 C1 H11 N 03 C2 H45 N0 C12 H22 010 C12 H42 01 C21 H42 04 C20 H42 011 C21 H42 05 C10 H8 04	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Not the top hit No the top hit No the top hit No the top hit Full match Full match Full match Full match Full match Full match Full match Full match Full match	Annotation Source: mcCloud Sarcher Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Fall match Fall match Fall match Fall match No match Not the top hit Not the top hit Not the top hit Not the top hit Not match Fall match No result No result Partial match Fall match Fall match Fall match Fall match Fall match	Annotation Source: MassList Match Full match Full match	FISh Coverage 14-91 	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 192,0425	RT [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 6.238 3.723	Area (Max.) 3457136.7 3189018.09 3134569.78 3131520.41 3032768.98 230984.25 2270151.36 2180416.19 2099593.48 2096363.33 1867381 15714399.28 15714399.28 15714399.28 157148199.14 1477574.46 1432077.92	# ChemSpid er Results 223 19 4 18 4 4 18 36 26 411 34 26 411 34 24 11 1 1 31 0 0 15 1 1 25 38	# mzCloud Results 2 3 3 2 2 6 6 10 5 1 1 2 2 2 2 4 4 6 6 2 2 4 4 8 8 8	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 5 87.7 84.6 93.2 87.8 88.8 87.9 90.8 87.9	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2309984.244 2270151.362 2180416.19 2099593.479 2096363.325 1867381 157429.278 1571849.911 1477574.46 1448182.689 1432077.925
Name 18-f-Olycyrrhetinic acid c-Ecostenic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexafocanamide 3-[2-(3-Hydroxyhenylahyl)- Bis(2-ethylhexyl) phthalate 2-Hydroxyhenylahaine Adenoisia 9-Oto-10(E),12(E)-octafocadii Givietino Givietino Givietino Docostamine D	Formula C30 H46 04 C18 H30 02 C18 H30 02 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C24 H38 04 C24 H38 04 C18 H30 03 C22 H22 010 C42 H72 013 C22 H22 010 C42 H72 013 C22 H42 010 C22 H42 010 C21 H22 04 C20 H42 011 C21 H22 04 C21 H22 05 C15 H10 04	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mcCloud Search Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Partial match Pail match Fail match Pail match Nor match Fail match Nor match Fail match Nor the top hit Partial match Nor match Fail match So results Partial match Fail match Fail match Fail match Fail match Fail match Fail match Fail match Fail match Fail match	Amortation Source: MassList Match Full match Full match	FISh Coverage 14-91 - - - - - - - - - - - - - - - - - -	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.065 294.2194 294.2194 339.3495 338.1515 458.2729 354.1463 192.0425 254.0577	RT [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 6.238 3.723 5.231	Area (Max.) 3457136.7 3189018.09 313184569.78 3131520.41 3032768.98 22567369.03 2420907.38 22099593.48 2009593.48 2009593.48 2009593.48 1571849.91 1477574.46 1448182.69 1432077.92 1268752.83	ChemSpid er Results 233 19 4 4 36 266 411 34 244 111 1 311 0 0 15 1 1 25 38 444	* mzCloud Results 2 3 3 2 2 3 3 2 2 3 3 2 2 3 3 2 2 5 10 0 0 5 11 2 2 2 4 4 6 6 2 2 2 8 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	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 82.7 82.7 82.7 82.7 82.7 82.7	Group Ares: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2309984.246 2270151.362 240907381 150984.246 2270151.362 1807181 167381 1573849.911 1477574.46 1448182.689 1433127.528.28
Name 18-f-Olycyrthetinic acid a-Eleostenic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hezadecasamide 3-12-(3-Hydroxyheryl)ethalate His(2-ethylHezyl) phthalate Bis(2-ethylHezyl) p	Formula C30 H46 04 C18 H30 02 C11 H10 04 C6 H9 N3 02 C16 H33 N 0 C16 H16 03 C24 H38 04 C9 H11 N 03 C1 H1 N 03 C1 H1 N 03 C1 H1 N 03 C2 H10 N2 03 C2 H45 N 0 C1 H2 04 C2 H45 N 0 C1 H2 04 C2 H45 N 0 C1 H2 04 C2 H45 N 0 C1 H2 04 C1 H10 04 C	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Not the top hit No match Full match	Annotation Source: mcCloud Sarcher Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Fall match Fall match Fall match Fall match No match Not the top hit Not the top hit Not the top hit Partial match No match So results Partial match Fall match Fall match Fall match Fall match Fall match Fall match Fall match Fall match	Annotation Source: MassList Match Full match Full match	FISh Coverage 14.91 	Molecular Weight 470.3392 278.2245 198.1255 198.1255 198.1255 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 238,1418	RT [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 6.994 13.084 6.994 13.084 6.994 8.159 6.238 3.723 5.231 2.866	Area (Max.) 3457136.7 3189018.09 3131820.41 30312620.41 3032768.98 2567369.03 2420907.38 230984.25 220151.36 2209151.36 209953.48 2096363.33 1574239.28 157124.99 1477574.46 1448182.69 14520779.21 208752.83 1146294.07 1268752.83 1146294.07 1268752.83 1269752.83 126875752.83 126875752.83 126875752.83 126875752.83 126875752.83 126875752.83 126875757575757575757575757575757575757575	# ChemSpid er Results 233 19 4 18 4 4 36 266 411 34 24 24 11 1 1 31 0 15 1 1 255 38 44	# mzCloud Results 2 3 3 2 2 3 3 2 2 3 3 2 2 3 6 6 10 5 1 1 2 2 2 4 4 6 6 2 2 4 8 8 8 8 8 8	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 95 5 87.7 84.6 93.2 87.9 90.8 87.9 90.8 87.9 90.8 87.9 90.6 81.2 2 83.8 81.2 8 83.8 8 83.8 8 83.8 8 83.8 8 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2309984.246 2270151.362 2180416.19 2099593.479 209958.375 1571849.911 1477574.46 1443182.689 1432077.925 1268752.828 1146294.075
Name 18-f-Olycyrrhetinic acid c-Ecostenic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide 3-(2-3)-Hydroxyhenylalanine Adenosine Aden	Formula C30 H46 04 C18 H30 02 C18 H30 02 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C24 H38 04 C18 H30 03 C19 H11 N 03 C10 H13 N5 04 C18 H30 03 C10 H13 N5 04 C18 H30 03 C12 H42 010 C22 H22 010 C22 H22 010 C22 H42 011 C20 H42 011 C20 H42 011 C21 H22 04 C10 H0 04 C15 H10 04 C10 H22 06 C13 H24 N2 0	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mcCloud Search Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Partial match Fall match Fall match Fall match Nor match Fall match Nor the top hit Partial match Nor match Fall match Partial match Fall match	Amortation Source: MassList Match Full match Full match	Fish Coverage 14.91	Molecular Weight 470.3392 278.2245 198.1255 155.0695 255.256 244.1097 390.2761 164.0475 267.0964 294.2194 294.2194 446.1211 766.4856 139.3495 338.1511 458.2729 354.1463 192.0425 254.0577 238.1418 224.1887	RT [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 6.238 3.723 5.231 2.866 6.574	Area (Max.) 3457136.7 3189018.09 31814569.78 3131520.41 3032768.98 203978.42 210017.18 2009593.48 2009593.48 2009593.48 1571849.91 1477574.46 1448182.69 1432077.92 1268752.83 1146294.07 1070298.00	ChemSpid er Results 233 19 4 4 36 26 41 34 34 24 4 11 1 31 0 0 15 15 1 25 388 44 4 4 1 6	# mzCloud Results 2 3 3 2 6 6 10 5 5 1 1 2 2 2 4 4 6 6 2 2 4 4 6 8 8 8 8 8 4 4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.8 8.1 80.9 95 87.7 84.6 93.2 89.8 87.9 90.8 87.9 90.6 8.7.9 90.0 8.8 87.9 90.0 8.8 9.0 9.0 8.8 9.0 9.0 8.8 9.0 9.0 8.9 9.0 9.0 8.9 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9.0 9	Group Ares: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2309984.246 2270151.362 218041619 2009636.335 1867381 1577849.911 1477574.69 1571849.911 1477574.89 1433127.699 1448152.689 1443152.689 1443152.689 144254.075 1268752.828 1146294.075 1268752.828 1146294.075 1070298.044
Name 18-f-Olycyrthetinic acid a-Eleostenic acid (35,47)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecasamide 3-12-(3-Hydroxyheryl)ethalate Elic2-ethyltexyl) phthalate Bic2-ethyltexyl) phthalate Bic2-ethyltexyl) phthalate Bic2-ethyltexyl) phthalate Bic2-ethyltexyl phthalate 1-Histidine Bic2-ethyltexyl phthalate D-(x)-Olutamine Docosanamide Licochalcome A PEG n10 Xantholumol 7,8-Dihydroxy-4-methylcouma Daideein PEG n2 NN-Dicyclobexylurea PEG n2 NN-Dicyclobexylurea	Formula C30 H46 04 C18 H30 02 C11 H10 04 C6 H9 N3 02 C16 H33 N 0 C16 H11 N 03 C15 H16 03 C24 H38 04 C9 H11 N 03 C18 H30 03 C22 H45 N 0 C12 H22 04 C22 H42 N10 C21 H22 04 C20 H42 011 C21 H22 05 C10 H3 04 C15 H10 04 C14 H20	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Nor the top hit Nor the top hit Nor the top hit Nor the top hit Full match Full match	Annotation Source: mcCloud Sarcher Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Fall match Fall match Fall match Fall match No match Not the top hit Not the top hit Partial match No match So results Partial match Fall match	Annotation Source: MassList Match Full match Full match	Fish Coverage 14.91 	Molecular Weight 470.3392 278.2245 198.1255 198.1255 255.256 244.1097 390.2761 164.0475 204.2194 446.1211 766.4856 146.0691 338.1515 458.2729 338.1515 458.2729 354.1463 192.0425 254.0577 238.1418 224.1887 60.290	RT [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 6.238 3.723 5.231 2.86 6.574 4.282	Area (Max.) 3457136.7 3189018.09 3181520.41 30312620.41 3032768.98 22070138 220908425 22070151.36 220905348 2096363.33 1574292.83 157124921 1477574.46 1448182.69 1445182.69 1445752.83 1146294.07 1070298.03 107390.05 105390	ChemSpid er Results 223 19 4 4 36 26 26 26 41 34 4 24 11 31 31 0 15 1 1 25 5 38 44 4 4 1 6 0 0	# mzCloud Results 2 3 3 2 2 6 10 5 1 1 2 2 4 4 6 6 2 2 4 4 6 8 8 8 8 8 8 8 4 4 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.9 88.1 80.9 95.5 87.7 84.6 93.2 89.8 87.9 90.8 87.9 90.6 81.2 93.3 87.9 90.6 81.2 93.3 87.9 90.6 93.3 87.9 90.6 93.3 87.9 93.5 87.9 93.5 87.9 93.5 87.9 93.5 87.9 93.5 87.9 93.5 87.9 93.5 87.9 93.5 87.5 93.5 87.5 93.5 87.5 93.5 87.5 93.5 87.5 94.5 94.5 94.5 94.5 94.5 94.5 94.5 94	Group Area: F2 3457136.704 3189018.093 3184569.784 31315120.407 3032768.978 2420907.381 2200954.242 210016.19 2009593.479 2009563.325 1867381 1574239.278 1571849.911 1477574.46 1443182.689 1432077.925 1268752.823 1146294.075 1070298.034 105300.00 1053000.00 1053000.00 10530
Name 18-f-Olycyrrhetinic acid c-Ecostenic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide 3-(2-3)-Hydroxyhenylehylyl 3-(2-3)-Hydroxyhenylehylyl 3-(2-3)-Hydroxyhenylalanine Adenosise Ade	Formula C30 H46 04 C18 H30 02 C18 H30 02 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C16 H38 04 C24 H38 04 C24 H38 04 C18 H30 03 C10 H13 N5 04 C18 H30 03 C12 H45 0 0 C22 H22 010 C24 H27 013 C12 H42 011 C20 H22 04 C20 H42 011 C21 H22 04 C10 H22 06 C15 H10 04 C10 H22 06 C13 H24 N2 0 C12 H42 005 C13 H24 N2 0 C12 H42 005 C13 H24 N2 0 C12 H42 005 C12 H42 005 C15 H10 005 C15 H10 005 C12 H42 005 C12 H42 005 C10 H4	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mcCloud Search Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match No match Fell match Fell match Fell match Not the top hit Not the top hit Not the top hit Not the top hit Not the top hit Partial match Fell match	Amortation Source: MassList Match Full match Full match	Fish Coverage 14.91	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 192.0425 254.0577 238.1418 224.1887 502.299	RT [min] 6.089 7.936 6.84 9.729 6.2 11.144 1.195 5.594 4.432 5.594 4.432 5.594 4.432 5.594 4.432 3.733 3.733 3.723 3.723 5.236 6.238 3.723 3.723 4.442	Area (Max.) 3457136.7 3185918.09 3184569.78 3131520.41 3032768.98 2567369.03 2420907.38 230984.25 2270151.36 2180416.19 2096363.33 1867381 1574239.25 1571849.91 1477574.46 1574239.25 1448182.69 1432077.92 14285752.83 1146294.07 107028.03 1053909.78 307616.92 307	ChemSpid er Results. 23 19 4 4 8 36 26 41 1 34 36 41 34 36 41 1 1 31 3 1 5 38 38 44 4 4 1 1 0 0 0 15 5 38 8 44 4 10 0 0 0 0 0 0 0 0 19 9 19 9 19 9	<pre># mzCloud Results 2 3 3 2 6 6 10 5 5 1 1 2 2 2 4 4 6 6 2 2 4 4 4 2 2 8 8 8 8 8 4 4 4 2</pre>	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.4 88.1 80.9 95 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 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 87.9 87.9 87.9 87.9 87.9 87.9 87	Group Area: F2 3457136.704 3189018.093 3184569.784 31313152.407 3032768.978 2420907381 2309944.246 2270151362 2180416.19 2099539.479 2099363.325 1867381 1577849.911 1477574.69 1537849.911 1477574.89 143312.689 144812.689 144812.689 144812.689 144812.689 144812.689 144812.689 14482.689 146294.075 1070298.034 1053909.777 005667 005767 005767 00590 105909 10590 105909 105909 105909 105909 105909 105909 105909 105909 105909 105909 105909 105909 105909 105909 105909 105909 105909 10590 105909 10590 105909 105909 10590 105909 10590 10590 105909 10590
Name 18-f-Olycyrthetinic acid a-Eleostearic acid (35,47)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide 3-12-(3-Hydroxyheryl)ethyl]-5 Bi(2-ethylHexyl) phthalate Bi(2-ethylHexyl) phthalate Bi(2-ethylHexyl) phthalate Bi(2-ethylHexyl) phthalate D-Ox-010(E),12(E)-octadecadii Ginsenoside Rg3 D-()-Gittamine Doccoanamide Liocchalcome A PEG n10 Xantholumol 7,8-Dihydroxy-4-methylcouma Daidzein PEG n2 NN-Dicyclobexylurea PEG n11 Naringenin	Formula C30 H46 04 C18 H30 02 C118 H20 04 C6 H9 N3 02 C16 H33 N 0 C16 H33 N 0 C16 H16 03 C24 H38 04 C9 H11 N 03 C18 H30 03 C22 H45 N 0 C18 H30 N2 03 C22 H45 N 0 C11 H22 04 C30 H42 011 C21 H22 05 C10 H18 04 C15 H10 04 C15 H10 04 C15 H10 04 C15 H10 04 C15 H10 04 C13 H24 N2 06 C13 H24 N2 06 C13 H24 N2 06 C13 H24 N2 06 C15 H12 05 C15 H10 205 C15 H10 C4 C15 H10 C4 C	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Nor the top hit Nor the top hit Nor the top hit Nor the top hit Full match Full match	Annotation Source: mcCloud Sarcher Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Fall match Fall match Fall match Fall match No match Not the top hit Partial match No match Not the top hit Partial match Fall match	Annotation Source: MassList Match Full match Full match	FISh Coverage 	Molecular           Weight           470.3392           278.2245           198.1255           155.0695           255.256           244.1097           390.2761           164.0475           294.2194           446.1211           766.4856           146.0691           338.1515           458.2729           354.1463           192.0425           254.1484           228.1418           290.220.683           474.067	RT [min] 6.089 7.936 6.84 0.828 8.9729 6.2 11.144 1.195 6.28 8.157 4.5594 0.948 8.157 4.5594 0.948 4.5594 0.948 4.5594 13.084 4.5594 2.5231 2.866 6.574 4.283 3.723 5.231	Area (Max.) 3457136.7 3189018.09 3184569.78 3134520.41 3032768.98 2309984.25 2309984.25 23099593.48 2006533.33 15714239.28 1571439.21 1477574.46 1477574.46 1477574.46 1477574.67 1477574.77 1477574.67 1477574.67 1477574.67 1477574.67 1477574.67 1477574.67 1477574.67 1477574.67 1477574.67 1477574.67 1477574.67 1477574.77 1477	ChemSpid or Results 233 19 4 4 18 4 36 26 41 34 36 41 13 4 11 1 1 31 0 0 15 15 38 38 44 4 16 6 0 0	# mzCloud Results 2 3 3 2 2 6 10 5 1 1 2 2 4 4 6 6 2 2 4 4 6 8 8 8 8 8 4 4 2 2 2 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	mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.8 8.1 80.9 95.8 87.7 84.6 93.2 89.8 87.9 90.6 81.2 93.3 87.9 90.6 81.2 93.3 87.9 90.6 93.3 87.9 90.6 93.8 87.9 90.6 93.8 87.9 93.8 93.8 87.9 93.8 94.8 87.9 94.8 94.8 94.8 94.8 94.8 94.8 94.8 94	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907.381 2200954.242 2100151.362 2210016.19 2009593.479 20096363.325 1867381 1574239.278 16771849.911 1477574.46 1448182.689 1432077.925 1268752.825 1146294.075 1070298.034 1053909.777 975615.82
Name 18-f-Olycyrrhetinic acid c-Ecostenic acid (38,4R)-3-(1-hydroxyhaeyl)-4- L-Histidine 12-(3-Hydroxyhaeylahyl)-3 3-(2-3)-Hydroxyhaeylahyl 3-(2-3)-Hydroxyhaeylahalate 2-Hydroxyhaeylahalate 2-Hydroxyhaeylahalate 3-Oso-10(E),12(E)-octadecadii Giviettin Ginsenoside Rg3 D-(-)-Giltamine Docosanamide Licochalcone A PEG n10 Nx-Dicyclohexylurea PEG n15 NX-Dicyclohexylurea PEG n11 Nariagenin 2-Hydroxyheeylalanine	Formula C30 H46 04 C18 H30 02 C18 H30 02 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C16 H38 04 C18 H30 03 C10 H13 N5 04 C18 H30 03 C10 H13 N5 04 C18 H30 03 C12 H42 010 C12 H42 010 C12 H42 011 C12 H42 011 C12 H42 011 C13 H24 N 0 C13 H24 N 0 C16 H10 04 C16 H12 06 C13 H24 N2 0 C15 H10 04 C15 H10 V3 C15 H10 V3 C16 H13 V5 C17 H10 V3 C17 H10	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mcCloud Search Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match No match Fell match Fell match Fell match Not the top hit Not the top hit Not the top hit Not the top hit Not match Fell match No match No match	Amortation Source: MassList Match Full match Full match	Fish Coverage 14.91	Nolecular           Weight           470.3392           278.2245           198.1255           198.1255           255.0695           255.256           244.1097           390.2761           164.0475           267.0965           294.2194           446.1211           766.4856           146.0691           339.3495           338.1515           525.254.0577           238.1416           224.1887           502.299           212.0683           164.0475	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 8.9729 6.2 8.157 4.432 5.594 6.054 4.594 6.238 3.723 5.231 2.866 6.574 4.447 0.886 6.574 4.447 0.886 6.574 4.447 0.886 6.574 6.288 6.574 6.288 6.574 6.288 6.574 6.288 6.574 6.288 6.574 6.288 6.574 6.288 6.574 6.288 6.5749 6.288 6.5749 6.288 6.5749 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 6.288 7.299 7.299 6.288 7.299 7.299 6.288 7.2997 7.299 7.299 7.299 7	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.41 3032768.98 2567369.03 242090738 2309984.25 22701513.62 2180416.19 2096383.33 1867381 1574239.25 1574239.25 1574239.25 1445182.69 1445182.69 1445182.69 1445182.69 1445182.69 142527.72 1268752.83 1146294.07 1070298.03 1053909.78 975615.82 857400.572	ChemSpid er Results. 23 19 4 4 18 36 26 41 34 36 41 31 31 31 31 31 31 31 338 44 41 6 6 46 41	# mzCloud Results 2 3 3 2 2 6 100 5 1 1 2 2 4 4 6 6 2 2 4 4 2 2 8 8 8 8 8 4 4 2 2 3 3 3 1 2 1 2 1 2 1 2 2 3 3 2 2 2 3 3 2 2 2 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 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 3 2 2 3	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mcClood Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 88.1 87.9 90.8 87.9 90.8 87.9 90.8 87.9 90.8 81.2 93.8 81.2 83.8 8.1 85.1 85.1 85.1 85.1 85.1 85.1 85.	Group Area: F2 3457136.704 3189018.093 3184569.784 31313152.407 3032768.978 2420907381 2309984.246 2270151.362 2180416.19 2099593.479 2099533.479 2099533.479 2099533.479 2099533.479 209953.479 209953.479 209953.479 2099553.478 1445182.689 1445182.689 14452.4572.828 1146294.075 21268752.828 1146294.075 21268752.828 1146294.075 22857402.958.034 1053909.777 975615.82 857402.4722
Name 18-f-Olycyrthetinic acid a-Eleostearic acid (35,47)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide 3-12-(3-Hydroxyheryl)ethalate Bic3-ethylbeyryl phthalate Bic3-ethylbeyryl phthalate Bic3-ethylbeyryl phthalate Bic3-ethylbeyryl phthalate Bic3-ethylbeyryl phthalate D-Ox-010(E),12(E)-octadecadii Givention D-(y-Gittamine Sakaranetin Sakaranetin Sakaranetin	Formula C30 H46 04 C18 H30 02 C11 H20 04 C6 H9 N3 02 C16 H33 N 0 C16 H16 03 C24 H38 04 C9 H11 N 03 C18 H30 03 C22 H45 N 0 C18 H30 03 C22 H45 N 0 C11 H22 04 C30 H42 01 C21 H22 05 C10 H13 N 04 C15 H10 04 C15 H10 04 C15 H12 05 C15 H12 05 C15 H12 05 C15 H12 05 C15 H12 05 C16 H14 05	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Nor the top hit Nor the top hit Nor the top hit Nor the top hit Full match Full match	Annotation Source: mcCloud Sarcher Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Fall match Fall match Fall match Fall match No match Not the top hit Partial match No match Not the top hit Partial match Fall match	Annotation Source: MassList Match Full match Full match	FISh Coverage 	Molecular           Weight           470.3392           278.2245           198.1255           155.0695           255.256           244.1097           390.276           294.2194           164.0475           294.2194           164.0475           393.1515           458.2729           338.1515           354.1463           392.0425           254.0577           238.1418           238.141887           502.299           272.0683           164.0475           286.08475	RT [min] 6.089 7.936 6.84 8.729 6.2 11.144 1.195 0.88 8.157 4.432 5.594 0.948 8.157 4.432 5.594 0.948 6.238 5.231 5.231 5.231 5.231 5.231 5.231 5.231 5.254 5.263	Area (Max.) 3457136.7 3189018.09 3184569.78 3134520.41 3032768.98 2369786.98 2369784.92 2270151.36 2180416.19 2009593.48 2006563.33 1867381 1574239.28 1571849.91 1477574.46 1477574.46 1477574.46 1477574.46 1477574.67 1452077.92 1268752.83 1146294.07 1070298.03 1073909.78 975615.82 857402.572	ChemSpid er Result 23 19 4 18 36 266 411 34 244 244 11 1 1 31 0 0 15 1 1 25 5 38 44 4 1 6 0 0 0 46 41 44	# mzCloud Results 2 3 3 2 2 6 6 10 0 5 1 1 2 2 4 4 6 6 2 2 4 4 6 8 8 8 8 8 8 8 8 4 4 2 2 2 3 3 7 2 10 0 5 10 10 5 10 10 10 5 10 10 10 10 10 10 10 10 10 10 10 10 10	# mzVaslt Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCood Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.8 8.8 1 80.9 9.9 9.9 8.7 9.9 9.0 8.7 9.9 9.0 8.7 9.9 9.0 8.7 9.9 9.0 8.7 9.9 9.0 8.7 9.3 8.7 9.9 2.2 9.3 8.7 8.7 9.2 2.2 9.3 8.7 8.7 8.7 8.7 8.7 8.7 8.7 8.7 8.7 8.7	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2420907381 22009584.242 210016.19 2099593.479 2099583.479 2099583.479 2099583.479 2099583.479 2099583.479 2099583.479 2099583.479 2099583.479 2099583.479 2099583.479 2095752.825 1146294.075 1070298.034 1145294.075 1070298.034 1145294.075 1070298.034 1145294.075 1070298.034 1145294.075 1070298.034 1145294.075 1070298.034 1145294.075 1070298.034 1145294.075 107528.034 1145294.075 107528.034 1145294.075 107528.034 1145294.075 107528.034 1055390.977 2759550.072 2759550.072 2759550.072 2759550.072 2759550.072 2759550.072 2759550.072 2759550.072 2759550.072 2759550.072 2759550.075 2759550.072 2759550.075 27595500.075 27595500.075 27595500.075 27595500.075 2759550000000000000000000000000000000000
Name 18-f-Olycyrrhetinic acid c-Ecostenic acid (38,4R)-3-(1-hydroxyhexyl)-4- L-Histidine 12-(3-Hydroxyhenylehyl)- 32-(2-3-Hydroxyhenylehyl)- Bis(2-chylhexyl) plethalate 2-Hydroxyhenylalanine Adenosine 9-Oxo-10(E),12(E)-octadecadii Giyetiin Oinsenoside Rg3 D-(-)-Gilutanine Docosanamide Licochalcone A PEG n10 Nx-Dicyclohexylurea PEG n5 NY-Dicyclohexylurea PEG n5 NY-Dicyclohexylurea PEG n1 Nariagenin 2-Hydroxybenylalanine Sakaranetin 1-Linolecyl glycerol	Formula C30 H46 04 C18 H30 02 C18 H30 02 C16 H33 N 0 C16 H33 N 0 C16 H33 N 0 C24 H38 04 C24 H38 04 C24 H38 04 C18 H30 03 C10 H13 N5 04 C18 H30 03 C12 H20 10 C22 H22 010 C22 H22 010 C22 H22 010 C22 H42 011 C21 H22 04 C20 H42 011 C15 H10 04 C15 H10 04 C15 H10 04 C15 H10 04 C15 H10 05 C22 H46 012 C15 H10 04 C15 H10 05 C22 H46 012 C15 H10 05 C15 H10 05 C12 H10 05 C15 H10 05 C12 H10 05 C12 H10 05 C12 H10 05 C15 H10 05 C12 H10 05 C15 H10 05 C12 H10 05 C15 C15 H10 05 C15 H10	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mcCloud Search Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match No match Fell match Fell match Fell match Not the top hit Not match Fell match No match Fell match No match Fell match No match Fell match No match Fell match	Amortation Source: MassList Match Full match Full match	FISh Coverage 14-91 	Molecular           Weight           470.3392           278.2245           198.1255           155.0695           254.256           244.1097           390.2761           164.0475           267.0665           294.2194           446.1211           766.4856           146.0691           339.3495           338.1515           454.272.0425           254.0577           238.1418           224.1887           502.299           272.0683           164.0475           286.0841           354.2766	RT [min] 6.089 7.936 6.84 9.729 6.2 9.729 6.2 9.729 6.2 8.8 1.144 1.195 0.828 8.157 4.432 5.594 4.432 5.594 4.159 6.238 3.723 5.231 2.86 6.574 4.457 0.886 5.223 4.447 0.886 5.2263 9.33	Area (Max.) 3457136.7 3189018.09 3184569.78 3131520.14 3032768.98 2567369.00 2180416.19 2009593.48 2009593.48 2009593.48 2009593.48 2009593.48 2009593.48 157124.99 1457374.46 1448182.09 1420577.24 1448182.09 107226.05 107226.05 107226.05 107226.05 107226.05 1072599.075 75559.154 285740.257 75559.0154 285740.257 75559.0154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 28599.076 775559.154 285740.257 285740.257 285740.257 285740.257 2857540.257 2857640.257 2857540.257540.257	ChemSpid or Results 23 19 4 4 34 6 266 41 134 4 4 4 4 11 1 1 31 0 15 38 38 44 4 4 1 1 6 6 0.00 466 6 41 1 44 4 5	# mzCloud Results 2 3 3 2 2 6 10 0 5 1 1 2 2 4 4 6 6 2 2 4 4 4 2 2 8 8 8 8 8 8 4 4 4 2 2 0 10 0 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	mcClood Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94 88.1 80.9 92.3 94 88.1 80.9 92.3 87.7 84.6 93.2 87.9 90.8 87.9 90.8 81.2 93.8 87.8 83.8 83.8 83.8 83.8 83.8 83.8 8	Group Area: F2 3457136.704 3189018.093 3184569.784 3131520.407 3032768.978 2402097381 2309984.246 2270151.362 2180416.19 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 2099593.479 209959.342 1146224.075 1146224.075 21268752.828 1146224.075 21268752.828 1146224.075 21268752.828 1146224.075 21268752.828 1146224.075 212689.044 212773589.1341
Name 18-F-Olycyrthetinic acid ac-Ecostenic acid (35,4R)-3-(1-hydroxyhexyl)-4- L-Histidine Hexadecanamide 3-12-(3-Hydroxyheryl)ethyl]-5 Bit(2-ethylHexyl) phthalate Bit(2-ethylHexyl) phthalate Bit(2-ethylHexyl) phthalate Ginsenoside Rg3 D-()-Giltamine Doccosanamide Licochalcone A PEG n10 Nambolumol 7.8-Dihydroxy-4-methylcouma Daidzein PEG n5 NN-Dicyclobexylurea PEG n1 Nariagenin 2-Hydroxyphenylalanine Sakaranetin 1-Linolecyl giycerol Leucyhprole	Formula C30 H46 04 C18 H30 02 C11 H10 04 C6 H9 N3 02 C16 H33 N 0 C16 H14 03 C24 H38 04 C24 H38 04 C29 H11 N 03 C18 H30 03 C22 H45 N 0 C11 H22 04 C20 H42 011 C21 H22 05 C10 H13 N 04 C15 H10 04 C15 H10 04 C15 H10 04 C15 H12 05 C13 H24 N20 C15 H12 05 C15 H12 05 C16 H14 05 C11 H20 N2 03	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Nor the top hit Nor the top hit Nor the top hit Nor the top hit Full match Full match	Annotation Source: mcCloud Sarcher Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Fall match Fall match Fall match Fall match No match No match No match No match No match Fall match Partial match Partial match	Annotation Source: MassList Match Full match Full match	FISh Coverage 14-91 	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           1339.3495           338.1515           458.2729           354.1463           192.0425           254.0677           328.1418           224.1847           592.292           254.0477           328.1418           244.1897           592.284.21847           592.292           226.0841           354.228.1475	RT [min] 6.089 7.936 6.082 9.729 6.2 11.144 1.195 6.28 8.8.157 4.432 5.594 0.948 8.8.157 4.432 0.948 8.8.157 4.432 5.594 0.948 8.559 4.159 6.298 5.231 2.86 6.574 4.283 5.231 2.86 6.574 4.283 5.243 2.99 9.33	Area (Max.) 3457136.7 3189018.09 3184569.78 3134520.41 3032768.98 2309984.25 2309984.25 2309984.25 23099593.48 2006563.33 15714239.28 15714239.28 15714239.28 15714239.28 15714239.28 157152.25 167552.83 1146294.07 1070298.03 1073909.78 975615.82 857402.572 7389958.015 734846.835 9.14846.25 734846.835 14489.14 1448.25 1457.25	ChemSpid er Result 23 19 4 4 18 36 266 41 34 34 24 41 11 1 31 0 15 1 1 1 255 38 34 44 11 6 0 0 0 46 41 14 4 5 6 6	<pre># mzCloud Results 2 3 2 2 3 2 2 3 2 6 6 10 0 5 1 1 2 2 2 4 4 6 6 2 2 8 8 4 4 4 2 2 2 10 3 7 7 2 4 4</pre>	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCloud Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.8 8.8 1 80.9 93.2 87.9 93.2 87.9 93.2 87.9 90.6 81.2 93.8 87.9 90.6 81.2 93.8 87.9 90.6 81.2 93.8 87.9 90.6 81.8 8.7 8.7 8.8 8.8 8.8 8.8 8.7 8.8 8.8 8	Group Area: F2 3457136.704 3189018.093 3184569.784 2367369.002 2420907381 2309984.246 2270151.362 2210416.19 2099593.479 2099563.325 1867381 1574239.278 1571849.911 1477574.46 1443182.689 1146274.075 1070298.034 1146294.075 1070298.034 1146294.075 1070298.034 1145294.075 1070298.034 1145294.075 1070298.034 1145294.075 1070298.034 1145294.075 1075389.134 115589.0762 2789959.0762 2789959.0762 2789959.0762 2789959.0762 2789959.0762 2789959.0762 2789959.0762 2789959.0762 2789959.0762 2789959.0762 2789959.0762 173484.63445 174444.63445 174444.63445 17445 17445 17445 17445 17445 17445 17445 17445 17445 17445 17445 174555 17455 17455 174555 17455 174555 17455 174555 174555
Name 18-f-Olycyrrhetinic acid c-Ecostenic acid (38, 4R)-3-(1-hydroxyhexyl)-4- L-Histidine 13-(2-3Hydroxyhenyl)-4hyd- 13-(2-3Hydroxyhenyl)-4hyd- 13-(2-3Hydroxyhenyl)-4hyd- Bis(2-athylhexyl) plathalate 2-Hydroxyhenylalanine Adenosine 9-Oxo-10(E),12(E)-octadecadi Giyettin Oinsenoside Rg3 D-()-Gitlatnine Docosanamide Licochalcone A PEG n10 Xantholumol 7,8-Dihydroxy-4-methylcoumat Daidzein PEG n5 NN-Dicyclohexylurea PEG n1 Nariagenin 2-Hydroxybenylalanine Sakaranetin 1-Linolecyl glycerol Leuxylproline Ouanine	Formula C30 H46 O4 C18 H30 02 C18 H30 02 C16 H33 N 0 C16 H33 N 0 C16 H38 O4 C24 H38 O4 C18 H30 O3 C24 H38 O4 C18 H30 O3 C22 H22 010 C42 H72 013 C22 H42 011 C22 H42 011 C24 H42 011 C21 H22 O4 C20 H42 011 C16 H10 O4 C13 H22 O5 C15 H10 O4 C13 H22 O5 C15 H10 O4 C13 H22 O5 C15 H10 O4 C13 H22 O5 C15 H10 O4 C13 H22 O5 C16 H14 O5 C12 H46 O12 C16 H14 O5 C12 H48 O4 C11 H20 N2 O3 C16 H14 O5 C12 H38 O4 C11 H20 N2 O3 C14 H45 O4 C11 H20 N2 O3 C14 H45 O4 C11 H20 N2 O3 C14 H35 O4 C11 H20 N2 O3 C14 H35 O4 C14 H20 N2 O3 C16 H10 N5 C14 H10 N5 C16 H1	Annotation Source: Predicted Compositions Full match Full match	Annotation Source: mcCloud Sarrob Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Partial match Fall match Fall match Fall match Not match Fall match No match Fall match No match Fall match	Amortation Source: MassList Match Full match Full match	FISh Coverage 14-91 	Molecular           Weight           470.3392           278.2245           198.1255           155.0695           254.256           244.1097           390.2761           164.0475           267.0665           294.2194           446.1211           766.4856           146.0691           339.3495           338.1515           454.224.0827           234.1463           192.0425           254.0577           234.1481           224.1887           504.272.0683           164.0475           286.0841           354.2766           281.475           151.0494	RT [min] 6.089 7.936 6.84 9.729 6.2 9.729 6.2 9.729 6.2 8.157 4.432 5.594 4.159 6.238 3.723 3.723 5.231 2.866 6.574 4.159 6.238 3.723 4.447 0.886 5.233 4.447 0.886 5.263 9.333 2.999 9.318 2.526 1.188	Area (Max.) 3457136.7 3189018.09 3184569.78 313152014.0 3032768.98 22673369.00 212099738 21309984.25 2270151.36 21309184.16 19 2009593.48 2009593.48 2009593.48 2009593.48 2009593.48 2009593.48 2165724.58 1445182.69 143277.92 1457354.61 1457354.95 1070286.05	ChemSpid or Results 23 19 4 4 34 6 266 41 134 4 4 4 4 11 1 1 31 0 15 1 1 255 38 44 4 4 1 1 6 6 46 41 325 38 44 4 1 9 6 6 6 6 6 6 20 0 0 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	mxCloud Results           2         3           2         3           2         2           3         2           6         10           10         5           11         2           2         4           6         2           4         2           4         2           10         3           7         2           4         4	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mcClood Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.4 88.1 80.9 94.5 87.7 84.6 93.2 87.9 90.8 87.9 90.8 87.9 90.8 81.2 83.8 83.8 83.8 83.8 83.8 83.8 84.1 80.7 90.8 85.1 85.1 85.1 85.1 85.1 85.1 85.1 85	Group Area: F2 3457136.704 3189018.093 3184569.784 31313152.407 3032768.978 2420907381 2309984.246 2270151.362 2180416.19 20099593.479 200954.240 200954.240 200954.240 200954.240 200954.240 200955.2828 146224.075 215598.040 200956.040 200956.040 200956.040 200956.040 200956.040 200956.040 200956.040 200956.040 200957.2828
Name 18-F-Olycyrthetinic acid ac-Ecostenic acid (35,4R)-3-(1-hydroxyhery)-4- L-Histidine Hexadocanamide 3-12-(3-Hydroxyhery)-hyl]-5 Bi(2-a-tyl)Heyl)-19 Bi(2-a-tyl)Heyl)-19 Discontine Docosanamide Licochalocone A PEG n10 Vantholumol 7,3-Dihydroxy-4-methylcouma Daidzein PEG n1 Naringenin 2-Hydroxyherylalanine Sakuranetin NN-Dicyclobexylurea PEG 01 Naringenin 2-Hydroxyherylalanine Sakuranetin 1-Linoleyl giycerol Leucylproline Cuanine Monobuty phthalate	Formula C30 H46 04 C18 H30 02 C11 H10 04 C6 H9 N3 02 C16 H33 N 0 C16 H14 03 C24 H38 04 C9 H11 N 03 C18 H30 03 C22 H45 N 0 C18 H30 03 C22 H45 N 0 C11 H22 04 C30 H42 011 C21 H22 05 C10 H3 04 C15 H10 04 C15 H10 04 C15 H10 04 C15 H12 05 C11 H22 06 C13 H24 N20 C15 H12 05 C15 H12 05 C15 H12 05 C15 H12 05 C15 H12 05 C16 H14 05 C11 H20 N2 03 C11 H20 N2 03 C1 H20 N2 N3 C1 H20 N3 C1 H20 N2 N3 C1 H20 N3 C	Annotation Source: Predicted Compositions Full match Full match Full match Full match Full match Nor the top hit Nor the top hit Nor the top hit Nor the top hit Full match Full match	Annotation Source: mcCloud Sarcher Full match Full match	Amotation Source: ChemSpider Search Partial match Partial match Fall match Fall match Fall match Fall match No match No match No match No match No match Partial match Partial match Fall match Partial match Partial match Partial match Partial match Partial match Partial match	Annotation Source: MassList Match Full match Full match	FISh Coverage 14-91 	Molecular Weight 470.3392 278.2245 198.1255 195.0695 255.256 244.1097 390.2761 164.0475 294.2194 446.1211 766.4856 146.0691 339.3495 338.1515 458.2729 354.1463 192.0425 254.0577 238.1418 224.1897 592.2492 272.0683 164.0475 286.0841 354.2766 228.1475 151.0494 222.089	RT [min] 6.089 7.936 6.84 0.828 9.729 6.2 11.144 1.195 6.88 8.157 4.432 5.594 0.948 8.8157 4.432 5.594 0.948 8.8157 4.459 6.238 5.594 0.948 6.397 4.159 6.238 5.231 2.86 6.574 4.4283 4.447 2.86 6.574 4.4283 2.99 9.138 6.331	Area (Max.) 3457136.7 3189018.09 3184569.78 3134520.41 3032768.98 2309984.25 2309984.25 2309984.25 23099593.48 2006563.33 15714239.28 15714239.28 15714239.28 15714239.28 1571249.21 1477574.46 1477574.46 1477574.46 1477574.46 1477574.46 1477574.46 1477574.46 1477574.46 1477574.46 1477574.87 1475752.83 15712928.03 1073298.03 1073909.78 975615.82 857402.572 734846.85 676845.058 6738454.058 6738757 675854.058 6758557 675857	ChemSpid or Results 23 199 4 4 36 26 26 41 34 4 4 34 4 11 1 1 31 1 0 5 15 1 38 8 44 4 11 3 1 9 0 0 46 45 26 0 0 0 20 20 20 20 20 20 20 20 20 20 20	<pre># mzCloud Results 2 3 2 2 3 2 2 3 3 2 2 6 6 10 0 5 1 1 2 2 2 2 2 4 4 4 2 2 2 8 8 8 8 4 4 4 2 2 2 3 3 7 2 6 6 10 0 10 5 5 11 2 2 2 3 3 2 2 6 6 6 10 10 5 5 10 10 10 5 5 10 10 10 10 10 10 10 10 10 10 10 10 10</pre>	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mcCood Best Match 96.9 92.2 83.8 90.1 91.9 92.3 94.8 8.8 1 80.9 93.2 87.9 93.2 87.9 93.2 87.9 93.2 87.9 90.6 81.2 93.8 87.9 90.6 81.2 93.8 87.9 90.6 81.2 93.8 87.9 90.6 81.5 80.5 81.5 80.5 81.5 80.5 81.5 80.5 81.5 81.5 81.5 81.5 81.5 81.5 81.5 81	Group Area: F2 3457136.704 3189018.093 3184569.784 2313520.407 3032768.978 2420907381 2200954.242 210016.19 2009593.479 2009563.325 1867381 1574239.278 1571849.911 1477574.46 1443122.689 1146274.075 107028.034 1146294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 1145294.075 107028.034 105390.077 107028.034 105390.077 1075655.252 107028.034 105390.077 1075655.252 107028.034 105390.077 1075655.252 107028.034 105390.077 1075655.252 107028.034 105390.077 1075655.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107565.252 107555 107555.252 107555 107555.252 107555.252 107555.255 107555.255 107555.255 107555.255 107555 107555.255 107555 107555.255 107555.255 107555.255 107555.255 1075555.255 107555.255 107555.255 107555.255 107555.255 107555.255 1075555.255 107555.255 1075555.255 1075555.255 1075555.255 1075555.255 1075555.255 107555.255 1075555.255 1075555.255 1075555.255 1075555.255 1075555.255 1075555.255 107555555 1075555.255 10755555555 107555555555555555555555555555555555555

(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	8.357	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	4.513	43149066.46	34	6	0	97.5	43149066.5
Hexamethylenetetrame	C6 H12 N4	Full match	Full match	Full match	No results	23.53	140.10596	14.469	36810028.01	3	2	0	97.5	36810028
L-Pyroglutamic acid	C5 H7 N O3	Full match	Full match	Not the top hit	Full match	-	129.04274	1.145	31014849.17	24	4	0	81.7	31014849.2
Choine DI Stechnologie	C5 HI3 N O	Full match	Full match	Partial match	Full match	-	143.00467	0.810	28080713.24	12	2	0	82.0	28080713.2
DL-Stachydrine	C/ HI3 N 02	No match	Full match	Partial match	Puil match	-	143.09407	0.82	23521925.51	52	4	0	02.5	23521925.5
L-Marlencine	C6 H13 N O2	Full match	Full match	Not the top hit	Full match	-	131.09474	1 357	21421231 76	56	10	0	\$93.5	21421231.8
Pinecolic acid	C6 HU N O2	Full match	Full match	Not the top hit	Full match		120 0701	0.055	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	1.096	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-methylpy	C6 H7 N O	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-fu	C6 H6 O3	Full match	Full match	Partial match	Full match	-	126.03195	2.037	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	11.764	4661529.045	3	3	0	95.9	4661529.04
18-β-Glycyrrhetinic ac	C30 H46 O4	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	4.271	3986402.448	47	12	0	93.5	3986402.45
α-Lactose	C12 H22 O11	Full match	Full match	Not the top hit	Full match	-	342.11555	5.593	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	1.069	3565462.707	34	2	0	89.8	3565462.71
L-Glutamine	C5 H10 N2 O3	No match	Invalid mass	No match	No match	-	129.04262	0.842	3447711.429	24	3	0	86.3	3447711.43
(3S,4R)-3-(1-hydroxyl	C11 H20 O4	No match	Invalid mass	No match	No results	-	198.12547	6.861	3107090.822	4	3	0	83.7	3107090.82
Betulin	C30 H50 O2	Full match	Full match	Partial match	Full match	-	442.38046	5.59	2850840.167	42	2	0	\$3.7	2850840.17
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
Name •	Formula C30 H50 O2	Annotation Source: Predicted Compositions Full match	Annotation Source: mzCloud Search Full match	Annotation Source: ChemSpider Search Partial match	Annotation Source: MassList Match Full match	FISh Coverage	Molecular Weight 442.38046	RT [min] 5.59	Area (Max.) 2850840.167	# ChemSpi der 42	# mzCloud Results 2	# mzVault Results 0	mzCloud Best Match 83.7	Group Area: F8 2850840.17
Name Betulin PEG n10	Formula C30 H50 O2 C20 H42 O11	Annotation Source: Predicted Compositions Full match Not the top hit	Annotation Source: mzCloud Search Full match Full match	Annotation Source: ChemSpider Search Partial match Full match	Annotation Source: MassList Match Full match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269	RT [min] 5.59 4.161	Area (Max.) 2850840.167 2782623.267	# ChemSpi der 42 1	# mzCloud Results 2 2	# mzVault Results 0 0	mzCloud Best Match 83.7 88.1	Group Area: F8 2850840.17 2782623.27
Name Betulin PEG n10 Maltol	Formula C30 H50 O2 C20 H42 O11 C6 H6 O3	Annotation Source: Predicted Compositions Full match Not the top hit Full match	Annotation Source: mzCloud Search Full match Full match Full match	Annotation Source: ChemSpider Search Partial match Full match Partial match	Annotation Source: MassList Match Full match Full match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195	RT [min] 5.59 4.161 2.799	Area (Max.) 2850840.167 2782623.267 2599740.77	# ChemSpi der 42 1 26	# mzCloud Results 2 2 12	# mzVault Results 0 0 0	mzCloud Best Match 83.7 88.1 89.2	Group Area: F8 2850840.17 2782623.27 2599740.77
Name Betulin PEG n10 Maltol PEG n11	Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12	Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit	Annotation Source: mzCloud Search Full match Full match Full match Full match	Annotation Source: ChemSpider Search Partial match Full match Partial match No results	Annotation Source: MassList Match Full match Full match Full match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909	RT [min] 5.59 4.161 2.799 4.284	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253	# ChemSpi der 42 1 26 0	# mzCloud Results 2 12 2 2	# mzVault Results 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3	Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13	Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit No match	Annotation Source: mzCloud Search Full match Full match Full match Full match Invalid mass	Annotation Source: ChemSpider Search Partial match Full match No results No match	Annotation Source: MassList Match Full match Full match Full match Full match No results	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533	RT [min] 5.59 4.161 2.799 4.284 5.588	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447	# ChemSpi der 42 1 26 0 1	# mzCloud Results 2 12 2 4	# mzVault Results 0 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5 83.2	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin	Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C22 H22 O10	Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit No match Not the top hit	Annotation Source: mzCloud Search Full match Full match Full match Full match Invalid mass Full match	Annotation Source: ChemSpider Search Partial match Full match Partial match No results No match Partial match	Annotation Source: MassList Match Full match Full match Full match No results Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822	# ChemSpi der 42 1 26 0 1 1 11	# mzCloud Results 2 2 12 2 4 2 4 2	# mzVault Results 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid	Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H46 O12 C42 H72 O13 C22 H22 O10 C5 H9 N O4	Annotation Source: Predicted Compositions Full match Not the top hit Not the top hit No match Not the top hit Full match	Annotation Source: mzCloud Search Full match Full match Full match Invalid mass Full match Full 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 No results Full match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833	# ChemSpi der 42 1 26 0 1 11 31	# mzCloud Results 2 2 2 12 2 4 2 4 2 5 5	# mzVault Results 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 82.7 82.7	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82 1748442.83
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutanie acid Bis(2-ethylhexyl) platha	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	Annotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit Not the top hit Full match Not the top hit	Annotation Source: mzCloud Search Full match Full match Full match Full match Full match Full match Full match Full match	Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Full match Full match	Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007	# ChemSpi der 42 1 26 0 1 11 31 26 0 26 0	# mzCloud Results 2 2 2 12 2 4 2 4 2 5 10	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 82.7 94.2 94.2	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82 1748442.83 1545042.01
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Ghttamic acid Bis(2-ethylhexyl) phth 7.8-Dihydroxy-4-meth	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 C10 H8 O4 C10 H8 O4	Annotation Source: Predicted Compositions Full match Not the top hit Not the top hit Not the top hit Full match Not the top hit Full match	Annotation Source: mzCloud Search Full match Full match Full match Full match Full match Full match Full match Full match	Annotation Source: ChemSpider Search Partial match Full match No results No match Partial match Full match Not the top hit	Annotation Source: MassList Match Full match Full match Full match Full match Full match Full match Full match Full match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762 192.04254	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 3.746	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919	# ChemSpi der 42 1 26 0 1 11 31 26 38	# mzCloud Results 2 2 2 12 2 4 2 5 10 8	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 82.7 94.2 88.1 21.2 88.1	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1783088.82 1788482.83 1545042.01 1252325.92
Name Betulin PEG n10 Mahol PEG n10 Ginsenoside Rg3 Glycitin L-Ghtranis acid Bis(2-ethylhexyl) phth N.N-Dicyclohexylurea DEC of DEC of	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 C10 H8 O4 C13 H24 N2 O C14 H24 N2 O	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	Annotation Source: mzCloud Search Full match Full match Full match Invalid mass Full match Full match Full match Full match Full match Full match	Annotation Source: ChernSpider Search Partial match Pull match No results No match Partial match Full match Full match Full match Full match	Annotation Source: MassList Match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 446.12103 147.05307 390.2762 192.04254 224.18852 238.14466	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.864	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1171308.019	# ChemSpi der 42 1 26 0 1 1 11 31 26 38 6 1	# mzCloud Results 2 2 2 12 2 4 2 5 10 8 1 1	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 92.7 94.2 88.1 91.5 86.1	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1788482.83 1545042.01 1252325.92 1171308.02
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamie acid Bis(2-ethylhexyl) phth 7.8-Dihydroxy-4-meth N.N-Dieyelohexylures PEG n5	Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C22 H22 010 C5 H9 N 04 C24 H38 04 C10 H8 04 C13 H24 N2 0 C19 H20 03	Amotation Source: Predicted Compositions Full match Not the top hit Full match Not the top hit Full match 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 Full match Full match	Annotation Source: ChemSpider Search Partial match Full match No results No match Partial match Full match Full match Full match Full match Full match Full match	Annotation Source: MassList Match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.584 2.895 7.395	Area (Max.) 2850840.167 2782623.267 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1171308.019 1165243.832	# ChemSpi der 42 1 26 0 0 1 111 311 26 338 6 1 24 4 24 24 24 24 24 24 24 24 24 24 24 2	# mzCloud Results 2 2 2 12 2 2 4 2 5 10 8 1 1 4 2 2 5 10 0 8 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5 83.2 86.7 82.7 82.7 94.2 88.1 91.5 86.4	Group Area: F8 2850840.17 2782623.27 2999740.77 2098519.25 1792976.45 1783088.82 1748442.83 1545042.01 1252325.92 1171308.02 1165243.83
Name Betulin PEG n10 Maltol PEG n10 Ginsenoside Rg3 Glyoritn L-Olutamic acid Bis(2-ethylhexyl) phth 7.8-Dhydroxy-4-meth N.N-Dicyclohexylurea PEG n5 9-Oxo-10(E),12(E)-ecl	Formula (30 H50 O2 (22 H42 O11 C6 H6 O3 (22 H46 O12 C42 H72 O13 (22 H22 O10 C5 H9 N O4 C10 H8 O4 C10 H8 O4 C10 H2 A2 O C10 H22 O6 C18 H13 O5	Amotation Source: Predited Compositions 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	Annotation Source: mzCloud Search Full match Full match	Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Full match Full match Full match Full match Not the top hit Full match Not the top hit Full match	Annotation Source: MassList Match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935 232.06833	RT [min] 5.59 4.161 2.799 4.284 5.88 4.439 0.852 11.155 3.746 6.584 2.895 7.232 4.445	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1171308.019 1171308.019 1165243.832 1003683.429	# ChemSpi der 42 1 266 0 1 1 111 311 266 338 6 1 244 446	# mzCloud Results 2 2 2 2 12 2 2 4 2 5 5 10 8 1 4 4 2 2 5 10 0 8 1 4 2 2 2 2 2 2 2 12 2 2 12 2 2 2 12 2 2 2 12 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	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 91.1 97.1	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 178208.82 1748442.83 1545042.01 1252325.92 1171308.02 1165243.83 1003683.43 0042563.43
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylicacyl) phth N-Dicyelohexylures PEG n5 9-Cox-10(E):12(E)-cc Naringenin Ghoren 1 icharobata	Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C22 H22 010 C5 H9 N 04 C13 H24 N2 0 C10 H2 06 C18 H30 03 C15 H12 05 C15 H1	Amotation Source: Predicted Compositions Full match Not the top hit Full match 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: mrCloud Search Full match Full match	Annotation Source: ChemSpider Search Full match Partial match No results No match Partial match Full match Pall match Full match Full match Full match Full match Full match Full match Full match Full match Full match	Annotation Source: MassList Match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935 272.06832 276.06832	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.852 7.232 4.445 7.232	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1171308.019 1165243.832 1003683.429 948756.3665 011408.6067	# ChemSpi der 42 1 26 0 1 11 11 31 26 38 6 6 1 24 46 29	# mzCloud Results 2 2 2 12 2 4 4 2 5 10 8 11 0 8 1 10 8 1 10 2 2 2 10 0 2 2 2 2 2 2 2 2 12 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	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 91.1 87.1 87.1 87.1	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82 1748442.83 1545042.01 1252325.92 1175243.83 1003683.43 948756.367 911409.607
Name PEG n10 PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylhexyl) phth 7.8-Dhydroxy-4-aneth N.N-Dicyclohexylurea PEG n5 9-Oxo-10(E).12(E)-oct Naringenin Glucous 1-phosphate	Formula (30 H50 O2 (22 0 H42 O11 C6 H6 O3 (22 H46 O12 C44 H72 O13 C24 H22 O10 C24 H22 O10 C24 H22 O10 C24 H38 O4 (13 H24 N2 O C10 H22 O6 C15 H13 O3 C15 H12 O5 C6 H13 O9 P C18 H13 O5	Aunotation Source Predicate 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 Pall match Pall match Pall match Full match Full match Pall match Pall match Full match Full match Full match Full match Full match Full match Full match	Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Full match Full match Full match Full match Not the top hit Full match Not the top hit Patl match Patla match Partial match Partial match	Annotation Source: MastList Match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935 272.06832 260.02962 283.29203	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 0.901 10.658	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1163243.832 1003683.429 911408.6067 911408.607 911408.707 911408.707 911408.7	# ChemSpi der 42 1 26 0 1 111 31 26 38 6 1 1 24 46 39 4 4	# mzCloud Results 2 2 2 2 2 2 2 2 4 4 2 5 5 10 0 8 8 1 1 4 2 2 10 0 2 2 10 2 2 2 2 2 2 2 2 2 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud 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 \$1 \$7.1	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82 1748442.83 1545042.01 1252325.92 171308.02 1167243.83 1003683.43 1003683.43 948756.367 911408.607 911408 911408 911408 911408 911408 911408 91
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glyotin L-Ghttamic acid Bis(2-ethylicetyl) phth N-Dicyelothexylurea PEG n5 9-Oxo-10(E).12(E)-oct Naringenin Glucose 1-phosphate Stearmide Stearmide	Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C2 H20 10 C2 H20 10 C2 H38 04 C13 H24 N2 0 C10 H20 06 C10 H20 03 C15 H12 05 C18 H30 03 C15 H12 05 C18 H37 N 0 C15 H437 N 0	Aunotation Source Predicted Compositions Fail match Not the top hit Not the top hit Not the top hit Fail match Not the top hit Fail match Fail match	Annotation Source: mcCloud Search Foll match Foll match	Annotation Source: ChemSpider Search Partial match Partial match No match Partial match No match Partial match Pail match Pail match Fail match Fail match Fail match Fail match Pail match	Annotation Source: MassList Match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.2900 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935 272.06832 260.02962 283.28703	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 0.901 10.658 0.971	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252325.919 1171308.019 1165243.832 1003683.429 948756.3665 911408.6067 855834.1188	# ChemSpi der 42 1 26 0 1 1 11 31 26 388 6 1 1 24 46 39 4 200	# m2Cloud Results 2 2 2 2 2 2 2 2 4 4 2 5 5 10 8 8 8 8 4 2 2 10 0 2 2 10 10 2 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	mzCloud Best Match \$3.7 \$8.1 \$9.2 \$8.5 \$3.2 \$8.5 \$3.2 \$8.7 \$2.7 94.2 \$8.4 91.1 \$7.1 \$7.1 \$7.1 \$7.1 \$7.1 \$7.2 \$7.2 \$7.2 \$7.2 \$7.2 \$7.2 \$7.2 \$7.2	Group Area: F8 2850840.17 2782623.27 2782623.27 1792976.45 1792976.45 1783088.82 1748442.83 1545042.01 1252325.92 1171308.02 1165243.83 1003683.43 948756.367 911408.607 885834.119 911408.607
Name Betulin PEG n10 Maliol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylhexyl) phth N.N-Dicyclohexylures PEG n5 9-Oxo-10(E).12(E)-oci Naringenin Glucous I-phosphate Stearamide Guanine Jasouthorofine	Formula C30 H50 O2 C20 H42 O11 C6 H6 O3 C22 H42 O13 C42 H72 O13 C22 H22 O10 C42 H72 O13 C24 H22 O10 C44 H72 O13 C24 H38 O4 C10 H8 O4 C10 H8 O4 C10 H8 O4 C10 H22 O6 C11 H20 O3 C15 H12 O5 C6 H13 O9 P C11 H20 N2 O3 C15 H37 N O C5 H8 N5 O C11 H20 N2 O3 C5 H8 N5 O	Aunotation Source Prediction Fold match Fold match Fold match Not the top hit Fold match Not the top hit Fold match Fold match	Annotation Source: mcCloud Search Foil match Foil match	Annotation Source: ChemSpider Search Partial match Partial match No match Partial match No match Partial match Full match Full match Not the top hit Full match Not the top hit Patla match Patla match Patlal match Patlal match Patlal match Patlal match Patlal match	Annotation Source: MaskList Match Full match	FISh Coverage	Molecular Weight 442.38046 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14852 272.06832 294.21935 272.06832 294.21935 3151.04936 278.14936	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 0.901 10.658 0.876 0.905	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 1748442.833 1545042.007 1252232.919 1173038.019 1165243.832 103683.429 948756.3665 911408.6667 885834.1188 840032.1577	# ChemSpi der 42 1 26 0 1 1 11 31 1 26 38 6 1 24 46 39 9 4 24 46 39 9 4 20 6 6	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match \$3,7 \$8,1 \$9,2 \$8,5 \$3,2 \$6,7 \$2,7 \$2,7 \$2,7 \$2,7 \$2,7 \$2,7 \$3,1 \$4,2 \$3,1 \$5,5 \$3,2 \$6,4 \$1,1 \$9,1 \$5,5 \$6,4 \$1,1 \$7,2 \$6,5 \$1,1 \$6,2 \$1,2 \$1,2 \$1,2 \$1,2 \$1,2 \$1,2 \$1,2 \$1	Group Area: F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1783088.82 1748442.83 1545042.01 1252325.92 1171308.02 1152534.83 103368.34 948755.367 911408.607 885834.119 840032.158 904372.548
Name Betulin PEG n10 Maltol PEG n10 Ginsenoside Rg3 Glyorin L-Olutamic acid Bis(2-ethylhexyl) phth 7.8-Dhydroxy-4-meth N.N-Dicyclohexylurea PEG n5 9-Oxo-10(E),12(E)-ec Naringenin Glucose 1-phosphate Stearamide Guanine Lewsylprofine PEG n13	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 H28 O4 C18 H30 O3 C15 H12 O5 C6 H13 O9 P C18 H37 N O C1 H120 N2 O3 C1 H120 N2 O3 C18 H37 N O	Aunotation Source Predicate 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: mr2Cloud Search Fuil match Pail match	Annotation Source: ChemSpider Search Partial match Partial match No match Partial match No match Partial match Partial match Pail match Pail match Fuil match Not the top hit Fuil match Not the top hit Fuil match Partial match Partial match Partial match Partial match Partial match	Annotation Source: MastList Match Full match	FISh Coverage	Molecular Weight 442,38046 458,27269 502,29909 766,48533 446,12103 147,05307 390,2762 2192,04254 224,18852 228,14166 294,21935 272,06832 260,02962 283,28703 151,04936 218,1476 509,35113	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 0.901 10.658 0.876 2.987 4.469	Area (Max.) 2850840.167 2782032.267 2599740.77 2098519.233 1792976.447 1783088.822 1748442.833 1748442.833 1748642.833 1748642.833 171308.019 845763.365 911408.6067 885834.1188 840032.1577 840307.6478 759721.2017.	# ChemSpi der 42 1 26 0 0 1 1 11 26 0 0 1 1 11 26 0 0 1 1 26 0 0 1 1 12 4 4 6 38 6 1 24 4 6 38 6 0 0 0 1 1 24 2 0 0 0 1 1 1 26 0 0 1 2 1 26 0 0 1 2 1 26 0 0 1 2 2 3 2 3 2 3 2 3 2 3 2 3 2 3 2 3 2 3	# mzCloud Results 2 2 2 2 2 2 2 2 4 4 4 5 5 10 8 8 11 2 2 12 2 10 2 2 10 2 4 4 4 4 4 10 2 2 10 2 2 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	mzCloud Best Match \$3.7 \$9.2 \$8.5 \$3.2 \$6.7 \$2.7 \$4.2 \$8.1 \$3.1 \$1.5 \$6.4 91.1 \$7.1 \$1.7 \$2.1 \$1.5 \$6.4 \$1.9 \$1.5 \$6.4 \$1.9 \$1.5 \$6.4 \$1.9 \$1.5 \$1.5 \$1.1 \$1.1 \$1.1 \$1.1 \$1.1 \$1.1	Group Area: F8 2850540.17 2782623.27 2782623.27 2782623.27 17820740.77 2098519.25 1782076.47 1782076.47 1782076.47 171408.627 911408.607 911408.607 911408.07 540032.158 804307.648 50407.648
Name PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylkeryl) phth N-Dicyclohexylurea PEG n5 9-Oxo-10(E),12(E)-oci Naringenin Glucous 1-phosphate Stearamide Guanine Leusylprofine PEG n13 Uraci	Formula C30 H50 02 C20 H42 011 C42 H42 012 C42 H47 013 C42 H47 013 C42 H47 013 C42 H47 013 C42 H47 013 C42 H48 04 C10 H8 04 C10 H22 06 C18 H37 N 0 C5 H12 05 C6 H13 09 P C18 H37 N 0 C5 H12 05 C6 H13 07 N C5 H12 05 C6 H13 07 N C5 H15 07 C1 H22 07 C2 H44 07 C2 C1 H22 07 C2 H47 07 C2 H4	Aunotation Source Prediction Compositions Fall match Not the top hit Fall match Not the top hit Fall match Not the top hit Fall match Fall match	Annotation Source: mcCloud Search Full match Full match	Annotation Source: ChemSpider Search Partial match Fall match No metals No match Partial match Fall match Fall match Fall match Fall match Fall match Fall match Fall match Patla match Partial match Partial match Partial match No results Fall match No results Fall match	Annotation Source: MaskList Match Full match	FISh Coverage	Molecular Weight 442.38046 458.27260 502.29009 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 228.14166 204.21935 272.06832 260.02962 283.124166 294.21935 272.06832 260.02962 283.28703 151.04936 228.1476 590.35113 112.02780	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 0.901 10.658 0.876 2.987 4.469	Area (Max.) 2850840.167 289740.77 2899740.77 2899740.77 2999740.77 1783088.822 1792976.447 1784842.831 1545042.007 12522325.919 1165243.832 117308.199 948756.3665 9948756.365 9948756.365 991408.6067 885834.1188 840032.1577 891408.2057	# ChemSpi der 42 1 266 0 0 1 1 11 31 266 388 6 6 1 1 24 4 6 39 4 20 0 6 0 0 28	# mzCloud Results 2 2 2 2 2 2 4 4 2 2 5 10 8 8 11 4 4 2 2 2 2 12 2 4 12 2 3 4 12 2 12 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match \$3,7 \$8,1 \$9,2 \$8,5 \$3,2 \$6,7 \$2,7 \$2,7 \$4,2 \$8,1 94,2 \$8,1 94,2 \$8,1 94,2 \$8,1 94,2 \$8,1 \$1,5 \$6,4 \$1,6 \$1,5 \$1,5 \$1,5 \$1,6 \$1,6 \$1,6 \$1,6 \$1,6 \$1,6 \$1,6 \$1,6	Group Ares: F8 2850840.17 2782023.27 2599740.77 2599740.77 2599740.77 2098519.25 1792076.45 1792076.45 1792076.45 1782076.02 1174542.83 1545042.01 1252325.92 1171308.82 1171308.02 1155245.83 154505.03 948755.367 911408.607 911408.607 911408.507 911408 911407 911408 91148 91148 91148 91148 91148 91148 91148 91148 91
Name PEG n10 PEG n10 PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylhexyl) phth 7.8-Dhydoxy-4-aneth N.N-Dicyclohexylurea PEG n5 9-Oxo-10(E).12(E)-oct Naringenin Glacose 1-phosphate Stearamide Guanine Leuxylproline PEG n13 Uracil Uracil	Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C24 H38 04 C10 H8 04 C13 H24 N2 0 C18 H30 03 C18 H30 N0 C18 H37 N0 C18 H37 N0 C18 H37 N0 C18 H37 N0 C18 H37 N0 C11 H20 N2 03 C11 H20 N2 03 C12 H34 014 C4 H4 N2 02 C4 H4 N2 04 C4 H4 N2 02 C4 H4 N2 04 C4 H4 N2 02 C4 H4 C4 H4 N2 02 C4 H4 C4 H4 N2 02 C4 H4 N2 04 C4 H4 N2 02 C4 H4 C4 H4 N2 02 C4 H4 H4 N2 04 C4 H4 N2 0	Aunotation Source: Predicator 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: mr2Coud Search Fuil match Pail match Pail match Pail match Fuil match Fuil match Pail match	Annotation Source: ChemSpider Search Partial match Partial match No match Partial match No match Full match Full match Full match Partial match	Annotation Source: MastList Match Full match	FISh Coverage	Molecular Weight 442,38046 445,27269 126,03195 502,29909 766,48533 446,12103 147,05307 390,2762 192,04254 224,18852 238,14166 294,21935 242,1835 260,02962 283,28703 151,04936 228,1876 390,35113 112,002769 222,0889	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 0.658 4.445 0.6576 2.987 4.469 1.094 6.327	Area (Max.) 2850840.167 2850940.167 2782032.867 2599740.77 2098519.233 1792976.447 1783088.822 1718408.832 171308.019 1165234.832 1003683.429 911408.0067 885834.1188 840032.1577 804307.6478 759721.2017 672279.754 662943.6763	# ChemSpi der 42 1 26 0 1 1 11 31 26 38 6 1 1 24 4 46 39 9 4 4 20 6 0 0 28 45 5	# mzCloud Results 2 2 2 2 2 2 2 4 4 2 5 5 10 8 11 10 8 11 10 8 11 10 2 2 10 10 2 2 11 10 10 10 10 10 10 10 10 10 10 10 10	# mzVauk Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match \$3.7 \$3.1 \$9.2 \$3.5 \$3.2 \$3.2 \$3.2 \$3.7 \$2.7 \$2.7 \$2.7 \$2.7 \$2.7 \$2.7 \$2.7 \$2	Group Area: F8 2850840.17 2782052.37 2599740.77 2098519.25 1782086.82 1782076.45 1783086.82 1784842.83 1784842.83 1784842.83 1748442.83 1545042.01 1252325.92 11545042.01 1252325.92 11545042.01 1252325.92 1171308.82 103683.43 948756.367 911408.607 858584.119 \$40032.158 804307.648 759721.202 672279.754 662043.676
Name PEG n10 Maltol PEG n10 L-Oltramic acid Bis(2-ethylicacyl) phth N-Disyelohexylurea PEG n5 9-Oxo-10(E),12(E)-occ Naringenin Glucose 1-phosphate Stearamide Guanine Lewsylprofine PEG n13 Uracil Monobutyl phthalate L-Histidine	Formula C30 H50 02 C20 H42 011 C6 H6 03 C42 H47 013 C42 H47 013 C42 H47 013 C42 H47 013 C42 H47 013 C44 H8 04 C10 H8 04 C10 H8 04 C18 H30 03 C15 H12 05 C6 H13 09 P C1 H20 N2 03 C26 H54 014 C14 H4 N2 02 C12 H4 04 C26 H9 N3 02 C12 H14 04 C12 H4 04 C12 H4 04 C12 H4 04 C26 H9 N3 02 C12 H14 04 C12 H4 04 C14	Aunotation Source Predicter Compositions Fail match Not the top hit Fail match Not the top hit Fail match Not the top hit Fail match Fail match	Annotation Source: mcCloud Search Foll match Foll match	Annotation Source: ChemSpider Search Patrial match Patrial match No results No match Patrial match Patrial match Full match Full match Full match Full match Full match Full match Patrial match	Annotation Source: MaskList Match Full match	FISh Coverage	Molecular Weight 442,38046 458,27269 126,03195 502,2900 766,48533 446,12103 147,05307 390,2762 192,04254 223,146 294,21935 272,06832 260,02962 283,28703 151,04936 228,1476 590,35113 112,02769 222,0889 125,06490	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.558 4.445 0.876 2.985 7.232 4.445 0.876 2.987 4.469 2.987 4.469 2.987 4.6327 0.834	Area (Max.) 2850840.167 2899740.77 2899740.77 2098510.233 1792976.447 1783088.822 1784042.837 1545042.007 1165243.832 1165243.832 1165243.832 1165243.832 1165243.832 1103683.429 948756.3665 941205.457 840032.1577 804307.6478 759721.2017	# ChemSpi der 42 1 266 0 0 1 111 311 266 388 6 1 1 244 46 399 4 200 6 0 0 28 45 18	# mzCloud Results 2 2 2 2 2 2 2 4 4 2 5 5 10 0 8 8 1 1 4 4 2 2 2 2 2 10 2 2 11 2 4 4 10 2 2 10 2 5 5 10 10 2 5 5 10 10 2 5 5 10 2 5 5 5 10 2 5 5 5 5 10 2 5 5 5 5 10 2 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match \$3.7 \$3.1 \$9.2 \$6.7 \$3.2 \$6.7 \$3.2 \$6.7 \$4.2 \$8.1 94.2 \$8.4 91.1 \$7.1 \$7.1 \$8.5 \$6.7 \$1.2 \$8.5 \$1.2 \$8.5 \$1.2 \$8.5 \$1.2 \$1.2 \$1.2 \$1.2 \$1.2 \$1.2 \$1.2 \$1.2	Group Ares: F8 2850840.17 2782623.27 2599740.77 2599740.77 2098519.25 1792976.45 1792976.45 1792976.45 1792976.45 1748442.83 1545042.01 1252325.92 1171308.02 1165243.43 948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 941408.56 3948756.367 3948756
Name PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylexyl) phth N.N-Dicyclohexylarea Bis(2-ethylexyl) phth N.N-Dicyclohexylarea Bis(2-ethylexyl) phth Stearamide Glucous 1-phosphate Stearamide Cusmine Leucylproline PEG n13 Uracil Monobutyl phthalate L-Histidine 2-Hydroxycinnamic ac	Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C42 H72 013 C5 H9 N 04 C13 H24 N2 00 C10 H22 06 C18 H30 03 C15 H12 05 C6 H13 09 P C15 H12 05 C6 H13 09 P C18 H37 N 0 C5 H5 N5 0 C11 H20 N2 03 C26 H54 014 C4 HA N2 02 C26 H54 014 C4 HA N2 02 C5 H14 04 C6 H9 N3 02 C9 H8 03 C5 H5 03	Aunotation Source: Prediction Foll match Not the top hit Full match Not match Not the top hit Full match Not the top hit Full match Full match	Annotation Source: mcCloud Search Foil match Foil match	Annotation Source: ChemSpider Search Partial match Partial match No match Partial match No match Partial match Full match Partial match Not the top hit Full match Partial match	Annotation Source: MaskList Match Full match	FISh Coverage	Molecular Weight 442,38046 458,27269 126,03195 502,29090 766,48533 446,12103 147,05307 390,2762 192,04254 224,18852 272,06832 204,21935 272,06832 260,0296 294,21935 272,06832 263,28703 151,04936 228,1476 590,35113 112,0276 590,35113 112,02689 155,06949 155,06949	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 0.876 0.876 0.876 4.699 1.094 4.6327 0.833 3.412	Ares (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.822 178448.283 1545042.007 1525325.919 1173308.429 91408.6067 88584.1188 840032.1577 804307.6478 759721.2017 672279.754 662943.6763 659854.4891 612912.9287	# ChemSpi der 42 1 266 0 0 1 1 111 31 266 388 6 1 1 24 4 40 0 0 6 0 0 0 288 45 18	# mzCloud Results 2 2 2 2 2 2 2 2 2 4 4 2 2 5 5 10 8 11 4 4 2 2 10 2 2 2 11 10 8 11 2 10 10 10 2 10 10 12 12 2 2 4 4 12 2 2 2 2 2 2 2 2 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match \$3.7 \$8.1 \$9.2 \$8.5 \$3.2 \$8.7 \$2.7 94.2 \$8.1 91.5 \$6.4 91.1 \$7.1 \$8.9 \$1.6 \$7.3 \$3.4 \$3.4 \$2.9 \$8.4 \$2.9 \$8.4 \$3.4 \$2.9 \$3.4 \$3.4 \$3.4 \$3.4 \$3.4 \$3.4 \$3.4 \$3.4	Group Area: F8 28508-01,7 2782-02-3,27 2599740,77 2098519,25 1792076.45 1783068.82 1748442.83 1545042.01 1545042.01 1545042.01 11522422.92 1171306.02 115224.58 1033068.34 948755.367 911408.607 858534.119 40032.158 804307.648 759721.202 672279.754 662943.376 659854.489 612912.292
Name Betulin PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Ghttanic acid Bis(2-ethylicstyl) phth N-Toiseyclohexylurea PEG n5 9-Oxo-10(E).12(E)-oct Naringenin Glucose 1-phosphate Stearamide Guanite Lewsylprofine PEG n13 Uracil Monobutyl phthalate L-Histidine 2-Hydroxycinnamis ac	Formula C30 H50 02 C20 H42 011 C6 H6 03 C42 H47 013 C42 H47 013 C42 H72 013 C42 H72 010 C5 H9 N 04 C10 H8 04 C10 H8 04 C10 H8 04 C18 H30 03 C15 H12 05 C18 H37 N0 C5 H5 N5 0 C1 H20 N2 03 C26 H54 014 C4 H4 N2 02 C12 H14 04 C6 H9 N3 02 C9 H8 03 C1 H18 N2 02 C9 H8 03 C9 H8 03 C9 H8 03 C1 H18 N2 02 C9 H8 03 C1 H18 N2 02 C1 H18 N2 02	Aunotation Source Prediction Compositions Fail match Not the top hit Fail match Not the top hit Fail match Not the top hit Fail match Fail match	Annotation Source: mrCloud Search Foll match Foll match	Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match Partial match Partial match Pail match Pail match Pail match Pail match Pail match Partial match	Annotation Source: MaskList Match Foll match	FISh Coverage	Molecular Weight 442,382469 458,272046 458,272046 502,29009 766,48533 446,12103 792,04224 147,05307 792,04224 224,18852 228,14166 204,21935 272,06832 228,1426 228,1426 228,1426 509,35113 151,04936 228,1426 509,35113 151,04936 228,1426 509,35113 151,04946 220,2689 151,044749 210,13866	RT [min] 5.59 4.161 2.799 4.284 5.588 4.439 0.852 11.155 3.746 6.852 7.232 4.445 0.801 10.658 0.876 2.987 4.469 1.094 6.327 0.833 3.412	Area (Max.) 2850840.167 2782623.267 2098710.273 2008710.273 2008710.273 1792976.447 1783088.822 1713086.19 1713086.19 11733088.422 1003683.429 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3665 948756.3675 948756.37555 948756.37555 948756.37555 948756.37555 948756.37555555 949756.375555 949755555	# ChemSpi der 42 1 26 0 1 1 11 31 31 26 6 33 8 6 1 1 24 4 6 39 4 20 6 0 0 28 45 18 8 45 18 8 8 45 18 8 8 45 18 9 9 45 18 19 18 18 18 18 18 18 18 18 18 18 18 18 18	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 5 0 0 8 8 1 1 4 4 2 2 2 10 0 8 8 11 2 4 4 2 2 5 5 10 12 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7, 83.1, 83.7, 83.2, 83.5, 83.2, 88.5, 85.4, 91.5, 86.4, 91.1, 87.1, 81.6,	Group Area: F8 F8 28508-01.2 258054-01.2 2599740.77 2098510.25 1792076.45 1792076.45 1793078.82 1748442.83 1545042.0 1155243.83 0030854.34 911408.607 911408.607 911408.607 672279.734 659854.489 612912.929 612912.929
Name PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ethylkeryl) phth N-Dicyclohexylurea PEG n5 9-Oxo-10(E),12(E)-eet Naringenin Gluccose 1-phosphate Stearamide Guanine Lewsylproline PEG n13 Urseil Monobutyl phthalate L-Histidine 2-Hydroxycinnamic ac Cyclo(leusylprolyl)	Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C42 H72 013 C42 H72 013 C42 H72 013 C5 H9 N 04 C10 H22 06 C18 H30 03 C18 H37 N 0 C5 H9 X02 C6 H13 09 P C11 H20 X2 03 C26 H54 014 C4 H4 N2 02 C12 H14 04 C6 H9 N3 02 C11 H18 N2 02 C11 H18 N2 03 C11 H18 N2 03 C11 H18 N2 03 C11 H18 N2 03 C12 H18 N2 03 C11 H18 N2 03 C12 H18 N2 03 C13 H18 N2 03 C13 H18 N2 03 C13 H18 N2 03 C13 H18 N2 03 C14 H18 N2 N2 N2 N2 N2 C14 H18 N2 N2 N2 C14 H18 N2 N2 N2 C14 H18 N2 N2	Aunotation Source: Predictions Foll 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 Foil match Foil match	Annotation Source: ChemSpider Search Partial match Partial match No match Partial match No meals Partial match Full match Full match Full match Partial match	Annotation Source: MaskList Match Full match	FISh Coverage	Molecular Weight 442.38044 4458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935 272.06832 260.02962 228.1476 590.35113 112.02769 222.0889 115.06949 115.06949 210.13686 339.34957	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 0.801 0.901 10.658 0.876 2.987 4.469 1.094 6.327 0.833 3.412 4.27 13.101	Area (Max.) 2850840.167 2782623.267 2599740.77 2098519.253 1792976.447 1783088.222 1748442.833 1792976.447 1783088.222 1748442.833 1792976.447 1173056.019 1173056.019 1165243.825 911408.6067 858384.1188 840032.1577 597213.2017 662943.6763 659854.4891 662943.6763 659854.4891 662943.8763 659854.4891 662943.8763 659854.4891 662943.8763 659854.4891 662943.8763 659854.4891 662943.8763 659854.4891 662943.8763 571451.973 446650.3856 19212.9257 571451.973 446650.3856 19212.9257 571451.973 446650.3856 19212.9257 571451.973 571455.975 571451.973 571455.975 571455	# ChemSpi der 42 1 1 26 0 0 1 1 11 31 26 38 6 1 1 11 26 38 6 1 1 24 4 6 39 4 20 0 0 28 45 18 8 41 28 0 0 1 11 28 6 0 1 11 12 6 0 0 1 11 12 6 12 10 10 10 10 10 10 10 10 10 10 10 10 10	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 2 3 5 100 8 8 1 4 4 2 2 0 0 2 2 2 2 1 1 3 4 4 2 2 0 2 2 2 1 2 2 2 2 2 2 2 2 2 2 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match \$3.7 \$8.1. \$9.2 \$8.5 \$3.2 \$8.5 \$3.2 \$8.1 91.5 \$6.4 91.1 \$7.1 \$8.9 \$1.6 \$7.3 \$3.4 \$2.9 \$1.6 \$3.3 \$3.4 \$3.3 \$3.4 \$3.5 \$3.5 \$3.5 \$3.5 \$3.5 \$3.5 \$3.5 \$3.5	Group Area: F8 2850840.17 2782623.27 2782623.27 2599740.77 2098519.25 1782076.45 1783088.82 1748442.83 1748442.83 1748048.23 1145243.83 1003683.43 948756.367 911408.607 885834.119 84092.2158 858534.119 94092.2158 858534.119 94092.2158 858534.119 94092.2158 858534.119 94092.2158 948756.367 911408.607 858534.119 94092.2158 948756.367 911408.607 858534.119 94092.2158 948756.367 911408.607 858534.119 94075.2158 948756.367 911408.607 858534.119 94075.2158 94575.2158575.2158 94575.2158 94575.2158 94575.2158 94575.
Name PEG n10 Maltol PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glystin L-Ghtramic acid Bis(2-ethylicetxyl) phth N-Dicyclothexylurea PEG n5 9-Oxo-10(E).12(E)-oct Naringenin Glucose 1-phosphate Stearamide Guasnine Leucylproline PEG n13 Urscil Monobutyl phthalate L-Histidine 2-Hydroxycinnamic ac 2-tylotycrolyn) Docosnamide Diphenylamine	Formula C30 H50 02 C20 H42 Ol1 C6 H6 03 C22 H42 Ol2 C42 H72 Ol3 C42 H72 Ol3 C42 H72 Ol3 C42 H72 Ol3 C42 H72 Ol3 C13 H24 N2 O C10 H22 O6 C18 H30 O3 C15 H12 O5 C18 H30 O3 C15 H12 O5 C11 H20 N2 O3 C26 H3 N O4 C11 H20 N2 O3 C26 H3 N O C11 H20 N2 O3 C26 H3 N O C11 H20 N2 O3 C26 H3 N O3 C11 H10 N2 O3 C26 H30 N3 O2 C9 H8 O3 C11 H18 N2 O2 C21 H45 N O C12 H11 N	Aunotation Source Prediction Compositions Fail match Not the top hit Not the top hit Not the top hit Pail match Not the top hit Pail match Fail match	Annotation Source: mrCloud Search Full match Full match	Annotation Source: ChemSpider Search Partial match No match Partial match No mesuits No match Full match Full match Full match Partial match Partial match Partial match Partial match Partial match Partial match Partial match Full match Partial match Partial match Full match Partial match	Annotation Source: MastList Match Full match	FISh Coverage	Molecular Weight 442,38044 458,27269 126,03195 502,29009 766,48533 446,12103 446,12103 192,04254 224,18852 228,14166 204,21935 272,06832 228,1476 590,35113 112,02769 228,0326 215,104936 215,104936 215,06949 155,06949 155,06949 155,06949 155,06949 164,04749 2210,13866 339,34957 169,08913	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 0.901 10.658 4.445 0.901 10.658 4.469 1.094 6.383 3.412 4.27 0.833 3.412 1.427 1.101 7.451	Area (Max.) 2850640.1267 289740.77 2008519.233 1792976.447 1783088.822 1783088.422 171308.019 1171308.019 1171308.019 1171308.019 1175308.420 911408.0067 885834.41188 84032.1577 840307.478 759721.2017 672279.754 662943.6763 659854.4891 612912.9287 571451.973 446630.3886 440857.50065.5886 440857.50065.5886 440857.5986 440857.50065.5886 440857.598	# ChemSpi der 42 1 26 0 1 1 11 31 1 26 38 6 1 1 24 4 46 39 4 4 20 6 6 0 0 28 45 5 18 18 18 18 10 18 28 28 20 10 28 28 20 28 20 28 20 28 20 20 20 28 20 20 20 20 20 20 20 20 20 20 20 20 20	# mzCloud Results 2 2 2 2 2 2 2 2 2 2 4 4 2 5 5 10 0 8 8 11 4 4 2 10 0 2 2 11 10 0 2 2 11 0 0 2 2 10 10 10 12 12 12 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 83.7 83.2 83.5 85.7 86.7 94.2 88.1 91.5 86.4 91.1 87.1 81.6 87.3 83.4 83.4 83.4 83.4 83.4 83.6 87.3 83.6 87.3 83.6 85.3 83.6 83.8 84.3 83.6 88.8 84.3 85.2 85.2 85.2 85.2 85.2 85.2 85.2 85.2	Group Area: F8 2850840.17 2783023.27 2599740.77 2599740.77 2098519.25 1792076.45 1792076.45 1783088.82 1738088.23 1738068.23 1738088.33 1030683.43 1030683.43 1030683.43 1030683.43 911408.607 885834.119 840032.158 804307.648 759721.202 672279.754 662943.676 659854.489 612912.929 571451.973 440653.039
Name PEG n10 Maltol PEG n10 Information of the second second L-Glutamic acid Bis(2-ethylhexyl) phth N-Dicyelohexylurea PEG n5 9-Oxo-10(E),12(E)-oct Naringenin Glucous 1-phosphate Stearamide Ouanine Lewsylproline PEG n13 Uracil Monobutyl phthalate L-Histidine 2-Hydroxycinnamic ac Cyclo(lewsylprolyl) Docosnamide Diphenylanine Pig,138-12-Oxophytod	Formula C30 H50 02 C20 H42 O11 C42 H42 O12 C42 H47 O13 C42 H47 O13 C42 H47 O13 C42 H72 O13 C42 H72 O13 C5 H9 N O4 C10 H8 O4 C10 H8 O4 C10 H8 O4 C10 H22 O6 C18 H37 N O C5 H3 O3 C6 H13 O9 P C6 H3 N5 O C1 H20 N2 O3 C26 H54 O14 C4 H4 N2 O2 C12 H14 O4 C6 H9 N3 O2 C9 H8 O3 C11 H18 N2 O2 C12 H11 N C12 H11 N C12 H11 N C18 H37 O C18 H37 O C12 H11 N C12 H11 N C18 H37 O C18 H37 O C18 H37 O C12 H11 N C12 H11 N C18 H37 O C18 H37 O C18 H37 O C18 H37 O C12 H11 N C12 H11 N C18 H37 O C18 H37 O C	Aunotation Source: Prediction Source: Predictions Fail match Not the top hit Fail match Not the top hit Fail match Not the top hit Fail match Fail match	Annotation Source: mcCloud Search Foll match Foll match	Annotation Source: ChemSpider Search Partial match Partial match No metals No match Partial match No metals Full match Full match Full match Full match Full match Full match Partial match	Annotation Source: MaskList Match Full match	FISh Coverage	Molecular Weight 442.38044 458.27269 126.03195 502.29909 766.48533 446.12103 147.05307 390.2762 192.04254 224.18852 238.14166 294.21935 224.18852 260.02962 283.28703 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 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 151.04936 228.1476 590.35113 151.04936 228.1476 228.1476 228.1476 239.34112 250.08913 192.20339 292.20339	RT [min] 5,59 4,161 2,799 4,44 5,588 4,439 0,852 11,155 3,746 6,584 2,895 7,232 4,445 0,901 10,658 0,876 0,876 0,876 0,876 0,876 0,873 3,445 1,098 7,459 1,3101 7,451 6,857	Area (Max.) 2850840.167 2782632.267 2599740.77 2098719.23 1792976.447 1783088.222 1748442.833 1792976.447 1783088.222 1748442.833 1792976.447 1783088.22 1748442.833 191292.25 191108.0067 858384.1188 840032.1577 859854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.4891 659854.491 659854.491 659854.491 659854.491 771475.1989 771475.7066 41073.1189 770475.7066 41073.1189 700475.7066 41073.1189 700475.7066 41073.1189 700475.7066 41073.1189 700475.7066 700475	# ChemSpi der 42 1 26 0 0 0 1 1 1 1 1 1 26 0 6 1 1 1 24 4 4 20 6 6 1 1 24 4 4 20 0 6 1 1 24 4 4 20 5 1 2 6 1 2 6 1 2 6 1 2 6 1 2 6 0 0 0 1 1 1 2 6 0 0 0 0 1 1 1 1 2 6 0 0 0 0 0 0 1 1 1 1 2 6 0 0 0 0 0 0 0 0 0 1 1 1 1 1 2 6 0 0 0 0 0 0 1 1 1 1 1 2 6 0 0 0 0 0 0 1 1 1 1 2 6 0 0 0 0 0 1 1 1 1 2 6 0 0 0 0 0 1 1 1 1 2 6 0 0 0 0 0 1 1 1 1 2 6 0 0 0 0 0 1 1 1 1 2 6 0 0 0 0 1 1 1 1 2 6 0 0 0 0 1 1 1 1 2 6 0 0 0 0 1 1 1 1 2 6 0 0 0 0 1 1 1 2 6 0 0 0 0 0 0 0 0 0 1 1 1 2 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	<pre># mzCloud Results 2 2 2 2 2 2 2 4 4 2 5 10 8 8 1 4 4 2 10 0 2 2 1 1 4 1 1 3 3 4 4 2 6 2 2 1 1 4 4 1 1 3 3 4 2 6 2 1 1 4 4 1 1 3 3 4 4 2 6 6 2 1 1 4 4 4 1 3 4 4 2 6 6 2 1 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4</pre>	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 83.1 83.7 83.2 86.7 94.2 85.7 94.2 85.7 94.2 85.7 94.2 85.7 94.2 85.7 94.2 85.7 94.2 85.4 91.1 87.1 87.1 83.9 92.1 83.4 83.9 81.6 85.3 83.4 83.4 83.6 85.3 85.3 85.3 85.3 85.3 85.3 85.3 85.3	Group Area: F8 2850840, F7 2782622, 27 2782622, 27 2599740, 77 2098519, 25 1792076, 45 1773078, 82 178308, 82 177308, 82 177508,
Name PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glycitin L-Glutamic acid Bis(2-ettylhextyl) phth. N.N-Dikyclohexylarea Bis(2-ettylhextyl) phth. PEG n5 9-Oxo-10(E).12(E)-oci Naringenin Glucose 1-phosphate Stearamide Guanine Leuxylproline PEG n13 Uracil Monobutyl phthalate L-Histidine 2-Hydroxycinnamie ac Cyclo(leuxylprolyf) Docosanamide Bijhenylamine 95,138-12-Oxophytod	Formula C30 H50 02 C20 H42 011 C6 H6 03 C22 H46 012 C42 H72 013 C42 H72 013 C5 H9 N 04 C13 H24 N2 00 C10 H22 06 C18 H37 N 0 C5 H5 N5 0 C11 H20 N2 03 C18 H37 N 0 C5 H5 N5 0 C11 H20 N2 03 C18 H37 N 0 C5 H5 N5 0 C11 H10 N2 03 C11 H18 N2 02 C22 H45 N 0 C12 H11 N C12 H11 N C12 H11 N C12 H11 N C18 H28 03 C11 H18 N2 02 C22 H45 N 0 C12 H11 N C18 H28 03 C11 H18 N2 02 C22 H45 N 0 C12 H11 N C18 H28 03 C11 H18 N2 02 C22 H45 N 0 C12 H11 N C18 H28 03 C11 H18 N2 02 C12 H11 N C18 H28 03 C11 H18 N2 02 C22 H45 N 0 C12 H11 N C18 H28 03 C12 H11 N C18 H28 03 C18 H28 04 C18 H28 H28 04 C18 H28 H28 H28 H28 H28 H28 H28 H28 H28 H2	Aunotation Source: Predictions Full match Not the top hit Full match No match No match Not me top hit Full match Full match	Annotation Source: mr2Coud Search Fuil match Pail match	Annotation Source: ChemSpider Search Partial match No match Partial match No results No match Partial match Full match Full match Full match Partial match	Annotation Source: MastList Match Full match	FISh Coverage	Molecular Weight 442,38044 458,27269 126,03195 502,29090 766,48533 446,12103 147,05307 390,2762 192,04254 224,18852 228,14166 294,21935 272,06832 220,81476 590,35113 112,002962 222,0889 155,06949 155,06949 150,06949 210,13686 339,34957 164,04749 210,13686 339,34957	RT [min] 5.59 4.161 2.799 4.45,588 4.439 0.852 7.232 4.445 7.232 4.445 0.901 10.658 0.876 0.876 1.094 4.669 1.094 4.469 1.094 4.465 1.3101 7.451 2.845 2.857 2.845 3.412	Area (Max.) 2850640.167 2850540.167 2098519.233 1792976.447 1783088.822 1748442.833 1545042.007 152325.919 1173308.129 1173308.129 1165243.825 911408.6067 885834.1188 84032.1577 804307.6478 7579212.1017 672279.754 662943.6763 659854.4891 612912.9278 571451.973 571451.973 571451.973 571451.973 571451.973 571451.973 571451.973 571451.973 571451.973 571451.973 571451.973 286344.3592 571451.973 286344.3592 571451.973 571451.97	# ChemSpi der 42 1 26 0 1 1 11 31 26 38 6 1 1 24 4 46 33 9 9 4 4 20 6 0 0 0 28 8 45 18 18 8 0 0 0 15 16 33 8	# mzCloud Results 2 2 2 2 2 2 2 2 2 4 4 2 5 5 10 8 8 11 4 4 2 2 00 2 2 11 4 4 2 2 10 2 2 11 2 2 12 12 2 2 5 5 12 12 2 2 2 2	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 88.1 83.7 88.5 86.7 82.7 94.2 88.1 91.5 86.4 91.1 87.1 87.1 81 92.1 81.6 87.3 83.4 83.4 83.4 83.4 82.9 88.8 84.3 83.8 85.3 85.3 85.3 85.3 85.3 85.3 85	Group Area: F8 F8 2850840.17 278302.32 2599740.77 2599740.77 2599740.77 2098519.25 178208519.25 1783088.82 1748042.83 1545042.01 1252325.92 1171308.02 1152343.83 1033085.43 91408.607 885834.119 804307.648 759721.202 672279.734 662943.676 659854.489 612912.292 571451.973 446630.389 430857.660 12912.292 571451.973 446630.389 430857.660 12912.292 571451.973 446630.389 430857.667 417031.149 386314.35 1.607
Name PEG n10 Maltol PEG n11 Ginsenoside Rg3 Glyotin L-Oltramic acid Bis(2-ethylkersyl) phth N-Disyelohexylurea PEG n5 9-Oxo-10(E),12(E)-occ Naringenin Glucose 1-phosphate Stearamide Ouanine Lewsylprofine PEG n13 Uracil Monobutyl phthalate L-Histidine 2-Hydroxycinnamic ac Cyclo(leuxylprolyf) Docosanamide Diphenylanine 95,138-12-Oxophytod Kojis acid Oleamide	Formula C30 H50 02 C20 H42 011 C42 H42 011 C42 H47 013 C42 H47 013 C42 H47 013 C42 H47 013 C42 H47 013 C44 H48 04 C10 H8 04 C18 H30 03 C18 H30 03 C18 H30 04 C18 H30 04 C18 H30 07 C6 H13 09 P C18 H30 07 C6 H13 09 P C18 H37 N 0 C5 H57 N 0 C5 H57 N 0 C6 H0 N3 02 C6 H0 N3 02 C1 H10 N2 02 C11 H10 N2 02 C11 H10 N2 02 C11 H18 N2 02 C12 H11 N C12 H11 N C18 H35 N 0	Aunotation Source Prediction Source Productors Fail match Not the top hit Fail match Not the top hit Fail match Not the top hit Fail match Fail match	Annotation Source: mcCloud Search Foll match Foll match	Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match No match Partial match Full match Full match Full match Full match Full match Full match Partial match	Annotation Source: MaskList Match Full match	FISh Coverage	Molecular Weight 442,38044 458,27269 126,03195 502,29909 766,48533 446,12103 147,05307 390,2762 192,04254 294,21935 224,18852 238,14166 294,21935 224,18852 238,14166 294,21935 212,02965 228,1476 210,13686 228,1476 319,24057 221,0275 281,27159 142,02675	RT [mm] 5,59 4,161 2,799 4,284 5,588 4,439 0,852 11,155 3,746 6,852 7,225 4,445 0,901 10,658 0,876 2,987 4,469 10,054 4,469 10,0576 4,297 4,469 10,0576 4,277 10,6876 7,2845 9,863	Area (Max.) 2850840.167 2782633.267 2098719.23 1792976.447 1783088.222 1748442.833 1792976.447 1783088.222 1748442.833 1792976.447 173308.822 1748442.833 179308.429 911405.4852 911408.6067 885884.1188 84032.1577 859824.4591 612912.9287 57714519.73 446630.385 571451.973 446630.3857.6066 417031.1489 386314.3502 367757.8594 15977.8594 159778.5494 159778.5494 159778.5494 159778.5494 28778.5494 29788 29788.544 29788.544 29788 29788.544 297888 29788 29788 29788 29788 297888 29788 29788 29788 29788 297888 29788 29788	# ChemSpi der 42 1 26 0 0 1 1 1 1 1 26 38 8 6 1 1 1 24 46 39 9 4 20 0 6 0 0 28 45 18 8 41 20 5 0 6 1 1 24 45 6 19 24 20 0 0 0 1 1 26 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	<pre># mzCloud Results 2 2 2 2 2 2 4 4 2 5 10 8 1 1 4 2 2 0 2 2 1 1 4 4 1 1 3 3 4 2 2 6 6 2 1 1 2 4 4 1 1 </pre>	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83.7 88.1 89.2 88.5 86.7 82.7 94.2 88.1 91.1 87.1 87.1 87.1 87.1 87.1 87.1 87.1 8	Group Area: F8 F8 2850840,17 2580240,27 2599740,77 2008519,25 1792076,45 1792076,45 1783088,82 1748442,83 1545042,01 1252325,92 1173108,60 1858384,110 944076,34 791708,08 944076,34 791704,80 672279,74 642043,676 659854,489 612912,929 571451,973 571451,973 571451,973 571451,973 571451,973 571451,973 571451,973 571451,973 571451,973 571451,973 57757,859 367757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757,859 37757 37757 37757 37757 37757 37757 37757 37757 37757 37757 37757 37777 37777 37777 37777 377777 377777 377777 377777777
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Name Betulin PEG n10 Maltol PEG n11 Ginsenovide Rg3 Glycitin L-Ghttamic acid Bis(2-etyl)factoryl ohth N-Toiseyclohexylurea PEG n5 9-Oxo-10(E).12(E)-oct Naringenin Glucoxe 1-phosphate Stearamide Guasine Lewsylproline PEG n13 Uracil Monobutyl phthalate L-Histidine 2-Hydroxycinnamis ac Cyclo(leuxylprolyl) Docosnamide 95,13R-12-Oxophytod Kojie acid Oleamide PEG n14 Genistin	Formula C30 H50 02 C20 H42 Ol1 C6 H6 03 C42 H42 Ol1 C42 H72 Ol3 C42 H72 Ol3 C42 H72 Ol3 C42 H72 Ol3 C42 H72 Ol3 C18 H38 Od C18 H38 Od C18 H38 Od C18 H37 NO C5 H5 N5 O C11 H20 N2 O3 C26 H54 Ol4 C18 H37 NO C5 H5 N5 O C11 H20 N2 O3 C26 H54 Ol4 C18 H37 NO C28 H58 O3 C11 H18 N2 O2 C12 H11 N C18 H28 O3 C6 H0 O4 C12 H13 N O C28 H58 NO C28 H58 NO C28 H58 S O15 C31 H20 O10	Aunotation Source Predictor Compositions Fail match Not the top hit Fail match Not the top hit Fail match Not the top hit Fail match Fail match	Annotation Source: mrCloud Search Foll match Foll match	Annotation Source: ChemSpider Search Partial match Partial match No results No match Partial match	Annotation Source: MaskList Match Foll match	FISh Coverage	Molecular Weight 442,38044 458,27269 126,03195 502,29009 766,48533 446,12103 147,05307 390,2762 192,04254 224,18852 224,18855 272,06832 260,02962 224,21935 272,06832 260,02962 228,1476 590,35113 112,02769 228,1476 339,34957 169,08913 155,06949 164,04749 210,13866 339,34957 169,08913 16	RT [min] 5,59 4,161 2,799 4,284 5,588 4,439 0,852 11,155 3,746 6,584 4,455 0,901 10,658 0,876 2,987 4,469 1,094 4,6327 0,833 3,3412 4,227 113,101 7,451 6,857 2,865 9,865 4,541 4,651	Area (Max.) 2850840.167 2782623.267 2098519.233 1792976.447 1783088.822 1748442.833 1792976.447 1783088.822 1748442.833 1792976.447 173308.192 1652543.832 0116326.365 911408.6067 85834.1188 84032.1577 85924.12017 662943.6763 662943.6763 662943.6763 662943.6763 662943.6763 662943.6763 659854.4891 612912.9287 571451.973 446630.3856 417031.1489 366314.4302 30615.8429 330615.8429 330615.8429 330649.1577 1849	# ChemSpi der 42 42 42 42 42 42 42 58 6 11 11 11 11 12 66 6 13 11 12 66 6 1 12 66 6 1 12 66 6 1 12 66 6 1 12 66 6 1 12 66 6 1 12 12 66 13 11 12 16 6 1 12 12 16 16 12 12 16 16 12 12 16 16 12 16 12 16 12 16 12 16 12 16 12 16 12 16 12 12 12 16 12 12 12 12 12 12 12 12 12 12	<pre># mzCloud Results 2 2 2 2 2 2 2 4 4 2 5 5 100 8 8 11 4 4 2 2 10 0 2 2 11 10 2 2 11 10 10 2 2 11 10 10 10 10 10 10 10 10 12 10 12 12 12 12 12 12 12 12 12 12 12 12 12</pre>	# mzVault Results 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	mzCloud Best Match 83,7 83,17 83,2 84,5 85,2 86,7 82,7 94,2 88,5 86,4 91,1 81 92,1 88,9 93,1 88,9 81,6 87,3 83,4 88,9 81,6 86,3 83,8 83,8 83,8 83,8 83,8 83,8 83	Group Area: F8 F8 2850840.17 2782623.27 2599740.77 2098519.25 1792976.45 1792976.45 1793085.82 1748442.83 1545042.01 1252325.92 1173108.02 1155243.83 0430756.367 911408.007 911408.007 659854.489 612912.929 672297.974 659854.489 612912.929 672297.974 63943.676 659854.489 612912.929 571451.973 446630.389 430857.607 571451.973 446630.389 430857.607 571451.973 330815.843

(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.

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