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综述

刘雨欣,秦雪梅, 高 丽 脑细胞衰老在阿尔茨海默症发病 机制中的潜在作用

研究论文

邢文慧, 龚宁波, 吕 杨等 吡罗昔康多晶型分子间相互作用的分 析研究





中国药学会 中国医学科学院药物研究所

药 学 学 报

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图文摘要

综述

1925

中药有效成分对 AD 相关认知功能的改善作用及其机制研究进展

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本篇综述总结了部分经典中药方和中药分子在阿尔茨海默病 (AD) 相关认知功能方面的 改善效应及相关分子机制,提出多靶点干预可能是防治 AD 的有效策略。



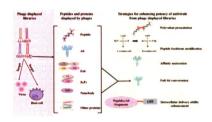
1937

噬菌体展示技术及其在抗病毒药物发现中的应用

许世琦, 贺子涵, 陶炳灼, 秦鑫*

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本文介绍了噬菌体展示技术的基本原理和常用于抗病毒药物发现的噬菌体展示文库, 对目前噬菌体展示文库来源的抗病毒药物的不足及其相关改进策略进行了讨论,并对 噬菌体展示技术在抗病毒药物开发中的应用前景进行了展望。



1946

脑细胞衰老在阿尔茨海默症发病机制中的潜在作用

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脑细胞衰老和阿尔茨海默症密切联系。

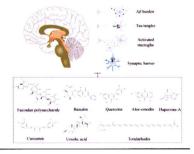
1954

阿尔茨海默症的临床治疗和天然来源潜在药物的研究进展

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本文探讨了目前临床研究中治疗阿尔茨海默症 (AD) 的方法并总结了近年报道的有潜力治疗 AD 的活性天然产物。



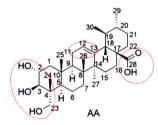
1962

积雪草酸的结构修饰与生物活性研究进展

刘斌 1,2, 唐文强 1,2, 仝红娟 1,2, 朱周静 1,2, 唐初 3*

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本综述对积雪草酸 (AA) 近 20 年来的结构修饰、生物活性、构效关系及作用机制的相关研究进行了归纳、总结。

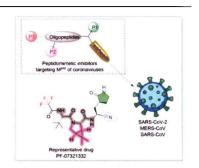


拟肽类冠状病毒主蛋白酶抑制剂的研究进展

刘玉1,明巍1,李陈宗1,朱园园2,古双喜1*

- (1. 武汉工程大学化工与制药学院, 绿色化工过程教育部重点实验室, 湖北 武汉 430205;
- 2. 武汉工程大学化学与环境工程学院, 湖北 武汉 430205)

根据药物设计策略中"warheads"(弹头)的不同,对拟肽类冠状病毒抑制剂进行分类综述,对抑制剂的设计思路、生物活性和 P1、P2 及 P3 片段的修饰与优化进行分析与总结,为冠状病毒抑制剂的进一步设计与开发提供有益的参考。



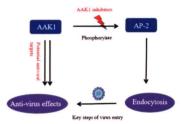
1991

衔接子相关蛋白激酶 1 (AAK1) 抑制剂抗病毒研究进展

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(杭州师范大学药学院, 浙江省榄香烯类抗癌中药重点实验室, 浙产中药材资源开发与应用 浙江省工程实验室, 浙江省浙八味等浙产中药材综合利用开发 2011 协同创新中心, 浙江 杭 州 311121)

AAK1 是调控 AP-2 蛋白 μ2 亚基 T156 磷酸化的特异性关键激酶,成为抗病毒的潜在靶点。 靶向 AAK1 有望开发出抗病毒药物。



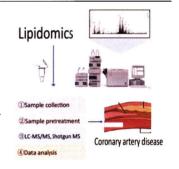
2003

基于脂质组学技术发现冠心病的脂质标志物和治疗靶点

杨冠林 1,3#, 翟琼 1#, 董馨 2, 布仁 2, 薛培凤 2, 赵芳新 1, 陆景坤 1*

(1. 内蒙古医科大学基础医学院, 内蒙古自治区 呼和浩特 010010; 2. 内蒙古医科大学药学院, 内蒙古自治区 呼和浩特 010010; 3. 枣庄市肿瘤医院, 山东 枣庄 277000)

脂质分子是心肌细胞结构重要组成部分,在心脏功能方面扮演重要角色,脂质组学技术越来越 多地被用于评估冠心病的风险等等相关研究。本文对利用脂质组学技术探究冠心病脂质小分子 标志物以及相关治疗靶点、药物研发策略进行了综述。



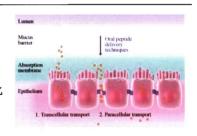
2012

肽类药物的口服递送研究进展

李琪, 陈宏达, 周天华, 刘祥瑞*

(浙江大学基础医学院, 浙江 杭州 310058)

针对肽类药物的口服递送展开综述, 总结归纳口服屏障、相关递送技术, 重点关注已产业化的专利, 并提出展望。



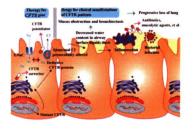
2024

囊性纤维化及其治疗方法的研究进展

林霖1, 王岩1, 吴传斌2, 朱春娥1*

(1. 广东药科大学中药学院, 广东 广州 510006; 2. 暨南大学药学院, 广东 广州 510032)

对囊性纤维化 (CF) 的致病原因、给药方法、药物的作用机制及新型治疗药物进行综述,为 CF 的治疗提供参考。



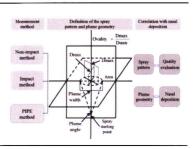
2032

鼻喷剂喷雾模式与羽流几何测量方法及其与鼻腔沉积的相关性

于铎, 孙影, 申欣, 张欣, 毛世瑞*

(沈阳药科大学药学院, 辽宁 沈阳 117004)

本文对鼻喷剂的喷雾模式与羽流几何的定义、测量方法及其与鼻腔沉积的相关性进行了系统综述。

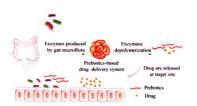


益生元在药物递送系统中的研究进展

任玲¹,郑稳生¹,何淑旺²,于昊杨¹,王璐璐¹*

(1. 中国医学科学院、北京协和医学院药物研究所, 北京 100050; 2. 北京达因高科儿童药物研究院, 北京 101149)

益生元构建药物递送系统的"双重作用":实现药物靶向释放,以及调节肠道菌而影响宿主健康和疾病治疗。



2049

诱导白色脂肪棕色化的靶向递送载体的研究进展

孙倩雯, 许雅琪, 陈微, 叶军, 王洪亮, 高丽丽, 高越, 刘玉玲, 杨艳芳'(中国医学科学院、北京协和医学院药物研究所, 北京 100050)

特异性配体修饰药物递送系统靶向白色脂肪组织,释放褐变剂上调棕色样基因表达,诱导白色脂肪细胞棕色化。



2057

我国金线兰资源特征及繁育技术研究进展

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(中国医学科学院、北京协和医学院药用植物研究所, 北京 100193)

本文对我国金线兰本草考证、资源分布、资源鉴定、化学及药理特征及人工繁育技术进行综述、旨在为金线兰资源可持续利用和后续深入研究提供参考。



研究论文

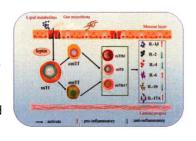
2068

姜黄素对肥胖小鼠溃疡性结肠炎记忆性滤泡性 T 细胞的调控作用

康增平1, 赵海梅2, 王梦雪1, 黄佳琦1, 钟友宝1,3*, 刘端勇4*

(1. 江西中医药大学研究生院, 江西 南昌 330004; 2. 江西中医药大学中医学院, 江西 南昌 330004; 3. 江西中医药大学动物科技中心, 江西 南昌 330004; 4. 江西中医药大学方证研究中心, 江西 南昌 330004)

姜黄素对葡聚糖硫酸钠 (DSS) 诱导的 ob/ob 小鼠结肠炎的治疗作用可能是通过调节 mTf 细胞亚群平衡实现的。



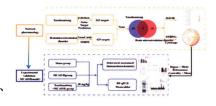
2077

基于网络药理学和实验验证的血栓通改善缺血性脑微循环障碍作用机制研究

王高瑞¹, 陈姿羽¹, 吴辉¹, 刘莹萍¹, 陈明², 赖树生², 吴晓俊^{1*}, 王峥涛¹

(1. 上海中医药大学中药研究所暨上海市复方中药重点实验室, 上海 201203; 2. 广西三七综合利用技术重点实验室, 广西 梧州 543002)

通过网络药理学和实验验证结合发现,血栓通可通过调节 PI3K、AKT、MMP-9、STAT3、caspase-3 相关通路改善缺血性再灌大鼠脑微循环障碍,减轻神经功能损伤。

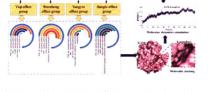


2087

敦煌医方大补脾汤对胃癌的体外活性及其配伍规律的计算机辅助药物设计分 析

李程豪 ¹, 张敏 ², 林佳 ², 张依茜 ², 刘昊 ², 王锐峰 ¹, 和建政 ¹, 李亚玲 ¹, 靳晓杰 ¹,²*, 刘永琦 ¹,³*

(1. 甘肃中医药大学,甘肃省高校重大疾病分子医学与中医药防治研究重点实验室,甘肃 兰州 730000; 2. 甘肃中医药大学药学院,甘肃 兰州 730000; 3. 甘肃中医药大学,敦煌医学与转化教育部重点实验室,甘肃 兰州 730000)



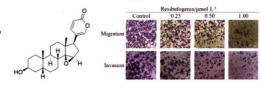
本研究基于计算机辅助药物设计结合复杂网络分析策略初步揭示了大补脾汤辅助防治胃癌的物质基础和分子机制,并探讨了大补脾汤不同功效组协同防治胃癌的科学内涵,为其临床应用提供化学生物信息学依据。



酯蟾毒配基抑制人肝癌细胞体外增殖和迁移侵袭研究

乔桐杉¹,周雯敏²,范欣悦²,张雨荃²,谢婷²,林晓琪²,乔山¹,郝利恒¹, 王猛1, 张建业2*

(1. 巴彦淖尔市医院, 肝胆外科, 内蒙古自治区 巴彦淖尔 015000; 2. 广 州医科大学药学院, 广东省分子靶标与临床药理学重点实验室, 广东 广 州 511436)



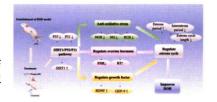
采用 MTT、划痕、Transwell、Western blot 评估酯蟾毒配基的抗肿瘤活性, 发现其可能通过 EMT 和 PI3K/AKT 信号通路抑制人 肝癌 MHCC-97H 细胞的体外增殖、转移和侵袭能力。

2108

左归丸联合西曲瑞克调节卵巢储备功能作用研究

李清瑜, 高晶晶, 付延津, 龙孟莎, 章依垚, 蒙祖玉, 林少姿, 秦佳佳* (暨南大学, 广东 广州 510632)

本文通过对比自然发育小鼠,以及受化疗药物暴露后经西曲瑞克、左归丸及其联合用药 处理后小鼠的卵巢功能、卵巢中生长因子、氧化反应产物的变化, 研究上述治疗药物通 过调控 SIRT1/P53/P21 通路调节卵巢激素的分泌, 从而保护卵巢功能的作用机制。



2115

一株蒲公英内生真菌 Epicoccum sorghinum 1-2 次级代谢产物研究

郝宝聪1,郑瑶瑶1,2,陈旭1,陈秋霞1,季若男1,陈敏1*

- (1. 扬州大学环境科学与工程学院, 海洋科学与技术研究所, 江苏 扬州 225127;
- 2. 中国海洋大学医药学院,海洋药物教育部重点实验室,山东 青岛 266003)

从蒲公英内生真菌 Epicoccum sorghinum 1-2 的发酵产物中分离并鉴定了 7 个化合 物, 其中化合物 1 和 2 为新化合物, 化合物 6 对 4 种金葡菌有显著抗菌作用。



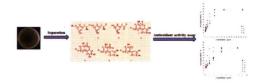
2120

海绵共附生真菌 Alternaria sp. F49 抗氧化次级代谢产物研究

陈雨实,冷佳荣,林舒婷,汪少芸,田永奇* (福州大学生物科学与工程学院, 福建 福州 350108)

利用色谱手段从海绵共附生真菌 Alternaria sp. F49 在 PDB 培养基中的代谢产 物中分离得到了7个化合物, 其中 (8R)-5-O-methyl-orcinotriol (1) 是新化合

物。体外抗氧化活性测定结果表明、化合物 4~7 具有强的 DPPH 自由基清除 活性; 化合物 $1 \sim 7$ 具有强的 ABTS 自由基清除活性。



2126

以对氨基水杨酸为母核的三分子缀合物的合成及其生物活性研究

任艳会 ¹, 范莉 ¹, 许峻旗 ², 谢建平 ²*, 代乐平 ¹, 毛丹 ¹, 杨茜 ¹, 杨大成 1*

(1. 西南大学化学化工学院, 重庆市高校应用化学重点实验室, 重庆 400715; 2. 西南大学 生命科学学院, 重庆 400715)

首次将三种抗结核药物片段缀合在单一分子中,设计并合成了2个系列16个目标分子;发现 了抗结核分枝杆菌及人致病菌的高活性目标分子,溶血性测试验证了分子的安全性; TM1a、 TM1h 和 TM2a 值得进一步研究。



TM1a MIC = 0.167 nmol·mL-1, S. aureus ATCC14125 TM1h

MIC = 0.329 nmol·mL-1. S. aureus ATCC14125 TM2a

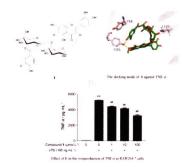
MIC = 0.63 nmol·mL⁻¹, Mycobacterium smegmatis

谷精草中 1 个新的黄酮苷类化合物

张勇 1,2,3, 阿吉艾克拜尔·艾萨 1,3, 朱维良 1,2,3*

(1. 中国科学院新疆理化技术研究所,省部共建新疆特有药用资源利用国家重点实验室培育基地,中国科学院干旱区植物资源化学重点实验室,新疆乌鲁木齐 830011; 2. 中国科学院上海药物研究所,新药研究国家重点实验室,中国科学院受体结构与功能重点实验室,上海 201203; 3. 中国科学院大学,北京 100049)

本研究从谷精草水提物中分离得到一个新的黄酮苷类化合物 1,分子对接结果显示化合物 1 具有潜在的 TNF-α 转换酶抑制活性,细胞实验证实化合物 1 可显著抑制 LPS 诱导的 RAW264.7 细胞中 TNF-α 的升高。



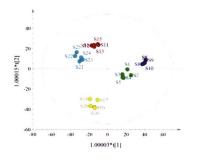
2146

基于指纹图谱结合化学计量学方法评价荆芥穗质量

张群, 罗沙, 李洁, 李贝, 牛文意, 谭睿*

(西南交通大学生命科学与工程学院, 四川 成都 610031)

本文通过指纹图谱、化学计量学方法及含量测定全面科学地评价了 25 批次中药荆芥穗的质量,以期为荆芥穗药材质量控制提供参考。



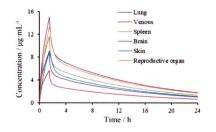
2153

基于生理药代动力学模型对盐酸莫西沙星有效性的研究

高婕 1,2, 冯芳 2, 王立新 1, 崇小萌 1, 王晨 1*, 尹利辉 1*

(1. 中国食品药品检定研究院, 北京 102629; 2. 中国药科大学, 江苏 南京 210009)

本研究基于生理药代动力学理论,利用机制性模型对抗感染药物在体内组织器官中暴露量进行计算,通过与病原菌药敏结果比较评估药物对不同适应证的有效性水平,并对研究的应用场景进行了讨论。



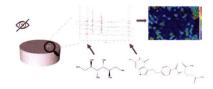
2158

共焦显微拉曼光谱成像技术探究冻干制剂-注射用培美曲塞二钠中药物分布均 匀性

韩静, 姚静, 董美阳, 施亚琴*, 孙葭北*

(中国食品药品检定研究院, 国家药品监督管理局化学药品质量研究与评价重点实验室, 北京 102629)

本研究采用共焦显微拉曼光谱成像技术评价了冻干制剂-注射用培美曲塞二钠中药物空间分布均匀性。

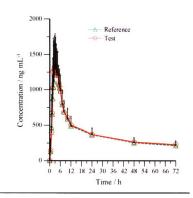


2166

依非韦伦片在中国健康受试者中空腹给药条件下的药代动力学和生物等效性研究 夏玉明 ^{1,2}, 许杨 ³, 马陶陶 ^{1*}

(1. 安徽医科大学药学院,安徽 合肥 230032; 2. 安徽贝克生物制药有限公司,安徽 合肥 230088; 3. 安徽万邦医药科技股份有限公司,安徽 合肥 230601)

通过依非韦伦片在中国健康受试者中空腹给药条件下的药代动力学和生物等效性研究,确认了本次试验受试药物及参比药物在空腹给药条件下依非韦伦具有生物等效性。

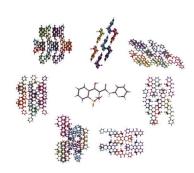


吡罗昔康多晶型分子间相互作用的分析研究

邢文慧, 邢逞, 喻红梅, 房政钰, 张丽, 龚宁波*, 吕扬*

(北京协和医学院、中国医学科学院药物研究所,晶型药物研究北京市重点实验室,北京100050)

本文对吡罗昔康 7 种晶型进行了构象分析、氢键分析、Hirshfeld 表面分析、Hirshfeld 指纹 图谱分析和分子间相互作用能分析。揭示分子间相互作用对多晶型的形成机制及性质差异 的重要作用。



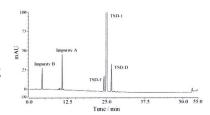
2177

新型 P2Y12 受体拮抗剂 TSD-1 的有关物质研究

王太禹 ^{1,2},杨洁 ²,杨海龙 ²,邬国栋 ¹,安明 ^{1*},徐学宇 ^{2*}

(1. 包头医学院, 内蒙古自治区 包头 014060; 2. 天士力控股集团有限公司天士力研究院, 天津 300410)

为评价新型 P2Y₁₂ 受体拮抗剂 TSD-1 的安全性,本研究采用半制备液相色谱仪分离和纯化 4 个主要杂质,并通过核磁共振波谱和高分辨质谱进行结构确证,并建立一种操作简单、专属性良好的高效液相色谱法用于测定 TSD-1 中有关物质的含量。



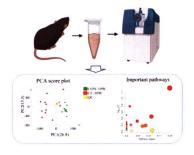
2183

基于代谢组学技术探讨间歇性禁食对小鼠粪便代谢物的影响

熊星¹, 熊微², 陈岩³, 鞠政财^{3*}

(1. 南通大学药学院, 江苏 南通 226000; 2. 福建农林大学动物科学学院, 福建 福州 350000; 3. 上海中医药大学教学实验中心, 上海 200120)

间歇性禁食显著改变健康小鼠的粪便代谢模型, 其主要影响小鼠的亚油酸代谢、胆汁酸生物合成及脂肪酸代谢等通路。本研究为间歇性禁食治疗相关代谢性疾病的机制提供一定的参考依据。

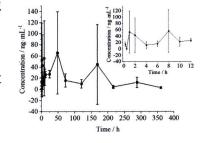


2191

黄体酮缓释制剂在 Beagle 犬中的血药浓度测定方法的建立及其药代动力学研究 王玥 ^{1,2},程艺 ²,张慧 ^{2*},郑爱萍 ^{1,2*}

(1. 徐州医科大学药学院, 江苏 徐州 221000; 2. 军事科学院军事医学研究院毒物药物研究所, 北京 100850)

本研究对黄体酮缓释微球注射液 Prosphere 进行了 Beagle 犬药代动力学研究, 并成功开发一种专属性强、灵敏度高的 LC-MS/MS 分析方法。



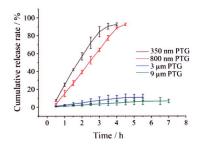
2197

紫杉醇温敏凝胶的制备、体外表征及其药代动力学研究

范冉冉1, 王增明2, 张慧2*, 李见春1*, 郑爱萍2*

(1. 蚌埠医学院药学院, 安徽 蚌埠 233030; 2. 军事科学院军事医学研究院毒物药物研究所, 北京 100850)

本研究构建了含有不同粒径紫杉醇的温敏凝胶给药系统, 结果表明粒径大小显著影响紫 杉醇温敏凝胶的释药速率。

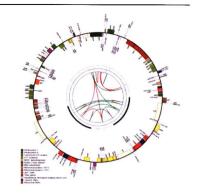


欧地笋叶绿体全基因组序列特征及其系统发育分析

杜清 1,2,3#*, 王立强 4#, 陈卓尔 2,5, 姜梅 6, 陈海梅 2, 曾晶 2,5, 王彬 5*, 刘昶 2

- (1. 青海民族大学药学院, 青海省青藏高原植物化学重点实验室, 青海 西宁 810007;
- 2. 中国医学科学院、北京协和医学院药用植物研究所生物信息中心, 北京 100193;
- 3. 清新天正 (北京) 国际科技有限责任公司, 北京 100097; 4. 菏泽学院药学院, 山东 菏泽 274015; 5. 湘南学院药学院, 湖南 郴州 423099; 6. 齐鲁工业大学药学院, 山东 济南 250200)

欧地笋叶绿体基因组全长 152 085 bp, 包括 132 个基因, 其中含有 88 个蛋白质编码基因、36 个 tRNA 基因和 8 个 rRNA 基因; 含有 34 个特征性 SSR 可用于区别和鉴定欧地笋植物。



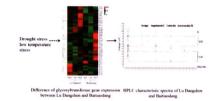
2216

基于转录组的不同产地党参糖基转移酶鉴定及分析

田星锐1, 吉姣姣1, 李建宽1, 姜峰1, 刘喆宇1, 高建平1,2*

(1. 山西医科大学药学院, 山西 太原 030001; 2. 山西省道地药材资源开发工程技术研究中心, 山西 太原 030001)

产地环境差异造成潞党参与白条党党参糖基转移酶基因表达存在显著差异,从而导致党参多糖、党参苷I及苍术内酯III代谢差异。

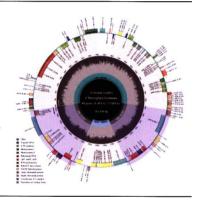


2224

葵花大蓟叶绿体基因组结构特征及系统发育分析

郑长远 ^{1,2}, 苏旭 ^{1,2,3}, 刘玉萍 ^{1,2*}, 刘涛 ^{1,2}, 王亚男 ^{1,2}, 苏丹丹 ^{1,2}, 张雨 ^{1,2}, 秦娜 ^{1,2} (1. 青海师范大学生命科学学院, 青海 西宁 810008; 2. 青海师范大学, 青海省青藏高原药用动植物资源重点实验室, 青海 西宁 810008; 3. 青海师范大学高原科学与可持续发展研究院, 青海 西宁 810016)

葵花大蓟 (C. souliei) 叶绿体基因组全长 152 470 bp, 为典型的环状四分体结构, 共编码 134 个基因。基于叶绿体基因组构建的系统发育树显示, 在管状花亚科 (Carduoideae) 46 种植物中, 葵花大蓟与蓟属的翼蓟 (C. vulgare) 的亲缘关系最近。



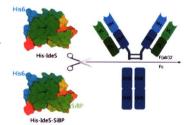
2234

免疫球蛋白降解酶 IdeS 在大肠杆菌中的表达、纯化及功能鉴定

周思含, 刘忞之, 杨燕, 王伟*

(中国医学科学院、北京协和医学院药物研究所,天然药物活性物质与功能国家重点实验室/国家卫生健康委员会天然药物生物合成重点实验室,北京 100050)

IdeS 在大肠杆菌中的异源表达及亲和层析标签对其表达产量和活性的影响研究。



新药发现与研究实例简析

2240

长效降血糖药物塞马鲁肽的研制

郭宗儒

(中国医学科学院、北京协和医学院药物研究所, 北京 100050)

ACTA PHARMACEUTICA SINICA

2022 July Volume 57 Number 7

Graphical Abstracts

Reviews

1925

Research progress on the effective components of traditional Chinese medicine for improving AD-related cognitive impairment

LEI Meng-yao, GAO Pei-pei, LONG Jian-gang*

(School of Life Science and Technology, Institute of Mitochondrial Biology and Medicine, Xi'an Jiaotong University, Xi'an 710049, China)

This review summarizes the improvement effects and related molecular mechanisms of partial classical Chinese prescriptions and traditional Chinese medicine molecules in Alzheimer's disease (AD)-related cognitive functions, and proposes that multi-target intervention may be an effective strategy to prevent AD.

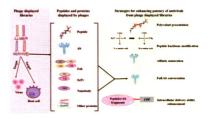


Phage display technology and its application in antivirals discovery

XU Shi-qi, HE Zi-han, TAO Bing-zhuo, QIN Xin*

(Department of Basic Medicine, Hubei University of Arts and Sciences, Xiangyang 441053, China)

The present review introduced the basic principle of phage display technology and the phage displayed libraries often used in antiviral drug discovery, discussed the strategies for enhancing the potency of antivirals derived from phage displayed libraries and prospected the future direction of antiviral drug research based on phage display technology.



1946

Potential role of brain cell senescence in the pathogenesis of Alzheimer's disease

LIU Yu-xin^{1,2,3}, OIN Xue-mei^{1,2,3*}, GAO Li^{1,2,3*}

(1. Modern Research Center for Traditional Chinese Medicine, Shanxi University, Taiyuan 030006, China; 2. The Key Laboratory of Chemical Biology and Molecular Engineering of Ministry of Education, Shanxi University, Taiyuan 030006, China; 3. The Key Laboratory of

Effective Substances Research and Utilization in TCM of Shanxi Province, Taiyuan 030006, China)

The senescence of brain cells is closely linked to Alzheimer's disease.

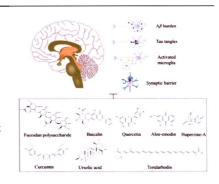
1954

Research progress in clinical treatment of Alzheimer's disease and potential drugs from natural products

ZHANG Ping¹, JI Hui², HU Qing-hua^{2*}

(1. Zhongshan Vocational College, Nanjing 210049, China; 2. School of Pharmacy, China Pharmaceutical University, Nanjing 211198, China)

The review discusses current clinical research approaches for the treatment of Alzheimer's disease (AD) and summarizes the active natural products reported in recent years with potential to treat AD.

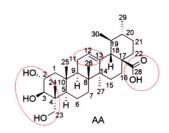


X Contents

1962

Advances in the study of structural modification and biological activities of asiatic acid LIU Bin^{1,2}, TANG Wen-qiang^{1,2}, TONG Hong-juan^{1,2}, ZHU Zhou-jing^{1,2}, TANG Chu^{3*} (1. School of Pharmacy, Shaanxi Institute of International Trade & Commerce, Xianyang 712046, China; 2. Collaborative Innovation Center of Green Manufacturing Technology for Traditional Chinese Medicine in Shaanxi Province, Xianyang 712046, China; 3. School of Life Science and Technology, Xidian University, Xi'an 710126, China)

This review summarizes the structural modification, biological activity, structure-activity relationship and mechanism studies of asiatic acid (AA) in recent twenty years.

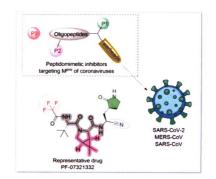


1977

Advances in peptidomimetic inhibitors of coronavirus main protease
LIU Yu¹, MING Wei¹, LI Chen-zong¹, ZHU Yuan-yuan², GU Shuang-xi^{1*}
(1. Key Laboratory for Green Chemical Process of Ministry of Education, School of

Chemical Engineering and Pharmacy, Wuhan Institute of Technology, Wuhan 430205, China; 2. School of Chemistry and Environmental Engineering, Wuhan Institute of Technology, Wuhan 430205, China)

Peptidomimetic inhibitors of coronavirus main protease were classified and reviewed according to the different "warheads" in design strategy. The molecular structures, biological activities and design ideas of the inhibitors were analyzed and discussed, which is aimed to provide useful reference for further design and development of coronavirus inhibitors.

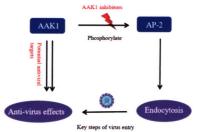


1991

Advances in antiviral research of adaptor-associated protein kinase 1 (AAK1) inhibitors

QI Xiang, JIANG Song-wei, YUAN Ying-hui, XU Li, HUI Zi*, YE Xiang-yang*, XIE Tian*

(Key Laboratory of Elemene Class Anti-Cancer Chinese Medicines, Engineering Laboratory of Development and Application of Traditional Chinese Medicines, Collaborative Innovation Center of Traditional Chinese Medicines of Zhejiang Province, School of Pharmacy, Hangzhou Normal University, Hangzhou 311121, China)



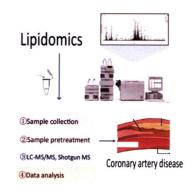
AAK1 is a specific key kinase regulating the phosphorylation of AP-2 protein μ2 subunit T156. It has potential to be an antiviral target. Targeting AAK1 might lead to antiviral therapy in the future.

2003

Lipid markers and targets of coronary artery disease based on lipidomics YANG Guan-lin^{1,3#}, ZHAI Qiong^{1#}, DONG Xin², BU Ren², XUE Pei-feng², ZHAO Fang-xin¹, LU Jing-kun^{1*}

- (1. School of Basic Medicine, Inner Mongolia Medical University, Hohhot 010010, China;
- 2. College of Pharmacy, Inner Mongolia Medical University, Hohhot 010010, China;
- 3. Zaozhuang Cancer Hospital, Zaozhuang 277000, China)

Lipids have an important role in maintaining the myocardial cell structure as well as cardiac function. Given the increasing application of lipidomics techniques for coronary artery disease, we provide a review of lipidomics technology, sensitive lipid markers, recent studies of therapeutic targets, and drug discovery for coronary artery disease.

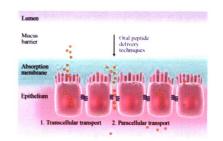


2012

Advances in the study of peptide drugs in oral drug delivery system LI Qi, CHEN Hong-da, ZHOU Tian-hua, LIU Xiang-rui*

(School of Basic Medical Sciences, Zhejiang University, Hangzhou 310058, China)

This review summarizes the main obstacles and challenges for oral peptide delivery as well as related delivery techniques, especially focusing on the commercialized patents. Our prospections are also included in this review.



Contents XI

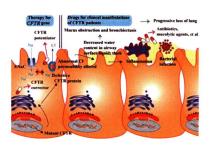
2024

Research progress of cystic fibrosis and its therapies

LIN Lin¹, WANG Yan¹, WU Chuan-bin², ZHU Chun-e^{1*}

(1. School of Chinese Materia Medica, Guangdong Pharmaceutical University, Guangzhou 510006, China; 2. School of Pharmaceutical Sciences, Jinan University, Guangzhou 510032, China)

This review summarizes pathogenic mechanisms of cystic fibrosis (CF), mechanisms of action of drugs, routes of administration, and new drug development as well as provides insights into the advanced treatment strategies for CF.

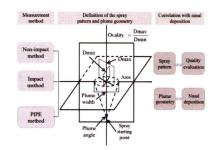


2032

Spray pattern and plume geometry measurement method of nasal spray and its correlation with nasal deposition

YU Duo, SUN Ying, SHEN Xin, ZHANG Xin, MAO Shi-rui* (School of Pharmacy, Shenyang Pharmaceutical University, Shenyang 117004, China)

This review systematically describes the definition and measurement methods of the spray pattern and plume geometry of nasal spray and their correlation with nasal deposition.

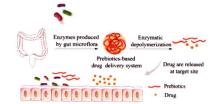


2041

Research progress of prebiotics in drug delivery system

REN Ling¹, ZHENG Wen-sheng¹, HE Shu-wang², YU Hao-yang¹, WANG Lu-lu^{1*} (1. Institute of Materia Medica, Peking Union Medical College, Chinese Academy of Medical Sciences, Beijing 100050, China; 2. Beijing Dyne High-tech Pediatric Pharmaceutical R&D Institute, Beijing 101149, China)

The dual function of prebiotics-based drug delivery system: targeted drug release combined with intestinal bacteria modification affecting host health and disease treatment.



2049

Advances of targeted delivery vectors for inducing browning of white adipose tissue SUN Qian-wen, XU Ya-qi, CHEN Wei, YE Jun, WANG Hong-liang, GAO Li-li,

GAO Yue, LIU Yu-ling, YANG Yan-fang*
(Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union

Drug delivery systems are modified with specific ligand for targeting white adipose tissue, then release browning agents to up regulate brown like gene expression and induce browning of white adipocytes.



2057

Resource characteristics and propagation techniques of $Anoectochilus\ roxburghii$ in China

LÜ Xin-kai, ZHOU Li-si*, GUO Shun-xing*

Medical College, Beijing 100050, China)

(Institute of Medicinal Plant Development, Chinese Academy of Medical Science and Peking Union Medical College, Beijing 100193, China)

This paper summarizes the distribution, identification, chemical and pharmacological characteristics and artificial propagation techniques of *A. roxburghii* in China. To provide a reference for sustainable development and subsequent mechanistic research.



XII Contents

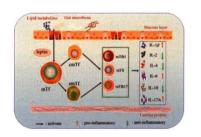
Original Articles

2068

Effects of curcumin on memory follicular T cells in obese mice with colitis KANG Zeng-ping¹, ZHAO Hai-mei², WANG Meng-xue¹, HUANG Jia-qi¹, ZHONG You-bao^{1,3*}, LIU Duan-yong^{4*}

(1. Graduate School, Jiangxi University of Chinese Medicine, Nanchang 330004, China; 2. College of Traditional Chinese Medicine, Jiangxi University of Chinese Medicine, Nanchang 330004, China; 3. Experimental Animal Science and Technology Center, Jiangxi University of Chinese Medicine, Nanchang 330004, China; 4. Formula-pattern Reasearch Center, Jiangxi University of Chinese Medicine, Nanchang 330004, China)

Curcumin-treatment of dextran sodium sulfate (DSS) induced *ob/ob* mice colitis may be achieved by regulating mTfh cell subpopulation balance.

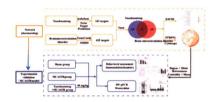


2077

Xueshuantong improves cerebral microcirculation disorder: action mechanism based on network pharmacology and experimental validation

WANG Gao-rui¹, CHEN Zi-yu¹, WU Hui¹, LIU Ying-ping¹, CHEN Ming², LAI Shu-sheng², WU Xiao-jun^{1*}, WANG Zheng-tao¹

(1. Institute of Chinese Materia Medica of Shanghai University of Traditional Chinese Medicine and Shanghai Key Laboratory of Compound Chinese Medicines, Shanghai 201203, China; 2. Guangxi Key Laboratory of Comprehensive Utilization Technology of Pseudo-ginseng, Wuzhou 543002, China)



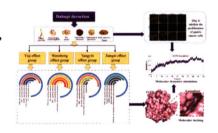
Network pharmacology and experimental validation *in vivo* found that Xueshuantong could improve ischemic cerebral microcirculation disorder and thereby reduce nerve damage in ischemia-reperfusion rats by regulating signaling pathways related with PI3K, AKT, MMP-9, STAT3 and caspase-3 in microvessels.

2087

Analysis of *in vitro* activity and compatibility of Dunhuang Yifang Dabupi Decoction on gastric cancer based on computer-aided drug design

LI Cheng-hao¹, ZHANG Min², LIN Jia², ZHANG Yi-xi², LIU Hao², WANG Rui-feng¹, HE Jian-zheng¹, LI Ya-ling¹, JIN Xiao-jie^{1,2*}, LIU Yong-qi^{1,3*}

(1. Gansu University Key Laboratory for Molecular Medicine and Chinese Medicine Prevention and Treatment of Major Diseases, Gansu University of Chinese Medicine, Lanzhou 730000, China; 2. College of Pharmacy, Gansu University of Chinese Medicine, Lanzhou 730000, China; 3. Key Laboratory of Dun Huang Medical and Transformation, Ministry of Education, Gansu University of Chinese Medicine, Lanzhou 730000, China)



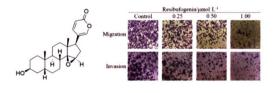
This study is based on computer-aided drug design combined with complex network analysis strategies to initially reveal the material basis and molecular mechanism of Dabupi Decoction in the prevention and treatment of gastric cancer. It also explores the scientific connotation of Dabupi Decoction in the prevention and treatment of gastric cancer with different efficacy groups, and its clinical application provide chemical bioinformatics basis.

2101

Resibufogenin suppresses human hepatocellular carcinoma cell proliferation, migration and invasion in vitro

QIAO Tong-shan¹, ZHOU Wen-min², FAN Xin-yue², ZHANG Yu-quan², XIE Ting², LIN Xiao-qi², QIAO Shan¹, HAO Li-heng¹, WANG Meng¹, ZHANG Jian-ye^{2*}

(1. Department of Hepatobiliary Surgery, Bayannur Hospital, Bayannur 015000, China; 2. Guangdong Key Laboratory of Molecular Target and Clinical Pharmacology, School of Pharmacy, Guangzhou Medical University, Guangzhou 511436, China)

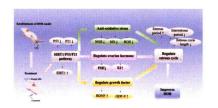


MTT, wound-healing, Transwell and Western blot assay were applied to evaluate the antitumor activity of resibufogenin, which found that it might inhibit the proliferation, metastasis and invasion of human hepatocellular carcinoma MHCC-97H cells *in vitro* through EMT and PI3K/AKT signaling pathway.

The regulation of ovarian reserve function by Zuogui pills combined with cetrorelix LI Qing-yu, GAO Jing-jing, FU Yan-jin, LONG Meng-sha, ZHANG Yi-yao,

MENG Zu-yu, LIN Shao-zi, QIN Jia-jia* (Jinan University, Guangzhou 510632, China)

This study compared normally developing mice to mice subjected to chemotherapeutic medicines treated with cetrorelix, Zuogui pills, and their combination. The alterations in ovarian function, growth factors, and oxidative reaction products were then investigated to determine the mechanism of action of the aforementioned therapeutic medications to protect ovarian function by regulating ovarian hormone production *via* the SIRT1/P53/P21 pathway.



2115

Secondary metabolites from the dandelion-derived endophytic fungus *Epicoccum* sorghinum 1-2

HAO Bao-cong¹, ZHENG Yao-yao^{1,2}, CHEN Xu¹, CHEN Qiu-xia¹, JI Ruo-nan¹, CHEN Min^{1*}

(1. Marine Science & Technology Institute, College of Environmental Science & Engineering, Yangzhou University, Yangzhou 225127, China; 2. Key Laboratory of Marine Drugs, the Ministry of Education of China, School of Medicine and Pharmacy, Ocean University of China, Qingdao 266003, China)



Seven compounds were isolated from the dandelion-derived fungus, *Epicoccum sorghinum* 1-2. Compounds 1 and 2 are new structures reported for the first time. Compound 6 showed significant antibacterial activity against 4 strains of *Staphylococcus aureus*.

2120

Research on the antioxidant activity of metabolites from a sponge-derived fungus *Alternaria* sp. F49

CHEN Yu-shi, LENG Jia-rong, LIN Shu-ting, WANG Shao-yun, TIAN Yong-qi $\mbox{^{\star}}$

(College of Biological Science and Engineering, Fuzhou University, Fuzhou 350108, China)



Seven compounds were isolated from the EtOAc extract of the deep-sea fungus *Alternaria* sp. F49 by chromatographic methods. (8R)-5-O-Methyl-orcinotriol (1) is a new compound. Compounds 4-7 showed strong DPPH free radical scavenging activity; whereas compounds 1-7 showed strong ABTS free radical scavenging activity.

2126

Synthesis and biological activities of three-molecule conjugates with para-aminosalicylic acid as parent nucleus

REN Yan-hui¹, FAN Li¹, XU Jun-qi², XIE Jian-ping^{2*}, DAI Le-ping¹, MAO Dan¹, YANG Xi¹, YANG Da-cheng^{1*}

(1. Key Laboratory of Applied Chemistry of Chongqing Municipality, School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715,
China; 2. College of Life Science, Southwest University, Chongqing 400715, China)

Three anti-tuberculosis drug fragments were conjugated in a single molecule for the first time, and 2 series of 16 target molecules were designed and synthesized. Highly active target molecules against *Mycobacterium tuberculosis* and human pathogenic bacteria were found, and the hemolytic test exhibited the safety of **TM1a/2a**, **TM1a**, therefore **TM1h** and **TM2a** deserve further study in the future.



TM1a MIC = 1.3 nmol·mL⁻¹, Mycobacterium smegmatis MIC = 0.167 nmol·mL⁻¹, S. aureus ATCC14125 TM1h

MIC = 0.329 nmol·mL⁻¹, S. aureus ATCC14125

TM2a

MIC = 0.63 nmol·mL⁻¹, Mycobacterium smegmatis

XIV Contents

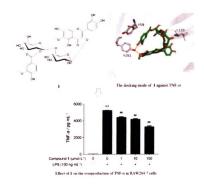
2139

A new flavone glycoside from Eriocaulon buergerianum

ZHANG Yong^{1,2,3}, HAJI Akber Aisa^{1,3}, ZHU Wei-liang^{1,2,3*}

(1. State Key Laboratory Basis of Xinjiang Indigenous Medicinal Plants Resource Utilization, CAS Laboratory of Chemistry of Plant Resources in Arid Regions, Xinjiang Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Urumqi 830011, China; 2. CAS Key Laboratory of Receptor Research, Stake Key Laboratory of Drug Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai 201203, China; 3. University of Chinese Academy of Sciences, Beijing 100049, China)

This study isolated and identified one new flavone glycoside from the water extract of *Eriocaulon buergerianum*. Molecular docking study showed that compound 1 is a potential inhibitor of TNF- α . Bioassay results revealed that 1 exhibited strong inhibitory activity against the LPS-induced expression of TNF- α in RAW264.7 cells *in vitro*.

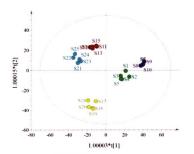


2146

Evaluation of spike quality of Schizonepeta tenuifolia based on fingerprint and chemometrics

ZHANG Qun, LUO Sha, LI Jie, LI Bei, NIU Wen-yi, TAN Rui* (School of Life Science and Engineering, Southwest Jiaotong University, Chengdu 610031, China)

This paper comprehensively and scientifically evaluated the quality of 25 batches of *Schizonepeta tenuifolia* by fingerprint, chemometrics and content determination, in order to provide reference for the quality control of *Schizonepeta tenuifolia*.



2153

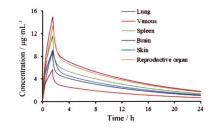
Evaluation on the efficacy of moxifloxacin hydrochloride based on physiological pharmacokinetic models

GAO Jie^{1,2}, FENG Fang², WANG Li-xin¹, CHONG Xiao-meng¹, WANG Chen^{1*}, YIN Li-hui^{1*}

(1. National Institutes for Food and Drug Control, Beijing 102629, China; 2. China Pharmaceutical University, Nanjing 210009, China)

This study is to establish mechanism models of anti-infective drug based on the theory of physiologically based pharmacokinetics (PBPK), and then to predict the distribution of anti-infective drug in human tissues and organs. The efficacy of anti-infective drugs

was quantified by comparing the pharmacokinetic parameters with the minimum inhibitory concentration of related pathogenic bacterium, and then discussed the application scenarios of research.



2158

Investigation of the API distribution homogeneity in lyophilized productpemetrexed disodium for injection by confocal micro-Raman spectroscopy mapping

HAN Jing, YAO Jing, DONG Mei-yang, SHI Ya-qin*, SUN Jia-bei* (NMPA Key Laboratory for Quality Research and Evaluation of Chemical Drugs, National Institutes for Food and Drug Control, Beijing 102629, China)



Evaluation of active pharmaceutical ingredient spatial distribution homogeneity in a lyophilized product-pemetrexed disodium for injection was achieved by confocal micro-Raman spectroscopy mapping.

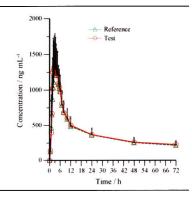
2166

Pharmacokinetics and bioequivalence study of efavirenz tablets in healthy Chinese subjects under fasting administration

XIA Yu-ming^{1,2}, XU Yang³, MA Tao-tao^{1*}

(1. School of Pharmacy, Anhui Medical University, Hefei 230032, China; 2. Anhui Bio-Pharmaceutical Co., Ltd., Hefei 230088, China; 3. Anhui Wanbang Pharmaceutical Technology Co., Ltd., Hefei 230601, China)

This clinic trial, aiming to study pharmacokinetics and bioequivalence of efavirenz tablets in healthy Chinese subjects under fasting administration, indicated that the main pharmacokinetic parameters of the test drug and the reference drug were similar, and the two preparations had bioequivalence.



Contents XV

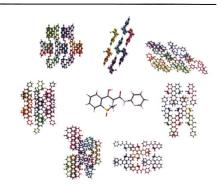
2171

Study of intermolecular interactions of piroxicam polymorphs

XING Wen-hui, XING Cheng, YU Hong-mei, FANG Zheng-yu, ZHANG Li, GONG Ning-bo*, LÜ Yang*

(Beijing Key Laboratory of Polymorphic Drugs, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100050, China)

Conformational analysis, hydrogen bond analysis, Hirshfeld surface analysis, Hirshfeld fingerprint analysis and intermolecular interaction energy analysis of piroxicam were studied. They are essential to reveal the formation mechanism and differences of polymorphs.

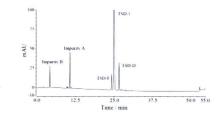


2177

Study on related substances of TSD-1 — a novel P2Y₁₂ receptor antagonist WANG Tai-yu^{1,2}, YANG Jie², YANG Hai-long², WU Guo-dong¹, AN Ming^{1*}, XU Xue-vu^{2*}

(1. Baotou Medical College, Baotou 014060, China; 2. Tasly Institute, Tasly Holding Group, Tianjin 300410, China)

In order to evaluate the safety of the novel P2Y₁₂ receptor antagonist TSD-1, four main impurities were isolated and purified by semi-preparative HPLC, and characterized by NMR and HR-MS. A simple and specific HPLC method was developed for the determination of TSD-1.



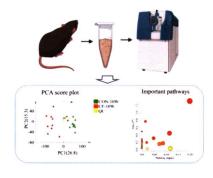
2183

Study on intermittent fasting changing fecal metabolism pattern of mice based on metabolomics technique

XIONG Xing¹, XIONG Wei², CHEN Yan³, JU Zheng-cai^{3*}

(1. School of Pharmacy, Nantong University, Nantong 226000, China; 2. College of Animal Sciences, Fujian Agriculture and Forestry University, Fuzhou 350000, China; 3. Teaching Experiment Center of Shanghai University of Traditional Chinese Medicine, Shanghai 200120, China)

Feces metabolome were significantly altered in intermittent fasting (IF) mice, and the most important metabolic pathways between control and IF mice were linoleic acid metabolism, bile acid biosynthesis, and fatty acid metabolism. This study might provide a valuable reference point for IF in the treatment of related metabolic diseases.



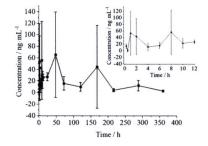
2191

Development of a method for determination of progesterone sustained-release formulation in Beagle dog plasma and its pharmacokinetic study

WANG Yue^{1,2}, CHENG Yi², ZHANG Hui^{2*}, ZHENG Ai-ping^{1,2*}

(1. School of Pharmacy, Xuzhou Medical University, Xuzhou 221000, China; 2. Institute of Pharmacology and Toxicology, Academy of Military Medical Sciences, Academy of Military Sciences, Beijing 100850, China)

In this study, we conducted a pharmacokinetic study on Prosphere, which is the sustained-release formulation in Beagle dogs. And a liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis method with strong specificity and high sensitivity was successfully developed.

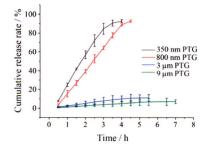


2197

Preparation, in vitro characterization and pharmacokinetics of paclitaxel thermosensitive gel

FAN Ran-ran¹, WANG Zeng-ming², ZHANG Hui^{2*}, LI Jian-chun^{1*}, ZHENG Ai-ping^{2*} (1. School of Pharmacy, Bengbu Medical College, Bengbu 233030, China; 2. Institute of Pharmacology and Toxicology, Academy of Military Medical Sciences, Academy of Military Sciences, Beijing 100850, China)

In this paper, a thermosensitive gel delivery system containing paclitaxel with different particle sizes was constructed. The results showed that the particle size significantly affected the release rate of paclitaxel thermosensitive gel.



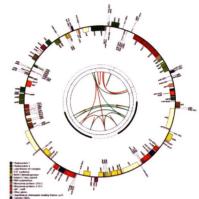
XVI Contents

2206

Characterization and phylogenetic analysis of the complete chloroplast genome of *Lycopus europaeus*

DU Qing^{1,2,3#*}, WANG Li-qiang^{4#}, CHEN Zhuo-er^{2,5}, JIANG Mei⁶, CHEN Hai-mei², ZENG Jing^{2,5}, WANG Bin^{5*}, LIU Chang²

(1. Key Laboratory of Medicinal Plant Resources of Qinghai-Tibetan Plateau in Qinghai Province, College of Pharmacy, Qinghai Minzu University, Xining 810007, China; 2. Institute of Medicinal Plant Development, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing 100193, China; 3. Fresh Sky-Right (Beijing) International Science and Technology Co. Ltd., Beijing 100097, China; 4. College of Pharmacy, Heze University, Heze 274015, China; 5. College of Pharmacy, Xiangnan University, Chenzhou 423099, China; 6. School of Pharmaceutical Sciences, Qilu University of Technology (Shandong Academy of Sciences), Jinan 250200, China)



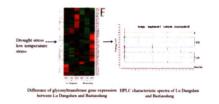
The total length of *Lycopus europaeus* chloroplast genome is 152 085 bp, including 132 genes with 88 protein coding genes, 36 tRNA genes, and 8 rRNA genes. It contains 34 characteristic SSR, which can be used to distinguish and identify the plants of *Lycopus europaeus*.

2216

Identification and analysis of glycosyltransferase in *Codonopsis pilosula* from different regions based on transcriptome

TIAN Xing-rui¹, JI Jiao-jiao¹, LI Jian-kuan¹, JIANG Feng¹, LIU Zhe-yu¹, GAO Jian-ping^{1,2*}

(1. School of Pharmaceutical Science, Shanxi Medical University, Taiyuan 030001, China; 2. Shanxi Province Daodi Medicinal Material Resources Development Engineering Technology Research Center, Taiyuan 030001, China)



The difference of producing area environment resulted in the significant difference of glycosyltransferase gene expression of *Codonopsis pilosula*, which led to the metabolic difference of *Codonopsis pilosula* polysaccharides, tangshenoside I and atractylenolide III.

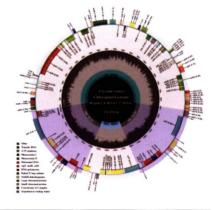
2224

Characteristics of complete chloroplast genome and phylogenetic analysis of *Cirsium souliei* (Asteraceae)

ZHENG Chang-yuan^{1,2}, SU Xu^{1,2,3}, LIU Yu-ping^{1,2*}, LIU Tao^{1,2}, WANG Ya-nan^{1,2}, SU Dan-dan^{1,2}, ZHANG Yu^{1,2}, QIN Na^{1,2}

(1. School of Life Sciences, Qinghai Normal University, Xining 810008, China; 2. Key Laboratory of Medicinal Animal and Plant Resources of the Qinghai-Tibet Plateau in Qinghai Province, Qinghai Normal University, Xining 810008, China; 3. Academy of Plateau Science and Sustainability, Qinghai Normal University, Xining 810016, China)

The complete chloroplast (cp) genome of *C. souliei* was a typical quadripartite circular structure of 152 470 bp in length, which encoded 134 genes, the result from phylogenetic analysis based on 46 cp genomes of Carduoideae showed that *C. souliei* and *C. vulgare* were sister species, and had the closest relationship.



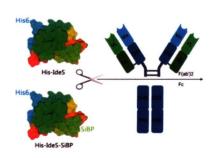
2234

Expression, purification, and functional identification of immunoglobulin degrading enzyme IdeS in *Escherichia coli*

ZHOU Si-han, LIU Min-zhi, YANG Yan, WANG Wei*

(State Key Laboratory of Bioactive Substance and Function of Natural Medicines, NHC Key Laboratory of Natural Drug Biosynthesis, Institute of Materia Medica, Peking Union Medical College and Chinese Academy of Medical Sciences, Beijing 100050, China)

Heterologous expression of IdeS in *E. coli* and investigation of the effect of different affinity tags on its yield and activity.



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