

藥科(二)Scifinder 報告-Caffeine

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1. 基本資訊

CAS Registry Number: 58-08-2

C8 H10 N4 O2

1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-

Caffeine (8CI); 1,3,7-Trimethyl-2,6-dioxopurine;

1,3,7-Trimethylxanthine; 3,7-Dihydro-1,3,7-trimethyl-1H-purine-2,6-dione;

7-Methyltheophylline; Alert-

Pep; Asia migrine; Cafalgine; Cafeina; Caffedrine; Caffein; Cafipel; DHCplus; Dasin;

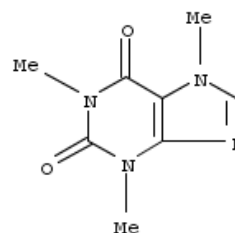
Diurex; Durvitan; Guaranine; Hycomine; Koffein; Mateina;

Methyltheobromine; Midron extra; Miudol; NSC 5036; New Cetamol; No-Doz;

Palergot-C; Phensal; Propoxyphene Compound 65; Refresh'n; SK 65

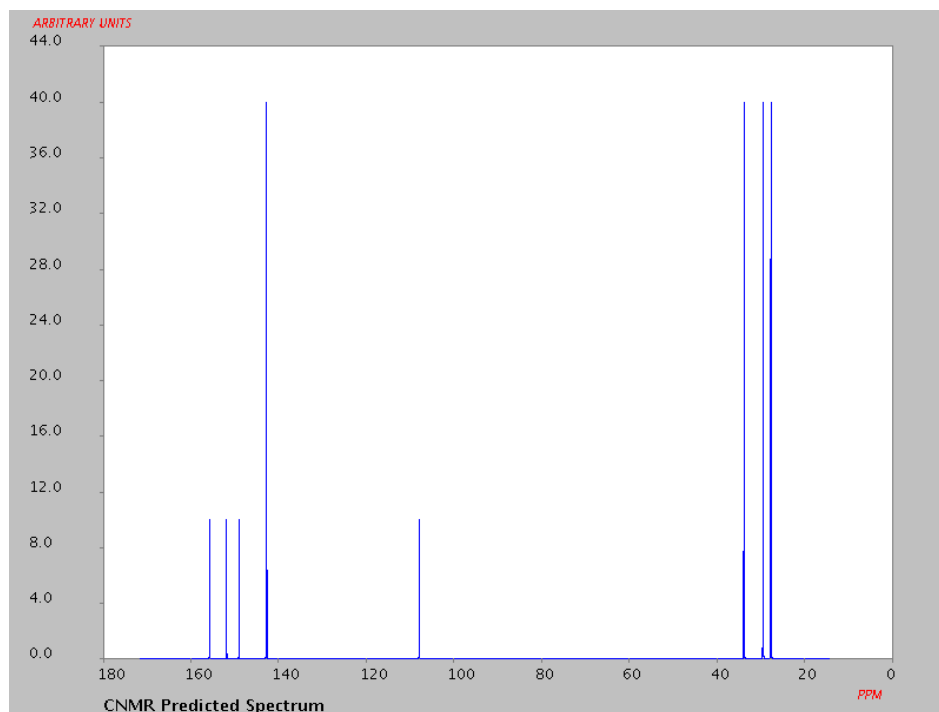
Compound; Shape Plus; Stay Alert; Stim; Synalgos; Thein; Theine; Tri-Aqua; Wigraine

Deleted CAS Registry Numbers: 71701-02-5, 95789-13-2

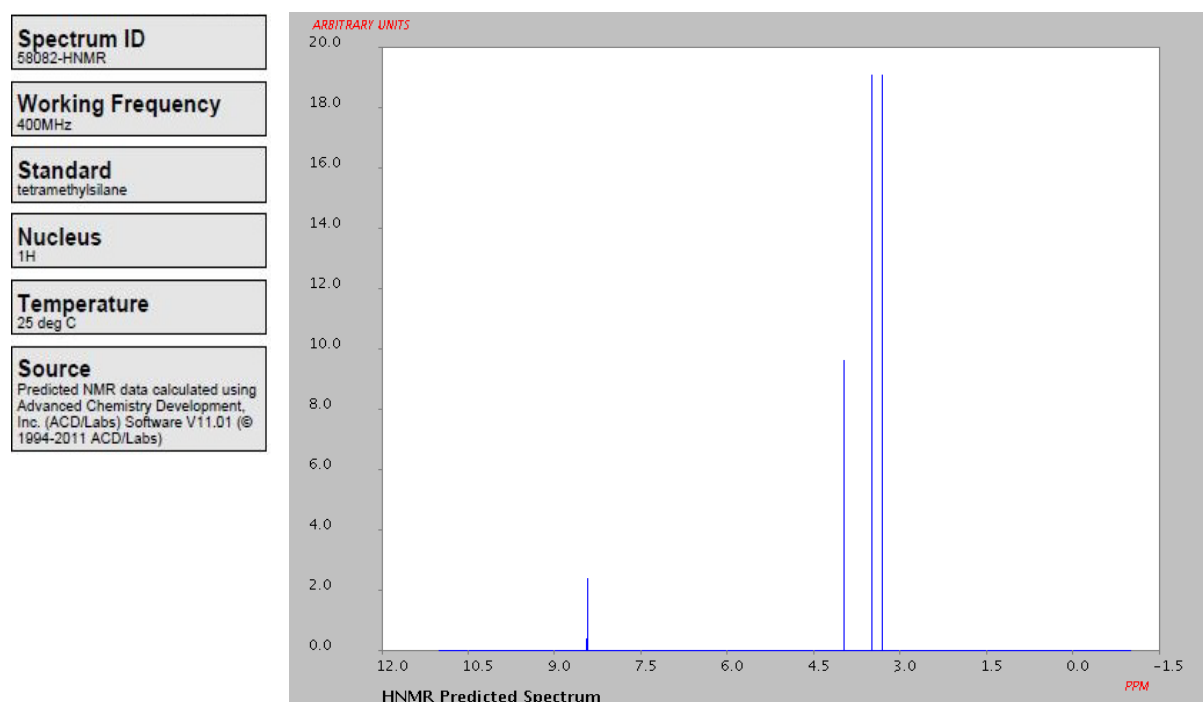


2. CNMR 資訊及圖譜：

Spectrum ID 68082-CNMR
Standard tetramethylsilane
Nucleus 13C
Temperature 25 deg C
Source Predicted NMR data calculated using Advanced Chemistry Development, Inc. (ACD/Labs) Software V11.01 (© 1994-2011 ACD/Labs)



3. HNMR 資訊及圖譜：



4. 疾病治療相關文章：

(1) Coffee as a functional beverage

By Taylor, Lem; Antonio, Jose

Edited By: Wildman, Robert E. C

From Handbook of Nutraceuticals and Functional Foods (2nd Edition) (2007),
453-465. Language: English, Database: CAPLUS

A review on coffee and its role as a functional beverage. A background on coffee and caffeine is presented, and the different types of coffee are discussed along with the ingredients in coffee, the effects of coffee on energy metab., and its role as a drink that can enhance various aspects of health and possibly prevent or reduce the risk of some diseases, including blood pressure, cardiovascular disease, diabetes, and cancer.

(2) Attenuation of cytotoxic natural product DNA intercalating agents by caffeine

By Hill, Gabrielle M.; Moriarity, Debra M.; Setzer, William N.

From ScientiaPharmaceutica (2011), 79(4), 729-747. Language: English, Database:
CAPLUS, DOI:10.3797/scipharm.1107-19

Many anti-tumor drugs function by intercalating into DNA. The xanthine alkaloid caffeine can also intercalate into DNA as well as form p-p mol. complexes with other planar alkaloids and anti-tumor drugs. The presence of caffeine could interfere with the intercalating anti-tumor drug by forming p-p mol. complexes with the drug, thereby blocking the planar arom. drugs from intercalating into the DNA and ultimately lowering the toxicity of the drug to the cancer cells. The cytotoxic activities of several known DNA intercalators (berberine, camptothecin, chelerythrine, doxorubicin, ellipticine, and sanguinarine) on MCF-7 breast cancer cells, both with and without caffeine present (200 mg/mL) were detd. Significant attenuation of the cytotoxicities by caffeine was found. Computational mol. modeling studies involving the intercalating anti-tumor drugs with caffeine were also carried out using d. functional theory (DFT) and the recently developed M06 functional. Relatively strong p-p interaction energies between caffeine and the intercalators were found, suggesting an "interceptor" role of caffeine protecting the DNA from intercalation.

(3) Caffeine-potentiated chemotherapy and function-preserving surgery for osteosarcoma: a long-term result in a single institute

By Tsuchiya, H.; Yamamoto, N.; Hayashi, K.; Takeuchi, A.; Yamauchi, K.; Tomita, K.
From UICC World Cancer Congress, Proceedings of the Free Papers, Washington, DC, United States, July 8-12, 2006 (2006), 33-36. Language: English, Database: CAPLUS

Introduction: We report on a long-term result of nonrandomized prospective study about caffeine-potentiated chemotherapy for osteosarcoma. Materials and Methods: Thirty-nine patients with non-metastatic osteosarcoma were treated with neoadjuvant chemotherapy consisting of cisplatin, adriamycin, and caffeine. Intraarterial chemotherapy was performed 3 to 5 times preoperatively. Results: Total tumor necrosis was histol. demonstrated in 31 patients (79%), more than 90% tumor necrosis in 5, and no response in 3. Overall effectiveness rate was 92%. Overall 5-yr survival rate was 93% and event-free survival 81% with a mean follow-up of 105 mo. Important anatomical structures were mostly preserved in 36 chemo-responders to improve limb function. Conclusions: Introduction of caffeine to osteosarcoma chemotherapy led to remarkable advancement of survival and surgical treatment in patients with osteosarcoma. Randomized trials of caffeine-potentiated chemotherapy will provide much more clear evidence in musculoskeletal sarcomas and other cancers.

(4) Catechins and caffeine in tea: A review of health risks and benefits

By Cooper, Raymond; Likimani, Talash A.; Morre, D. James; Morre, Dorothy M.

Edited By: Smith, Barry D.; Gupta, Uma; Gupta, B. S

From Caffeine and Activation Theory (2007), 351-364. Language: English, Database: CAPLUS

A review. Catechins are polyphenols comprising epigallocatechingallate, epigallocatechin, epicatechingallate, and epicatechin. Oxidn. results in the formation of higher mol. wt. condensed polyphenolic constituents known as theaflavins. Caffeine is a methylxanthine compd. and a known stimulant of the central nervous system. Low to moderate doses of caffeine are widely considered to enhance mental alertness and phys. performance pos. in some individuals. Doses most often assocd. with increased alertness, energy, and concn. are generally in the 100- to 600-mg range. Since green tea ext. may stimulate thermogenesis to an extent greater than can be attributed to its caffeine content, the thermogenic properties of green tea may be due to an interaction between caffeine and its high content of catechin-polyphenols. The probable mechanism explaining the thermogenic effect of green tea is through an increase in levels of norepinephrine. Catechin-polyphenols are known to inhibit catechol-o-methyltransferase, the enzyme that degrades norepinephrine.

(5) The influence of caffeine analogues and antagonists on the Ca^{2+} -accumulation by sarcoplasmic reticulum

By Alekseeva, Olga M.; Kim, Yuri A.; Rykov, Vladimir A.

Edited By: Lekishvili, Nodar; Zaikov, Gennady; Howell, Bob

From Advanced Biologically Active Polyfunctional Compounds and Composites (2010), 25-33. Language: English, Database: CAPLUS

This study investigates the actions of caffeine analogs and antagonists to the main Ca^{2+} -depo in the rabbit skeletal muscle - sarcoplasmic reticulum. The efficiency of Ca^{2+} -accumulation by vesicles of heavy fragmented sarcoplasmic reticulum was greatly changed by caffeine analogs and antagonist: cordiamin, camphor, bemegrid, 8-methylcaffeine, teophylline, theobromine, midocalm. All tested substances have some similar characteristics at its mol. structure. The carbonyl oxygen and Me groups are of a great importance for "caffeine effect" of these substances.

(6) Pharmacology and use of methylxanthines and doxapram for the treatment of neonatal apnea

By Boutroy, Marie-Jeanne

Edited By:Jacqz-Aigrain; Choonara, Imti

From Paediatric Clinical Pharmacology (2006), 417-423. Language: English, Database: CAPLUS

A review. A review. Apnea is a transient cessation of breathing. In neonates, it may be attributed to immaturity of the respiratory command system or to specific disorders. The methylxanthines (theophylline and caffeine) are the first-line therapeutic agents for treating apnea in neonates. The efficacy, therapeutic drug monitoring, pharmacokinetics, dose guidelines, and toxicity for methylxanthines and doxapram are discussed.

(7) Coffee and caffeine suppress the development of type 2 diabetes in mouse models

By Horio, Fumihiko; Kobayashi, Misato

Edited By:Smith, Barry D.; Gupta, Uma; Gupta, B. S

From Baio Saiensu to Indasutori (2011), 69(6), 452-457. Language: Japanese, Database: CAPLUS

A review on epidemiol. of assocn. coffee intake and onset of type 2 diabetes, discussing the identification of caffeine as an active ingredient in coffee, antidiabetic effect of coffee and caffeine in spontaneously type 2 diabetic kk-Ay mice, and in another type of type 2 diabetic mice induced by high-fat diet.

(8) Efficacy of caffeine-potentiated chemotherapy for high-grade soft tissue sarcoma

By Takeuchi, A.; Tsuchiya, H.; Yamamoto, N.; Hayashi, K.; Yamauchi, K.; Tomita, K.

Edited By:Smith, Barry D.; Gupta, Uma; Gupta, B. S

From UICC World Cancer Congress, Proceedings of the Free Papers, Washington, DC, United States, July 8-12, 2006 (2006), 27-32. Language: English, Database: CAPLUS

A nonrandomized prospective clin. trial was initiated for the treatment of non-metastatic (Stage II) or metastatic (Stage III) high-grade soft tissue sarcoma (STS) to assess the efficacy of caffeine-potentiated chemotherapy. Seventy-two patients

(49 extremities, 19 trunks, 4 retroperitoneal) were enrolled. Following doxorubicin or ifosfamide-based caffeine-potentiated chemotherapy with or without radiotherapy, they were treated surgically. A radio-graphic and histol. response to chemotherapy was assessed. Forty-eight (66.7%) patients were evaluated for an objective radiog. responder. Histol.response was obsd. in 37 (52.9%) patients. The local recurrences were obsd. in 14 patients 0(26.4y) at Stage II. The lung metastases were newly developed in 18 (34.0%) patients at stage II. With a median follow-up period of 49 mo, the overall 5-yr cumulative survival rate of the patients with non-metastatic STS was 75.6%.

In conclusion, caffeine-potentiated chemotherapy resulted in a favor radiog. response and prolonged survival of the patients at stage II.

(9) Evaluation of the efficacy of caffeine cessation, nortriptyline, and topiramate therapy in vestibular migraine and complex dizziness of unknown etiology

By Mikulec, Anthony A.; Faraji, Farhoud; Kinsella, Laurence J.

Edited By:Smith, Barry D.; Gupta, Uma; Gupta, B. S

From American Journal of Otolaryngology (2012), 33(1), 121-127. Language: English,

Database: CAPLUS,

DOI:10.1016/j.amjoto.2011.04.010

Objective: The aim of this study was to evaluate the efficacy of a therapeutic pathway for vestibular migraine (VM) and complex dizziness of undetd. etiol. (CDUE) with caffeine cessation and pharmacotherapy. **Study Design:** This study is a retrospective chart review. **Intervention(s):** Patients were recommended to stop intake of caffeine and other putative migraine-triggering agents. **Pharmacotherapy** was initiated with nortriptyline or topiramate if symptoms persisted despite diet modification. **Main Outcome Measure:** Self-reported dizziness is the main outcome measure. **Results:** Vestibular migraine and CDUE were considered contributing factors to dizziness in 34 and 10, resp., of 156 patients. Fourteen percent of patients reported improvement in symptoms upon caffeine cessation, whereas 46% of patients reported a redn. in dizziness after nortriptyline therapy ($P = .007$). Topiramate reduced symptoms in 25% of patients. In total, 75% of VM patients and 56% of patients with CDUE received sufficient benefit from this therapeutic pathway to not progress to other treatments. **Conclusions:** Vestibular migraine and CDUE can be treated effectively with a therapeutic pathway consisting of caffeine cessation followed by pharmacotherapy.

(10) Menstrual endocrinology and pathology: caffeine, physiology, and PMS

By Vo, Hoa T.; Smith, Barry D.; Elmi, Solmaz

Edited By:Smith, Barry D.; Gupta, Uma; Gupta, B. S

From Caffeine and Activation Theory (2007), 181-197. Language: English, Database: CAPLUS

A review on caffeine and its role in premenstrual syndrome (PMS). An overview of the link between caffeine intake and PMS is presented, including the biol. and environmental variables underlying caffeine, the menstrual cycle, PMS, premenstrual dysphoric disorder (PMDD), etiol. of PMS and PMDD, and role of caffeine in the menstrual cycle.

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5. 心得

這三小時的課程非常充實，講者不僅用 **power point** 說明了如何利用此平台搜尋資料，更實際示範所有我們目前最需要的基礎功能，並將教學與自由操作時間分割數段，使我們不會一時間獲得太多知識而無法完整吸收。除了詳細解說外，自由操作時間也不少，可以讓我們立刻嘗試，有使用的經驗記憶會比較清楚，以後能更順手地使用 **Scifinder**。至於 **Scifinder** 此平台，使用起來非常方便，現在如遇到不熟悉的化學結構或物質，我就會想用 **Scifinder** 搜尋，因其內容專業無須擔心資訊有誤，且在課堂上用過之後便深深認識到它的便利性。