# 科技部補助產學合作研究計畫成果精簡報告

## 快速測定安定劑中高級脂肪酸

計畫類別：開發型
計畫編號：MOST 104-2622-M-041-001-CC2
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執行單位：嘉藥學校財團法人嘉南藥理大學醫藥化學系

計畫主持人：王來好
共同主持人：凌櫻玫
計畫參與人員：此計畫無其他參與人員

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中華民國 105 年 03 月 16 日

中文摘要：利用紅外線光譜儀快速測定脂肪酸 (辛酸(Octanoic acid)、壬酸(Nonanoic acid)、癸酸(Decanoic acid)、月桂酸(Lauric acid)、肉豆蔻酸(Myristic acid)、棕櫚酸(Palmitic acid)、硬脂酸(Stearic acid)、苯甲酸(Benzoic acid)、對叔丁基苯甲酸(4-tert-butylbenzoicacid)與油酸(Oleic acid), 與測定合成其相對應之甲基脂肪酸酯類，建立各別的脂肪酸與其相對應甲基脂肪酸酯類的指紋分析資料圖譜。同時利用氣相層析儀與高解析氣相層析質譜儀(GC-HRMS)測定相對應之甲基脂肪酸酯類。比對紅外線光譜之資料圖譜得知市售脂肪酸原料之純度。

中文關鍵詞：傳立葉轉換紅外線；氣相層析及氣相層析連線質譜；高級脂肪酸。

英文摘要：A rapid nondestruction analysis method is established to qualitatively detect of ten kinds fatty acids, containing octanoic acid, nonanoic acid, decanoic acid, lauric acid, myristic acid, palmitic acid, stearic acid, benzoic acid, 4-tert-butylbenzoicacid, oleic acid, which uses Fourier transform spectroscopy to determine the IR spectrogram of fatty acids and their methyl esters. Comparison with results obtained from gas chromatography and gas chromatography with mass spectrometry detection.
The spectrogram of fingerprint data is applied for the compare with commercial raw materials of fatty acid samples for the purity.

英文關鍵詞：Fourier transform mid-infrared spectroscopy, gas chromatography and gas chromatography/mass spectrometry; higher fatty acids.

# 科技部補助專題研究計畫成果報告

（□期中進度報告/■期末報告）

（計畫名稱）

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執行機構及系所：嘉南藥理大學 醫藥化學系

計畫主持人：王來好
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中　華　民　國 105 年 3 月 16 日

# 快速測定安定劑中高級脂肪酸

# Rapid determination of the stabilizers higher fatty acids

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## 中文摘要

利用紅外線光譜儀快速測定脂肪酸 (辛酸(Octanoic acid)、壬酸(Nonanoic acid)、癸酸(Decanoic acid)、月桂酸(Lauric acid)、肉豆蔻酸(Myristic acid)、棕櫚酸(Palmitic acid)、硬脂酸(Stearic acid)、苯甲酸(Benzoic acid)、對叔丁基苯甲酸(4-tert-butylbenzoicacid)與油酸(Oleic acid), 與測定合成其相對應之甲基脂肪酸酯類，建立各別的脂肪酸與其相對應甲基脂肪酸酯類的指紋分析資料圖譜。同時利用氣相層析儀與高解析氣相層析質譜儀(GC-HRMS)測定相對應之甲基脂肪酸酯類。比對紅外線光譜之資料圖譜得知市售脂肪酸原料之純度。

**關鍵詞**：傅立葉轉換紅外線；氣相層析及氣相層析連線質譜；高級脂肪酸。

## 英文摘要

A rapid nondestruction analysis method is established to qualitatively detect of ten kinds fatty acids, containing octanoic acid, nonanoic acid, decanoic acid, lauric acid, myristic acid, palmitic acid, stearic acid, benzoic acid, 4-tert-butylbenzoicacid, oleic acid, which uses Fourier transform spectroscopy to determine the IR spectrogram of fatty acids and their methyl esters. Comparison with results obtained from gas chromatography and gas chromatography with mass spectrometry detection.

The spectrogram of fingerprint data is applied for the compare with commercial raw materials of fatty acid samples for the purity.

**Keywords:** Fourier transform mid-infrared spectroscopy, gas chromatography and gas chromatography/mass spectrometry; higher fatty acids.

## 內容

## 前言

Poly(vinyl chloride), commonly abbreviated to PVC, is the third most widely used thermoplastic polymer after polyethylene and polypropylene. The most important thermal stabilizers for PVC are those metal soaps like Pb-, Cd-, Ba-,Ca-, and Zn-carboxylates. The mixed Ca/Zn thermal stabilizers at an appropriate ratio exhibit synergetic effects with both acceptable initial color and long-term stability for PVC products [1-2]. Higher fatty acids $C_{6-18}$, Ca (Zn) oxides, and catalysts are heats at melting to prepare heat stabilizers [3-4]. An experimental study of the influence of carboxylic acid additives in various thermoplastics in rheometers is described [5].

## 研究目的

Various methods have been proposed for determining fatty acids: gas chromatographic analysis of the acetonyl esters of higher fatty acids is reported [6], individual derivatization of volatile fatty acids with N-(1-naphthyl)ethylenediamine(EDAN) followed can be determined by gas chromatography [7], After methyl esterification treatment fatty acids in seed, and esterification trans fatty acids using boron trifluoride in methanol in animal and vegetable oils were identified by gas chromatography-mass spectroscopy (GC-MS) [8-11]. In the literature there are several references about the use of spectroscopy technique to analyze fatty acid composition, e.g. Fourier transform mid-infrared spectroscopy (MID-FTIR) in milk control [12], MID-FTIR spectroscopy coupled with partial least square algorithm (PLS-1) was used to predict total fat, fish oil, fatty acid composition [13-14], investigating polyunsaturated fatty acids distribution in mouse retina and brain tissue with FTIR [15-16], methyl oleate and methyl linoleate in fats and oils were analyzed by GC–MS and GC–FTIR [17]. However, these studies [12-17] reports that fatty acids in foods. There are only one FTIR applied to stearic acid in styrenic polymer [18]. In this report, the application of FTIR spectroscopy will be described ten long –chain fatty acid esterified compounds and corresponding to non- esterified fatty acids, and esterified compounds were compared to GC and GC-MS.

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## 研究方法

### Materials and apparatus

The commercial sample fatty acids investigated

were provided by Kim Yu-long Ltd.

Pure standard substances were purchased from biomedical supply houses: octanoic acid, decanoic acid, benzoic acid from Acros Organics (Geel, Belgium); and nonanoic acid, stearic acid from Tokyo Chemical Industry Co., Ltd.(Tokyo, Japan). Oleic acid, lauric acid, myristic acid, palmitic acid were obtained from Showa Chemical Co., Ltd., 4-tert-butylbenzoicacid was from Alfa Aesar (Ward Hill, MA, USA).The mixture methyl esters of fatty acids were determined using a gas chromatography-flame ionization detector (GC-FID) (Model GC-2014 GC; Shimadzu Technologies). The absorption spectra of fatty acids and its methyl ester were determined using a fourier transform infrared spectrophotometer (FTIR Perkin Elmer Spectrum RX 1 (RX-1; Perkin-Elmer, Fremont, CA, USA) with a potassium bromide window. All other chemicals were analytical reagent grade.

### Methylesterfication and gas chromatography and GC/MS analysis

The analysis of methyl esters of fatty acids was carried out GC and GC/MS. The Shimadzu

GC-2014 chromatograph equipped with FID and Agilent HP-5 column (30 m × 0.32 mm, film thickness 0.25 μm) was used to for quantitative analysis. Methylester of fatty acids was prepared by adding 8 ml of hydrochloric acid/methanol (5:95); the mixture was then placed in water bath with temperature set at 75° C for 1,2,3 and 4 hour, respectively. A methylestered fatty acid was neutralized of 2 % sodium carbonate, later extracted in hexane and dried under nitrogen gas. Prepared methylesters were then dissolved in hexane and a 0.5 uL sample of the clear solution injected in a HP-5 capillary column. The oven temperature was programmed: held isothermal at 80 ºC for 3 min, then from 80 ºC -290 ºC at 30 ºC/min (stay in 130 ºC, 200 ºC, 270 ºC for 2 min and 280 ºC for 1 min, 280 ºC for 2min), injector temperature, 290 ºC; detector temperature, 290 ºC. Carrier gas nitrogen at a 1 mL/min; splitless. Analysis by GC-MS was performed using a chromatograph Shimadzu QP-2010 mass spectrometer instrument at 70 eV and 250 ºC. The temperature was from 50-270 ºC at 6 mL/min. Helium gas was used as carrier at a flow rate of 0.80 mL/min.

*Free fatty acids and methyl esters of fatty acids using FTIR analysis*

Infrared spectra were recorded in liquid, using KBr cell (a single -beam). Because of the high signal-to-noise ratio on this instrument, 10 scans (in the range of 4000-400 $cm^{-1}$) at 4 $cm^{-1}$ resolution were sufficient to obtain spectra adequate for quantitation.

## 結果與討論

### Gas chromatography

The development of the sensitive GC technique to the higher-boiling fatty acids, we have preferred to use the methyl esters rather than the free acids, as difficulty was encountered in finding a stationary phase for the column that would prevent dimerization of the free acids. It is not possible to cover the whole range of saturated, unsaturated straight chain aliphatic acids and aromatic acids from $C_6$-$C_{18}$ by operating the column at any one temperature. Therefore, temperature programming was used to good separation methyl esters of fatty acids. In Table 1 were given the retention times of methyl esters of a variety of acids using GC-FID and GC-MS . The 10 components of methyl esters of fatty acids were identified by comparing the retention time and comparision of the obtained mass spectra of the chromatographic peaks with those of authentic standard and with spectra of the NIST 05 library. Molecular weight and retention times were listed in Table1. Fig. 1 shows a typical gas chromatogram of mixed methyl esters fatty acid obtained by esterifying hexane-soluble extract of reaction products. The GC analysis of aliphatic acids and aromatic acids from $C_6$-$C_{18}$ higher fatty acids can be achieved by the use of their methyl derivatives. Esterification reaction yields were obtained using this procedure as those described in experimental section and listed in Table 2. The methyl derivatives show good chromatographic properties and excellent yields were observed (yields ranging from 98.5 ± 0.26 to 104.5 ± 0.67). The analytical features of the GC were evaluated under the optimal experimental condition. Regression equations, calibration ranges, retention times and limit of detections of analytes were listed in Table 3. From the Fig. 2, the linearity was validated in the range 0.5~80 mg $L^{-1}$ for methyl octanoate, methyl laurinate, methyl myristate, methyl palmitate, methyl oleate, methyl stearate, 0.8~80 mg $L^{-1}$ for methyl nonanoate, 3.0~80 mg $L^{-1}$ for methyl benzoate, methyl decanoate, respectively. Linear regression coefficients ranged from 0.9993 to 0.9997. The detection of limit (LOD) and quantification of limit(LOQ) were estimated using the classical 3δ, i.e. calculation of LOD and LOQ through analysis of the standard deviation of blank measurements(n=3).Limits of detection obtained with GC-FID system were in the range0.06 – 0.23 mg $L^{-1}$ for injection 0.5 $\mu$L. The proposed GC-FID method was used to determine purity in commercial benzoic acid and oleic acid, and content (w/w, %) were 76.6 ±2.52 and 72.3±2.08, respectively.

**FTIR spectroscopy**

The MID-FTIR spectra of higher fatty acids show different bands absorptions that are a function of the molecular bonds. Table 4 shows the MID-FTIR bands interpretation in spectra of the benzoic acid, 4-tert-butylbenzoic, $C_8$-$C_{18}$ saturated, unsaturated straight chain aliphatic acids, so all species of higher fatty acids have a ‘‘fingerprint’’ spectrum related to their chemical structure. The regions that show a suitable correlations between fatty acid structure and spectral response were the following: 3411 – 3447 $cm^{-1}$ very broad, 2958 – 2966 $cm^{-1}$, 2918 – 2936 $cm^{-1}$, 2846- 2876 $cm^{-1}$, 1709- 1685 $cm^{-1}$, 1640 – 1605 $cm^{-1}$, 1428-1407 $cm^{-1}$, 1285 – 1297 $cm^{-1}$, and 932-941 $cm^{-1}$ [19-21]. Carboxylic acids -C(==O)-OH are characterized by the OH stretch bands, the C=O stretch bands, the C-O stretch bands, the OH in plane bend bands, and the OH out-of plane wag bands. These bands are all sensitive to the hydrogen-bonding state of the COOH group, which can exist as unbonded monomer, the carboxylic acid dimmer form or sometimes in a hydrogen-bonded polymeric form [19].

From Fig. 3 can been seen, the spectra in the high wavenumber region reveal the strong O–H stretching modes of fatty acid ca 3429 $cm^{-1}$. The asymmetric stretching $(OH…O=C)_2$ mode for structure fatty acids are very broad over the range 2985-3690 with subsidiary maxima, which are due to combination and overtones in Fermi resonance with asymmetric stretching $(OH…O=C)_2$ [20]. Table 4 lists the IR frequency data for the asymmetric stretch $CH_3$, asymmetric $CH_2$ and symmetric $CH_2$ stretching frequencies for $C_8H_{16}O_2$ (octanoic acid) to $C_{18}H_{36}O_2$ (stearic acid). A study of the IR data and figures show that asymmetric stretch $CH_3$ generally decreases as the number of carbon atoms increases in the order $C_8$ to $C_{18}$ . For n-alkanes $C_8H_{16}O_2$, to $C_{18}H_{36}O_2$, the asymmetric stretch $CH_3$ occurs in the range 2954 -2948 $cm^{-1}$. Carboxylic acid group on aromatic rings absorb in the range 1710-1660 $cm^{-1}$ [19]. The C=O stretching frequencies for these fatty acids decrease in frequency in the order for octanoic acid (1709 $cm^{-1}$) to stearic acid (1685 $cm^{-1}$). The C=O stretching frequencies of 4-tert-butylbenzoic (1682 $cm^{-1}$ ) is lower than benzoic acid (1688 $cm^{-1}$) and n-alkanes $C_8$ to $C_{18}$ fatty acids (1709 $cm^{-1}$ and 1685 $cm^{-1}$) because of strong electron-donating group of hydrogen-bonding group on the benzene ring can lower the C=O stretching frequencies. IR bands in the range 1428-1407 $cm^{-1}$ are assigned to C-OH in plane bend , in the range 1285 - 1297 $cm^{-1}$ are assigned to C-O stretch and in the range 932-941 $cm^{-1}$ are assigned to Out-of –plane wag. The stretching C=C mode for 1-alkanes (R-CH=CH2) occur in the region 1641-1650 $cm^{-1}$ [20].Oleic acid has the formula $CH_3(CH_2)_7CH=CH(CH_2)_7COOH$ (18:1 cis -9). It overlapped bands at 1639 $cm^{-1}$, are due to the combination of double bond and carbonyl group of oleic acid. The distinctive bonds of oleic acid at 1054 $cm^{-1}$ and 1013 $cm^{-1}$ significantly higher than the stearic acid which reveal the presence of –HC = CH– (cis) bending out of plane (Fig 4). The ester and acid carbonyl (C=O) functional groups show characteristic stretching bands of methyl ester and free fatty acids and shown in Table 5. Representative FT-IR spectra in methyl laurate and free lauric acid (Fig.5) at 1742 $cm^{-1}$ and 1696 $cm^{-1}$, respectively (Fig. 5). This Fig.5 also shows the C=O stretching frequencies change or shift with change in the molecular structure [20]. Carboxylic acid ester has two very strong IR bands in the region between 1300 and 1050 $cm^{-1}$ [21]. Commercial raw materials of fatty acid samples are analysed by IR spectrometry to detect the purity of fatty acid. In Fig. 6 these spectra (4-tert-Butylbenzoic acid, benzoic acid, octanoic acid, decanoic acid, lauric acid, stearic acid, and oleic acid.) are compared with the standard fatty acids. Based on spectra comparison, commercial sample at 3200-3500 $cm^{-1}$ (OH stretch) is not obvious. Decanoic acid is found the most similar to the standard. However, oleic acid spectrum does not meet of standard because of commercial raw material mixed other myristic acid, palmitic acid and stearic acid.

### 誌謝

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### 成果報告自評表

本計畫研究快速測定安定劑中高級脂肪酸，近一年經由科技部計畫之執行，**已完成**目標如下：

1. 利用紅外線光譜儀快速測定 10 種常使用脂肪酸包括:辛酸(Octanoic acid)、壬酸(Nonanoic acid)、癸酸(Decanoic acid)、月桂酸(Lauric acid)、肉豆蔻酸(Myristic acid)、棕櫚酸(Palmitic acid)、硬脂酸(Stearic acid)、苯甲酸(Benzoic acid)、對叔丁基苯甲酸(4-tert-butylbenzoicacid)與油酸(Oleic acid)。並合成其相對應之甲基酯類，建立 10 種的脂肪酸與其 10 種甲基脂肪酸酯類的指紋分析資料圖譜。比對資料圖譜得知市售脂肪酸原料之純度。合成脂肪酸酯類之圖譜有助於公司塑化劑的研發。

2. 利用氣相層析儀同時測定 10 種合成的甲基脂肪酸酯類，並用高解析氣相層析質譜儀鑑定合成的酯類結構。建立 10 條甲基脂肪酸酯類之檢量線，用於實際樣品之純度測定。

Table 1 Methyl esters of fatty acids identification using a gas chromatography-flame ionization detector (GC-FID) and gas chromatography-mass spectroscopy (GC-MS)

| Methyl esters of fatty acids | Identification methods | | |
|---|---|---|---|
| | GC-FID Retention time ( min) | GC-MS | |
| | | Retention time (min) | Molecular weight |
| Methyl benzoate | 7.64 | 10.5 | 136 |
| Methyl octanoate | 7.88 | 11.1 | 158 |
| Methyl nonanoate | 9.03 | 13.7 | 172 |
| Methyl decanoate | 10.2 | 16.2 | 186 |
| Methyl 4-tert-butylbenzoate | 11.6 | 19.1 | 192 |
| Methyl laurinate | 12.1 | 20.8 | 214 |
| Methyl myristate | 13.7 | 24.8 | 242 |
| Methyl palmitate | 15.2 | 28.6 | 270 |
| Methyl oleate | 16.4 | 31.5 | 296 |
| Methyl stearate | 16.6 | 31.9 | 298 |

Table 2 Yields of 2.5 m M fatty acids with hydrochloric acid/methanol (5:95) reaction 4 hour using GC-FID

| Methyl ester of fatty acids | Yields (%)N=3[a] |
|---|---|
| Methyl benzoate | 99.3 ± 1.27[b] |
| Methyl octanoate | 101.8 ± 0.34 |
| Methyl nonanoate | 100.8 ± 1.83 |
| Methyl decanoate | 102.1 ± 2.44 |
| Methyl 4-tert-butylbenzoate | 101.8 ± 0.66 |
| Methyl laurinate | 98.5 ± 0.26 |
| Methyl myristate | 103.8 ± 1.33 |
| Methyl palmitate | 99.5 ± 2.02 |
| Methyl oleate | 104.5 ± 0.67 |
| Methyl stearate | 100.7 ± 1.47 |

[a] Number of determination

[b] Standard deviation

Table 3. Statistical evaluation of the calibration data obtained by GC- FID detection

| Methyl esters of fatty acids | y= aX+b | R | Range of linearity (mg $L^{-1}$) | LOD (mg $L^{-1}$) |
|---|---|---|---|---|
| Methyl benzoate | y = 9273.9x - 25412 | 0.9993 | 3.0~80 | 0.06 |
| Methyl octanoate | y = 9366.6x - 5150 | 0.9993 | 0.5~80 | 0.11 |
| Methyl nonanoate | y = 9329.4x + 983 | 0.9996 | 0.8~80 | 0.06 |
| Methyl decanoate | y = 11315x - 1045 | 0.9996 | 3.0~80 | 0.23 |
| Methyl 4-tert-butylbenzoate | y = 11556x - 3314 | 0.9996 | 0.8~80 | 0.15 |
| Methyl laurinate | y = 9880.1x + 2289 | 0.9996 | 0.5~80 | 0.06 |
| Methyl myristate | y = 10380x - 20690 | 0.9996 | 0.5~80 | 0.13 |
| Methyl palmitate | y = 10676x + 1356 | 0.9997 | 0.5~80 | 0.12 |
| Methyl oleate | y = 11188x + 14585 | 0.9993 | 0.5~80 | 0.08 |
| Methyl stearate | y = 8469.7x + 17058 | 0.9993 | 0.5~80 | 0.14 |

a, =slope; b = intercept on ordinate; R = correlation coefficient;
LOD = limit of detection.

.

Table 4 MID-FTIR bands assignments for functional groups found in spectra of $C_8$-$C_{18}$ higher fatty acids

| Frequency of bands ($cm^{-1}$) | Absorption intensity | Assignment |
|---|---|---|
| 3411 – 3447 very broad | Strong | OH stretch |
| 2958 – 2966 | Weak | $CH_3$ asymmetric stretch |
| 2918 - 2936 | Medium | $CH_2$ asymmetric stretch |
| 2846- 2876 | Medium | $CH_2$ symmetric stretch |
| 1709- 1685 | Strong | C=O asymmetric stretch |
| 1640 - 1605 | Weak | C=O symmetric stretch |
| 1428-1407 | Medium | C-OH in plane bend |
| 1285 - 1297 | Strong | C-O stretch |
| 932-941 | Medium | Out-of –plane wag |

Table 5 The carbonyl frequencies for $C_8$-$C_{18}$ higher methyl ester fatty acids

| Methyl ester fatty acids | C=O ester ($cm^{-1}$) | C-O ester very strong 1318 – 1010 ($cm^{-1}$) |
|---|---|---|
| Methyl 4-tert-butylbenzoate | 1721 | 1315,1282,1186,1117,1019 |
| Methyl benzoate | 1721 | 1318,1279,1192,1174,1111 |
| Methyl octanoate | 1739 | 1255,1198,1168,1108,1010 |
| Methyl nonanoate | 1742 | 1252,1198,1165,1111,1010 |
| Methyl decanoate | 1742 | 1246,1198,1168,1111,1010 |
| Methyl laurinate | 1742 | 1246,1195,1168,1111,1075 |
| Methyl myristate | 1742 | 1246,1195,1168,1114,1013 |
| Methyl palmitate | 1742 | 1237,1218,1185,1167,1117 |
| Methyl stearate | 1742 | 1241,1190,1167,1111,1087 |
| ethyl oleate | 1742 | 1246,1195,1171,1120,1016 |

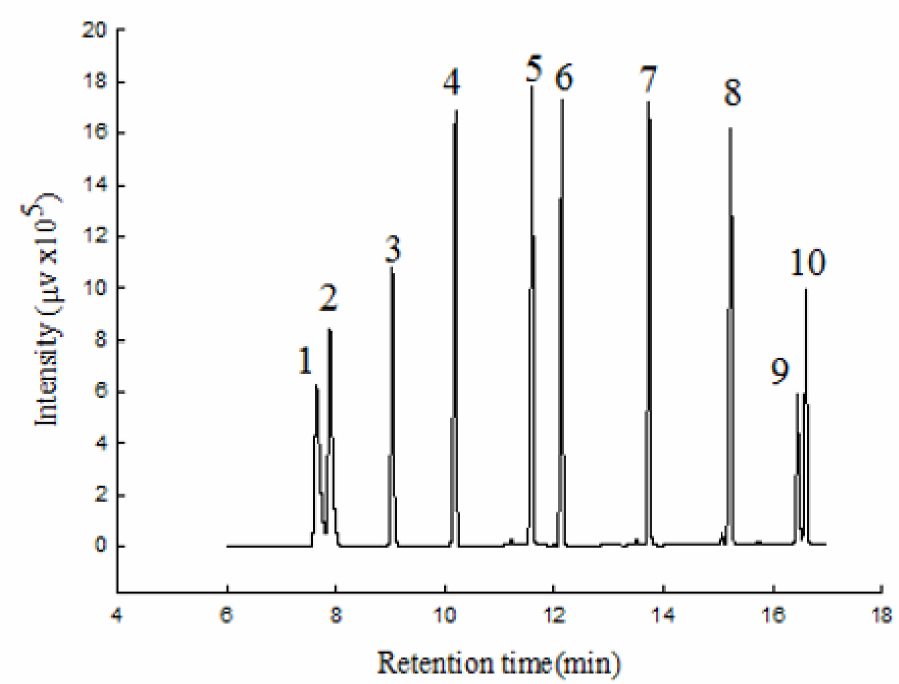


Fig. 1 A typical gas chromatogram of mixed methyl esters fatty acid (20 mgL$^{-1}$) obtained by esterifying hexane-soluble extract of products. Peak identification: 1, methyl benzoate; 2, methyl octanoate; 3, methyl nonanoate; 4, methyl decanoate; 5, methyl 4-tert-butylbenzoate; 6, methyl laurinate; 7, methyl myristate; 8, methyl palmitate; 9, methyl oleate; 10, methyl stearate.

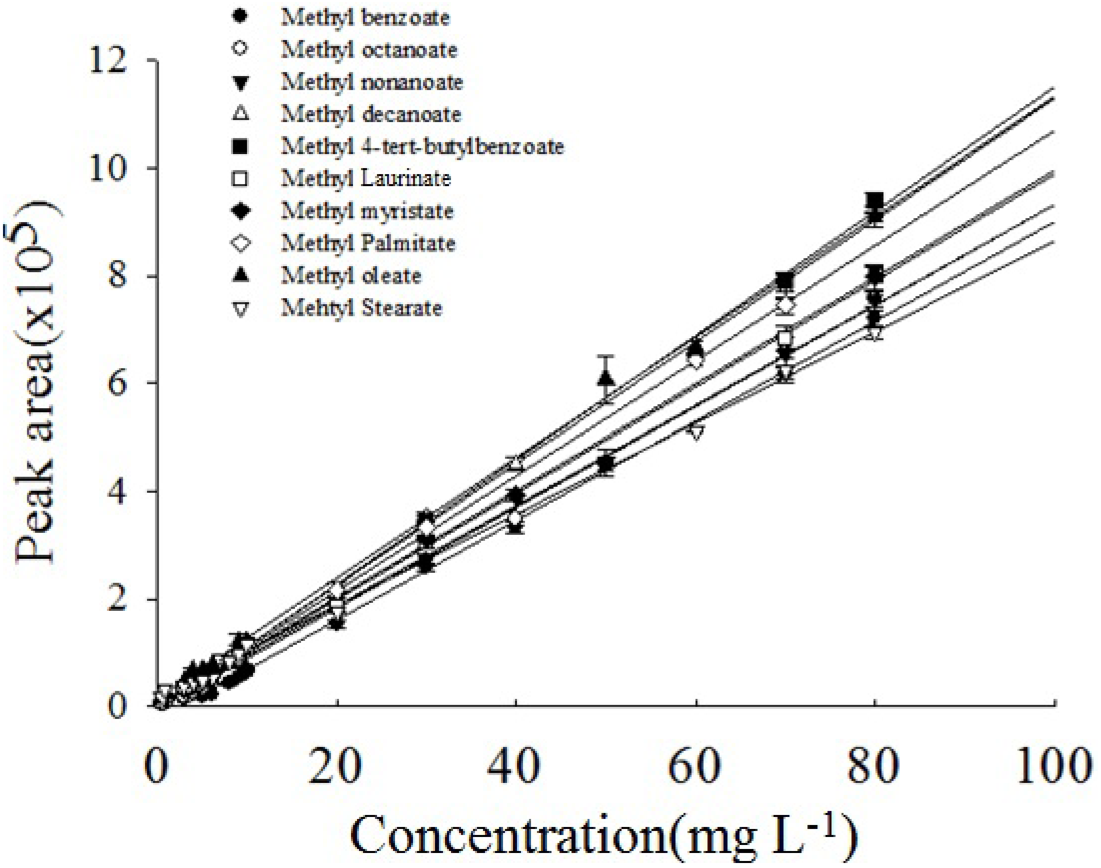


Fig. 2 The linearity of peak area versus concentration of methyl ester of fatty acids.

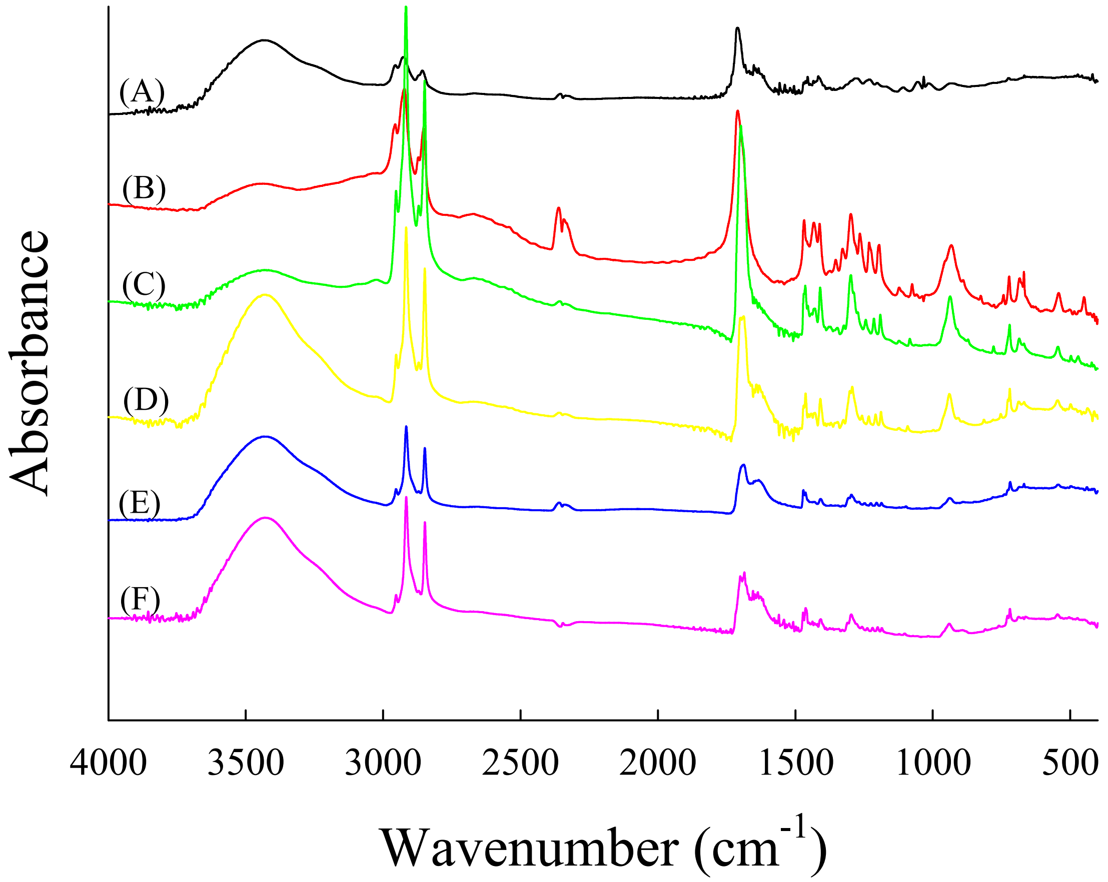


Fig. 3 The FT-IR of fatty acid (A) octanoic acid; (B) decanoic acid; (C) lauric acid; (D) myristic acid ;(E) palmitic acid ; (F) stearic acid.

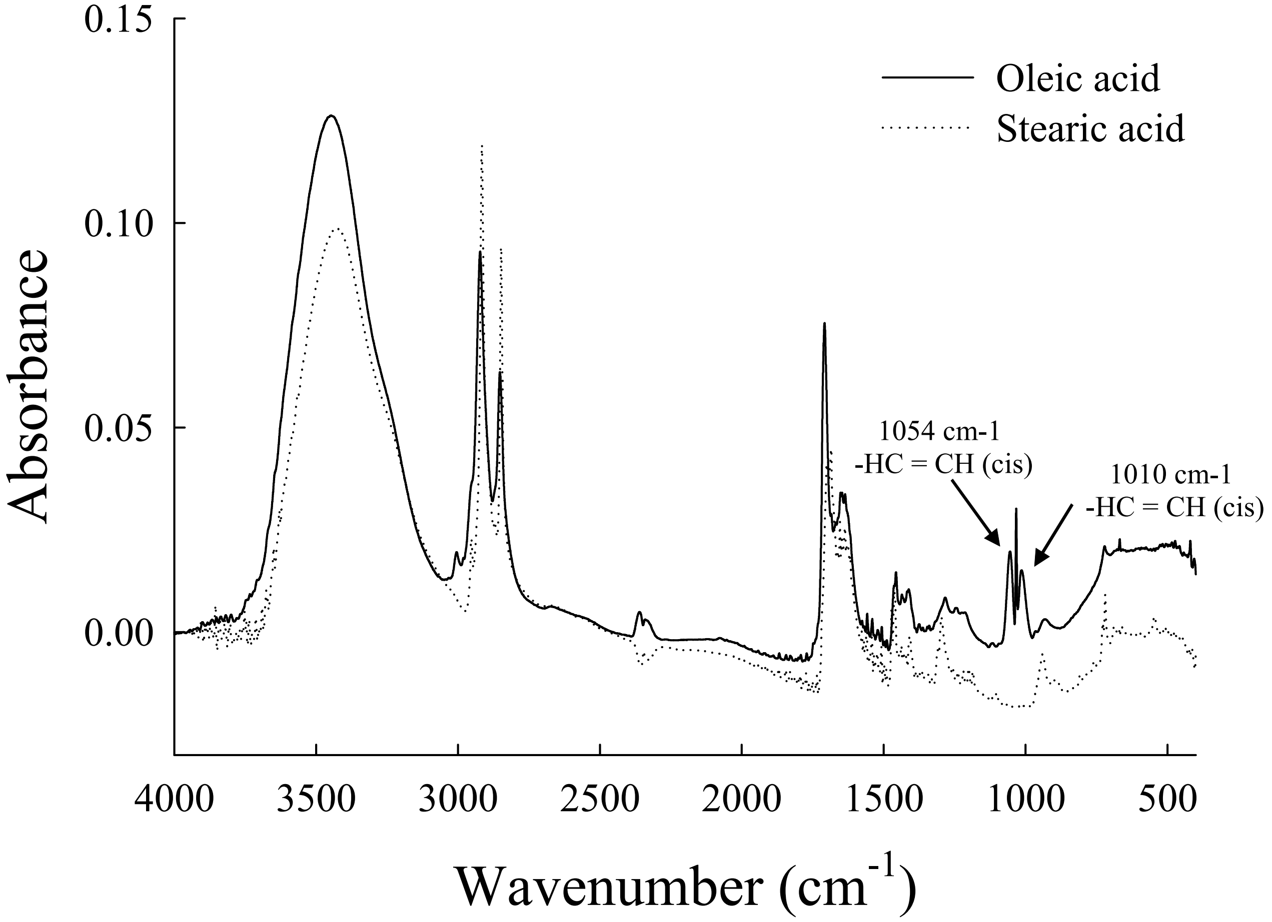


Fig. 4 Compare with saturated (stearic acid) and unsaturated (oleic acid) straight chain aliphatic acids.

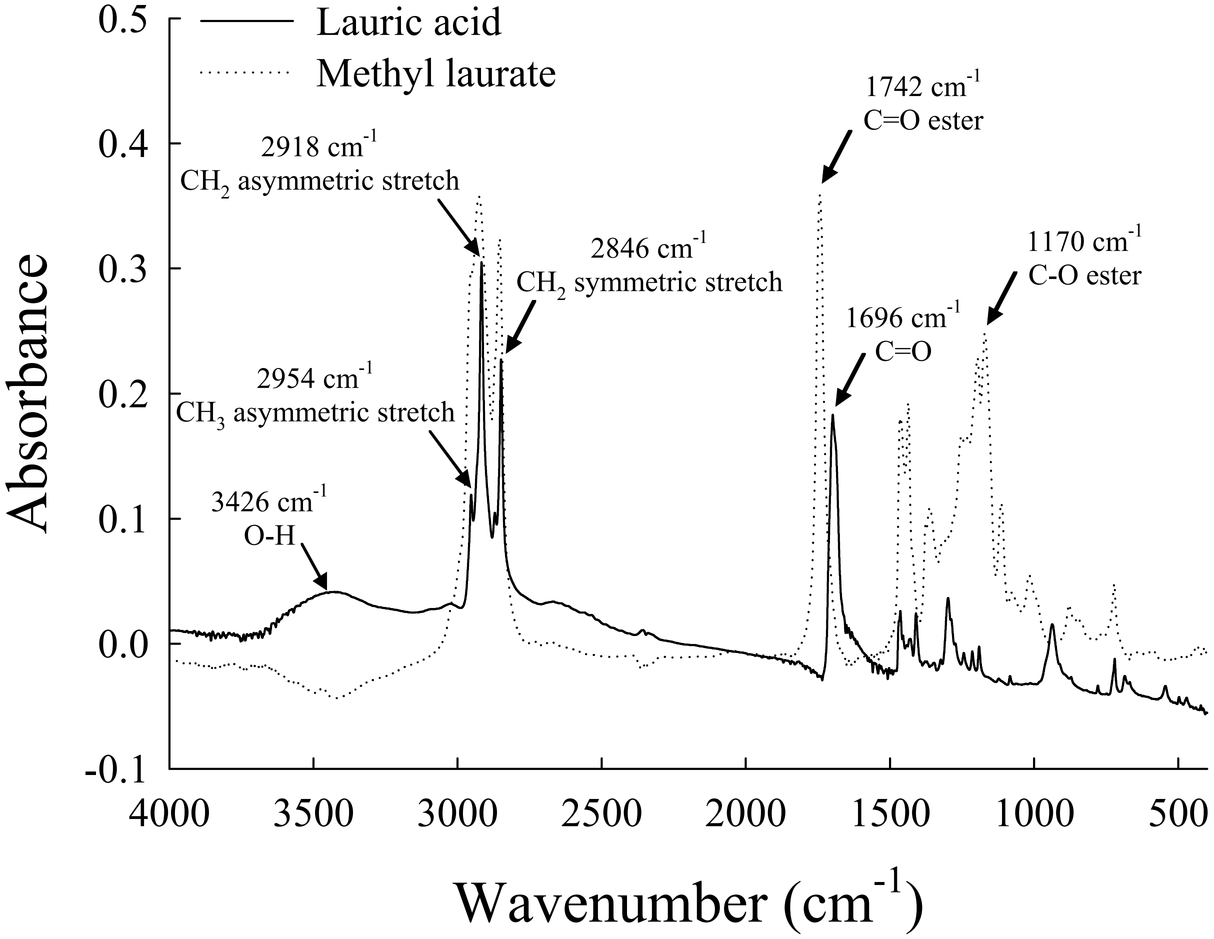
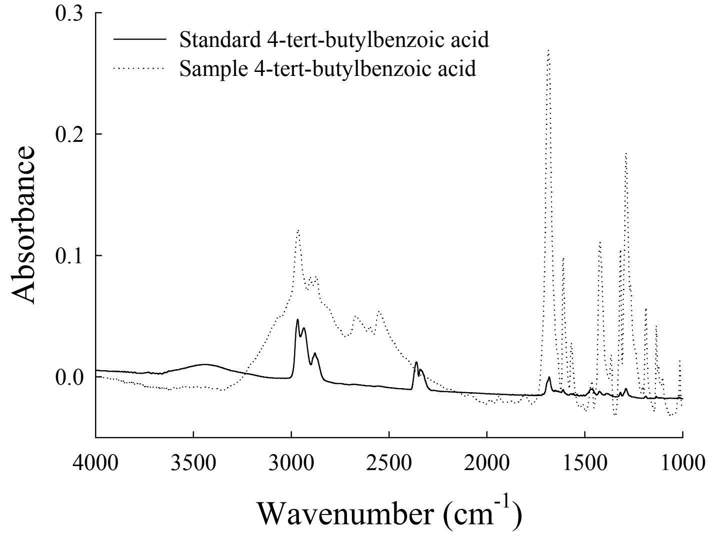
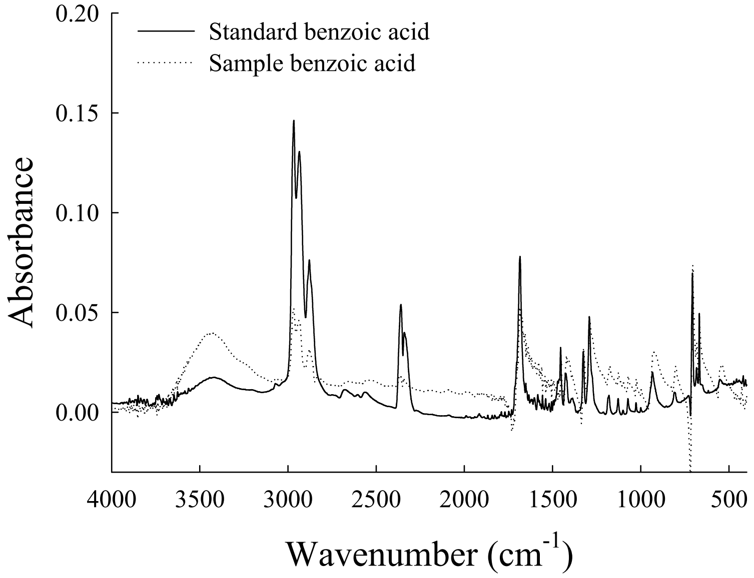


Fig 5 Compare with lauric acid and its methyl ester.

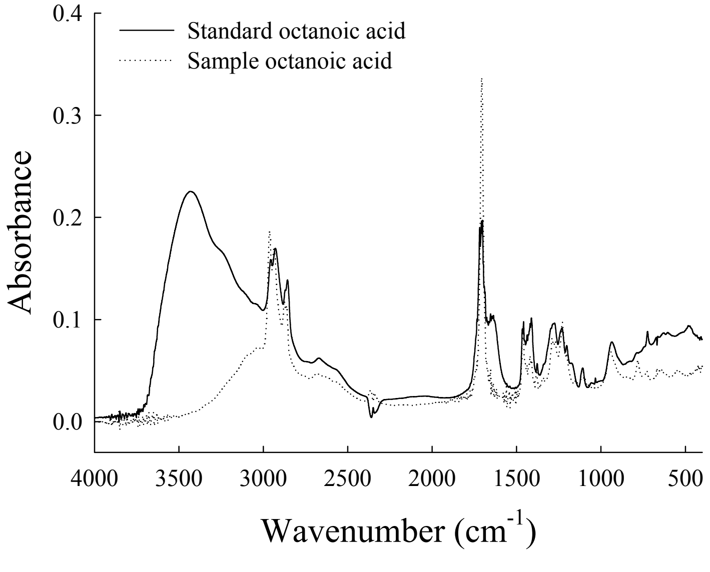
(A)



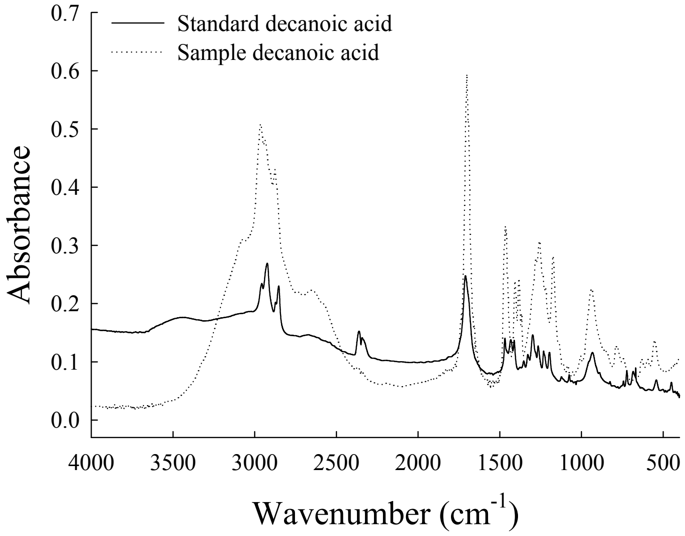
(B)


Standard benzoic acid
Sample benzoic acid
Absorbance
0.20
0.15
0.10
0.05
0.00
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm$^{-1}$)

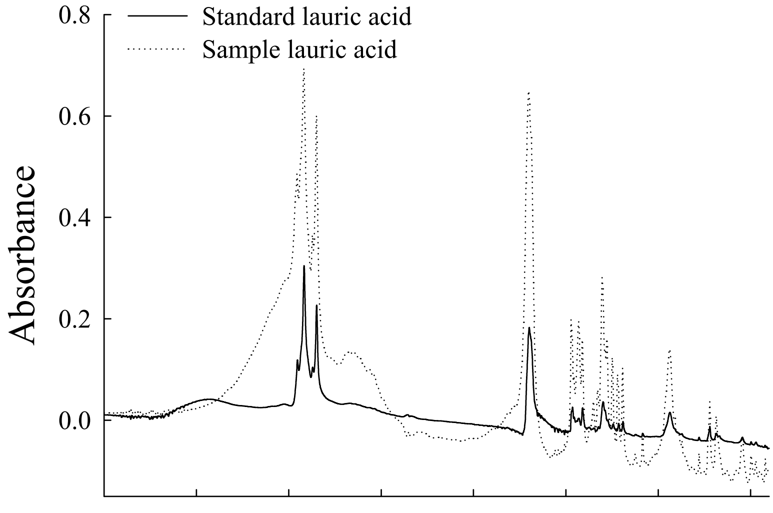
**(C)**


Standard octanoic acid
Sample octanoic acid
Absorbance
0.4
0.3
0.2
0.1
0.0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm$^{-1}$)

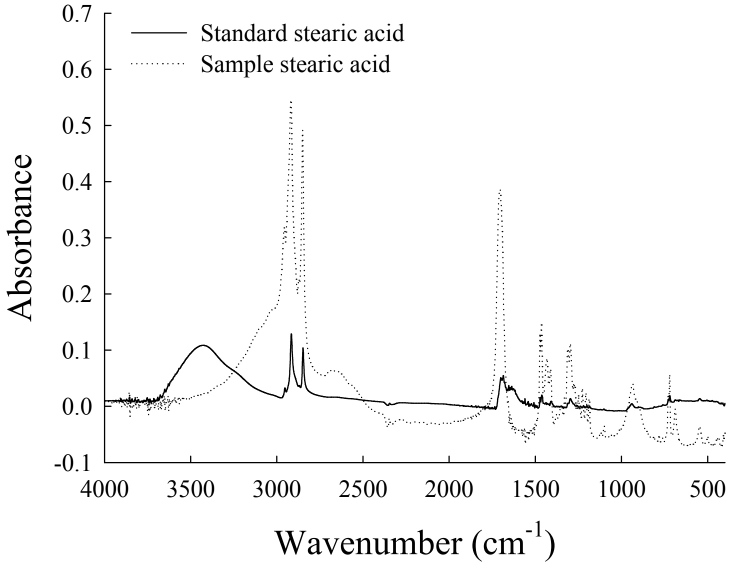
**(D)**


Standard decanoic acid
Sample decanoic acid
Absorbance
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

(E)


Standard lauric acid
Sample lauric acid
Absorbance
0.8
0.6
0.4
0.2
0.0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

(F)



(G)

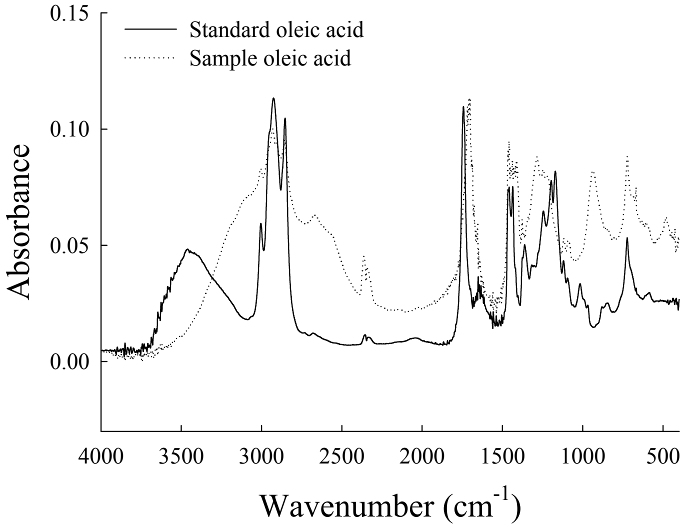


Fig. 6 FTIR spectra of commercial samples in comparison to standard fatty acids, (A) 4-tert- butylbenzoic acid; (B) benzoic acid; (C) octanoic acid; (D) decanoic acid; (E) lauric acid; (F) stearic acid; (G) oleic acid.

# 科技部補助計畫衍生研發成果推廣資料表

日期:2016/03/15

| | |
|---|---|
| 科技部補助計畫 | 計畫名稱: 快速測定安定劑中高級脂肪酸 |
| | 計畫主持人: 王來好 |
| | 計畫編號: 104-2622-M-041-001-CC2 學門領域: 分析化學 |

無研發成果推廣資料

# 104年度專題研究計畫研究成果彙整表

| | |
|---|---|
| **計畫主持人：**王來好 | **計畫編號：**104-2622-M-041-001-CC2 |
| **計畫名稱：**快速測定安定劑中高級脂肪酸 | |

| 成果項目 | | | 量化 | | | 單位 | 備註（質化說明：如數個計畫共同成果、成果列為該期刊之封面故事...等） |
|---|---|---|---|---|---|---|---|
| | | | 實際已達成數（被接受或已發表） | 預期總達成數（含實際已達成數） | 本計畫實際貢獻百分比 | | |
| 國內 | 論文著作 | 期刊論文 | 0 | 0 | 100% | 篇 | |
| | | 研究報告/技術報告 | 0 | 0 | 100% | | |
| | | 研討會論文 | 0 | 0 | 100% | | |
| | | 專書 | 0 | 0 | 100% | 章/本 | |
| | 專利 | 申請中件數 | 0 | 0 | 100% | 件 | |
| | | 已獲得件數 | 0 | 0 | 100% | | |
| | 技術移轉 | 件數 | 0 | 0 | 100% | 件 | |
| | | 權利金 | 0 | 0 | 100% | 千元 | |
| | 參與計畫人力（本國籍） | 碩士生 | 0 | 0 | 100% | 人次 | |
| | | 博士生 | 0 | 0 | 100% | | |
| | | 博士後研究員 | 0 | 0 | 100% | | |
| | | 專任助理 | 0 | 0 | 100% | | |
| 國外 | 論文著作 | 期刊論文 | 0 | 0 | 100% | 篇 | |
| | | 研究報告/技術報告 | 0 | 0 | 100% | | |
| | | 研討會論文 | 0 | 0 | 100% | | |
| | | 專書 | 0 | 0 | 100% | 章/本 | |
| | 專利 | 申請中件數 | 0 | 0 | 100% | 件 | |
| | | 已獲得件數 | 0 | 0 | 100% | | |
| | 技術移轉 | 件數 | 0 | 0 | 100% | 件 | |
| | | 權利金 | 0 | 0 | 100% | 千元 | |
| | 參與計畫人力（外國籍） | 碩士生 | 0 | 0 | 100% | 人次 | |
| | | 博士生 | 0 | 0 | 100% | | |
| | | 博士後研究員 | 0 | 0 | 100% | | |
| | | 專任助理 | 0 | 0 | 100% | | |
| 其他成果（無法以量化表達之成果如辦理學術活動、獲得獎項、重要國際合作、研究成果國際影響力及其他協助產業技術發展之具體效益事項等，請以文字敘述填列。） | 本計畫研究快速測定安定劑中高級脂肪酸，近一年經由科技部計畫之執行，已完成目標如下：<br>1. 利用紅外線光譜儀快速測定10種常使用脂肪酸包括:辛酸(Octanoic acid)、壬酸(Nonanoic acid)、癸酸(Decanoic acid)、月桂酸(Lauric acid)、肉豆蔻酸(Myristic acid)、棕櫚酸(Palmitic acid)、硬脂酸(Stearic acid)、苯甲酸(Benzoic acid)、對叔丁基苯甲酸(4-tert-butylbenzoicacid)與油酸(Oleic acid)。並合成其相對應之甲基酯類，建立10種的脂肪酸與其10種甲基脂肪酸酯類的指紋分析資料圖譜。比對資料圖譜得知市售脂肪酸原料之純度。合成脂肪酸酯類之圖譜有助於公司塑化劑的研發。 | | | | | | |

| | |
|---|---|
| | 2. 利用氣相層析儀同時測定10種合成的甲基脂肪酸酯類，並用高解析氣相層析質譜儀鑑定合成的酯類結構。建立10條甲基脂肪酸酯類之檢量線，用於實際樣品之純度測定。 |

| | **成果項目** | **量化** | **名稱或內容性質簡述** |
|---|---|---|---|
| **科教處計畫加填項目** | 測驗工具(含質性與量性) | 0 | |
| | 課程/模組 | 0 | |
| | 電腦及網路系統或工具 | 0 | |
| | 教材 | 0 | |
| | 舉辦之活動/競賽 | 0 | |
| | 研討會/工作坊 | 0 | |
| | 電子報、網站 | 0 | |
| | 計畫成果推廣之參與（閱聽）人數 | 0 | |

# 本產學合作計畫研發成果及績效達成情形自評表

| 成果項目 | | 本產學合作計畫預估研究成果及績效指標（作為本計畫後續管考之參據） | 計畫達成情形 |
|---|---|---|---|
| 技術移轉 | | 預計技轉授權 0 項 | 完成技轉授權 0 項 |
| 專利 | 國內 | 預估 0 件 | 提出申請 0 件，獲得 0 件 |
| | 國外 | 預估 0 件 | 提出申請 0 件，獲得 0 件 |
| 人才培育 | | 博士 0 人，畢業任職於業界 0 人 | 博士 0 人，畢業任職於業界 0 人 |
| | | 碩士 0 人，畢業任職於業界 0 人 | 碩士 0 人，畢業任職於業界 0 人 |
| | | 其他 0 人，畢業任職於業界 0 人 | 其他 0 人，畢業任職於業界 0 人 |
| 論文著作 | 國內 | 期刊論文 0 件 | 發表期刊論文 0 件 |
| | | 研討會論文 0 件 | 發表研討會論文 0 件 |
| | | SCI論文 0 件 | 發表SCI論文 0 件 |
| | | 專書 0 件 | 完成專書 0 件 |
| | | 技術報告 0 件 | 完成技術報告 0 件 |
| | 國外 | 期刊論文 0 件 | 發表期刊論文 0 件 |
| | | 學術論文 0 件 | 發表學術論文 0 件 |
| | | 研討會論文 0 件 | 發表研討會論文 0 件 |
| | | SCI/SSCI論文 0 件 | 發表SCI/SSCI論文 0 件 |
| | | 專書 0 件 | 完成專書 0 件 |
| | | 技術報告 0 件 | 完成技術報告 0 件 |
| 其他協助產業發展之具體績效 | | 新公司或衍生公司 0 家 | 設立新公司或衍生公司(名稱)： |
| 計畫產出成果簡述：請以文字敘述計畫非量化產出之技術應用具體效益。（限600字以內） | | 本計畫研究快速測定安定劑中高級脂肪酸，近一年經由科技部計畫之執行，已完成目標如下：<br>1. 利用紅外線光譜儀快速測定10種常使用脂肪酸包括:辛酸(Octanoic acid)、壬酸(Nonanoic acid)、癸酸(Decanoic acid)、月桂酸(Lauric acid)、肉豆蔻酸(Myristic acid)、棕櫚酸(Palmitic acid)、硬脂酸(Stearic acid)、苯甲酸(Benzoic acid)、對叔丁基苯甲酸(4-tert-butylbenzoicacid)與油酸(Oleic acid)。並合成其相對應之甲基酯類，建立10種的脂肪酸與其10種甲基脂肪酸酯類的指紋分析資料圖譜。比對資料圖譜得知市售脂肪酸原料之純度。合成脂肪酸酯類之圖譜有助於公司塑化劑的研發。<br>2. 利用氣相層析儀同時測定10種合成的甲基脂肪酸酯類，並用高解析氣相層析質譜儀鑑定合成的酯類結構。建立10條甲基脂肪酸酯類之檢量線，用於實際樣品之純度測定。 | |