application note

萨特勒红外谱库在中药成分解析中的应用

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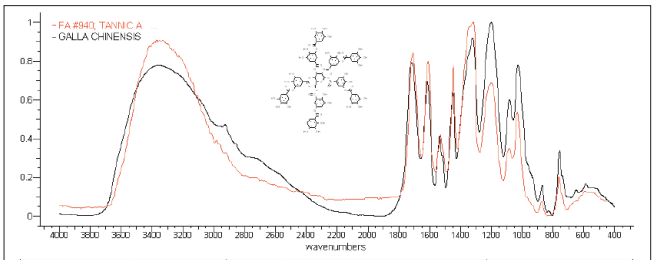
中药的研究是一个庞大复杂的体系，其分析研究与质量控制一直是科研和实践领域的重大难题。清华大学孙素琴教授著名地多年从事应用红外光谱技术解析中药。她在这方面的研究是领域里的“金标”；最近她出书《复杂混合物的红外光谱学：在食品的中药分析中的应用》[1]。下面是她友好地共享应用我公司25万多张萨特勒红外谱图对照一个个中药谱图的例子。图片中红色的谱图来自萨特勒标准谱库，黑色谱图是中药样品。

五倍子

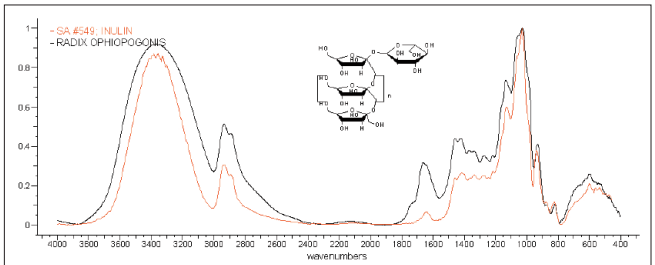
通过样品谱图和萨特勒谱库谱图对比，我们清楚地看到这一药品的主要成分是单宁。



Name	Value	Unit
Source of Sample	THE MATHESON COMPANY, INC., EAST RUTHERFORD, NEW JERSEY	
Melting Point	210-215C	
Flash Point	198C	
CAS Registry Number	1401-55-4	
Comments	Description= FAINT CHARACTERISTIC ODOR, ASTRINGENT TASTE Physical Description= YELLOWISH- WHITE TO LIGHT BROWN, AMORPHOUS, BULKY POWDER OR FLAKES, OR SPONGY MASSES	单宁
Synonyms	TANNIN GALLOTANNIN QUERCUS	
FEMA Number	3042	

麦冬

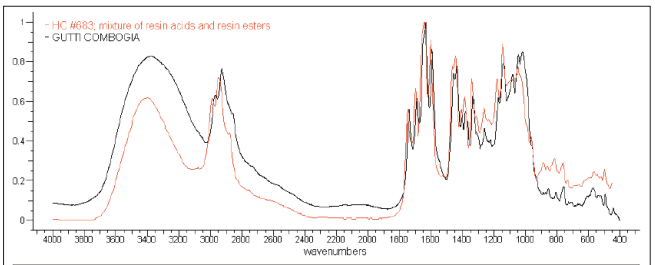
光谱对比显示麦冬主成分之一是菊粉。



Name	Value	Unit
Name	INULIN	
Source of Sample	FLUKA CHEMIE AG, BUCHS, SWITZERLAND	
Technique	KBr WAFER	
CAS Registry Number	9005-80-5	
Synonyms	INULIN, HYDRATE	
Formula		

藤黄

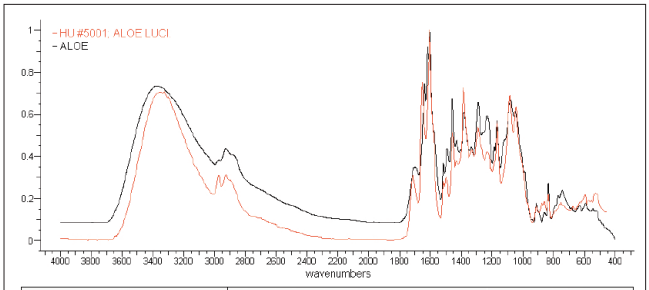
下面这个例子是藤黄光谱和产于斯里兰卡、泰国、柬埔寨的藤黄光谱对比。



Name	Value	Unit
Name	mixture of resin acids and resin esters	
Source of Sample	from Garcinia morella (Sri Lanka, Thailand, Cambodia)	藤黄
Technique	KBr pellet	
Comments	HUMMEL DECIMAL NUMBER= 141(+)412 Description= APPEARANCE=red brown resin	
Synonyms	gambogi	

芦荟

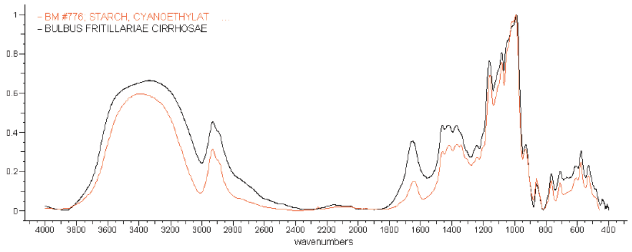
芦荟样品被这种方法鉴定。



Name	Value	Unit
Source of Sample	DRIED SAP FROM THE LEAVES OF SOME ALOE SPECIES	
Technique	FILM (CAST FROM ETHANOL)Spectrometer Recording Technique=DIGILAB FTS13C	
Comments	HUMMEL/SCHOLL "INFRARED ANALYSIS OF POLYMERS, RESINS AND ADDITIVES, AN ATLAS" VOLUME 1 (1969), SPECTRUM #682 Composition=MIXTURE OF POLYSACCHARIDES, RESIN ACIDS AND AROMATIC ALIPHATIC COMPOUNDS (ALOIN) Description=NATURAL PRODUCT Description=CARBOHYDRATE	
Source of Spectrum	SADTLER (SAMPLE AND PROPERTIES PROVIDED BY PROFESSOR DOCTOR DIETER O. HUMMEL)	

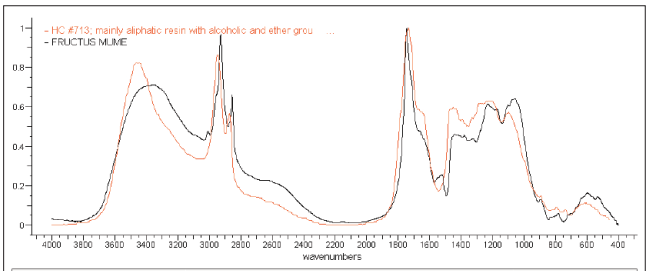
BIO-RAD

川贝



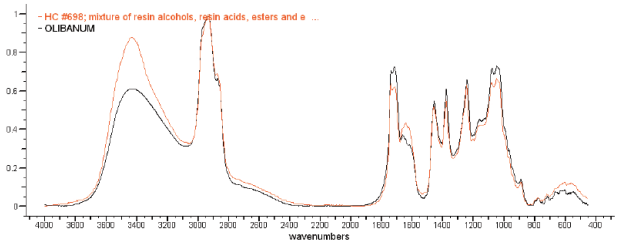
Name	Value	Unit
Name	STARCH, CYANOETHYLATED	
Source of Sample	POLYSCIENCES, INC., WARRINGTON, PENNSYLVANIA	
Technique	KBr WAFER	
Comments	Chemical Description= CYANOETHYLATED STARCH	
Synonyms	STARCH, CYANOETHYL ETHER	
Classification	MISCELLANEOUS CARBOHYDRATE DERIVATIVES	

乌梅



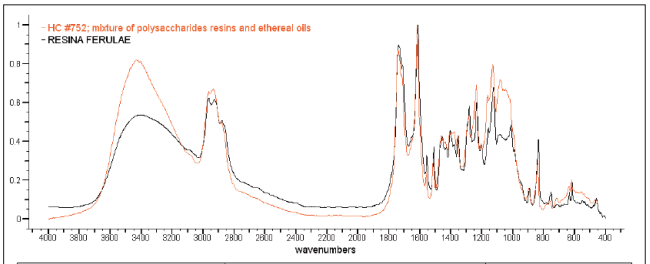
Name	Value	Unit
Name	mainly aliphatic resin with alcoholic and ether groups	
Source of Sample	A. BURMESTER, TU BERLIN	
Technique	finely shaved substance in KBr	
Comments	HUMMEL DECIMAL NUMBER= 1416Description= APPEARANCE=brown lacquer fragments	
Synonyms	Japanese lacquer (Japan black, pre-1850)	

乳香



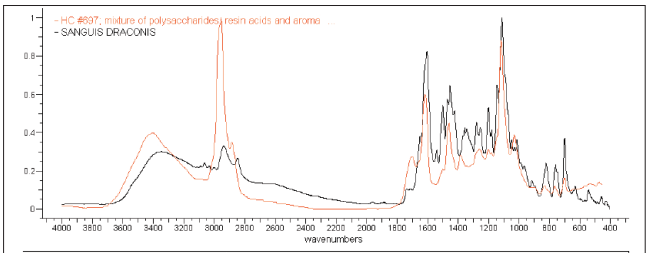
Name	Value	Unit
Name	mixture of resin alcohols, resin acids, esters and ethereal oils	
Source of Sample	sap from Burseraceae (Eritrea)	
Technique	KBr pellet	
Comments	HUMMEL DECIMAL NUMBER= 1415+1411 H2O sublimate(s)Description= APPEARANCE=ochre-colored, opaque resin	
Synonyms	olibanum	

阿魏



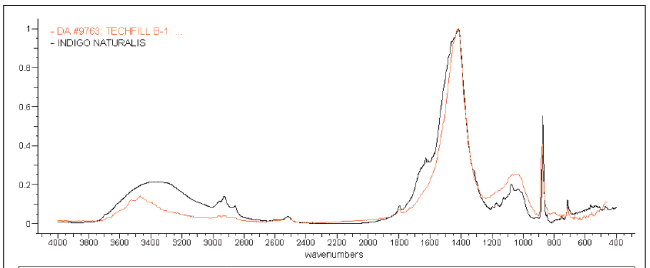
Name	Value	Unit
Name	mixture of polysaccharides resins and ethereal oils	
Source of Sample	dried Ferula resin sap	
Technique	KBr pellet	
Comments	HUMMEL DECIMAL NUMBER= 1432 Description= APPEARANCE=dirty- brown resin	
Synonyms	galbanum	

血竭



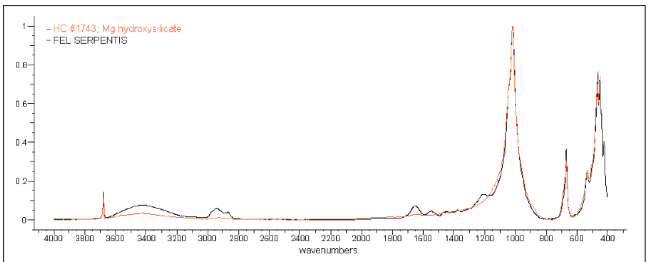
Name	Value	Unit
Name	mixture of polysaccharides, resin acids and aromatic bodies	
Source of Sample	from the fruit of the palm Calamus draco (Southeast India), from C.E. Roeger	
Technique	KBr pellet	
Comments	HUMMEL DECIMAL NUMBER= 1413+1411Description= APPEARANCE=dark red-brown resin	
Synonyms	dragon's blood	

青黛



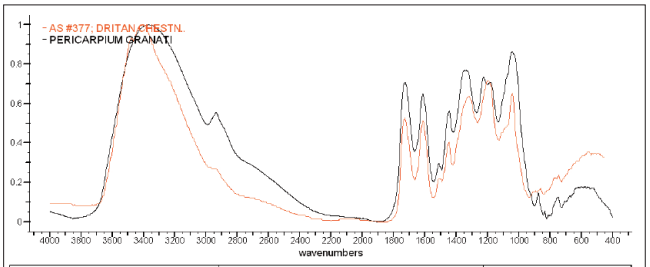
Name	Value	Unit
Name	TECHFILL B-105	
Source of Sample	GREAT LAKES MINERALS COMPANY	
Technique	KBr WAFER	
Density	(Specific Gravity)= 0.95-1.0	
Comments	Chemical Description= LIGHTWEIGHT CALCIUM CARBONATE	
Classification	MONOMERS - MISCELLANEOUS MONOMERS	

蛇胆汁



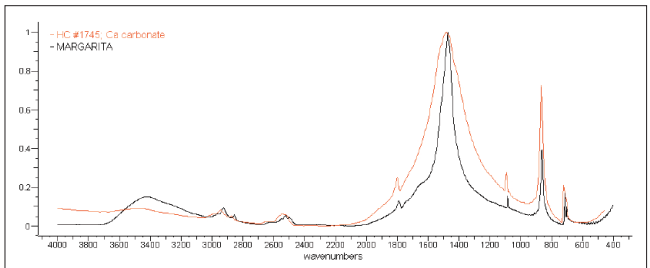
Name	Value	Unit
Name	Mg hydroxysilicate	
Source of Sample	Merck	
Technique	KBr pellet	
Formula	$MgSiO_3(OH)_2H_2O$	
Comments	HUMMEL DECIMAL NUMBER= 19172Description= APPEARANCE=colorless solid	
Synonyms	talc	

石榴皮



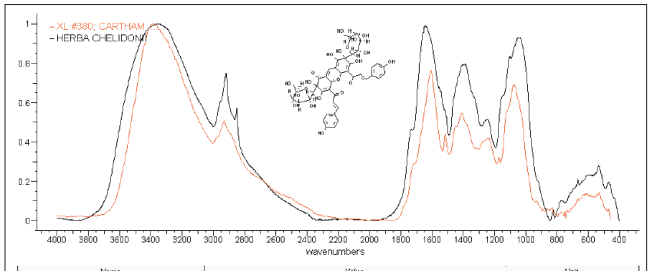
Name	Value	Unit
Name	DRITAN CHESTNUT	
Source of Sample	RICHARD HODGSON & SONS,LTD., ENGLAND	
Technique	KBr WAFER	

珍珠



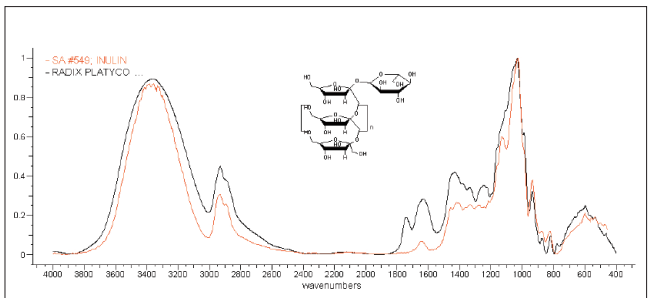
Name	Value	Unit
Name	Ca carbonate	
Source of Sample	collector's find	
Technique	KBr pellet	
Formula	CaCO3	
Comments	HUMMEL DECIMAL NUMBER=-19122Description= APPEARANCE=colorless crystals	
Synonyms	Aragonite	

白屈菜



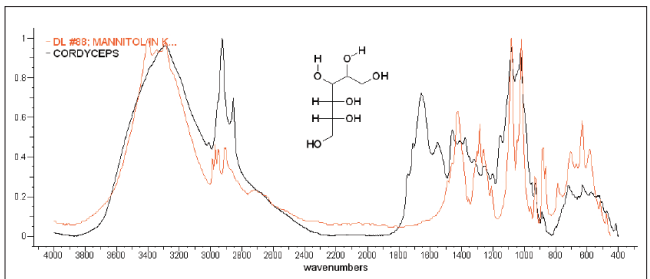
Name	Value	Unit
Name	CARTHAMIN	
Source of Sample	TOKYO KASEI KOGYO COMPANY, LTD., TOKYO, JAPAN	
Technique	KBr WAFER	
Mol Weight	818.83	
CAS Registry Number	36338-96-2	
Formula	C29H32O21	
Comments	Chemical Description= NATURAL, 5,6-DIHYDROXY- 6-(beta-D-GLUCOPYRANOSYL)- 2-[[3-(beta-D-GLUCOPYRANOSYL)- 5-(p-	
Use	RED DYE FOR SILK AND COTTON	
Synonyms	5,6-DIHYDROXY- 6-(beta-D-GLUCOPYRANOSYL)- 2-[[3-(beta-D-GLUCOPYRANOSYL)- 5-(p-HYDROXYCINNAMOYL)- 6-OXO-2,3,4-TRIHYDROXY- 1,4-CYCLOHEXADIEN- 1-YLMETHYLENE]- 4-(p-	
Color Properties	Color and Crystallization= DARK RED POWDER WITH GREEN LUSTER Colour Index Name= NATURAL RED 26Colour Index Number= 75140	
Classification	Dyes NATURAL	

桔梗



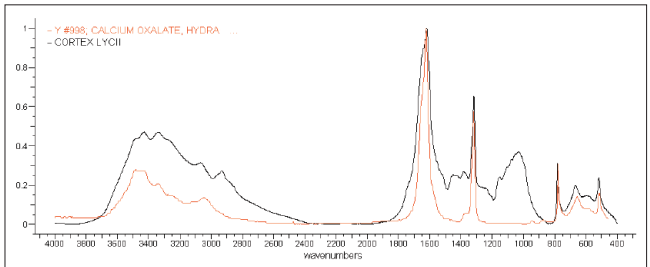
Name	Value	Unit
Name	INULIN	
Source of Sample	FLUKA CHEMIE AG, BUCHS, SWITZERLAND	
Technique	KBr WAFER	
CAS Registry Number	9005-80-5	
Synonyms	INULIN, HYDRATE	
Formula		

冬虫夏草



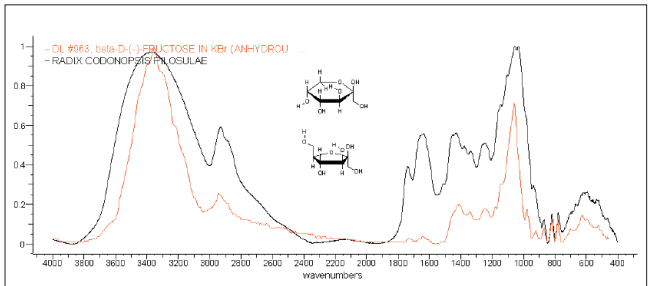
Name	Value	Unit
Name	MANNITOL IN KBr	
Technique	KBr PELLETS	
Mol Weight	182.17 (182.08)	
Formula	C6H14O6	
Use	DIURETIC	
Synonyms	D- MANNITOL MANNITEMANNA SUGARTrade Name= MANICOL, MANNIDEX, DIOSMOL, OSMITROL, OSMOSAL	

地骨皮（用一级微分的方法）



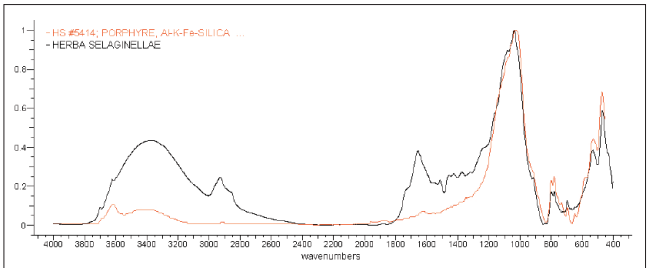
Name	Value	Unit
Name	CALCIUM OXALATE, HYDRATE	
Source of Sample	THE MATHESON COMPANY, INC., EAST RUTHERFORD, NEW JERSEY	
Technique	KBr WAFER	
Mol Weight	146.12	
Formula	C2H2O5C5	
Comments	Chemical Description= CALCIUM OXALATE, HYDRATE	

党参



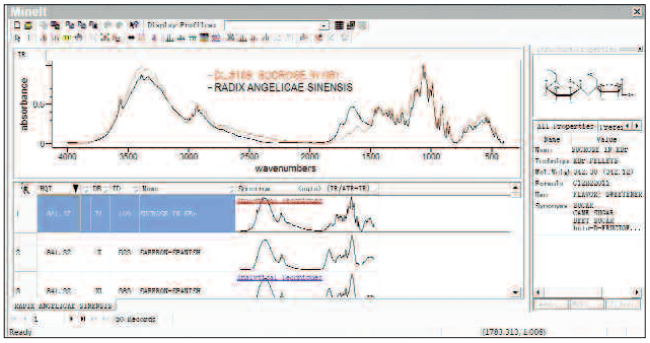
Name	Value	Unit
Name	beta-D-(-)-FRUCTOSE IN KBr (ANHYDROUS)	
Technique	KBr PELLETS	
Mol Weight	180.16 (180.06)	
Formula	C6H12O6	
Use	SUGAR	
Synonyms	D- FRUCTOSE beta-D- FRUCTOSE LEVULOSE FRUIT	

卷柏

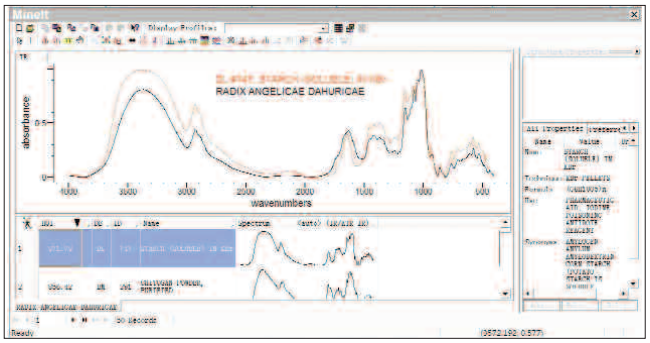


Name	Value	Unit
Name	PORPHYRE, Al-K-Fe-SILICATE	
Source of Sample	LEON	
Technique	KBr (2/1000)	
Comments	Description= FILLER - CLAY MINERAL, MICA	
Source of Spectrum	SCHOLL	
Synonyms	Trade Name= PORPHYR	
Classification	Scholl= INORGANIC FILLERS AND PIGMENTS	

当归



白芷



由这些例子看到，萨特勒红外谱库适用于中药化学成分的鉴定、确认或归类。

参考书籍

1. 孙素琴，周群，陈建波，著。《复杂混合物的红外光谱学：在食品和中药分析中的应用》第一版。李晓红，任慧敏,编辑。化学工业出版社：北京，中国，2011。

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