CUMCM-2021 Problem E

Identification of Traditional Chinese Medicine

The spectral characteristics of different traditional Chinese medicine are quite different. Even the same medicinal material from different origins will show different spectra under the irradiation of near-infrared and mid-infrared spectra due to the differences in the chemical composition of inorganic elements and organic substances. These features can be used to identify the types and origins of traditional Chinese medicines.

It is relatively easy to identify the types of traditional Chinese medicine, and the differences in the spectra between different types of medicines are obvious. Fig.1 is the mid-infrared spectroscopy data of two different medicinal materials. It is easy to see that the difference between them is quite large.

The authenticity of traditional Chinese medicine is mainly indicated by its original place of production, and the identification of the original place of production is particularly important for the quality control of medicine. However, the spectra of the same type of medicine from different origins are relatively close, which makes the identification of the original place quite difficult. In addition, some traditional Chinese medicines have obvious near-infrared differences, while other medicines have more obvious mid-infrared differences (see Fig.2 and Fig.3 for the near-infrared and mid-infrared spectral data curves of a certain type of medicine from 5 different origins). When the samples are not sufficient, we can comprehensively identify the origins of traditional Chinese medicines by combining both near-infrared and mid-infrared spectral data.

Appendix 1 to 4 are the near-infrared or mid-infrared spectroscopy data of some traditional Chinese medicines. The “No” column is the order of the medicines, the “Class” column indicates the types of traditional Chinese medicines, the “OP” column indicates the original place of the medicines, and the first row of the remaining columns is the wavenumber of the spectrum with unit of cm^{-1}. The data after the second line represents the absorbance of the medicines in the corresponding band under the spectrum irradiation (Note: the absorbance is the value after a certain correction, therefore negative values are possible). Please build mathematical models to solve the following problems.

Problem 1. Based on the mid-infrared spectroscopy data of several traditional Chinese medicine in Appendix 1, study the characteristics and differences of different types of medicines, and identify the types of medicines.

Problem 2. Based on the mid-infrared spectroscopy data of a certain type of medicine in Appendix 2, analyze the characteristics and differences of medicines from different origins, try to identify the origins of medicines, and fill in the corresponding identification results into the following table.

No	3	14	38	48	58	71	79	86	89	110	134	152	227	331	618
OP															

Problem 3. Based on the near-infrared and mid-infrared data of a certain type of traditional Chinese medicine in Appendix 3, try to identify the origins of the medicines, and fill in the corresponding identification results into the table below.

No	4	15	22	30	34	45	74	114	170	209
OP										

Problem 4. Appendix 4 gives the near-infrared spectroscopy data of several traditional Chinese medicines. Try to identify the types and origins of medicines, and fill in the corresponding identification results into the table.

No	94	109	140	278	308	330	347
Class							
OP							

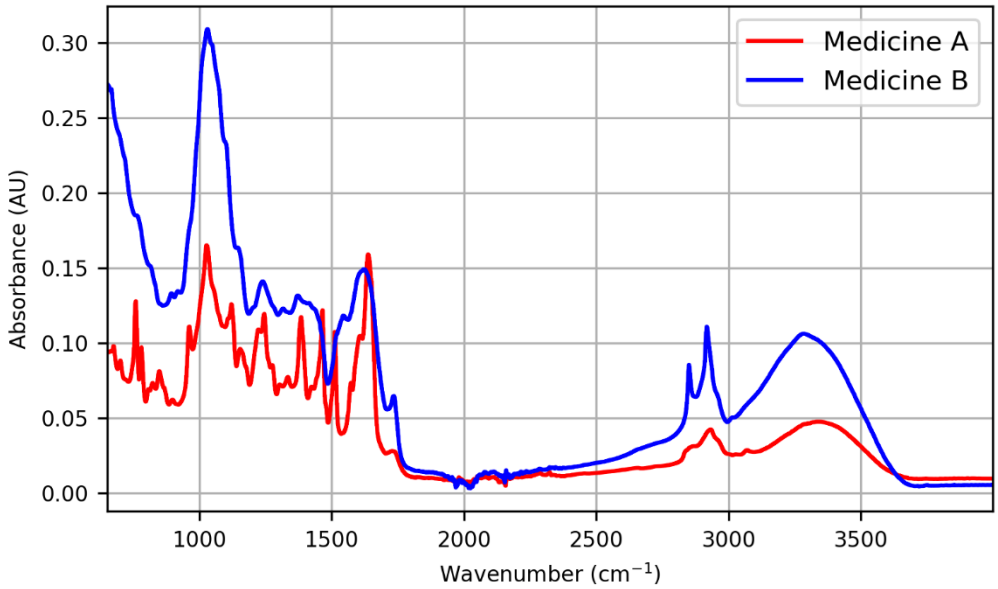

Fig.1 Mid-infrared spectroscopy curves of two different traditional Chinese medicines

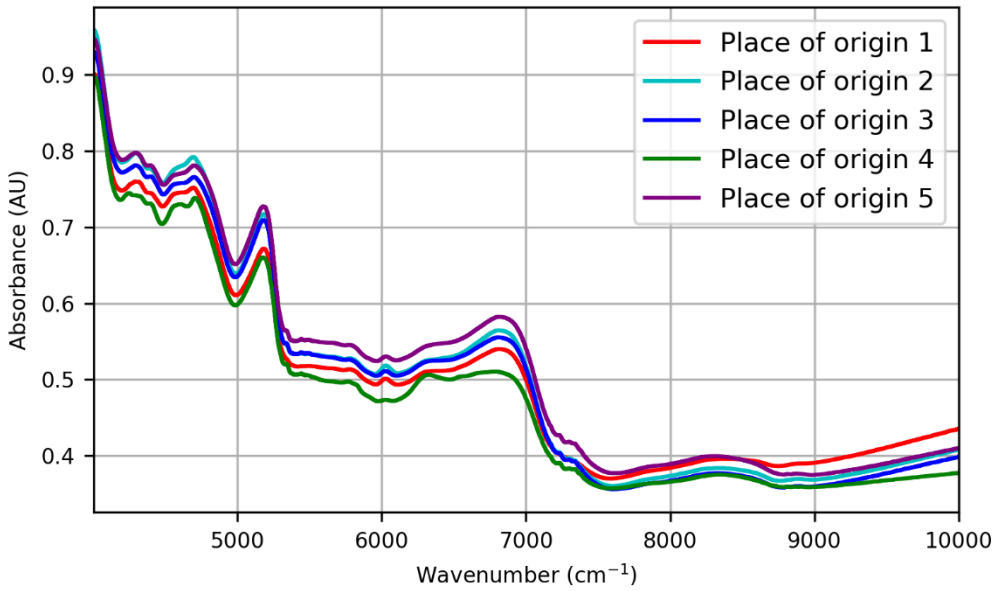

Fig.2 Near-infrared spectra of a certain type of traditional Chinese medicine from different origins

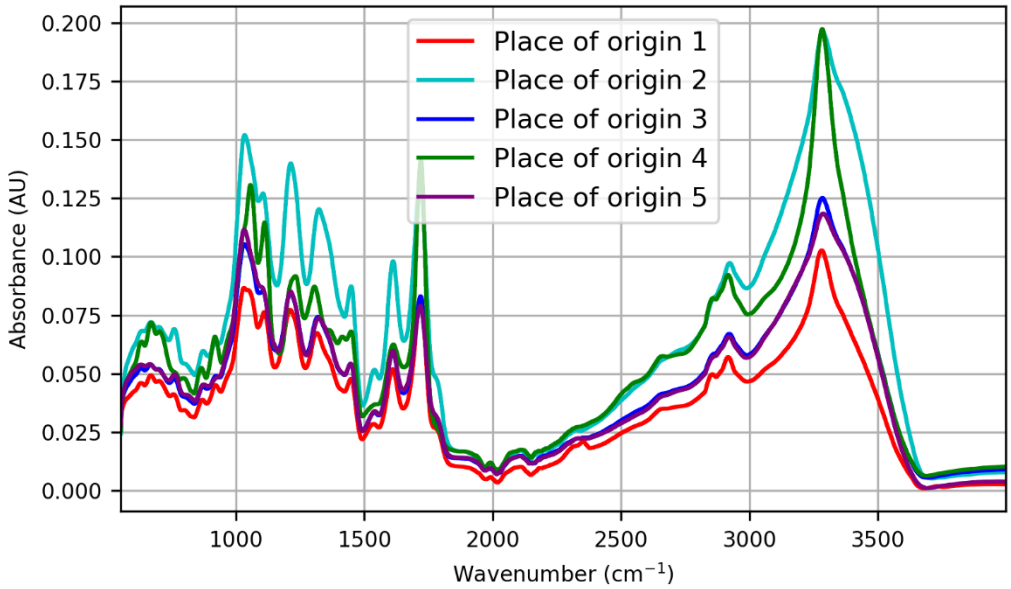

Fig.3 Mid-infrared spectra of a certain type of raditional Chinese medicine from different origins

Note 1. For information on authentic medicines, please refer to Baidu Encyclopedia (https://baike.baidu.com/item/%E9%81%93%E5%9C%B0%E8%8D%AF%E6%9D%90/1950482?fr=aladdin).

Note 2. For information on infrared spectroscopy analysis, please refer to Baidu Encyclopedia (https://baike.baidu.com/item/%E7%BA%A2%E5%A4%96%E5%85%89%E8%B0%B1%E5%88%86%E6%9E%90).