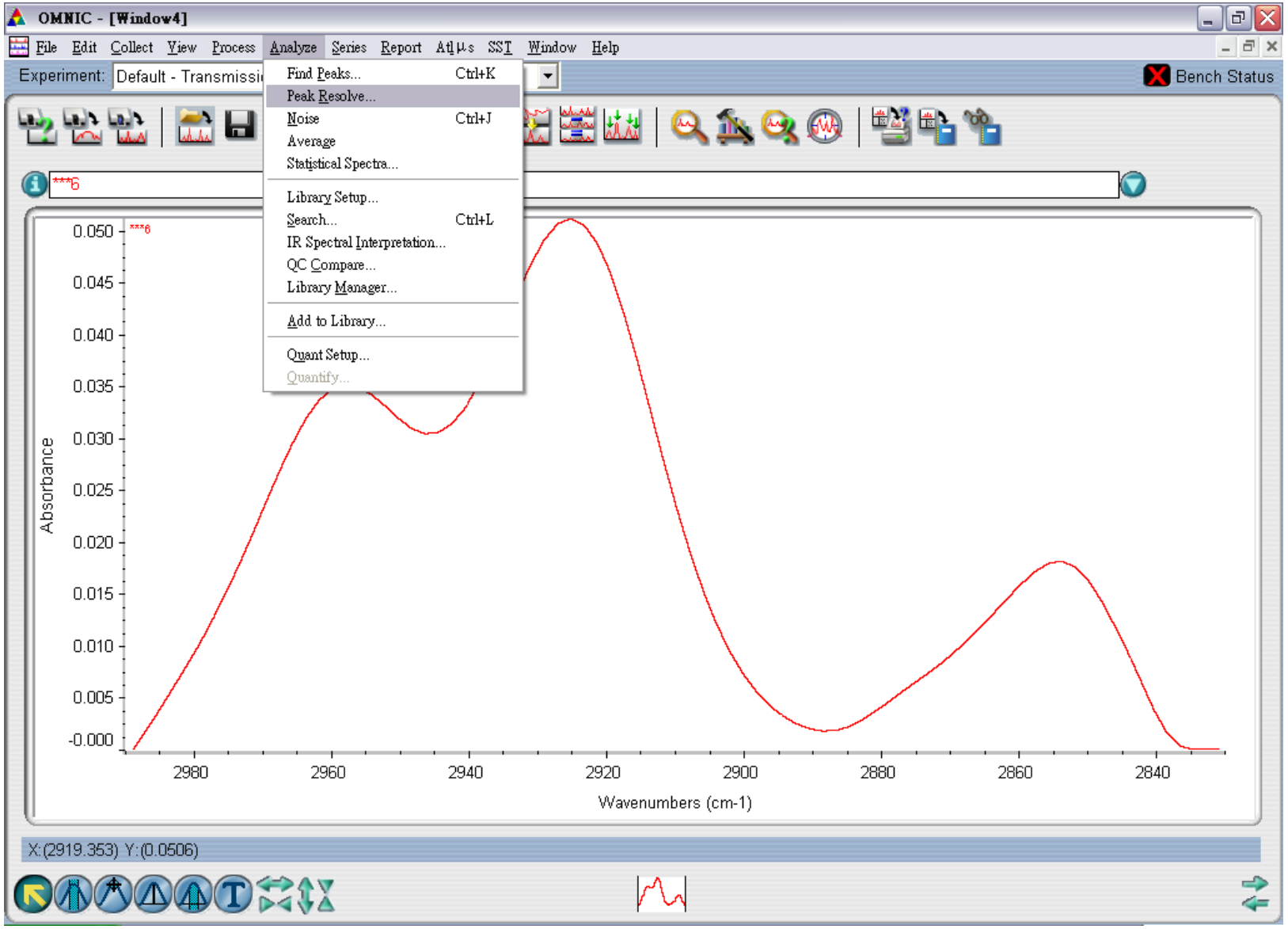
Curve Fitting in IR Spectroscopy

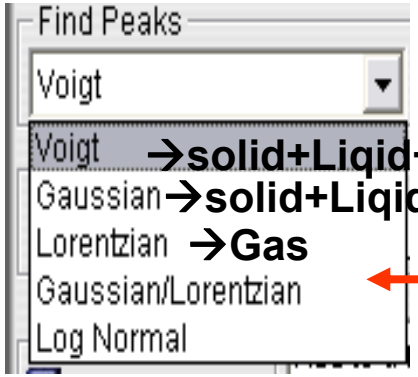
-Peak resolve in OMNIC software

TLS 14A1 IR Microspectroscopy ES

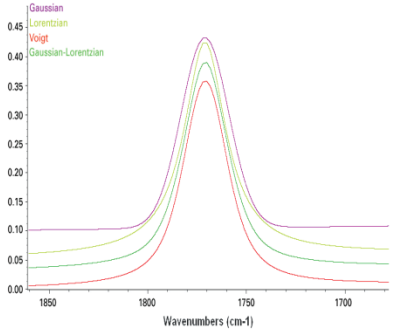
Truncate data set in the spectra range 2800-3000 cm^{-1} using peak resolve to analysis spectra



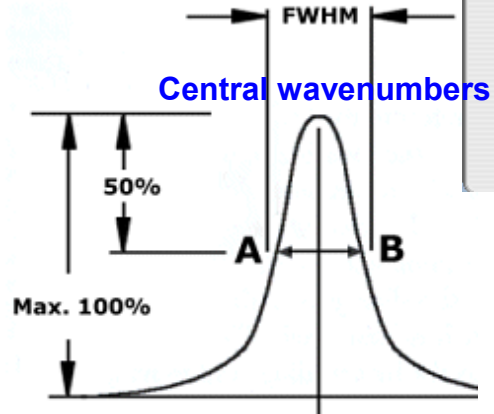
Set up Peak Resolve method→ Find Peaks→ Fit peaks

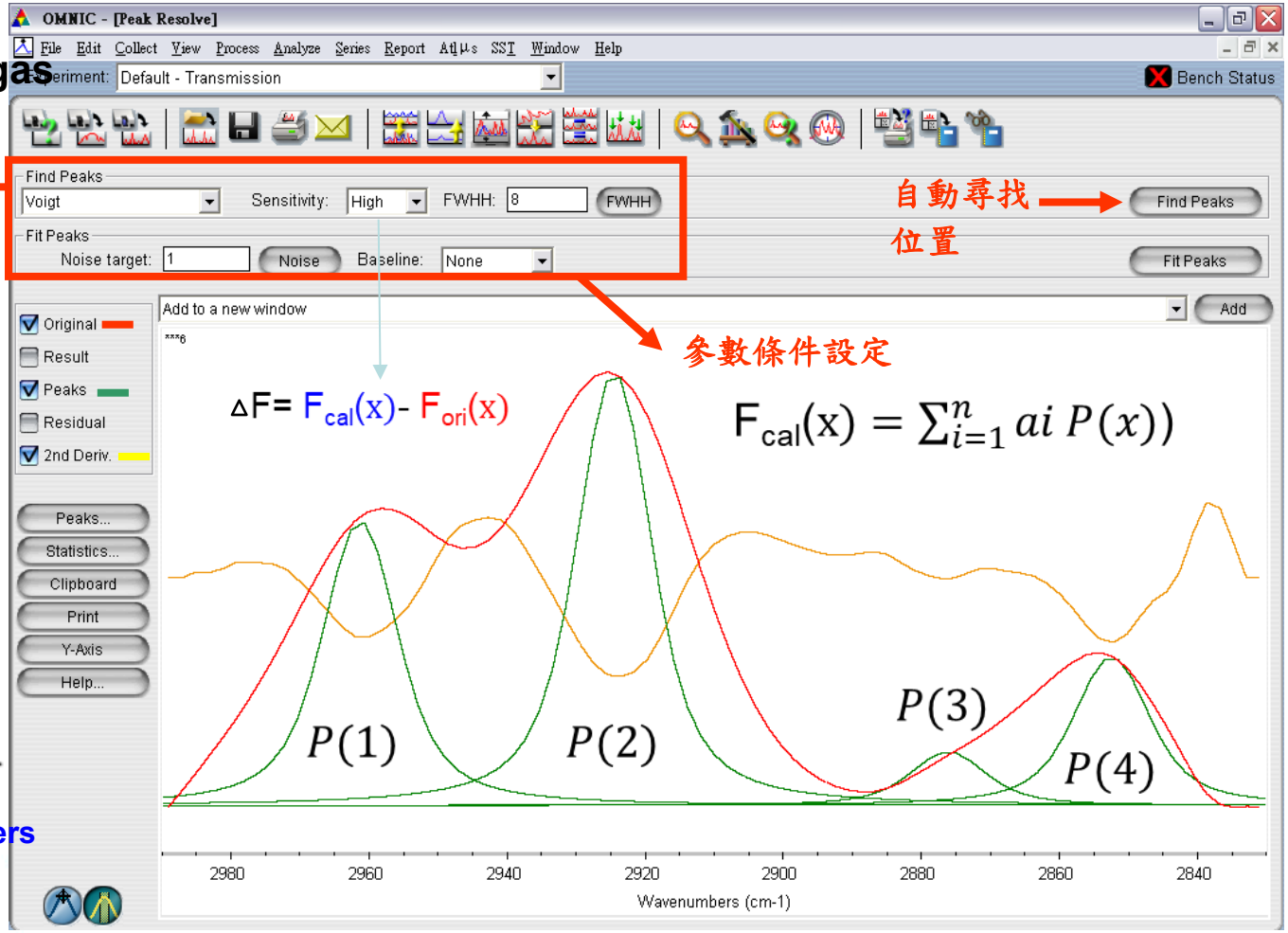


Fit method



Full width at half maximum

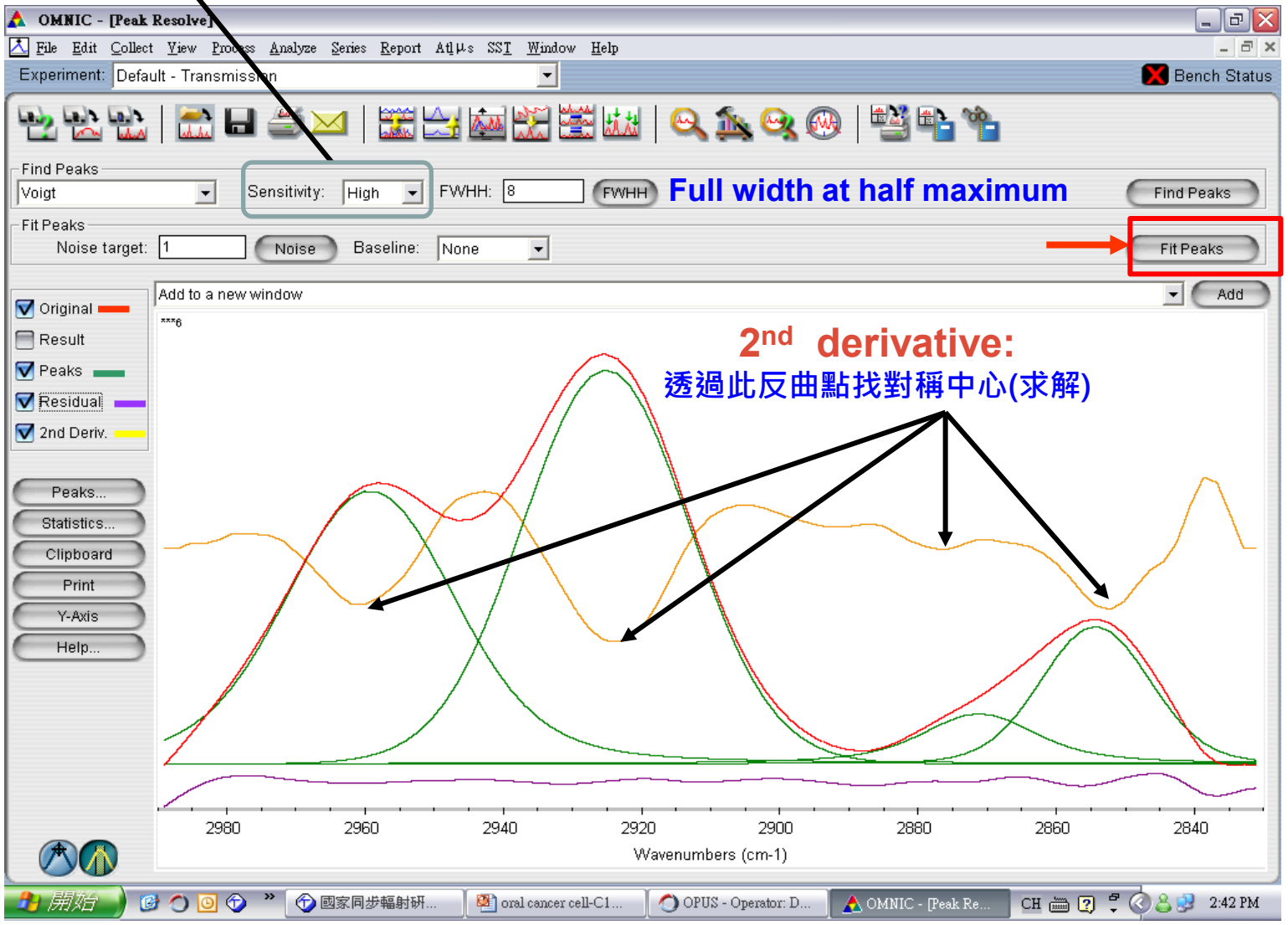




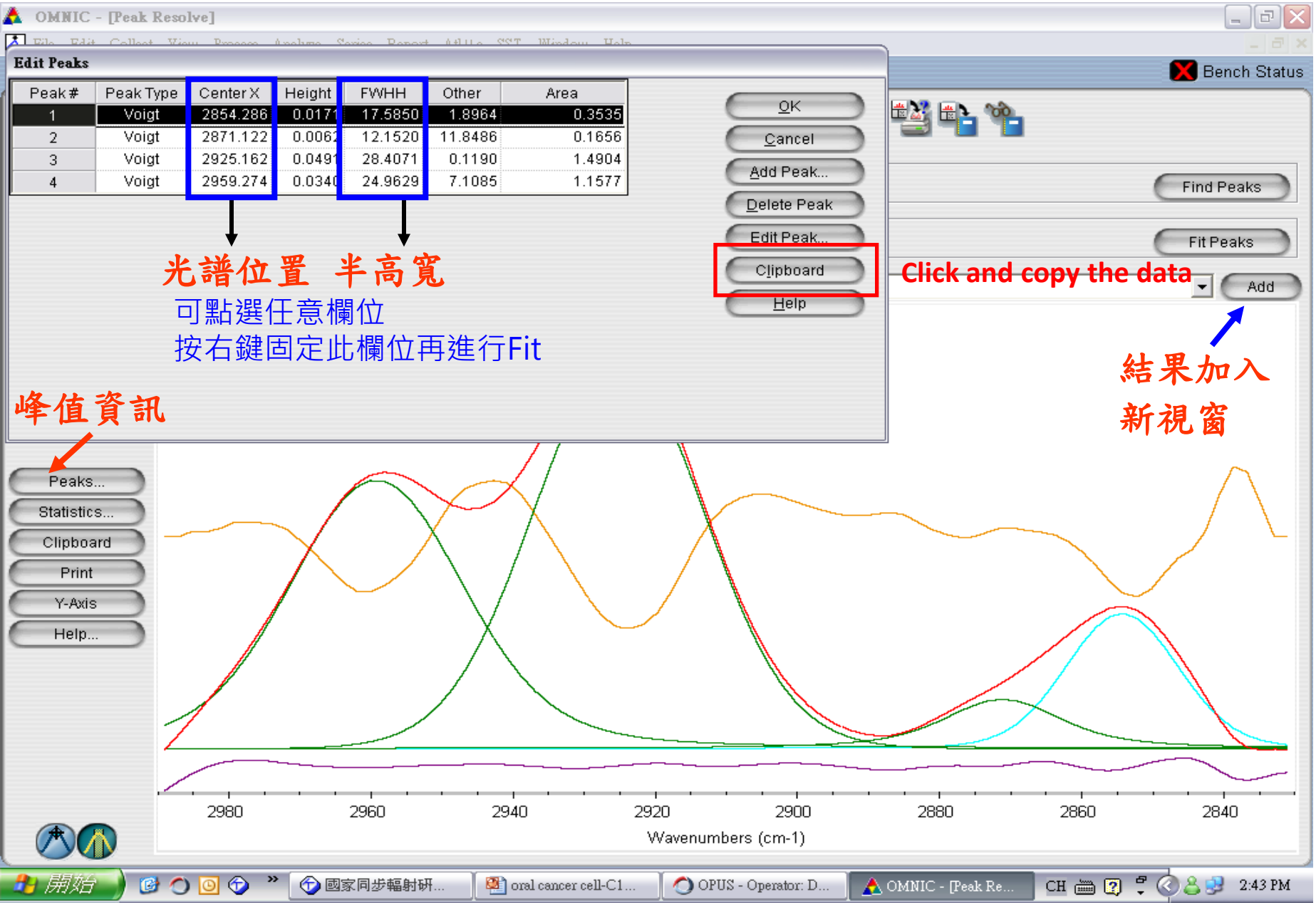
Sensitivity	Polynomial Order
Low	3
Medium	5
High	6

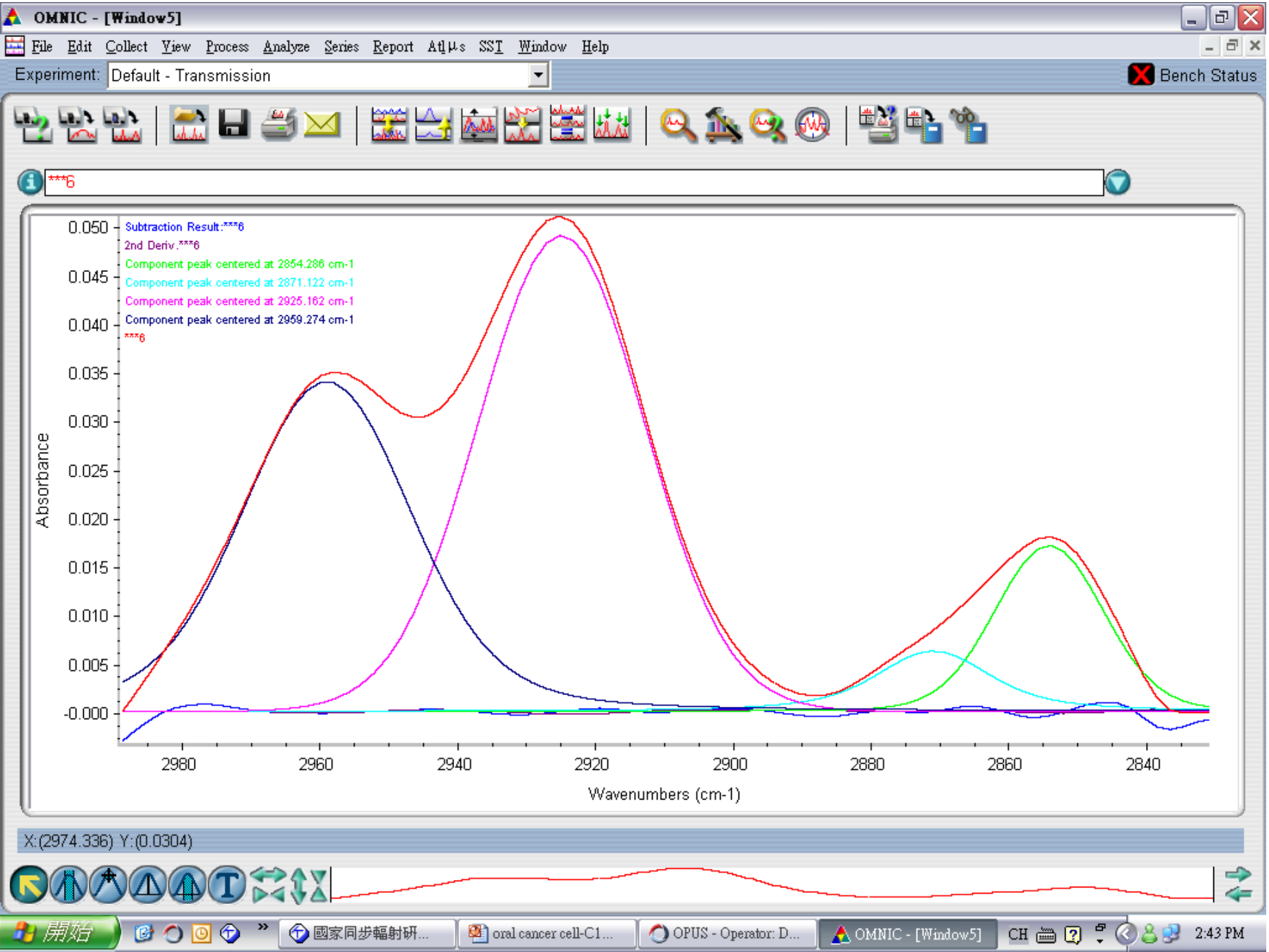
Result of Fit peak

$\Delta F = F_{cal}(x) - F_{ori}(x)$ Sensitivity愈高，兩函數差愈小，Fit程度也愈好



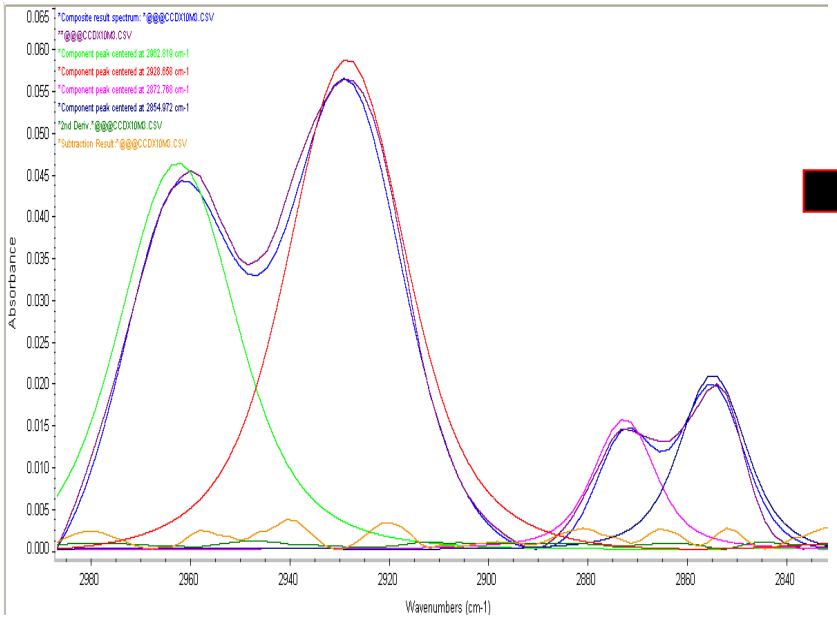
Information of peaks



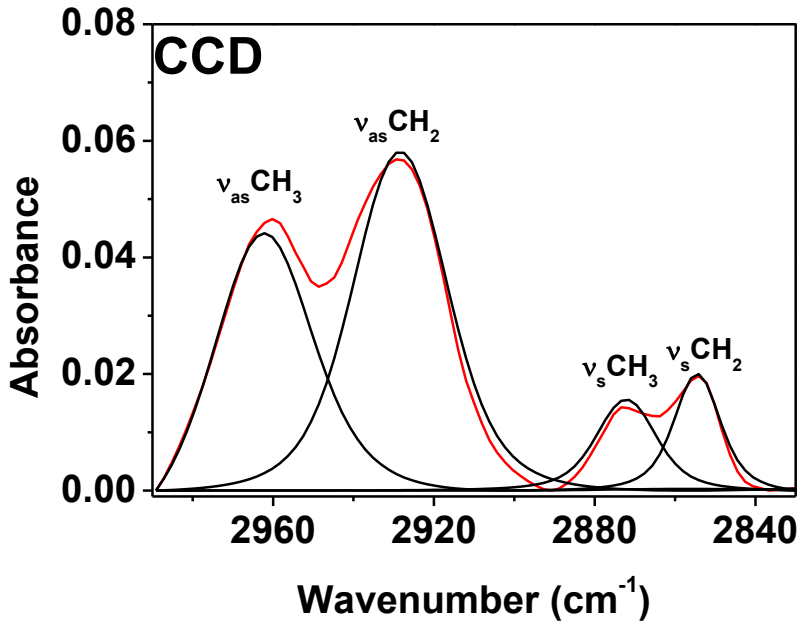

OMNIC - [Window5]
File Edit Collect View Process Analyze Series Report Atl μs SST Window Help
Experiment: Default - Transmission
Bench Status
***6
Subtraction Result:***6
2nd Deriv.***6
Component peak centered at 2854.286 cm-1
Component peak centered at 2871.122 cm-1
Component peak centered at 2925.162 cm-1
Component peak centered at 2959.274 cm-1
***6
0.050
0.045
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
-0.000
Absorbance
2980
2960
2940
2920
2900
2880
2860
2840
Wavenumbers (cm-1)
X:(2974.336) Y:(0.0304)
開始
國家同步輻射研...
oral cancer cell-C1...
OPUS - Operator: D...
OMNIC - [Window5]
CH
2:43 PM

Data plot by Origin software

Display in OMNIC window



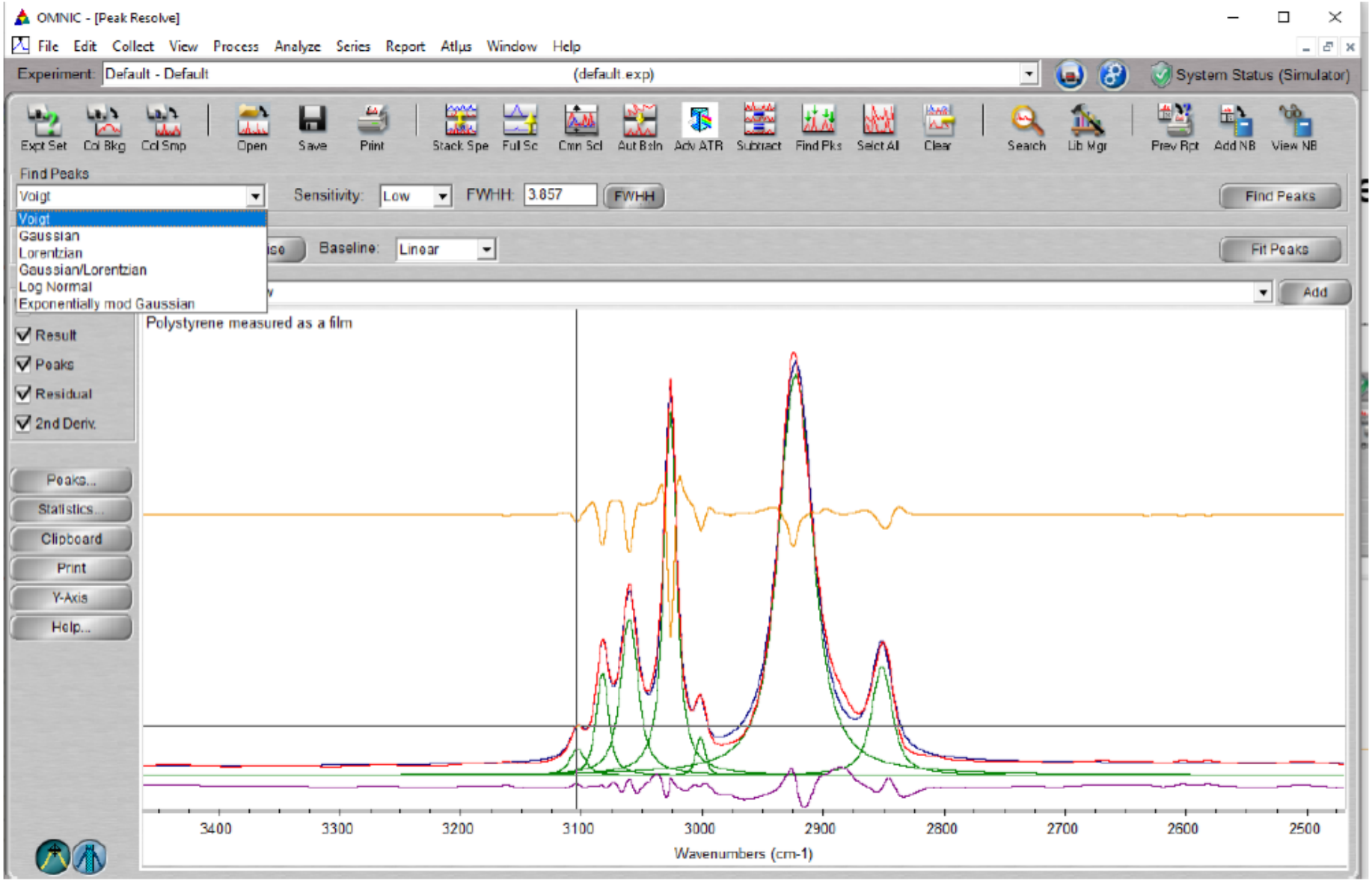
Display in Origin window



amount/total = percentage

Peak #	Peak Type	Center X	Height	FWHH	Other	Area	%
1	Voigt	2854.972	0.0217	9.6991	9.9321	0.4751	9.27
2	Voigt	2872.768	0.0157	9.4737	8.5312	0.3125	6.09
3	Voigt	2928.658	0.0617	17.7705	17.7423	2.4311	47.45
4	Voigt	2962.819	0.0492	17.7251	17.2272	1.9049	37.18

OMNIC Peak Fitting Analysis of Polystyrene Film FTIR Spectrum



Key Concepts and Parameters of Line Shapes and Peak Fitting in Vibrational Spectroscopy (IR/Raman)

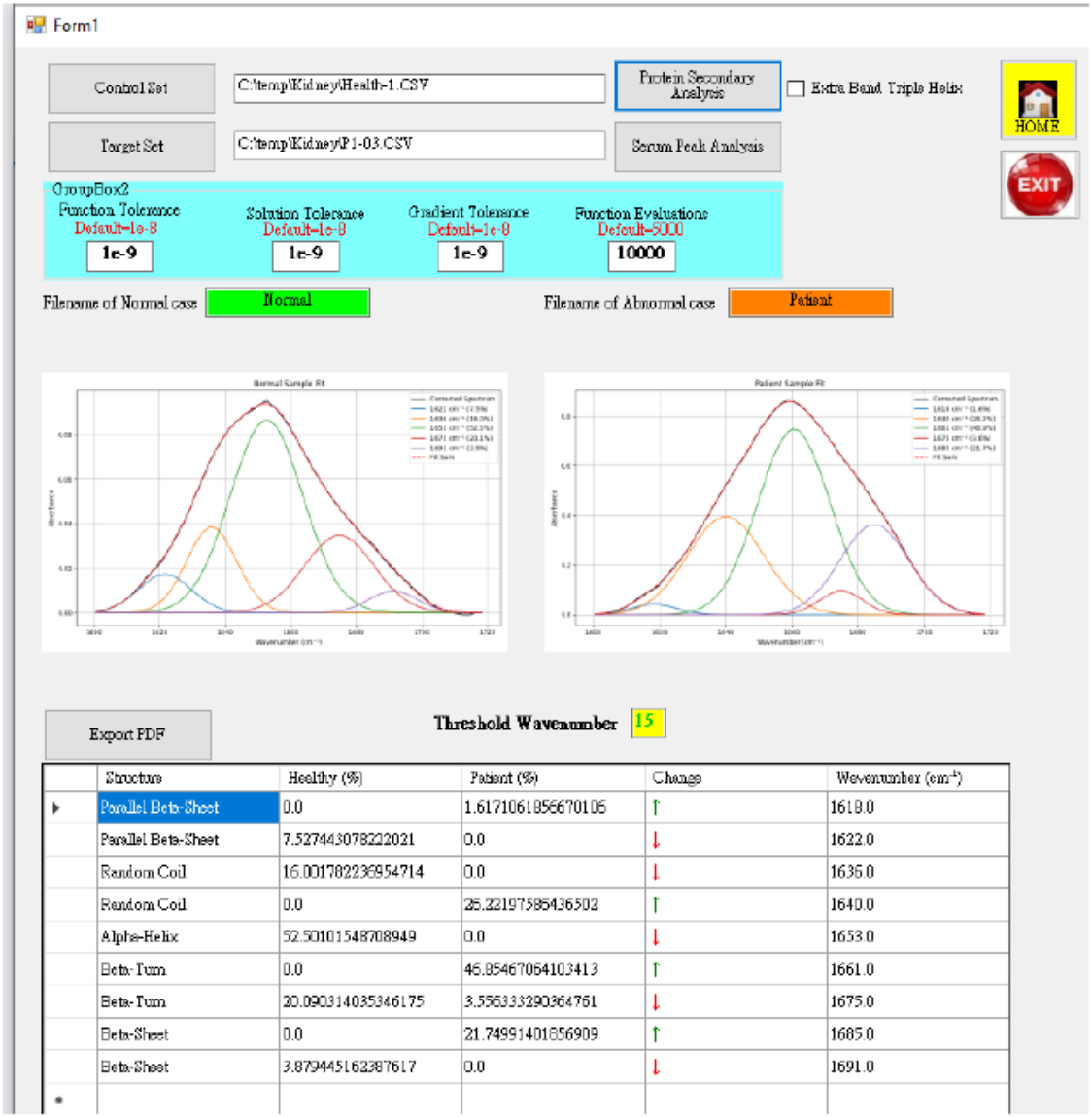
Key Concepts and Parameters of Line Shapes and Peak Fitting in Vibrational Spectroscopy (IR/Raman)

Function	Description
Gaussian	Typical in solids; static environment; produces broader, symmetric peaks.
Lorentzian	Common in gases; sharp central peak with longer wings due to collisions and rotations.
Voigt	A convolution of Gaussian and Lorentzian shapes; often used for liquids, combining both features.
Gaussian/Lorentzian	Weighted sum or mix of Gaussian and Lorentzian; allows flexible fitting between the two extremes.
Log Normal	Asymmetric peak shape, often seen in Raman or chromatographic peaks.
Exponentially mod Gaussian	Gaussian profile modified by an exponential decay, used for asymmetric peaks often found in IR/Raman spectra.

Key Concepts and Parameters of Line Shapes and Peak Fitting in Vibrational Spectroscopy (IR/Raman)

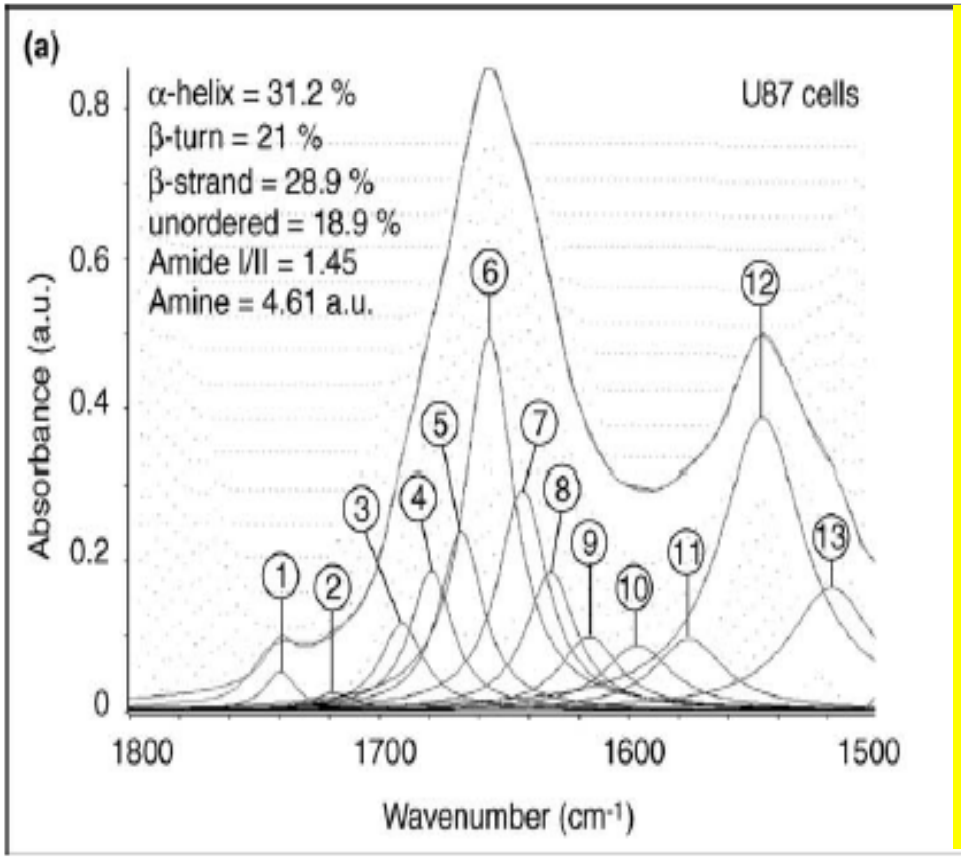
Other Key Parameters	Description
Peak Position	Location of the peak maximum (center).
Intensity	Height of the peak; less accurate for concentration than area.
FWHH	Full width at half height; relates to dynamics and lifetime.
Peak Area	More reliably reflects molecular concentration than intensity alone.
Peak Width	Broader peaks indicate faster dynamics and shorter lifetimes.

Comparative Analysis of Protein Secondary Structures in Serum Samples Using Spectral Deconvolution



	Structure	Healthy (%)	Patient (%)	Change	Wavenumber (cm^{-1})
▶	Parallel Beta-Sheet	0.0	1.6171061856670105	↑	1618.0
	Parallel Beta-Sheet	7.527443078222021	0.0	↓	1622.0
	Random Coil	16.001782236954714	0.0	↓	1636.0
	Random Coil	0.0	25.22197585436502	↑	1640.0
	Alpha-Helix	52.50101548708949	0.0	↓	1653.0
	Beta-Turn	0.0	46.05467054103413	↑	1661.0
	Beta-Turn	20.090314035346175	3.556333290364761	↓	1675.0
	Beta-Sheet	0.0	21.74991401856909	↑	1685.0
	Beta-Sheet	3.879445162387617	0.0	↓	1691.0
*					

Spectral Curve Fitting in IR Spectroscopy for determining the secondary of protein



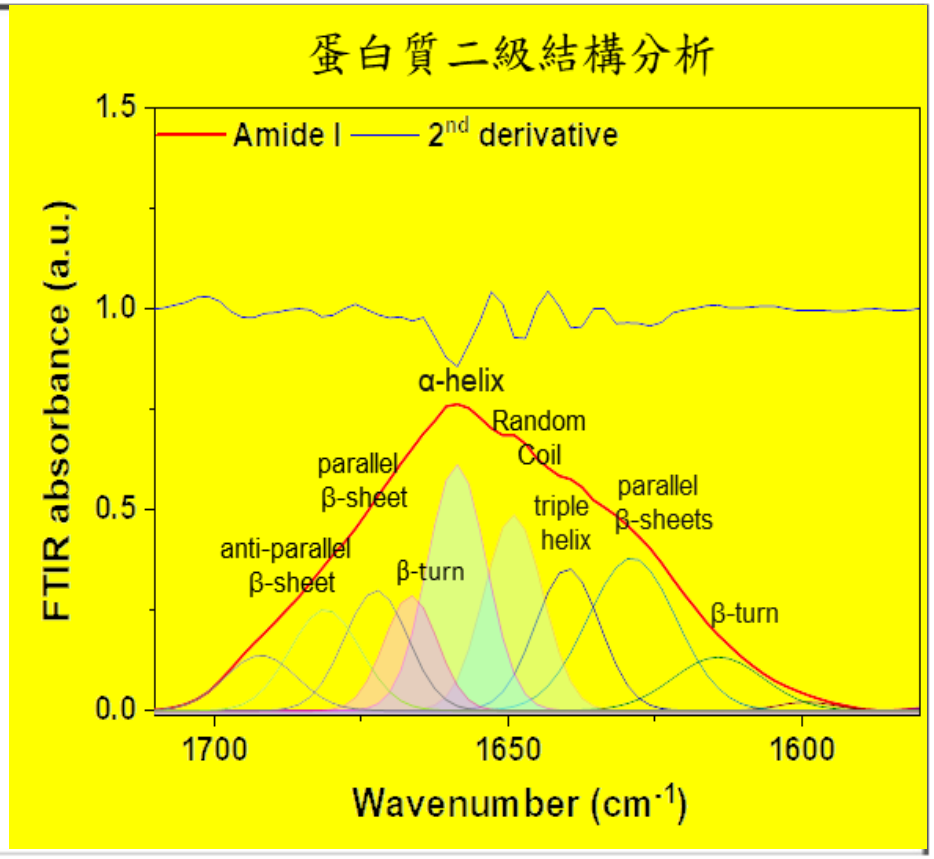


Figure 3. Spectral curve-fitting of the 1800–1500 cm^{-1} spectral interval of cell FT-IR spectra for determining the secondary structure of proteins. The IR absorption bands can be assigned as follows. ν(C=O): (1) acid esters, 1739 cm^{-1}; (2) lipid esters,1718 cm^{-1}; (3) anti-parallel β-strand, 1690 cm^{-1}; (4) parallel β-strand, 1678 cm^{-1}; (5) β-turn, 1666 cm^{-1}; (6) α-helix, 1654 cm^{-1}; (7) unordered structure, 1642 cm^{-1}; (8) parallel β-strand, 1630 cm^{-1}; (9) β-turn, 1615 cm^{-1}. δ(NH_2): (10) amine, 1595 cm^{-1}. δ(N–H): (11) amide II, 1575 cm^{-1}; (12) amide II, 1546 cm^{-1}; (13) tyrosine ring, 1518 cm^{-1}. The bands are used for determining the secondary structure.

Olinger J.M., Hill D.M., Jakobsen R.J. and Brody R.S., *Biochem. Biophys. Acta,* 869, 89(1986).
Levitt M. and Greer J., *J. Mol. Biol.* 114, 181(1977).

GAUSSIAN FUNCTION

Gaussian function, often referred as a Gaussian, is a function of the form

$$f(x) = ae^{-\frac{(x-b)^2}{2c^2}}$$

For arbitrary real constants a, b and non-zero c.

The graph of a Gaussian is a characteristic symmetric bell shaped curve. The parameter 'a' is the height of the curve's peak, 'b' is the position of the center of the peak and 'c', the standard deviation, controls the width of bell.