Atlas of Metabolite SERS Fingerprints obtained by means of q-Gaussian deconvolutions and Fityk Software

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Abstract: This atlas is proposing the fingerprints of the SERS (Surface-Enhanced Raman Spectroscopy) spectra of metabolites, published by Sherman et al. in Talanta, 2020, in an article entitled "A surface-enhanced Raman spectroscopy database of 63 metabolites". The atlas of fingerprints is based on q-Gaussian deconvolutions and Fityk software. Comparison with data available in literature is also proposed.

Introduction

In Sparavigna 2023, we considered three of the Surface-Enhanced Raman spectra of metabolites (L-Cysteine, Cysteamine and Homocysteine), among the 63 spectra provided by Sherman et al., 2020. The aim was to investigate the line shapes of SERS peaks by means of the q-Gaussian functions. These functions are considered by the author (AC Sparavigna) fundamental for any deconvolution of Raman spectra, as shown by several cases (see for instance, Sparavigna, 2023, 2024). In November 2023, we proposed the fingerprints of some of the Sherman et al.'s SERS spectra, to show the relevance of gaining information from them. The fingerprints had been derived from spectra according to a method based on the first derivative behavior, that is on the "first derivative spectrum" (Mosier-Boss et al., 1995). To determine the position of the peaks, details of the method are given in Sparavigna, 2023. Here we propose the fingerprints of the Sherman and coworkers' 63 SERS spectra of metabolites, all obtained by means of q-Gaussian deconvolutions. The used software is Fityk.

Fingerprints

The first use of the term "fingerprint" in relation to the Raman spectroscopy, to the best of my knowledge, is in an article published in 1947 about the Raman spectra of hydrocarbons by Fenske and coworkers. Fenske et al., 1947, wrote that the bands of the Raman spectrum, "which are called Raman lines, are characteristic of the substance illuminated and are therefore a "fingerprint" of that substance". From that time on, the points of identification, such as positions of peaks, shoulders and valleys create the characteristic spectral pattern which is known as the "Raman fingerprint" of a given material. This pattern allows the material classification, "without any preliminary information about composition and structural origin of the individual features" (D'Ippolito et al., 2015).

SERS Data

Sherman et al. provide the SERS spectra of metabolites organized in alphabetical order, with their classification, and formulae. Here we use the same alphabetic order, providing fingerprints in the form of spectra and tables. ***Many thanks to Sherman and coworkers for providing access to their precious data.***

About metabolites

The abstract of the article by Sherman et al., 2020, explains that "Metabolomics, the study of metabolic profiles in a biological sample, has seen rapid growth due to advances in measurement technologies such as mass spectrometry (MS). While MS metabolite reference libraries have been generated for metabolomics applications, mass spectra alone are unable to unambiguously identify many metabolites in a sample; these unidentified compounds are typically annotated as "features". Surface-enhanced Raman spectroscopy (SERS) is an interesting technology for metabolite identification based on vibrational spectra. However, no reports have been published that present SERS metabolite spectra from chemical libraries". Sherman and coworkers, in their article of 2020, "demonstrate that an untargeted approach utilizing citrate-capped silver nanoparticles yields SERS spectra for 20% of 80 compounds chosen randomly from a commercial metabolite library. Furthermore, prescreening of the metabolites according to chemical functionality allowed for the efficient identification of samples within the library that yield distinctive SERS spectra under our experimental conditions".

The Atlas

Using the data provided by Sherman et al., pmc.ncbi.nlm.nih.gov, we propose the fingerprints of metabolites by means of q-Gaussian deconvolutions. Deconvolutions are obtained using Fityk software (Wojdyr, 2010). The centers of the peaks and the parameters of the components are given in files .peaks by Fityk. The q-Gaussians are defined by Sparavigna in a script for this software. In some cases, the first-derivative spectrum has been already considered in Sparavigna, 2023. In the method based on the first-derivative spectrum, to evaluate the peak positions, some data smoothing is necessary; here, the data are used as they are. Baseline corrections are necessary to avoid negative values of intensity.

q-Gaussian function and its asymmetric q-BWF form

The fitting of Raman spectra with q-Gaussian line shapes has been proposed for the first time in 2023 by A. C. Sparavigna. The q-Gaussian line shape is a function based on the Tsallis q-form of the exponential function (Tsallis, 1988). This exponential form is characterized by a q-parameter. When q is equal to 2, we have the Lorentzian function. If q is close to 1, we have a Gaussian function. For values of q between 1 and 2, we have a bell-shaped symmetric function with power-law wings ranging from Gaussian to Lorentzian tails.

The q-Gaussian is given as $f(x) = Ce_q(-\gamma x^2)$, where $e_q(.)$ is the q-exponential function and C a scale constant (Hanel et al., 2009). The q-exponential has expression: $e_q(u) = [1 + (1-q)u]^{1/(1-q)}$. For spectroscopy, we write the q-Gaussian function with the center of the band at x_o:

$$q\text{-}Gaussian = Cexp_q(-\gamma(x-x_o)^2) = C\,[1+(q-1)\gamma(x-x_o)^2]^{1/(1-q)}.$$

We can apply q-Gaussian functions by means of Fityk software. In Fityk, a q-Gaussian function can be defined in the following manner:

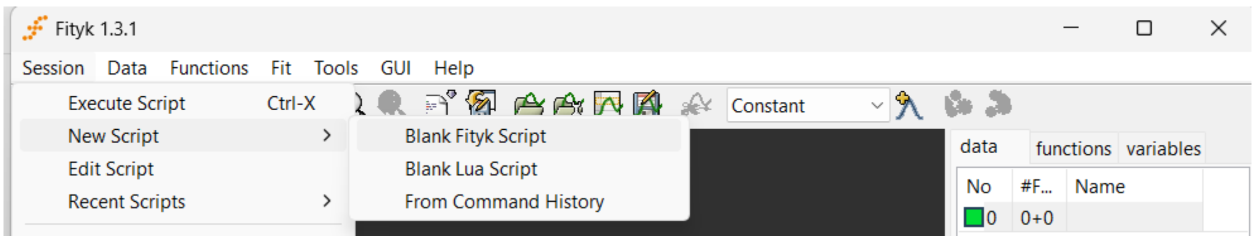
```
define Qgau(height, center, hwhm, q=1.5) = height*(1+(q-1)*((x-center)/hwhm)^2)^(1/(1-q))
```

where q=1.5 is the initial guessed value of the q-parameter. Parameter hwhm is the half width at half maximum of the line, in the case of a Lorentzian function. In fact, when q=2, the q-Gaussian turns into a Lorentzian function, that we can find defined in Fityk as:

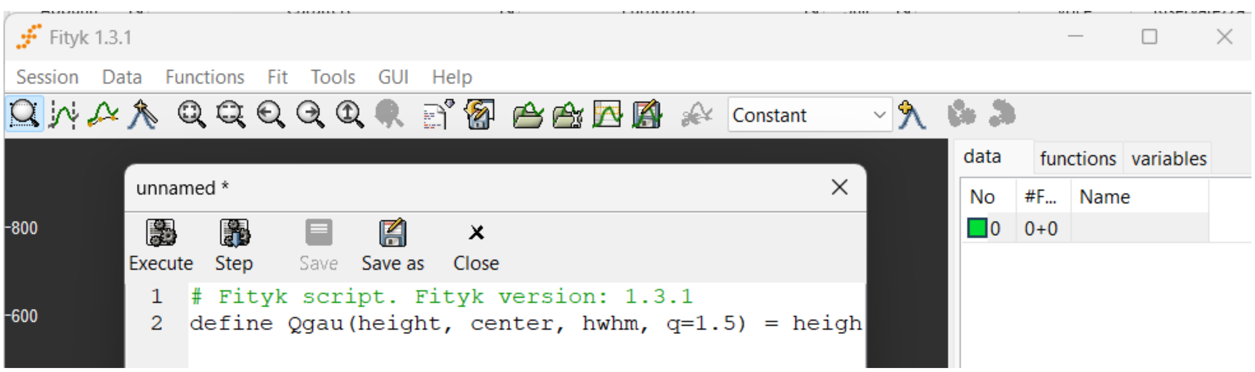
```
Lorentzian(height, center, hwhm) = height/(1+((x-center)/hwhm)^2)
```

When q is close to 1, the q-Gaussian becomes a Gaussian function.

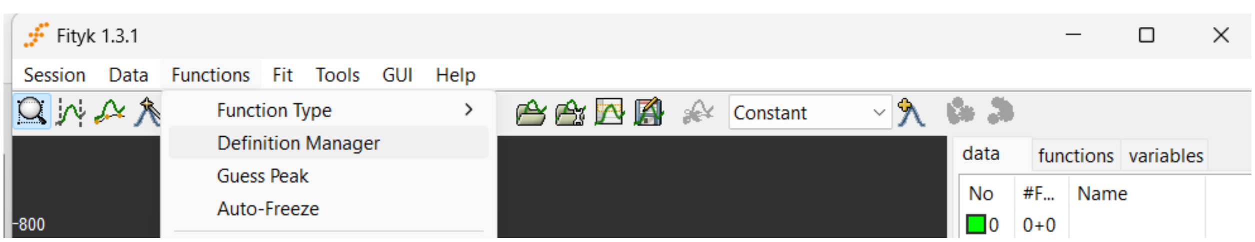
In Fityk, to define a function, use please Session > New Script > Blank Fityk Script



In the Blank Fityk Script paste the "define" of the function, for instance the Qgau given above.



Then, save the Script, and execute it. Using Functions > Definition Manager, in the list of the functions, it will be the q-Gaussian function too.



As shown on many occasions, the q-Gaussians are suitable for fitting Raman spectra (by examples proposed in SSRN to the SERS cases, for instance). For applying the q-Gaussians to asymmetric bands, we can define also an asymmetric function, turning the Breit-Wigner-Fano (BWF) function into a q-BWF function (Sparavigna, 2023). Let us write the BWF as follow:

$$\text{BWF}(x) = C\,\frac{\left[1-\xi\gamma^{1/2}(x-x_o)\right]^2}{[1+\gamma(x-x_o)^2]}$$

When asymmetry parameter ξ is zero, BWF becomes a symmetric Lorentzian function. Note that the center of the line does not correspond to the position of the peak of the function. As in Sparavigna, 2023, we can define the q-BWF function in the following manner:

$$\text{q-BWF} = C\left[1-\xi\gamma^{1/2}(q-1)^{1/2}(x-x_o)\right]^2[1+(q-1)\gamma(x-x_o)^2]^{1/(1-q)}$$

In fact, the Lorentzian function is substituted by a q-Gaussian function.
In Fityk, the q-Breit-Wigner-Fano (q-BWF) can be defined as:

```
Qbreit(height, center, hwhm, q=1.5, xi=0.1) = (1-xi*(q-1)*(x-center)/hwhm)^2 * height*(1+(q-1)^0.5 *((x-center)/hwhm)^2)^(1/(1-q))
```

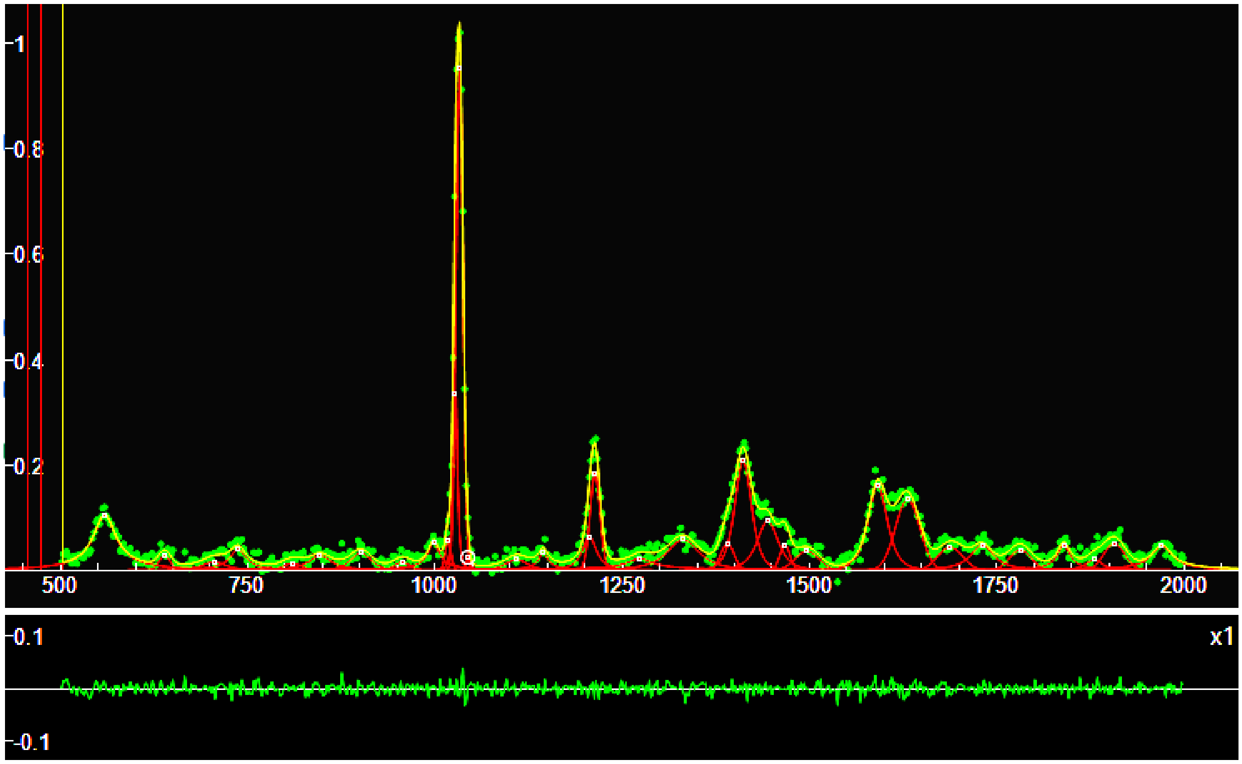
And the BWF can be defined as:

```
Breit(height, center, hwhm, xi=0.1 ) = (1-xi*(x-center)/hwhm)^2 * height/(1+((x-center)/hwhm)^2)
```

Using +xi instead of −xi does not change the fitting results in Fityk.
In the following Atlas, we provide for each metabolite, a screenshot of Fityk software, where the green dots are data from Sherman et al., 2020, red curves the q-Gaussian components, yellow curve the sum of components. In the lower part of the screenshot, the misfit is given (difference between data and yellow curve).
Supplementary material is providing two folders containing the Fityk files name_metabolite.fit and name_metabolite-fingerprint.peaks.

1-Methylnicotinamide

As told by Sherman and coworkers, "While a spectrum of this molecule has not been previously reported to our knowledge, comparable spectra have been published for the analogous nicotinamide" in Jaworska, et al., 2012.



PeakType Center Parameters: Height Center hwhm q (height > 0.045, **Bold** h>0.10)
The position of the centers is in cm^{-1}, intensity in arbitrary unit.

%_8	**Qgau**	**558.953**	**0.105979**	**558.953**	**18.2871**	**2.26664**
%_14	Qgau	998.287	0.0554683	998.287	8.86794	2.61864
%_43	Qgau	1017.85	0.0582474	1017.85	5.32125	1.07878
%_42	**Qgau**	**1027.14**	**0.365554**	**1027.14**	**3.48534**	**1.56505**
%_1	**Qgau**	**1032.98**	**0.954419**	**1032.98**	**6.49359**	**1.00002**
%_13	Qgau	1206.29	0.0648222	1206.29	11.6139	1.88741
%_3	**Qgau**	**1213.78**	**0.185379**	**1213.78**	**9.1399**	**1.07241**
%_38	Qgau	1331.26	0.059443	1331.26	26.5227	1.81559
%_19	Qgau	1390.5	0.0518422	1390.5	12.6854	0.999816
%_4	**Qgau**	**1411.48**	**0.20852**	**1411.48**	**14.7099**	**1.42494**
%_9	Qgau	1444.25	0.0947042	1444.25	17.9707	1.57323
%_31	Qgau	1467.22	0.0485978	1467.22	9.69591	1.00166
%_5	**Qgau**	**1590.96**	**0.162519**	**1590.96**	**16.7199**	**1.50445**
%_6	**Qgau**	**1631.12**	**0.135273**	**1631.12**	**23.168**	**0.999633**
%_34	Qgau	1730.76	0.0484485	1730.76	18.6942	2.03091
%_17	Qgau	1839.67	0.0493608	1839.67	10.3953	2.34436
%_11	Qgau	1907.18	0.0516374	1907.18	20.0302	0.999874
%_21	Qgau	1970.8	0.0478351	1970.8	16.1983	2.44148

Therefore, the centers are: (in cm^{-1}):

558.953(m)	998.287	1017.85	1027(s)	1032.98(vs)	1206.29
1213.78(m)	1331.26	1390.5	1411.48(m)	1444.25	1467.22
1590.96(m)	1631.12(m)	1730.76	1839.67	1907.18	1970.8

In Jaworska, et al., 2012, we find the following fingerprints for nicotinamide (solid state and solutions). In ***bold***, the peaks which are corresponding to q-Gaussian centers given above, within +/− 5 cm^{-1} (in *italic*, within +/− 10 cm^{-1}):

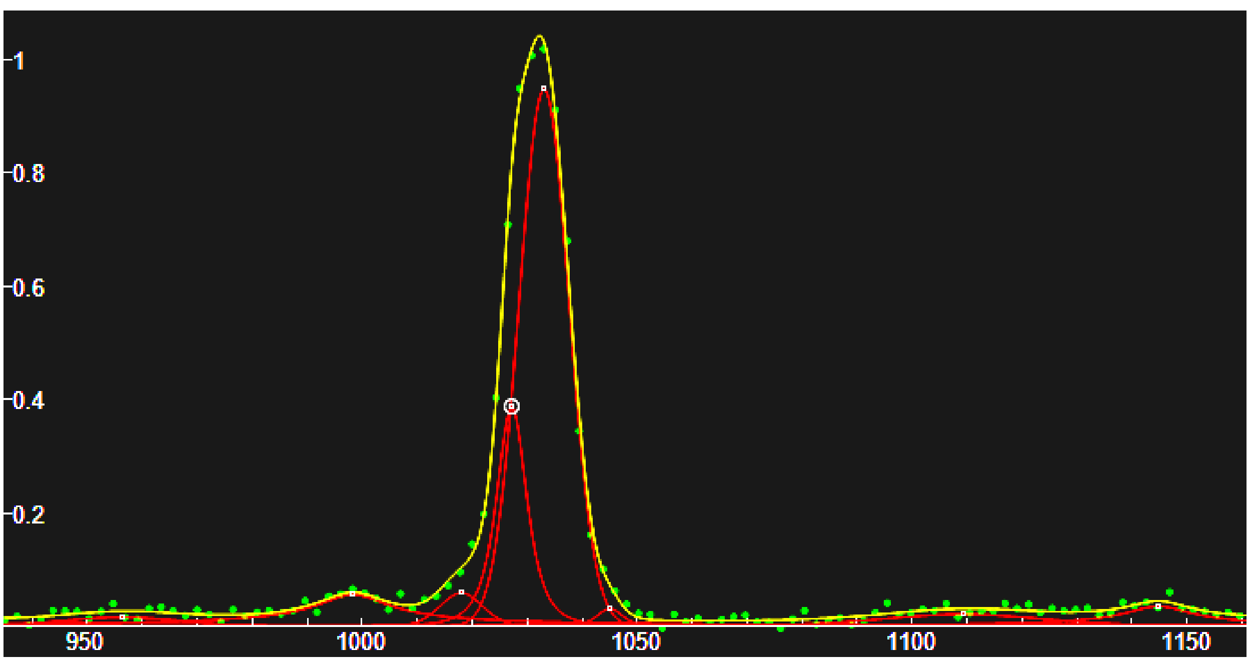
Solid: 390 629 789 ***994*** *1043(vs)* 1094 1124 1161 ***1211*** ***1393*** 1579 1597 1616 1677

Solution (pH=12): 394 631 787 847 ***997*** ***1032(vs)*** *1042(vs)* 1101 1154 ***1202*** ***1395*** 1424 ***1441*** 1489 1574 *1597* 1672

Solution (pH=2): 368 621 779 836 *990* ***1030(s)*** 1046(vs) 1107 1157 1267 1368 1424(s) 1605 *1641(s)* 1695

SERS pH=9: 789 *992* ***1032(vs)*** 1078 1371 ***1410*** ***1439*** 1489 ***1586*** 1601

According to Jaworska and coworkers, "the normal FT-Raman spectrum of the aqueous solution at low pH reveals the presence of two bands at 1030 and 1046 cm^{-1}, which are attributed to vibrations 1 and 12 of the pyridine ring, respectively. Mode 1 originates from the trigonal bend of the ring (breathing), while mode 12 is a combination of the ring C-C and C-N stretches". If we consider Figure 3 in Jaworska et al., we can note that the intensity of the peak at 1030 cm^{-1} changes according to pH.



A detail of the two q-Gaussian components at 1027 and 1033 cm^{-1}.

In Majzner et al., 2016, among the supplementary information, we can find the Raman spectra of arachidonic acid (AA) and 1-methyl-nicotinamide (MNA).
The fingerprint provided by Majzner and coworkers is:

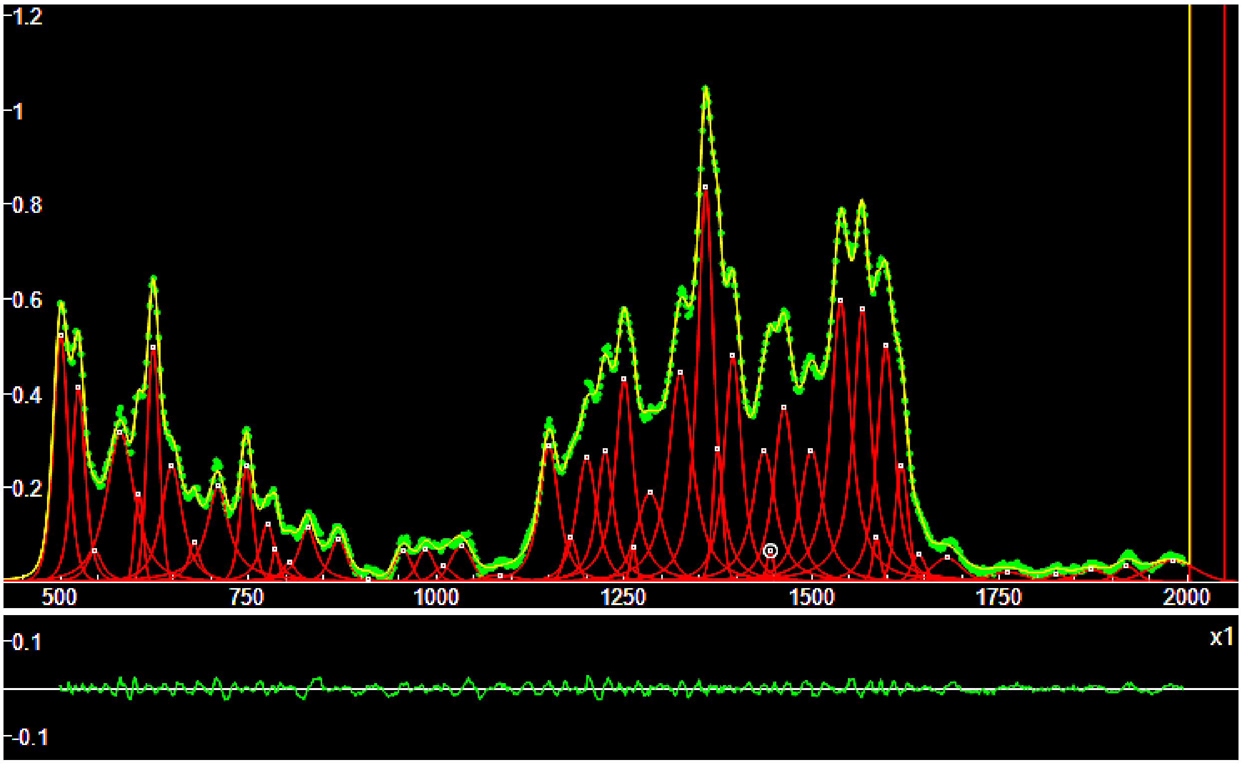
209 233 367 398 525 643 739 845 899 ***1030(vs)*** 1129 1194 1289 *1399(s)*
1503 ***1586*** *1639* 1682 2588 2803 2951 3067

Let us repropose the SERS fingerprint, and compare within 5 cm^{-1} (bold) and within 10 cm^{-1} (italic):

558.953(m)	998.287	1017.85	***1027(s)***	***1032.98(vs)***	1206.29
1213.78(m)	1331.26	*1390.5*	1411.48(m)	1444.25	1467.22
1590.96(m)	*1631.12(m)*	1730.76	1839.67	1907.18	1970.8

1-naphthylamine

As told in Sherman et al., "SERS spectra have previously been reported for this molecule" by Alvarez-Puebla et al., 2007.



# PeakType		Center	Parameters: Height	Center	HWHM	q (height > 0.25 **Bold** h>0.40)
%_48	**Qgau**	**499.592**	**0.522043**	**499.592**	**13.1201**	**1.34321**
%_14	**Qgau**	**522.941**	**0.41493**	**522.941**	**11.4354**	**1.51673**
%_19	Qgau	579.012	0.317255	579.012	23.6034	1.68347
%_8	**Qgau**	**622.498**	**0.497027**	**622.498**	**11.4899**	**1.03955**
%_20	Qgau	1149.7	0.290043	1149.7	16.123	1.74769
%_23	Qgau	1200.06	0.264314	1200.06	17.416	1.57414
%_15	Qgau	1224.54	0.277563	1224.54	13.4779	1.88233
%_11	**Qgau**	**1250.08**	**0.43203**	**1250.08**	**14.3411**	**1.95591**
%_13	**Qgau**	**1324.93**	**0.445613**	**1324.93**	**19.9008**	**1.82074**
%_5	**Qgau**	**1358.43**	**0.835659**	**1358.43**	**13.1081**	**1.80107**
%_16	Qgau	1374.18	0.284494	1374.18	8.7291	1.23907
%_10	**Qgau**	**1394.67**	**0.480097**	**1394.67**	**14.4381**	**1.74448**
%_18	Qgau	1436.06	0.279891	1436.06	18.5879	1.91098
%_12	Qgau	1462.82	0.370136	1462.82	17.1288	1.69961
%_17	Qgau	1499.18	0.280505	1499.18	19.2749	1.78655
%_7	**Qgau**	**1538.37**	**0.595345**	**1538.37**	**16.1571**	**1.94248**
%_6	**Qgau**	**1566.92**	**0.580069**	**1566.92**	**13.717**	**2.08098**
%_9	**Qgau**	**1598.48**	**0.500772**	**1598.48**	**14.5671**	**1.69709**

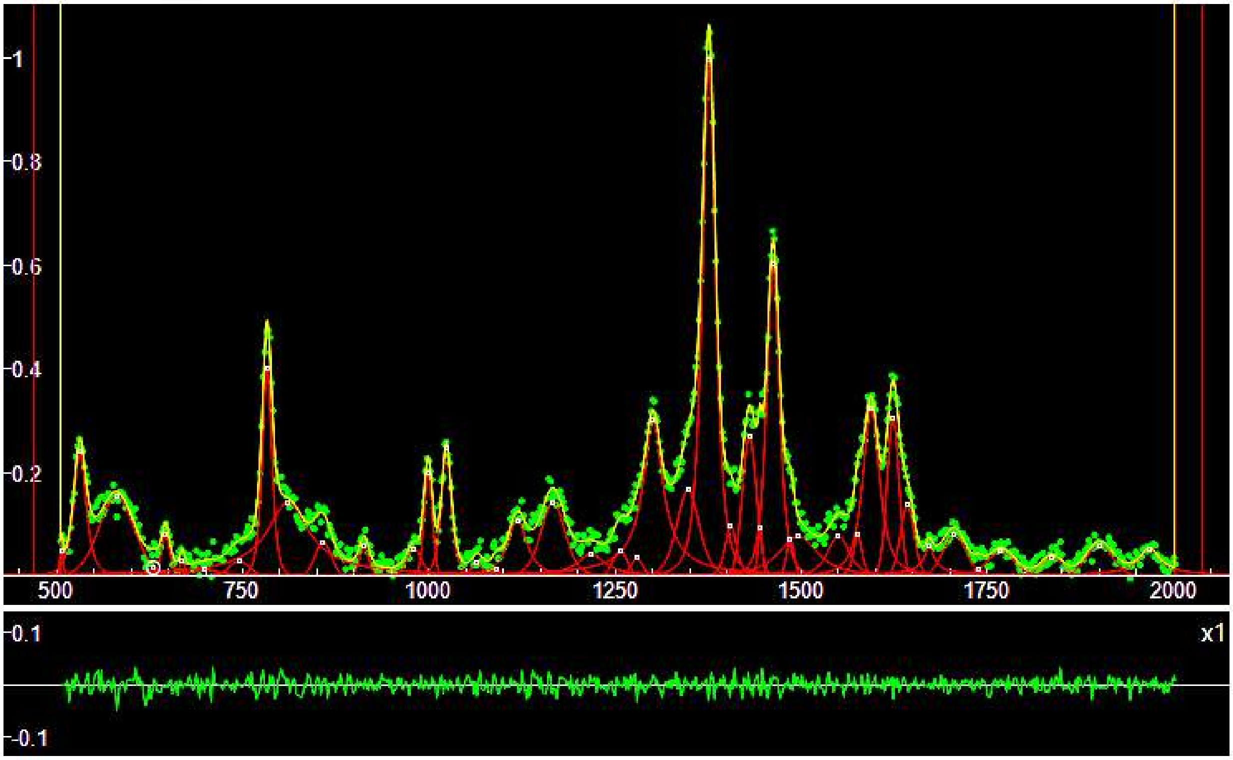
Therefore, the centers are:

499.592(s)	522.941(s)	579.012	622.498(s)	1149.7	1200.06
1224.54	1250.08(s)	1324.93(s)	1358.43(vs)	***1374.18***	1394.67(s)
1436.06	***1462.82***	1499.18	1538.37(s)	***1566.92(s)***	1598.48(s)

In bold, the centers which are corresponding to data in Alvarez-Puebla et al., within +/− 5 cm^{-1}.
In Alvarez-Puebla et al., 2007, we find the study of two "important environmental pollutants, 1-naphthylamine (1NA) and pyridine (PYR)". "The Raman and SERS spectra (with the pollutant added before and after the preparation of the nanoparticles) of 1NA and PYR are shown in Fig. 5 [of Alvarez-Puebla et al.]. Raman spectra of 1NA (Fig. 5A) is dominated by ring stretching (1575 and 1454 cm^{-1}), and C–N stretching (1376 cm^{-1}). 1NA SERS spectra on HA–AuNP … is characterized by ring stretching (1575, ***1567***, ***1462*** and 1454 cm^{-1}), C=C and C–N stretching (***1377*** cm^{-1})".
Let us add data from the IR spectrum from the NIST/EPA Gas-Phase Infrared Database, available at https://webbook.nist.gov/cgi/cbook.cgi?ID=C134327&Mask=80. The main peaks are:

563.3 769.5 1015.5 1086 1285 1379 1414 ***1461*** 1515 1590 1625

2-Quinolinecarboxilic Acid

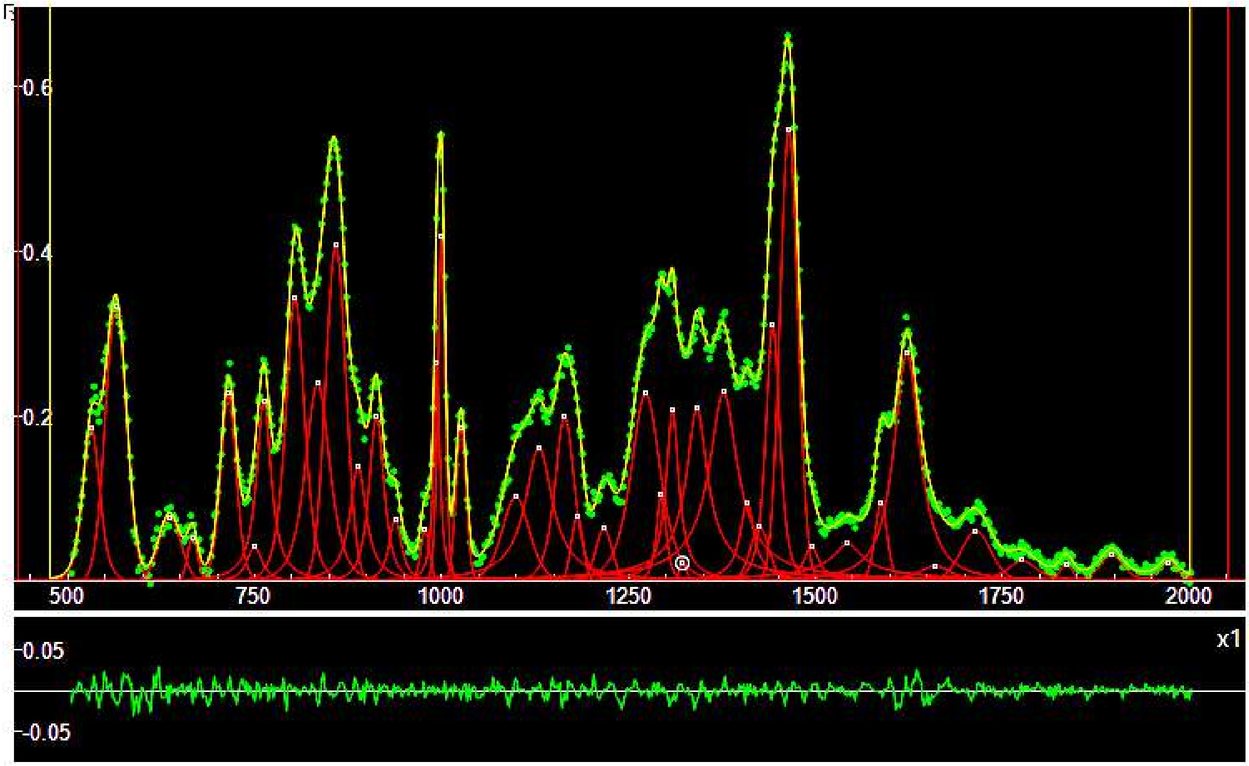


PeakType Center Parameters: Height Center HWHM q (height > 0.1 **Bold** characters for height > 0.30)

#	PeakType	Center	Height	Center	HWHM	q
%_8	Qgau	531.131	0.240283	531.131	10.7482	1.58802
%_13	Qgau	580.413	0.152971	580.413	33.2128	1.06819
%_3	**Qgau**	**782.538**	**0.403204**	**782.538**	**8.56315**	**1.3799**
%_14	Qgau	810.648	0.142473	810.648	33.846	2.24916
%_10	Qgau	998.892	0.20039	998.892	7.84557	0.999979
%_9	Qgau	1023.39	0.24717	1023.39	8.77852	1.45528
%_15	Qgau	1118.53	0.107309	1118.53	16.5132	1.76095
%_50	Qgau	1166.47	0.142384	1166.47	21.7435	1.2464
%_5	**Qgau**	**1300.66**	**0.302995**	**1300.66**	**15.7266**	**2.26704**
%_11	Qgau	1347.79	0.166581	1347.79	20.2771	1.253
%_1	**Qgau**	**1375.95**	**0.999205**	**1375.95**	**11.3259**	**1.57419**
%_7	Qgau	1430.13	0.26981	1430.13	13.412	0.999849
%_2	**Qgau**	**1461.89**	**0.6015**	**1461.89**	**11.1805**	**1.47625**
%_6	**Qgau**	**1593.72**	**0.323765**	**1593.72**	**14.0857**	**1.69766**
%_4	**Qgau**	**1623.15**	**0.305301**	**1623.15**	**11.169**	**1.06056**
%_19	Qgau	1642.29	0.136353	1642.29	12.6886	1.077

3'-5'-Cyclic AMP

3', 5'-cyclic adenosine monophosphate (AMP).



PeakType Center Parameters: Height Center HWHM q
(h > 0.15, bold h > 0.25)

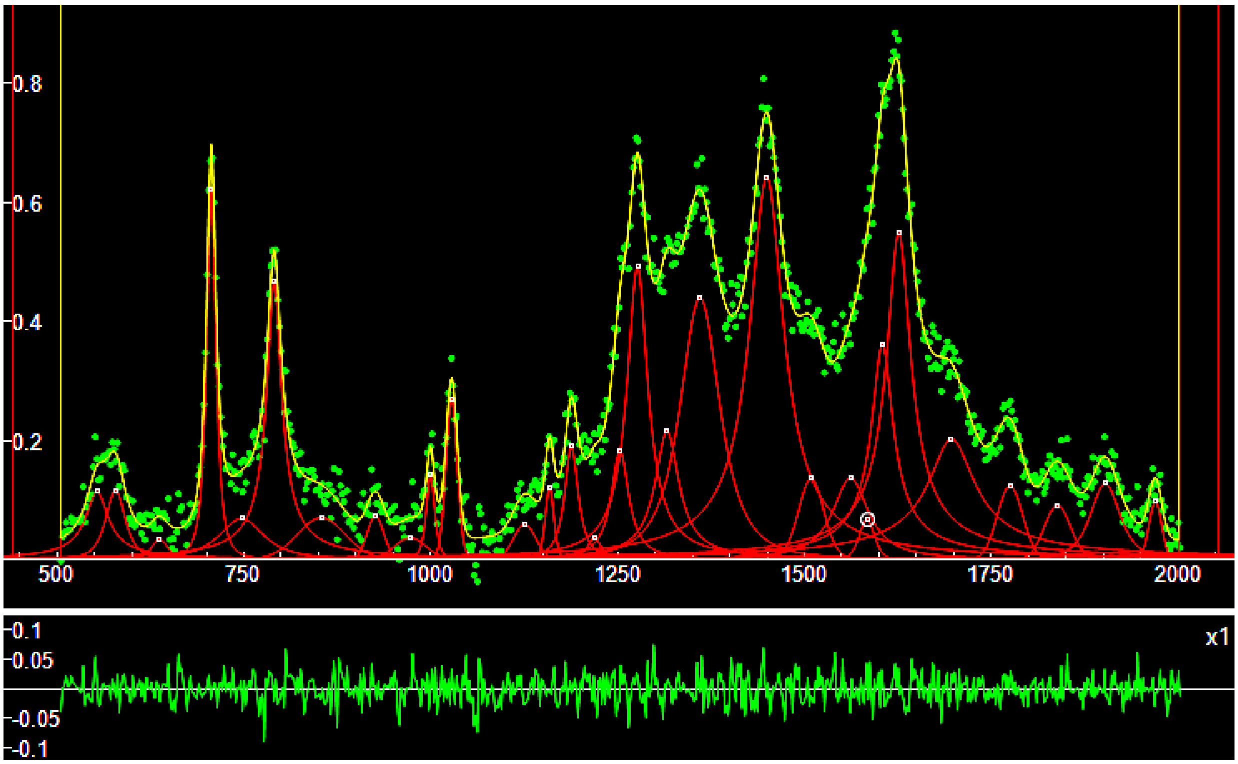
%_17	Qgau	531.5	0.186584	531.5	14.9697	1.30829
%_5	**Qgau**	**564.412**	**0.334314**	**564.412**	**19.8898**	**0.999887**
%_8	Qgau	714.877	0.22756	714.877	13.9872	1.21092
%_9	Qgau	762.265	0.220584	762.265	11.8189	1.94594
%_7	**Qgau**	**804.158**	**0.344244**	**804.158**	**16.3874**	**1.40253**
%_33	Qgau	834.133	0.239719	834.133	21.2652	1.44203
%_32	**Qgau**	**858.453**	**0.4075**	**858.453**	**19.0275**	**0.999746**
%_15	Qgau	913.046	0.200361	913.046	12.5196	1.62419
%_13	**Qgau**	**993.445**	**0.274204**	**993.445**	**4.84623**	**1.90005**
%_2	**Qgau**	**999.917**	**0.423528**	**999.917**	**6.40414**	**1.21384**
%_11	Qgau	1025.87	0.186371	1025.87	9.6439	0.999989
%_37	Qgau	1130.08	0.162462	1130.08	21.9856	2.08123
%_36	Qgau	1164.55	0.200073	1164.55	17.0445	1.39851
%_38	Qgau	1272.96	0.227295	1272.96	25.3669	1.45812
%_39	Qgau	1308.71	0.208174	1308.71	10.2481	2.06841
%_40	Qgau	1341.54	0.21001	1341.54	16.9198	2.44676
%_41	Qgau	1376.98	0.229396	1376.98	22.8388	2.27672
%_46	**Qgau**	**1442.82**	**0.313052**	**1442.82**	**11.9285**	**1.52154**
%_45	**Qgau**	**1464.54**	**0.548247**	**1464.54**	**16.9416**	**0.999707**
%_49	**Qgau**	**1622.33**	**0.27668**	**1622.33**	**21.2343**	**1.87109**

3-Methoxytyramine

As told by Sherman and coworkers, the SERS spectrum of 3-methoxytyramine have previously been reported Lee et al. 1988. The following Table is proposing their results.

SERS shifts (cm^{-1})

ν_{C-O}	ν_3	ν_{19a}		ν_{8a}	ν_{8b}
1273	1363	1441	1507	1578	1601



PeakType Center Parameters Height Center hwhm q (height > 0.13, **bold** h > 0.40)

%_4	**Qgau**	**706.307**	**0.629718**	**706.307**	**7.63984**	**1.7298**
%_5	**Qgau**	**790.396**	**0.467177**	**790.396**	**11.8253**	**2.41048**
%_10	Qgau	999.562	0.142311	999.562	7.16415	1.56206
%_7	Qgau	1027.74	0.269247	1027.74	10.2847	1.12087
%_28	Qgau	1188.19	0.189406	1188.19	11.1802	1.87053
%_6	Qgau	1253.12	0.183342	1253.12	14.1057	2.02955
%_34	**Qgau**	**1276.41**	**0.493423**	**1276.41**	**16.6394**	**2.15852**
%_35	Qgau	1316.07	0.215772	1316.07	19.3529	2.15666
%_29	**Qgau**	**1360.2**	**0.439941**	**1360.2**	**33.4662**	**1.67333**
%_2	**Qgau**	**1449.46**	**0.64263**	**1449.46**	**27.6449**	**2.24146**
%_30	Qgau	1508.99	0.135781	1508.99	23.4604	1.11215
%_22	Qgau	1561.55	0.136789	1561.55	28.9504	1.96478
%_21	Qgau	1604.21	0.362019	1604.21	17.7133	2.51739
%_1	**Qgau**	**1626.1**	**0.549836**	**1626.1**	**19.5846**	**2.46796**
%_14	Qgau	1696.77	0.202231	1696.77	38.3693	2.58073

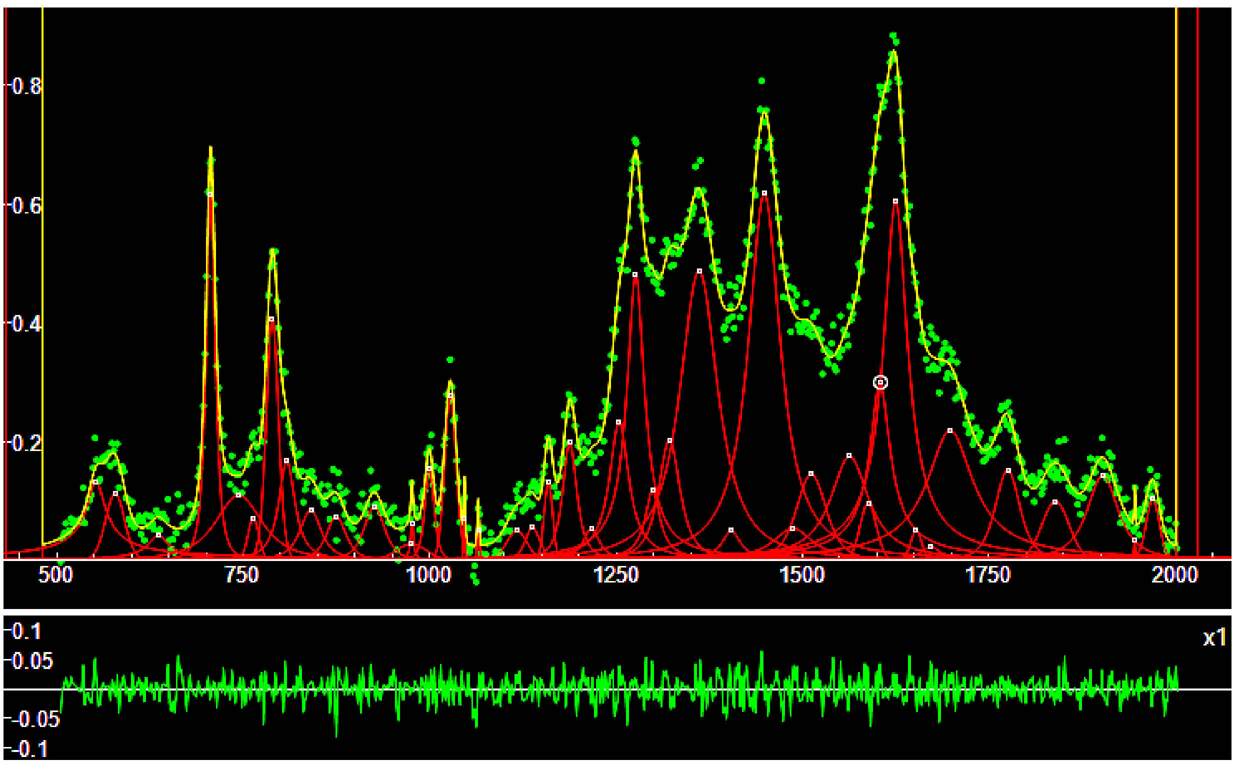
Therefore, the q-Gaussian centers are:

706.307(s)	790.396(s)	999.562	1027.74(m)	1188.19	1253.12
1276.41(s)	1316.07	1360.2(s)	1449.46(s)	1508.99	1561.55
1604.21(m)	1626.1(s)	1696.77			

As previously told, in Lee et al. we find the SERS shifts (in bold, the peaks which are corresponding to centers given above, within +/− 5 cm^{-1}, and in italic, within +/− 10 cm^{-1}):

1273 ***1363*** *1441* ***1507*** 1578 ***1601***

As we can see from the Table given in the previous page, we have some q-Gaussian components which have a q-parameter greater than 2. That is, we have fat tails of the line shape. To reduce the role of the tail, we can try to add further components. The fit is proposed in the following image. We can find just some small improvement of the misfit.



# PeakType	Center	Parameters	Height	Center hwhm q (height > 0.13, bold h > 0.40)
%_9 Qgau	552.375	x	x	0.132223 552.375 16.3061 2.94561
%_4 Qgau	**706.247**	**x**	**x**	**0.621548 706.247 7.66745 1.66303**
%_5 Qgau	**788.847**	**x**	**x**	**0.410713 788.847 11.021 1.15093**
%_11 Qgau	808.323	x	x	0.167201 808.323 13.4801 1.83597
%_10 Qgau	999.509	x	x	0.153592 999.509 8.11765 1.4459
%_7 Qgau	1027.72	x	x	0.278812 1027.72 10.8717 1.00793
%_27 Qgau	1159.04	x	x	0.131124 1159.04 8.09418 0.999914

%_28 Qgau	1187.74	x	x	0.198444	1187.74	11.7757	1.74643
%_6 Qgau	1253.9	x	x	0.233884	1253.9	15.6213	2.06796
%_34 Qgau	**1276.21**	**x**	**x**	**0.482606**	**1276.21**	**14.179**	**2.18849**
%_35 Qgau	1321.26	x	x	0.202588	1321.26	18.2082	1.70216
%_29 Qgau	**1360.98**	**x**	**x**	**0.487771**	**1360.98**	**31.4059**	**1.8383**
%_2 Qgau	**1448.7**	**x**	**x**	**0.618138**	**1448.7**	**26.1096**	**1.95863**
%_30 Qgau	1511.67	x	x	0.145332	1511.67	26.2348	1.41157
%_22 Qgau	1562.98	x	x	0.175103	1562.98	31.0861	1.9807
%_21 Qgau	1603.76	x	x	0.299136	1603.76	16.4645	2.48782
%_1 Qgau	**1624.68**	**x**	**x**	**0.605469**	**1624.68**	**19.2242**	**2.24542**
%_14 Qgau	1697.84	x	x	0.219136	1697.84	37.2766	2.22763
%_8 Qgau	1774.85	x	x	0.15245	1774.85	21.4257	1.46477
%_12 Qgau	1902.38	x	x	0.143522	1902.38	25.9448	1.75693

We have used the same thresholds for height (height $>$ 0.13, bold h $>$ 0.40). The centers are:

552.375	706.247(s)	788.847(s)	808.323	999.509	1027.72(m)
1159.04	1187.74	1253.9(m)	1276.21(s)	1321.26	1360.98(s)
1448.7(s)	1511.67	1562.98	1603.76(m)	1624.68(s)	1697.84
1774.85	1902.38				

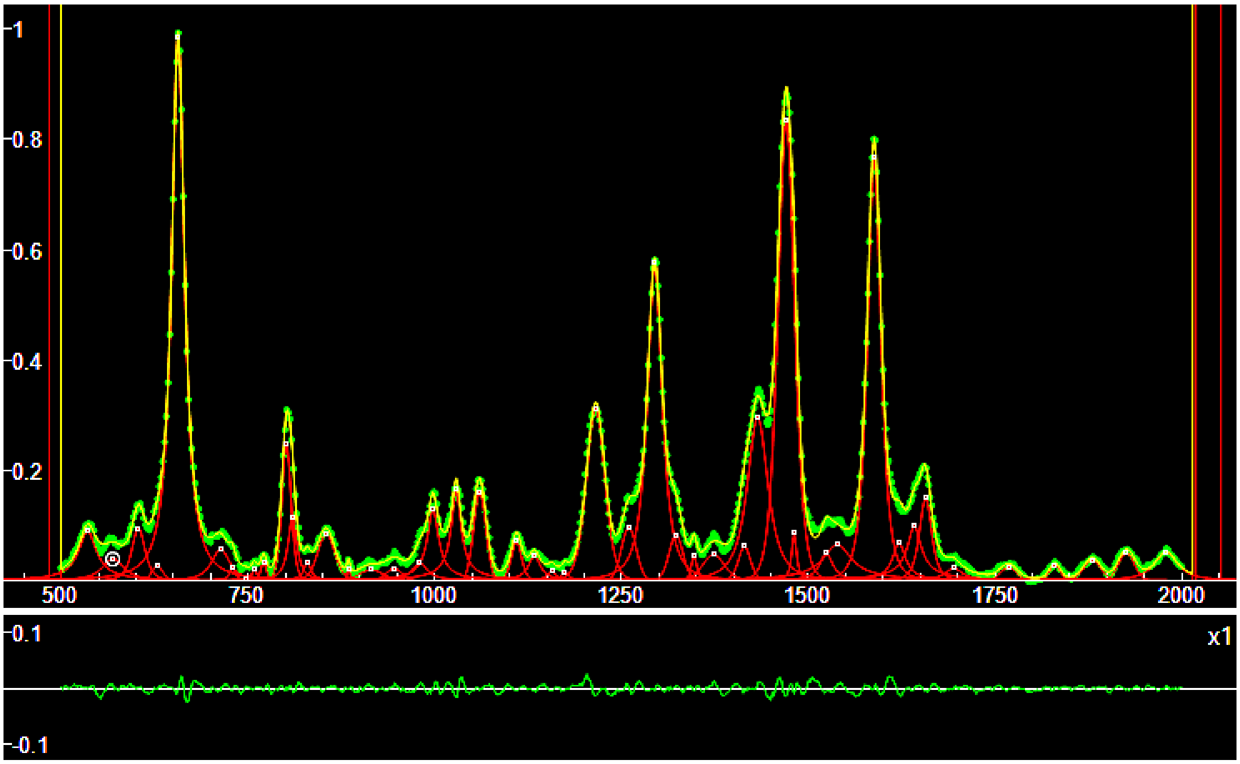
We can compare with the centers obtained before, which are:

706.307(s)	790.396(s)	999.562	1027.74(m)	1188.19	1253.12
1276.41(s)	1316.07	1360.2(s)	1449.46(s)	1508.99	1561.55
1604.21(m)	1626.1(s)	1696.77			

The largest variation of the center position is 5 cm^{-1}, from 1316 to 1321 cm^{-1}. In fact, a further component is present between the two strong peaks at 1276 and 1361 cm^{-1}.

3-Methyladenine

Sherman and coworkers tell that the SERS spectra for 3-Methyladenine have previously been reported by Harroun et al., 2017, and by Nguyen et al., 2017.



#	PeakType	Center	Parameters Height	Center	hwhm	q (h > 0.08, **bold** h > 0.20.)
%_19	Qgau	535.109	0.0897919	535.109	14.4715	2.1924
%_26	Qgau	603.185	0.0957003	603.185	11.3101	1.53316
%_1	**Qgau**	**656.303**	**0.988356**	**656.303**	**10.3341**	**1.8972**
%_5	**Qgau**	**801.295**	**0.247788**	**801.295**	**8.35259**	**1.24499**
%_24	Qgau	809.351	0.115062	809.351	7.07465	1.97317
%_14	Qgau	854.773	0.0847764	854.773	15.8237	1.14921
%_47	Qgau	997.673	0.129678	997.673	9.04125	2.25515
%_16	Qgau	1028.71	0.166022	1028.71	7.673	2.37184
%_9	Qgau	1060.25	0.160606	1060.25	11.6573	0.999862
%_6	**Qgau**	**1215.37**	**0.312233**	**1215.37**	**16.6507**	**1.22759**
%_13	Qgau	1259.83	0.0965649	1259.83	14.0671	0.999658
%_4	**Qgau**	**1294.45**	**0.577864**	**1294.45**	**12.2958**	**1.74939**
%_12	Qgau	1322.95	0.0828656	1322.95	13.0129	1.09422
%_7	**Qgau**	**1432.24**	**0.296223**	**1432.24**	**17.3177**	**1.71632**
%_2	**Qgau**	**1470.45**	**0.834111**	**1470.45**	**14.8157**	**1.28347**
%_28	Qgau	1481.06	0.0869664	1481.06	3.80723	1.96985
%_3	**Qgau**	**1588.19**	**0.767821**	**1588.19**	**11.638**	**1.54062**
%_48	Qgau	1641.93	0.0992832	1641.93	11.2123	2.47543
%_49	Qgau	1657	0.150396	1657	10.404	1.57514

Therefore, the centers are at:

535.109	603.185	656.303(vs)	801.295	809.351	854.773
997.673	1028.71(m)	1060.25(m)	1215.37(s)	1259.83	1294.45(s)
1322.95	1432.24(s)	1470.45(vs)	1481.06	1588.19(vs)	1641.93
1657(m)					

Harroun et al., 2017, are providing in their Table 3 the following SERS peaks (assignments are also given):

486(s)	***533***	***600(m)***	*646(s)*	693	743	789
826(s)	***850***	924(s)	962	*1021*	1048	1140
1209	1244	1272	***1291***	***1323(s)***	1364	1396
1409	1421	*1461(s)*	***1476(vs)***	1528	1567	*1632*

As previous cases, we have marked the correspondences of q-Gaussian centers and peaks, in bold within +/− 5 cm^{-1}, and in italic, within +/− 10 cm^{-1}.

The Raman peaks given by Harroun et al. are (for comparison with the q-Gaussian centers, in bold within +/− 5 cm^{-1}, and in italic, within +/− 10 cm^{-1}):

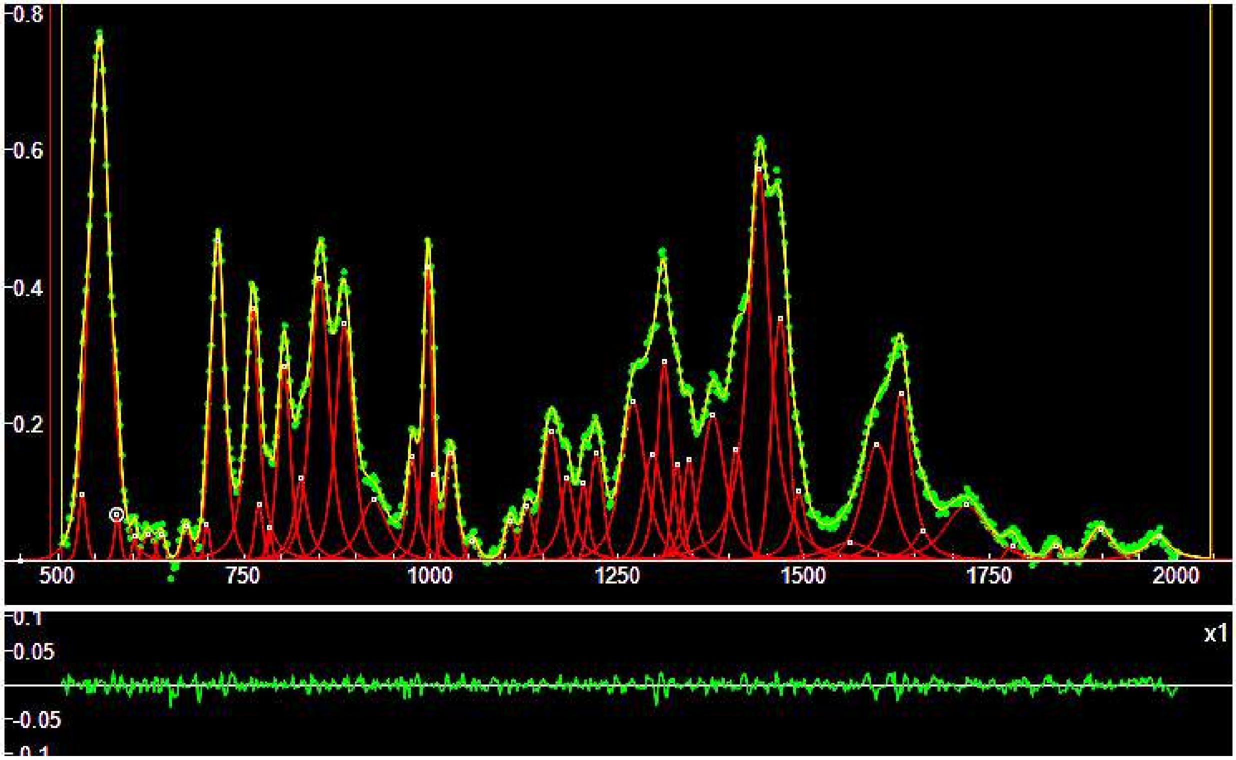
481(s)	***539***	583	617	*664(vs)*	694	732
796	*817*	828	886	928	955	***1059***
1112	1178	***1212***	*1254*	*1285(s)*	*1316*	1367
1408	***1431***	1457	***1471***	1529	1575	***1641***

Nguyen et al., 2017, are providing ***Raman and SERS*** on Au data (for comparison with q-Gaussian centers, in bold, within +/− 5 cm^{-1}, and in italic, within +/− 10 cm^{-1}):

481	580	***660(vs)***	***803***	956	*1053*	1106
1167	1240	*1267(s)*	***1322***	1410(s)	1457	1519
1567(s)	1628	(***Raman***)				

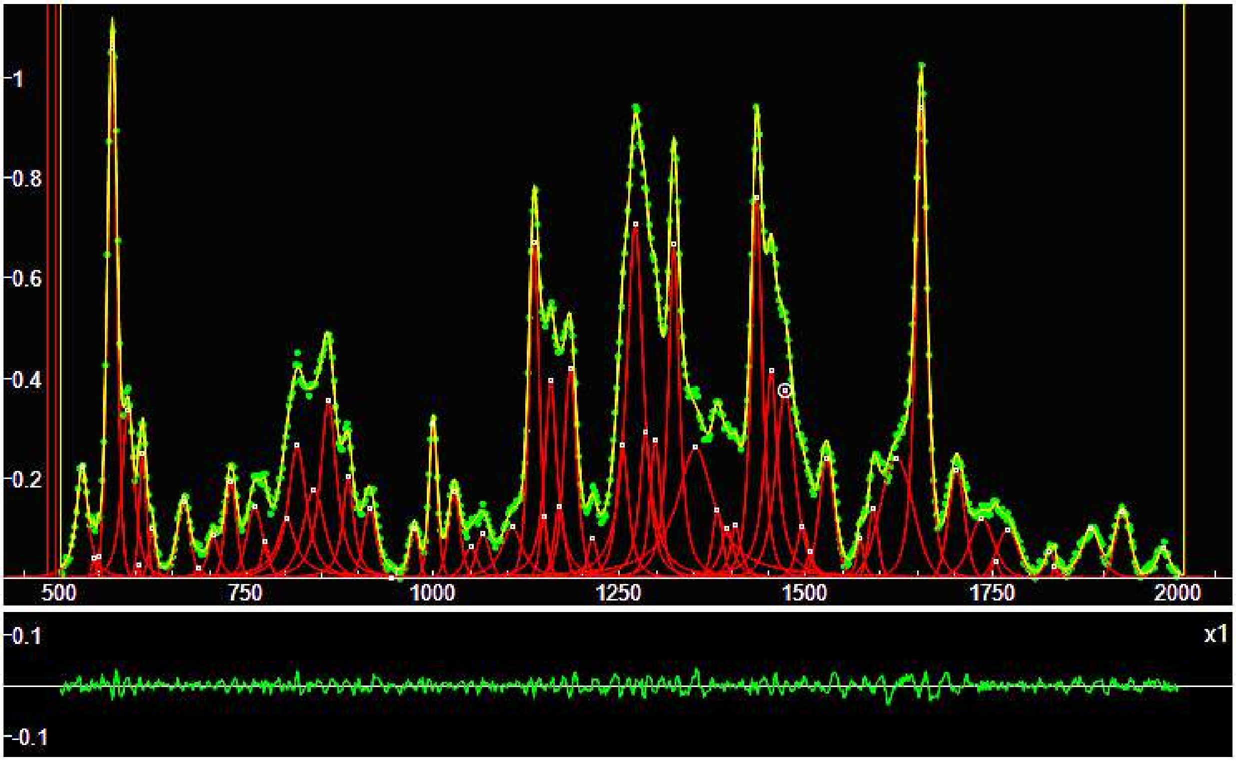
503	*597*	642(s)	***812(s)***	940	*1034(s)*
1128	1165	*1223*	***1258(s)***	*1329(vs)*	1416
1470(s)	1531(vs)	1572(s)	***1639(s)***	(***SERS on Au***)	

4-Imidazoleacetic acid



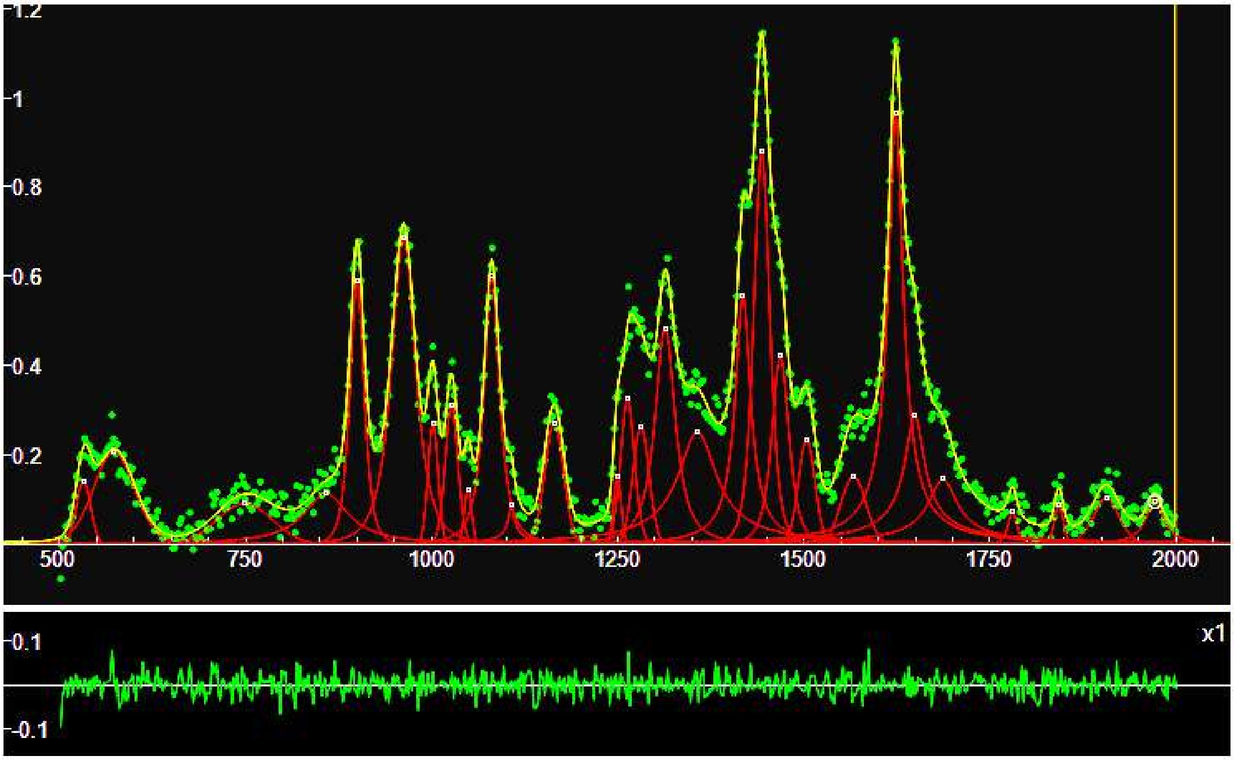
#	PeakType	Parameters	Height	Center	hwhm	q
			(height > 0.15, **bold** h > 0.34)			
%_1	**Qgau**	**555.252**	**0.764792**	**555.252**	**17.93**	**1.40203**
%_3	**Qgau**	**713.995**	**0.468404**	**713.995**	**11.9505**	**1.38044**
%_7	**Qgau**	**760.418**	**0.370185**	**760.418**	**10.7779**	**1.8768**
%_4	**Qgau**	**850.971**	**0.412089**	**850.971**	**16.4771**	**1.44034**
%_11	Qgau	802.976	0.283064	802.976	11.1995	1.31442
%_9	**Qgau**	**883.791**	**0.345797**	**883.791**	**14.8631**	**1.51016**
%_16	Qgau	974.925	0.152207	974.925	8.70443	1.92419
%_5	**Qgau**	**995.636**	**0.434743**	**995.636**	**7.16485**	**1.69447**
%_17	Qgau	1027.03	0.159663	1027.03	10.8022	1.10759
%_45	Qgau	1160.65	0.190324	1160.65	16.5144	0.999652
%_18	Qgau	1221.97	0.157471	1221.97	12.8491	0.999793
%_48	Qgau	1297.28	0.155587	1297.28	18.7029	1.20064
%_12	Qgau	1271.12	0.231336	1271.12	21.0803	1.53804
%_6	Qgau	1312.81	0.289805	1312.81	12.2031	1.47017
%_49	Qgau	1378.03	0.212151	1378.03	20.4595	1.58675
%_50	Qgau	1409.66	0.162721	1409.66	13.5699	1.01189
%_2	**Qgau**	**1440.34**	**0.572245**	**1440.34**	**17.772**	**1.86828**
%_8	**Qgau**	**1468.1**	**0.353439**	**1468.1**	**15.9704**	**0.999734**
%_15	Qgau	1598.85	0.170455	1598.85	26.1734	1.35947
%_10	Qgau	1630.28	0.246575	1630.28	16.5975	1.76537

5-oxo-L-proline



#	PeakType	Center	Parameters	Height	Center	HWHM	q	(height > 0.15, **bold** h > 0.40)
%_16	Qgau	528.376		0.224202	528.376	9.23023	1.91342	
%_1	**Qgau**	**568.666**		**1.06175**	**568.666**	**8.58585**	**1.1483**	
%_7	Qgau	589.823		0.339663	589.823	10.2177	1.68003	
%_19	Qgau	609.842		0.254816	609.842	6.35479	1.17895	
%_17	Qgau	727.871		0.193114	727.871	10.5156	1.09687	
%_15	Qgau	816.969		0.264728	816.969	15.3226	1.76945	
%_50	Qgau	859.092		0.356304	859.092	13.3166	1.8101	
%_51	Qgau	885.448		0.202675	885.448	8.85459	2.0062	
%_10	Qgau	999.791		0.309807	999.791	7.17605	1.30205	
%_55	**Qgau**	**1135.27**		**0.669826**	**1135.27**	**9.25538**	**1.35581**	
%_56	Qgau	1157.69		0.394534	1157.69	9.67869	1.96836	
%_12	**Qgau**	**1183.75**		**0.421502**	**1183.75**	**11.0511**	**1.40259**	
%_66	Qgau	1253.9		0.265053	1253.9	9.95135	1.77494	
%_58	**Qgau**	**1270.66**		**0.711915**	**1270.66**	**13.5148**	**1.87724**	
%_59	Qgau	1284.51		0.293077	1284.51	9.29025	1.97957	
%_68	Qgau	1298.04		0.277126	1298.04	9.12413	1.64683	
%_6	**Qgau**	**1322.94**		**0.666514**	**1322.94**	**9.00307**	**1.84737**	
%_14	Qgau	1351.85		0.261353	1351.85	29.2274	2.12759	
%_62	**Qgau**	**1434.18**		**0.762772**	**1434.18**	**9.57799**	**1.59745**	
%_63	**Qgau**	**1453.44**		**0.417919**	**1453.44**	**10.2565**	**2.05014**	
%_39	Qgau	1472.4		0.37552	1472.4	16.3574	1.52171	
%_18	Qgau	1528.17		0.238252	1528.17	14.0235	1.16648	
%_11	Qgau	1622.01		0.239853	1622.01	30.9479	0.999241	
%_2	**Qgau**	**1655.26**		**0.93971**	**1655.26**	**9.83303**	**1.58128**	
%_64	Qgau	1702.53		0.214659	1702.53	14.9946	1.079	

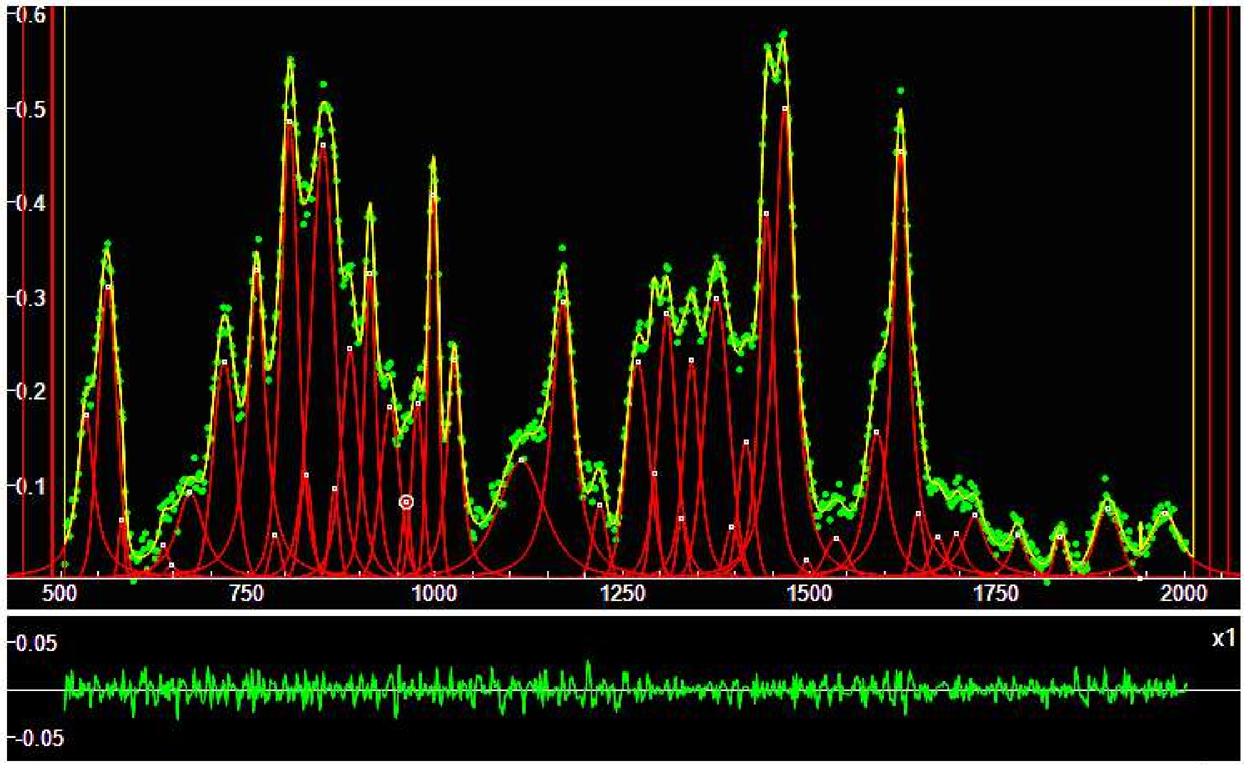
Agmatine Sulfate



#	PeakType	Parameters	Height	Center	HWHM	q (height > 0.14, **bold** h >0.40)
%_18	Qgau	531.981	0.141439	531.981	13.6065	0.999929
%_15	Qgau	572.887	0.207158	572.887	38.6744	1.10126
%_6	**Qgau**	**899.53**	**0.590259**	**899.53**	**12.48**	**1.45465**
%_3	**Qgau**	**962.038**	**0.687379**	**962.038**	**20.6693**	**1.59863**
%_13	Qgau	1001.56	0.273127	1001.56	9.40753	1.0002
%_11	Qgau	1026.6	0.31235	1026.6	11.7838	1.12164
%_5	**Qgau**	**1080.54**	**0.600028**	**1080.54**	**12.9321**	**1.76471**
%_12	Qgau	1164.45	0.273022	1164.45	17.8005	0.999546
%_21	Qgau	1249.18	0.153476	1249.18	7.28787	1.00039
%_8	Qgau	1263.06	0.326839	1263.06	12.8507	1.15016
%_16	Qgau	1281.07	0.264179	1281.07	15.3649	0.999829
%_7	**Qgau**	**1313.54**	**0.485759**	**1313.54**	**16.7005**	**1.81503**
%_14	Qgau	1356.9	0.251929	1356.9	31.6421	2.29504
%_4	**Qgau**	**1418.07**	**0.55933**	**1418.07**	**12.4194**	**2.1354**
%_1	**Qgau**	**1443.39**	**0.87945**	**1443.39**	**14.0127**	**1.40472**
%_9	**Qgau**	**1468.42**	**0.422695**	**1468.42**	**14.7778**	**1.53927**
%_19	Qgau	1503.74	0.235537	1503.74	15.7858	0.999895
%_17	Qgau	1566.57	0.152636	1566.57	23.8556	0.99957
%_2	**Qgau**	**1623.31**	**0.969752**	**1623.31**	**12.0288**	**2.27352**
%_10	Qgau	1648.89	0.289271	1648.89	16.2633	2.69073
%_26	Qgau	1686.76	0.146647	1686.76	24.1083	2.53812

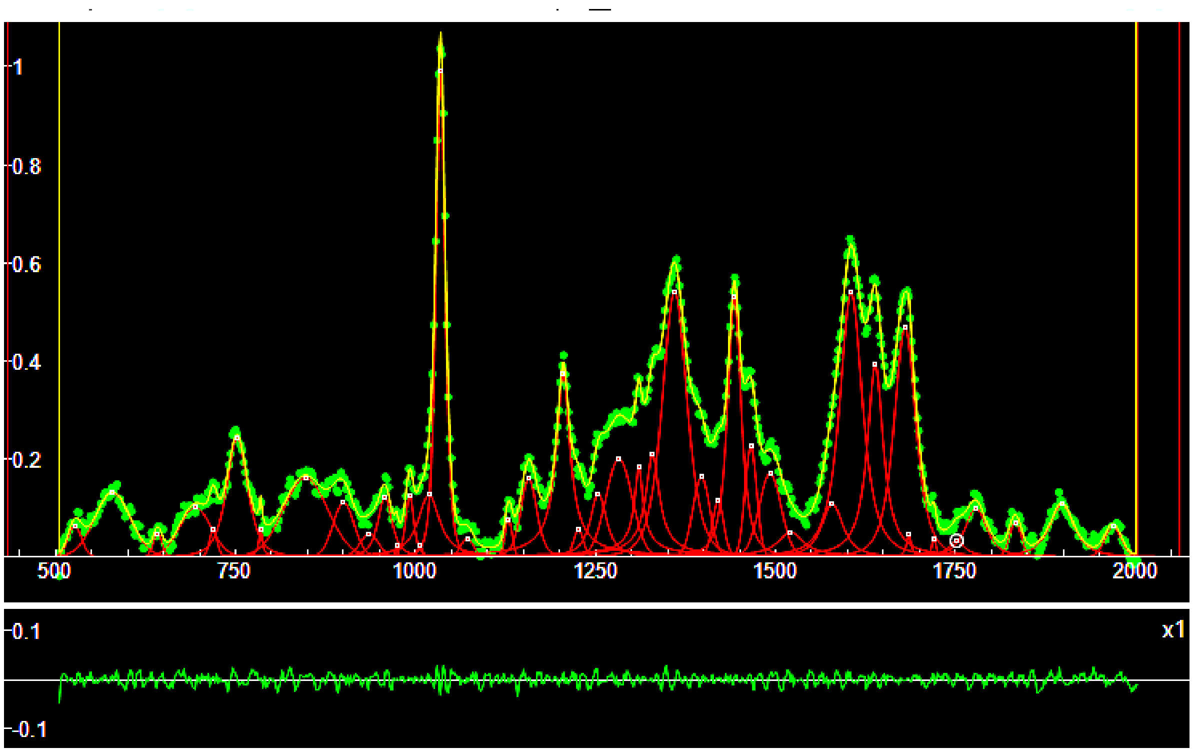
Biliverdin

According to Sherman et al., spectra of biliverdin have been proposed by Celis et al.,2016.



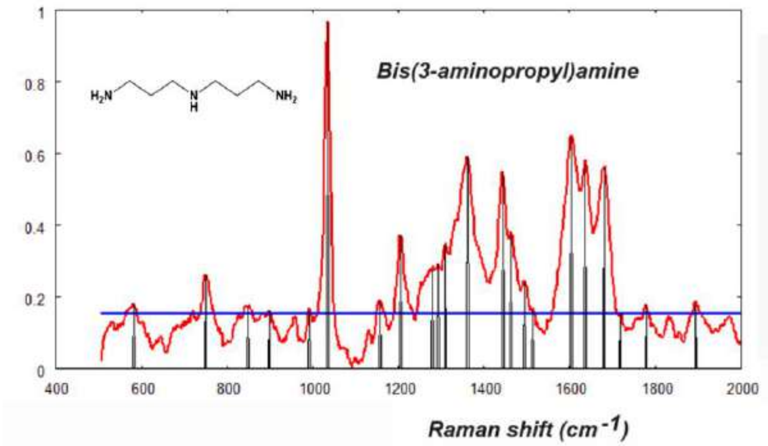
#	PeakType	Center	Parameters Height	Center	HWHM	q (Height > 0.15, bold h > 0.30)
%_20	Qgau	533.17	0.174925	533.17	13.156	2.10512
%_8	**Qgau**	**562.325**	**0.3109**	**562.325**	**17.5031**	**0.999854**
%_13	Qgau	717.943	0.230636	717.943	20.4684	0.999767
%_10	**Qgau**	**761.161**	**0.327309**	**761.161**	**14.1227**	**1.97741**
%_2	**Qgau**	**805.309**	**0.4853**	**805.309**	**15.0605**	**1.37269**
%_4	**Qgau**	**849.804**	**0.46121**	**849.804**	**20.691**	**1.3117**
%_15	Qgau	886.358	0.244251	886.358	15.4334	1.50217
%_7	**Qgau**	**912.946**	**0.325374**	**912.946**	**10.0145**	**1.55505**
%_19	Qgau	939.655	0.182866	939.655	17.7734	1.05464
%_31	Qgau	976.137	0.187003	976.137	10.9601	0.99991
%_5	**Qgau**	**997.166**	**0.407926**	**997.166**	**9.84068**	**1.00002**
%_16	Qgau	1025.11	0.233371	1025.11	11.5146	1.79901
%_9	Qgau	1169.97	0.293996	1169.97	18.2218	1.82655
%_14	Qgau	1270.02	0.229655	1270.02	21.4019	0.999217
%_12	Qgau	1309.02	0.281782	1309.02	15.9272	1.42901
%_17	Qgau	1342.05	0.231364	1342.05	13.6724	1.57671
%_11	Qgau	1375.8	0.296836	1375.8	23.0032	0.999329
%_1	**Qgau**	**1465.91**	**0.499978**	**1465.91**	**17.0584**	**1.77127**
%_6	**Qgau**	**1442.35**	**0.387912**	**1442.35**	**12.5895**	**1.62978**
%_18	Qgau	1589.69	0.155373	1589.69	17.9558	1.77618
%_3	**Qgau**	**1621.32**	**0.456948**	**1621.32**	**13.1644**	**1.96945**

Bis(3-aminopropyl)amine



#	PeakType	Center		Parameters	Height	Center	HWHM	q (H > 0.09, **Bold** H>0.2)
%_14	Qgau	579.14	x	x	0.130698	579.14	34.7279	1.01466
%_21	Qgau	694.096	x	x	0.100422	694.096	30.8049	0.999445
%_9	**Qgau**	**752.297**	**x**	**x**	**0.242158**	**752.297**	**18.8103**	**1.48545**
%_13	Qgau	847.294	x	x	0.160348	847.294	43.3934	0.998588
%_23	Qgau	900.084	x	x	0.110346	900.084	20.65	0.999714
%_20	Qgau	957.422	x	x	0.122052	957.422	12.4786	1.62887
%_41	Qgau	991.932	x	x	0.126049	991.932	7.30613	1.49002
%_42	Qgau	1018.49	x	x	0.126318	1018.49	18.2717	1.88191
%_1	**Qgau**	**1034.71**	**x**	**x**	**0.992971**	**1034.71**	**8.27992**	**1.43966**
%_11	Qgau	1157.24	x	x	0.16046	1157.24	14.7725	1.3027
%_6	**Qgau**	**1205.03**	**x**	**x**	**0.376324**	**1205.03**	**10.9745**	**2.25702**
%_15	Qgau	1253.94	x	x	0.12978	1253.94	13.7609	1.81443
%_30	**Qgau**	**1282.55**	**x**	**x**	**0.200504**	**1282.55**	**25.6306**	**0.999089**
%_29	Qgau	1310.01	x	x	0.18663	1310.01	6.98851	2.72594
%_28	**Qgau**	**1329.17**	**x**	**x**	**0.209496**	**1329.17**	**11.2987**	**2.30499**
%_3	**Qgau**	**1359.87**	**x**	**x**	**0.540645**	**1359.87**	**22.6112**	**1.402**
%_32	Qgau	1396.93	x	x	0.162643	1396.93	16.5709	0.999655
%_35	Qgau	1420.03	x	x	0.114052	1420.03	10.8879	1.10331
%_31	**Qgau**	**1442.77**	**x**	**x**	**0.531637**	**1442.77**	**11.6138**	**1.68907**
%_34	**Qgau**	**1465.67**	**x**	**x**	**0.225919**	**1465.67**	**11.3358**	**0.999893**
%_10	Qgau	1492.34	x	x	0.170111	1492.34	21.4431	1.03815
%_18	Qgau	1578.86	x	x	0.107916	1578.86	18.7236	1.6849
%_2	**Qgau**	**1604.88**	**x**	**x**	**0.540546**	**1604.88**	**19.8346**	**1.64896**
%_7	**Qgau**	**1638.54**	**x**	**x**	**0.393314**	**1638.54**	**13.4776**	**1.9372**
%_5	**Qgau**	**1679.79**	**x**	**x**	**0.46947**	**1679.79**	**19.3682**	**1.50165**
%_19	Qgau	1778.16	x	x	0.0990565	1778.16	19.0525	1.61508
%_16	Qgau	1897.68	x	x	0.106957	1897.68	21.2605	1.67011

Bis(3-aminpropyl)amine has been already investigated in Sparavigna, 2023. Here in the following image, the peaks are determined with the first-derivative spectrum. The blue line represents a threshold.



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
581.50	0.18	1361.50	0.59
749.00	0.26	1444.00	0.55
849.00	0.17	1462.50	0.37
897.50	0.16	1495.00	0.24
991.50	0.16	1513.00	0.16
1035.00	0.97	1604.00	0.64
1157.50	0.19	1636.00	0.57
1204.00	0.37	1680.00	0.56
1280.00	0.27	1717.50	0.16
1292.50	0.29	1778.00	0.18
1309.50	0.34	1894.50	0.17

Let us compare the positions in the Table given above with the centers of the q-Gaussians given below. Some little differences exist.

581.50	749.00	849.00	897.50	991.00	1035.00
1157.50	1204.00	1280.00	1292.50	1309.50	1361.50
1444.00	1462.50	1495.00	1513.00	1604.00	1636.00
1680.00	1717.00	1778.00	1894.50		

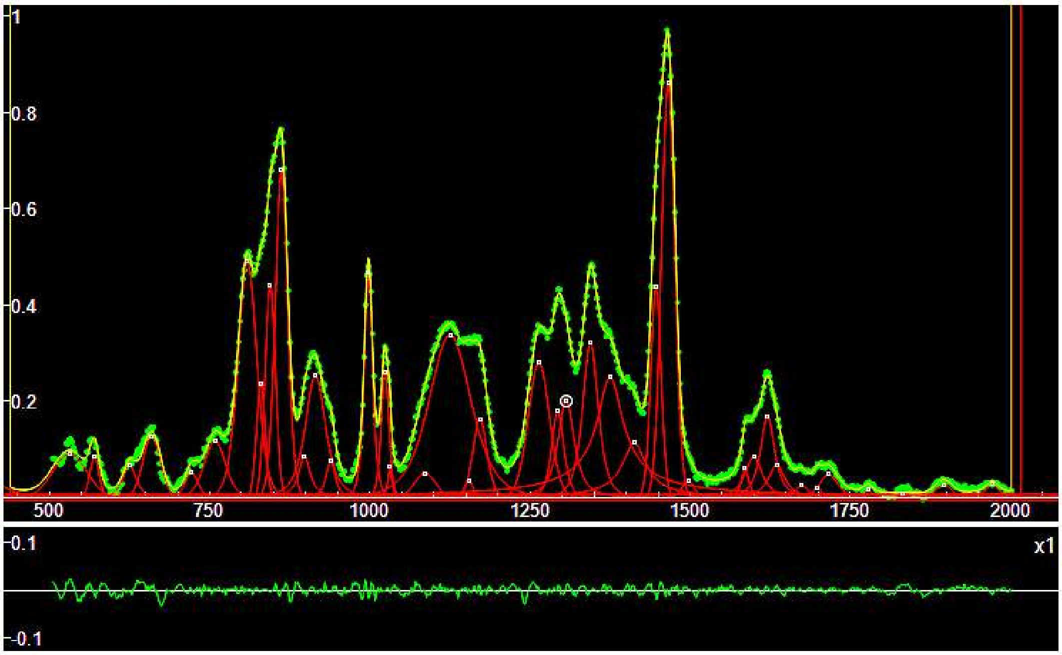
579.14	694.096	752.297(m)	847.294	900.084	957.422
991.932	1018.49	1034.71(vs)	1157.24	1205.03(s)	1253.94
1282.55(m)	1310.01(m)	1329.17 (m)	1359.87(s)	1396.93	1420.03
1442.77(s)	1465.67(m)	1492.34	1578.86	1604.88(s)	1638.54(s)
1679.79(s)	1778.16	1897.68			

For other metabolites proposed in Sparavigna, 2023, we can observe differences. Differences are due to the involved methods, that is, deconvolution in components of the spectrum, and use of the first-derivative spectrum. Moreover, further differences come from the used baselines.

Regarding literature, let us suggest the article by Dongil et al., 2014, about the insertion of bis (3-aminopropyl) amine into graphite oxide.

Caffeine

SERS spectra have previously been reported (Sherman et al., 2020) in the literature (Pavel et al., 2003, Alharbi et al, 2015, Zheng et al., 2016). Let us also add Edwards et al., 2005, Baranska and Proniewicz, 2008, Hédoux et al., 2011, Kang et al., 2011, and Zareef et al., 2020.



# PeakType	Center	Parameters Height	Center	HWHM	q (height above 0.08, **Bold** h > 0.30)
%_16 Qgau	531.467	0.0914161	531.467	37.4459	0.999352
%_24 Qgau	569.994	0.085199	569.994	9.80618	1.18148
%_14 Qgau	659.489	0.127382	659.489	19.6592	0.999786
%_21 Qgau	758.035	0.119518	758.035	22.6832	1.18291
%_40 Qgau	**808.885**	**0.493561**	**808.885**	**19.6707**	**1.22397**
%_41 Qgau	829.743	0.237029	829.743	9.62846	0.999943
%_37 Qgau	**844.438**	**0.444253**	**844.438**	**11.1953**	**1.00685**
%_36 Qgau	**862.005**	**0.682168**	**862.005**	**13.2155**	**1.12924**
%_42 Qgau	897.898	0.0880217	897.898	10.8249	1.99505
%_10 Qgau	914.965	0.255041	914.965	20.1982	1.56256
%_19 Qgau	938.797	0.0769385	938.797	9.1078	1.69223
%_4 Qgau	**997.683**	**0.469875**	**997.683**	**8.54077**	**1.39884**
%_11 Qgau	1023.56	0.261468	1023.56	8.03156	1.26004
%_34 Qgau	**1125.1**	**0.339096**	**1125.1**	**43.4381**	**1.38016**
%_15 Qgau	1171.76	0.164507	1171.76	14.7999	1.24373
%_17 Qgau	1263.71	0.28104	1263.71	23.0412	1.07572
%_32 Qgau	1293.27	0.179753	1293.27	12.5303	1.41733
%_35 Qgau	1306.26	0.202028	1306.26	15.9324	1.76058
%_3 Qgau	**1344.26**	**0.323139**	**1344.26**	**15.5518**	**1.52349**
%_8 Qgau	1374.9	0.251476	1374.9	24.763	2.66219
%_54 Qgau	1412.57	0.114308	1412.57	22.75	2.28797
%_53 Qgau	**1446.46**	**0.437509**	**1446.46**	**11.0786**	**1.0769**
%_49 Qgau	**1465.53**	**0.865632**	**1465.53**	**14.6203**	**0.999798**
%_2 Qgau	1620.66	0.169268	1620.66	13.8408	1.7399

Therefore, the q-Gaussian centers are:

531.467	569.994	659.489	758.035	808.885(s)	829.743
844.438(s)	862.005(vs)	897.898	914.965(m)	938.797	997.683(s)
1023.56(m)	1125.1(s)	1171.76	1263.71(m)	1293.27	1306.26
1344.26(s)	1374.9(m)	1412.57	1446.46(s)	1465.53(vs)	1620.66

In the following, these centers are compared with data from literature (bold, within 5 cm^{-1}, and italic. within 10 cm^{-1}).

Pavel et al. give the following peaks for SERS pH 2.5:

375 392 450 488(m) 555 611 648(m) 693 745(m) ***806***

926 980 ***1028*** 1066 1078 1237(m) *1253* *1285* 1325(vs) 1362

1390 ***1414*** *1436* 1555 1604(m) 1657 1712(m)

And for SERS pH 8.5 (Pavel et al.):

316 366 420 472 *526* ***570(s)*** 613 640(s) 686(m) ***754*** *800*

926 952 1036 1063 1075 ***1130*** *1162(m)* 1223 1236(m) ***1311(vs)***

1359(vs) *1384(s)* 1398(m) ***1414(s)*** 1496 1540 1607(vs) 1649

Pavel et al. are also proposing Raman data:

223 314 367 391 444 483 555(vs) 609 643 698 740 *801* 927 974 ***1021***

1073 1134 1191 1214 1241 1251 *1283* 1327(vs) 1359 1391 ***1409*** 1431 *1454* ***1470*** 1488

1552 1599(s) 1654 1698(s)

Alharbi et al., 2015, are providing the SERS peaks at:

509 650 693 1006 1247 1450 1672

Zheng et al., 2016:

556(vs) 644(s) 741(s) *801(s)* 928 974 ***1020*** 1239 *1284* 1328(vs) *1410* 1601 (Raman)

607 *658* ***807(vs)*** 958(s) 1040(vs) ***1269*** 1327 ***1415*** 1593 (SERS)

Edwards et al., 2005:

391 442 483 555(s) 647 744 *890* *930* 1076 1242 1255 ***1290*** 1333(s) 1361 ***1409***
1445 *1475* 1551 1605(s) 1698(s) (Raman, Caffeine hydrate)

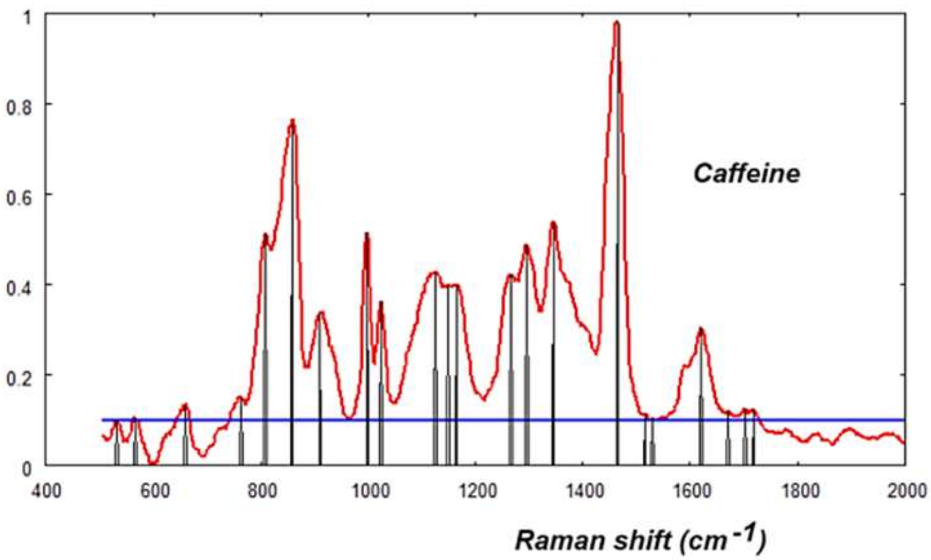
390 442 484 556(s) 644 741 928 1073 1241 1251 1284 1328 1360 1408 *1456*
1470 1554 1600(s) 1654 1698(s) (Raman, Anhydrous caffeine)

Baranska and Proniewicz (2008):

555(s) 647 *890* *930* 1076 *1255* *1290* 1333(s) 1361 ***1409*** 1605(s) 1698(s) (Caffeine hydrate)

556(s) 644 928 1073 *1284* 1328(s) 1360 ***1408*** 1554 1600 1656 1698(s) (Anhydrous caffeine)

Caffeine has been already investigated in [Sparavigna, 2023](). Here in the following image, the peaks are determined with the first-derivative spectrum. The blue line represents a threshold.



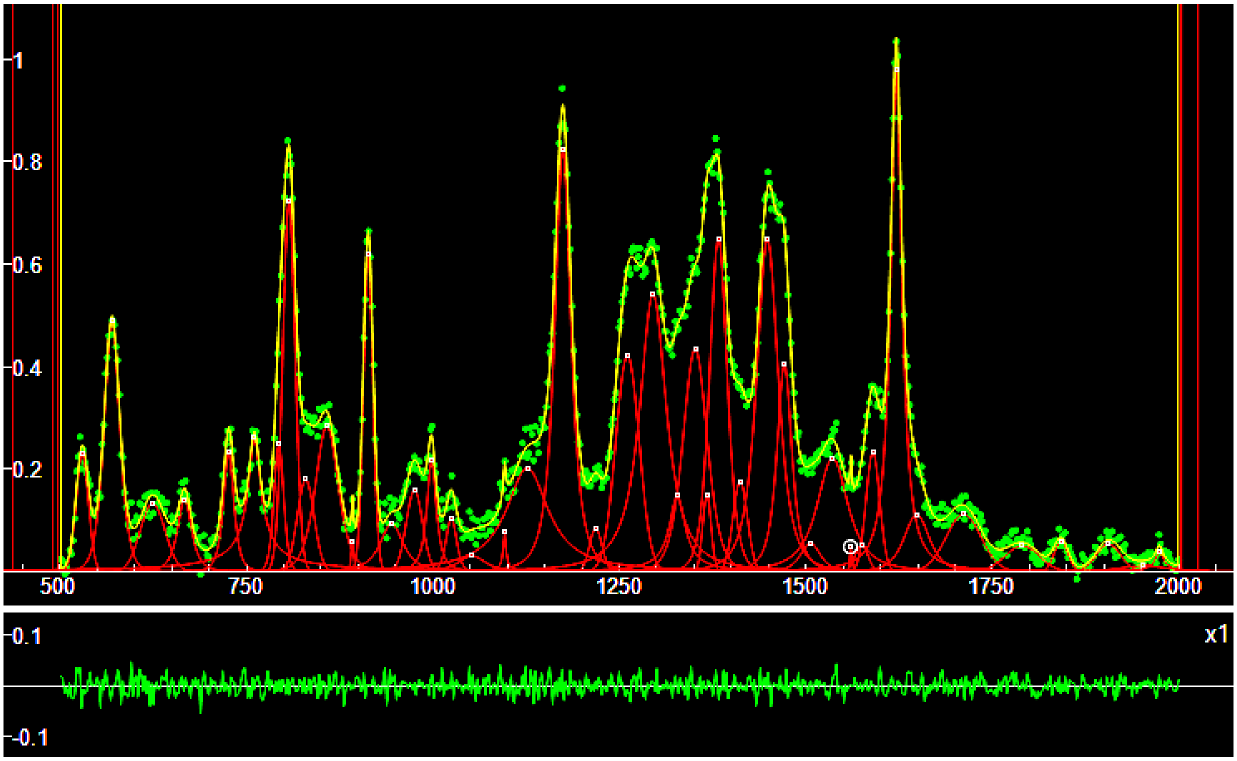
Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
531.50	0.10	1164.00	0.40
565.50	0.11	1265.50	0.42
659.00	0.13	1294.50	0.49
762.50	0.15	1344.50	0.54
809.00	0.51	1464.50	0.98
858.00	0.75	1515.00	0.11
911.00	0.34	1529.50	0.10
998.00	0.51	1620.00	0.31
1024.00	0.36	1670.00	0.12
1125.50	0.43	1701.50	0.12
1149.00	0.40	1717.50	0.12

Let us compare the peaks with the q-Gaussian centers:

531.50	565.50	659.00	762.50	809.00	858.00
911.00	998.00	1024.00	1125.50	1149.00	1164.00
1265.50	1294.50	1344.50	1464.50	1515.00	1529.50
1620.00	1670.00	1701.50	1717.50		

531.467	569.994	659.489	758.035	808.885(s)	829.743
844.438(s)	862.005(vs)	897.898	914.965(m)	938.797	997.683(s)
1023.56(m)	1125.1(s)	1171.76	1263.71(m)	1293.27	1306.26
1344.26(s)	1374.9(m)	1412.57	1446.46(s)	1465.53(vs)	1620.66

Carbamoyl phosphate

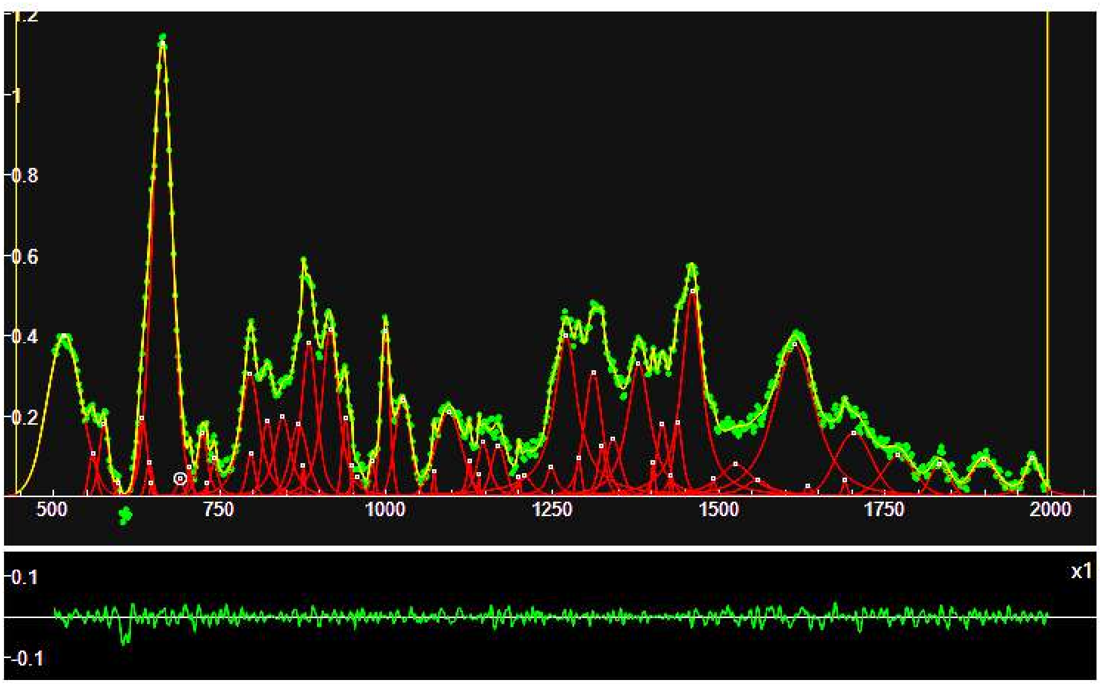


# PeakType		Center	Parameters	Height	Canter	HWHM	q (height > 0.15)
%_19	Qgau	529.632		0.2308	529.632	11.8033	0.999936
%_9	**Qgau**	**569.467**		**0.490629**	**569.467**	**14.0025**	**1.33428**
%_15	Qgau	725.927		0.233332	725.927	9.02135	1.54307
%_18	Qgau	760.699		0.265129	760.699	10.3407	2.68279
%_22	Qgau	793.269		0.248517	793.269	8.83712	1.20726
%_4	**Qgau**	**806.832**		**0.723814**	**806.832**	**11.4589**	**1.04653**
%_23	Qgau	829.329		0.180475	829.329	16.0023	0.999889
%_13	Qgau	857.749		0.284789	857.749	20.336	1.34815
%_6	**Qgau**	**913.15**		**0.620673**	**913.15**	**8.87531**	**1.04599**
%_32	Qgau	975.079		0.159856	975.079	15.4962	0.999819
%_36	Qgau	998.132		0.216574	998.132	7.77219	1.82106
%_16	Qgau	1126.44		0.202827	1126.44	34.3326	2.01955
%_2	**Qgau**	**1174.09**		**0.825171**	**1174.09**	**13.5993**	**1.65408**
%_10	**Qgau**	**1260.74**		**0.42221**	**1260.74**	**22.0917**	**0.999168**
%_7	**Qgau**	**1295.13**		**0.542871**	**1295.13**	**22.0708**	**1.83263**
%_8	**Qgau**	**1351.43**		**0.435548**	**1351.43**	**21.822**	**1.29374**
%_41	Qgau	1367.29		0.151474	1367.29	7.95077	0.999968
%_3	**Qgau**	**1382.71**		**0.652717**	**1382.71**	**15.6097**	**1.32574**
%_25	Qgau	1411.9		0.176713	1411.9	13.5878	0.99981
%_5	**Qgau**	**1448.45**		**0.649994**	**1448.45**	**18.4651**	**1.57792**
%_12	**Qgau**	**1471.16**		**0.406851**	**1471.16**	**12.4476**	**1.65054**
%_17	Qgau	1535.79		0.221965	1535.79	25.8216	1.74478
%_11	Qgau	1589.78		0.233724	1589.78	13.0755	0.999927
%_1	**Qgau**	**1621.16**		**0.989627**	**1621.16**	**9.11309**	**1.96347**

Bold characters for peaks with height > 0.40.

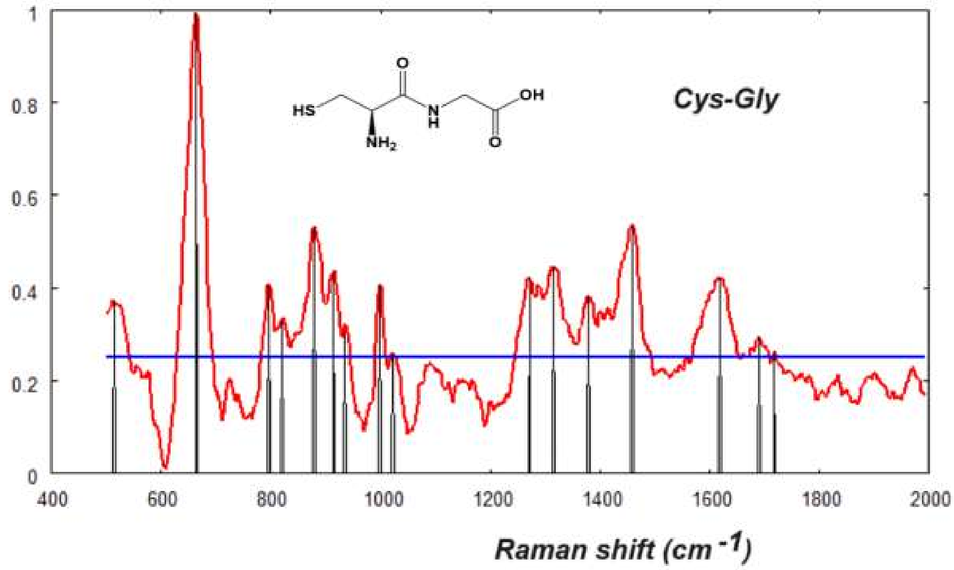
Cys-Gly

Literature from Sherman et al. for L-cysteine-L-glycine (Cys-Gly) is Dong and Lam, 2011. Let us add literature about L-methionine (Met), L-cysteine (Cys), L-glycine (Gly), L-leucine (Leu), L-phenylalanine (Phe), L-proline (Pro) and their homodipeptides Met-Met, Cys-Cys, Gly-Gly, LeuLeu, Phe-Phe, and Pro-Pro in Podstawka et al., 2004.



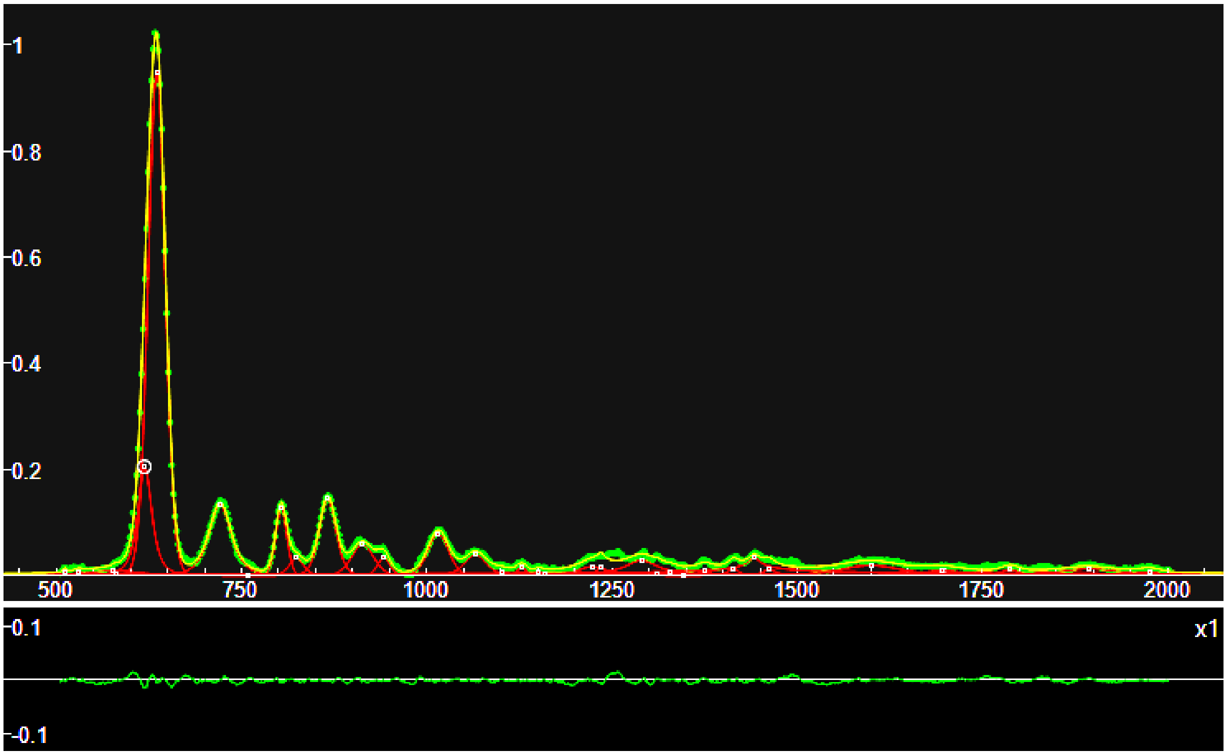
#	PeakType	Parameters	Height	Center	HWHM	q (height > 0.15, **Bold h>** 0.30.)
%_9	**Qgau**	**516.208**	**0.40208**	**516.208**	**36.0095**	**0.999502**
%_19	Qgau	575.76	0.179343	575.76	10.326	1.08231
%_30	Qgau	633.528	0.194436	633.528	10.2605	0.999985
%_1	**Qgau**	**663.469**	**1.12826**	**663.469**	**20.6749**	**1.09642**
%_37	Qgau	724.519	0.159834	724.519	8.42838	1.72293
%_7	**Qgau**	**795.423**	**0.30453**	**795.423**	**18.0011**	**1.60324**
%_35	Qgau	821.7	0.188433	821.7	11.6658	0.999944
%_36	Qgau	844.294	0.198055	844.294	15.2784	1.73081
%_5	Qgau	868.75	0.180306	868.75	17.5994	1.26083
%_2	**Qgau**	**884.198**	**0.381497**	**884.198**	**14.8583**	**1.43791**
%_11	**Qgau**	**915.966**	**0.416355**	**915.966**	**15.5626**	**1.65283**
%_23	Qgau	938.925	0.193715	938.925	7.20694	1.00005
%_6	**Qgau**	**998.637**	**0.412255**	**998.637**	**9.53423**	**1.03149**
%_15	Qgau	1024.93	0.240581	1024.93	16.5256	0.999827
%_14	Qgau	1093.86	0.210649	1093.86	27.4441	0.999073
%_39	**Qgau**	**1270.57**	**0.400027**	**1270.57**	**20.5671**	**2.11077**
%_4	**Qgau**	**1311.35**	**0.310678**	**1311.35**	**17.1461**	**1.41395**
%_10	**Qgau**	**1379.98**	**0.331637**	**1379.98**	**21.538**	**1.7499**
%_42	Qgau	1415.37	0.181311	1415.37	10.3524	1.60629
%_41	Qgau	1439.05	0.184089	1439.05	8.51605	1.70917
%_3	**Qgau**	**1460**	**0.513357**	**1460**	**18.1175**	**1.9337**
%_8	**Qgau**	**1614.33**	**0.376848**	**1614.33**	**39.1264**	**1.61849**
%_17	Qgau	1703.33	0.158477	1703.33	37.9622	0.999093

Cys-Gly has been already investigated in Sparavigna, 2023. Here in the following image, the peaks are determined with the first-derivative spectrum. The blue line represents a threshold.



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
514.00	0.37	1023.00	0.26
663.50	0.99	1271.50	0.42
795.50	0.40	1315.50	0.44
820.00	0.33	1379.50	0.38
879.50	0.53	1460.00	0.53
914.50	0.44	1619.50	0.42
934.00	0.30	1691.00	0.29
999.00	0.41	1718.50	0.26

Cysteamine



#	PeakType	Center	Parameters	Height	Center	HWHM	q
%_53	**Qgau**	**619.372**		**0.204235**	**619.372**	**11.9654**	**1.60872**
%_52	**Qgau**	**635.414**		**0.952468**	**635.414**	**15.8847**	**1.07473**
%_3	**Qgau**	**721.027**		**0.133766**	**721.027**	**19.2694**	**1.49283**
%_4	**Qgau**	**803.55**		**0.127846**	**803.55**	**10.303**	**1.10061**
%_15	Qgau	824.036		0.0328436	824.036	12.9071	1.3223
%_2	**Qgau**	**866.25**		**0.144842**	**866.25**	**15.1942**	**1.22946**
%_7	**Qgau**	**913.294**		**0.0581742**	**913.294**	**20.6005**	**1.14986**
%_12	Qgau	941.912		0.0333498	941.912	11.5504	1.15299
%_6	**Qgau**	**1015.42**		**0.0785633**	**1015.42**	**19.3324**	**1.107**
%_10	Qgau	1065.66		0.0396224	1065.66	18.9899	1.40754
%_14	Qgau	1128.24		0.0145713	1128.24	9.26353	1.14423
%_17	Qgau	1223.44		0.0170236	1223.44	24.0621	1.80948
%_40	Qgau	1235.28		0.0169896	1235.28	5.69847	3.09605
%_37	Qgau	1289.88		0.0289994	1289.88	26.7493	2.12131
%_42	Qgau	1413.84		0.0139418	1413.84	8.35939	1.92051
%_43	Qgau	1442.05		0.0345895	1442.05	10.7688	5.08741
%_46	Qgau	1462.52		0.0120811	1462.52	10.3275	2.05886
%_47	Qgau	1599.2		0.0193048	1599.2	53.817	1.52384
%_45	Qgau	1787.63		0.0114776	1787.63	16.2027	1.4014
%_16	Qgau	1894.5		0.0128305	1894.5	53.4924	1.77827

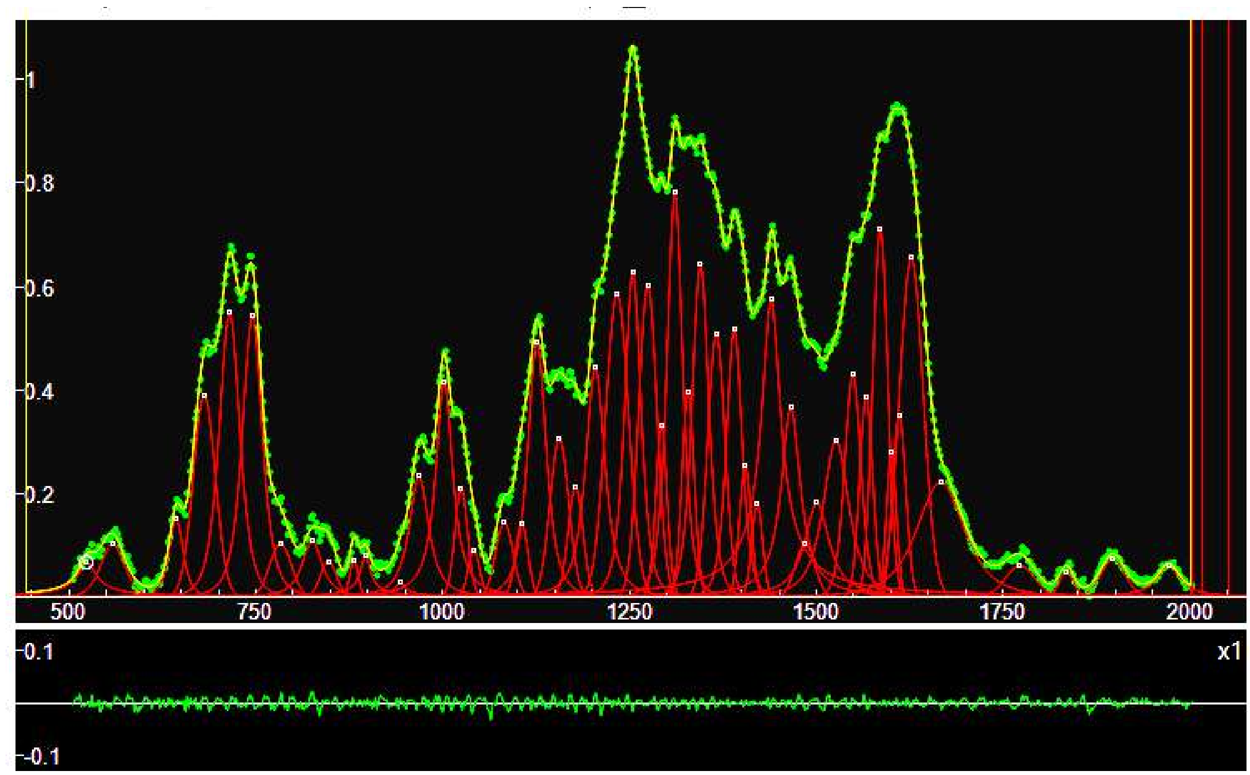
Bold characters for peaks with height above 0.05.

Literature given by Sherman et al. for this molecule is Michota et al., 2000, 2001, 2002, Goto and Watarai, 2010, and Jiang et al., 2013. Let us add Kudelski and Hill, 1999. Cysteamine has been investigated in [Sparavigna, 2023](). Let us compare the data from first-derivative spectrum (first line), the q-Gaussian deconvolution by Fityk (second line) and literature:

Sherman et al.,	634	721	804.5	866.5	910	1015.5				
Sherman et al.,	619.5	635.5	721.0	803.5	824.0	866.25	913.3	941.9	1015.42	1065.7
Jiang et al., 2013, Cys/silver:	387	640	831	978	1047					
Jiang et al., 2013, Cys powder:	510	661	793	987	1045					
Kudelski and Hill, 1999, Cys solid	758	938	1012							
Kudelski and Hill, 1999, Cys sol	510	666	753	817	936	1013				
Kudelski and Hill, 1999, Cys mono	509	640	726	946	1014					

Cytochrome C

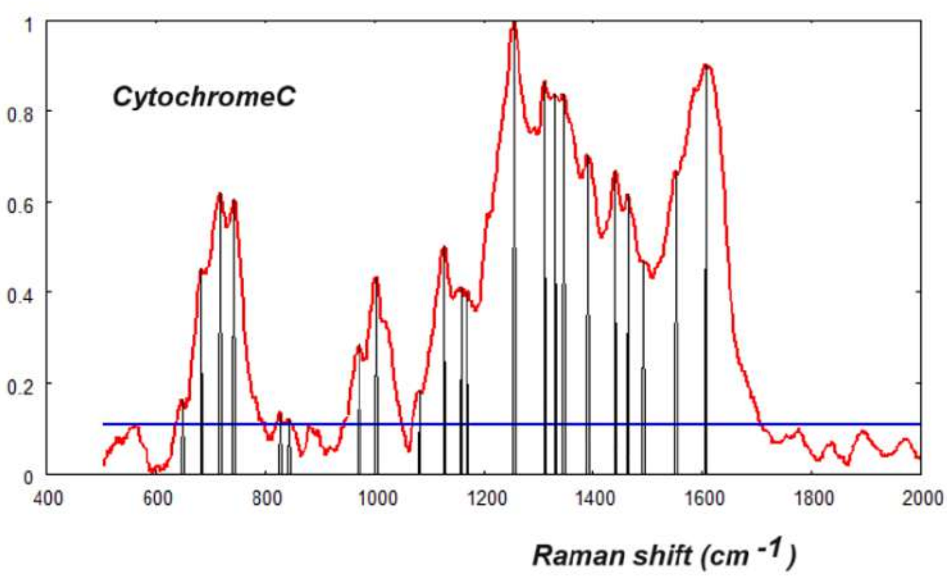
Literature reported for this molecule by Sherman et al. are Delfino et al., 2005, and Qu et al., 2013. Let us add Strekas and Spiro, 1972, Murgida and Hildebrandt, 2004, Brazhe et al., 2015.



#	PeakType	Center	Parameters	Height	Center	HWHM	q
%_19	Qgau	524.007		0.0665223	524.007	15.4766	2.65571
%_14	Qgau	558.22		0.102031	558.22	21.8446	1.2526
%_30	Qgau	643.299		0.15255	643.299	12.0515	1.53655
%_21	Qgau	680.953		0.389964	680.953	20.8036	0.999835
%_10	Qgau	714.676		0.549271	714.676	18.0899	1.40682
%_16	Qgau	745.247		0.543089	745.247	17.1963	1.49251
%_38	Qgau	782.973		0.103346	782.973	20.3319	0.999729
%_39	Qgau	825.162		0.10808	825.162	16.9665	1.73982
%_40	Qgau	846.971		0.0694217	846.971	14.8549	1.05378
%_41	Qgau	881.247		0.071215	881.247	7.99838	1.00014
%_42	Qgau	896.626		0.0798935	896.626	8.31753	2.58221
%_43	Qgau	943.359		0.0275413	943.359	8.47648	3.08027
%_24	Qgau	968.248		0.233349	968.248	16.1786	1.77344
%_17	Qgau	1001.9		0.416649	1001.9	13.7546	1.88213
%_27	Qgau	1024.56		0.21091	1024.56	11.6871	1.08861
%_44	Qgau	1041.69		0.0902759	1041.69	11.073	0.99988
%_29	Qgau	1082.3		0.144294	1082.3	16.3373	0.999685
%_37	Qgau	1105.64		0.142968	1105.64	11.7425	0.999916
%_15	Qgau	1126.05		0.492147	1126.05	15.7547	1.558
%_26	Qgau	1155.92		0.306745	1155.92	17.5873	1.00102
%_45	Qgau	1177.57		0.213898	1177.57	14.0123	0.999713
%_46	Qgau	1204.12		0.443974	1204.12	16.126	1.69247
%_7	Qgau	1233.29		0.586131	1233.29	21.599	0.999393

%_1	Qgau	1254.25	0.629822	1254.25	14.1421	1.45585
%_12	Qgau	1274.22	0.603109	1274.22	17.2482	0.99957
%_47	Qgau	1292.44	0.332256	1292.44	10.4378	1.05884
%_3	Qgau	1310.41	0.781752	1310.41	13.7177	1.4388
%_18	Qgau	1328.28	0.394971	1328.28	11.4888	1.01836
%_5	Qgau	1344.82	0.644361	1344.82	14.6778	1.35589
%_13	Qgau	1366.09	0.509742	1366.09	16.1313	1.02208
%_8	Qgau	1390.07	0.521596	1390.07	13.4729	1.39543
%_23	Qgau	1404.69	0.253934	1404.69	10.9671	1.00553
%_32	Qgau	1420.65	0.181244	1420.65	10.1295	1.00002
%_9	Qgau	1439.28	0.575297	1439.28	15.366	2.43357
%_48	Qgau	1465.68	0.366737	1465.68	15.5325	2.0157
%_51	Qgau	1484.82	0.104432	1484.82	18.1162	0.999736
%_33	Qgau	1500.77	0.182177	1500.77	19.8606	1.95793
%_22	Qgau	1526.15	0.303098	1526.15	21.6399	1.66666
%_11	Qgau	1548.56	0.430224	1548.56	14.7971	1.21239
%_20	Qgau	1566.47	0.386362	1566.47	12.4199	1.00012
%_4	Qgau	1585.35	0.713699	1585.35	14.1155	0.999965
%_36	Qgau	1600.18	0.280777	1600.18	9.33993	0.999949
%_2	Qgau	1610.71	0.352325	1610.71	12.4385	1.00108
%_6	Qgau	1626.96	0.655939	1626.96	22.3783	0.999763
%_25	Qgau	1666.03	0.221657	1666.03	40.9672	1.54301
%_34	Qgau	1772.46	0.0608262	1772.46	27.8928	0.99964
%_50	Qgau	1834.45	0.0488929	1834.45	13.6795	0.999914
%_35	Qgau	1896.62	0.0732631	1896.62	22.1991	1.17009
%_52	Qgau	1971.16	0.0606333	1971.16	18.9365	2.08492

Cytochrome C has been already investigated in Sparavigna, 2023. Here in the following image, the peaks are determined with the first-derivative spectrum. The blue line represents a threshold.



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
647.50	0.16	1170.00	0.40
683.50	0.45	1255.00	1.00
717.50	0.62	1311.50	0.86
742.00	0.60	1330.00	0.84
827.00	0.13	1344.50	0.84
842.50	0.12	1390.50	0.70
972.00	0.28	1439.50	0.66
1002.50	0.43	1464.50	0.62
1082.50	0.18	1493.00	0.47
1127.50	0.50	1551.50	0.66
1157.50	0.41	1606.00	0.90

In Delfino et al., 2005, Figs. 1,3,6, and Table 1, we can find the following data:

750 ***1128*** ***1172*** ***1230*** ***1313*** ***1363*** *1398* ***1544*** ***1584*** *1621* 1639 (Raman, liquid)

746 ***1127*** *1170* *1226* ***1310*** *1358* *1396* 1488 *1539* ***1584*** *1621* (Raman, solid)

674 ***750*** 804 ***1130*** ***1174*** ***1232*** *1314* *1375* *1400* 1408 1501 *1540* 1568 ***1587*** ***1605*** ***1626*** 1640 (Delfino et al. Table 1, Raman data from literature)

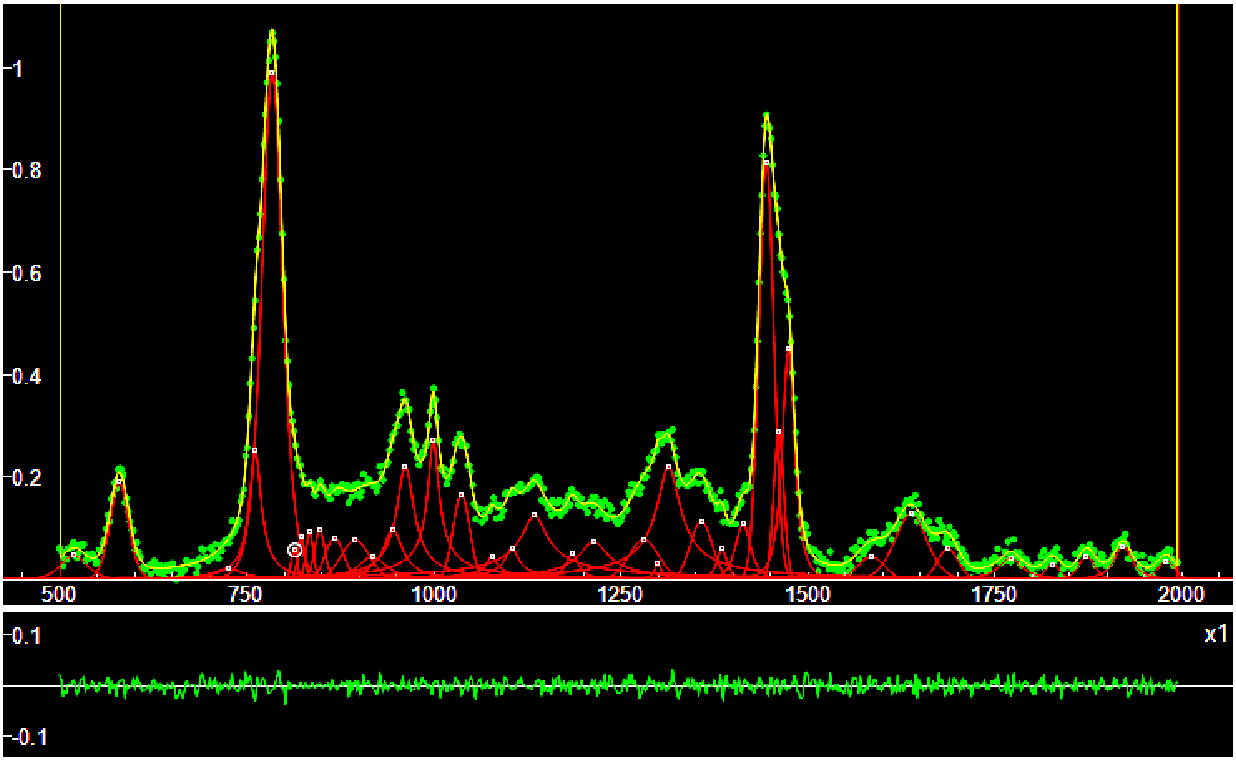
674 804 1144 ***1312*** *1360* ***1391*** 1498 ***1584*** ***1622*** (SERS: aver. 1800 spectra)

667 *1167* ***1310*** *1360* 1398 1483 *1534* ***1562*** ***1604*** 1640 (SERS, averaged 500 spectra)

These data are compared with the q-Gaussian centers (bold, within +/− 5 cm^{-1}, italic, within +/− 10 cm^{-1}). Here the q-Gaussian centers for h>0.2, given for the reader's convenience.

680.953	714.676(s)	745.247(s)	968.248	1001.9(s)	1024.56
1126.05(s)	1155.92	1177.57	1204.12(s)	1233.29(s)	1254.25(s)
1274.22(s)	1292.44	1310.41(vs)	1328.28(s)	1344.82(vs)	1366.09(s)
1390.07(s)	1404.69	1439.28(s)	1465.68	1526.15	1548.56(s)
1566.47	1585.35(vs)	1600.18	1610.71	1626.96(vs)	1666.03

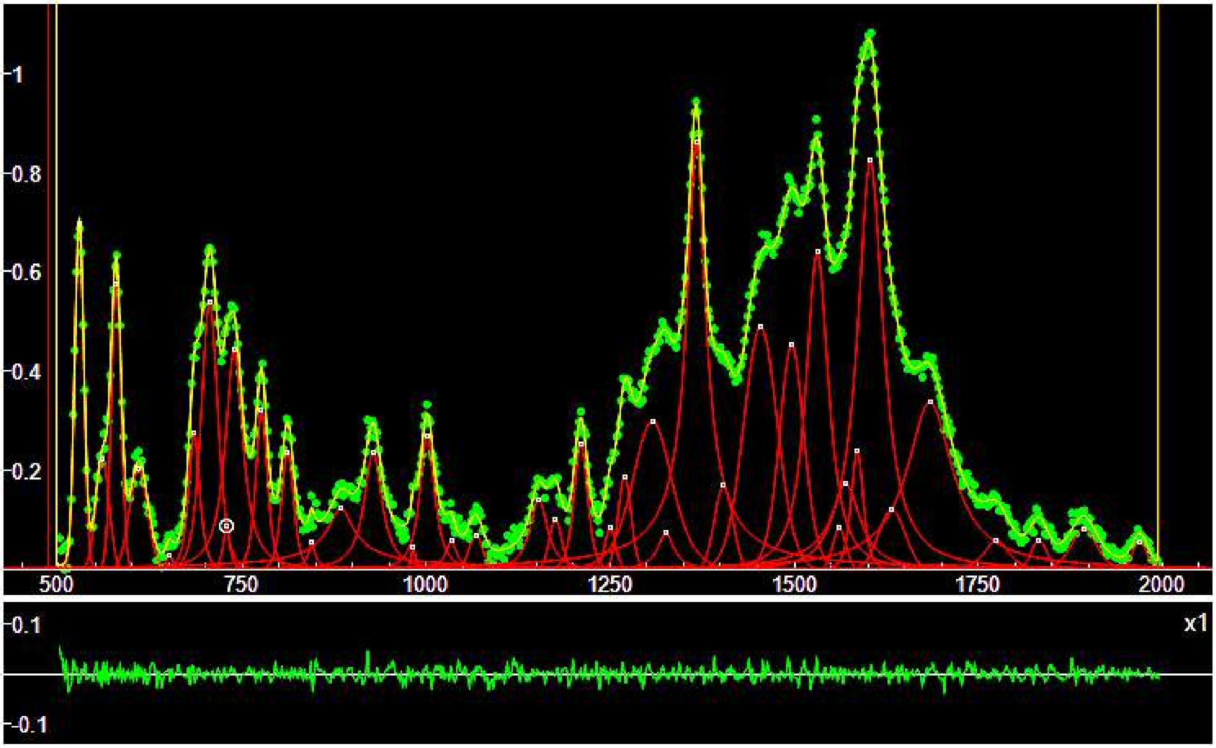
Dethiobiotin



#	PeakType	Parameters	Height	Center	HWHM	q (height above 0.07)
%_7	**Qgau**	**578.68**	**0.190438**	**578.68**	**16.921**	**1.19041**
%_38	**Qgau**	**760.673**	**0.252403**	**760.673**	**9.65629**	**2.26665**
%_1	Qgau	783.367	0.99309	783.367	18.3984	1.33456
%_12	Qgau	822.016	0.0854246	822.016	6.46117	1.06604
%_45	Qgau	833.28	0.0930614	833.28	6.80514	1.04078
%_46	Qgau	846.752	0.0979455	846.752	9.1957	1.25281
%_47	Qgau	866.47	0.0821213	866.47	17.3897	0.999762
%_26	Qgau	894.455	0.0775728	894.455	27.2074	0.999583
%_24	Qgau	944.662	0.0987189	944.662	15.9579	2.21752
%_48	**Qgau**	**961.429**	**0.222232**	**961.429**	**14.068**	**2.3805**
%_25	**Qgau**	**998.843**	**0.274798**	**998.843**	**8.86197**	**2.82286**
%_15	**Qgau**	**1036.23**	**0.166533**	**1036.23**	**15.8576**	**0.999817**
%_29	**Qgau**	**1133.98**	**0.125745**	**1133.98**	**22.331**	**3.08859**
%_31	Qgau	1213.26	0.0742828	1213.26	25.0431	2.67602
%_13	Qgau	1280.39	0.078985	1280.39	27.851	1.04968
%_4	**Qgau**	**1313.43**	**0.220736**	**1313.43**	**19.5478**	**2.68583**
%_11	**Qgau**	**1357.22**	**0.114636**	**1357.22**	**20.8055**	**0.999752**
%_41	**Qgau**	**1413.03**	**0.109597**	**1413.03**	**12.9737**	**1.59281**
%_2	**Qgau**	**1444.12**	**0.818909**	**1444.12**	**13.9328**	**1.01764**
%_39	**Qgau**	**1460.83**	**0.288385**	**1460.83**	**9.54964**	**1.00154**
%_6	**Qgau**	**1473.8**	**0.451347**	**1473.8**	**10.505**	**1.65764**
%_9	**Qgau**	**1637.53**	**0.128455**	**1637.53**	**29.6106**	**1.19058**

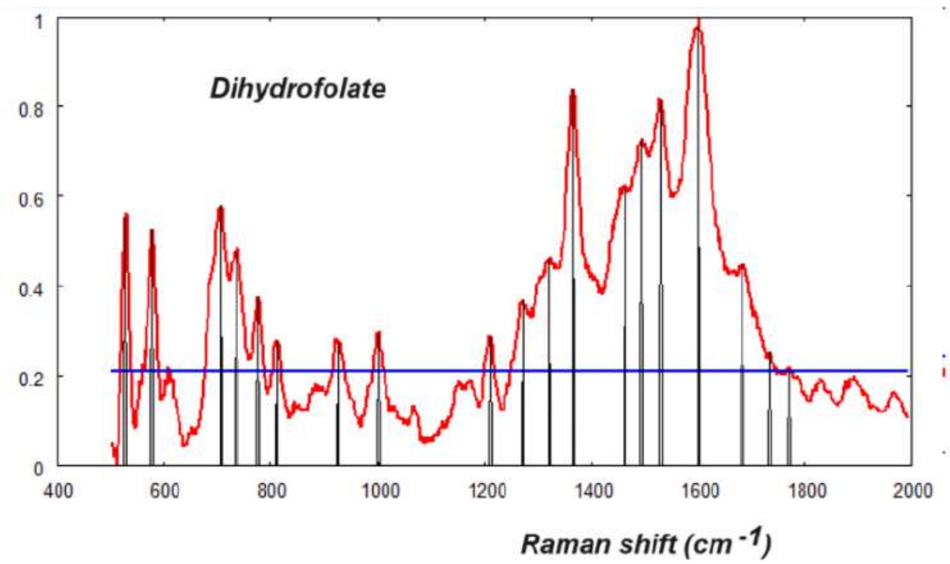
Bold characters for peaks with height above 0.10**.**

Dihydrofolate



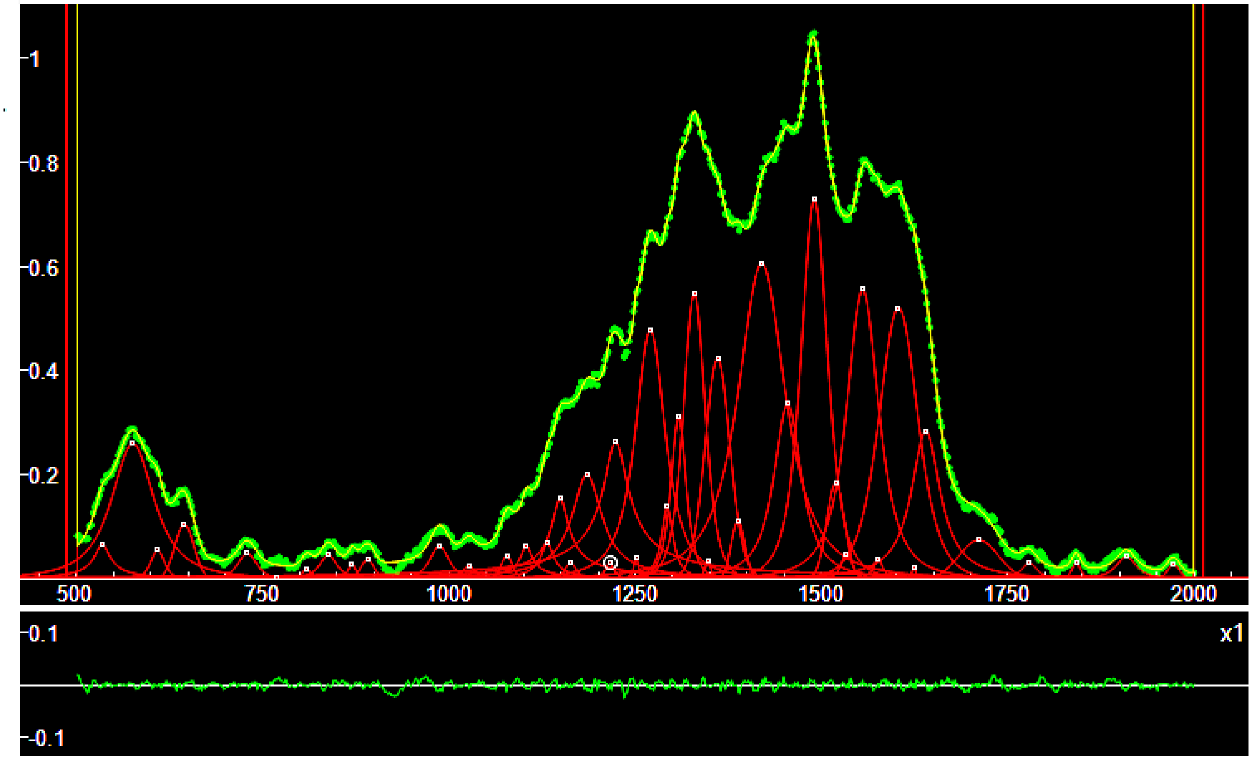
# PeakType		Center	Parameters	Height	Center	HWHM	q (h > 0.10)
%_4	Qgau	528.205		0.697782	528.205	8.65267	1.00005
%_18	Qgau	559.681		0.223815	559.681	12.6656	0.99996
%_7	Qgau	578.362		0.583572	578.362	9.31023	0.999993
%_17	Qgau	608.8		0.205068	608.8	17.2193	0.999883
%_34	Qgau	684.291		0.275614	684.291	9.81341	1.50131
%_37	Qgau	705.346		0.539975	705.346	14.7896	1.35482
%_16	Qgau	738.75		0.444069	738.75	14.707	1.87372
%_11	Qgau	776.017		0.324381	776.017	10.144	1.44044
%_15	Qgau	811.299		0.239531	811.299	11.0422	1.32977
%_22	Qgau	883.682		0.124332	883.682	22.5751	3.00253
%_13	Qgau	927.545		0.237626	927.545	14.7601	1.94793
%_12	Qgau	1001.11		0.271069	1001.11	12.4548	1.77097
%_19	Qgau	1152.67		0.142714	1152.67	14.7877	1.86662
%_29	Qgau	1175.46		0.101007	1175.46	12.0616	0.999841
%_14	Qgau	1209.84		0.252755	1209.84	12.355	1.33154
%_21	Qgau	1269.41		0.189598	1269.41	12.0718	1.07746
%_9	Qgau	1307.06		0.299586	1307.06	36.2467	1.27972
%_2	Qgau	1366.73		0.863951	1366.73	15.2401	2.43106
%_3	Qgau	1531.22		0.640838	1531.22	18.7888	1.81117
%_23	Qgau	1403.9		0.169579	1403.9	17.4865	0.999731
%_8	Qgau	1454.19		0.489505	1454.19	32.0238	1.06053
%_6	Qgau	1496.6		0.453765	1496.6	22.8429	1.17814
%_43	Qgau	1570.01		0.173565	1570.01	24.2429	1.94286
%_20	Qgau	1585.59		0.240223	1585.59	10.7385	1.45946
%_1	Qgau	1603.55		0.824487	1603.55	21.0216	1.96897
%_42	Qgau	1632.72		0.121448	1632.72	25.5122	0.999496
%_10	Qgau	1684.36		0.33811	1684.36	37.6321	2.11617

Dihydrofolate has been already investigated in Sparavigna, 2023. Here in the following image, the peaks are determined with the first-derivative spectrum. The blue line represents a threshold.



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
527.50	0.55	1321.50	0.46
577.50	0.53	1367.50	0.84
706.50	0.58	1464.00	0.62
735.50	0.47	1494.50	0.72
775.50	0.38	1531.00	0.81
811.00	0.28	1601.50	0.98
925.50	0.27	1683.00	0.45
1001.50	0.29	1734.00	0.25
1210.50	0.29	1771.50	0.21
1271.50	0.37		

Dopamine



#	PeakType	Center	Parameters:	Height	Center	HWHM	q (height > 0.05)
%_18	Qgau	534.576		0.0672526	534.576	13.2355	2.66539
%_11	Qgau	575.637		0.260624	575.637	35.6865	1.76787
%_28	Qgau	608.927		0.0561813	608.927	12.0024	1.47542
%_15	Qgau	644.773		0.105925	644.773	18.2131	0.999819
%_21	Qgau	729.245		0.049647	729.245	16.5314	1.54131
%_42	Qgau	986.91		0.0641393	986.91	16.1713	1.6481
%_41	Qgau	1103.72		0.065592	1103.72	9.64448	2.97502
%_25	Qgau	1131.79		0.0705868	1131.79	10.1616	2.64804
%_40	Qgau	1149.17		0.155478	1149.17	14.3976	2.91933
%_39	Qgau	1184.99		0.201346	1184.99	24.5155	2.17509
%_38	Qgau	1223.72		0.263353	1223.72	21.6693	2.84917
%_5	Qgau	1270.06		0.478972	1270.06	25.0395	1.74123
%_19	Qgau	1292.81		0.139714	1292.81	9.24206	2.00442
%_12	Qgau	1307.9		0.310811	1307.9	13.3339	1.55029
%_49	Qgau	1329.14		0.549262	1329.14	19.4215	1.37303
%_8	Qgau	1360.27		0.424096	1360.27	23.063	1.1419
%_22	Qgau	1387.63		0.112341	1387.63	12.8744	0.999797
%_46	Qgau	1419.65		0.606993	1419.65	39.8152	1.71804
%_45	Qgau	1490.15		0.729414	1490.15	22.8775	1.49893
%_10	Qgau	1518.73		0.185404	1518.73	17.067	0.999727
%_47	Qgau	1555.12		0.556087	1555.12	27.1367	1.67997
%_7	Qgau	1603.08		0.521465	1603.08	34.8251	1.34361
%_13	Qgau	1639.73		0.285107	1639.73	23.8022	1.96959
%_16	Qgau	1710.88		0.0755049	1710.88	37.3299	0.999049

Sherman et al. report literature: Wang et al., 2015, and McGlashen et al., 1990.

Data from Wang et al, are:
591 635 771 816 1267 1358 1424 1482 (SERS, Wang et al., 2015)

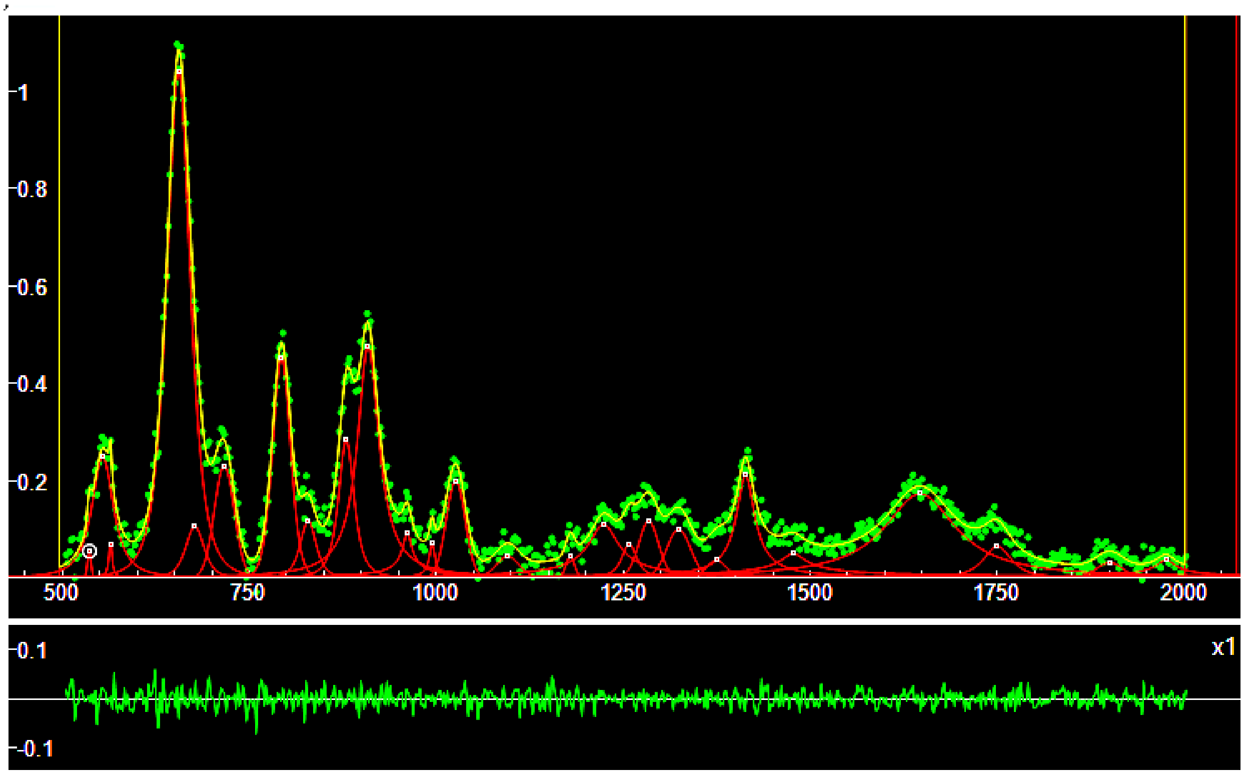
In McGlashen et al., we find mentioned the C—O stretch mode at 1269 cm^{-1} and v_{19b} at 1479 cm^{-1} "which is primarily a phenyl C—C stretch".

Here the q-Gaussian centers for comparison:

534.576	575.637(m)	608.927	644.773	729.245	986.91
1103.72	1131.79	1149.17	1184.99(m)	1223.72(m)	***1270.06(s)***
1292.81	1307.9(m)	1329.14(s)	***1360.27(s)***	1387.63	***1419.65(vs)***
1490.15(vs)	1518.73	1555.12(s)	1603.08(s)	1639.73(m)	1710.88

Some centers have been marked, in ***bold*** for correspondence within +/− 5 cm^{-1}.

Glutathione



#	PeakType	Center		Parameters	Height	Center	HWHM	q (height > 0.05)
%_27	Qgau	536.007	x	x	0.0547519	536.007	3.24141	1.00018
%_5	**Qgau**	**553.927**	**x**	**x**	**0.249743**	**553.927**	**17.8992**	**1.77739**
%_24	Qgau	564.306	x	x	0.0837745	564.306	2.06509	2.24099
%_1	**Qgau**	**655.401**	**x**	**x**	**1.04599**	**655.401**	**20.3839**	**1.49549**
%_16	Qgau	677.241	x	x	0.105765	677.241	16.0279	1.45826
%_7	**Qgau**	**716.463**	**x**	**x**	**0.230702**	**716.463**	**18.7528**	**0.999787**
%_3	**Qgau**	**793.173**	**x**	**x**	**0.453925**	**793.173**	**16.3589**	**1.17664**
%_11	Qgau	828.748	x	x	0.117624	828.748	13.6246	1.52802
%_4	**Qgau**	**879.585**	**x**	**x**	**0.284483**	**879.585**	**13.0842**	**1.62667**
%_2	**Qgau**	**909.018**	**x**	**x**	**0.4779**	**909.018**	**17.5125**	**2.02669**
%_13	Qgau	961.236	x	x	0.0918966	961.236	8.14201	2.95923
%_25	Qgau	994.473	x	x	0.0708151	994.473	4.53895	2.3707
%_8	**Qgau**	**1025.87**	**x**	**x**	**0.20019**	**1025.87**	**17.8638**	**0.99994**
%_14	Qgau	1223.66	x	x	0.110315	1223.66	24.5172	2.50792
%_22	Qgau	1257.96	x	x	0.0699137	1257.96	12.6826	1.70807
%_10	Qgau	1283.86	x	x	0.117212	1283.86	18.2406	1.11297
%_12	Qgau	1323.99	x	x	0.0997824	1323.99	22.6173	0.999256
%_6	**Qgau**	**1413.39**	**x**	**x**	**0.211364**	**1413.39**	**14.7713**	**2.29633**
%_9	Qgau	1646.89	x	x	0.173046	1646.89	58.2366	2.0528
%_15	Qgau	1750.11	x	x	0.0646977	1750.11	23.5459	1.71593

Literature provided by Sherman et al.: Huang et al., 2009, and Podstawka et al., 2004.

Here the centers of the q-Gaussian components (in cm^{-1}):

536.007	553.927(m)	564.306	655.401(vs)	677.241	716.463(m)
793.173(s)	828.748	879.585(m)	909.018(s)	961.236	994.473
1025.87(m)	1223.66	1257.96	1283.86	1323.99	1413.39(m)
1646.89	1750.11				

In De Gelder et al., 2007, we find the following Raman peaks for Glutathione (in bold, the peaks which are corresponding to centers, within +/− 5 cm^{-1} of the q-Gaussians given above; in italic, within +/− 10 cm^{-1}):

400(s), 446(w), 523(w), ***550(m),*** 625(vs), 643(m), ***660(s), 679(vs),*** *722(w),* 776(s), 811(m), ***828(m),*** 867(m), 885(s), *917(m),* 931(s), *953(m),* 972(m), *988(m),* 1015(m), 1041(m), 1074(w), 1117(w), 1143(w), 1169(m), ***1224(m),*** 1235(m), ***1255(w), 1280(s),*** 1309(m), *1334(m),* 1368(m), 1403(m), ***1415(m),*** 1443(m), 1455(m), 1536(w), 1629(m), 1660(w), 1703(w)

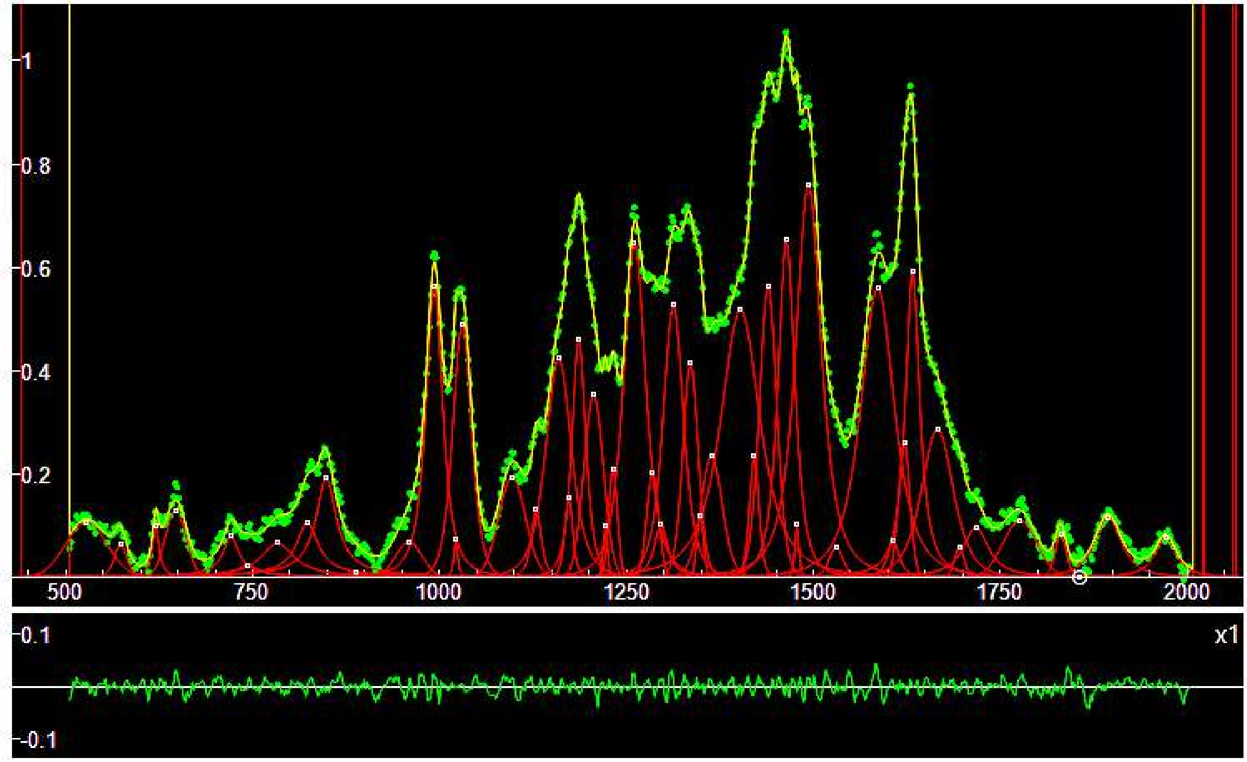
As told by De Gelder and coworkers, "in the spectrum of glutathione, intense bands are related to the presence of the Sulphur atom: (1) (C–S) stretching causes intense bands in the region 600–700 cm^{-1} and (2) the band at 400 cm^{-1} can be assigned to υ(C–S) deformations. Furthermore, the (C-O) stretching of amide and carboxylic groups gives rise to a broad band at 1630 cm^{-1}".
In Huang et al., 2009, a reference suggested by Sherman et al., we have the possibility of a further comparison with the spectrum obtained by means of the "heat-induced surface-enhanced Raman scattering sensing method". Then, let us propose once more the fingerprint obtained from the Sherman et al.'s data (in bold, the centers which are corresponding, within +/− 5 cm^{-1}, to peaks given by Huang et al.):

536.007	553.927(m)	564.306	***655.401***(vs)	677.241	***716.463***(m)
793.173(s)	828.748	***879.585***(m)	***909.018***(s)	961.236	994.473
1025.87(m)	1223.66	***1257.96***	1283.86	1323.99	***1413.39***(m)
1646.89	1750.11	(q-Gaussian centers)			

231 539 ***660*** ***717*** ***795*** 838 ***880*** ***905*** 1007 1034 1053 1125 ***1258*** ***1414***
(Fingerprint from the Table 1, in Huang et al.).

As in De Gelder et al., 2007, Huang and coworkers assign the peak at 660 cm^{-1}, here at 655.4 cm^{-1}, to C-S stretching. Centers at 716.5 and 793.2 cm^{-1} are due to the -COO^{-} deformation and the -COO^{-} bending. Center 879.6 cm^{-1} is coming from the C-C stretching. Component at 909 (905) is assigned by Huang and coworkers to C-COO^{-} stretching. Component with center at 1258 is assigned to amide III. And 1413.4 is assigned to -COO^{-} symmetric stretching.

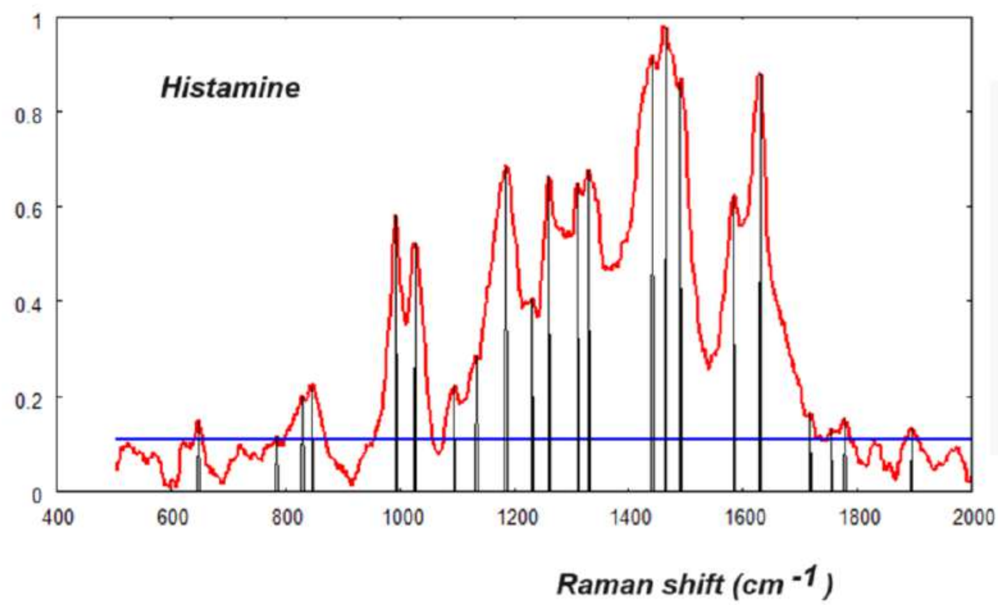
Histamine



#	PeakType	Center	Parameters	Height	Center	HWHM	q ...
%_23	Qgau	527.49	0.106677	527.49	39.0871	0.999351	
%_37	Qgau	573.294	0.0642975	573.294	10.8441	1.44455	
%_36	Qgau	620.383	0.101789	620.383	5.35963	2.04651	
%_19	Qgau	647.079	0.130199	647.079	19.573	0.999995	
%_41	Qgau	720.936	0.0797191	720.936	12.5386	2.39696	
%_42	Qgau	743.498	0.0230481	743.498	18.6459	2.43694	
%_34	Qgau	783.33	0.066663	783.33	26.7276	2.13613	
%_43	Qgau	822.937	0.107349	822.937	17.1129	2.3569	
%_16	Qgau	848.298	0.192326	848.298	16.4116	2.20556	
%_44	Qgau	887.244	0.00907325	887.244	16.6555	2.05575	
%_26	Qgau	958.864	0.0685701	958.864	24.9426	0.999448	
%_9	Qgau	992.868	0.564799	992.868	14.0947	1.70675	
%_35	Qgau	1021.62	0.0748717	1021.62	2.99341	1.77457	
%_11	Qgau	1030.24	0.490134	1030.24	16.9603	1.28823	
%_18	Qgau	1097.03	0.193857	1097.03	25.3574	0.999462	
%_33	Qgau	1129.21	0.133754	1129.21	8.27595	1.59216	
%_13	Qgau	1159.09	0.424256	1159.09	22.468	1.44395	
%_46	Qgau	1172.73	0.153148	1172.73	7.08702	1.42382	
%_4	Qgau	1186.23	0.460229	1186.23	11.936	1.51547	
%_15	Qgau	1205.99	0.354122	1205.99	18.325	0.999479	
%_39	Qgau	1221.55	0.100407	1221.55	4.08317	1.12604	
%_24	Qgau	1231.98	0.21309	1231.98	8.16037	0.999894	
%_7	Qgau	1260.7	0.648215	1260.7	19.0229	1.54029	
%_20	Qgau	1284.93	0.202691	1284.93	11.1322	0.999797	

%_47	Qgau	1296.13	0.104465	1296.13	10.828	1.85523
%_12	Qgau	1312.57	0.527497	1312.57	17.8226	1.45387
%_6	Qgau	1335.63	0.415372	1335.63	13.9069	1.16535
%_30	Qgau	1348.48	0.120394	1348.48	6.29783	1.00758
%_17	Qgau	1363.68	0.235544	1363.68	19.4888	1.16656
%_10	Qgau	1402.3	0.518257	1402.3	33.3744	1.64757
%_49	Qgau	1420.65	0.237078	1420.65	8.34639	1.28701
%_3	Qgau	1439.23	0.564621	1439.23	15.6618	1.18327
%_1	Qgau	1463.9	0.652849	1463.9	14.4634	1.57659
%_50	Qgau	1477.97	0.103674	1477.97	3.25385	1.54925
%_5	Qgau	1493.39	0.761118	1493.39	21.4964	1.66263
%_31	Qgau	1530.22	0.0582327	1530.22	12.8113	1.22813
%_8	Qgau	1585.76	0.559376	1585.76	29.0512	1.59228
%_29	Qgau	1606.85	0.0710362	1606.85	9.44842	1.83661
%_48	Qgau	1621.35	0.263186	1621.35	10.6001	1.05289
%_2	Qgau	1632.61	0.59483	1632.61	11.5678	1.85976
%_14	Qgau	1665.79	0.287285	1665.79	27.7981	1.42708
%_38	Qgau	1695.14	0.0581424	1695.14	9.12184	1.06787
%_28	Qgau	1717.23	0.0974879	1717.23	20.3347	1.99417
%_21	Qgau	1776.11	0.110208	1776.11	32.0432	0.999364
%_32	Qgau	1830.54	0.0838345	1830.54	10.1602	1.19316
%_51	Qgau	1855.88	0.00111574	1855.88	9.07953	1.47953
%_22	Qgau	1894.02	0.117205	1894.02	22.4857	1.69743
%_27	Qgau	1970.96	0.0774743	1970.96	17.5982	1.8575

Histamine has been investigated in Sparavigna, 2023. Here in the following image, the peaks are determined with the first-derivative spectrum. The blue line represents a threshold.



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
647.50	0.15	1311.50	0.65
784.50	0.11	1330.00	0.68
829.00	0.20	1442.00	0.91
847.00	0.22	1464.50	0.98
994.00	0.58	1491.00	0.86
1026.50	0.52	1584.00	0.62
1095.50	0.22	1630.00	0.88
1134.00	0.28	1717.50	0.16
1185.00	0.68	1755.00	0.13
1231.50	0.40	1778.00	0.15
1261.00	0.66	1894.50	0.13

SERS spectra reported by Sherman et al. are Gao et al., 2015, Lin et al., 2012, Janči et al., 2017. Let us mention Chen et al., 2022, 2024, Torreggiani et al., 2003, and Itabashi et al., 1982, too.

In Gao et al., 2015, we can find that "SERS spectral collection was conducted by 10 s exposure times to increase the signal-to-noise ratio. … Featured bands at 1267, 1304, 1317 and 1576 cm^{-1} in the SERS spectra … The enhancement factor based on Raman band of histamine at 1576 cm^{-1} was calculated to be ~104. As the structural analogue of histamine, L-histidine did not show a high SERS activity … Moreover, the band positions could further facilitate distinguishing L-histidine from histamine".
In the Supplementary Data by Gao et al., 2015, we can find the peak assignment of histamine in normal Raman spectroscopy:

1105	*1164*	***1232***	*1267*	*1305*	1320	*1356*	1383	***1440***	1481	1570

That we can compare with the q-Gaussian centers (h>0.15):

848.298	992.868(s)	1030.24(s)	1097.03	1159.09(s)	1172.73
1186.23(s)	1205.99	1231.98	1260.7(vs)	1284.93	1312.57(s)
1335.63	1363.68	1402.3 (s)	1420.65	1439.23(s)	1463.9(vs)
1493.39(vs)	1585.76(s)	1621.35	1632.61(s)	1665.79	

Again, in bold within +/−5 cm^{-1}, in italic within +/−10 cm^{-1}.
Let us consider the data from Lin et al., 2012, from their Table 2, which contains also assignments.

279.66	390.32	634.24	727.24	775.55	819.23
854.01	897.29	927.45	953.21	*983.17*	***1025.78***
1085.07	*1164.85*	***1235.59***	***1289.27***	***1318.03***	*1342.6*
1407.75	*1448.20*	*1472.38*	1536.46	***1623.82***	(Raman)
226.95	407.22	547.88	672.97	***1024.73***	1084.05
1358.07	1378.46	1455.46	1567.1		(SERS)

In the Figure 1 by Janči et al., 2017, we find the peaks at:

1264	*1320*	***1437***	1570	(SERS)

In the Table 1 by Torreggiani et al., 2003, we have the "Wavenumbers and Assignments of Main Raman Bands of Free Hmand Cu(II)-Hm (M/L 1) Aqueous System at pH 9 and 6".

359	379	***989***	***1093***	*1165(m)*		*1230(m)*
1250(sh)	1274(s)	1455(m)	1569(m)	1599		(Raman, pH 9)
289(vs)	394	464	490	536	980	1005(m)
1088	*1270(s)*	***1435(m)***	*1579*	***1590(m)***	***1618***	***1630***
						(Raman, pH 6)

In Itabashi et al., 1982, we find the data (with assignments):

482	630	646(m)	860(m)	940	970
990(m)	1004	*1036*	1075	1090	1102(m)
1160(m)	***1230(m)***	*1268(s)*	*1306(m)*	*1320(m)*	*1354*
1442(m)	***1490(m)***	1570(s)	1590		(Raman, pH 11.85)

480	630	648(m)	852	894	953(m)
990(m)	1006	***1032***	*1090*	1108	***1160(m)***
1230(m)	*1278(vs)*	*1328(m)*	***1360***	1385	1450(m)
1495(m)	1574(s)				(Raman, pH 8,52)

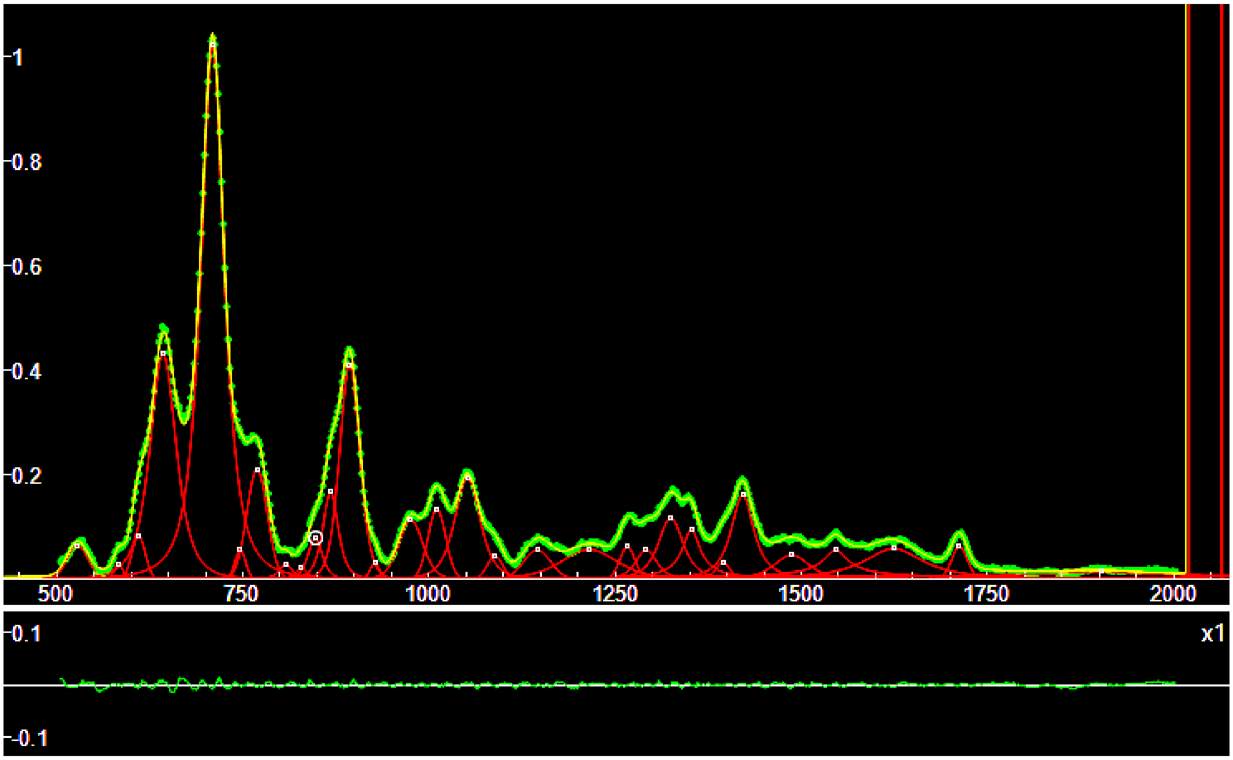
480	630(m)	652	***852***	*958*	***994(m)***
1038	***1098***	*1196(s)*	*1269(vs)*	*1446(m)*	***1498(vs)***
1634(s)					(Raman, pH 3.44)

As previously, in bold within +/−5 cm^{-1}, in italic within +/−10 cm^{-1}, the data compared with the q-Gaussian centers (h>0.15), here given again for reader's convenience:

848.298	992.868(s)	1030.24(s)	1097.03	1159.09(s)	1172.73
1186.23(s)	1205.99	1231.98	1260.7(vs)	1284.93	1312.57(s)
1335.63	1363.68	1402.3 (s)	1420.65	1439.23(s)	1463.9(vs)
1493.39(vs)	1585.76(s)	1621.35	1632.61(s)	1665.79	

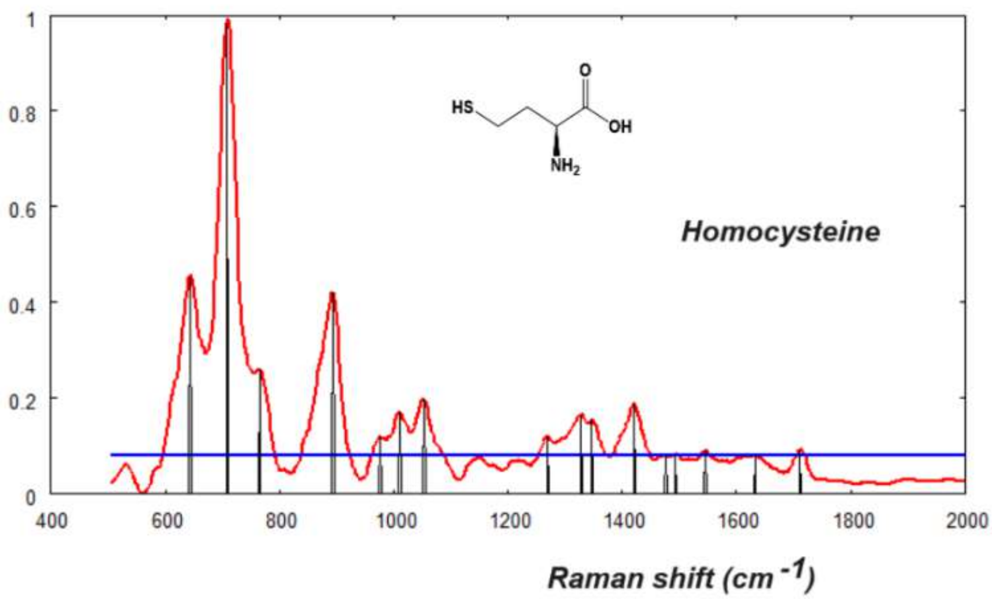
Homocysteine

Literature : Zheng et al., 2023.



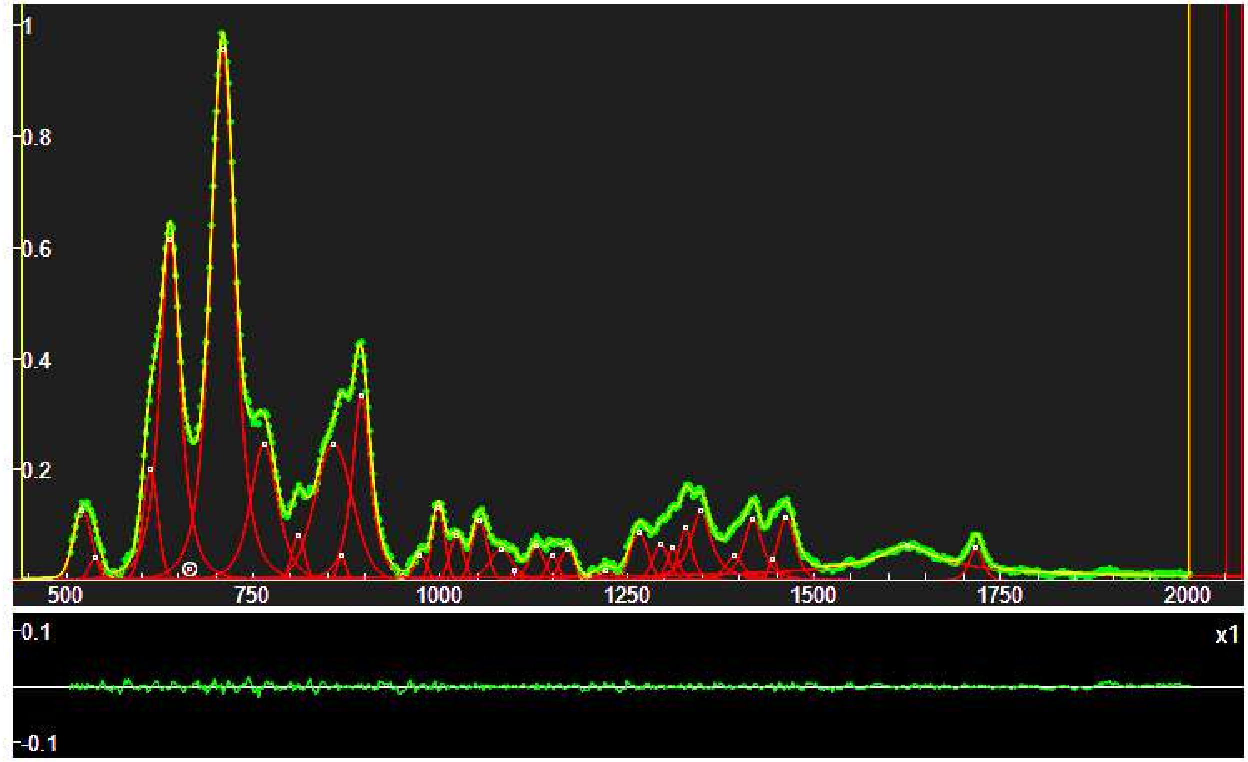
#	Center	Parameters		Height	Center	HWHM	q
(height > 0.04, bold h >0.08)							
%_12	Qgau	528.117 x	x	0.0650858	528.117	19.608	0.999837
%_16	**Qgau**	**609.987 x**	**x**	**0.0839277**	**609.987**	**12.5643**	**1**
%_3	**Qgau**	**642.893 x**	**x**	**0.431558**	**642.893**	**22.8363**	**1.51267**
%_2	**Qgau**	**709.421 x**	**x**	**1.0244**	**709.421**	**19.6631**	**1.65678**
%_18	Qgau	746.607 x	x	0.0568473	746.607	9.95242	0.999993
%_5	**Qgau**	**769.083 x**	**x**	**0.210457**	**769.083**	**19.3797**	**0.999792**
%_8	Qgau	847.176 x	x	0.0783994	847.176	12.9028	1.38805
%_11	**Qgau**	**867.714 x**	**x**	**0.167157**	**867.714**	**13.4385**	**1.4915**
%_4	**Qgau**	**893.428 x**	**x**	**0.411221**	**893.428**	**18.2392**	**1.217**
%_13	**Qgau**	**975.586 x**	**x**	**0.113782**	**975.586**	**21.9833**	**1.19494**
%_20	**Qgau**	**1010.61 x**	**x**	**0.134285**	**1010.61**	**16.7956**	**0.999746**
%_6	**Qgau**	**1051.6**	**x**	**0.195153**	**1051.6**	**22.1978**	**1.44431**
%_21	Qgau	1088.59 x	x	0.0447134	1088.59	14.719	0.999844
%_22	Qgau	1145.13 x	x	0.0563891	1145.13	25.637	0.999135
%_15	Qgau	1215.2 x	x	0.0574025	1215.2	49.74	1.37894
%_14	Qgau	1266.39 x	x	0.0625667	1266.39	14.4205	1.00002
%_25	Qgau	1291.61 x	x	0.0569048	1291.61	18.1939	1.51948
%_24	**Qgau**	**1324.59 x**	**x**	**0.117217**	**1324.59**	**21.3606**	**1.5667**
%_23	**Qgau**	**1352.17 x**	**x**	**0.0954933**	**1352.17**	**14.5949**	**2.30727**
%_26	**Qgau**	**1420.98 x**	**x**	**0.161467**	**1420.98**	**18.9969**	**1.7664**
%_30	Qgau	1486.94 x	x	0.0465937	1486.94	31.1235	1.43307
%_28	Qgau	1546.1 x	x	0.0566472	1546.1	20.1668	2.99065
%_29	Qgau	1623.94 x	x	0.0588805	1623.94	49.0563	1.91071
%_9	Qgau	1712.31 x	x	0.0636533	1712.31	14.4229	1.11057

Homocysteine has been investigated in Sparavigna, 2023. Here in the following image, the peaks are determined with the first-derivative spectrum. The blue line represents a threshold.



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
643.00	0.45	1328.00	0.16
708.50	0.98	1347.00	0.16
764.50	0.26	1421.00	0.19
893.00	0.42	1476.50	0.08
976.50	0.12	1493.00	0.08
1011.00	0.17	1545.50	0.09
1052.50	0.20	1632.00	0.08
1269.50	0.12	1711.50	0.09

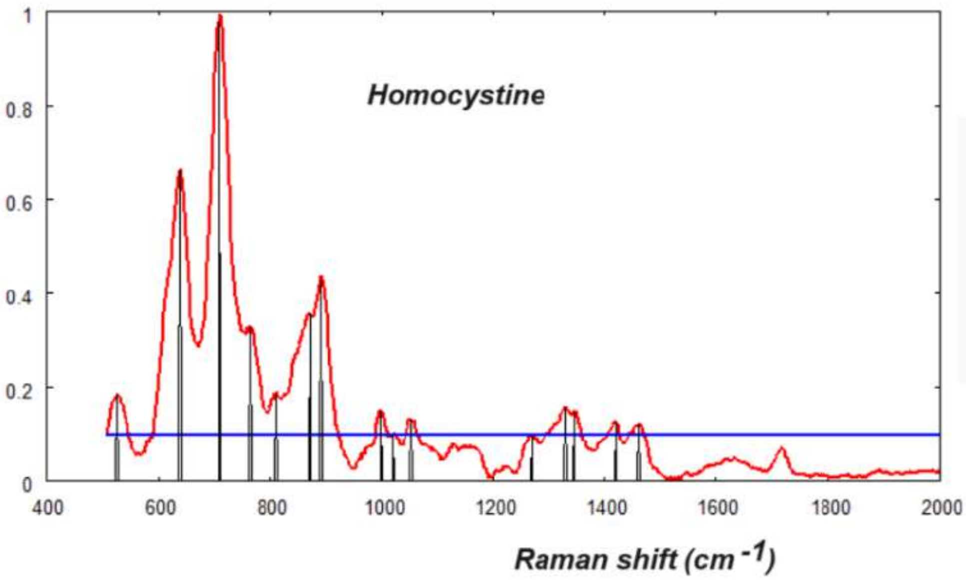
Homocystine



#		Center	Parameters		Height	Center	HWHM	q	(height above 0.05)
%_8	**Qgau**	**521.854**	**x**	**x**	**0.125228**	**521.854**	**17.3184**	**0.99988**	
%_10	**Qgau**	**612.221**	**x**	**x**	**0.19999**	**612.221**	**14.0269**	**1.06507**	
%_2	**Qgau**	**638.784**	**x**	**x**	**0.614286**	**638.784**	**17.6191**	**1.58923**	
%_1	**Qgau**	**709.235**	**x**	**x**	**0.955922**	**709.235**	**20.9581**	**1.48294**	
%_5	**Qgau**	**764.481**	**x**	**x**	**0.247401**	**764.481**	**23.3945**	**1.44433**	
%_4	**Qgau**	**857.325**	**x**	**x**	**0.246369**	**857.325**	**35.1213**	**1.08865**	
%_20	Qgau	810.09	x	x	0.0806111	810.09	12.1146	0.999908	
%_3	**Qgau**	**894.601**	**x**	**x**	**0.332444**	**894.601**	**15.6921**	**1.60249**	
%_25	**Qgau**	**997.638**	**x**	**x**	**0.133169**	**997.638**	**11.8242**	**0.999874**	
%_26	Qgau	1022.06	x	x	0.0800839	1022.06	13.0029	0.999889	
%_27	**Qgau**	**1052.55**	**x**	**x**	**0.107437**	**1052.55**	**14.2564**	**0.999813**	
%_28	Qgau	1081.37	x	x	0.0571147	1081.37	20.841	1.26932	
%_30	Qgau	1128.62	x	x	0.0621891	1128.62	13.5369	1.35247	
%_19	Qgau	1169.82	x	x	0.0580814	1169.82	13.4674	0.999738	
%_33	Qgau	1265.85	x	x	0.0862004	1265.85	16.9907	0.999635	
%_34	Qgau	1294.9	x	x	0.0659788	1294.9	13.4772	1.34765	
%_44	Qgau	1311.16	x	x	0.0594297	1311.16	9.72223	1.62565	
%_45	Qgau	1328.15	x	x	0.0947884	1328.15	11.0467	1.62116	
%_46	**Qgau**	**1348.67**	**x**	**x**	**0.124694**	**1348.67**	**16.7369**	**1.9626**	
%_39	**Qgau**	**1418.37**	**x**	**x**	**0.112329**	**1418.37**	**15.4447**	**1.8054**	
%_40	**Qgau**	**1463**	**x**	**x**	**0.114044**	**1463**	**16.1805**	**1.33128**	
%_17	Qgau	1624.7	x	x	0.0631931	1624.7	49.5056	3.52736	
%_12	Qgau	1716.46	x	x	0.0587963	1716.46	12.2933	1.39666	

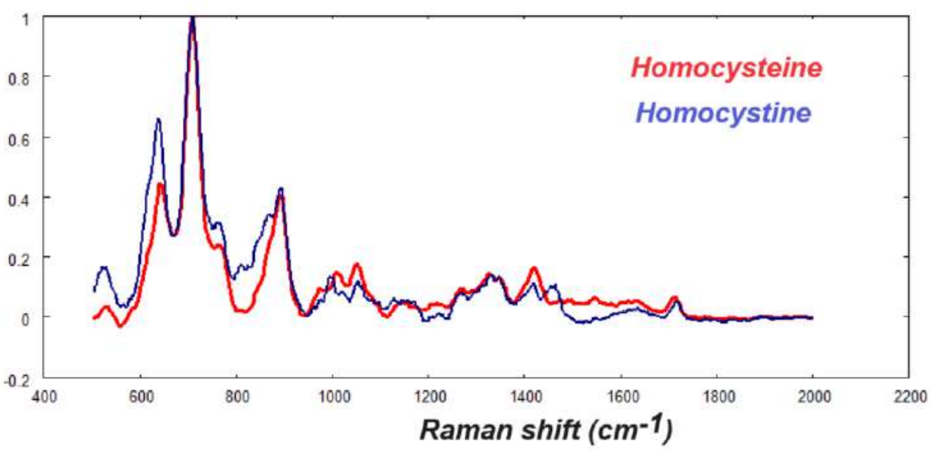
Bold characters for peaks with height above 0.10**.**

Homocystine has been investigated in [Sparavigna, 2023](). Here in the following image, the peaks are determined with the first-derivative spectrum. The blue line represents a threshold.



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
524.50	0.18	1020.00	0.10
638.50	0.66	1052.50	0.13
708.50	0.98	1267.50	0.10
762.50	0.33	1330.00	0.16
811.50	0.19	1344.50	0.15
871.00	0.35	1419.00	0.13
891.00	0.43	1460.00	0.12
998.00	0.15		

It is interesting to compare the two SERS spectra of homocysteine and homocystine as in the following plot.



According to the fingerprints obtained from the first-derivative spectrum in Sparavigna, [2023](), within the uncertainty of plus/minus 2 cm^{-1}, the comparison is as follows:

Homocysteine		643	**708.5**	**764.5**			**893**	976.5	1011
Homocystine	524.5	638.5	**708.5**	**762.5**	811.5	871	**891**	998	1020

Homocysteine	**1052.5**			**1269.5**	**1328**	**1347**	**1421**	1476.5	1493	1545.5		**1632**	**1711.5**
Homocystine	**1052.5**	1129.5	1149	**1267.5**	**1330**	**1344.5**	**1419**	1460			1620	**1634**	**1715.5**

Let us repeat the comparison with the data obtained by means of the q-Gaussian deconvolutions.

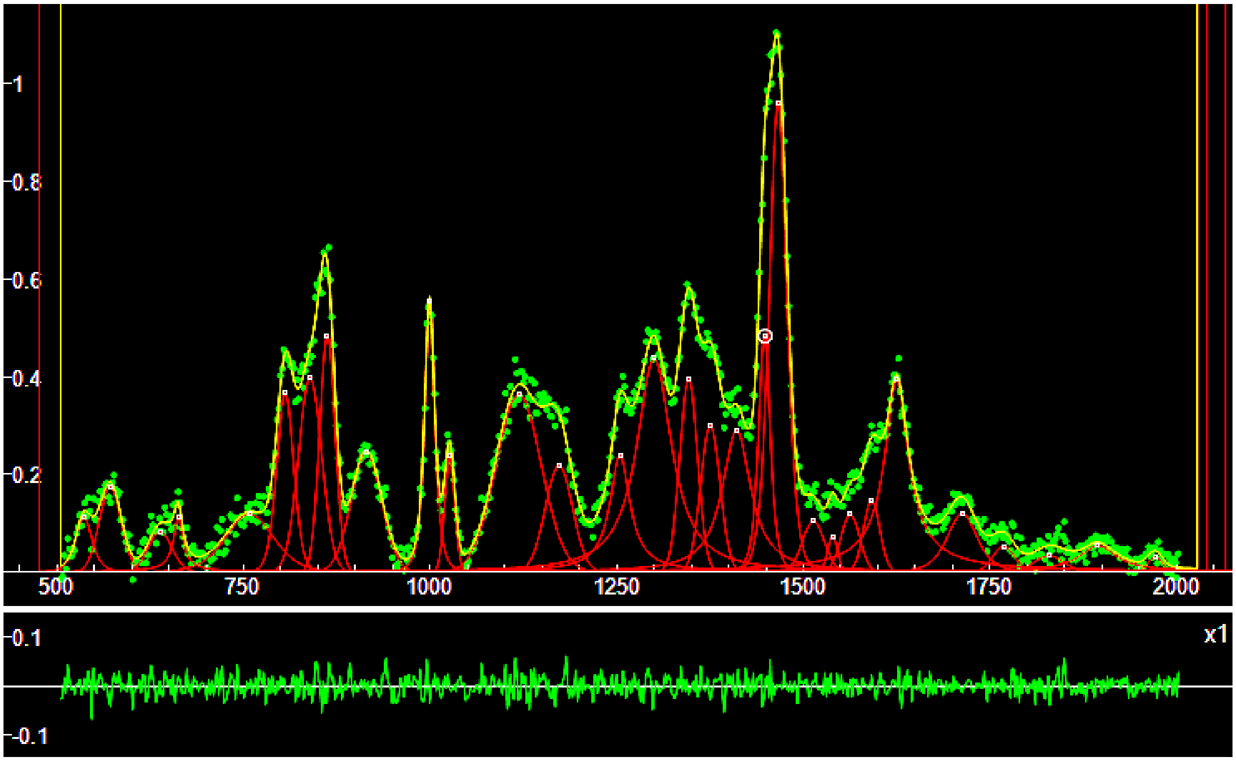
Homocysteine

%_12 Qgau	528.117
%_16 Qgau	**609.987**
%_3 Qgau	**642.893**
%_2 Qgau	**709.421**
%_18 Qgau	746.607
%_5 Qgau	**769.083**
%_8 Qgau	847.176
%_11 Qgau	**867.714**
%_4 Qgau	**893.428**
%_13 Qgau	**975.586**
%_20 Qgau	**1010.61**
%_6 Qgau	**1051.6**
%_21 Qgau	1088.59
%_22 Qgau	1145.13
%_15 Qgau	1215.2
%_14 Qgau	1266.39
%_25 Qgau	1291.61
%_24 Qgau	**1324.59**
%_23 Qgau	**1352.17**
%_26 Qgau	**1420.98**
%_30 Qgau	1486.94
%_28 Qgau	1546.1
%_29 Qgau	1623.94
%_9 Qgau	1712.31

Homocystine

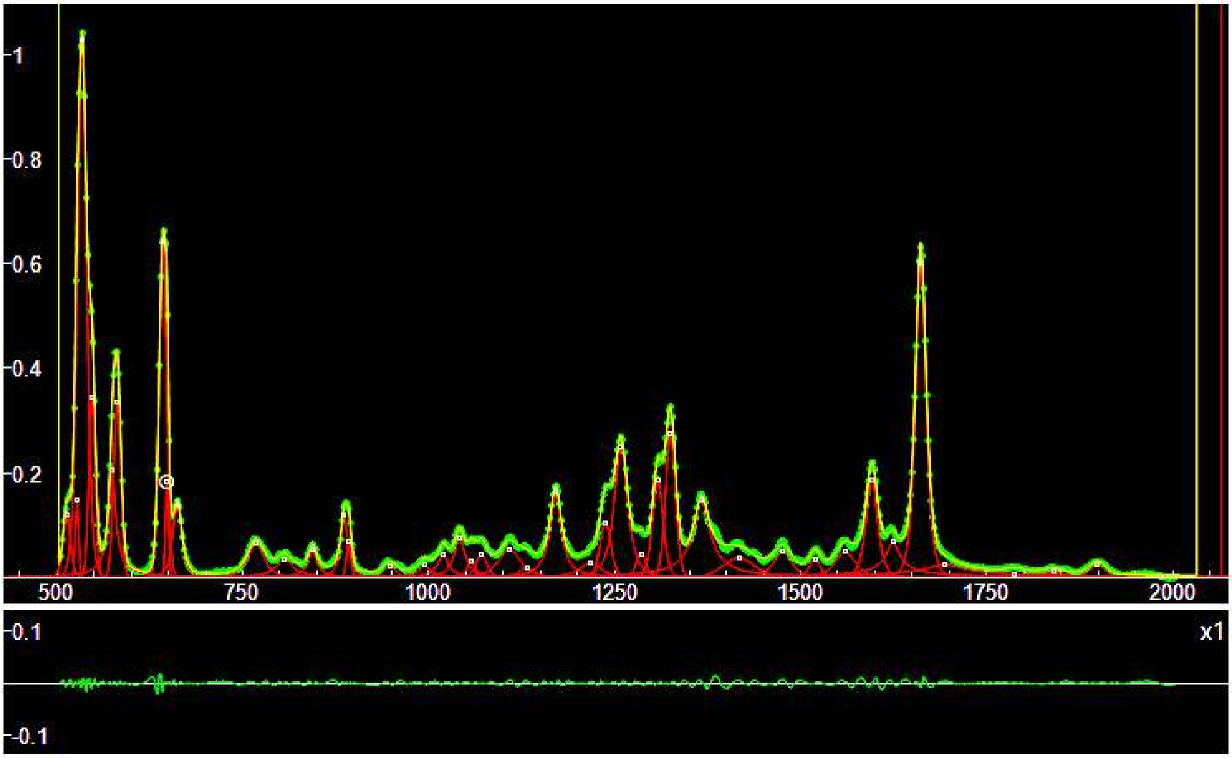
%_8 Qgau	**521.854**
%_10 Qgau	**612.221**
%_2 Qgau	**638.784**
%_1 Qgau	**709.235**
%_5 Qgau	**764.481**
%_4 Qgau	**857.325**
%_20 Qgau	810.09
%_3 Qgau	**894.601**
% 25 Qgau	**997.638**
%_26 Qgau	1022.06
%_27 Qgau	**1052.55**
%_28 Qgau	1081.37
%_30 Qgau	1128.62
%_19 Qgau	1169.82
%_33 Qgau	1265.85
%_34 Qgau	1294.9
%_44 Qgau	1311.16
%_45 Qgau	1328.15
%_46 Qgau	**1348.67**
%_39 Qgau	**1418.37**
%_40 Qgau	**1463**
%_17 Qgau	1624.7
%_12 Qgau	1716.46

Indole-3-acetic acid



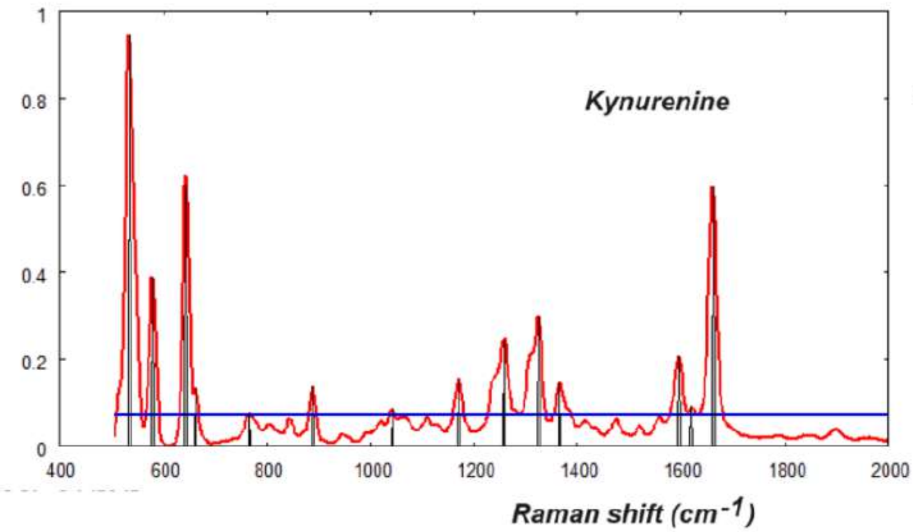
#	PeakType	Center	Parameters:	Height	Center	HWHM	q	(height > 0.1, **bold** h>0.2)
%_10	Qgau	536.045		0.11237	536.045	14.4895	1.44512	
%_39	Qgau	571.395		0.17417	571.395	20.6907	0.999854	
%_31	Qgau	662.54		0.112366	662.54	7.46312	2.31789	
%_30	Qgau	757.939		0.11894	757.939	43.5302	1.21908	
%_29	**Qgau**	**805.728**		**0.366326**	**805.728**	**15.6099**	**1.14596**	
%_37	**Qgau**	**839.153**		**0.398191**	**839.153**	**22.0377**	**0.999809**	
%_26	**Qgau**	**862.307**		**0.486219**	**862.307**	**14.5255**	**0.999848**	
%_13	**Qgau**	**914.488**		**0.244159**	**914.488**	**28.991**	**0.999366**	
%_4	**Qgau**	**999.297**		**0.556612**	**999.297**	**8.61866**	**1.54358**	
%_14	**Qgau**	**1026.08**		**0.238881**	**1026.08**	**9.44412**	**1.00819**	
%_8	**Qgau**	**1118.59**		**0.363919**	**1118.59**	**42.7171**	**0.997795**	
%_15	**Qgau**	**1172.45**		**0.218078**	**1172.45**	**25.7108**	**0.999255**	
%_16	**Qgau**	**1254.19**		**0.239651**	**1254.19**	**15.9635**	**2.12635**	
%_5	**Qgau**	**1300.08**		**0.438246**	**1300.08**	**28.5262**	**1.94179**	
%_3	**Qgau**	**1346.24**		**0.394952**	**1346.24**	**16.8054**	**0.99973**	
%_34	**Qgau**	**1375.45**		**0.300744**	**1375.45**	**18.2939**	**0.999588**	
%_24	**Qgau**	**1410.44**		**0.290442**	**1410.44**	**23.2548**	**1.98403**	
%_2	**Qgau**	**1447.82**		**0.488318**	**1447.82**	**10.1738**	**1.44222**	
%_1	**Qgau**	**1466.14**		**0.961573**	**1466.14**	**15.8595**	**1.25248**	
%_38	Qgau	1513.36		0.104628	1513.36	20.7551	0.999577	
%_35	Qgau	1562.77		0.117879	1562.77	17.6498	0.999782	
%_21	Qgau	1591.41		0.146861	1591.41	15.367	1.00009	
%_22	**Qgau**	**1625.02**		**0.394003**	**1625.02**	**18.9762**	**2.28608**	
%_17	Qgau	1712.65		0.119672	1712.65	26.4446	1.40234	

Kynurenine



#	PeakType	Center	Parameters		Height	Center	HWHM	q (h>0.05, bold h>0.12)
%_27	**Qgau**	**513.373**	**x**	**x**	**0.120626**	**513.373**	**6.39926**	**1.31922**
%_1	**Qgau**	**527.236**	**x**	**x**	**0.150343**	**527.236**	**3.06483**	**1**
%_49	**Qgau**	**533.966**	**x**	**x**	**1.02852**	**533.966**	**8.26442**	**1.23945**
%_9	**Qgau**	**547.572**	**x**	**x**	**0.345901**	**547.572**	**6.06794**	**0.999983**
%_14	**Qgau**	**574.455**	**x**	**x**	**0.205883**	**574.455**	**5.53224**	**2.3934**
%_4	**Qgau**	**581.202**	**x**	**x**	**0.336568**	**581.202**	**6.79711**	**0.99998**
%_2	**Qgau**	**642.715**	**x**	**x**	**0.644034**	**642.715**	**6.93595**	**1.07326**
%_5	**Qgau**	**648.11**	**x**	**x**	**0.187777**	**648.11**	**2.81833**	**1.00004**
%_13	**Qgau**	**662.074**	**x**	**x**	**0.142319**	**662.074**	**7.79482**	**1.57131**
%_18	Qgau	767.698	x	x	0.0648257	767.698	14.0522	1.64255
%_24	Qgau	843.914	x	x	0.0529193	843.914	6.93109	2.30171
%_11	**Qgau**	**886.252**	**x**	**x**	**0.120842**	**886.252**	**5.45849**	**2.00578**
%_34	Qgau	892.572	x	x	0.0700003	892.572	4.42244	0.999996
%_40	Qgau	1041.5	x	x	0.0745293	1041.5	8.99635	2.02773
%_23	Qgau	1108.11	x	x	0.0551641	1108.11	18.92	1.59997
%_8	**Qgau**	**1170.42**	**x**	**x**	**0.163397**	**1170.42**	**9.15875**	**2.0382**
%_21	Qgau	1237.46	x	x	0.105451	1237.46	10.4151	1.10047
%_44	**Qgau**	**1258.26**	**x**	**x**	**0.250496**	**1258.26**	**11.1443**	**1.69562**
%_15	**Qgau**	**1307.82**	**x**	**x**	**0.186777**	**1307.82**	**9.53921**	**1.28567**
%_46	**Qgau**	**1325.01**	**x**	**x**	**0.277907**	**1325.01**	**9.05506**	**1.14314**
%_10	**Qgau**	**1366.68**	**x**	**x**	**0.148191**	**1366.68**	**13.2945**	**2.40961**
%_7	**Qgau**	**1595.44**	**x**	**x**	**0.188057**	**1595.44**	**10.0265**	**1.49582**
%_19	Qgau	1623.71	x	x	0.0685103	1623.71	11.3866	2.94344
%_3	**Qgau**	**1661.26**	**x**	**x**	**0.608047**	**1661.26**	**9.08178**	**1.44948**

Using the first-derivative spectrum, in [Sparavigna, 2023](), we obtained the following peaks:



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
533.50	0.94	1170.00	0.15
579.50	0.39	1257.00	0.24
643.00	0.60	1324.00	0.30
661.00	0.13	1365.50	0.14
767.00	0.07	1596.00	0.21
889.00	0.14	1620.00	0.09
1041.50	0.08	1662.00	0.60

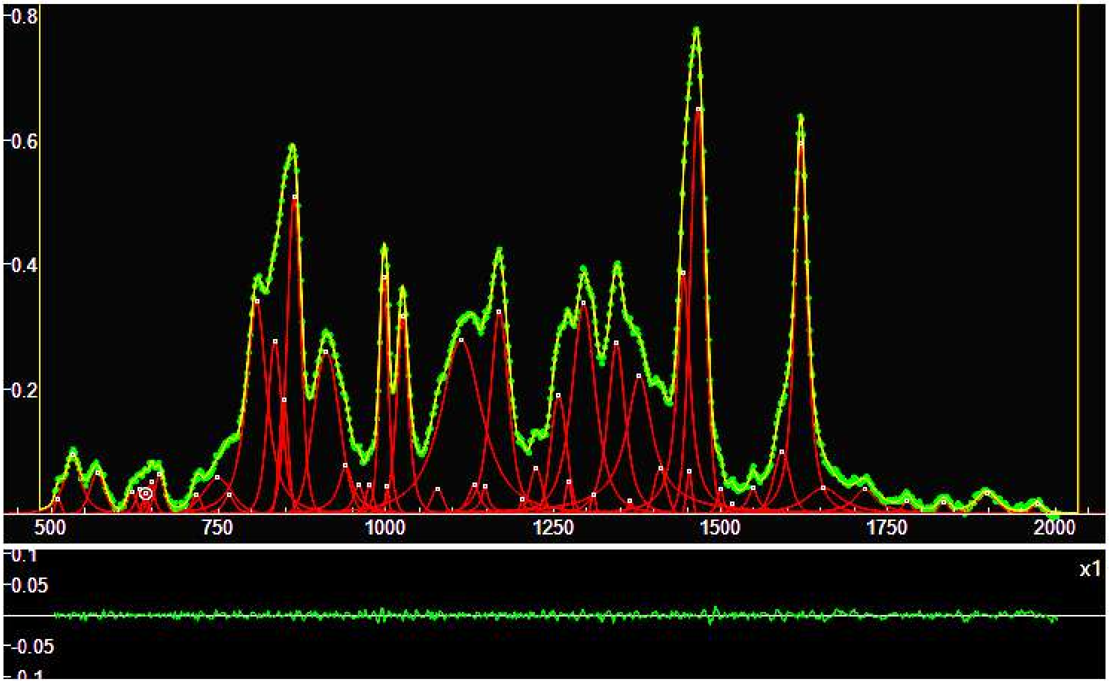
We can compare these peaks with the q-Gaussian centers obtained from deconvolution:

513.373	527.236(m)	533.966(vs)	547.572(s)	574.455(m)	581.202(s)
642.715(vs)	648.11(m)	662.074(m)	767.698	843.914	886.252
892.572	1041.5	1108.11	1170.42(m)	1237.46	1258.26(m)
1307.82(m)	1325.01(m)	1366.68	1595.44(m)	1623.7	1661.26(vs)

As told by Sherman et al., SERS spectra have previously been reported for this molecule by Nie et al., 1990. Let us add here a discussion from the recent work by Das et al., 2021. The abstract of their review is proposing the Surface-Enhanced Raman spectroscopy (SERS) as “a powerful tool for biosensing applications owing to its *fingerprint recognition*, high sensitivity, multiplex detection, and biocompatibility” (Das et al., 2021). According to the authors, their review is offering “an overview of the most significant aspects of SERS for biomedical and biosensing applications” (Das et al., 2021). In the review, kynurenine is mentioned as follow. “Intrinsic SERS signals can be used to detect specific biomarkers or physiologically relevant biomolecular species inside or near individual cells, such as important metabolites in normal and tumor cells, or other cellular components such as exosomes. The application of SERS to identify the presence of extracellular metabolites, secreted by cancer cells and relevant to tumor biology, including tryptophan, *kynurenine*, and purine derivatives, has been demonstrated by Plou et al., 2020”. (Das and coworkers are mentioning Plou et al., 2020). In Figure 7 in Das et al., 2021, the Panel (e) allows a “comparison of Raman and SERS spectra for kynurenine (Kyn) and tryptophan (Trp)”. The nanoparticles are of gold.
From the plot by Plou et al. in Das et al., 2021, we can obtain the peaks above a certain threshold at positions that we can compare with those given by Sherman et al. (in cm^{-1}):

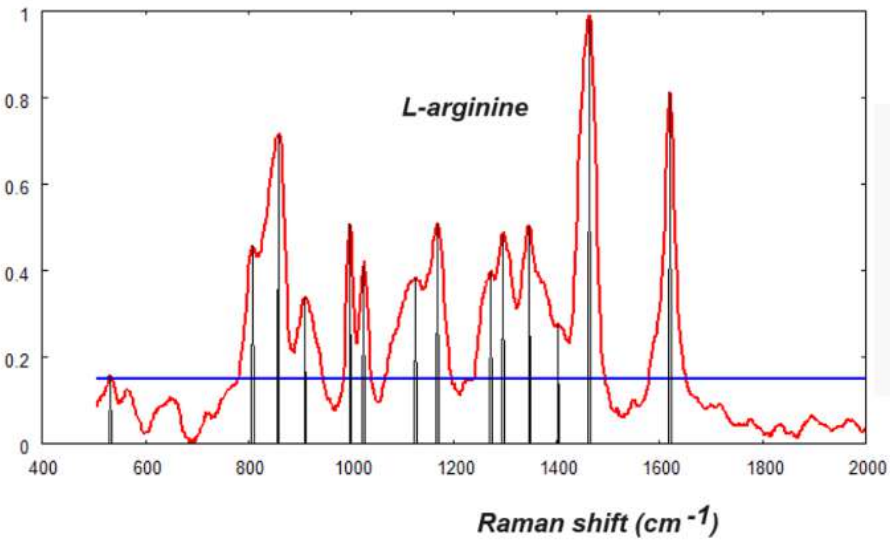
562.5	***664.0***	938.0	999.5	***1039.5***	*1227.0*
1350.5	1378.0				(Plou et al.)

L-arginine



#	Center		Parameters		Height	Center	HWHM	q ... (h > 0.05**, bold** h>0.15)
%_18	Qgau	531.445	x	x	0.0965466	531.445	14.87	1.80809
%_22	Qgau	568.693	x	x	0.067613	568.693	15.5271	1.15328
%_60	Qgau	648.893	x	x	0.0537662	648.893	5.80739	1.69304
%_59	Qgau	661.492	x	x	0.0646335	661.492	9.74302	1.31092
%_23	Qgau	748.598	x	x	0.0589676	748.598	29.0783	1.26032
%_9	**Qgau**	**806.805**	**x**	**x**	**0.342536**	**806.805**	**18.4342**	**1.77269**
%_17	**Qgau**	**833.798**	**x**	**x**	**0.277945**	**833.798**	**14.3488**	**1.31045**
%_52	**Qgau**	**847.229**	**x**	**x**	**0.185334**	**847.229**	**9.2883**	**0.999971**
%_51	**Qgau**	**862.433**	**x**	**x**	**0.511955**	**862.433**	**13.59**	**1.20707**
%_12	**Qgau**	**910.998**	**x**	**x**	**0.260015**	**910.998**	**27.1723**	**0.999464**
%_50	Qgau	939.937	x	x	0.0789916	939.937	12.5899	2.22329
%_6	**Qgau**	**997.102**	**x**	**x**	**0.379254**	**997.102**	**8.59164**	**1.35778**
%_58	Qgau	1002.38	x	x	0.0511441	1002.38	2.71727	1.42405
%_10	**Qgau**	**1024.87**	**x**	**x**	**0.320029**	**1024.87**	**11.0673**	**1.51015**
%_11	**Qgau**	**1112.46**	**x**	**x**	**0.278516**	**1112.46**	**38.6364**	**1.70718**
%_5	**Qgau**	**1169.38**	**x**	**x**	**0.326181**	**1169.38**	**17.4575**	**1.53757**
%_24	Qgau	1224.5	x	x	0.0747978	1224.5	13.0212	1.00834
%_13	**Qgau**	**1257.89**	**x**	**x**	**0.190121**	**1257.89**	**16.4587**	**0.999551**
%_32	Qgau	1272.13	x	x	0.0547543	1272.13	5.81358	1.05179
%_8	**Qgau**	**1295.3**	**x**	**x**	**0.338162**	**1295.3**	**22.5636**	**1.58389**
%_7	**Qgau**	**1344.56**	**x**	**x**	**0.274593**	**1344.56**	**16.4393**	**1.6293**
%_14	**Qgau**	**1378.47**	**x**	**x**	**0.221544**	**1378.47**	**23.0369**	**2.27487**
%_21	Qgau	1409.98	x	x	0.0739174	1409.98	13.1975	1.02703
%_15	**Qgau**	**1444.85**	**x**	**x**	**0.387734**	**1444.85**	**11.1535**	**2.06092**
%_41	Qgau	1453.23	x	x	0.0684554	1453.23	5.67164	0.999979
%_2	**Qgau**	**1465.65**	**x**	**x**	**0.652393**	**1465.65**	**15.1134**	**1.12798**
%_16	Qgau	1591.48	x	x	0.100745	1591.48	16.3948	1.352
%_3	**Qgau**	**1620.29**	**x**	**x**	**0.595589**	**1620.29**	**11.7483**	**1.73734**

L-arginine has been investigated in Sparavigna, 2023. Here in the following table the peaks as have been determined with the first-derivative spectrum (with height above a given threshold):



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
531.50	0.16	1168.00	0.51
809.00	0.46	1271.50	0.40
858.00	0.71	1294.50	0.48
911.00	0.34	1347.00	0.50
998.00	0.51	1402.50	0.28
1024.00	0.41	1462.50	0.98
1125.50	0.38	1620.00	0.81

We can compare the Table given above with the centers of the q-Gaussians given before:

%_18 Qgau	531.445	0.0965466	%_11 Qgau	1112.46	0.278516
%_22 Qgau	568.693	0.067613	%_5 Qgau	1169.38	0.326181
%_60 Qgau	648.893	0.0537662	%_24 Qgau	1224.5	0.0747978
%_59 Qgau	661.492	0.0646335	%_13 Qgau	1257.89	0.190121
%_23 Qgau	748.598	0.0589676	%_32 Qgau	1272.13	0.0547543
%_9 Qgau	806.805	0.342536	%_8 Qgau	1295.3	0.338162
%_17 Qgau	833.798	0.277945	%_7 Qgau	1344.56	0.274593
%_52 Qgau	847.229	0.185334	%_14 Qgau	1378.47	0.221544
%_51 Qgau	862.433	0.511955	%_21 Qgau	1409.98	0.0739174
%_12 Qgau	910.998	0.260015	%_15 Qgau	1444.85	0.387734
%_50 Qgau	939.937	0.0789916	%_41 Qgau	1453.23	0.0684554
%_6 Qgau	997.102	0.379254	%_2 Qgau	1465.65	0.652393
%_58 Qgau	1002.38	0.0511441	%_16 Qgau	1591.48	0.100745
%_10 Qgau	1024.87	0.320029	%_3 Qgau	1620.29	0.595589

In De Gelder et al., 2007, we find the following Raman peaks (in bold, the peaks which are corresponding to q-Gaussian centers, within +/− 5 cm^{-1}):

376(w), 410(w), 490(mw), 551(m), 577(m), 613(m), ***849(m),*** 879(mw), 922(m), 982(vs), 1036(mw), 1067(s), 1100(m), 1122(m), 1189(m), 1264(mw), ***1298(m),*** 1330(m), ***1377(mw),*** 1436(s), 1475(m), 1713(w)

As told by Sherman et al., SERS spectra of L-arginine have previously been reported in the literature for this molecule, Aliaga et al., 2010, Garrido et al., 2013. Let us add Botta and Bansal, 2015, Dummitt, 2023.

In Aliaga et al., 2010, we find the following SERS fingerprint (in cm^{-1}):

535	611	***665***	781	*839*	891	*934*	978	***993***
1088	***1171***	1325	1355	***1412***	***1444***	1479	1569	1653

that we compared with the q-Gaussian centers (bold, within +/− 5 cm^{-1}, and in italic, within +/− 10 cm^{-1}), here given again below for reader's convenience:

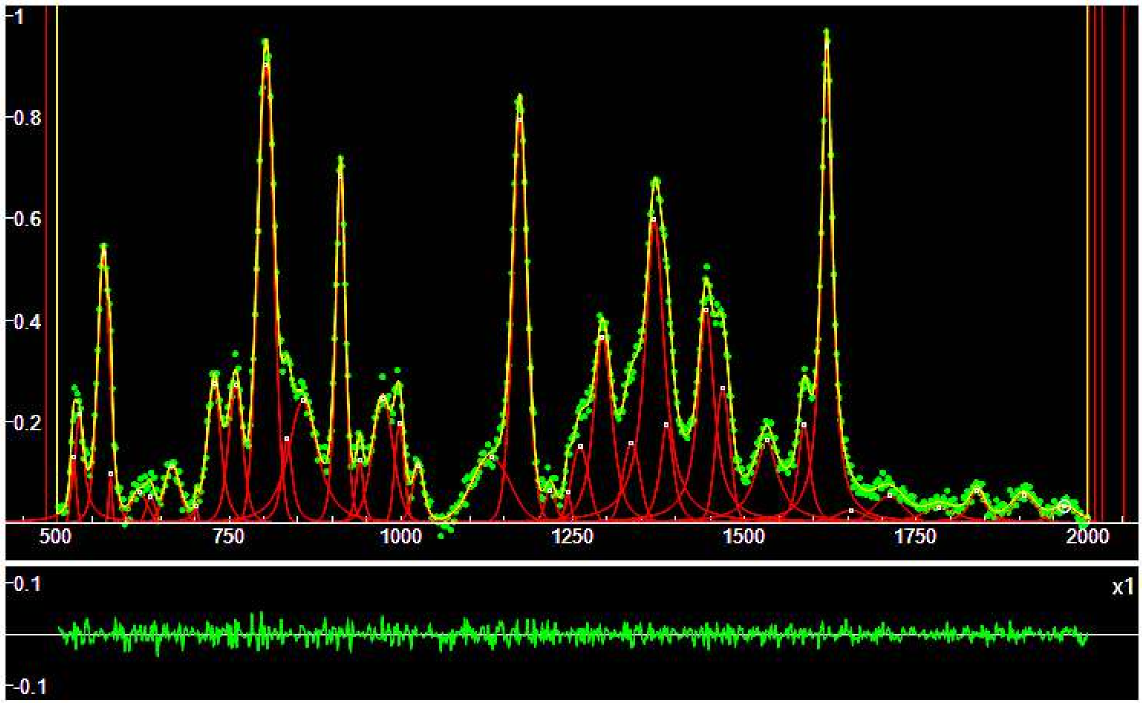
531.445	568.693	648.893	661.492	748.598	806.805
833.798	847.229	862.433	910.998	939.937	997.102
1002.38	1024.87	1112.46	1169.38	1224.5	1257.89
1272.13	1295.3	1344.56	1378.47	1409.98	1444.85
1453.23	1465.65	1591.48	1620.29		

In Aliaga et al., the Raman spectrum is also given. And, again, we can compare:

389	455	*524*	***571***	613	675	***746***	759	793	***848***	***858***	899	971
997	***1020***	1046	1069	1085	1135	*1218*	***1268***	1287	1309	1316	1327	1358
1392	***1410***	***1443***	***1457***	***1466***	1523	*1598*	1650	1680				

L-asparagine

Literature reported by Sherman et al.: Guicheteau et al., 2006, Kuang et al., 2016.



#	PeakType	Center	Parameters :		Height	Center	HWHM	q (h > 0.09, **bold** h>0.2)
%_12	Qgau	523.163	x	x	0.131469	523.163	5.39448	0.999987
%_24	**Qgau**	**531.614**	**x**	**x**	**0.219004**	**531.614**	**7.22798**	**2.26907**
%_6	**Qgau**	**567.174**	**x**	**x**	**0.534704**	**567.174**	**11.4564**	**1.31481**
%_32	Qgau	576.735	x	x	0.0971789	576.735	2.99727	1.00011
%_23	Qgau	666.598	x	x	0.110831	666.598	15.9135	1.1181
%_16	**Qgau**	**727.566**	**x**	**x**	**0.277827**	**727.566**	**12.8277**	**1.52387**
%_10	**Qgau**	**758.962**	**x**	**x**	**0.273718**	**758.962**	**13.6352**	**1.30942**
%_2	**Qgau**	**803.082**	**x**	**x**	**0.907411**	**803.082**	**16.5992**	**0.999851**
%_30	Qgau	833.783	x	x	0.168009	833.783	9.13045	1.76691
%_13	**Qgau**	**856.947**	**x**	**x**	**0.240812**	**856.947**	**26.8927**	**1.64773**
%_4	**Qgau**	**911.64**	**x**	**x**	**0.685165**	**911.64**	**9.24071**	**1.33083**
%_21	Qgau	939.395	x	x	0.125517	939.395	6.92238	1.5623
%_15	**Qgau**	**973.267**	**x**	**x**	**0.245038**	**973.267**	**20.5676**	**1.19895**
%_9	Qgau	997.55	x	x	0.196653	997.55	9.73733	0.999915
%_27	Qgau	1024.64	x	x	0.111826	1024.64	11.4238	1.19612
%_19	Qgau	1130.96	x	x	0.129617	1130.96	38.9454	0.998045
%_3	**Qgau**	**1172.86**	**x**	**x**	**0.79788**	**1172.86**	**14.4206**	**1.20295**
%_20	Qgau	1260.19	x	x	0.150347	1260.19	17.4823	0.999474
%_8	**Qgau**	**1293.33**	**x**	**x**	**0.3682**	**1293.33**	**16.976**	**1.56586**
%_18	Qgau	1335.31	x	x	0.158077	1335.31	17.3152	0.999649
%_5	**Qgau**	**1368.83**	**x**	**x**	**0.598571**	**1368.83**	**16.5794**	**1.95342**
%_25	Qgau	1386.63	x	x	0.195043	1386.63	12.3302	1.59385
%_7	**Qgau**	**1443.77**	**x**	**x**	**0.42044**	**1443.77**	**13.8196**	**2.04867**
%_14	**Qgau**	**1468.05**	**x**	**x**	**0.266218**	**1468.05**	**14.4949**	**1.0691**
%_17	**Qgau**	**1531.98**	**x**	**x**	**0.162975**	**1531.98**	**19.7601**	**2.07346**
%_11	Qgau	1586.42	x	x	0.193293	1586.42	10.6437	1.71602
%_1	**Qgau**	**1619.76**	**x**	**x**	**0.940533**	**1619.76**	**9.38334**	**1.98005**

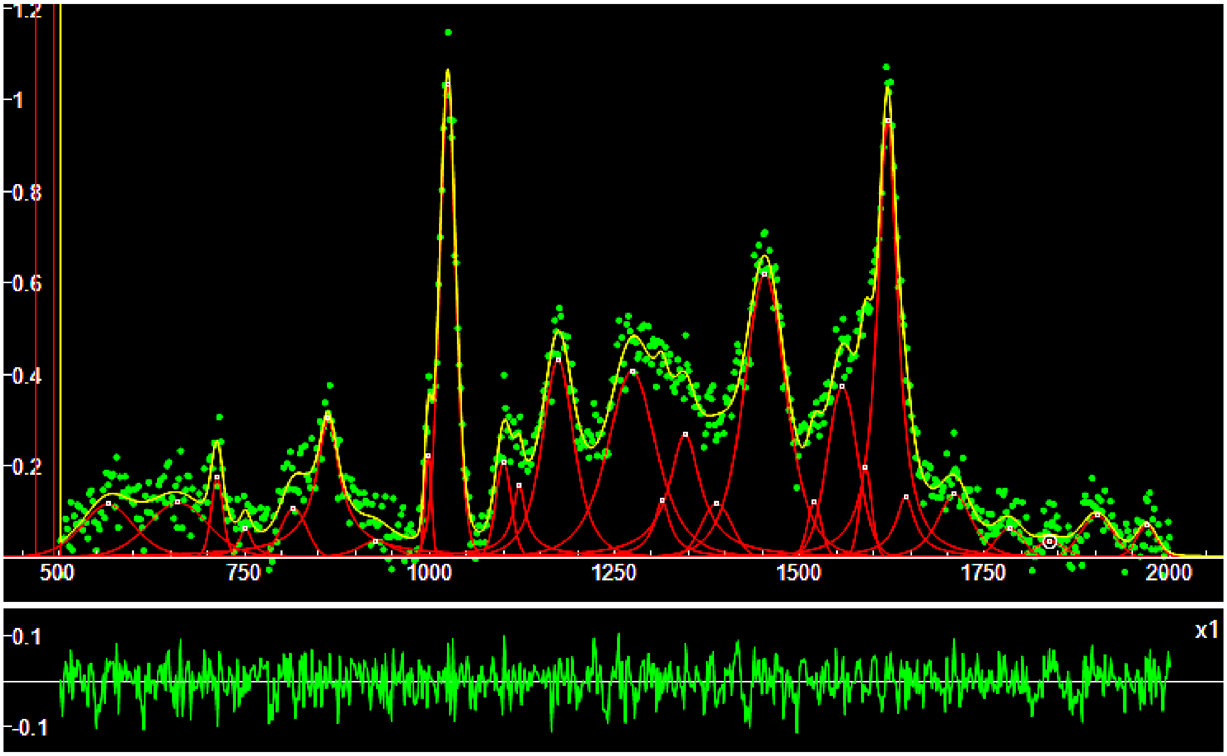
In Guicheteau et al., 2006, we can find the following data about asparagine:

450	***539***	*752*	876	***940***	1072	1111	1158	***1261***	***1330***	1415	***1622***	(Raman)
610	772	862	925	1048	1320	*1396*	***1619***					(SERS)

that we compared with the q-Gaussian centers (bold, within +/− 5 cm^{-1}, and in italic, within +/− 10 cm^{-1}), here given below:

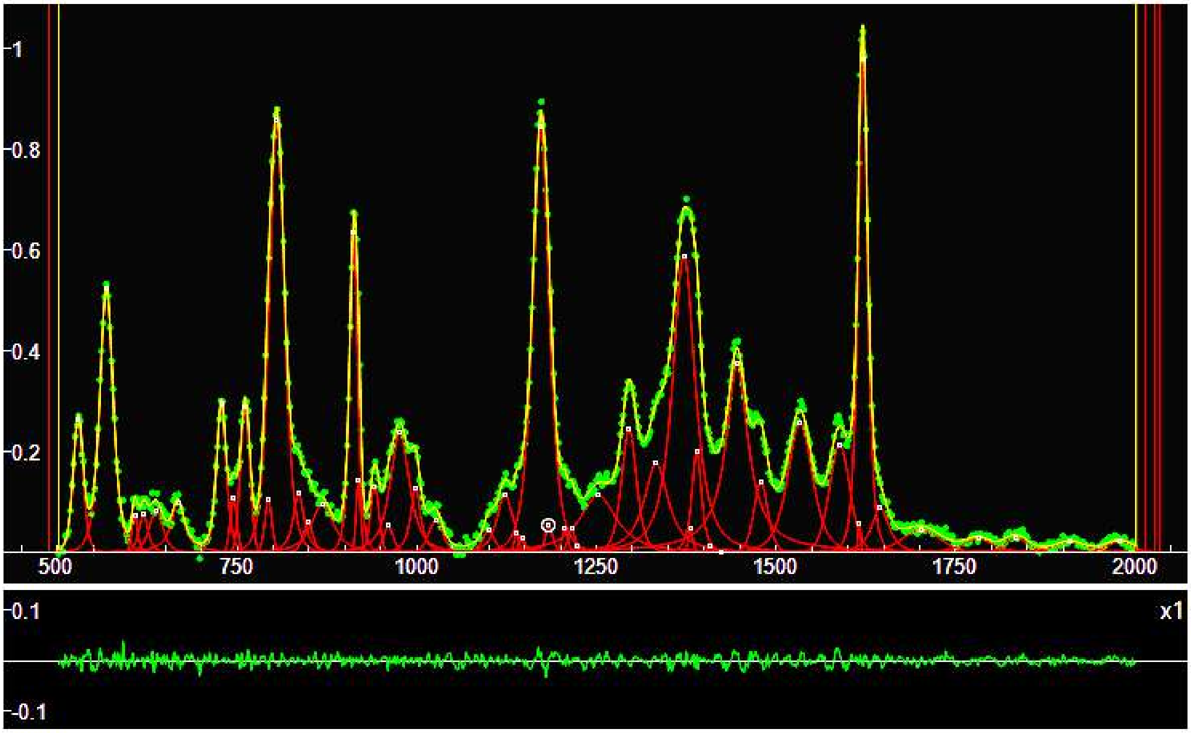
523.163	531.614	567.174(s)	576.735	666.598	727.566(m)
758.962(m)	803.082(vs)	833.783	856.947(m)	911.64(s)	939.395
973.267	997.55	1024.64	1130.96	1172.86(vs)	1260.19
1293.33(s)	1335.31	1368.83(s)	1386.63	1443.77(s)	1468.05(m)
1531.98	1586.42	1619.76(vs)			

L-cystathionine



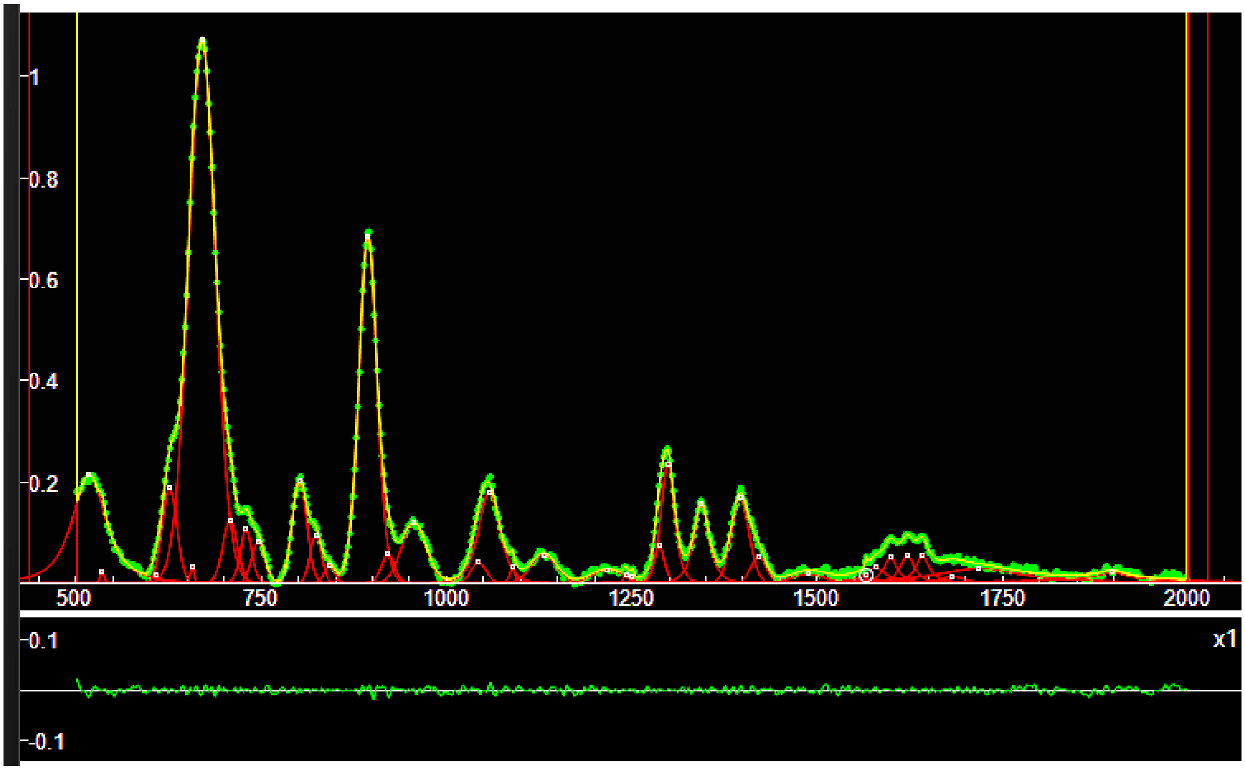
# PeakType		Center	Parameters		Height	Center	HWHM	q ...
%_16	Qgau	565.307	x	x	0.117311	565.307	47.7822	1.30952
%_13	Qgau	660.167	x	x	0.120867	660.167	56.4195	1.20144
%_9	**Qgau**	**712.853**	**x**	**x**	**0.176985**	**712.853**	**10.7676**	**1.24603**
%_27	Qgau	751.204	x	x	0.065869	751.204	9.81566	2.44543
%_14	Qgau	816.455	x	x	0.108378	816.455	25.0885	0.999715
%_7	**Qgau**	**862.873**	**x**	**x**	**0.305153**	**862.873**	**18.1504**	**2.47705**
%_15	Qgau	927.743	x	x	0.0376464	927.743	30.7411	1.65527
%_12	**Qgau**	**997.939**	**x**	**x**	**0.224521**	**997.939**	**6.40355**	**1.00028**
%_1	**Qgau**	**1024.45**	**x**	**x**	**1.0343**	**1024.45**	**14.9149**	**1.23089**
%_8	**Qgau**	**1099.95**	**x**	**x**	**0.209668**	**1099.95**	**14.5022**	**1.14466**
%_22	**Qgau**	**1121.07**	**x**	**x**	**0.158742**	**1121.07**	**10.1405**	**2.77454**
%_4	**Qgau**	**1173.64**	**x**	**x**	**0.43261**	**1173.64**	**27.8784**	**1.52489**
%_5	**Qgau**	**1273.37**	**x**	**x**	**0.408106**	**1273.37**	**43.021**	**1.46442**
%_26	Qgau	1314.28	x	x	0.125951	1314.28	12.9957	2.37511
%_10	**Qgau**	**1345.08**	**x**	**x**	**0.270214**	**1345.08**	**25.375**	**2.13761**
%_29	Qgau	1387.97	x	x	0.11889	1387.97	29.8497	0.998951
%_3	**Qgau**	**1453.37**	**x**	**x**	**0.620411**	**1453.37**	**37.2699**	**1.39333**
%_30	Qgau	1520.11	x	x	0.123095	1520.11	12.9016	1.19186
%_6	**Qgau**	**1557.93**	**x**	**x**	**0.372912**	**1557.93**	**28.4327**	**1.12524**
%_24	**Qgau**	**1589.29**	**x**	**x**	**0.197464**	**1589.29**	**11.0825**	**1.16038**
%_2	**Qgau**	**1619.01**	**x**	**x**	**0.956956**	**1619.01**	**16.6636**	**1.89993**
%_21	Qgau	1643.35	x	x	0.13425	1643.35	15.0647	2.40336
%_11	Qgau	1709.76	x	x	0.139364	1709.76	30.1015	1.52098
%_20	Qgau	1783.86	x	x	0.0658436	1783.86	25.8645	0.999594
%_31	Qgau	1838.52	x	x	0.0363917	1838.52	29.0288	0.999536
%_17	Qgau	1901.86	x	x	0.0924939	1901.86	31.3436	0.999499
%_18	Qgau	1969.03	x	x	0.0714026	1969.03	19.0599	1.19281

L-cysteic acid



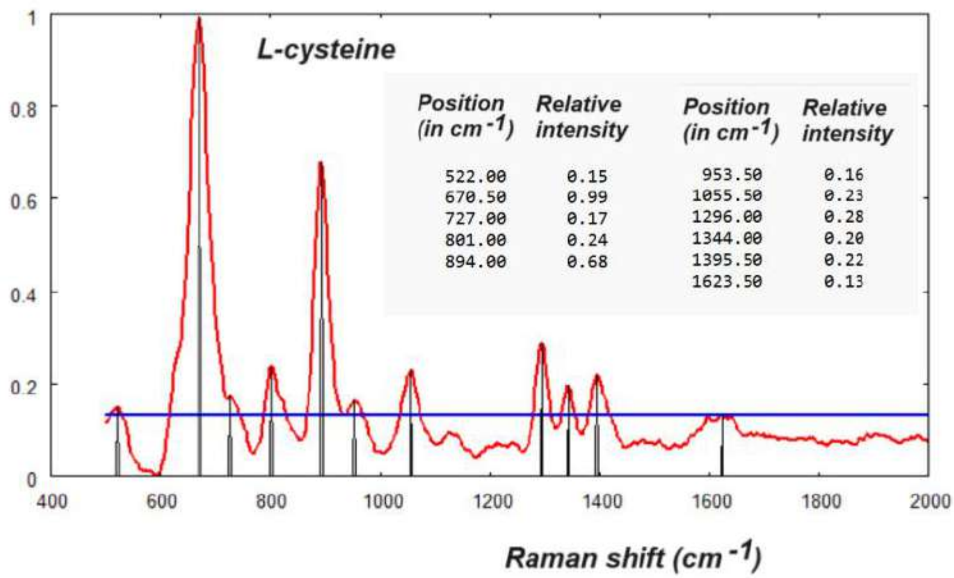
#	PeakType	Center	Parameters		Height	Center	HWHM	q (h>0.10)
%_13	**Qgau**	**528.456**	**x**	**x**	**0.264731**	**528.456**	**9.24909**	**1.27096**
%_6	**Qgau**	**567.873**	**x**	**x**	**0.524611**	**567.873**	**12.1217**	**1.41245**
%_30	Qgau	667.455	x	x	0.100476	667.455	11.1299	2.01952
%_9	**Qgau**	**727.744**	**x**	**x**	**0.299078**	**727.744**	**8.69307**	**1.41494**
%_32	Qgau	744.761	x	x	0.107725	744.761	6.6484	0.999973
%_11	**Qgau**	**760.745**	**x**	**x**	**0.291412**	**760.745**	**9.18634**	**0.999947**
%_25	Qgau	793.054	x	x	0.106112	793.054	6.58518	1.19774
%_3	**Qgau**	**805.067**	**x**	**x**	**0.861605**	**805.067**	**14.0118**	**1.33369**
%_19	Qgau	835.394	x	x	0.117068	835.394	9.33487	1.8188
%_5	**Qgau**	**912.046**	**x**	**x**	**0.642778**	**912.046**	**7.2332**	**1.44717**
%_17	Qgau	918.484	x	x	0.144886	918.484	4.29933	1.00516
%_18	Qgau	941.125	x	x	0.131053	941.125	8.38408	0.999938
%_12	**Qgau**	**976.174**	**x**	**x**	**0.237162**	**976.174**	**16.8716**	**1.64137**
%_21	Qgau	998.296	x	x	0.126757	998.296	8.83525	1.69441
%_43	Qgau	1122.63	x	x	0.114515	1122.63	14.2397	1.60913
%_2	**Qgau**	**1172.82**	**x**	**x**	**0.846428**	**1172.82**	**15.0219**	**1.45483**
%_22	Qgau	1252.31	x	x	0.113621	1252.31	31.5817	1.85037
%_8	**Qgau**	**1295.35**	**x**	**x**	**0.244584**	**1295.35**	**13.8456**	**1.35137**
%_15	Qgau	1333.15	x	x	0.176704	1333.15	20.7628	1.84705
%_4	**Qgau**	**1371.63**	**x**	**x**	**0.590362**	**1371.63**	**19.4286**	**1.68897**
%_53	**Qgau**	**1389.5**	**x**	**x**	**0.202911**	**1389.5**	**8.37401**	**1.60401**
%_7	**Qgau**	**1445.82**	**x**	**x**	**0.376284**	**1445.82**	**18.2567**	**2.13228**
%_16	Qgau	1478.92	x	x	0.141138	1478.92	12.9108	1.27985
%_10	**Qgau**	**1533.48**	**x**	**x**	**0.257518**	**1533.48**	**22.6134**	**1.41156**
%_14	**Qgau**	**1588.55**	**x**	**x**	**0.213888**	**1588.55**	**19.3352**	**1.17707**
%_1	**Qgau**	**1620.99**	**x**	**x**	**0.991819**	**1620.99**	**8.48004**	**1.46199**

L-cysteine



#	PeakType	Center			Parameters	Height	Center	HWHM	q	(h > 0.04)
%_4	**Qgau**	**517.445**	**x**	**x**		**0.213922**	**517.445**	**28.7274**	**1.65581**	
%_9	**Qgau**	**625.967**	**x**	**x**		**0.188652**	**625.967**	**14.0799**	**1.00008**	
%_1	**Qgau**	**669.797**	**x**	**x**		**1.07352**	**669.797**	**25.026**	**1.07137**	
%_31	Qgau	707.701	x	x		0.125674	707.701	13.459	1.11066	
%_32	Qgau	729.214	x	x		0.10742	729.214	10.241	1.2183	
%_37	Qgau	745.601	x	x		0.0813513	745.601	12.7323	0.999991	
%_6	**Qgau**	**801.425**	**x**	**x**		**0.203425**	**801.425**	**13.7443**	**0.999897**	
%_18	Qgau	823.342	x	x		0.0935258	823.342	11.1204	0.999935	
%_2	**Qgau**	**893.798**	**x**	**x**		**0.685963**	**893.798**	**16.4834**	**1.15393**	
%_36	Qgau	920.819	x	x		0.0589538	920.819	11.7514	1.2019	
%_10	Qgau	955.778	x	x		0.119422	955.778	23.4839	0.999521	
%_17	Qgau	1043.05	x	x		0.0416432	1043.05	14.4385	1.06833	
%_5	**Qgau**	**1057.47**	**x**	**x**		**0.180427**	**1057.47**	**19.1766**	**1.37861**	
%_13	Qgau	1130.91	x	x		0.0569785	1130.91	23.7926	1.09622	
%_16	Qgau	1286.9	x	x		0.0765448	1286.9	8.72292	1.38671	
%_3	**Qgau**	**1298.28**	**x**	**x**		**0.235413**	**1298.28**	**12.107**	**1.37223**	
%_8	**Qgau**	**1343.87**	**x**	**x**		**0.1553**	**1343.87**	**13.2249**	**1.567**	
%_7	**Qgau**	**1395.99**	**x**	**x**		**0.168389**	**1395.99**	**16.4244**	**1.09507**	
%_22	Qgau	1420.63	x	x		0.0535573	1420.63	14.5872	0.999806	
%_30	Qgau	1598.76	x	x		0.0510395	1598.76	10.941	1.98585	
%_28	Qgau	1621.39	x	x		0.0551901	1621.39	11.9534	1.84365	
%_24	Qgau	1641.97	x	x		0.0548389	1641.97	10.7495	2.09447	

L-cysteine has been investigated in Sparavigna, 2023. Here in the following table the peaks as have been determined with the first-derivative spectrum (with height above a given threshold):



Literature about L-cysteine: Diaz Fleming et al., 2009, Jing and Fang, 2007, Brolo et al., 2002, Graff and Bukowska, 2005, Yao and Huang, 2018.

Let us consider the centers of the q-Gaussians that we have given before, and compare with data from literature in the table given below. In bold within +/−5 cm^{-1}, in italic within +/−10 cm^{-1}, the q-Gaussian centers which are close to the peaks.

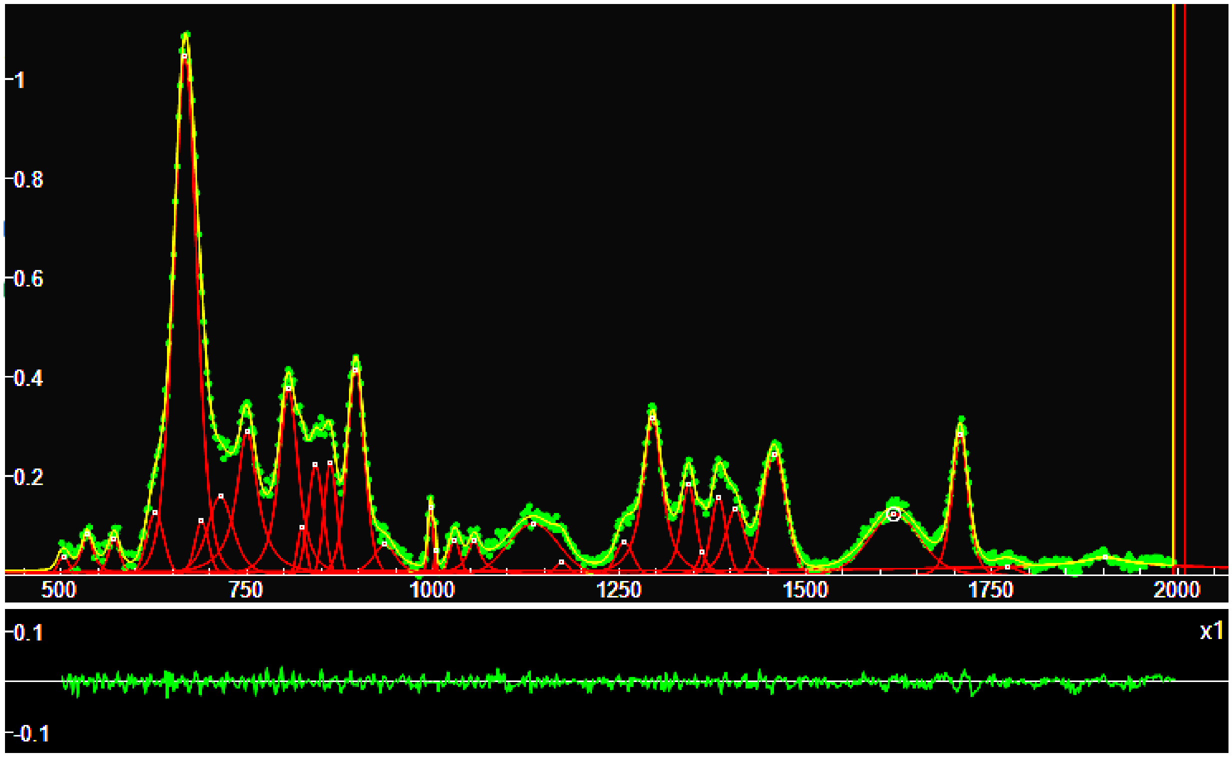
517.445 625.967 ***669.797*** 707.701 ***729.214*** 745.601 801.425 823.342 ***893.798*** 920.819 955.778 *1043.05* **1057.47** *1130.91* 1286.9 *1298.28* **1343.87** **1395.99** 1420.63 1598.76 1621.39 1641.97

In the following table, data from literature.

Diaz Fleming et al., 2009.	667		778	815		903	947	1002	1058		1200		1292	1347	1402
Jing and Fang, 2007.	663	725				908			1033				1291	1341	1395
Graff and Bukowska, 2005.	670	725				890									1395
Yao and Huang, 2018.	673		789		832	900	949		1050	1125		1232	1292	1339	1391

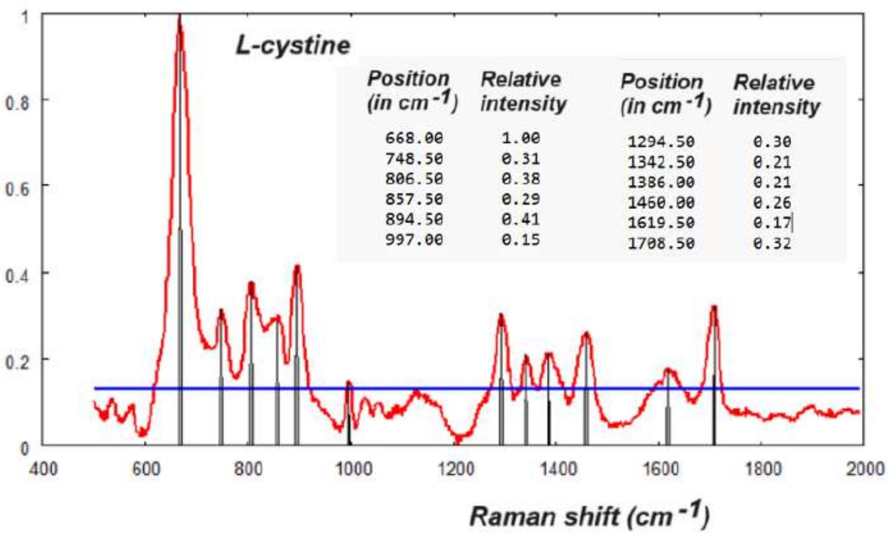
L-cystine

Literature on L-cystine: Lee et al., 1991, Su et al., 2022, Itoh and Hanari, 2022.

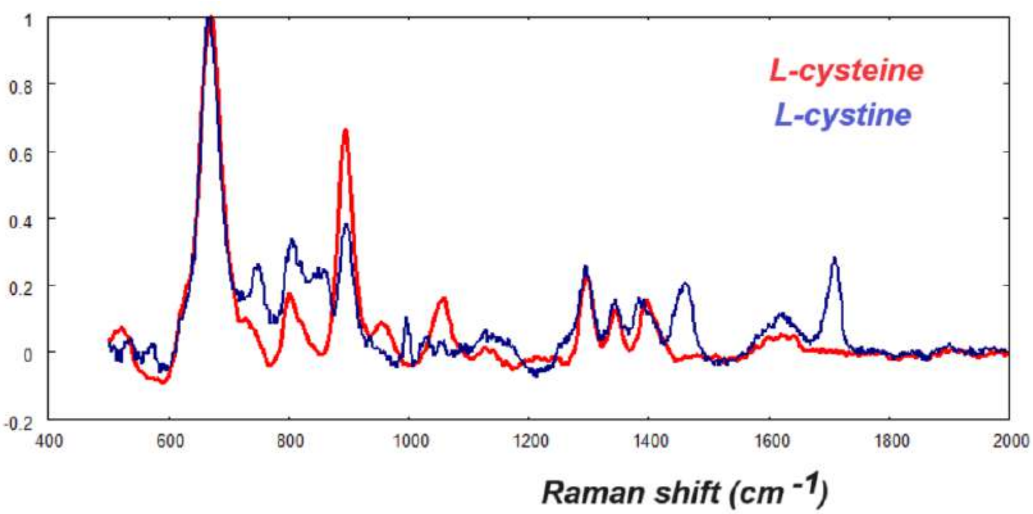


#	PeakType	Center	Parameters		Height	Center	HWHM	q ... (h > 0.10)
%_15	Qgau	535.434	x	x	0.082677	535.434	9.70627	2.08344
%_14	Qgau	626.648	x	x	0.125887	626.648	16.5337	1.01067
%_1	**Qgau**	**666.885**	**x**	**x**	**1.04685**	**666.885**	**20.7877**	**1.26573**
%_7	Qgau	689.062	x	x	0.109095	689.062	12.8326	1.15127
%_19	Qgau	714.089	x	x	0.159291	714.089	22.7415	1.42957
%_30	**Qgau**	**750.062**	**x**	**x**	**0.290384**	**750.062**	**16.8527**	**1.9841**
%_29	**Qgau**	**805.709**	**x**	**x**	**0.37457**	**805.709**	**16.3025**	**1.63571**
%_3	Qgau	823.484	x	x	0.0961291	823.484	8.34062	1.00529
%_20	**Qgau**	**842.099**	**x**	**x**	**0.222777**	**842.099**	**14.2008**	**0.999995**
%_9	**Qgau**	**861.879**	**x**	**x**	**0.225927**	**861.879**	**11.7972**	**0.999892**
%_2	**Qgau**	**895.911**	**x**	**x**	**0.41584**	**895.911**	**15.8149**	**1.23523**
%_10	Qgau	996.541	x	x	0.139399	996.541	4.6311	1.16102
%_12	Qgau	1134.49	x	x	0.104714	1134.49	47.6545	0.99704
%_4	**Qgau**	**1294.84**	**x**	**x**	**0.316848**	**1294.84**	**16.0032**	**1.80115**
%_13	Qgau	1343.31	x	x	0.182575	1343.31	12.7225	1.59931
%_32	Qgau	1383.39	x	x	0.156429	1383.39	14.0507	1.10228
%_33	Qgau	1405.83	x	x	0.134175	1405.83	16.8948	1.63444
%_6	**Qgau**	**1458.09**	**x**	**x**	**0.243735**	**1458.09**	**21.9402**	**1.05254**
%_11	Qgau	1619.71	x	x	0.123442	1619.71	47.0623	1.1741
%_5	**Qgau**	**1707.73**	**x**	**x**	**0.283449**	**1707.73**	**14.3828**	**1.36595**

L-cystine has been investigated in Sparavigna, 2023. Here in the following plot and table the peaks as have been determined with the first-derivative spectrum (with height above a given threshold):



As we did for homocysteine and homocysteine, let us compare the spectra.



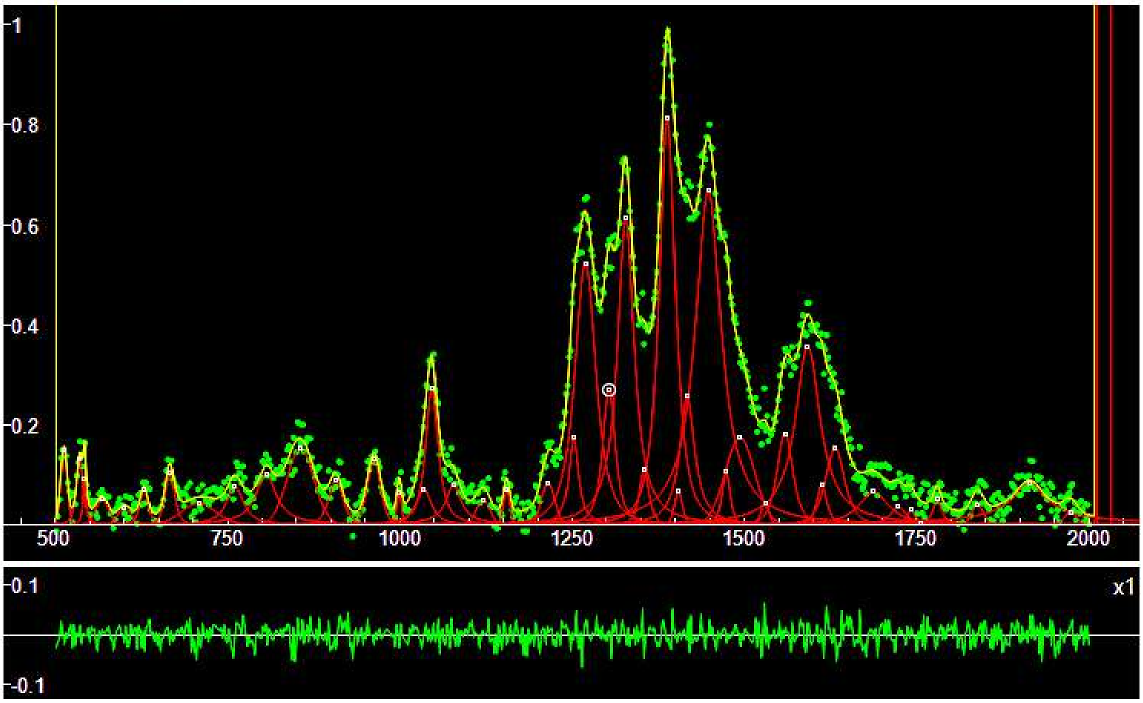
Comparing the fingerprints (in bold characters, the centers which have close values, within +/− 5 cm^{-1}):

L-cysteine
517.445 **625.967** **669.797** 707.701 729.214 745.601 **801.425** **823.342** **893.798** 920.819 955.778 1043.05 1057.47 **1130.91** 1286.9 **1298.28** **1343.87** 1395.99 1420.63 1598.76 **1621.39** 1641.97

L-cystine
535.434 **626.648** **666.885** 689.062 714.089 750.062 805.709 **823.484** 842.099 861.879 **895.911** 996.541 **1134.49** **1294.84** **1343.31** 1383.39 1405.83 1458.09 **1619.71** 1707.73

Leucine

Sherman and coworkers propose references Stewart and Fredericks, 1999, and Negri and Schultz, 2014.



#	PeakType	Center	Parameters		Height	Center	HWHM	q (h > 0.80)
%_14	**Qgau**	**512.18**	**x**	**x**	**0.150056**	**512.18**	**6.4972**	**0.999984**
%_12	Qgau	535.347	x	x	0.132432	535.347	5.9648	1.72617
%_27	Qgau	542.377	x	x	0.112065	542.377	2.03594	2.1105
%_16	Qgau	665.997	x	x	0.105326	665.997	8.6785	1.54874
%_33	Qgau	805.709	x	x	0.102214	805.709	17.5525	2.13158
%_9	**Qgau**	**855.465**	**x**	**x**	**0.152539**	**855.465**	**27.6916**	**0.999423**
%_35	Qgau	907.031	x	x	0.0894207	907.031	13.9381	1.39074
%_15	Qgau	962.224	x	x	0.131395	962.224	12.7988	1.27383
%_7	**Qgau**	**1046.31**	**x**	**x**	**0.274086**	**1046.31**	**10.8575**	**1.85383**
%_18	Qgau	1214.92	x	x	0.0837155	1214.92	13.6064	0.999949
%_13	**Qgau**	**1252.19**	**x**	**x**	**0.174106**	**1252.19**	**8.36908**	**2.02458**
%_4	**Qgau**	**1269.09**	**x**	**x**	**0.522888**	**1269.09**	**19.3881**	**1.6368**
%_45	**Qgau**	**1303.37**	**x**	**x**	**0.26926**	**1303.37**	**11.4275**	**1.70702**
%_3	**Qgau**	**1327.72**	**x**	**x**	**0.612553**	**1327.72**	**14.5944**	**1.96967**
%_47	Qgau	1354.33	x	x	0.110775	1354.33	9.17224	1.53178
%_1	**Qgau**	**1388**	**x**	**x**	**0.814109**	**1388**	**14.6941**	**1.70734**
%_6	**Qgau**	**1416.87**	**x**	**x**	**0.258597**	**1416.87**	**13.1672**	**1.97903**
%_2	**Qgau**	**1447.43**	**x**	**x**	**0.670485**	**1447.43**	**22.7853**	**1.98122**
%_10	Qgau	1473.3	x	x	0.106807	1473.3	7.45322	1.56356
%_8	**Qgau**	**1493.37**	**x**	**x**	**0.173821**	**1493.37**	**30.3714**	**0.999063**
%_11	**Qgau**	**1558.76**	**x**	**x**	**0.182376**	**1558.76**	**14.8433**	**1.52328**
%_5	**Qgau**	**1591.89**	**x**	**x**	**0.35613**	**1591.89**	**22.0416**	**2.03853**
%_39	Qgau	1612.2	x	x	0.0821004	1612.2	9.18521	1.59104
%_40	**Qgau**	**1631.57**	**x**	**x**	**0.155174**	**1631.57**	**17.7204**	**1.51022**
%_17	Qgau	1913.83	x	x	0.0840255	1913.83	29.8215	2.70657

The q-Gaussian centers:

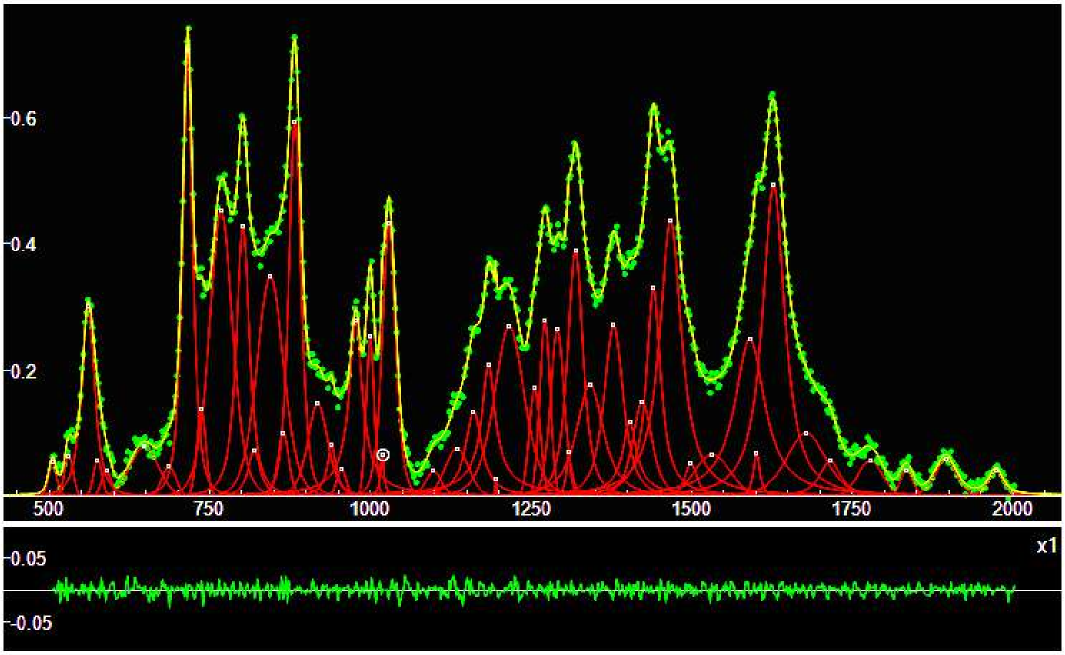
512.18	535.347	542.377	665.997	805.709	855.465(m)
907.031	962.224	1046.31(m)	1214.92	1252.19	1269.09(s)
1303.37(m)	1327.72(vs)	1354.33	1388(vs)	1416.87(m)	1447.43(vs)
1473.3	1493.37	1558.76	1591.89(s)	1612.2	1631.57
1913.83					

Table 4 from Stewart and Fredericks, 1999, provides data and assignments. The reported peaks are:

620	718	835	845	928	944	962	1130	1342	1410	1455

L-Histidine

Sherman and coworkers propose as literature: Stewart and Fredericks, 1999, Lim et al., 2008, Martusevičius et al., 1996.



#	PeakType	Center		Parameters	Height	Center	HWHM	q (h > 0.1)
%_17	**Qgau**	**560.408**	**x**	**x**	**0.301956**	**560.408**	**12.8061**	**1.63981**
%_1	**Qgau**	**715.172**	**x**	**x**	**0.71107**	**715.172**	**10.0375**	**1.61021**
%_34	Qgau	736.561	x	x	0.137551	736.561	10.0535	1.00014
%_8	**Qgau**	**767.334**	**x**	**x**	**0.452209**	**767.334**	**24.1083**	**1.26779**
%_5	**Qgau**	**801.304**	**x**	**x**	**0.428227**	**801.304**	**12.6506**	**1.69634**
%_12	**Qgau**	**843.892**	**x**	**x**	**0.349469**	**843.892**	**28.134**	**1.21357**
%_50	Qgau	864.236	x	x	0.100737	864.236	11.4838	1.24183
%_2	**Qgau**	**882.367**	**x**	**x**	**0.597978**	**882.367**	**12.3898**	**1.42412**
%_25	Qgau	917.819	x	x	0.147573	917.819	20.8349	1.31545
%_46	**Qgau**	**976.972**	**x**	**x**	**0.278196**	**976.972**	**12.203**	**2.24447**
%_45	**Qgau**	**999.425**	**x**	**x**	**0.25302**	**999.425**	**8.7543**	**1.00972**
%_9	**Qgau**	**1028.68**	**x**	**x**	**0.433691**	**1028.68**	**13.5383**	**1.35414**
%_48	Qgau	1160.51	x	x	0.135096	1160.51	15.3214	1.99569
%_13	Qgau	1183.64	x	x	0.209011	1183.64	12.4847	2.48762
%_16	**Qgau**	**1216.02**	**x**	**x**	**0.268593**	**1216.02**	**31.2931**	**1.32521**
%_24	Qgau	1255.5	x	x	0.171643	1255.5	12.0003	0.999855
%_10	**Qgau**	**1271.44**	**x**	**x**	**0.278802**	**1271.44**	**11.2618**	**0.999853**
%_14	**Qgau**	**1290.8**	**x**	**x**	**0.264102**	**1290.8**	**14.1843**	**1.26923**
%_6	**Qgau**	**1318.7**	**x**	**x**	**0.392091**	**1318.7**	**15.0808**	**1.62196**
%_20	Qgau	1341.48	x	x	0.177248	1341.48	26.4153	1.68352
%_49	**Qgau**	**1378.39**	**x**	**x**	**0.272027**	**1378.39**	**18.8562**	**1.62214**
%_51	Qgau	1403.31	x	x	0.11858	1403.31	12.9751	2.34933
%_18	Qgau	1423.13	x	x	0.150462	1423.13	19.6822	1.46038
%_4	**Qgau**	**1440.4**	**x**	**x**	**0.331913**	**1440.4**	**13.2271**	**1.99065**
%_7	**Qgau**	**1466.89**	**x**	**x**	**0.436676**	**1466.89**	**20.5567**	**1.94772**
%_15	**Qgau**	**1590.2**	**x**	**x**	**0.249331**	**1590.2**	**28.3836**	**1.98963**
%_3	**Qgau**	**1627.35**	**x**	**x**	**0.493789**	**1627.35**	**21.2911**	**1.85602**
%_22	Qgau	1677.84	x	x	0.100635	1677.84	40.7983	1.32226

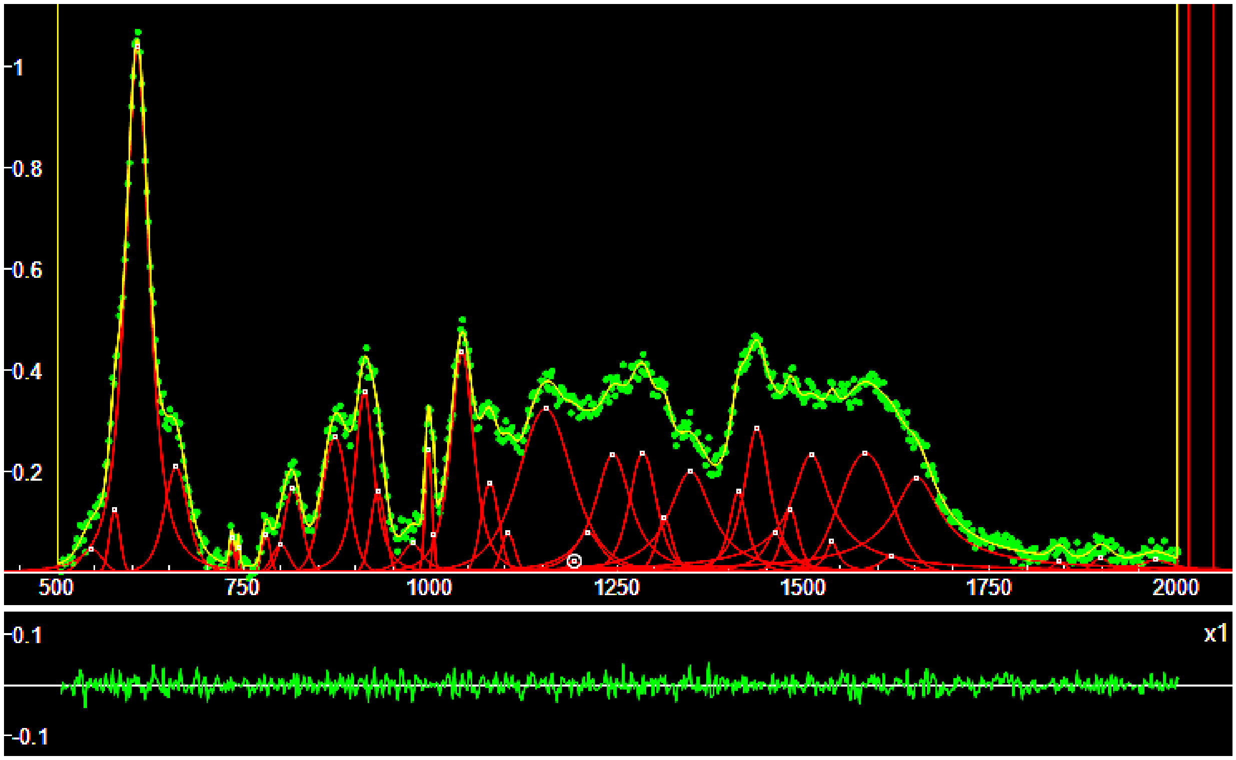
Therefore, the centers of the component are:

560.408(s)	715.172(vs)	736.561	767.334(s)	801.3048s)	843.892(s)
864.236	882.367(vs)	917.819	976.972(m)	999.425(m)	1028.68(s)
1160.51	1183.64	1216.02(m)	1255.5	1271.44(m)	1290.8
1318.7	1341.48	1378.39	1403.31	1423.13	1440.4(s)
1466.89(s)	1590.2(m)	1627.35(s)	1677.84		

In De Gelder et al., 2007, we find the following Raman peaks (in bold, the peaks which are corresponding to centers, within +/− 5 cm^{-1}, in italic within +/−10 cm^{-1}).

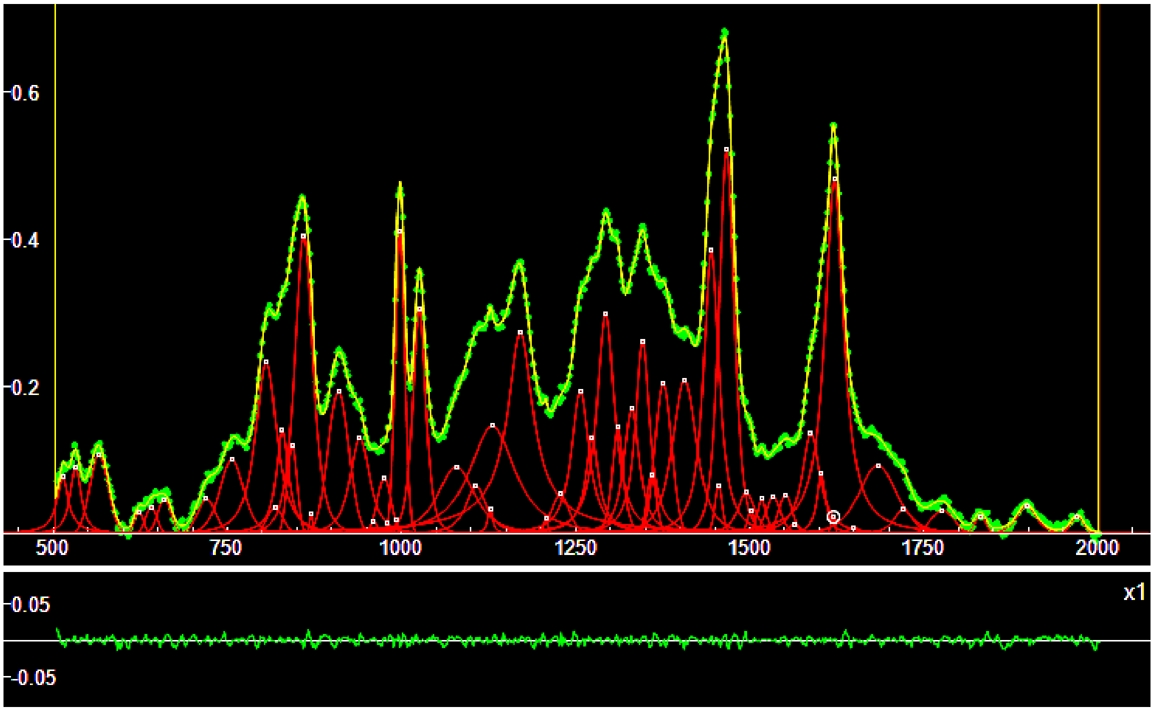
404(m), 422(mw,sh), 540(mw), 623(mw), 656(m), 680(w), ***731(mw),*** 784(mw), ***804(m),*** 824(mw), 852(m), ***918(m),*** 929(mw,sh), *963(m),* ***976(m),*** 1061(m), 1087(s), 1111(m), 1140(mw), 1174(m), *1224(m),* ***1250(m), 1271(s), 1317(vs),*** *1336(m)*, *1347(m)*, ***1407(m)***, *1430(m)*, *1476(mw)*, 1498(m), 1538(w), 1571(m), 1608(w), 1639(w)

Lipoamide



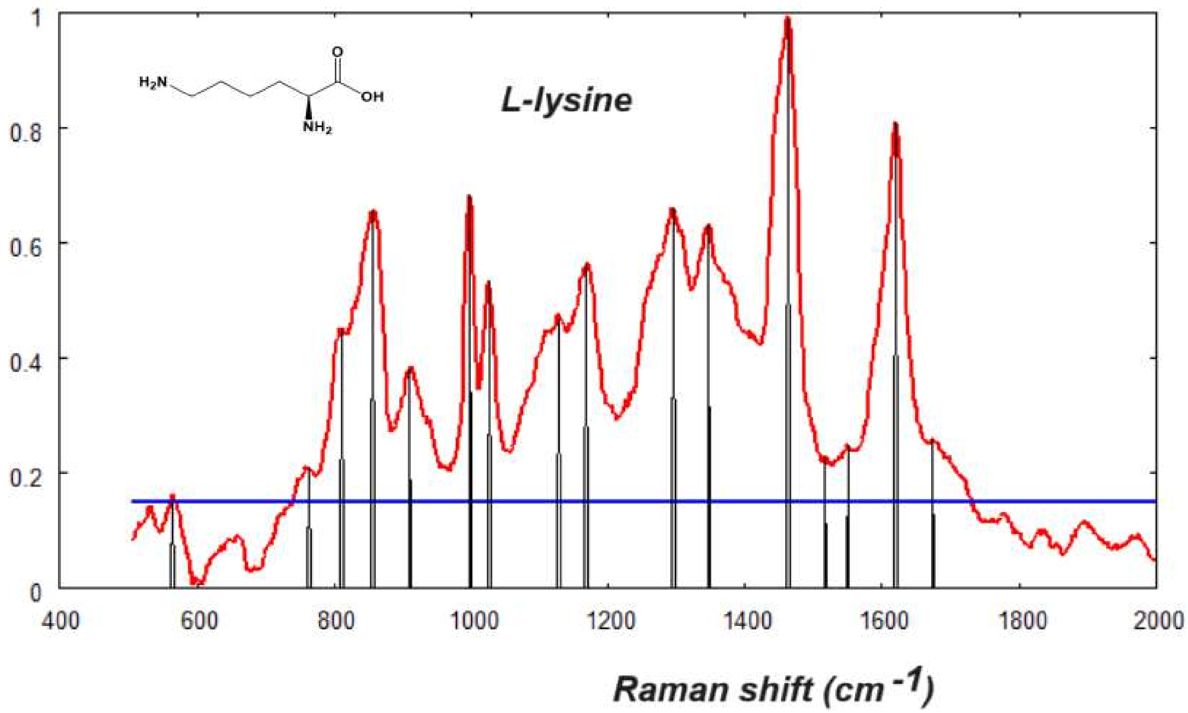
#	PeakType	Center	Parameters		Height	Center	HWHM	q (h > 0.08)
%_16	Qgau	576.709	x	x	0.123722	576.709	9.89256	0.999953
%_1	**Qgau**	**606.867**	**x**	**x**	**1.04181**	**606.867**	**20.1998**	**1.67159**
%_14	**Qgau**	**659.002**	**x**	**x**	**0.208648**	**659.002**	**20.8459**	**1.37568**
%_15	Qgau	815.616	x	x	0.167216	815.616	16.6678	1.14561
%_11	**Qgau**	**872.054**	**x**	**x**	**0.268494**	**872.054**	**23.9697**	**1.07415**
%_4	**Qgau**	**911.35**	**x**	**x**	**0.358155**	**911.35**	**15.8095**	**1.69298**
%_22	Qgau	929.301	x	x	0.161215	929.301	13.5887	1.01223
%_10	**Qgau**	**997.431**	**x**	**x**	**0.242576**	**997.431**	**6.32839**	**0.999962**
%_33	**Qgau**	**1004.43**	**x**	**x**	**0.0815081**	**1004.43**	**2.91366**	**1.19068**
%_2	**Qgau**	**1042.29**	**x**	**x**	**0.438237**	**1042.29**	**19.5897**	**1.59738**
%_57	Qgau	1079.64	x	x	0.177668	1079.64	16.6888	0.999848
%_55	**Qgau**	**1153.96**	**x**	**x**	**0.324393**	**1153.96**	**48.0996**	**1.37703**
%_5	Qgau	1210.99	x	x	0.080018	1210.99	22.894	2.00186
%_9	**Qgau**	**1244.76**	**x**	**x**	**0.234593**	**1244.76**	**29.5433**	**1.85521**
%_3	**Qgau**	**1284.78**	**x**	**x**	**0.237381**	**1284.78**	**24.3565**	**1.3597**
%_6	Qgau	1313.62	x	x	0.107375	1313.62	13.9962	1.41333
%_7	**Qgau**	**1348.48**	**x**	**x**	**0.200406**	**1348.48**	**35.0018**	**2.014**
%_19	Qgau	1412.66	x	x	0.160123	1412.66	15.495	1.69246
%_43	**Qgau**	**1437.77**	**x**	**x**	**0.286492**	**1437.77**	**21.7964**	**1.71896**
%_44	Qgau	1482.34	x	x	0.125877	1482.34	14.2173	1.50771
%_47	**Qgau**	**1583.11**	**x**	**x**	**0.236639**	**1583.11**	**49.499**	**0.997912**
%_49	**Qgau**	**1510.16**	**x**	**x**	**0.234007**	**1510.16**	**30.9031**	**2.49847**
%_48	Qgau	1652.17	x	x	0.188699	1652.17	38.7433	2.60028

L-lysine



#	PeakType	Center	Parameters		Height	Center	HWHM	q	(h > 0.09)
%_34	Qgau	565.568x	x	x	0.10804	565.568	18.501	0.999872	
%_37	Qgau	756.229x	x	x	0.100926	756.229	23.002	1.27844	
%_8	**Qgau**	**805.665x**	**x**	**x**	**0.232742**	**805.665**	**19.1429**	**1.70557**	
%_39	Qgau	828.89 x	x	x	0.141639	828.89	10.3958	2.02729	
%_48	Qgau	842.797x	x	x	0.120523	842.797	10.0273	0.999998	
%_38	**Qgau**	**859.672x**	**x**	**x**	**0.404788**	**859.672**	**16.6498**	**1.48266**	
%_10	Qgau	909.254x	x	x	0.19314	909.254	21.0803	0.999673	
%_49	Qgau	940.185x	x	x	0.130523	940.185	17.7422	1.66115	
%_3	**Qgau**	**997.706x**	**x**	**x**	**0.412654**	**997.706**	**9.47971**	**1.04221**	
%_6	**Qgau**	**1025.43x**	**x**	**x**	**0.306007**	**1025.43**	**11.9403**	**1.47385**	
%_11	Qgau	1130.33x	x	x	0.146155	1130.33	40.4937	1.76785	
%_40	**Qgau**	**1170.57x**	**x**	**x**	**0.273028**	**1170.57**	**21.9174**	**2.35852**	
%_59	Qgau	1256.63x	x	x	0.193161	1256.63	15.5182	1.88178	
%_60	Qgau	1273.6 x	x	x	0.1312	1273.6	11.0605	2.18907	
%_42	**Qgau**	**1293.05x**	**x**	**x**	**0.299483**	**1293.05**	**15.3753**	**1.85177**	
%_61	Qgau	1310.54x	x	x	0.145755	1310.54	10.0839	1.46135	
%_69	Qgau	1330.44x	x	x	0.169957	1330.44	13.7983	1.7912	
%_62	**Qgau**	**1346.05x**	**x**	**x**	**0.260804**	**1346.05**	**12.3055**	**1.88846**	
%_64	**Qgau**	**1375.79x**	**x**	**x**	**0.204261**	**1375.79**	**16.6304**	**1.00062**	
%_65	**Qgau**	**1406.25x**	**x**	**x**	**0.208702**	**1406.25**	**22.1551**	**1.57464**	
%_1	**Qgau**	**1466.7 x**	**x**	**x**	**0.520765**	**1466.7**	**14.2637**	**1.39675**	
%_67	**Qgau**	**1444.73x**	**x**	**x**	**0.384747**	**1444.73**	**13.4068**	**1.81615**	
%_4	Qgau	1587.84x	x	x	0.136498	1587.84	15.4859	1.90074	
%_2	**Qgau**	**1621.36x**	**x**	**x**	**0.482424**	**1621.36**	**16.0409**	**1.95601**	
%_14	Qgau	1683.74x	x	x	0.0933717	1683.74	35.5198	1.39384	

L-lysine has been investigated in [Sparavigna, 2023](), with the first derivative spectrum.

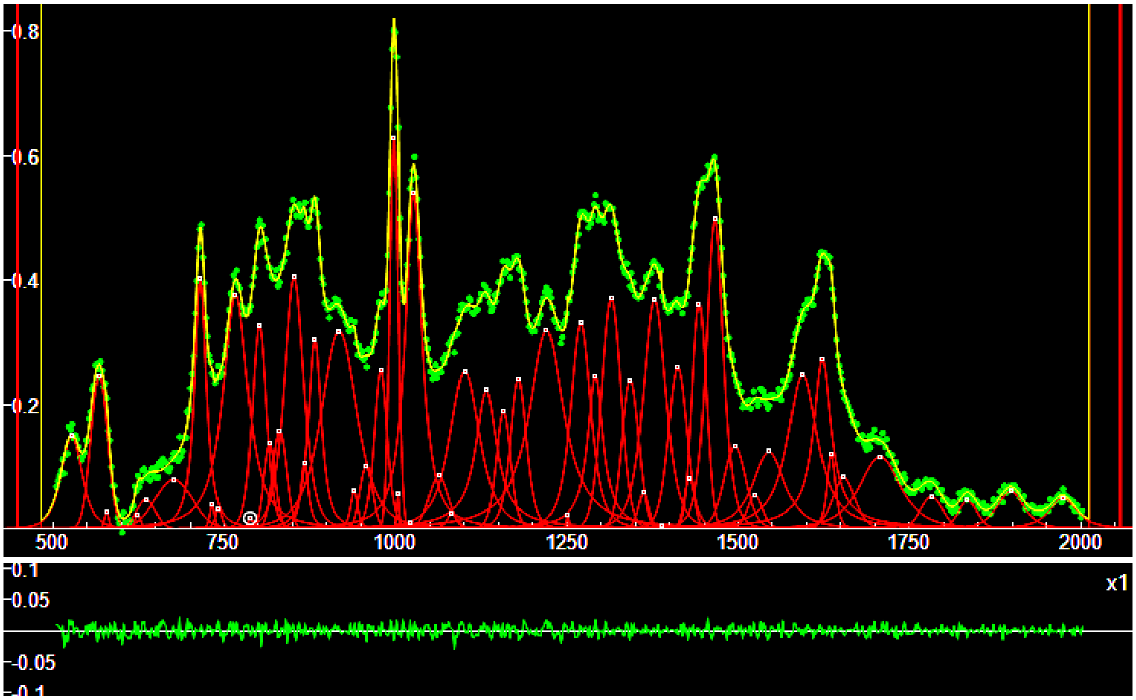


Here in the following table the peaks as have been determined with the first-derivative spectrum (with height above a given threshold):

Position (in cm $^{-1}$)	Relative intensity	Position (in cm $^{-1}$)	Relative intensity
563.50	0.15	1168.00	0.56
762.50	0.21	1294.50	0.66
811.50	0.45	1347.00	0.63
855.50	0.66	1462.50	0.99
911.00	0.38	1517.50	0.23
998.00	0.68	1549.50	0.25
1026.50	0.53	1620.00	0.81
1127.50	0.47	1674.00	0.26

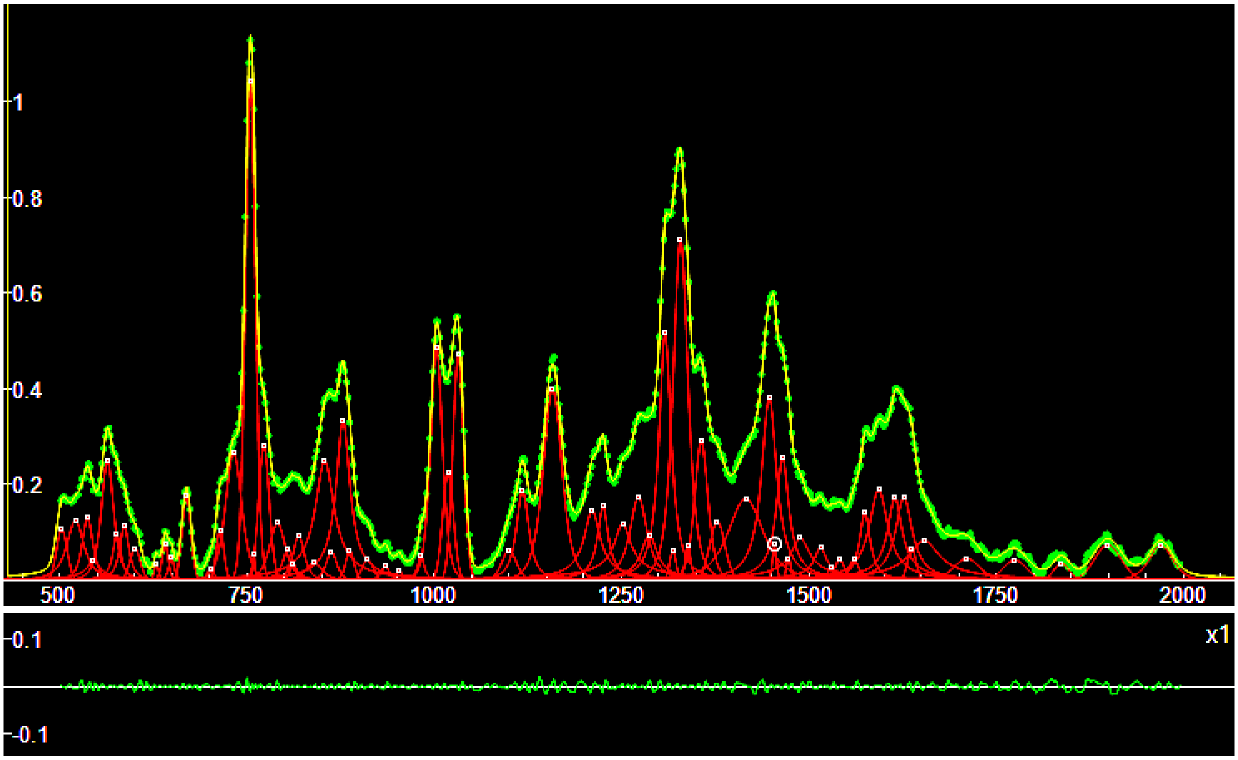
According to Sherman et al., SERS spectra have previously been reported for this molecule: Sengupta et al., 2005, Aliaga et al., 2009. Let us add Aboltaman et al., 2023, Yao and Huang, 2022, Das et al., 2020.

L-methionine sulfoximine



#	PeakType	Center	Parameters		Height	Center	HWHM	q	(H > 0.14)
%_27	Qgau	527.315	x	x	0.149161	527.315	20.1785	1.43966	
%_22	Qgau	567.702	x	x	0.245674	567.702	17.0966	0.999868	
%_7	**Qgau**	**715.231**	**x**	**x**	**0.404512**	**715.231**	**10.659**	**1.76735**	
%_15	**Qgau**	**766.572**	**x**	**x**	**0.37676**	**766.572**	**22.5161**	**1.79231**	
%_8	**Qgau**	**801.468**	**x**	**x**	**0.327621**	**801.468**	**13.7434**	**1.27653**	
%_44	Qgau	831.053	x	x	0.156774	831.053	14.1163	0.999929	
%_6	**Qgau**	**851.902**	**x**	**x**	**0.404492**	**851.902**	**18.4409**	**1.40661**	
%_5	**Qgau**	**882.233**	**x**	**x**	**0.306169**	**882.233**	**11.6769**	**1.6926**	
%_18	**Qgau**	**917.711**	**x**	**x**	**0.317793**	**917.711**	**33.7592**	**1.46679**	
%_26	Qgau	978.435	x	x	0.256376	978.435	12.6119	1.2873	
%_1	**Qgau**	**997.85**	**x**	**x**	**0.634351**	**997.85**	**8.53498**	**1.01857**	
%_3	**Qgau**	**1026.4**	**x**	**x**	**0.541391**	**1026.4**	**14.9146**	**1.86747**	
%_19	Qgau	1100.93	x	x	0.253897	1100.93	27.7559	1.56325	
%_16	Qgau	1132.51	x	x	0.222467	1132.51	18.5632	2.09692	
%_24	Qgau	1157.51	x	x	0.189082	1157.51	14.2477	1.18223	
%_12	Qgau	1179.25	x	x	0.24053	1179.25	15.2514	1.38356	
%_17	**Qgau**	**1220.37**	**x**	**x**	**0.319163**	**1220.37**	**31.0505**	**1.8751**	
%_13	**Qgau**	**1270.32**	**x**	**x**	**0.330432**	**1270.32**	**18.621**	**1.51841**	
%_4	Qgau	1291.56	x	x	0.246453	1291.56	13.7163	2.00897	
%_9	**Qgau**	**1314.81**	**x**	**x**	**0.369974**	**1314.81**	**19.1453**	**1.10784**	
%_23	Qgau	1342.57	x	x	0.23917	1342.57	17.3359	0.999594	
%_14	**Qgau**	**1377.95**	**x**	**x**	**0.369049**	**1377.95**	**21.4707**	**1.4216**	
%_21	Qgau	1411.87	x	x	0.259938	1411.87	18.3481	1.21004	
%_10	**Qgau**	**1443.18**	**x**	**x**	**0.362973**	**1443.18**	**14.7193**	**0.999781**	
%_2	**Qgau**	**1465.85**	**x**	**x**	**0.498816**	**1465.85**	**16.1384**	**1.39126**	
%_46	Qgau	1593.96	x	x	0.248012	1593.96	26.8812	1.80829	
%_11	Qgau	1622.85	x	x	0.2729	1622.85	15.1407	2.20583	

L-tryptophan



#	PeakType	Center	Parameters			Height	Center	HWHM	q	(h > 0.05)
%_23	Qgau	502.867	x	x	x	0.107574	502.867	9.93948	1.00007	
%_39	Qgau	520.892	x	x	x	0.125706	520.892	14.2531	1.79517	
%_37	Qgau	537.089	x	x	x	0.131668	537.089	8.98731	1.64037	
%_30	Qgau	563.662	x	x	x	0.251177	563.662	10.5553	1.55644	
%_31	Qgau	576.086	x	x	x	0.100255	576.086	5.95915	2.19609	
%_32	Qgau	586.032	x	x	x	0.115546	586.032	7.47295	1.88147	
%_33	Qgau	600.507	x	x	x	0.0661625	600.507	9.95468	1.02793	
%_34	Qgau	629.01		x	x	0.0348737	629.01	4.22579	1.00018	
%_35	Qgau	640.758	x	x	x	0.0782045	640.758	5.33358	1.3205	
%_36	Qgau	649.08		x	x	0.0492128	649.08	4.4669	1.65484	
%_14	Qgau	669.16		x	x	0.178679	669.16	8.27613	1.00002	
%_25	Qgau	713.926	x	x	x	0.106949	713.926	7.0626	1.00007	
%_13	Qgau	732.014	x	x	x	0.26742	732.014	14.3535	1.34556	
%_1	Qgau	754.478	x	x	x	1.04483	754.478	9.16089	1.09287	
%_42	Qgau	758.901	x	x	x	0.057346	758.901	2.29903	1.00998	
%_2	Qgau	772.585	x	x	x	0.282608	772.585	9.68552	1.122	
%_3	Qgau	790.633	x	x	x	0.120398	790.633	13.7032	1.48374	
%_9	Qgau	804.674	x	x	x	0.0678834	804.674	8.38702	1.97615	
%_7	Qgau	818.888	x	x	x	0.0942258	818.888	9.6279	1.61582	
%_46	Qgau	853.641	x	x	x	0.250971	853.641	15.1664	2.25154	
%_20	Qgau	862.638	x	x	x	0.0604697	862.638	9.21011	1.48268	
%_43	Qgau	878.059	x	x	x	0.337346	878.059	10.8218	2.19526	
%_17	Qgau	887.058	x	x	x	0.0638588	887.058	7.21831	1.34542	
%_48	Qgau	982.281	x	x	x	0.0545629	982.281	4.90071	2.01813	
%_8	Qgau	1002.85	x	x	x	0.488488	1002.85	10.4945	1.34517	

%_74	Qgau	1018.32	x	x	x	0.226792	1018.32	10.0937	0.99997
%_49	Qgau	1031.98	x	x	x	0.472751	1031.98	10.0827	1.00001
%_29	Qgau	1099.83	x	x	x	0.0642398	1099.83	13.0443	1.27293
%_12	Qgau	1117.77	x	x	x	0.188738	1117.77	10.0907	1.81205
%_5	Qgau	1157.77	x	x	x	0.400763	1157.77	16.2389	1.43101
%_50	Qgau	1210.81	x	x	x	0.146988	1210.81	12.7999	2.39824
%_51	Qgau	1225.25	x	x	x	0.155778	1225.25	8.47001	2.2198
%_52	Qgau	1251.39	x	x	x	0.12004	1251.39	13.3395	2.88279
%_18	Qgau	1272.62	x	x	x	0.175359	1272.62	14.1611	1.80673
%_75	Qgau	1286.89	x	x	x	0.0960407	1286.89	12.8974	2.28344
%_55	Qgau	1308.14	x	x	x	0.519178	1308.14	9.73966	1.92027
%_54	Qgau	1318.38	x	x	x	0.0632579	1318.38	6.06906	1.00005
%_53	Qgau	1328.8		x	x	0.716256	1328.8	12.6213	1.51458
%_24	Qgau	1338.7		x	x	0.0747675	1338.7	4.10607	1.92211
%_21	Qgau	1356.39	x	x	x	0.292399	1356.39	11.6362	1.40396
%_28	Qgau	1377.71	x	x	x	0.123692	1377.71	14.1372	1.07609
%_56	Qgau	1415.64	x	x	x	0.170769	1415.64	30.1941	1.55756
%_57	Qgau	1446.99	x	x	x	0.382592	1446.99	12.4754	1.95744
%_59	Qgau	1454.04	x	x	x	0.0758626	1454.04	3.66327	1.25291
%_58	Qgau	1465.25	x	x	x	0.257199	1465.25	9.85173	2.23797
%_61	Qgau	1488.68	x	x	x	0.0889039	1488.68	15.574	2.75942
%_63	Qgau	1515.66	x	x	x	0.0702154	1515.66	9.78447	2.85423
%_69	Qgau	1574.75	x	x	x	0.141918	1574.75	8.63019	2.02981
%_68	Qgau	1593.2		x	x	0.190361	1593.2	15.1006	2.1287
%_66	Qgau	1614.92	x	x	x	0.173896	1614.92	11.4481	2.3822
%_67	Qgau	1626.91	x	x	x	0.173924	1626.91	13.5143	2.11237
%_44	Qgau	1637.3		x	x	0.0680258	1637.3	7.9811	1.00006
%_71	Qgau	1653.97	x	x	x	0.0838281	1653.97	25.0152	2.54035
%_72	Qgau	1899.31	x	x	x	0.074355	1899.31	25.058	1.05671
%_22	Qgau	1969.93	x	x	x	0.0741344	1969.93	20.9099	1.40791

Further reducing the considered components:

#	PeakType	Center		Parameters		Height	Center	HWHM	q (h > 0.10, **bold** 0.15)
%_23	Qgau	502.867	x	x	x	0.107574	502.867	9.93948	1.00007
%_39	Qgau	520.892	x	x	x	0.125706	520.892	14.2531	1.79517
%_37	Qgau	537.089	x	x	x	0.131668	537.089	8.98731	1.64037
%_30	**Qgau**	**563.662**	**x**	**x**	**x**	**0.251177**	**563.662**	**10.5553**	**1.55644**
%_31	Qgau	576.086	x	x	x	0.100255	576.086	5.95915	2.19609
%_32	Qgau	586.032	x	x	x	0.115546	586.032	7.47295	1.88147
%_14	**Qgau**	**669.16**		**x**	**x**	**0.178679**	**669.16**	**8.27613**	**1.00002**
%_25	Qgau	713.926	x	x	x	0.106949	713.926	7.0626	1.00007
%_13	**Qgau**	**732.014**	**x**	**x**	**x**	**0.26742**	**732.014**	**14.3535**	**1.34556**
%_1	**Qgau**	**754.478**	**x**	**x**	**x**	**1.04483**	**754.478**	**9.16089**	**1.09287**
%_2	**Qgau**	**772.585**	**x**	**x**	**x**	**0.282608**	**772.585**	**9.68552**	**1.122**
%_3	Qgau	790.633	x	x	x	0.120398	790.633	13.7032	1.48374
%_46	**Qgau**	**853.641**	**x**	**x**	**x**	**0.250971**	**853.641**	**15.1664**	**2.25154**
%_43	Qgau	878.059	x	x	x	0.337346	878.059	10.8218	2.19526
%_8	**Qgau**	**1002.85**	**x**	**x**	**x**	**0.488488**	**1002.85**	**10.4945**	**1.34517**
%_74	Qgau	1018.32	x	x	x	0.226792	1018.32	10.0937	0.99997
%_49	**Qgau**	**1031.98**	**x**	**x**	**x**	**0.472751**	**1031.98**	**10.0827**	**1.00001**
%_12	**Qgau**	**1117.77**	**x**	**x**	**x**	**0.188738**	**1117.77**	**10.0907**	**1.81205**
%_5	**Qgau**	**1157.77**	**x**	**x**	**x**	**0.400763**	**1157.77**	**16.2389**	**1.43101**
%_50	Qgau	1210.81	x	x	x	0.146988	1210.81	12.7999	2.39824
%_51	**Qgau**	**1225.25**	**x**	**x**	**x**	**0.155778**	**1225.25**	**8.47001**	**2.2198**

%_52	Qgau	1251.39	x	x	x	0.12004	1251.39	13.3395	2.88279
%_18	**Qgau**	**1272.62**	**x**	**x**	**x**	**0.175359**	**1272.62**	**14.1611**	**1.80673**
%_55	**Qgau**	**1308.14**	**x**	**x**	**x**	**0.519178**	**1308.14**	**9.73966**	**1.92027**
%_53	**Qgau**	**1328.8**		**x**	**x**	**0.716256**	**1328.8**	**12.6213**	**1.51458**
%_21	**Qgau**	**1356.39**	**x**	**x**	**x**	**0.292399**	**1356.39**	**11.6362**	**1.40396**
%_28	Qgau	1377.71	x	x	x	0.123692	1377.71	14.1372	1.07609
%_56	**Qgau**	**1415.64**	**x**	**x**	**x**	**0.170769**	**1415.64**	**30.1941**	**1.55756**
%_57	**Qgau**	**1446.99**	**x**	**x**	**x**	**0.382592**	**1446.99**	**12.4754**	**1.95744**
%_58	**Qgau**	**1465.25**	**x**	**x**	**x**	**0.257199**	**1465.25**	**9.85173**	**2.23797**
%_69	Qgau	1574.75	x	x	x	0.141918	1574.75	8.63019	2.02981
%_68	**Qgau**	**1593.2**		**x**	**x**	**0.190361**	**1593.2**	**15.1006**	**2.1287**
%_66	**Qgau**	**1614.92**	**x**	**x**	**x**	**0.173896**	**1614.92**	**11.4481**	**2.3822**
%_67	**Qgau**	**1626.91**	**x**	**x**	**x**	**0.173924**	**1626.91**	**13.5143**	**2.11237**

Therefore, the centers of the components are:

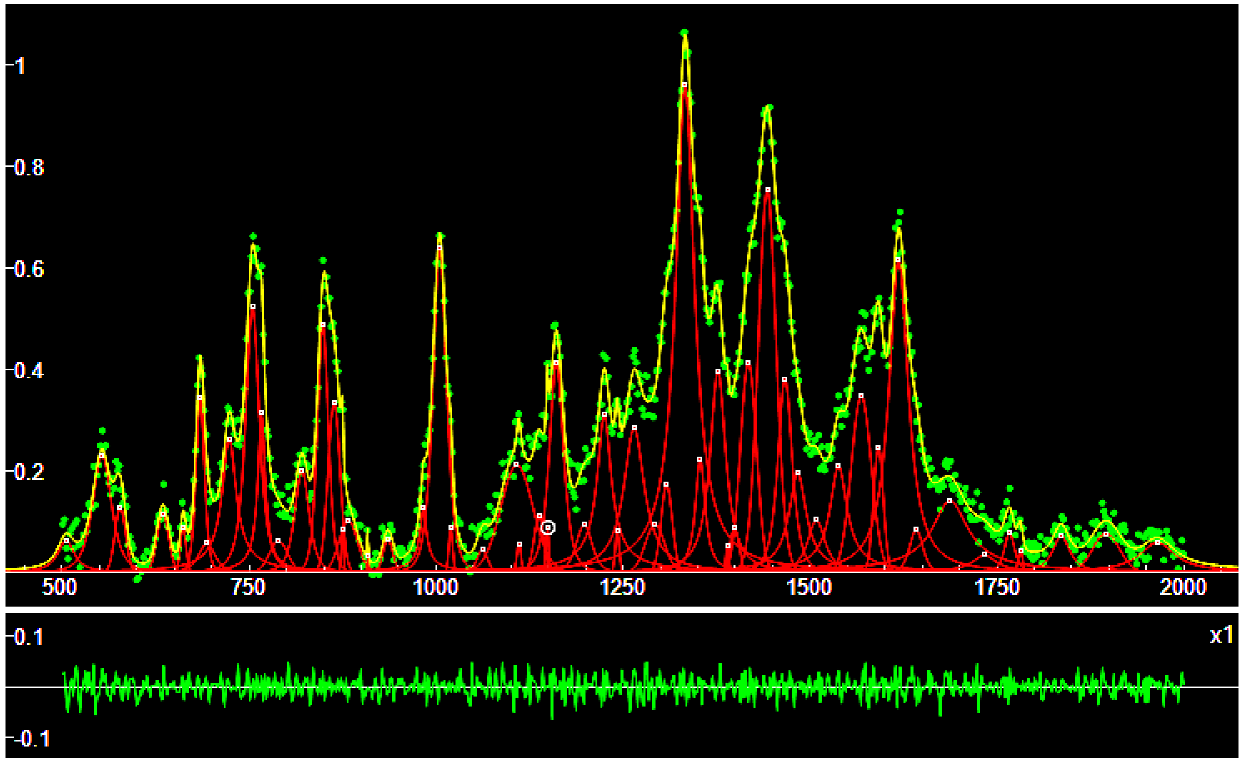
502.867	520.892	537.089	563.662(m)	576.086	586.032
669.16(m)	713.926	732.014(m)	754.478 (vs)	772.585(s)	790.633
853.641(m)	878.059(s)	1002.85(s)	1018.32(m)	1031.98(s)	1117.77(m)
1157.778(s)	1210.81	1225.25(m)	1251.39	1272.62	1308.1(s)
1328.8(vs)	1356.39(m)	1377.71	1415.64	1446.99 (s)	1465.25(m)
1574.75	1593.2(m)	1614.92	1626.91		

In De Gelder et al., 2007, we find the following Raman peaks (in **bold**, the peaks which are corresponding to q-Gaussian centers, within +/− 5 cm^{-1}, and in italic, within +/− 10 cm^{-1}):

393(w), 425(w), 456(w), 498(m), *509(m)*, ***534(m)***, 548(w), ***574(m),*** *596(m)*, 626(m), 683(w), *706(m)*, *741(m)*, ***755(vs),*** *766(m)*, *778(m)*, 802(w), 840(m), *848(m)*, 865(m), ***874(s),*** 988(w), *1009(vs)*, 1046(w), 1076(w), 1103(w), ***1118(m), 1160(w), 1207(w),*** *1231(m)*, ***1253(w),*** *1278(w)*, ***1309(w),*** *1314(m)*, ***1328(m),*** 1338(s), ***1358(s),*** *1423(s)*, ***1450(m),*** 1457(m), 1486(m), 1556(s), ***1576(m), 1616(m)***

Sherman et al. are mentioning the SERS spectra reported in Aliaga et al., 2009, Qu et al., 2012. Let us add Aboltaman et al., 2023, Gao et al., 2023, Xu et al., 2022, Gautam et al., 2022.

L-tryptophanamide

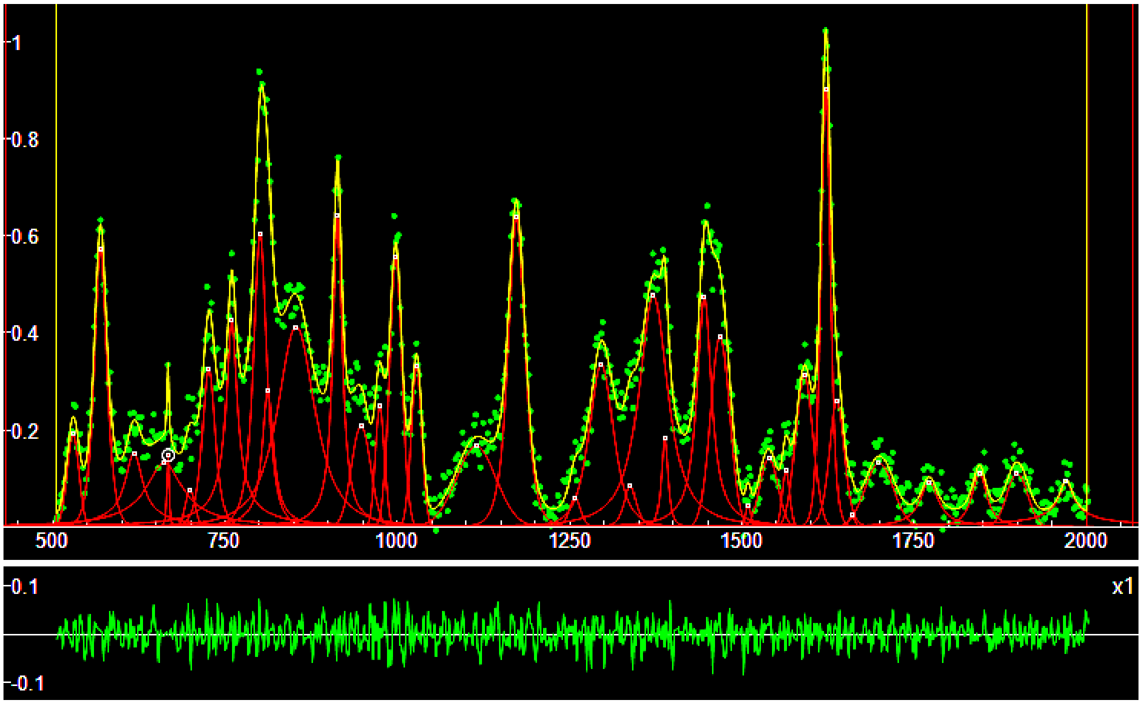


#	PeakType	Center	Parameters		Height	Center	HWHM	q ...
%_40	Qgau	505.14	x	x	0.0635918	505.14	13.5069	1.98942
%_18	Qgau	553.287	x	x	0.231473	553.287	16.1335	1.54068
%_34	Qgau	577.613	x	x	0.12871	577.613	10.0293	1.00001
%_26	Qgau	634.543	x	x	0.11583	634.543	11.041	1
%_31	Qgau	661.759	x	x	0.0890779	661.759	5.05891	1.16878
%_13	Qgau	684.503	x	x	0.346232	684.503	7.51814	1.31307
%_33	Qgau	693.323	x	x	0.0580727	693.323	13.9694	1.57172
%_19	Qgau	723.23	x	x	0.265304	723.23	11.1941	2.28803
%_5	Qgau	754.312	x	x	0.526487	754.312	11.4236	1.59839
%_23	Qgau	766.47	x	x	0.314042	766.47	5.76137	2.24499
%_35	Qgau	789.225	x	x	0.0622217	789.225	17.2845	1.00058
%_24	Qgau	820.509	x	x	0.201405	820.509	12.4435	1.50152
%_6	Qgau	848.619	x	x	0.489313	848.619	9.75321	1.30424
%_16	Qgau	863.585	x	x	0.335422	863.585	11.3583	0.999947
%_56	Qgau	874.664	x	x	0.108265	874.664	1.6102	1.19827
%_30	Qgau	882.657	x	x	0.102388	882.657	17.4521	1.00245
%_57	Qgau	908.42	x	x	0.0581179	908.42	0.612662	1.00285
%_37	Qgau	935.571	x	x	0.0653727	935.571	9.20733	1.00013
%_28	Qgau	982.964	x	x	0.128768	982.964	5.17918	2.71766
%_4	Qgau	1004.89	x	x	0.64004	1004.89	11.773	1.44036

%_38	Qgau	1019.56	x	x	0.0912701	1019.56	3.5143	1.00006
%_42	Qgau	1061.74	x	x	0.0451848	1061.74	10.0478	1.00011
%_17	Qgau	1107.98	x	x	0.212184	1107.98	30.1725	1.0569
%_58	Qgau	1110.56	x	x	0.0611348	1110.56	3.71738	1.00424
%_43	Qgau	1137.38	x	x	0.111894	1137.38	8.88737	1.17111
%_55	Qgau	1148.6	x	x	0.122926	1148.6	1.40327	1.76001
%_10	Qgau	1160.8	x	x	0.414775	1160.8	12.0726	1.51343
%_44	Qgau	1197.89	x	x	0.0948247	1197.89	14.0258	1.39427
%_11	Qgau	1224.72	x	x	0.311512	1224.72	11.2145	2.3611
%_53	Qgau	1242.08	x	x	0.0866367	1242.08	3.59074	1.00006
%_14	Qgau	1264.63	x	x	0.285693	1264.63	16.5368	2.06985
%_54	Qgau	1292.5	x	x	0.0949248	1292.5	18.331	0.999611
%_25	Qgau	1308.16	x	x	0.17389	1308.16	10.4585	1.00011
%_1	Qgau	1332.76	x	x	0.964426	1332.76	14.9919	2.11178
%_21	Qgau	1353.08	x	x	0.22717	1353.08	7.68316	2.01288
%_9	Qgau	1376.67	x	x	0.398508	1376.67	12.7339	1.92893
%_45	Qgau	1389.35	x	x	0.057847	1389.35	2.66674	1.00011
%_32	Qgau	1398.88	x	x	0.0890905	1398.88	8.55639	1.00009
%_7	Qgau	1417.47	x	x	0.415649	1417.47	15.0396	1.0001
%_2	Qgau	1442.55	x	x	0.756666	1442.55	16.4938	1.08408
%_46	Qgau	1466.44	x	x	0.383445	1466.44	12.1773	1.53446
%_47	Qgau	1483.25	x	x	0.196612	1483.25	13.8754	2.19354
%_52	Qgau	1508.27	x	x	0.103671	1508.27	14.5502	1.78408
%_20	Qgau	1537.91	x	x	0.211039	1537.91	13.5995	2.27228
%_8	Qgau	1568.3	x	x	0.348625	1568.3	18.9488	0.999984
%_15	Qgau	1591.17	x	x	0.248545	1591.17	9.17014	1.00003
%_3	Qgau	1618.2	x	x	0.618341	1618.2	15.6178	1.95411
%_48	Qgau	1641.71	x	x	0.0848378	1641.71	11.7919	1.3621
%_22	Qgau	1687.13	x	x	0.141623	1687.13	29.3284	2.28653
%_51	Qgau	1733.19	x	x	0.0344621	1733.19	19.347	2.3059
%_29	Qgau	1766.61	x	x	0.0792541	1766.61	8.66777	1.60466
%_50	Qgau	1781.16	x	x	0.0449193	1781.16	4.12127	1.00002
%_36	Qgau	1835.76	x	x	0.0726922	1835.76	14.0365	1.93869
%_27	Qgau	1895.7	x	x	0.0770053	1895.7	25.4399	0.999792
%_49	Qgau	1964.34	x	x	0.0596845	1964.34	28.455	2.12914

Lumichrome

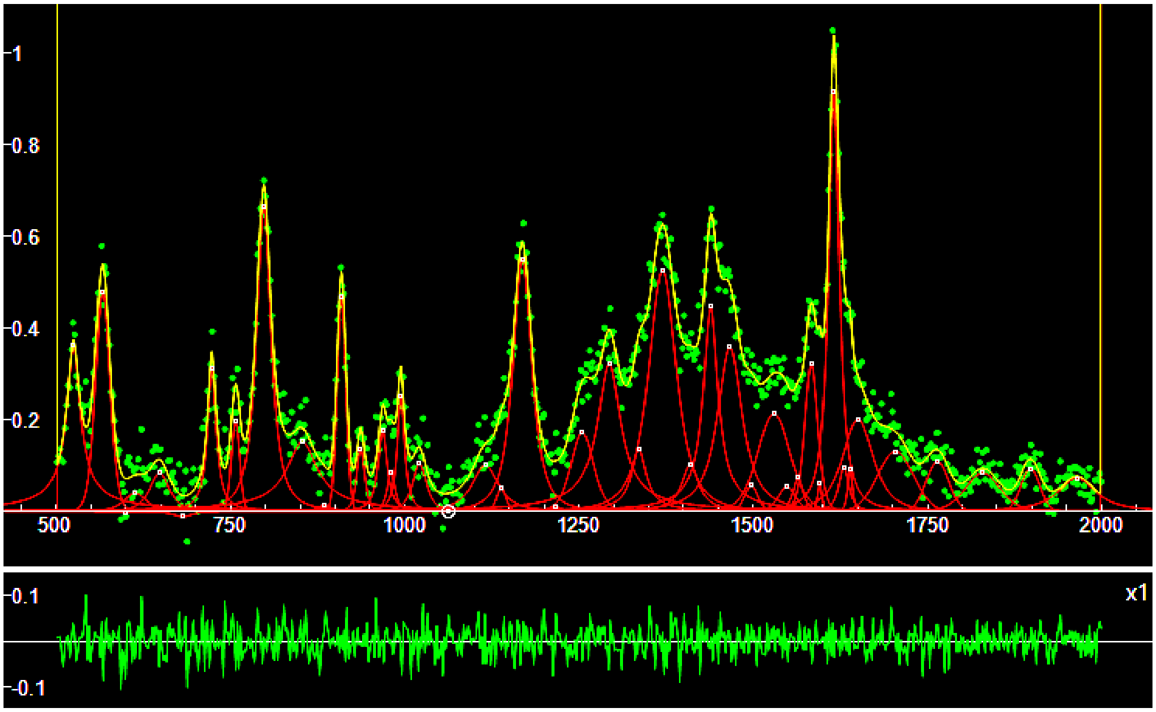
Sherman et al. give reference to Lee et al., 1986.



#	PeakType	Center	Parameters		Height	Center	HWHM	q (h > 0.11)
%_25	Qgau	529.263	x	x	0.191893	529.263	12.2125	1
%_12	**Qgau**	**569.273**	**x**	**x**	**0.573458**	**569.273**	**12.1165**	**1.39518**
%_29	Qgau	617.621	x	x	0.152104	617.621	15.5966	2.40316
%_22	Qgau	661.859	x	x	0.132478	661.859	32.6555	2.22068
%_36	Qgau	667.147	x	x	0.161773	667.147	1.72378	1.8424
%_16	**Qgau**	**726.358**	**x**	**x**	**0.327096**	**726.358**	**12.2655**	**1.45395**
%_14	**Qgau**	**759.654**	**x**	**x**	**0.429026**	**759.654**	**9.40073**	**2.46767**
%_7	**Qgau**	**800.885**	**x**	**x**	**0.605471**	**800.885**	**12.3191**	**1.60198**
%_18	**Qgau**	**811.997**	**x**	**x**	**0.281086**	**811.997**	**9.58003**	**2.14663**
%_15	**Qgau**	**853.288**	**x**	**x**	**0.41283**	**853.288**	**34.2347**	**1.67934**
%_8	**Qgau**	**913.169**	**x**	**x**	**0.646509**	**913.169**	**7.71212**	**2.09087**
%_24	**Qgau**	**947.251**	**x**	**x**	**0.208278**	**947.251**	**19.6533**	**0.999693**
%_30	**Qgau**	**974.688**	**x**	**x**	**0.24934**	**974.688**	**9.32502**	**0.999947**
%_11	**Qgau**	**997.734**	**x**	**x**	**0.557776**	**997.734**	**12.856**	**0.999836**
%_23	**Qgau**	**1027.81**	**x**	**x**	**0.332632**	**1027.81**	**10.8187**	**0.999923**
%_27	Qgau	1114.36	x	x	0.166784	1114.36	40.5208	1.04924
%_9	**Qgau**	**1173**	**x**	**x**	**0.638079**	**1173**	**16.0399**	**1.40173**
%_19	**Qgau**	**1295.88**	**x**	**x**	**0.336211**	**1295.88**	**22.8326**	**1.49312**
%_17	**Qgau**	**1371.55**	**x**	**x**	**0.477605**	**1371.55**	**25.7745**	**1.82464**
%_13	Qgau	1387.99	x	x	0.185364	1387.99	5.8118	1.71749
%_10	**Qgau**	**1445.27**	**x**	**x**	**0.476587**	**1445.27**	**12.5856**	**1.98786**
%_20	**Qgau**	**1468.22**	**x**	**x**	**0.393554**	**1468.22**	**19.4237**	**0.999698**
%_28	Qgau	1539.08	x	x	0.14157	1539.08	18.4489	0.999811
%_21	**Qgau**	**1590.49**	**x**	**x**	**0.313518**	**1590.49**	**17.8876**	**0.999812**
%_6	**Qgau**	**1621.46**	**x**	**x**	**0.910754**	**1621.46**	**9.33016**	**1.28042**
%_26	**Qgau**	**1637.63**	**x**	**x**	**0.260213**	**1637.63**	**14.4352**	**1.26338**
%_1	Qgau	1699.09	x	x	0.132134	1699.09	29.0974	0.999473

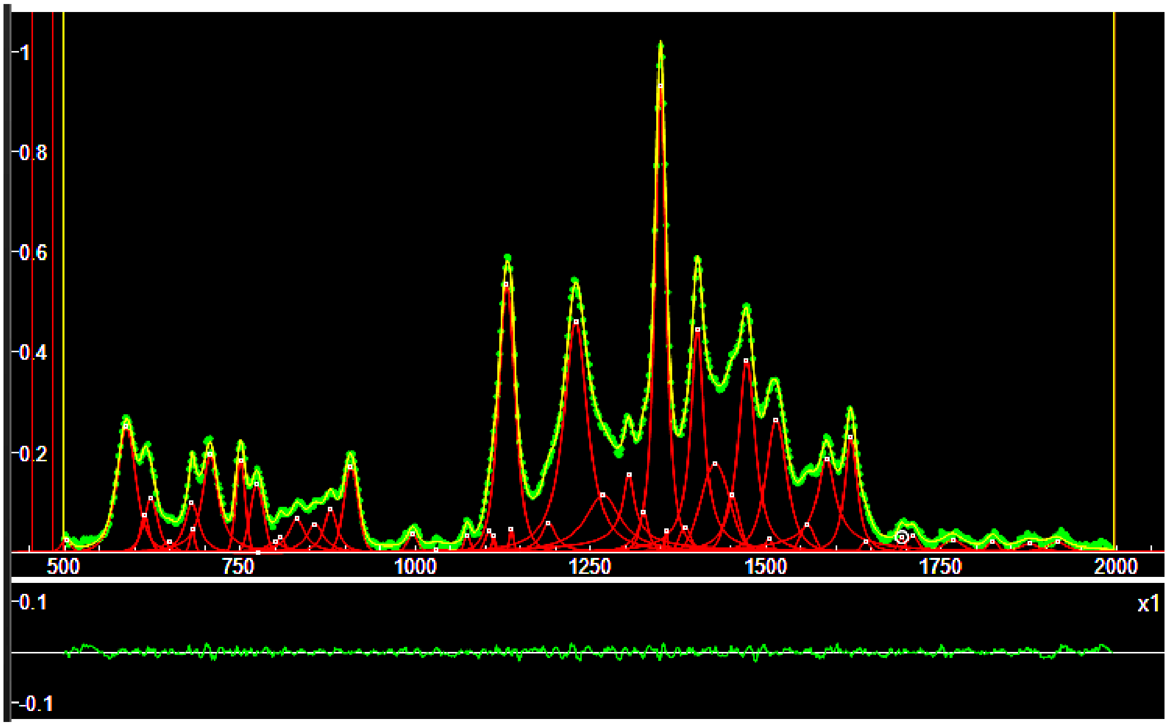
Mandelic acid

According to Sherman and coworkers, SERS spectra have been reported by Horváth et al., 2000.



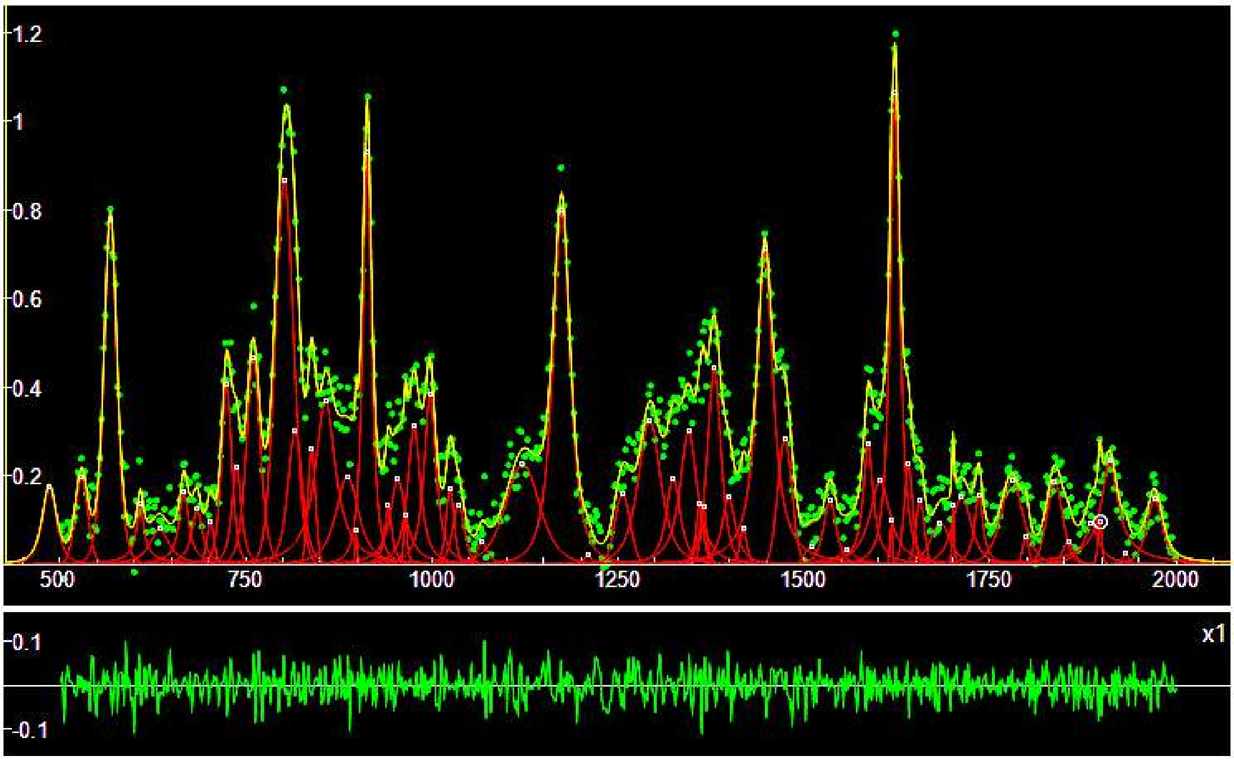
#	PeakType	Center	Parameters		Height	Centers	HWHM	q (H > 0.10)
%_11	**Qgau**	**524.529**	**x**	**x**	**0.365171**	**524.529**	**11.2507**	**2.5227**
%_6	**Qgau**	**566.541**	**x**	**x**	**0.479937**	**566.541**	**13.9895**	**1.18403**
%_12	**Qgau**	**723.073**	**x**	**x**	**0.316977**	**723.073**	**7.24003**	**2.01453**
%_15	Qgau	757.128	x	x	0.195239	757.128	8.50441	0.999953
%_2	**Qgau**	**797.531**	**x**	**x**	**0.66494**	**797.531**	**12.8894**	**1.80022**
%_18	Qgau	852.753	x	x	0.151301	852.753	26.5972	2.34901
%_7	**Qgau**	**909.106**	**x**	**x**	**0.467348**	**909.106**	**8.8247**	**1.03973**
%_26	Qgau	936.711	x	x	0.139689	936.711	7.21454	1.5055
%_36	Qgau	968.12	x	x	0.177547	968.12	7.83097	1.90477
%_34	**Qgau**	**994.365**	**x**	**x**	**0.256618**	**994.365**	**6.29576**	**1.88754**
%_35	Qgau	1021.09	x	x	0.10411	1021.09	12.5927	1.64582
%_21	Qgau	1115.46	x	x	0.100056	1115.46	23.8332	1.72481
%_5	**Qgau**	**1168.66**	**x**	**x**	**0.549587**	**1168.66**	**16.9933**	**1.67855**
%_17	Qgau	1254.65	x	x	0.171751	1254.65	21.9679	1.23955
%_9	**Qgau**	**1293.29**	**x**	**x**	**0.322068**	**1293.29**	**19.8282**	**2.25154**
%_19	Qgau	1335.77	x	x	0.135986	1335.77	12.6415	2.20283
%_4	**Qgau**	**1369.8**	**x**	**x**	**0.525523**	**1369.8**	**25.1006**	**1.62799**
%_20	Qgau	1409.63	x	x	0.101278	1409.63	14.9265	2.0152
%_3	**Qgau**	**1438.89**	**x**	**x**	**0.445378**	**1438.89**	**12.3982**	**2.21022**
%_8	**Qgau**	**1466.5**	**x**	**x**	**0.357661**	**1466.5**	**21.8518**	**1.82244**
%_16	**Qgau**	**1529.52**	**x**	**x**	**0.21281**	**1529.52**	**31.6469**	**1.18723**
%_52	**Qgau**	**1583.17**	**x**	**x**	**0.321356**	**1583.17**	**12.3455**	**1.29218**
%_1	**Qgau**	**1615.71**	**x**	**x**	**0.918467**	**1615.71**	**9.29086**	**1.88638**
%_13	**Qgau**	**1650.1**	**x**	**x**	**0.200951**	**1650.1**	**28.0185**	**1.56811**
%_23	Qgau	1704.11	x	x	0.130274	1704.11	36.3519	0.999087
%_29	Qgau	1764.26	x	x	0.107772	1764.26	23.0615	0.999667

Methyl indole-3-acetate



#	PeakType	Center	Parameters		Height	Center	HWHM	q (H > 0.05)
%_6	**Qgau**	**587.705**	**x**	**x**	**0.251383**	**587.705**	**17.4293**	**1.50447**
%_49	Qgau	613.762	x	x	0.0744421	613.762	8.12969	1.55447
%_48	Qgau	622.562	x	x	0.10947	622.562	12.397	1.56293
%_19	Qgau	681.063	x	x	0.0987309	681.063	12.8094	1.82762
%_47	Qgau	681.578	x	x	0.050551	681.578	3.63483	1.6864
%_10	Qgau	707.353	x	x	0.195081	707.353	13.5362	2.0279
%_11	Qgau	750.392	x	x	0.184711	750.392	9.4841	1.00001
%_32	Qgau	773.722	x	x	0.135549	773.722	13.4343	1.00518
%_21	Qgau	830.468	x	x	0.0678266	830.468	13.8736	2.1235
%_22	Qgau	856.753	x	x	0.0576086	856.753	14.5445	2.02527
%_23	Qgau	878.945	x	x	0.0873483	878.945	11.4623	1.84409
%_14	Qgau	907.939	x	x	0.171559	907.939	14.0262	1.12558
%_2	**Qgau**	**1130.33**	**x**	**x**	**0.538634**	**1130.33**	**15.0269**	**1.4652**
%_28	Qgau	1189.78	x	x	0.0606854	1189.78	12.1902	2.27186
%_27	**Qgau**	**1228.48**	**x**	**x**	**0.461948**	**1228.48**	**20.7024**	**1.84966**
%_16	Qgau	1267.58	x	x	0.115456	1267.58	30.6072	2.00414
%_15	Qgau	1304.09	x	x	0.157821	1304.09	9.88416	3.09823
%_40	Qgau	1325.7	x	x	0.0806286	1325.7	7.68489	1.95988
%_1	**Qgau**	**1349.49**	**x**	**x**	**0.930018**	**1349.49**	**9.93448**	**1.70866**
%_42	Qgau	1384.61	x	x	0.0511604	1384.61	11.6827	1.12939
%_3	**Qgau**	**1402.12**	**x**	**x**	**0.447755**	**1402.12**	**10.9205**	**2.17268**
%_13	Qgau	1427.76	x	x	0.178449	1427.76	28.6062	0.999055
%_35	Qgau	1451.56	x	x	0.115117	1451.56	13.214	1.44806
%_37	**Qgau**	**1472.49**	**x**	**x**	**0.384839**	**1472.49**	**14.8663**	**1.83988**
%_8	**Qgau**	**1514.6**	**x**	**x**	**0.26406**	**1514.6**	**19.1907**	**1.56329**
%_36	Qgau	1559	x	x	0.0570507	1559	14.1959	0.999821
%_12	Qgau	1586.17	x	x	0.188604	1586.17	15.0541	2.58803
%_9	**Qgau**	**1621.26**	**x**	**x**	**0.231608**	**1621.26**	**10.864**	**1.81801**

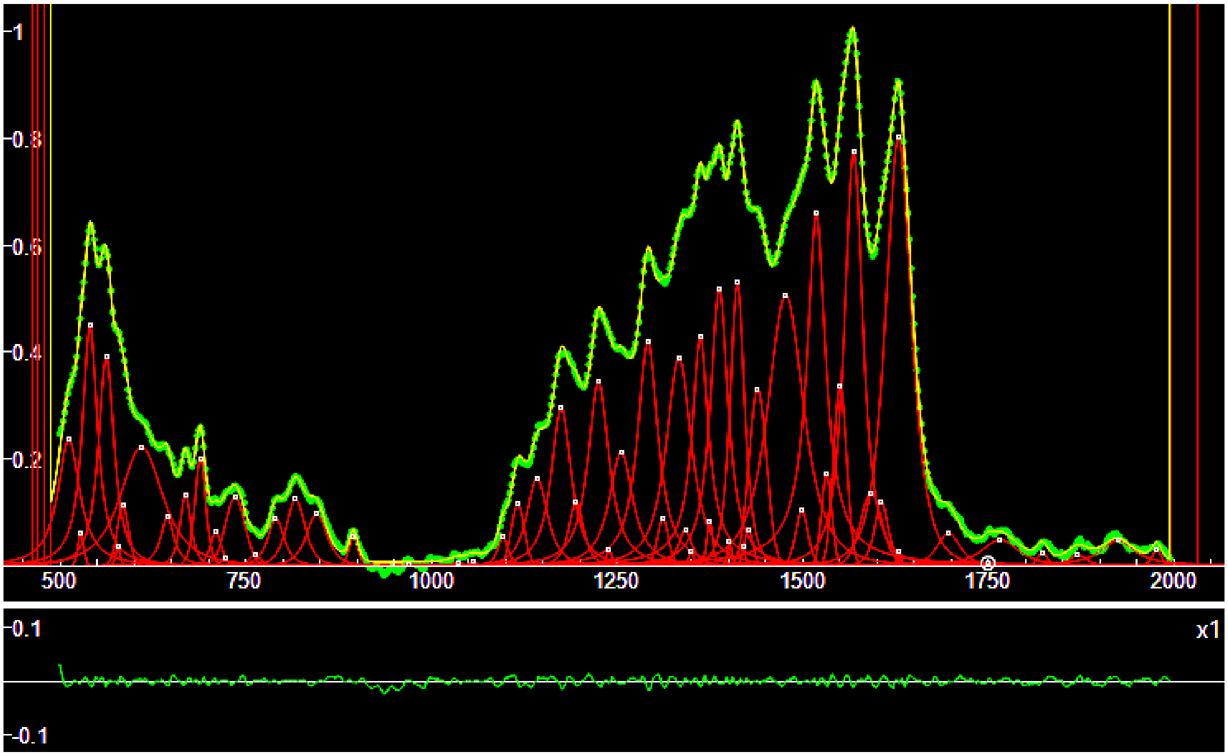
Methylguanidine



#	PeakType	Center	Parameters		Height	Center	HWHM	q ...
%_21	Qgau	380.221	x	x	2.26793e-019	380.221	9.508	1.42925
%_26	Qgau	486.009	x	x	0.175891	486.009	12.3142	1.58318
%_25	Qgau	529.115	x	x	0.200361	529.115	11.4244	1.17945
%_5	Qgau	567.917	x	x	0.777713	567.917	11.5302	1.31799
%_28	Qgau	607.996	x	x	0.136977	607.996	5.68909	2.61944
%_39	Qgau	633.933	x	x	0.0813946	633.933	15.6503	1.95416
%_37	Qgau	666.652	x	x	0.164329	666.652	7.77852	2.15031
%_38	Qgau	684.35	x	x	0.12638	684.35	8.37423	2.05434
%_40	Qgau	702.35	x	x	0.0984983	702.35	6.72031	1.11333
%_10	Qgau	723.965	x	x	0.406471	723.965	9.15019	1.36816
%_41	Qgau	737.35	x	x	0.221594	737.35	8.04174	1.66472
%_8	Qgau	760.011	x	x	0.468505	760.011	12.0451	1.34548
%_2	Qgau	801.686	x	x	0.865385	801.686	17.1636	1.07365
%_23	Qgau	816.174	x	x	0.303486	816.174	12.8788	1.37851
%_33	Qgau	838.36	x	x	0.264243	838.36	6.98722	1.02848
%_12	Qgau	856.9	x	x	0.371377	856.9	16.4765	1.97883
%_17	Qgau	886.217	x	x	0.199694	886.217	18.9812	1.69621
%_56	Qgau	898.113	x	x	0.0813316	898.113	1.29951	1.96001
%_3	Qgau	912.985	x	x	0.933013	912.985	7.36945	1.6743
%_34	Qgau	941.226	x	x	0.136694	941.226	5.62644	1.93994
%_42	Qgau	954.25	x	x	0.193467	954.25	12.6503	1.99792
%_62	Qgau	964.351	x	x	0.11547	964.351	2.29854	2.15031

%_43	Qgau	975.95	x	x	0.313867	975.95	10.4429	1.80568
%_9	Qgau	997.563	x	x	0.387431	997.563	9.53023	1.85126
%_60	Qgau	1024.39	x	x	0.17376	1024.39	7.14289	1.34075
%_31	Qgau	1035.63	x	x	0.135082	1035.63	10.7066	1.33393
%_45	Qgau	1067.66	x	x	0.05347	1067.66	8.26765	1.98829
%_19	Qgau	1121.82	x	x	0.227896	1121.82	30.336	1.35982
%_4	Qgau	1174.17	x	x	0.800285	1174.17	14.6342	1.62878
%_46	Qgau	1209.15	x	x	0.0223393	1209.15	6.5983	1.31246
%_49	Qgau	1256.15	x	x	0.159168	1256.15	14.6483	0.999755
%_15	Qgau	1292.36	x	x	0.32545	1292.36	19.4564	1.56107
%_48	Qgau	1324.2	x	x	0.196522	1324.2	11.6503	1.7747
%_11	Qgau	1344.79	x	x	0.302508	1344.79	14.2081	1.84529
%_59	Qgau	1359.77	x	x	0.141439	1359.77	5.57259	1.78942
%_35	Qgau	1365.09	x	x	0.133922	1365.09	4.28472	1.85644
%_7	Qgau	1379.25	x	x	0.443481	1379.25	12.0594	1.42095
%_22	Qgau	1398.78	x	x	0.151967	1398.78	11.0331	1.90259
%_50	Qgau	1418.41	x	x	0.0832363	1418.41	5.94746	1.50099
%_6	Qgau	1447.42	x	x	0.714055	1447.42	12.8736	1.97582
%_14	Qgau	1474.17	x	x	0.283767	1474.17	13.4361	0.999836
%_36	Qgau	1509.65	x	x	0.0405841	1509.65	12.2835	1.07511
%_30	Qgau	1534.75	x	x	0.144376	1534.75	10.9817	1.55146
%_44	Qgau	1557.35	x	x	0.0339916	1557.35	13.5326	2.12933
%_13	Qgau	1586.26	x	x	0.272961	1586.26	7.90517	2.12249
%_47	Qgau	1602.13	x	x	0.189393	1602.13	16.8083	1.93285
%_61	Qgau	1616.88	x	x	0.121284	1616.88	1.69186	1.21858
%_1	Qgau	1622.27	x	x	1.06382	1622.27	8.07002	1.72279
%_18	Qgau	1640.37	x	x	0.227147	1640.37	7.71289	1.23825
%_53	Qgau	1655.75	x	x	0.144365	1655.75	8.33815	1.0004
%_54	Qgau	1683.05	x	x	0.0942756	1683.05	17.4917	1.47222
%_63	Qgau	1700.19	x	x	0.135289	1700.19	1.95181	1.0004
%_55	Qgau	1711.99	x	x	0.153413	1711.99	16.4496	1.57175
%_32	Qgau	1734.75	x	x	0.161512	1734.75	6.63531	2.00777
%_24	Qgau	1779.51	x	x	0.188855	1779.51	19.7034	1.39568
%_52	Qgau	1797.85	x	x	0.0620914	1797.85	5.88268	1.00419
%_27	Qgau	1836.87	x	x	0.188305	1836.87	14.1711	1.24294
%_57	Qgau	1854.95	x	x	0.0526337	1854.95	9.70946	1.58191
%_58	Qgau	1885.95	x	x	0.0923679	1885.95	11.6503	2.15031
%_64	Qgau	1897.43	x	x	0.105291	1897.43	2.875	1.5
%_20	Qgau	1910.74	x	x	0.235188	1910.74	13.3455	2.35588
%_51	Qgau	1932.21	x	x	0.0259798	1932.21	4.5499	1.72832
%_29	Qgau	1971.27	x	x	0.148456	1971.27	13.7997	1.48835

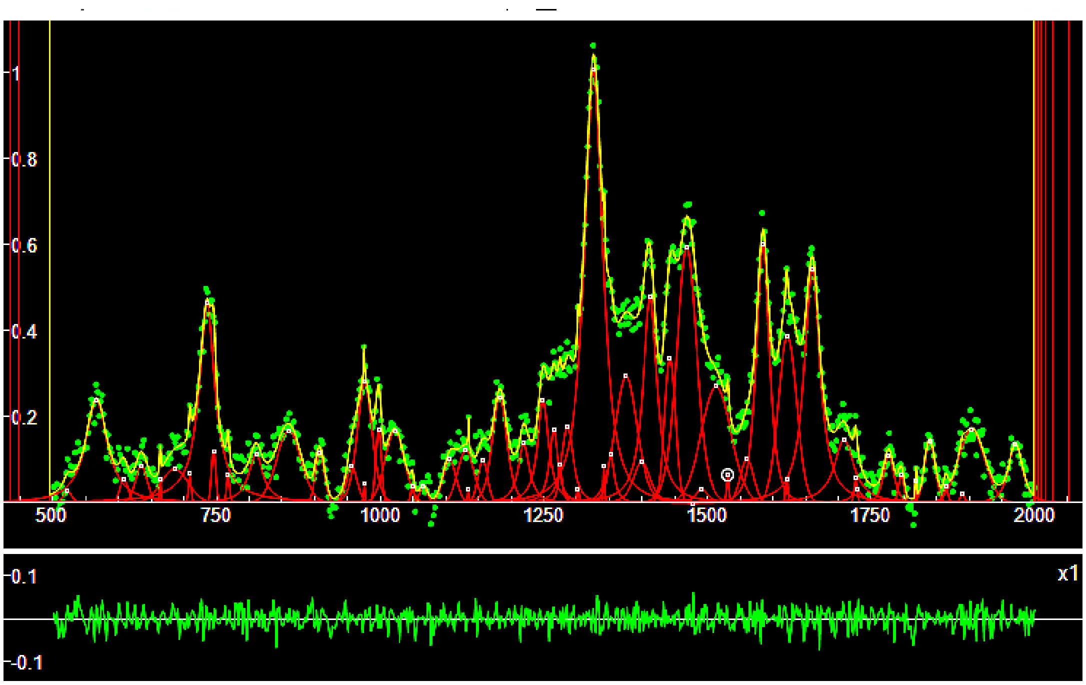
N, N-dimethyl-1, 4-phenylenediamine



# PeakType	Center	Parameters		Height	Center	HWHM	q ...
%_18 Qgau	511.218	x	x	0.237455	511.218	18.0746	1.95281
%_31 Qgau	527.361	x	x	0.0634541	527.361	5.69372	1.05507
%_2 Qgau	539.588	x	x	0.450965	539.588	12.2852	1.94725
%_11 Qgau	561.611	x	x	0.392325	561.611	13.0867	1.78821
%_58 Qgau	577.204	x	x	0.0375793	577.204	3.59901	1.62663
%_17 Qgau	583.86	x	x	0.114061	583.86	10.5929	1.11475
%_20 Qgau	609.221	x	x	0.223596	609.221	36.2761	1.65227
%_35 Qgau	643.893	x	x	0.0930664	643.893	10.7807	1.97722
%_59 Qgau	668.386	x	x	0.13511	668.386	9.21516	1.64766
%_19 Qgau	688.328	x	x	0.203018	688.328	9.70535	1.29485
%_60 Qgau	709.08	x	x	0.0641537	709.08	10.0053	1.37163
%_62 Qgau	721.572	x	x	0.0172454	721.572	5.75234	1.37132
%_25 Qgau	735.203	x	x	0.129681	735.203	18.459	1.05175
%_61 Qgau	761.748	x	x	0.0223779	761.748	10.0284	1.63998
%_39 Qgau	790.159	x	x	0.0900468	790.159	13.9555	1.65077
%_40 Qgau	816.833	x	x	0.125537	816.833	16.3898	1.49903
%_41 Qgau	845.12	x	x	0.0982779	845.12	18.0716	1.55843
%_34 Qgau	894.746	x	x	0.0566441	894.746	7.93439	1.3527
%_42 Qgau	968.982	x	x	0.00258298	968.982	5.80692	0.999968
%_44 Qgau	1034.95	x	x	0.00714393	1034.95	10.6523	1.52448
%_45 Qgau	1055.4	x	x	0.00817658	1055.4	9.35502	0.999909
%_46 Qgau	1095.93	x	x	0.0552341	1095.93	8.58569	1.74222

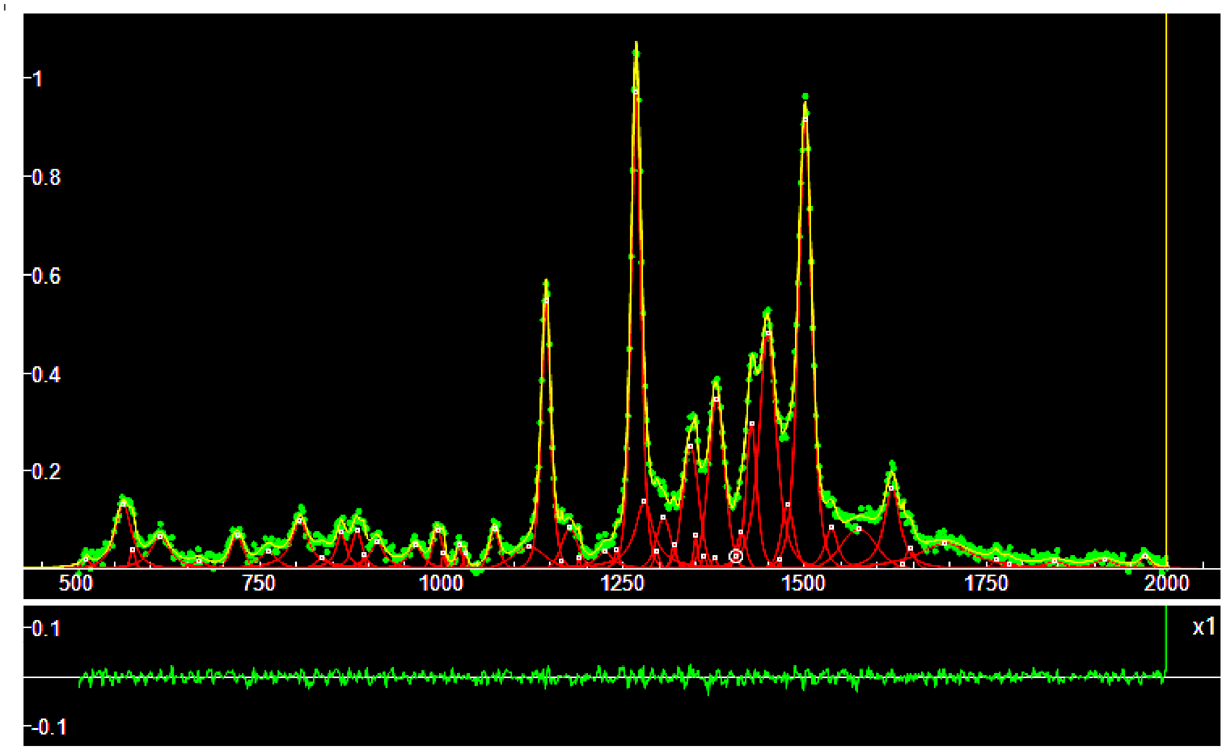
%_27	Qgau	1115.95	x	x	0.116957	1115.95	12.4712	1.00041
%_21	Qgau	1142.01	x	x	0.164436	1142.01	17.7638	1.66853
%_13	Qgau	1174.56	x	x	0.296231	1174.56	16.7473	1.80818
%_63	Qgau	1194.7	x	x	0.120601	1194.7	12.8406	1.61304
%_12	Qgau	1224.77	x	x	0.345681	1224.77	17.2622	1.88517
%_16	Qgau	1255.13	x	x	0.214504	1255.13	19.4786	1.85079
%_65	Qgau	1238.95	x	x	0.0303601	1238.95	5.2366	1.4716
%_9	Qgau	1291.2	x	x	0.421153	1291.2	16.8181	1.9224
%_28	Qgau	1311.58	x	x	0.0904004	1311.58	10.0277	1.25388
%_10	Qgau	1333.07	x	x	0.389996	1333.07	21.2507	1.77283
%_43	Qgau	1341.67	x	x	0.0688247	1341.67	11.165	1.93075
%_66	Qgau	1349.67	x	x	0.0280837	1349.67	4.1684	1.50245
%_6	Qgau	1361.93	x	x	0.43158	1361.93	13.0773	2.16953
%_52	Qgau	1374.73	x	x	0.0856462	1374.73	5.46905	1.18463
%_7	Qgau	1387.39	x	x	0.519892	1387.39	14.7532	1.88326
%_55	Qgau	1401.33	x	x	0.0491415	1401.33	3.23568	1.54424
%_5	Qgau	1411.82	x	x	0.529875	1411.82	12.3821	1.54755
%_57	Qgau	1419.91	x	x	0.0368023	1419.91	3.22568	1.62564
%_32	Qgau	1426.98	x	x	0.0687054	1426.98	8.2502	0.999923
%_15	Qgau	1439.27	x	x	0.333004	1439.27	16.6637	0.99971
%_49	Qgau	1477.05	x	x	0.507274	1477.05	30.8445	1.61313
%_51	Qgau	1498.7	x	x	0.104448	1498.7	11.1682	1.27025
%_4	Qgau	1518.27	x	x	0.660069	1518.27	14.8299	2.18083
%_50	Qgau	1532	x	x	0.172831	1532	9.74282	0.999915
%_14	Qgau	1550.24	x	x	0.338104	1550.24	12.498	0.999867
%_1	Qgau	1568.51	x	x	0.77766	1568.51	15.4493	1.72148
%_37	Qgau	1592.11	x	x	0.137356	1592.11	20.2359	1.15503
%_64	Qgau	1605.88	x	x	0.121702	1605.88	11.9043	1.51075
%_3	Qgau	1629.06	x	x	0.801973	1629.06	22.603	1.51661
%_67	Qgau	1629.79	x	x	0.027013	1629.79	2.98114	1.4716
%_47	Qgau	1696.31	x	x	0.0623808	1696.31	19.9916	1.60516
%_53	Qgau	1749.46	x	x	0.00592445	1749.46	5.43899	1.35691
%_30	Qgau	1765.95	x	x	0.0501081	1765.95	31.3847	1.76796
%_36	Qgau	1822.89	x	x	0.0251595	1822.89	9.91636	1.06761
%_22	Qgau	1870.56	x	x	0.0216385	1870.56	16.839	1.33899
%_29	Qgau	1924.23	x	x	0.0483515	1924.23	27.9641	2.10525
%_48	Qgau	1976.87	x	x	0.030918	1976.87	8.40067	1.43904

N-acetyl-d-tryptophan



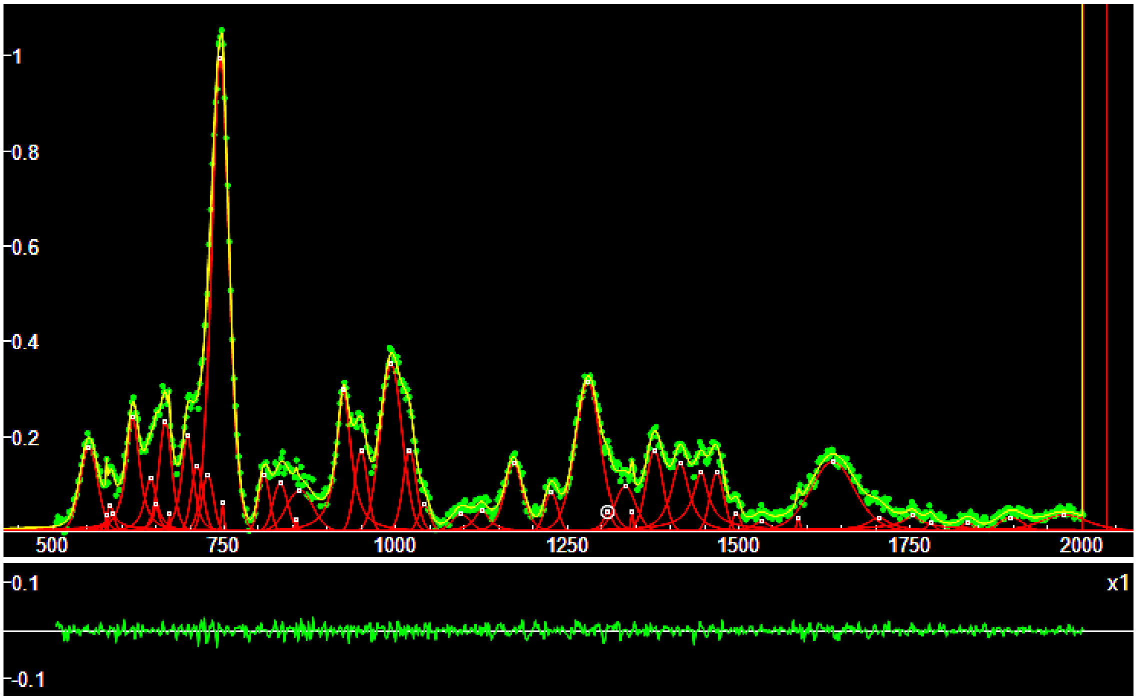
#	PeakType	Center		Parameters	Height	Center	HWHM	q (H>0.12)
%_13	**Qgau**	**566.159**	**x**	**x**	**0.238088**	**566.159**	**20.5046**	**1.90188**
%_7	**Qgau**	**735.258**	**x**	**x**	**0.464463**	**735.258**	**14.1891**	**2.09541**
%_20	Qgau	745.307	x	x	0.127765	745.307	4.32428	0.999991
%_18	Qgau	860.083	x	x	0.167362	860.083	26.0335	1.05043
%_9	**Qgau**	**976.135**	**x**	**x**	**0.28157**	**976.135**	**15.2194**	**1.22712**
%_15	Qgau	997.245	x	x	0.172615	997.245	5.97995	1.00001
%_24	Qgau	1021.97	x	x	0.16649	1021.97	20.8565	0.999547
%_19	Qgau	1130.72	x	x	0.122403	1130.72	17.2462	0.999623
%_14	**Qgau**	**1182.27**	**x**	**x**	**0.244736**	**1182.27**	**15.1304**	**1.26637**
%_27	Qgau	1219.12	x	x	0.137989	1219.12	10.431	1.86536
%_40	**Qgau**	**1248.62**	**x**	**x**	**0.239511**	**1248.62**	**10.1853**	**1.88892**
%_43	Qgau	1264.89	x	x	0.169383	1264.89	7.91133	1.86551
%_41	Qgau	1285.8	x	x	0.17776	1285.8	11.0698	1.69996
%_1	**Qgau**	**1325.74**	**x**	**x**	**1.00679**	**1325.74**	**17.5039**	**1.73405**
%_10	**Qgau**	**1375.68**	**x**	**x**	**0.295182**	**1375.68**	**22.8088**	**1.1836**
%_4	**Qgau**	**1412.02**	**x**	**x**	**0.478279**	**1412.02**	**12.7893**	**1.89073**
%_8	**Qgau**	**1442.52**	**x**	**x**	**0.337078**	**1442.52**	**11.604**	**0.999891**
%_2	**Qgau**	**1468.22**	**x**	**x**	**0.59377**	**1468.22**	**20.709**	**1.19245**
%_12	**Qgau**	**1512.98**	**x**	**x**	**0.270307**	**1512.98**	**32.0195**	**1.00364**
%_3	**Qgau**	**1584.57**	**x**	**x**	**0.599338**	**1584.57**	**12.8996**	**1.50883**
%_6	**Qgau**	**1622.15**	**x**	**x**	**0.387661**	**1622.15**	**19.8076**	**0.999716**
%_5	**Qgau**	**1659.95**	**x**	**x**	**0.544218**	**1659.95**	**14.6554**	**1.85321**
%_17	Qgau	1708.65	x	x	0.14685	1708.65	18.2156	1.92442
%_22	Qgau	1839.45	x	x	0.143121	1839.45	11.2783	1.03953
%_16	Qgau	1903.57	x	x	0.169793	1903.57	27.9599	0.999607
%_25	Qgau	1970.49	x	x	0.137654	1970.49	13.5719	1.58799

N-acetyl-DL-glutamic acid



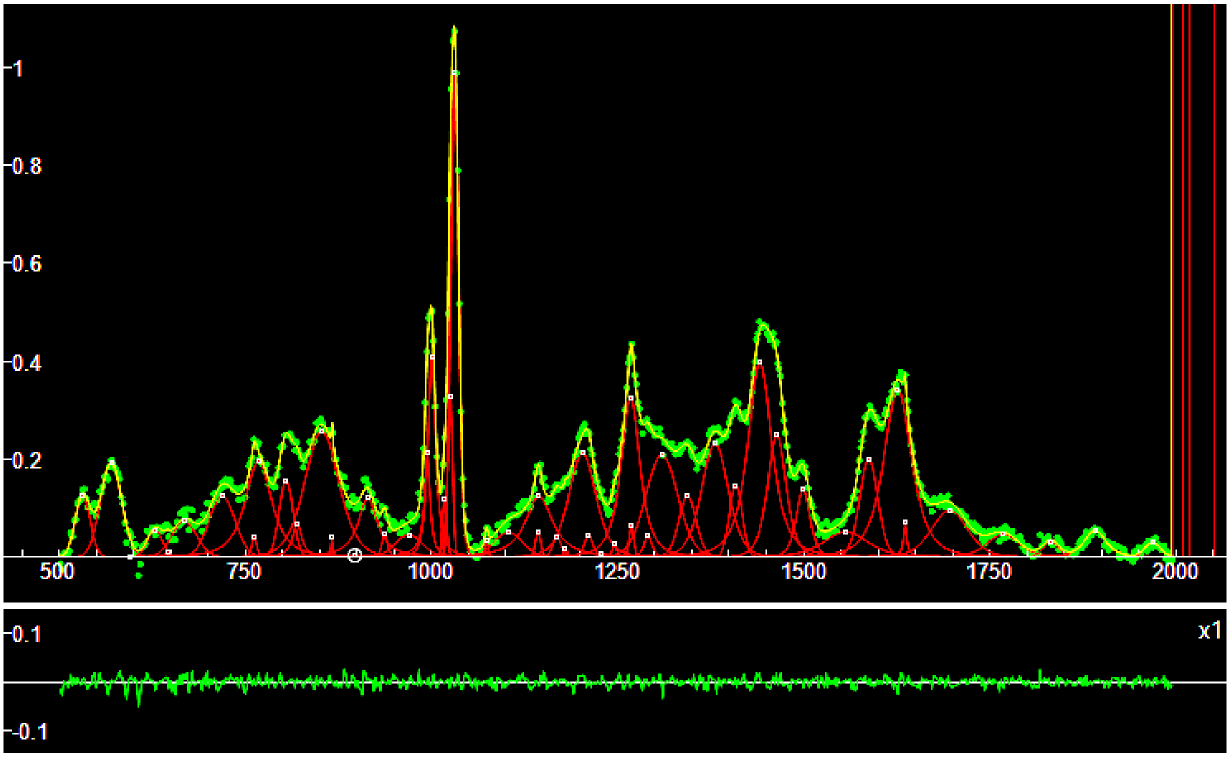
#	PeakType	Center	Parameters		Height	Area	HWHM	q (H>0.05)
%_10	Qgau	561.792	x	x	0.130981	561.792	14.4509	1.72753
%_19	Qgau	612.72	x	x	0.06741	612.72	16.083	2.0049
%_20	Qgau	718.489	x	x	0.0680714	718.489	12.1424	1.27442
%_11	Qgau	804.996	x	x	0.100692	804.996	13.616	2.20951
%_43	Qgau	861.882	x	x	0.0754135	861.882	8.01757	2.21677
%_41	Qgau	883.556	x	x	0.0784469	883.556	9.29368	1.72265
%_42	Qgau	911.218	x	x	0.0555484	911.218	11.6176	2.21757
%_18	Qgau	994.634	x	x	0.0796551	994.634	9.66433	1.16306
%_15	Qgau	1073.03	x	x	0.0821542	1073.03	8.50122	1.49405
%_3	**Qgau**	**1144.05**	**x**	**x**	**0.555617**	**1144.05**	**8.24552**	**1.47139**
%_16	Qgau	1176.69	x	x	0.0841257	1176.69	15.2414	1.19612
%_1	**Qgau**	**1268**	**x**	**x**	**0.97632**	**1268**	**8.723**	**1.39839**
%_9	Qgau	1279.23	x	x	0.138706	1279.23	14.5256	2.18581
%_17	Qgau	1305.96	x	x	0.106047	1305.96	13.1706	1.33162
%_47	Qgau	1319.89	x	x	0.0518296	1319.89	4.47132	1.57001
%_7	**Qgau**	**1343.27**	**x**	**x**	**0.250564**	**1343.27**	**15.0899**	**1.09785**
%_49	Qgau	1349.9	x	x	0.0699548	1349.9	2.78309	2.07977
%_5	**Qgau**	**1378.87**	**x**	**x**	**0.34629**	**1378.87**	**15.0291**	**1.1903**
%_27	Qgau	1413.01	x	x	0.0754615	1413.01	8.87905	1.21956
%_6	**Qgau**	**1426.9**	**x**	**x**	**0.301433**	**1426.9**	**9.11204**	**1.5211**
%_4	**Qgau**	**1449.2**	**x**	**x**	**0.483928**	**1449.2**	**14.8371**	**1.5752**
%_12	Qgau	1476.62	x	x	0.133119	1476.62	11.4538	1.3507
%_2	**Qgau**	**1500.85**	**x**	**x**	**0.916663**	**1500.85**	**12.0313**	**1.41525**
%_22	Qgau	1536.87	x	x	0.0852476	1536.87	10.9458	1.78915
%_14	Qgau	1574.71	x	x	0.082228	1574.71	33.6128	1.07167
%_8	Qgau	1620.55	x	x	0.16742	1620.55	12.8811	1.93442
%_21	Qgau	1693.8	x	x	0.0527822	1693.8	45.4537	1.97743

N-acetyl-L-cysteine



#	PeakType	Center	Parameters		Height	Center	HWHM	q (H>0.05)
%_7	**Qgau**	**552.486**	**x**	**x**	**0.178097**	**552.486**	**17.318**	**1.19613**
%_15	Qgau	583.686	x	x	0.0549244	583.686	7.35758	1.3303
%_10	Qgau	616.626	x	x	0.239406	616.626	12.1678	1.8131
%_32	Qgau	642.406	x	x	0.111981	642.406	10.5435	1.96506
%_47	Qgau	650.523	x	x	0.059506	650.523	4.22838	2.79642
%_31	**Qgau**	**663.997**	**x**	**x**	**0.232677**	**663.997**	**12.6839**	**1.3009**
%_30	**Qgau**	**696.042**	**x**	**x**	**0.203241**	**696.042**	**10.9957**	**1.60167**
%_16	Qgau	710.527	x	x	0.13825	710.527	12.4424	1.00078
%_46	Qgau	725.871	x	x	0.11755	725.871	11.6761	1.00002
%_1	**Qgau**	**744.198**	**x**	**x**	**0.996585**	**744.198**	**17.6012**	**1.12076**
%_17	Qgau	747.326	x	x	0.0614731	747.326	2.28378	1.64501
%_33	Qgau	807.831	x	x	0.118021	807.831	11.3575	0.99991
%_34	Qgau	831.472	x	x	0.102681	831.472	15.2871	0.999839
%_35	Qgau	860.098	x	x	0.0883044	860.098	26.9004	1.08333
%_5	**Qgau**	**924.056**	**x**	**x**	**0.297648**	**924.056**	**12.4654**	**1.98146**
%_36	**Qgau**	**949.246**	**x**	**x**	**0.17002**	**949.246**	**13.4865**	**0.999884**
%_2	**Qgau**	**993.148**	**x**	**x**	**0.352332**	**993.148**	**22.3778**	**0.999706**
%_14	**Qgau**	**1020.13**	**x**	**x**	**0.171473**	**1020.13**	**12.8986**	**1.19879**
%_24	Qgau	1041.61	x	x	0.0563601	1041.61	12.2394	0.999838
%_12	**Qgau**	**1171.76**	**x**	**x**	**0.146485**	**1171.76**	**17.1149**	**1.40455**
%_19	Qgau	1226.38	x	x	0.0821971	1226.38	13.3951	1.0018
%_3	**Qgau**	**1280.01**	**x**	**x**	**0.31356**	**1280.01**	**25.2227**	**1.18028**
%_39	Qgau	1334.46	x	x	0.096516	1334.46	21.2649	1.1041
%_40	**Qgau**	**1376.98**	**x**	**x**	**0.171341**	**1376.98**	**17.3761**	**1.06051**
%_41	**Qgau**	**1414.29**	**x**	**x**	**0.144339**	**1414.29**	**16.4206**	**1.8446**
%_42	Qgau	1444.62	x	x	0.126566	1444.62	12.8319	2.59585
%_13	Qgau	1468.12	x	x	0.124049	1468.12	14.3668	1.01987
%_9	**Qgau**	**1636.83**	**x**	**x**	**0.147639**	**1636.83**	**44.0961**	**1.20693**

Nicotinamide



# PeakType		Center		Parameters		Height Center HWHM q (H>0.02)
%_22	Qgau	531.399	x	x	x	0.125903 531.399 14.145 0.999909
%_16	Qgau	569.655	x	x	x	0.193152 569.655 19.938 0.99982
%_53	Qgau	595.418	x	x	x	1.47569e-020 595.418 5.4813 1.4813
%_41	Qgau	628.361	x	x	x	0.0556148 628.361 14.3144 0.999935
%_42	Qgau	667.803	x	x	x	0.0730052 667.803 23.6366 0.999683
%_24	Qgau	718.626	x	x	x	0.125024 718.626 24.4777 0.999691
%_50	Qgau	761.968	x	x	x	0.0416537 761.968 4.24972 1.46967
%_12	Qgau	767.523	x	x	x	0.196617 767.523 22.3676 1.6416
%_18	Qgau	804.556	x	x	x	0.157106 804.556 12.9647 1.00042
%_34	Qgau	819.487	x	x	x	0.068052 819.487 7.76789 1.88528
%_8	Qgau	852.64	x	x	x	0.257228 852.64 31.0114 1.24758
%_52	Qgau	866.586	x	x	x	0.0477409 866.586 1.34342 1.00004
%_20	Qgau	914.409	x	x	x	0.120255 914.409 15.8232 1.90932
%_39	Qgau	937.21	x	x	x	0.0462378 937.21 4.73374 1.62284
%_27	Qgau	969.374	x	x	x	0.0454543 969.374 25.891 0.999393
%_19	Qgau	994.363	x	x	x	0.212977 994.363 4.37771 1.92428
%_4	Qgau	1000.44	x	x	x	0.419098 1000.44 5.96068 1.87595
%_40	Qgau	1017.64	x	x	x	0.121863 1017.64 4.01566 1.092
%_11	Qgau	1025.12	x	x	x	0.336157 1025.12 4.29255 0.999988
%_3	Qgau	1031.37	x	x	x	1.01279 1031.37 6.74749 1.2302
%_48	Qgau	1073.93	x	x	x	0.0353491 1073.93 3.06342 1.00041
%_31	Qgau	1103.18	x	x	x	0.0504122 1103.18 27.0008 0.999084

%_47	Qgau	1143.34	x	x	x	0.0514052	1143.34	5.18398	0.999971
%_17	Qgau	1144.55	x	x	x	0.124191	1144.55	22.391	1.83628
%_49	Qgau	1168.7	x	x	x	0.0410206	1168.7	7.90221	1.22869
%_9	Qgau	1202.65	x	x	x	0.213277	1202.65	24.1825	1.30879
%_51	Qgau	1211.05	x	x	x	0.0457326	1211.05	7.32896	1.41471
%_58	Qgau	1245.82	x	x	x	0.025622	1245.82	3.5813	1.4813
%_6	Qgau	1267.29	x	x	x	0.325947	1267.29	16.0877	1.61865
%_46	Qgau	1268.56	x	x	x	0.0661173	1268.56	4.05555	1.18226
%_45	Qgau	1290.83	x	x	x	0.0451052	1290.83	6.51408	1.60236
%_15	Qgau	1309.43	x	x	x	0.20916	1309.43	29.8791	1.07275
%_26	Qgau	1343.87	x	x	x	0.12467	1343.87	16.0375	1.1186
%_10	Qgau	1380.8	x	x	x	0.231691	1380.8	24.2869	1.24386
%_23	Qgau	1408.82	x	x	x	0.146871	1408.82	12.0612	0.999862
%_5	Qgau	1441.07	x	x	x	0.397916	1441.07	20.365	1.60867
%_14	Qgau	1463.98	x	x	x	0.249206	1463.98	16.4405	1.36307
%_21	Qgau	1499.14	x	x	x	0.138123	1499.14	12.2157	1.37644
%_35	Qgau	1556.39	x	x	x	0.0517027	1556.39	39.1539	1.40357
%_13	Qgau	1587.36	x	x	x	0.199638	1587.36	16.8835	1.10636
%_7	Qgau	1626.3	x	x	x	0.341006	1626.3	24.1771	1.53539
%_44	Qgau	1636.25	x	x	x	0.0733193	1636.25	2.17551	2.48556
%_25	Qgau	1695.92	x	x	x	0.0954512	1695.92	32.9793	1.19805
%_32	Qgau	1767.93	x	x	x	0.0466644	1767.93	29.0374	1.29335
%_38	Qgau	1832.18	x	x	x	0.0308424	1832.18	15.451	0.999891
%_30	Qgau	1891.43	x	x	x	0.0544543	1891.43	18.6632	1.54473
%_37	Qgau	1969.06	x	x	x	0.0293224	1969.06	14.91	0.99995

Nicotinamide has been investigated in Sparavigna, 2023, with the first derivative spectrum. The following table provides the peaks above a given threshold.

Position (in cm $^{-1}$)	Relative intensity	Position (in cm $^{-1}$)	Relative intensity
532.00	0.16	1204.50	0.29
571.00	0.20	1267.50	0.43
724.00	0.16	1342.50	0.28
764.50	0.24	1379.50	0.30
808.50	0.25	1408.50	0.34
850.50	0.27	1443.50	0.50
912.00	0.17	1496.50	0.25
999.00	0.48	1589.00	0.34
1029.50	0.95	1631.00	0.41
1145.00	0.22	1685.00	0.18

Literature about SERS spectrum and fingerprint of nicotinamide is: Xu et al., 2022, Gautam et al., 2022, Jaworska et al., 2012, Castro et al., 2013, Pal et al., 1998, Hernandez et al., 2020.

Let us consider the q-Gaussian centers

531.399	569.655(m)	595.418(vs)	628.361	667.803	718.626
761.968	767.523(m)	804.556	819.487	852.64(m)	866.586
914.409	937.21	969.374	994.363(m)	1000.44(s)	1017.64
1025.12(m)	1031.37(vs)	1073.93	1103.18	1143.34	1144.55
1168.7	1202.65(m)	1211.05	1245.82	1267.29(m)	1268.56
1290.83	1309.43(m)	1343.87	1380.8(m)	1408.82	1441.07(s)
1463.98(m)	1499.14	1556.39	1587.36	1626.3(s)	1636.25
1695.92	1767.93	1832.18	1891.43	1969.06	

As previously told, in Jaworska, et al., 2012, we have the fingerprints for nicotinamide in solid state and solutions. In ***bold***, the peaks which are corresponding to q-Gaussian centers given above, within +/− 5 cm^{-1} (in *italic*, within +/− 10 cm^{-1}):

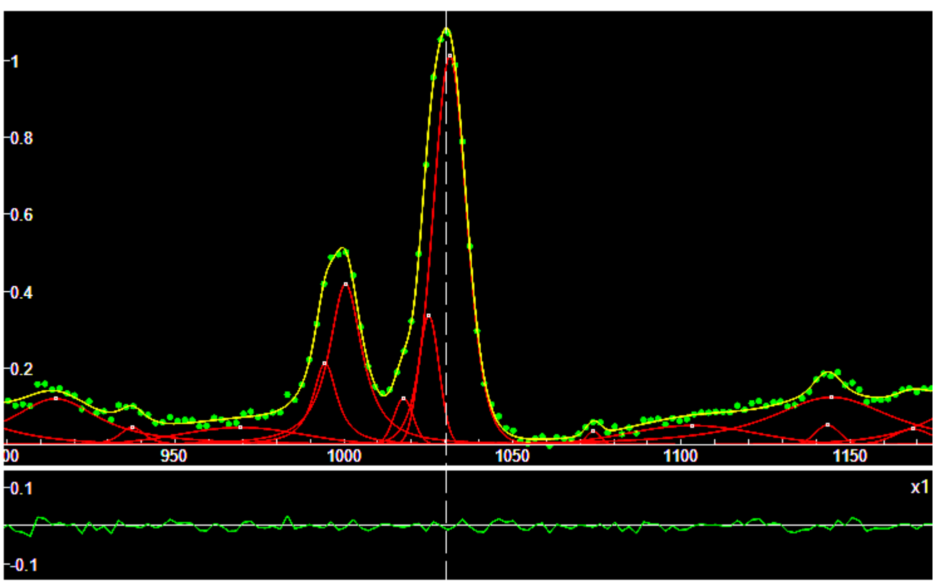
Solid: 390 ***629*** 789 ***994*** 1043(vs) 1094 1124 *1161* ***1211*** 1393 ***1579*** *1597* *1616* 1677

Solution (pH=12): 394 ***631*** 787 *847* ***997*** ***1032(vs)*** 1042(vs) ***1101*** 1154 ***1202*** 1395 1424 ***1441*** *1489* 1574 *1597* 1672

Solution (pH=2): 368 *621* 779 836 ***990*** ***1030(s)*** 1046(vs) ***1107*** 1157 ***1267*** 1368 1424(s) 1605 ***1641(s)*** ***1695***

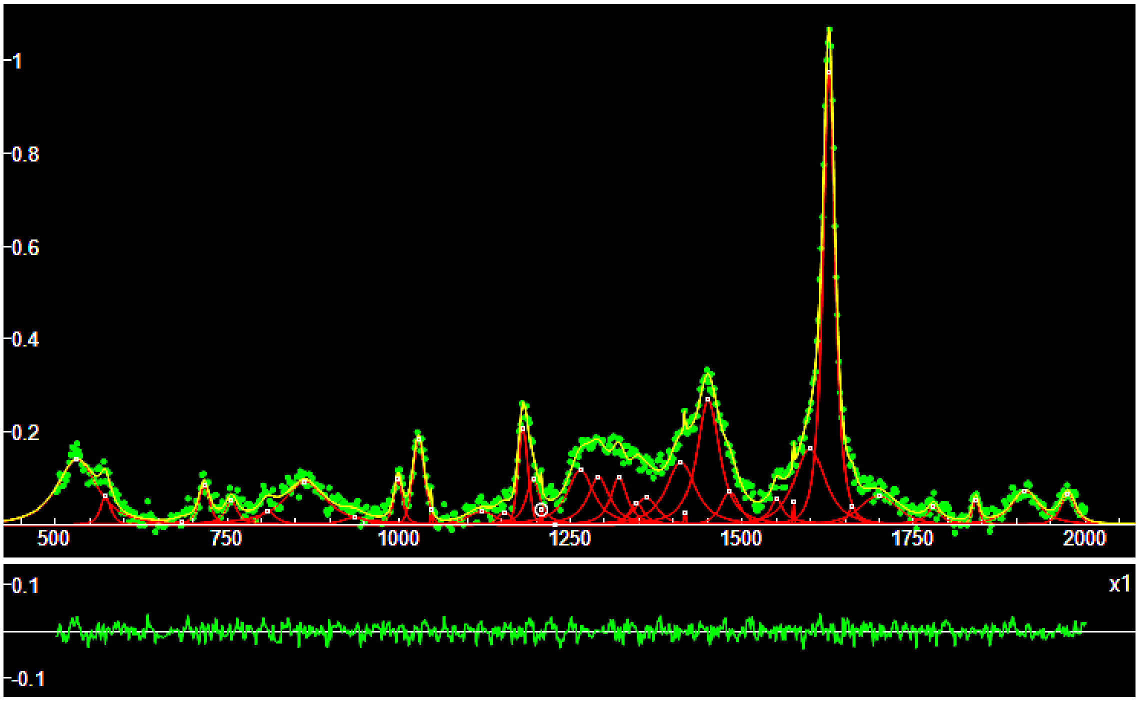
SERS pH=9: 789 992 ***1032(vs)*** ***1078*** *1371* ***1410*** ***1439*** *1489* ***1586*** 1601

Again, as told by to Jaworska and coworkers, “the normal FT-Raman spectrum of the aqueous solution at low pH reveals the presence of two bands at 1030 and 1046 cm^{-1}, which are attributed to vibrations 1 and 12 of the pyridine ring, respectively”.



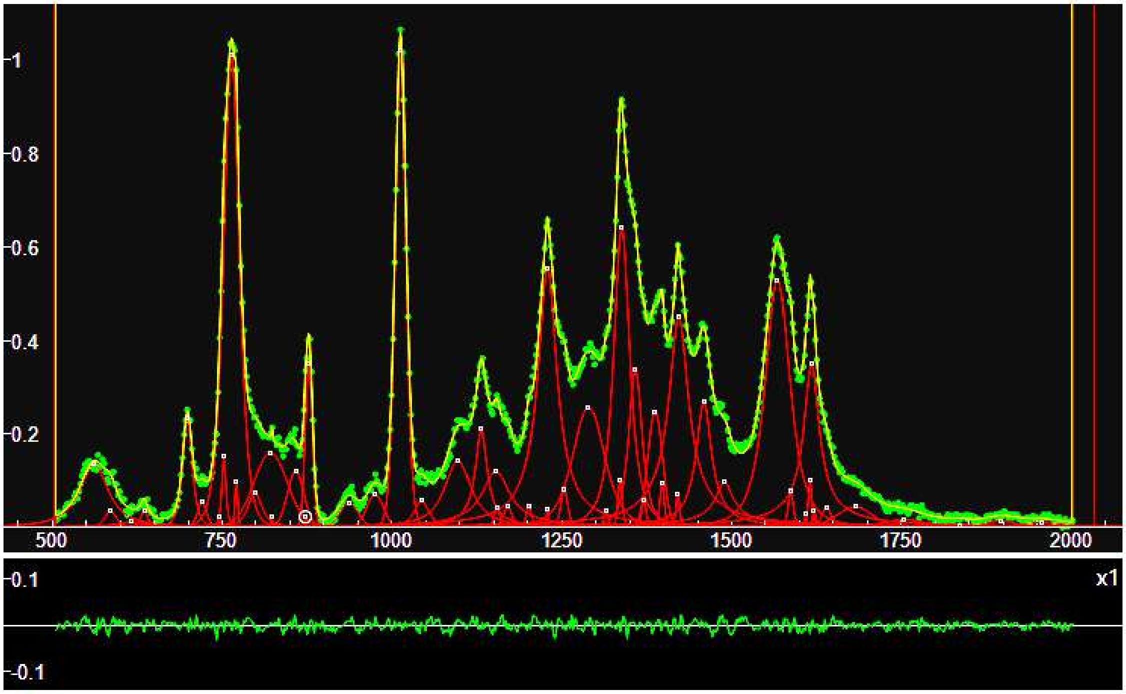
Detail of the peak at 1030 cm^{-1}.

N-methyl-D-aspartic acid



# PeakType		Center			Parametrs Height Center HWHM q (H>0.05)
%_31	Qgau	517.963	x	x	0.0435458 517.963 7.88891 1.01326
%_7	Qgau	531.168	x	x	0.13991 531.168 36.6984 1.64766
%_23	Qgau	572.878	x	x	0.0626833 572.878 9.5503 1.75143
%_33	Qgau	603.001	x	x	0.0386237 603.001 2.75744 1.00016
%_24	Qgau	966.33	x	x	0.0582535 966.33 37.8635 1.1583
%_11	Qgau	716.495	x	x	0.0844223 716.495 10.0296 1.64554
%_19	Qgau	756.132	x	x	0.0510117 756.132 10.8519 2.16395
%_26	Qgau	863.168	x	x	0.0930458 863.168 36.97 1.95842
%_29	Qgau	914.293	x	x	0.0969944 914.293 10.4379 1.71008
%_12	Qgau	999.104	x	x	0.102057 999.104 7.42456 1.74841
%_4	Qgau	1029.19	x	x	0.184373 1029.19 11.8274 1.16463
%_34	Qgau	1053.88	x	x	0.0354625 1053.88 12.6901 1.13105
%_3	Qgau	1181.24	x	x	0.206947 1181.24 9.86171 1.07092
%_13	Qgau	1195.64	x	x	0.0999497 1195.64 11.8958 1.89646
%_9	Qgau	1264.42	x	x	0.115033 1264.42 23.6764 1.87046
%_34	Qgau	1291.2	x	x	0.102664 1291.2 19.4024 2.00134
%_35	Qgau	1320.5	x	x	0.0995863 1320.5 14.8963 1.91443
%_18	Qgau	1360.54	x	x	0.0547264 1360.54 22.741 1.50189
%_8	Qgau	1410.81	x	x	0.12984 1410.81 26.4992 1.86448
%_2	Qgau	1450.87	x	x	0.267468 1450.87 20.3539 1.8288
%_16	Qgau	1482.46	x	x	0.0678135 1482.46 17.9272 1.5517
%_20	Qgau	1550.66	x	x	0.0567171 1550.66 10.7574 2.65249
%_6	Qgau	1598.88	x	x	0.160389 1598.88 28.8732 1.55264
%_1	Qgau	1626.72	x	x	0.9767 1626.72 11.2821 1.60688
%_15	Qgau	1698.98	x	x	0.0625437 1698.98 36.6713 1.39126
%_21	Qgau	1840.47	x	x	0.0543642 1840.47 6.41342 1.40115
%_14	Qgau	1912.5	x	x	0.0730464 1912.5 24.5547 1.8238
%_17	Qgau	1975.06	x	x	0.0656699 1975.06 14.1818 1.51452

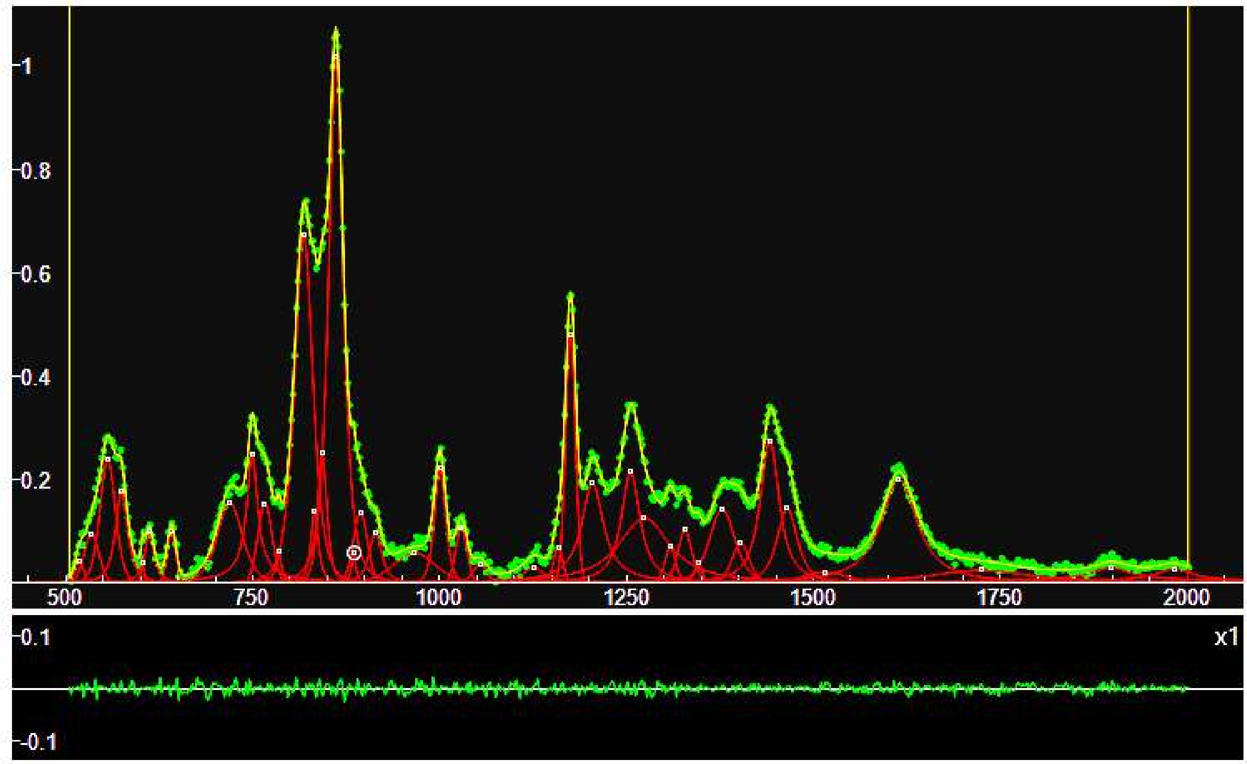
N-methyltryptamine



# PeakType		Center		Parameters	Height Center HWHM q (h>0.08)
%_26	Qgau	561.4	x	x	0.134713 561.4 25.5486 1.89271
%_40	**Qgau**	**699.042**	**x**	**x**	**0.233325 699.042 9.18402 1.52421**
%_35	Qgau	752.354	x	x	0.151638 752.354 3.73642 1.63
%_2	Qgau	763.601	x	x	1.01118 763.601 15.5096 1.32631
%_37	Qgau	770.779	x	x	0.106519 770.779 2.66518 1.15183
%_29	Qgau	821.225	x	x	0.159966 821.225 33.7875 1.0895
%_30	Qgau	858.079	x	x	0.120028 858.079 17.0484 1.05807
%_8	**Qgau**	**877.644**	**x**	**x**	**0.353709 877.644 7.50384 0.999958**
%_1	**Qgau**	**1012.71**	**x**	**x**	**1.02165 1012.71 10.5105 1.18048**
%_42	Qgau	1097.12	x	x	0.142649 1097.12 23.9291 1.89838
%_10	**Qgau**	**1131.18**	**x**	**x**	**0.210747 1131.18 10.3241 2.22062**
%_22	Qgau	1152.96	x	x	0.11987 1152.96 25.198 2.20381
%_4	**Qgau**	**1228.77**	**x**	**x**	**0.55574 1228.77 16.9604 2.15886**
%_44	Qgau	1253.67	x	x	0.0808227 1253.67 7.24395 1.12166
%_12	**Qgau**	**1289.46**	**x**	**x**	**0.257267 1289.46 30.8255 1.40265**
%_39	Qgau	1335.74	x	x	0.102179 1335.74 4.18793 1.34656
%_3	**Qgau**	**1338.12**	**x**	**x**	**0.64293 1338.12 14.8228 1.68607**
%_45	**Qgau**	**1358.45**	**x**	**x**	**0.340383 1358.45 12.6028 1.62667**
%_11	**Qgau**	**1387.37**	**x**	**x**	**0.246597 1387.37 15.1946 0.999705**
%_36	Qgau	1397.27	x	x	0.0940129 1397.27 4.31351 1.3619
%_6	**Qgau**	**1421.99**	**x**	**x**	**0.451131 1421.99 17.6854 2.30716**
%_15	Qgau	1489.25	x	x	0.0958895 1489.25 16.4234 2.74589
%_9	**Qgau**	**1459.28**	**x**	**x**	**0.268988 1459.28 13.7275 2.15659**
%_5	**Qgau**	**1567.64**	**x**	**x**	**0.530499 1567.64 23.0139 1.61247**
%_46	Qgau	1615.27	x	x	0.101896 1615.27 3.15844 1.63893
%_7	**Qgau**	**1617.5**	**x**	**x**	**0.350319 1617.5 13.7012 2.42038**

Octopamine

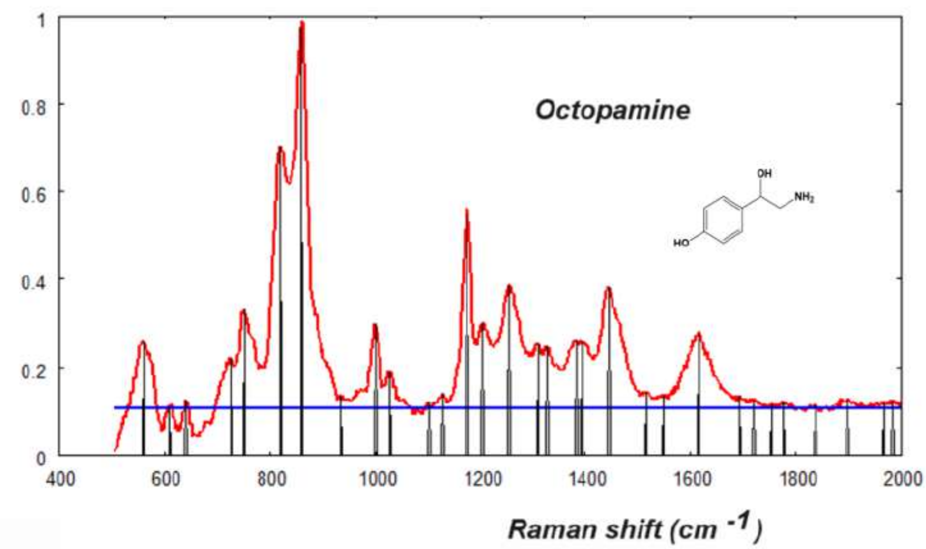
Literature suggested by Sherman et al.: Kang et al., 2015.



#	PeakType	Center			Parameters	Height	Cenetr	HWHM	q ...
%_23	Qgau	534.581	x	x	x	0.0943118	534.581	14.042	0.999988
%_7	Qgau	556.03		x	x	0.239062	556.03	13.8763	1.23213
%_13	Qgau	574.692	x	x	x	0.176836	574.692	10.1368	1.73239
%_21	Qgau	611.806	x	x	x	0.0991465	611.806	7.54415	1.86854
%_19	Qgau	641.544	x	x	x	0.100883	641.544	7.82287	1.00009
%_15	Qgau	719.455	x	x	x	0.154469	719.455	22.3249	1.333
%_6	Qgau	749.245	x	x	x	0.25062	749.245	8.51345	2.28563
%_16	Qgau	766.412	x	x	x	0.153169	766.412	13.4552	0.999912
%_40	Qgau	784.701	x	x	x	0.0632523	784.701	3.80176	2.30088
%_41	Qgau	818.179	x	x	x	0.675322	818.179	16.0616	1.41331
%_42	Qgau	832.731	x	x	x	0.139912	832.731	6.16523	1.76309
%_39	Qgau	843.014	x	x	x	0.250871	843.014	7.96939	1.47273
%_1	Qgau	861.346	x	x	x	1.01902	861.346	12.432	1.55903
%_2	Qgau	885.057	x	x	x	0.0623427	885.057	2.85633	2.00338
%_17	Qgau	893.902	x	x	x	0.134897	893.902	13.3741	0.999883
%_8	Qgau	1000.65	x	x	x	0.222643	1000.65	9.93112	1.33788
%_18	Qgau	1029.04	x	x	x	0.105675	1029.04	10.8818	0.999875
%_27	Qgau	1125.75	x	x	x	0.0305317	1125.75	16.5196	1.95867
%_35	Qgau	1158.6		x	x	0.0698835	1158.6	8.68287	0.999971
%_3	Qgau	1174.92	x	x	x	0.479423	1174.92	9.34428	1.00003
%_10	Qgau	1204.52	x	x	x	0.192813	1204.52	17.634	2.04474

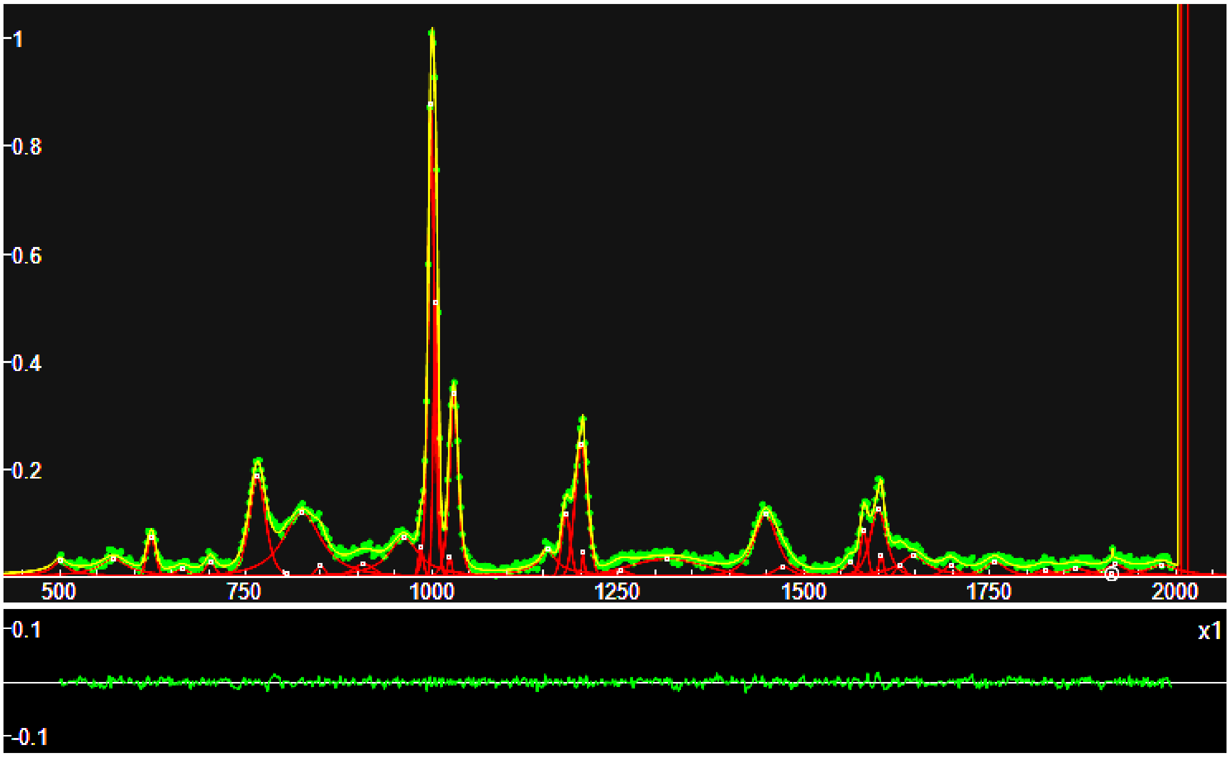
%_4	Qgau	1255.54	x	x	x	0.214385	1255.54	15.374	1.87486
%_12	Qgau	1273.72	x	x	x	0.125666	1273.72	41.531	1.90634
%_36	Qgau	1308.38	x	x	x	0.0706802	1308.38	9.34209	1.28782
%_37	Qgau	1328.16	x	x	x	0.102547	1328.16	12.0596	1.41574
%_38	Qgau	1346.05	x	x	x	0.0381563	1346.05	6.43078	1.5037
%_11	Qgau	1377.98	x	x	x	0.142586	1377.98	22.4149	1.35635
%_22	Qgau	1402.59	x	x	x	0.0761776	1402.59	16.1271	1.10173
%_5	Qgau	1441.5		x	x	0.274676	1441.5	15.526	1.83857
%_14	Qgau	1464.97	x	x	x	0.144184	1464.97	17.4861	1.57269
%_28	Qgau	1514.96	x	x	x	0.0204935	1514.96	40.232	0.998413
%_30	Qgau	1724.43	x	x	x	0.0246363	1724.43	80.0925	1.89938
%_32	Qgau	1982.37	x	x	x	0.0268359	1982.37	31.4431	2.61452
%_9	Qgau	1614.5		x	x	0.200112	1614.5	29.7312	1.89637
%_26	Qgau	1898.41	x	x	x	0.0297512	1898.41	31.8323	3.19416

Octopamine has been investigated in Sparavigna, 2023, with the first derivative spectrum. The following table provides the peaks above a given threshold.



Position (in cm^{-1})	Relative intensity	Position (in cm^{-1})	Relative intensity
559.00	0.26	1326.00	0.25
609.00	0.11	1382.00	0.26
640.50	0.12	1392.50	0.26
726.50	0.22	1444.00	0.38
751.00	0.33	1515.00	0.14
820.00	0.70	1547.50	0.14
860.00	0.97	1614.00	0.28
935.00	0.13	1693.50	0.13
1000.50	0.30	1719.50	0.12
1028.50	0.19	1753.00	0.11
1102.00	0.12	1776.50	0.12
1129.50	0.14	1836.50	0.11
1174.50	0.55	1898.50	0.12
1204.00	0.30	1967.00	0.12
1255.00	0.39	1984.00	0.12
1309.50	0.25		

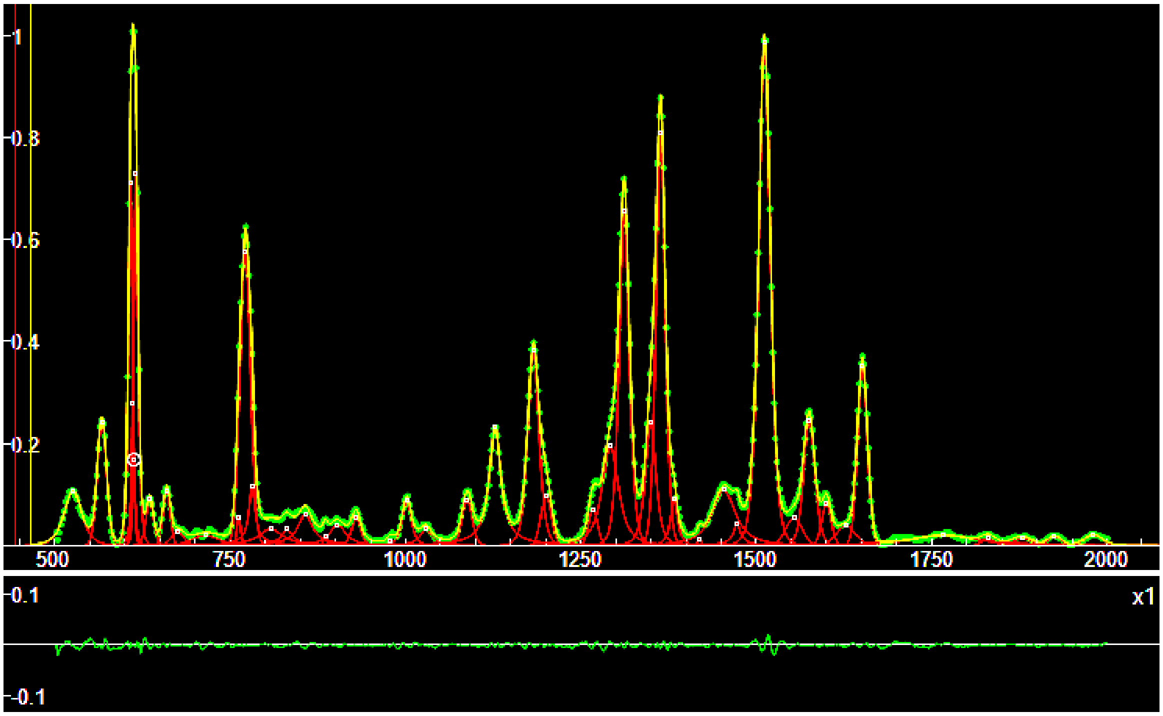
Phenethylamine



#	PeakType	Center	Parameters		Height	Center	HWHM	q (h > 0.025)
%_21	Qgau	499.203	x	x	0.0296734	499.203	11.3121	3.01484
%_16	Qgau	571.506	x	x	0.0345262	571.506	22.5921	2.44381
%_9	Qgau	622.301	x	x	0.0735304	622.301	8.39485	0.999963
%_18	Qgau	701.797	x	x	0.028208	701.797	8.42292	1.58481
%_5	Qgau	765.079	x	x	0.186653	765.079	14.5652	1.36454
%_8	Qgau	825.152	x	x	0.11909	825.152	32.3426	1.77195
%_10	Qgau	961.85	x	x	0.0736342	961.85	24.4669	2.09934
%_30	Qgau	984.89	x	x	0.0559441	984.89	4.67277	1.00001
%_1	Qgau	998.769	x	x	0.890332	998.769	5.22143	1.39229
%_23	Qgau	1023.6	x	x	0.0387287	1023.6	3.73817	0.999989
%_2	Qgau	1029.18x	x	x	0.339725	1029.18	7.50594	1.45743
%_3	Qgau	1005.04x	x	x	0.510854	1005.04	4.38144	1.10491
%_13	Qgau	1155.45x	x	x	0.0509014	1155.45	12.8783	2.9206
%_11	Qgau	1180.01x	x	x	0.117717	1180.01	8.23121	1.04485
%_4	Qgau	1200.53x	x	x	0.246188	1200.53	11.8521	0.999789
%_37	Qgau	1202.93x	x	x	0.0471643	1202.93	2.2154	1.57446
%_32	Qgau	1315.93x	x	x	0.0340446	1315.93	72.8711	1.00043
%_7	Qgau	1448.63x	x	x	0.116213	1448.63	19.84	1.70228
%_12	Qgau	1580.53x	x	x	0.0858522	1580.53	6.78397	1.11554
%_24	Qgau	1561.78x	x	x	0.0272248	1561.78	10.1286	2.22663
%_6	Qgau	1599.99x	x	x	0.127023	1599.99	13.7709	1.56274
%_15	Qgau	1647.36x	x	x	0.0404801	1647.36	22.0027	2.42609
%_38	Qgau	1603.79x	x	x	0.0434236	1603.79	3.8896	1.3996
%_35	Qgau	1756.79x	x	x	0.0285283	1756.79	18.2903	1.9903

Pipecolate

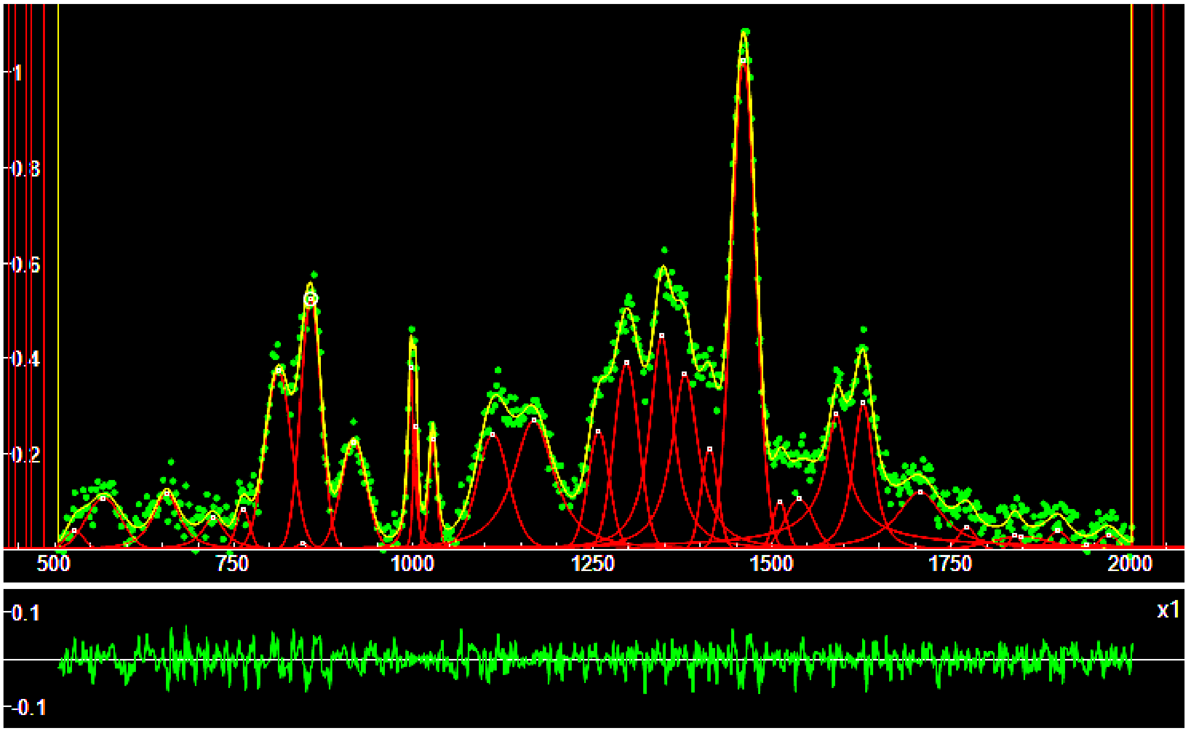
Literature suggested by Sherman and coworkers: Sobolewski et al., 2013.



# PeakType		Center			Parameters Height	Center	HWHM	q (H>0.08)
%_17	Qgau	525.658	x	x	0.107164	525.658	16.4909	1.45034
%_10	Qgau	566.969	x	x	0.245009	566.969	9.05357	1.09504
%_48	Qgau	607.494	x	x	0.724982	607.494	3.70661	1.44435
%_60	Qgau	610.926	x	x	0.30266	610.926	2.3295	1.45049
%_61	Qgau	612.686	x	x	0.170363	612.686	2.29879	1.62251
%_47	Qgau	615.518	x	x	0.759812	615.518	3.90097	1.47981
%_25	Qgau	635.15	x	x	0.0933598	635.15	6.81644	1.39659
%_15	Qgau	659.07	x	x	0.107092	659.07	7.39882	0.999978
%_5	Qgau	771.301	x	x	0.577051	771.301	10.3826	1.05255
%_20	Qgau	780.936	x	x	0.118469	780.936	4.84892	2.43667
%_19	Qgau	1001.65	x	x	0.0890385	1001.65	7.95042	1.63077
%_18	Qgau	1087.66	x	x	0.089509	1087.66	9.72184	1.19786
%_11	Qgau	1127.63	x	x	0.234263	1127.63	9.49611	2.13266
%_6	Qgau	1182.13	x	x	0.383138	1182.13	10.3769	1.35778
%_21	Qgau	1200.36	x	x	0.097444	1200.36	10.6803	0.99989
%_12	Qgau	1291.79	x	x	0.194602	1291.79	14.7779	1.68326
%_4	Qgau	1311.7	x	x	0.656908	1311.7	9.32303	1.35255
%_13	Qgau	1349.18	x	x	0.242106	1349.18	9.55428	1.54093
%_3	Qgau	1363.65	x	x	0.813406	1363.65	8.82116	1.19224
%_30	Qgau	1382.58	x	x	0.0918508	1382.58	6.2555	1.76298
%_14	Qgau	1453.64	x	x	0.109455	1453.64	20.4829	1.80865
%_2	Qgau	1511.67	x	x	0.989075	1511.67	10.8917	1.35315
%_8	Qgau	1575.62	x	x	0.248463	1575.62	10.5212	1.28703
%_22	Qgau	1600.1	x	x	0.0838386	1600.1	9.08983	1.14286
%_7	Qgau	1651.47	x	x	0.356433	1651.47	9.68638	1.07625

Pterin

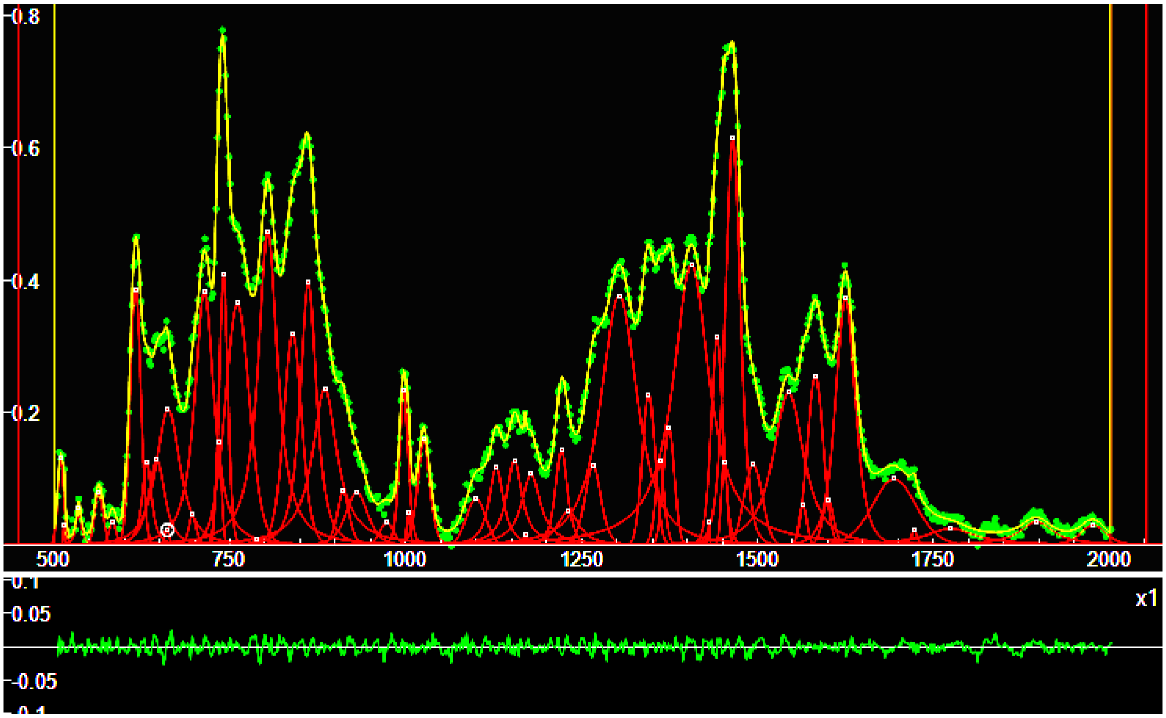
Literature: Stevenson et al., 2009, and Smyth et al., 2011.



#	PeakType	Center			Parameters Height	Center	HWHM	q (H>0.05)
%_19	Qgau	568.145	x	x	0.108662	568.145	34.2892	0.999428
%_17	Qgau	655.598	x	x	0.118245	655.598	23.2323	1.77128
%_24	Qgau	721.401	x	x	0.0677716	721.401	18.8381	1.98337
%_29	Qgau	762.45	x	x	0.0855823	762.45	13.6063	0.999885
%_7	Qgau	811.803	x	x	0.37319	811.803	26.1716	0.999517
%_3	Qgau	857.229	x	x	0.526094	857.229	20.0844	0.999748
%_14	Qgau	916.805	x	x	0.223026	916.805	25.1967	0.999503
%_5	Qgau	996.37	x	x	0.386768	996.37	4.80498	2.01139
%_20	Qgau	1002.94	x	x	0.266496	1002.94	3.7477	1.52563
%_12	Qgau	1027.05	x	x	0.23558	1027.05	7.20219	1.38291
%_8	Qgau	1111.04	x	x	0.242265	1111.04	29.902	1.21041
%_11	Qgau	1167.75	x	x	0.269769	1167.75	35.1487	1.81618
%_13	Qgau	1258.26	x	x	0.249236	1258.26	20.3862	1.10646
%_4	Qgau	1297.03	x	x	0.390469	1297.03	24.5585	0.999038
%_2	Qgau	1346.22	x	x	0.446987	1346.22	20.1724	1.88986
%_10	Qgau	1378.61	x	x	0.367035	1378.61	22.7317	1.91667
%_15	Qgau	1412.86	x	x	0.211936	1412.86	16.1267	0.999771
%_1	Qgau	1460.45	x	x	1.02224	1460.45	23.517	0.999473
%_25	Qgau	1510.8	x	x	0.101862	1510.8	13.6612	0.999831
%_18	Qgau	1537.78	x	x	0.106561	1537.78	27.4154	1.04051
%_9	Qgau	1590	x	x	0.28391	1590	17.9072	2.85701
%_6	Qgau	1627.07	x	x	0.306108	1627.07	18.0633	1.64725
%_16	Qgau	1706.21	x	x	0.121738	1706.21	38.6929	1.9528

Riboflavin

Literature: Liu et al., 2012, Bailey and Schultz, 2016, Dendisová-Vyškovská et al., 2013.



#	PeakType	Center		Parameters	Height	Center	HWHM	q (h>0.13, **bold** h>0.20)
%_20	Qgau	509.548	x	x	0.132844	509.548	6.38009	0.999991
%_6	**Qgau**	**615.63**	**x**	**x**	**0.388069**	**615.63**	**10.6448**	**0.999941**
%_16	**Qgau**	**662.036**	**x**	**x**	**0.205646**	**662.036**	**21.4606**	**1.69231**
%_12	**Qgau**	**713.545**	**x**	**x**	**0.384037**	**713.545**	**16.7399**	**1.78736**
%_33	Qgau	733.814	x	x	0.157629	733.814	5.56765	1.00005
%_1	**Qgau**	**740.705**	**x**	**x**	**0.409706**	**740.705**	**8.39408**	**1.14401**
%_8	**Qgau**	**760.54**	**x**	**x**	**0.365545**	**760.54**	**23.3775**	**1.17989**
%_4	**Qgau**	**803.766**	**x**	**x**	**0.473947**	**803.766**	**16.7303**	**1.91826**
%_9	**Qgau**	**839.139**	**x**	**x**	**0.319764**	**839.139**	**17.2136**	**1.22164**
%_36	**Qgau**	**884.683**	**x**	**x**	**0.236503**	**884.683**	**21.1573**	**2.00948**
%_3	**Qgau**	**861.291**	**x**	**x**	**0.396463**	**861.291**	**14.4233**	**1.65361**
%_14	**Qgau**	**996.936**	**x**	**x**	**0.233248**	**996.936**	**8.18527**	**1.30717**
%_19	Qgau	1025.27	x	x	0.16103	1025.27	11.3529	1.32021
%_21	Qgau	1220.98	x	x	0.143912	1220.98	11.1476	1.51304
%_11	**Qgau**	**1303.11**	**x**	**x**	**0.376702**	**1303.11**	**32.7884**	**1.67156**
%_23	**Qgau**	**1345.03**	**x**	**x**	**0.228627**	**1345.03**	**12.8569**	**1.00495**
%_43	Qgau	1360.9	x	x	0.130955	1360.9	8.24518	1.22131
%_5	Qgau	1373.82	x	x	0.177525	1373.82	11.0558	1.001
%_7	**Qgau**	**1405.66**	**x**	**x**	**0.424245**	**1405.66**	**31.0457**	**1.96519**
%_15	**Qgau**	**1442.17**	**x**	**x**	**0.314003**	**1442.17**	**10.8292**	**1.27372**
%_2	**Qgau**	**1464.65**	**x**	**x**	**0.613821**	**1464.65**	**14.2401**	**1.33739**
%_30	**Qgau**	**1543.71**	**x**	**x**	**0.230789**	**1543.71**	**27.058**	**1.78597**
%_29	**Qgau**	**1581.87**	**x**	**x**	**0.255827**	**1581.87**	**15.8048**	**0.999805**
%_10	**Qgau**	**1624.64**	**x**	**x**	**0.373628**	**1624.64**	**18.3203**	**1.42289**

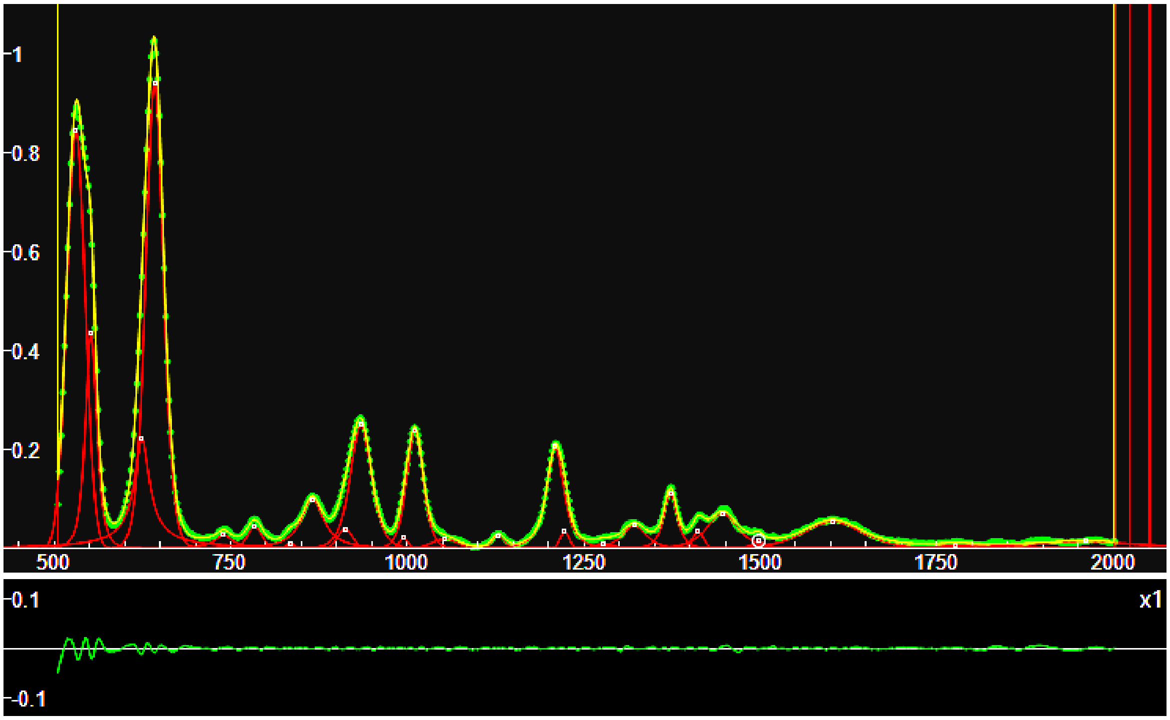
The centers of the q-Gaussians are:

509.548	615.63	662.036	713.545	733.814	***740.705***
760.54	803.766	839.139	884.683	861.291	996.936
1025.27	1220.98	1303.11	***1345.03***	1360.9	1373.82
1405.66	1442.17	***1464.65***	1543.71	1581.87	***1624.64***

In De Gelder et al., 2007, we find the following Raman peaks (in bold, the peaks which are corresponding to centers, within +/− 5 cm^{-1}):

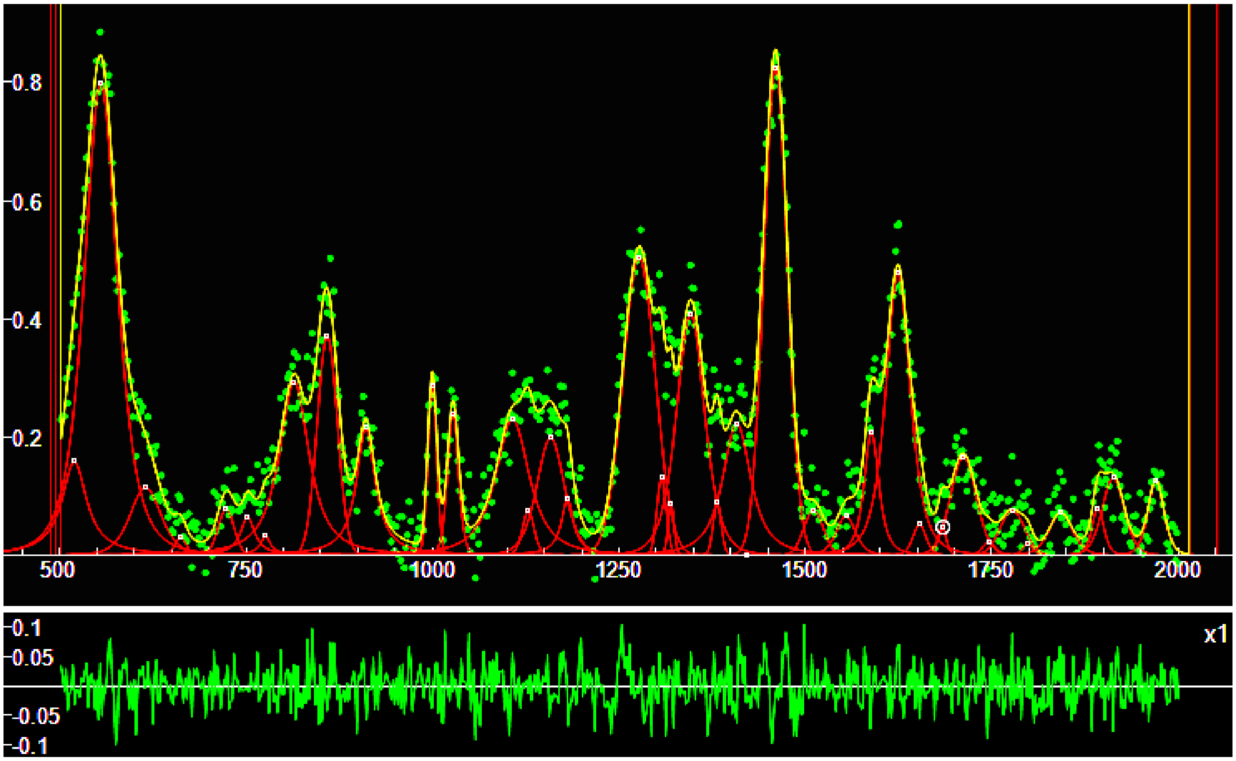
422(w), 451(w), 502(m), 531(w), 603(w), 677(w), ***742(m),*** 785(m), 1158(m), 1184(m), 1226(s), 1253(w), ***1345(vs), 1402(m), 1464(m),*** 1496(m), 1534(m), 1576(m), ***1621(w),*** 1658(w), 1704(w)

Selenocystamine



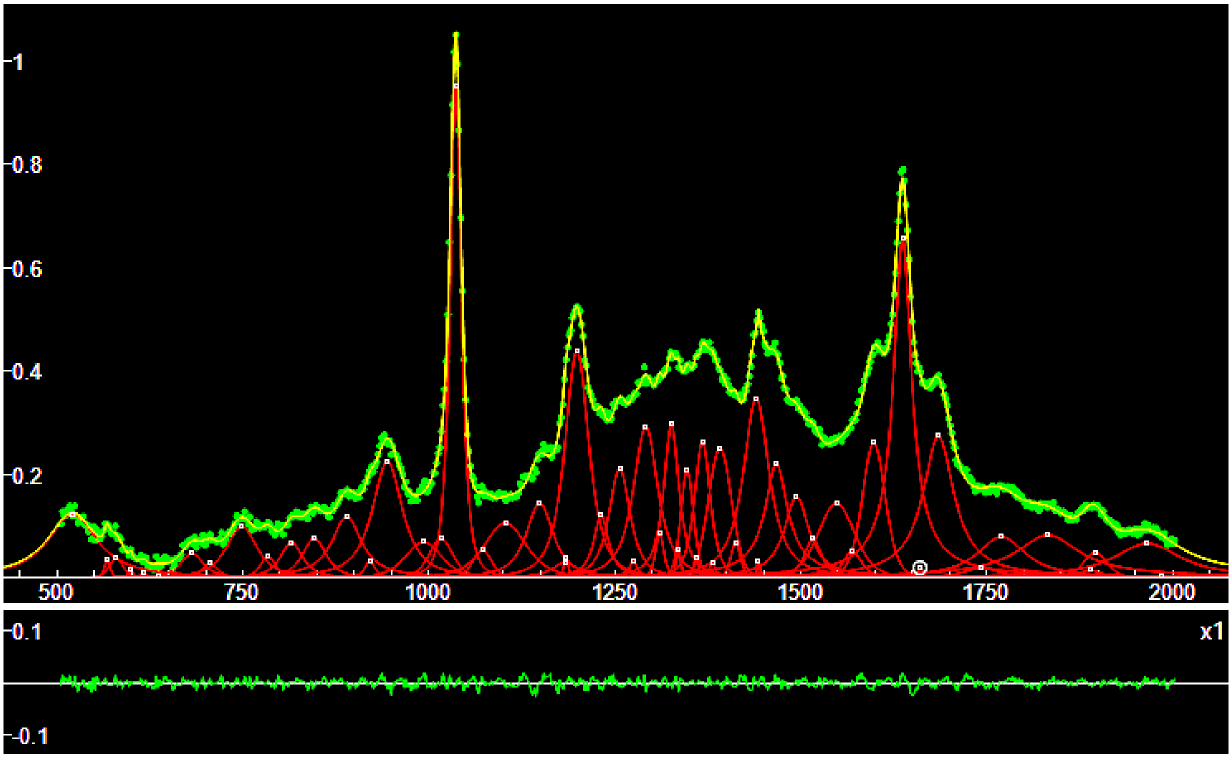
# PeakType		Center		Parameters	Height	Center	HWHM	q ...
%_2	Qgau	530.64	x	x	0.847653	530.64	18.4971	0.999842
%_3	Qgau	552.191	x	x	0.43485	552.191	10.3452	1.51614
%_7	Qgau	624.131	x	x	0.223044	624.131	12.917	2.40854
%_1	Qgau	642.114	x	x	0.943585	642.114	16.9689	1.1943
%_17	Qgau	739.864	x	x	0.0273157	739.864	15.1287	2.39113
%_12	Qgau	783.9	x	x	0.0441947	783.9	14.0605	1.16538
%_23	Qgau	834.409	x	x	0.0106968	834.409	9.0093	0.999943
%_9	Qgau	865.664	x	x	0.0998369	865.664	19.3645	1.92659
%_16	Qgau	911.967	x	x	0.0395918	911.967	14.9142	0.999886
%_4	Qgau	934.223	x	x	0.250479	934.223	19.8478	1.34842
%_26	Qgau	994.645	x	x	0.0207419	994.645	8.91478	0.999949
%_5	Qgau	1010.6	x	x	0.23874	1010.6	15.6565	1.29529
%_24	Qgau	1052.91	x	x	0.01921	1052.91	26.8769	0.999199
%_19	Qgau	1128.82	x	x	0.0251368	1128.82	12.9014	0.999805
%_6	Qgau	1209.48	x	x	0.206013	1209.48	15.1887	1.66881
%_20	Qgau	1222.88	x	x	0.033979	1222.88	9.24872	0.999885
%_25	Qgau	1278.44	x	x	0.0094367	1278.44	21.0128	0.999262
%_13	Qgau	1321.26	x	x	0.046481	1321.26	21.7214	1.56834
%_8	Qgau	1372.55	x	x	0.112534	1372.55	11.8888	1.61565
%_18	Qgau	1411.56	x	x	0.0339854	1411.56	11.3182	0.999873
%_10	Qgau	1445.8	x	x	0.070841	1445.8	28.3946	1.53804
%_28	Qgau	1497.13	x	x	0.0158504	1497.13	9.44661	2.23175
%_11	Qgau	1602.65	x	x	0.0544409	1602.65	55.1025	1.37757
%_27	Qgau	1776.78	x	x	0.00744753	1776.78	32.4871	3.98511
%_22	Qgau	1959.77	x	x	0.0146226	1959.77	86.1106	2.71729

Selenomethionine



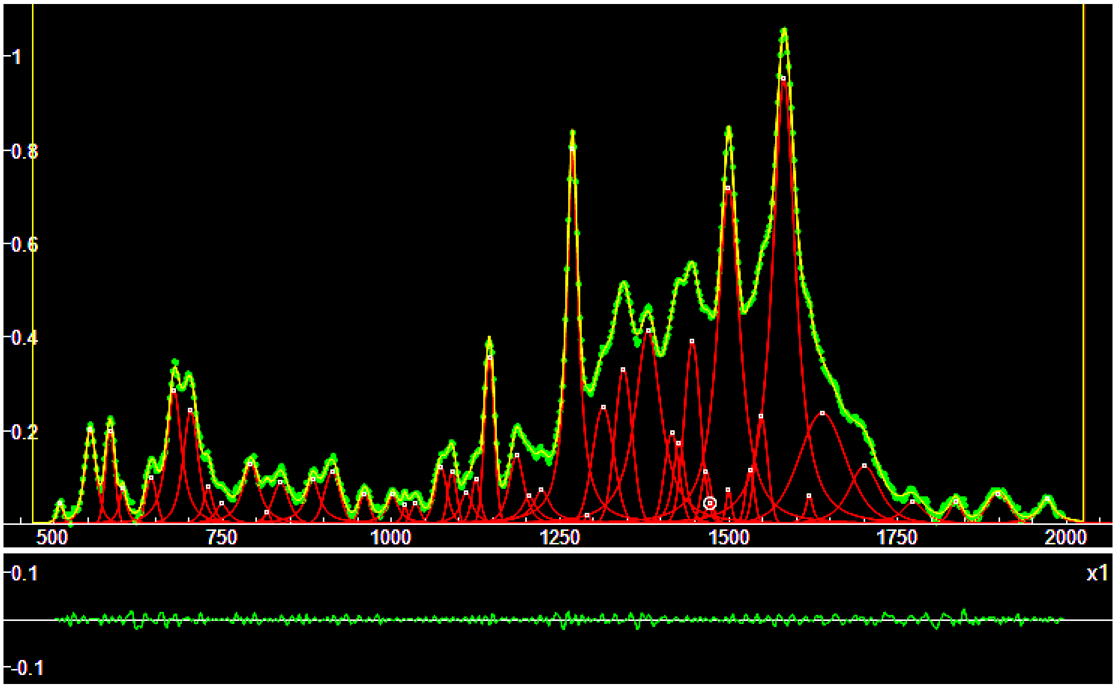
#	PeakType	Center	Parameters		Height	Center	HWHM	q (h>0.08)
%_15	Qgau	519.359	x	x	0.159045	519.359	20.1139	2.03809
%_1	Qgau	554.958	x	x	0.797872	554.958	28.746	1.50041
%_18	Qgau	615.003	x	x	0.11468	615.003	27.8742	1.32456
%_7	Qgau	814.295	x	x	0.293294	814.295	24.7806	1.79844
%_5	Qgau	858.718	x	x	0.37126	858.718	19.0781	0.999727
%_14	Qgau	910.428	x	x	0.215692	910.428	15.3376	1.9974
%_9	Qgau	999.567	x	x	0.290363	999.567	8.38493	0.999942
%_11	Qgau	1027.27	x	x	0.239793	1027.27	10.0181	1.21226
%_10	Qgau	1107.03	x	x	0.230338	1107.03	28.169	1.72529
%_8	Qgau	1158.25	x	x	0.198651	1158.25	24.7318	1.29899
%_28	Qgau	1180.8	x	x	0.0951656	1180.8	9.89773	2.11022
%_4	Qgau	1276.94	x	x	0.50432	1276.94	30.9281	0.998411
%_30	Qgau	1307.11	x	x	0.131914	1307.11	8.77823	0.999881
%_20	Qgau	1319.7	x	x	0.0887815	1319.7	5.40437	1.10437
%_6	Qgau	1345.99	x	x	0.407982	1345.99	25.1496	1.35555
%_32	Qgau	1381.8	x	x	0.0896634	1381.8	7.40437	1.10437
%_12	Qgau	1407.97	x	x	0.22268	1407.97	23.5294	1.72906
%_2	Qgau	1460.1	x	x	0.824643	1460.1	22.3084	0.999468
%_13	Qgau	1588.64	x	x	0.207902	1588.64	12.6857	1.60668
%_3	Qgau	1624.27	x	x	0.477812	1624.27	21.0842	1.50003
%_16	Qgau	1711.89	x	x	0.166713	1711.89	23.9374	1.112
%_35	Qgau	1892.43	x	x	0.0802105	1892.43	10.6907	1.32815
%_17	Qgau	1913.01	x	x	0.131007	1913.01	20.2139	1.19799
%_23	Qgau	1970.23	x	x	0.12608	1970.23	14.5486	1.29808

Spermidine



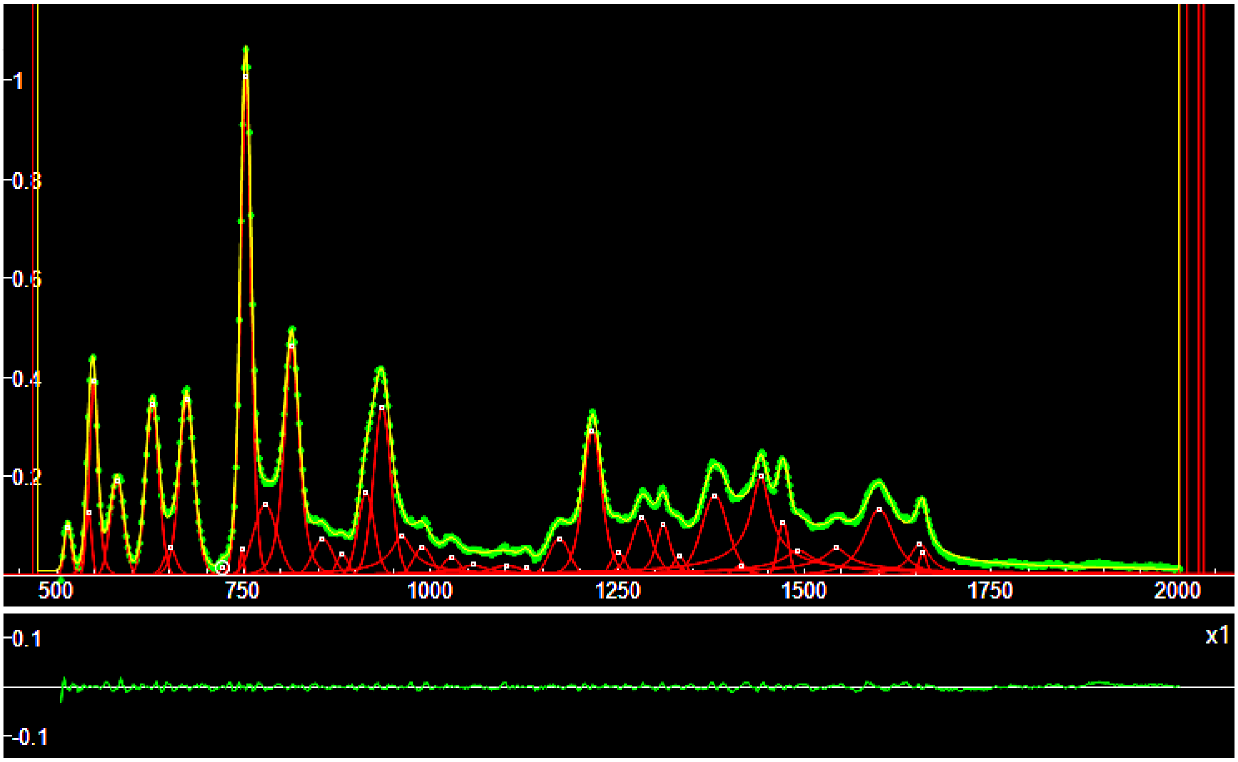
# PeakType		Center			Parameters	Height	Center	HWHM	q (h>0.08)
%_18	Qgau	520.775	x	x		0.122775	520.775	40.4705	1.91163
%_17	Qgau	748.249	x	x		0.0994429	748.249	26.0612	1.65247
%_48	Qgau	889.335	x	x		0.118396	889.335	24.2851	1.97284
%_13	Qgau	944.186	x	x		0.225544	944.186	24.9729	1.79914
%_1	Qgau	1036.03	x	x		0.963732	1036.03	9.54562	1.61564
%_41	Qgau	1102.73	x	x		0.106019	1102.73	37.1723	1.39964
%_43	Qgau	1148.94	x	x		0.144489	1148.94	22.6281	1.76855
%_3	Qgau	1198.98	x	x		0.440486	1198.98	20.3334	1.63656
%_45	Qgau	1231.49	x	x		0.122883	1231.49	11.7865	1.98138
%_44	Qgau	1256.34	x	x		0.211051	1256.34	18.0749	1.65218
%_7	Qgau	1291.51	x	x		0.292228	1291.51	20.7111	1.73551
%_27	Qgau	1310.33	x	x		0.0862096	1310.33	7.19528	1.5202
%_6	Qgau	1325.99	x	x		0.298761	1325.99	12.396	1.88855
%_15	Qgau	1347.23	x	x		0.2086	1347.23	11.5378	1.22579
%_5	Qgau	1367.66	x	x		0.264787	1367.66	13.5809	1.55559
%_10	Qgau	1391.3	x	x		0.25148	1391.3	21.5855	1.07021
%_4	Qgau	1440.05	x	x		0.347634	1440.05	21.4145	1.82966
%_46	Qgau	1467.1	x	x		0.221386	1467.1	18.2052	2.25507
%_47	Qgau	1494.38	x	x		0.15765	1494.38	20.0245	2.02432
%_19	Qgau	1547.98	x	x		0.14409	1547.98	33.0461	1.26059
%_8	Qgau	1598.1	x	x		0.261202	1598.1	20.9476	1.2309
%_9	Qgau	1685.06	x	x		0.274725	1685.06	25.0606	2.08978
%_2	Qgau	1636.82	x	x		0.65994	1636.82	14.3417	2.22483
%_40	Qgau	1832.3	x	x		0.0827289	1832.3	51.6759	2.21761

Tetrahydrofolate



#	PeakType	Center			Parameters	Height	Center	HWHM	q	)h>0.08)
%_14	Qgau	553.823	x	x		0.20531	553.823	10.4983	1.54255	
%_13	Qgau	582.964	x	x		0.20274	582.964	9.56396	1.00007	
%_24	Qgau	643.74	x	x		0.0997166	643.74	11.2105	0.99997	
%_9	Qgau	677.741	x	x		0.287546	677.741	13.2324	1.83211	
%_12	Qgau	702.355	x	x		0.244454	702.355	14.3129	1.49719	
%_20	Qgau	791.53	x	x		0.128869	791.53	15.2612	1.91217	
%_22	Qgau	835.635	x	x		0.088785	835.635	15.917	1.3718	
%_25	Qgau	882.993	x	x		0.0975354	882.993	11.9181	2.29348	
%_19	Qgau	911.965	x	x		0.112932	911.965	15.878	1.11731	
%_42	Qgau	1072.98	x	x		0.123056	1072.98	11.8921	1.3579	
%_43	Qgau	1089.57	x	x		0.114432	1089.57	9.0659	0.999925	
%_45	Qgau	1124.73	x	x		0.09848	1124.73	8.17193	1.40926	
%_8	Qgau	1144.68	x	x		0.360314	1144.68	10.1961	0.999883	
%_15	Qgau	1184.92	x	x		0.147978	1184.92	14.0185	1.56921	
%_3	Qgau	1268.55	x	x		0.805086	1268.55	10.212	2.06036	
%_10	Qgau	1313.9	x	x		0.250937	1313.9	22.2029	1.00534	
%_5	Qgau	1344.09	x	x		0.332053	1344.09	17.7606	1.04235	
%_7	Qgau	1380.4	x	x		0.415672	1380.4	23.4879	1.8625	
%_16	Qgau	1415.67	x	x		0.195055	1415.67	15.3098	0.999847	
%_21	Qgau	1426.59	x	x		0.175185	1426.59	11.4525	1.63671	
%_6	Qgau	1446.04	x	x		0.391116	1446.04	16.612	1.04045	
%_49	Qgau	1466.54	x	x		0.113508	1466.54	10.7509	1.01522	
%_4	Qgau	1499.81	x	x		0.721518	1499.81	20.3961	1.82659	
%_51	Qgau	1531.29	x	x		0.115961	1531.29	9.31122	1.00006	
%_17	Qgau	1548.13	x	x		0.230385	1548.13	13.0543	0.999854	
%_2	Qgau	1581.71	x	x		0.95351	1581.71	20.8756	1.775	
%_11	Qgau	1638.44	x	x		0.238333	1638.44	46.7953	1.22994	
%_23	Qgau	1701.01	x	x		0.124496	1701.01	29.7112	1.54596	

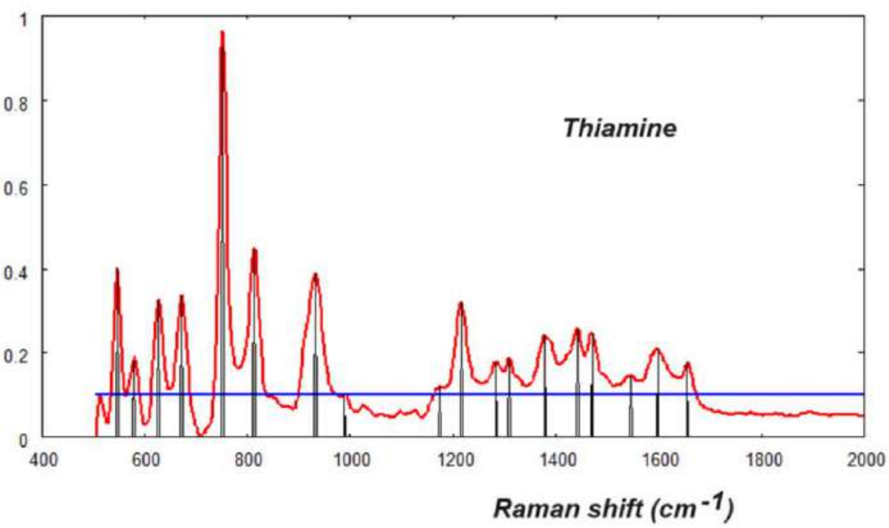
Thiamine



#	PeakType	Center	Parameters			Height	Center	HWHM	q ...
%_19	Qgau	514.651	x	x	x	0.0981844	514.651	6.65867	0.999983
%_22	Qgau	542.196	x	x	x	0.130684	542.196	5.62575	1.00008
%_3	Qgau	548.963	x	x	x	0.395916	548.963	7.31937	1.45626
%_10	Qgau	580.073	x	x	x	0.190877	580.073	12.6792	1.00002
%_6	Qgau	627.386	x	x	x	0.347156	627.386	12.5156	1.04543
%_26	Qgau	651.274	x	x	x	0.0569842	651.274	10.7599	1.3389
%_5	Qgau	673.312	x	x	x	0.357291	673.312	13.0119	1.27956
%_27	Qgau	722.056	x	x	x	0.0159725	722.056	6.54317	1.00002
%_18	Qgau	747.027	x	x	x	0.0567107	747.027	3.08345	1.29763
%_1	Qgau	752.458	x	x	x	1.0079	752.458	9.63899	1.218
%_16	Qgau	778.623	x	x	x	0.144437	778.623	22.0782	1.05659
%_2	Qgau	813.996	x	x	x	0.465423	813.996	12.8653	1.51543
%_21	Qgau	855.565	x	x	x	0.0747697	855.565	19.1588	0.999721
%_29	Qgau	881.733	x	x	x	0.0436283	881.733	11.1736	0.999962
%_12	Qgau	913.484	x	x	x	0.168029	913.484	15.1273	1.12966
%_4	Qgau	935.005	x	x	x	0.341054	935.005	16.0221	1.11645
%_32	Qgau	961.236	x	x	x	0.0815373	961.236	16.7052	2.87961
%_31	Qgau	988.98	x	x	x	0.058477	988.98	16.9669	1.05715
%_30	Qgau	1027.56	x	x	x	0.0375431	1027.56	16.8787	0.999719
%_33	Qgau	1056.85	x	x	x	0.0219195	1056.85	22.9807	3.74143

%_25	Qgau	1101.29	x	x	x	0.0207686	1101.29	32.4881	0.99873
%_34	Qgau	1127.6	x	x	x	0.0163769	1127.6	8.11052	0.999959
%_20	Qgau	1172.02	x	x	x	0.0757417	1172.02	19.3703	0.999456
%_7	Qgau	1216.14	x	x	x	0.294854	1216.14	16.3539	1.38769
%_24	Qgau	1250.71	x	x	x	0.0476886	1250.71	13.972	0.999678
%_14	Qgau	1282.4	x	x	x	0.116689	1282.4	18.3748	1.4764
%_17	Qgau	1311.16	x	x	x	0.104741	1311.16	12.2129	1.78325
%_28	Qgau	1332.49	x	x	x	0.0401341	1332.49	11.9499	1.10426
%_9	Qgau	1380.08	x	x	x	0.163005	1380.08	23.9056	1.27475
%_37	Qgau	1414.41	x	x	x	0.0205421	1414.41	14.1617	1.0032
%_8	Qgau	1441.4	x	x	x	0.201211	1441.4	15.8368	2.93324
%_36	Qgau	1471.65	x	x	x	0.109265	1471.65	9.96138	0.999902
%_35	Qgau	1491.99	x	x	x	0.0516749	1491.99	25.375	3.6521
%_23	Qgau	1542.95	x	x	x	0.056347	1542.95	20.9342	3.96312
%_11	Qgau	1600.1	x	x	x	0.135232	1600.1	25.1752	1.74137
%_15	Qgau	1654.41	x	x	x	0.0646294	1654.41	16.7576	2.20697
%_13	Qgau	1658.36	x	x	x	0.0481326	1658.36	6.77852	1.58572

Thiamine has been investigated in Sparavigna, 2023, with the first derivative spectrum. The following table provides the peaks above a given threshold.



Position (in cm-1)	Relative intensity	Position (in cm-1)	Relative intensity
547.50	0.40	1217.00	0.32
579.50	0.18	1284.00	0.18
627.00	0.33	1309.50	0.18
672.50	0.34	1380.00	0.24
751.00	0.93	1442.00	0.26
813.50	0.45	1470.50	0.25
932.50	0.39	1545.50	0.14
989.50	0.10	1598.00	0.21
1174.50	0.12	1656.00	0.18

Sherman et al. provide the following reference: Leopold et al., 2005.

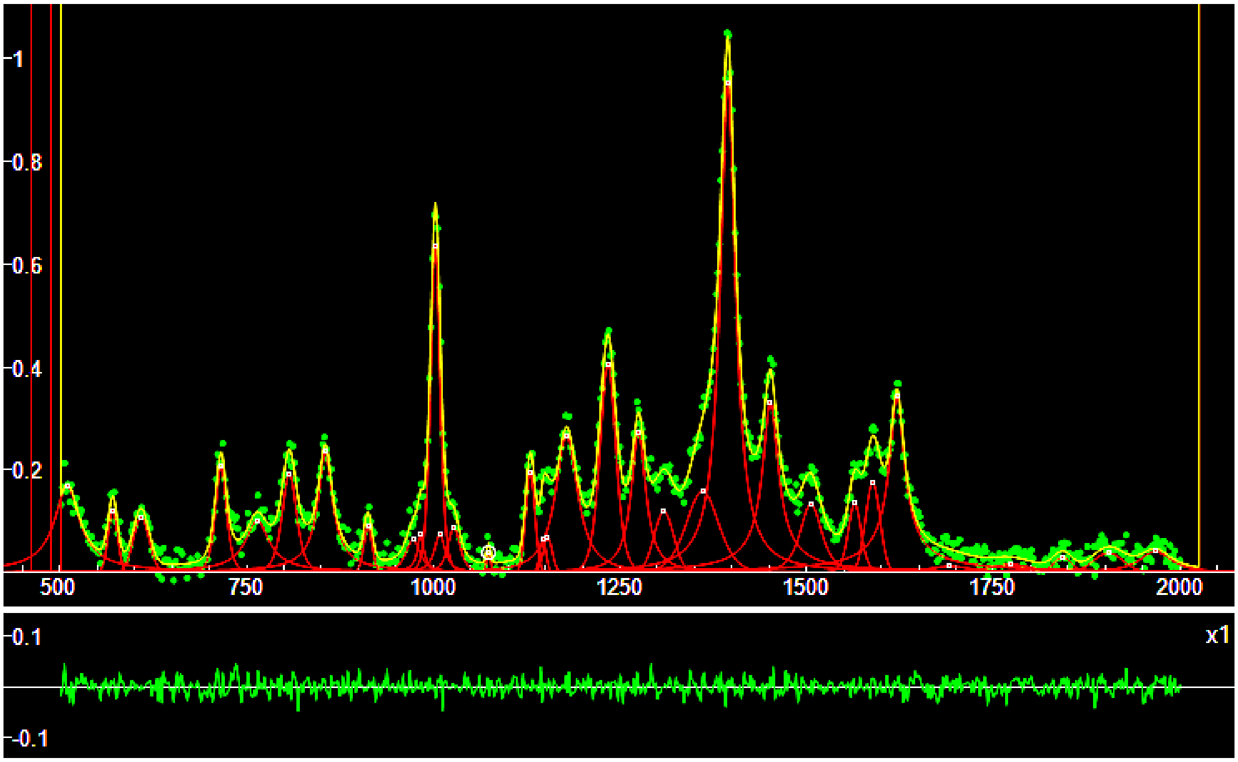
342(m)	408	***515***	***543(m)***	***583(s)***	***632(m)***	667
755(vs)	***778***	*804*	825	***881***	*922*	*942(s)*
1064(m)	*1108(m)*	**1177**	***1229(m)***	***1254(m)***	1297(m)	***1313***
1340(m)	***1380(s)***	1400(s)	***1439***	*1447*	1456	*1484(s)*
1514(m)	*1550*	***1597(s)***	1628	***1657(vs)***	(Raman, pH 4)	

341(m)	417	***512***	***548(m)***	592(m)	639	***678***
760(vs)	***780***	803	826	***878***	921	*941(s)*
1059(m)	*1107(m)*	***1170***	*1210(m)*	1239(m)	***1255(m)***	*1290(m)*
1311	1341	1366	***1375(s)***	1398	***1436***	1442
1450	*1483(s)*	1564	***1603(vs)***	1633	***1654***	(Raman, pH 7)

We have marked in ***bold***, the peaks which are corresponding to the q-Gaussian centers, within +/− 5 cm^{-1}, and in *italic*, within +/− 10 cm^{-1}). Here below, the q-Gaussian centers as obtained from deconvolution.

514.651	542.196	548.963(s)	580.073(m)	627.386(s)	651.274
673.312(s)	722.056	747.027	752.458(vs)	778.623	813.996(s)
855.565	881.733	913.484	935.005(s)	961.236	988.98
1027.56	1056.85	1101.29	1127.6	1172.02	1216.14(s)
1250.71	1282.4	1311.16	1332.49	1380.08(m)	1414.41
1441.4(m)	1471.65	1491.99	1542.95	1600.1(m)	1654.41
1658.36					

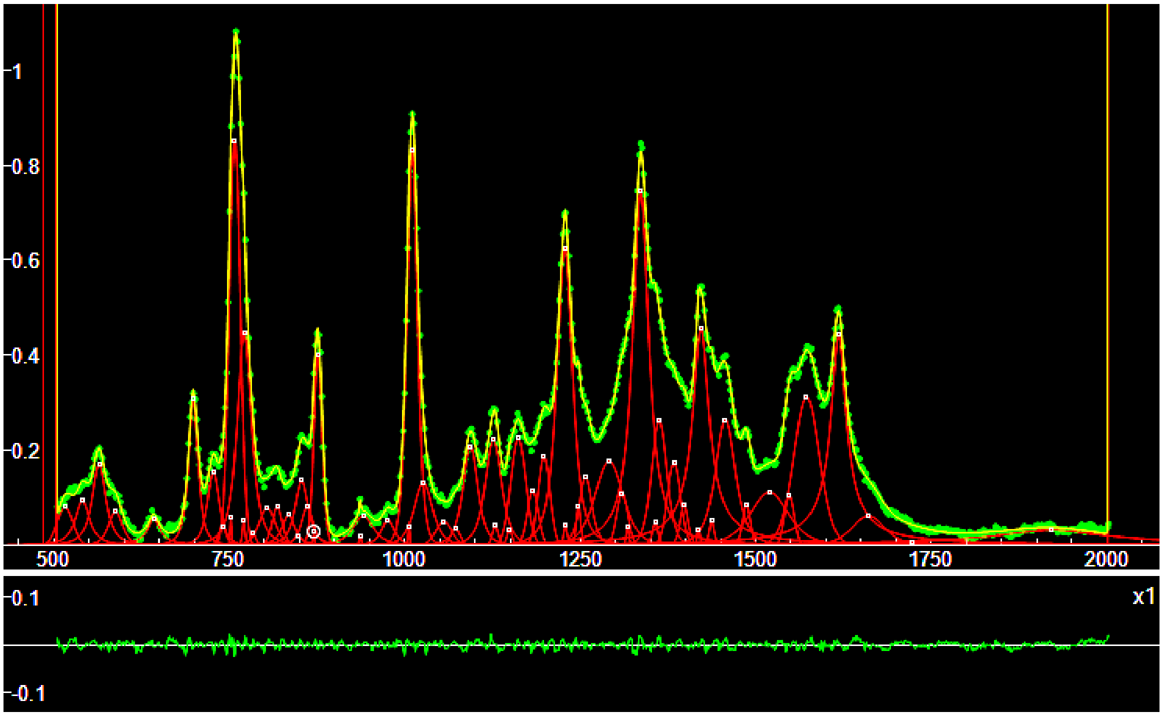
Thyrotropin releasing hormone



#	PeakType	Center		Parameters		Height	Center	HWHM	q (h>0.08)
%_14	Qgau	509.451	x	x	x	0.169585	509.451	20.0768	2.2471
%_16	Qgau	570.5	x	x	x	0.121276	570.5	8.83928	1.04773
%_21	Qgau	608.556	x	x	x	0.107961	608.556	15.0003	0.999888
%_9	**Qgau**	**715.399**	**x**	**x**	**x**	**0.206903**	**715.399**	**9.77513**	**1.41387**
%_17	Qgau	764.035	x	x	x	0.101505	764.035	19.2871	2.24503
%_11	Qgau	807.135	x	x	x	0.192888	807.135	12.7175	1.43095
%_8	**Qgau**	**855.098**	**x**	**x**	**x**	**0.236309**	**855.098**	**11.5824**	**2.3082**
%_20	Qgau	912.464	x	x	x	0.0912671	912.464	7.6276	1.11554
%_2	**Qgau**	**1002.41**	**x**	**x**	**x**	**0.636373**	**1002.41**	**8.37746**	**1.33764**
%_32	Qgau	1027.54	x	x	x	0.0889135	1027.54	10.4485	1.52575
%_13	Qgau	1129.75	x	x	x	0.195296	1129.75	8.65717	0.999969
%_7	**Qgau**	**1178.42**	**x**	**x**	**x**	**0.266843**	**1178.42**	**18.3167**	**1.86749**
%_3	**Qgau**	**1233.8**	**x**	**x**	**x**	**0.406305**	**1233.8**	**14.2879**	**1.27711**
%_6	**Qgau**	**1274.79**	**x**	**x**	**x**	**0.272666**	**1274.79**	**11.7658**	**2.00364**
%_22	Qgau	1308.79	x	x	x	0.119219	1308.79	18.5998	0.999489
%_12	Qgau	1360.45	x	x	x	0.158611	1360.45	29.5975	1.22262
%_1	**Qgau**	**1394.41**	**x**	**x**	**x**	**0.953371**	**1394.41**	**12.3319**	**2.03324**
%_4	**Qgau**	**1451.54**	**x**	**x**	**x**	**0.332646**	**1451.54**	**12.8114**	**2.37118**
%_15	Qgau	1505.72	x	x	x	0.133996	1505.72	18.3823	1.56691
%_19	Qgau	1564.28	x	x	x	0.135086	1564.28	11.6919	1.24706
%_10	Qgau	1588.55	x	x	x	0.175214	1588.55	13.7735	0.99984
%_5	**Qgau**	**1621.05**	**x**	**x**	**x**	**0.345333**	**1621.05**	**12.2902**	**2.52062**

Tryptamine

Literature: Hussain and Pang, 2015.



#	PeakType	Center	Parameters		Height	Center	HWHM	q (h>0.10)
%_16	Qgau	564.333	x	x	0.172682	564.333	11.821	1.79201
%_11	**Qgau**	**698.484**	**x**	**x**	**0.307853**	**698.484**	**8.40896**	**1.66452**
%_22	Qgau	727.198	x	x	0.155806	727.198	10.871	1.54796
%_1	**Qgau**	**757.668**	**x**	**x**	**0.85938**	**757.668**	**10.9925**	**0.999922**
%_14	**Qgau**	**771.24**	**x**	**x**	**0.44952**	**771.24**	**12.6216**	**1.63912**
%_38	Qgau	852.947	x	x	0.137068	852.947	11.8014	1.66714
%_7	**Qgau**	**876.163**	**x**	**x**	**0.404248**	**876.163**	**8.0608**	**1.12587**
%_2	**Qgau**	**1010.33**	**x**	**x**	**0.83245**	**1010.33**	**9.86063**	**1.32082**
%_23	Qgau	1026.16	x	x	0.132476	1026.16	17.0774	1.45389
%_18	**Qgau**	**1093.2**	**x**	**x**	**0.208945**	**1093.2**	**13.5646**	**1.51456**
%_12	**Qgau**	**1126.03**	**x**	**x**	**0.223271**	**1126.03**	**14.9481**	**1.50902**
%_13	**Qgau**	**1161.47**	**x**	**x**	**0.225258**	**1161.47**	**15.0958**	**0.999678**
%_30	Qgau	1182.13	x	x	0.114423	1182.13	11.1471	1
%_19	Qgau	1198.17	x	x	0.187216	1198.17	11.8825	0.999843
%_4	**Qgau**	**1227.66**	**x**	**x**	**0.627591**	**1227.66**	**13.8941**	**1.59592**
%_46	Qgau	1257.33	x	x	0.14357	1257.33	11.8272	1.43074
%_45	Qgau	1290.85	x	x	0.177242	1290.85	26.7959	1.3069
%_44	Qgau	1309.55	x	x	0.109989	1309.55	11.1071	0.999811
%_41	**Qgau**	**1335.94**	**x**	**x**	**0.748472**	**1335.94**	**13.7204**	**1.93957**
%_42	**Qgau**	**1362.27**	**x**	**x**	**0.262833**	**1362.27**	**14.6226**	**1.2566**
%_43	Qgau	1383.28	x	x	0.173901	1383.28	13.1771	0.999785
%_5	**Qgau**	**1421.64**	**x**	**x**	**0.457833**	**1421.64**	**13.9182**	**2.29627**
%_9	**Qgau**	**1456.49**	**x**	**x**	**0.265396**	**1456.49**	**18.2553**	**1.54057**
%_20	Qgau	1519.13	x	x	0.112283	1519.13	35.9609	1.38954
%_24	Qgau	1547.62	x	x	0.105761	1547.62	9.72981	0.999968
%_8	**Qgau**	**1572.25**	**x**	**x**	**0.312963**	**1572.25**	**25.2684**	**1.12261**
%_6	**Qgau**	**1617.77**	**x**	**x**	**0.442489**	**1617.77**	**13.0105**	**2.42514**

The centers of the q-Gaussian components are:

564.333	698.484(m)	727.198	757.668(vs)	771.24(s)	852.947
876.163(s)	1010.33(vs)	1026.16	1093.2	1126.03	1161.47
1182.13	1198.17	1227.66(s)	1257.33	1290.85	1309.55
1335.94(vs)	1362.27(m)	1383.28	1421.64(s)	1456.49(m)	1519.13
1547.62	1572.25(m)	1617.77(s)			

In Hussain and Pang, 2015, in their Fig. 6, we can find data. The figure caption tells: "SERS of (a) tryptophan (TRP) and (b) tryptamine (TMN) with the CT gold colloid, and SERS of (c) TRP, (d) TMN, and (e) 3-indolepropionic acid (IPA) with the BH gold colloid". The same concentration was used for SERS measurements.

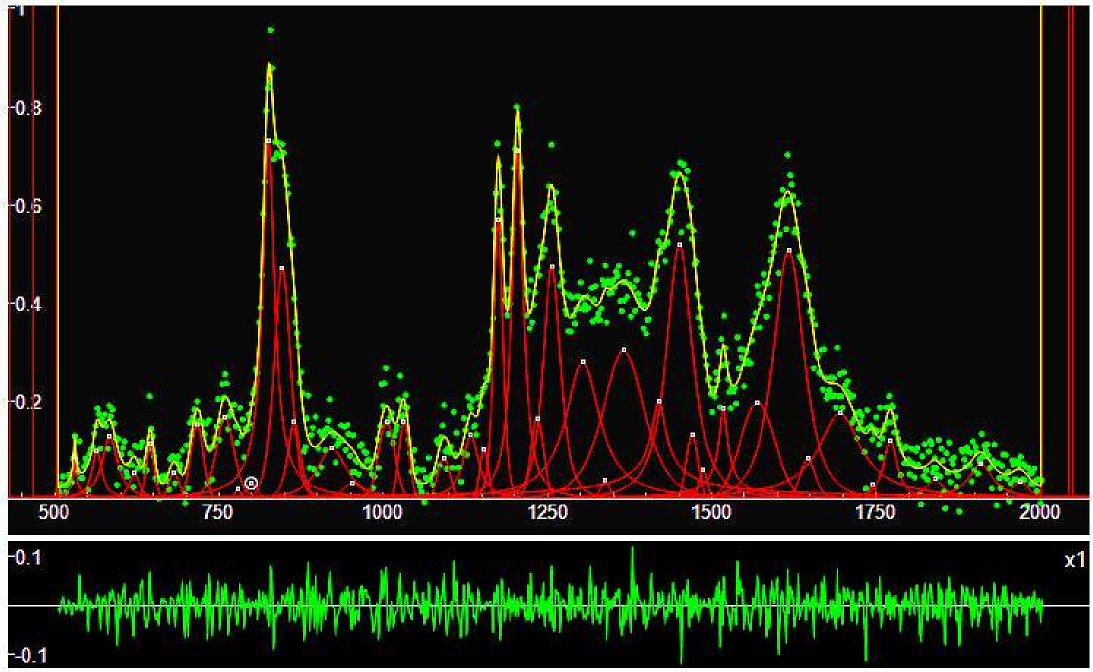
759(m)	***871***	991(m)	*1112*	*1220(m)*	1347(m)
1417(m)	1534(m)	1598(s)			(b, TMN)

711(m)	818	1144(s)	***1259(m)***	*1342(s)*	1434(s)
1534(s)	1600(vs)				(d, TMN)

Bold and *italic* used to guide the comparison.

Tyramine

Literature: Buccolieri et al., 2018, Wang et al., 2018)



#	PeakType	Center	Parameters		Height	Center	HWHM	q (H > 0.10)
%_26	Qgau	530.442	x	x	0.10213	530.442	1.84259	3.4022
%_14	Qgau	563.983	x	x	0.100269	563.983	8.28542	2.25087
%_1	Qgau	583.686	x	x	0.127025	583.686	14.5714	1.99546
%_28	Qgau	645.425	x	x	0.113699	645.425	7.77892	1.31453
%_21	Qgau	716.465	x	x	0.152091	716.465	13.7628	0.999904
%_12	Qgau	758.874	x	x	0.167819	758.874	18.1039	1.34726
%_36	**Qgau**	**825.149**	**x**	**x**	**0.731402**	**825.149**	**10.6879**	**2.16381**
%_8	**Qgau**	**846.23**	**x**	**x**	**0.472515**	**846.23**	**16.6335**	**1.28713**
%_46	Qgau	864.236	x	x	0.158068	864.236	12.447	1.52734
%_17	Qgau	921.784	x	x	0.103437	921.784	28.1791	1.78405
%_11	Qgau	1004.91	x	x	0.158673	1004.91	17.1785	0.999703
%_23	Qgau	1031.47	x	x	0.159879	1031.47	10.9004	0.999884
%_19	Qgau	1133.02	x	x	0.131978	1133.02	14.2528	2.01934
%_27	Qgau	1153.19	x	x	0.102969	1153.19	8.86784	0.999902
%_6	**Qgau**	**1174.84**	**x**	**x**	**0.570733**	**1174.84**	**9.21034**	**1.38342**
%_2	**Qgau**	**1204.34**	**x**	**x**	**0.708924**	**1204.34**	**10.4567**	**1.92392**
%_13	Qgau	1234.15	x	x	0.164892	1234.15	13.8575	0.999674
%_3	**Qgau**	**1256.39**	**x**	**x**	**0.476833**	**1256.39**	**16.8452**	**1.55883**
%_15	**Qgau**	**1303.53**	**x**	**x**	**0.279396**	**1303.53**	**31.4566**	**2.01095**
%_32	**Qgau**	**1365.77**	**x**	**x**	**0.302625**	**1365.77**	**41.7873**	**1.43511**
%_33	**Qgau**	**1419.15**	**x**	**x**	**0.200111**	**1419.15**	**14.1194**	**3.3823**
%_5	**Qgau**	**1450.71**	**x**	**x**	**0.517782**	**1450.71**	**24.815**	**1.71351**
%_34	Qgau	1470.14	x	x	0.131468	1470.14	12.515	0.999855
%_16	Qgau	1517.36	x	x	0.184965	1517.36	8.5515	2.77753
%_9	Qgau	1569.62	x	x	0.197798	1569.62	36.7295	0.998817
%_4	**Qgau**	**1616.88**	**x**	**x**	**0.506827**	**1616.88**	**30.1246**	**1.53338**
%_10	Qgau	1694.91	x	x	0.175337	1694.91	38.6235	2.17556
%_20	Qgau	1771.85	x	x	0.119136	1771.85	12.5948	1.94615

Therefore, the q-Gaussian centers (h>0.15) are:

716.465	758.874	825.149(vs)	846.23(s)	864.236
1004.91	1031.47	1174.84(s)	1204.34(vs)	1234.15
1256.39(s)	1303.53(m)	1365.77(m)	1419.15	1450.71(s)
1517.36	1569.62	1616.88(s)	1694.91	

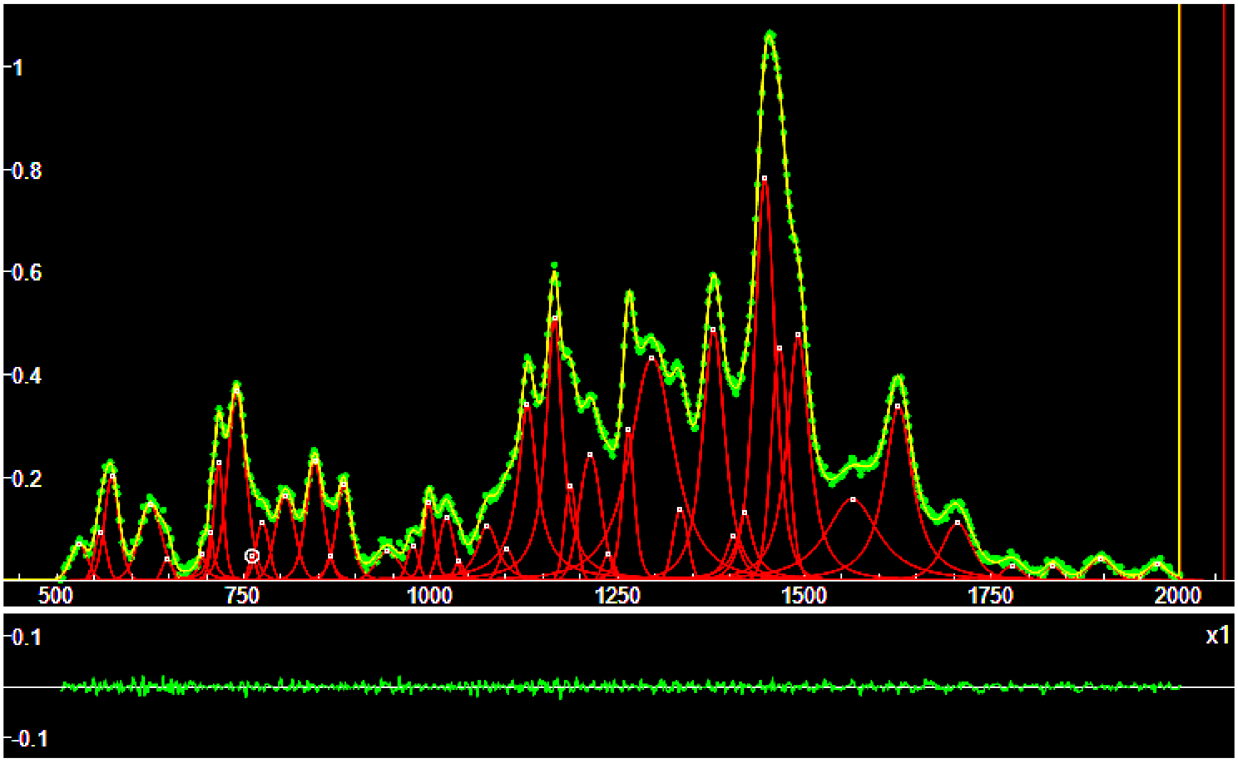
In Wang et al., we can find data in their Fig.2. The figure caption tells: "AgNPs mediated SERS responses of Tyr bands after derivatization at the presence of different salts, excited by 532 (A), 633 (B) and 785 (C) nm lasers, respectively". Then let us use the values of the Raman shift given in this figure.

667(m)	*815(vs)*	1215(s)	1548(s)	1613(m)	(A)
770(m)	*834(vs)*	1046(m)	*1187(s)*	*1214(vs)*	
1243(s)	***1453(m)***	***1621(m)***	1645(m)		(B)
649(s)	*764(m)*	***830(s)***	***1006(m)***	1108(m)	
1211(m)	1262				(C)

Again, in bold within +/−5 cm^{-1}, in italic within +/−10 cm^{-1}.

Vitamin B12

Literature: Radu et al., 2016, Zhang et al., 2009.



#	PeakType	Center		Parameters		Height	Center	HWHM	q ...
%_28	Qgau	529.825	x	x	x	0.0714747	529.825	15.8532	1.04531
%_38	Qgau	558.372	x	x	x	0.0952555	558.372	11.2125	1.00013
%_13	Qgau	573.28	x	x	x	0.203419	573.28	13.047	1.21121
%_20	Qgau	625.083	x	x	x	0.14817	625.083	20.9654	1.15306
%_29	Qgau	647.422	x	x	x	0.0415624	647.422	9.63803	1.00012
%_45	Qgau	694.683	x	x	x	0.0521468	694.683	4.64109	2.90725
%_34	Qgau	705.993	x	x	x	0.0955493	705.993	4.37714	2.55202
%_15	Qgau	716.242	x	x	x	0.228502	716.242	8.60174	1.3029
%_9	**Qgau**	**740.383**	**x**	**x**	**x**	**0.368613**	**740.383**	**16.481**	**1.27377**
%_41	Qgau	761.257	x	x	x	0.0483728	761.257	7.12263	1.00095
%_36	Qgau	775.037	x	x	x	0.1144	775.037	12.3865	1.0001
%_21	Qgau	805.186	x	x	x	0.165116	805.186	18.3794	1.07195
%_12	Qgau	844.681	x	x	x	0.23305	844.681	14.9289	1.34732
%_46	Qgau	865.36	x	x	x	0.0473498	865.36	7.1077	1.51564
%_18	Qgau	883.559	x	x	x	0.186477	883.559	12.7702	1.49984
%_27	Qgau	942.221	x	x	x	0.0576988	942.221	22.7553	0.999539
%_32	Qgau	975.896	x	x	x	0.0691548	975.896	10.9884	0.999919
%_19	Qgau	997.508	x	x	x	0.151457	997.508	9.74574	1.35655
%_25	Qgau	1020.85	x	x	x	0.123601	1020.85	13.8814	1.09805
%_44	Qgau	1037.65	x	x	x	0.0396675	1037.65	8.41204	1.17912

%_24	Qgau	1075.93	x	x	x	0.10844	1075.93	17.129	1.81601
%_39	Qgau	1101.34	x	x	x	0.0617912	1101.34	13.957	0.999878
%_7	**Qgau**	**1129.37**	**x**	**x**	**x**	**0.343905**	**1129.37**	**14.8124**	**2.21726**
%_2	**Qgau**	**1165.13**	**x**	**x**	**x**	**0.513594**	**1165.13**	**13.0329**	**2.0495**
%_10	Qgau	1186.97	x	x	x	0.185994	1186.97	11.4388	0.999907
%_17	Qgau	1213.28	x	x	x	0.244906	1213.28	20.3585	0.999423
%_30	Qgau	1237.85	x	x	x	0.0527564	1237.85	11.1325	0.99996
%_4	Qgau	1264.12	x	x	x	0.29286	1264.12	10.0595	1.5034
%_5	**Qgau**	**1295.97**	**x**	**x**	**x**	**0.434188**	**1295.97**	**37.2735**	**1.65659**
%_16	Qgau	1333.95	x	x	x	0.139905	1333.95	13.7307	0.999965
%_3	**Qgau**	**1378.29**	**x**	**x**	**x**	**0.488688**	**1378.29**	**18.6686**	**1.65704**
%_22	Qgau	1404.8	x	x	x	0.0867957	1404.8	13.0301	1.95863
%_33	Qgau	1420.02	x	x	x	0.133195	1420.02	12.5208	2.29538
%_1	**Qgau**	**1446.75**	**x**	**x**	**x**	**0.78199**	**1446.75**	**17.8931**	**1.4098**
%_26	**Qgau**	**1466.7**	**x**	**x**	**x**	**0.453422**	**1466.7**	**15.5772**	**1.14397**
%_6	**Qgau**	**1491.36**	**x**	**x**	**x**	**0.477513**	**1491.36**	**18.096**	**1.83906**
%_14	Qgau	1563.62	x	x	x	0.15996	1563.62	42.9472	1.82076
%_8	**Qgau**	**1625.68**	**x**	**x**	**x**	**0.338702**	**1625.68**	**22.7747**	**1.91937**
%_23	Qgau	1704.07	x	x	x	0.112433	1704.07	26.2109	1.4487
%_37	Qgau	1778.03	x	x	x	0.02948	1778.03	18.9254	1.13484
%_42	Qgau	1832.34	x	x	x	0.029044	1832.34	14.8205	1.06322
%_31	Qgau	1896.11	x	x	x	0.0424228	1896.11	21.5254	1.30385
%_35	Qgau	1971.5	x	x	x	0.0334599	1971.5	16.4355	1.64012

In **bold**, h > 0.3

In Radu et al., 2016, Fig. 2, we can find the pH dependence of the SERS signal of B2 and B12. For B12, we can find reported peaks at 1270, 1495 and 1580 cm^{-1}. In the Fig.3 of Radu et al., the "fingerprints" of B2 and B12 are given.

The q-Gaussian centers are (for h>0.1):

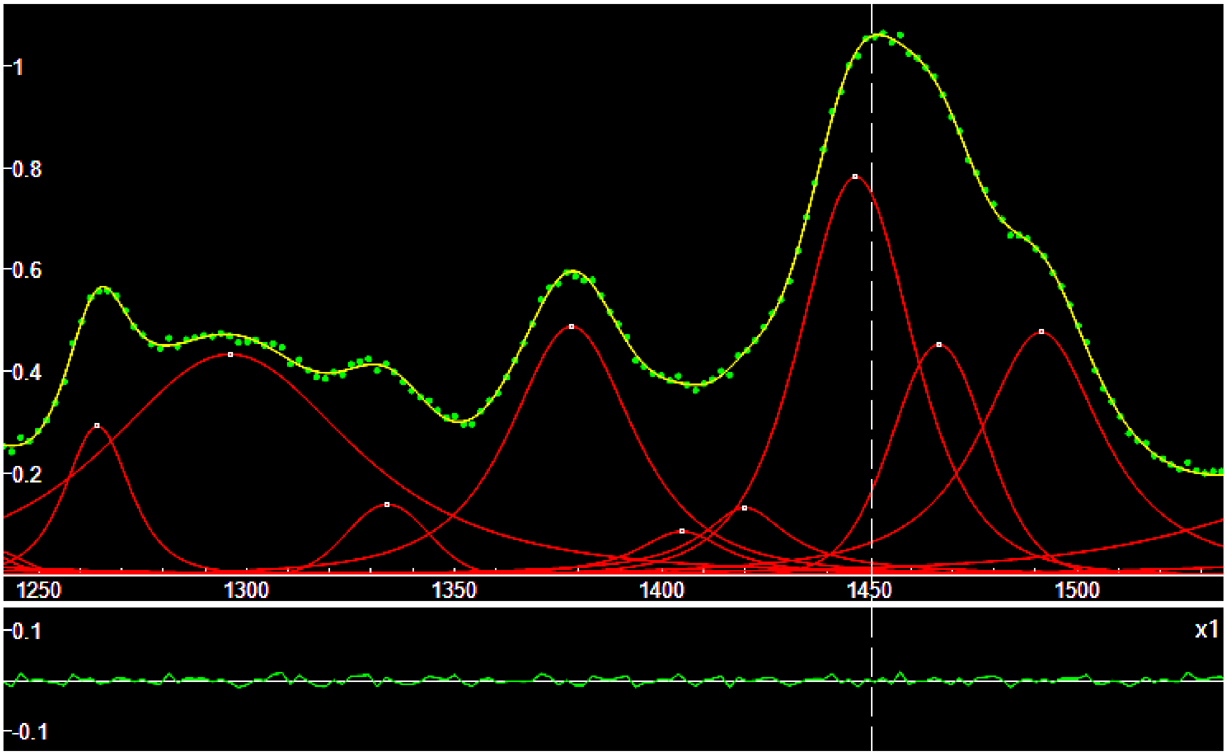
573.28	625.083	716.242	740.383(m)	775.037	805.186
844.681(m)	883.559	997.508	1020.85	1075.93	1129.37(m)
1165.13(s)	1186.97	1213.28(m)	1264.12(m)	1295.97(s)	1333.95
1378.29(s)	1420.02	1446.75(vs)	1466.7(s)	1491.36(s)	1563.62
1625.68(m)	1704.07				

In Zhang et al., 2009, we find Raman and SERS data, and compare (in ***bold***, the peaks which are corresponding to q-Gaussian centers given above, within +/− 5 cm^{-1}, in *italic*, within +/− 10 cm^{-1}):

320	457	481	587	*633*	*726(m)*
841	***882***	***1163(s)***	*1206(m)*	1350(s)	1394(m)
1454(m)	*1498(vs)*	1602(m)			(Raman)

383	611	***716***	1008(m)	1052	1159
1239(m)	***1337***	1395(s)	***1493(s)***	1601	(SERS, Ag sol)

272	310(m)	452(m)	496(m)	608	672(vs)
732	**848**	949	1006	1060	*1140*
1170(s)	1224	1258	1356(m)	1400	*1473(m)*
1507(vs)	1595(s)				(SERS, Ag)



A detail of the spectrum given before.

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