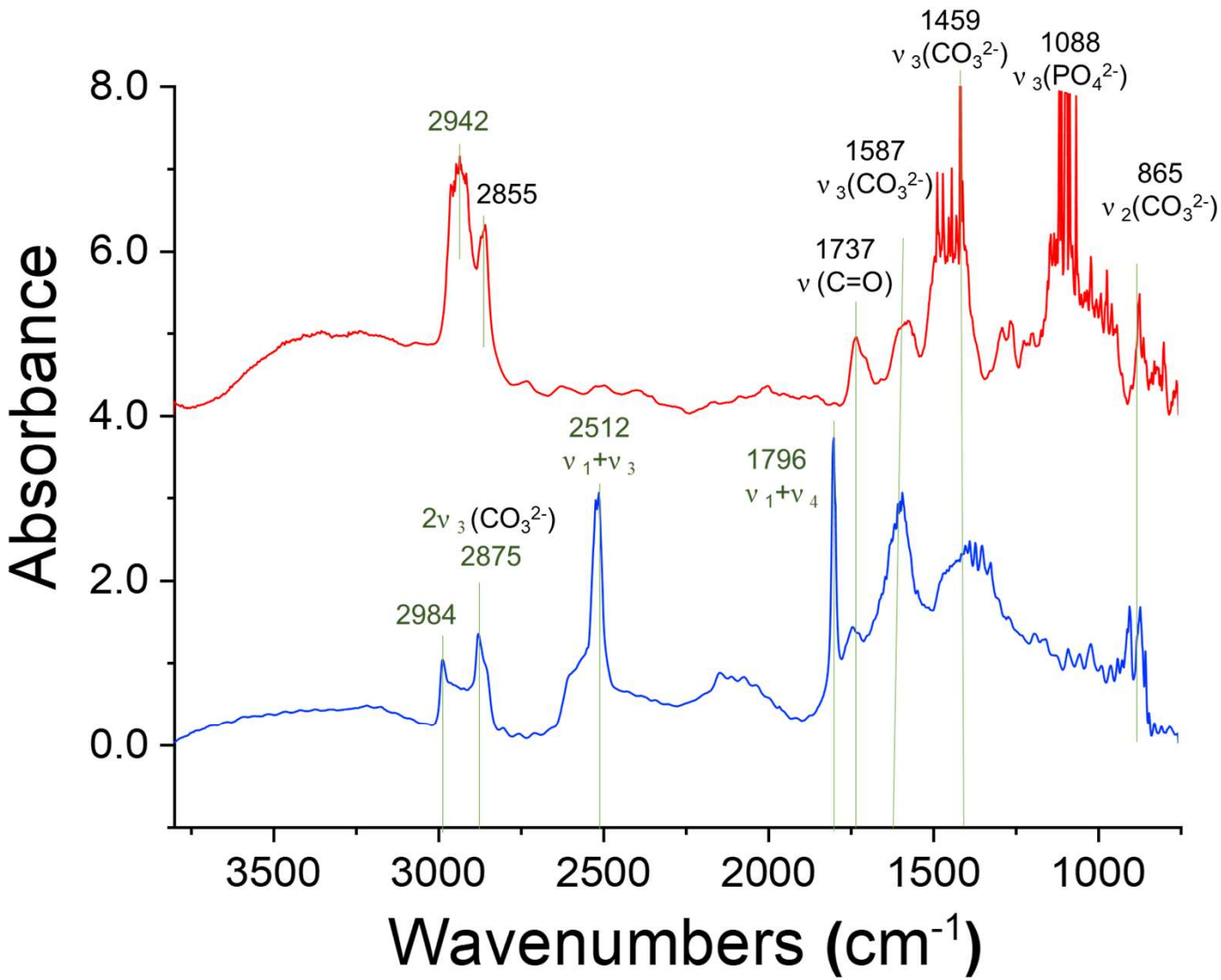
Calcite and Hydrocarbon Remain



Bone Matrix	Skin	Assignments
Wavenumbe (cm^{-1})		
865	-	$\nu_2(CO_3^{2-})$
875		$\nu_2(CO_3^{2-})$
966	-	$\nu_1(PO_4^{3-})$, Bone matrix
1012	-	$\nu_{3c}(PO_4^{3-})$, Bone matrix
1035	1037	
1051	-	$\nu_{3a}(PO_4^{3-})$, Bone matrix
-	1077	
1088	-	$\nu_3(PO_4^{3-})$, Bone matrix
1095	-	
1124	1107	$\nu_3(PO_4^{3-})$, Bone matrix
1262	1259	
1278	-	
1286	1281	Nitrogen-containing Compound
1292	-	
1433	1448	$\nu_3(CO_3^{2-})$
1457	1452	Amorphous calcium carbonate (ACC)
1555	-	Coupling of CNH stretching and NH being, Amide II, Protein
1587	-	$\nu_3(CO_3^{2-})$
1651		ν C=O, Amide I, Protein
1727		ν_s (C=O)
1736	-	ν_s (C=O)
1796		$\nu_1+\nu_4(CO_3^{2-})$, Calcite
2512	2516	$\nu_1+\nu_3(CO_3^{2-})$, Calcite
2856	2861	ν_s CH_2,Hydrocarbon remain
2870	2875	$2\nu_1(CO_3^{2-})$, Calcite
2927	2930	ν_{as} CH_2,Hydrocarbon remain
2960	2968	ν_{as} CH_3,Hydrocarbon remain
2984	-	(CO_3^{2-}), Calcite
3291		ν NH, Amide A, Protein
3676	3682	ν OH bone matrix

Table 1. Band assignment

Liver / Peak	Control	White LED	Blue LED	Assignments
	Wavenumber (cm^{-1})			
1	1035	1034	1035	δC-O-C (bending of Carbohydrate)
2	1081	1080	1081	δC-O-C (bending of Carbohydrate), $\nu_s PO_2^-$ (PO_2^- symmetric stretching vibration of DNA)
3	1154	1154	1155	δC-O-H (bending of Carbohydrate)
4	1240	1237	1238	$\nu_{as} PO_2^-$ (PO_2^- antisymmetric stretching vibration of DNA)
5	1399	1396	1396	δ COO^-, δ CH_3 (COO^-, CH_3 antisymmetric bending, lipids and proteins)
6	1451	1453	1453	δ CH_2 (CH_2 antisymmetric bending, lipids and proteins)
7	1542	1540	1541	Amide II (vibration motion coupled C-N stretching vibration and C-N-H bending vibration)
8	1654	1651	1651	Amide I (C=O stretching vibration, proteins)
9	2850	2852	2852	$\nu_s CH_2$ (CH_2 symmetric stretching vibration, dominant contribution from lipids)
10	2874	2876	2873	$\nu_s CH_3$ (CH_3 symmetric stretching vibration, dominant contribution from proteins)
11	2926	2927	2926	$\nu_{as} CH_2$ (CH_2 antisymmetric stretching vibration, dominant contribution from lipids)
12	2959	2960	2959	$\nu_{as} CH_3$ (CH_3 antisymmetric stretching vibration, dominant contribution from proteins)
13	3072	3066	3065	Amide B (overtone of amide II)
14	3293	3293	3286	Amide A (N-H stretching vibration)

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The amide III absorption between 1340 and 1300 cm^{-1} corresponds to α-helix structure;

The amide III absorption between 1290 and 1260 cm^{-1} corresponds to unordered structure;

The amide III absorption between 1250 and 1220 cm^{-1} corresponds to the β-sheet structure.

1. Singh, Bal Ram *et.al.*, SPIE. 1890, 47, 1993 10.1117/12.145242.

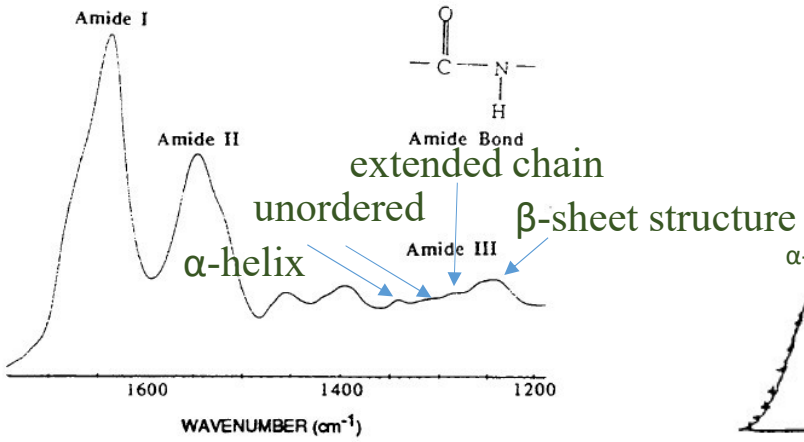


Figure 1. FT-IR spectrum of α-chymotrypsin showing amide I, amide II and amide III spectral region
Amide I 1600-1700 cm^{-1} : C=O stretch weakly coupled with C-N stretch and N-H bending.
Amide II 1500-1600 cm^{-1} : C-N stretch strongly coupled with N-H bending.
Amide III 1200-1350 cm^{-1} : N-H in plane bending coupled with C-N stretching; also C-H a deformation vibrations.

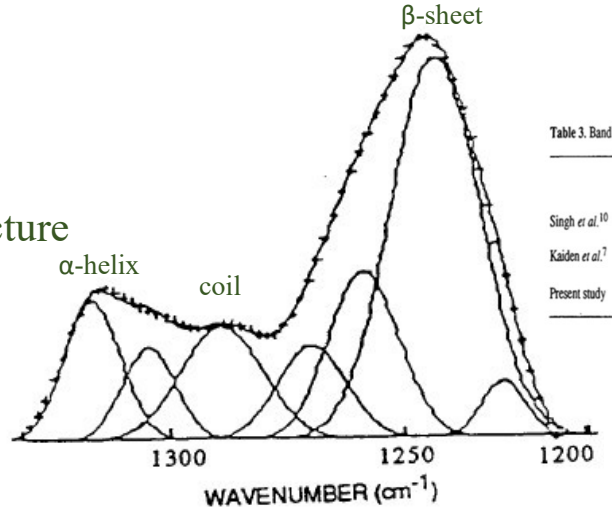
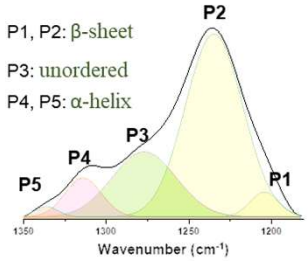


Figure 5. Amide III curve-fitted spectrum of type A botulinum neurotoxin.

Table 3. Band assignments for Amide III frequencies.

	α-helix	β-sheet	random coil
Singh *et al.*[10]	1317 - 1280 cm^{-1}	1245 - 1230 cm^{-1}	1271 - 1245 cm^{-1}
Kaiden *et al.*[7]	1300 - 1250 cm^{-1}	1240 - 1230 cm^{-1}	1270 - 1240 cm^{-1}
Present study	1320 - 1295 cm^{-1}	1255 - 1225 cm^{-1}	1294 - 1255 cm^{-1}



The amide III mode of a protein is the in-phase combination of the C-N-H bending and the C-N stretching vibration with small contributions from the C=O in-plane bending and the C-C stretching vibration

3. Kai Griebenow *et.al.*, Proc. Natl. Acad. Sci. USA, 92, 10969-10976, 1995

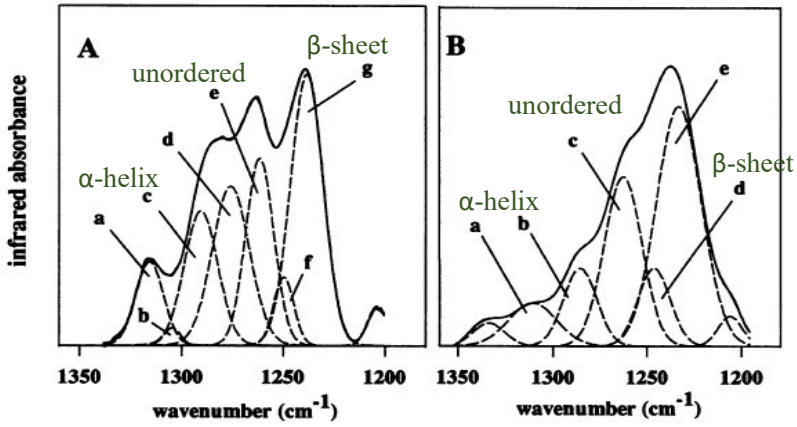


FIG. 2. FTIR spectra of BPTI in aqueous solution at pH 3.5 (*A*) and the powder lyophilized from that solution (*B*) after the Gaussian curve-fitting process. The results of the added Gaussian bands and the original spectra (solid lines) are superimposed and are nearly identical. The area of the individual Gaussian bands (broken lines) has been used to calculate the secondary structure content. The individual bands were assigned as follows: (*A*) a, b, and c, α-helix; d and e, unordered; f and g, β-sheet; (*B*) a, α-helix; b and c, unordered; d and e, β-sheet. The bands at ≈1205 cm^{-1} are not an amide III vibration (21) and are presented solely for the fit. The band at around 1340 cm^{-1} in the spectrum of the powder (*B*), which is of an unknown origin and not found in the BPTI spectrum in aqueous solution, was not assigned to any secondary structural element.

3. Results and discussion

The amide III mode of a protein is the in-phase combination of the N-H bending and the C-N stretching vibration with small contributions from the C=O in plane bending and the C-C stretching vibration [5]. Like amide I mode, different protein secondary structures have different amide III absorptions. Based on the general assignments made by Griebenow and Klibanov, an amide III absorption between 1320 and 1300 cm^{-1} corresponds to α-helix structure; an amide III absorption between 1280 and 1260 cm^{-1} corresponds to unordered structure; an amide III absorption between 1250 and 1240 cm^{-1} corresponds to extended chain; an amide III between 1240 and 1220 cm^{-1} corresponds to β-sheet structure [8].

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peak resolve 光譜指派@ Amide III