

Supplementary Materials

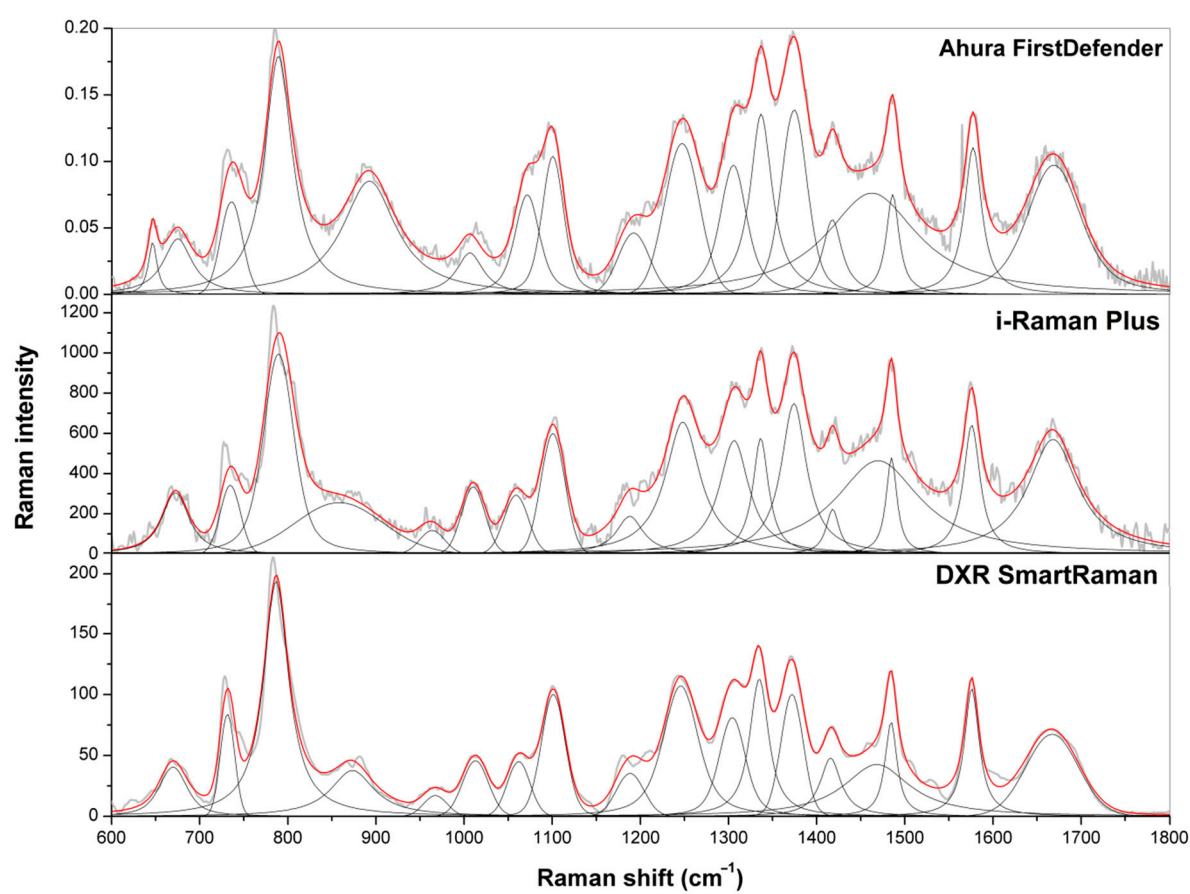


Figure S1. Peak decomposition of the Raman spectra of calf thymus DNA obtained with handheld (top), modular (middle), and laboratory (bottom) instruments.

Table S1. Raman band assignments for the reference compounds [29–34,36–39,41,42].

Reference compound	Instrument/Raman shift (cm ⁻¹)*			Vibrational mode	Moiety
	Ahura	i-Raman Plus	SmartRaman		
Calf Thymus DNA	1662	1664	1663	$\nu(\text{C=O})$	C, T
	1577	1574	1576	$\nu(\text{C=C})$	A, G
	1530	1529	1528	$\nu(\text{C=N})$	C
	sh	sh	1504	$\delta(\text{NH}_2)$, ring	A
	1485	1482	1484	ring	G, A
	sh	sh	1462	$\delta(5'\text{CH}_2)$	dRib
	1419	1416	1418	$\delta(2'\text{CH}_2)$	dRib
	1372	1370	1371	ring, $\delta_s(\text{CH}_3)$	T, A, C
	1335	1332	1334	$\nu(\text{C=N})$	A, G
	1306	1306	1310	ring	A, C
	1242	1241	1242	ring	C, T
	1209	1205	1207	ring	C, T
	1182	1179	1179	ring	G, T, C
	1099	1100	1100	$\nu_s(\text{PO}_2^-)$	P
	sh	1060	1066	$\nu(\text{C-O})$	dRib
	1013	1010	1009	ring, $\nu(\text{C-O})$	T, G, C, dRib
	962	956	967	$\nu(\text{C-O})$	dRib
	890	876	881, 867	$\nu(\text{C-O})$	dRib-P
	786	781	783	ring breath	T, C
	sh	sh	744	ring breath	T
	733	728	728	ring breath	A
	670	671	667	ring breath	G
Human Serum Albumin (HSA)	1659	1655	1655	amide I	backbone
	1615	1618	1615	$\nu(\text{C=C})$	Tyr, Trp, Phe
	1606	1605	1606	$\nu(\text{C=C})$	Tyr, Trp, Phe
	1584	1584	1585	$\nu(\text{C=C})$	Phe, Trp
	1451	1449	1449	$\delta(\text{CH}_2)$, $\delta_{as}(\text{CH}_3)$	side chains
	1340	1339	1337	$\delta(\text{C}_\alpha\text{-H})$	backbone, Trp
	sh	1319	1317	$\tau(\text{CH}_2)$	side chains
	sh	1275	1270	amide III	CONH
	1209	1209	1208	$\delta(\text{C-H})$	Phe, Tyr
	1171	1178	1174	$\delta(\text{C-H})$	Tyr
	1157	1161	1158	$\nu(\text{C-C})$, $\nu(\text{C-N})$	backbone
	1124	1126	1126	$\nu(\text{C-C})$, $\nu(\text{C-N})$	Trp
	1103	1104	1102	$\nu(\text{C-C})$, $\nu(\text{C-N})$	backbone
	1075	1083	1081	$\nu(\text{C-C})$, $\nu(\text{C-N})$	backbone
	sh	1056	1053	$\nu(\text{C-C})$, $\nu(\text{C-N})$	backbone
	1032	1032	1032	ring	Phe
	1004	1003	1003	ring breath	Phe
	960	960	960	$\nu(\text{C-C})$	Trp, Val
	940	938	939	$\nu(\text{C-C})$	backbone
	900	894	894	$\nu(\text{C-C})$	backbone
	854	851	866,851	ring	Trp, Tyr
	828	827	827	ring breath	Tyr
	749	744	744	$\rho(\text{CH}_2)$	side chains, Trp
	672	667	667	$\nu(\text{C-S})$	Cys
	647	644	644	ring	Tyr
	623	622	622	ring	Phe

Reference compound	Instrument/Raman shift (cm ⁻¹)			Vibrational mode	Moiety
	Ahura	i-Raman Plus	SmartRaman		
Rat Tail Collagen Type I	1672br	1672	1676	amide I	backbone
		1604	1605	$\nu_{as}(\text{CO}_2^-)$	Asp, Glu
	1556	1553	1556	indole ring	Trp
	1453	1449	1449	$\nu(\text{C}=\text{N})$, $\delta(\text{CH}_2)$	backbone, Pro, Hyp
	1342	1342	1331	$\omega(\text{CH}_2)$, $\omega(\text{CH}_3)$	Pro, Ala
		1320	1308	$\tau(\text{CH}_3)$	side chains
	1268	1270	1268	amide III, $\omega(\text{CH}_2)$	backbone, Pro, Hyp
	1246	1245	1239	amide III	backbone
	1216	1207	1214	ω , $\tau(\text{CH}_2)$	Pro
	1195	1181	1178	$\omega(\text{CH}_2)$, $\rho(\text{CH}_3)$	Pro, Ala
	1097	1101	1097	$\rho(\text{CH}_2)$	Pro
	1066	1062	1067	$\omega(\text{CH}_2)$, $\nu(\text{CN})$	Pro, Hyp
	1032	1032	1033	ring breath	Pro, Phe
	1002	1003	1004	ring breath	Pro, Phe
	sh	sh	976	$\nu(\text{C}-\text{C})$	backbone
	948	936	939	$\nu(\text{C}-\text{C})$	backbone
	925	921	920	ring	Pro
	sh	872	881	ring	Hyp
	862	854	867	ring	Pro
	816	818	816	$\nu(\text{C}-\text{C})$	backbone
	790	779	788	$\nu(\text{C}-\text{C})$	backbone
Bacterial Sodium Hyaluronate	1656	1655	1652	amide I	N-Ac
	sh	1455	1456	$\delta(\text{CH}_2)$, $\delta_{as}(\text{CH}_3)$	GlcNAc
	1410	1410	1410	$\nu_s(\text{CO}_2^-)$	GlcA
	1371	1376	1374	$\delta_s(\text{CH}_3)$	N-Ac
	sh	sh	1328	amide III, $\delta(\text{C}-\text{H})$, $\delta(\text{C}-\text{OH})$	N-Ac
	1273	1269	1269	$\omega(\text{CH}_2)$, $\delta(\text{C}-\text{CH})$,	GlcNAc, ring
	1209	1206	1206	$\tau(\text{CH}_2)$, $\delta(\text{C}-\text{CH})$, $\delta(\text{C}-\text{OH})$	GlcNAc, ring
	1124	1124	1125	$\nu(\text{C}-\text{O})$, $\nu(\text{C}-\text{C})$, $\delta(\text{C}-\text{OH})$	pyranoid ring
	1084	1002	1097	$\nu_{as}(\text{C}-\text{O}-\text{C})$	glycosidic bond
	sh	1045	1048	$\nu(\text{C}-\text{O})$, $\nu(\text{C}-\text{C})$, $\delta(\text{C}-\text{OH})$	pyranoid ring
	948	947	947	amide V	N-Ac
	900	897	896	$\nu_s(\text{C}-\text{O}-\text{C})$, $\delta(\text{C1}-\text{H})$	glycosidic bond
	804	810	807	$\delta(\text{CO}_2^-)$	GlcA

* br, broad; sh, shoulder; ν , stretching; δ , bending; τ , twisting; ω , wagging; A, G, C, and T, nucleic bases; P, phosphate diester, dRib, deoxyribose.

Table S2. Contribution of biological macromolecules in the Raman spectra of normal colon tissue [43–46,50–53].

Instrument/Raman shift (cm ⁻¹)*			Reference compounds			
Ahura	i-Raman Plus	SmartRaman	DNA	HSA	Collagen I	HA
1656	1657	1657		+		+
	sh	1636sh			+	
sh	1617	1617		+		
sh	1580	1582	+			
1553	1558	1569, 1553			+	
1531	sh	1540, 1520				
	sh	1486sh	+			
1446	1447	1446		+		
1395	sh	1396		+	+	
	1381	1381			+	
sh	sh	1363				+
1340	1339	1335		+	+	
	1320	1314	+			+
1304	1301	1303				
1267	1271	1267		+	+	+
	1262	1257		+		
		1245sh	+		+	
	1207	1209	+	+		+
	1175	1175	+	+	+	
1157	sh	1159, 1150				
	1125	1124		+		+
	1106	sh	+	+		+
1075	1086	1082			+	
	1065	1068	+			+
sh	1032	1034		+		
1005	1002	1004		+	+	
973	981	974	+		+	
	958	960		+		+
		940		+	+	
929	934	930			+	
	907	sh				+
882	874	880	+		+	
		865	+		+	+
854	853	851		+		
	832	832		+		
818		823			+	+
		801				
790	785	786	+		+	
		773				
	761	760			+	
751		744	+	+		+
	sh	726	+			
713	714	713				
680	695	694			+	
	673	666	+	+		
649	646	646		+	+	
615	622	622		+	+	