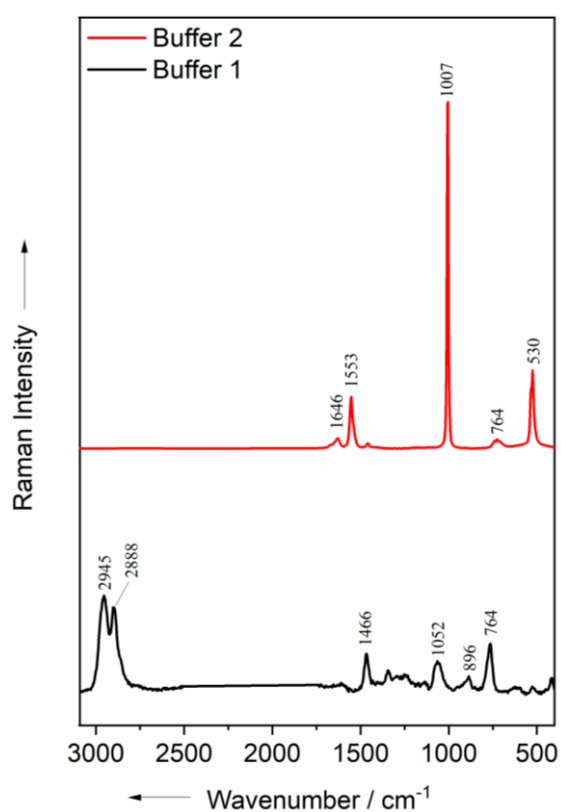


## Supplementary Materials Raman Stable Isotope Probing of Bacteria in Visible and Deep UV-Ranges



**Figure S1.** Mean Raman spectra of DNA extraction buffers.

**Table S1.** Red-shifts in the Raman bands of bacteria labeled with various isotopes. (/): new band red-shift observed in this work; no previous reference.

532 nm					
Isotope	Raman band of unlabeled cells / cm <sup>-1</sup>	Raman band of red-shift / cm <sup>-1</sup>	Extent of Raman shift / cm <sup>-1</sup>	Tentative assignement (Assignment from literature)	Reference for red-shift
D	2936	2172	764	C–H stretching vibration of all biomolecules [1]	[2]
<sup>18</sup> O	1667	1656	11	C=O stretching vibration of amide I (1663 cm <sup>-1</sup> ) [1,3]	[3-5]
<sup>13</sup> C		1628	39		
<sup>15</sup> N	1574	1565	9	C=N stretching vibration of guanine and adenine (1577 cm <sup>-1</sup> ) [6]	[3,5]
<sup>13</sup> C	1244	1236	8	C–N stretching vibration of amide III (1241 cm <sup>-1</sup> ) [7]	[3,5]
<sup>15</sup> N		1232	12		
<sup>13</sup> C	1007	962	39	Phe ring breathing (1007 cm <sup>-1</sup> ) [3,8,9]	[3,5]
D		962	39		
<sup>15</sup> N	728	713	12	Ring breathing of adenine (723 cm <sup>-1</sup> ) [3]	[3,5]
D	479	449	30	Adenine (473 cm <sup>-1</sup> )	/
244 nm					
Isotope	Raman band of unlabeled cells / cm <sup>-1</sup>	Raman band of red-shift / cm <sup>-1</sup>	Extent of Raman shift / cm <sup>-1</sup>	Tentative assignement (Assignment from literature)	Reference for red-shift
<sup>13</sup> C	1618	1564	54	C=C stretching vibration of Tyr, Trp, and Phe (1609 cm <sup>-1</sup> ) [10]	/
<sup>13</sup> C	1576	1563	13	C=C and C=N stretching vibrations of guanine and adenine (1578 cm <sup>-1</sup> ) [10,11]	/
<sup>15</sup> N		1563	13		
<sup>15</sup> N	1534	1521	13	Cytosine (1533 cm <sup>-1</sup> ) [12]	/
<sup>13</sup> C	1485	1455	30	N9C8 and C8N7 stretching vibrations along the long axis of purine bases (1485 cm <sup>-1</sup> ) [13,14]	/
<sup>15</sup> N		1470	15		
<sup>13</sup> C	1420	1384	36	CH <sub>2</sub> -deformation vibration of Adenine (1420 cm <sup>-1</sup> ) [15,16]	/
<sup>15</sup> N		1405	15		
<sup>13</sup> C	1334	1314	20	C–N stretching vibration of guanine, adenine, and tryptophan (1334 cm <sup>-1</sup> ) [11]	/
<sup>15</sup> N		1311	23		

**Table S2.** Peaks from oligonucleotide spectrum from both excitation wavelengths. A: adenine, T: thymine, C: cytosine, G: guanine, (/): no peak appearance.

	532 nm			244 nm		
Oligonucleotide	Band / cm <sup>-1</sup>	Tentative assignement	Reference	Band / cm <sup>-1</sup>	Tentative assignement	Reference
Poly-A	473			735		
	524	Vibration of ribose phospate	[15]	1242		
	611			1257		
	725	Ring breathing vibration of adenine	[3,5,16]	1311		
	776			1422	CH <sub>2</sub> -deformation vibration	[17]
	806	Ribose phosphodiester symmetric stretching	[15]	1485	N9C8 and C8N7 stretching vibrations along the long axis of purine bases	[13,14]
	1022			1581	NH <sub>2</sub> deformation virbration	[14]
	1100	PO <sub>2</sub> -streching vibration	[17]	/	/	/
	1328	C5N7, N7C8 stretching vibration	[14]	/	/	/
	1409	C4N9, C8H deformation vibration	[13]	/	/	/
	1508			/	/	/
	1553			/	/	/
	2891	CH <sub>2</sub> symmetric streching vibration	[18]	/	/	/
	2951	CH <sub>2</sub> asymmetric streching vibration	[18]	/	/	/

	532 nm			244 nm		
Oligonucleotide	Band / cm <sup>-1</sup>	Tentative assignement	Reference	Band / cm <sup>-1</sup>	Tentative assignement	Reference
Poly-T	494			675		
	563	Vibration of ribose phospate	[15]	771		
	659	Ribose phosphodiester symmetric stretching	[15]	795	PO <sub>2</sub> symmetrick streching vibration	[17]
	725	Ring breathing vibration of adenine	[3,5]	1188	C-C and C-N stretching vibration	[14]
	788	PO <sub>2</sub> symmetric streching vibration	[17]	1242	C6H deformation vibration, C4N4	[13]
	839	O—P—O streching vibration	[17]	1377	C6H bending vibration, ring stretching viration	[14]
	1016	Vibration of ribose	[15]	1485	N9C8 and C8N7 stretching vibrations along the long axis of purine bases	[13,14]
	1091	PO <sub>2</sub> -streching vibration	[17]	1656	C4=O-C4C5 streching vibration	[13,14]
	1184	C-C and C-N stretching vibration	[14]	/	/	/
	1235			/	/	/
	1373	C6H bending vibration	[14]	/	/	/
	1430	CH <sub>2</sub> -deformation vibration	[17]	/	/	/
	1667	C=O stretchichng vibration	[16]	/	/	/
	2954	CH <sub>2</sub> asymmetric streching vibration	[18]	/	/	/

	532 nm			244 nm		
Oligonucleotide	Band / cm <sup>-1</sup>	Tentative assignement	Reference	Band / cm <sup>-1</sup>	Tentative assignement	Reference
Poly-C	533			795	PO <sub>2</sub> -stretching vibration	[17]
	572			1296		
	725	Ring breathing vibration of adenine	[3,5]	1485	N9C8 and C8N7 stretching vibrations along the long axis of purine bases	[13,14]
	785	PO <sub>2</sub> symmetric streching vibration, Ring breathing vibration	[13,16]	1527		
	836	O—P—O streching vibration	[17]	1647	C2=O stretching vibration	[13]
	965		[17]	/	/	/
	1010	Vibration of ribose phospate	[15]	/	/	/
	1097	PO <sub>2</sub> -stretching vibration	[13]	/	/	/
	1259	C6H deformation vibration, C4N4	[17]	/	/	/
	1388	C4N, N2C2 stretching vibration	[13]	/	/	/
	1430	CH <sub>2</sub> -deformation viration	[14]	/	/	/
	1541	N3=C4 vibration	[17]	/	/	/
	1667	C=O stretching	[13]	/	/	/
	2894	CH <sub>2</sub> symmetric streching vibration	[18]	/	/	/
	2954	CH <sub>2</sub> asymmetric streching vibration	[18]	/	/	/

	532 nm				244 nm		
Oligonucleotide	Band / cm <sup>-1</sup>	Tentative assignement	Reference	Band / cm <sup>-1</sup>	Tentative assignement	Reference	
Poly-G	497	Vibration of ribose phosphate	[15]	1328	C–N stretching vibration	[11,13]	
	581	Vibration of ribose phosphate	[15]	1362	N7C8, N1C6, N5N7 stretching vibration	[14]	
	686	Ring breathing vibration	[16]	1485	N9C8 and C8N7 stretching vibrations along the long axis of purine bases	[13,14]	
	725	Ring breathing vibration of adenine	[3,5]	1578	NH <sub>2</sub> deformation vibration	[14]	
	785	PO <sub>2</sub> -streching vibration	[13,16]	/	/	/	
	839	O–P–O stretching vibration	[16]	/	/	/	
	1016	Vibration of ribose		/	/	/	
	1094	PO <sub>2</sub> -streching vibration	[17]	/	/	/	
	1175	C-C and C-N streching vibration	[15]	/	/	/	
	1328	C5N7, N7C8 stretching vibration	[14]	/	/	/	
	1361	N7C8, N1C6, N5N7 stretching vibration	[14]	/	/	/	
	1430	CH <sub>2</sub> -deformation vibration	[17]	/	/	/	
	1478	N9C8 and C8N7 stretching vibrations along the long axis of purine bases	[13,14]	/	/	/	

	532 nm			244 nm		
<b>Poly-G</b> <b>(continued)</b>	1577	NH <sub>2</sub> deformation vibration	[14]	/	/	/
	1712	C6=O stretch	[13]		/	
	2894	CH <sub>2</sub> symmetric stretching vibration	[18]	/		/
	2954	CH <sub>2</sub> asymmetric stretching vibration	[18]	/	/	/

**Table S3.** Peaks from oligonucleotide spectrum that appear at both excitation wavelengths. A: adenine, T: thymine, C: cytosine, G: guanine, (/): no peak appearance.

A		T		C		G	
532 nm	244 nm	532 nm	244 nm	532 nm	244 nm	532 nm	244 nm
725 cm <sup>-1</sup>	735 cm <sup>-1</sup>	1184 cm <sup>-1</sup>	1188 cm <sup>-1</sup>	785 cm <sup>-1</sup>	795 cm <sup>-1</sup>	1328 cm <sup>-1</sup>	1326 cm <sup>-1</sup>
/	/	1235 cm <sup>-1</sup>	1242 cm <sup>-1</sup>	1667 cm <sup>-1</sup>	1647 cm <sup>-1</sup>	1361 cm <sup>-1</sup>	1362 cm <sup>-1</sup>
/	/	1667 cm <sup>-1</sup>	1656 cm <sup>-1</sup>	/	/	1478 cm <sup>-1</sup>	1485 cm <sup>-1</sup>
/	/	/	/	/	/	1577 cm <sup>-1</sup>	1578 cm <sup>-1</sup>



**Table S4** Red-shifts in the UV Raman bands of DNA isolated from bacteria incubated with isotopes.

Isotope	Raman band of unlabeled cells / $\text{cm}^{-1}$	Raman band of red-shift / $\text{cm}^{-1}$	Extent of Raman shift / $\text{cm}^{-1}$	Assignment
$^{13}\text{C}$	1334	<b>1314</b>	20	C–N stretching vibration of guanine, adenine, and tryptophan
$^{15}\text{N}$		<b>1311</b>	23	
$^{13}\text{C}$	1485	<b>1455</b>	30	N9C8 and C8N7 stretching vibrations along the long axis of purine bases
$^{15}\text{N}$		<b>1470</b>	15	

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