

Evaluation of the Cytotoxic Effect of Pd₂Spm Against Prostate Cancer Through Vibrational Microspectroscopies

Raquel C. Laginha ¹, Clara B. Martins ¹, Ana L. Brandão ¹, Joana Marques ¹, M. Paula M. Marques ^{1,2},
Luís A.E. Batista de Carvalho ^{1*}, Inês P. Santos ^{1,†} and Ana L.M. Batista de Carvalho ^{1,†}

¹ Molecular Physical-Chemistry R&D Unit, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal

² Department of Life Sciences, Faculty of Science and Technology, University of Coimbra, 3000-456 Coimbra, Portugal

Supplementary material

* Correspondence: labc@ci.uc.pt; Tel.: +351 239 854 462

† These authors contributed equally to this work

Table S1: Raman and infrared bands for human healthy and cancer prostate cells (PNT-2, LNCaP and PC-3). Features from specific drug-prompted DNA and protein conformational rearrangements are presented in red. The signals exclusively detected by infrared are shaded in grey.

Bands (cm ⁻¹)	*Assignment			
	Nucleic acids	Proteins	Lipids	Carbohydrates
1716-1701	A-DNA ($\nu(\text{C=O})$)			
1688-1687		$\nu(\text{C=O})_{\text{amino acid side chain}}$		
1691-1669		Amide I/ β -sheet, antiparallel		
1660-1648		Amide I/random coil		
1639		Amide I/ β -sheet, parallel		
1659-1653	DNA ($\delta(\text{NH})$)	Amide I ($\nu(\text{C=O})$)/ α -helix	$\nu(\text{C=C})$	
1617	A ($\nu(\text{CC})_{\text{ring}}$), C ($\delta(\text{NH}_2)$)	Phe, Tyr, Trp ($\nu(\text{C=C})$), $\delta(\text{NH}_2)$		
1605	T ($\nu(\text{CC})_{\text{ring}}$)	Phe ($\delta(\text{C=CH})$)		
1586-1582		$\nu(\text{C=C})$, $\nu(\text{C=N})$	$\nu(\text{C=C})$, $\nu(\text{C=N})$	
1577-1575	A, G ($\nu(\text{CC})_{\text{ring}}$)			
1555	G ($\nu(\text{CC})_{\text{ring}}$)	Trp ($\nu(\text{CC})_{\text{ring}}$), $\nu(\text{C=C})_{\text{porphyrin}}$		
1545		Amide II ($(\delta(\text{CN-H})/\nu(\text{CN}))$)		
1521		$\nu(\text{C=C})_{\text{porphyrin}}$		
1467-1465		$\delta(\text{CH}_2)$, $\delta(\text{CH}_3)$	$\delta(\text{CH}_2)$, $\delta(\text{CH}_3)$, aromatic lipids	$\delta(\text{CH}_2)$
1455-1442			$\delta(\text{CH}_2)$	
1416	A-DNA ($\delta(\text{CH}_2)$)			
1398-1395		$\delta(\text{CH}_2)$, $\rho(\text{CH}_2)$	membrane lipids ($\delta(\text{CH}_2)$)	$\delta(\text{CH}_2)$, $\rho(\text{CH}_2)$
1379	A, G, T ($\nu(\text{CC})_{\text{ring}}$)	glycoproteins ($\delta(\text{CH}_3)$)	lipids/acyl chains ($\delta(\text{CH}_3)$)	saccharides ($\delta(\text{CH}_2)$)
1340-1339	G ($\nu(\text{CC})_{\text{ring}}$)			
1314-1309	G ($\nu(\text{CC})_{\text{ring}}$)	$\delta(\text{CH}_2)$	$\delta(\text{CH}_2)$	$\delta(\text{CH}_2)$
1306-1303	RNA/A, C ($\nu(\text{CC})_{\text{ring}}$)			
1280-1279		amide III/ α -helix	$\delta(\text{CH}_2)$, $\omega(\text{CH}_2)$, t(CH_2)	$\delta(\text{CH}_2)$, $\omega(\text{CH}_2)$, t(CH_2)
1260-1251	A, T ($\nu(\text{CC})_{\text{ring}}$)	$\delta(\text{CH}_2)$, $\delta(\text{C=C-H})$	$\delta(\text{C=C-H})_{\text{phospholipids}}$	$\delta(\text{CH}_2)$, $\omega(\text{CH}_2)$, t(CH_2)
1252-1240		amide III/random coil		
1238	B-DNA ($\nu_{\text{as}}(\text{PO}_2^-)$)			
1230-1225		amide III/ β -sheet		
1221-1220		amide III ($\delta(\text{NH})$, $\nu(\text{CN})$)		
1209		Hyp, Phe, Tyr ($\nu(\text{CC})$)		
1175-1167	C, G, T ($\nu(\text{CC})_{\text{ring}}$)	Tyr, Phe ($\delta(\text{CH})$)		
1158-1157		$\nu(\text{CC})$, $\nu(\text{CN})$, $\delta(\text{CH}_2)$	$\delta(\text{CH}_2)$, $\nu(\text{C=C})_{\text{conjugated}}$	$\delta(\text{CH}_2)$
1129-1126	RNA/ribose ($\nu(\text{CO})$)	$\nu(\text{CN})$	$\nu(\text{CC})_{\text{acyl}}$ (<i>trans</i> conformation)	$\nu(\text{CO})$, $\nu(\text{CC})$
1096-1091	B-DNA ($\nu_{\text{as}}(\text{PO}_2^-)$)			
1083-1077		$\nu(\text{CC})$, $\nu(\text{CN})$	phospholipids ($\nu_{\text{as}}(\text{PO}_2^-)$)	glycogen ($\nu(\text{CC})$, $\nu(\text{CO})$)
1063-1058	B-DNA/deoxyribose ($\nu(\text{CO})$)	$\nu(\text{CC})$, $\nu(\text{CN})$	$\nu(\text{CC})$, $\nu(\text{CO})$	$\nu(\text{CC})$, $\nu(\text{CO})$, $\delta(\text{OCH})$
1051-1050	RNA ($\nu(\text{OPO})$)		phosphate esters ($\nu_{\text{as}}(\text{OPO})$)	$\nu(\text{C-OH})$
1035-1031		Phe ($\delta(\text{CH})$), $\nu(\text{O-CH}_3)$	$\nu(\text{CC})$, phospholipids ($\delta(\text{CH})$)	$\nu(\text{CC})$, $\nu(\text{CO})$, $\nu(\text{C-OH})$
1004		Phe ($\nu_{\text{as}}(\text{CC})_{\text{ring}}$)		
980		$\nu(\text{CC})$ (β -sheet)	$\delta(\text{C=CH})$	
962-961	DNA ($\nu(\text{CC})/\nu(\text{CO})_{\text{backbone}}$)			polysaccharides ($\delta(\text{C=O})$)
945-944	RNA/ribose ($\nu(\text{CC})_{\text{ring}}$)			polysaccharides (skeletal modes)
937-935		$\nu(\text{CC})$ (α -helix)	glycolipids ($\nu(\text{COC})$)	$\nu(\text{COC})_{\text{glycosidic}}$
903-897	deoxyribose ($\nu(\text{CC})_{\text{ring}}$)	$\nu(\text{CC})$	fatty acids ($\nu(\text{CC})$, $\nu(\text{CO})$)	$\nu(\text{COC})$
884-883		$\rho(\text{CH}_2)$		
855-854		Pro, Tyr, Val ($\nu(\text{CC})$, $\delta(\text{CCH})$)		polysaccharides ($\gamma(\text{COC})$)
833-831	B-DNA ($\nu(\text{OPO})_{\text{backbone}}$)	Pro, Tyr ($\nu(\text{CC})$)		
816-813	RNA ($\nu(\text{OPO})_{\text{backbone}}$)	Pro, Tyr ($\nu(\text{CC})$)		
787-784	C, T, U ($\nu(\text{CC})_{\text{ring}}$)			
753-750	Z-DNA ($\nu(\text{OPO})_{\text{backbone}}$)			
752-750	B-DNA/dT ($\nu(\text{CC})_{\text{ring}}$)	Trp ($\nu_{\text{as}}(\text{CC})_{\text{ring}}$)		
731-726	B-DNA/A ($\nu(\text{CC})_{\text{ring}}$)	Trp ($\nu_{\text{as}}(\text{CC})_{\text{ring}}$)		
679-677	B-DNA/A, G, T, C ($\nu(\text{CC})_{\text{ring}}$)	Trp ($\nu(\text{CC})_{\text{ring}}$)		
670	A-DNA/dG ($\nu(\text{CC})_{\text{ring}}$)			
668	B-DNA/G, T ($\nu(\text{CC})_{\text{ring}}$)			
645-644		$\nu(\text{CS})$, Tyr (t($\text{CC})$)		
626-623	Z-DNA/dG ($\nu(\text{CC})_{\text{ring}}$)			
624-623		Phe (t($\text{CC})$)		

*A – adenine; C – cytosine; dG – deoxyguanine; dT – deoxythymine; G – guanine; Glu – glucose; Hyp – hydroxyproline; Met – methionine; Phe – phenylalanine; Pro – proline; T – thymine; Trp – tryptophan; Tyr – tyrosine; U – uracil; Val – valine. δ – in-plane deformation; γ – out-of-plane deformation; ν – stretching; ρ – rocking; t – twisting; ω – wagging; s – symmetric; as – anti-symmetric.