Supplementary Material

Monitoring of Biochemical Changes of Neuroblastoma Cells in Early-Stages after X-ray Exposure by Using Fourier Transform Infrared Spectroscopy

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Table S1

FT-IR peaks observed in the spectrum of control cells, with assignments in agreement with the data reported in the literature [S1-S6]; abbreviation: as = asymmetric, s = symmetric, ν = stretching, δ = bending, sc = scissoring, vbr = vibration, a. a. = free amino acids, c = carbohydrates, p = proteins, l = lipids. The indicated position of every peak is the center of the relative pseudo-Voigt function obtained from the deconvolution fit.

Peak Position (cm^{-1}) for control sample fixed at t = 0h	Assignment	Cellular Element
3434	O-H ν	c
3286	Amide A (-N-H ν) O-H ν	p, c
3178	$-NH_3+$ as. ν (a. a.)	p
3069	Amide B (-N-H ν) O-H ν	p, c
2954	CH_3 as. ν	p, l
2929	CH_2 as. ν	l
2866	CH_3 s. ν	p, l
2846	CH_2 s. ν	l
Amide I region (C=O ν, C-N ν)		
1694	Antiparallel β-sheet	p
1679	β-turn	P
1674	β-turn	P
1661	α-helix	P
1652	α-helix	P
1644	unordered structures	P
1636	parallel β-sheet	P
1624	parallel β-sheet	P
1614	antiparallel β-sheet	P
Amide II region (C-N ν, N-H δ)		
1575	Amide II (C-N ν, C-NH δ, α-helix)	
1539	Amide II (C-N ν, C-NH δ, β-sheets)	p
1453	CH_3 as. δ, CH2 sc.	p, l
1389	$COO-$ s. ν	p
Amide III region		
1314	α-helix	p
1294	α-helix	p
1281	random coil	p
1256	random coil	p
1242	$PO^{2}-$ as. ν	DNA, l, p

1231	PO^{2}– as. ν β-sheet	DNA, p
1220	β-sheet	DNA, p
1204	C-H ring δ, β-sheet	DNA, p
1192	β-sheet	p
1175	sugar-phosphate backbone vbr	DNA
1161	CO-O-C s. as. ν	l
1148	ribose C-O ν	DNA
1119	ν -C-O	DNA
1104	P-O-C s. ν	DNA
1082	PO^{2}– s. ν C-O-P ν	DNA, p
1053	ν -C-O	DNA
972	PO^{4}– s. ν C-0 ν, C=C ν (a.a.)	DNA, p

Table S2

Average FTIR peaks position for control and samples treated with the different doses of X-rays fixed immediately after irradiation (t_0 cells). Bold values indicate shifts greater than the spectral resolution of the instrument 4 cm^{-1}.

Peak position (cm^{-1}) for control samples fixed at t = 0h	Peak position (cm^{-1}) for 2Gy irradiated samples fixed at t = 0h	Peak position(cm^{-1}) for 4Gy irradiated samples fixed at t = 0h
3434	**3443**	3433
3286	3289	3286
3178	3178	**3170**
3069	**3059**	**3068**
2954	**2959**	2954
2929	**2923**	**2923**
2866	2866	2866
2846	2846	2846
	Amide I region	
1694	1694	1694
1679	1680	1680
1674	**1680**	1674
1661	1664	**1666**
1652	1654	1653
1644	1648	1644
1636	1638	1637
1624	1626	1624
1614	1614	1614
	Amide II region	
1575	1575	1575
1539	1539	1539
1453	1450	1453
1389	**1398**	**1394**
	Amide III region	
1314	**1305**	**1305**
1294	1295	**1285**
1281	1281	1283
1256	**1261**	**1262**
1242	1239	1242
1231	**1225**	1229
1220	1216	1220
1204	1204	1206
1192	1193	1191
1175	1175	1173
1161	1161	1161
1148	**1138**	**1142**

1119	**1129**	**1126**
1104	1105	1103
1082	1081	1081
1053	1053	**1059**
972	**958**	**965**

Table S3

Average FTIR peaks position for control and samples treated with the different doses of X-rays fixed 2 hours after irradiation (t_2 cells). Bold values indicate shifts greater than the spectral resolution of the instrument 4 cm^{-1}.

Peak position (cm^{-1}) for control samples fixed at t = 2h	Peak position (cm^{-1}) for 2Gy irradiated samples fixed at t = 2h	Peak position (cm^{-1}) for 4Gy irradiated samples fixed at t = 2h
3441	3443	**3433**
3287	3286	3286
3178	3178	3178
3061	3059	3061
2959	2960	**2964**
2923	2922	**2929**
2866	2866	**2876**
2846	2846	**2855**
	Amide I region	
1685	1686	**1694**
1679	1679	1676
1674	1673	1674
1664	1661	1667
1656	1652	1655
1644	1644	1642
1634	1636	1632
1627	1624	1624
1614	1614	1614
1612	1614	1614
	Amide II region	
1576	1575	1575
1539	1539	1539
1453	1453	1453
1394	1396	1395
	Amide III region	
1312	1312	1314
1295	1295	1295
1283	1283	1283
1261	1265	1263
1239	1242	1240
1225	**1230**	**1231**
1214	1218	1218
1202	1203	1203
1194	1190	**1199**
1168	1169	1166
1162	**1169**	1166

1140	**1148**	1141
1120	**1126**	1121
1101	1100	1098
1084	**1090**	1081
1062	**1057**	**1055**
962	965	962

Table S4

Average FTIR peaks position for control and samples treated with the different doses of X-rays fixed 4 hours after irradiation (t_4 cells). Bold values indicate shifts greater than the spectral resolution of the instrument 4 cm^{-1}.

Peak position (cm^{-1}) for control samples fixed at t = 4h	Peak position (cm^{-1}) for 2Gy irradiated samples fixed at t = 4h	Peak position (cm^{-1}) for 4Gy irradiated samples fixed at t = 4h
3443	3443	**3438**
3290	3289	3287
3178	3178	3178
3059	3059	**3069**
2958	2958	2960
2922	2922	**2927**
2866	2866	2866
2846	2846	2846
	Amide I region	
1694	1694	1694
1680	1680	1680
1674	1673	1674
1664	1662	1665
1652	1653	1652
1644	1644	1643
1636	1635	1636
1624	**1631**	1627
1614	1614	1615
	Amide II region	
1575	1575	1575
1539	1539	1539
1453	1453	1453
1393	**1399**	1394
	Amide III region	
1308	**1314**	**1314**
1295	1294	**1289**
1282	**1274**	1283
1263	1266	1259
1242	1240	**1233**
1231	1231	1233
1219	1218	1216
1204	1200	1203
1194	**1200**	1194
1167	1171	**1161**
1169	1171	**1174**
1138	1139	1141

1123	1127	1127
1101	1099	1102
1089	**1082**	1086
1053	1054	1053
958	959	958

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