applied sciences

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Supplementary Materials: An FTIR microspectroscopy ratiometric approach for monitoring X-ray irradiation effects on SH-SY5Y human neuroblastoma cells

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Table S1. Fourier transform infrared (FTIR) peaks observed in the spectrum of control cells, with assignments in accordance with the data reported in the literature [10,12,13,39,44]. Abbreviations: as = asymmetric, s = symmetric, ν = stretching, δ = bending, sc = scissoring, vbr = vibration, a. a. = free amino acids. The indicated position of every peak is the center of the relative Lorentzian function obtained from the deconvolution fit.

Peak	ASSIGNMENT			
cm^{-1}	DNA/RNA	Protein	Lipid	Carbohydrate
3438				O–H ν
3296		Amide A (–N–H ν)		O–H ν
3159		$–NH_3^+$ as. ν (a. a.)		
2955		CH_3 as. N	CH_3 as. ν	
2922			CH_2 as. ν	
2870		CH_3 s. ν	CH_3 s. ν	
2851			CH_2 s. ν	
1652		Amide I (C=O ν, C-N ν)		
1553		Amide II (C–N ν, C–NH δ, α-helix)		
1527		Amide II (C–N ν, C–NH δ, β-structure)		
1455		CH_3 as. δ, CH_2 sc.	CH_3 as. δ, CH_2 sc.	
1396		COO^- s. ν		
1246	PO_2^- as. N	C–O–P ν		
1082	PO_2^- s. ν	C–O–P ν		

Table S2. Amide I deconvolution results for control and irradiated sample fixed immediately after irradiation, with assignments in accordance with the data reported in the literature [37–39]; the ratio between the secondary structures peaks area and the area of the entire Amide I peak, as a percentage, are reported in the table.

Control	Assignments	2 Gy	4 Gy	6 Gy	8 Gy	10 Gy
Peak (cm^{-1})		Peak (cm^{-1})	Peak (cm^{-1})	Peak (cm^{-1})	Peak (cm^{-1})	Peak (cm^{-1})
1617	Antiparallel β-sheets	1617	1618 (+1)	1617	1618 (+1)	1619 (+2)
%A = 4.6 ± 0.3		%A = 7.4 ± 0.3	%A = 8.0 ± 0.6	%A = 7.2 ± 0.8	%A = 10.0 ± 1.6	%A = 11.8 ± 1.2
1626	Parallel β-sheets	1627 (+1)	1627	1627	1628 (+1)	1628 (+1)
%A = 8.1 ± 0.8		%A =10.8 ± 0.3	%A = 9.3 ± 1.2	%A = 9.4 ± 1.0	%A = 9.9 ± 0.8	%A = 9.8 ± 0.7
1635	Parallel β-sheets	1637 (+2)	1637 (+2)	1637 (+2)	1638 (+3)	1638 (+3)
%A = 13.2 ± 1.0		%A = 17.7 ± 0.8	%A = 18.6 ± 0.8	%A = 23.3 ± 0.9	%A = 18 ± 3	%A = 18.1 ± 1.2
1647	Unordered	1647	1647	1649	1647	1648
%A = 25.7 ± 1.0		%A = 17.0 ± 1.7	%A = 19.5 ± 0.6	%A = 19.0 ± 1.0	%A = 15 ± 2	%A = 20.2 ± 1.1
1661	α-helix	1659 (−2)	1660 (−1)	1660 (−1)	1658 (−3)	1660 (−1)
%A = 26.8 ± 0.9		%A = 19.7 ± 0.3	%A = 20.1 ± 0.8	%A = 14.9 ± 0.7	%A = 22.7 ± 1.0	%A = 20.8 ± 1.4
1674	β –turn	1672 (−2)	1673 (−1)	1671 (−3)	1672 (−2)	1675 (+1)
%A = 10.7 ± 0.5		%A = 14.8 ± 1.2	%A = 15.5 ± 0.4	%A = 13.4 ± 0.5	%A = 15.0 ± 1.3	%A = 13.6 ± 0.6
1686	β –turn	1685 (−1)	1687 (+1)	1684 (−2)	1686	1688 (+2)
%A = 6.9 ± 0.4		%A = 7.2 ± 0.7	%A = 5.5 ± 0.4	%A = 9.7 ± 0.9	%A = 6.7 ± 0.6	%A = 3.6 ± 0.8
1697	Antiparallel β-sheets (weak)	1698 (+1)	1698 (+1)	1699 (+2)	1698 (+1)	1698 (+1)
%A = 3.4 ± 0.3		%A = 4.5 ± 0.3	%A = 3.0 ± 0.8	%A = 2.6 ± 0.3	%A = 2.0 ± 1.0	%A = 1.7 ± 0.4

Table S3. Amide I deconvolution results for control and irradiated sample fixed 24 h after irradiation, with assignments in accordance with the data reported in the literature [37–39]; the ratio between the secondary structures peaks area and the area of the entire Amide I peak, as a percentage, are reported in the table.

Control	**Assignments**	**2 Gy**	**4 Gy**	**6 Gy**	**8 Gy**	**10 Gy**
Peak (cm^{-1})		Peak (cm^{-1})	Peak (cm^{-1})	Peak (cm^{-1})	Peak (cm^{-1})	Peak (cm^{-1})
1619	Antiparallel β-sheets	1619	1618 (−1)	1620 (+1)	1619	1617 (−2)
%A = 12.3 ± 0.7		%A = 10.5 ± 0.8	%A = 8.3 ± 0.5	%A = 12.7 ± 0.7	%A = 9.8 ± 0.5	%A = 8.3 ± 1.9
1628	Parallel β-sheets	1629 (+1)	1628	1630 (+2)	1629 (+1)	1626 (−2)
%A = 13.4 ± 0.5		%A = 10.6 ± 1.4	%A = 8.7 ± 1.2	%A = 14.1 ± 0.6	%A = 12.7 ± 0.3	%A = 11.9 ± 1.9
1639	Parallel β-sheets	1639	1640 (+1)	1641 (+2)	1639	1635 (−4)
%A = 19.1 ± 0.4		%A = 22.7 ± 1.7	%A = 28 ± 3	%A = 20.8 ± 1.6	%A = 19.5 ± 0.4	%A = 16.5 ± 1.0
1650	Unordered	1650	1652 (+2)	1651 (+1)	1651 (+1)	1647 (−3)
%A = 20.30 ± 0.12		%A =19.9 ± 0.3	%A = 18.8 ± 1.2	%A = 18.2 ± 1.4	%A = 20.8 ± 0.2	%A = 22.4 ± 1.1
1662	α-helix	1662	1663 (+1)	1662	1662	1659 (−3)
%A = 17.0 ± 0.2		%A = 17.0 ± 0.2	%A = 16.1 ± 0.8	%A = 16.4 ± 0.9	%A = 17.8 ± 0.3	%A = 26.0 ± 0.5
1673	β –turn	1673	1674 (+1)	1673	1674 (+1)	1675 (+2)
%A = 9.4 ± 0.2		%A = 10.44 ± 0.07	%A = 10.7 ± 0.6	%A = 7.5 ± 0.4	%A = 10.0 ± 0.4	%A = 7.8 ± 0.2
1682	β –turn	1683 (+1)	1683 (+1)	1681 (−1)	1683 (+1)	1684 (+2)
%A = 4.3 ± 0.2		%A = 5.3 ± 0.6	%A = 4.3 ± 0.8	%A = 4.7 ± 0.7	%A = 3.8 ± 0.4	%A = 5.0 ± 0.7
1692	Antiparallel β-sheets (weak)	1695 (+3)	1695 (+3)	1690 (−2)	1693 (+1)	1696 (+4)
%A = 3.5 ± 0.4		%A = 3.4 ± 0.2	%A = 4.3 ± 0.6	%A = 4.9 ± 1.0	%A = 4.7 ± 0.2	%A = 2.0 ± 0.6

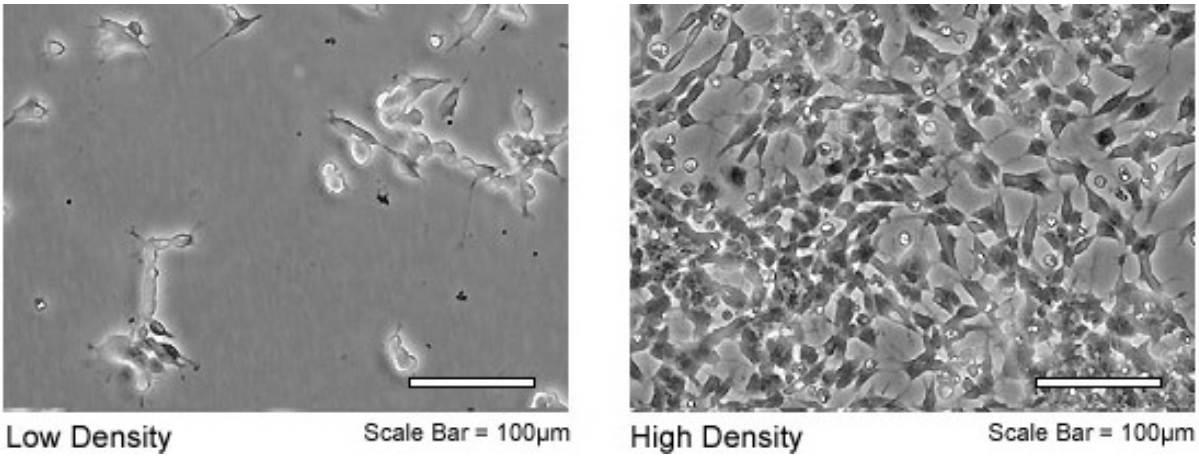

Figure S1. SH-SY5Y cells at different culture density (ATCC, American type culture collection).

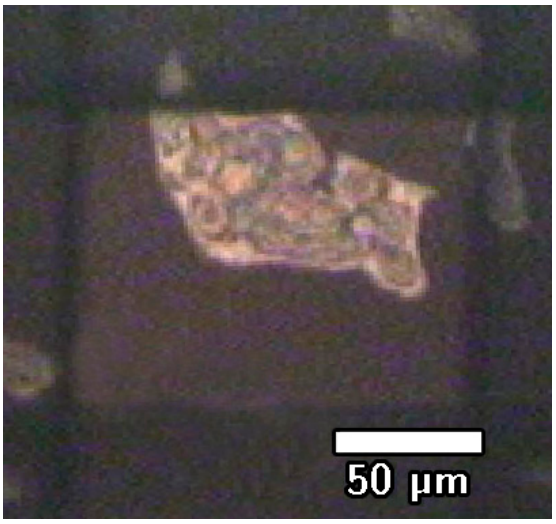

Figure S2. Micrograph at 10× magnification of SH-SY5Y cells control sample adherent to the MirrIR slide. A cell cluster is visible in the brighter area that is manually selected for collecting the signal for Fourier transform infrared (FTIR) spectroscopy.