

Supplementary Materials for

# Metabolomic Insight into Implications of Induction Chemotherapy Followed by Concomitant Chemoradiotherapy in Locally Advanced Head and Neck Cancer

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**The characteristics of the acquired spectra, as well as the pulse sequence parameters.**

- NOESY (nuclear Overhauser effect spectroscopy)—an overview of all types of molecules;
- CPMG (Carr–Purcell–Meiboom–Gill)—information on only low-molecular-weight metabolites.
- DIFF (diffusion-edited)—mainly macromolecular signals.
- Two-dimensional (2D) JRES (J-resolved)—a visualization of scalar couplings and improved metabolite identification.

Table S1. NMR pulse sequence parameters.

Pulse program	NOESYGPPR1D	CPMGPR1D	LEDBPGPPR2S1D	JRESGPPRQF
<b>TD</b>	65536	65536	65536	8192
<b>SW</b> [ppm]	30	20	30	16.62
<b>AQ</b> [sec]	2.73	4.09	2.73	0.62
<b>D1</b> [sec]	4	4	4	2
<b>D8</b> [sec]	0.01	-	-	-
<b>D16</b> [sec]	-	-	0.0002	0.0002
<b>D20</b> [sec]	-	0.0003	0.12	-
<b>D21</b> [sec]	-	-	0.005	-
<b>DS</b>	4	4	4	16
<b>L4</b>	-	126	-	-
<b>NS</b>	32	64	64	1
<b>DELTA1</b> [sec]	-	-	0.11572488	-
<b>DELTA2</b> [sec]	-	-	0.004172	-

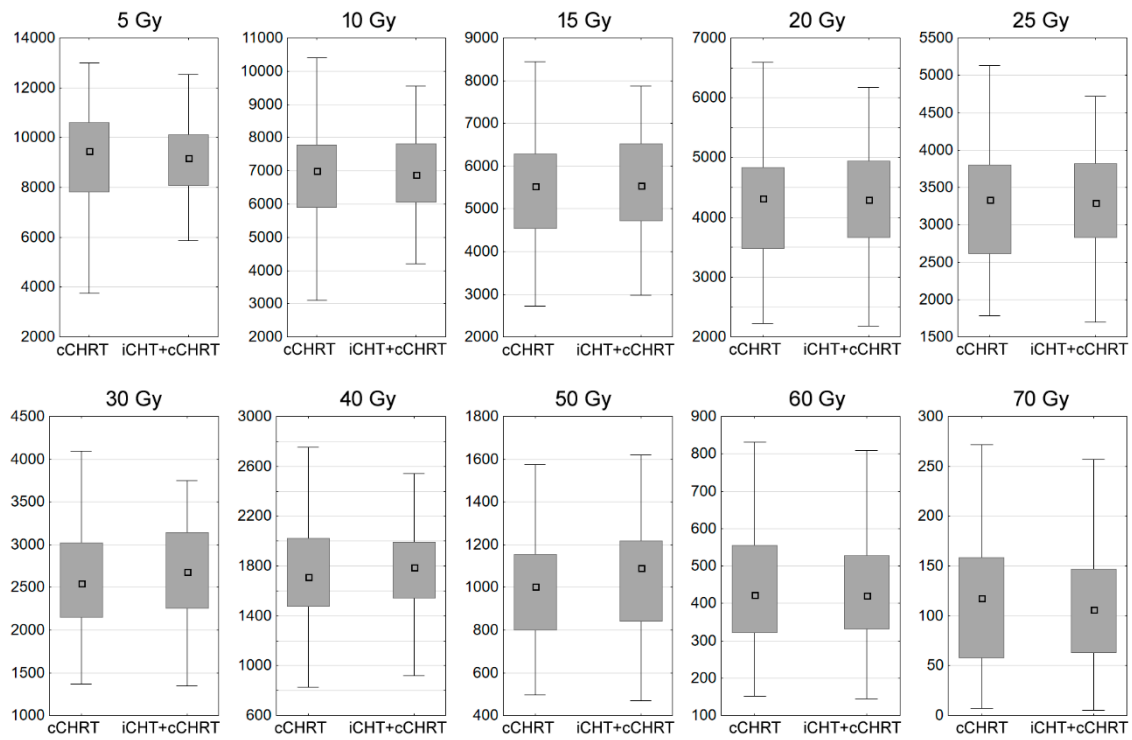


Figure S1. Box plot comparison of the tissue volumes receiving a particular dose of radiation. No statistically significant differences are observed. Point—median; box—25-75 percentile; whiskers—the minimum and maximum values.