

A quantitative assessment of Geant4 for predicting the yield and distribution of positron-emitting fragments in ion beam therapy: Supplementary Material

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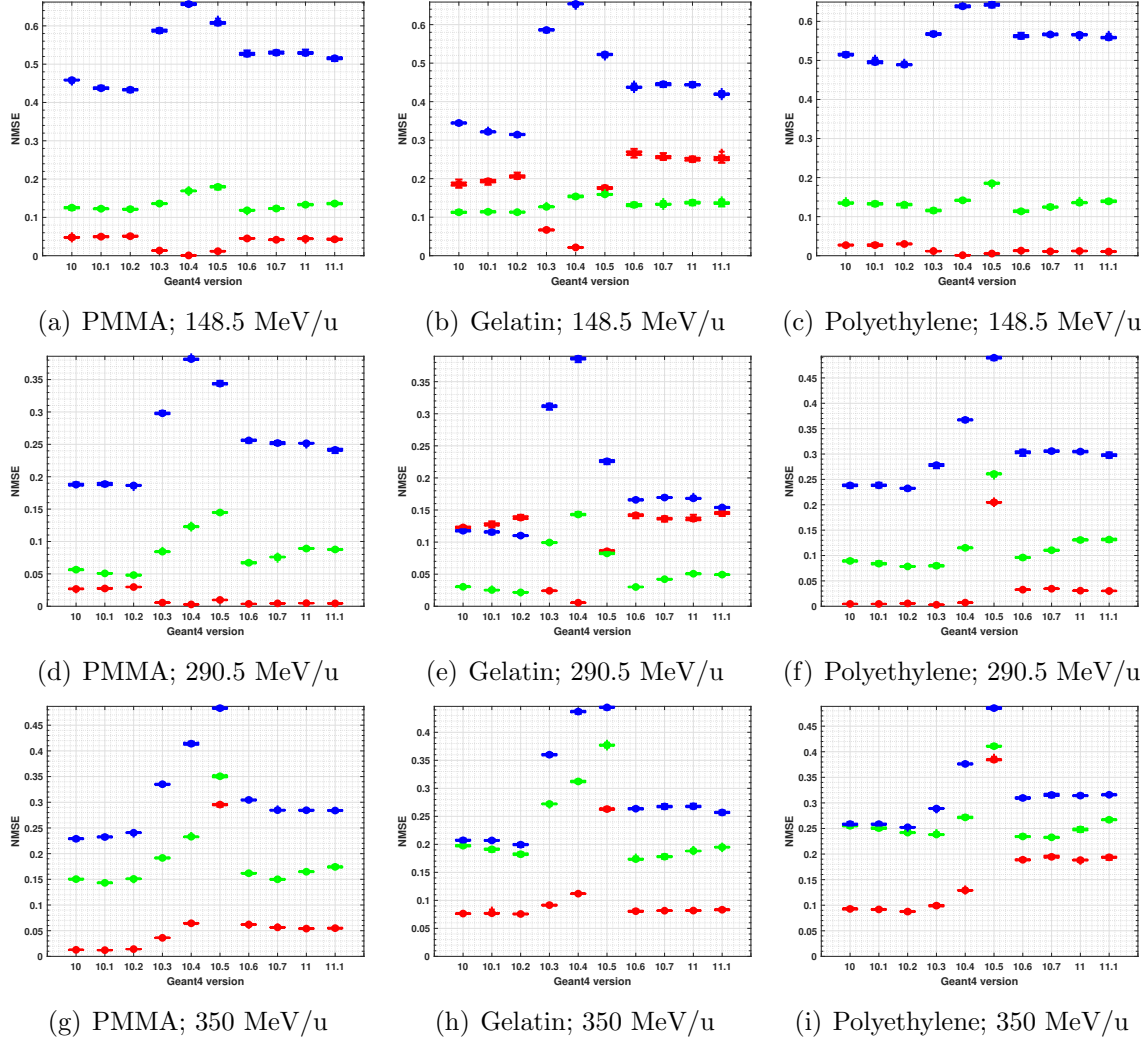
24 **1. Overview**

25 The normalised mean squared errors (NMSEs) and Pearson cross-correlation coefficients
26 (CCCs) for each test case are presented in the following sections, organised by region
27 (entrance, build up / Bragg peak and tail) and ion species (carbon and oxygen). NMSEs
28 are plotted with box-and-whisker plots, showing the median, interquartile range (IQR),
29 mean, minimum and maximum; in most instances the spread is quite small and hence
30 the IQR, mean and median are very close together.

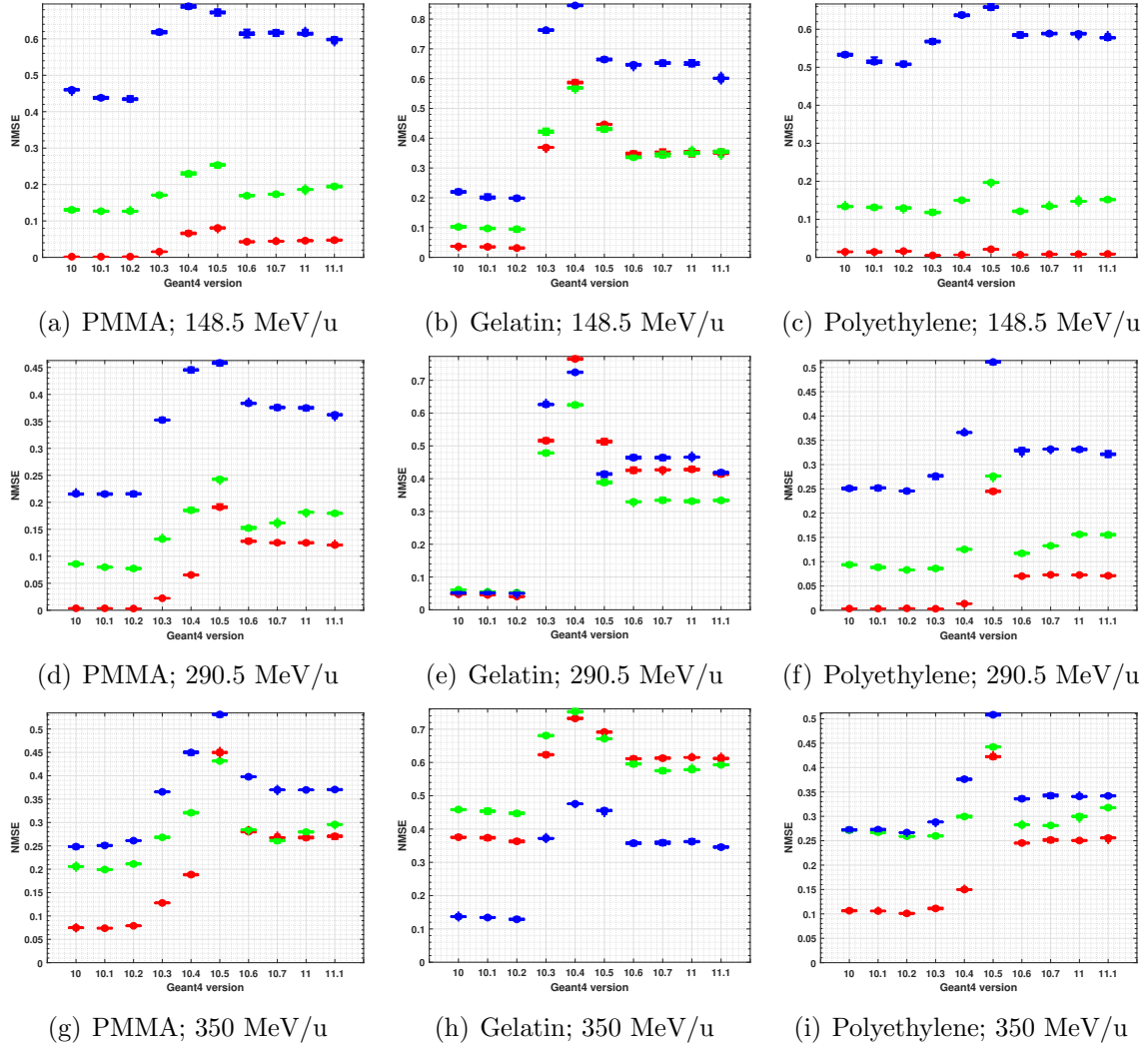
2. Entrance region

2.1. Carbon ion irradiation

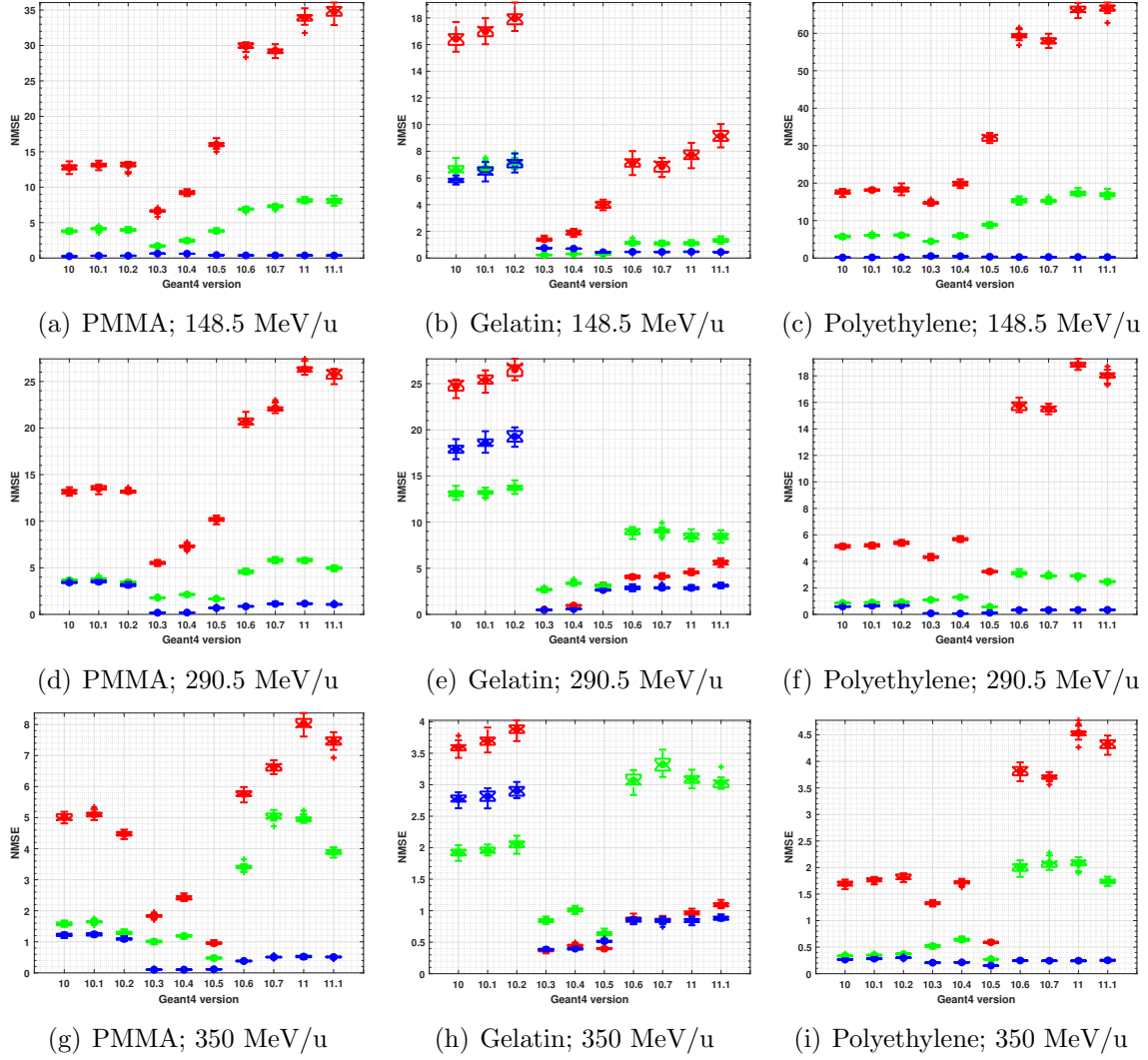
2.1.1. *NMSE* The NMSEs for total positron annihilation yield in the entrance region for carbon ion irradiation is presented in Supplementary Figure 1; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 2-4.



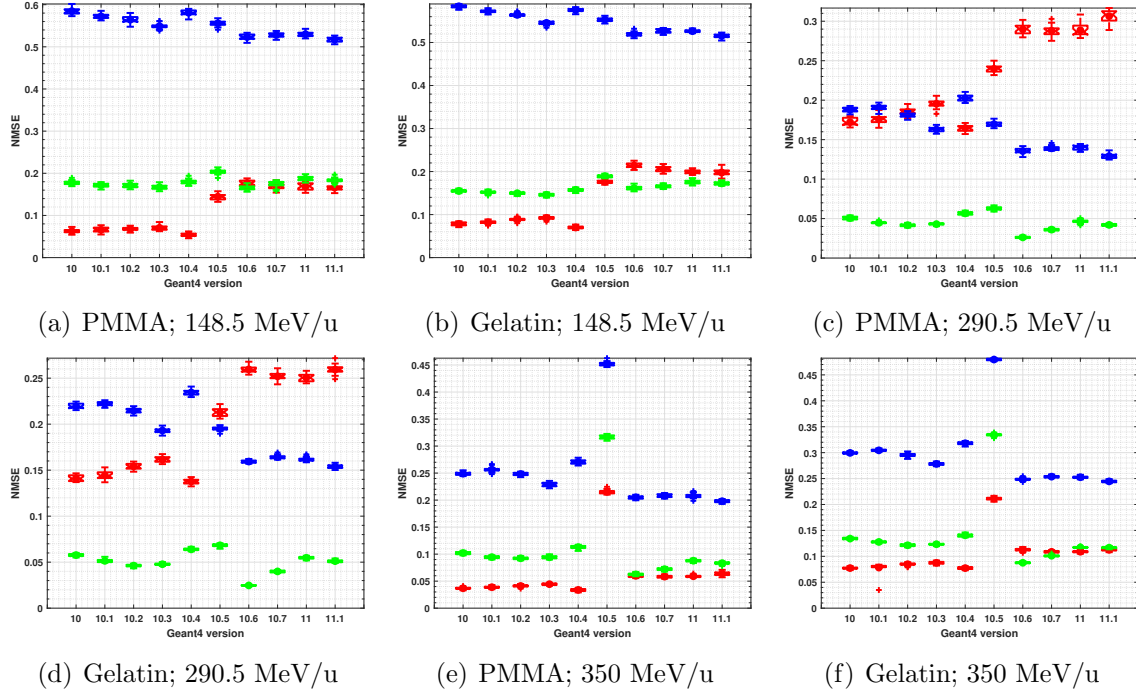
Supplementary Figure 1: NMSE between simulation and experimental measurements of total positron annihilations in the entrance region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 2: NMSE between simulations and experimental measurements of ^{11}C fragment production in the entrance region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

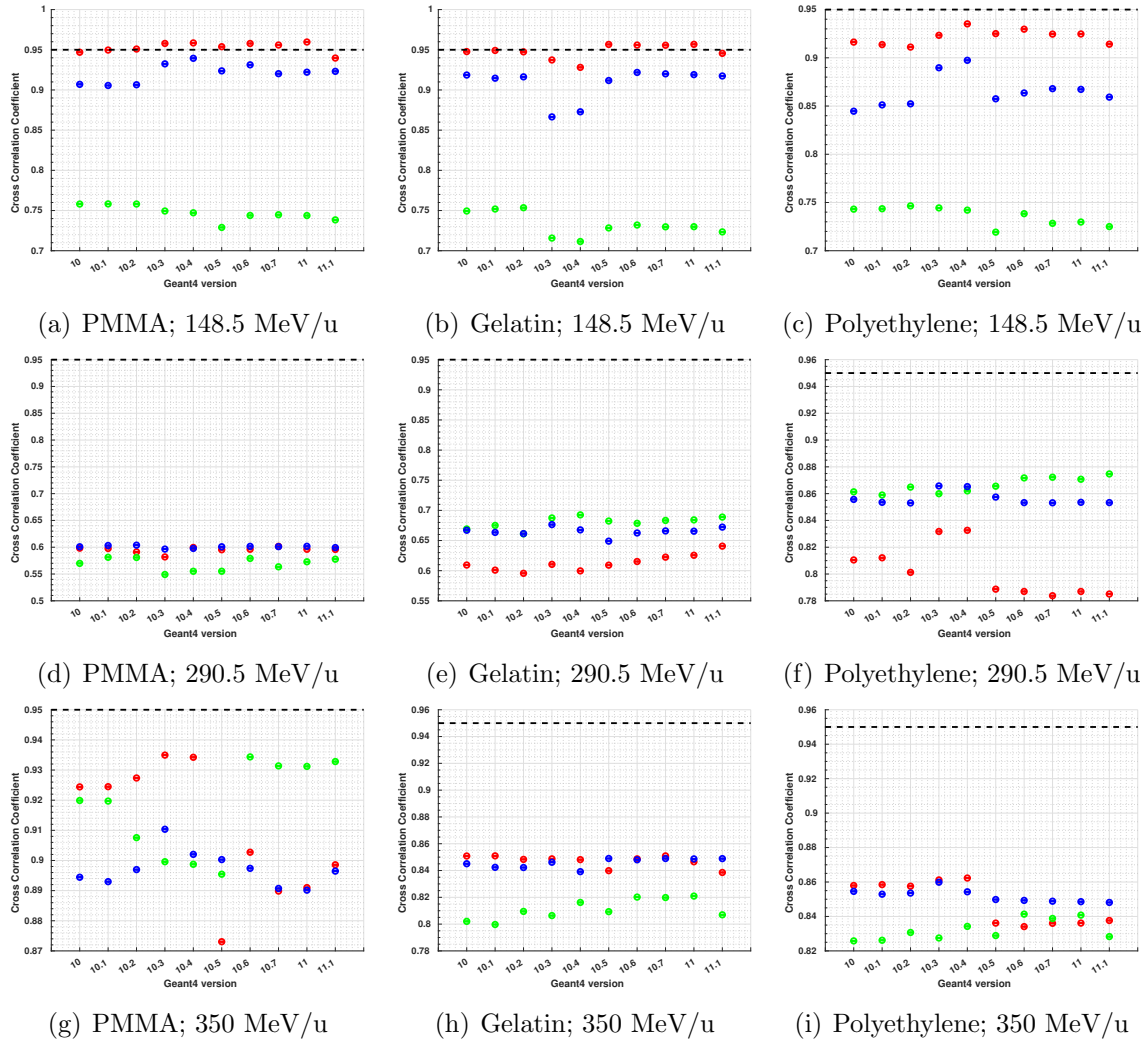


Supplementary Figure 3: NMSE between simulations and experimental measurements of ^{10}C fragment production in the entrance region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

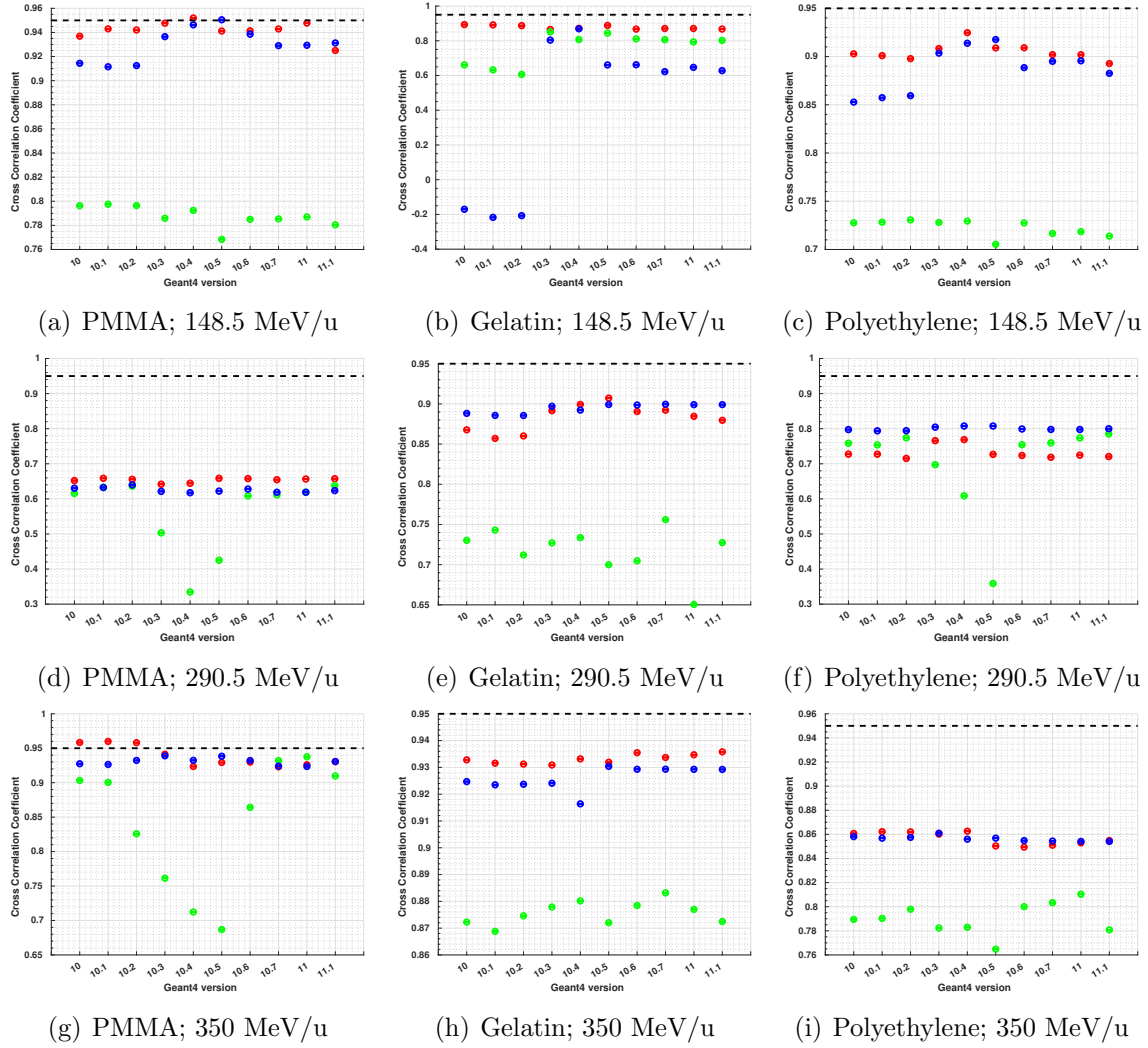


Supplementary Figure 4: NMSE between simulations and experimental measurements of ^{15}O fragment production in the entrance region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

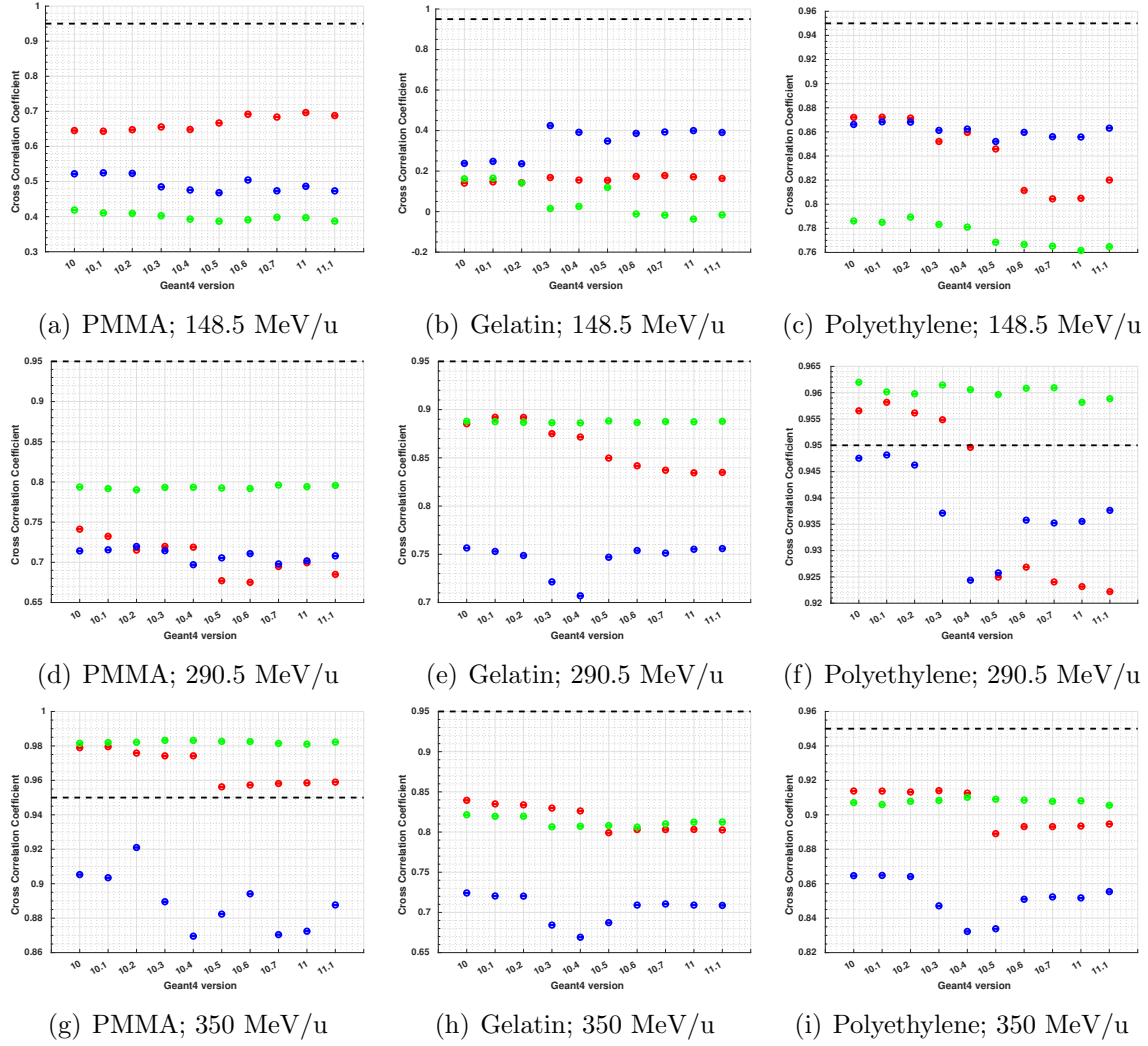
2.1.2. *Pearson CCC* The Pearson CCCs for total positron annihilation yield in the entrance region for carbon ion irradiation is presented in Supplementary Figure 5; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 6-8.



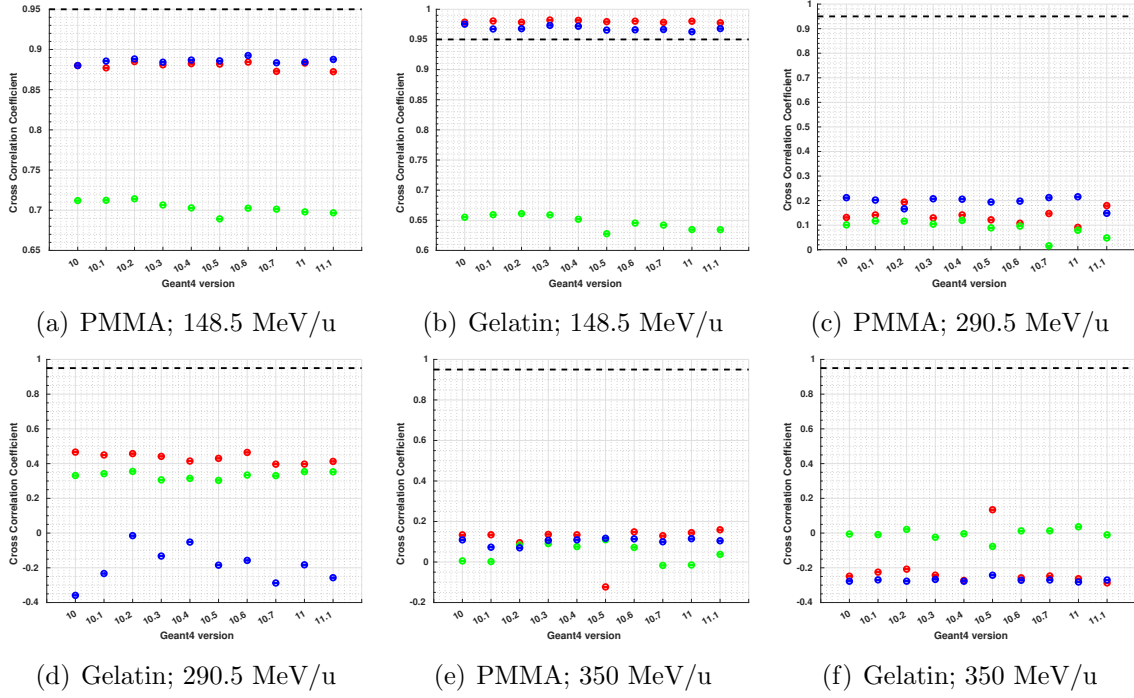
Supplementary Figure 5: Pearson CCC between simulation and experimental measurements of total positron annihilations in the entrance region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 6: Pearson CCC between simulations and experimental measurements of ^{11}C fragment production in the entrance region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



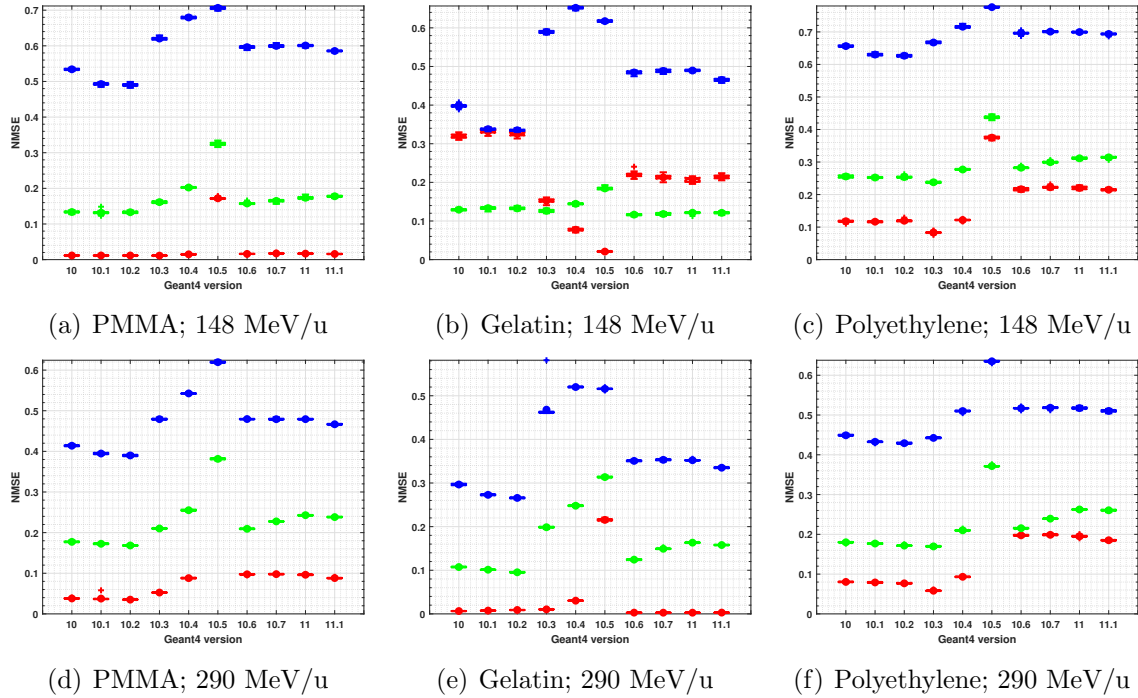
Supplementary Figure 7: Pearson CCC between simulations and experimental measurements of ^{10}C fragment production in the entrance region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



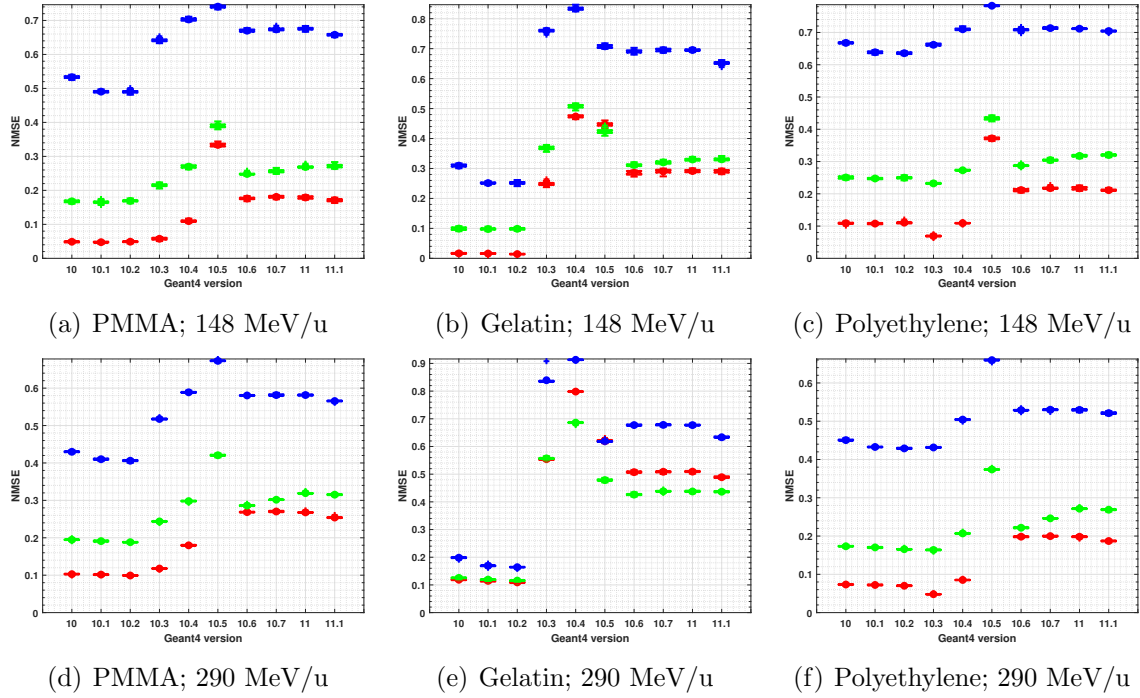
Supplementary Figure 8: Pearson CCC between simulations and experimental measurements of ^{15}O fragment production in the entrance region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

2.2. Oxygen ion irradiation

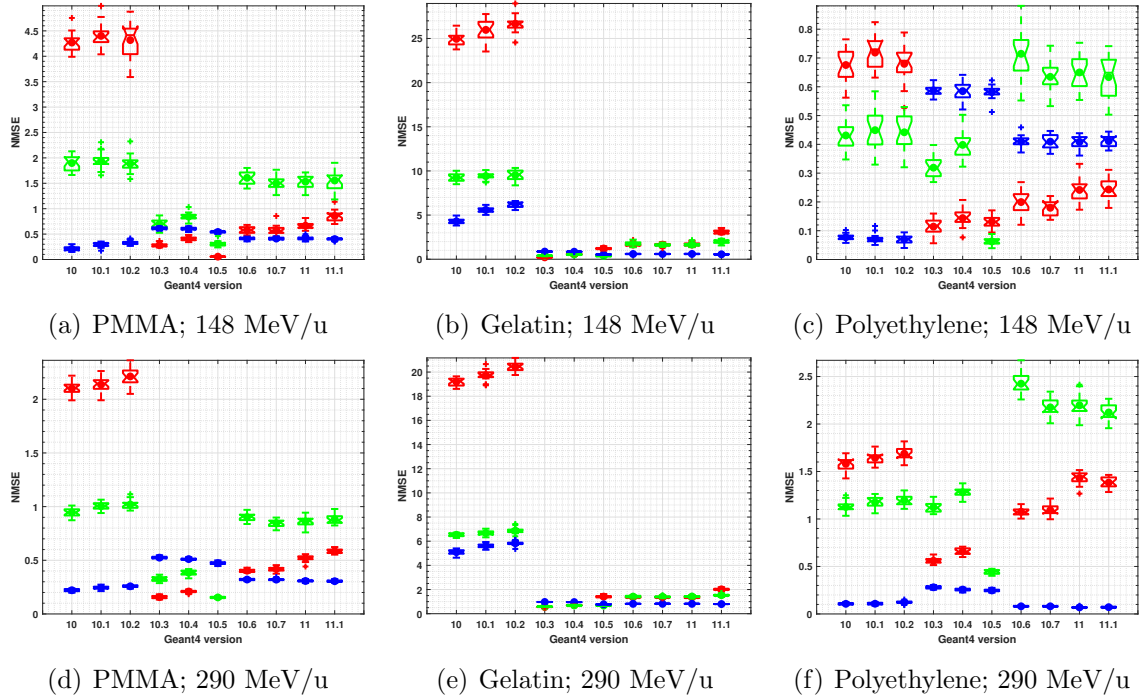
2.2.1. NMSE The NMSEs for total positron annihilation yield in the entrance region for oxygen ion irradiation is presented in Supplementary Figure 9; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 10-12.



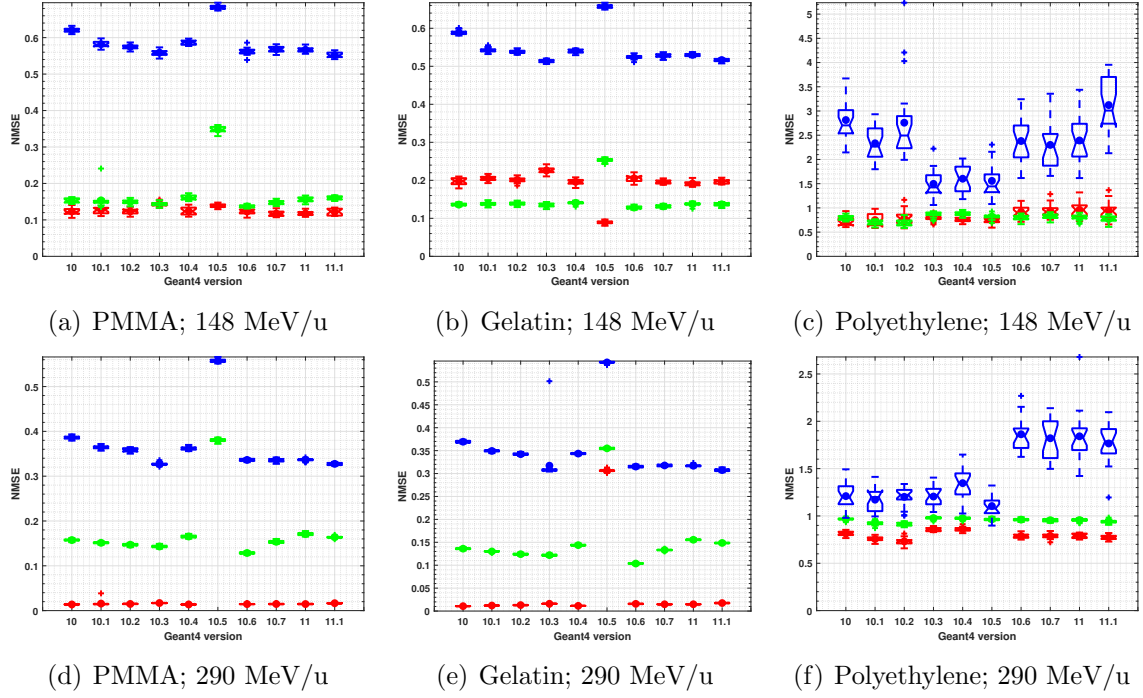
Supplementary Figure 9: NMSE between simulation and experimental measurements of total positron annihilations in the entrance region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 10: NMSE between simulations and experimental measurements of ^{11}C fragment production in the entrance region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

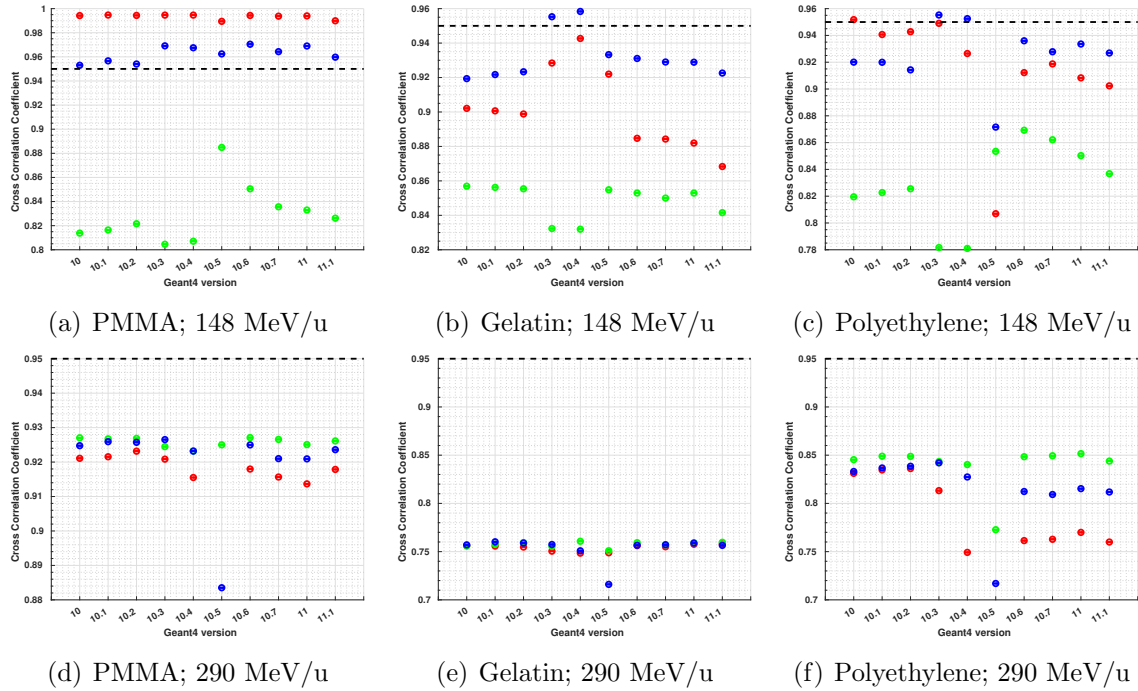


Supplementary Figure 11: NMSE between simulations and experimental measurements of ^{10}C fragment production in the entrance region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

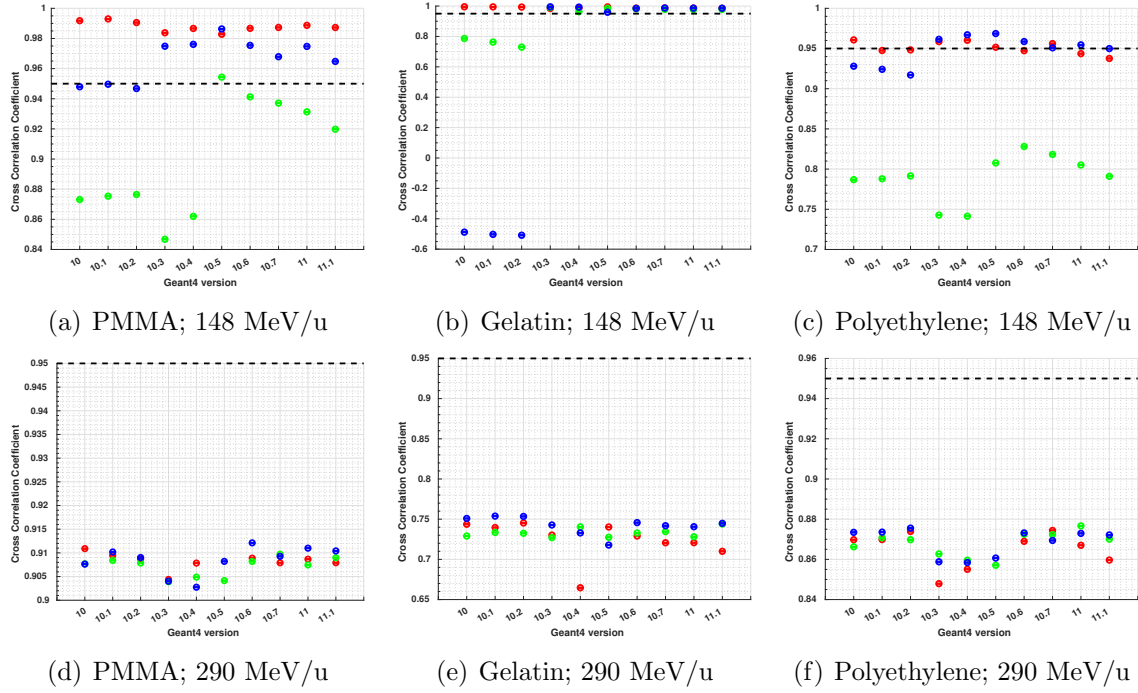


Supplementary Figure 12: NMSE between simulations and experimental measurements of ^{15}O fragment production in the entrance region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

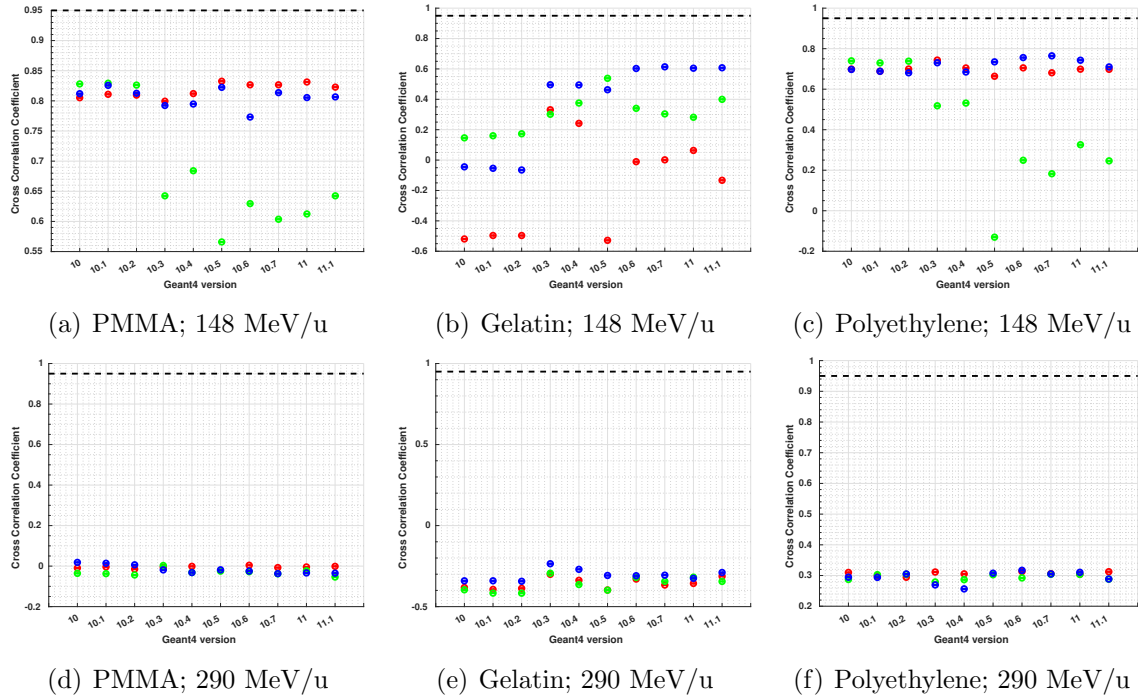
2.2.2. *Pearson CCC* The Pearson CCCs for total positron annihilation yield in the entrance region for oxygen ion irradiation is presented in Supplementary Figure 13; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 14-16.



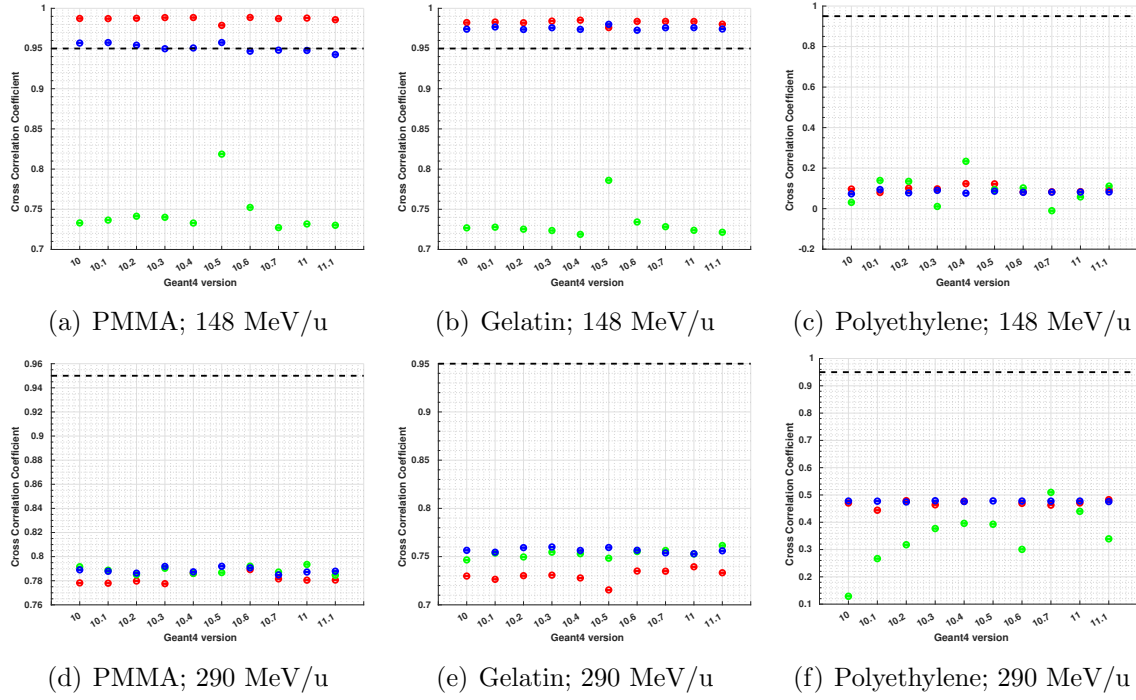
Supplementary Figure 13: Pearson CCC between simulation and experimental measurements of total positron annihilations in the entrance region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 14: Pearson CCC between simulations and experimental measurements of ^{11}C fragment production in the entrance region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 15: Pearson CCC between simulations and experimental measurements of ^{10}C fragment production in the entrance region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

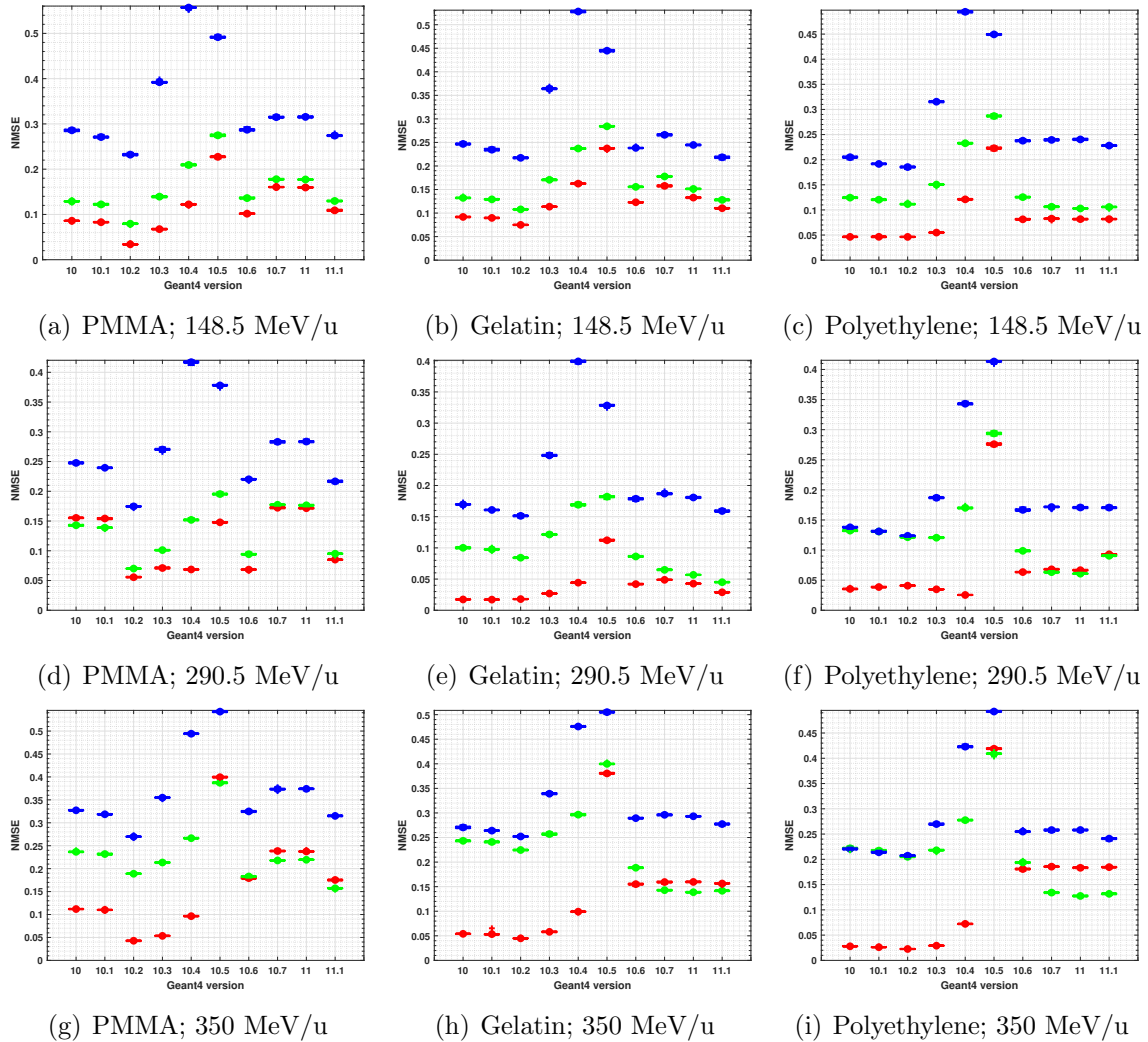


Supplementary Figure 16: Pearson CCC between simulations and experimental measurements of ^{15}O fragment production in the entrance region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

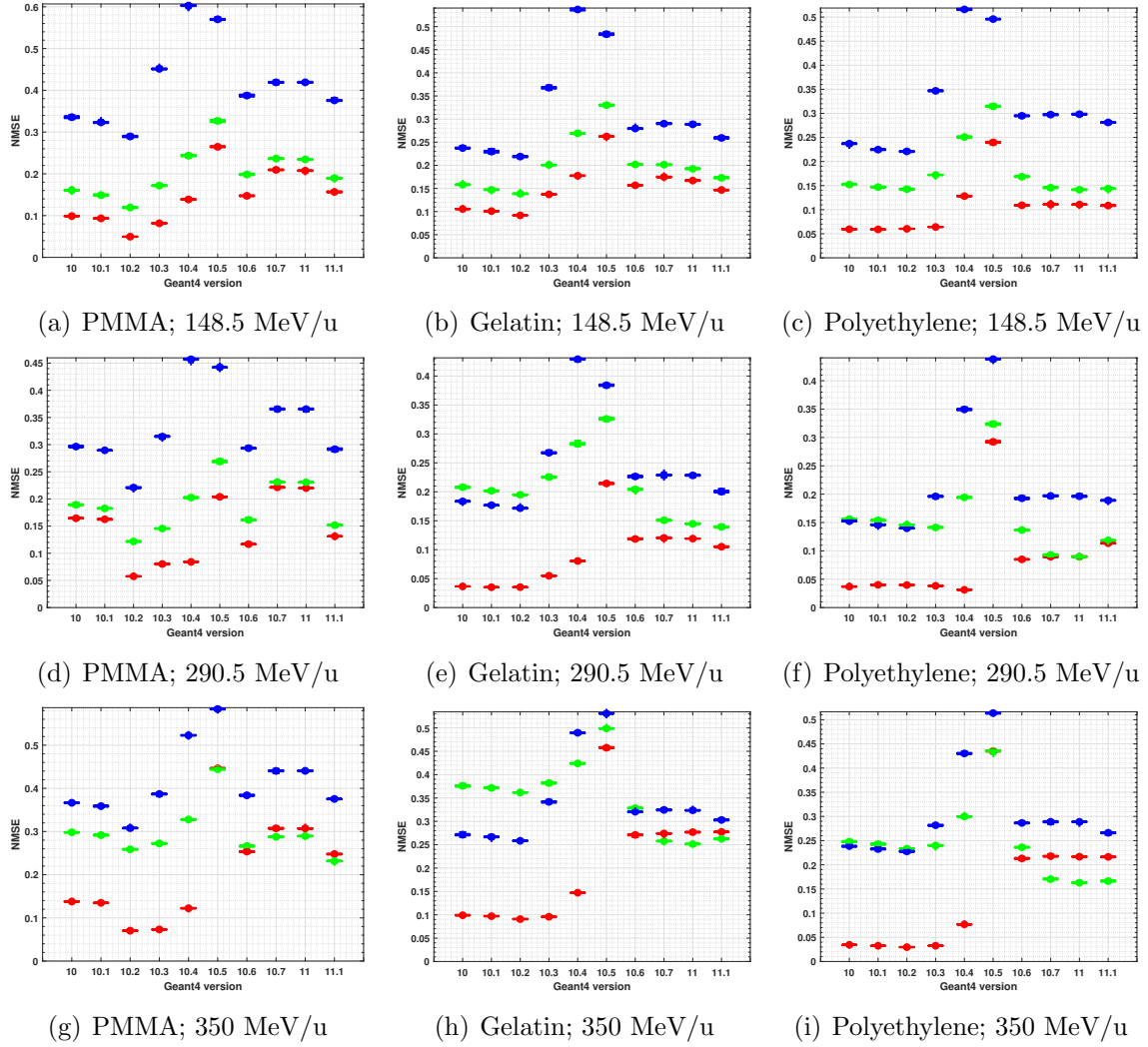
3. Build-up and Bragg peak region

3.1. Carbon ion irradiation

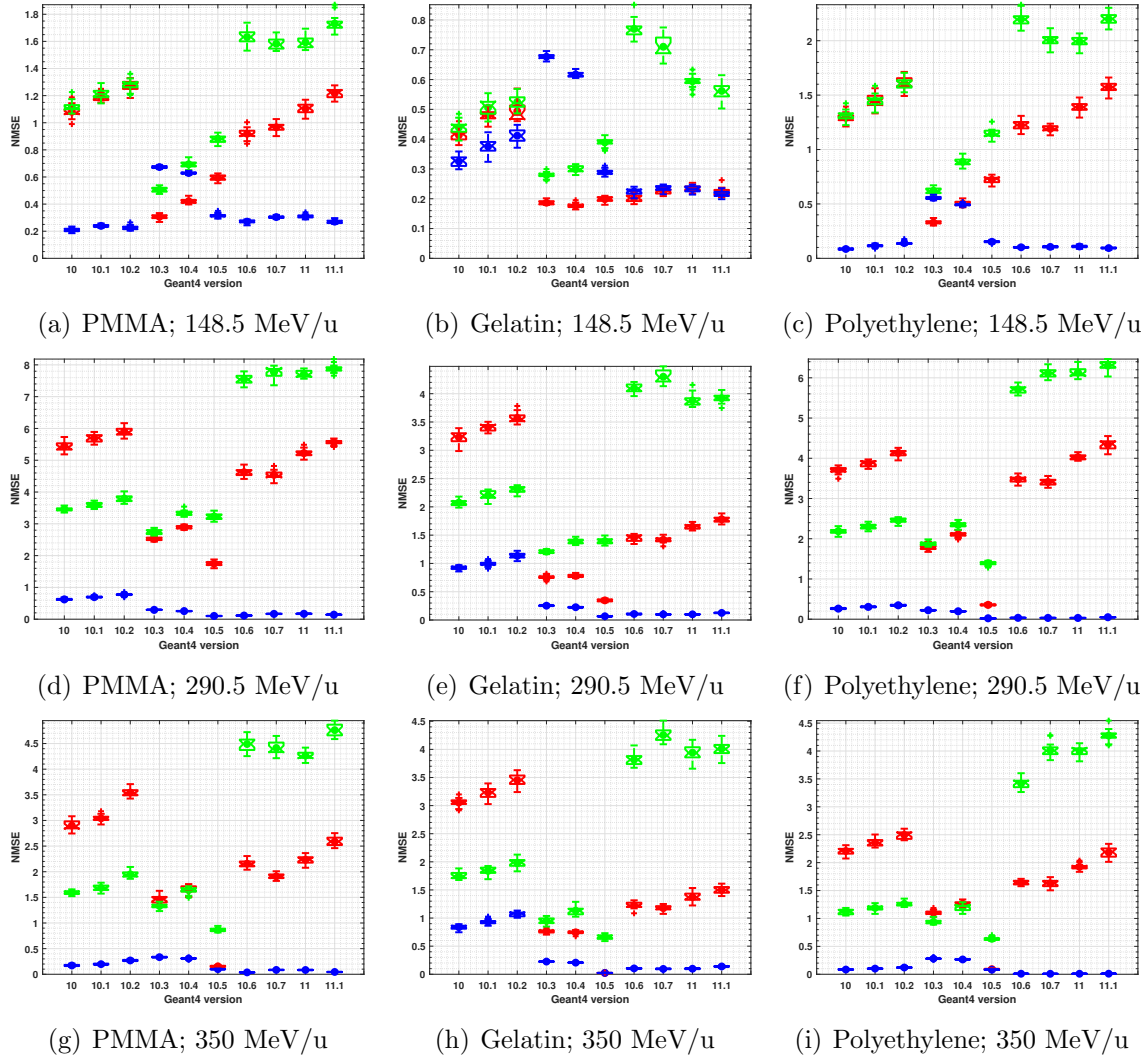
3.1.1. *NMSE* The NMSEs for total positron annihilation yield in the build-up and Bragg peak region for carbon ion irradiation is presented in Supplementary Figure 17; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 18-20.



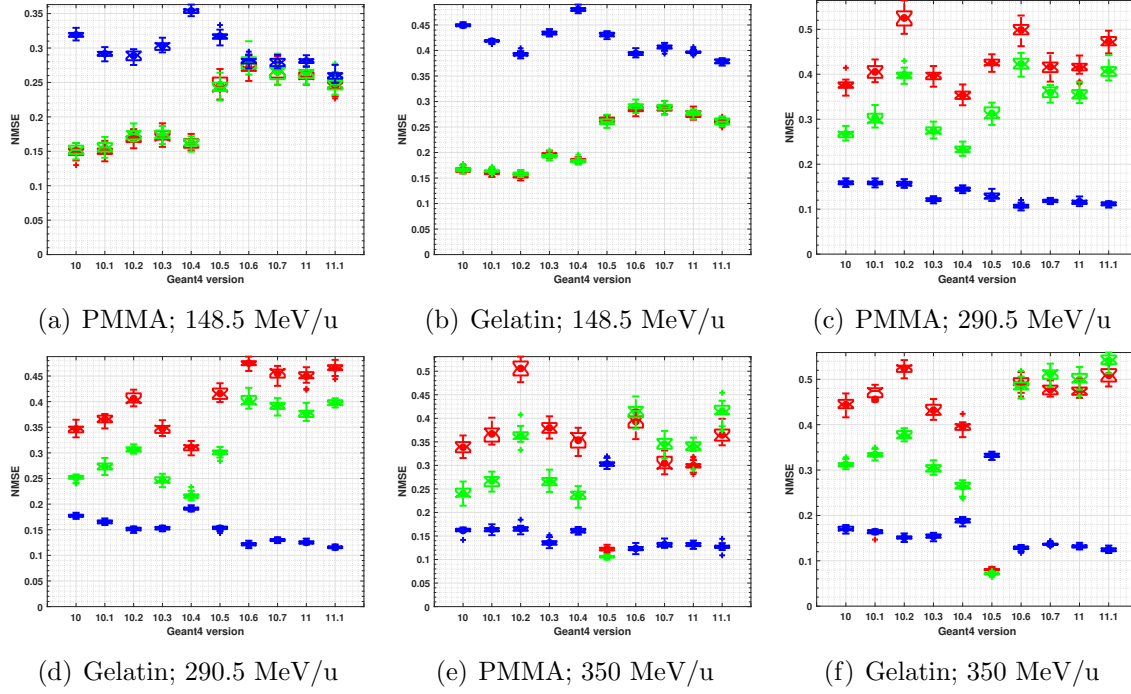
Supplementary Figure 17: NMSE between simulation and experimental measurements of total positron annihilations in the build-up and Bragg peak region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 18: NMSE between simulations and experimental measurements of ^{11}C fragment production in the build-up and Bragg peak region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

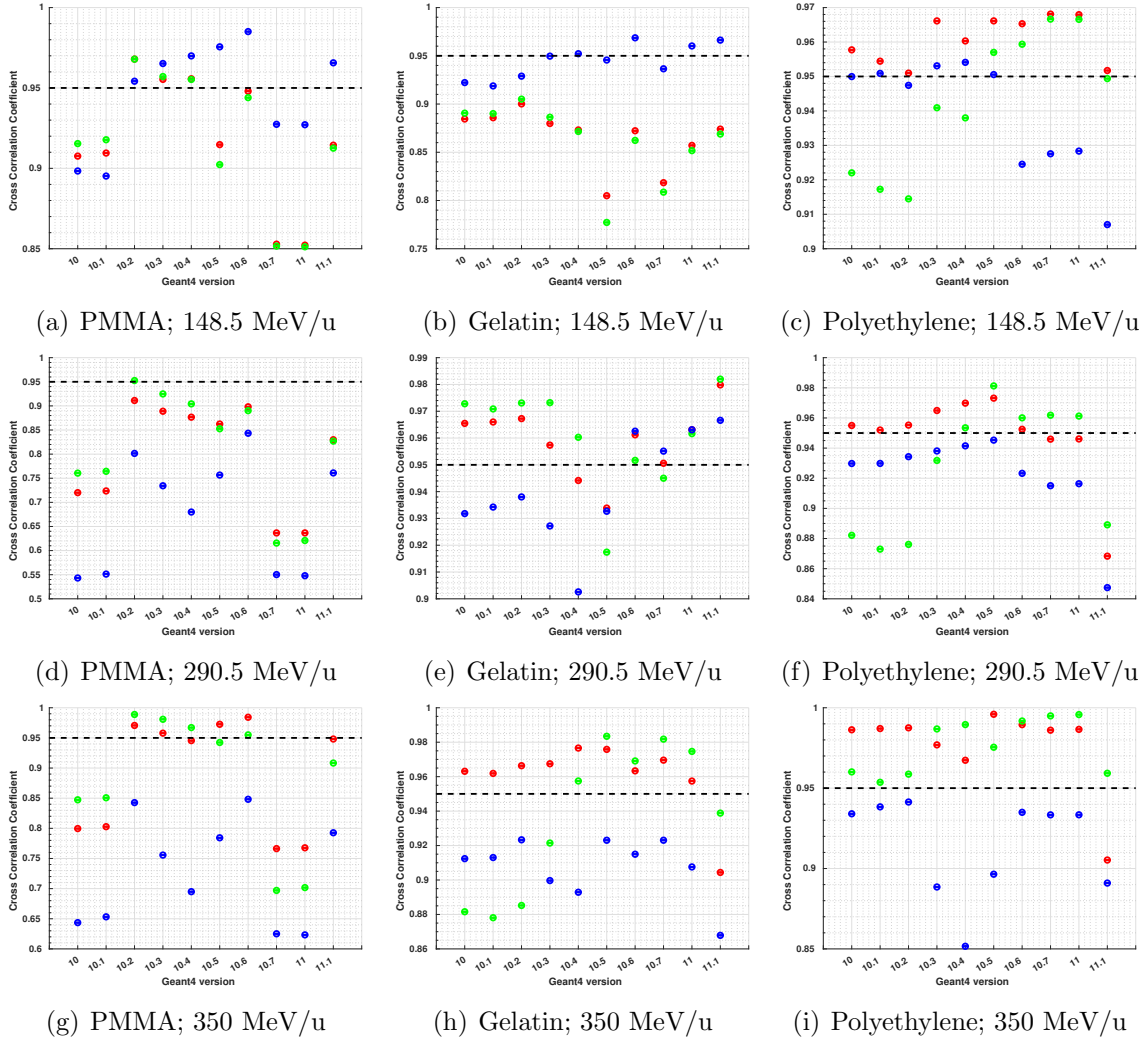


Supplementary Figure 19: NMSE between simulations and experimental measurements of ^{10}C fragment production in the build-up and Bragg peak region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

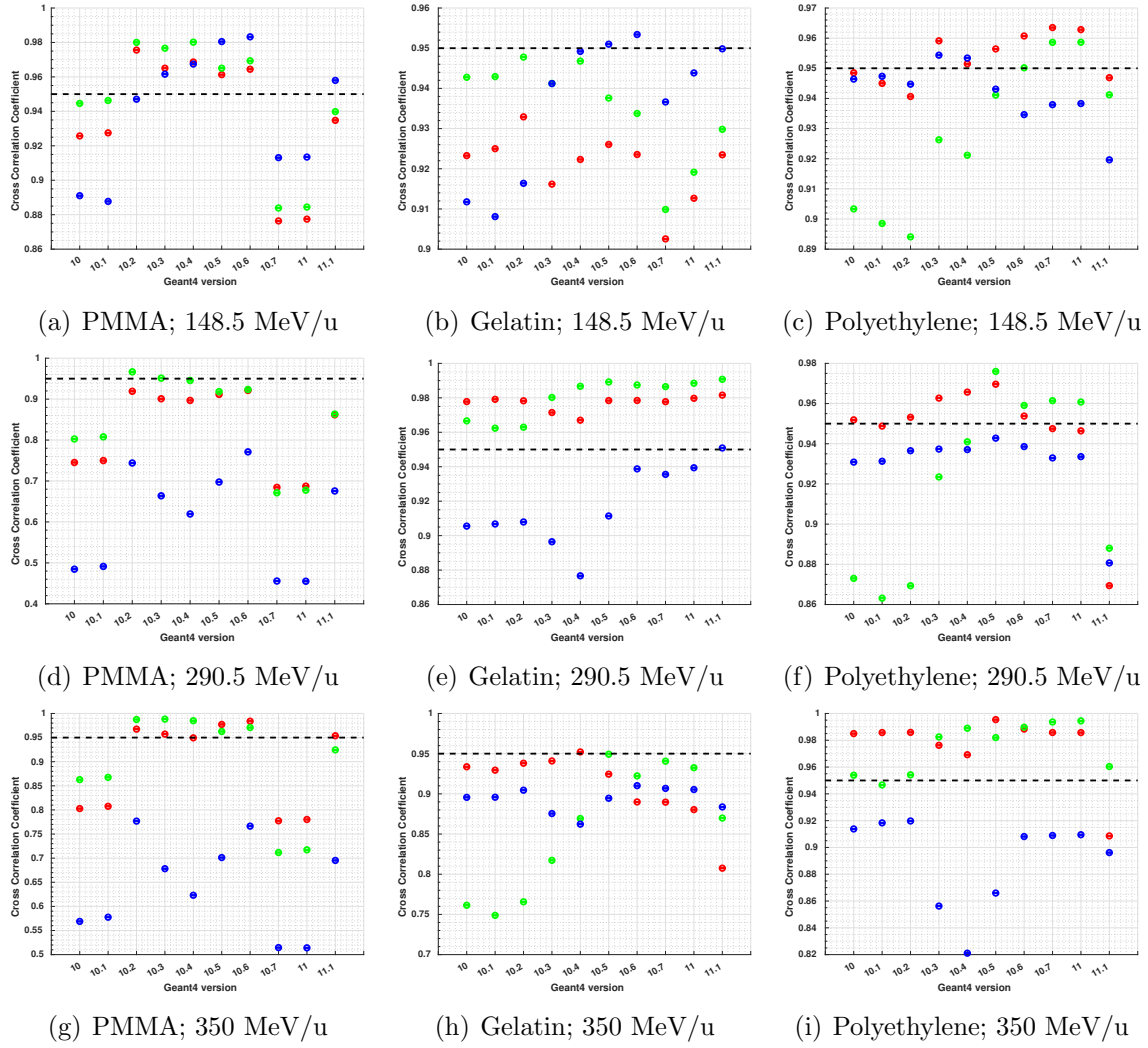


Supplementary Figure 20: NMSE between simulations and experimental measurements of ^{115}O fragment production in the build-up and Bragg peak region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

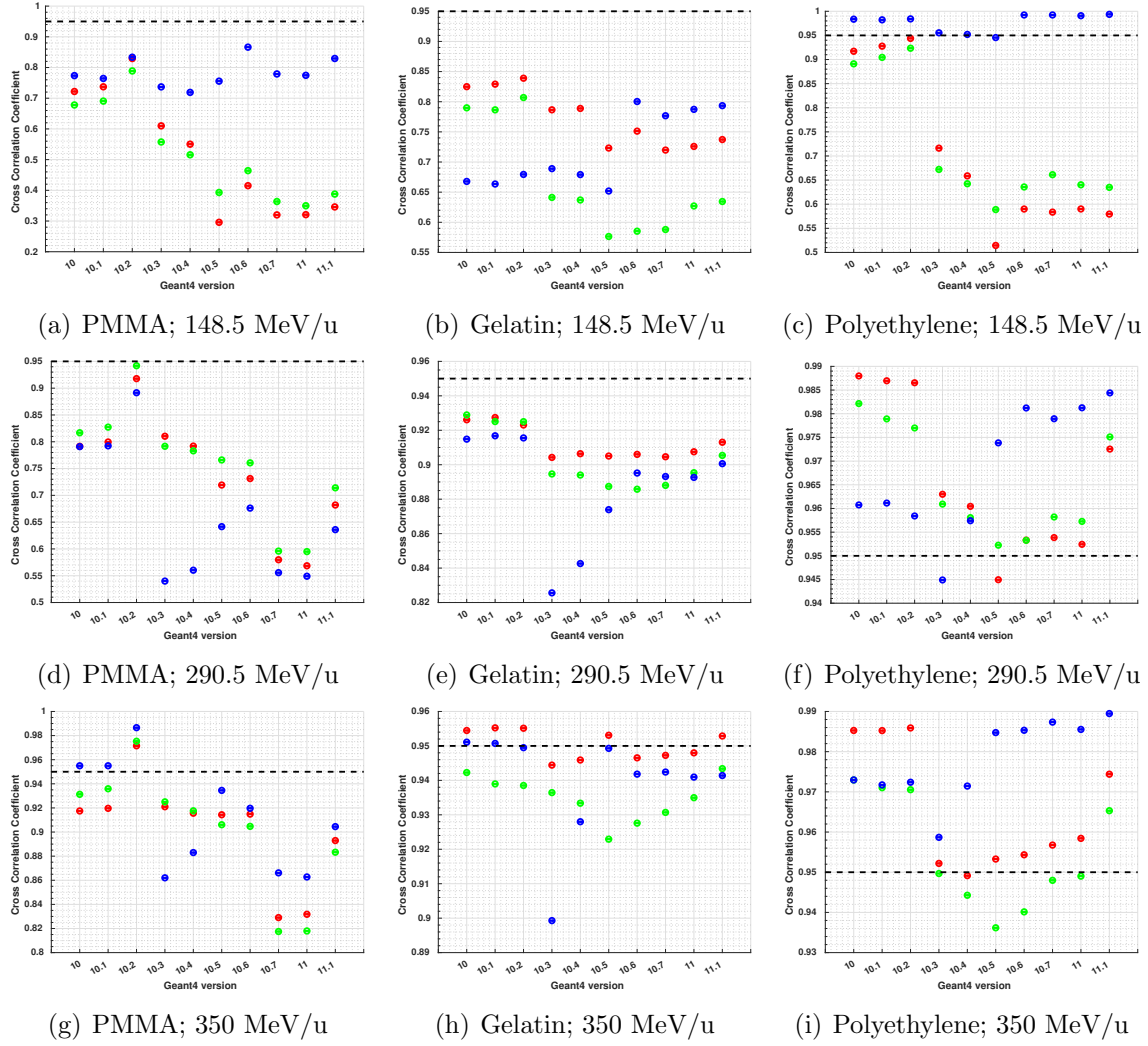
3.1.2. *Pearson CCC* The Pearson CCCs for total positron annihilation yield in the build-up and Bragg peak region for carbon ion irradiation is presented in Supplementary Figure 21; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 22-24.



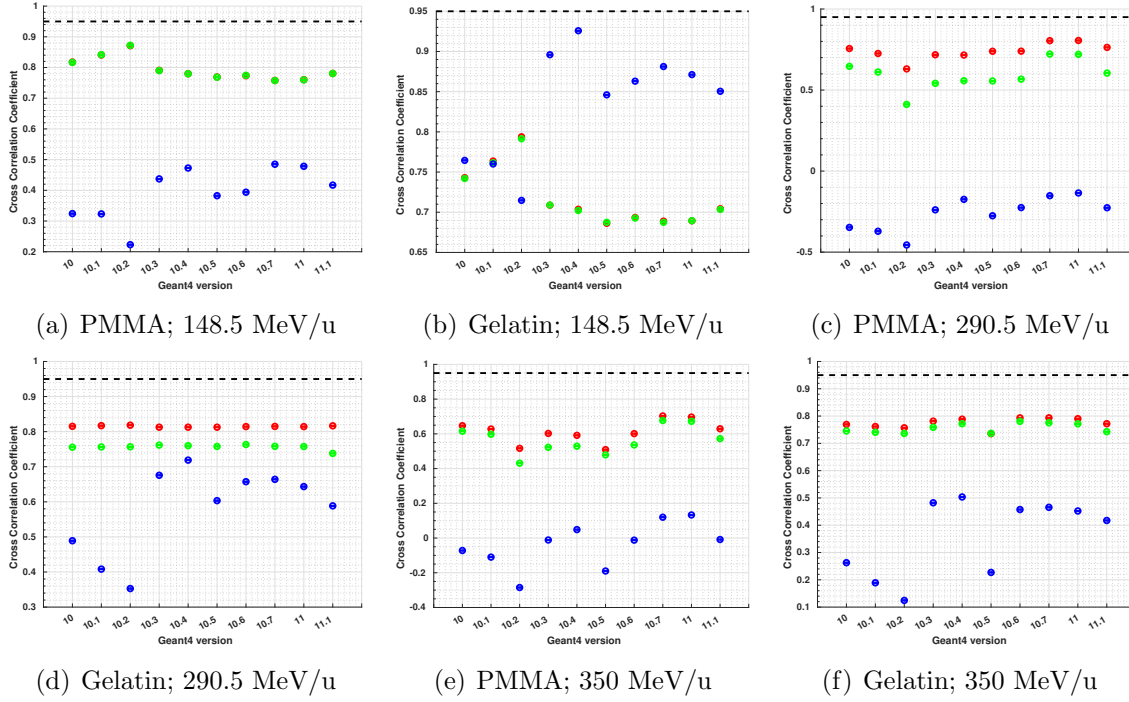
Supplementary Figure 21: Pearson CCC between simulation and experimental measurements of total positron annihilations in the build-up and Bragg peak region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 22: Pearson CCC between simulations and experimental measurements of ^{11}C fragment production in the build-up and Bragg peak region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



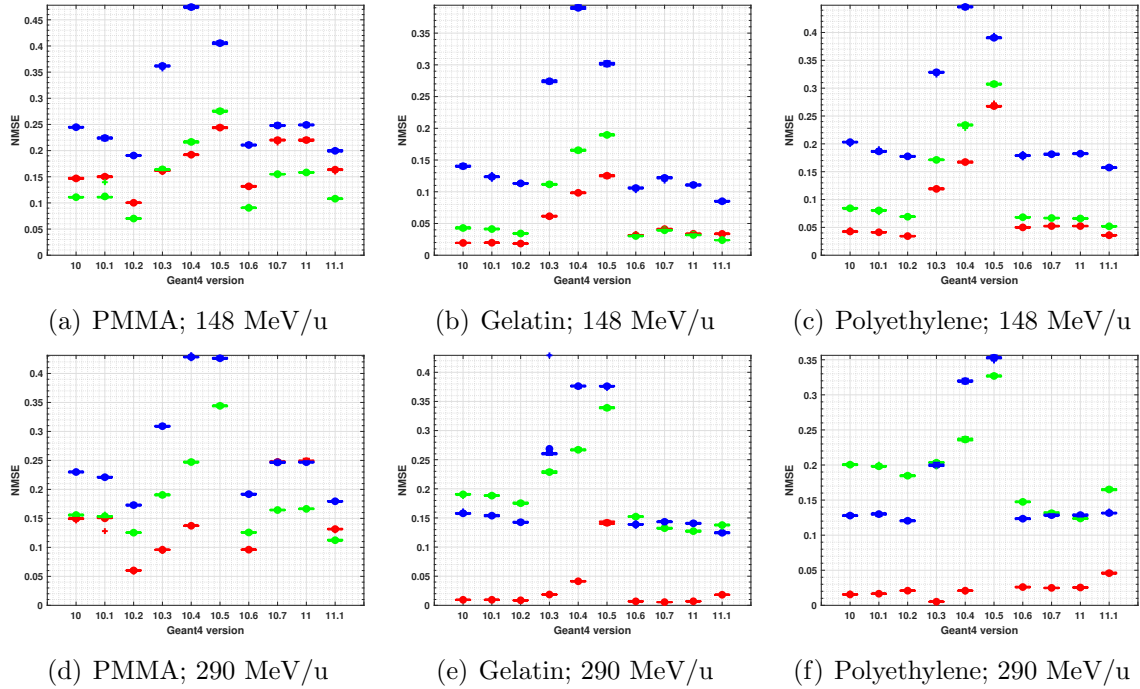
Supplementary Figure 23: Pearson CCC between simulations and experimental measurements of ^{10}C fragment production in the build-up and Bragg peak region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



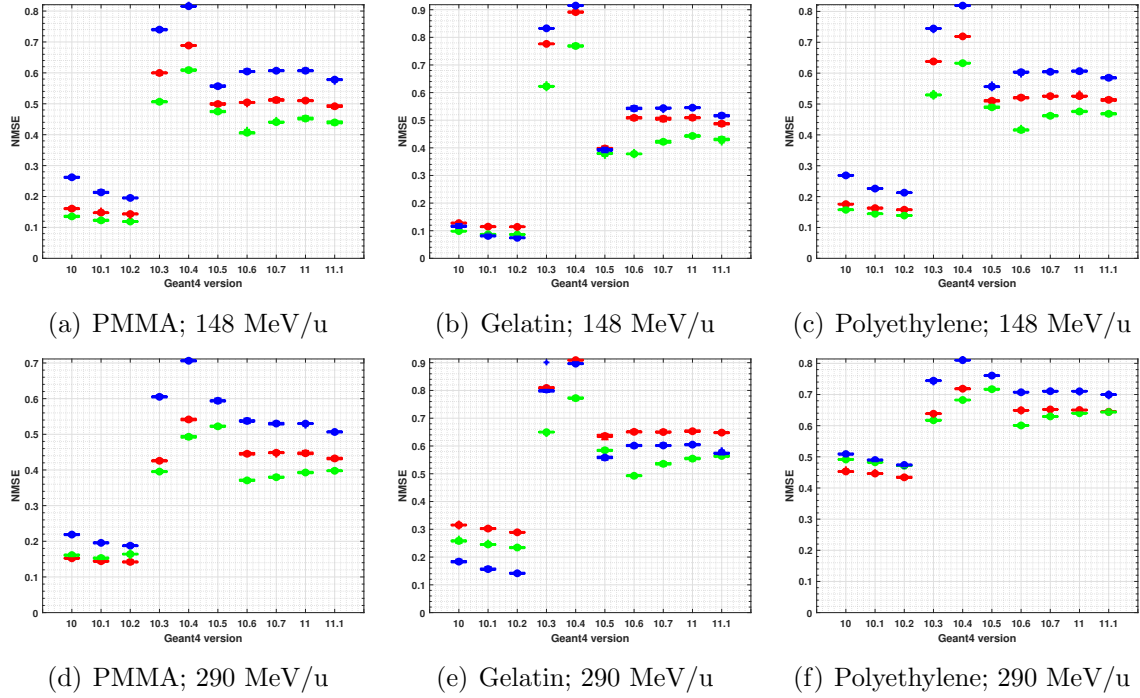
Supplementary Figure 24: Pearson CCC between simulations and experimental measurements of ^{15}O fragment production in the build-up and Bragg peak region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

3.2. Oxygen ion irradiation

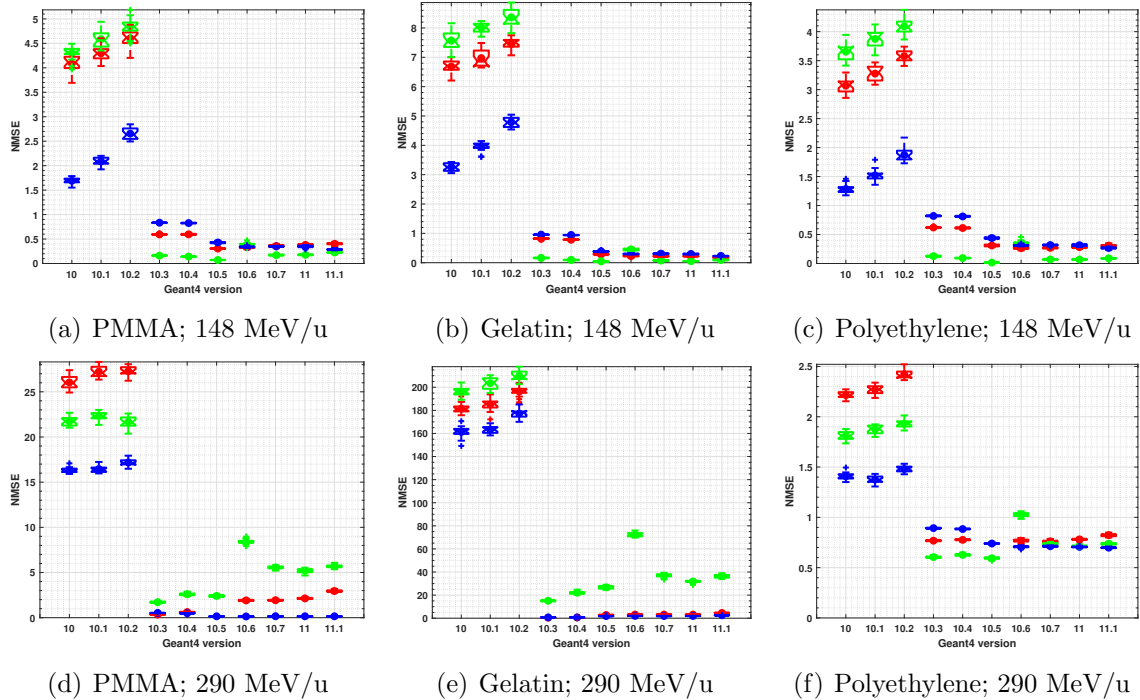
3.2.1. *NMSE* The NMSEs for total positron annihilation yield in the build-up and Bragg peak region for oxygen ion irradiation is presented in Supplementary Figure 25; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 26-28.



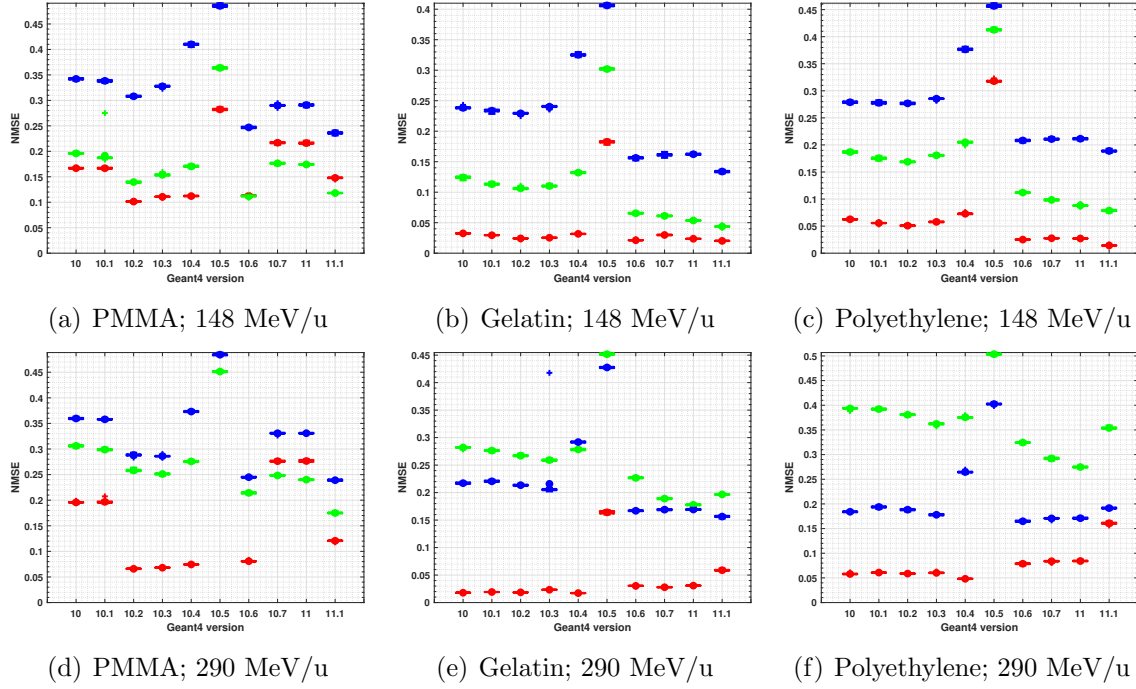
Supplementary Figure 25: NMSE between simulation and experimental measurements of total positron annihilations in the build-up and Bragg peak region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 26: NMSE between simulations and experimental measurements of ^{11}C fragment production in the build-up and Bragg peak region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

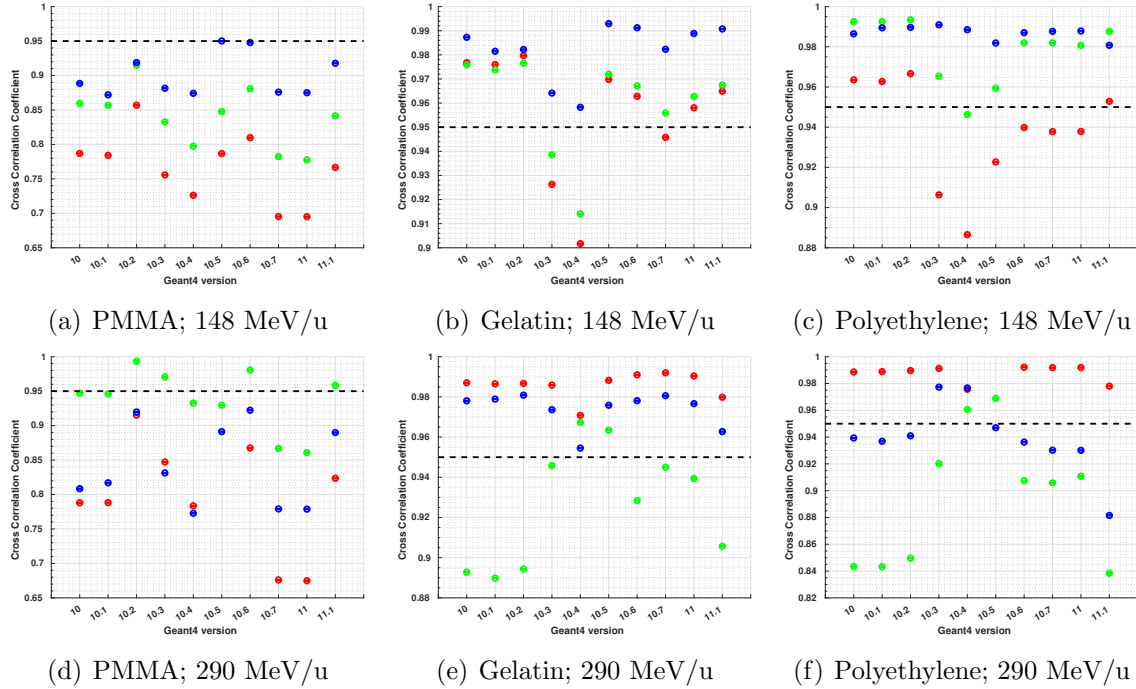


Supplementary Figure 27: NMSE between simulations and experimental measurements of ^{10}C fragment production in the build-up and Bragg peak region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

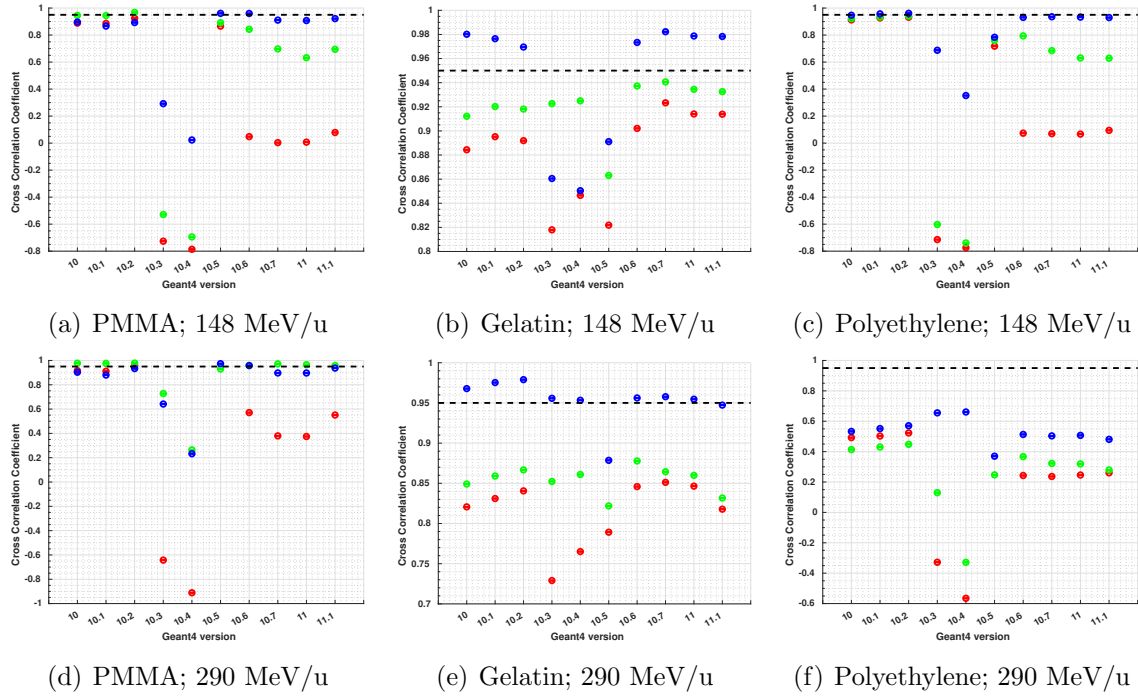


Supplementary Figure 28: NMSE between simulations and experimental measurements of ^{15}O fragment production in the build-up and Bragg peak region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

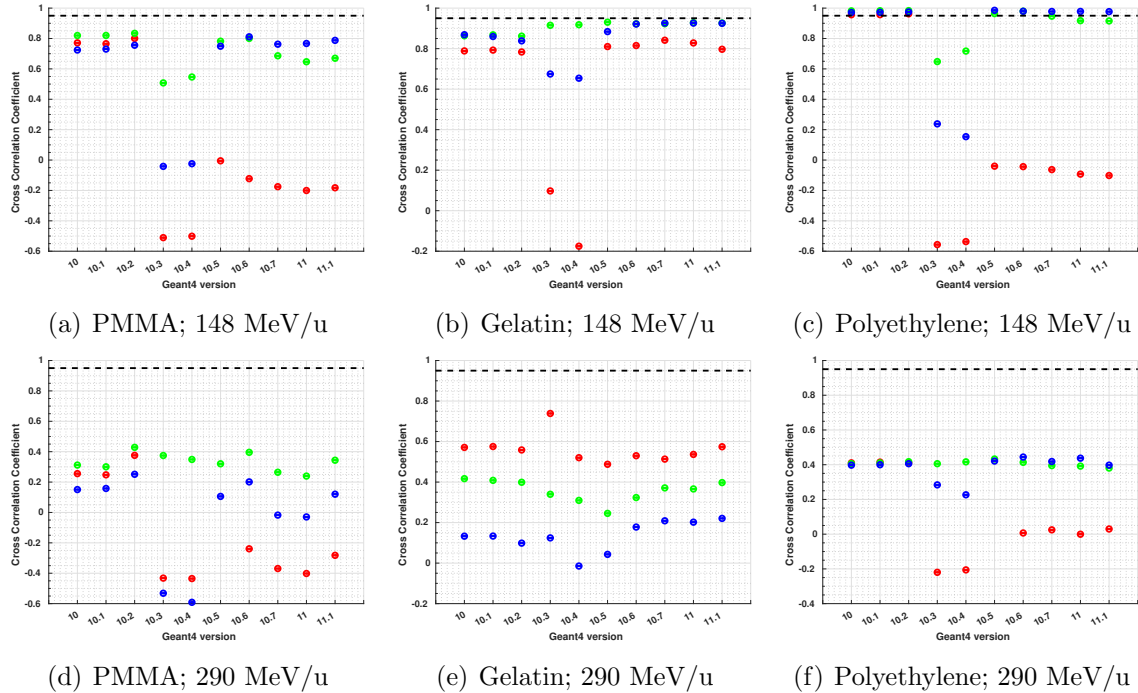
63 **3.2.2. Pearson CCC** The Pearson CCCs for total positron annihilation yield in the
 64 build-up and Bragg peak region for oxygen ion irradiation is presented in Supplementary
 65 Figure 29; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in
 66 Supplementary Figure 30-32.



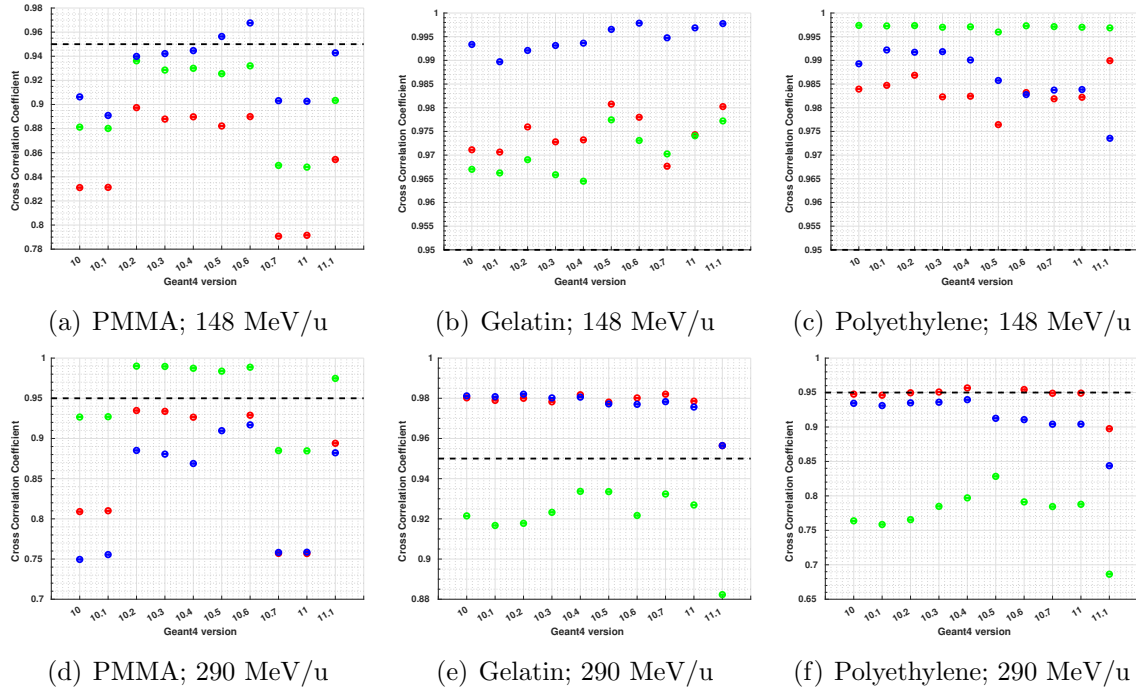
Supplementary Figure 29: Pearson CCC between simulation and experimental measurements of total positron annihilations in the build-up and Bragg peak region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 30: Pearson CCC between simulations and experimental measurements of ^{11}C fragment production in the build-up and Bragg peak region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 31: Pearson CCC between simulations and experimental measurements of ^{10}C fragment production in the build-up and Bragg peak region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

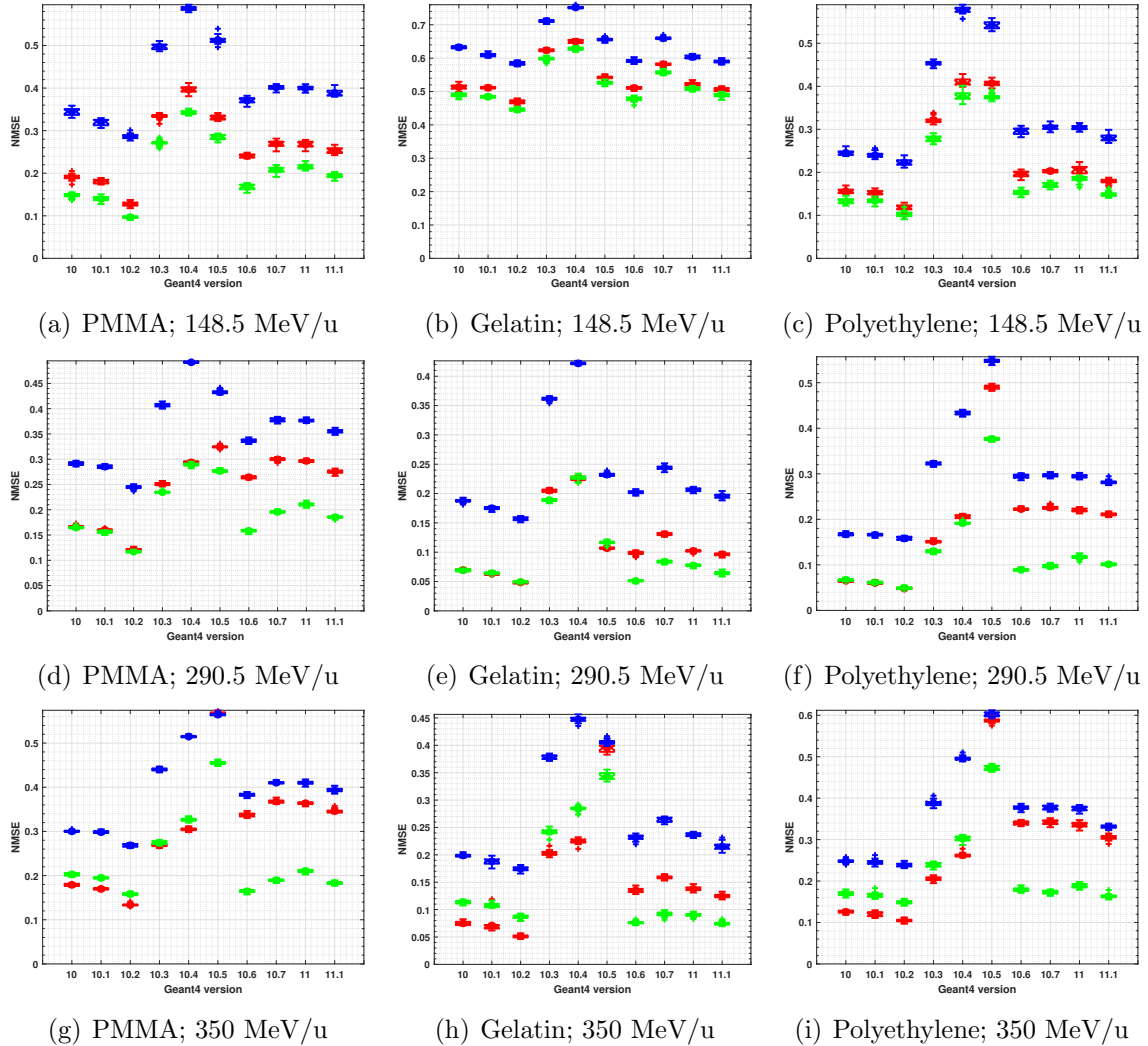


Supplementary Figure 32: Pearson CCC between simulations and experimental measurements of ^{15}O fragment production in the build-up and Bragg peak region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

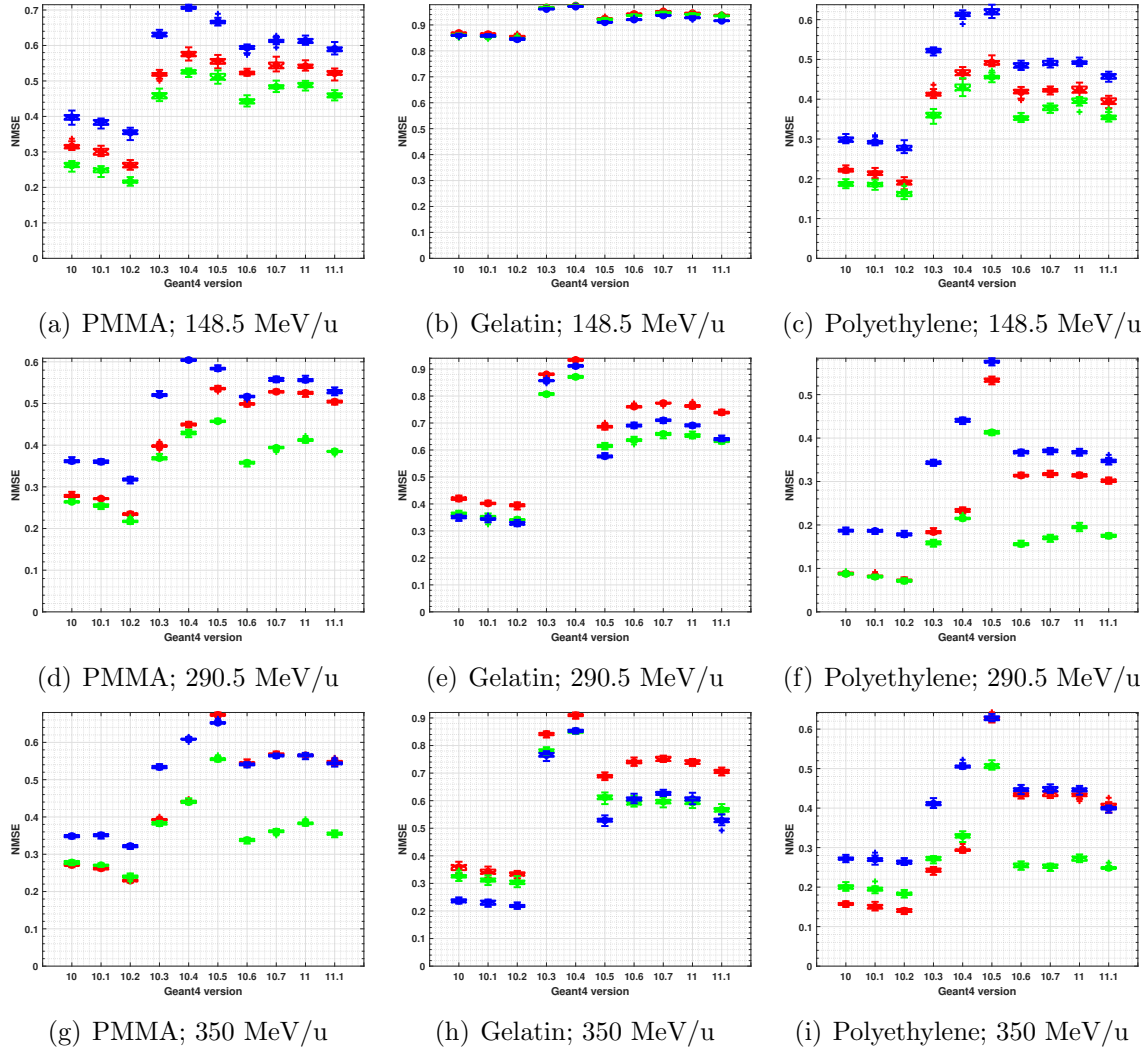
4. Tail region

4.1. Carbon ion irradiation

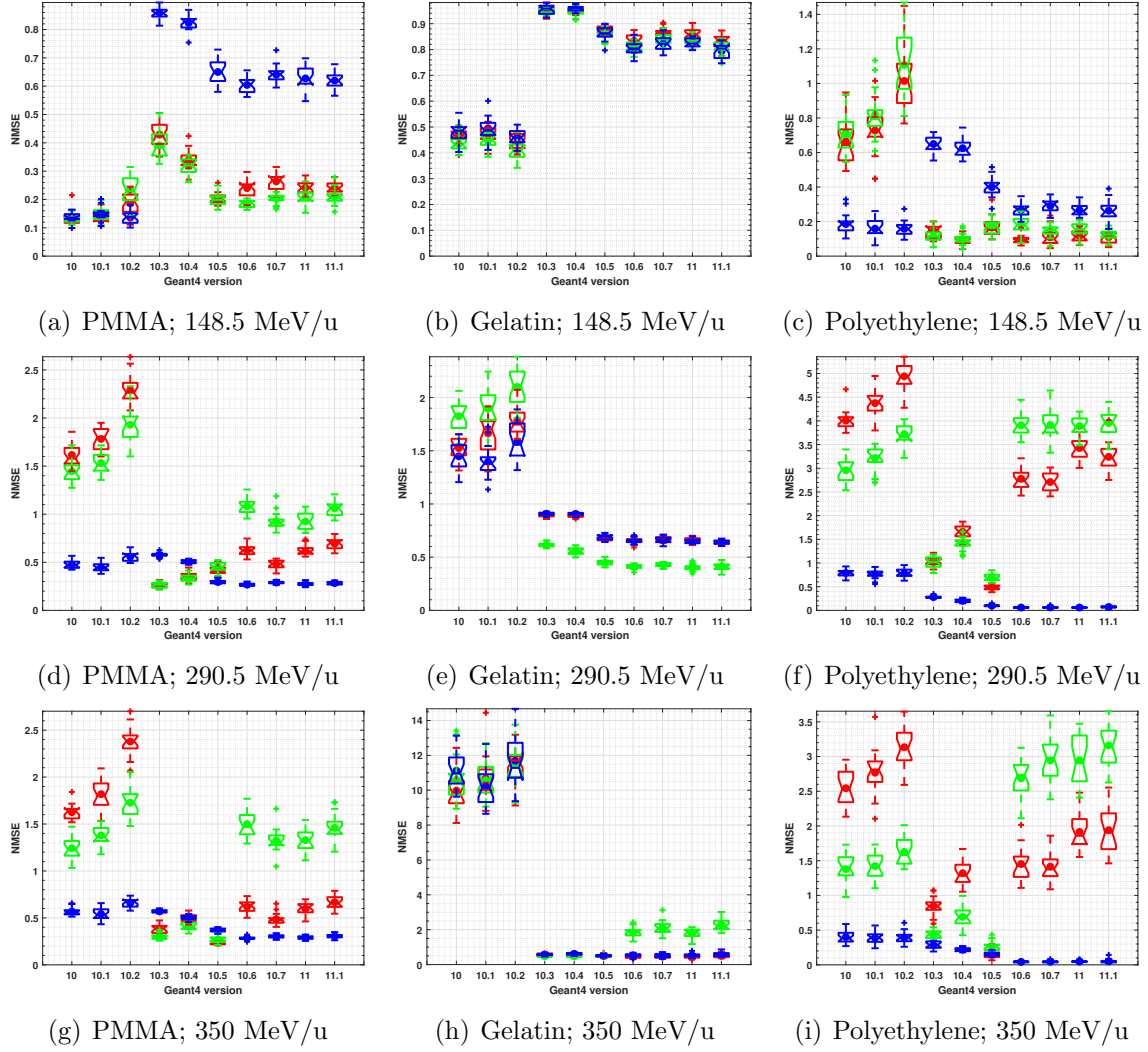
4.1.1. *NMSE* The NMSEs for total positron annihilation yield in the tail region for carbon ion irradiation is presented in Supplementary Figure 33; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 34-36.



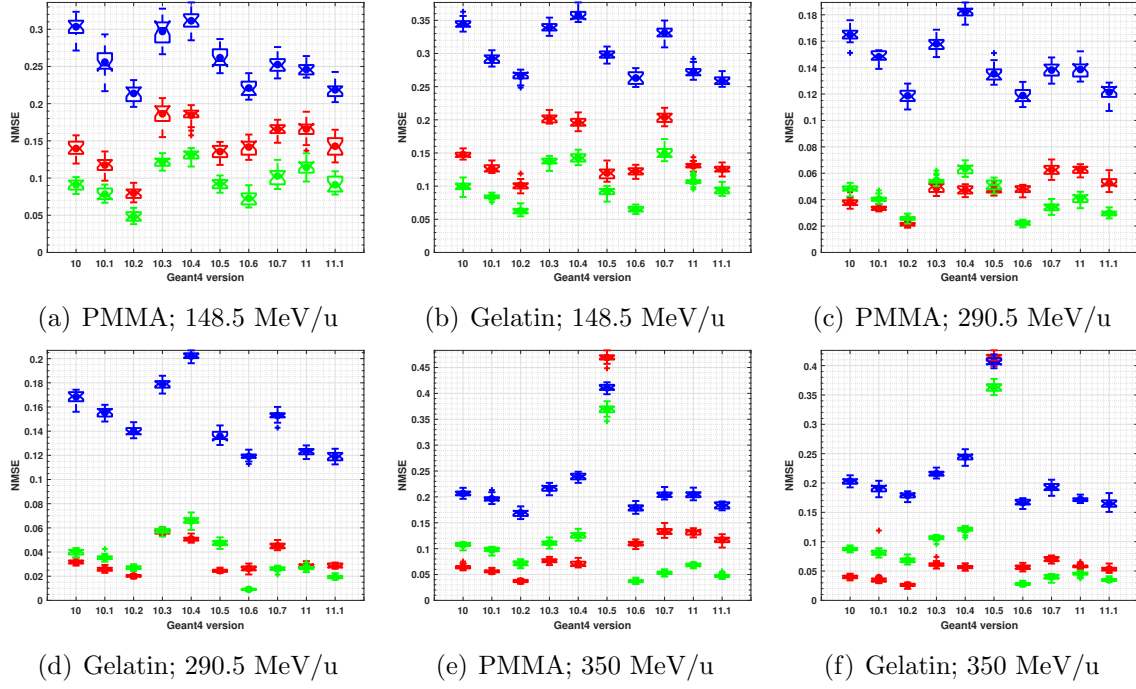
Supplementary Figure 33: NMSE between simulation and experimental measurements of total positron annihilations in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 34: NMSE between simulations and experimental measurements of ^{11}C fragment production in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

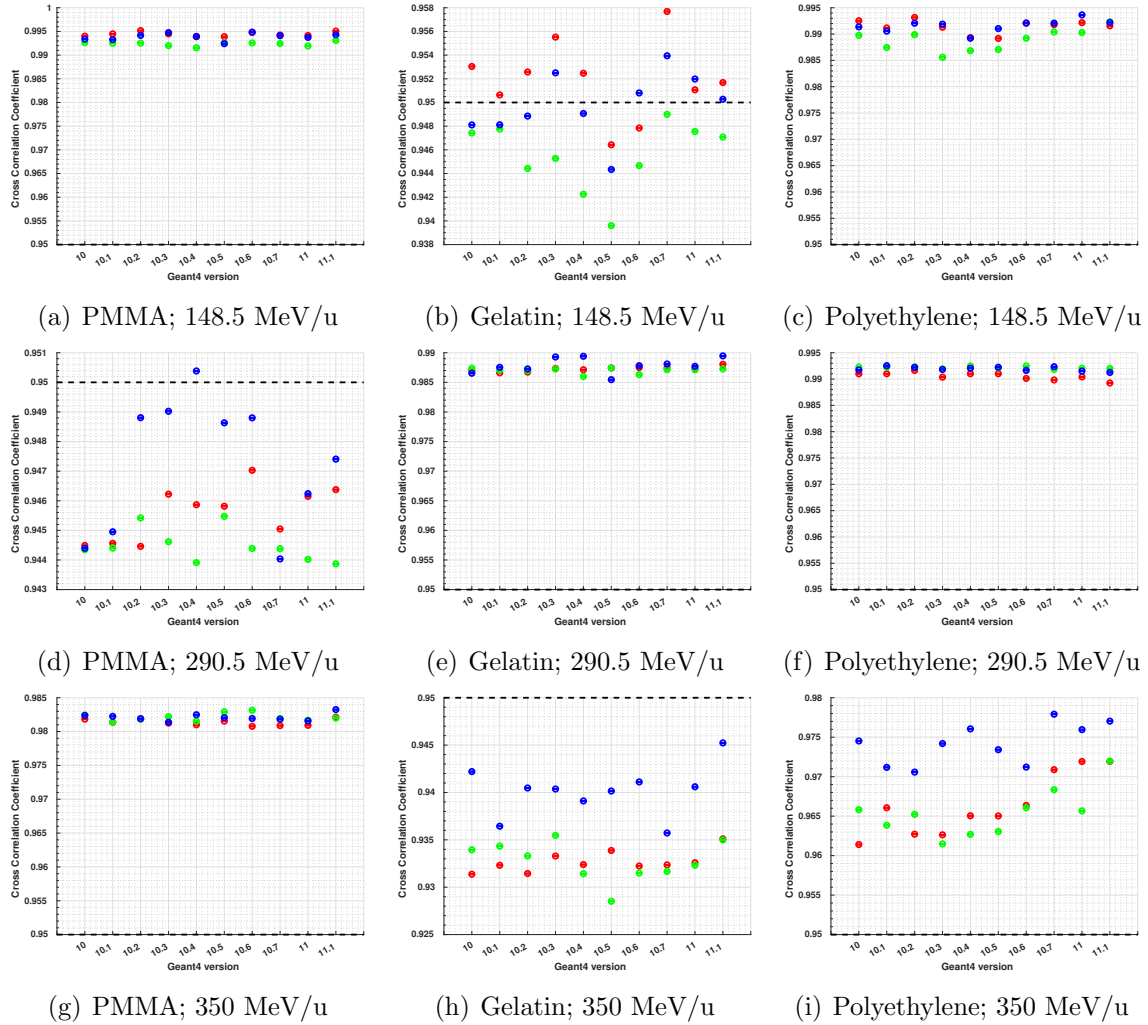


Supplementary Figure 35: NMSE between simulations and experimental measurements of ^{10}C fragment production in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

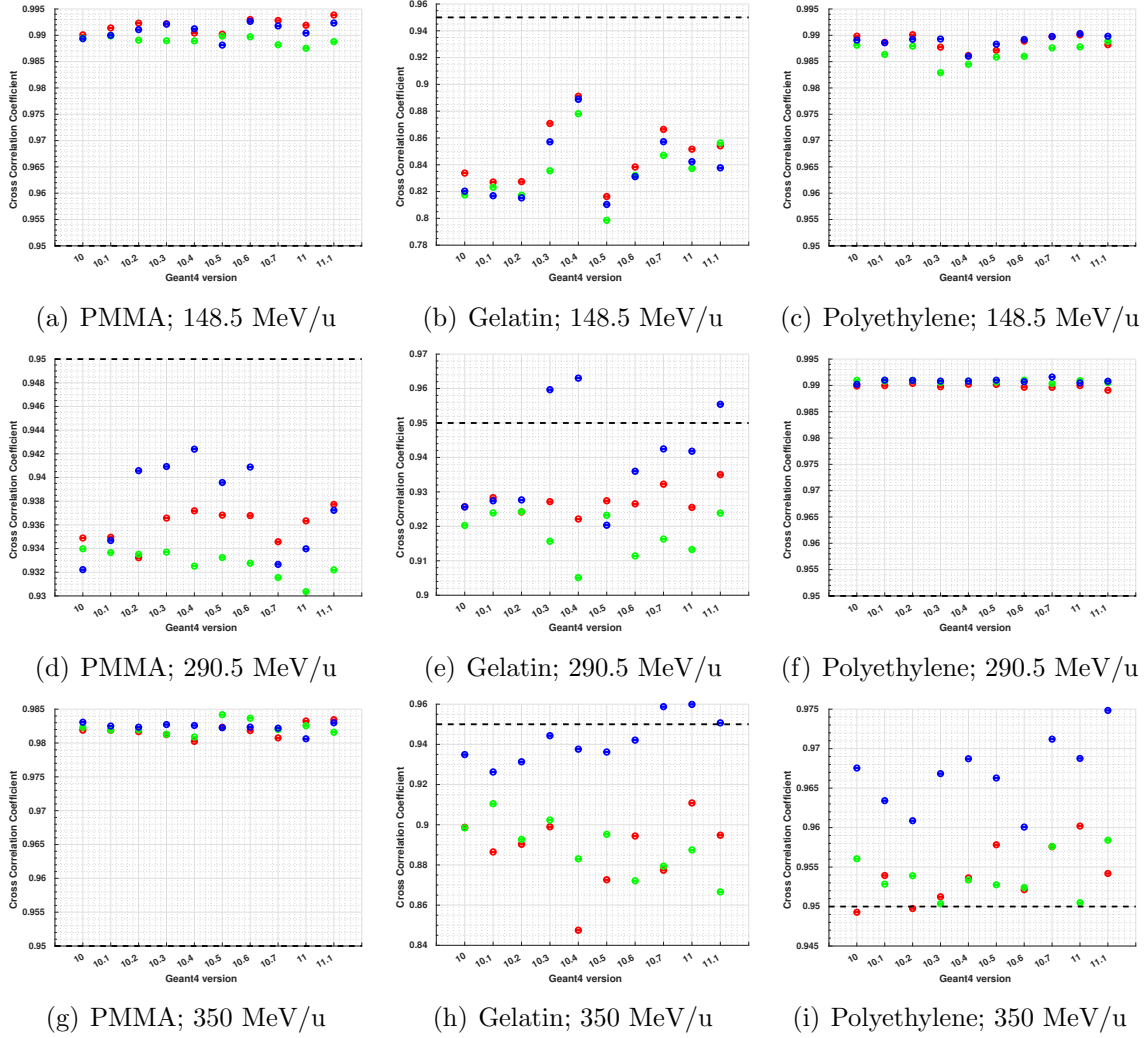


Supplementary Figure 36: NMSE between simulations and experimental measurements of ^{15}O fragment production in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

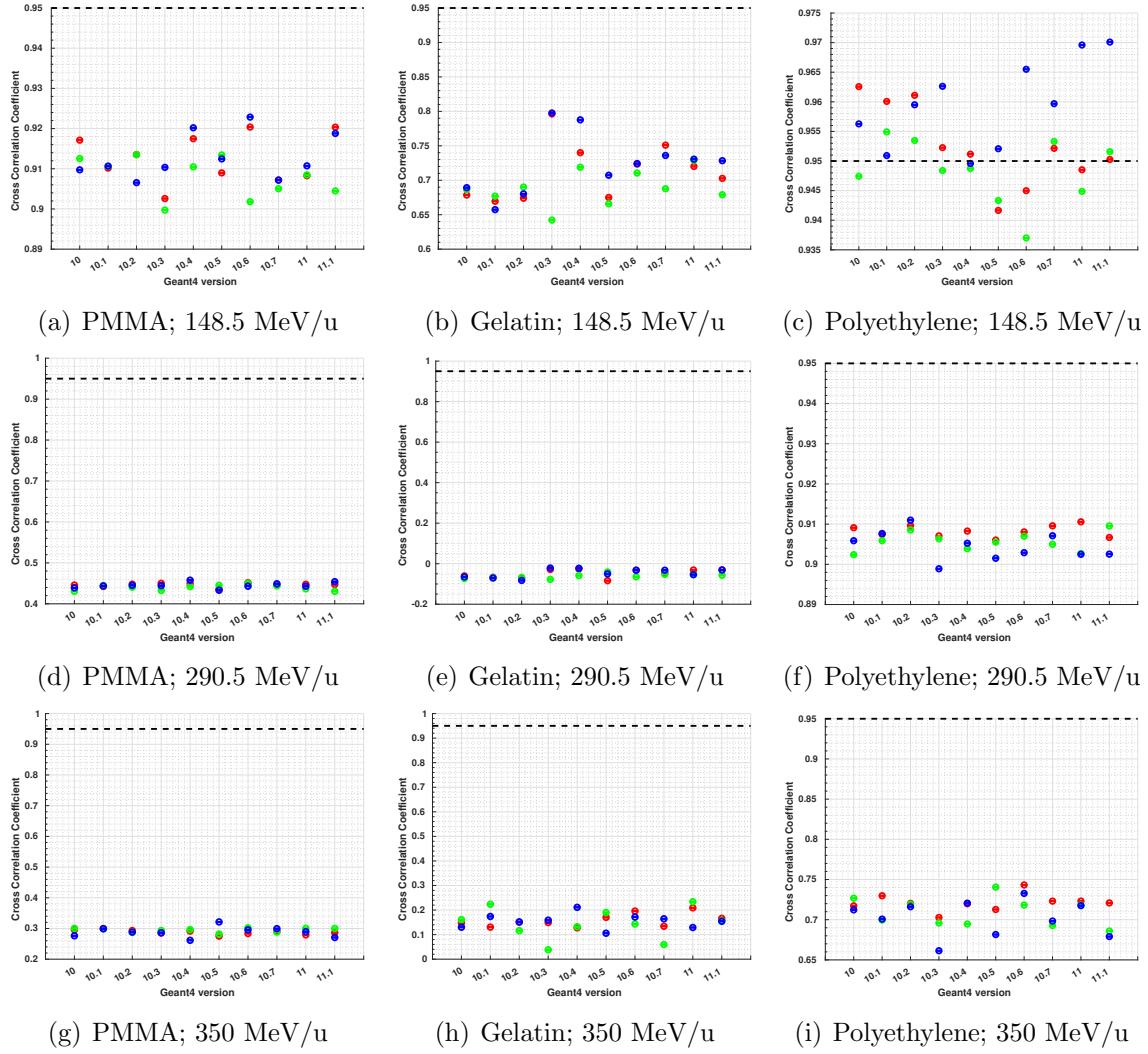
4.1.2. *Pearson CCC* The Pearson CCCs for total positron annihilation yield in the tail region for carbon ion irradiation is presented in Supplementary Figure 37; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 38-40.



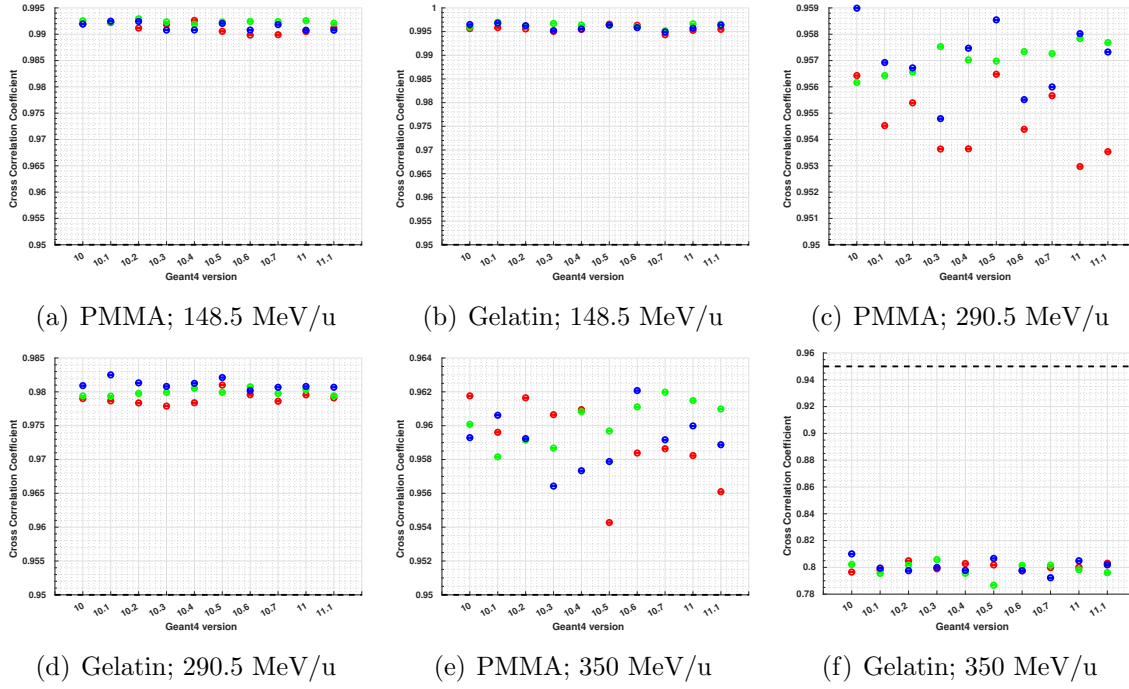
Supplementary Figure 37: Pearson CCC between simulation and experimental measurements of total positron annihilations in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 38: Pearson CCC between simulations and experimental measurements of ^{11}C fragment production in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



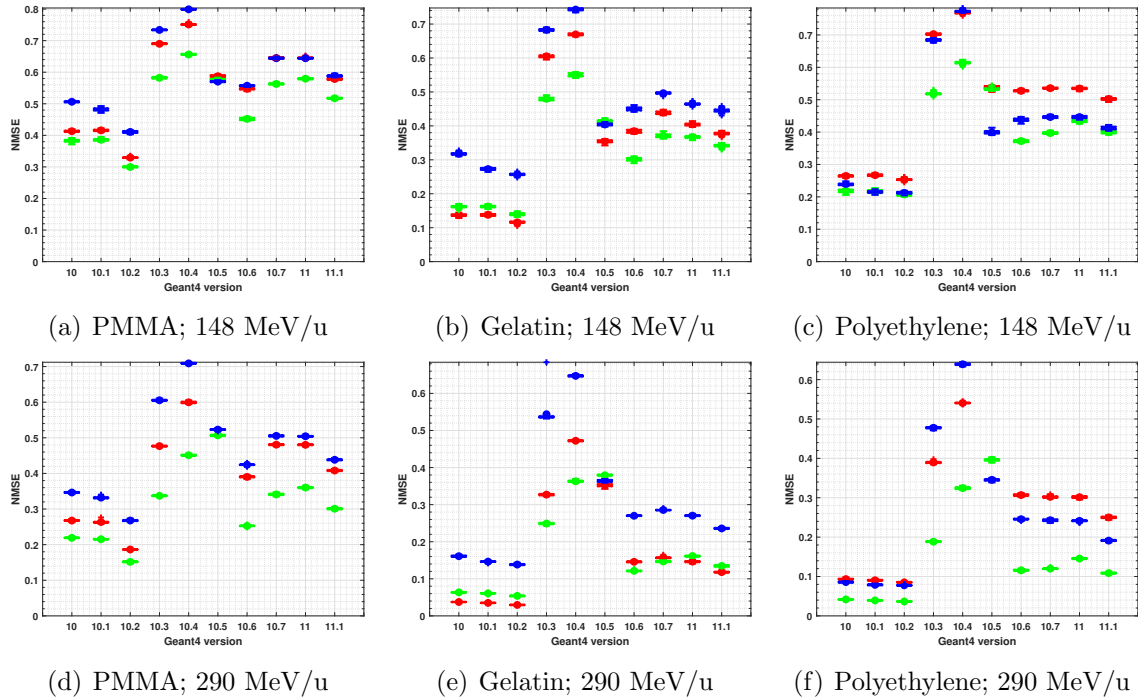
Supplementary Figure 39: Pearson CCC between simulations and experimental measurements of ^{10}C fragment production in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



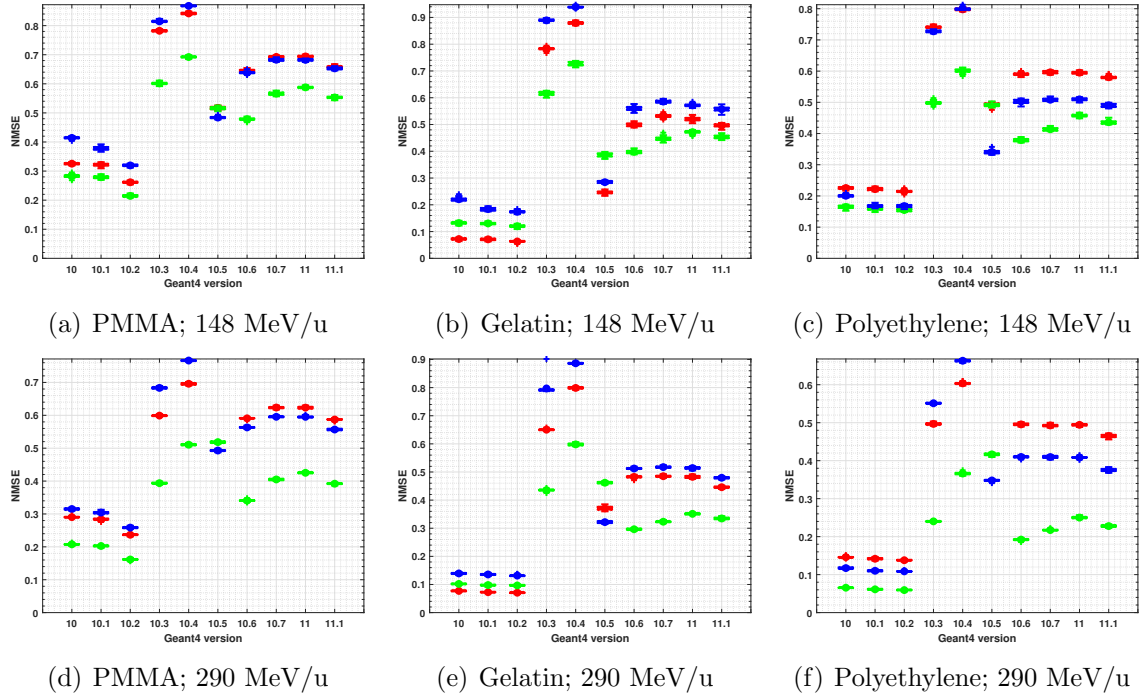
Supplementary Figure 40: Pearson CCC between simulations and experimental measurements of ^{15}O fragment production in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.

4.2. Oxygen ion irradiation

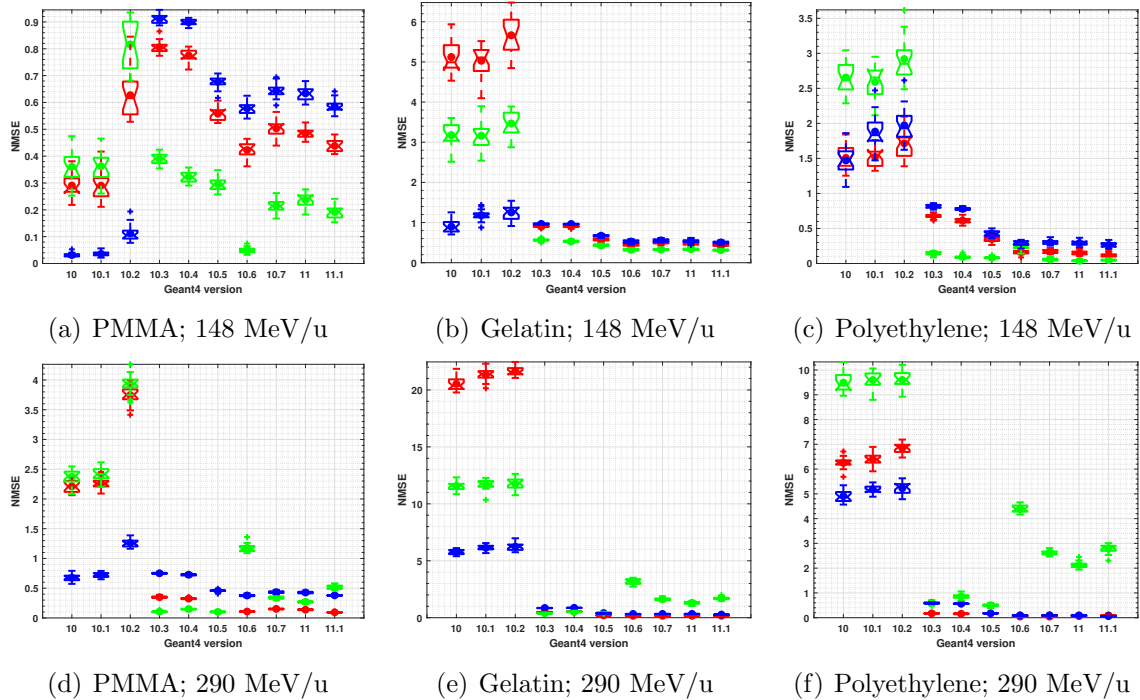
4.2.1. *NMSE* The NMSEs for total positron annihilation yield in the tail region for oxygen ion irradiation is presented in Supplementary Figure 41; the individual contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 42-44.



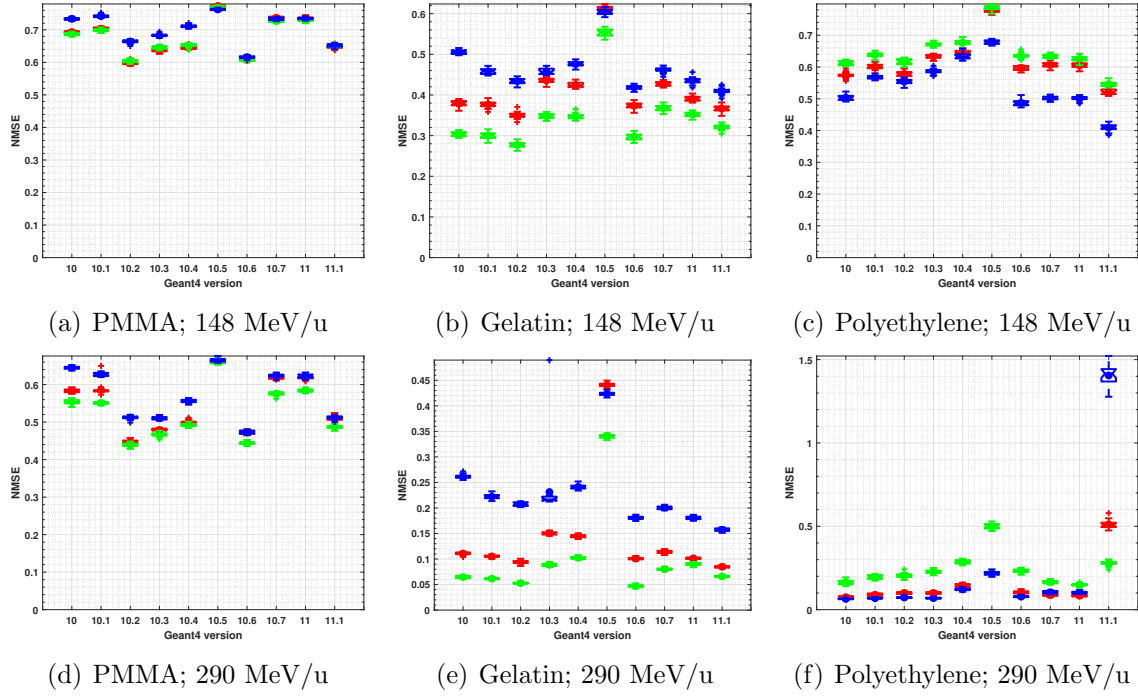
Supplementary Figure 41: NMSE between simulation and experimental measurements of total positron annihilations in the tail region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 42: NMSE between simulations and experimental measurements of ^{11}C fragment production in the tail region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

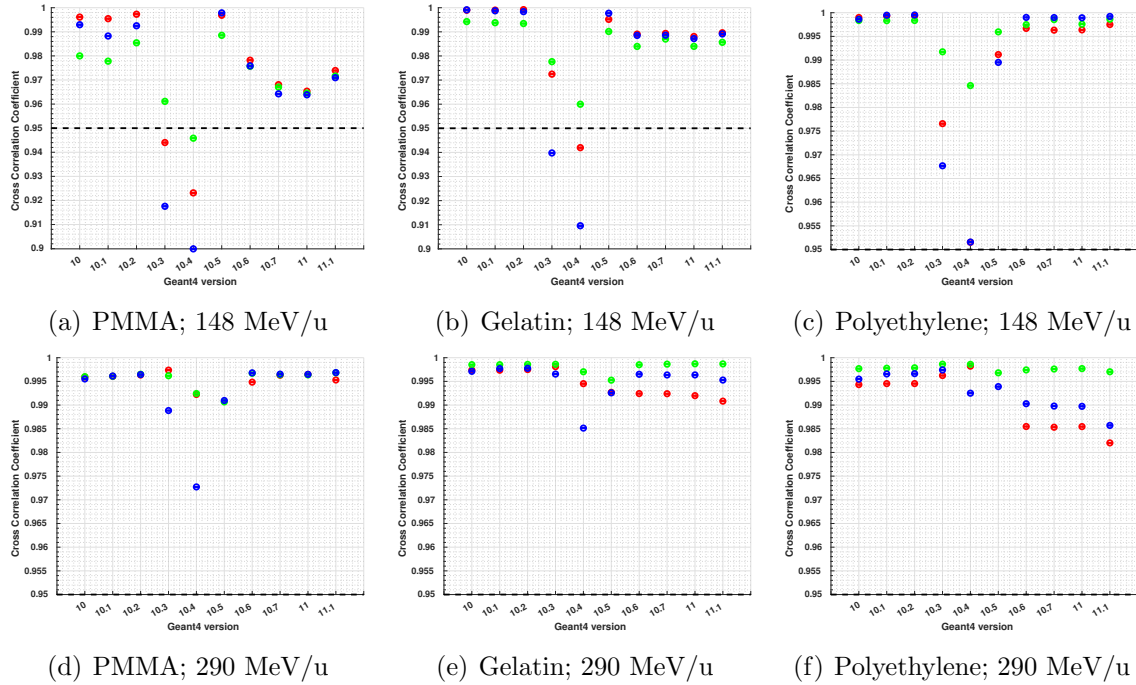


Supplementary Figure 43: NMSE between simulations and experimental measurements of ^{10}C fragment production in the tail region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

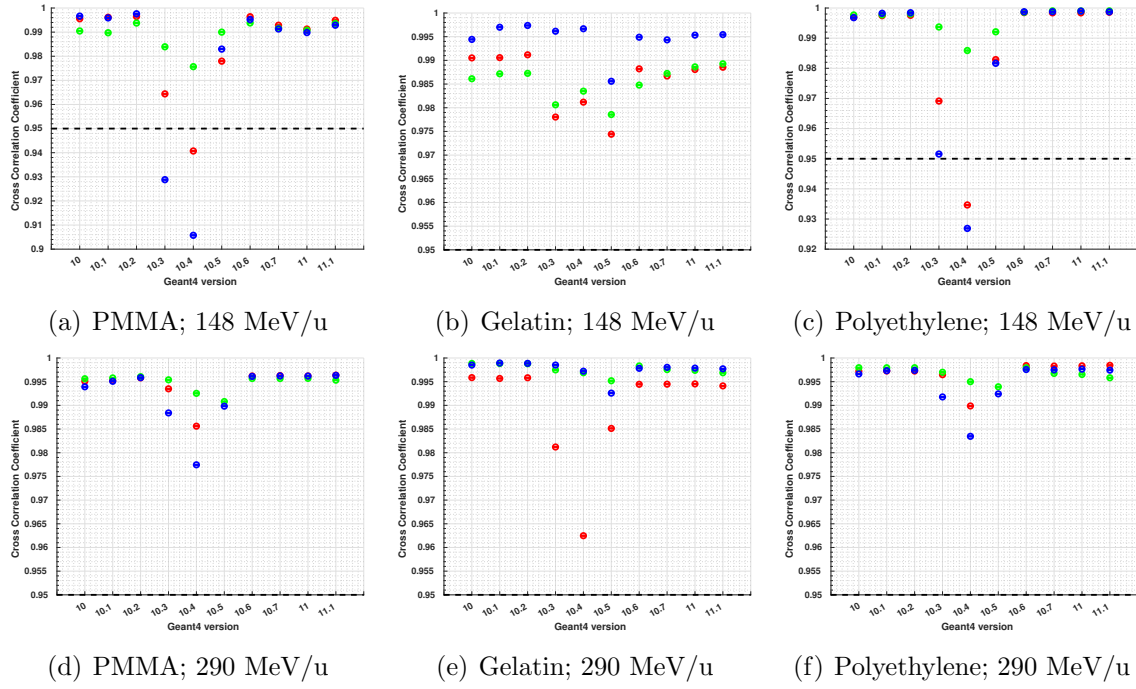


Supplementary Figure 44: NMSE between simulations and experimental measurements of ^{15}O fragment production in the tail region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.

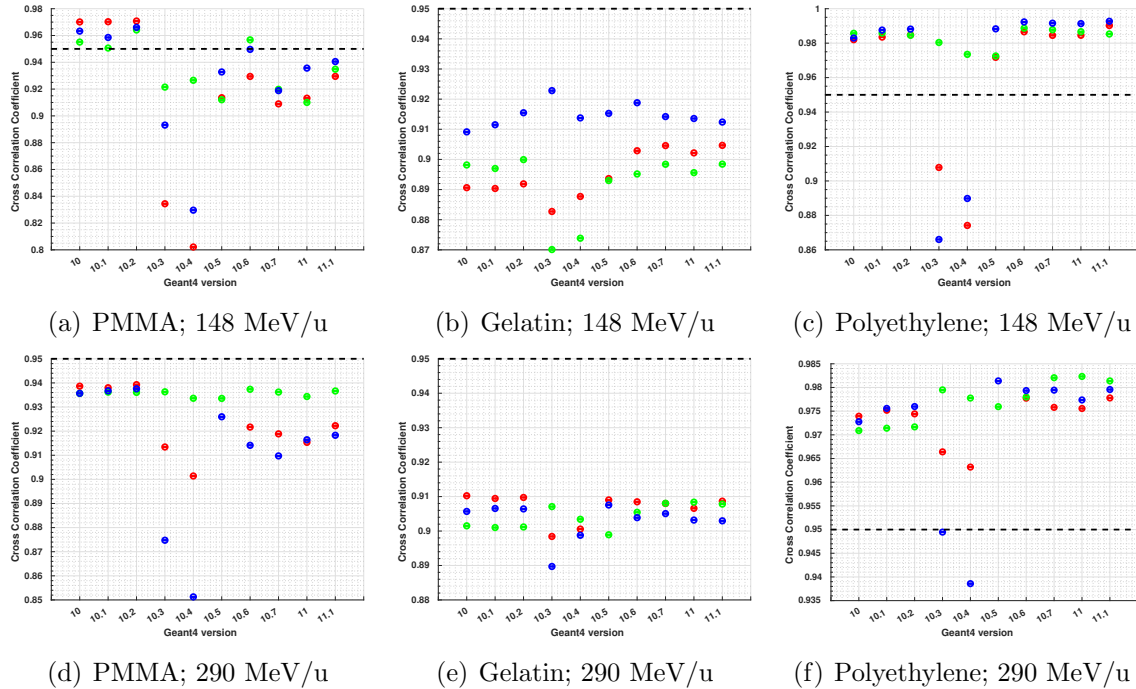
79 4.2.2. *Pearson CCC* The Pearson CCCs for total positron annihilation yield in the tail
 80 region for oxygen ion irradiation is presented in Supplementary Figure 45; the individual
 81 contributions from ^{11}C , ^{10}C and ^{15}O are presented in Supplementary Figure 46-48.



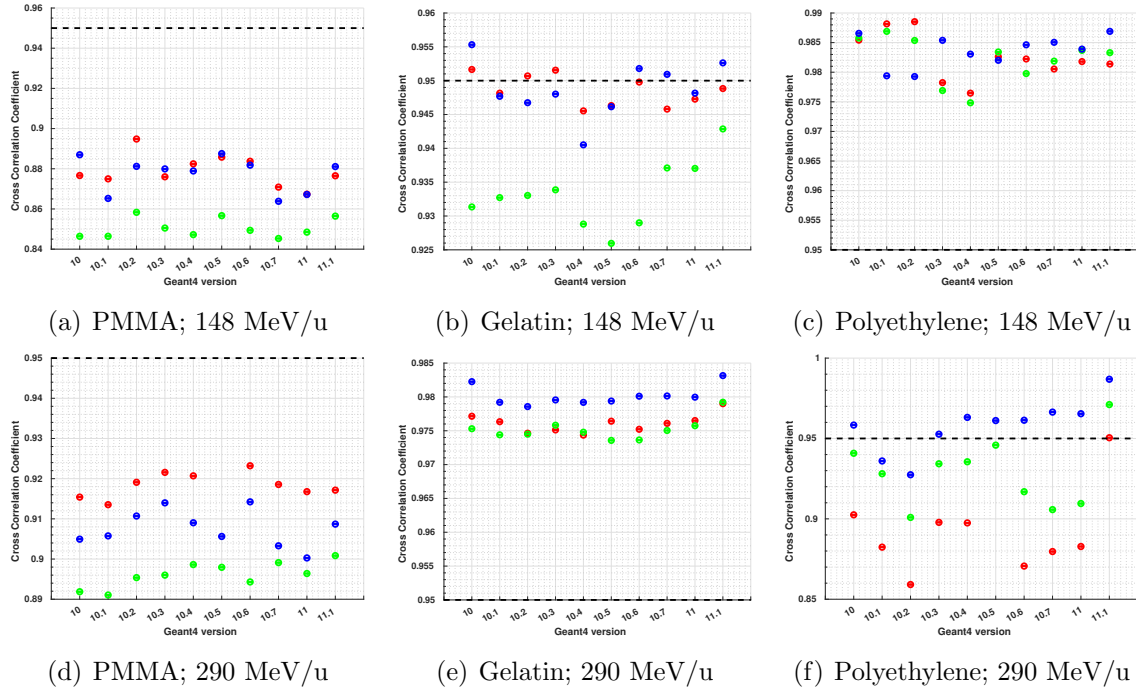
Supplementary Figure 45: Pearson CCC between simulation and experimental measurements of total positron annihilations in the tail region following carbon ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 46: Pearson CCC between simulations and experimental measurements of ^{11}C fragment production in the tail region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 47: Pearson CCC simulations and experimental measurements of ^{10}C fragment production in the tail region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.



Supplementary Figure 48: Pearson CCC simulations and experimental measurements of ^{15}O fragment production in the tail region following oxygen ion irradiation. Red = BIC, green = QMD and blue = INCL.