TOPAS-nBio v3.0 (OpenTOPAS v4.0)
Regression testing (cf. TOPAS-nBio v2.0 (TOPAS v3.9))*

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Table of Contents II

DBSCAN - TsEmDNAPhysics

Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. *Comput Methods Programs Biomed.* 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

DBSCAN - g4em-dna_opt2

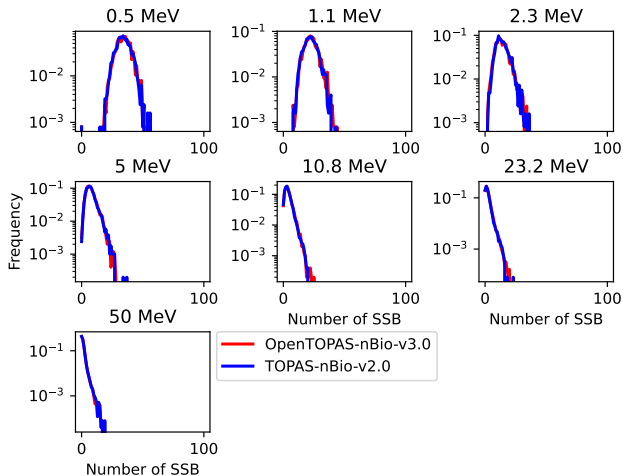|	OpenTOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	407.4 +/- 103.5	642.5 +/- 137.4
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. *Comput Methods Programs Biomed*. 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012
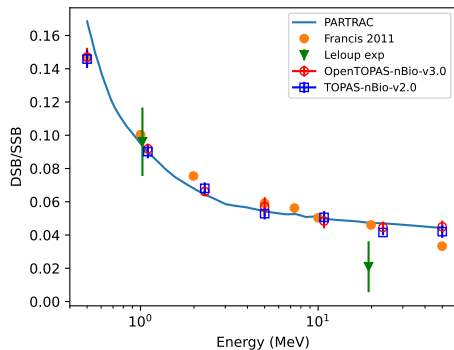
DBSCAN - g4em-dna_opt4

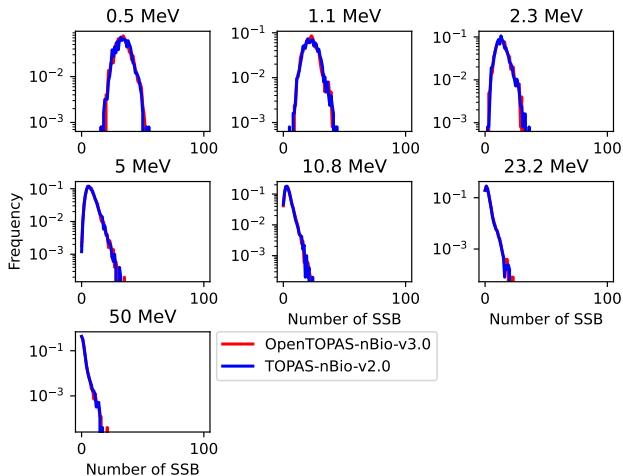|	OpenTOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	1812.7 +/- 478.4	2244.2 +/- 181.3
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. *Comput Methods Programs Biomed.* 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012
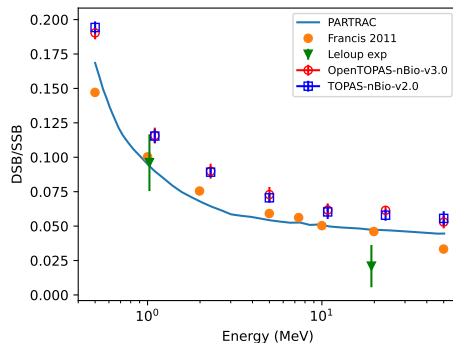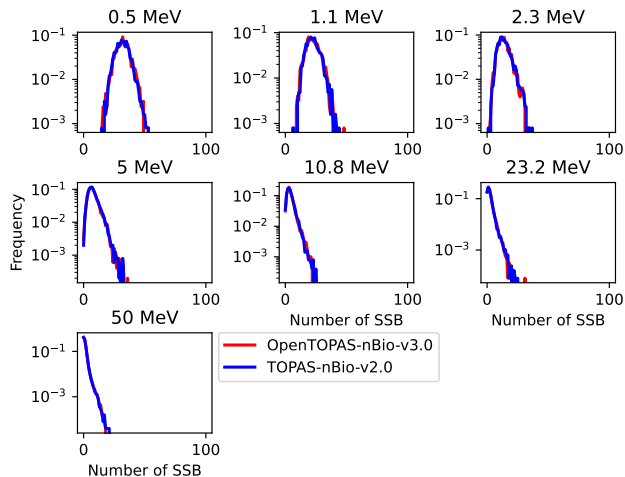
DBSCAN - g4em-dna_opt6
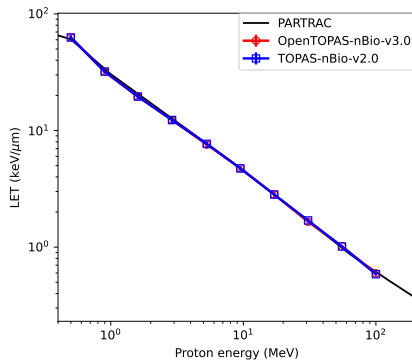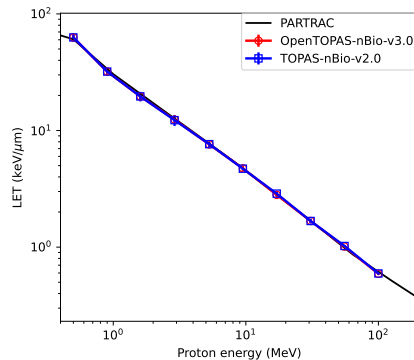

Francis Z, Villagrasa C, Clairand I. Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm. *Comput Methods Programs Biomed.* 2011; 101(3):265-270. doi:10.1016/j.cmpb.2010.12.012

LET I

	OpenTOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	717.5 +/- 89.6	1192.6 +/- 183.2
Final.	0.0 +/- 0.0	0.0 +/- 0.0

	OpenTOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	650.2 +/- 212.9	773.9 +/- 211.8
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ LET as a function of proton energy for TsEmDNAPhysics (left) and g4em-dna_opt2 (right).

LET II

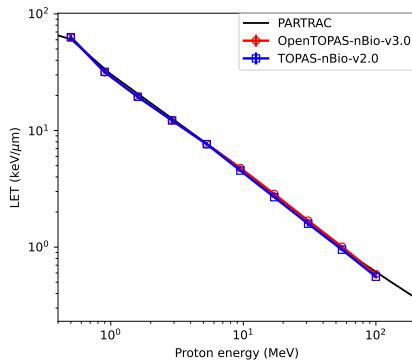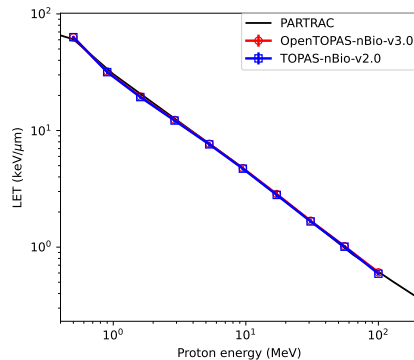|	OpenTOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	2811.8 +/- 334.0	2544.5 +/- 803.2
Final.	0.0 +/- 0.0	0.0 +/- 0.0

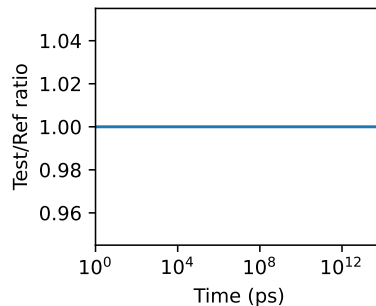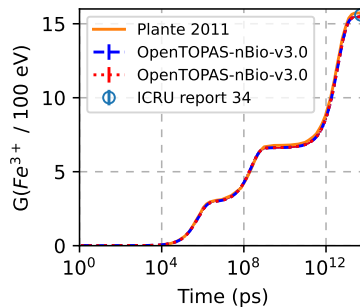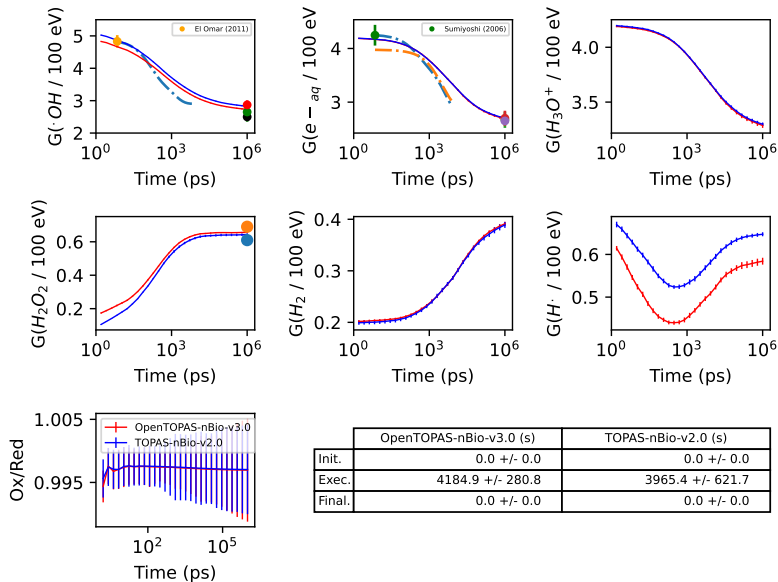|	OpenTOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	596.7 +/- 137.6	2763.6 +/- 384.7
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ LET as a function of proton energy for g4em-dna_opt4 (left) and g4em-dna_opt6 (right).

Fricke: IRT

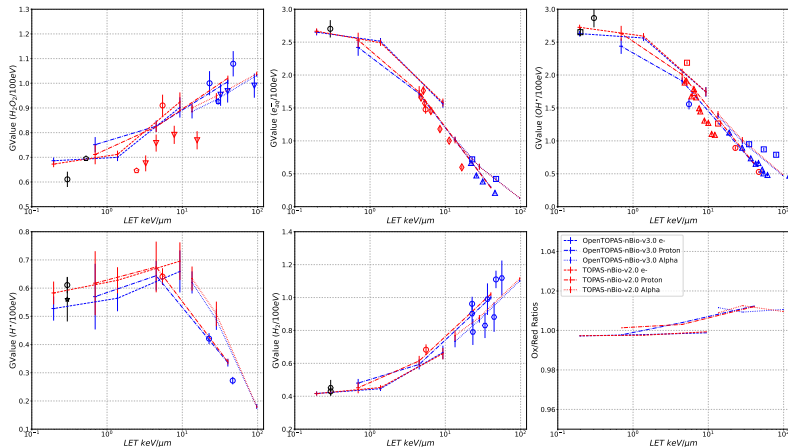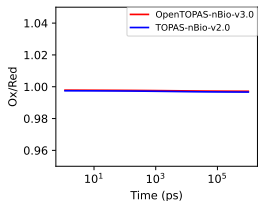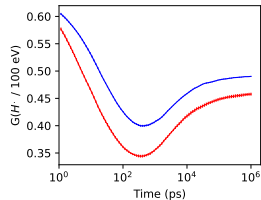|	OpenTOPAS-nBio-v3.0	OpenTOPAS-nBio-v3.0
Init. (s)	0.024 +/- 0.005	0.024 +/- 0.005
Exec. (s)	16.564 +/- 4.157	16.564 +/- 4.157
Final. (s)	0.030 +/- 0.016	0.030 +/- 0.016
Value (/100eV)	15.466 +/- 0.053	15.466 +/- 0.053

G-value: step-by-step

	OpenTOPAS-nBio-v3.0 (s)	TOPAS-nBio-v2.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	4184.9 +/- 280.8	3965.4 +/- 621.7
Final.	0.0 +/- 0.0	0.0 +/- 0.0

G-value vs. LET: step-by-step

	TOPAS-nBio-v2.0	OpenTOPAS-nBio-v3.0
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	3218.36 +- 390.17	3041.16 +- 688.34
Sys (s)	0.0 +- 0.0	0.0 +- 0.0

G-value: IRT
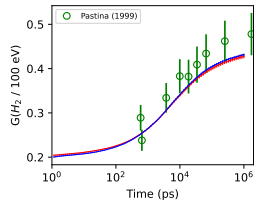
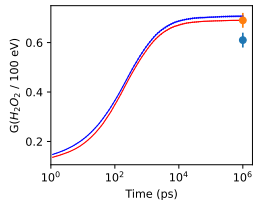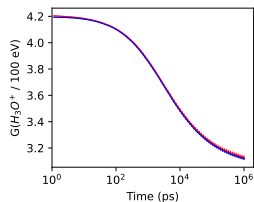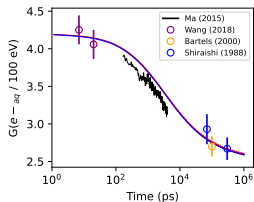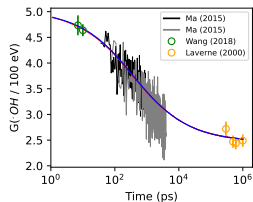# G-value vs. LET: IRT
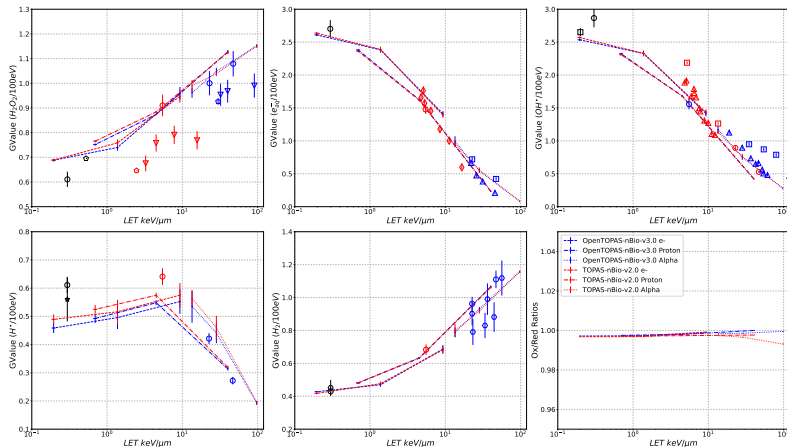
	TOPAS-nBio-v2.0	OpenTOPAS-nBio-v3.0
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	194.56 +- 14.74	146.19 +- 16.05
Sys (s)	0.0 +- 0.0	0.0 +- 0.0

G-value of H$_2$O$_2$: IRT
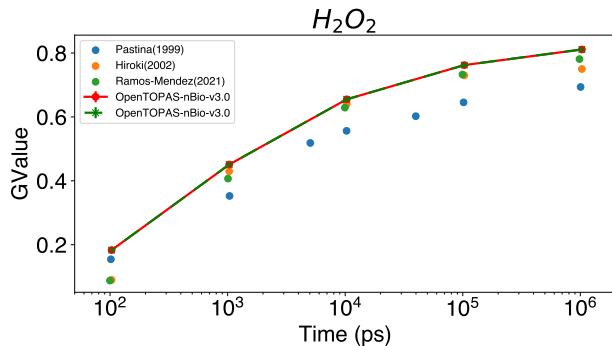
	Reference	Under Test
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	2442.34 +- 1003.79	2442.34 +- 1003.79
Sys (s)	0.0 +- 0.0	0.0 +- 0.0

G-value of H: IRT
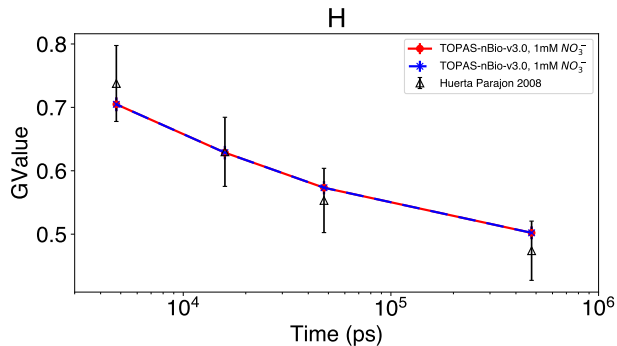
	Reference	Under Test
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	441.61 +- 165.61	441.61 +- 165.61
Sys (s)	0.0 +- 0.0	0.0 +- 0.0

G-value and Temperature I: IRT

G-value and Temperature II: IRT

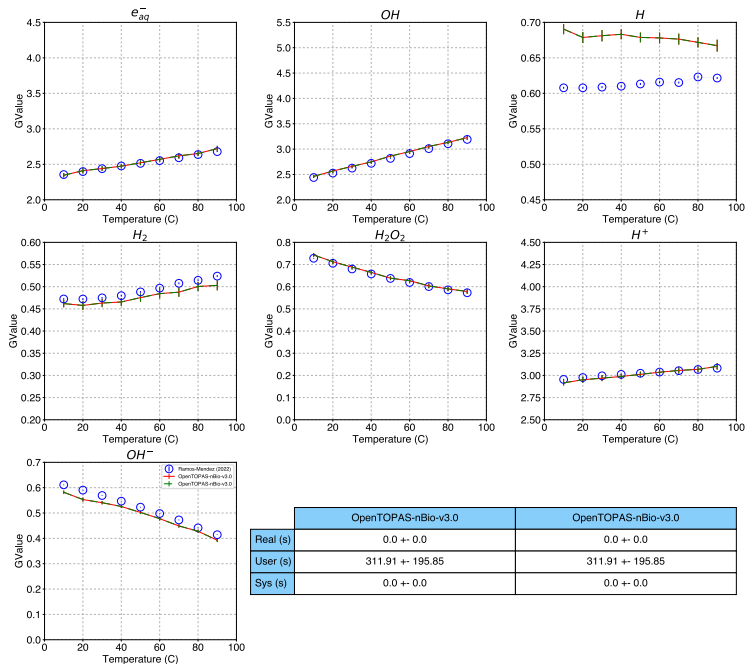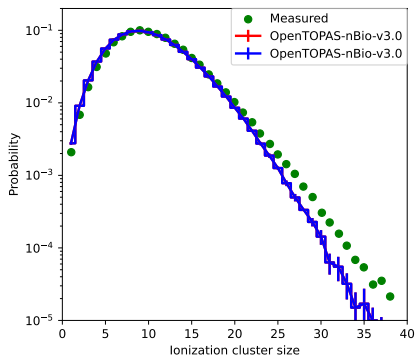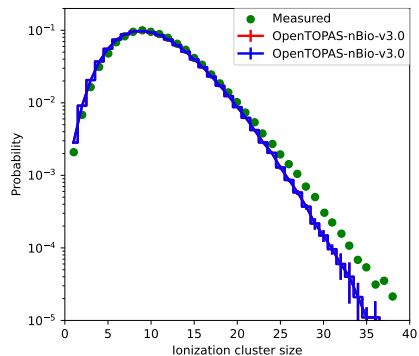|	OpenTOPAS-nBio-v3.0	OpenTOPAS-nBio-v3.0
Real (s)	0.0 +- 0.0	0.0 +- 0.0
User (s)	311.91 +- 195.85	311.91 +- 195.85
Sys (s)	0.0 +- 0.0	0.0 +- 0.0
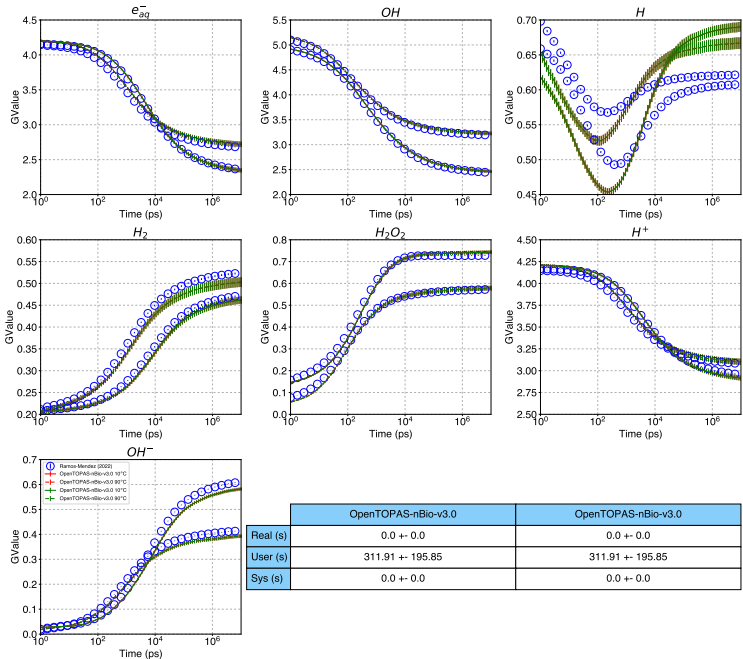
Nanodosimetry I: TsEmDNAPhysics and g4em-dna_opt2

	OpenTOPAS-nBio-v3.0 (s)	OpenTOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	23500.3 +/- 3503.6	23500.3 +/- 3503.6
Final.	0.0 +/- 0.0	0.0 +/- 0.0

	OpenTOPAS-nBio-v3.0 (s)	OpenTOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	22220.2 +/- 4455.1	22220.2 +/- 4455.1
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry I: g4em-dna_opt4 and g4em-dna_opt6

Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry II: TsEmDNAPhysics and g4em-dna_opt2
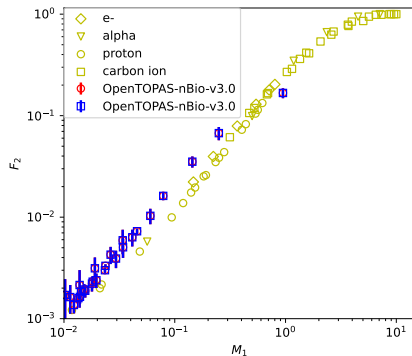
	OpenTOPAS-nBio-v3.0 (s)	OpenTOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	411.2 +/- 7.4	411.2 +/- 7.4
Final.	0.0 +/- 0.0	0.0 +/- 0.0

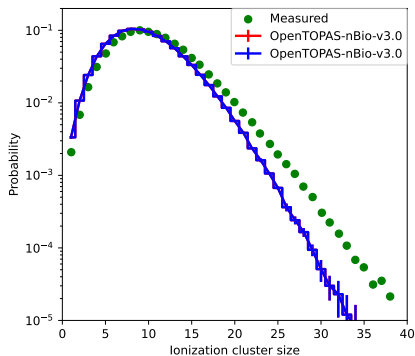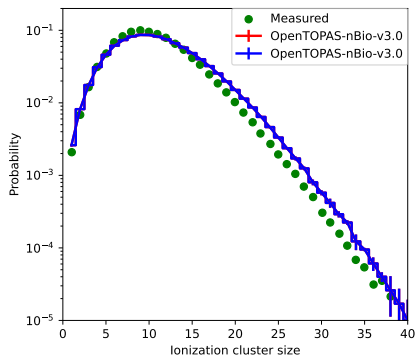|	OpenTOPAS-nBio-v3.0 (s)	OpenTOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	336.0 +/- 69.6	336.0 +/- 69.6
Final.	0.0 +/- 0.0	0.0 +/- 0.0

▶ Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry II: g4em-dna_opt4 and g4em-dna_opt6

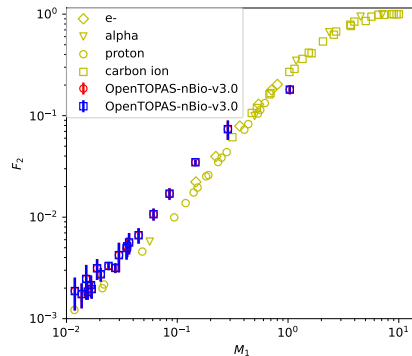|	OpenTOPAS-nBio-v3.0 (s)	OpenTOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	4989.0 +/- 765.6	4989.0 +/- 765.6
Final.	0.0 +/- 0.0	0.0 +/- 0.0

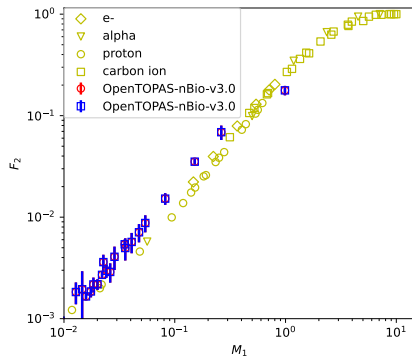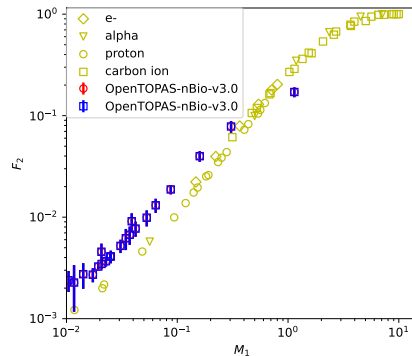|	OpenTOPAS-nBio-v3.0 (s)	OpenTOPAS-nBio-v3.0 (s)
Init.	0.0 +/- 0.0	0.0 +/- 0.0
Exec.	3740.6 +/- 1041.7	3740.6 +/- 1041.7
Final.	0.0 +/- 0.0	0.0 +/- 0.0

► Conte V, Selva A, Colautti P, et al., Nanodosimetry: Towards a new concept of radiation quality. *Radiat Prot Dosimetry*. 2018;180(1-4):150-156. doi:10.1093/rpd/ncx175

Nanodosimetry III: TsEmDNAPhysics
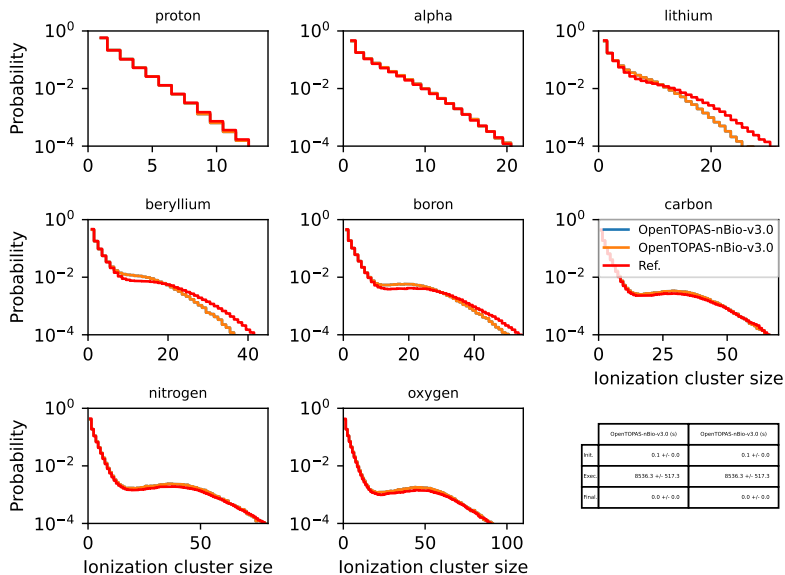
▶ Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. *Phys Med Biol*. 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee

Nanodosimetry III: g4em-dna_opt2
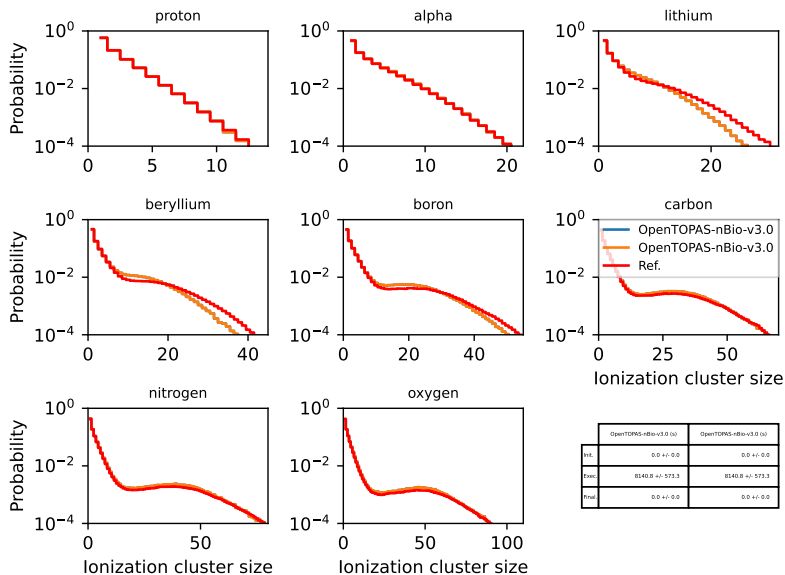
▶ Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. *Phys Med Biol*. 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee

Nanodosimetry III: g4em-dna_opt4

▶ Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. *Phys Med Biol.* 2018;63(23):235015. doi:10.1088/1361-6560/aaeeee
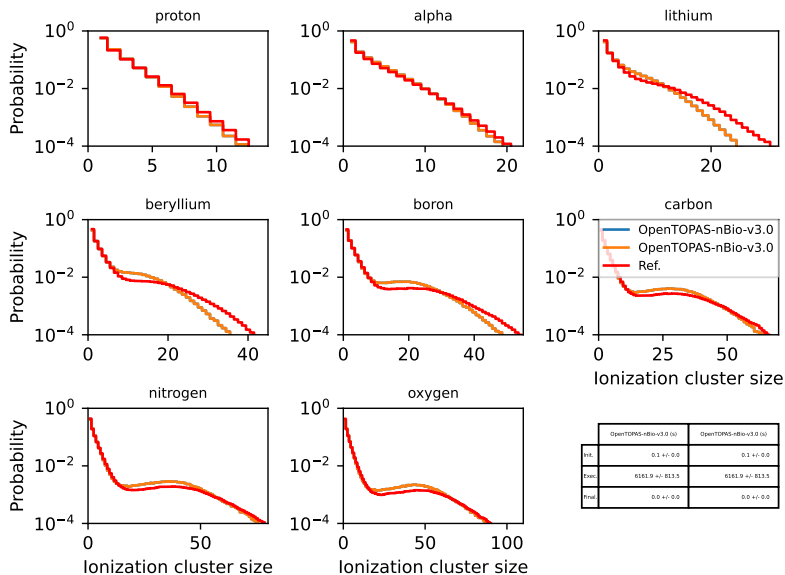
Nanodosimetry III: g4em-dna_opt6

Ramos-Méndez J, Burigo LN, Schulte R, Chuang C, Faddegon B. Fast calculation of nanodosimetric quantities in treatment planning of proton and ion therapy. *Phys Med Biol*. 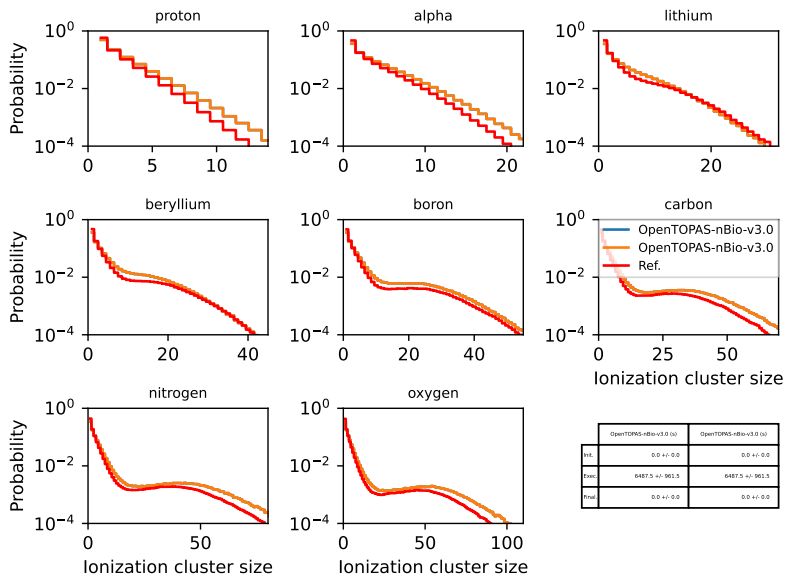2018;63(23):235015. doi:10.1088/1361-6560/aaeeee