Analysis of available PHITS simulations

produced by L. Heilbronn

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PC simulated data sets produced with PHITS by Lawrence Heilbronn

https://phits.jaea.go.jp/

(1) June 2022 from 0 pc to 24 pc full set 0,12,16,18,19,20,21,22,24; initial particle statistics 1.E+9

(2) September 2022 cold pc, low statistics, 0,12,16,18,20,22,24 pc (not full set)

(3) Oct.-Dec. 2022; High improved statistics 1E+10, pc set 12,16,18,20,22,24 (no zero)

- Overall normalization of three sets is not compatible (only within one set)

Set (1)

Passed to detector without any interactions

Number of PC	Initial n's
0	1.E+08
12	1.E+09
16	1.E+09
18	1.E+09
19	1.E+09
20	1.E+09
21	1.E+09
22	1.E+09
24	1.E+09

# PC	pass counts	Error	Fit†
0*	1.8755E+07	43307.04	1.2077E+08
12	325873	570.85	305928.81
16	42663	206.55	41703.86
18	15358	123.93	15397.64
19	9354	96.72	9356.06
20	5721	75.64	5685.02
21	3488	59.06	3454.39
22	2105	45.88	2098.99
24	744	27.28	774.98

* scaled up × 10

† fit for last 6 points 18-24 PC with 2 parameters

Set (2) Cold

Number of pcs	Initial ns
0	1.E+6
12	1.E+8
16	1.E+8
18	1.E+8
20	1.E+8
22	1.E+8
24	1.E+8

Passed to detector without any interactions

#pc	Counts †	Error	Fit *
0	1.56083E+08	3.951E+05	1.56080E+08
12	265950	1630.7974	266352.25
16	34450	586.9412	33731.1289
18	12010	346.5544	12134.042
20	4230	205.6696	4396.3647
22	1510	122.8821	1604.3062
24	660	81.2404	589.6273
†	scaled up		
*	fit all 7 points with 3 parameters		

Set (3) High Statistics

Number of pcs	Initial ns
12	1.E+10
16	1.E+10
18	1.E+10
20	1.E+10
22	1.E+10
24	1.E+10

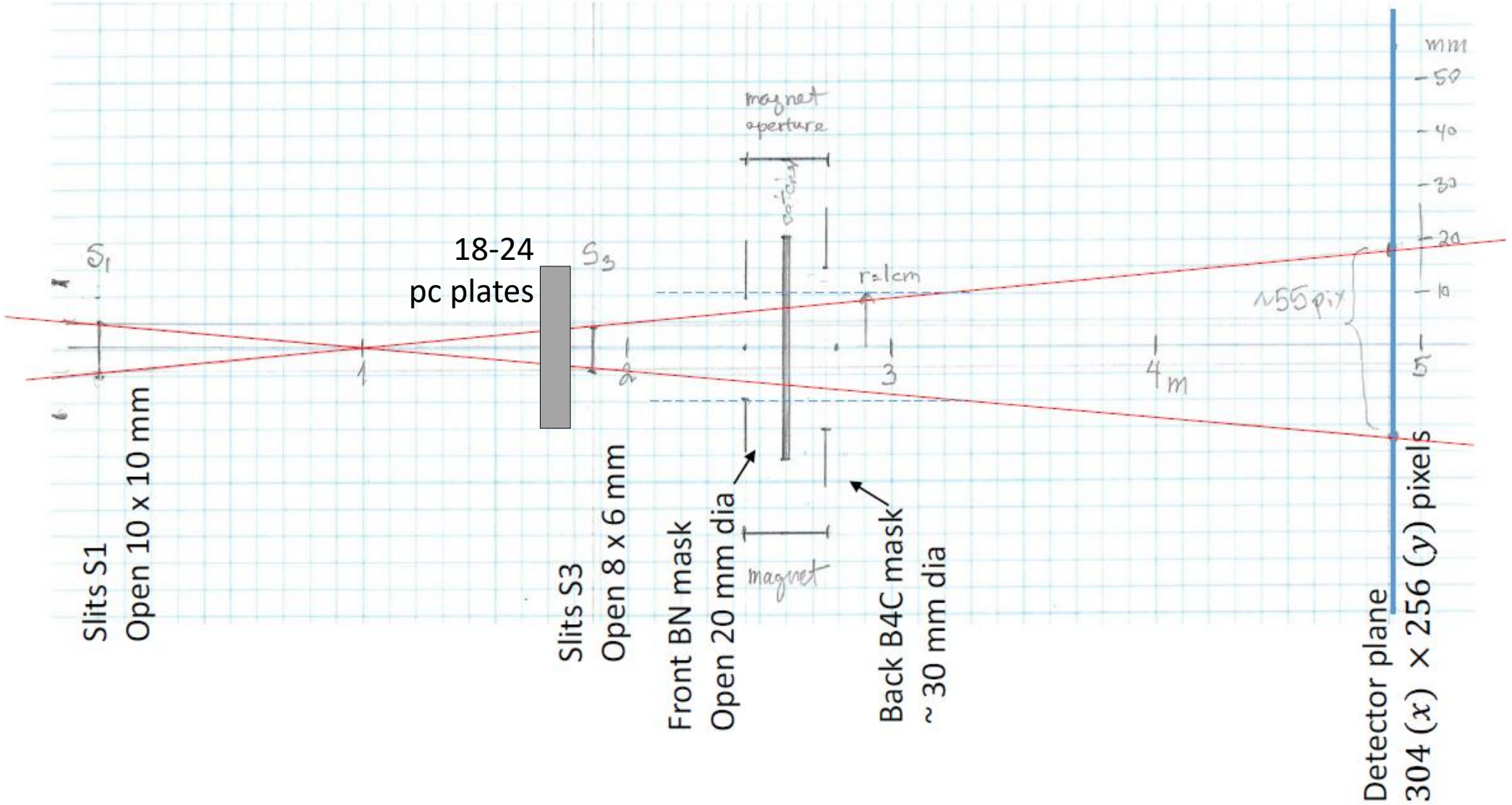
Passed to detector without any interactions

# PC	Counts	Error	Fit (5 -2)
12	4.522E+07	6.724E+03	4.517E+07
16	1.363E+07	3.692E+03	1.370E+07
18	7.520E+06	2.742E+03	7.541E+06
20	4.163E+06	2.040E+03	4.152E+06
22	2.000E+05	4.473E+02	-
24	1.284E+06	1.133E+03	1.259E+06

$$F = F_0 \cdot [\eta]^n$$
$$F_0 = 1.62059 \times 10^9 \pm 9.5 \times 10^5$$
$$\eta = 0.74205 \pm 0.00003$$
$$\chi^2/DOF = 340.8 \quad \text{(5-2)}$$

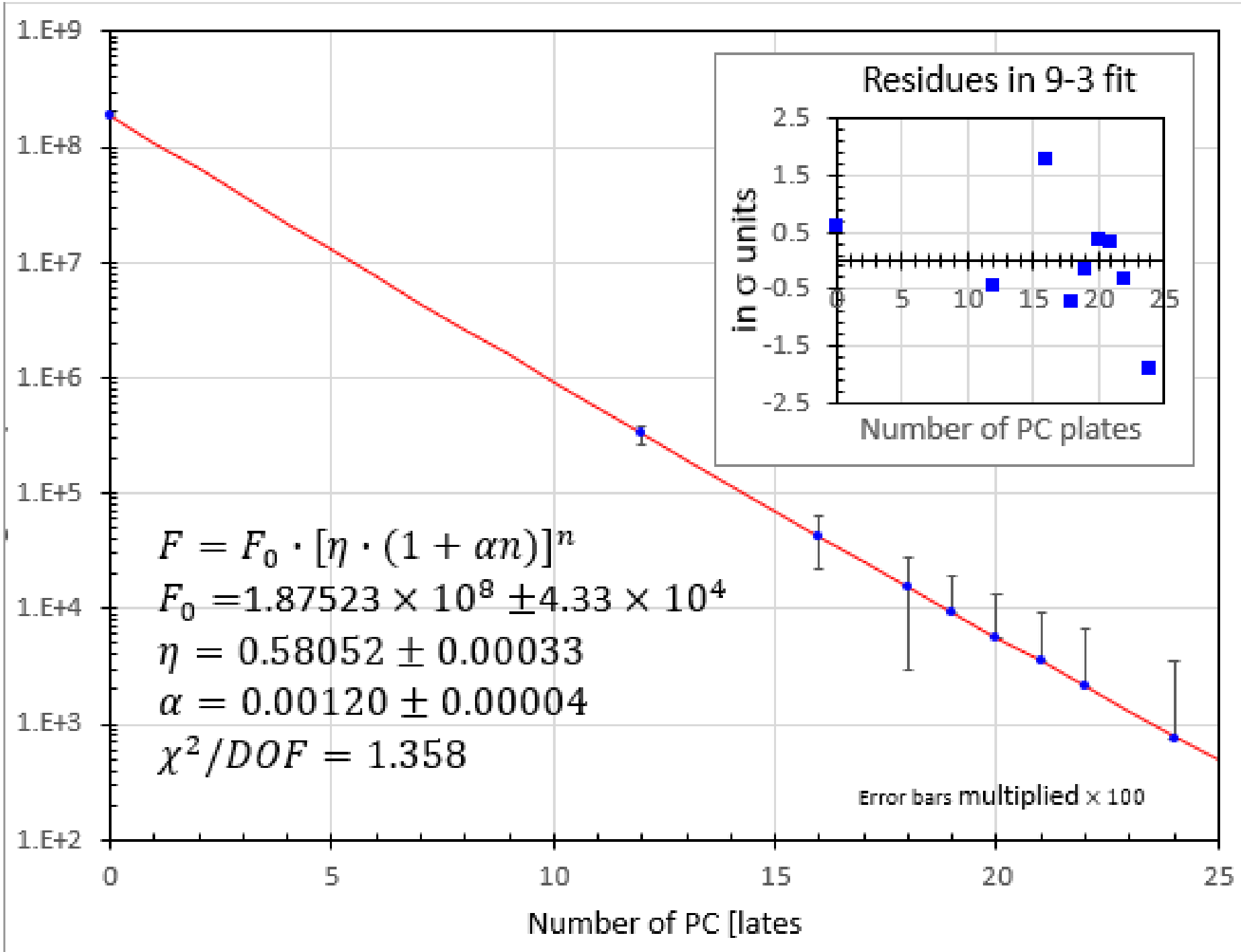
MAGREF SNS Beam Line 4A Configuration

All beam tracks are within the cylinder with r = 1 cm inside the magnet



Simulation set (1)

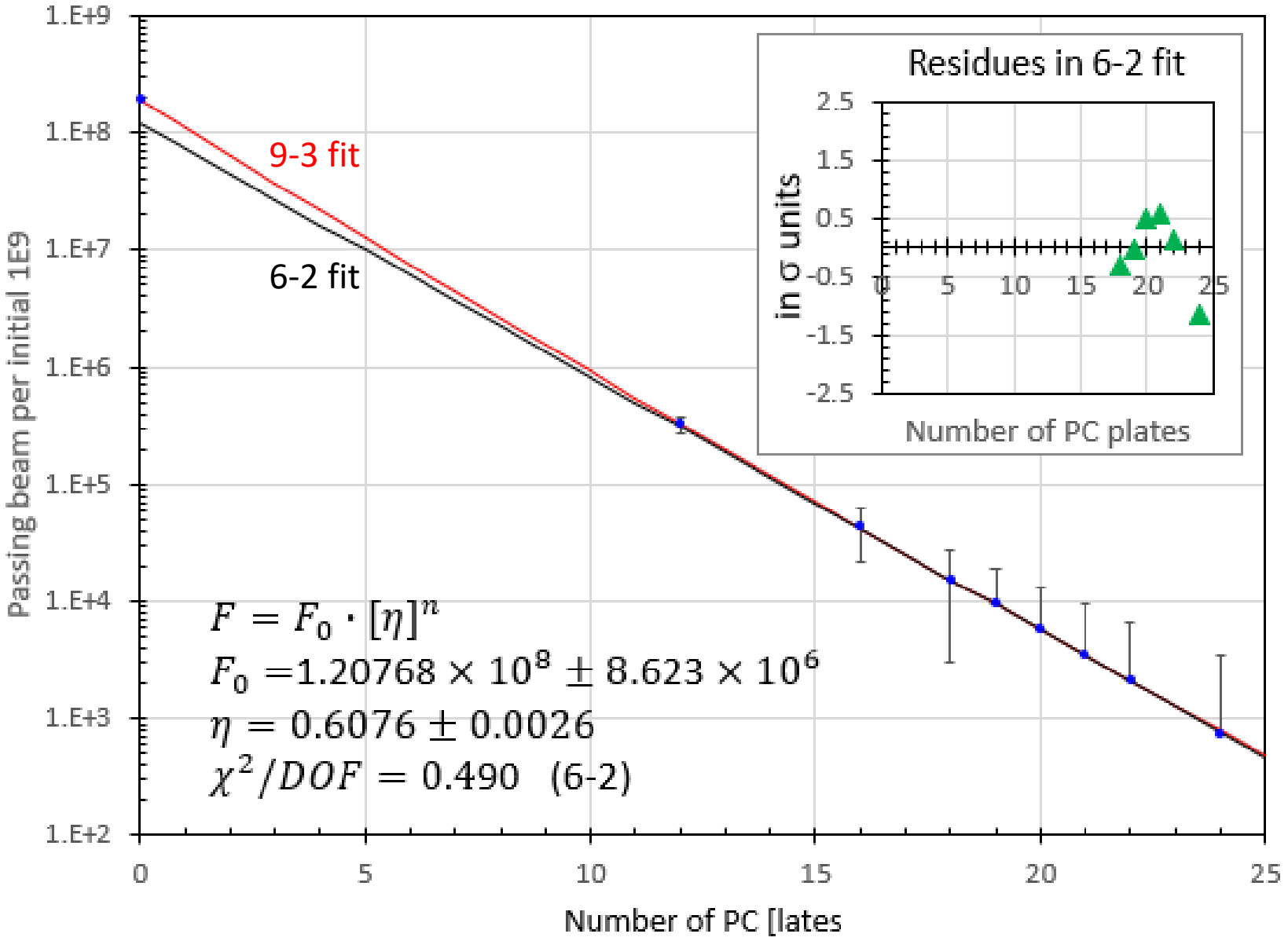
9 points, 3 parameters



Simulation set (1)

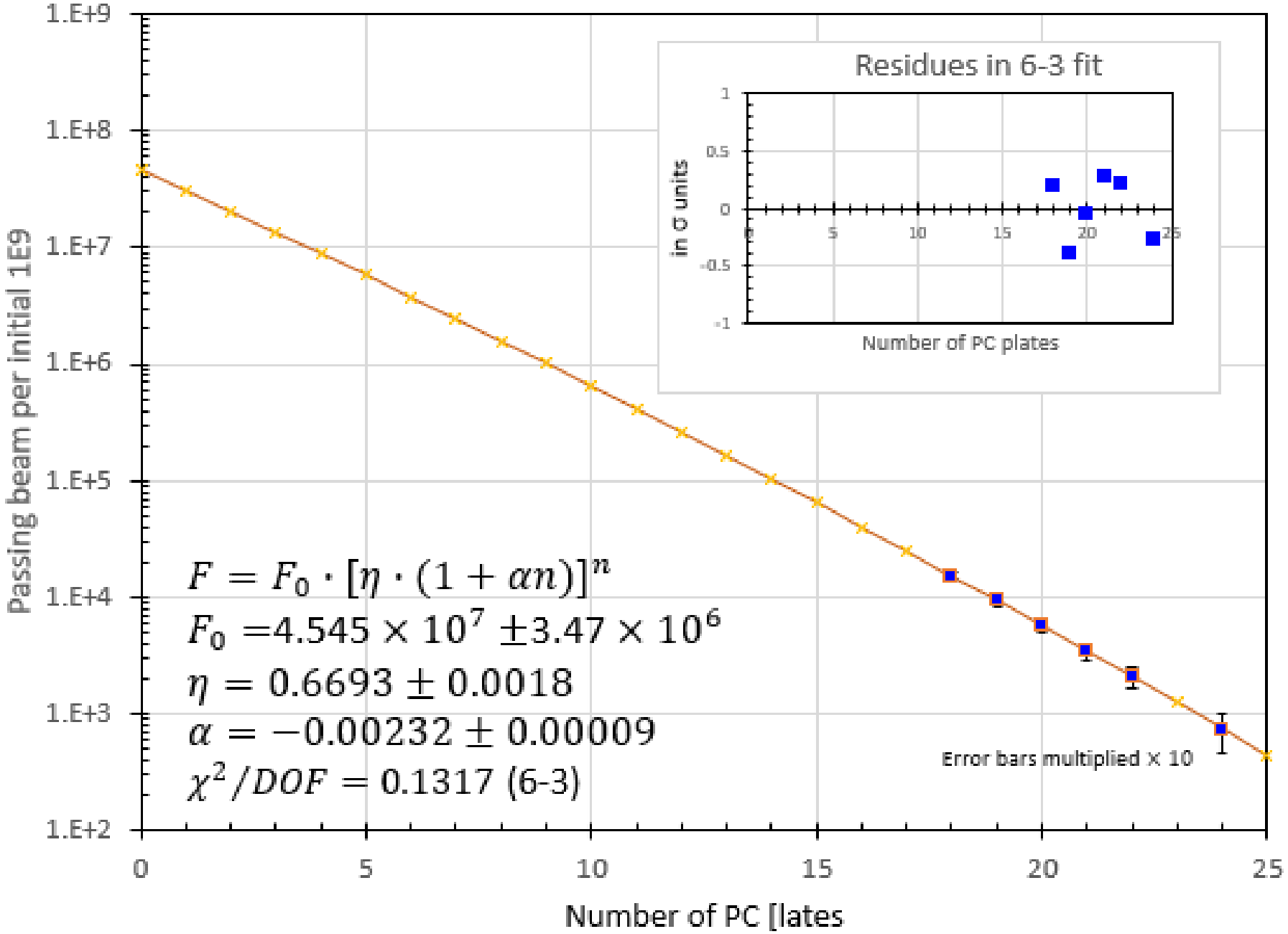
6 points, 2 parameters

(like with exp. data)



Simulation set (1)

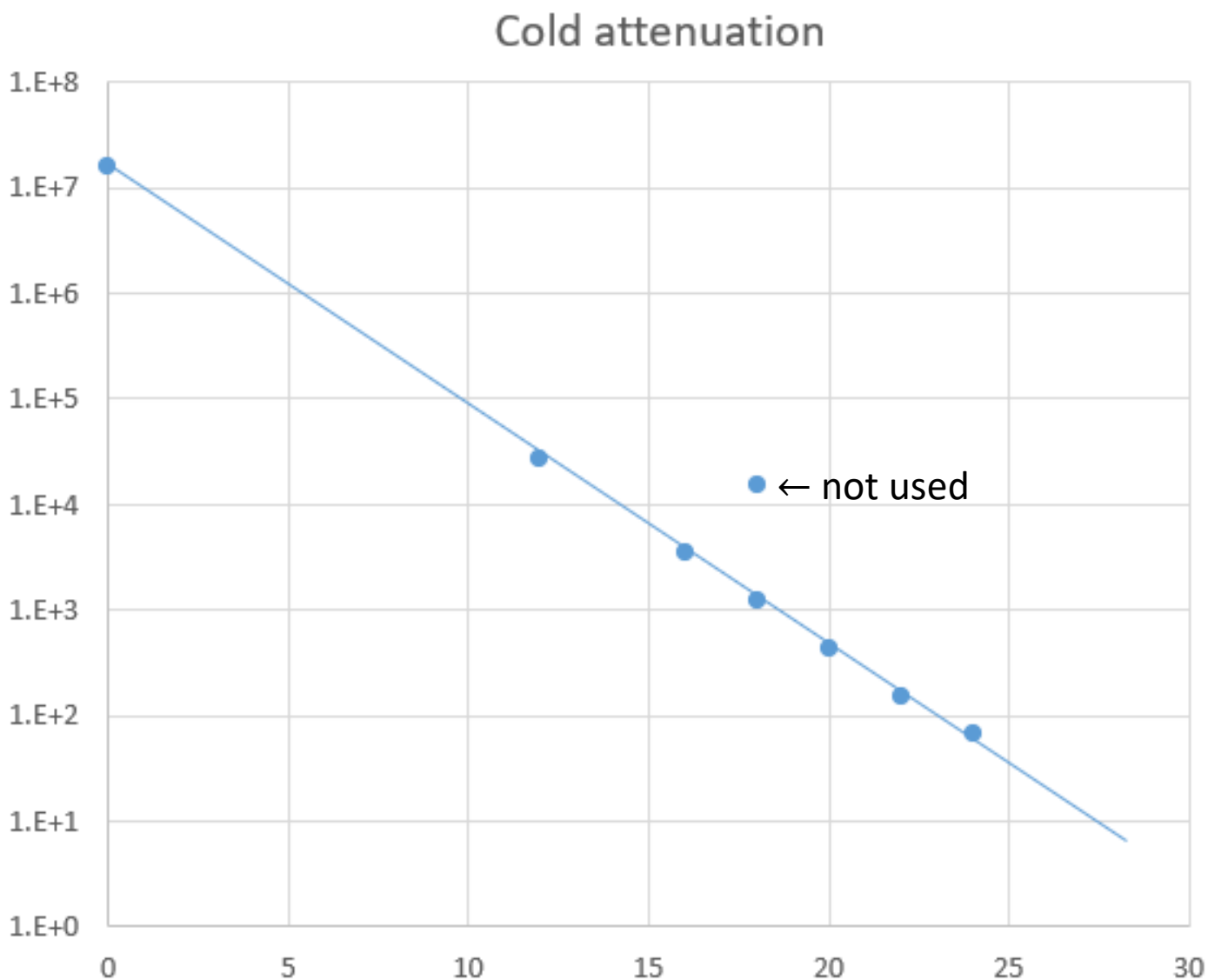
6 points, 3 parameters



Cold files

# pc	Ver	initial #	Ntotal	Pass	Scattered	Gauss tot X	Gaugg tot Y	chi^2 x	chi^2 y	constant	Gauss peak	constant	Gauss peak	Sigma x	Sigma y
0		1.00E+08	156842	15608300	759	286	388	0.764184	0.664042	1.574138	2.263283	1.235872	2.248492	2.807769	4.993311
12		1.00E+08	87262	26595	59286	2040	1902	1.115838	0.956659	195.42	18.85	195.88	20.39	3.62	3.17
16		1.00E+08	67707	3445	63253	1557	1410	1.011779	0.918175	209.01	13.10	209.51	13.54	3.82	3.35
18	A	1.00E+08	66791	1201	64755	1260	1175	0.983281	0.791863	214.43	9.97	214.71	11.37	3.88	3.30
18	B	1.00E+08	67553	15358	52195	3372	3367	0.991818	1.144091	162.74	37.99	162.76	39.25	3.23	3.07
20		1.00E+08	67100	423	65992	1067	1243	0.964496	0.962851	218.70	8.17	218.11	10.10	3.81	3.79
22		1.00E+08	67816	151	67140	766	1014	0.946457	0.971936	223.00	5.65	222.17	7.11	3.43	4.08
24		1.00E+08	68614	66	68092	613	1216	0.9399	1.05529	226.45	4.47	224.44	6.61	2.99	5.48

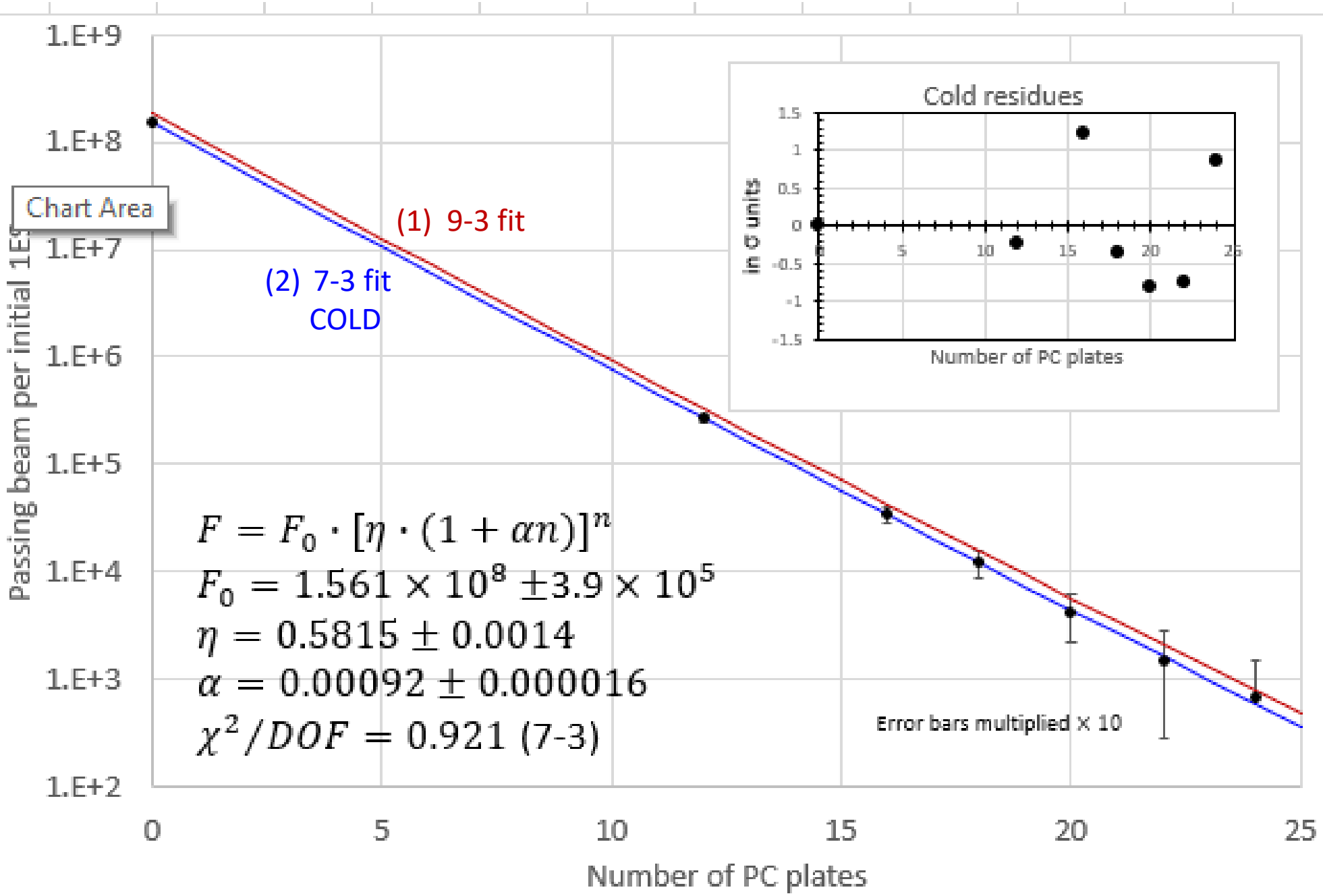
Cold data


Cold attenuation
1.E+8
1.E+7
1.E+6
1.E+5
1.E+4
1.E+3
1.E+2
1.E+1
1.E+0
0
5
10
15
20
25
30
← not used

Simulation set (2) COLD

7 points, 3 parameters

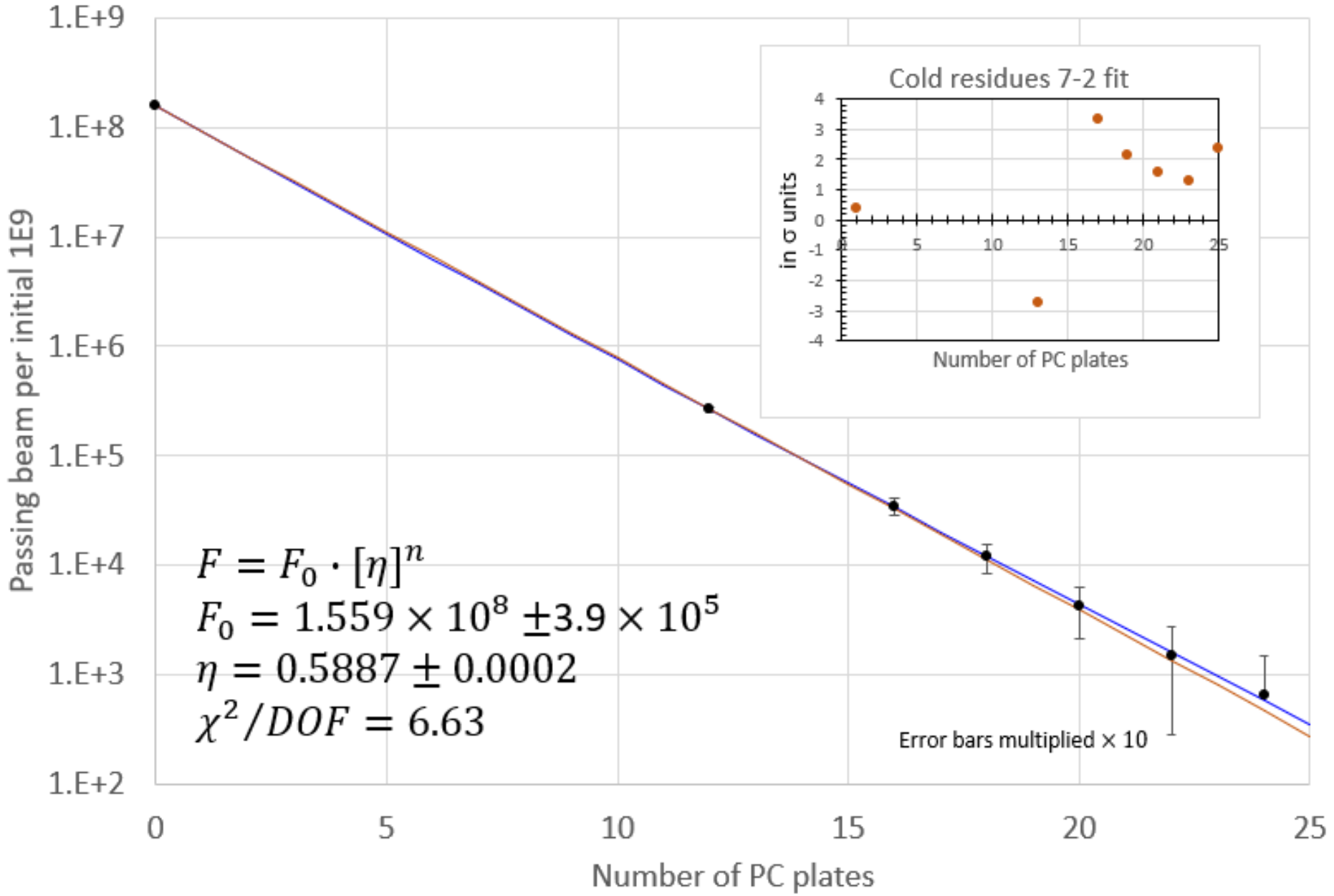
For comparison with (1)
Statistics scaled up by x10
0-point by factor 1,000



Simulation set (2) COLD

7 points, 2 parameters

For comparison with (1)
Statistics scaled up by x10;
0-point by factor 1,000



Fit (1) comparisons

F_0 is known as $1.8755 \times 10^8 \pm 4.3 \times 10^4$

Fit 9 points with 3 parameters

$F = F_0 \cdot [\eta \cdot (1 + \alpha n)]^n$

$F_0 = 1.87523 \times 10^8 \pm 4.33 \times 10^4$

$\eta = 0.58052 \pm 0.00033$

$\alpha = 0.00120 \pm 0.00004$

$\chi^2/DOF = 1.358$ (9-3)

Fit last 6 points with 2 parameters

$F = F_0 \cdot [\eta]^n$

$F_0 = 1.20768 \times 10^8 \pm 8.623 \times 10^6$

$\eta = 0.6076 \pm 0.0026$

$\chi^2/DOF = 0.490$ (6-2)

Fit last 6 points with 3 parameters

$F = F_0 \cdot [\eta \cdot (1 + \alpha n)]^n$

$F_0 = 4.545 \times 10^7 \pm 3.47 \times 10^6$

$\eta = 0.6693 \pm 0.0018$

$\alpha = -0.00232 \pm 0.00009$

$\chi^2/DOF = 0.1317$ (6-3)

Fit (2) cold for comparisons

Cold fit 7 points with 3 par.

$F = F_0 \cdot [\eta \cdot (1 + \alpha n)]^n$

$F_0 = 1.561 \times 10^8 \pm 3.9 \times 10^5$

$\eta = 0.5815 \pm 0.0014$

$\alpha = 0.00092 \pm 0.000016$

$\chi^2/DOF = 0.921$ (7-3)

Cold fit 7 points with 2 par.

$F = F_0 \cdot [\eta]^n$

$F_0 = 1.559 \times 10^8 \pm 3.9 \times 10^5$

$\eta = 0.5887 \pm 0.0002$

$\chi^2/DOF = 6.63$

Cold fit 4 points with 2 parameters

$F = F_0 \cdot [\eta]^n$

$F_0 = 1.327 \times 10^8 \pm 1.064 \times 10^8$

$\eta = 0.5969 \pm 0.0206$

$\chi^2/DOF = 589.4$

Reconstruction of beam intensity from the experimental 6 pc-attenuated points with per Coulomb normalization using simulated fit of same 6 points with 2 parameters and with correction factor

$$F = F_0 \cdot [\eta]^n$$

Correction factor obtained from simulation			
F0 (initial)	1.88E+08	±	4.30E+04
F0 (fit)	1.21E+08	±	8.62E+06
Correction	1.5530	±	0.1109

Update on η from Matt Frost PC plates measurements 5/17/2021 (update 5/27/2021)

One PC plate thickness: 1.270 mm $\pm$ 0.0173 mm
Ave PC density: 1.1947 $\pm$ 0.0085 g/cm3
$\bar{\lambda}$ =3.216 Å

Weight [g]	Thickness [mm]	Width [mm]	Height [mm]	Volume [cc]	Density
8.867	1.28	76.21	75.57	7.372	1.203
8.563	1.25	76.50	75.51	7.221	1.186
9.103	1.28	76.50	77.80	7.618	1.195
Average:	**1.270**				**1.195**

density	1.195	g/cm3	thick	1.27	mm	1 u	1.66E-27	kg	lambda ave	3.216Å
				u/mol	x-sec, b	abs, b	abs_x	# at/cm2	nΣi	
C	16	12.0107	u	192.1712	5.551	0.0035	0.0062598	5.75E+21	0.0319591	
O	3	15.999	u	47.997	4.232	0.00019	0.0003398	1.08E+21	0.00456368	
H	14	1.00784	u	14.10976	82.02	0.3326	0.5948551	5.03E+21	0.41571912	
				254.278	g/mol	6.02E+23	#/mol	tot nΣ	0.4522419	
				0.151765	g/cm2	3.59E+20	#	exp(-nΣ)	**0.63620025**	

The difference between measured and theoretical η values remains

New Value

$$\eta_{calc} = 0.63620 \pm 0.0039$$

Only Matt's measurement accuracies are included (dominant is thickness measurement)
Cross sections are assumed have no errors.
Matt's measurements errors will be improved.

Attenuation obtained from the data

$$\eta(1) = 0.6724 \pm 0.0053$$
$$\eta(2) = 0.67520 \pm 0.00053$$
$$\eta(3) = 0.6713 \pm 0.0123$$

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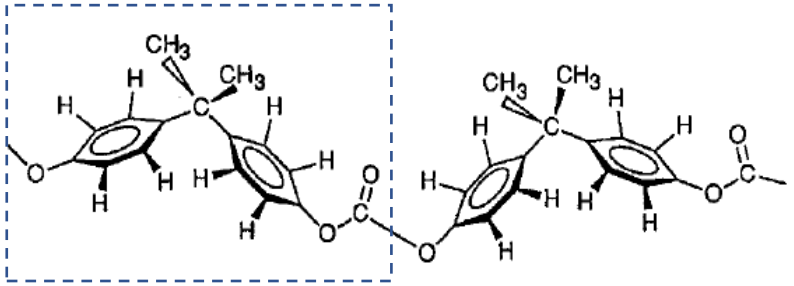
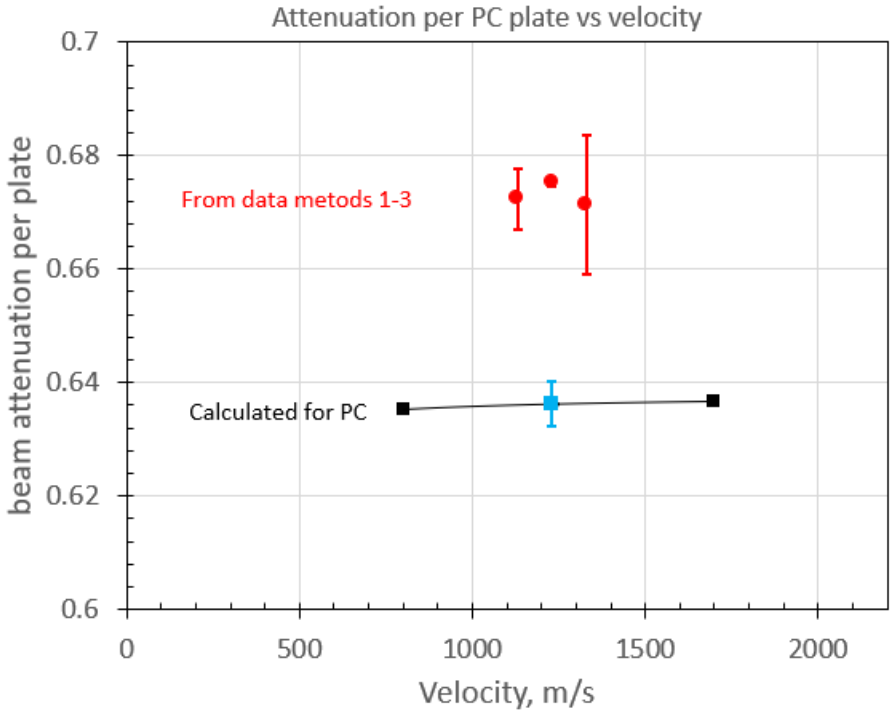
Spatial correlations in polycarbonates: Neutron scattering and simulation

J. Eilhard and A. Zirkel
Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany *et al.*

H-BPA-PC



$(C_{16}O_3H_{14})_n$



Theoretical calculation of η (2021) and comparison with η reconstructed from the 2019 data analysis as a fit to function $F_k = F_0 \cdot (\eta)^k$

η value

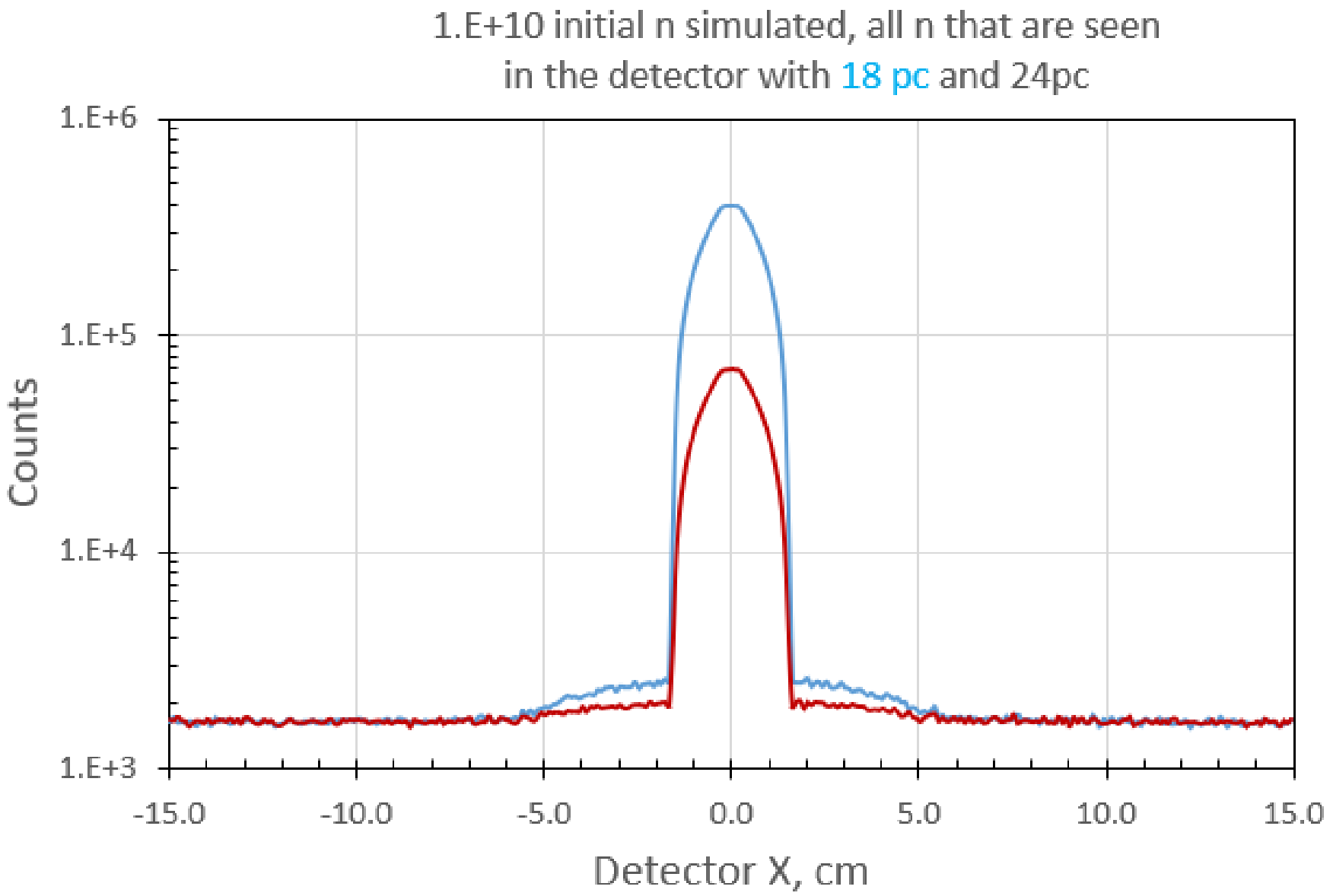
Calculation for average λ in spectrum was made in 2021 after Matt's PC weight/thickness revision

density	1.195	g/cm3	thick	1.27	mm	1 u	1.66E-27	kg	lambda ave	3.216Å
				u/mol	x-sec, b	abs, b	abs_x	# at/cm2	nΣi	
C	16	12.0107	u	192.1712	5.551	0.0035	0.0062598	5.75E+21	0.0319591	
O	3	15.999	u	47.997	4.232	0.00019	0.0003398	1.08E+21	0.00456368	
H	14	1.00784	u	14.10976	82.02	0.3326	0.5948551	5.03E+21	0.41571912	
				254.278	g/mol	6.02E+23	#/mol	tot nΣ	0.4522419	
2021	YK			0.151765	g/cm2	3.59E+20	#	exp(-nΣ)	**0.63620025**	

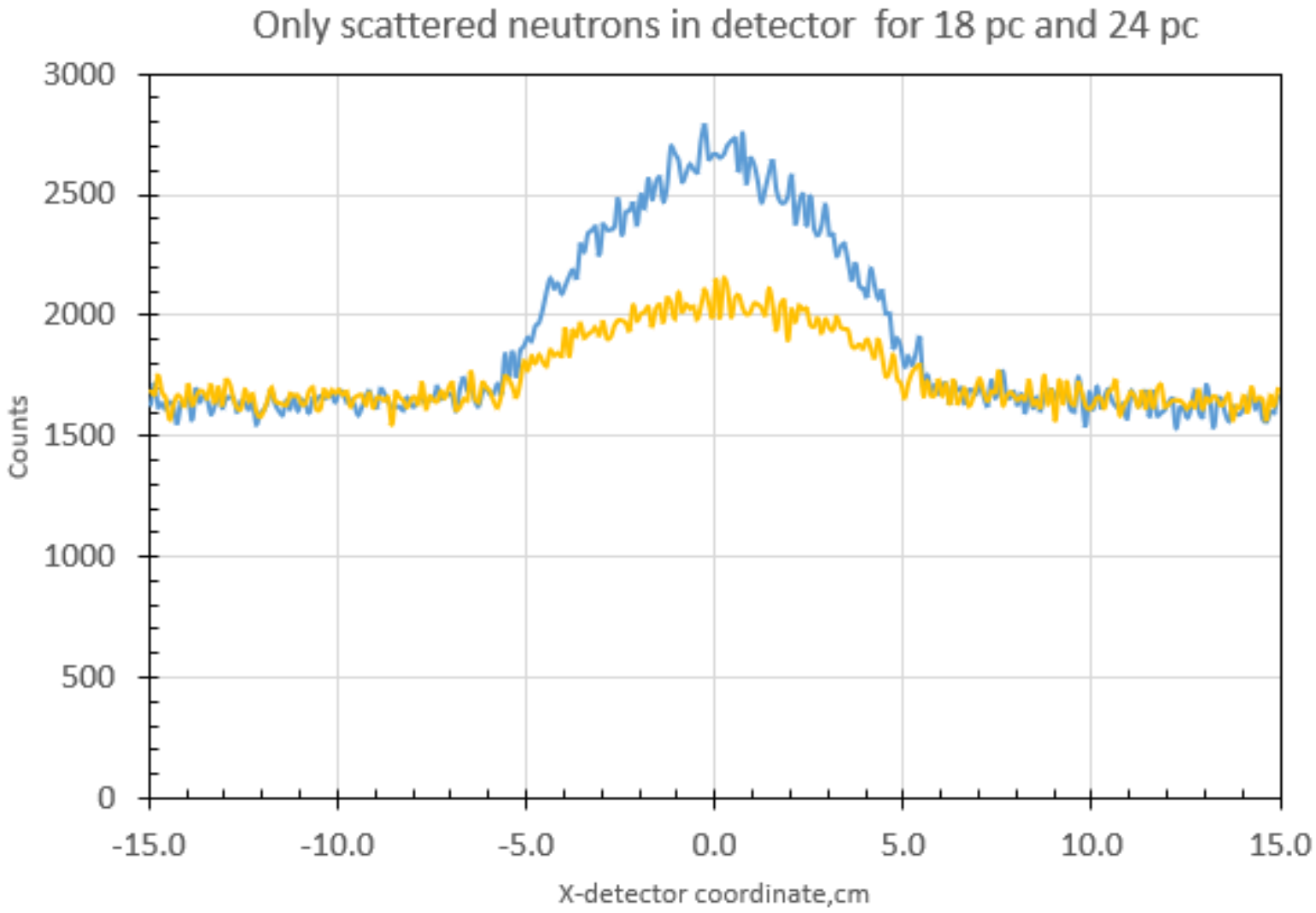
Fit parameter η from June 2022 (1) and cold (2) simulation fits

Fit type	η	Error η	
(1) 9-3 fit	0.58052	0.00033	
(1) 6-2 fit	0.6067	0.0026	
(1) 6-3 fit	0.6693	0.0018	$\leftarrow negative\ \alpha$
(2) 7-3 fit COLD	0.5815	0.0014	
(2) 7-2 fit COLD	0.5887	0.0002	

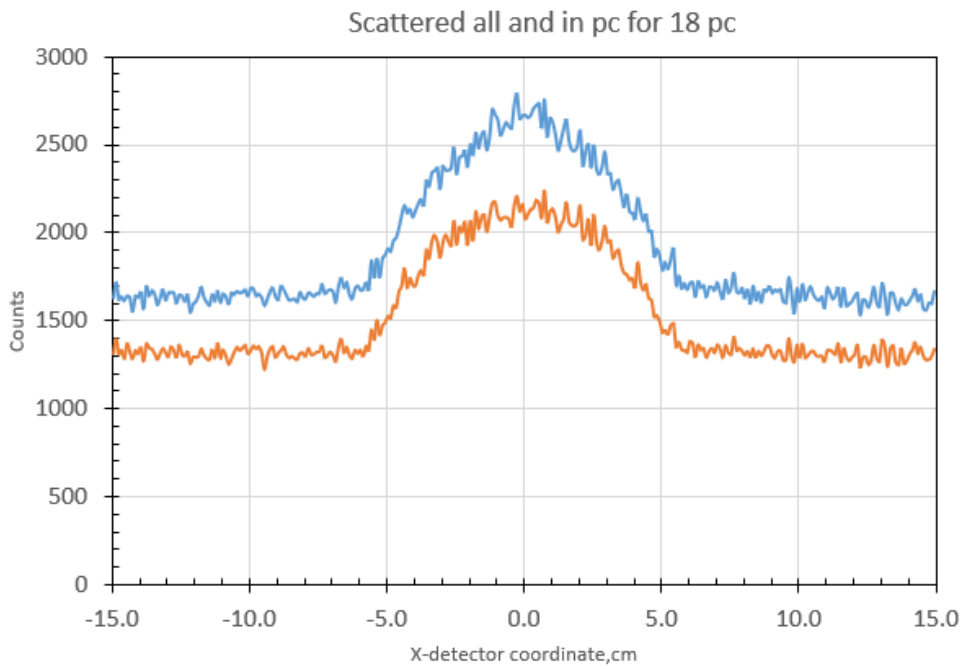
High-statistics data

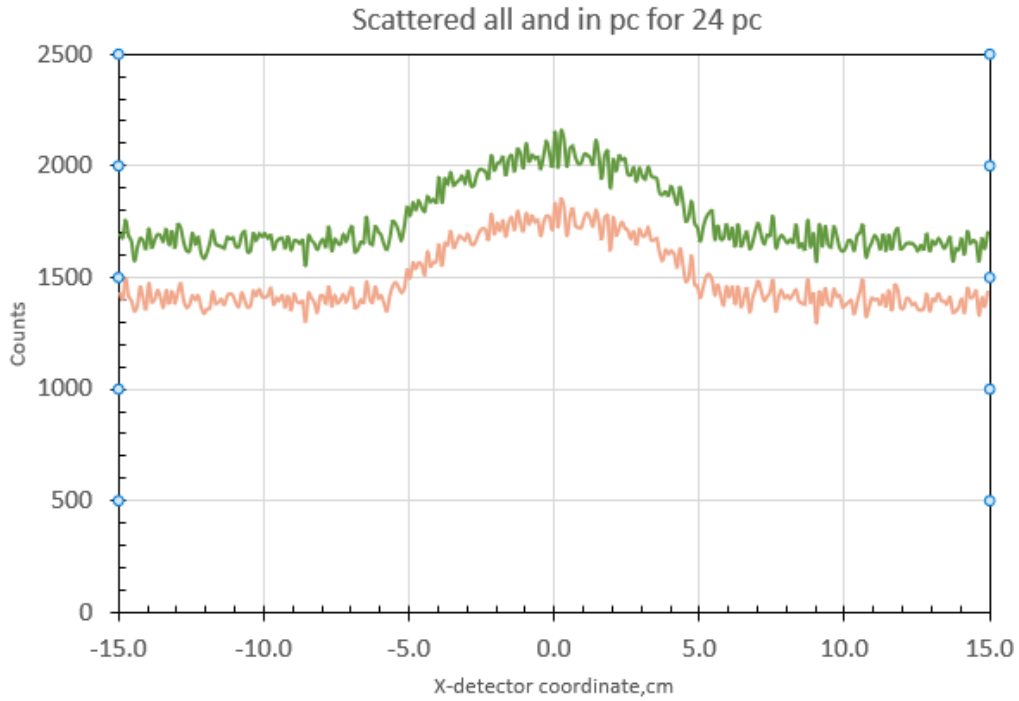

1.E+10 initial n simulated, all n that are seen
in the detector with 18 pc and 24pc
1.E+6
1.E+5
1.E+4
1.E+3
Counts
-15.0
-10.0
-5.0
0.0
5.0
10.0
15.0
Detector X, cm

Scattered background includes scattering on S3 collimator, in pc, in air, and beam diaphragm

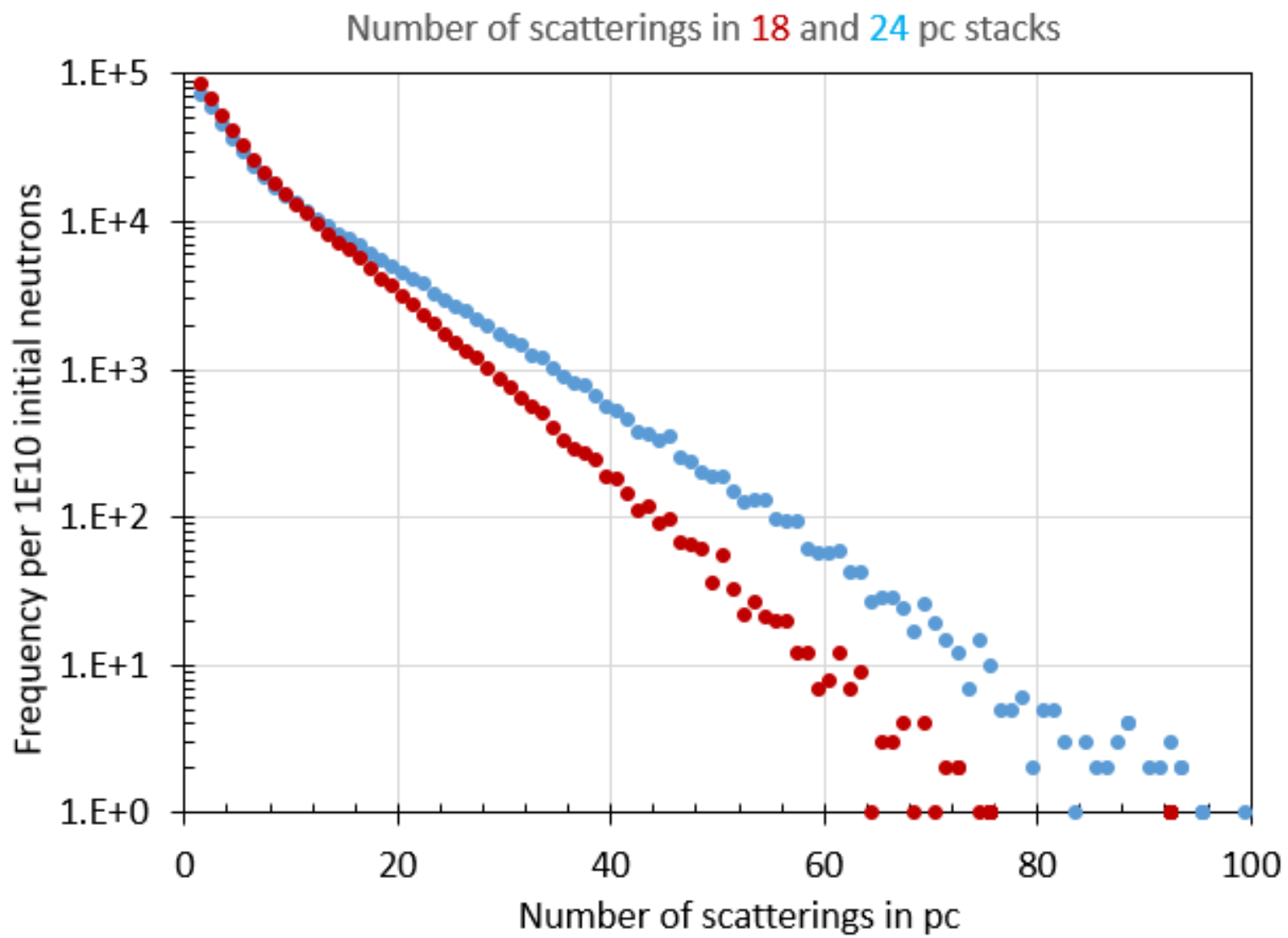


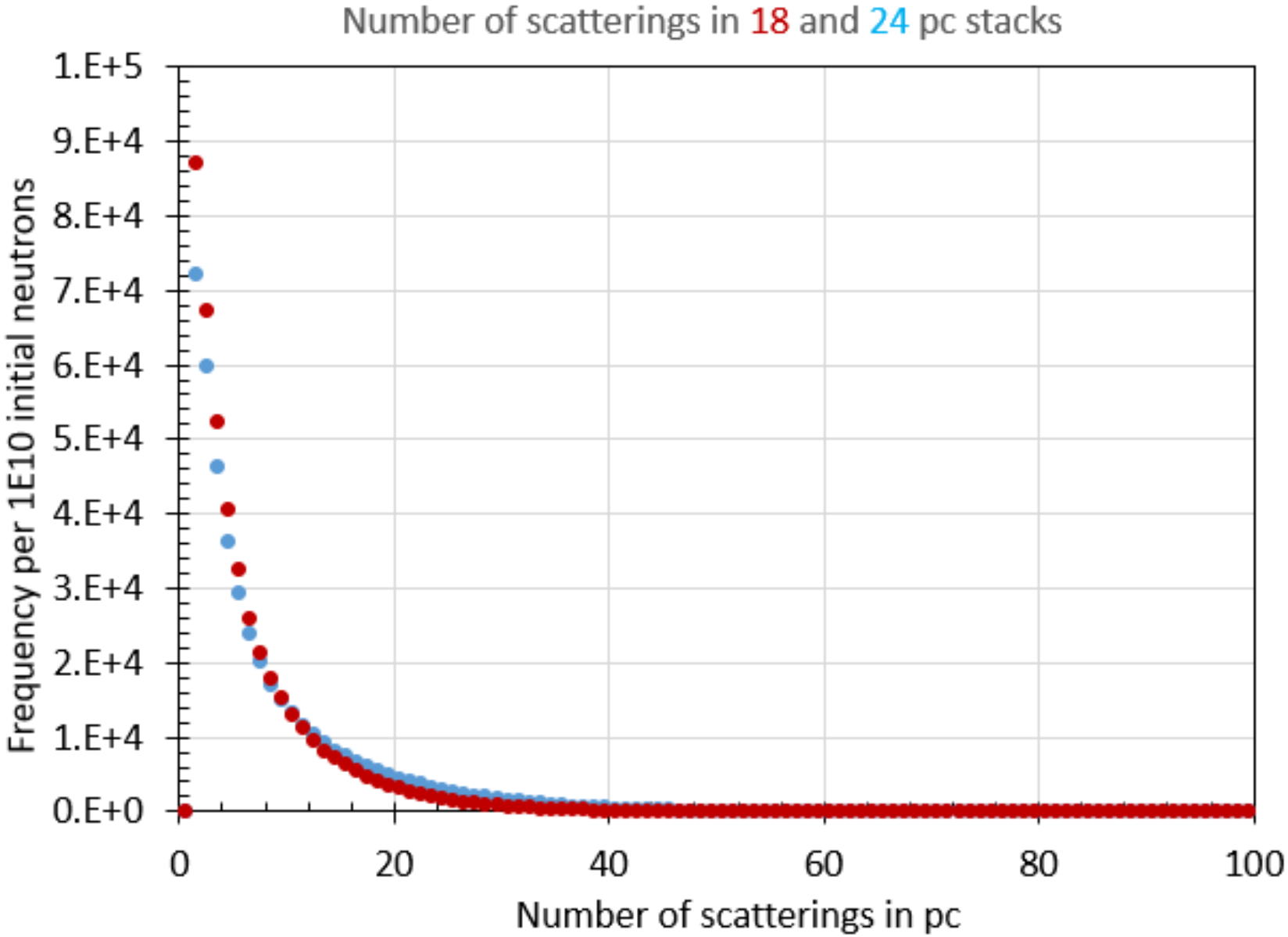
Background including all scattering and bkgr of scattering in pc only (lower curves)

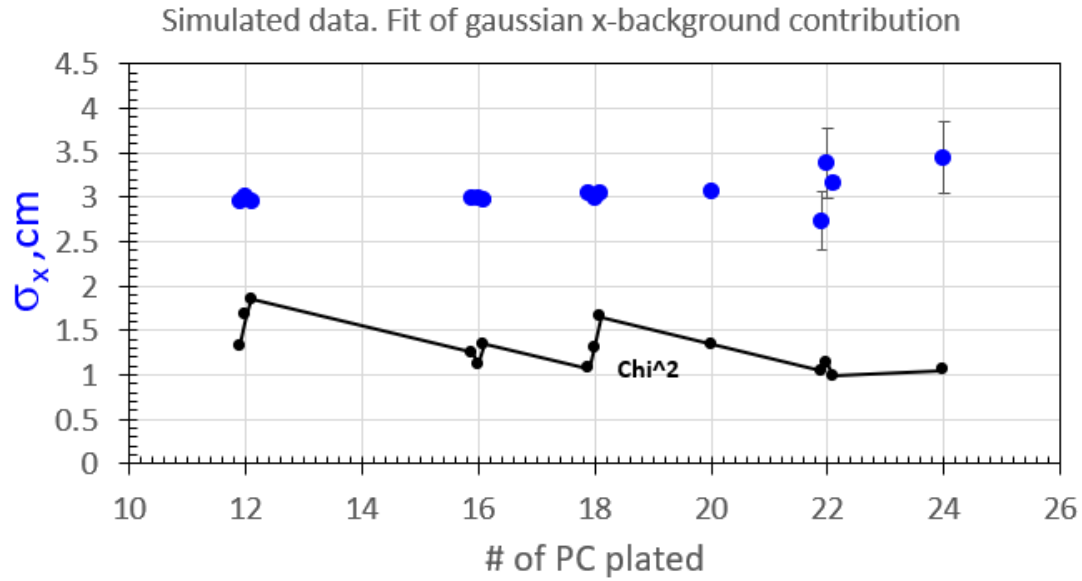


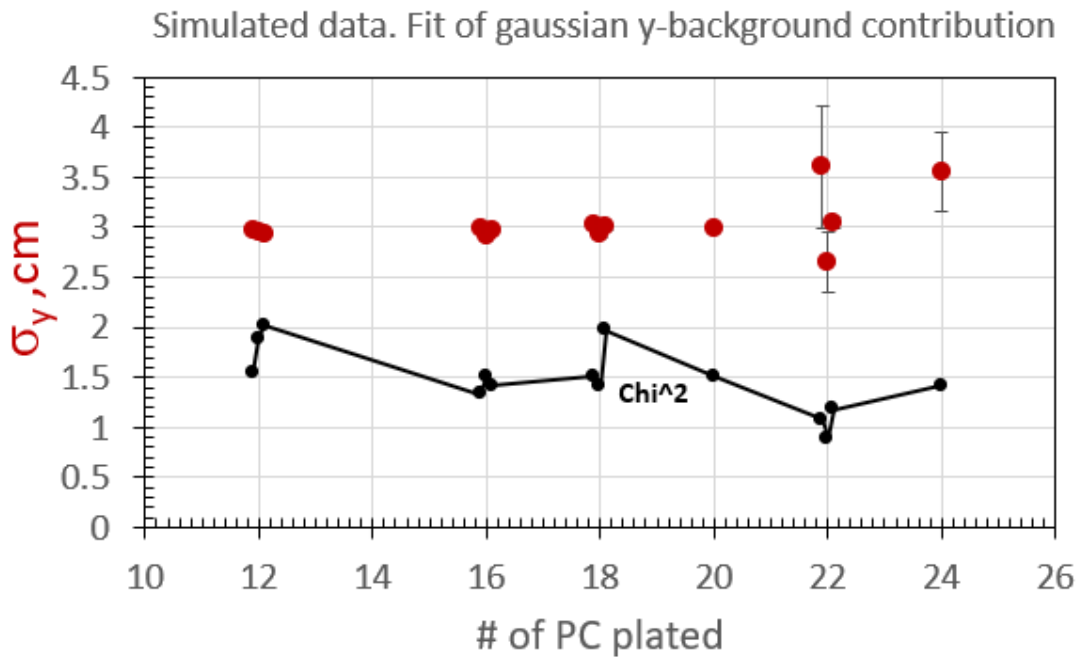


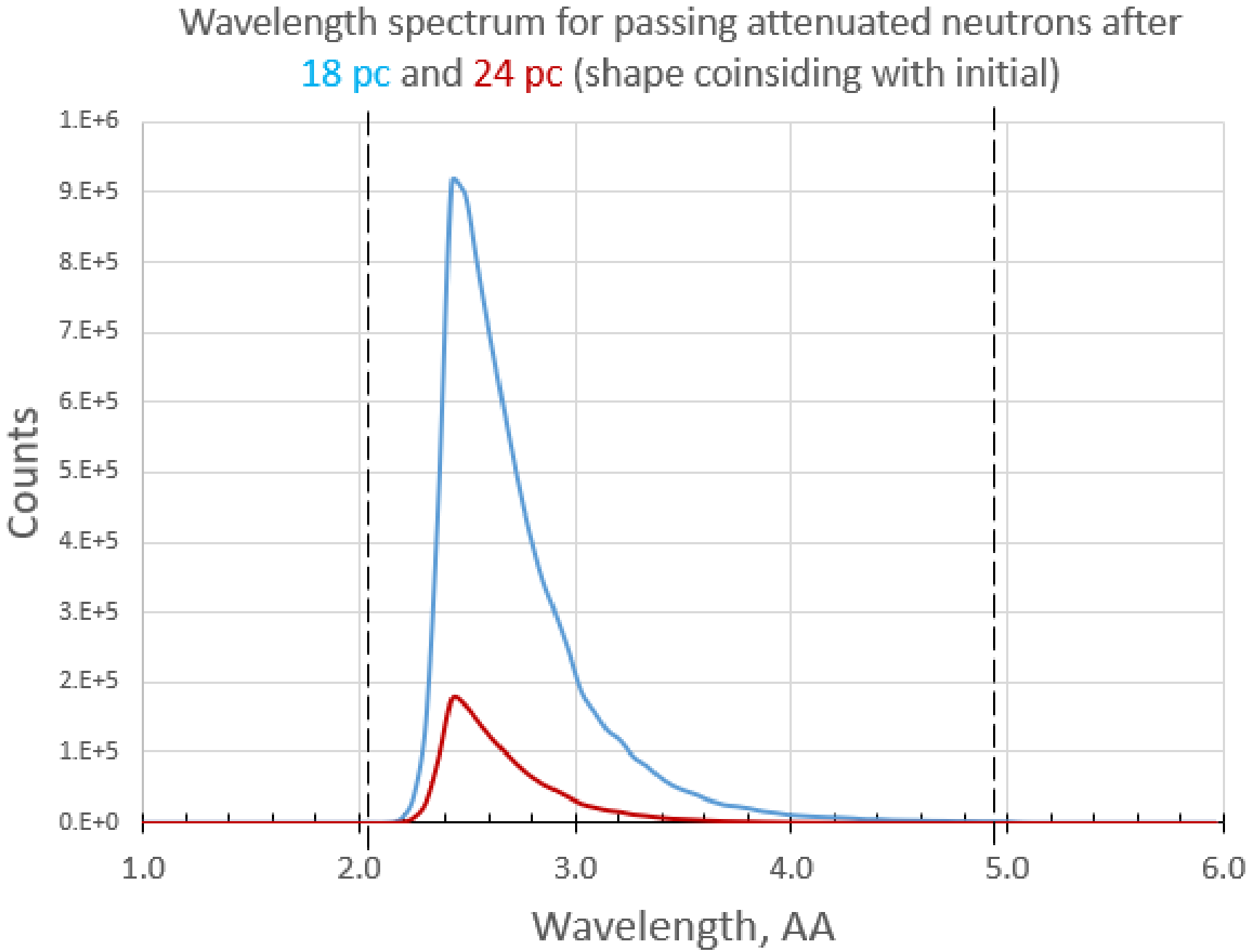
								x	x	y	y			
# pc	st#	initial #	Ntotal	Pass	TOT-PASS	Gauss tot X	Gaugg tot Y	constant	Gauss peak	constant	Gauss peak	GPeak X/Y	Const X/Y	
18	C	1.00E+10	8088753	7520114	568639	82820	82251	1619.39	1081.93	1621.29	1085.51	0.9967	0.9988	
18	C	1.00E+10	8088753	7520114	7520114	69529	68862	1296.85	903.47	1299.08	903.57	0.9999	0.9983	c2=bkgr
24	0	1.0E+10	1813608	1284221	529387	34335	33202	1650.17	429.32	1653.95	428.69	1.0015	0.9977	
24	0	1.0E+10	1813608	1284221	529387	32078	30798	1391.91	400.24	1396.17	395.66	1.0116	0.9969	c2=bkgr

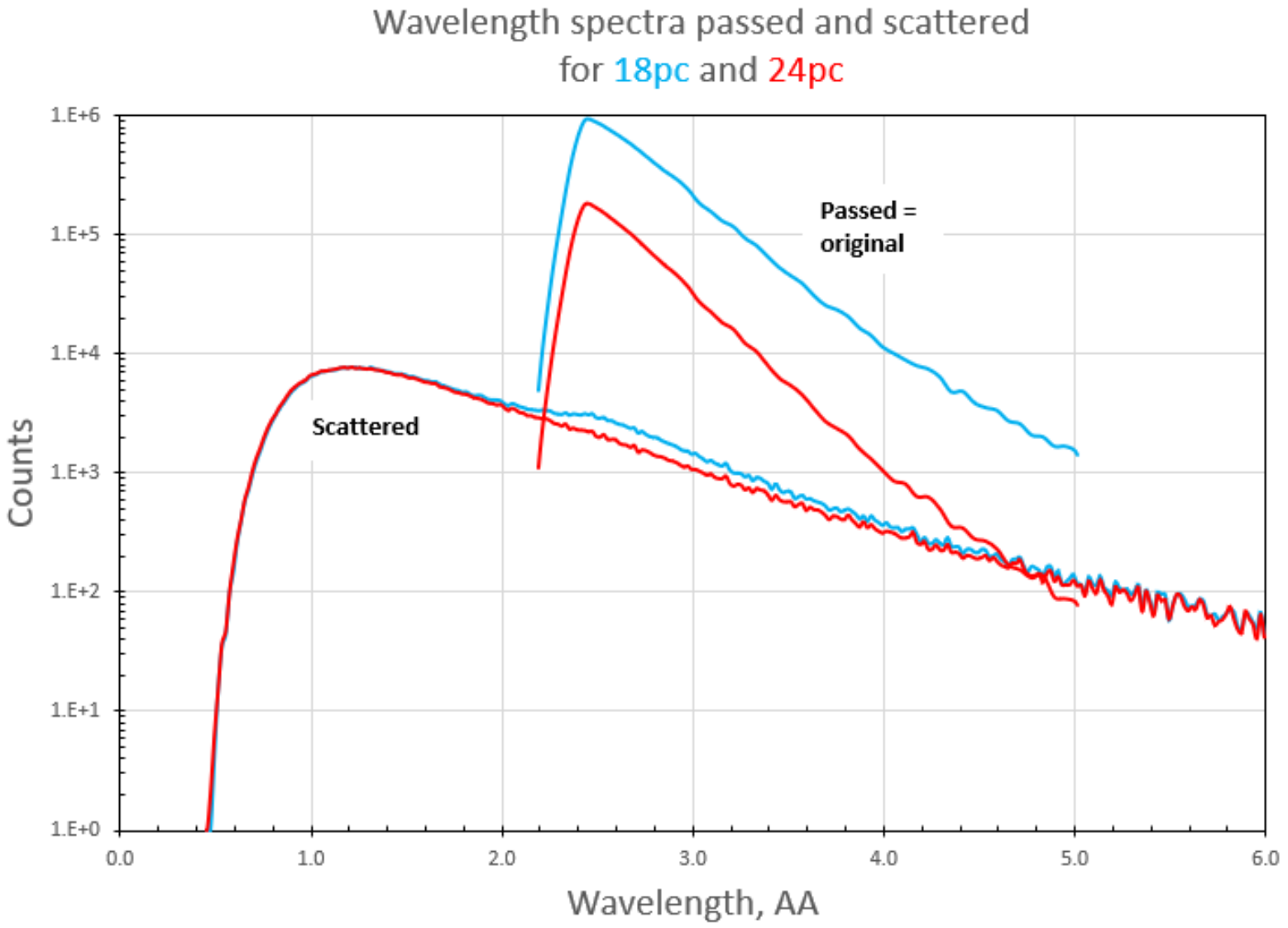

Number of scatterings in 18 and 24 pc stacks
1.E+5
1.E+4
1.E+3
1.E+2
1.E+1
1.E+0
Frequency per 1E10 initial neutrons
0
20
40
60
80
100
Number of scatterings in pc


Number of scatterings in 18 and 24 pc stacks
Frequency per 1E10 initial neutrons
1.E+5
9.E+4
8.E+4
7.E+4
6.E+4
5.E+4
4.E+4
3.E+4
2.E+4
1.E+4
0.E+0
0
20
40
60
80
100
Number of scatterings in pc

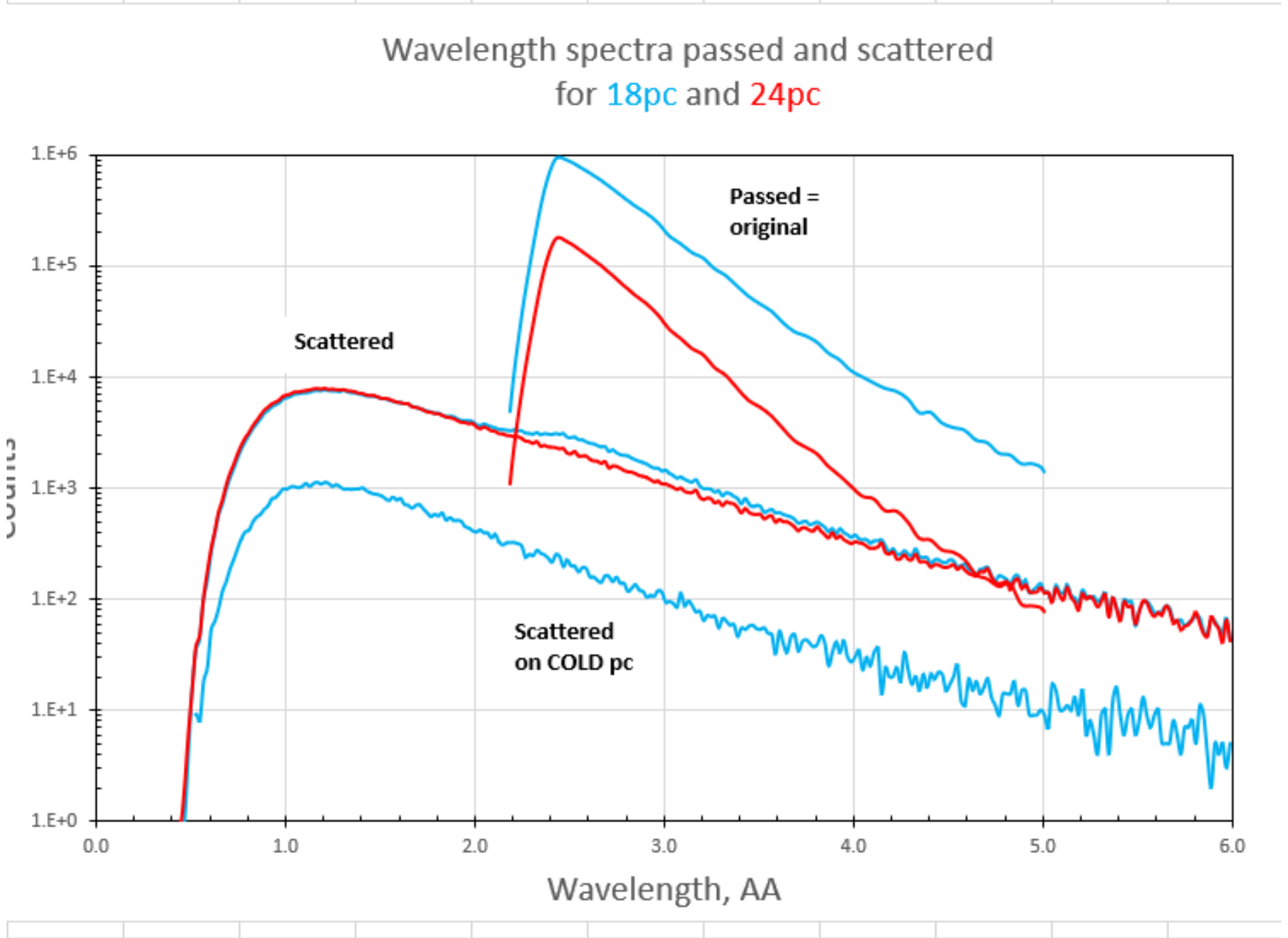

Simulated data. Fit of gaussian x-background contribution
σx,cm
Chi^2
# of PC plated

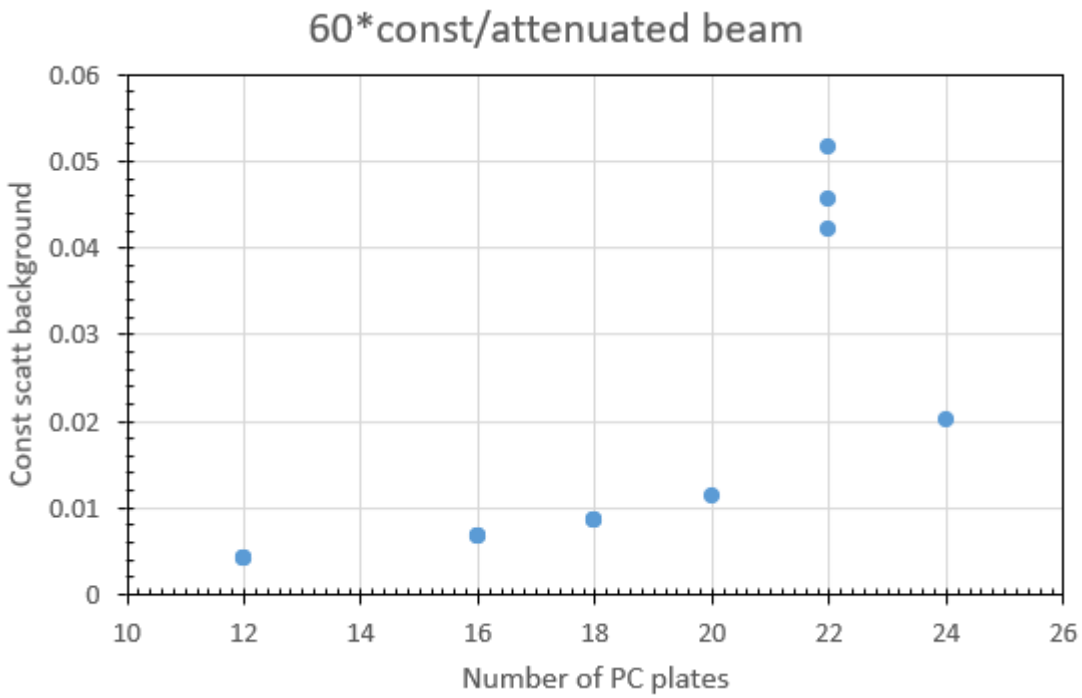

Simulated data. Fit of gaussian y-background contribution
σy,cm
Chi^2
# of PC plated

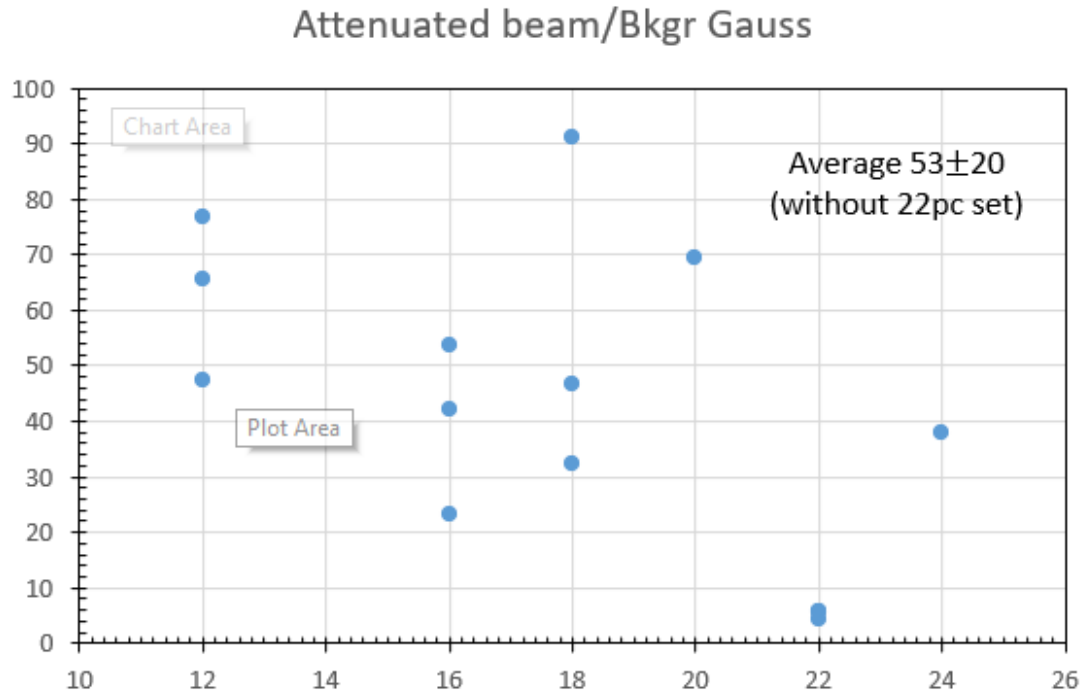

Wavelength spectrum for passing attenuated neutrons after
18 pc and 24 pc (shape coinsiding with initial)
Counts
1.E+6
9.E+5
8.E+5
7.E+5
6.E+5
5.E+5
4.E+5
3.E+5
2.E+5
1.E+5
0.E+0
1.0
2.0
3.0
4.0
5.0
6.0
Wavelength, AA

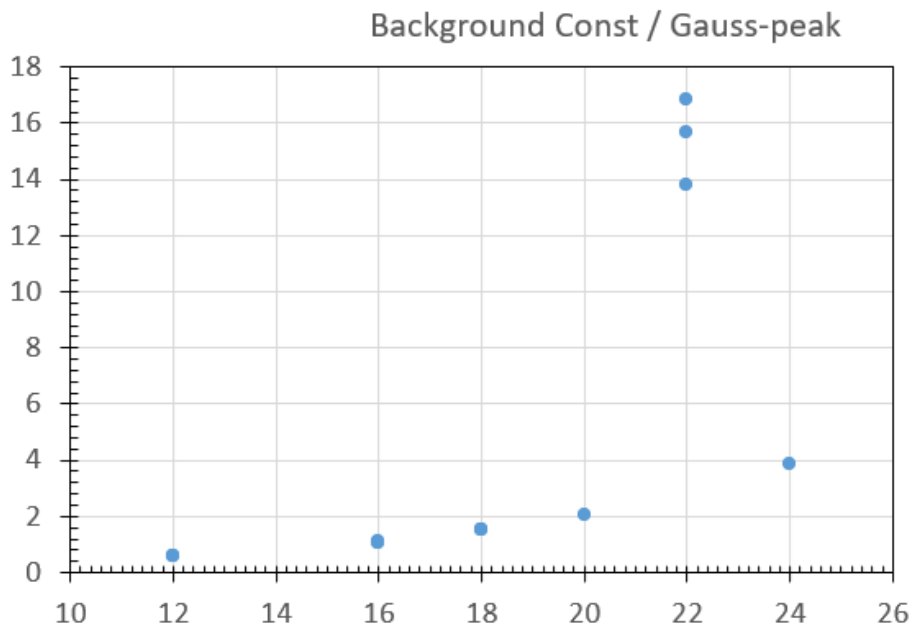


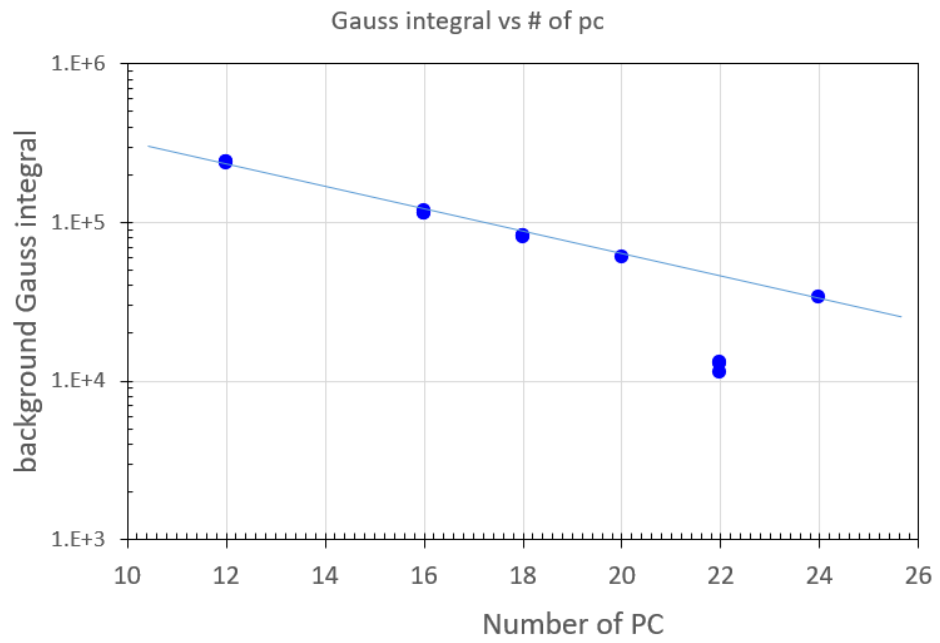
Theoretical calculation of η can be possible with scattered λ spectra for all n


Wavelength spectra passed and scattered
for 18pc and 24pc
1.E+6
1.E+5
1.E+4
1.E+3
1.E+2
1.E+1
1.E+0
Passed =
original
Scattered
Scattered
on COLD pc
0.0
1.0
2.0
3.0
4.0
5.0
6.0
Wavelength, AA


60*const/attenuated beam
Const scatt background
0.06
0.05
0.04
0.03
0.02
0.01
0
10
12
14
16
18
20
22
24
26
Number of PC plates


Attenuated beam/Bkgr Gauss
100
90
80
70
60
50
40
30
20
10
0
Chart Area
Plot Area
Average 53±20
(without 22pc set)
10
12
14
16
18
20
22
24
26


Background Const / Gauss-peak
18
16
14
12
10
8
6
4
2
0
10
12
14
16
18
20
22
24
26


Gauss integral vs # of pc
background Gauss integral
1.E+6
1.E+5
1.E+4
1.E+3
10
12
14
16
18
20
22
24
26
Number of PC