Overview and performance of low energy hadronic models in Geant4. Need of interfacing to evaluated data libraries for specific applications

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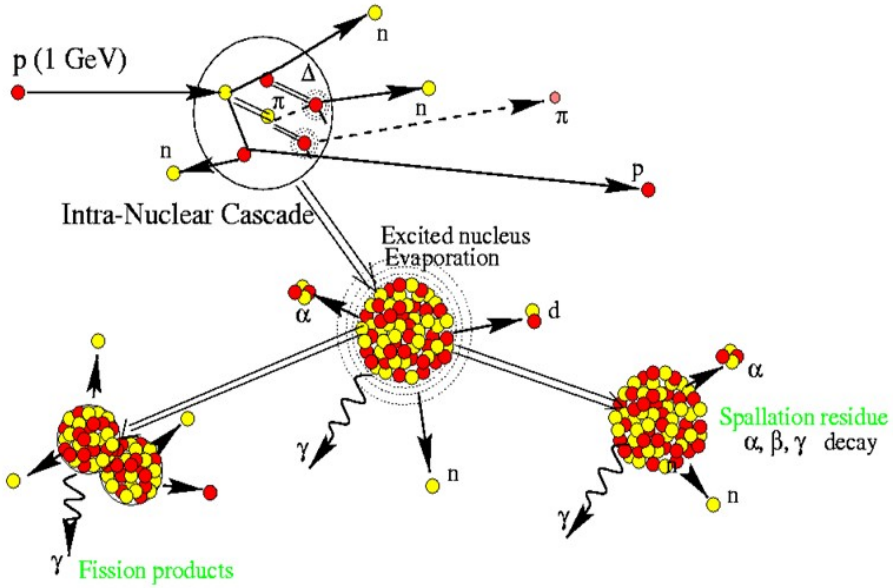
Workshop on low energy neutron libraries in Geant4
Madrid, March 21-23, 2011

Overview of low energy hadronic models in Geant4

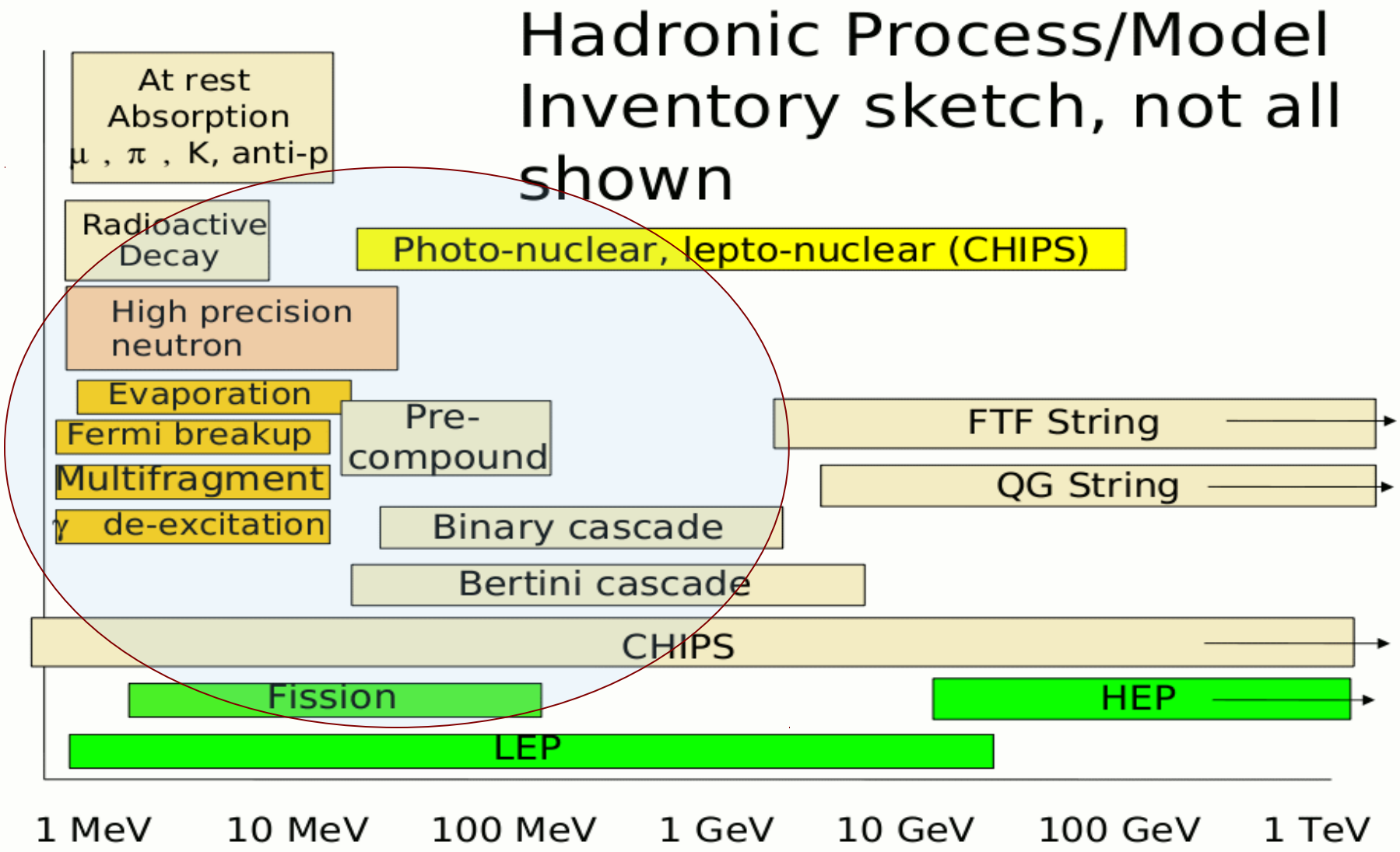
- Cascade models
  - Binary Cascade
    - Binary Light Ion *
  - Bertini cascade
  - INCL



- Non cascade models:
  - QMD*
  - CHIPS

(*): valid for nucleus-nucleus reactions

Geant4 Hadronic Models (outdated)



Geant4 Cascade Models

- **Binary Cascade**:
  - a time-dependent model which depends as little as possible on parameterization and therefore can be expected to be more predictive
  - is an *in house* development, including its own precompound and evaporation models.

NATIVE

- **Bertini Cascade**:
  - it came from the INUCL code which was intended as an all-inclusive model
  - it came with its own pre-compound and de-excitation models. Neither of these are very different in origin from those in Binary, but the implementations are different.

IAEA benchmark

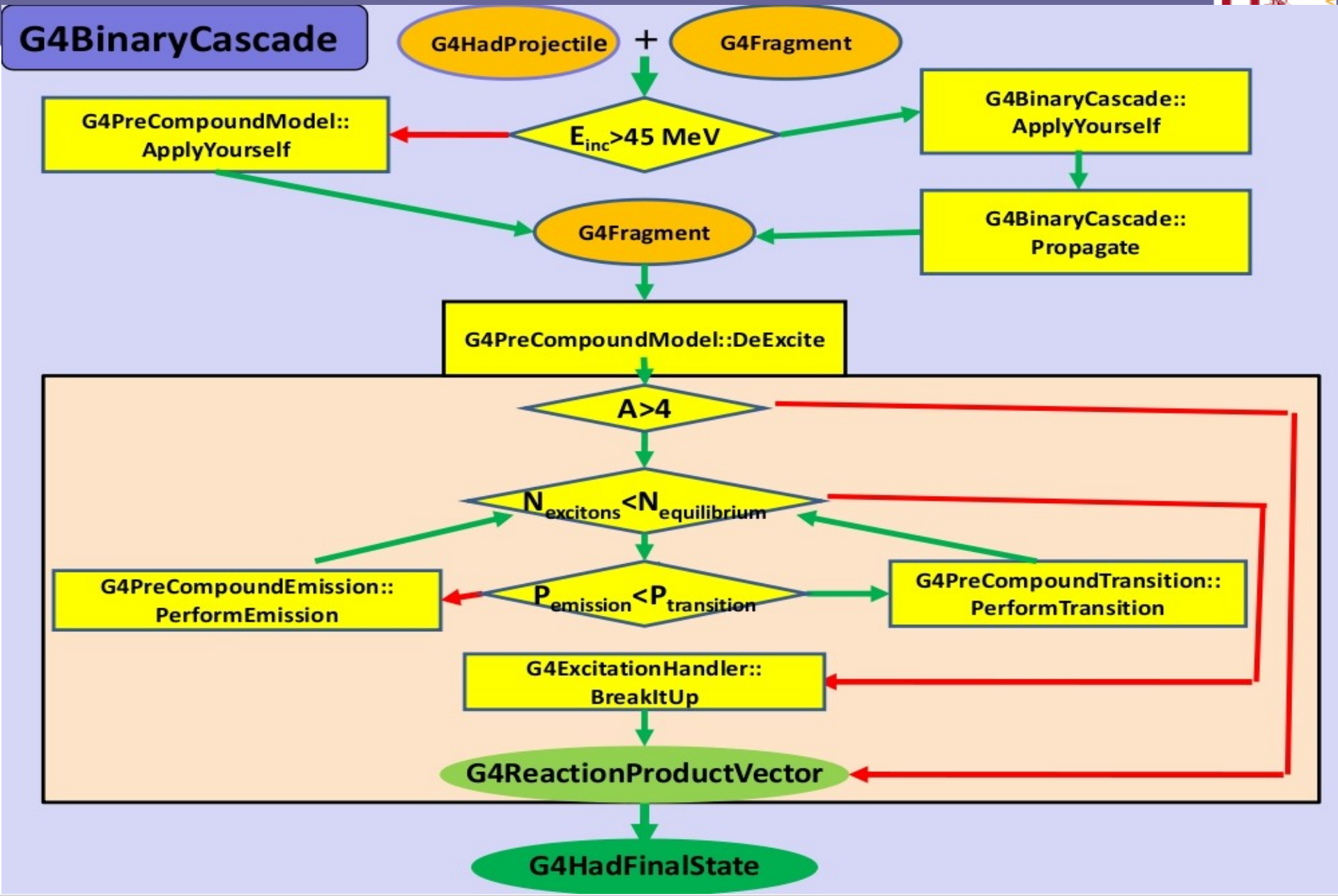
- **INCL/ABLA**:
  - C++ translation of INCL (v4.2) intranuclear cascade code
  - C++ translation of ABLA (v3p) evaporation/fission code

Geant4 *Non*-Cascade Models

- **Chiral Invariant Phase Space Model (CHIPS):**
  - Quark-level event generator for the fragmentation of hadronic systems into hadrons.

- **Quantum Molecular Dynamics Model (QMD) :**
  - Is a quantum extension of classical molecular-dynamics model.

Pre-equilibrium



Pre-equilibrium

- After Binary Cascade stage *native* pre-equilibrium follows

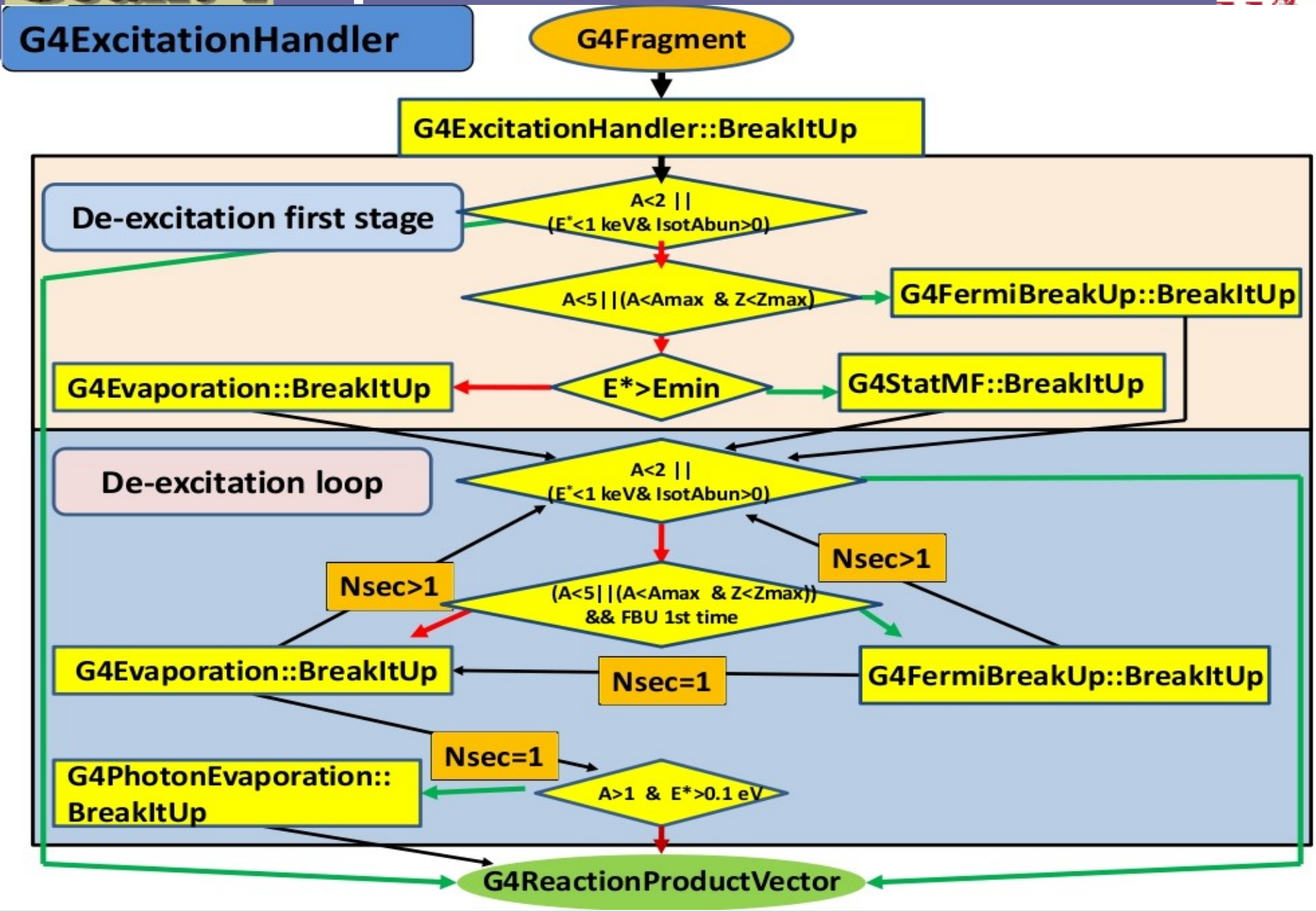
- Native pre-equilibrium model in Geant4 is a version of standard exciton model.

Key ingredients:

- Internal transition rates:
  - CEM (Cascade Exciton Model, Gudima et al). Default
  - Blann-Machner's parameterization.

- Emission rates:
  - Nucleon emission in standard exciton formulation.
  - Complex particle emission (d,t,^{3}He, ^{4}He) from CEM.

Equilibrium De-excitation



Equilibrium De-excitation

Five processes are considered:

Alternates:

- **Fermi Breakup , for Z<9, A<17 (Botvina *et al*)**
- **Statistical Multifragmentation, for E*/A > 3 MeV (Botvina *et al*)**

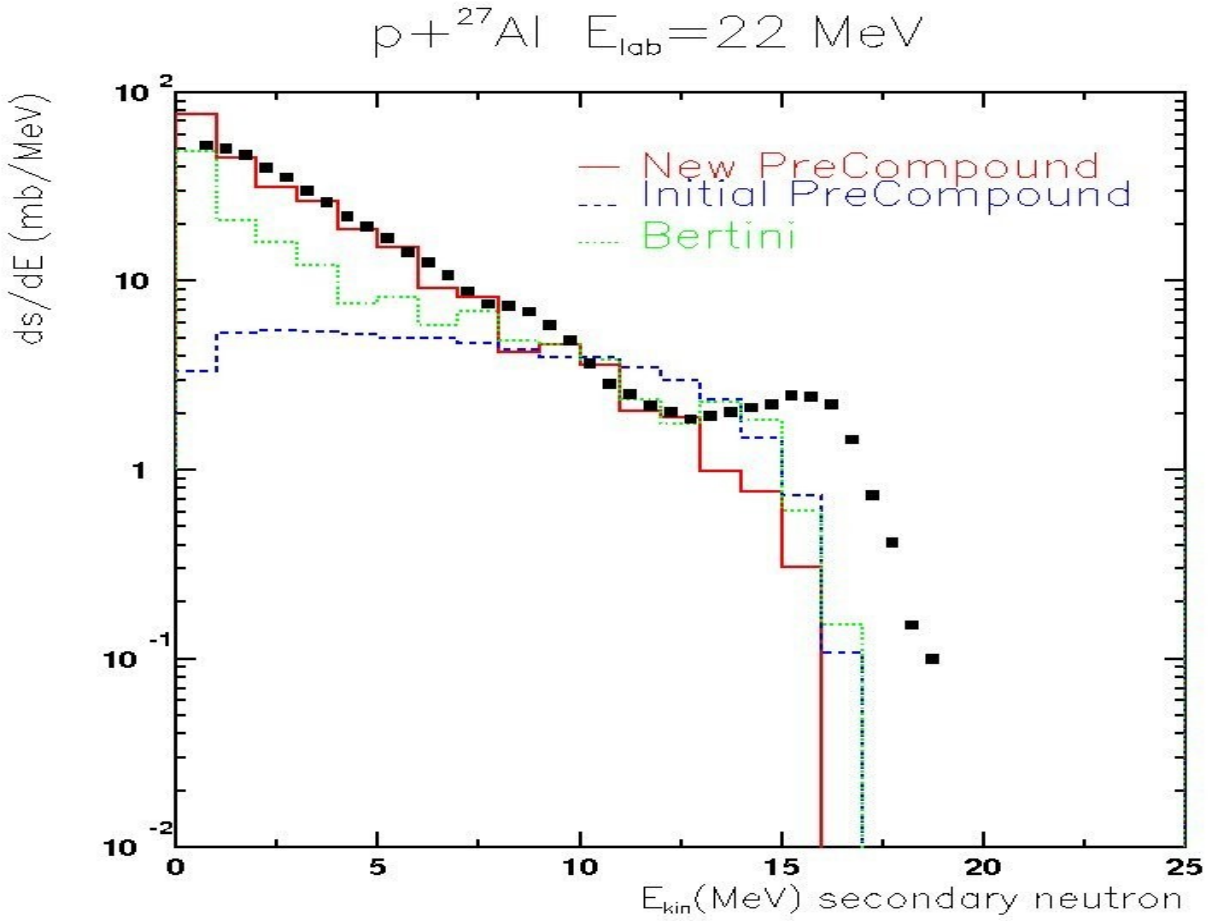
Competitors:

- **Fission (Bohr-Wheeler model + Amelin prescript.)**
- **Particle Evaporation:**
  - **Evaporation Model WE (Weisskopf-Ewing)**
  - **Generalized Evaporation Model GEM (Furihata).**
- **Photon Evaporation:**
  - **Discrete (tabulated E1,M1, E2)**
  - **Continuum (GDR strength)**

RESULTS

Test30 : incident nucleons from ~10 MeV up to ~500 MeV)

In 2007 the situation was not good with regard to native pre-equilibrium & de-excitation models in Geant4 in several cases:



IAEA benchmark of spallation models (p, n from ~60 MeV - 3GeV)

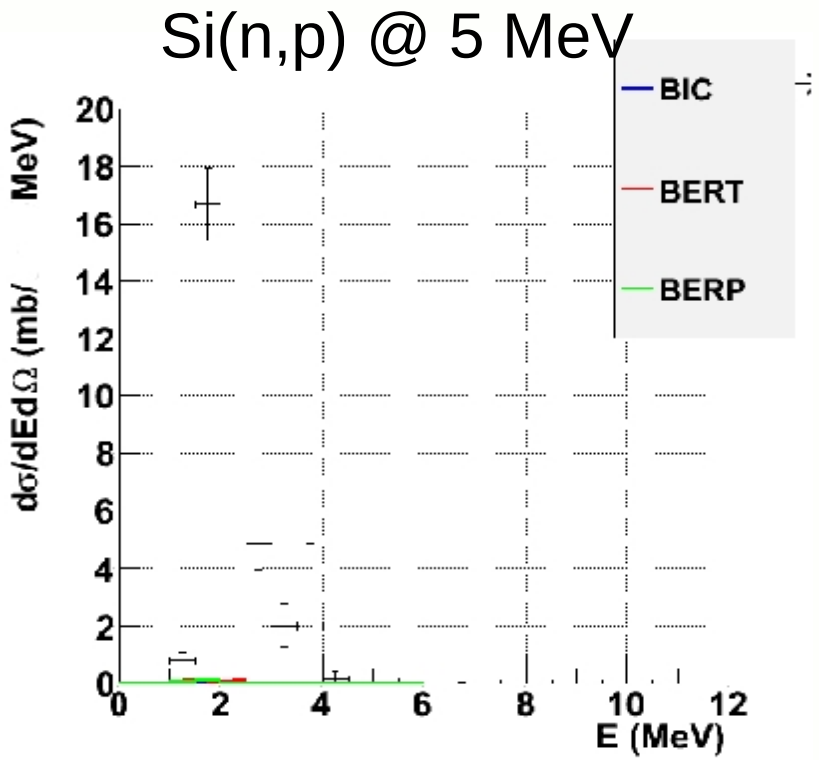
Initially the situation was bad in two critical aspects:

- Almost no cluster (d, t, ^{3}He, α) emission
- Almost no residuals from fission

Improvements

Many, during the last 3 years, but ..

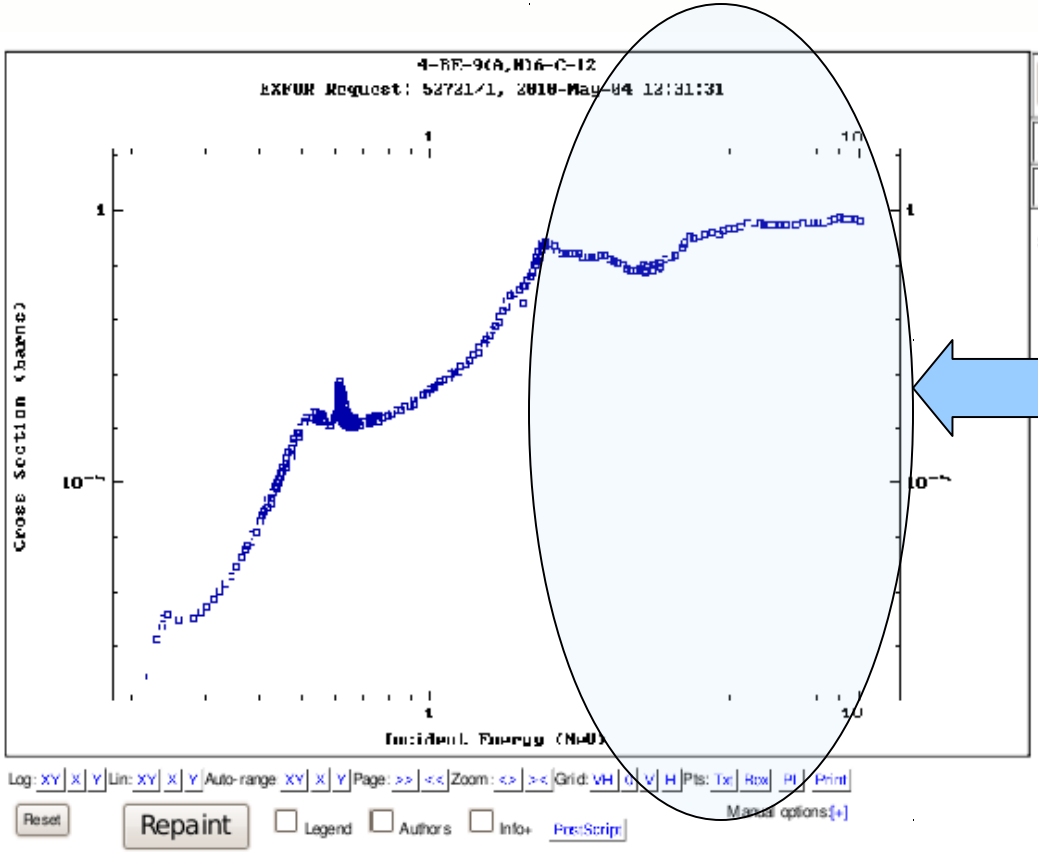
In principle, one shouldn't expect very good results for very low energies, where subtle nuclear structure effects show up



This is a typical situation where evaluated data are needed

$^{9}Be(\alpha,n)^{12}C$

In general one cannot expect much from models in specific channels which are ***privileged by*** **nuclear structure**



α–Be source
E_n ~5.5 MeV

"Theoretical perversions" (according to Daniel's terminology) will hardly be capable of describing such data (very light systems, very low energy …) on a general base

2009: request of support by PhD student (Consuelo Guardiola) from CNM-IMB (National Centre of Microelectronics, Barceloma, Spain)

Geant4 simulations of thermal neutrons irradiation on pad detectors with converter layers

Part 2 (with corrections: Quesada's files *)

- Detector Efficiency
- Spectrums of energy deposited on planar detector convered by converter layer (boron clusters)

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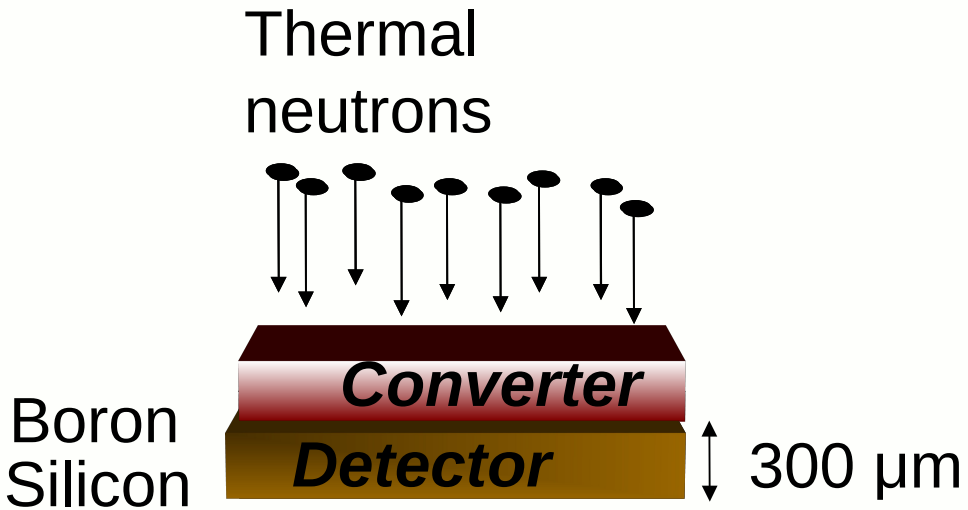
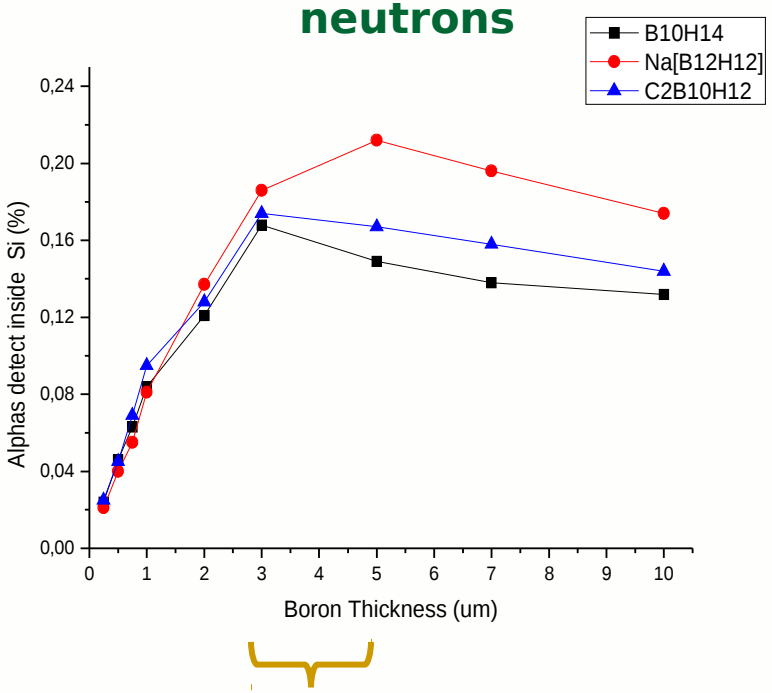
$^{10}B(n,\alpha)^{7}LI$ Detector Efficiency



$$^{10}B + n \rightarrow \alpha(1.47\,MeV) + {}^{7}Li(0.84\,MeV) + \gamma(0.48\,MeV) \quad 93.7\%$$

$$^{10}B + n \rightarrow \alpha(1.78\,MeV) + {}^{7}Li(1.01\,MeV) \quad 6.3\%$$

10^6 thermal neutrons



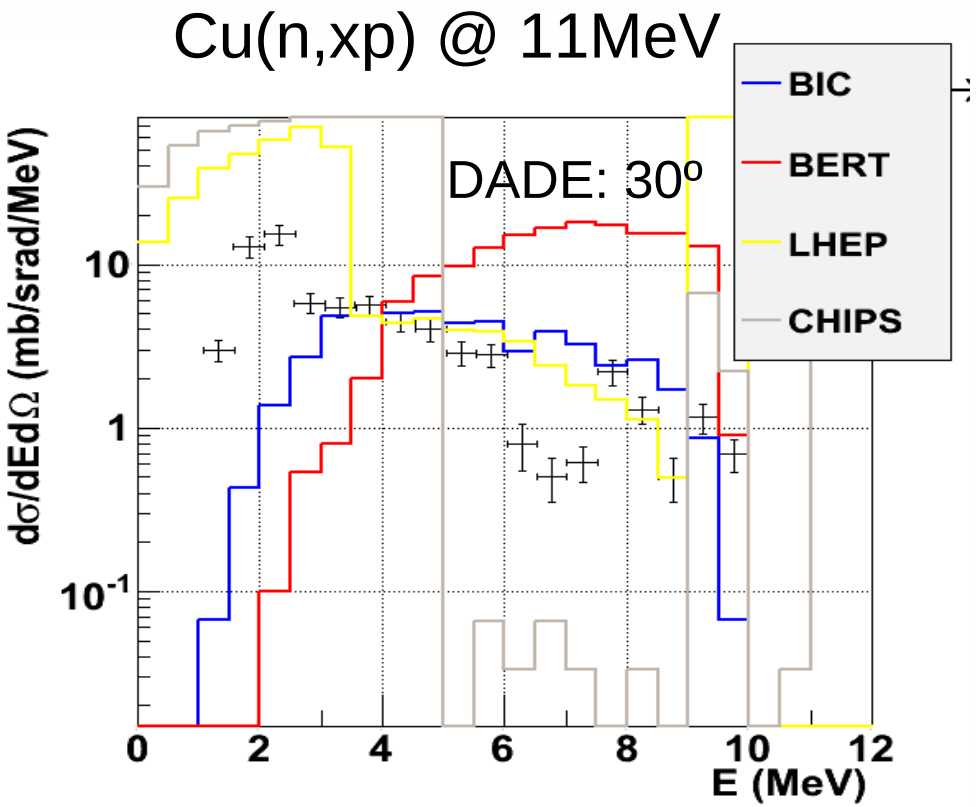
range 3–5 μm detection efficiency maximized

Quesada's files ("G4FermiFragmentsPool.cc" and "G4ExcitationHandler.cc")

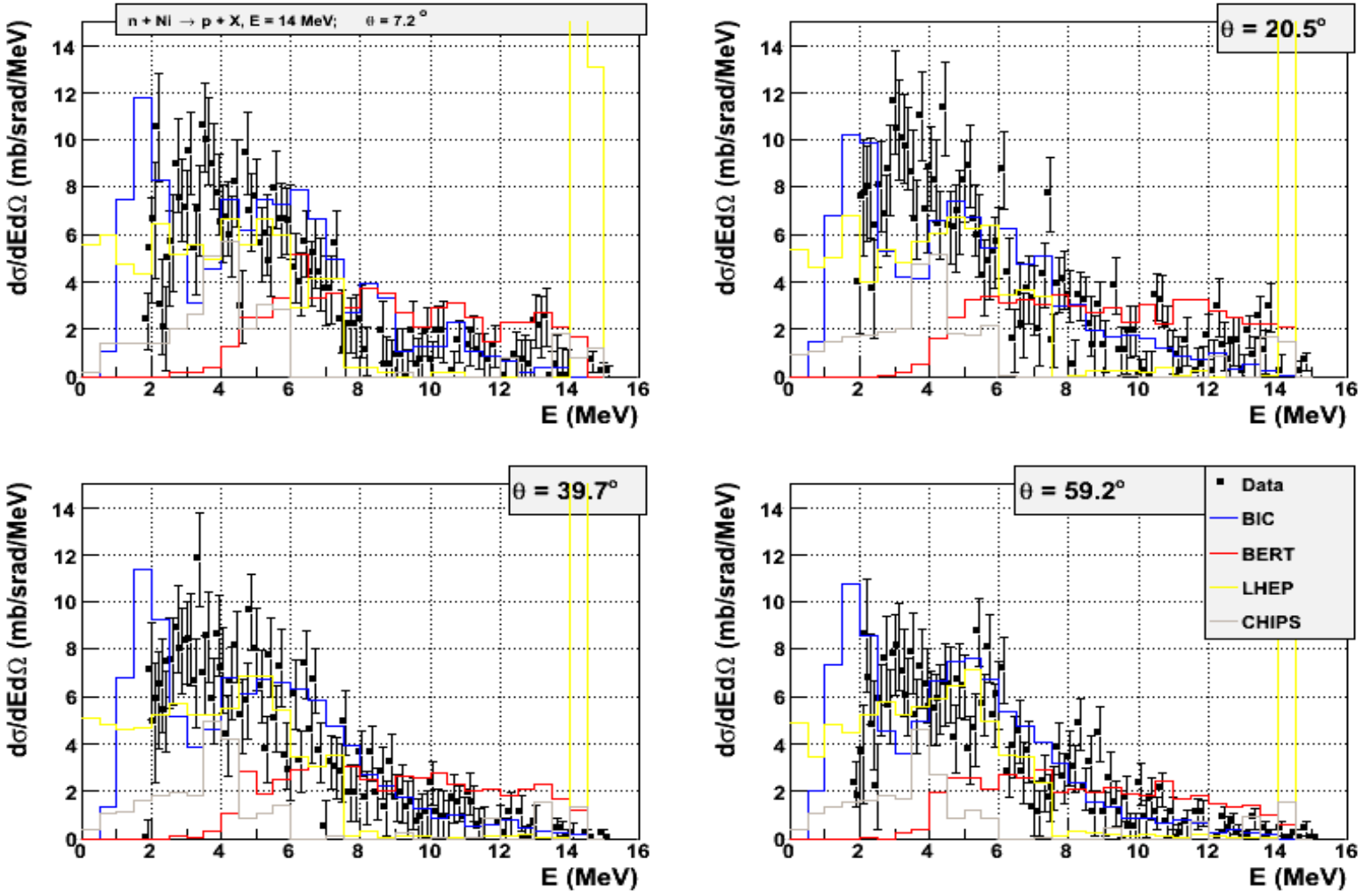
Spectrums simulated with optimized thickness

Cu(n,xp) @ 11 MeV

As the energy increases, the situation improves and statistical models are capable of doing their job



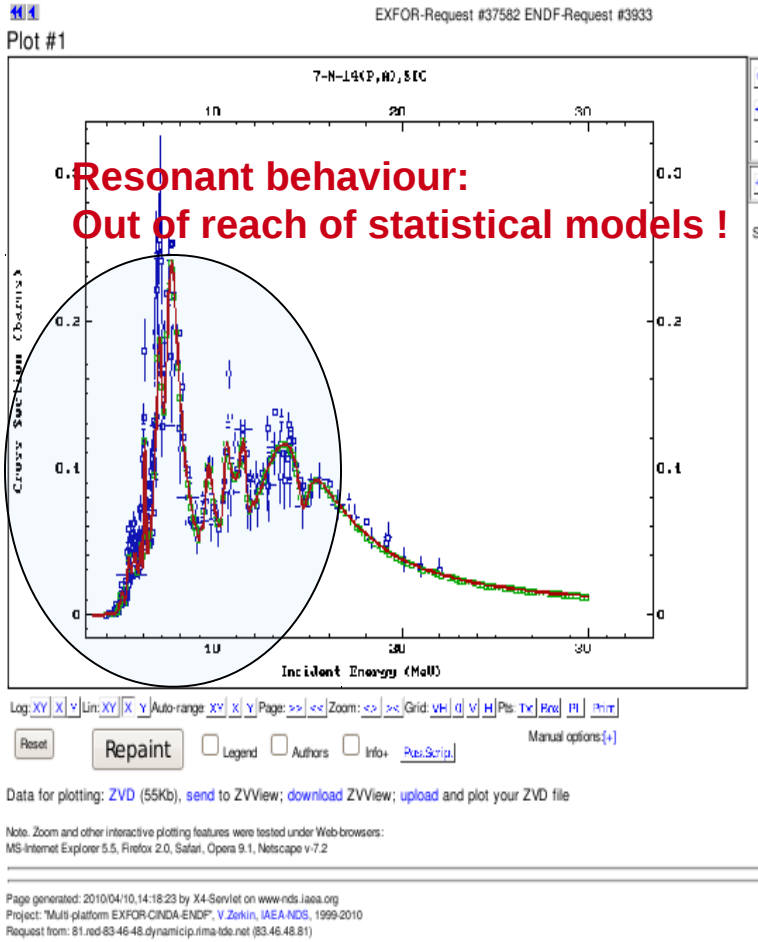
Ni(n,xp) @ 14 MeV


n + Ni → p + X, E = 14 MeV; θ = 7.2°
θ = 20.5°
θ = 39.7°
θ = 59.2°
Data
BIC
BERT
LHEP
CHIPS
dσ/dEdΩ (mb/srad/MeV)
E (MeV)

$^{14}N(p,\alpha)^{18}F$

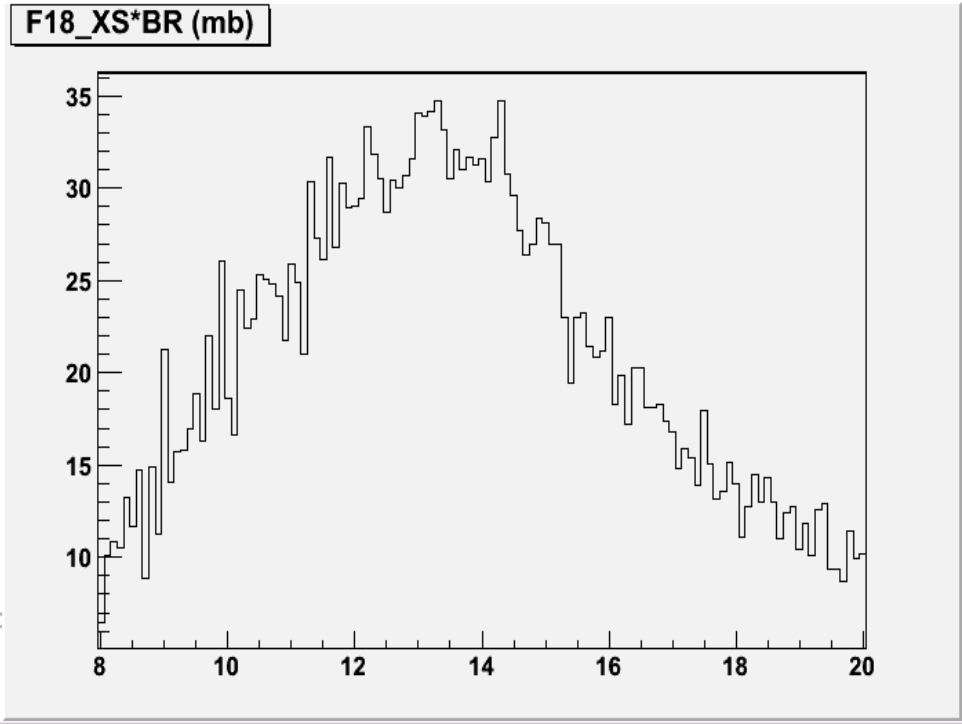
But unfortunately not always..

http://www-nds.iaea.org/exfor/servlet/X4sProcess...

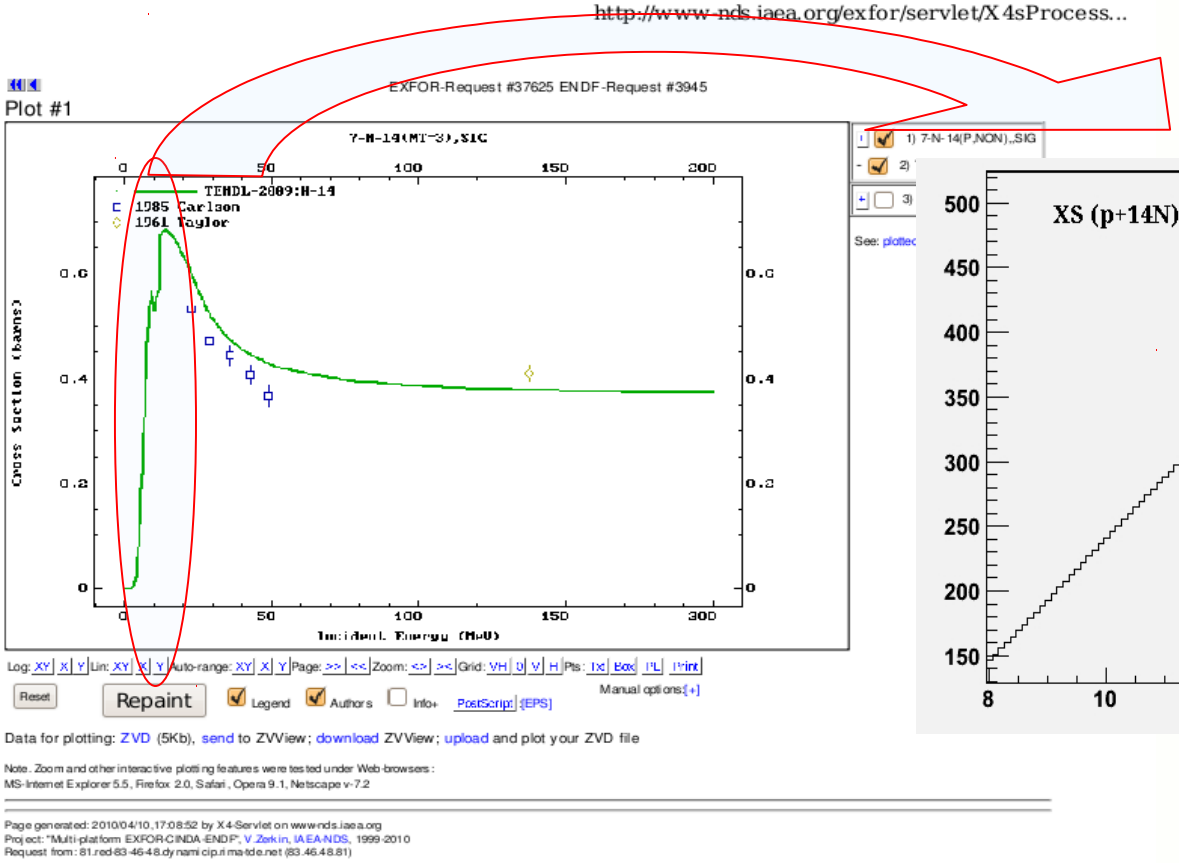


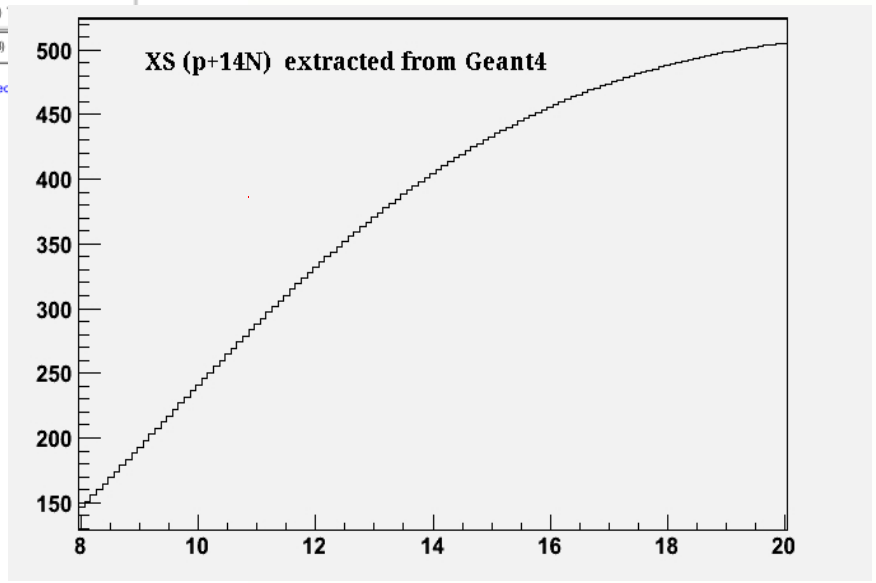
Resonant behaviour:
Out of reach of statistical models !

Production cross section, as product of:
1) XS: total reaction cross section (data)
2) BR: branching ratios (nuclear models)



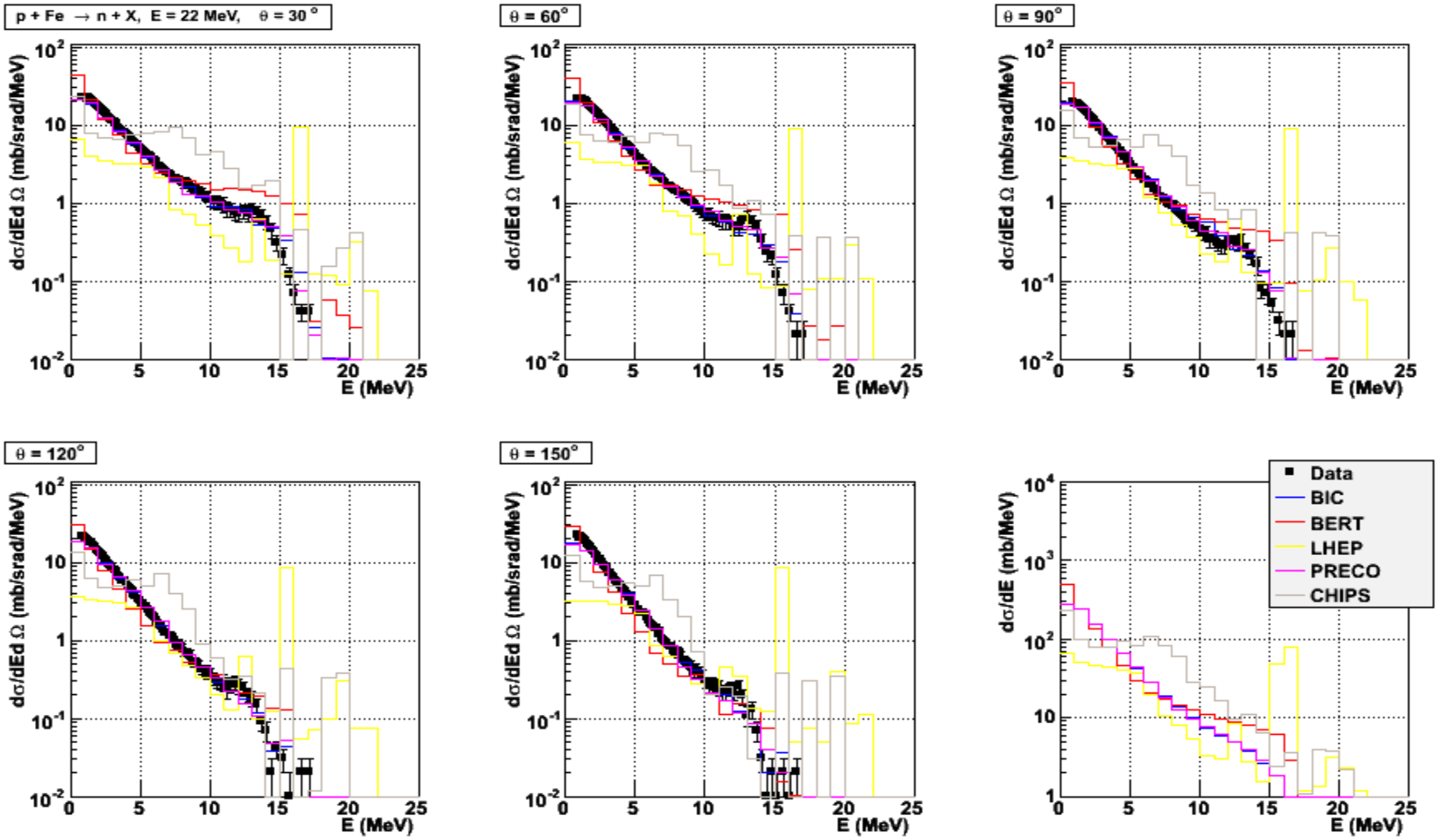
Reaction cross sections (not well known at such low energies) are partially responsible, but the description of reaction mechanisms (branching ratios) is the main source of discrepacy with exp. results





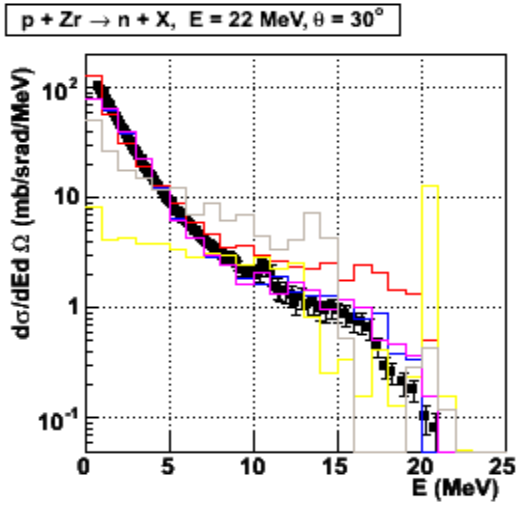
Fe(p,xn) @ 22 MeV

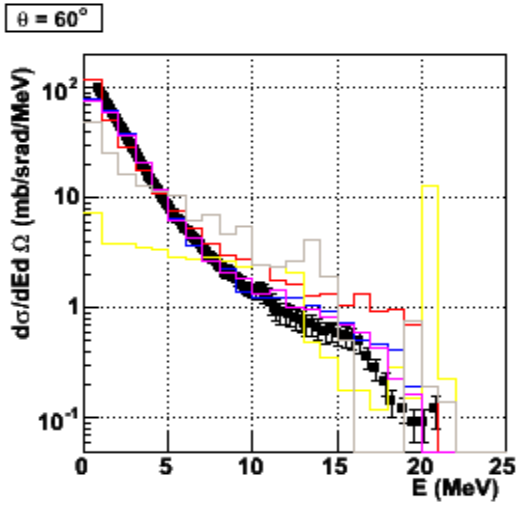
At higher energies generally the results improve:

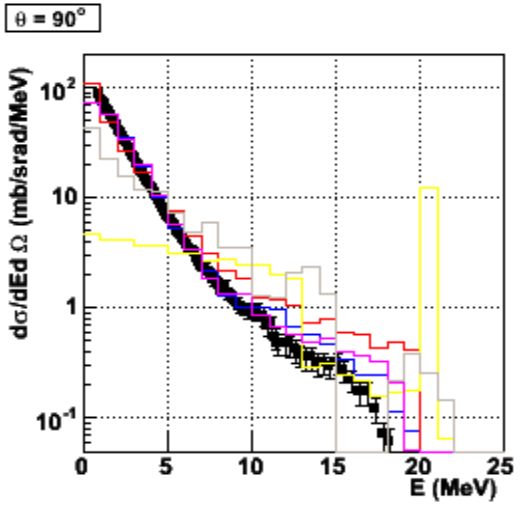


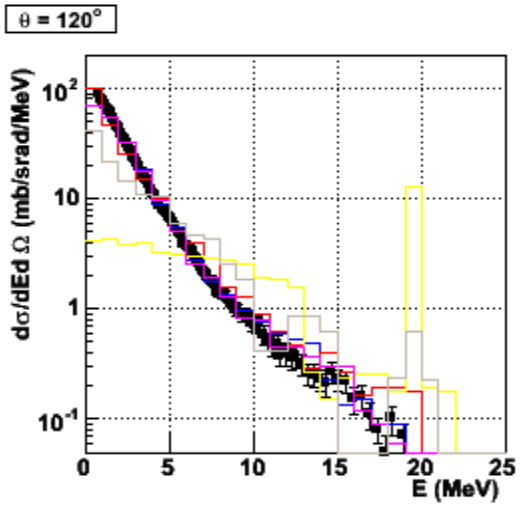
Zr(p,xn) @ 22 MeV

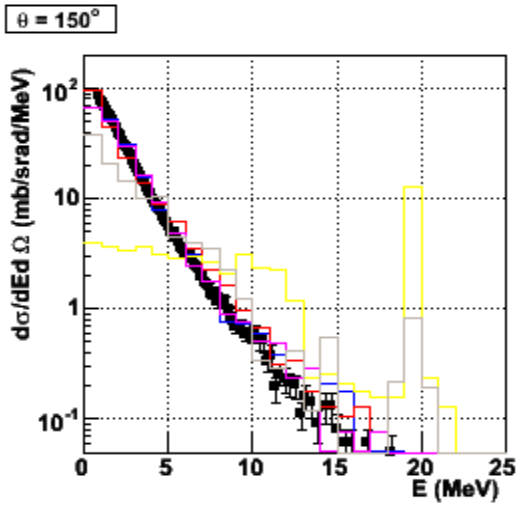
And here too:

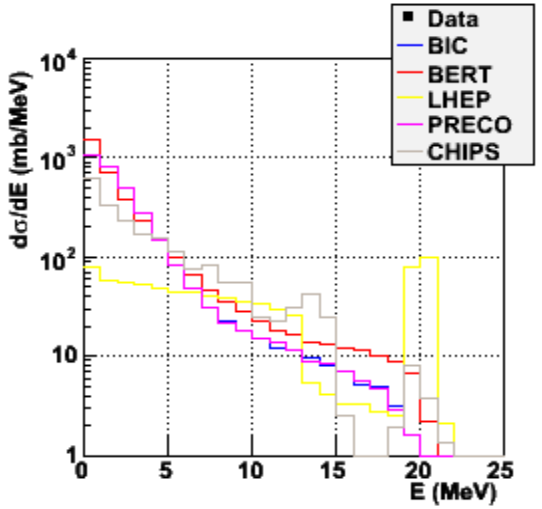






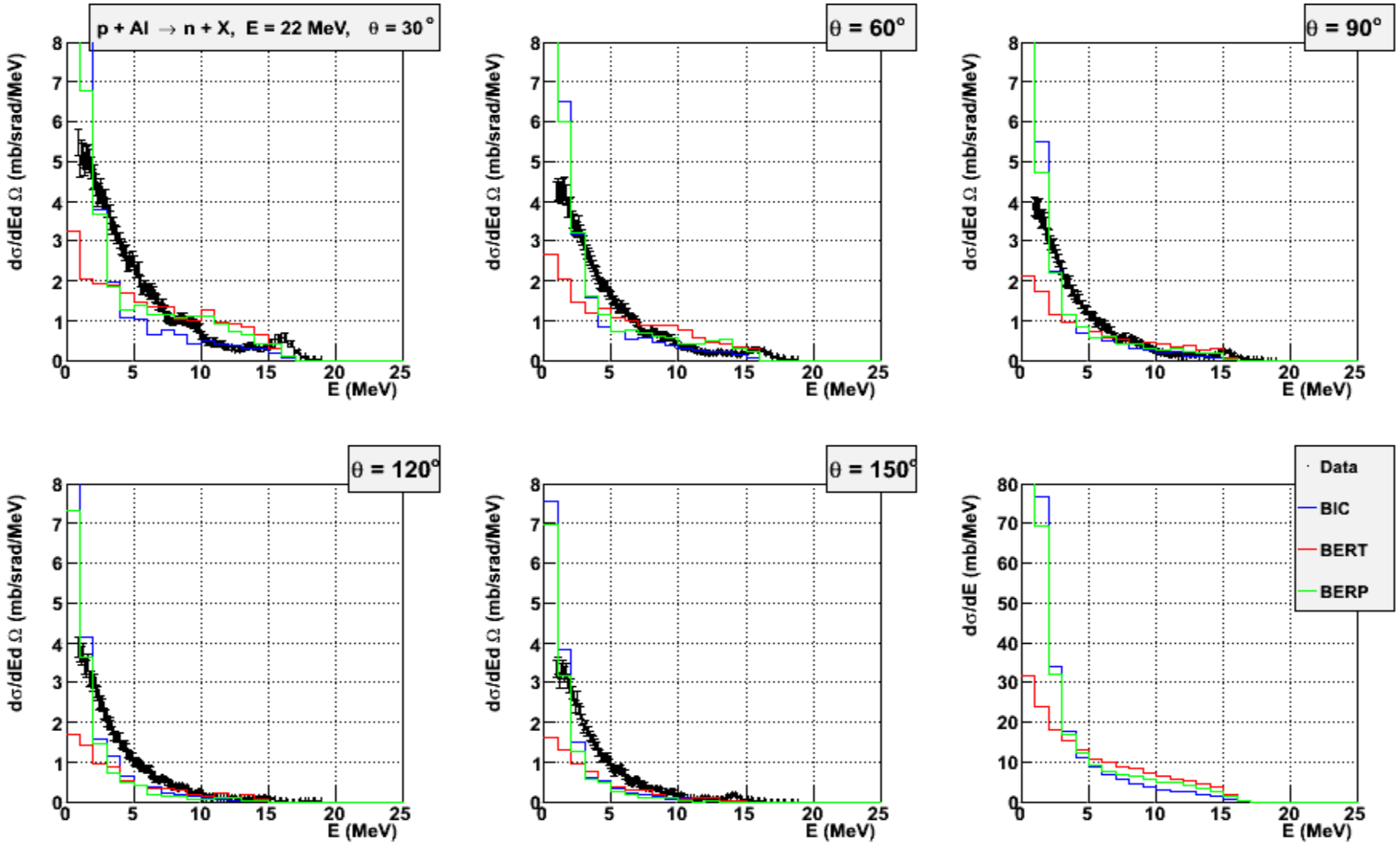






Al(p,xn) @ 22 MeV

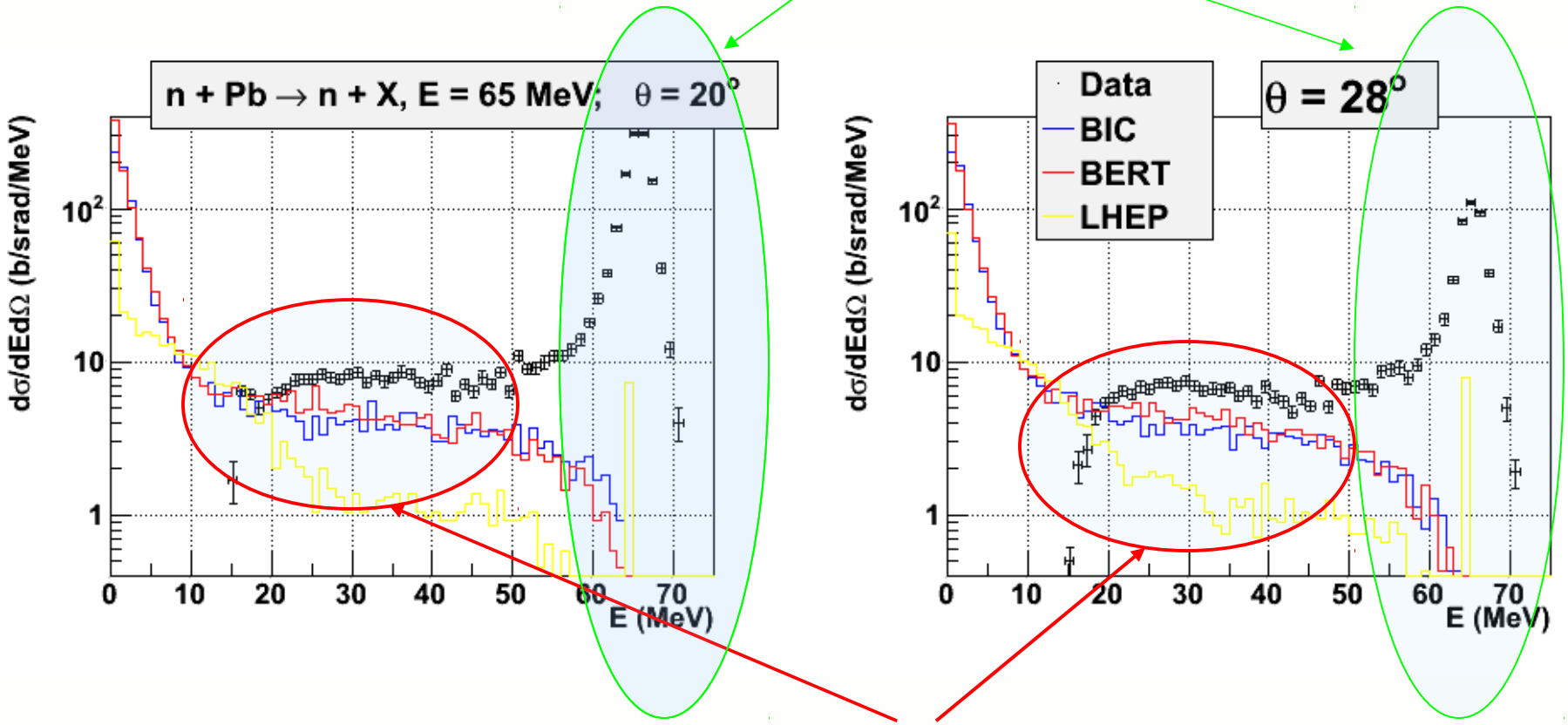
But there are exceptions, as here:



Pb(n,xn) @ 65 MeV

and here:

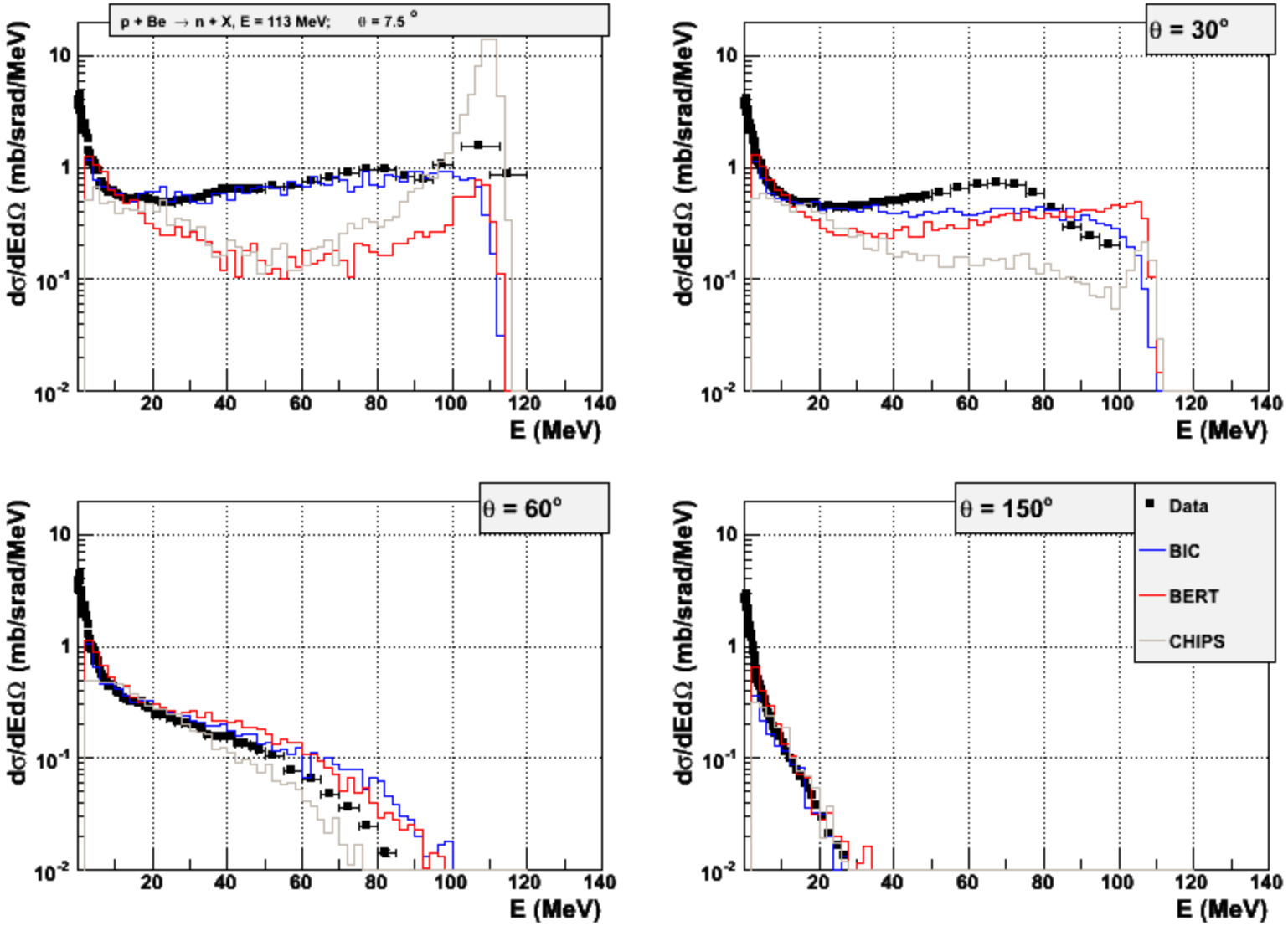
This is the elastic peak (no problem)



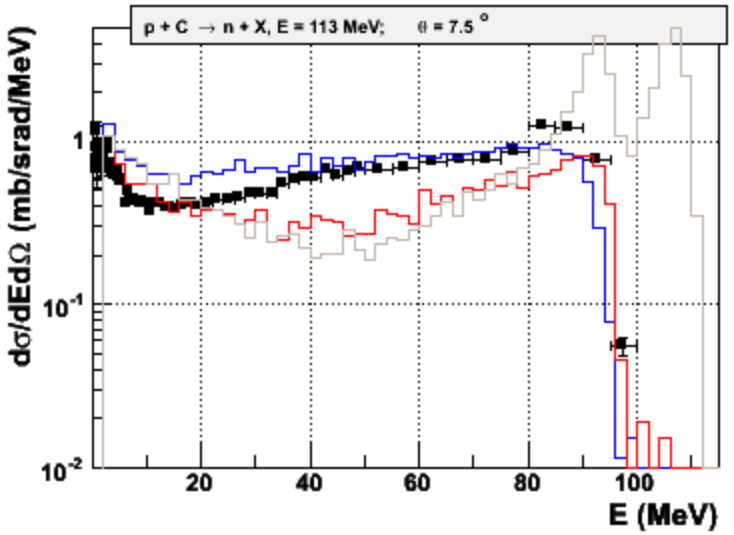
Pre-equlibrium emission is underestimated

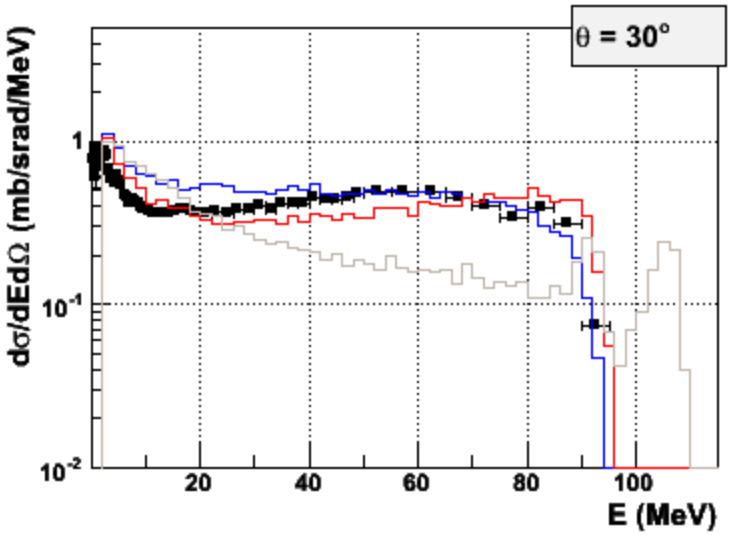
Geant4 *internal* benchmark “test30”

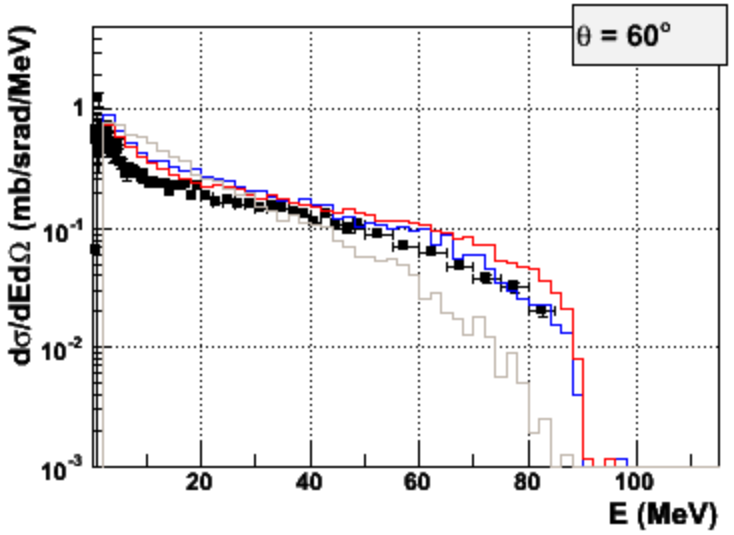
Be(p,xn) @ 113 MeV

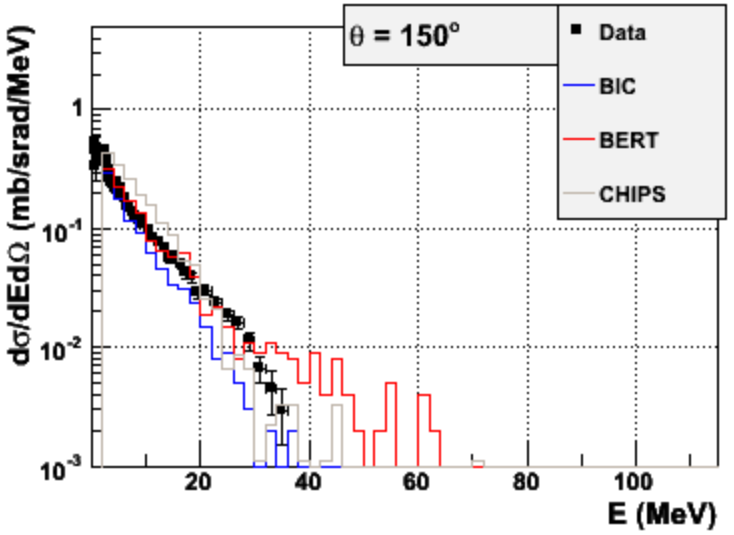


C(p,xn) @ 113 MeV

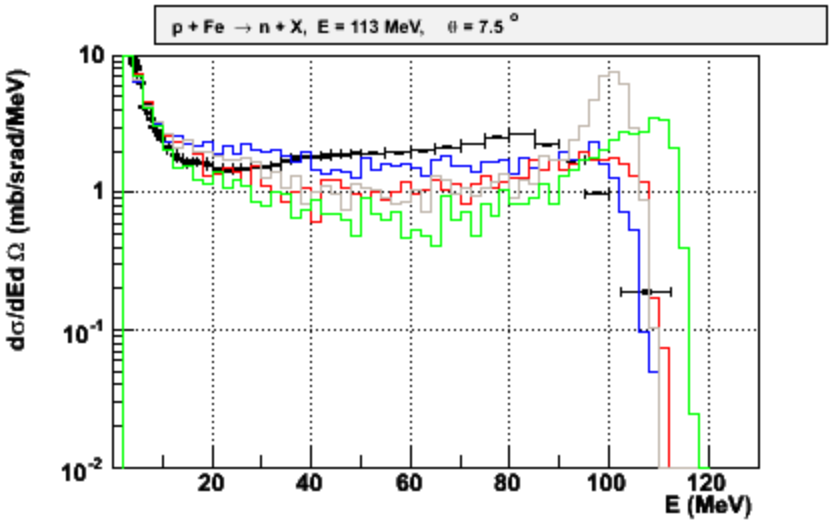

p + C → n + X, E = 113 MeV; θ = 7.5°
dσ/dEdΩ (mb/srad/MeV)
E (MeV)

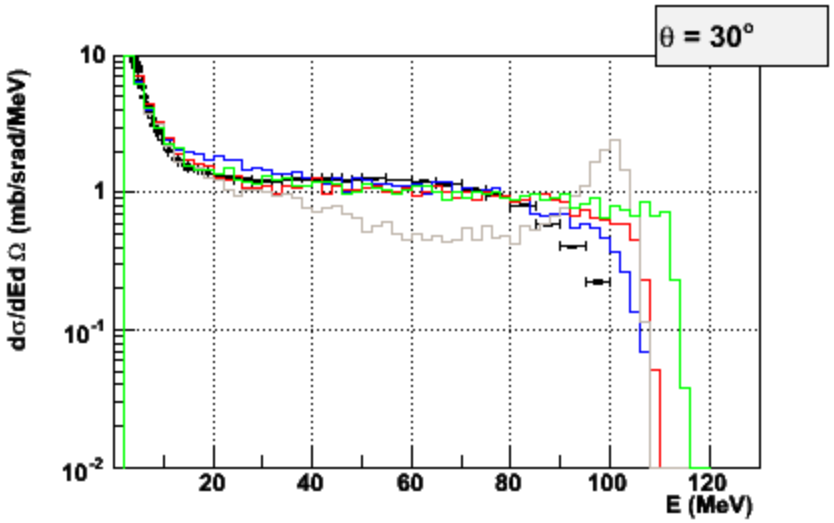

θ = 30°
dσ/dEdΩ (mb/srad/MeV)
E (MeV)

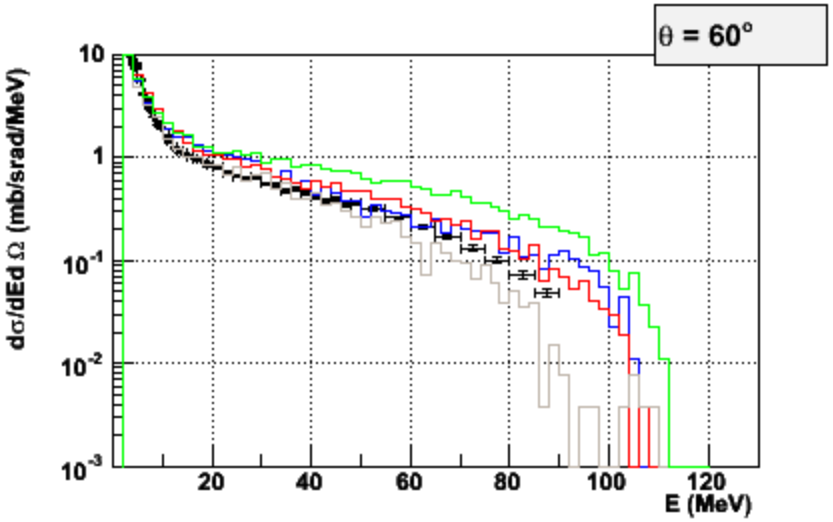

θ = 60°
dσ/dEdΩ (mb/srad/MeV)
E (MeV)

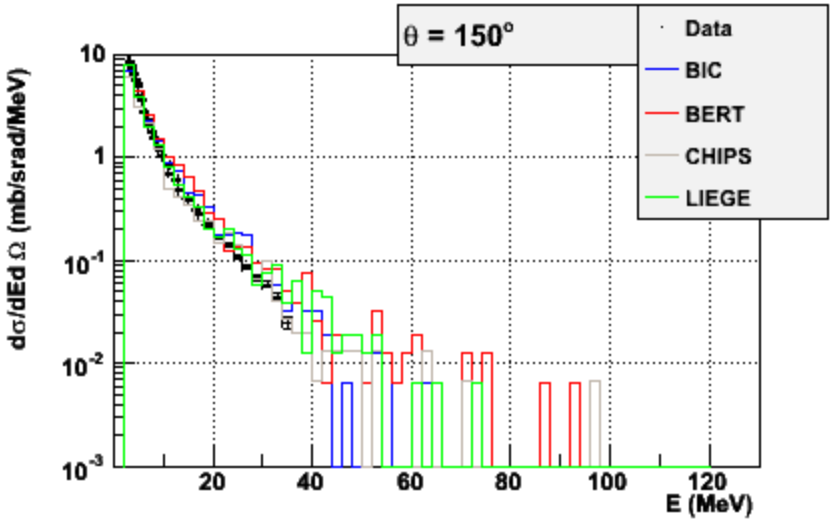

θ = 150°
Data
BIC
BERT
CHIPS
dσ/dEdΩ (mb/srad/MeV)
E (MeV)

Fe(p,xn) @ 113 MeV

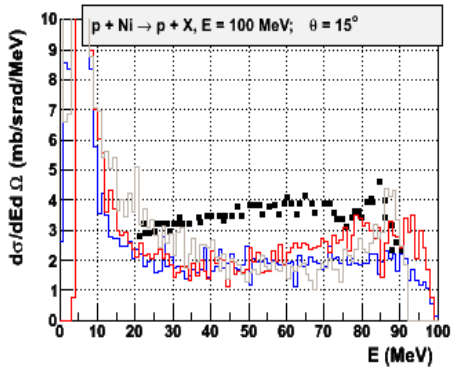


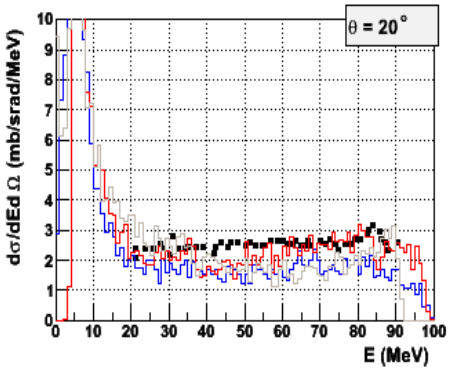


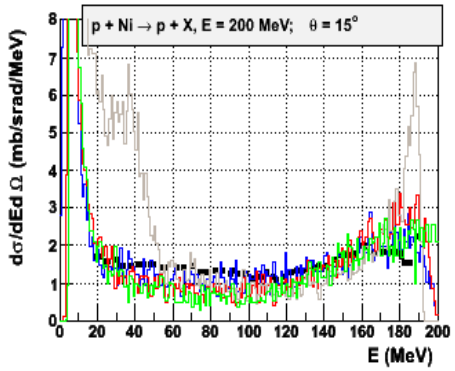


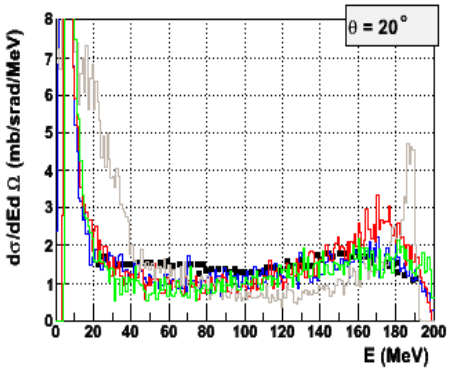


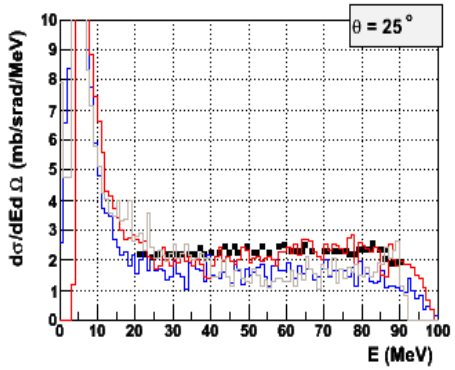
Ni(p,xn) @ 113MeV , 256 MeV

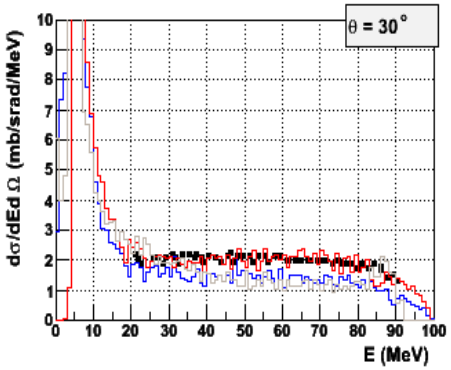


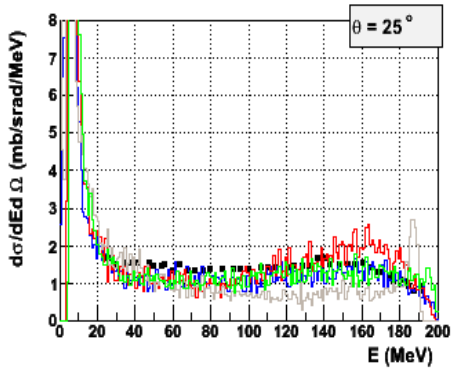


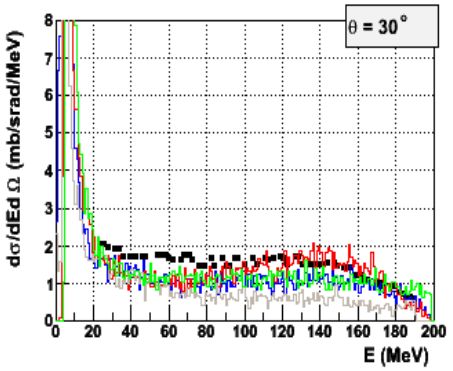


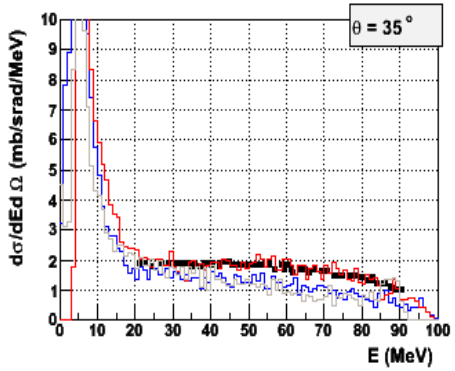


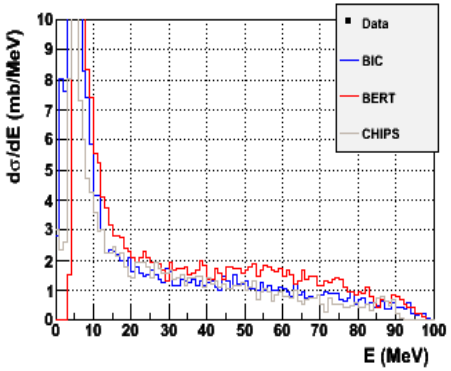


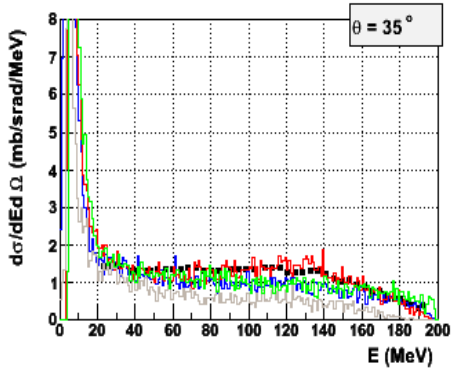


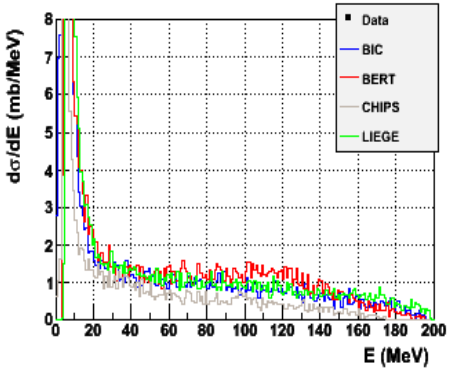




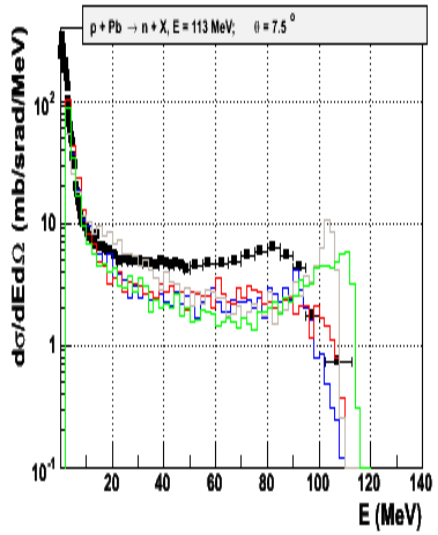


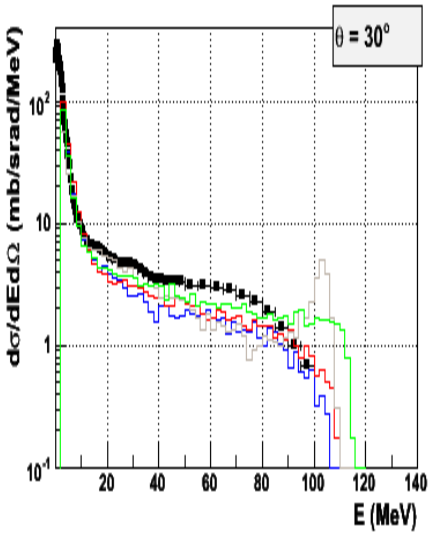


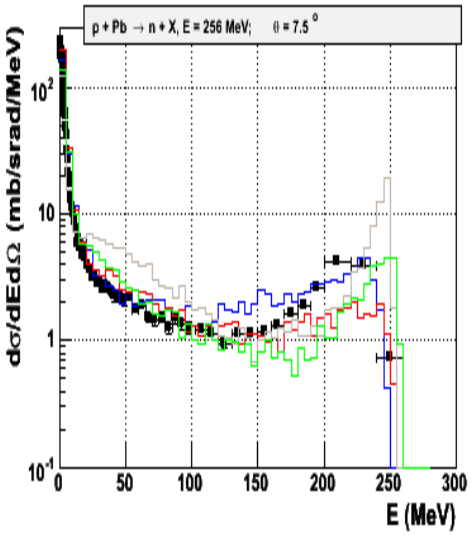


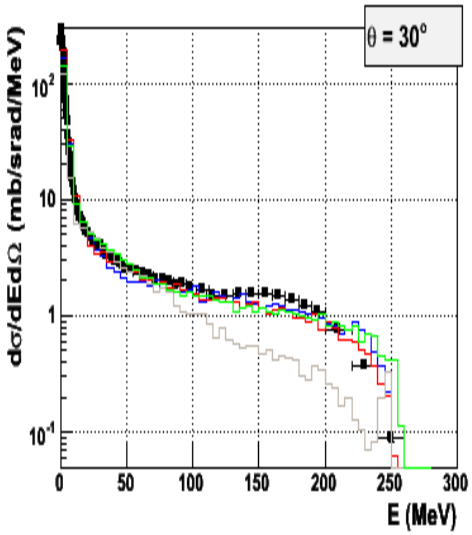


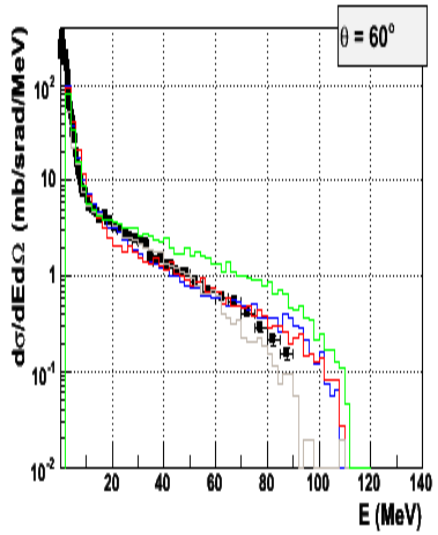
Pb(p,xn) @ 113, 256 MeV

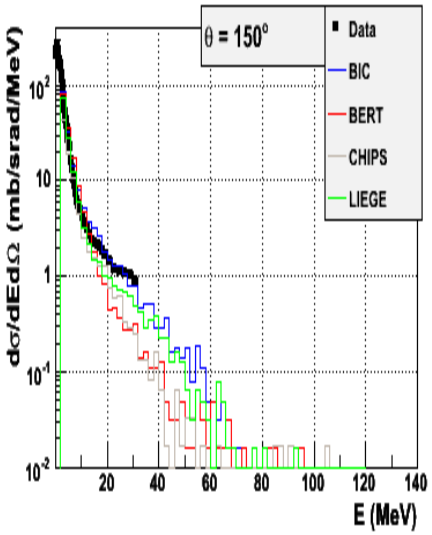


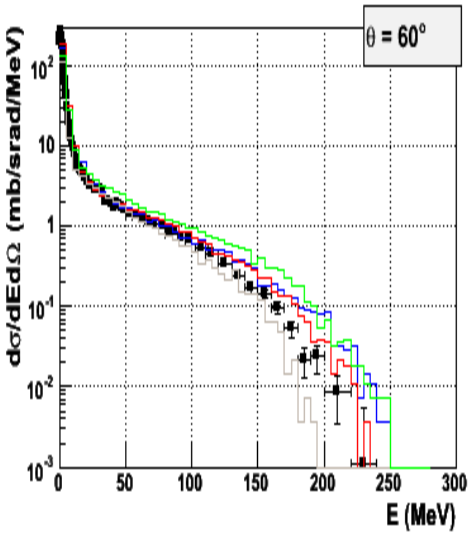


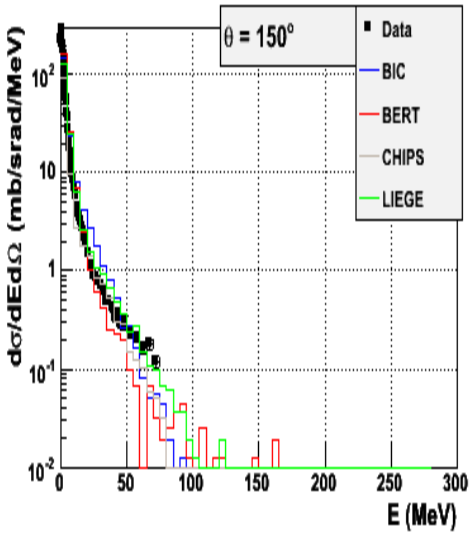






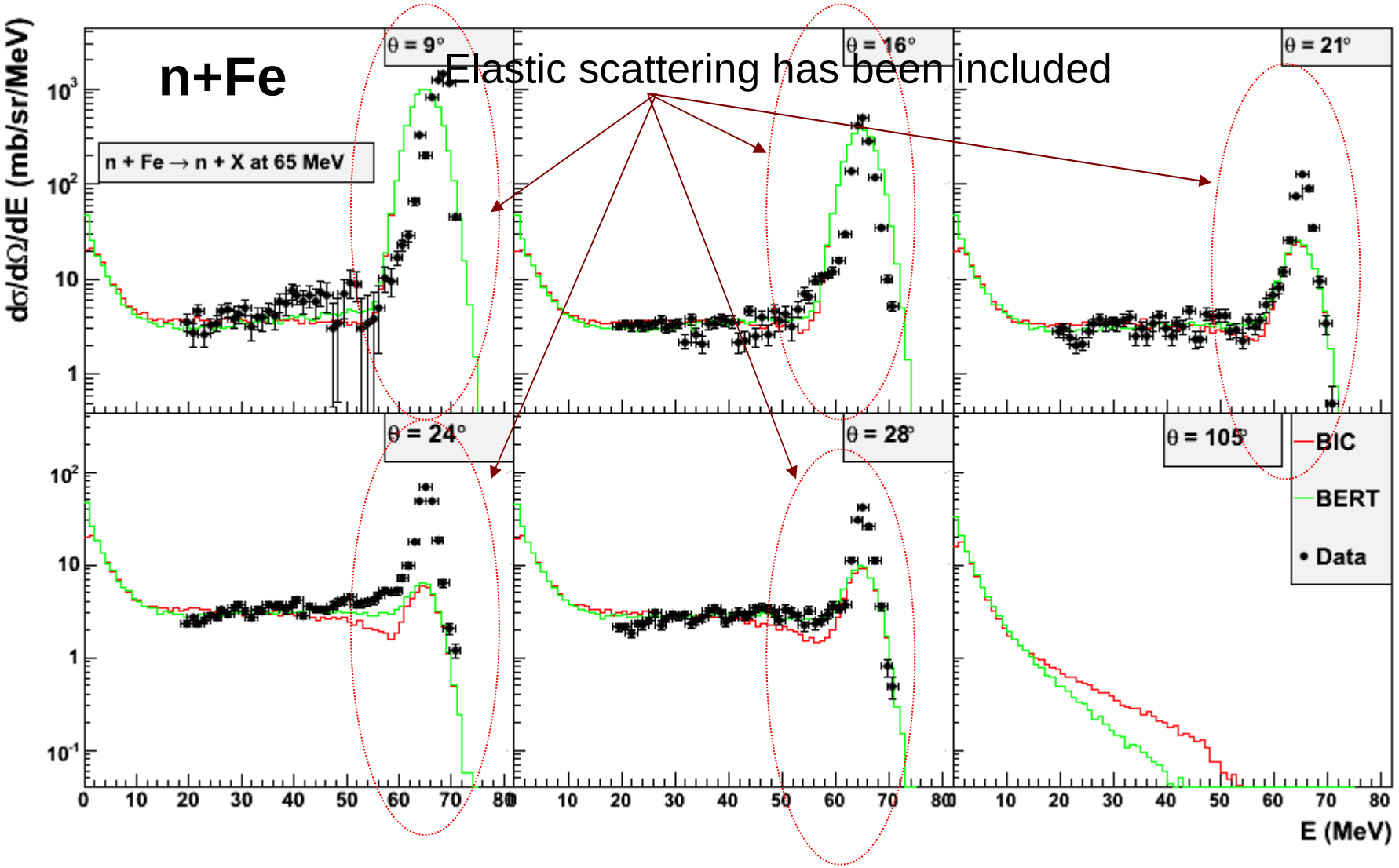




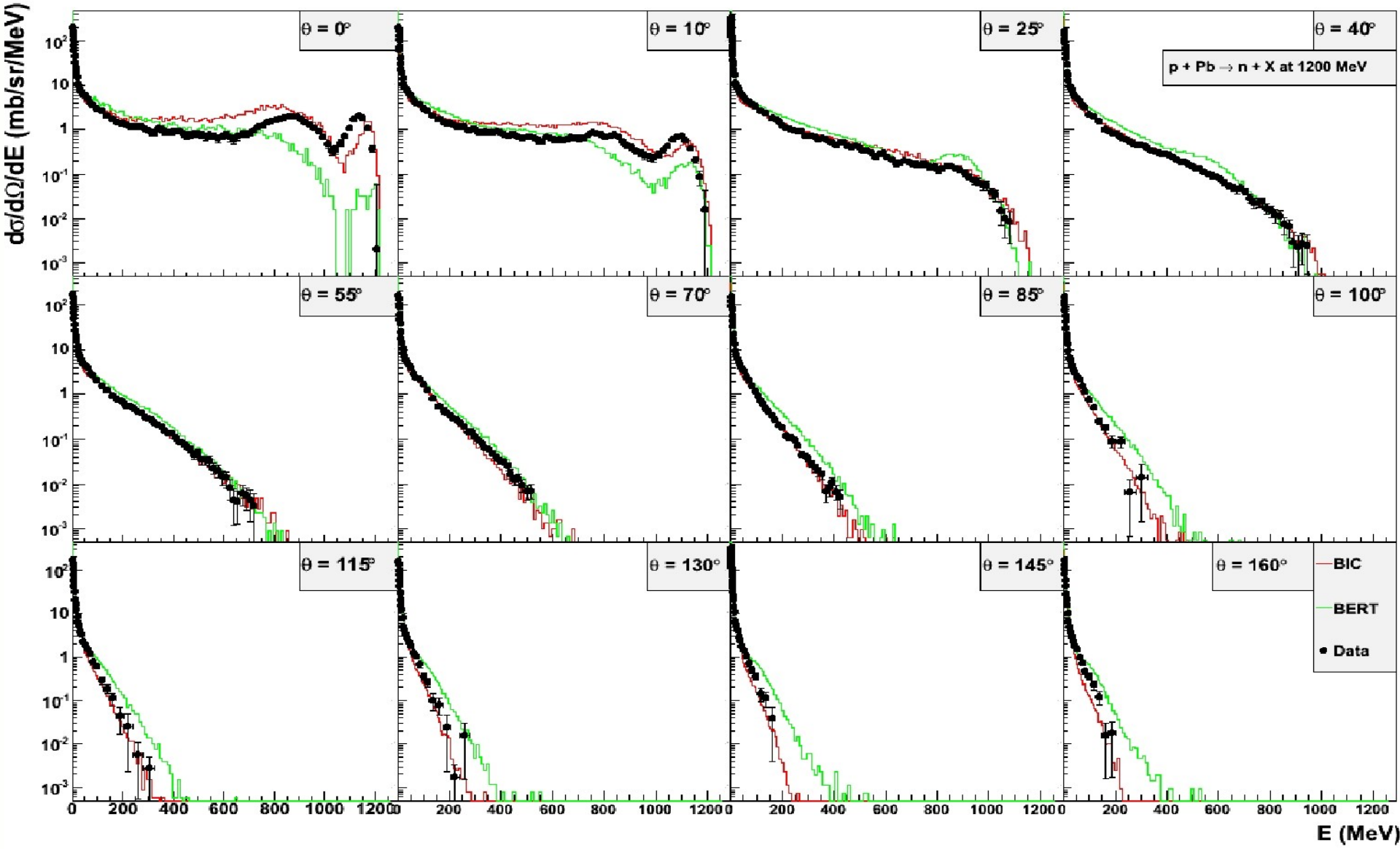


IAEA spallation benchmark

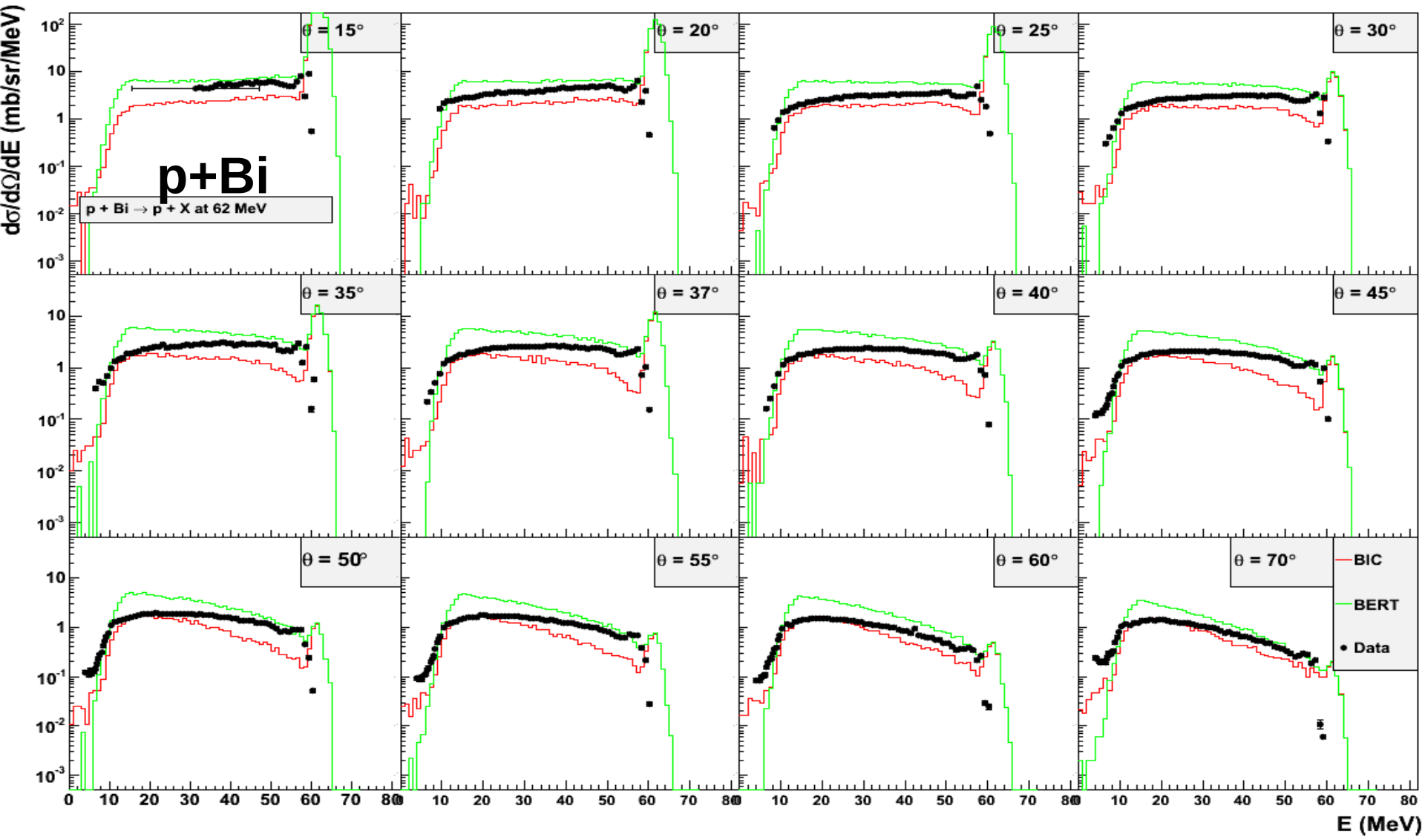
Neutron production at 65 MeV



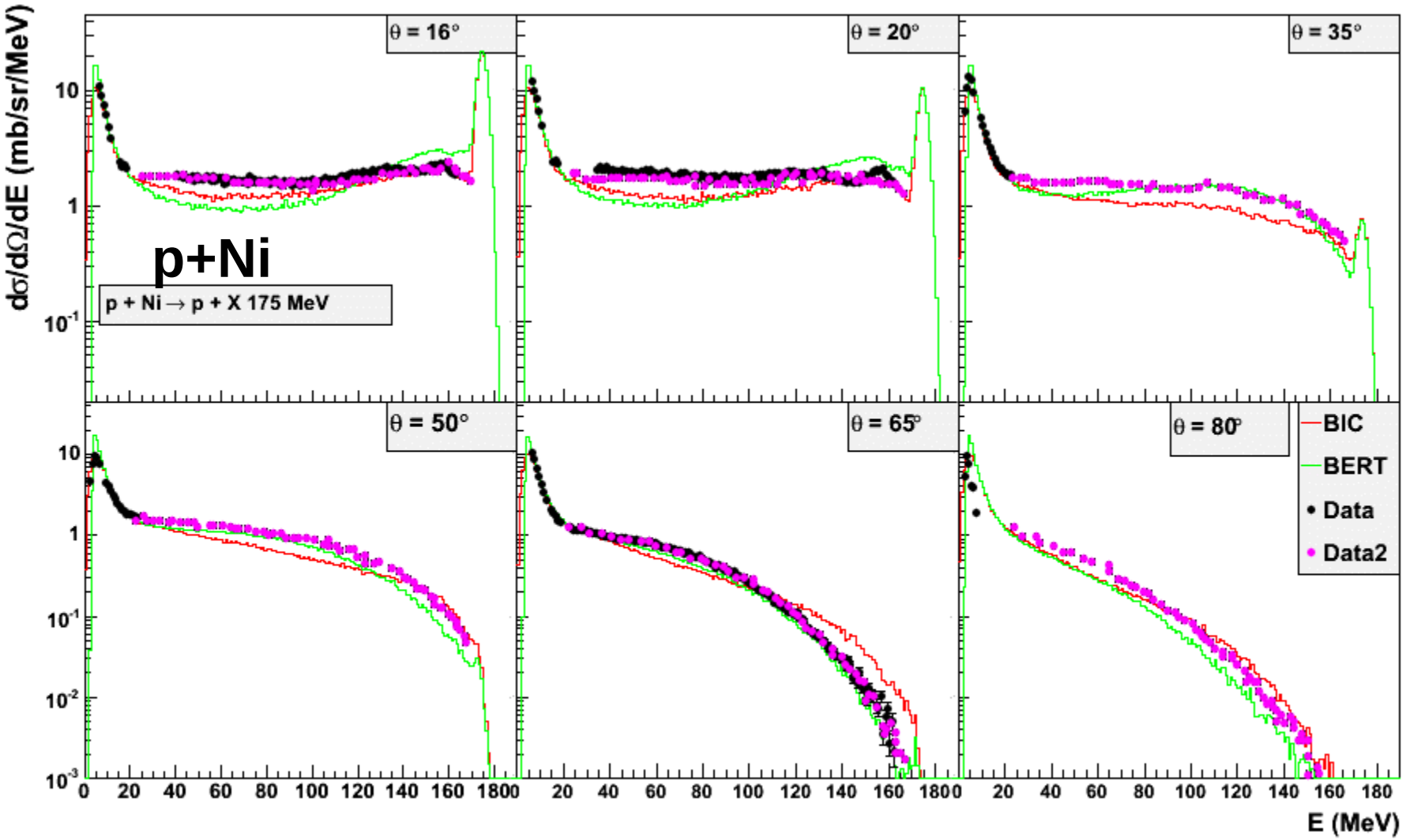
Neutron production at 1200 MeV



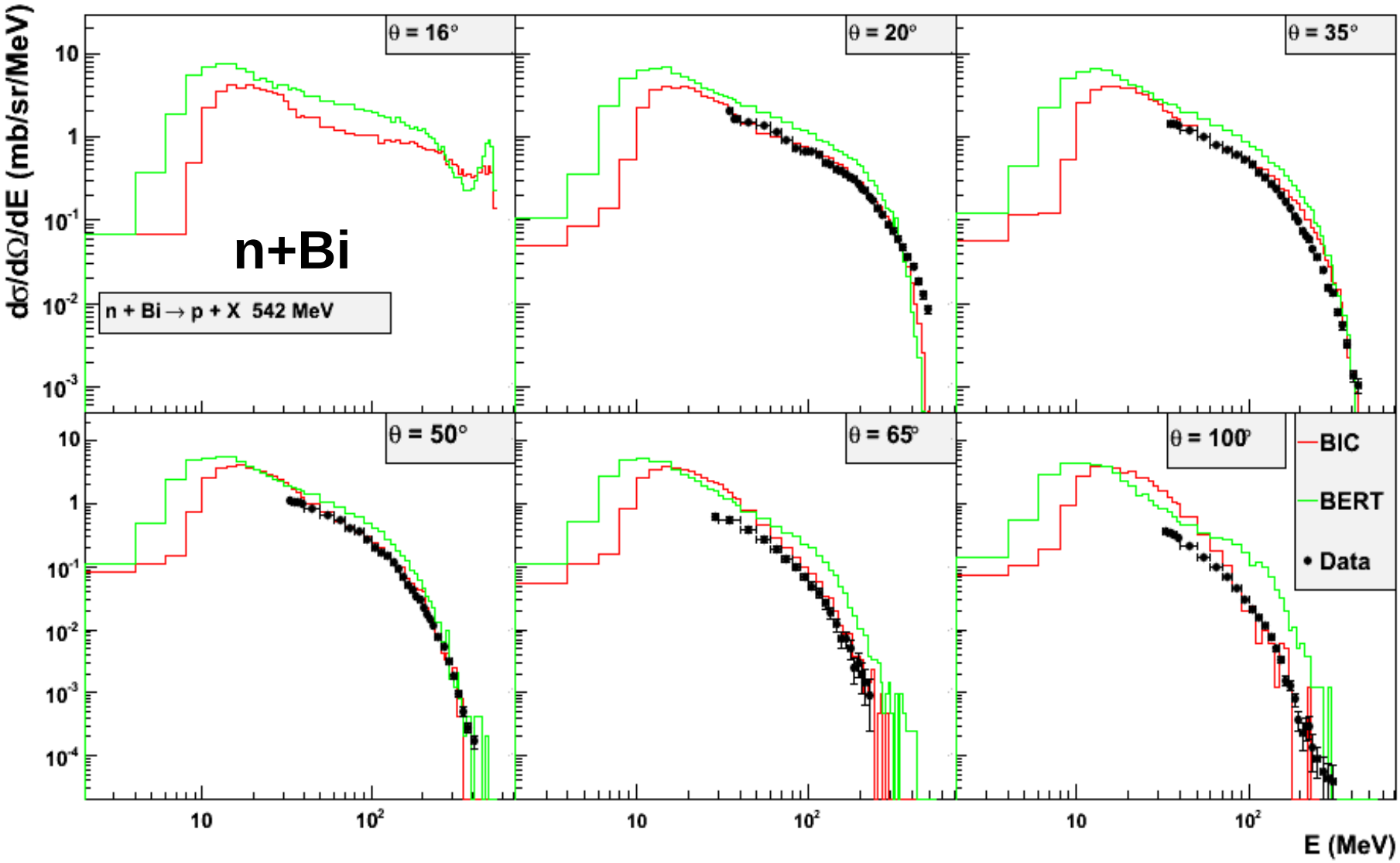
Proton production at 62 MeV



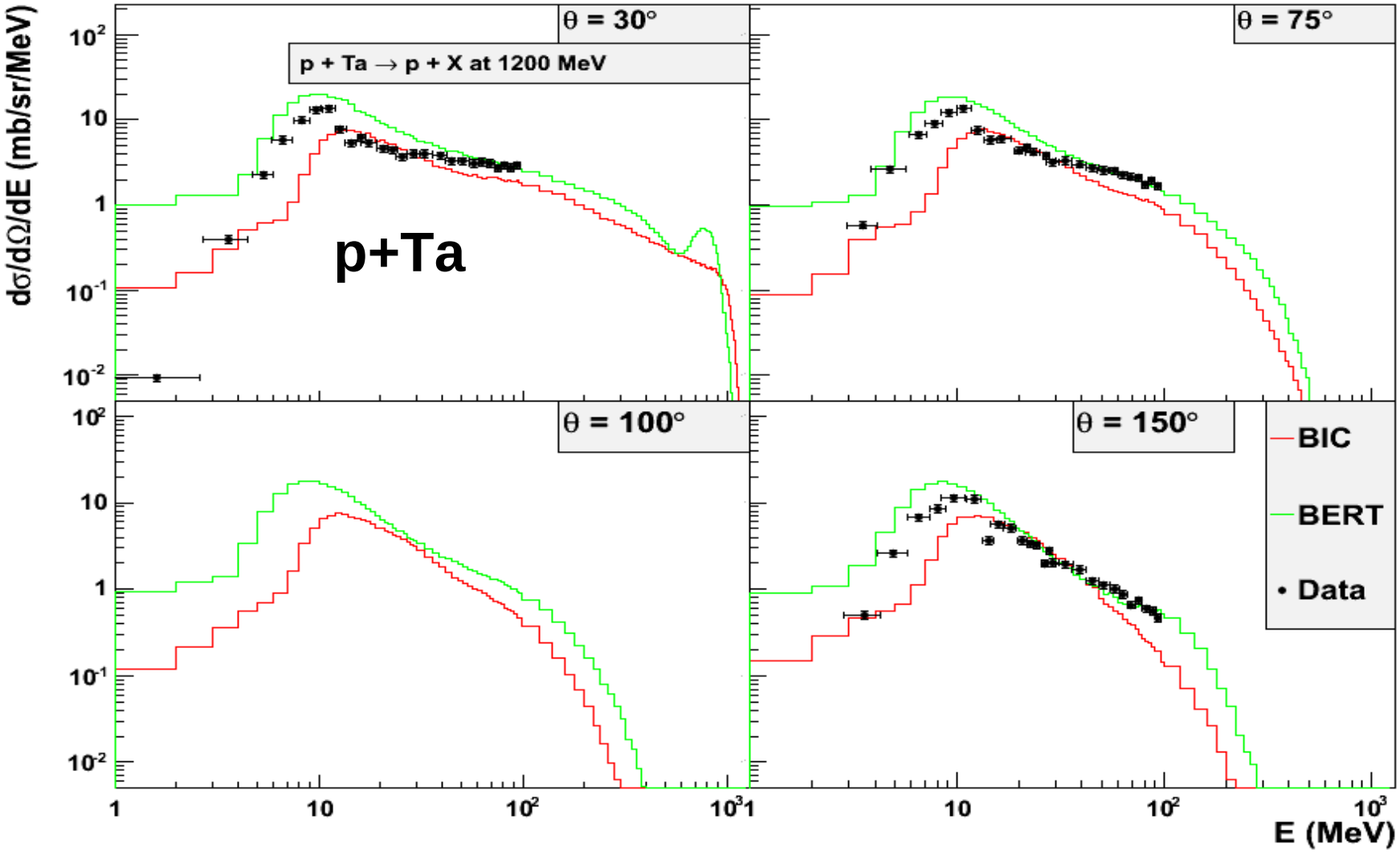
Proton production at 175 MeV



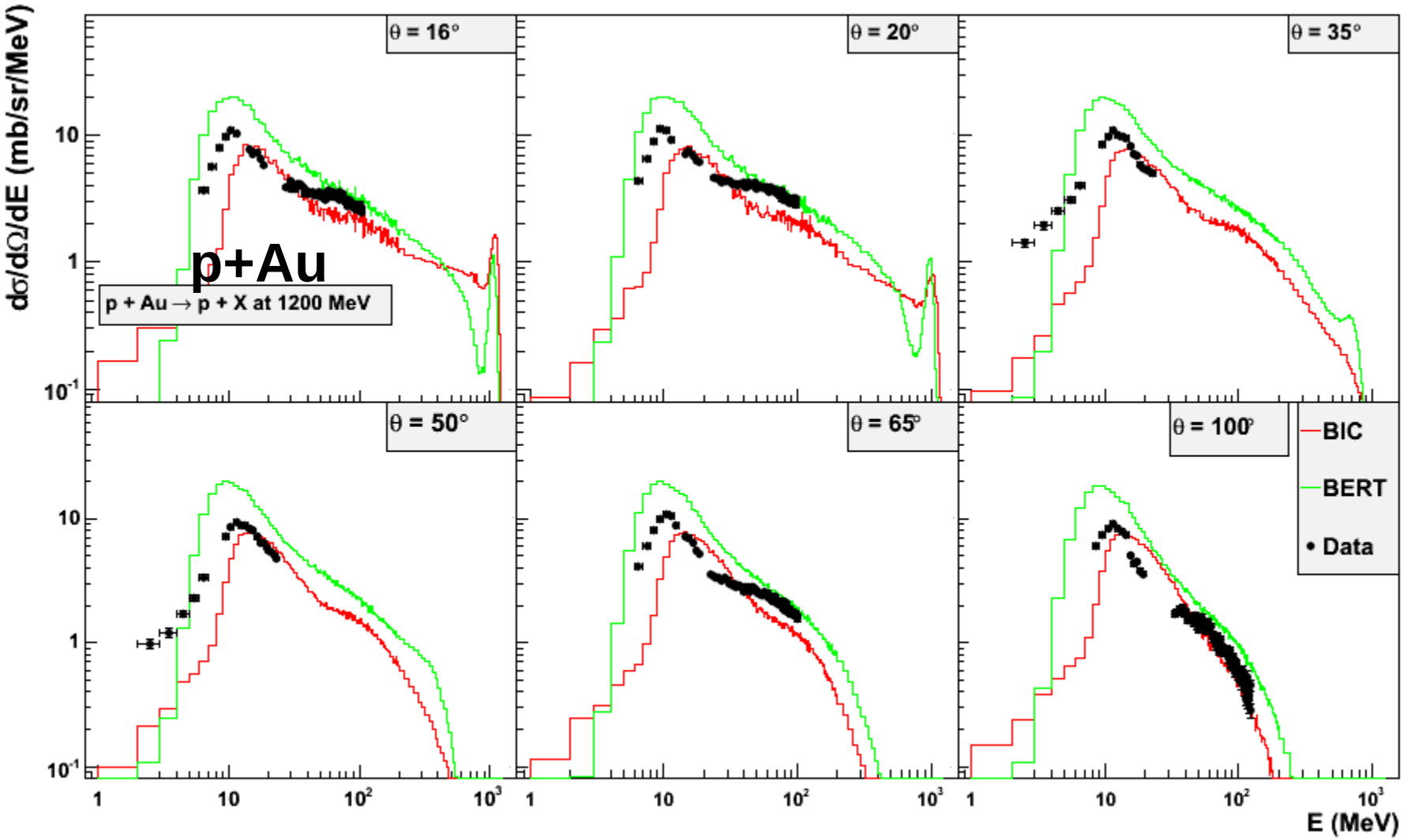
Proton production at 542 MeV



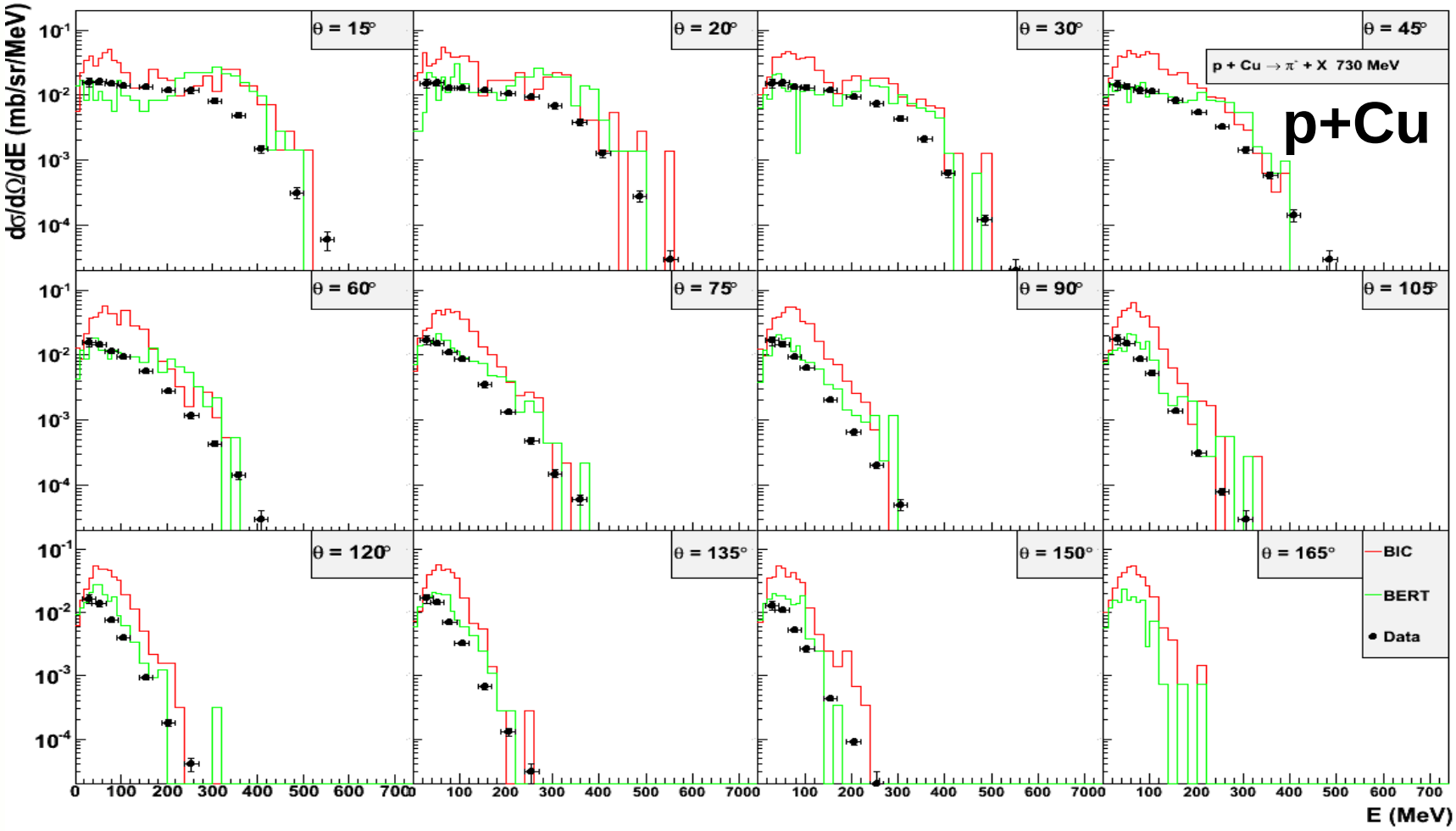
Proton production at 1200 MeV



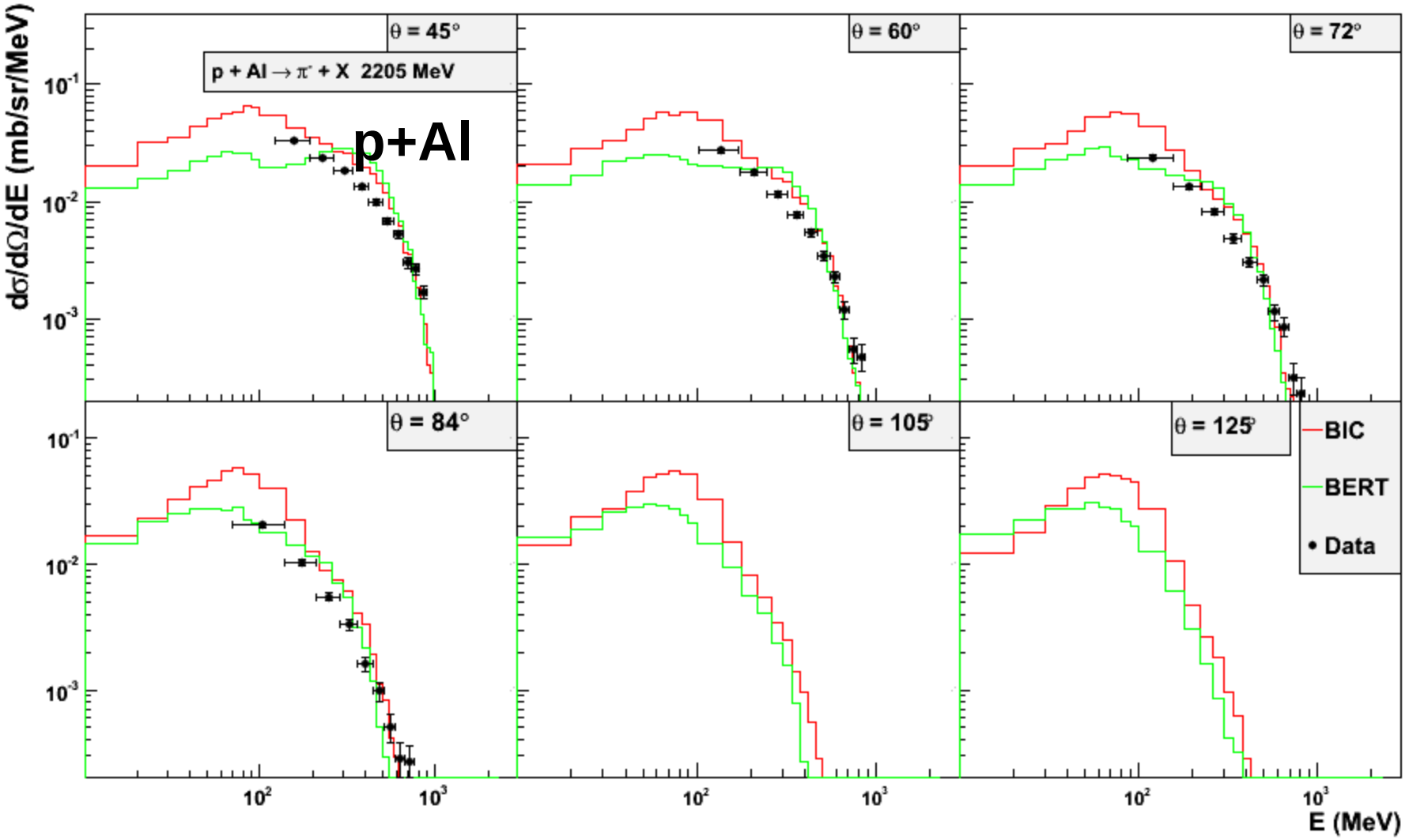
Proton production at 1200 MeV



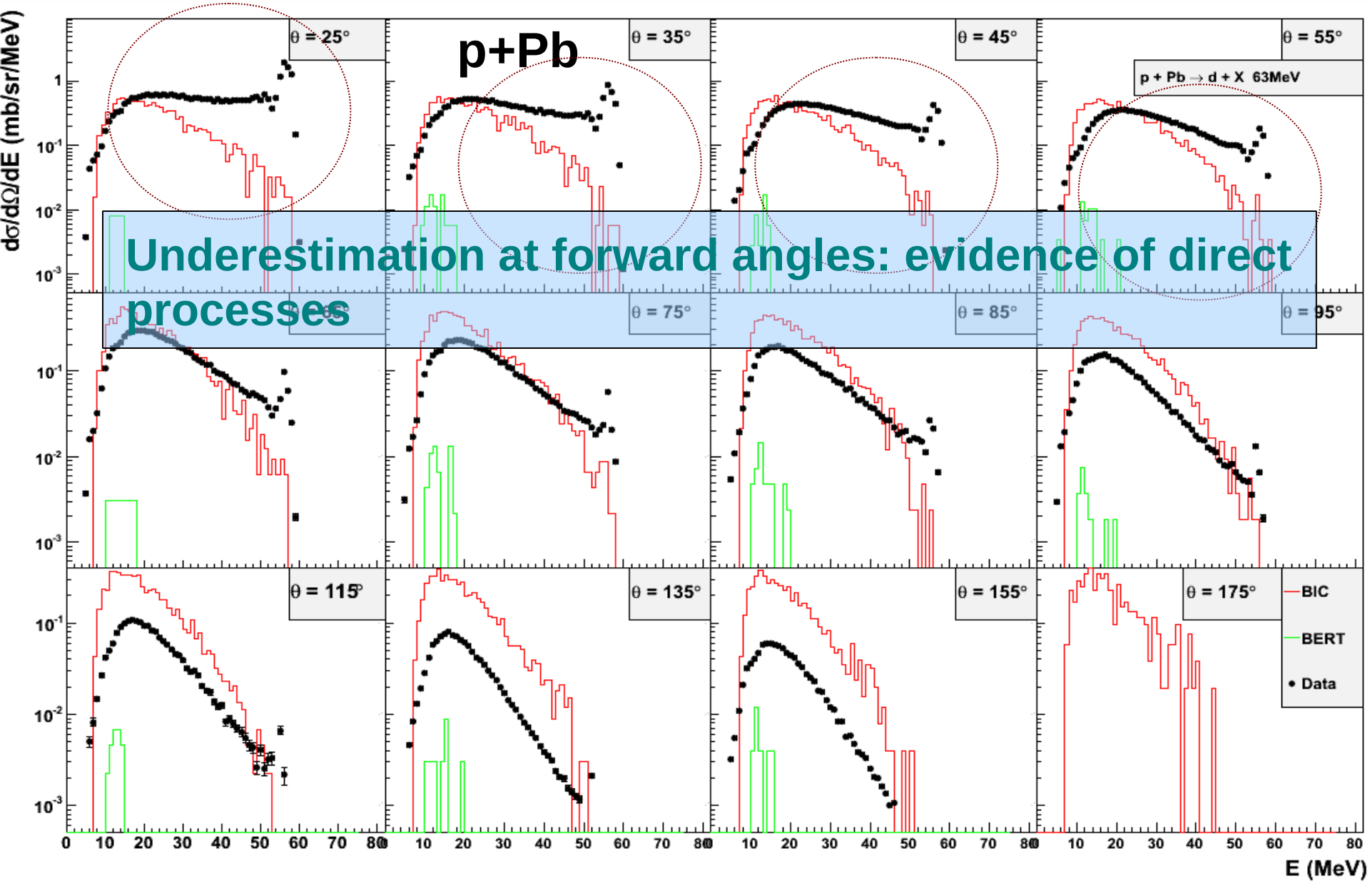
Pion production at 730 MeV



Pion production at 2205 MeV

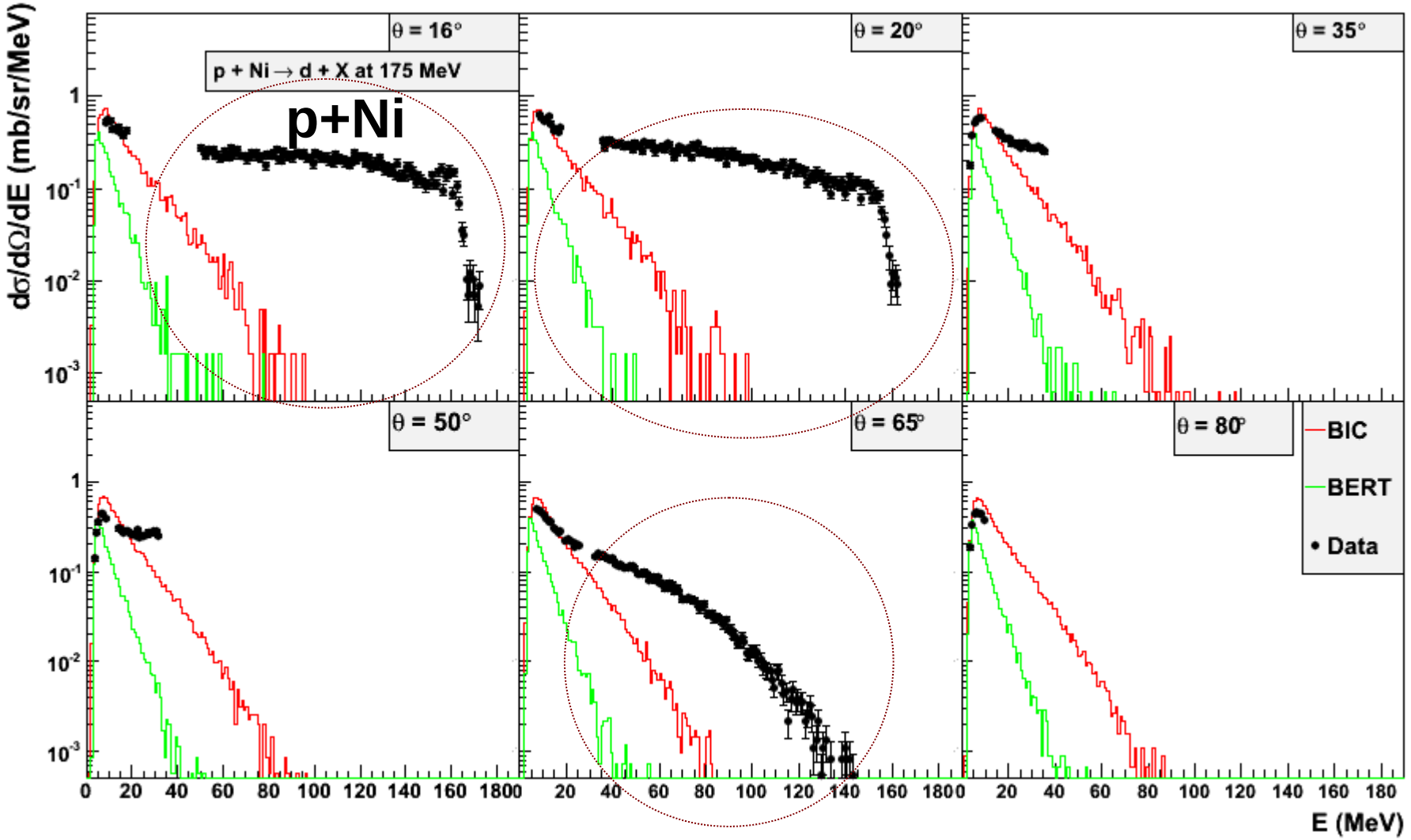


Deuteron production at 63 MeV

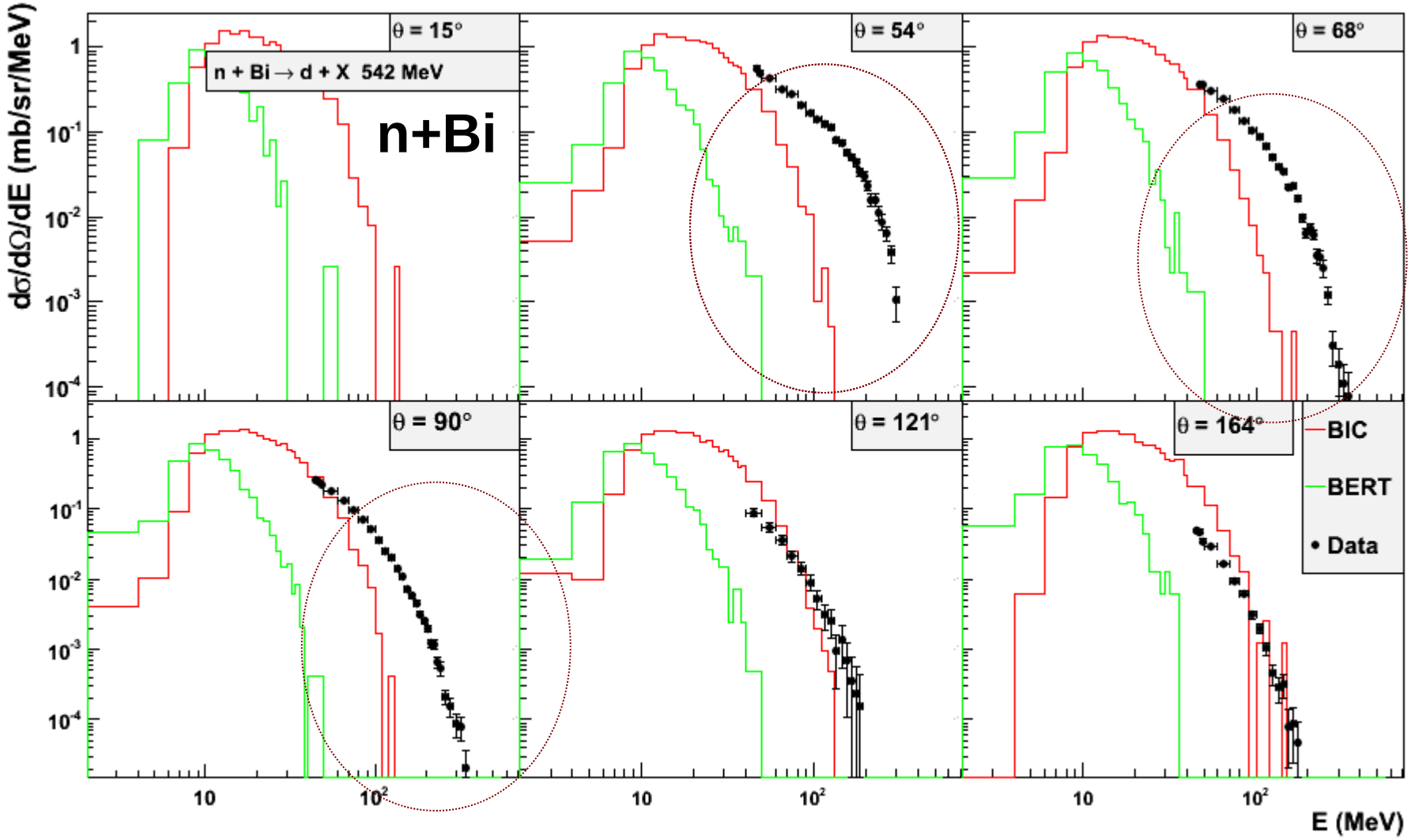


Underestimation at forward angles: evidence of direct processes

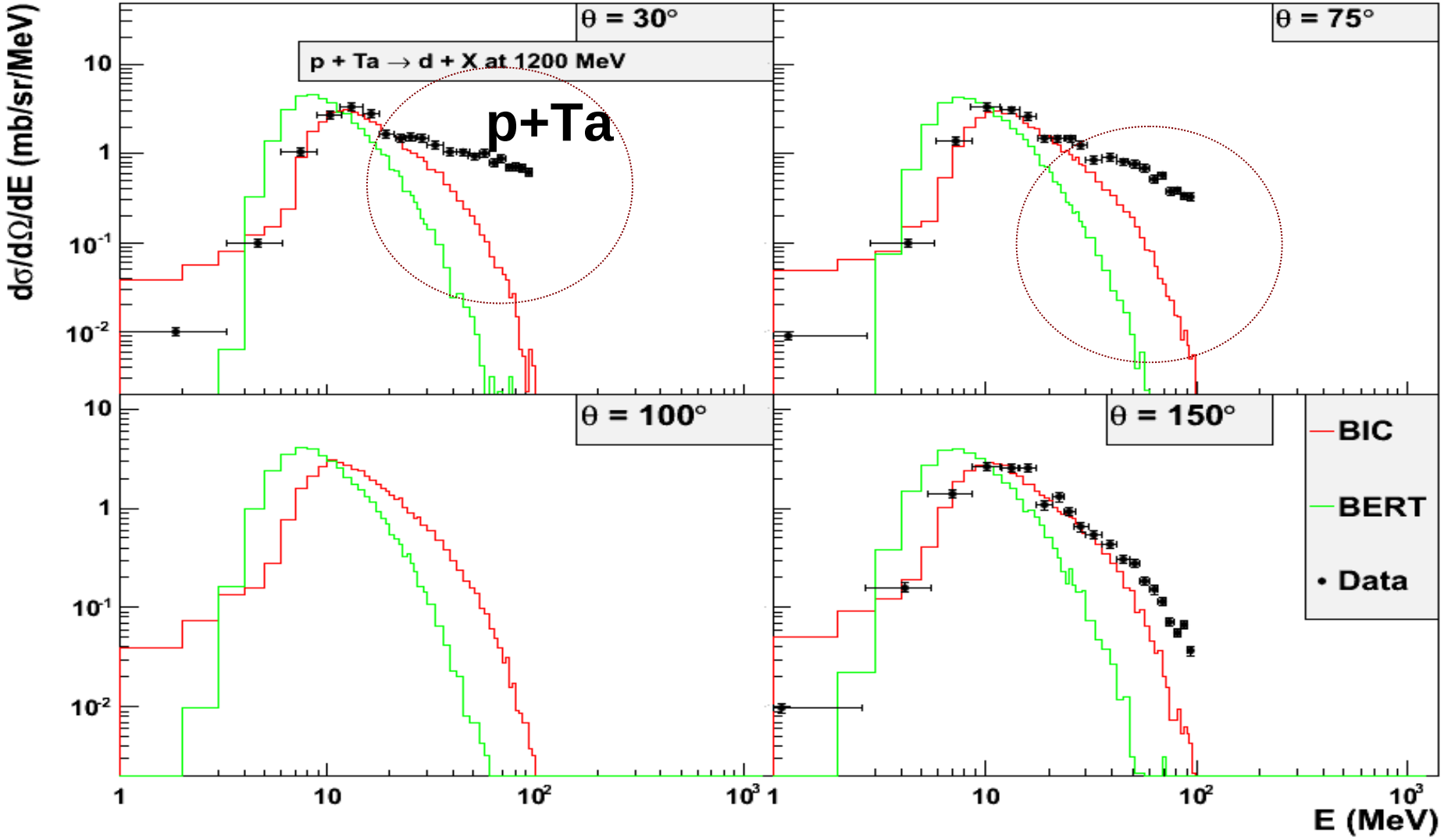
Deuteron production at 175 MeV



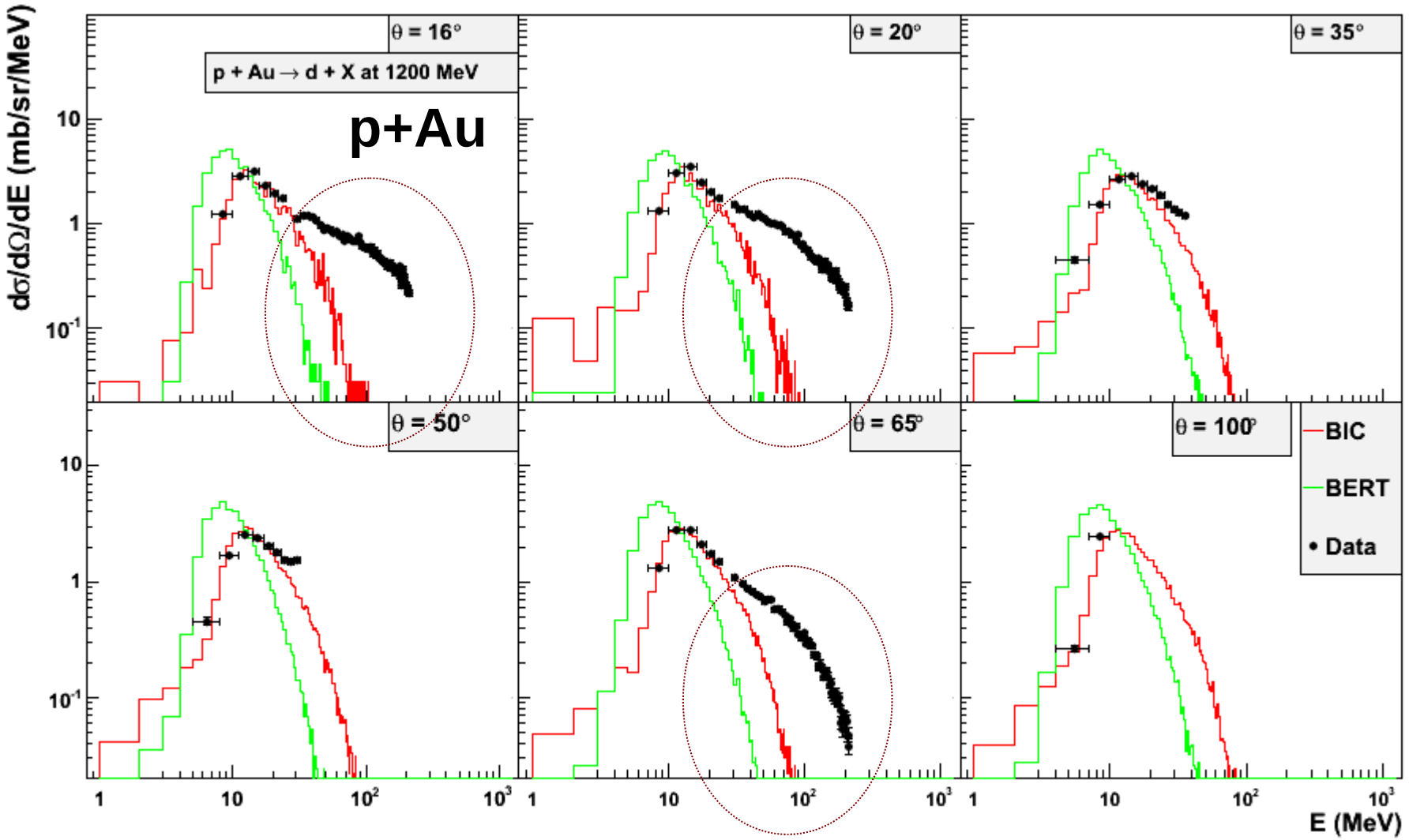
Deuteron production at 542 MeV



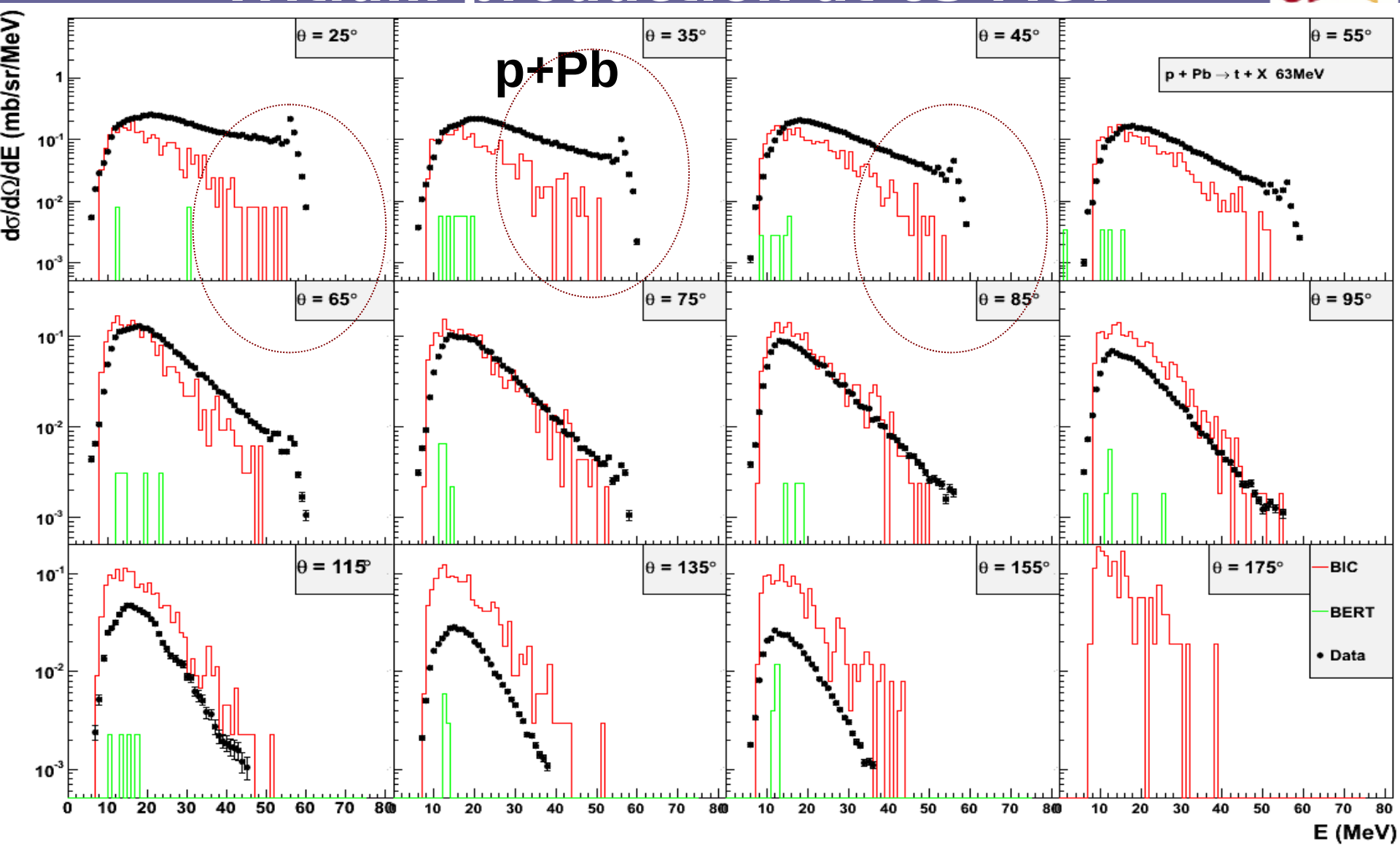
Deuteron production at 1200 MeV



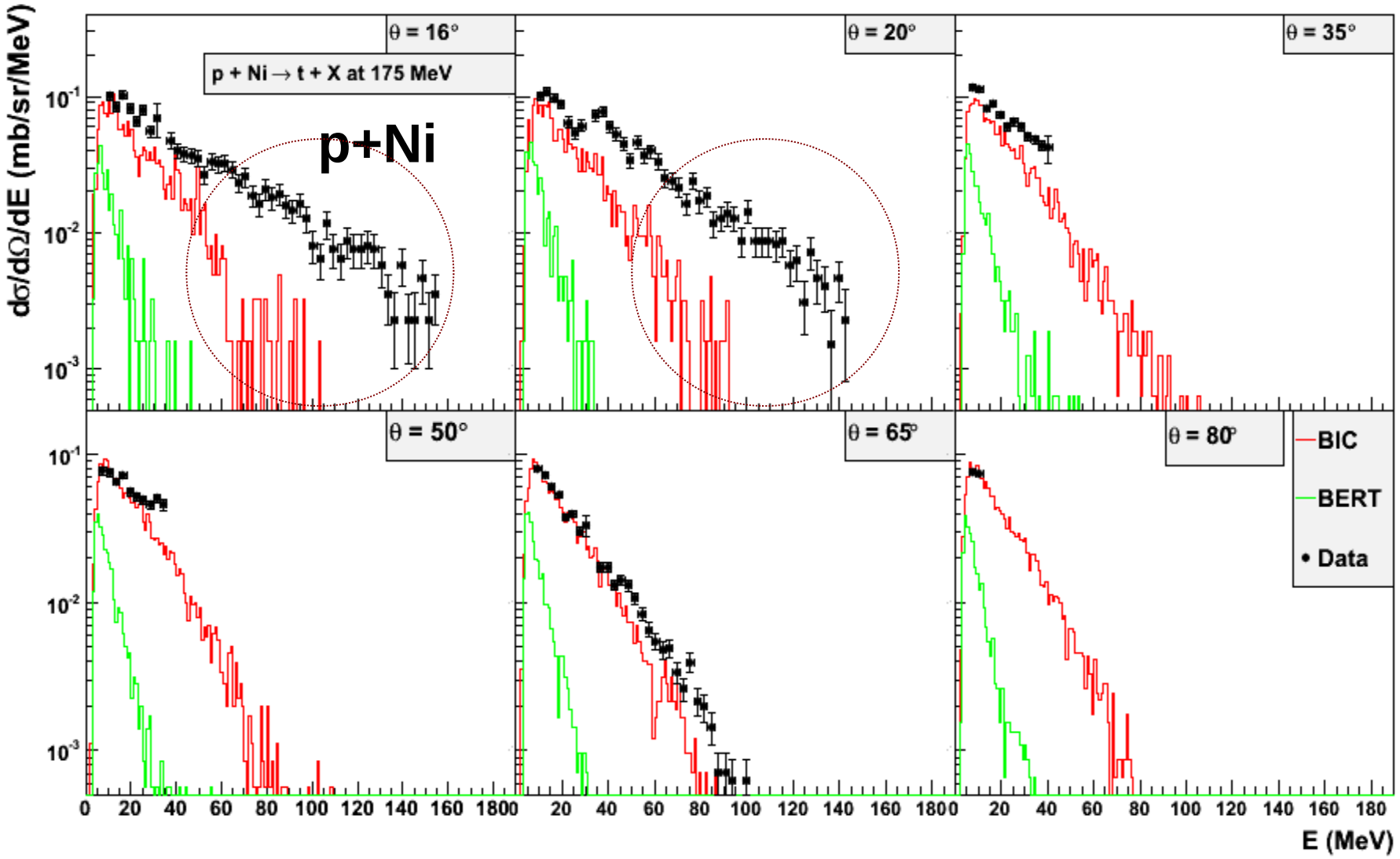
Deuteron production at 1200 MeV



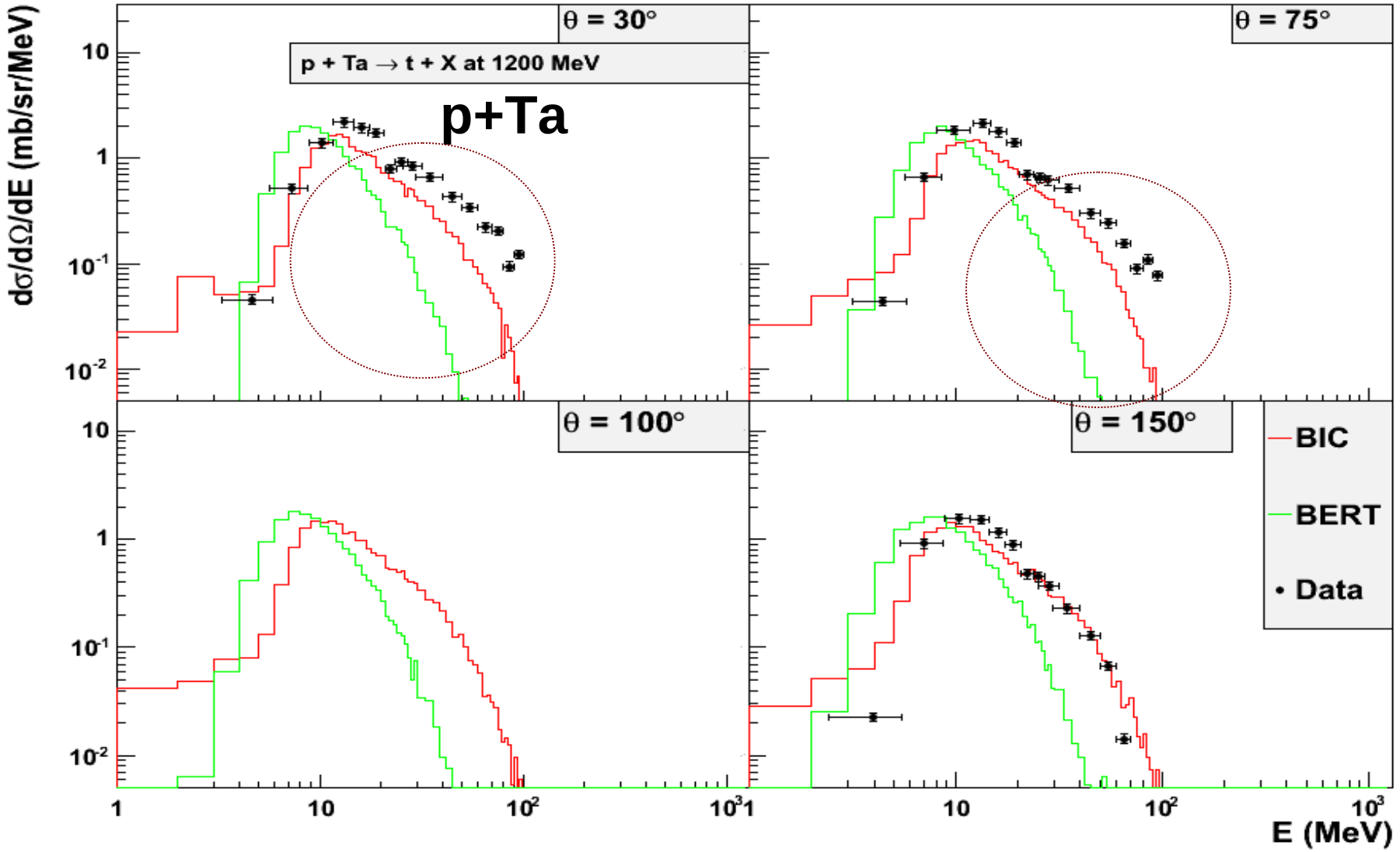
Tritium production at 63 MeV



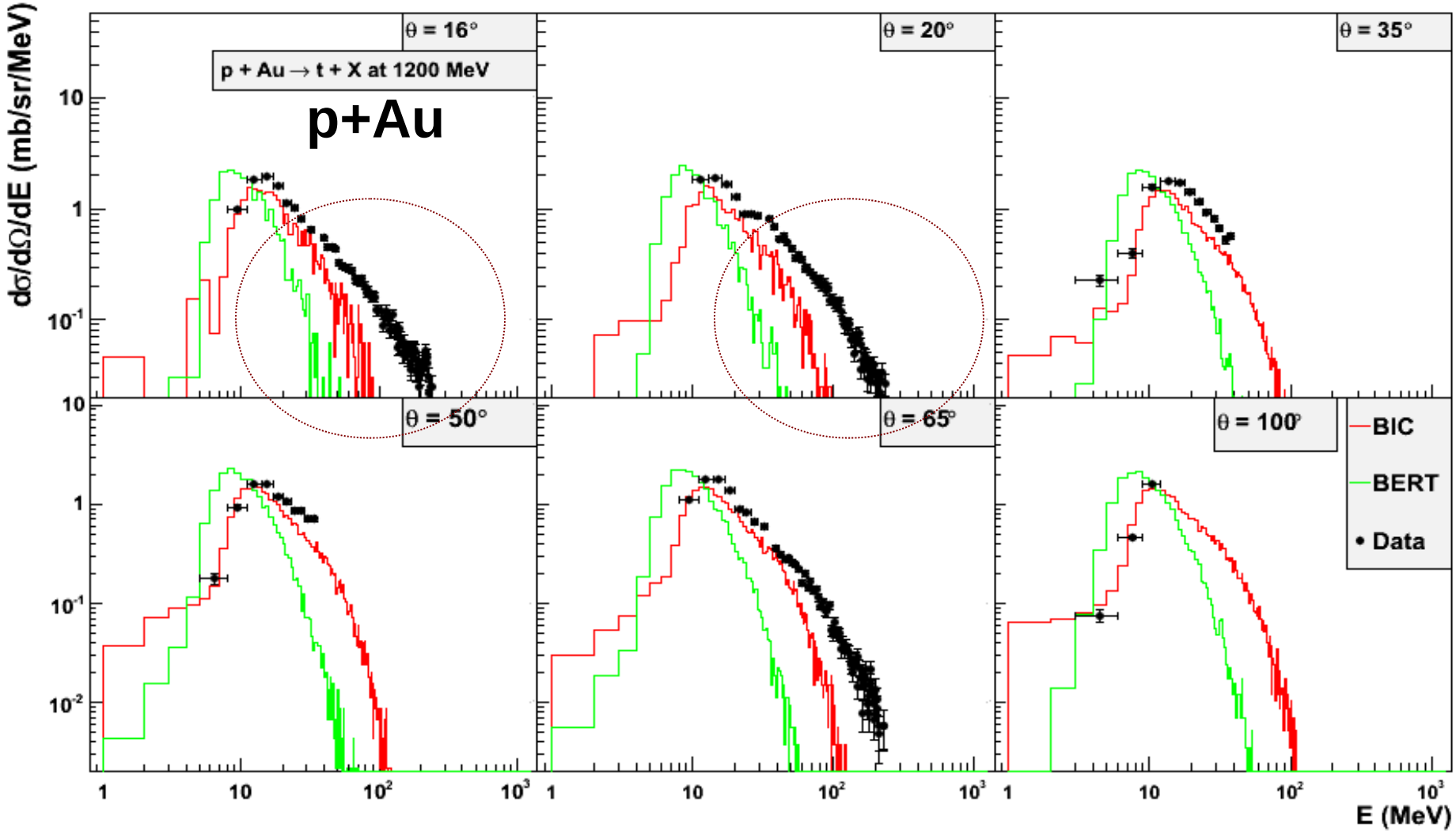
Tritium production at 175 MeV



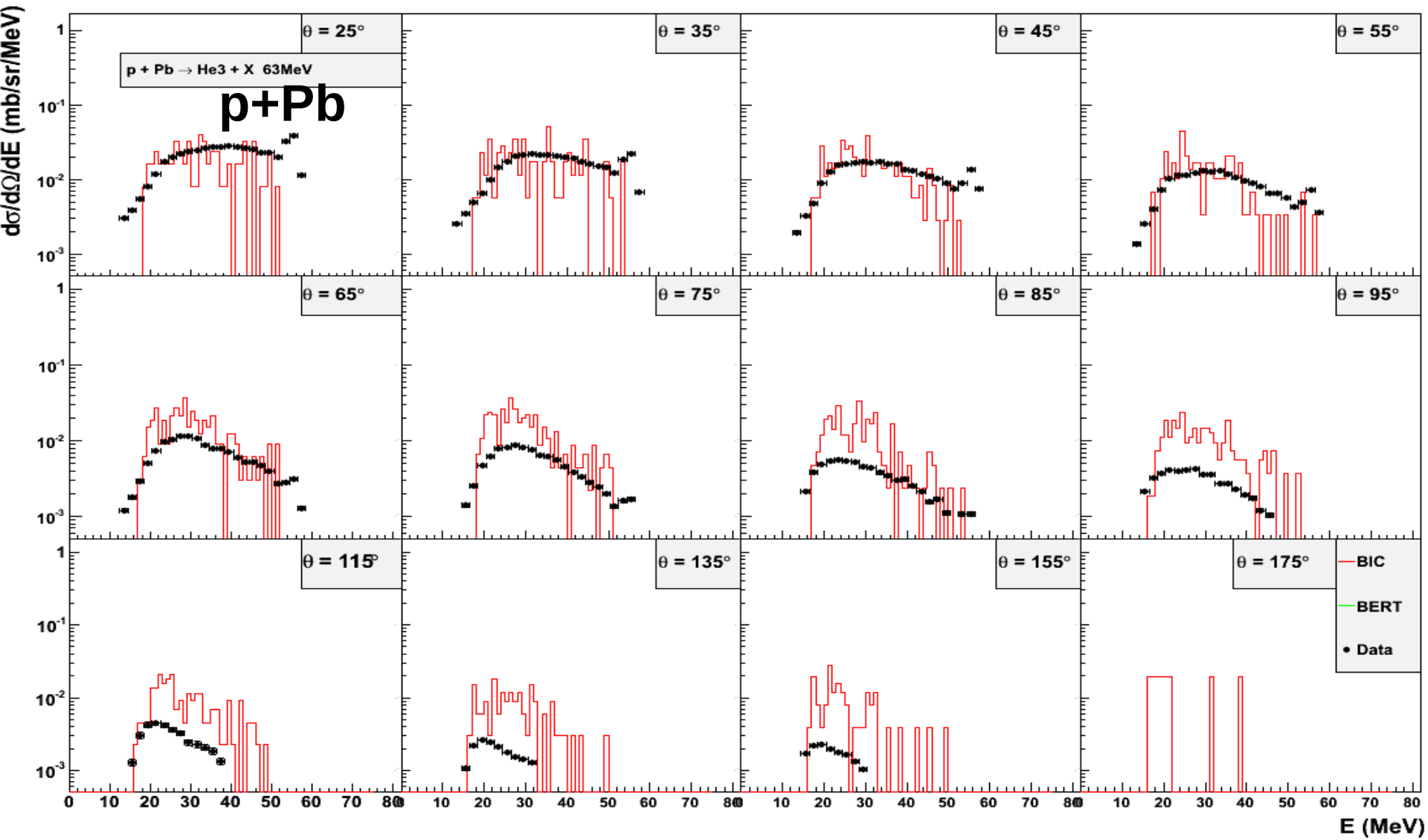
Tritum production at 1200 MeV



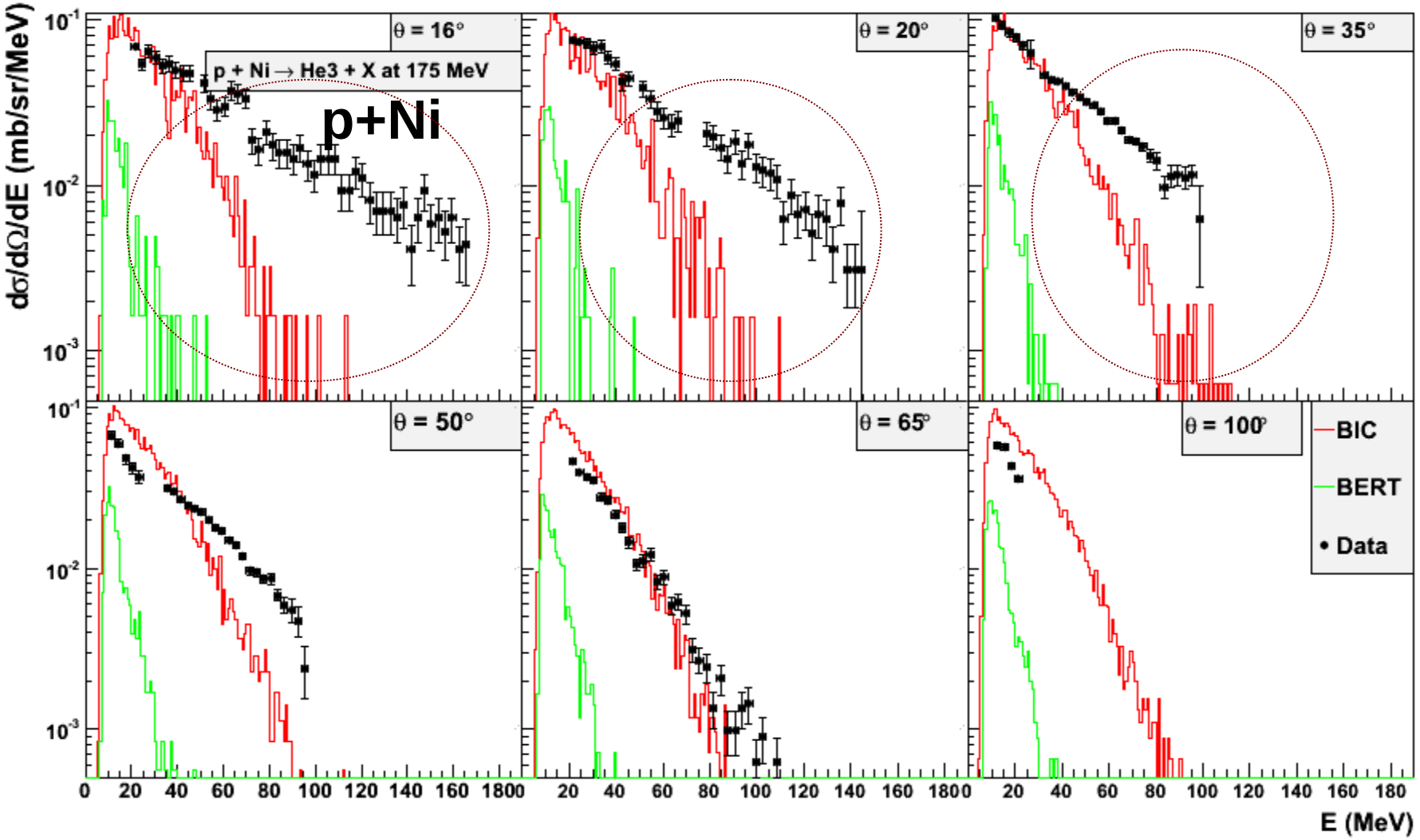
Tritium production at 1200 MeV



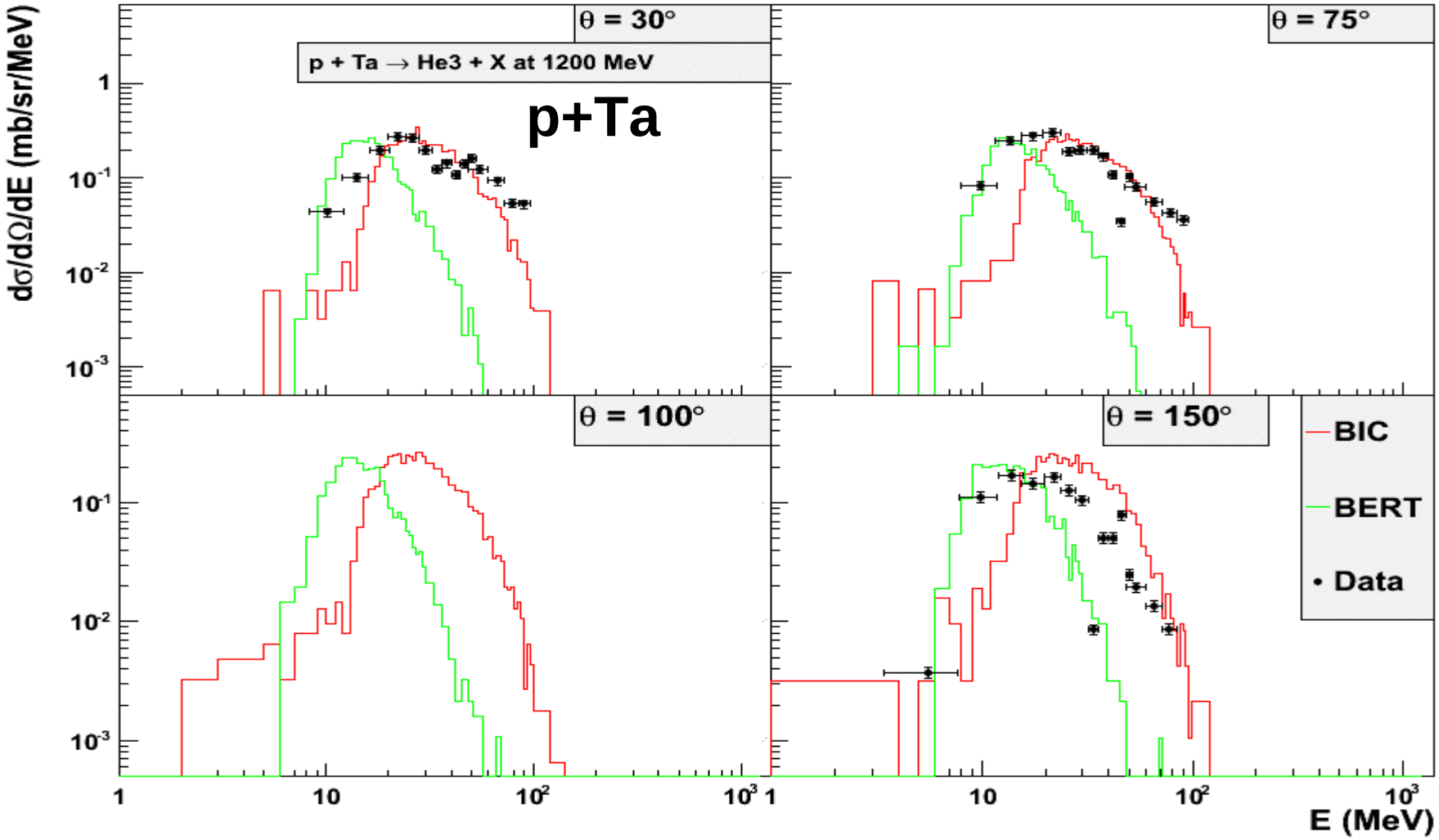
^{3}He production at 63 MeV



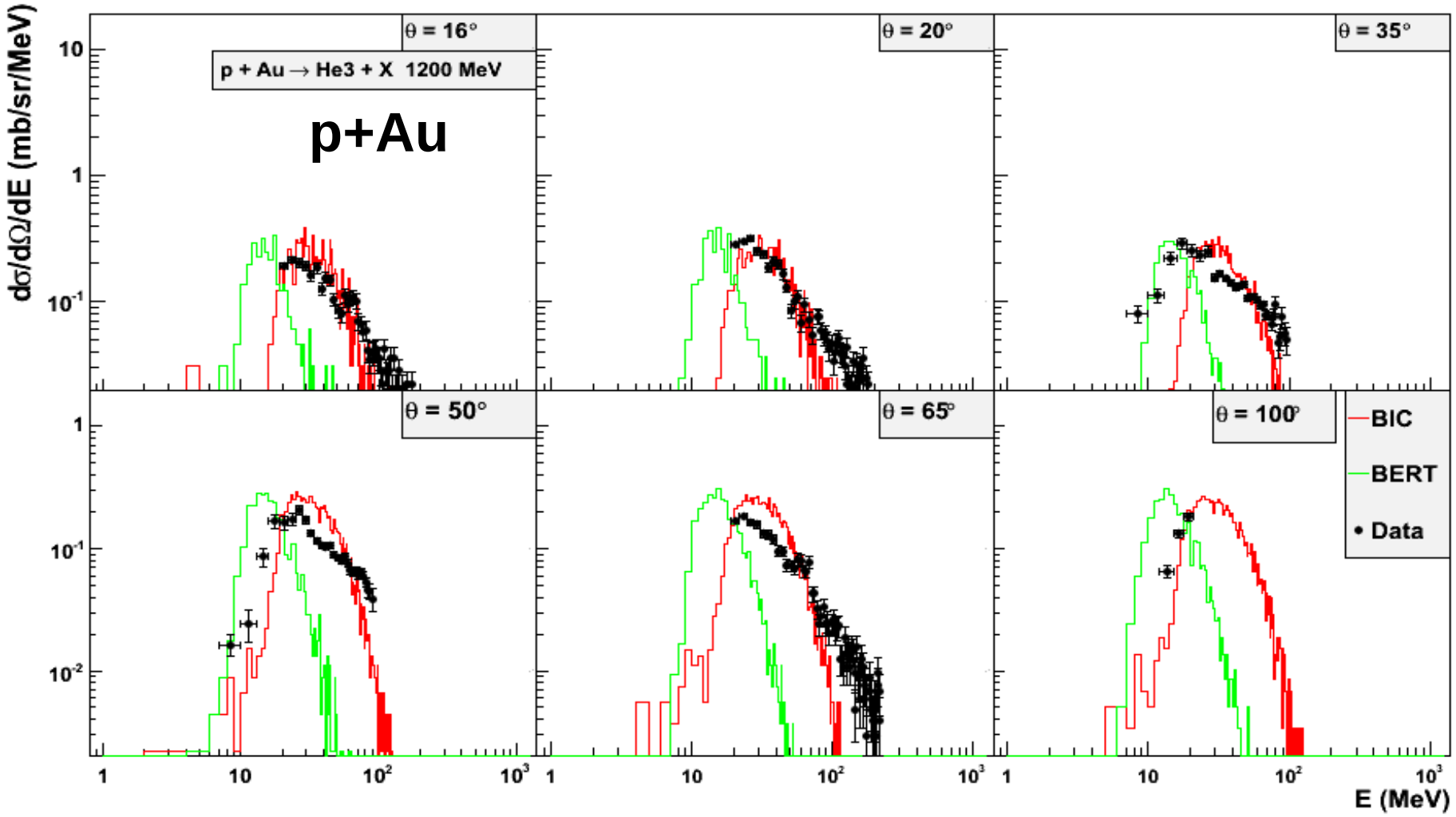
^{3}He production at 175 MeV



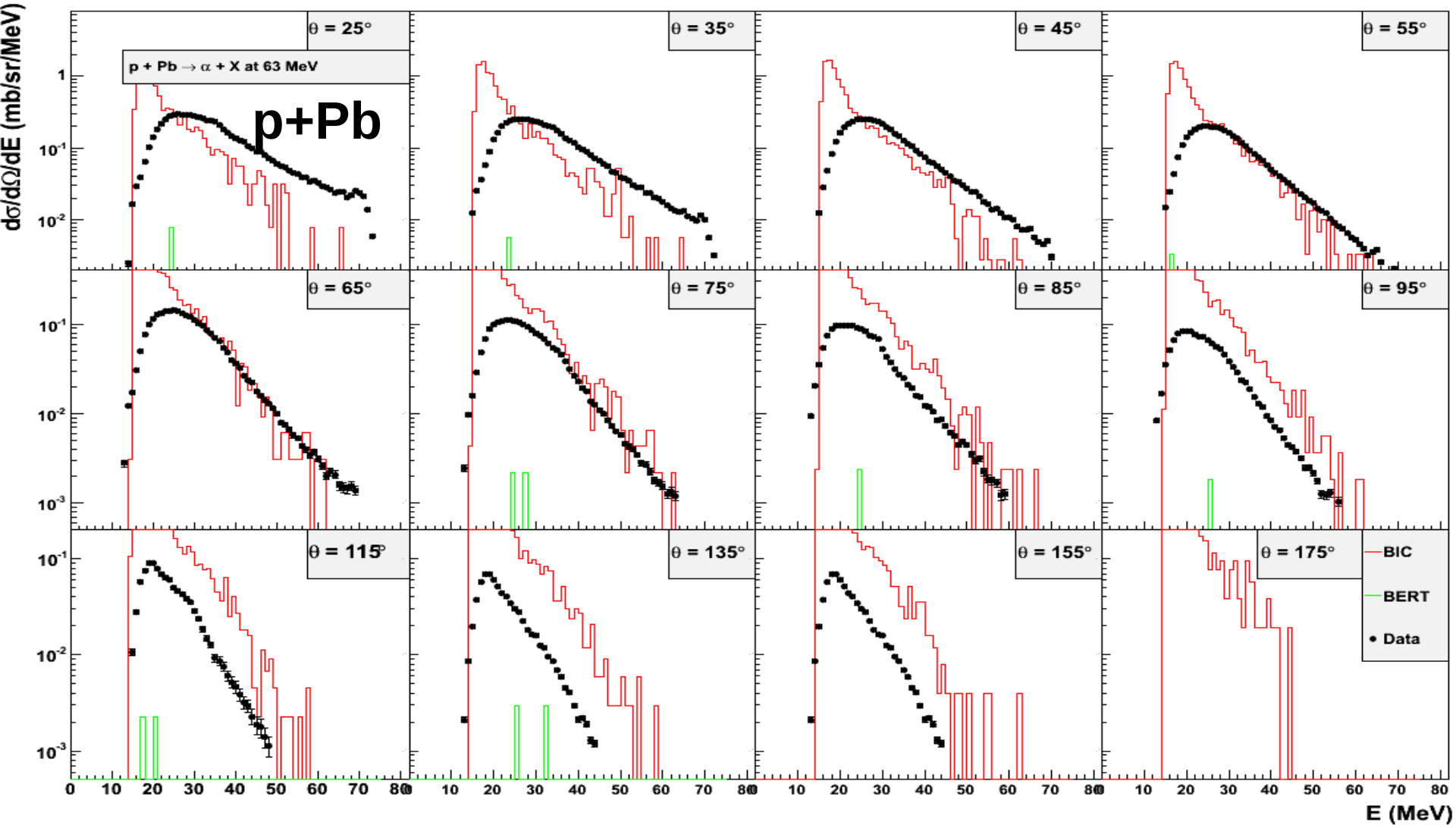
^{3}He production at 1200 MeV



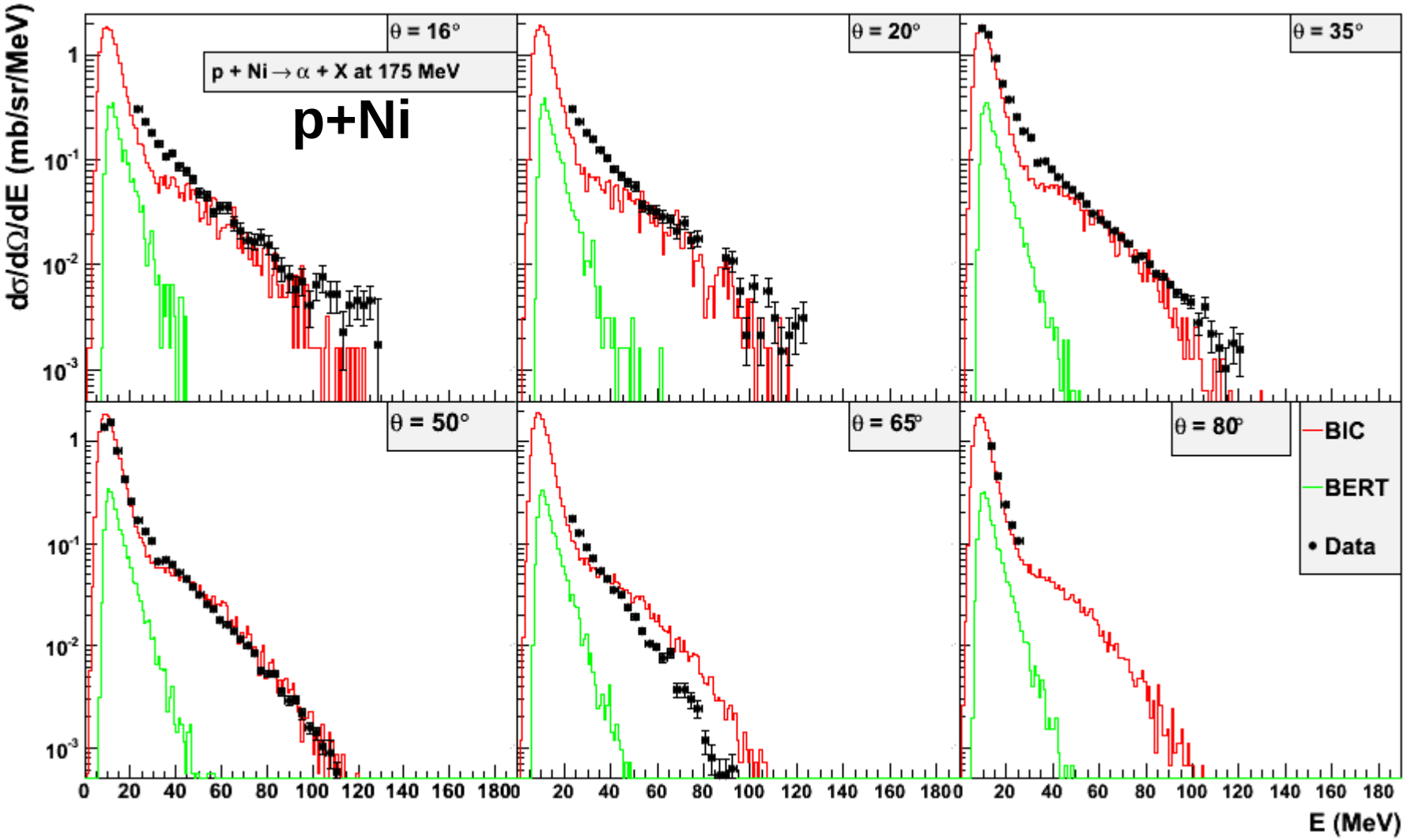
^{3}He production at 1200 MeV



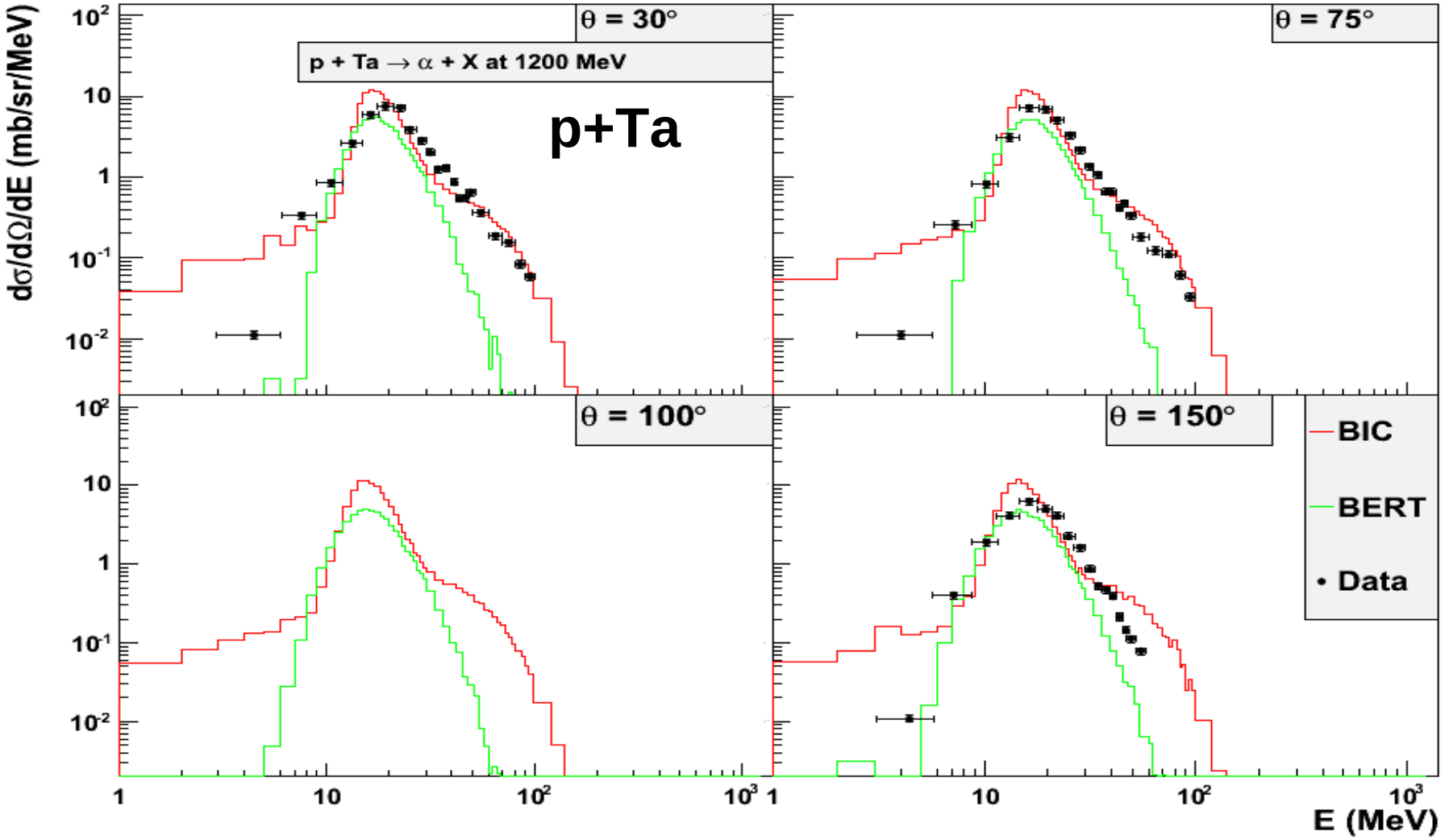
Alpha production at 63 MeV



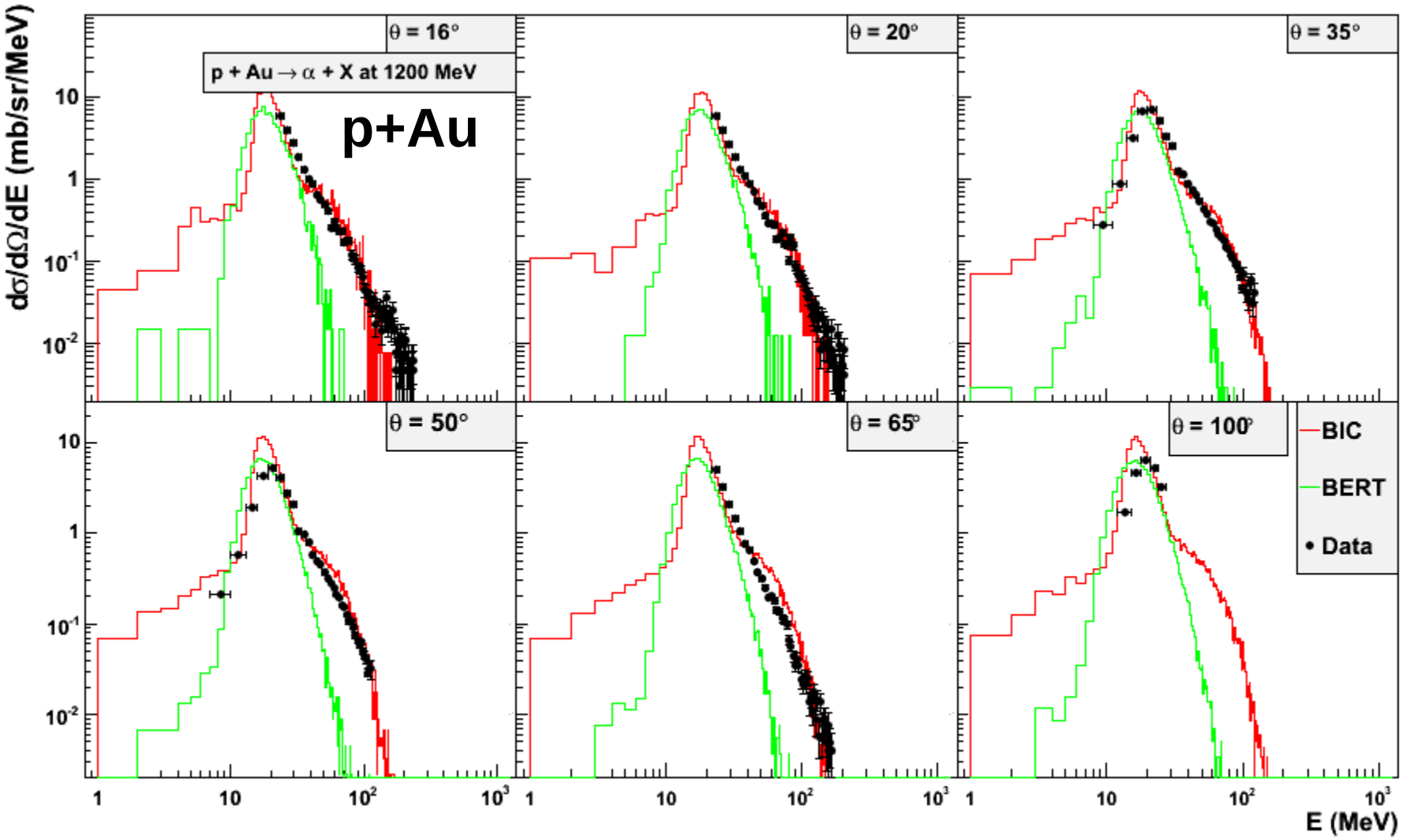
Alpha production at 175 MeV



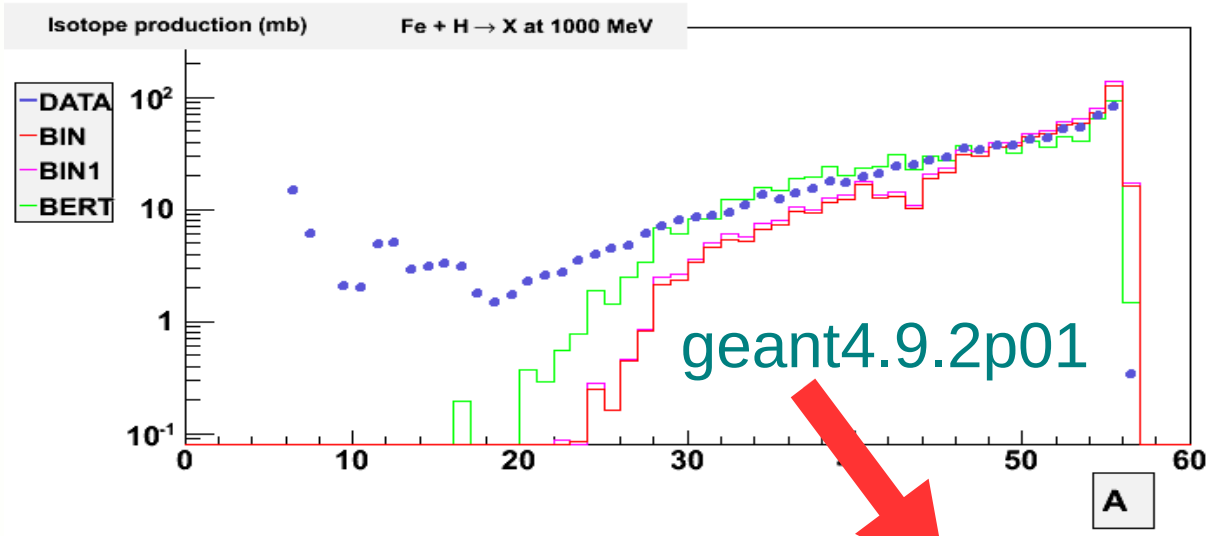
Alpha production at 1200 MeV



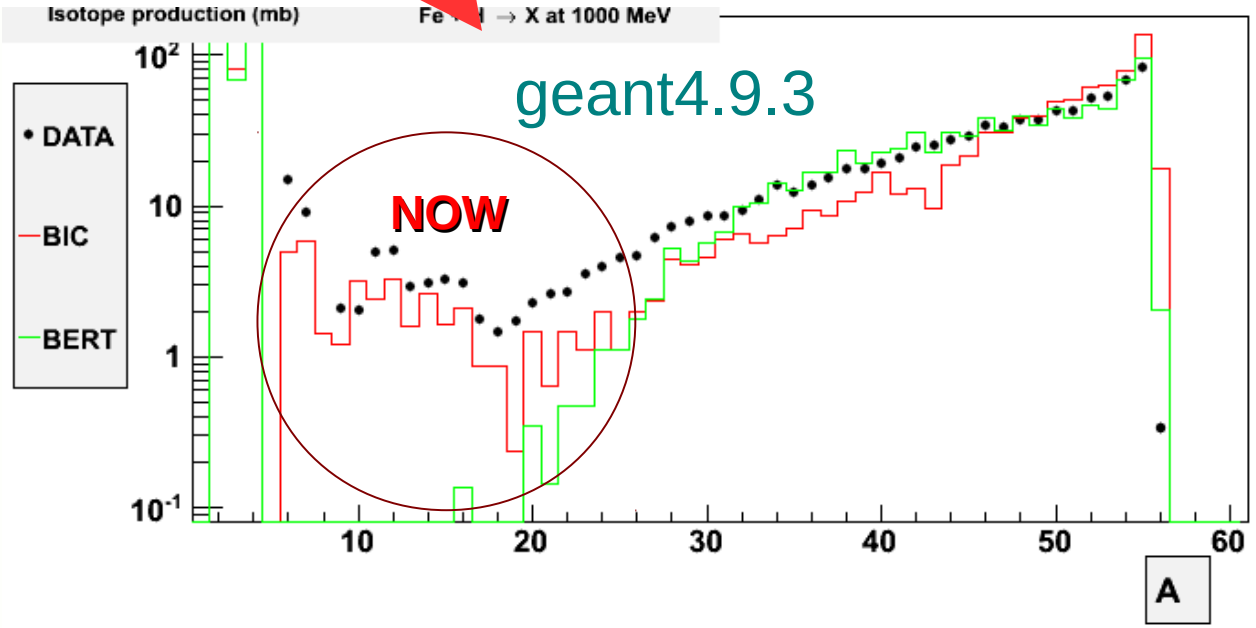
Alpha production at 1200 MeV



Isotopic distibution at 1 GeV

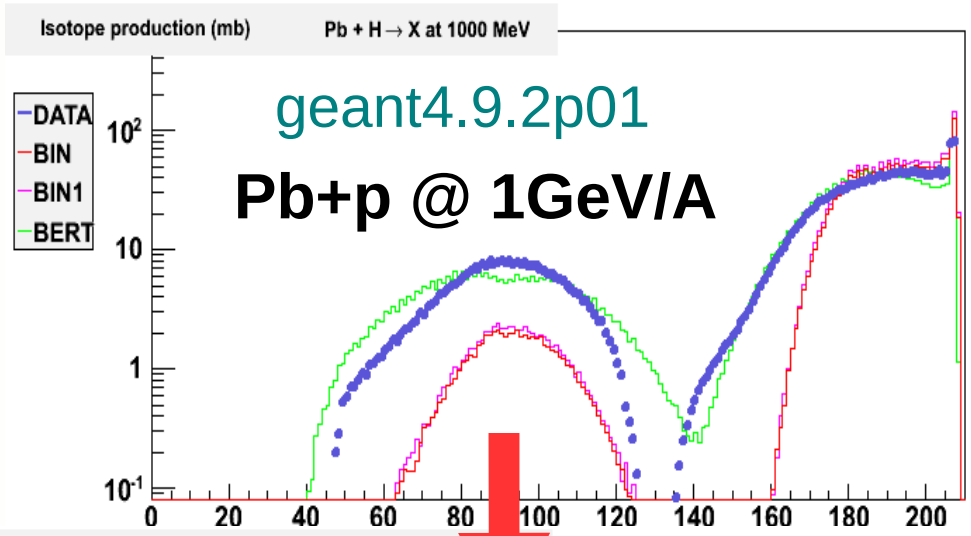


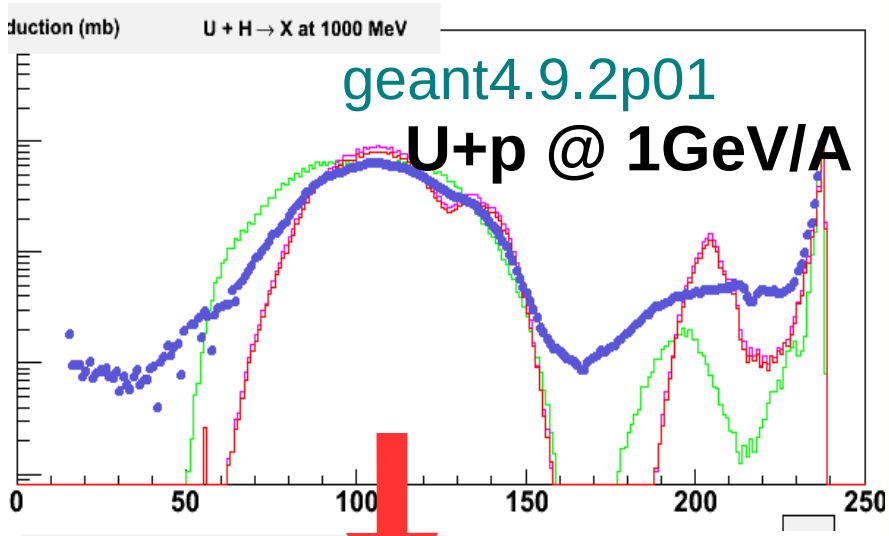
Fe+p @ 1GeV/A

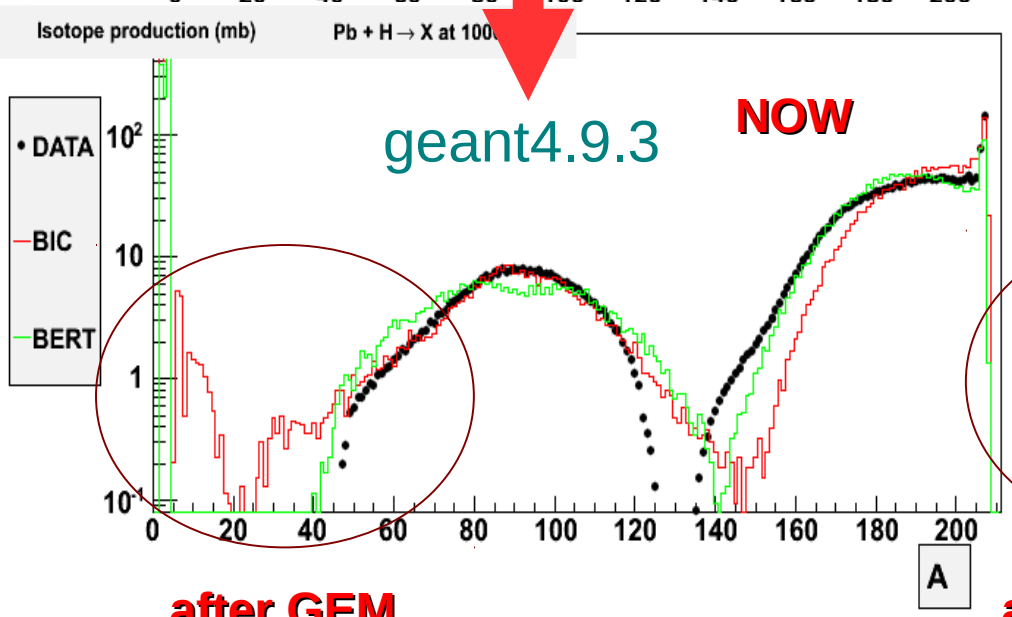


after GEM inclusion

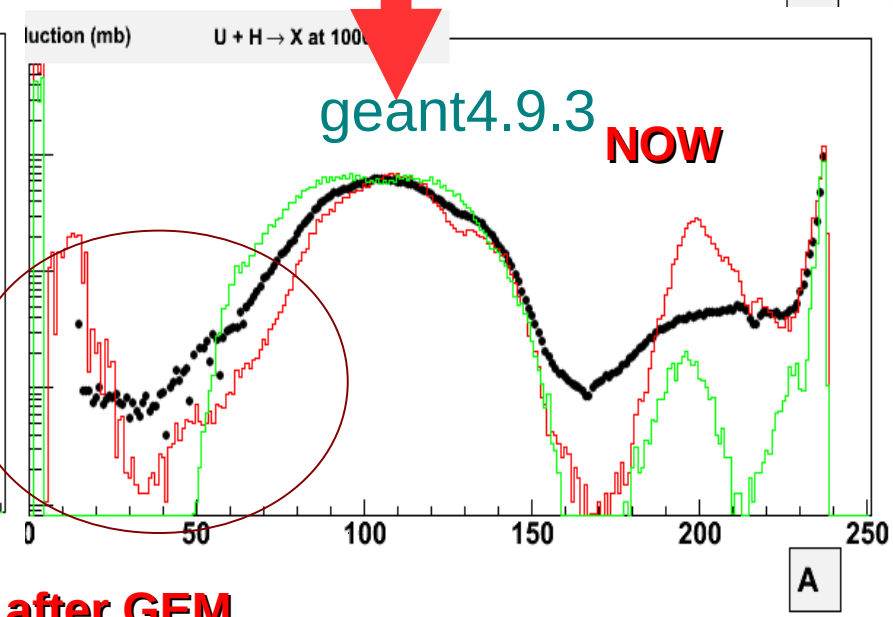
Isotopic distibution at 1 GeV





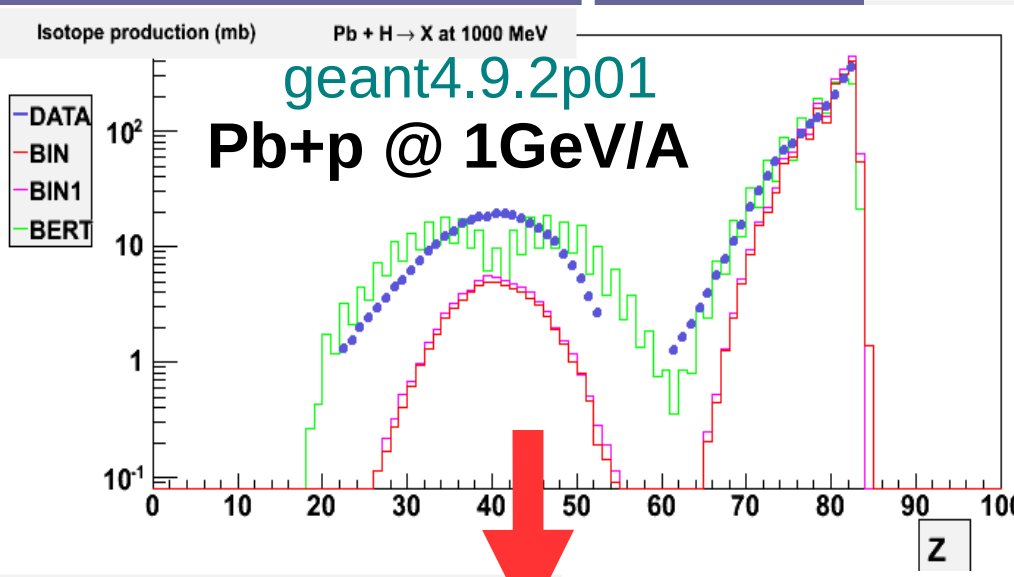


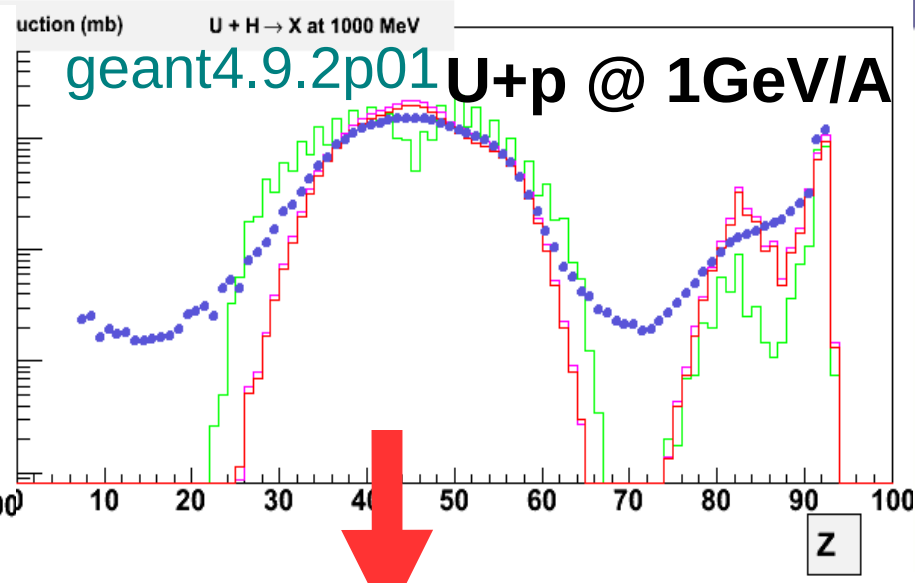
after GEM inclusion

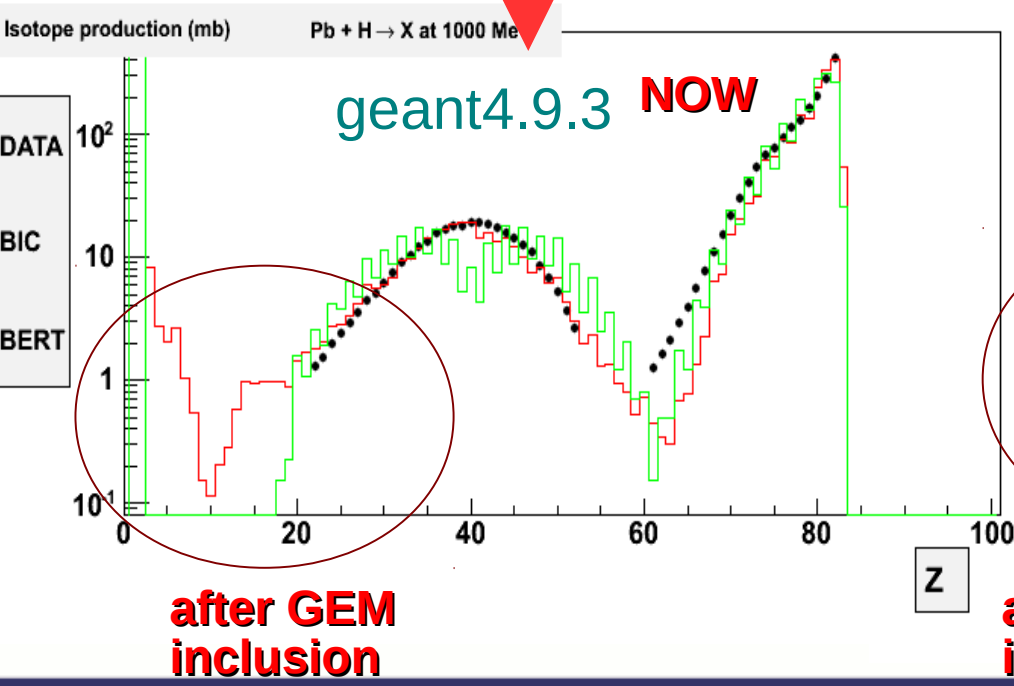


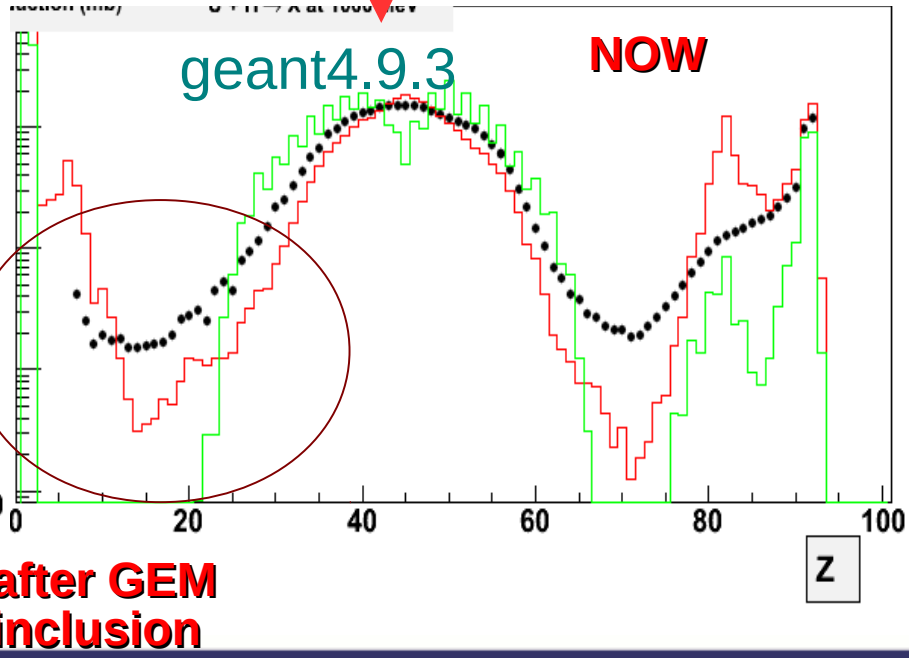
after GEM inclusion

Isotopic distribution at 1 GeV

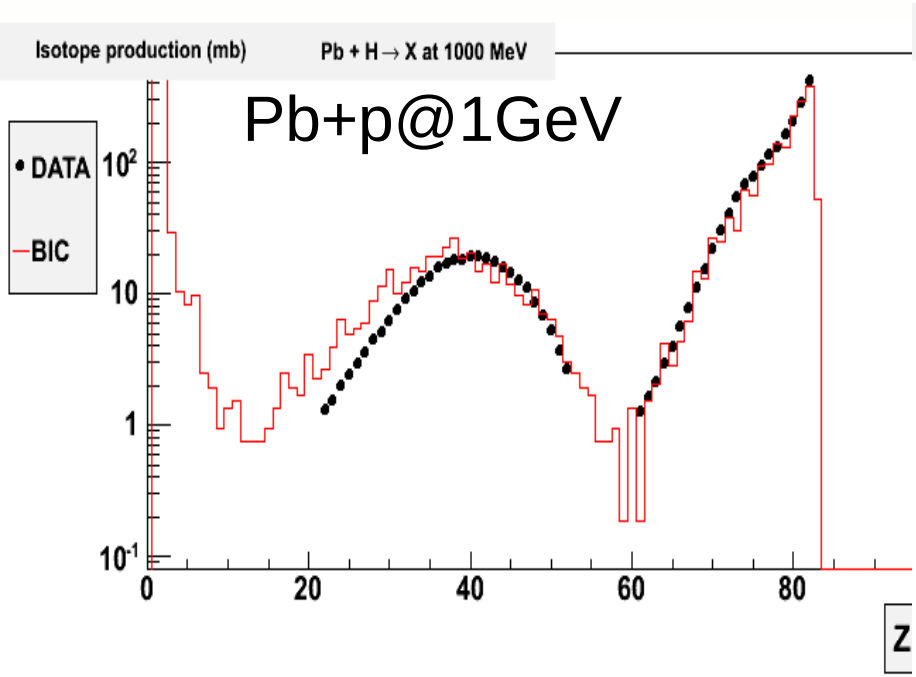


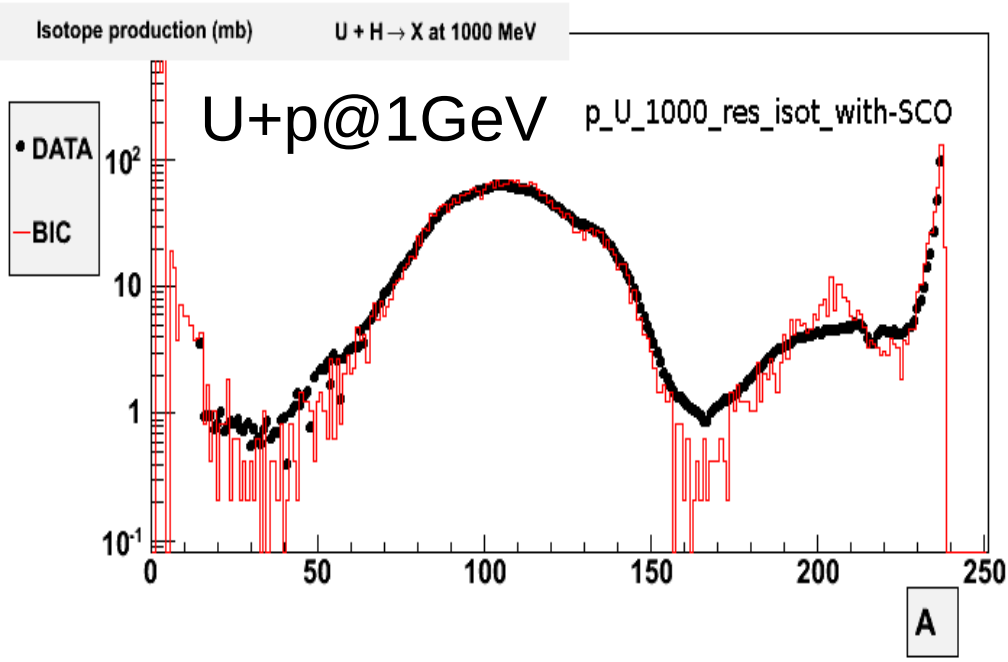






Development version
there is room for improvements

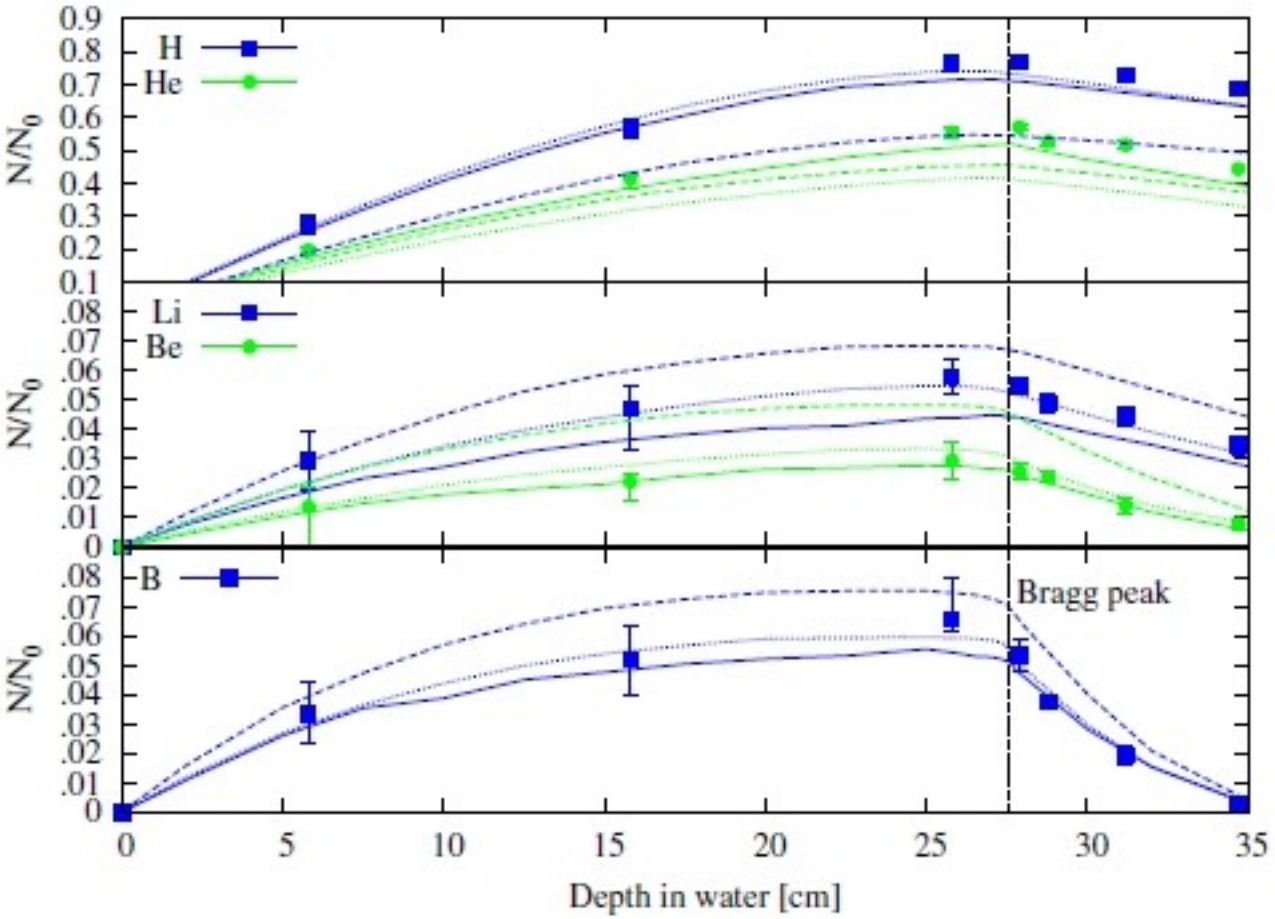




- “soft cut-off” ON
- Fission parameters have been fitted
- The situation at pre-equlibrium is quite the same
- CPU time increase (factor ~ 1.5)

Benchmark on nuclear models of FLUKA and Geant4 for carbon ion therapy

Thick target experiment
C on water



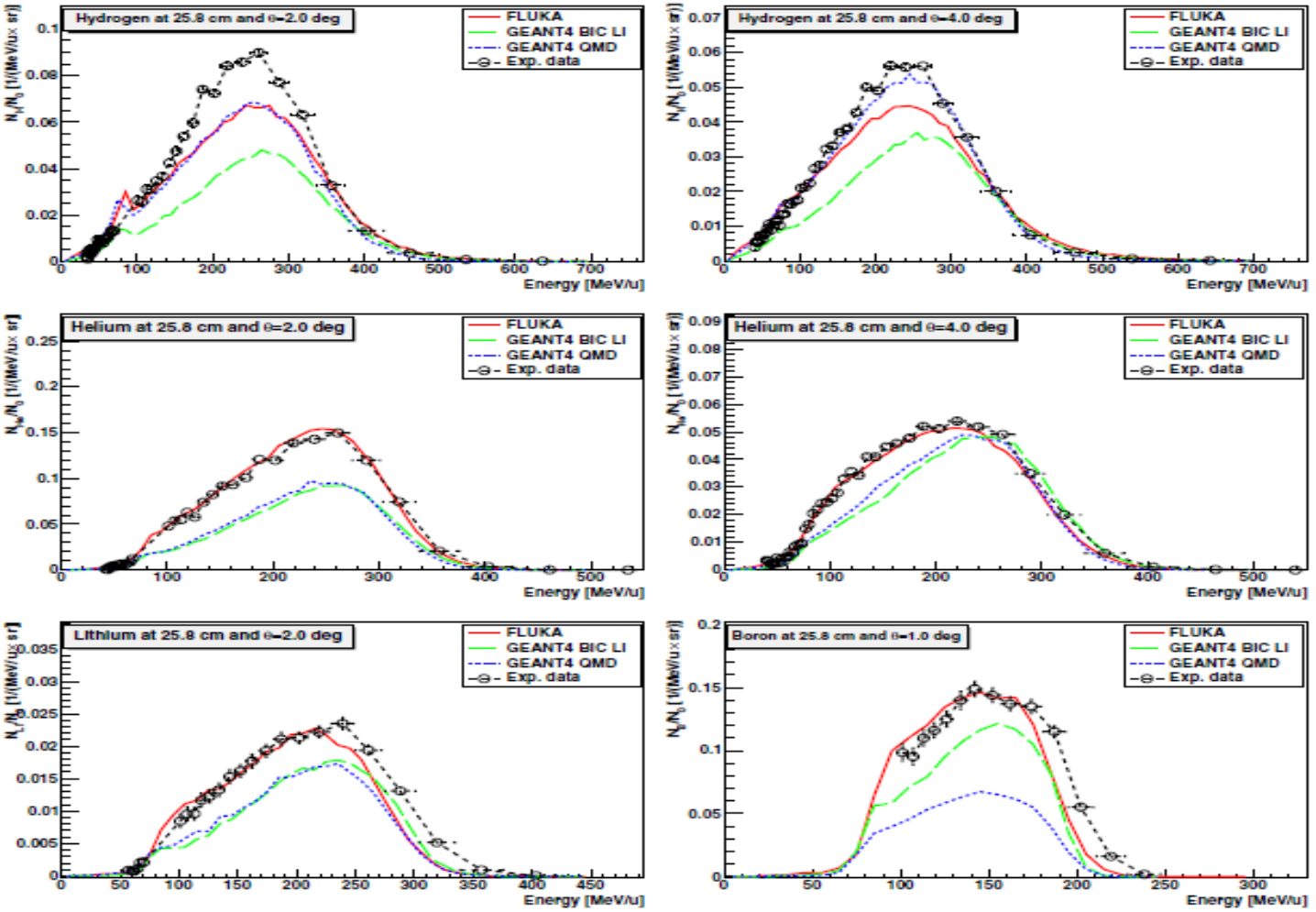
FLUKA

BIC LI

QMD

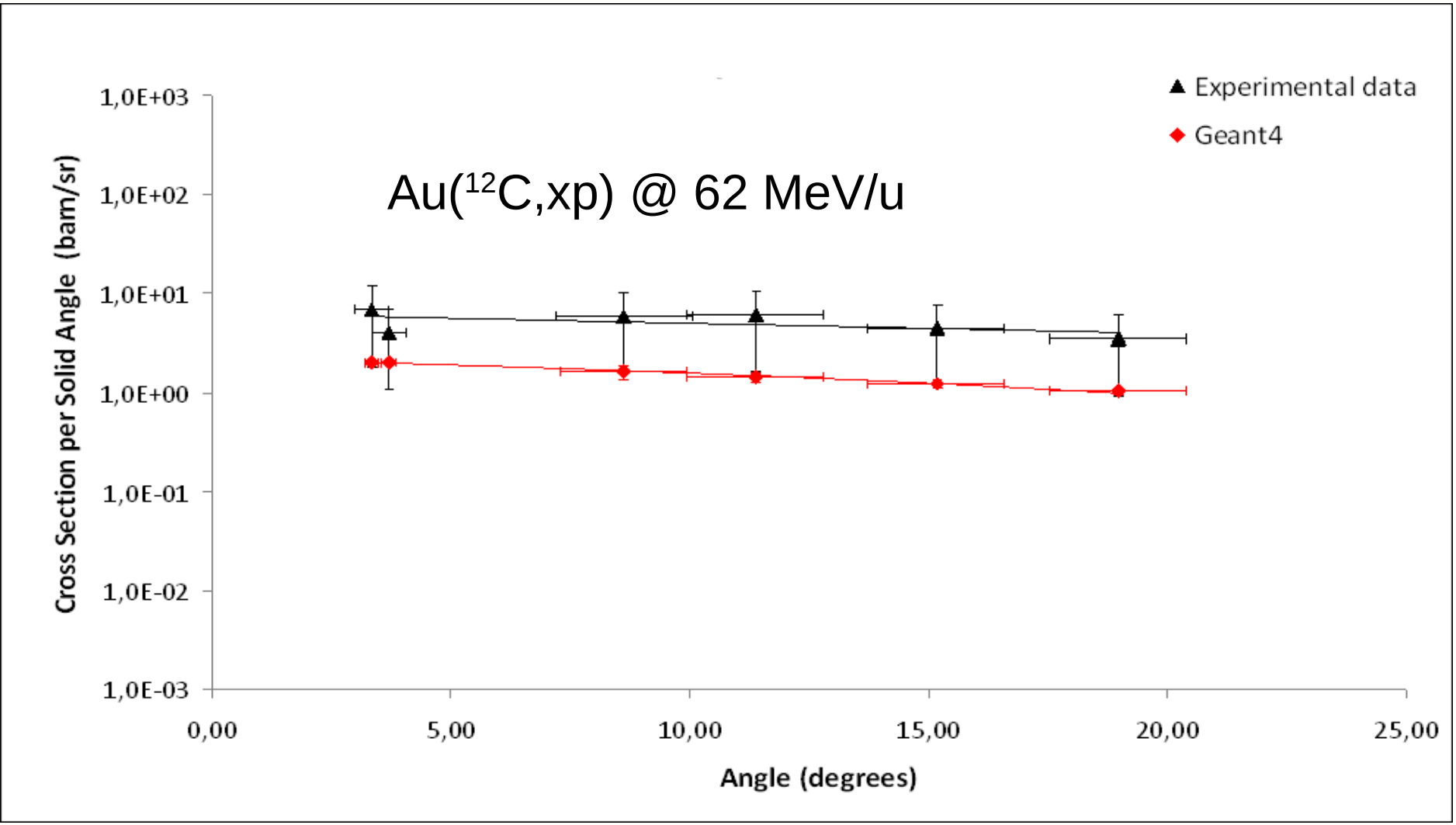
Fragment build-up curves in water of a 400 MeV/u carbon beam as a fraction of primary carbon ions N/N0. Simulations done for FLUKA (solid) and for GEANT4 using the BIC LI (dashed) and the G4QMD (dotted) model are displayed as lines. The dashed vertical line indicates the position of the Bragg peak.
T T Böhlen, F Cerutti , M Dosanjh , A Ferrari , I Gudowska , A Mairani and J M Quesada, "Nuclear models of FLUKA and GEANT4 for carbon ion therapy", Phys.. Med. Biol. (2010) 5833–5847

Thick target experiment
C on water



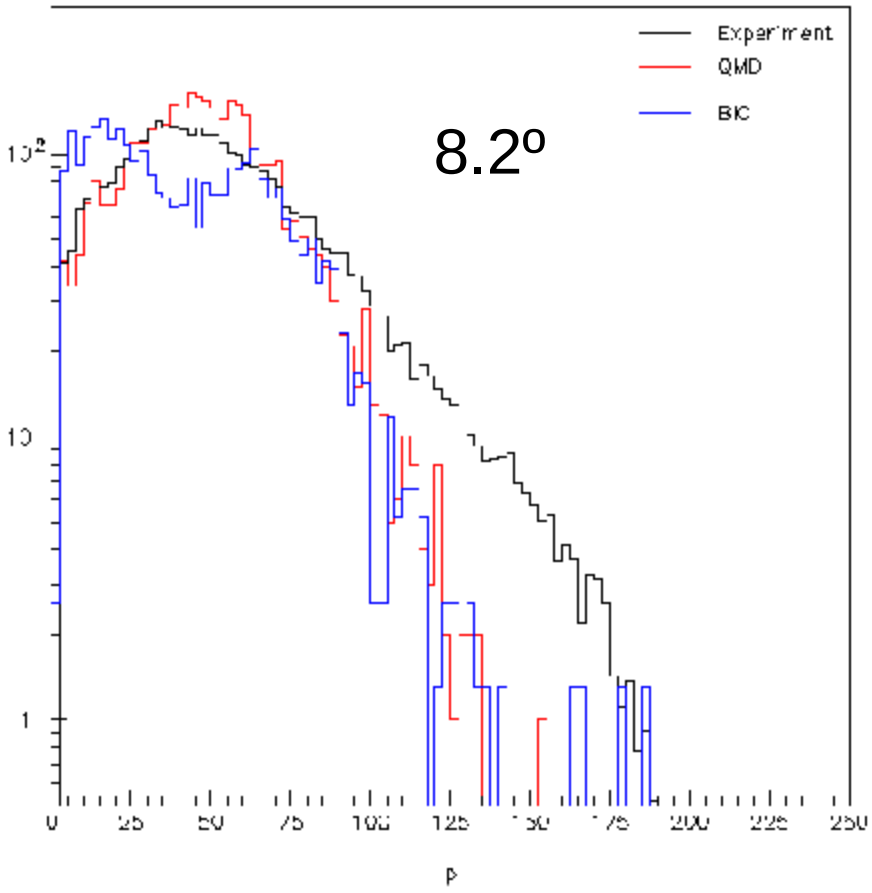
Number of ion fragments per steradian per MeV/u normalized to the number of incident particles N0 versus fragment energy are shown as produced by a 400 MeV/u carbon beam in water.Graphs are for a water-equivalent thickness of 25.8 cm and show H, He, Li and B fragments at selected angles.

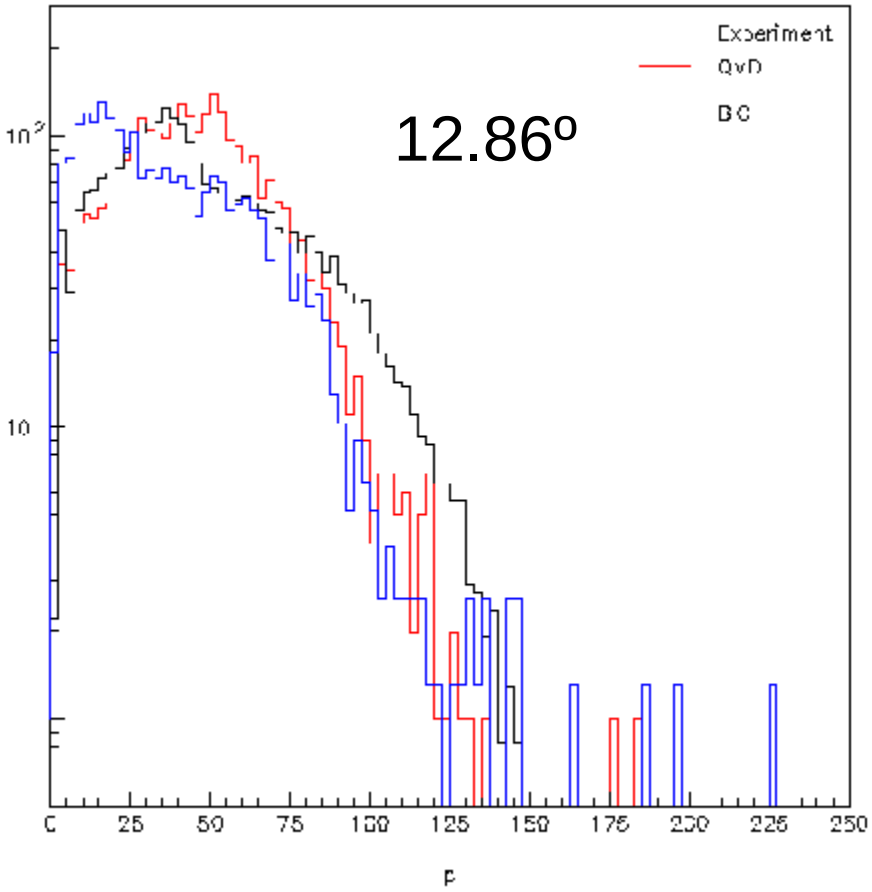
Hadrontherapy application
LNS-Catania's Geant4 group



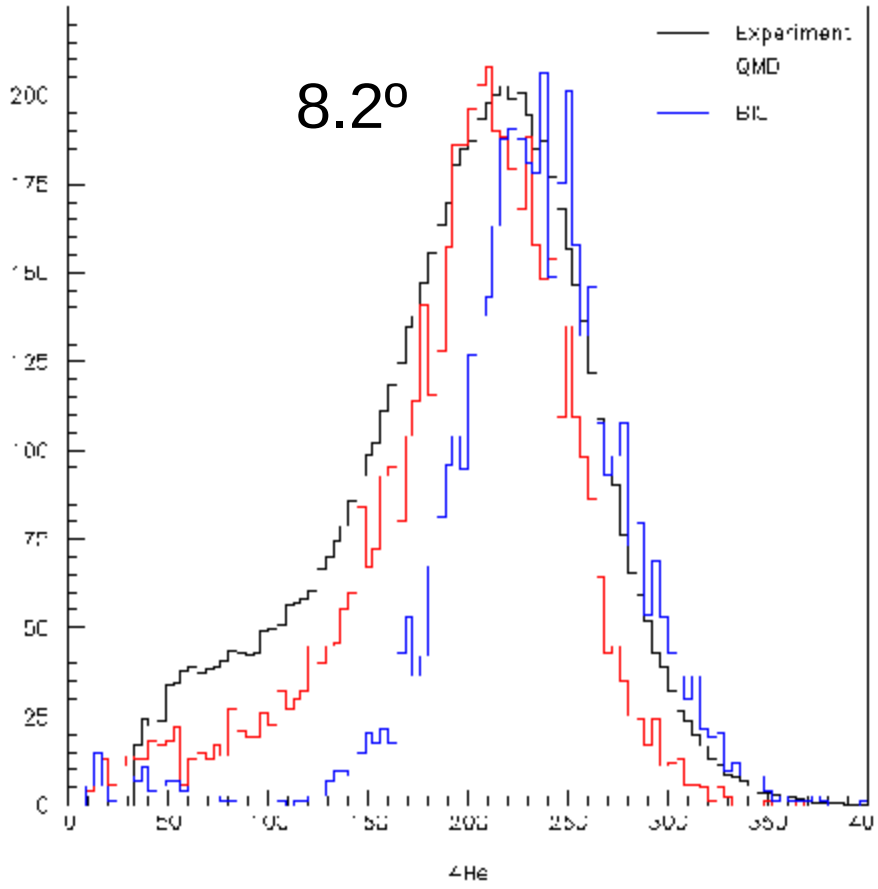
Angular distributions of proton production cross section for ^{12}C ions at gold target.

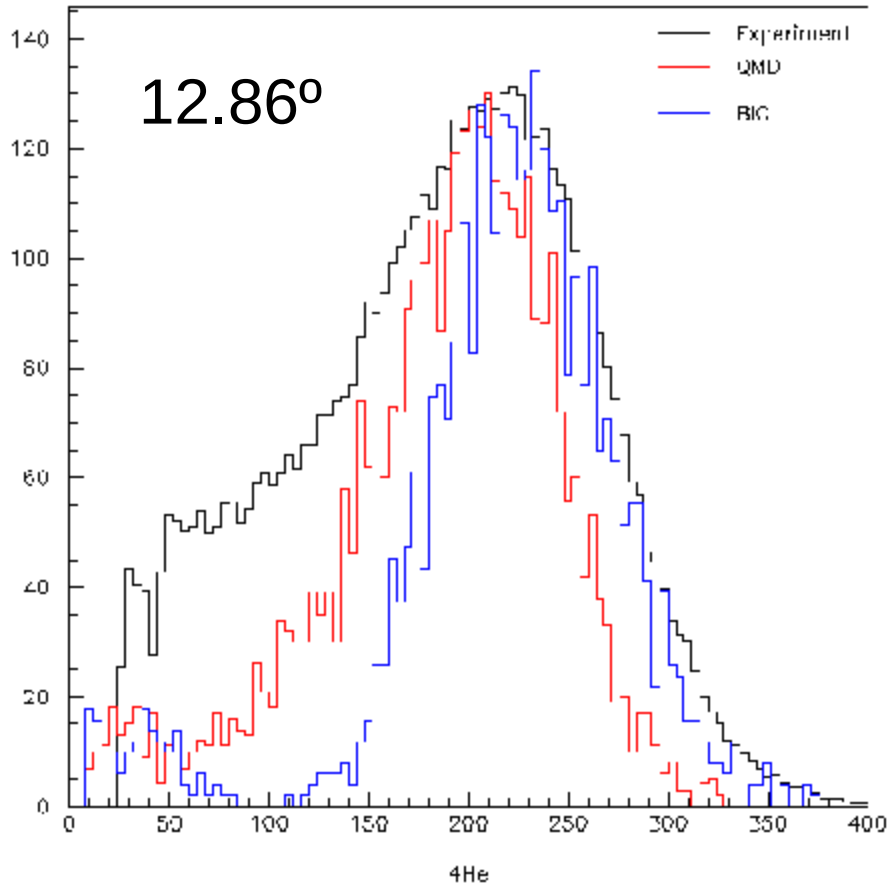
Au(^{12}C,xp) @ 62 MeV/u





Au(^{12}C,xp) @ 62 MeV/u





Thanks for your attention