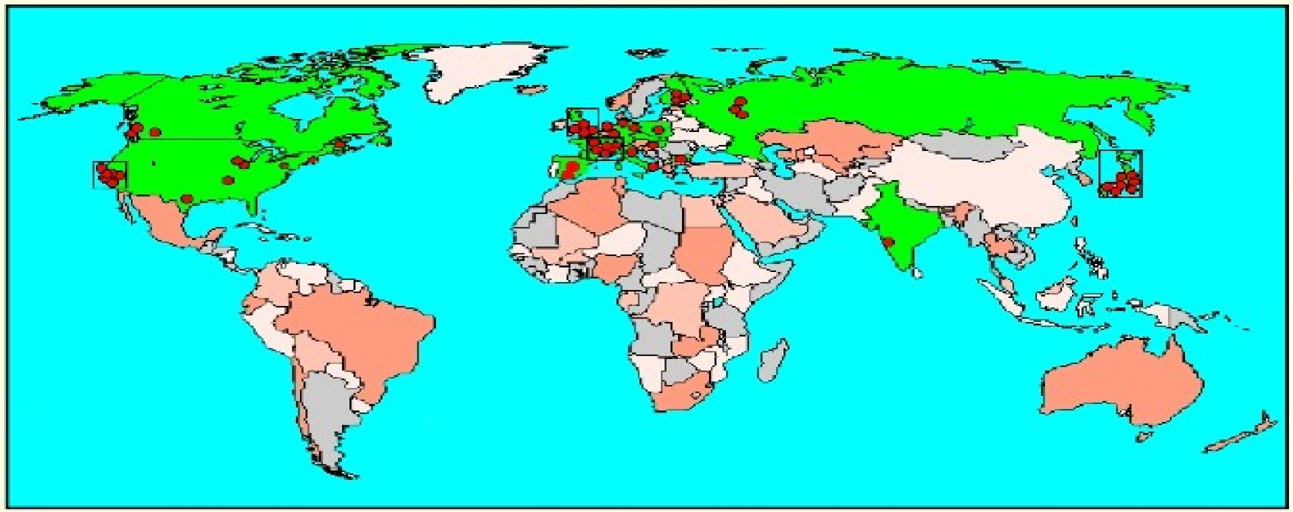
# Recent Developments in Pre-equilibrium and De-excitation Models in Geant4

J. M. Quesada
on behalf of the Geant4 Hadronic Group

V Encuentro de Física Nuclear
El Escorial, 27 de Septiembre de 2010

# Geant4 around the Word

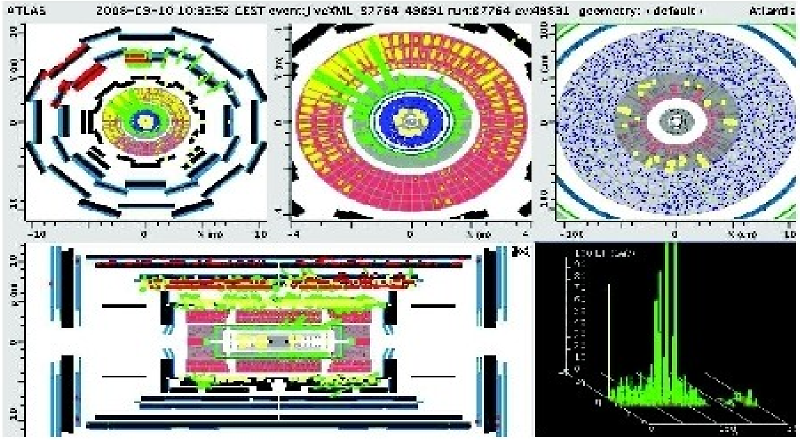
## Geant4 Collaboration

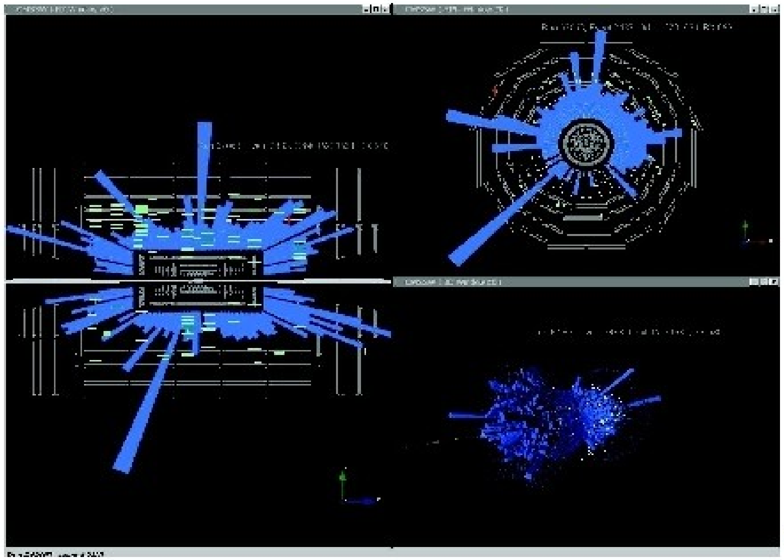


Collaborators also from non-member institutions, including
Budker Inst. of Physics
IHEP Protvino
MEPHI Moscow
Pittsburg University
University of Sevilla
CIEMAT

# Geant4 brief History

- Dec'94 : Project started
- Dec'98: First public release
- Geant4 was used by BaBar experiment at SLAC since 2000
- Geant4 is used for Monte Carlo simulation of particle transport for ATLAS, CMS, LHCb since 2004.
- Hadronic physics packages are an important part of Geant4 for LHC:
  - Signal acceptance
  - Background estimation



# What is Geant4?

- Geant4 is the C++ successor to Geant3

- Designed primarily with high energy physics in mind
  - but now used in medical an space physics as well

- It is a toolkit:
  - large degree of functionality and flexibility are provided
  - many different models provided, including alternates covering the same regions of applicability
  - choice of which to use is up to user, but guidance provided by Geant4 developers

- All major physics processes covered :
  - electromagnetic, hadronic, decay, photo- and electro-nuclear

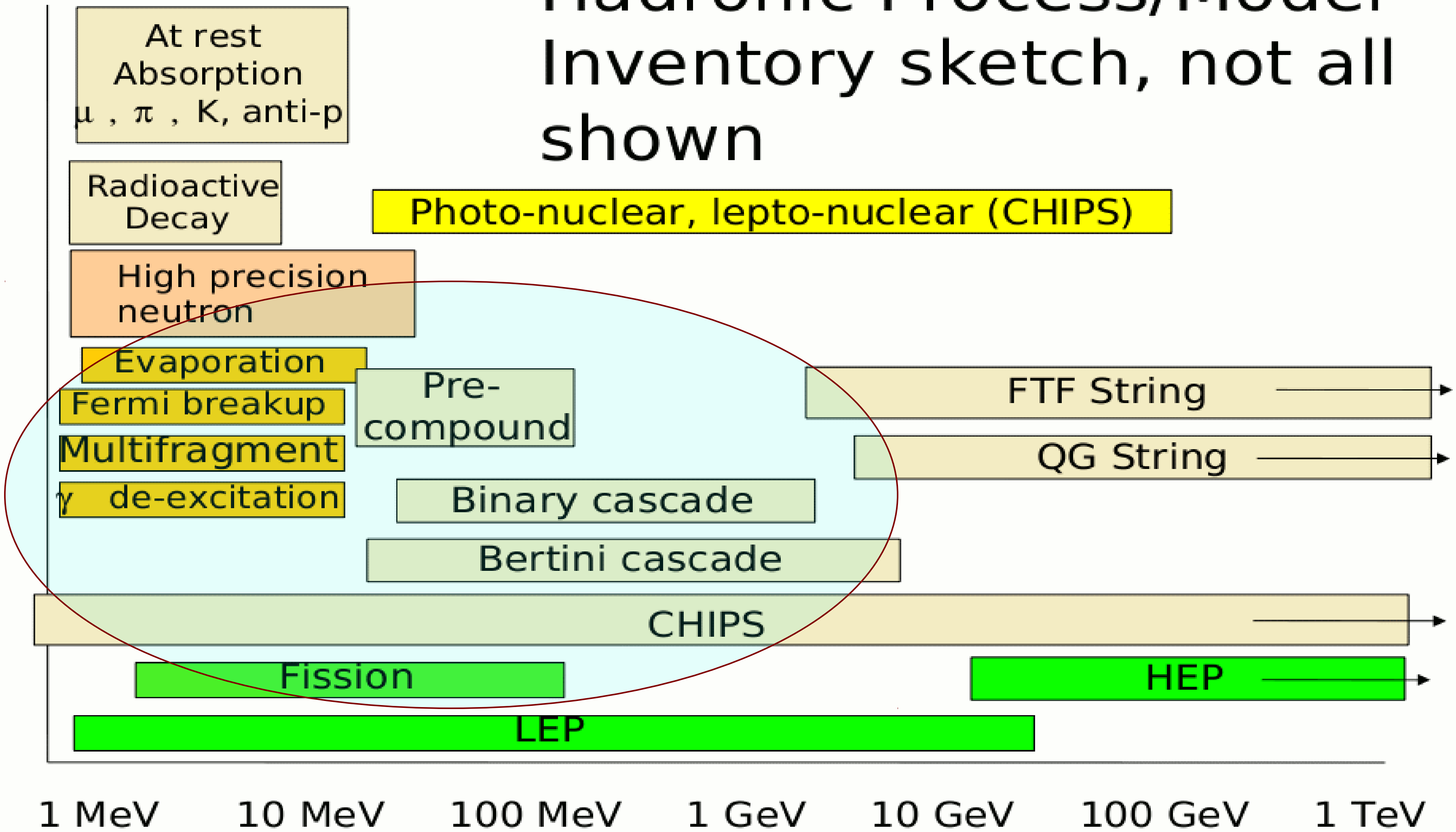
# Geant Hadronic Processes and Models

- Hadronic processes include:
  - Elastic
  - Inelastic
  - Capture at rest
  - Neutron capture
  - Neutron-induced fission
  - Lepton-nuclear
  - Gamma-nuclear

- Each of the above processes is implemented by one or more:
  - models (which contain the physics algorithm)
  - cross sections (which determine mean free path, etc.)

# Geant4 Hadronic Models

## Hadronic Process/Model Inventory sketch, not all shown



# Geant4 Cascade Models

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

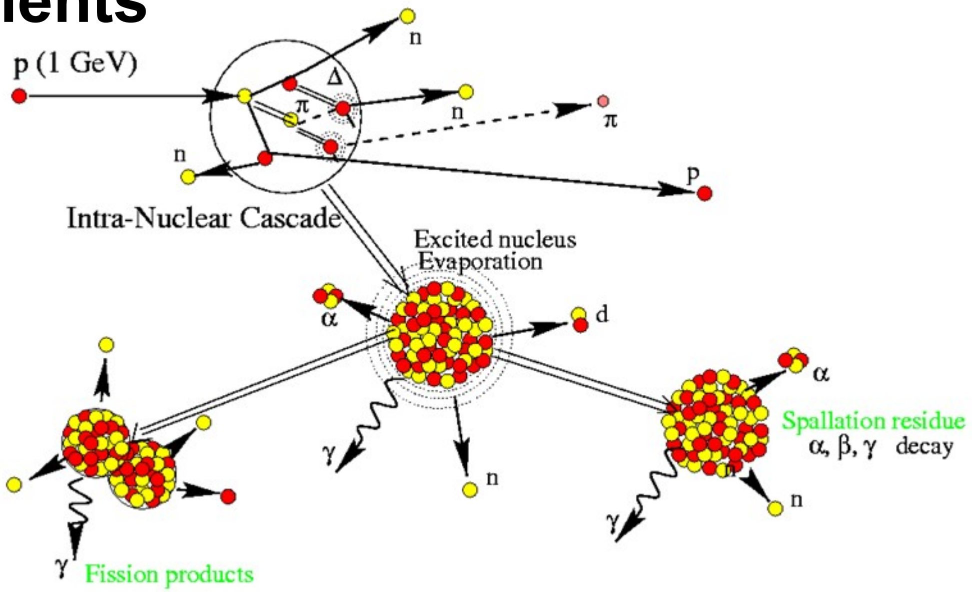
# Geant4 *Non*-Cascade Models

- **CHIPS**:
  - Quark-level event generator for the fragmentation of hadronic systems into hadrons.

- **QMD** :
  - Is a quantum extension of classical molecular-dynamics model.

# IAEA Benchmark on Spallation Reactions

- The benchmark is organised under the auspices of IAEA
- To assess the prediction capabilities of the spallation models
- To understand the reason for the success or deficiency of the models
- To reach a consensus, if possible, on some of the physics ingredients



# Origin and applicability of Binary Cascade

- H.P. Wellisch and G. Folger (CERN)
- Henning Weber (Frankfurt group)
- Based in part on Amelin's kinetic model
- Incident p, n
  - $0 < E < 3$ GeV
- light ions
  - $0 < E < 3$ GeV/A
- $\pi$
  - $0 < E < 1.5$ GeV

# Binary Cascade Model (1)

- Hybrid between classical cascade and full QMD model

- Detailed model of nucleus
  - nucleons placed in space according to nuclear density
  - nucleon momentum according to Fermi gas model

- Nucleon momentum is taken into account when evaluating cross sections, i.e. collision probability

- Collective effect of nucleus on participant nucleons described by optical potential
  - Participant particle's equations of motion are integrated numerically.

# Binary Cascade Model (2)

- Nucleon-nucleon scattering (t-channel) resonance excitation cross-sections are derived from p-p scattering using isospin invariance, and the corresponding Clebsch-Gordan coefficients
- Meson-nucleon inelastic (except true absorption) scattering modelled as s-channel resonance excitation. Breit-Wigner form used for cross section.
- Resonances may interact or decay
- Pauli blocking implemented in its classical form
- Coulomb barrier taken into account for charged hadrons

# Transition to preequilibrium

- If primary below 45 MeV, no cascade, just precompound
- Cascade stops when mean energy of all scattered particles is below 0.2*A-dependent cut for the average kinetic energies of secondaries, which means :
  - 18 MeV for A <31
  - 14 MeV for A<61
  - 10 MeV for A<121
  - 9 MeV for A>120
- When cascade stops, the properties of the residual exciton system and nucleus are evaluated, and passed to pre-equilibrium de-excitation class

I

# Pre-equilibrium

- Native pre-equilibrium de-excitation 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.

# Exciton Model Fundamentals

- The transition rates (for $\Delta n = -2, 0, +2$):

$$\lambda_{\Delta n}(p, h, E^*) = \frac{2\pi}{\hbar}|M_{\Delta n}|^2 \omega_{\Delta n}(p, h, E^*)$$

- The **total** transition rate:

$$\lambda_{total}(p, h, E^*) = \sum_{\Delta n=-2,0,+2} \lambda_{\Delta n}(p, h, E^*)$$

- The "j" particle (nucleon) emission probability distribution:

$$\mathcal{W}_c^j(p, h, E^*, \epsilon) = \frac{2s_j + 1}{\pi^2 \hbar^3} \mu_j \mathcal{R}_j(p, h) \frac{\omega(p-1, h, E^* - B_j - \epsilon)}{\omega(p, h, E^*)} \epsilon \sigma_{inv}(\epsilon)$$

- The "j" particle (cluster) emission probability distribution:

$$\mathcal{W}_c^j(p, h, E^*, \epsilon) = \frac{2s_j + 1}{\pi^2 \hbar^3} \mu_j \mathcal{R}_j(p, h) \gamma_j \frac{\omega(p - p_j, h, E^* - B_j - \epsilon)}{\omega(p, h, E^*)} \frac{\omega(p_j, 0, B_j + \epsilon)}{g_j} \epsilon \sigma_{inv}(\epsilon)$$

- The **total** emission rate:

$$\Gamma_c(p, h, E^*) = \sum_i \int_{V_i^c}^{E^* - B_j} \mathcal{W}_c^j(p, h, E^*, \epsilon) d\epsilon$$

# New inverse reaction cross sections

- Inverse reaction cross sections play a mayor role in the calculation of (competing) emission probabilities.

- Theory driven *old* parameterization (Dostrovski et al, 1959) (kept as option)

- NEW: More realistic parameterization of reaction cross sections (after release 9.2)
  - Chatterjee at al: Calculated with global optical model potentials, in turn fitted to reproduce available experimental data
  - Kalbach's retuning (PRECO code)
  - Wellisch's parameterization of proton reaction cross sections by direct fitting to experimental data
  - Default option combines the best combination of inverse cross sections (Wellisch's parameterization for protons and Kalbach's one for the rest)

# Transition from Pre-equilibrium to De-excitation

- **The transition from pre-equilibrium to equilibrium de-excitation should take place when:**

$$\lambda_{+}(p,h,E) \;=\; \lambda_{-}(p,h,E)$$

- **Which can be roughly estimated as:**

$$n_{eq} = \sqrt{2gE^{*}}$$

- **The practical need of less pre-equilibrium emission led to the introduction following probability :**

$$P_{pe}(n/n_{eq}) = 1 - e^{-\frac{1}{2\sigma_{pre}^{2}}\left(\frac{n}{n_{eq}}-1\right)^{2}}$$

**for $n<n_{eq}$ and equal to cero *for $n>n_{eq}$ , with*** $\sigma_{pre} \approx 0.4$

# Equilibrium De-excitation

Four processes are considered:

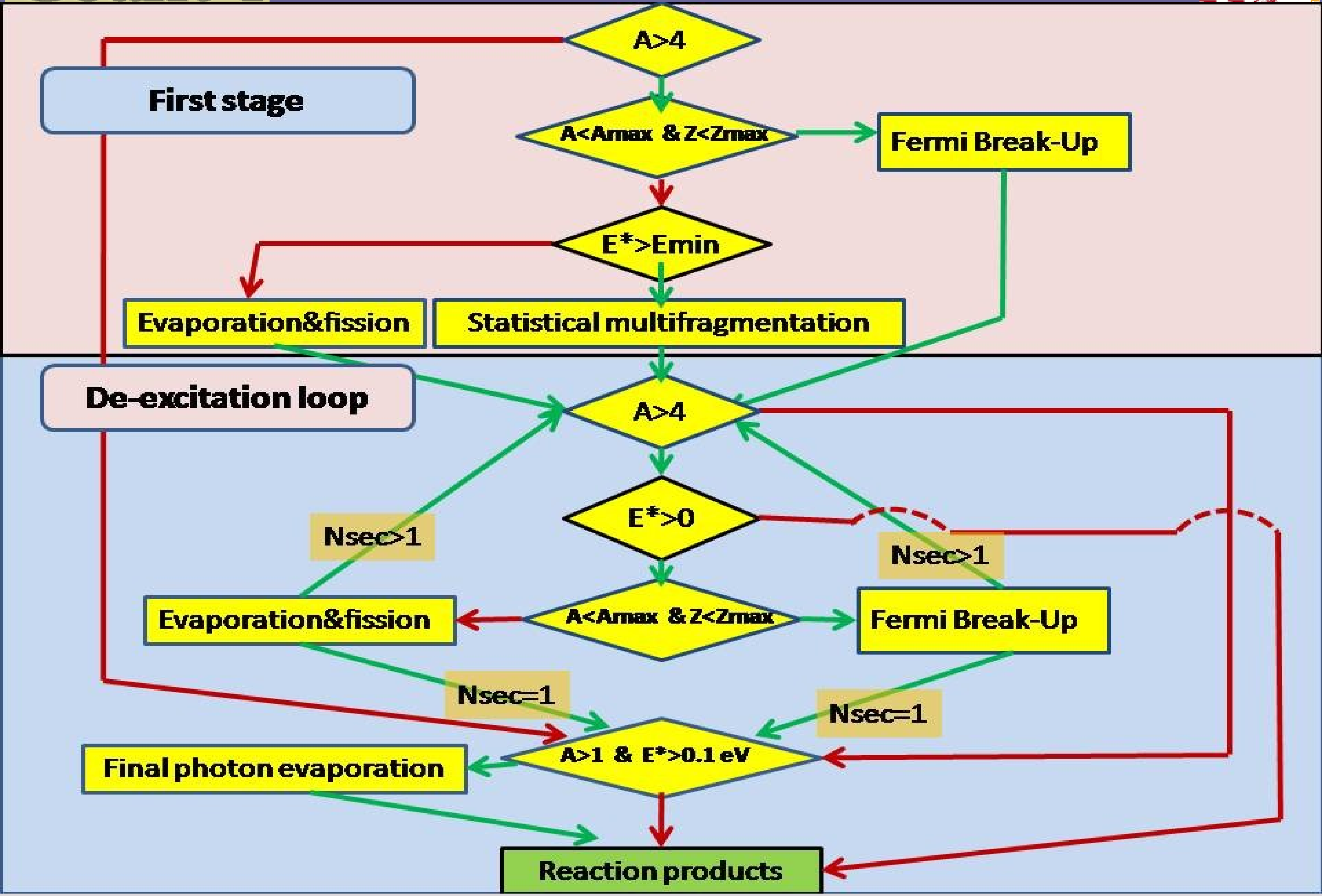
**Alternative:**

- Fermi break-up , 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)

# Equilibrium De-excitation



# Evaporation models

- WE: evaporation of particles (n,p,d,t,$^3$He, alphas) from a completely degenerated Fermi gas (excited compound nucleus)

$$\Gamma_c^j(E^*,\epsilon) = \frac{2s_j+1}{\pi^2\hbar^3}\mu_j \frac{exp[2\sqrt{a_0(E^*-S_n-\delta_0-\epsilon)}]}{exp[2\sqrt{a_0(E^*-\delta_0)}]}\epsilon\sigma_{inv}(\epsilon)$$

- GEM: generalization for including heavier ejected fragments
  (Z>13 , A<29)

- NEW: Combination of *improved* WE for evaporation of n,p,d,t,$^3$He, alpha and GEM for heavier fragments. (default)

# Preliminary results in AccApp'09 Conference

## (related to geant4.9.2p01 official release results )

- No *ad hoc* tuning of level density parameter ratio $a_{fis}/a_{evap}$. (preliminary trials show that it is critical, as reported in previous works).
- No *soft transition* from pre-equilibrium (i.e. increment of equilibium at the expenses of pre-equilibrium) .
- Very important: parameters tuned in a “model suite” shouldn’t be assumed to work in a different *environment*, i.e. with different *coupled* models.

↓

Ad hoc tuning of parameters was clearly necessary in order to reproduce fission data. (Done in next release)

# Progress after AccApp'09 Conference

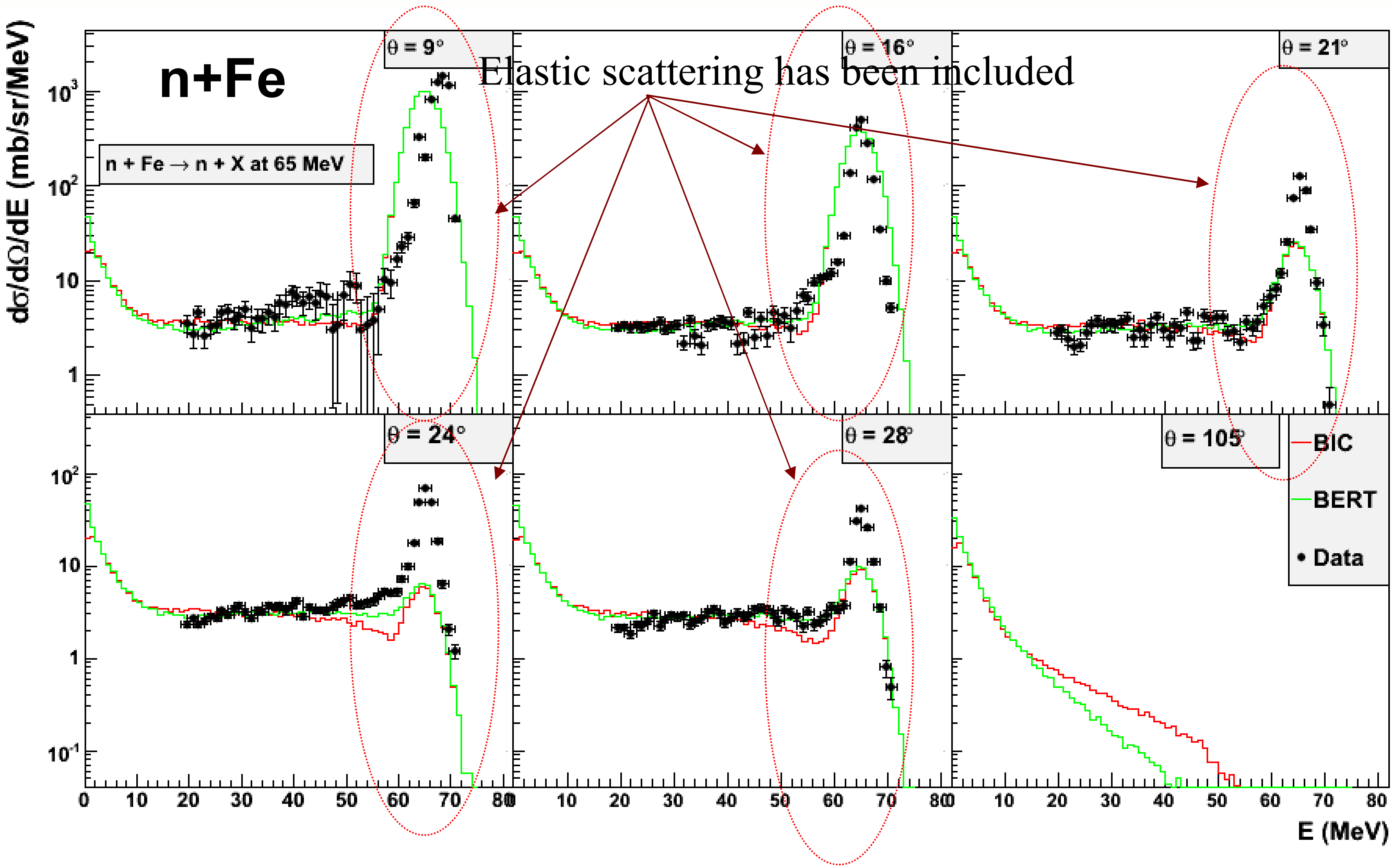
## (included in geant4.9.3 official release )

- Transition probabilities at pre-equilibrium (exciton model) have been calculated according to CEM version of model
- Combined WE-GEM model has been implemented in de-excitation (allows description of IMF production)
- First retuning of parameters now undertaken using two example reactions
  - Tuning of level density parameter ratio $a_{fis}/a_{evap}$.
  - Tuning of the width of symmetric component of fission fragment distribution

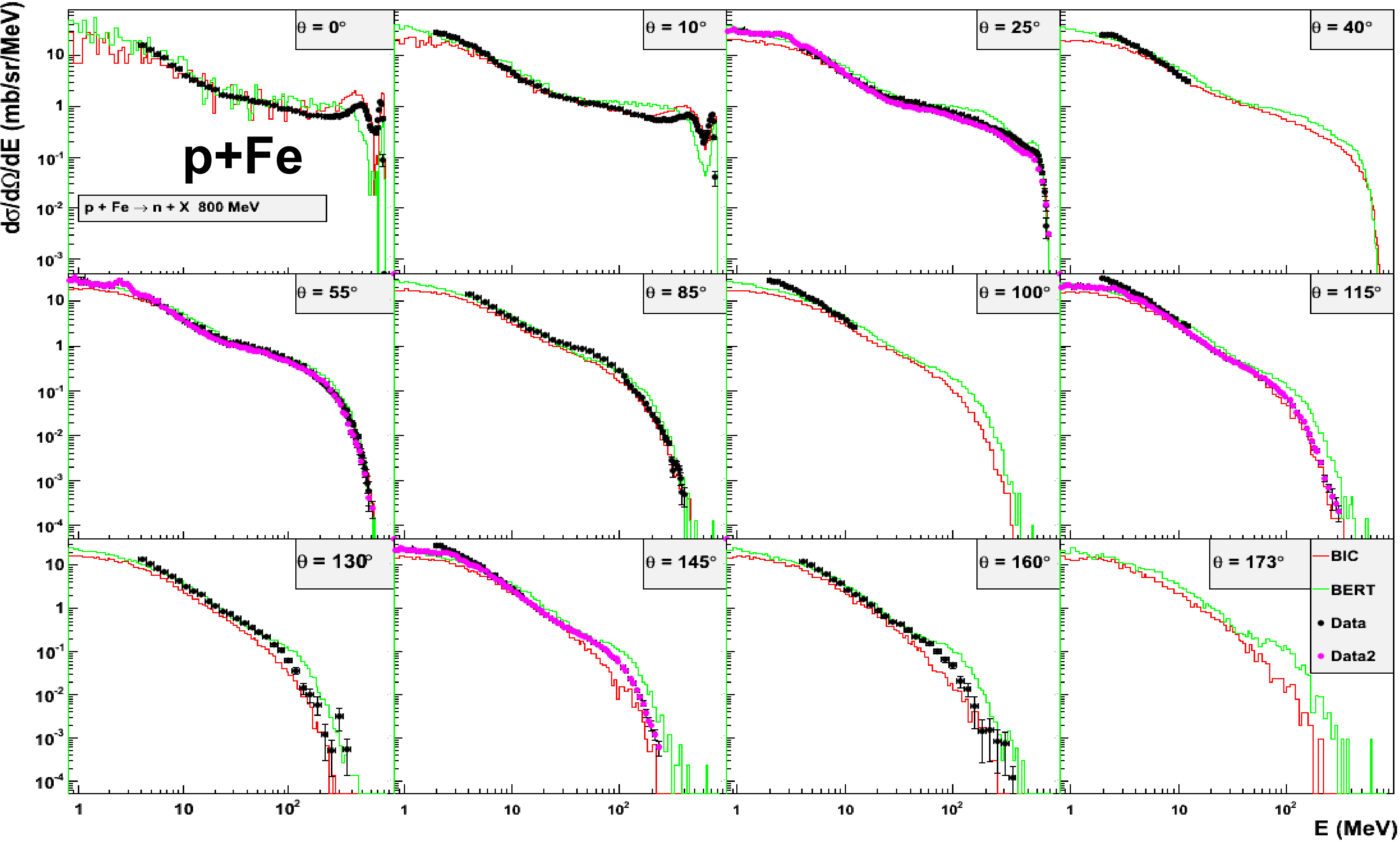
# RESULTS

(Geant4 release 9.3)

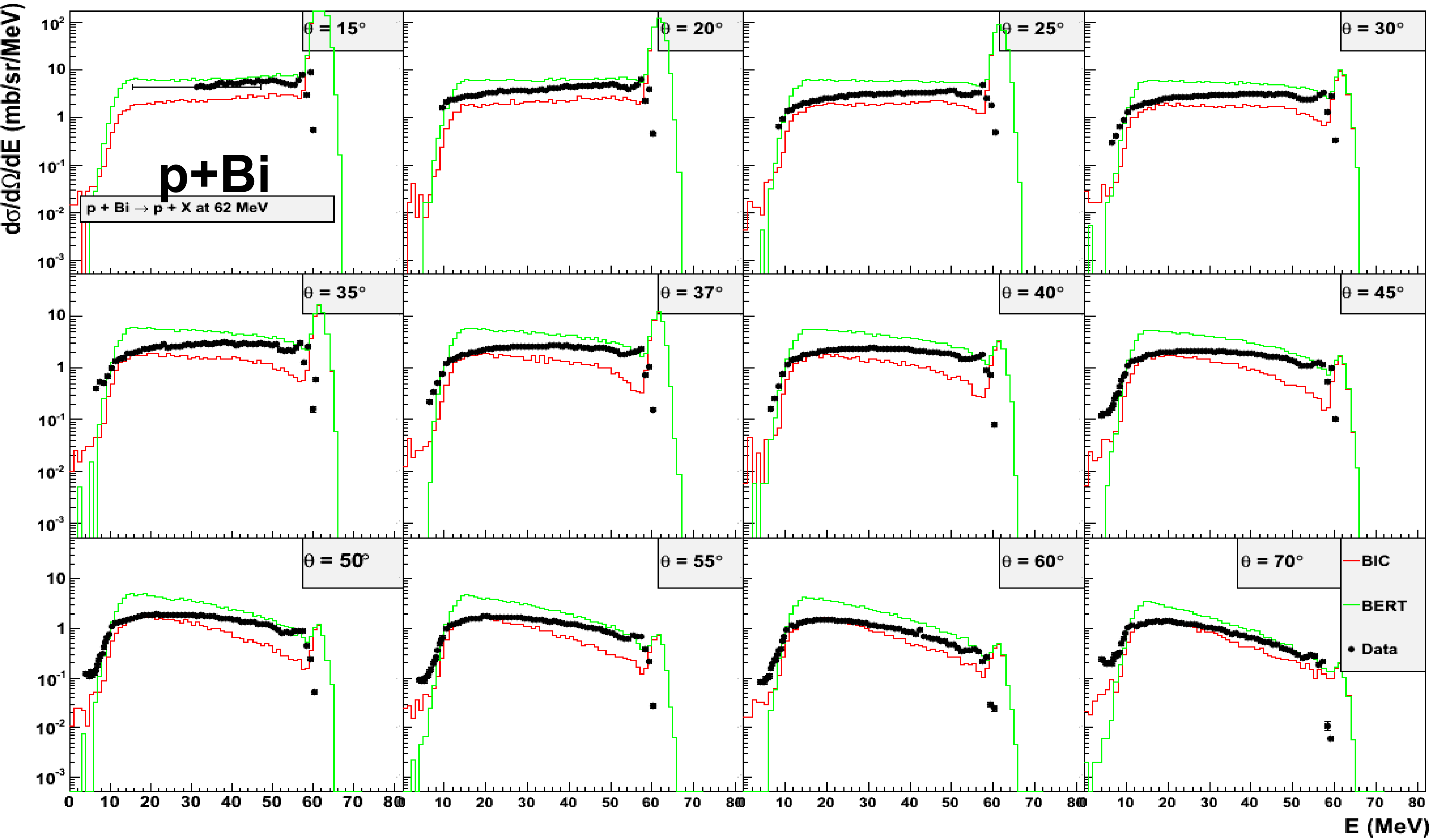
# Neutron production at 63 MeV



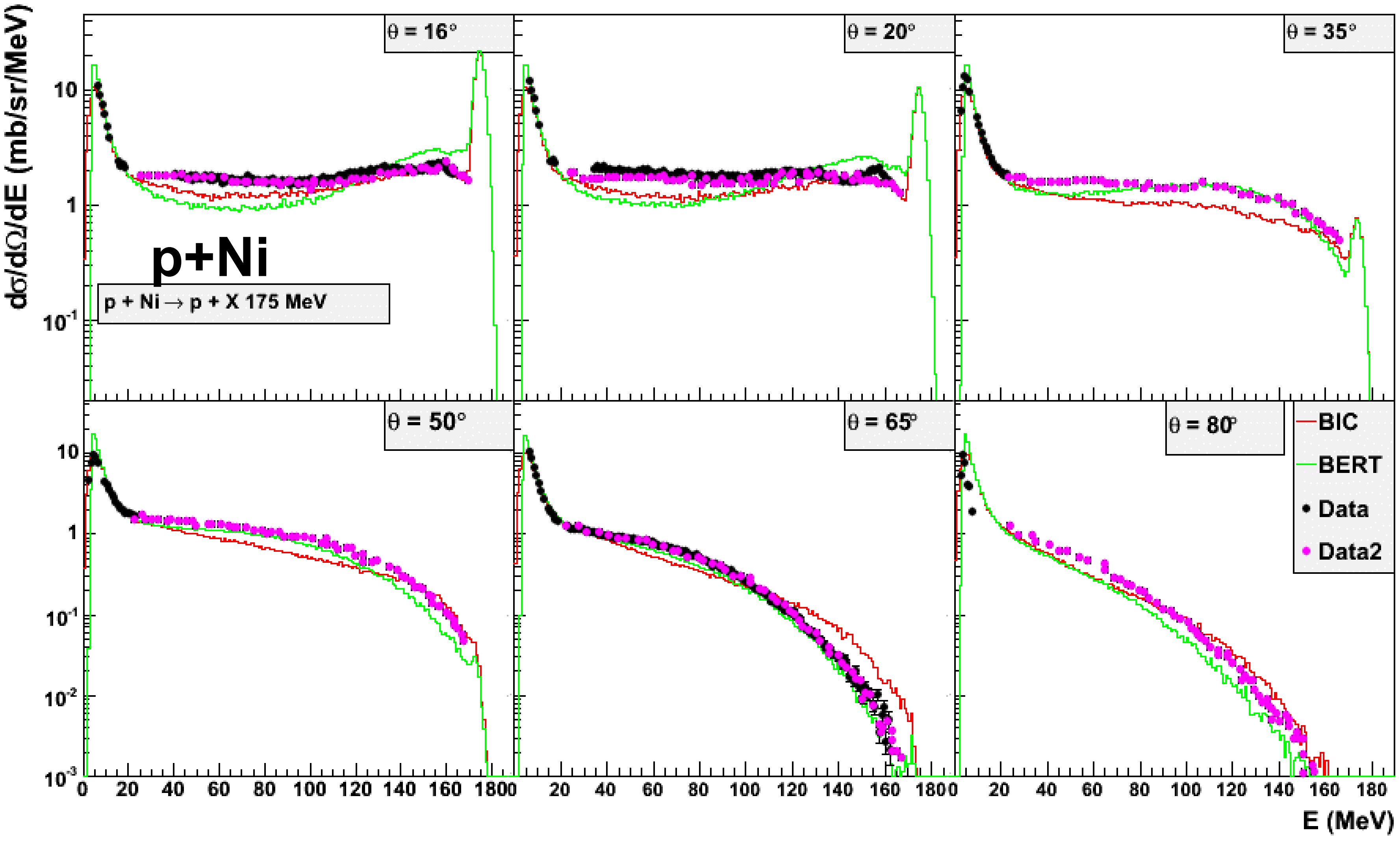
# Neutron production at 1200 MeV



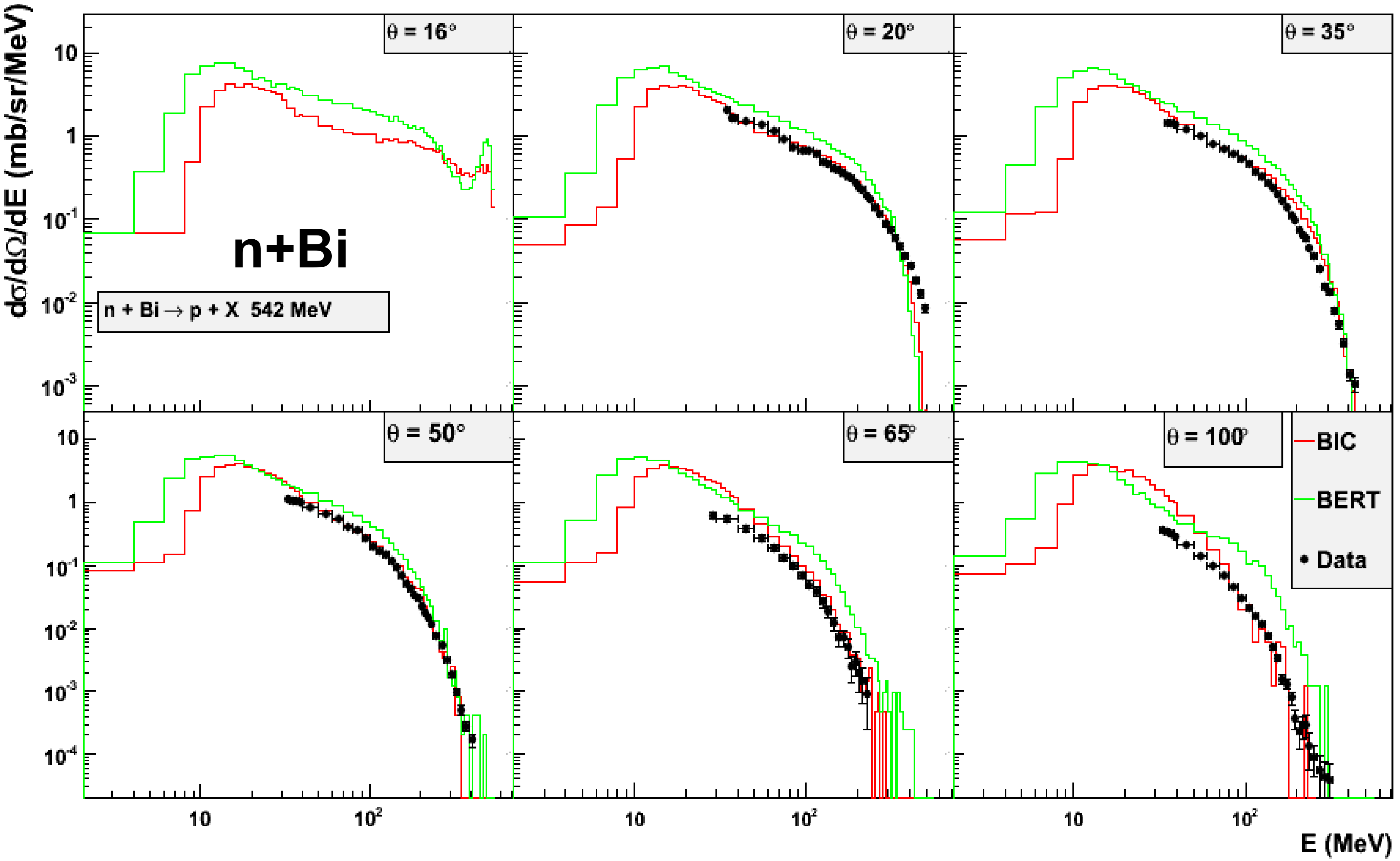
# Proton production at 62 MeV



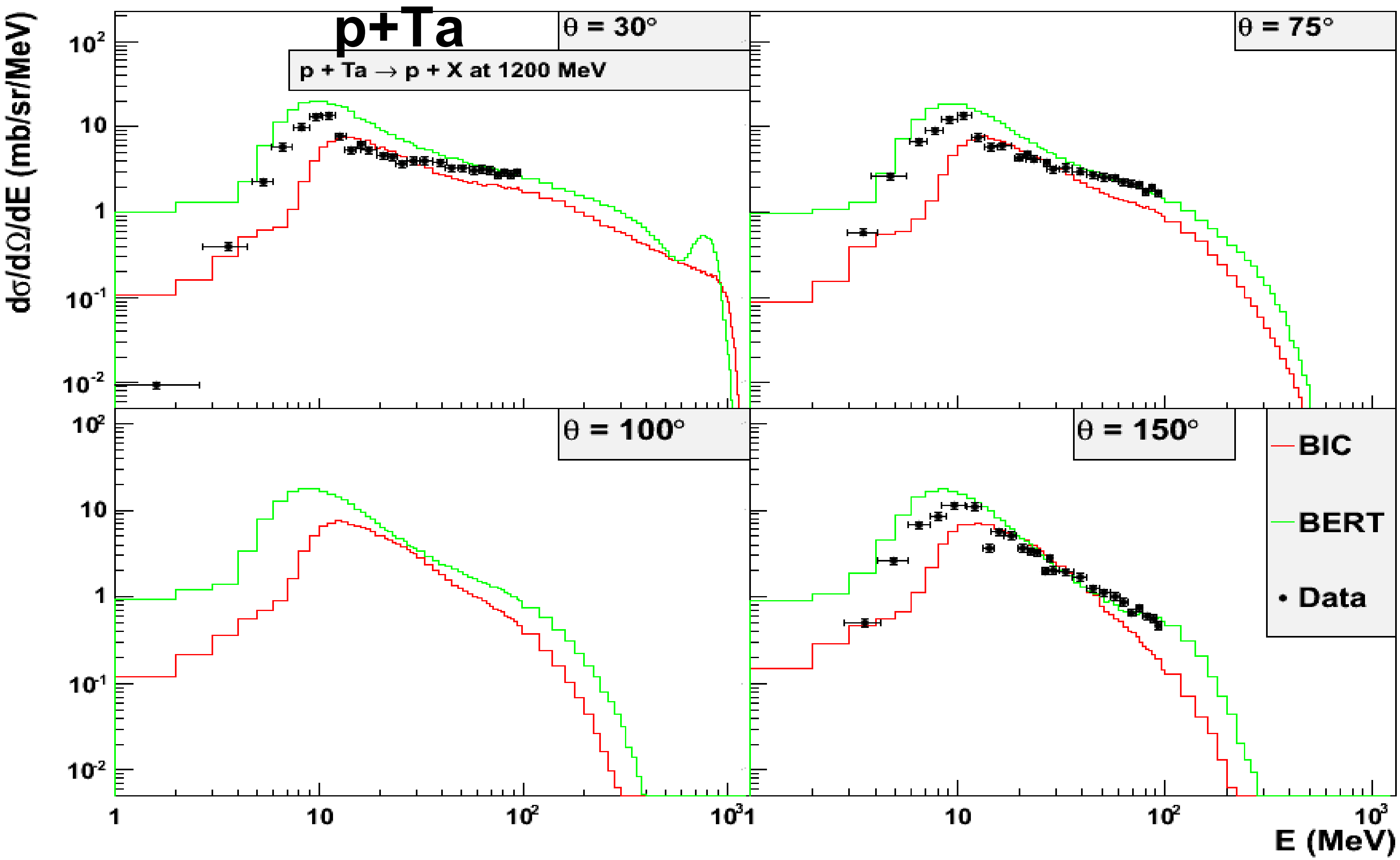
# Proton production at 175 MeV



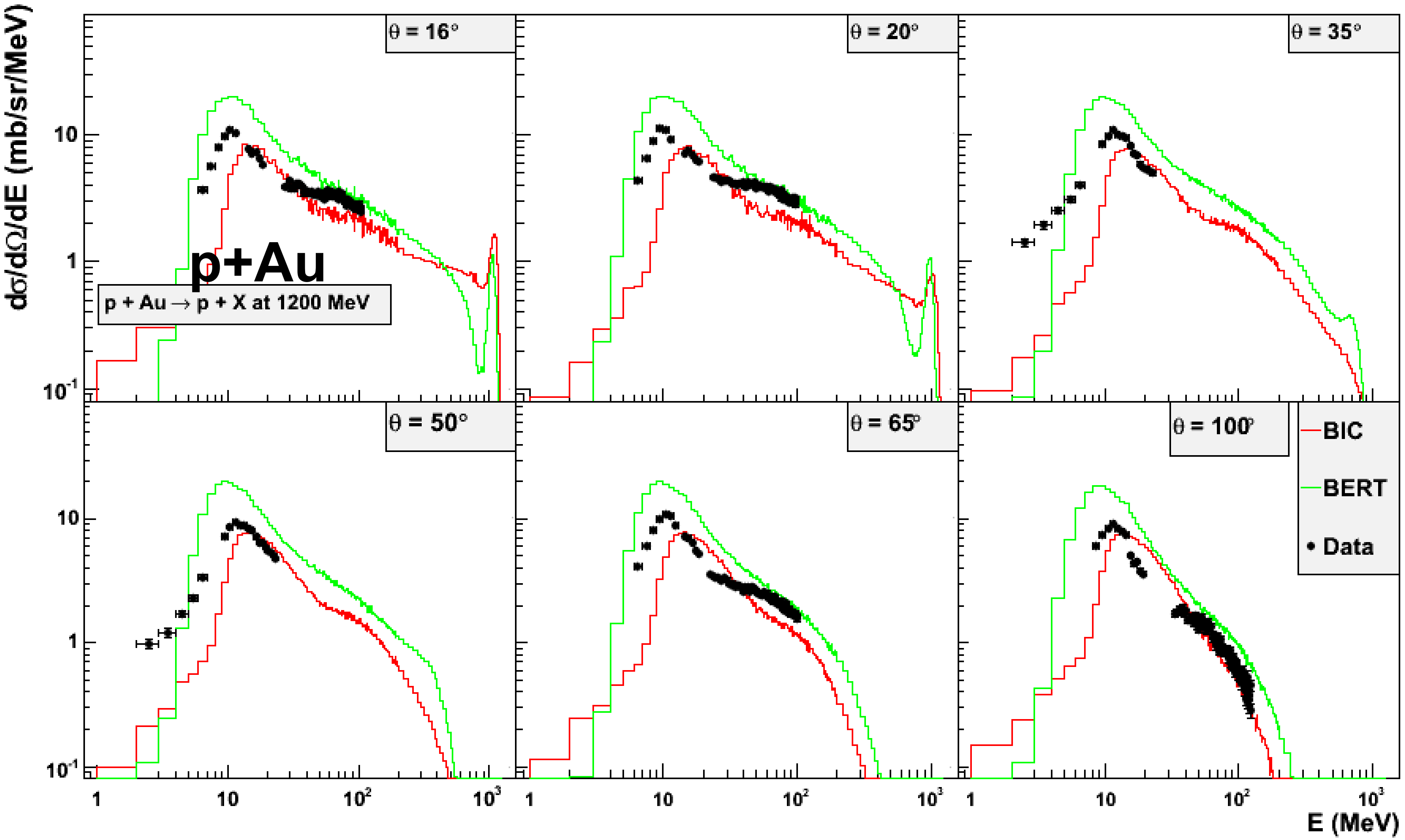
# Proton production at 542 MeV



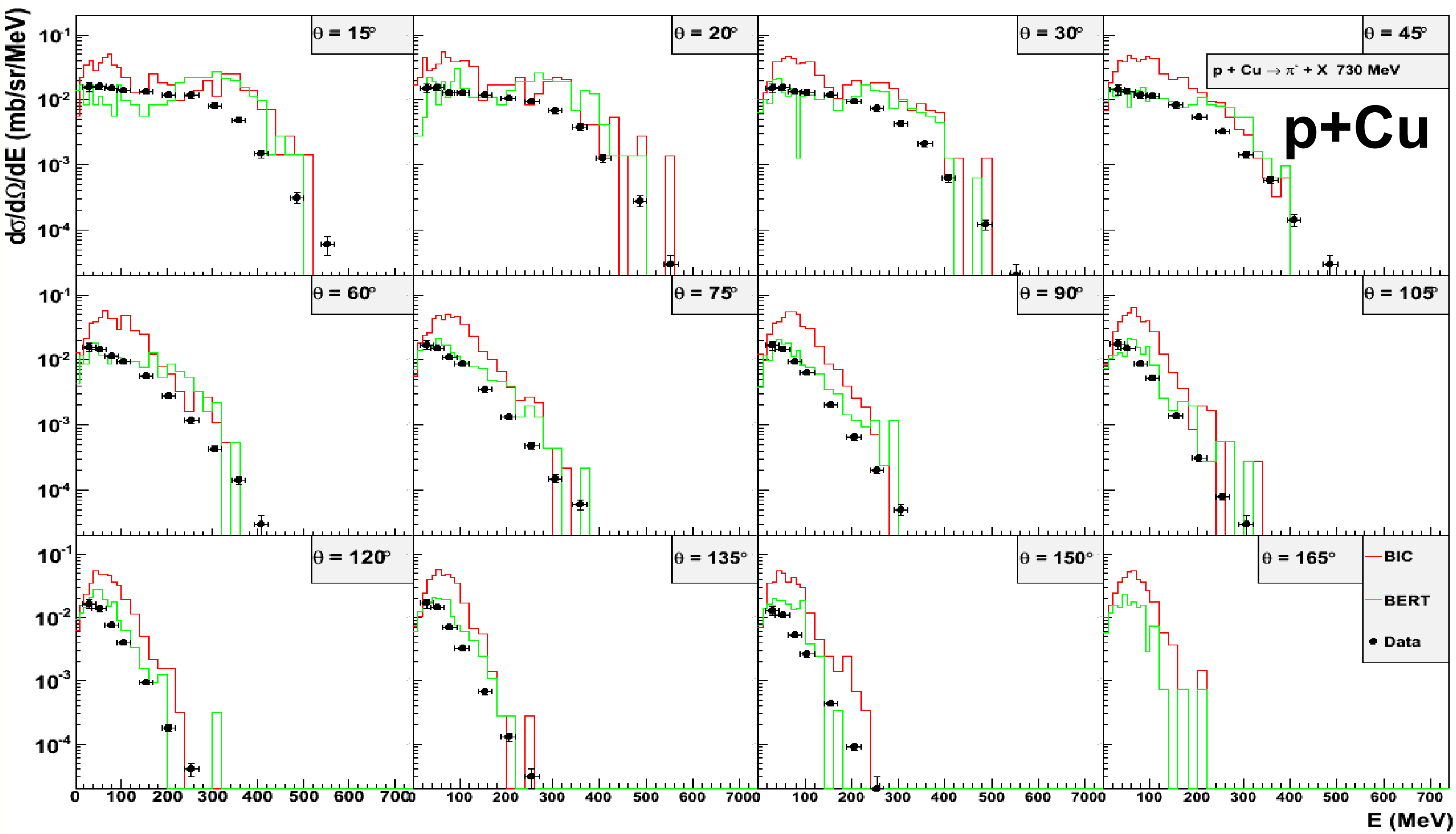
# Proton production at 1200 MeV



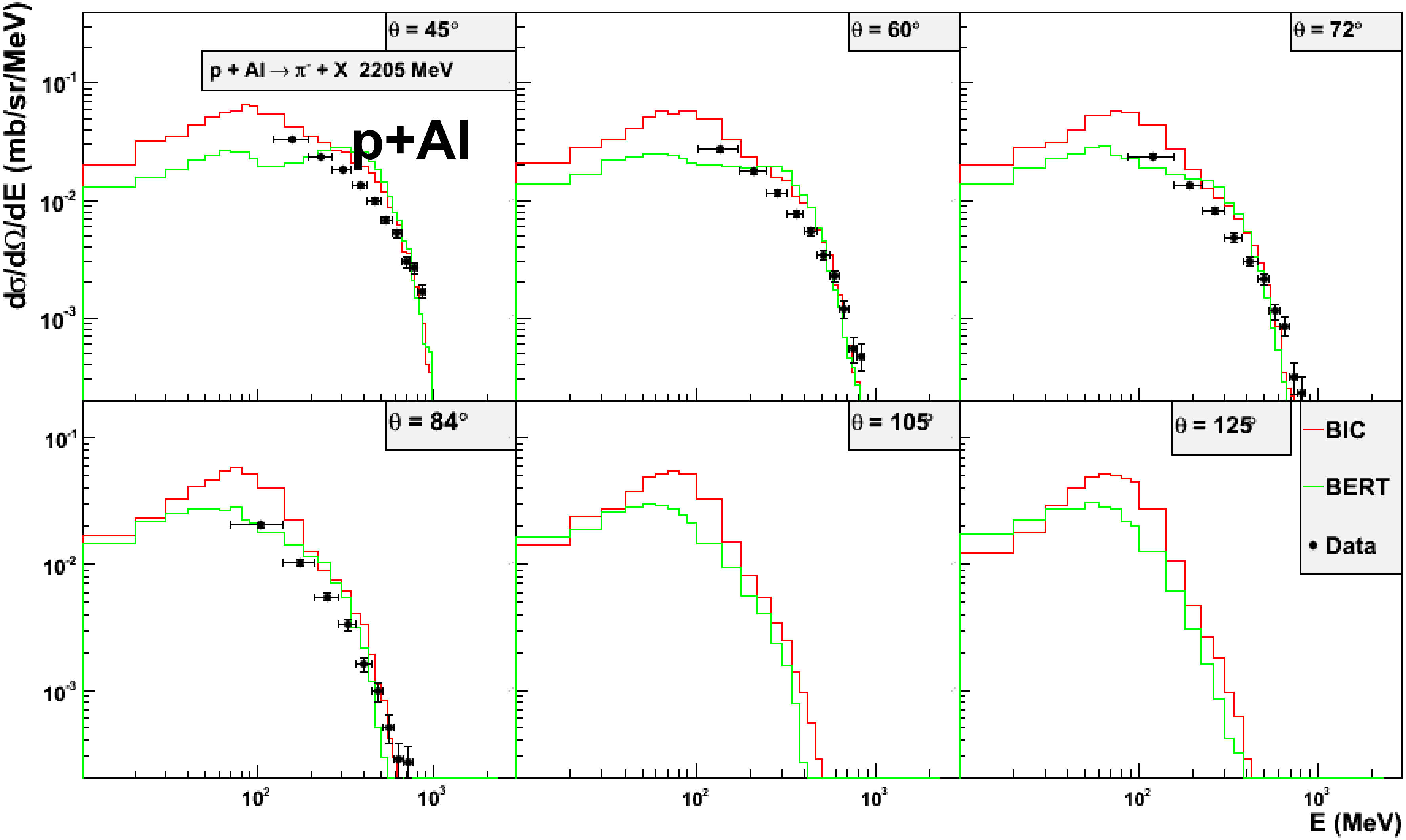
# Proton production at 1200 MeV



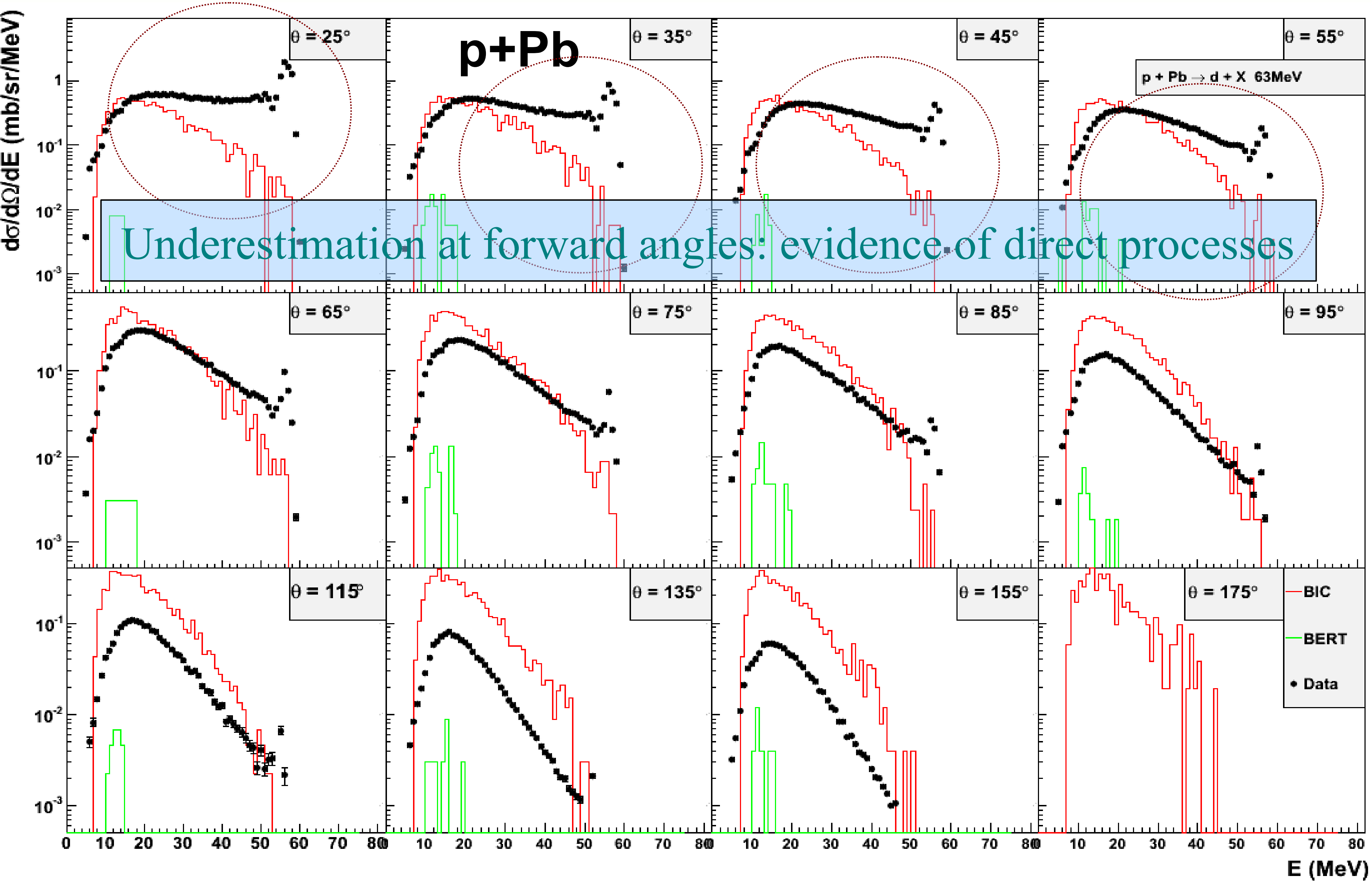
# Pion production at 730 MeV



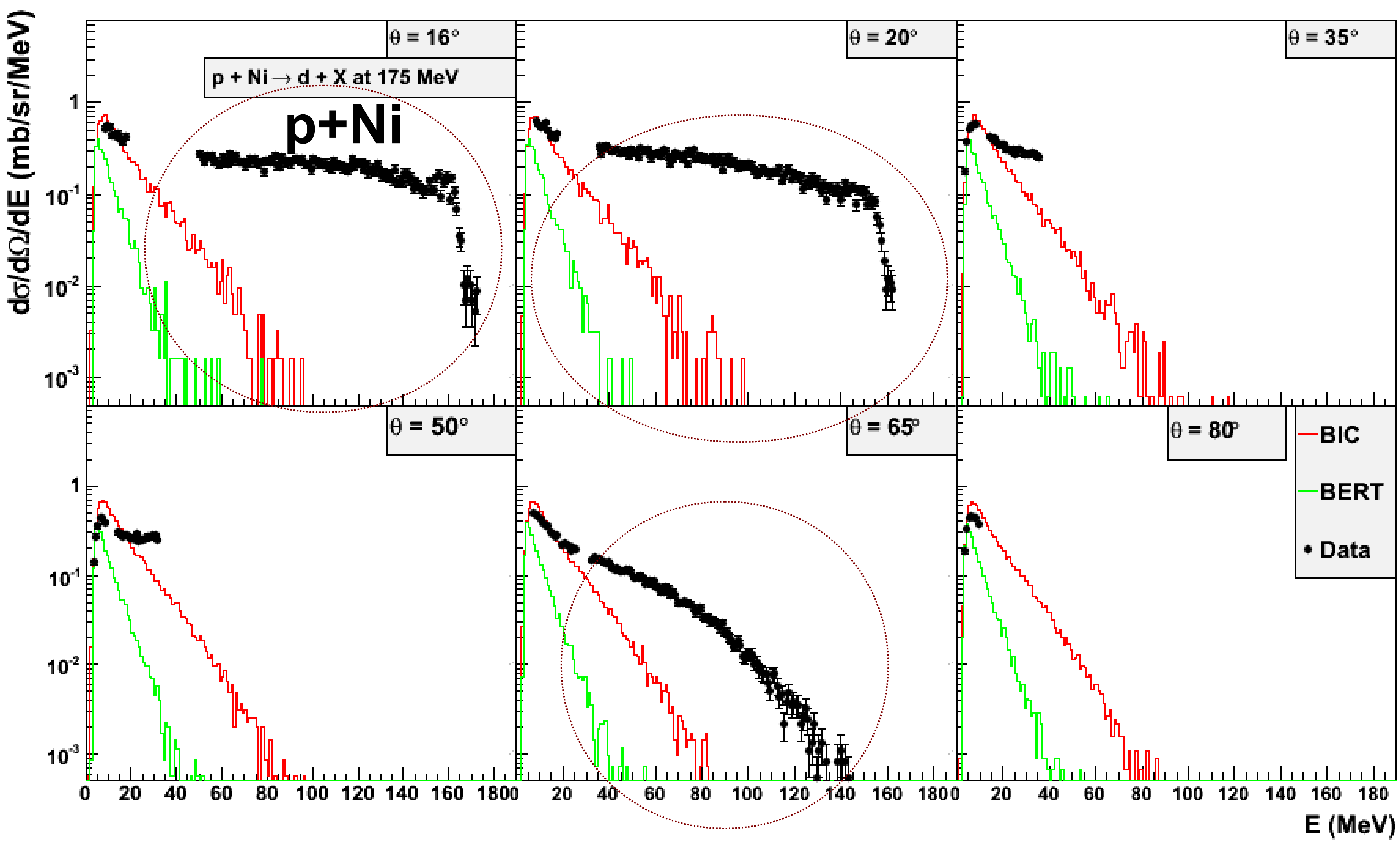
# Pion production at 2205 MeV



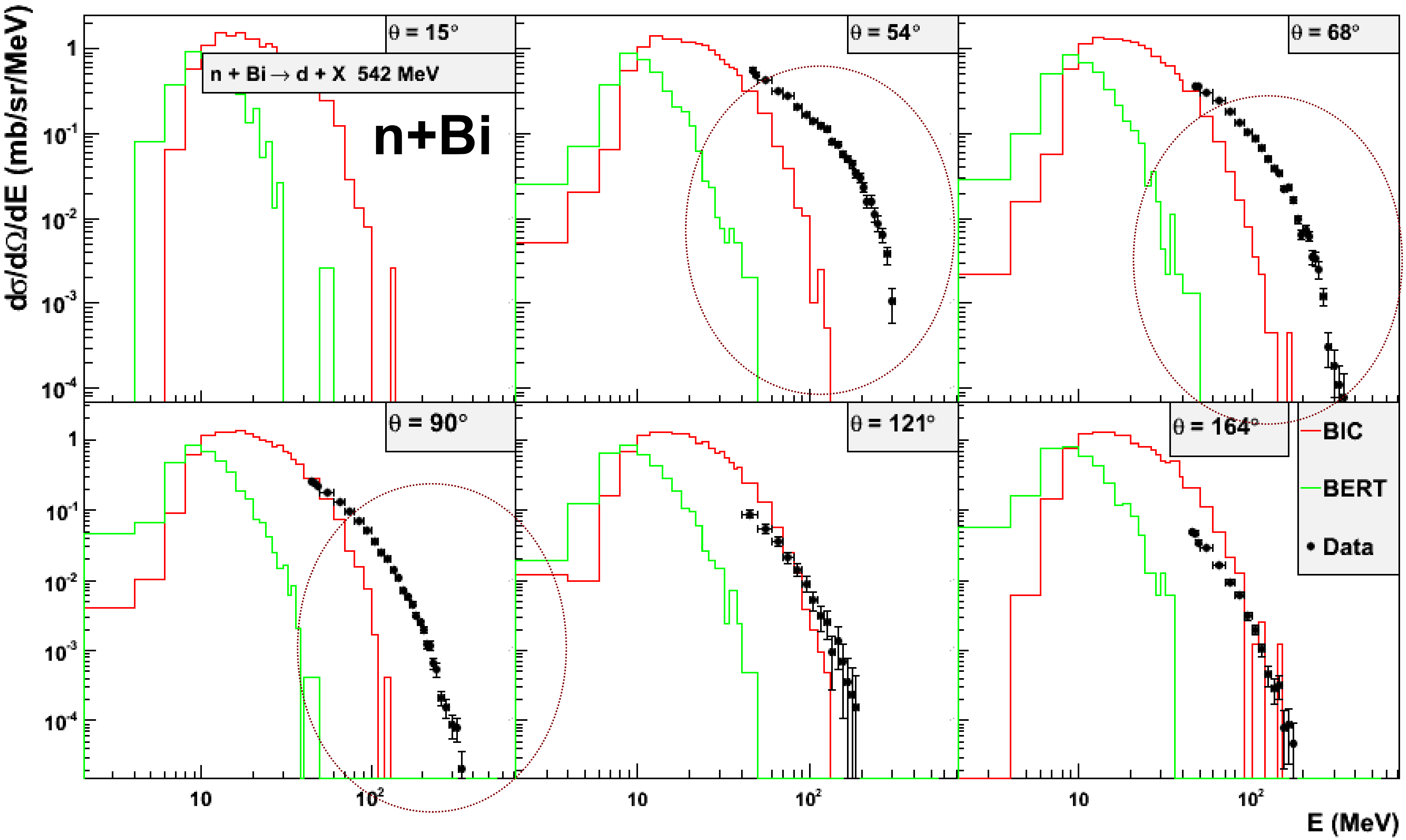
# Deuteron production at 63 MeV



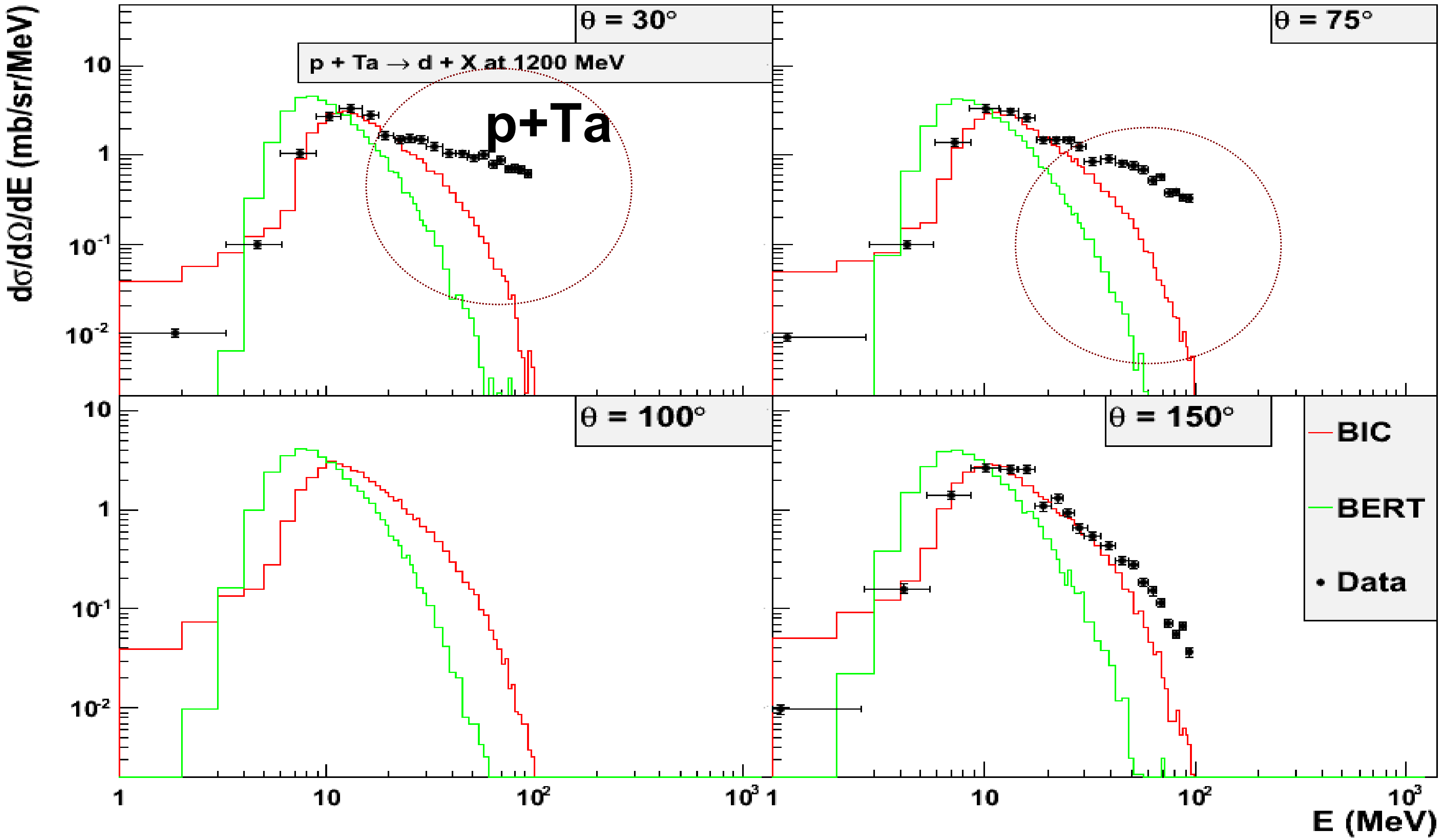
# Deuteron production at 175 MeV



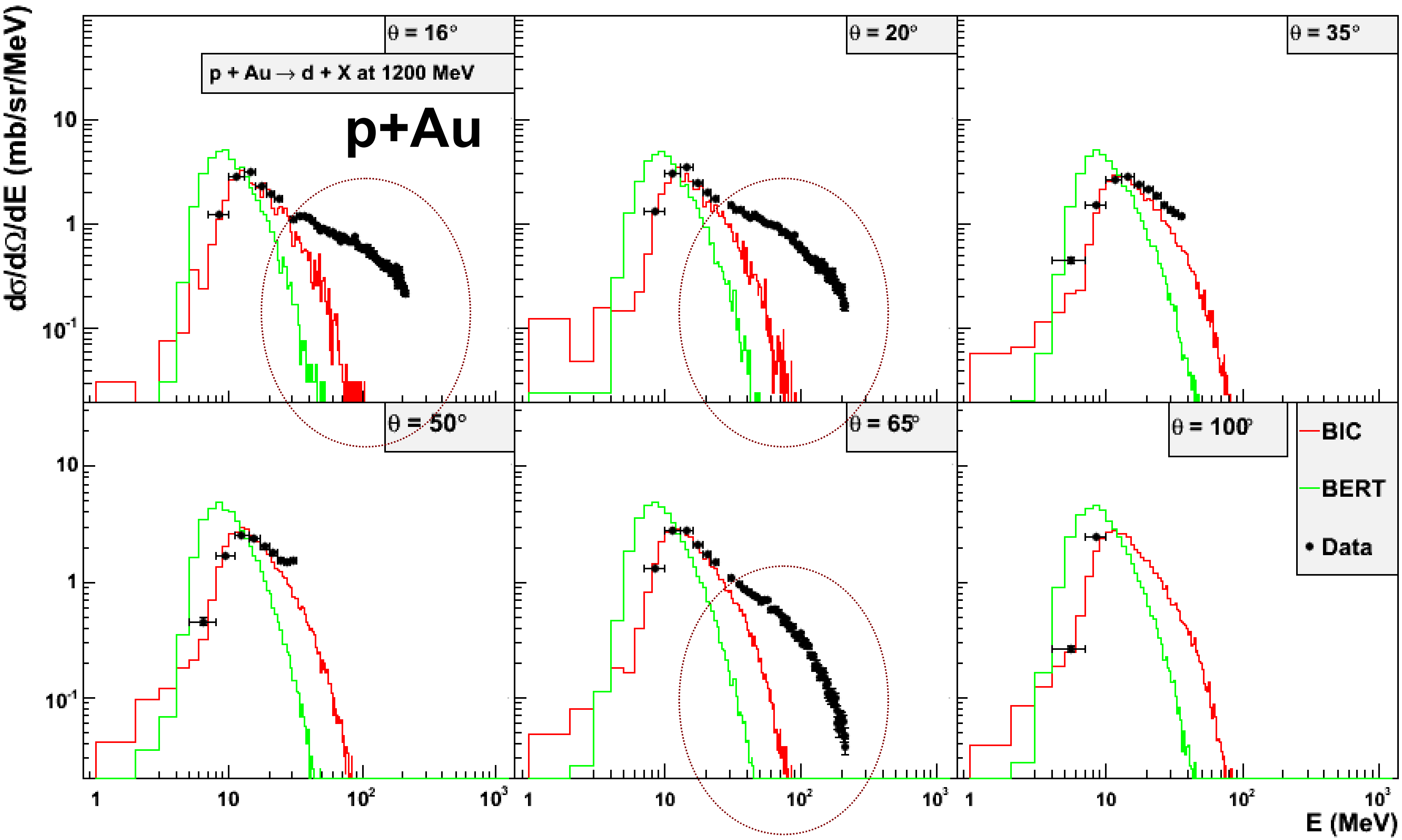
# Deuteron production at 542 MeV



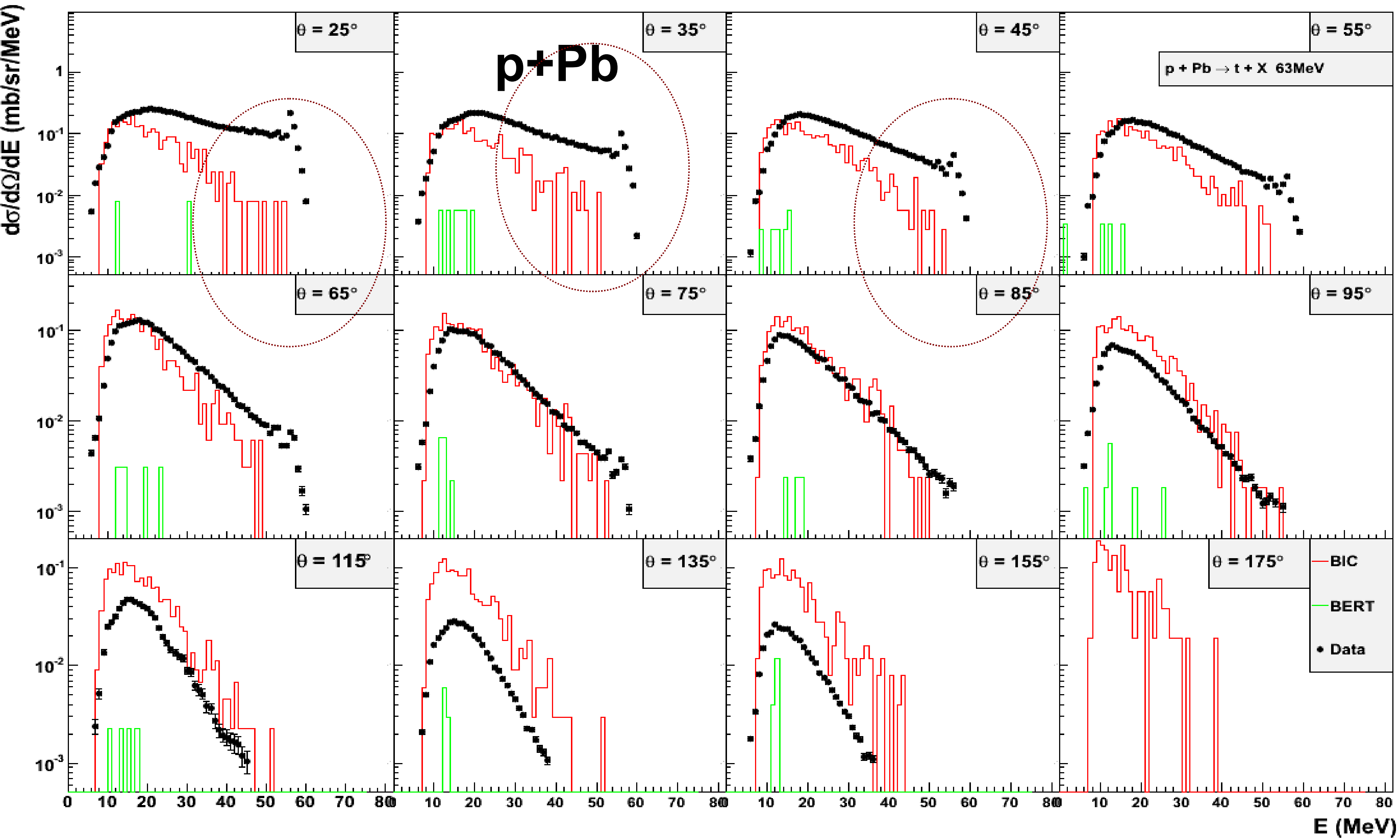
# Deuteron production at 1200 MeV



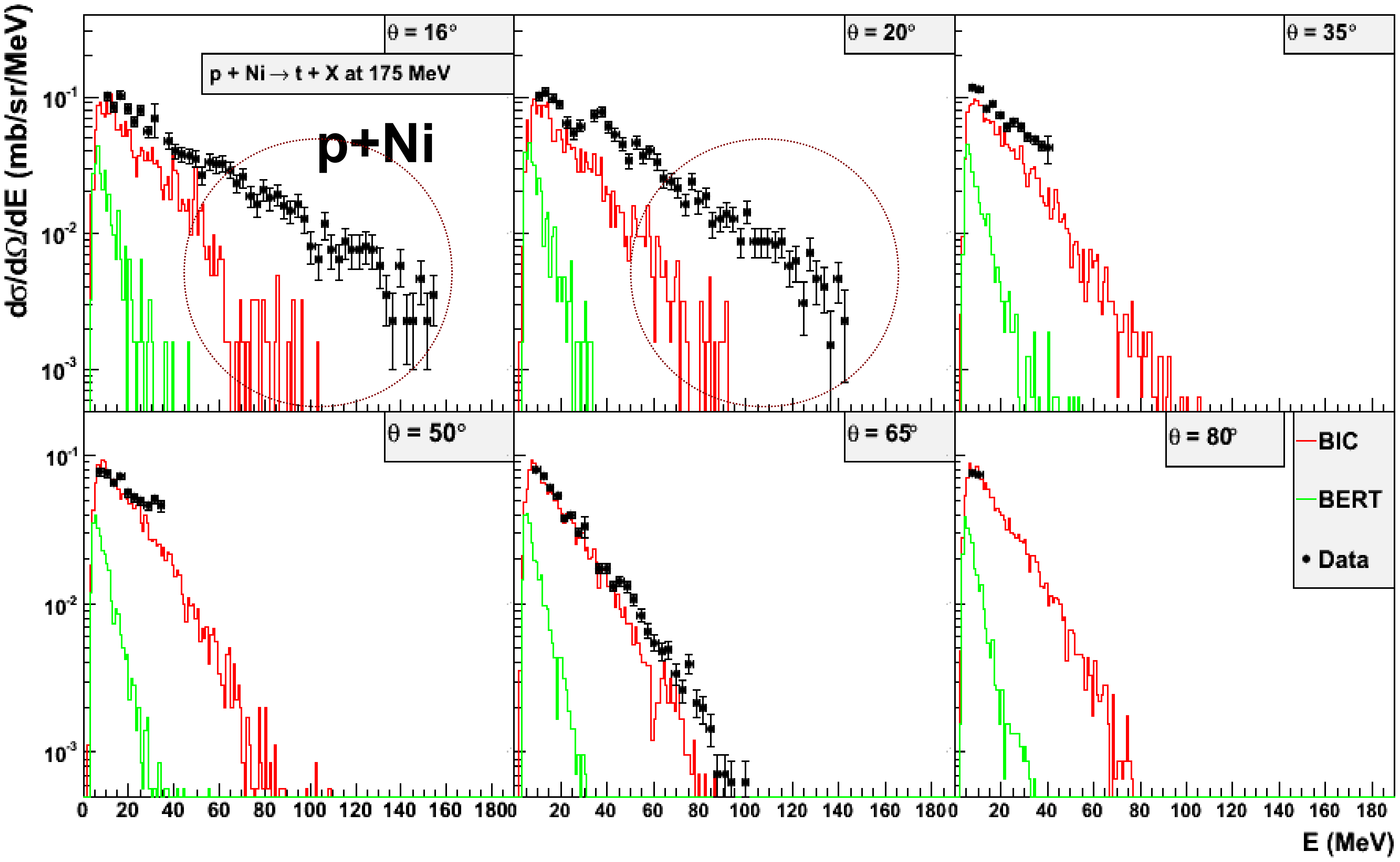
# Deuteron production at 1200 MeV



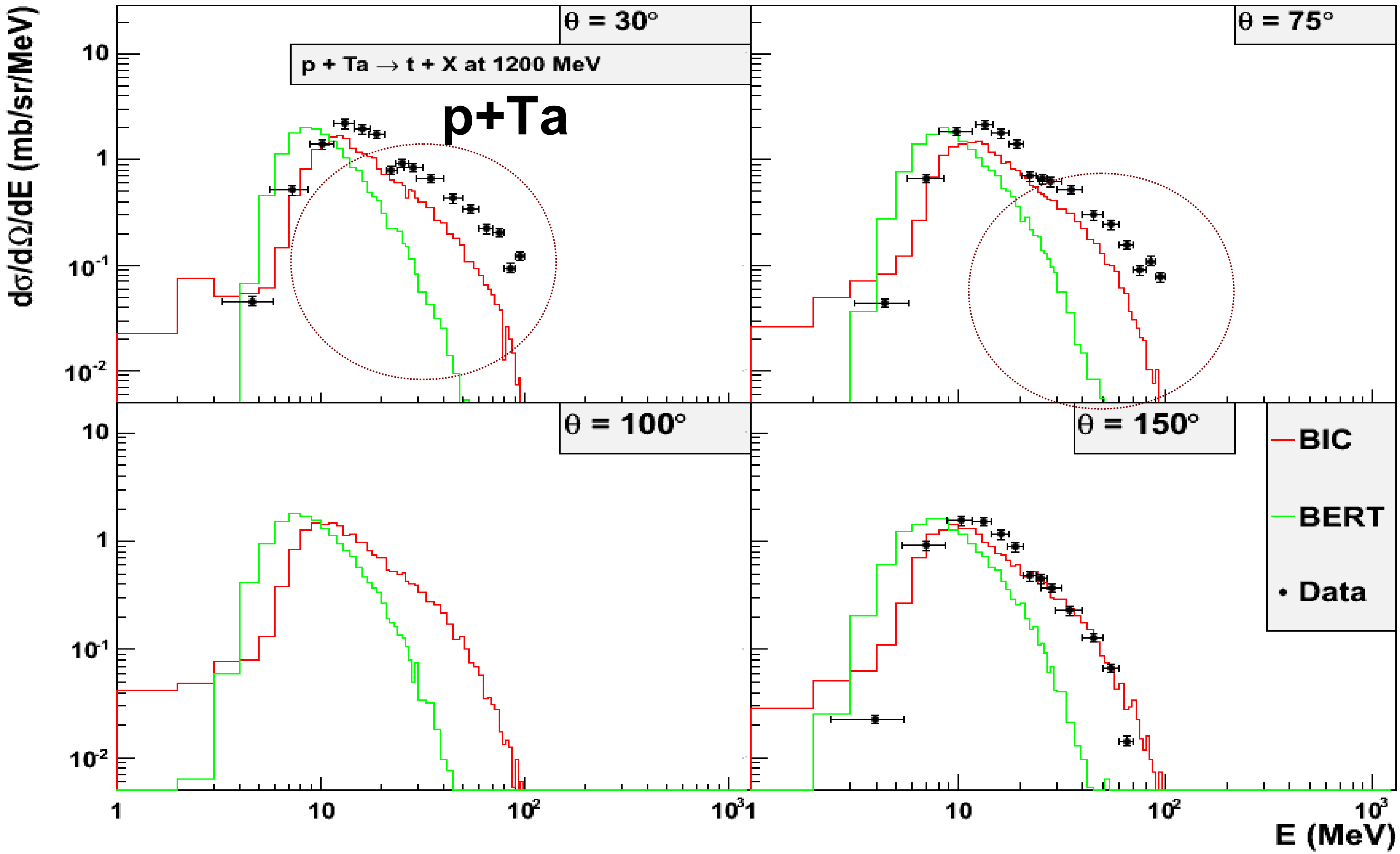
# Tritium production at 63 MeV



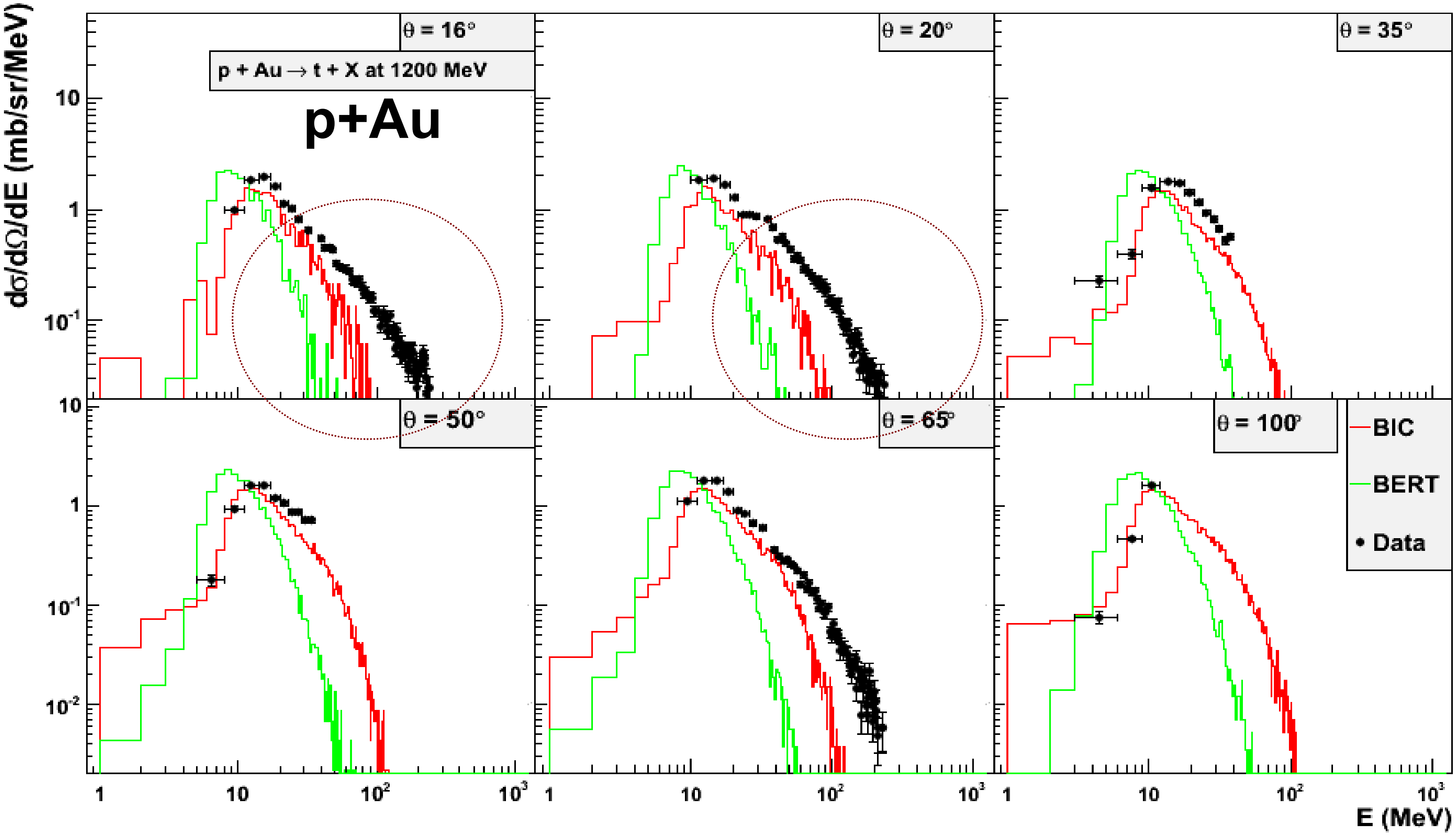
# Tritium production at 175 MeV



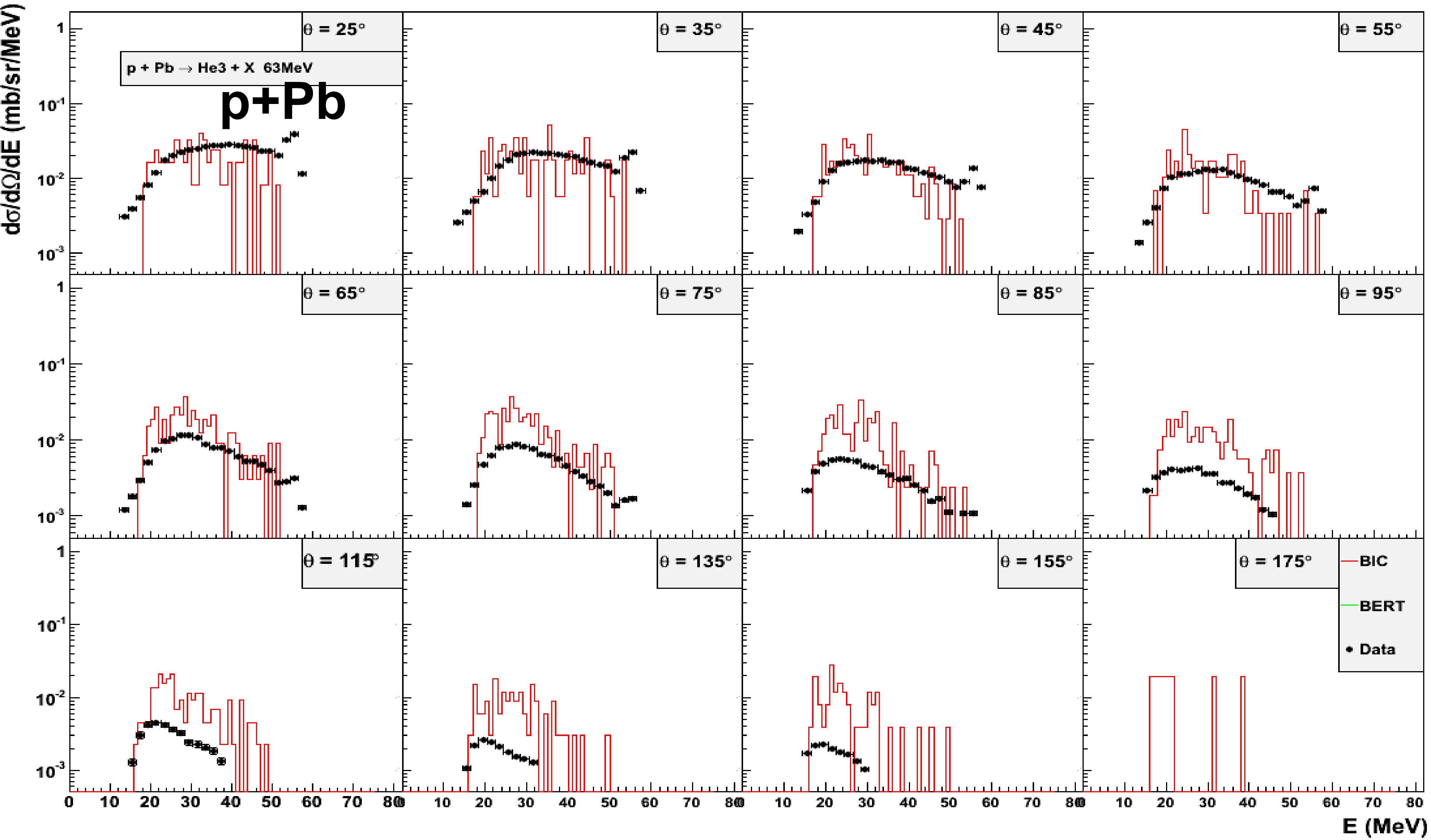
# Tritum production at 1200 MeV



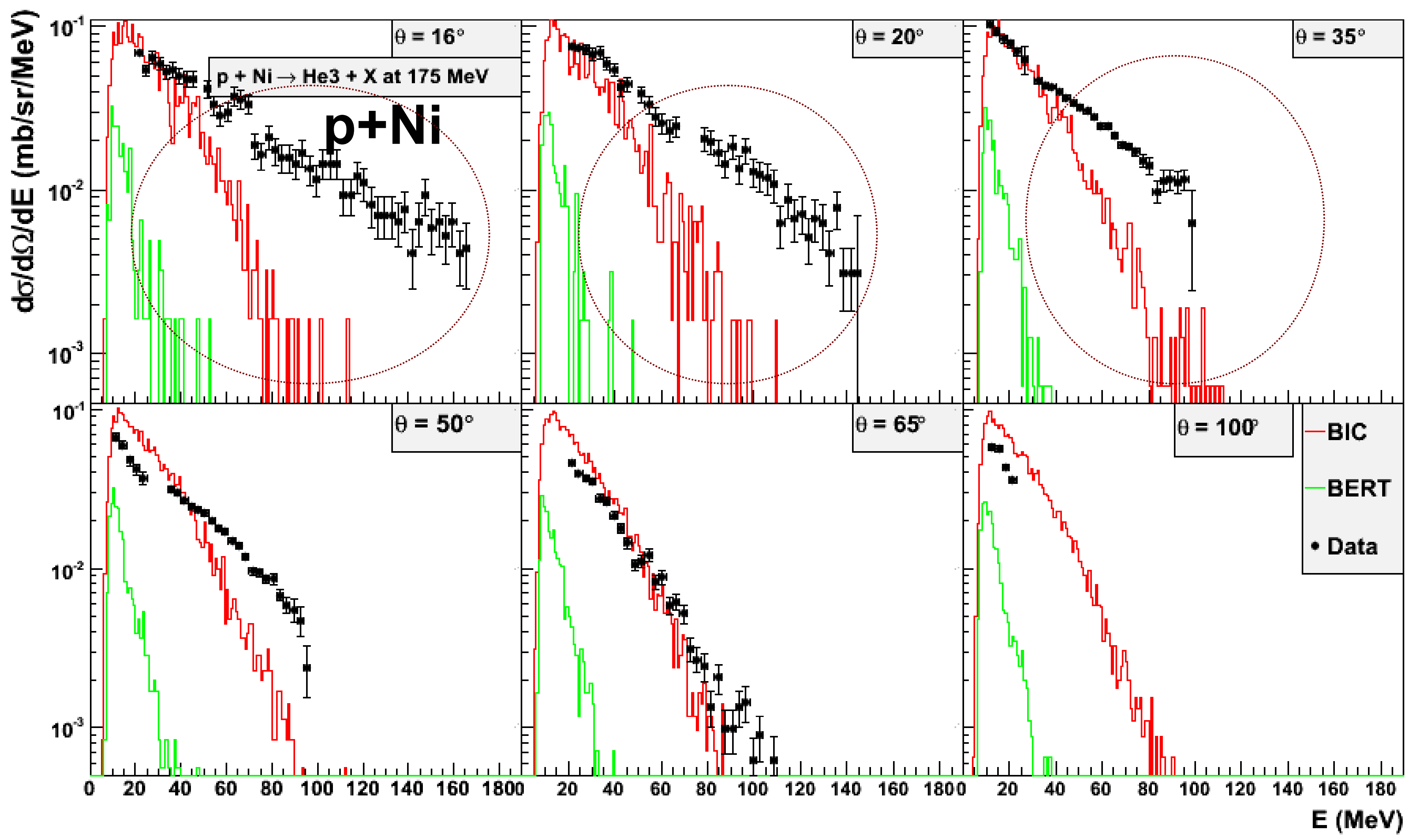
# Tritium production at 1200 MeV



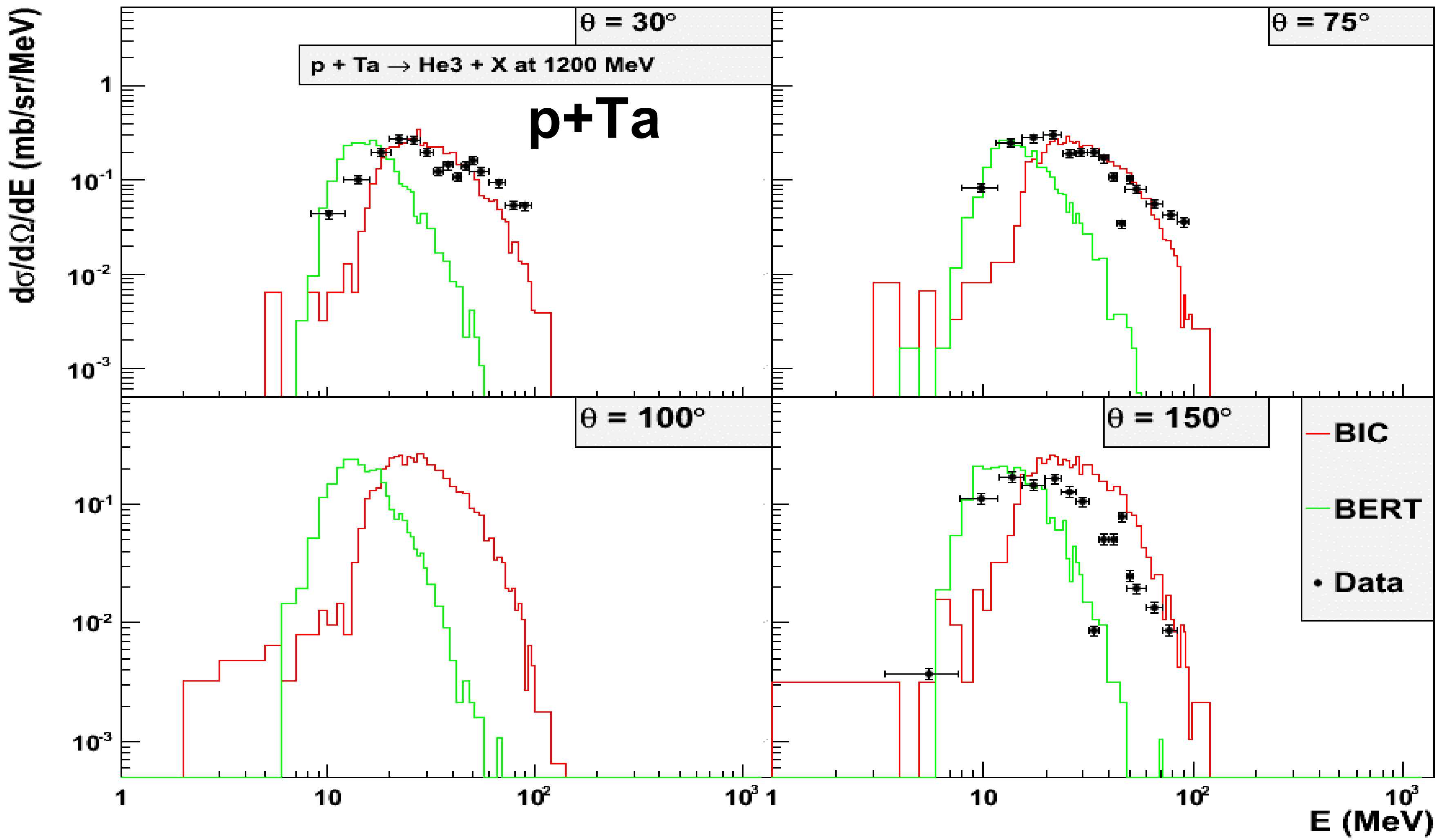
# $^3He$ production at 63 MeV



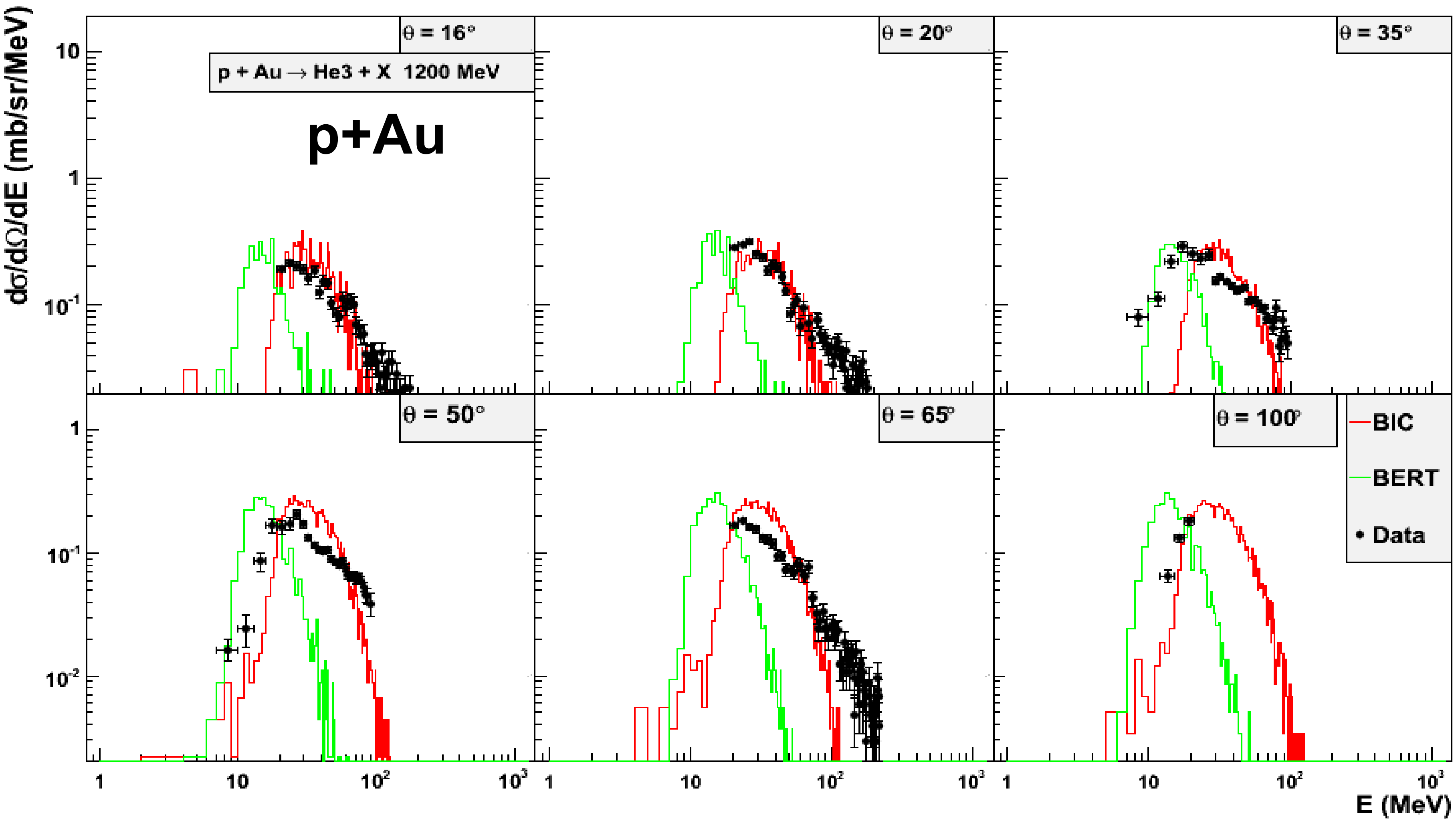
# $^{3}$He production at 175 MeV



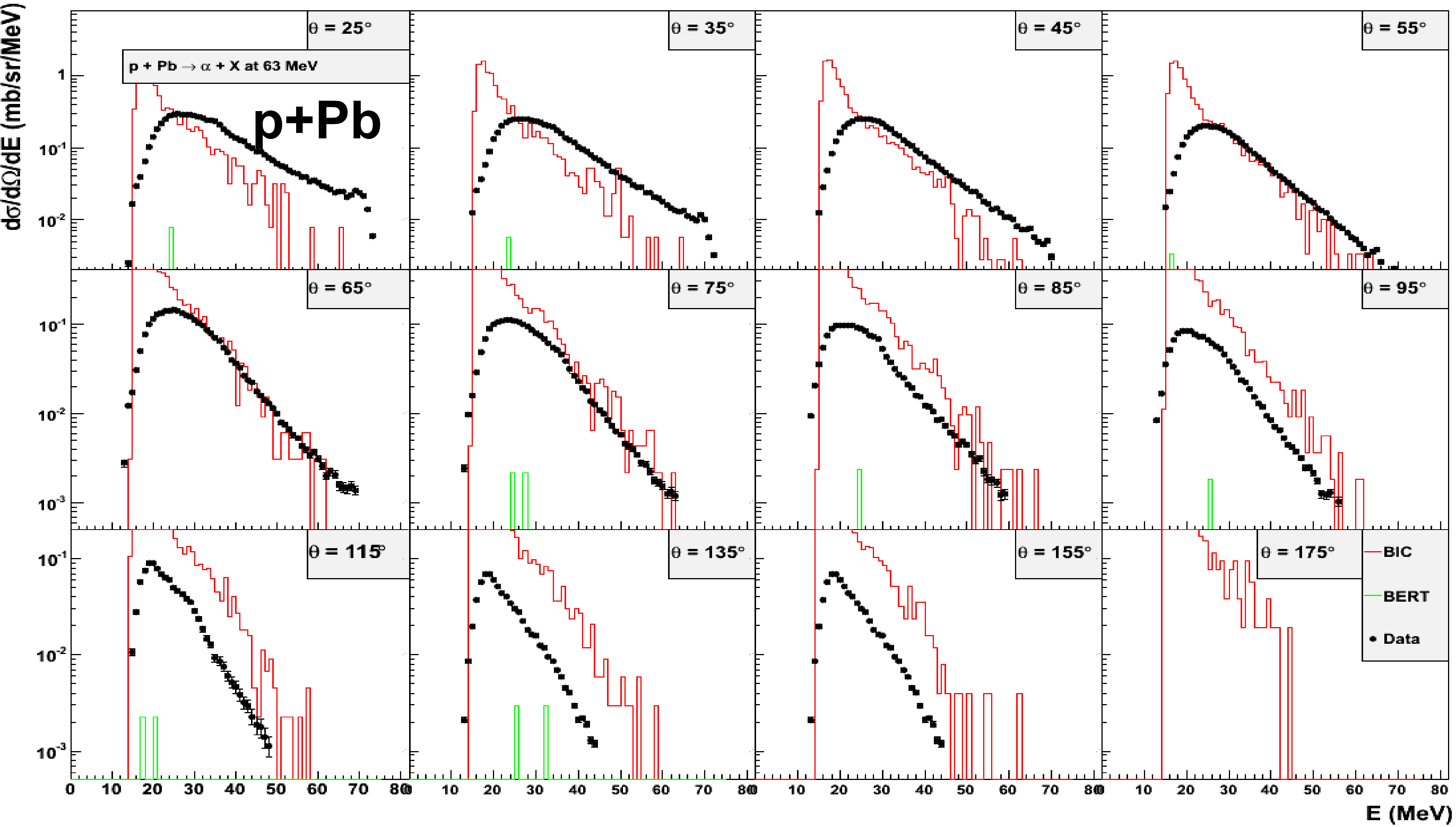
# $^{3}$He production at 1200 MeV



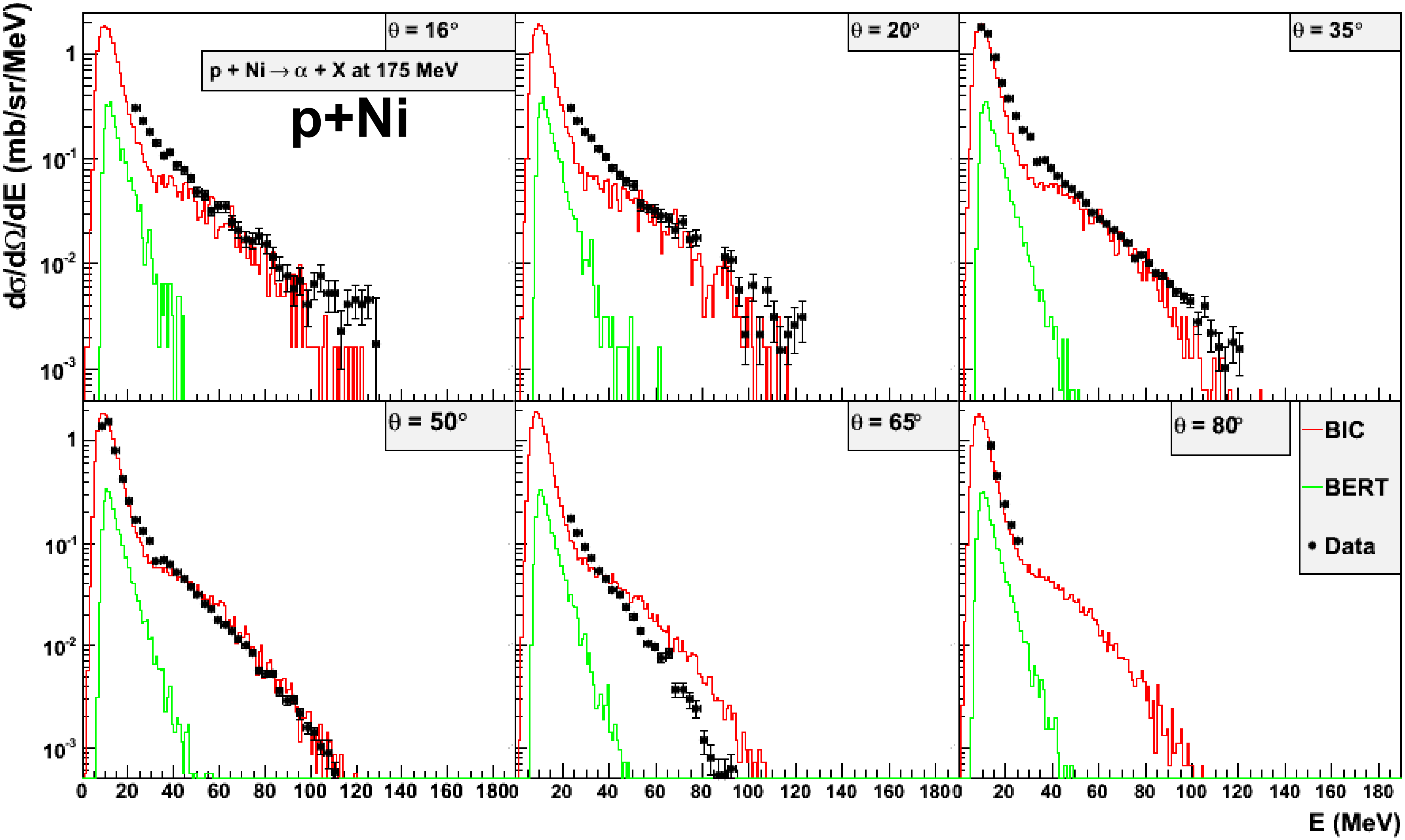
# $^{3}He$ production at 1200 MeV



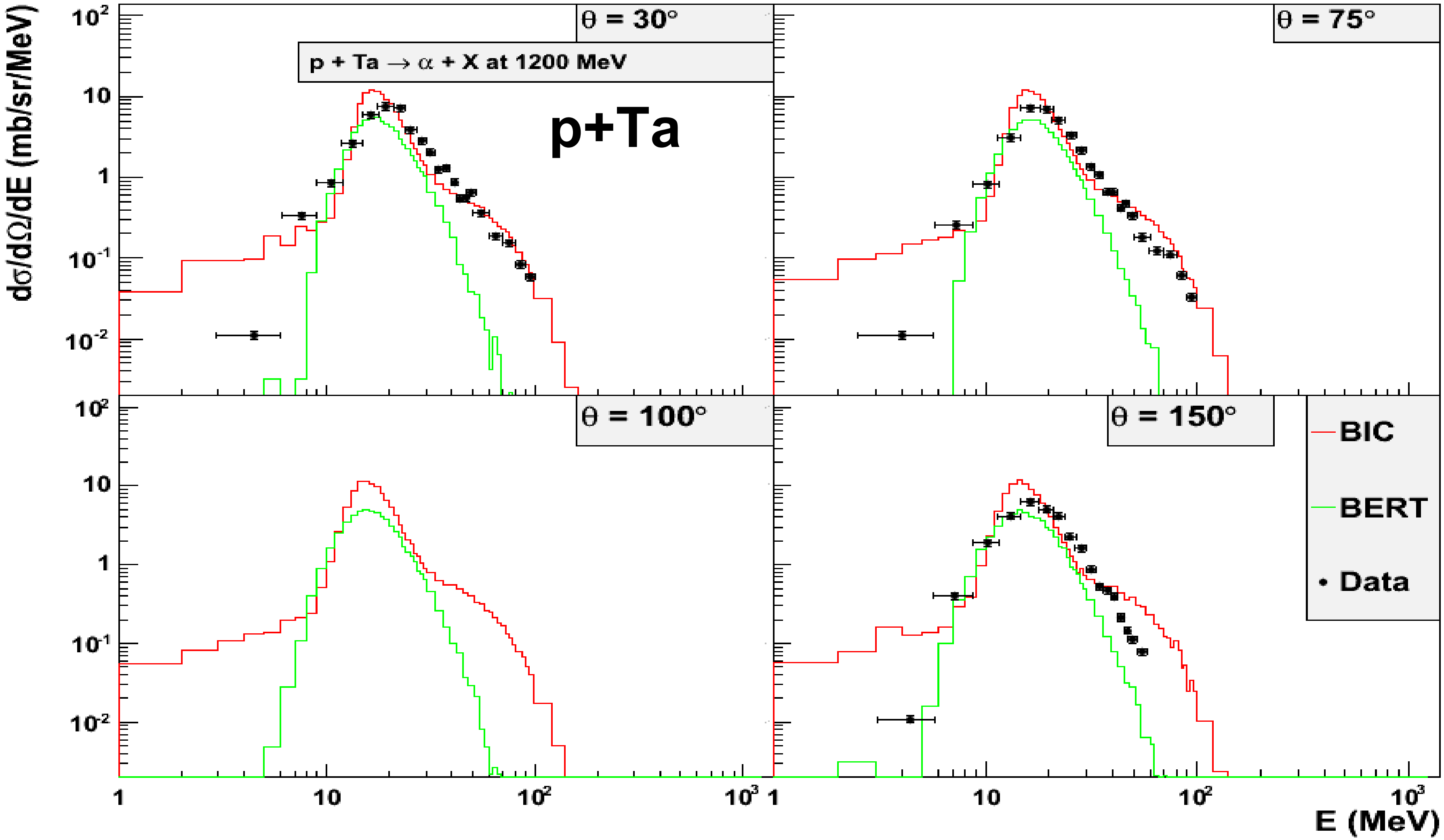
# Alpha production at 63 MeV



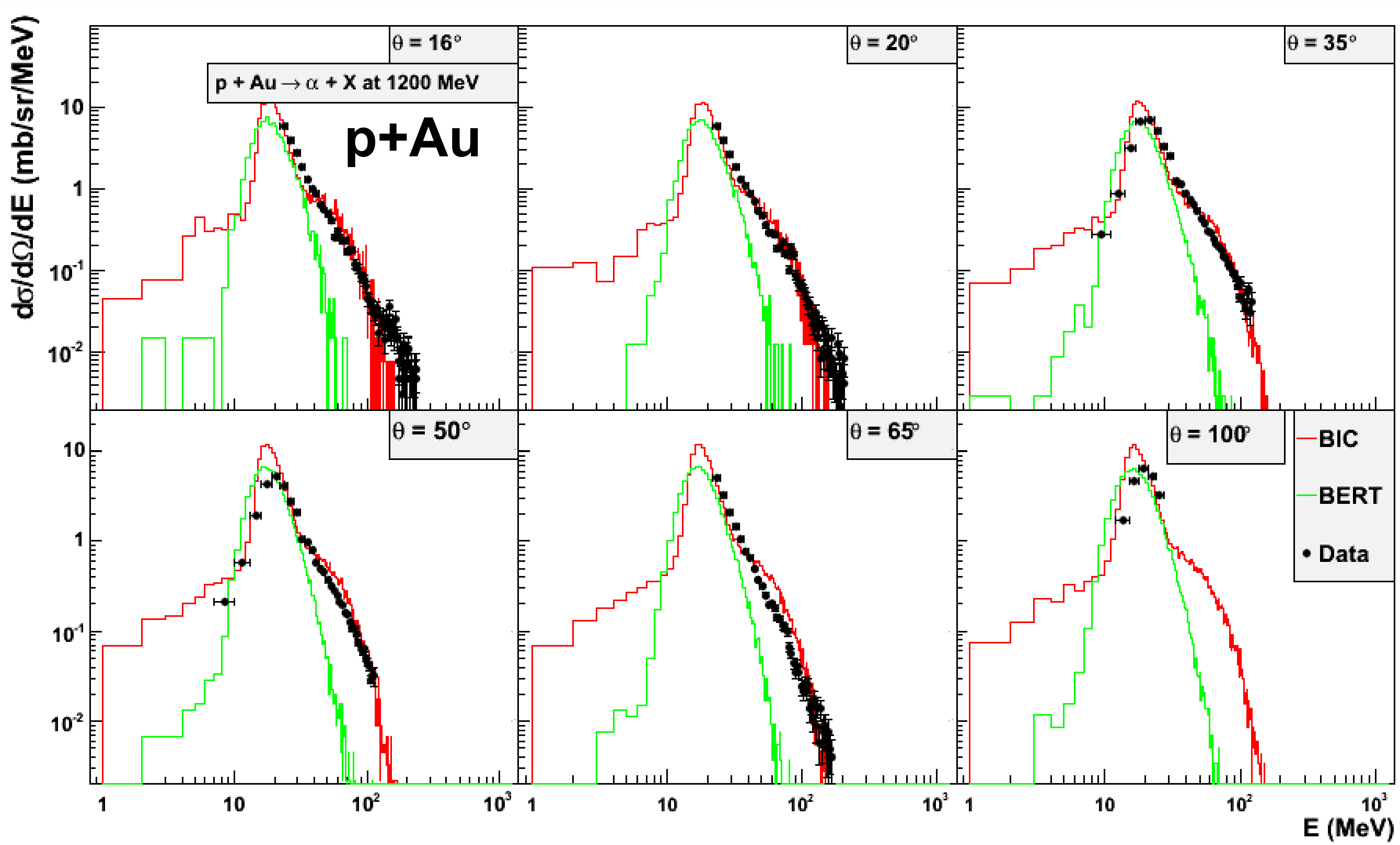
# Alpha production at 175 MeV



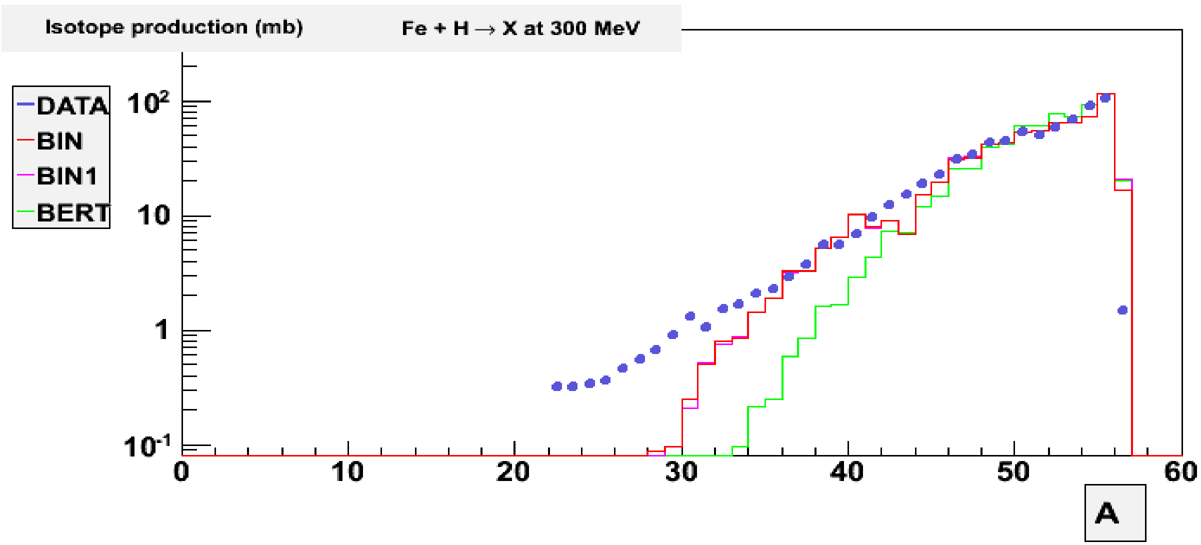
# Alpha production at 1200 MeV



# Alpha production at 1200 MeV

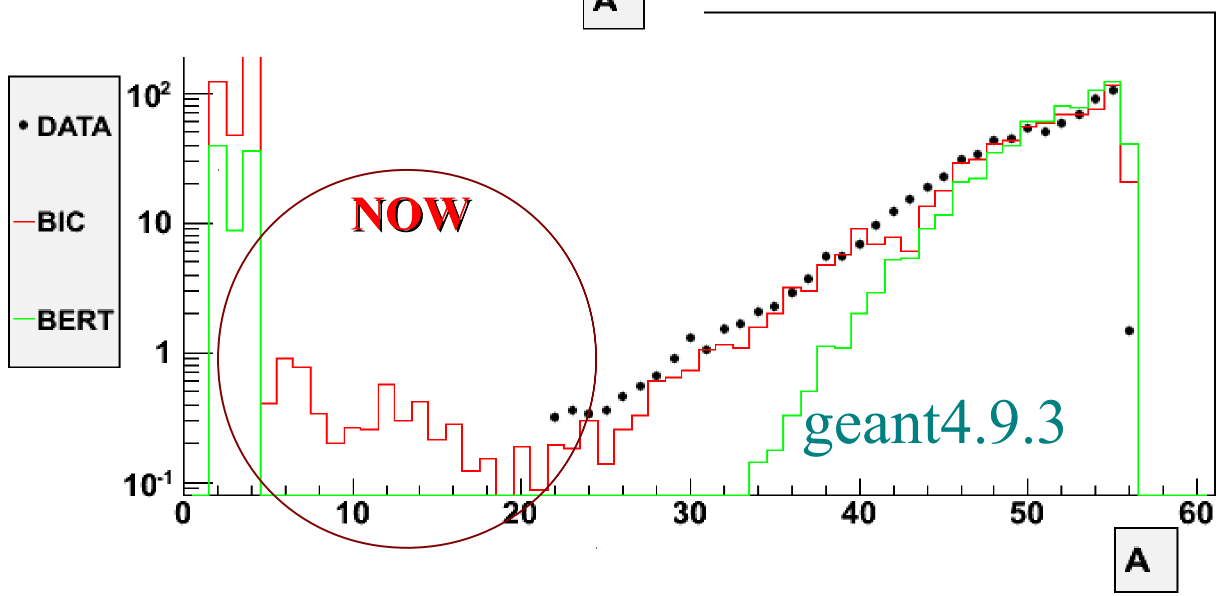


# Isotopic distribution at 0.3 GeV

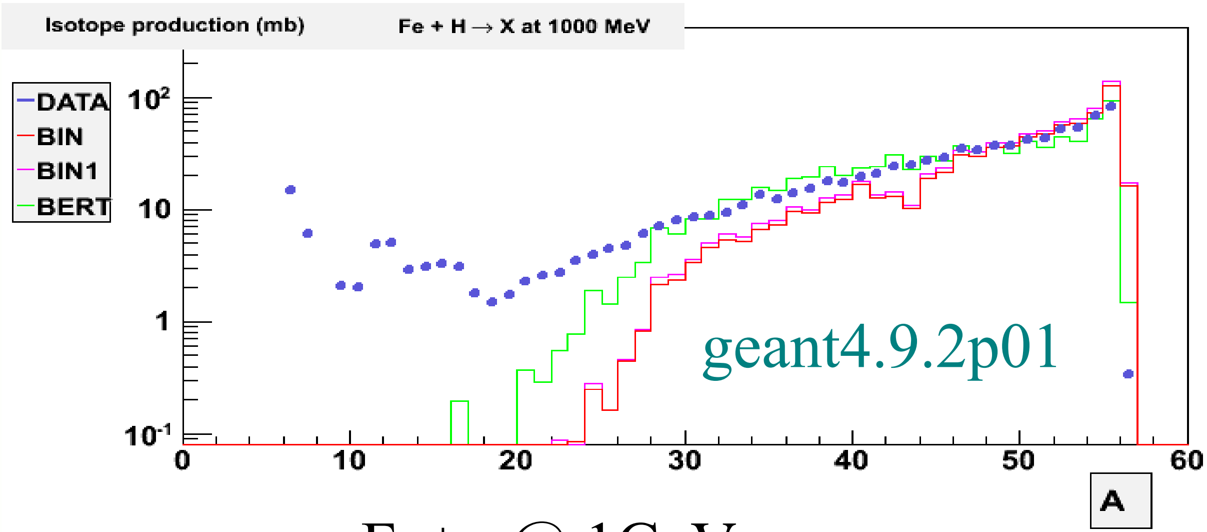



Fe+p @ 0.3 GeV

after GEM inclusion

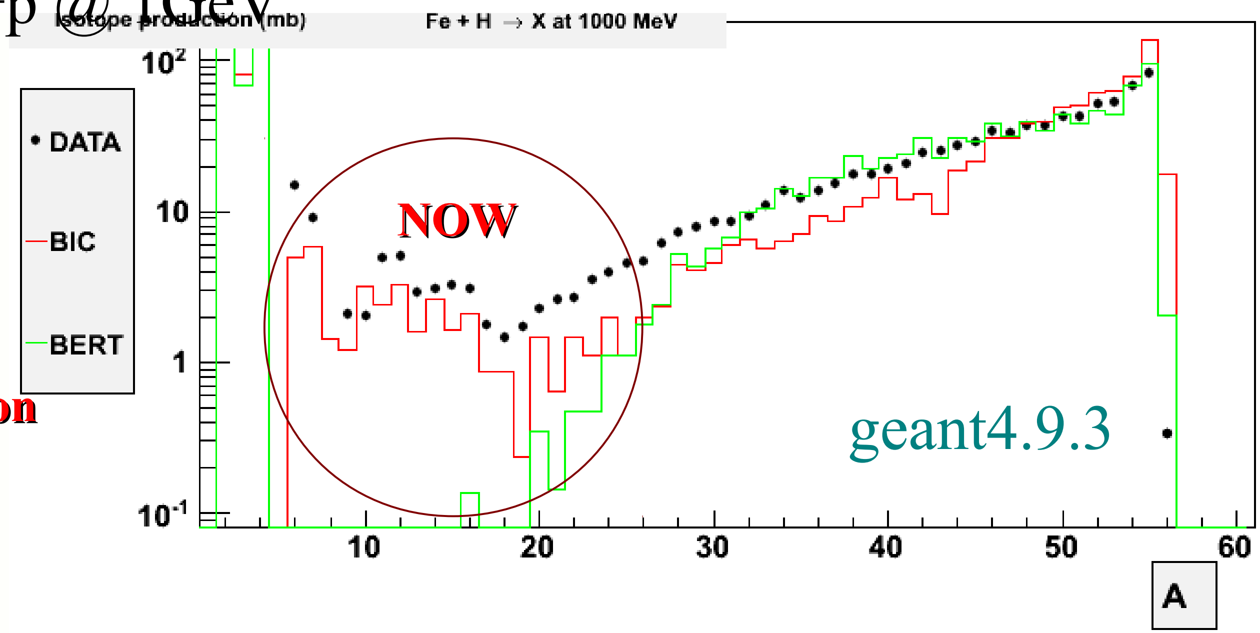


# Isotopic distibution at 1 GeV



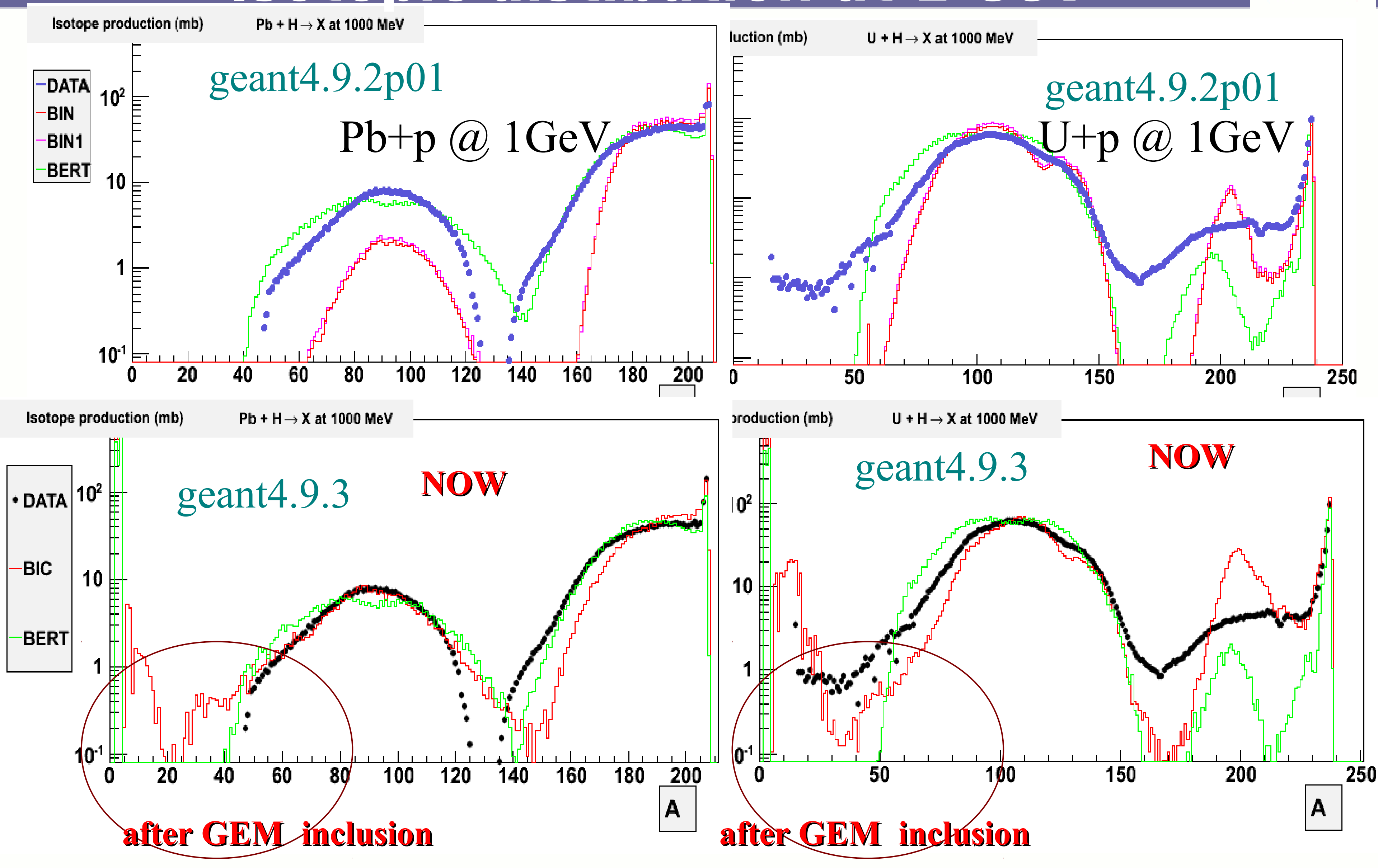

p+Fe

Fe+p @ 1GeV

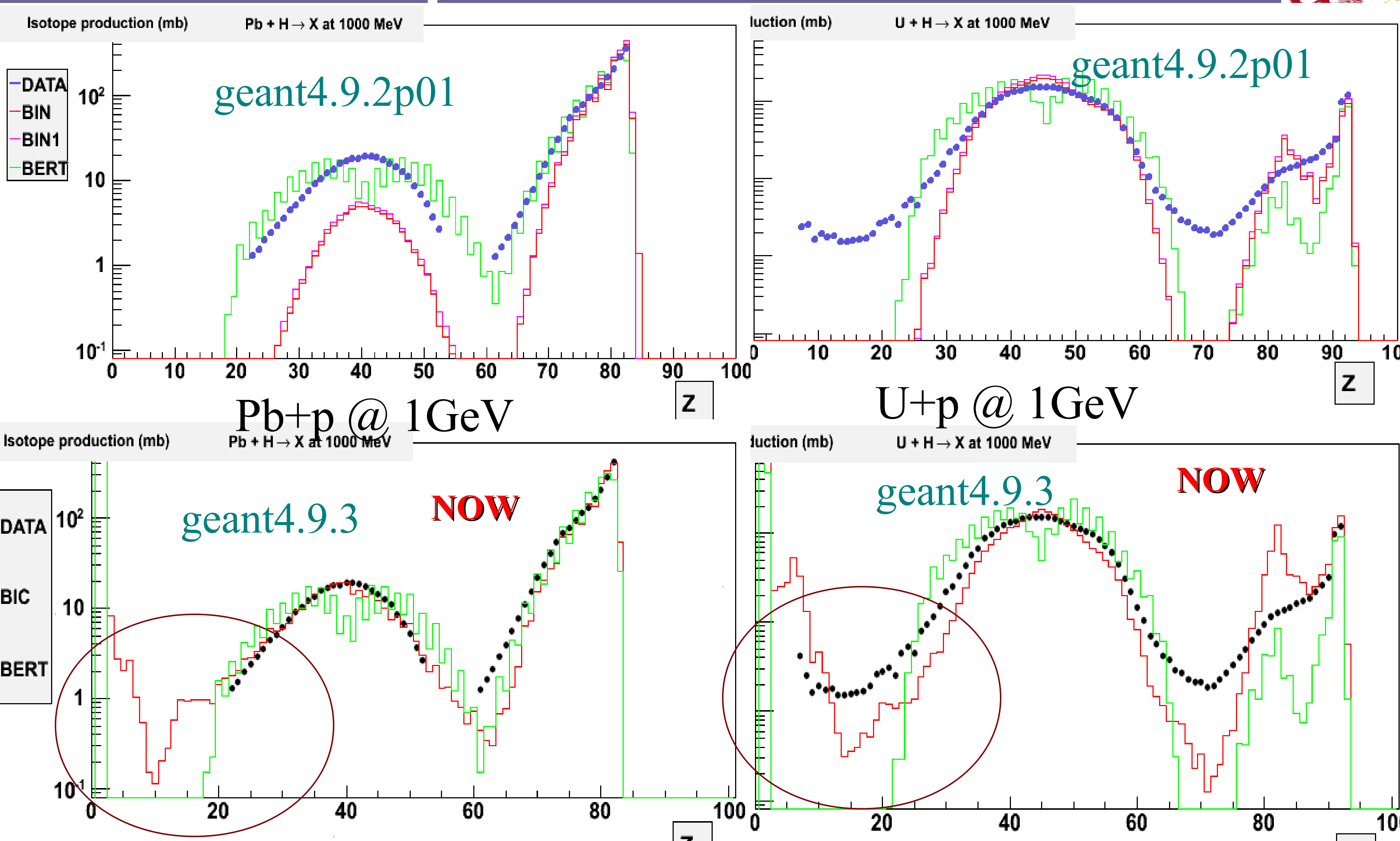



**after GEM inclusion**

# Isotopic distibution at 1 GeV



# Isotopic distribution at 1 GeV




**after GEM inclusion** **after GEM inclusion**

# Work in progress (I)

## (in development version, yet under testing)

- **There was still room for improvements,specially in the spallation products region**

- ***Soft cut-off* transition from pre-equilibrium cures this problem, but, in our case, it worsens performance at fission and at pre-equilibrium**

- **A new version of the s*oft cut-off* algorithm with $n_{eq}$ strictly calculated according to**

$$\lambda_+(p,h,E) = \lambda_-(p,h,E)$$

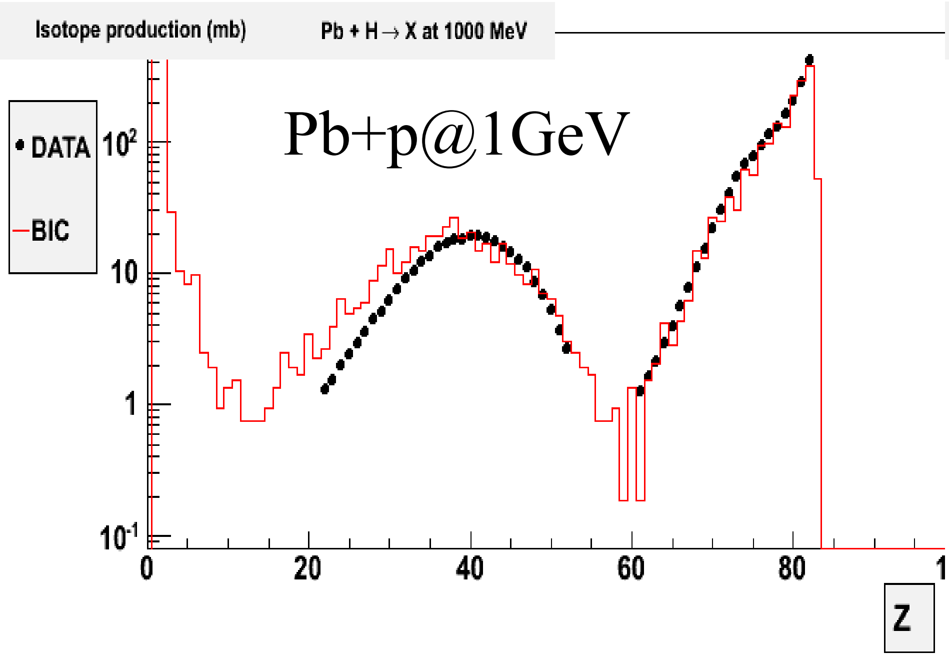
- **The *diffusivity* ($\sigma_{pre}$) of the transition has been drastically reduced (i.e. transition is now sharper)**

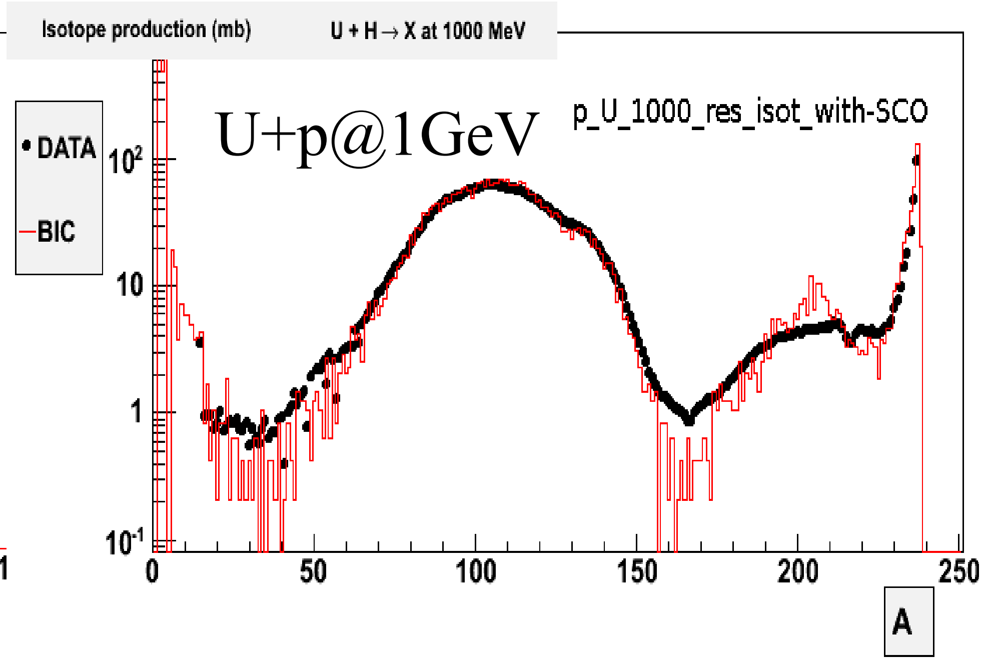
# Work in progress (II)

(in development version, yet under testing )

- **No chance for a global set of parameters (optimal for any combination of models)**
- **Different sets of fission parameters were fitted for each choice (with/without *soft cut-off*) .**
- **They are automatically selected**

# Development version




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

# Conclusions (I)

- The review of the native pre-equilibrium and de-excitation models of Geant4 recently performed has led to an overall satisfactory reproduction of experimental data set of IAEA nuclear spallation reactions benchmark:
    - recently made improvements to pre-compound:
        - More *physically sound* transition to equilibrium has been implemented
    - recently made improvements to evaporation:
        - Inverse reaction cross sections
        - IMF evaporation (GEM model)
    - recently made improvements to fission:
        - Fission parameters have been tuned
- Additional development work is in progress.

# Conclusions (II)

- Additional development work is in progress.
  - *Soft transition* to de-excitation and fine parameter tuning (specific interest: spallation reactions)
  - CPU performance and code cleanup (interest: all applications)
  - Fermi Breakup and Photon Evaporation (specific interest: Hadrontherapy)

# Thanks for your attention