Results obtained with nuclear models of Geant4 in IAEA Benchmark of Spallation

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on behalf of the Geant4 Hadronic Group
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General Introduction

What is Geant4?

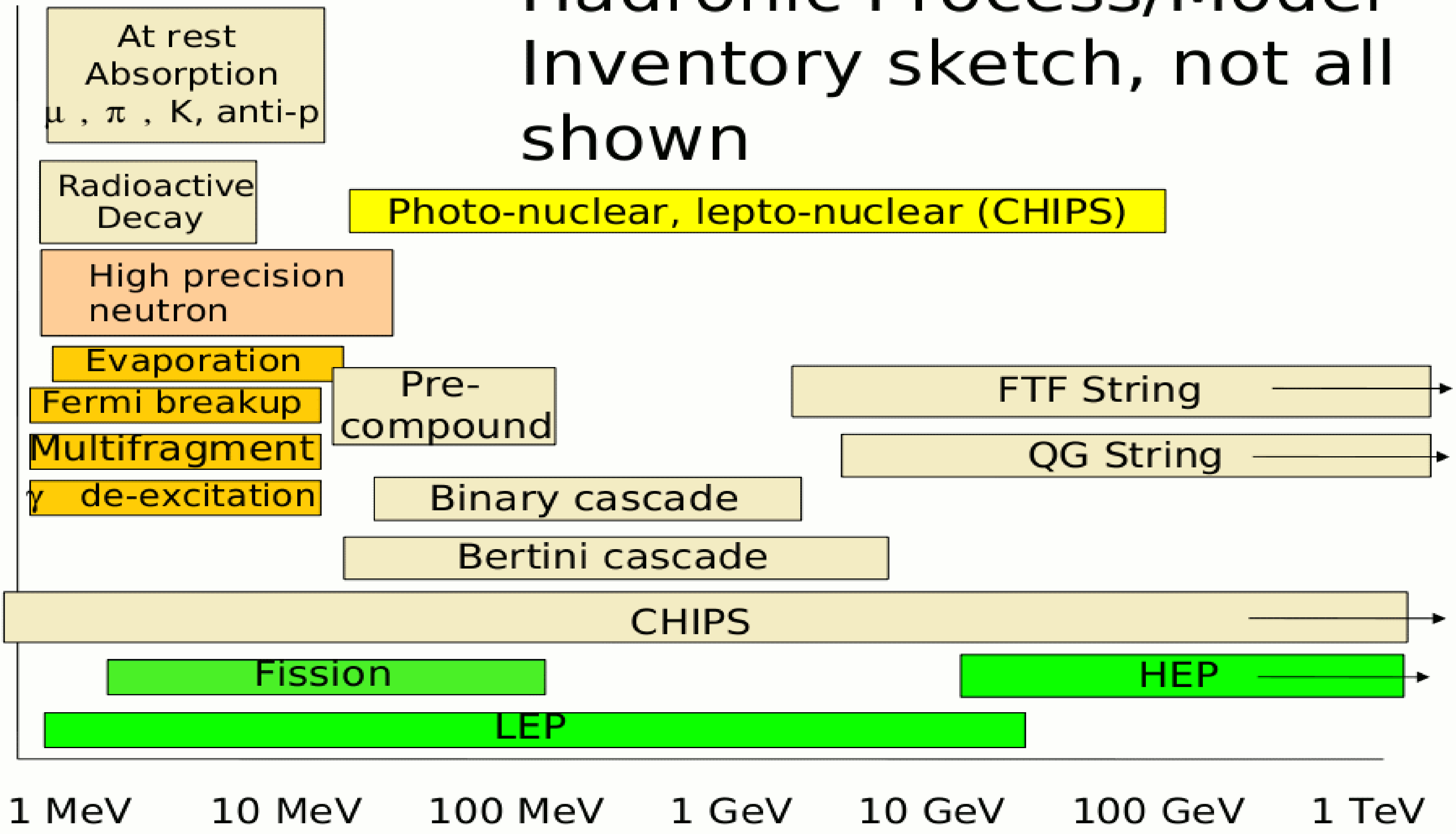
- Geant4 is the C++, object-oriented successor to GEANT3
- Designed primarily with high energy physics in mind
  - but now used in medical and space applications as well
- It is a toolkit:
  - large degree of functionality and flexibility are provided
  - many different codes provided, including alternates 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

Geant4 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



At rest Absorption
μ , π , K, anti-p

Radioactive Decay

Photo-nuclear, lepto-nuclear (CHIPS)

High precision neutron

Evaporation

Fermi breakup

Multifragment

γ de-excitation

Pre-compound

FTF String

QG String

Binary cascade

Bertini cascade

CHIPS

Fission

HEP

LEP

1 MeV 10 MeV 100 MeV 1 GeV 10 GeV 100 GeV 1 TeV

Geant4 Cascade Models

- The large energy region considered in this benchmarking includes different interaction regimes.
- In order to predict the production cross sections, different reaction mechanisms must be considered
  - Cascade
  - Pre-equilibrium
  - Equilibrium de-excitation
- Bertini Cascade has its own pre-compound and de-excitation models
- Binary cascade uses the native Geant4 pre-compound and de-excitation models.

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:
  - came from the INUCL code which was intended as an all-inclusive model.
  - It came with its own precompound and evaporation models. Neither of these are very different in origin from those in Binary, but the implementations are different.

Geant4 ongoing developments not included in this benchmark

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

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

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

Geant4 Bertini Cascade: Origin and applicability

- A re-engineered version of the INUCL code of N. Stepanov (ITEP)
- Employs many of the standard INC methods developed by Bertini (1968)
  - using free particle-particle collisions within cascade
  - step-like nuclear density
- Inelastic scattering of p, n, π , K, Λ , Σ , Ξ
- Incident energies: 0 < E < 10 GeV
  - upper limit determined by lack of partial final state cross sections and the end of the cascade validity region
  - lower limit due to inclusion of internal nuclear de-excitation models

Bertini Cascade Model

- **The Bertini model is a classical cascade:**
  - **It is a solution to the Boltzmann equation on average**
  - **No scattering matrix calculated**

- **Core code:**
  - **Elementary particle collider: uses free cross sections**
  - **Up to and including 9-body final state partial cross sections for pi+p, pi-p, pp, pn from the CERN compilations.**
  - **K+, K- partial cross sections.**
  - **pi+n, pi-n, nn cross sections are obtained through isospin arguments**
  - **Partial cross sections have been reviewed and partially changed.**
  - **Generated secondaries:**
    - **pions, nucleons, kaons, hyperons.**
    - **No resonances**
    - **Deuterons, tritons, 3He, alphas (from evaporation phase only)**
  - **Cascade in nuclear medium**
  - **Final steps: pre-equilibrium and equilibrium decay of residual nucleus**

Bertini Cascade Modelling Sequence (1)

- Nuclear entry point sampled over projected area of nucleus
- Incident particle is transported in density dependent nuclear medium
  - mean free path from total particle-particle cross sections
  - Nucleus modeled as 3 concentric, constant-density shells plus reflection/transmission shell boundaries.
  - nucleons have Fermi gas momentum distribution
  - Pauli exclusion invoked
- Projectile interacts with a single nucleon
  - hadron-nucleon interactions based on free cross sections and angular distributions
  - pions can be absorbed on quasi-deuterons

Bertini Cascade Modelling Sequence (2)

- Each secondary from initial interaction is propagated in nuclear potential until it interacts or leaves nucleus
  - can have reflection from density shell boundaries
  - Coulomb barrier added for all phases
- As cascade collisions occur, exciton states are built up, leading to equilibrated nucleus
  - selection rules for p-h state formation: $\Delta p = 0, +/-1$, $\Delta h = 0, +/-1$, $\Delta n = 0, +/-2$
- Model uses its own exciton routine based on that of Griffin
  - Kalbach matrix elements used
  - level densities parametrized vs. Z and A

Bertini Cascade Modelling Sequence (3)

- Cascade ends and exciton model takes over when secondary KE drops below 20% of its original value or 7 X nuclear binding energy
- Nuclear evaporation follows for most nuclei
  - emission continues as long as excitation is large enough to remove a particle.
- For light, highly excited nuclei, Fermi breakup
- Fission included in phenomenological way for heavy elements

Origin and Applicability of the 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
- π
  - $0 < E < 1.5$ GeV

Binary Cascade Model

- 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 Modelling Sequence(1)

- Nucleon-nucleon scattering (t-channel) resonance excitation cross-sections are derived from p-p scattering using isospin invariance, and the corresponding Clebsch-Gordan coefficients
  - elastic N-N scattering included
- 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
  - nominal PDG branching ratios used for resonance decay
  - masses sampled from Breit-Wigner form
- Developed in collaboration with Frankfurt group, broadly similar to UrQMD

Binary Cascade Modelling Sequence(2)

- Calculate imaginary part of the R-matrix using free 2-body cross-sections from experimental data and parameterizations
- For resonance re-scattering, the solution of an in-medium BUU equation is used.
  - The Binary Cascade at present takes the following strong resonances into account:
    - The delta resonances with masses 1232, 1600, 1620, 1700, 1900, 1905, 1910, 1920, 1930, and 1950 MeV
    - Excited nucleons with masses 1440, 1520, 1535, 1650, 1675, 1680, 1700, 1710, 1720, 1900, 1990, 2090, 2190, 2220, and 2250 MeV

Binary Cascade Modelling Sequence(3)

- Nucleon-nucleon elastic scattering angular distributions taken from :
  - Arndt phase shift analysis of experimental data up to 1.2 GeV
  - at higher energies PDG data are used
- Pauli blocking implemented in its classical form
  - final state nucleons occupy only states above Fermi momentum
- Coulomb barrier taken into account for charged hadrons

Geant 4

Binary Cascade Modelling Sequence(4)

- 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
- Pre-equilibrium: exciton model

Binary Cascade Modelling Sequence (5): Pre- equilibrium

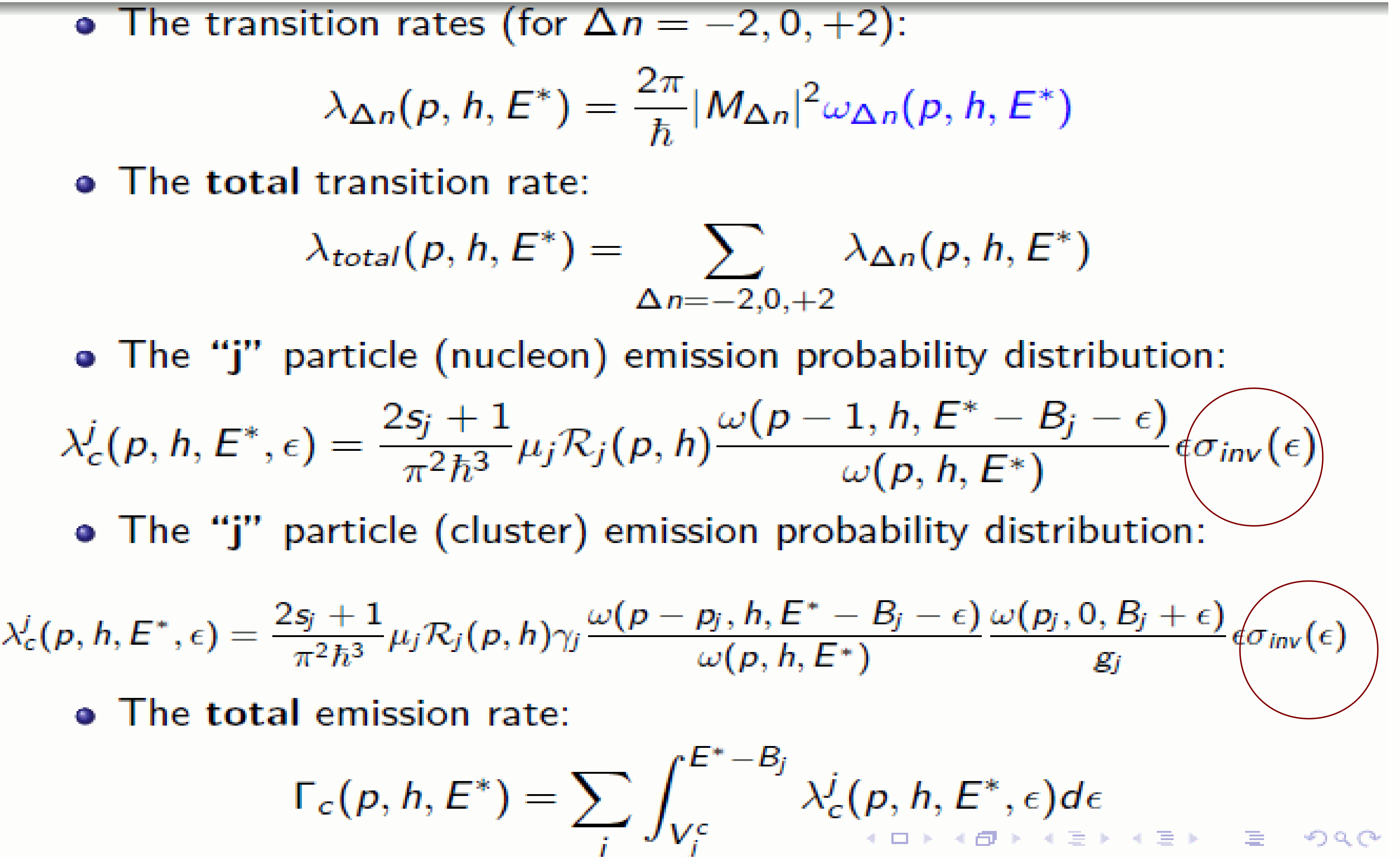
- Native pre-equilibrium de-excitation model in Geant4 is a version of standard exciton model.

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.

Pre- equilibrium :
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:

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

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

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

- The **total** emission rate:

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

Pre-equilibrium & Equilibrium

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 parameterization (after release 9.2)

- More realistic parameterization of reaction cross sections:
  - 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)

Binary Cascade Modelling Sequence(6): Transition from pre-equilibrium to equilibrium

- En principle, the transition from pre-equilibrium to equilibrium de-excitation should take place when the following condition is fulfilled: $\lambda_+(p,h,E) = \lambda_-(p,h,E)$

- 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* $\sigma_{pre} \approx 0.4$

Binary Cascade Modelling Sequence(7) : Equilibrium

After pre-equilibrium the properties of the residual nucleus are evaluated, and passed to the equilibrium de-excitation handler.

Four processes are considered:

- 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).

Equilibrium
Evaporation models

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

improved

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

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

- Combination of *improved* WE for evaporation of n,p,d,t,^{3}He,α and GEM for heavier fragments. DEFAULT

- Break down in explosive scenarios:
  - Very light systems → Fermi break-up
  - High excitation energies → Statistical Multifragmentation

Equilibrium
Fermi break-up

- For very light systems even a relatively small E^* may be comparable with their total binding energy.

- Fermi model does the partitioning of excited light nuclei ($Z<9$, $A<17$) and the sampling of their kinetic energies, based on very basic physical grounds (phase space availability).

- It does not have any impact in present benchmark.

- It is relevant in reactions involving light compound nuclei (hadrontherapy)

Equilibrium

Statistical multifragmentation

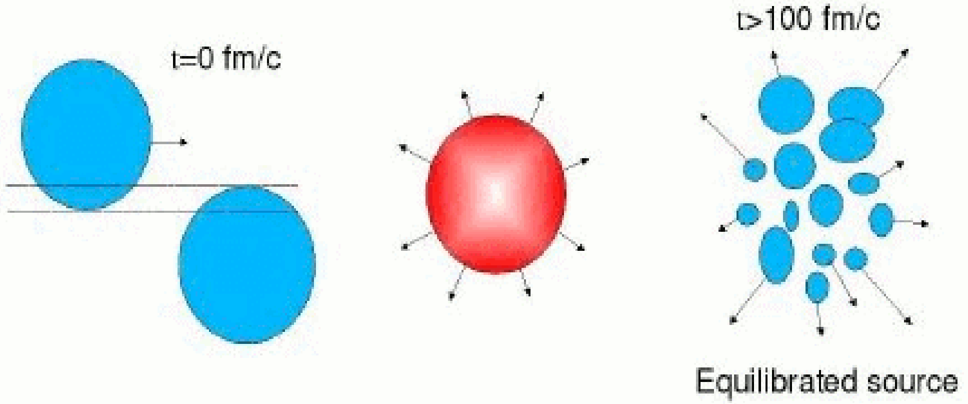
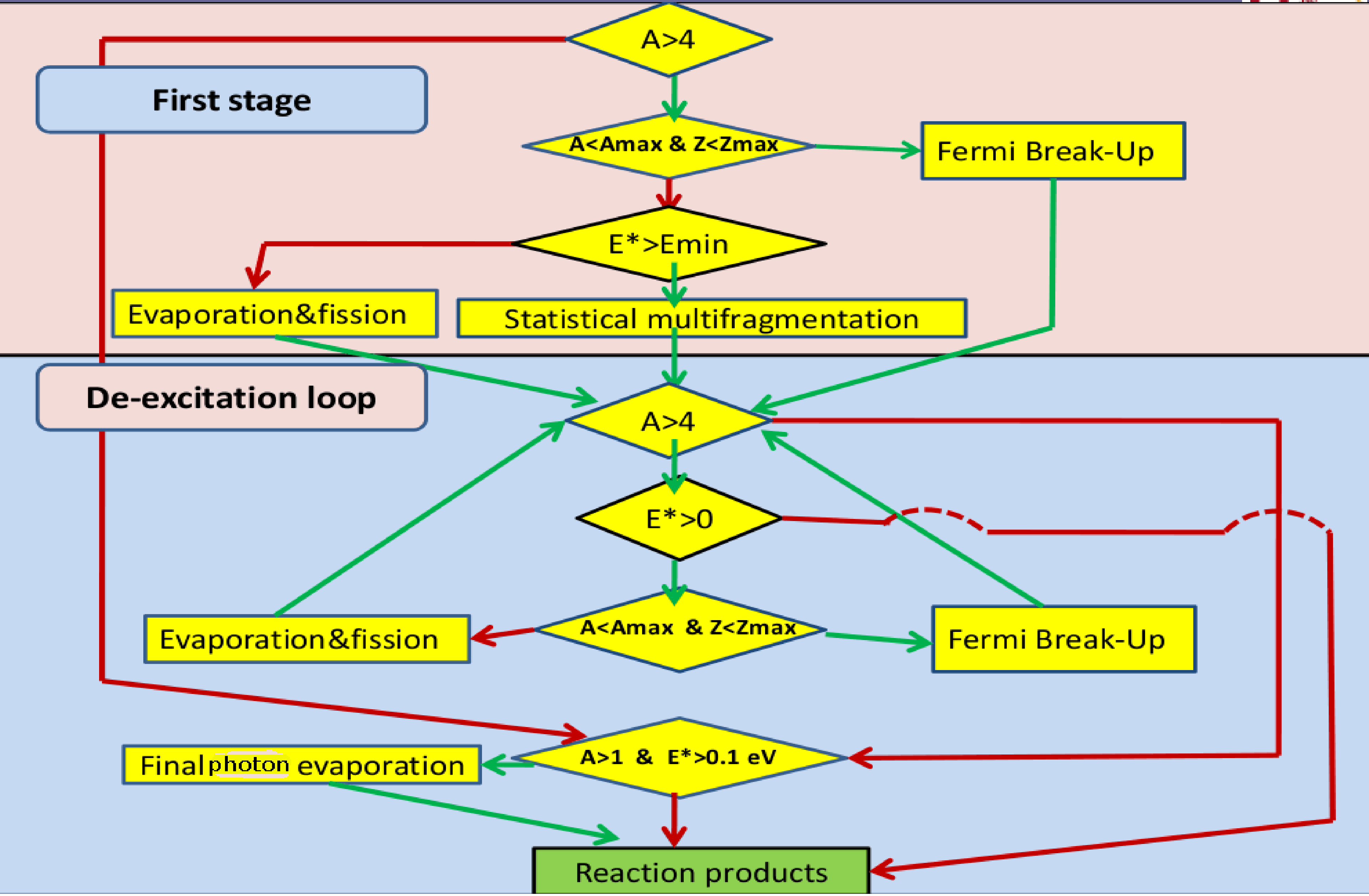


Figure: For $E^*/A \geq 3\ MeV$

- Implementation of Statistical Multifragmentation Model, developed since the seventies by Mishustin-Botvina.

- Igor Psenishnov (FIAS) has validated it against original FORTRAN code.

Equilibrium de-excitation models



First stage

A>4

A<Amax & Z<Zmax

Fermi Break-Up

E*>Emin

Evaporation&fission

Statistical multifragmentation

De-excitation loop

A>4

E*>0

A<Amax & Z<Zmax

Evaporation&fission

Fermi Break-Up

A>1 & E*>0.1 eV

Final photon evaporation

Reaction products

Remarks in AccApp'09 (Satellite Meeting on Spallation Reactions)

(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

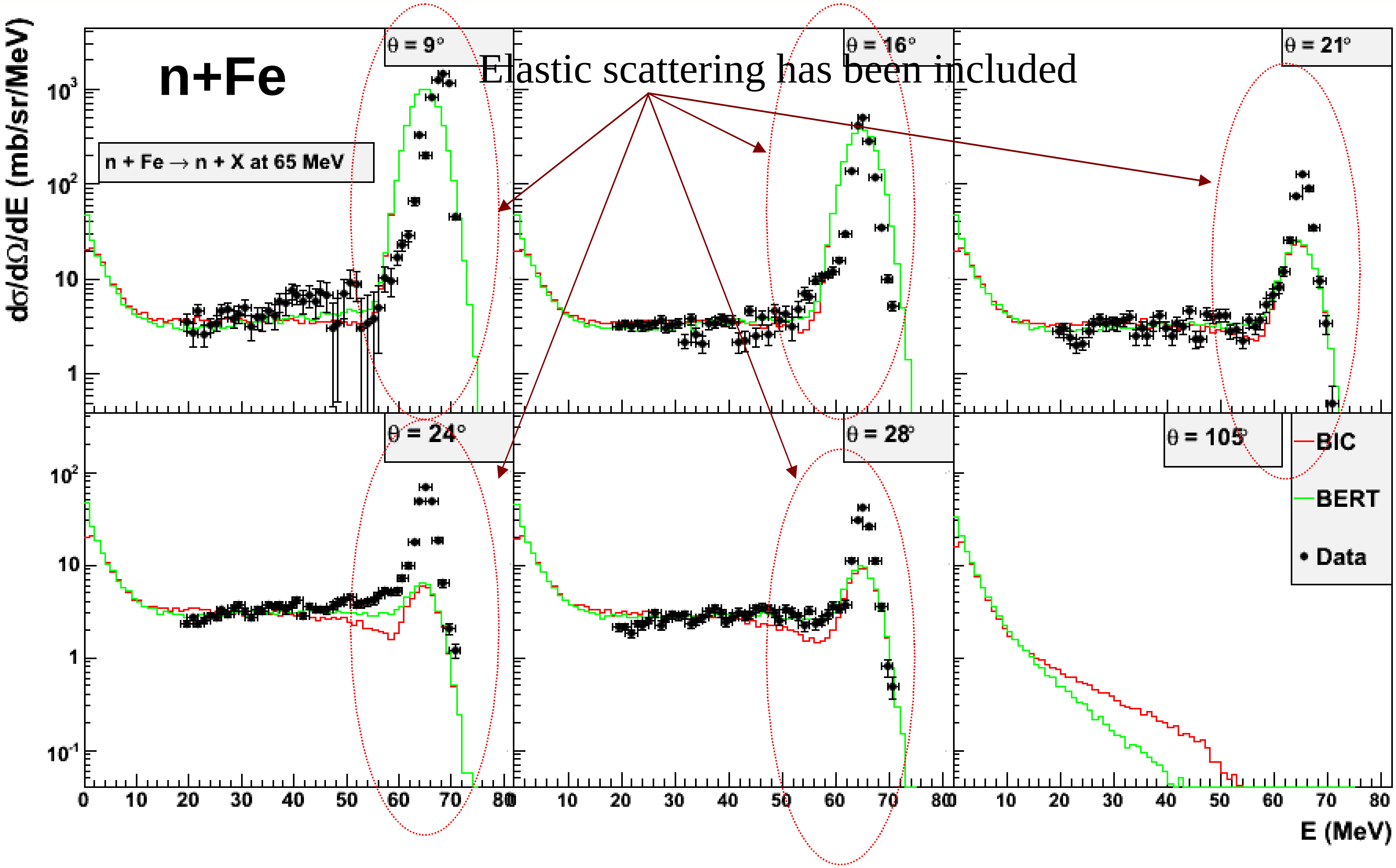
(included in geant4.9.3 official release)

- 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

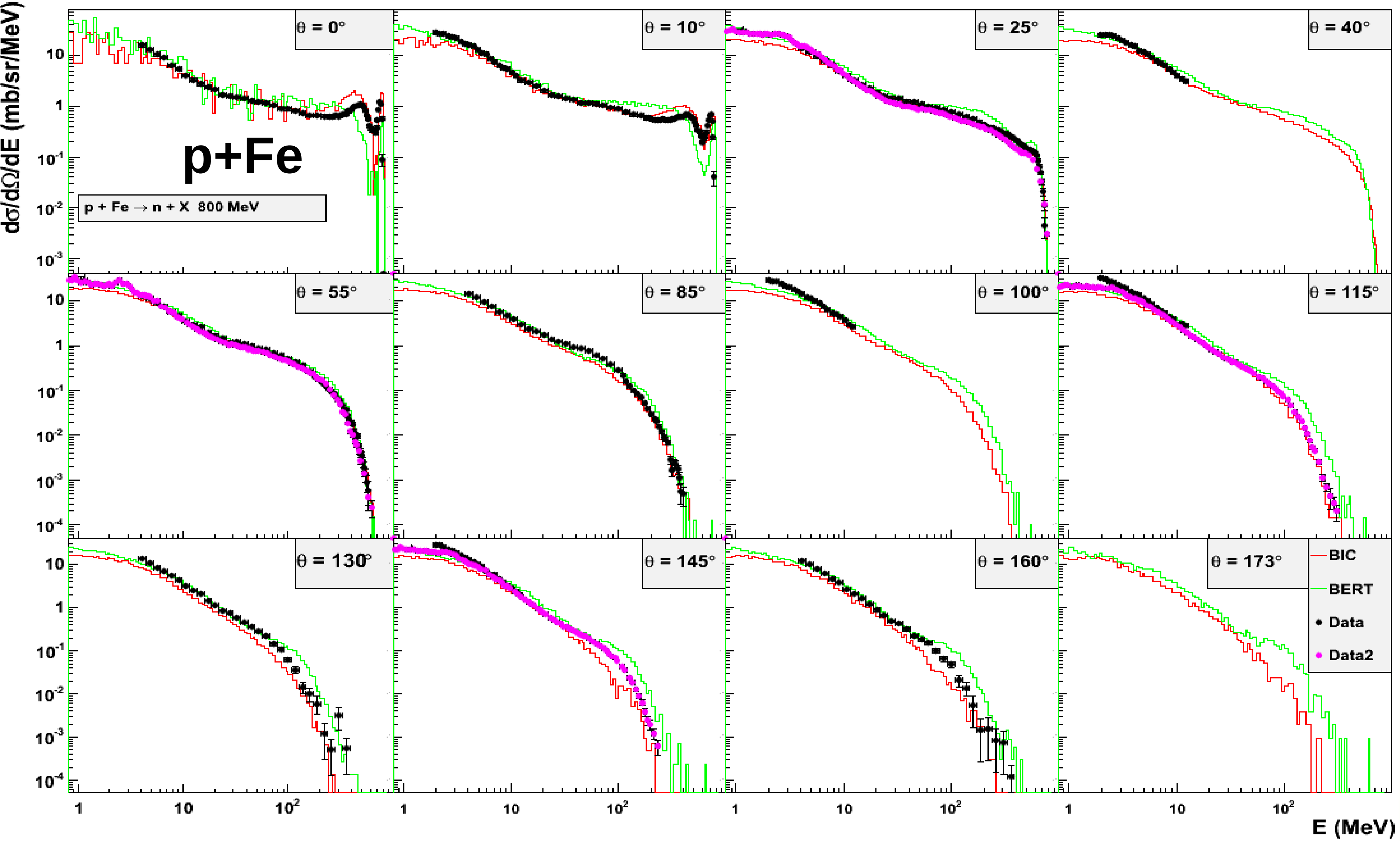
(Geant4 release 9.3)

Neutron production at 63 MeV

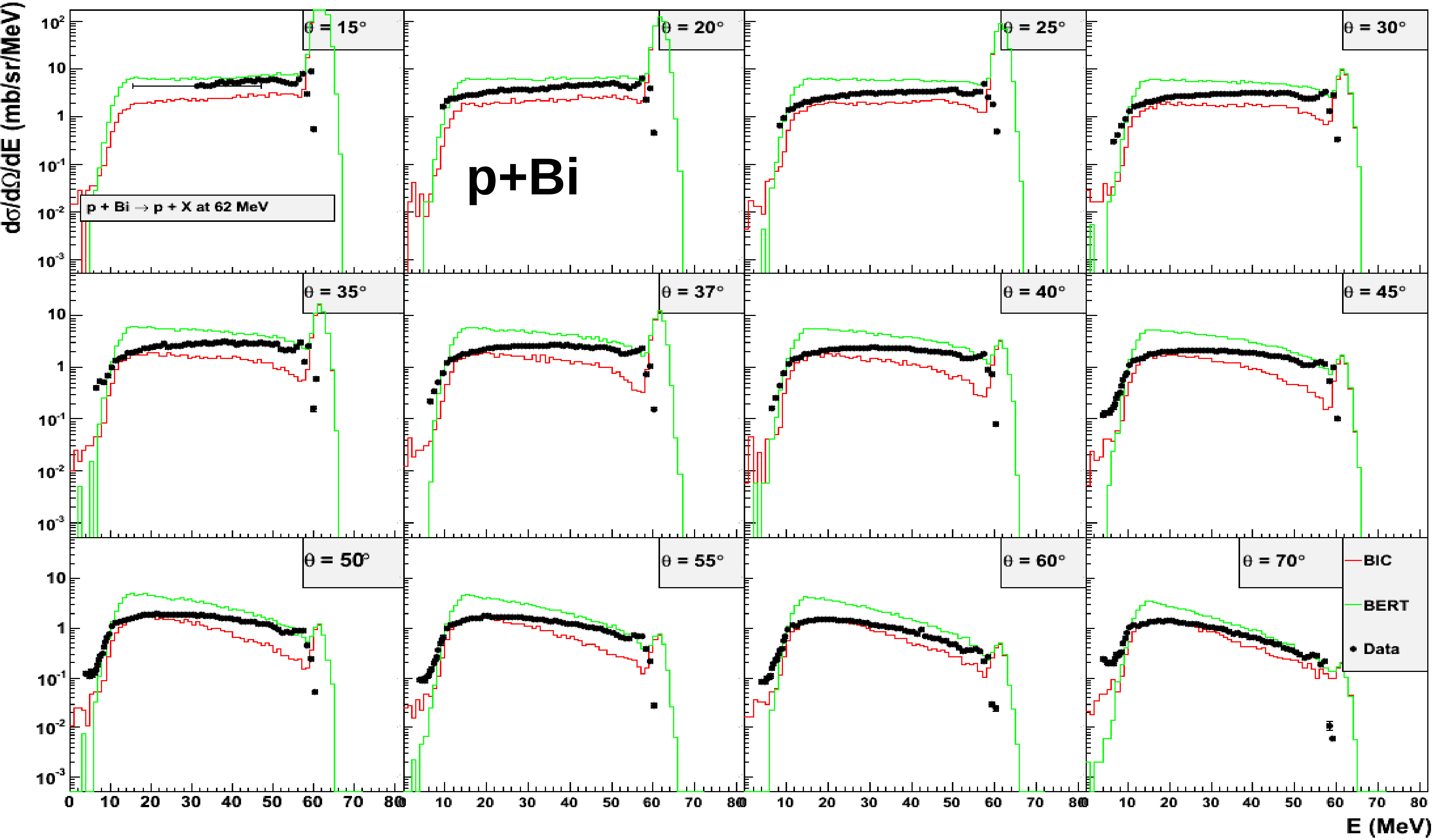


Elastic scattering has been included

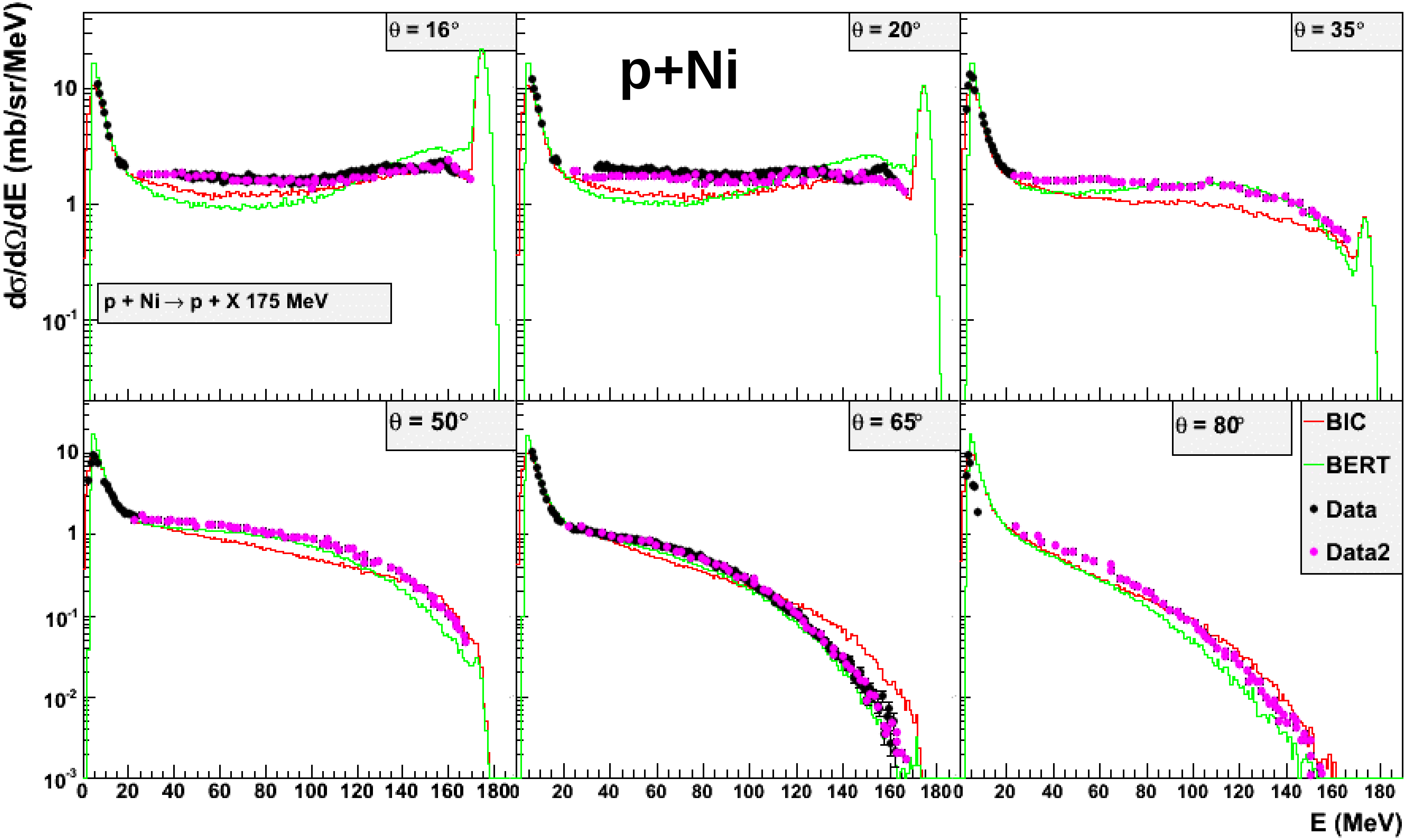
Neutron production at 1200 MeV



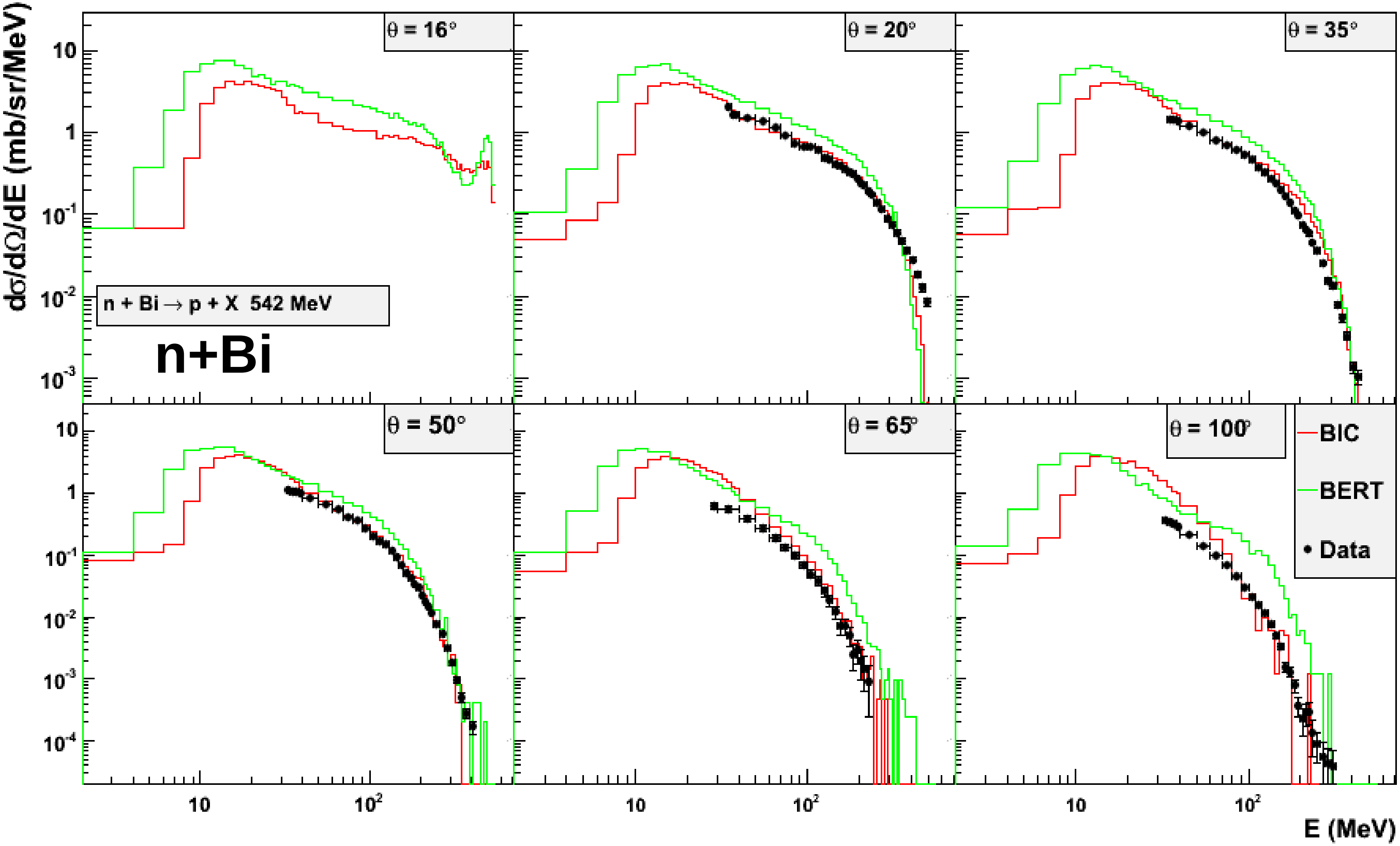
Proton production at 62 MeV



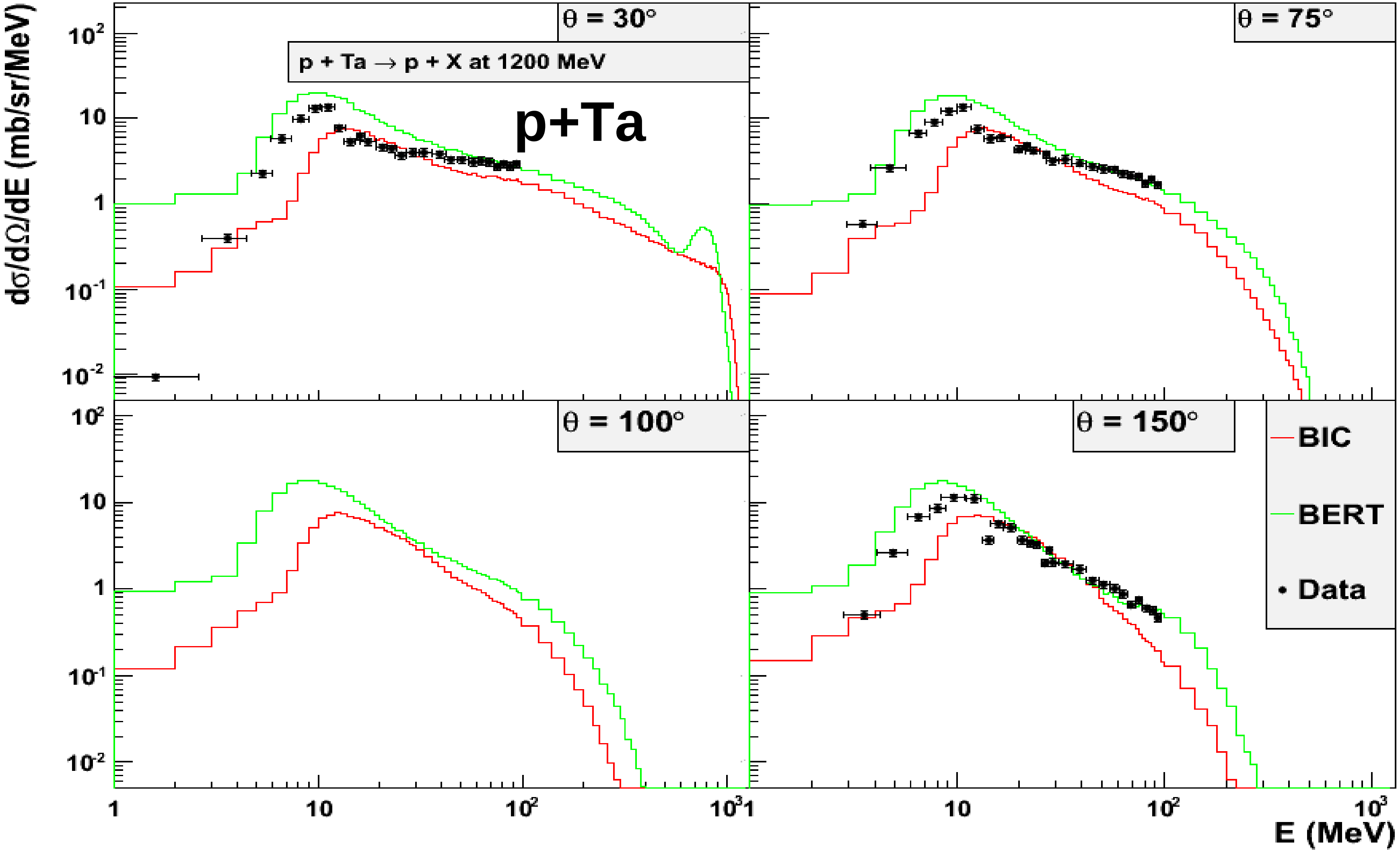
Proton production at 175 MeV



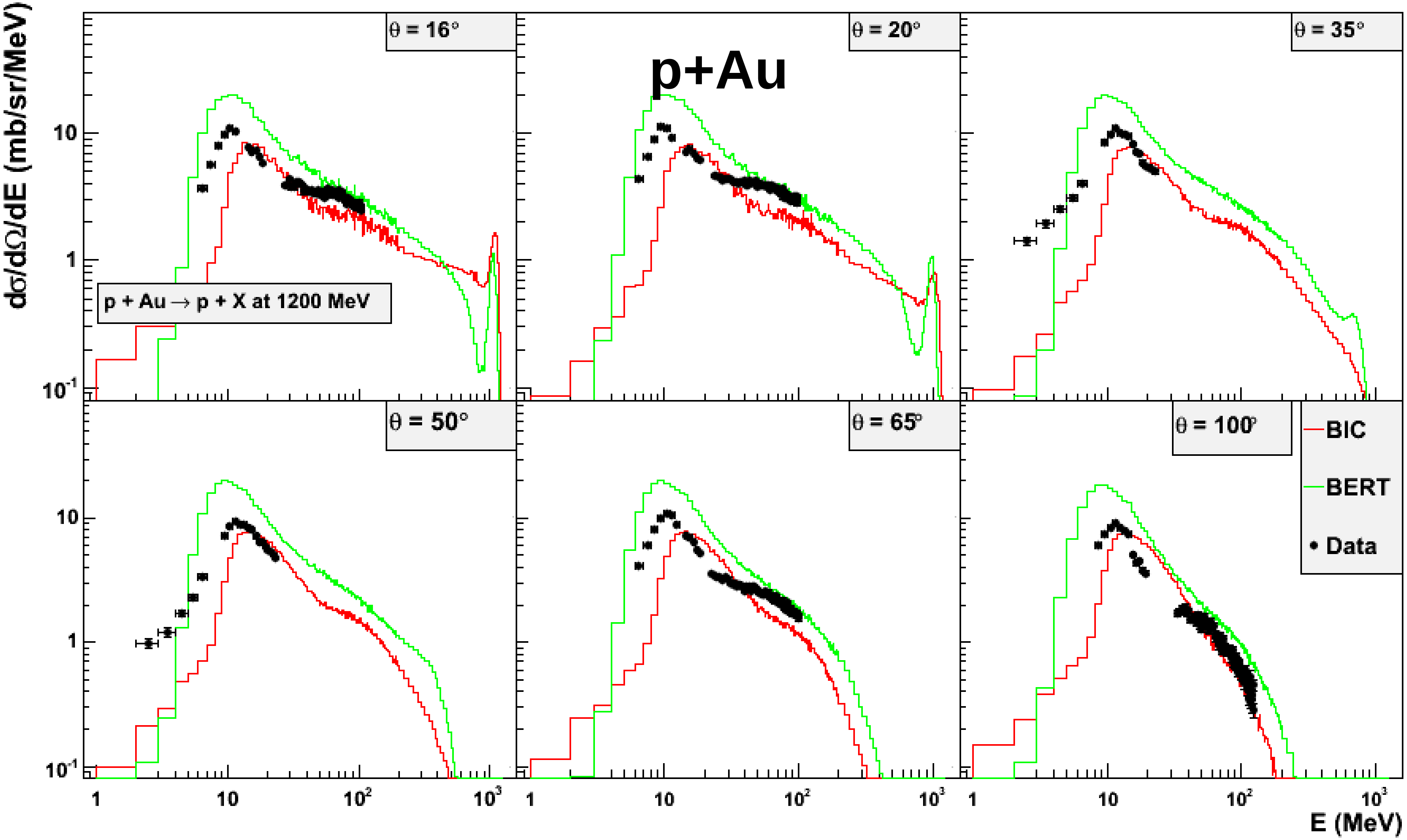
Proton production at 542 MeV



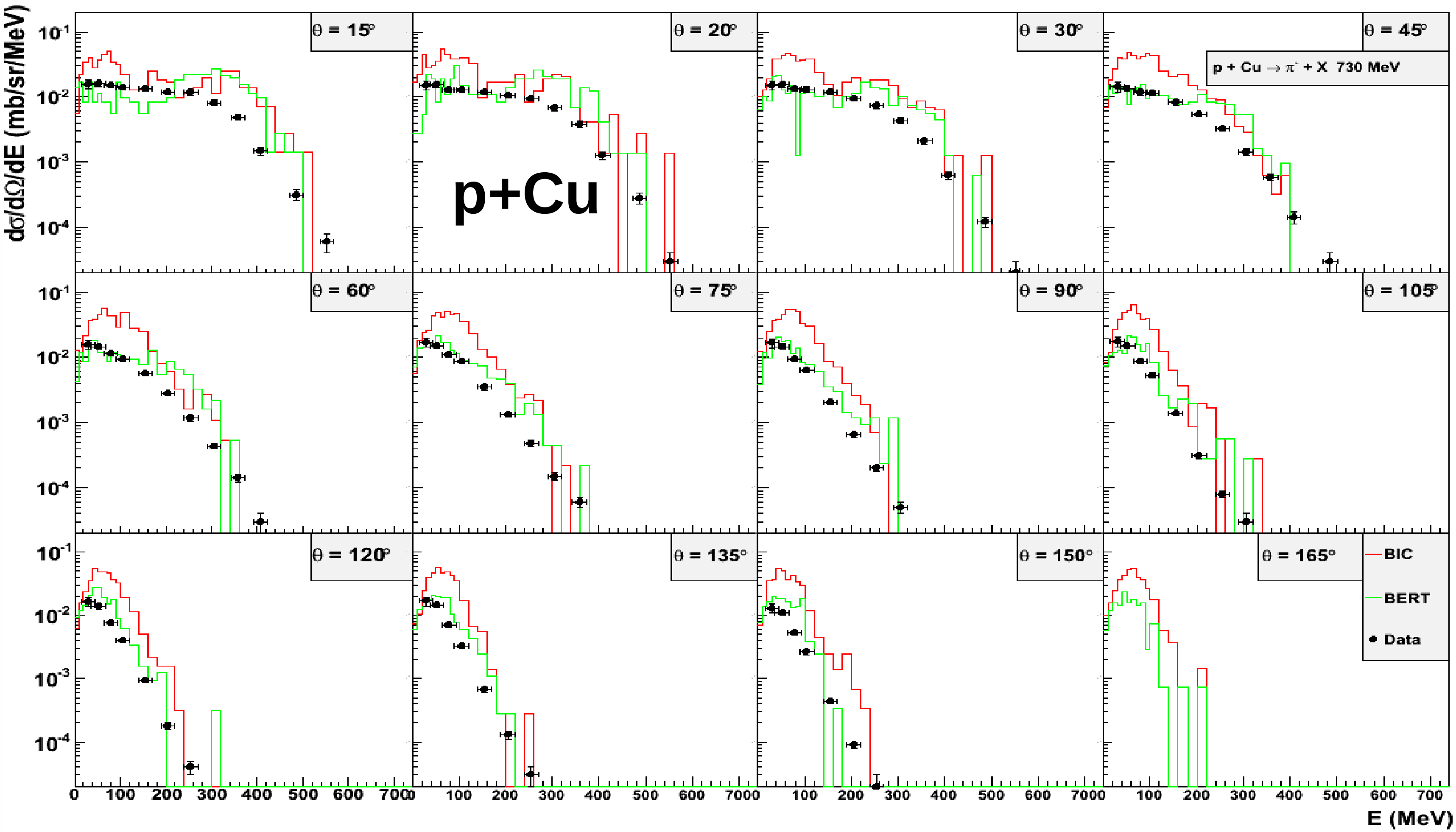
Proton production at 1200 MeV



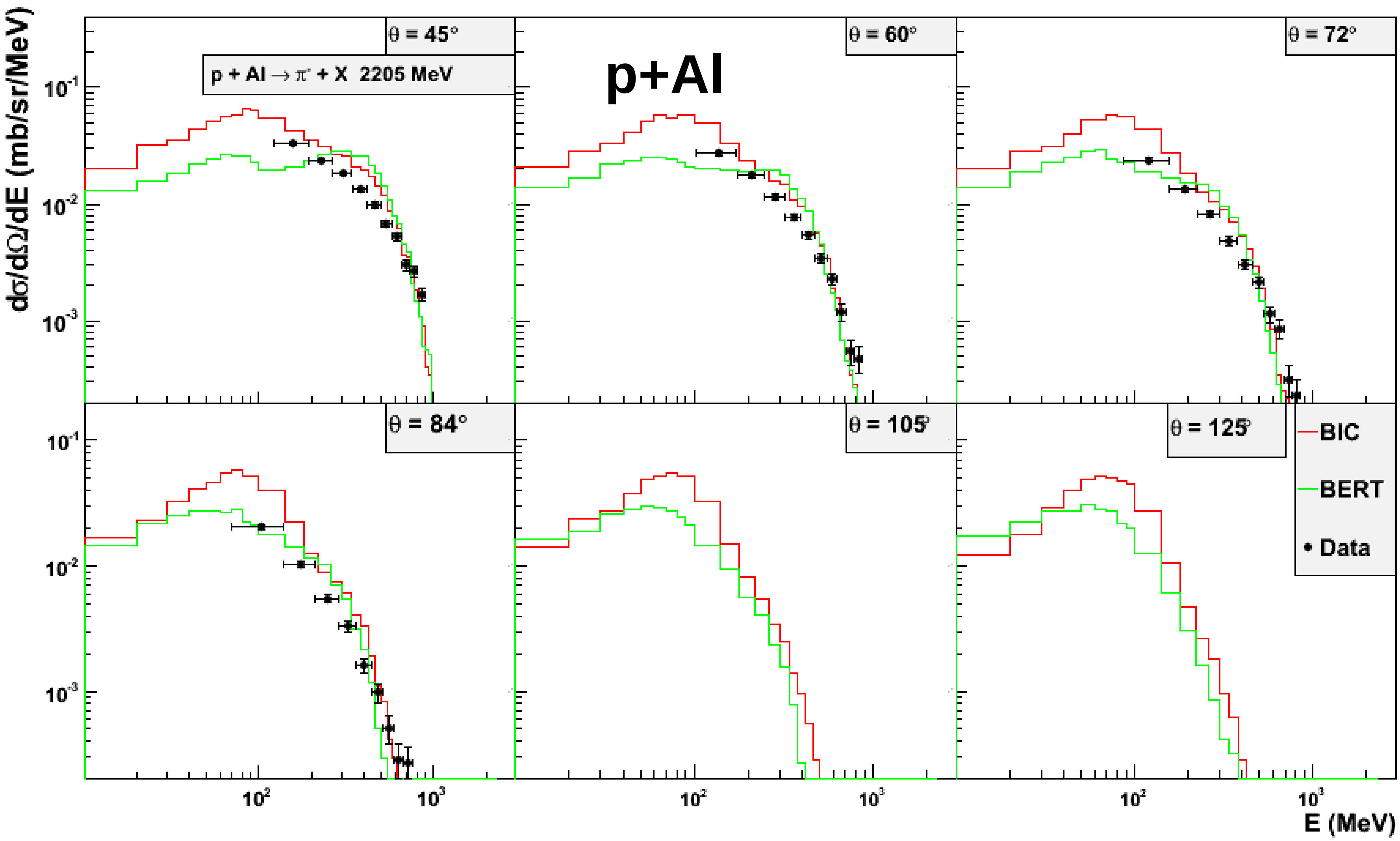
Proton production at 1200 MeV



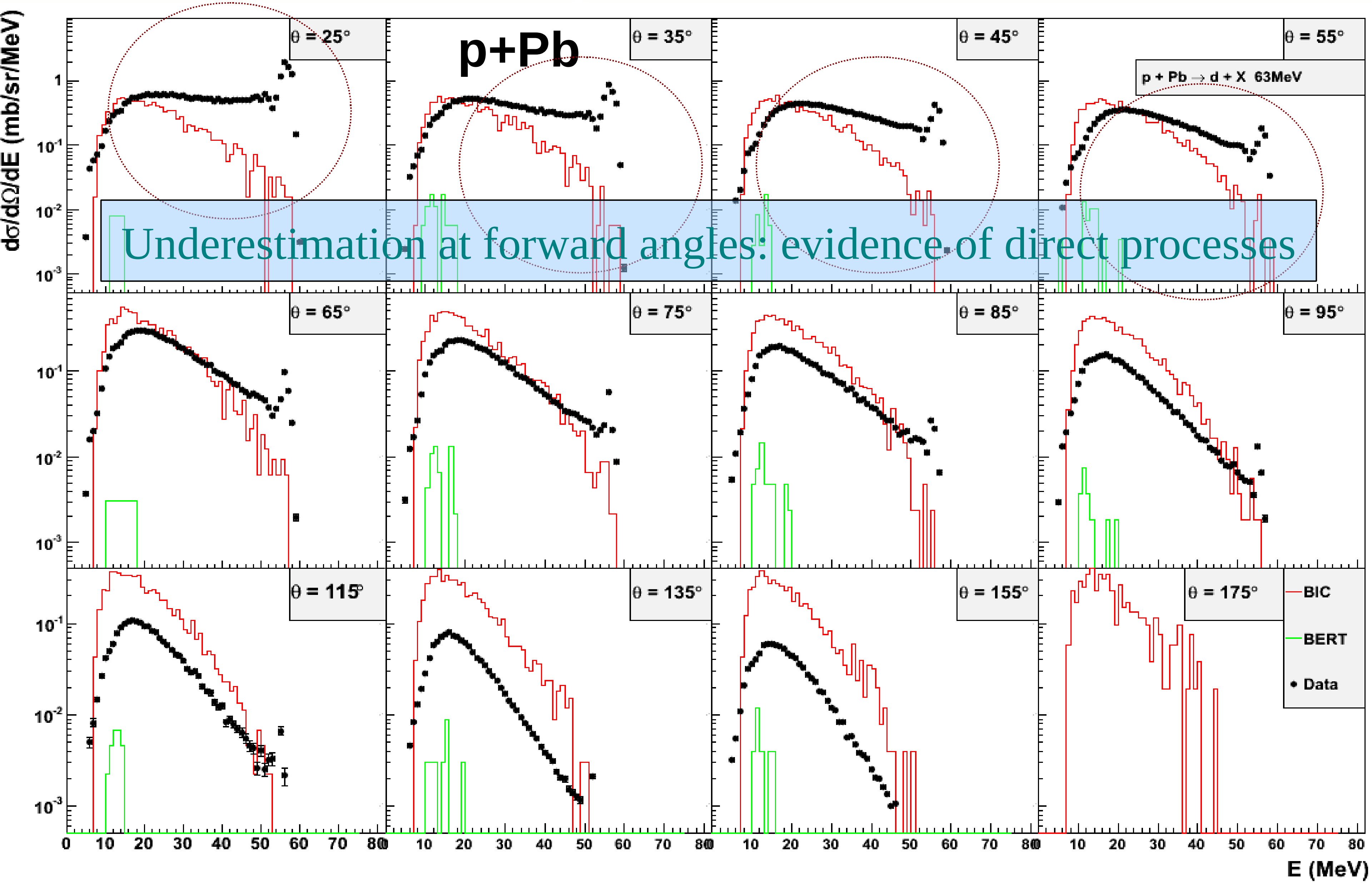
Pion production at 730 MeV



Pion production at 2205 MeV

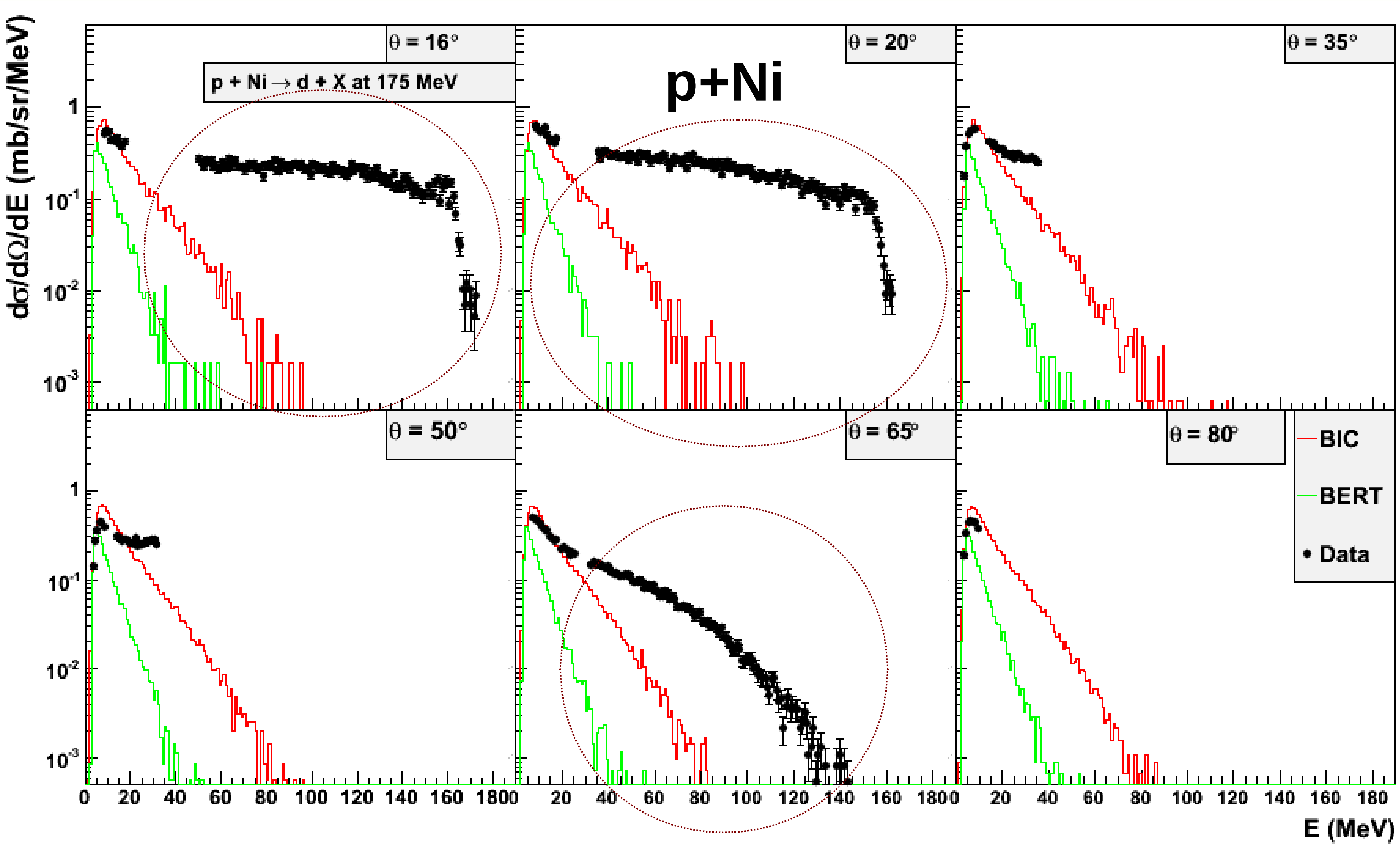


Deuteron production at 63 MeV

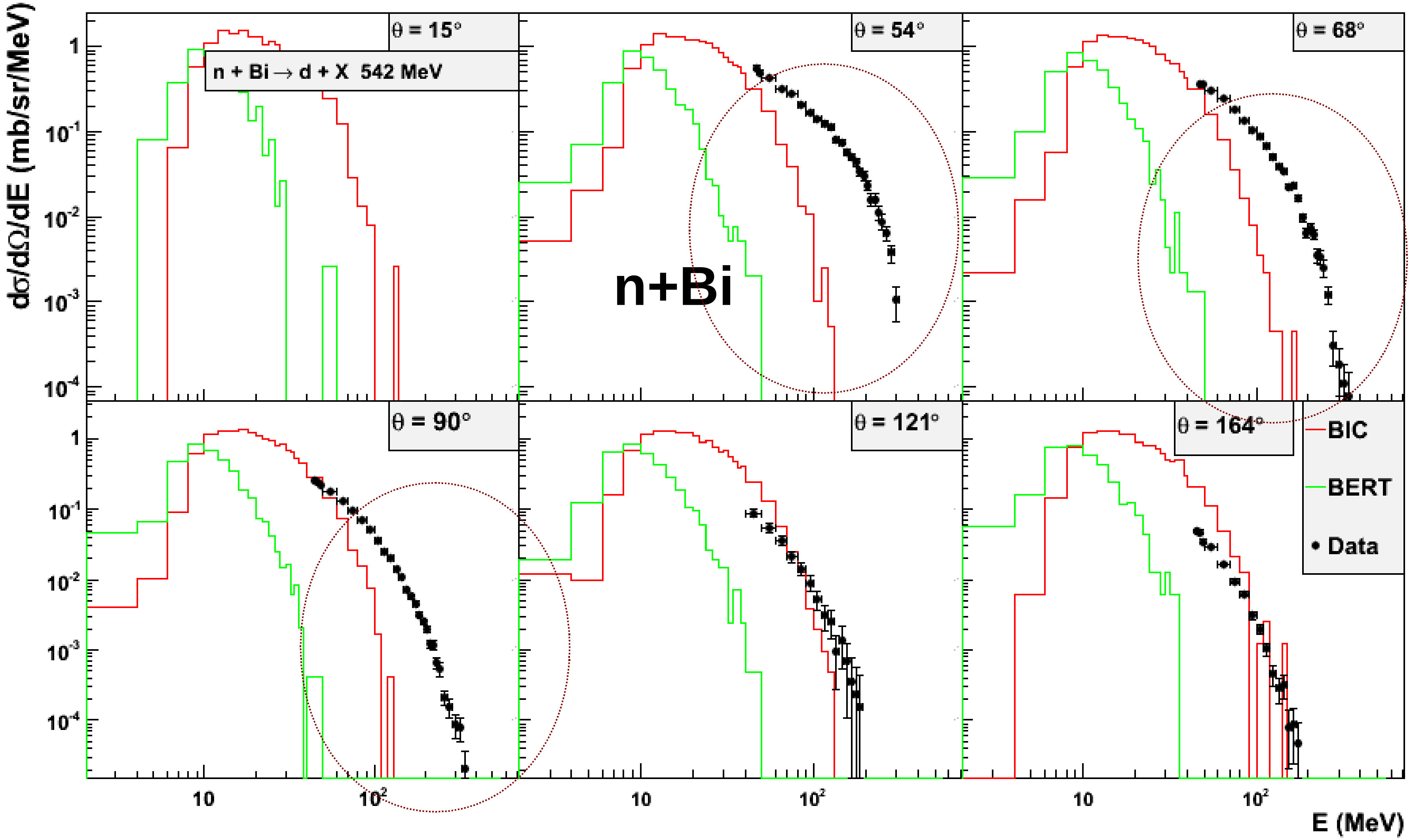


Underestimation at forward angles: evidence of direct processes

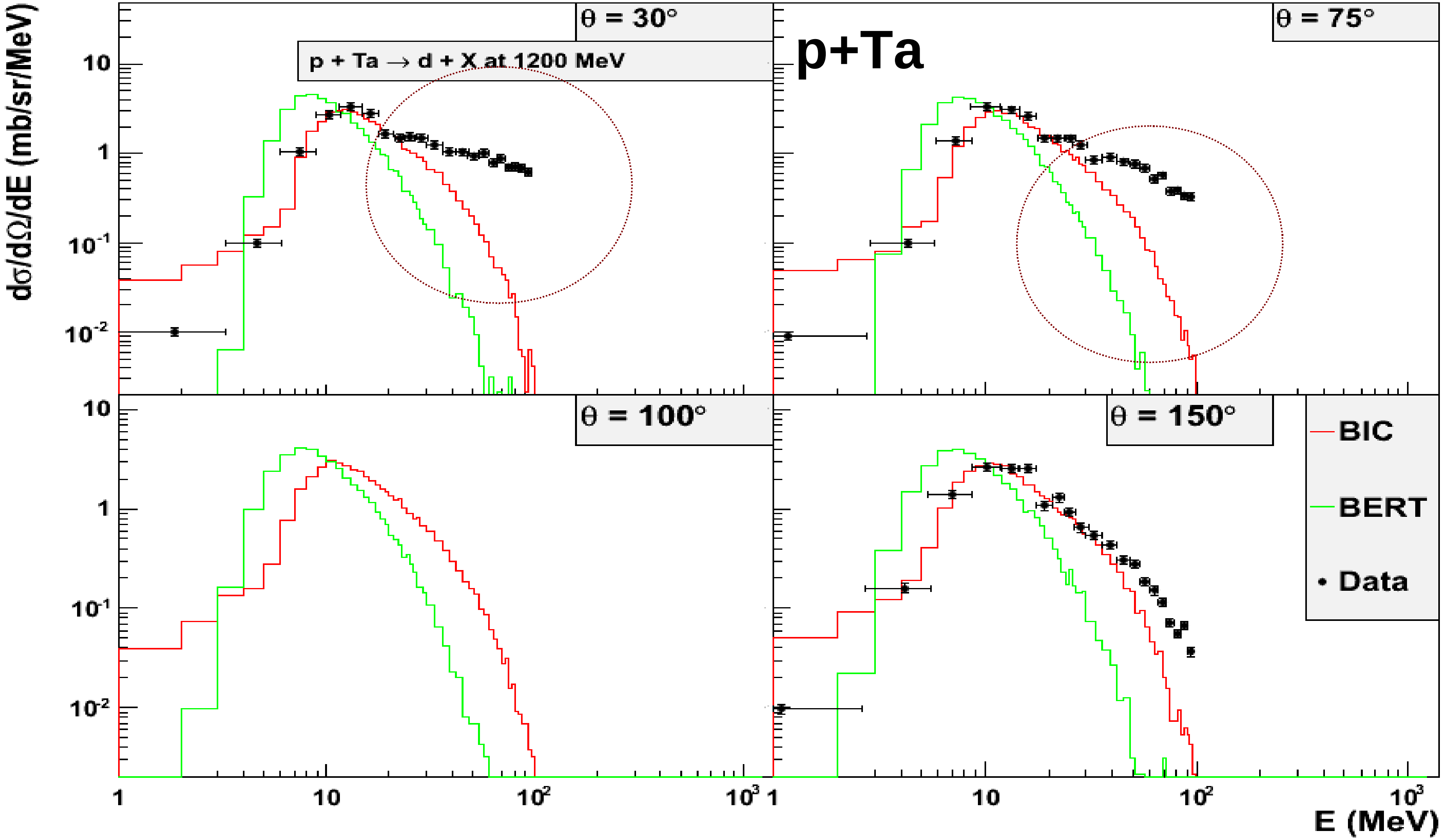
Deuteron production at 175 MeV



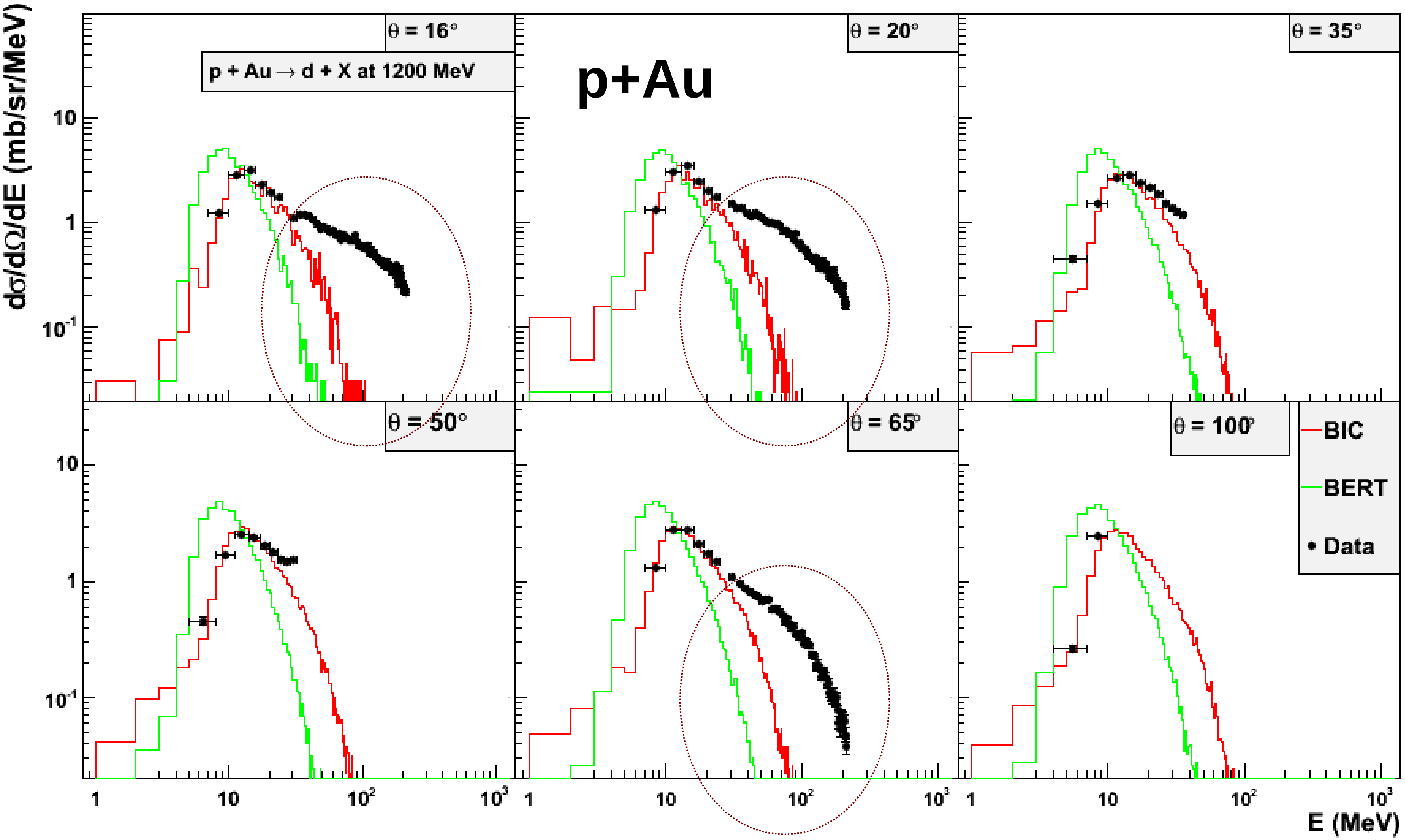
Deuteron production at 542 MeV



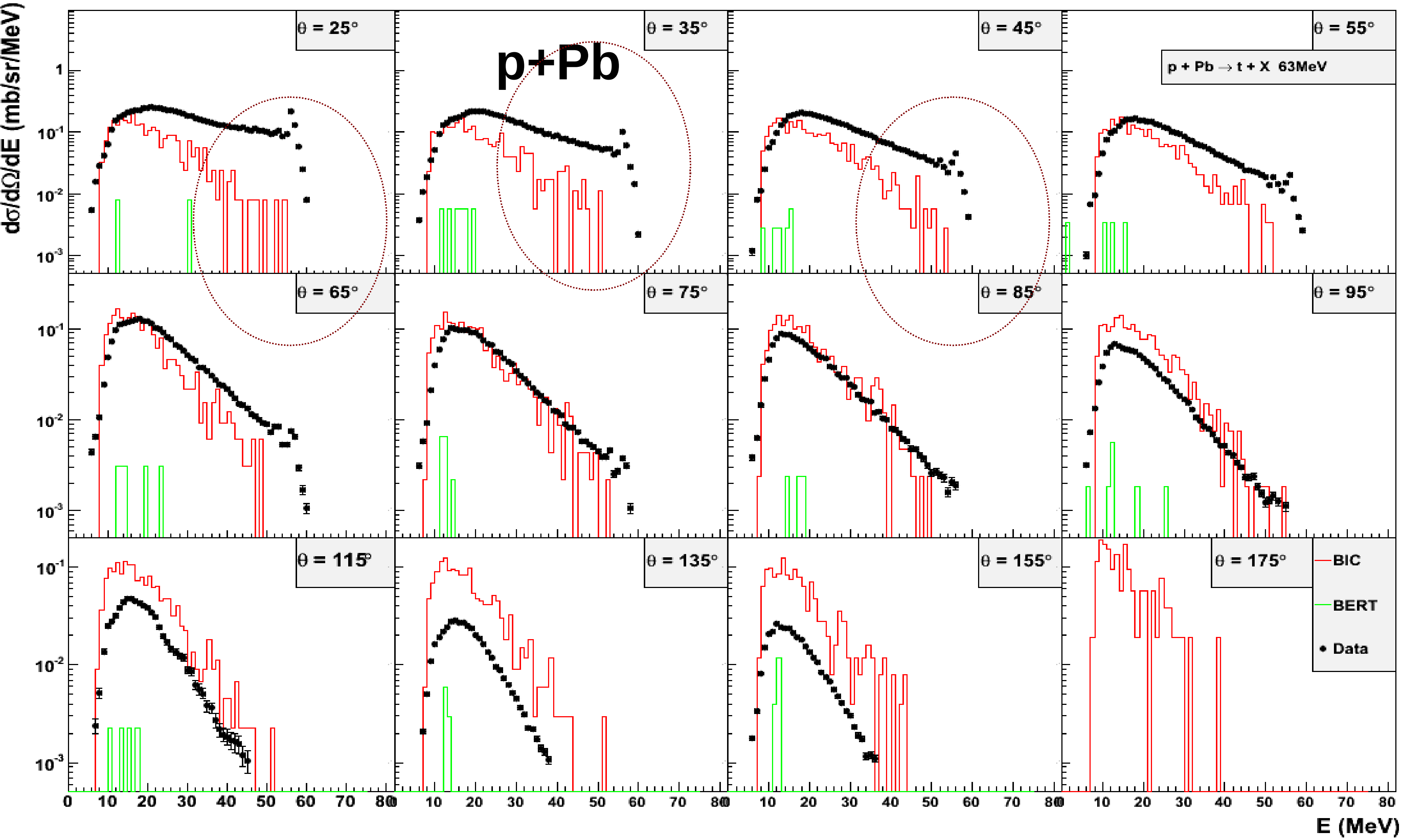
Deuteron production at 1200 MeV



Deuteron production at 1200 MeV



Tritium production at 63 MeV



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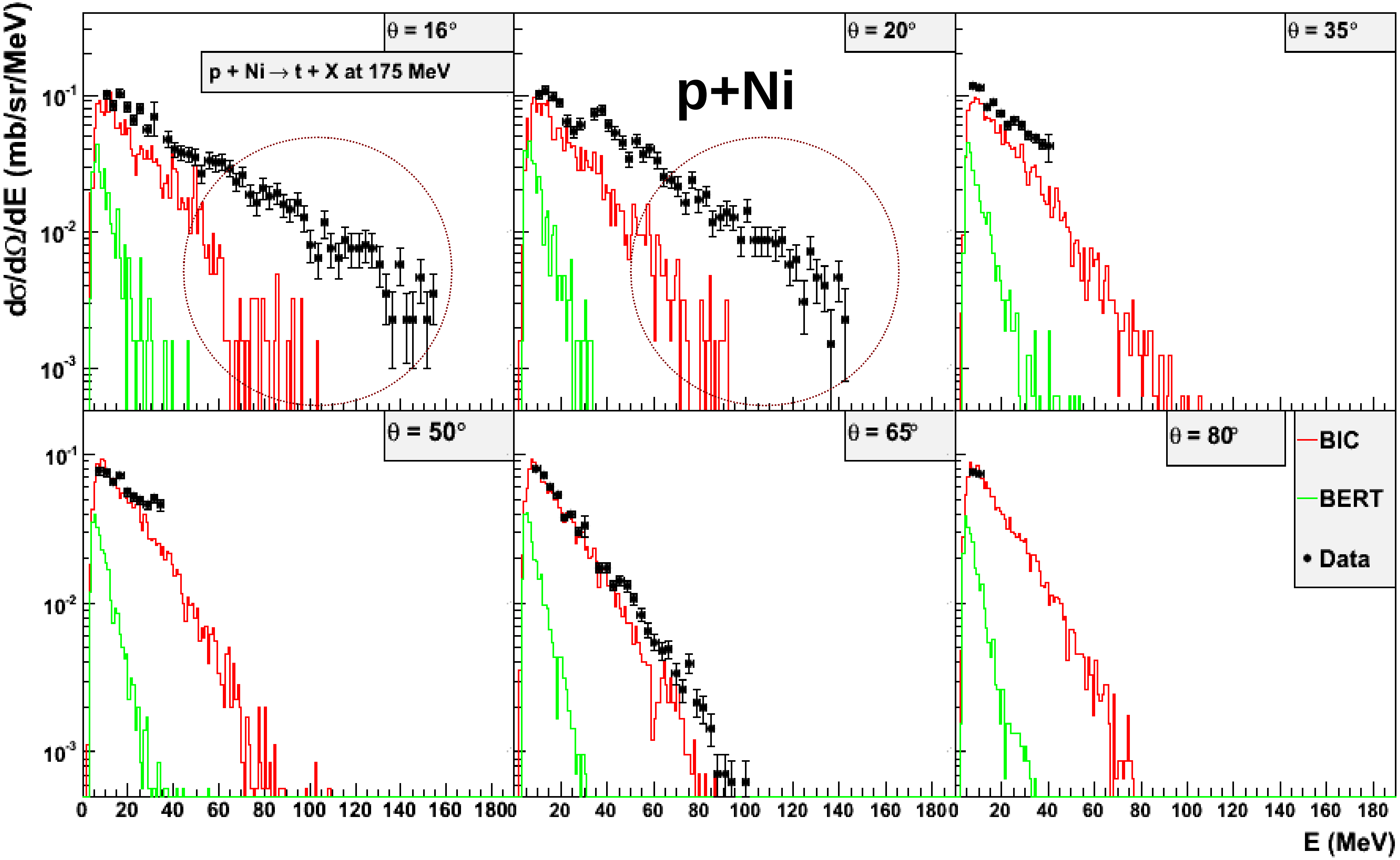
Tritium production at 175 MeV



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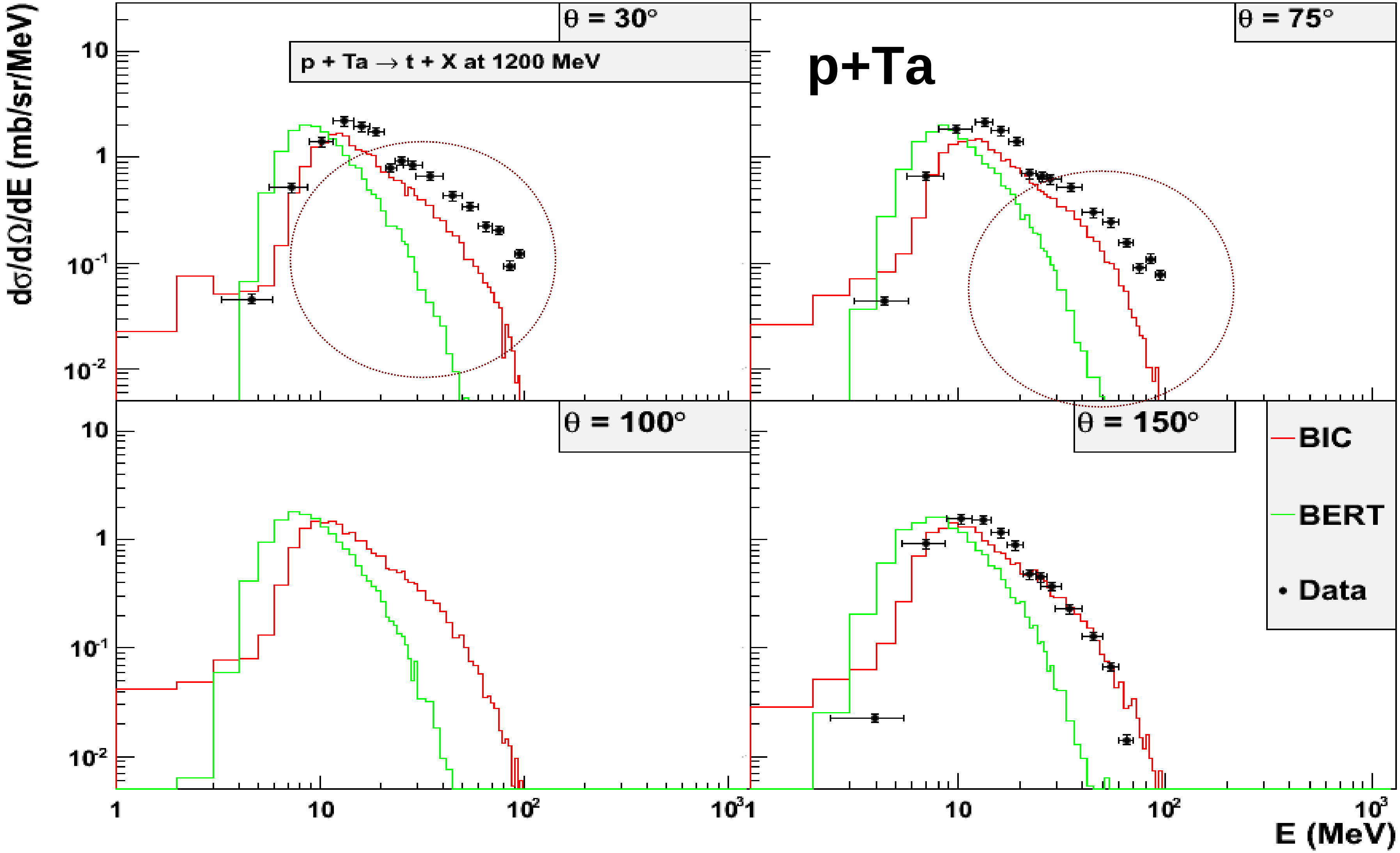
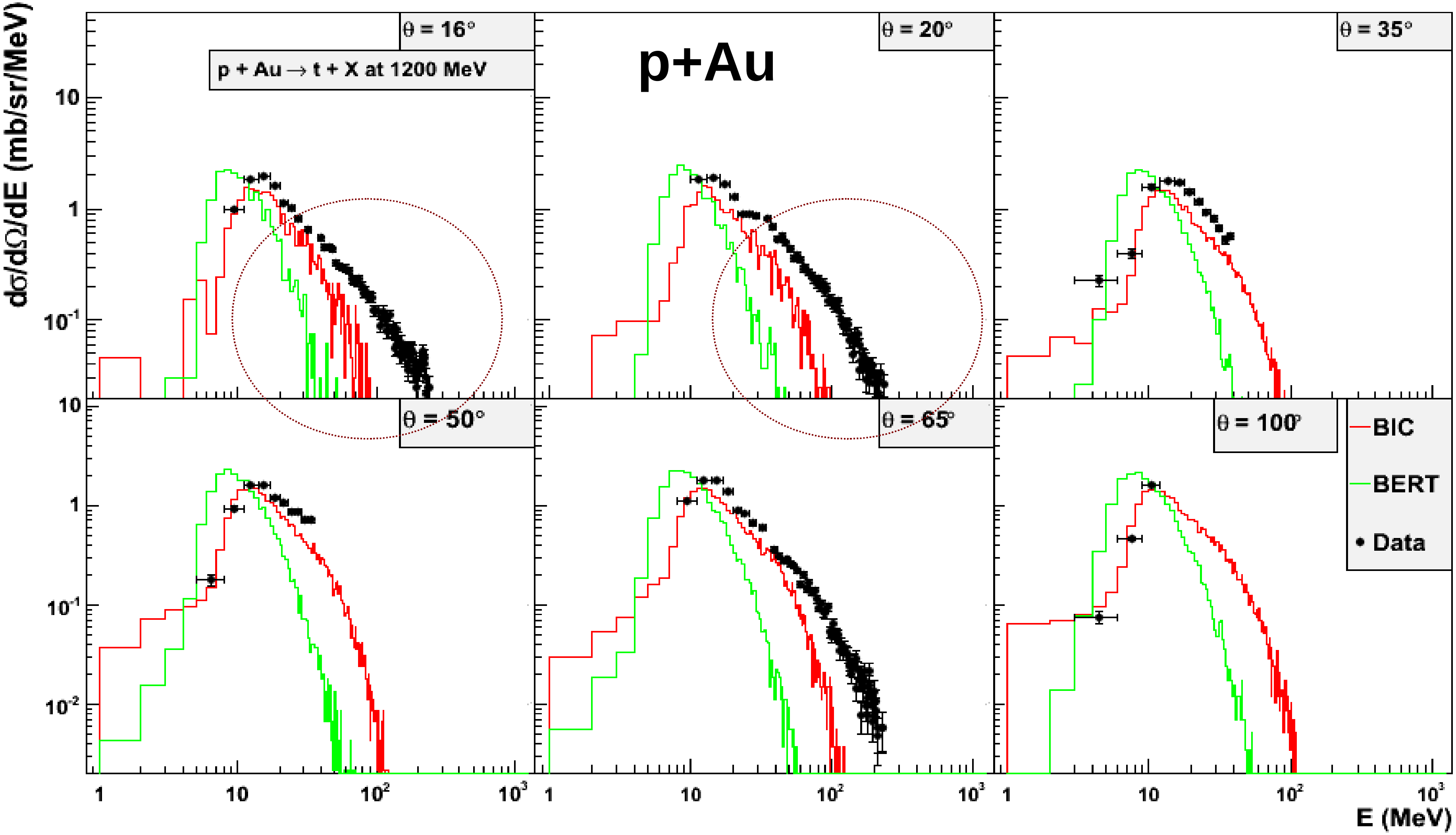
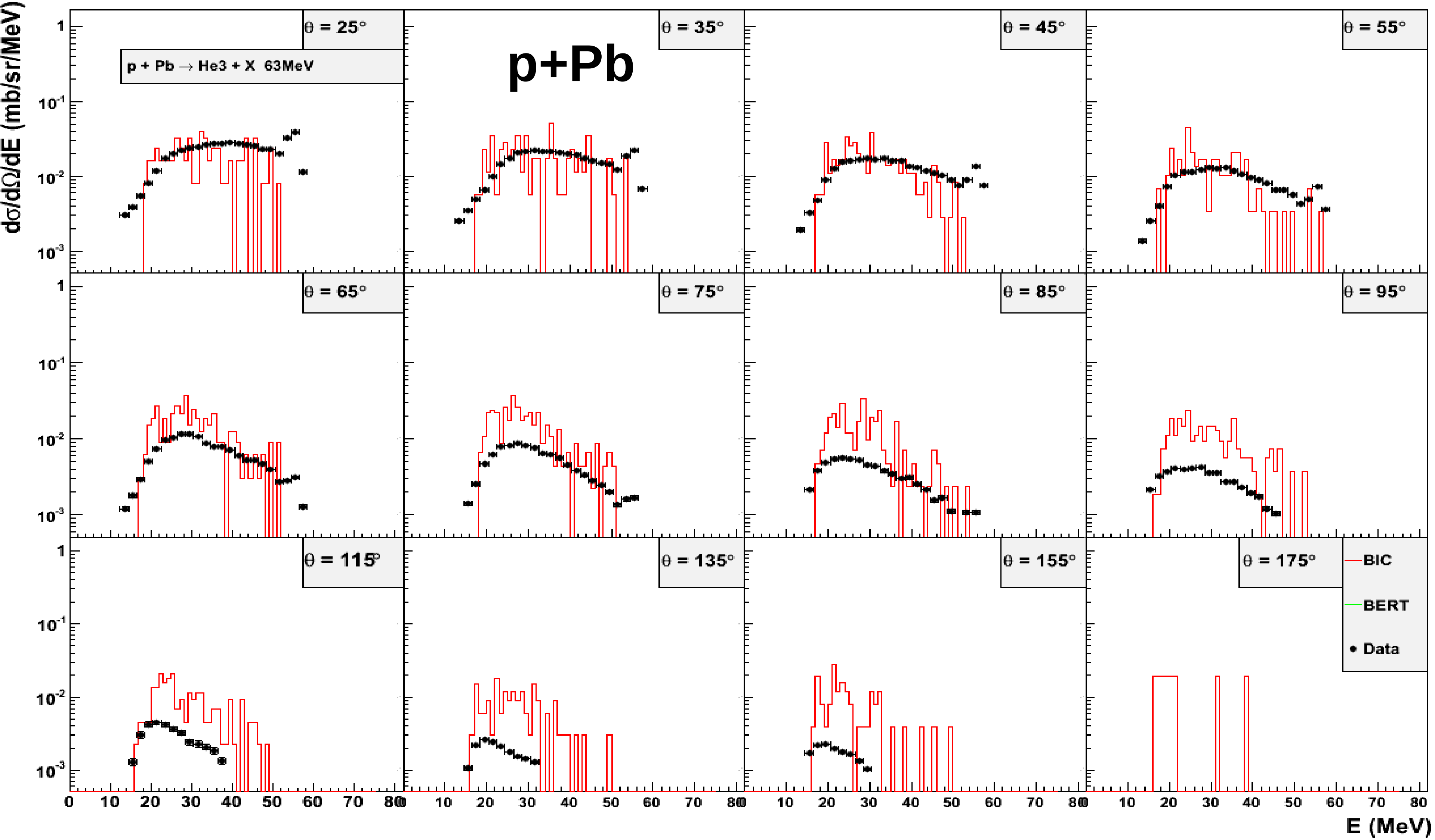
Tritium production at 1200 MeV



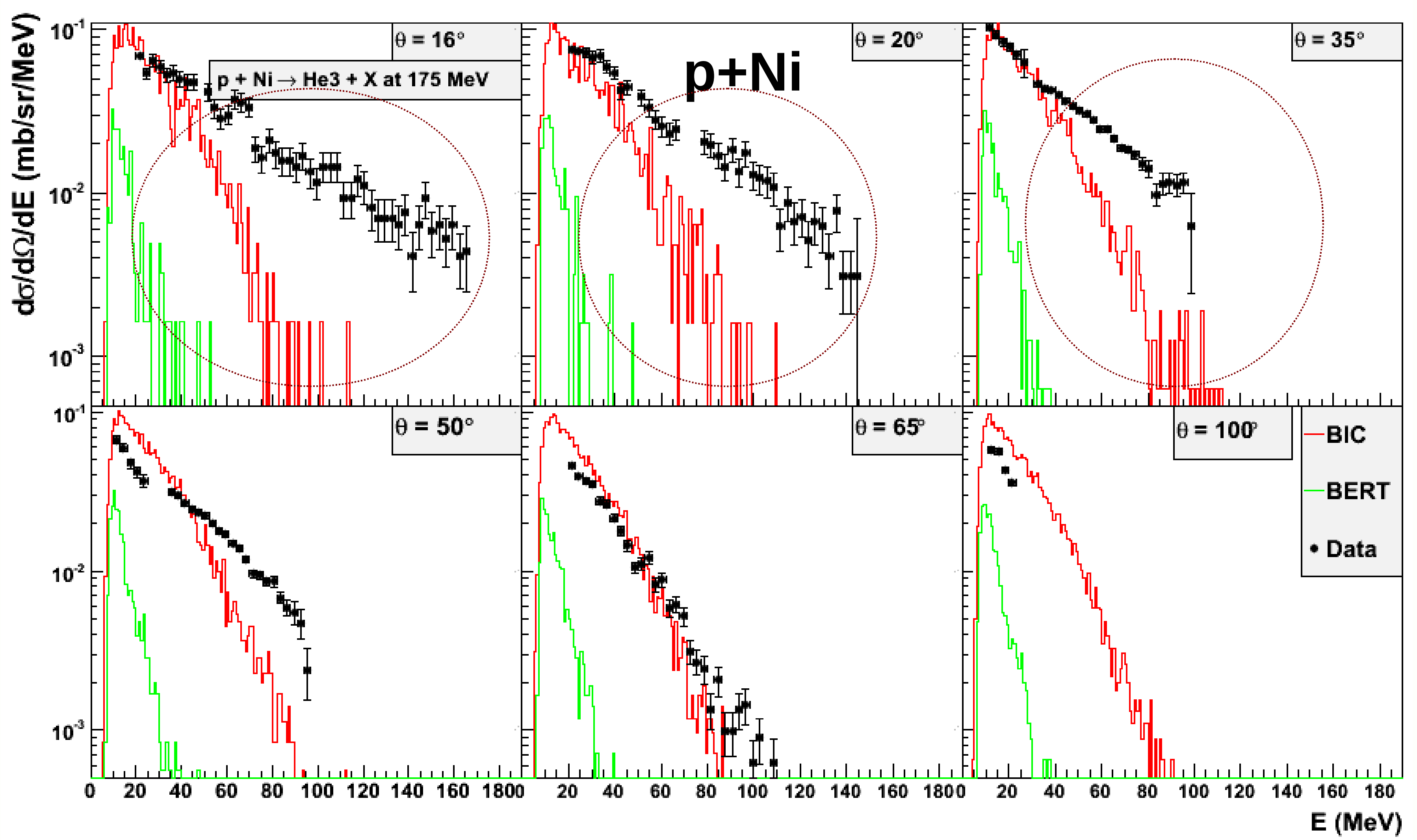
Tritium production at 1200 MeV



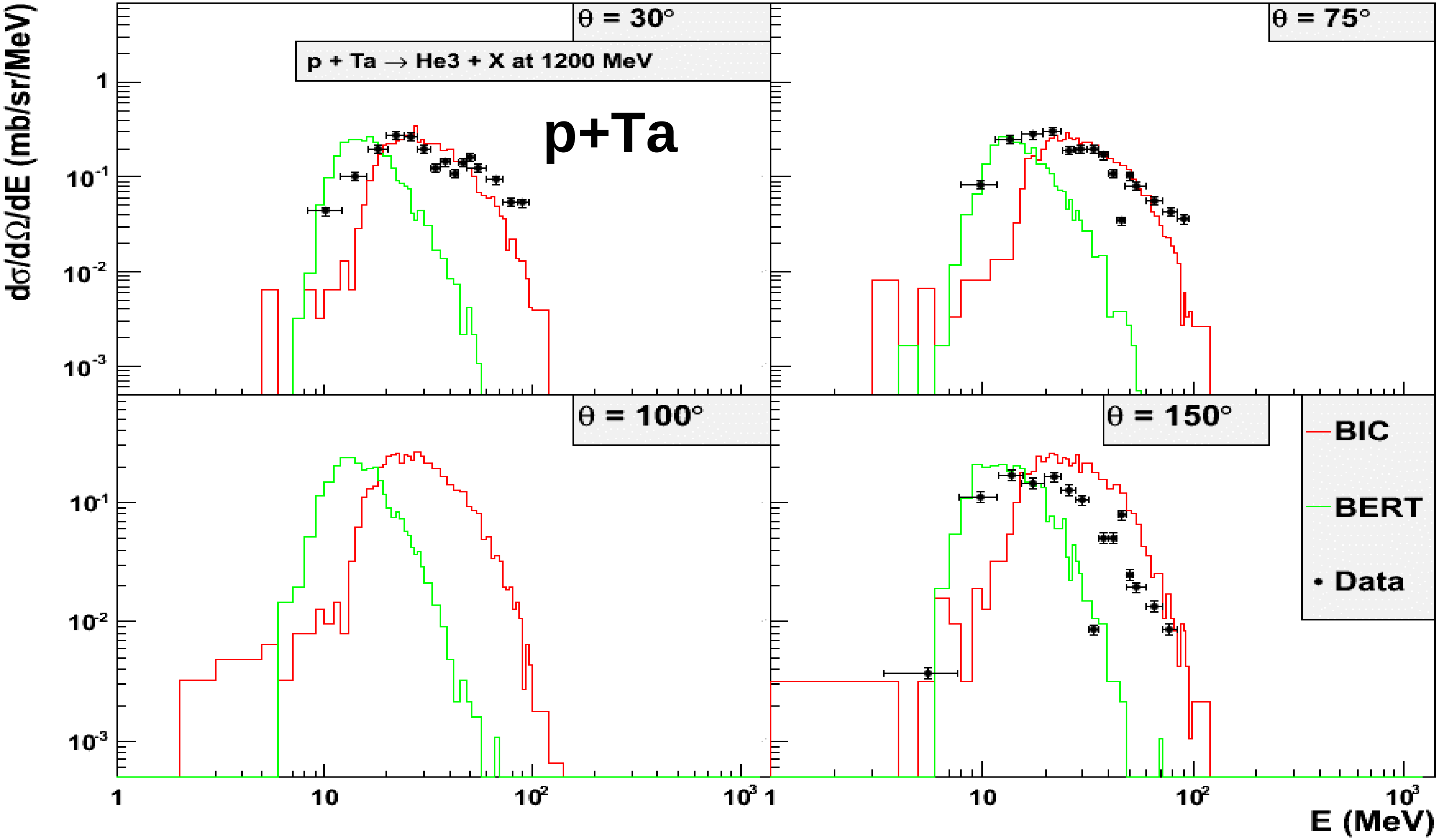
^{3}He production at 63 MeV



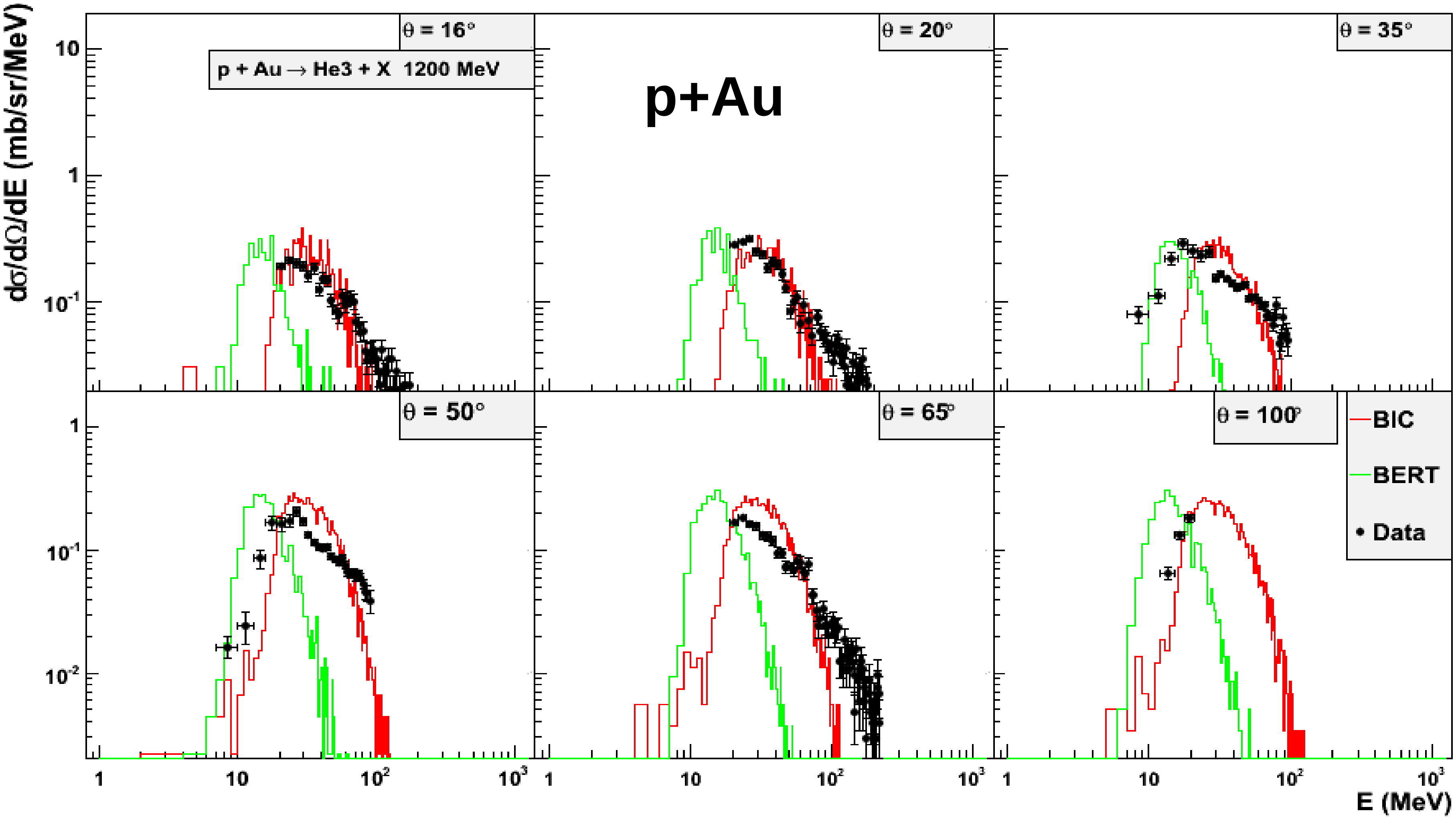
^{3}He production at 175 MeV



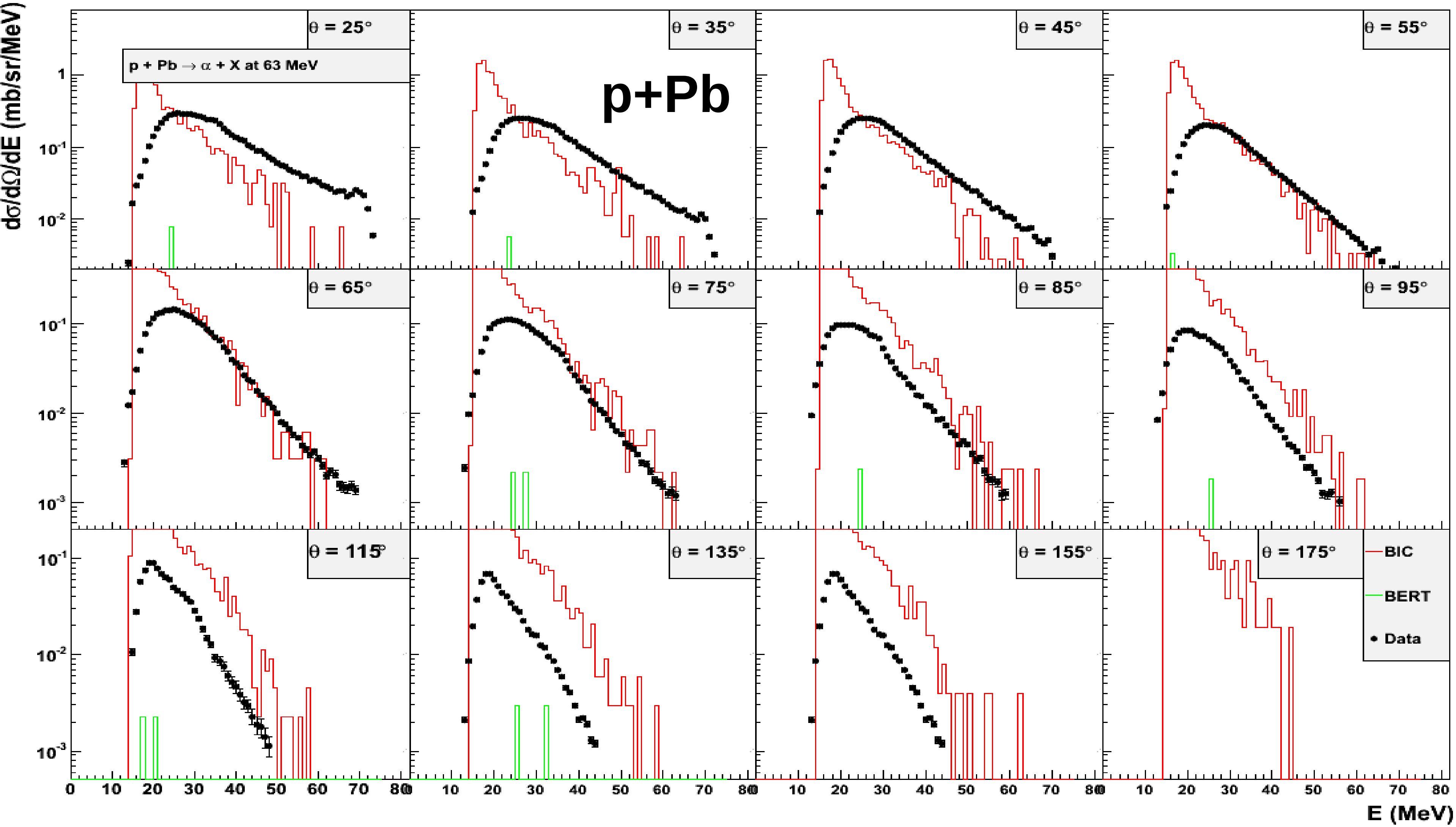
^{3}He production at 1200 MeV



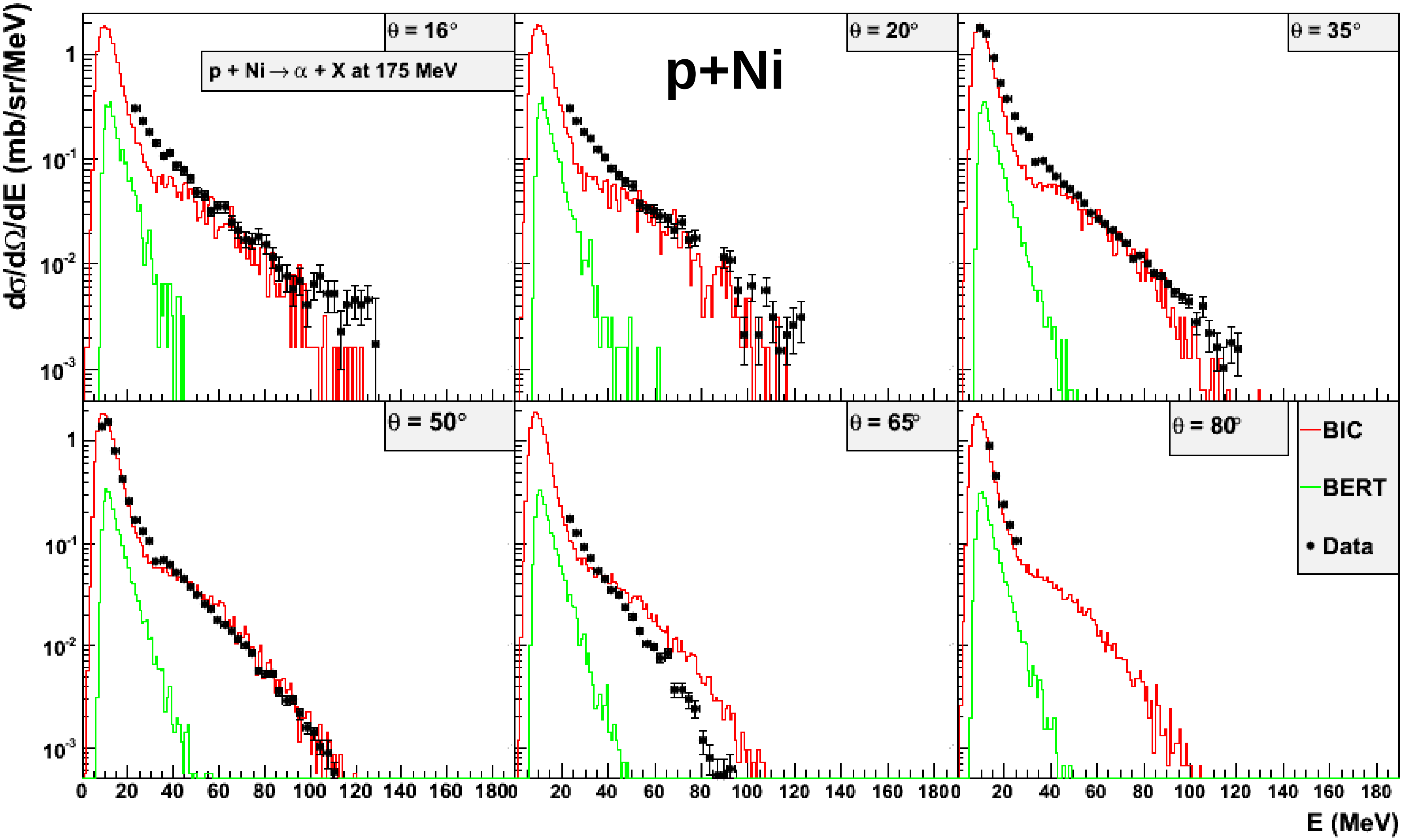
^{3}He production at 1200 MeV



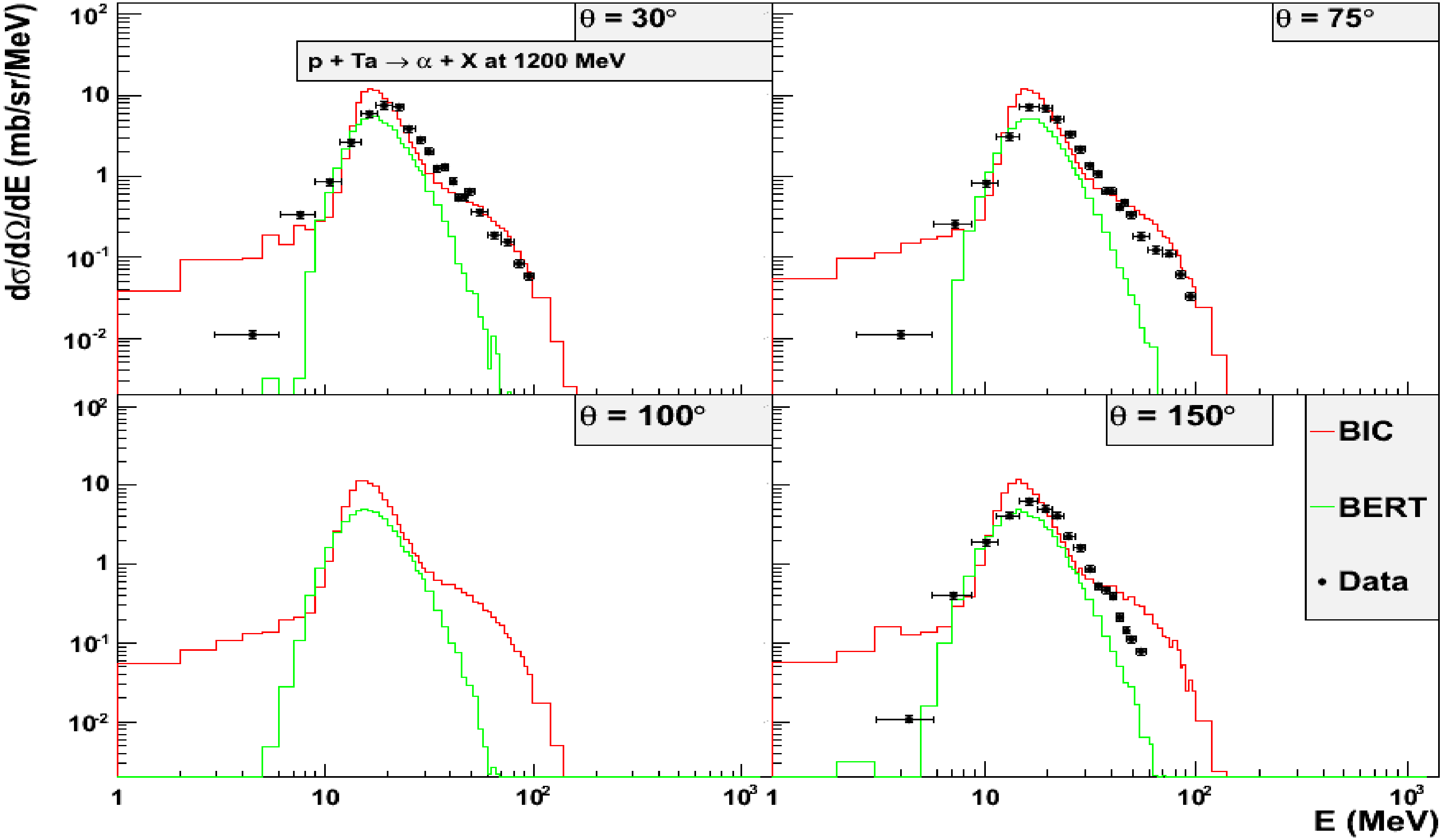
Alpha production at 63 MeV



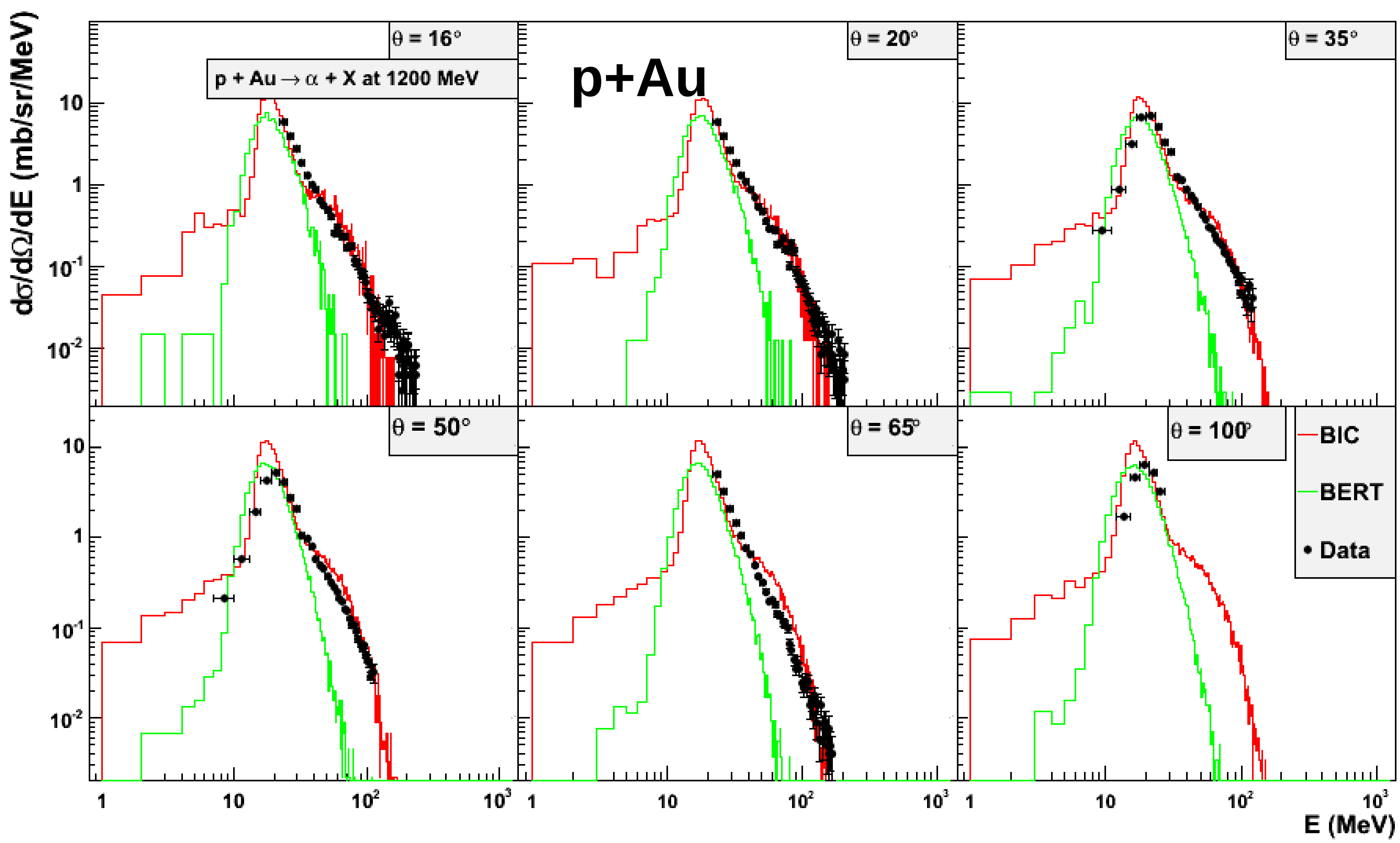
Alpha production at 175 MeV



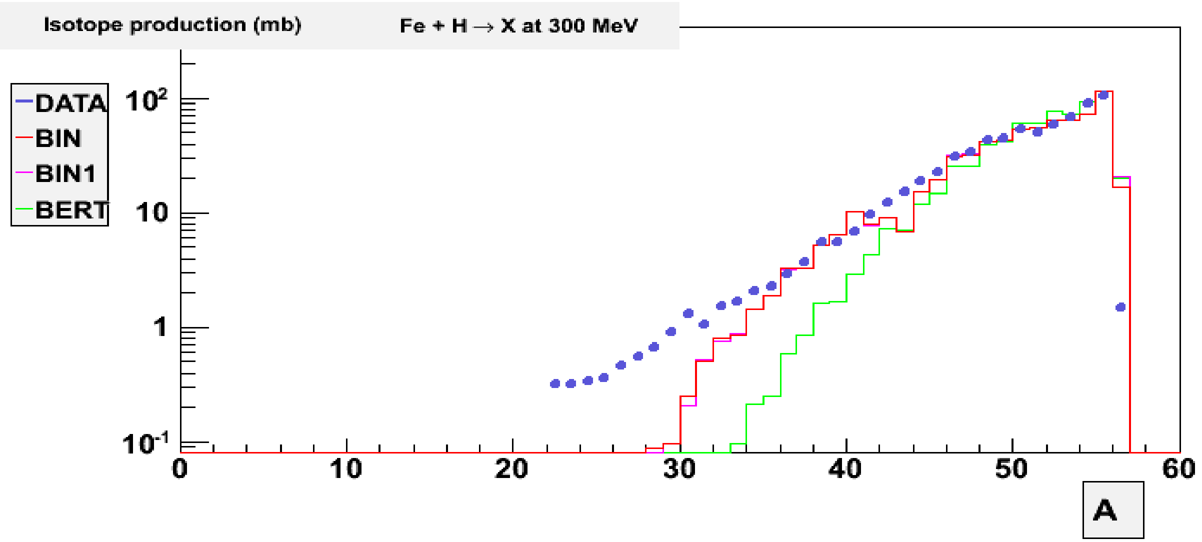
Alpha production at 1200 MeV



Alpha production at 1200 MeV

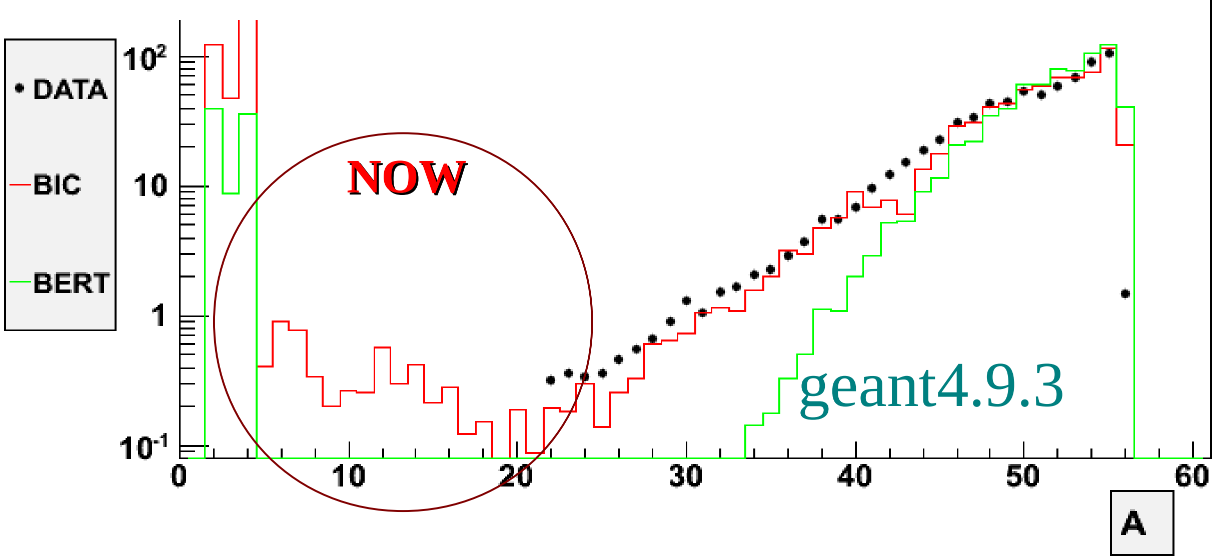


Isotopic distribution at 0.3 GeV



Fe+p @ 0.3 GeV

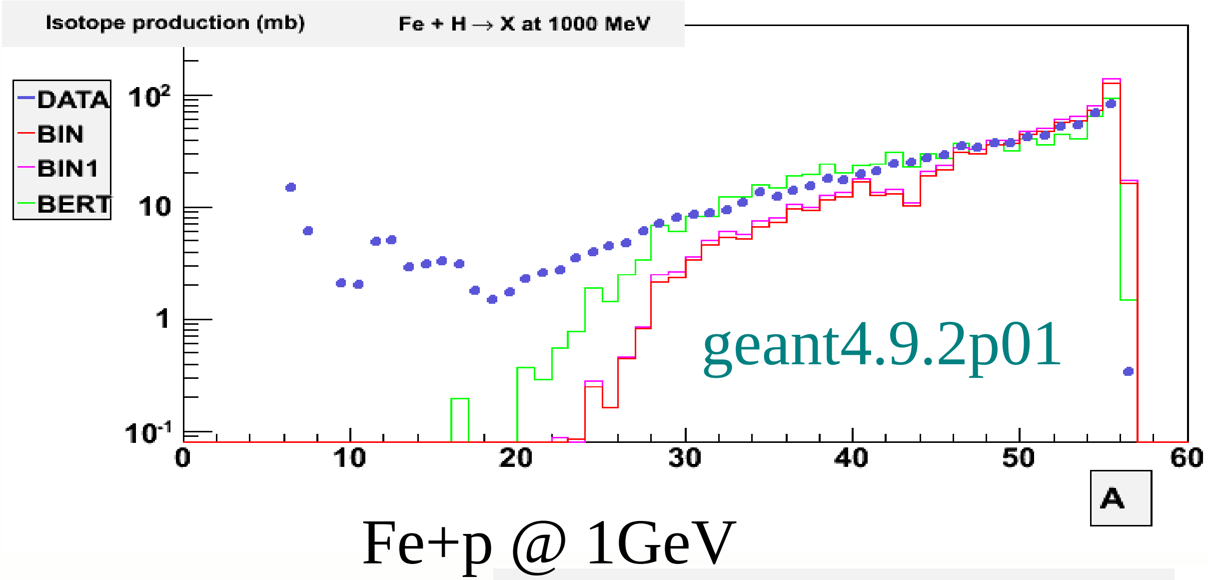
after GEM inclusion



NOW

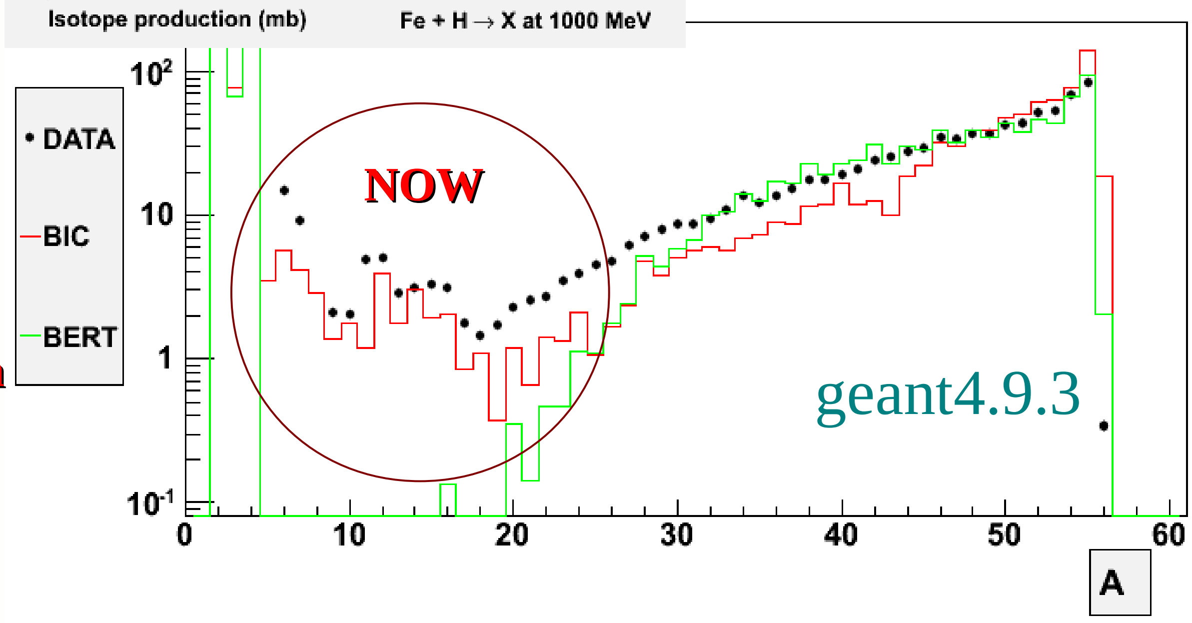
geant4.9.3

Isotopic distribution at 1GeV



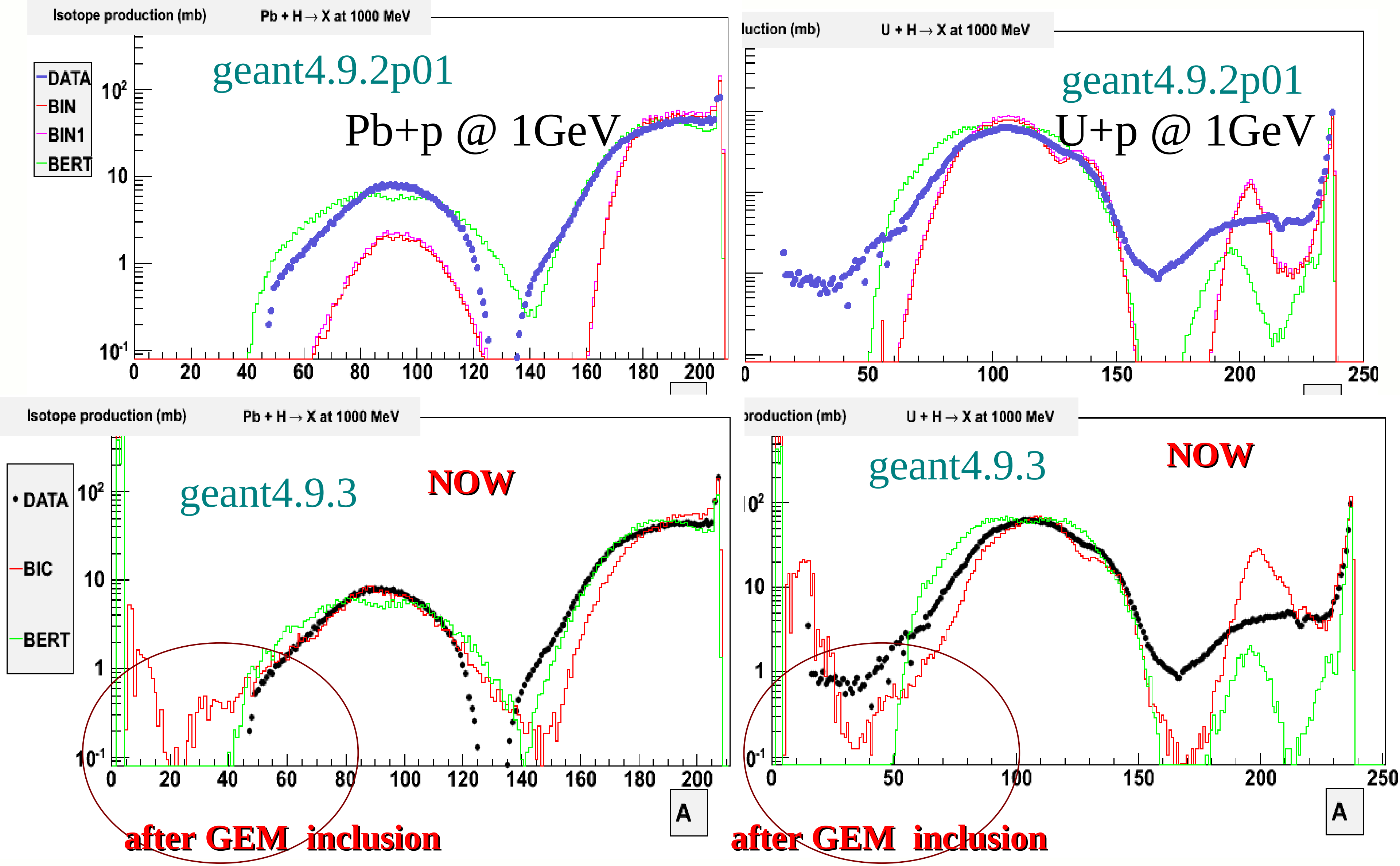
p+Fe

Fe+p @ 1GeV



after GEM inclusion

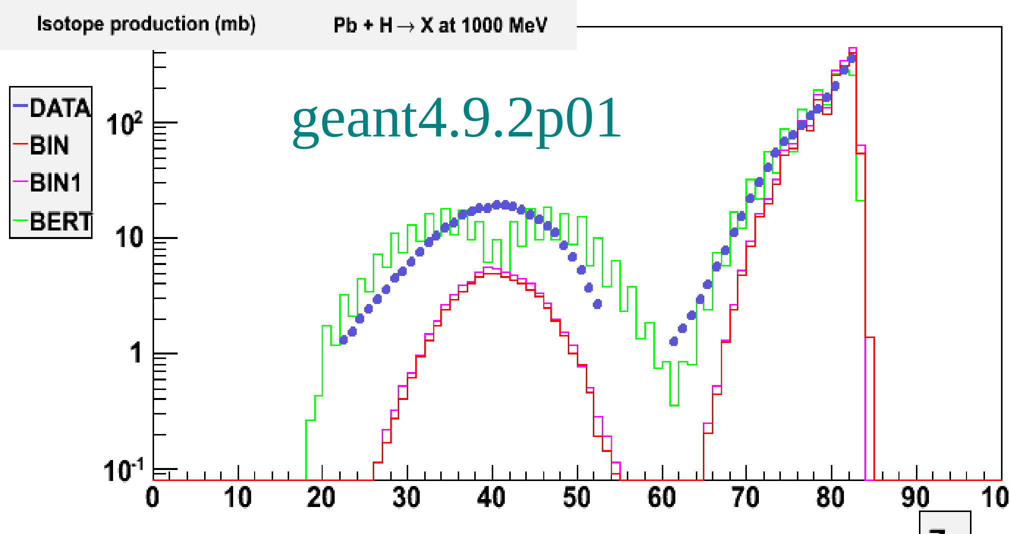
Isotopic distribution at 1 GeV



after GEM inclusion

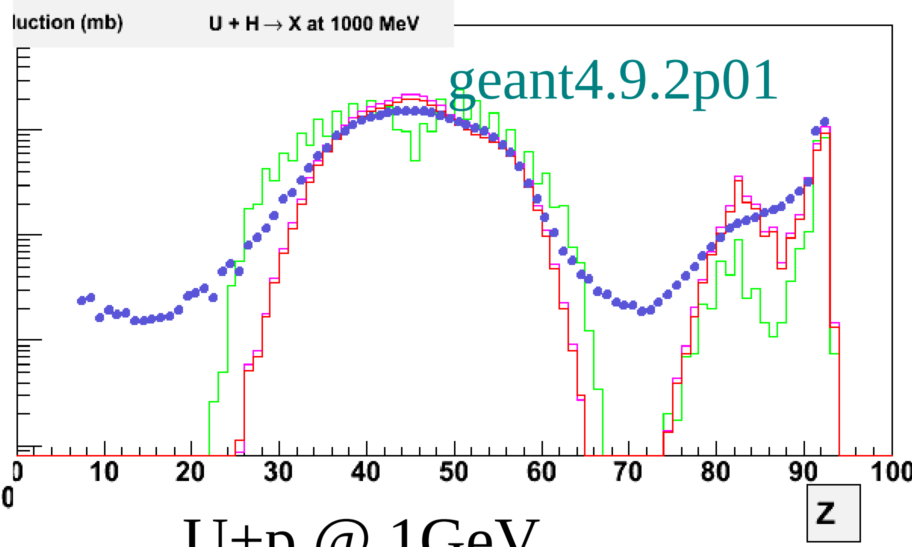
after GEM inclusion

Isotopic distribution at 1 GeV



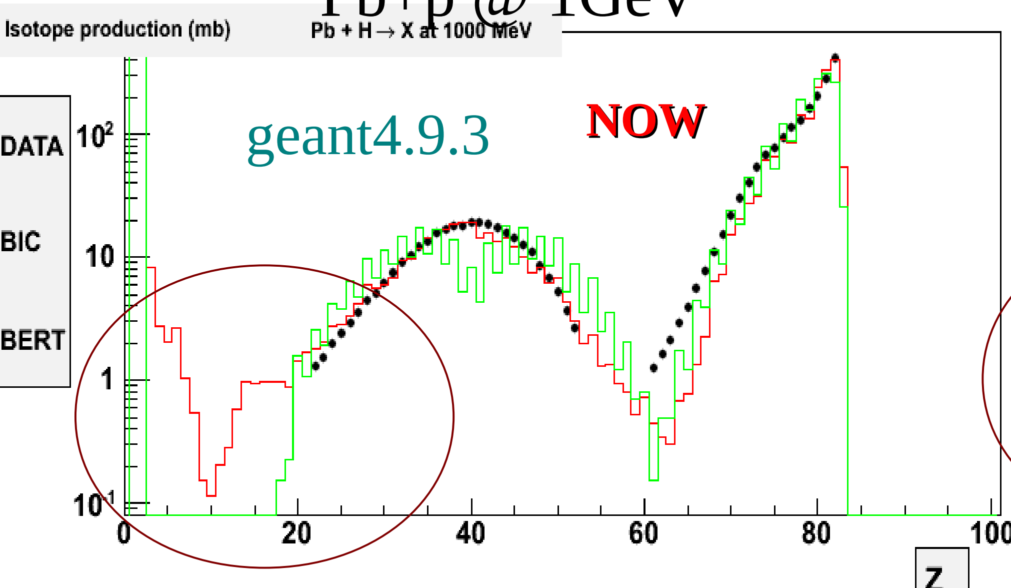
geant4.9.2p01

Pb+p @ 1GeV



geant4.9.2p01

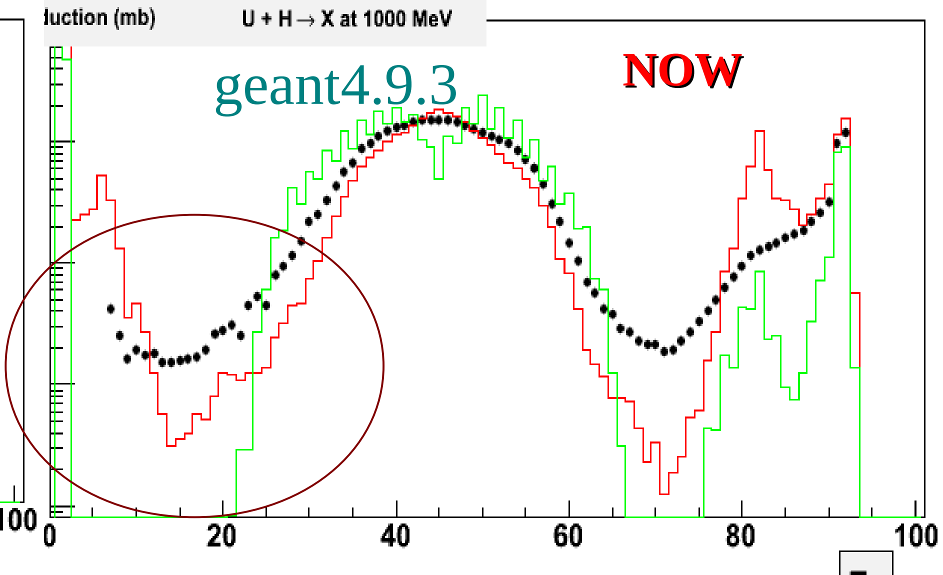
U+p @ 1GeV



geant4.9.3

NOW

after GEM inclusion



geant4.9.3

NOW

after GEM inclusion

Work in progress (I)

(in development version, not yet in official release)

- 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 makes performance at fission worse.

- A new algorithm for n_{eq} has been implemented (based on physical criterion of equilibration of transition probabilities, i.e. *exact* calculation for each fragment) , instead of

$$n_{eq} \sim \sqrt{2gU}$$

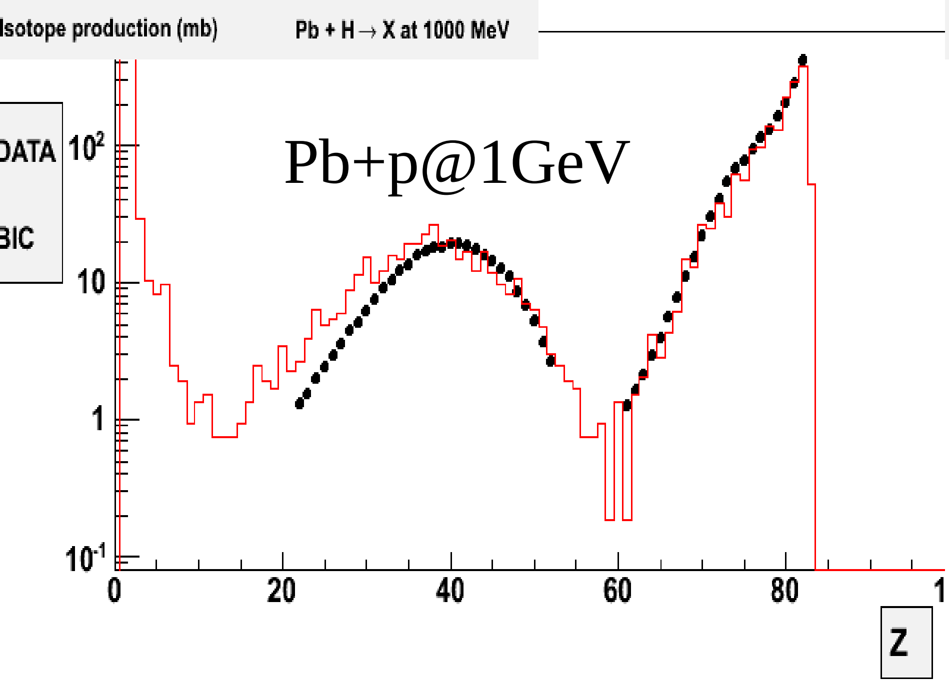
- The *diffusivity* (σ_{pre}) of the transition has been drastically reduced (i.e. transition is now sharper)

Work in progress (II)

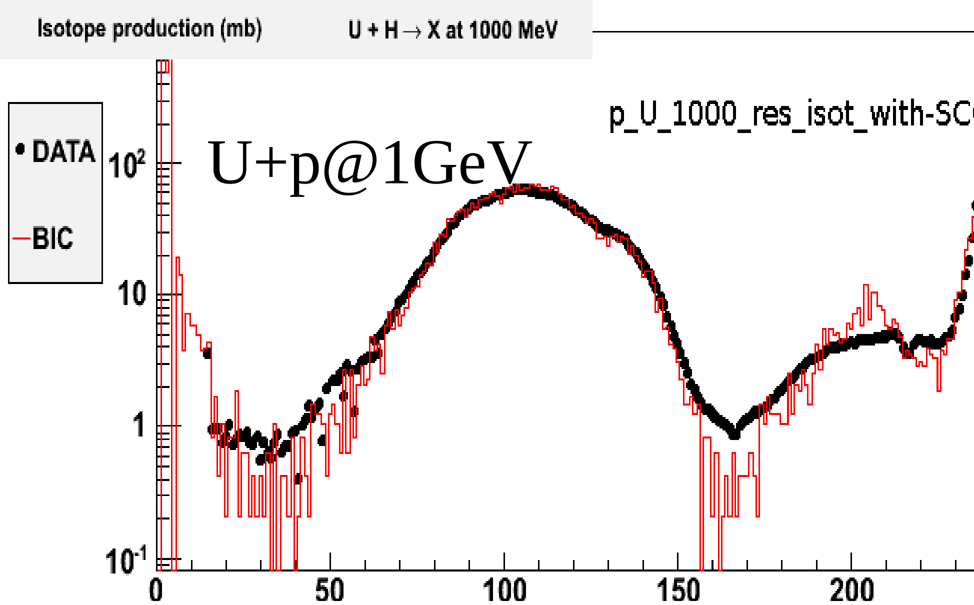
(in development version, not yet in official release)

- 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

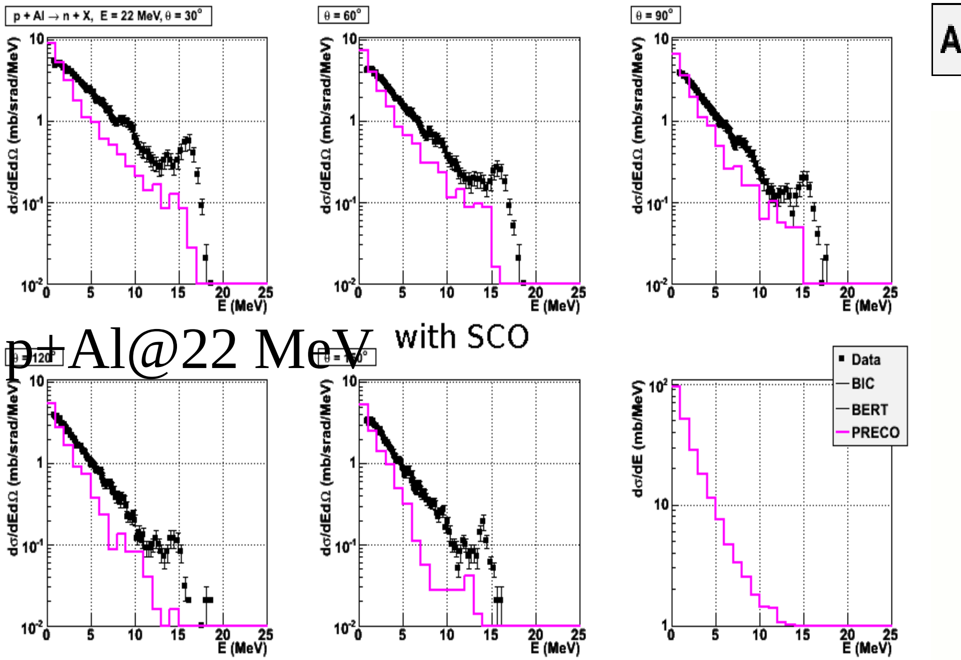
Present situation (preliminary results)



Pb+p@1GeV



U+p@1GeV



p+Al@22 MeV

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

J.

Conclusions (1)

- Bertini agrees better with data for:
  - pion production (high and low energy)

- Binary agrees better with data for:
  - neutron production
  - low and medium energy protons
  - light ion production
  - isotopic distribution

    (price to pay: BIC is abut 9 times slower than Bertini for Pb+H @ 1GeV)

- Cases where neither model is better overall
  - one model may be better for forward angles, the other for backward angles
- The fact that we cannot say that one model is clearly better than the other emphasizes the need for alternate models in same energy range

Conclusions (2)

- This benchmark study demonstrated areas where improvement is needed. As a result:
  - recently made **improvements to pre-compound**
    - *soft* transition to equilibrium has been tuned
  - recently made **improvements to de-excitation**:
    - IMF evaporation (GEM model)
  - recently made **improvements to fission**
    - fission parameters have been tuned
    - improvements are still possible (angular momentum dependence of fission barrier?)
- plan to add **coalescence models for cascade stage:**
  - The underestimation in the fast cluster yield (especially deuterons) at small angles clearly points to the direct mechanism of complex particle production

Thanks for your attention