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

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on behalf of the Geant4 Hadronic Group
IAEA, Vienna, 05.05.2009

General Introduction

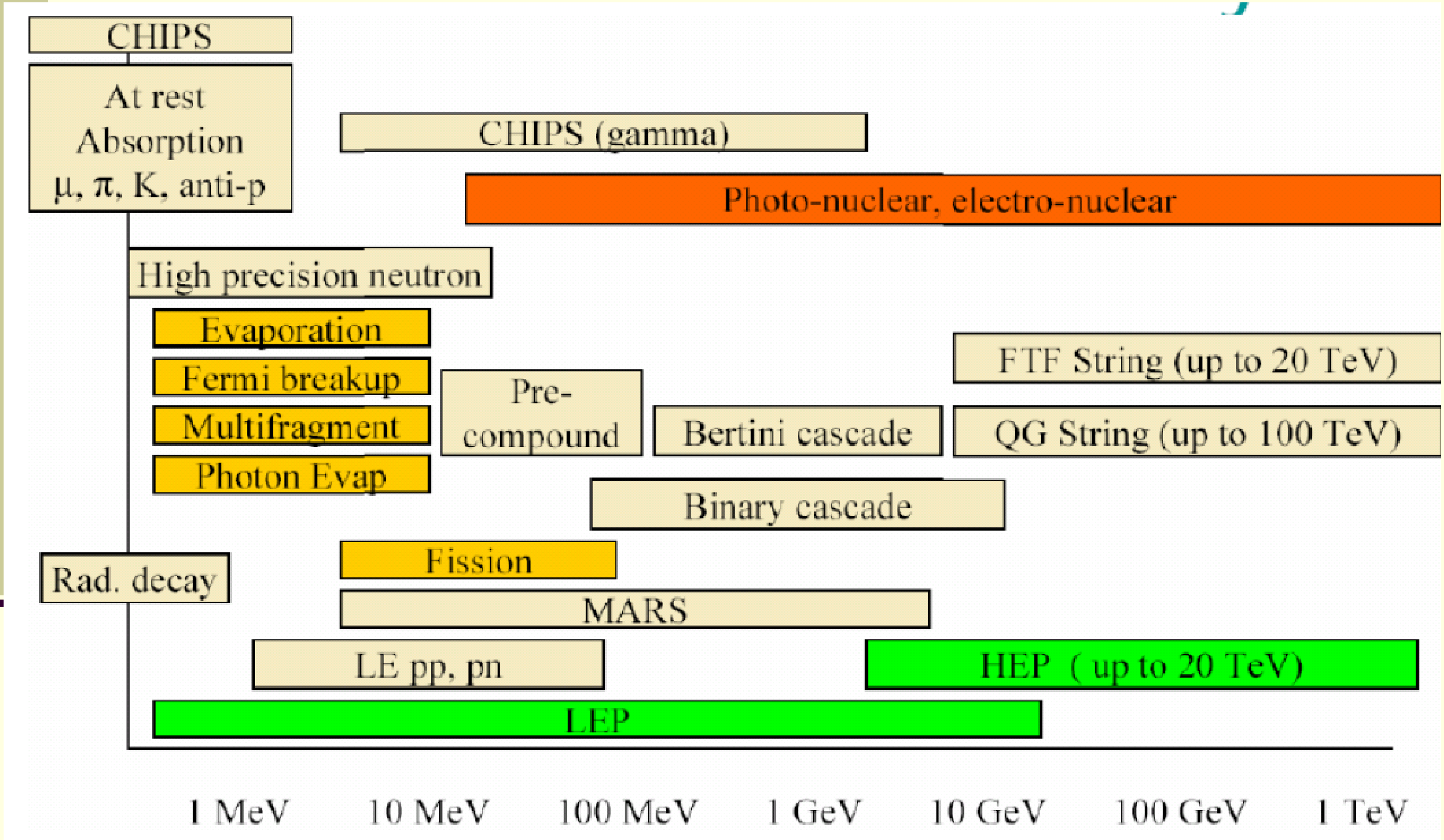
What is Geant4?

- 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



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

- Cascade models all have nuclear de-excitation models embedded in them

Why several 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**, Chiral invariant phase space, :
  - Quark-level event generator for the fragmentation of hadronic systems into hadrons.
  - Includes nonrelativistic phase space of nucleons to explain evaporation

- **INCL/ABLA** :
  - C++ translation of INCL intranuclear cascade code
  - C++ translation of ABLA evaporation/fission code

Geant4 Bertini Cascade: Origin

- 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
- Similar methods used in many different intra-nuclear transport codes

Applicability of the Bertini Cascade

- 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
- in principle, can be extended to:
  - anti-baryons
  - ion-ion collisions

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
  - numerically integrated equation of motion

The Nuclear model

- Nucleon momenta are sampled assuming Fermi gas model
- Nuclear density
  - harmonic oscillator for A < 17
  - Woods-Saxon for others
- Sampling is done in a correlated manner:
  - local phase-space densities are constrained by Pauli principle
  - sum of all nucleon momenta must equal zero

Inverse reaction cross sections (preequilibrium & equilibrium)

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

- Theory driven (old) parameterization (Dostrovski et al, 1959)

New parameterization:

- More realistic parameterization of reaction cross sections (Kalbach), calculated with global optical model potentials, in turn fitted to reproduce available experimental data (angular distributions, elastic scattering, total cross sections, etc..).

Remarks

- 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) .

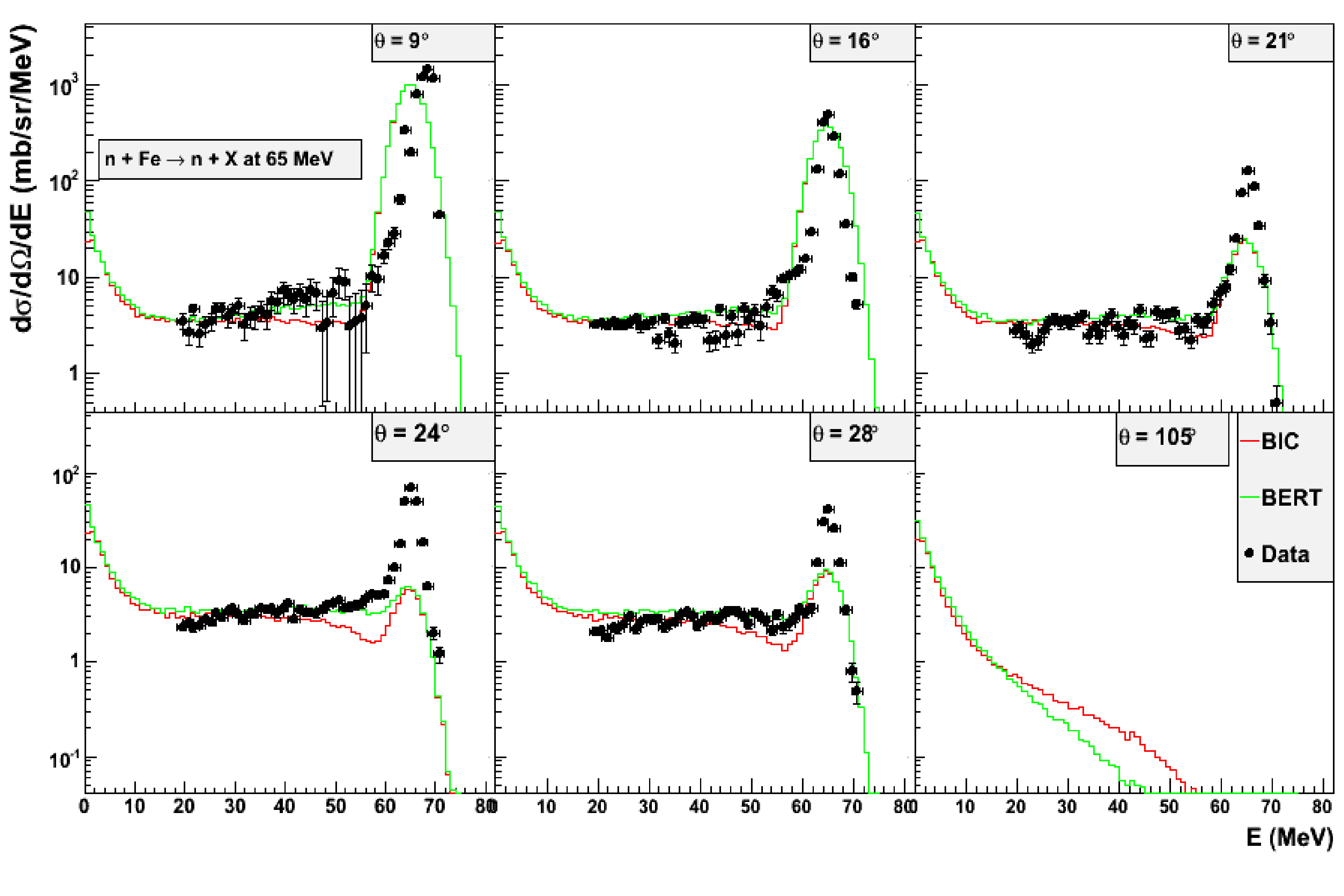
- Very important: parameters tuned in a “model suite” shuldn’t be assumed to work in a different *environment*, i.e. with different coupled models.

Quite likely, ad hoc tuning of parameters will be necessary in order to reproduce fission data.

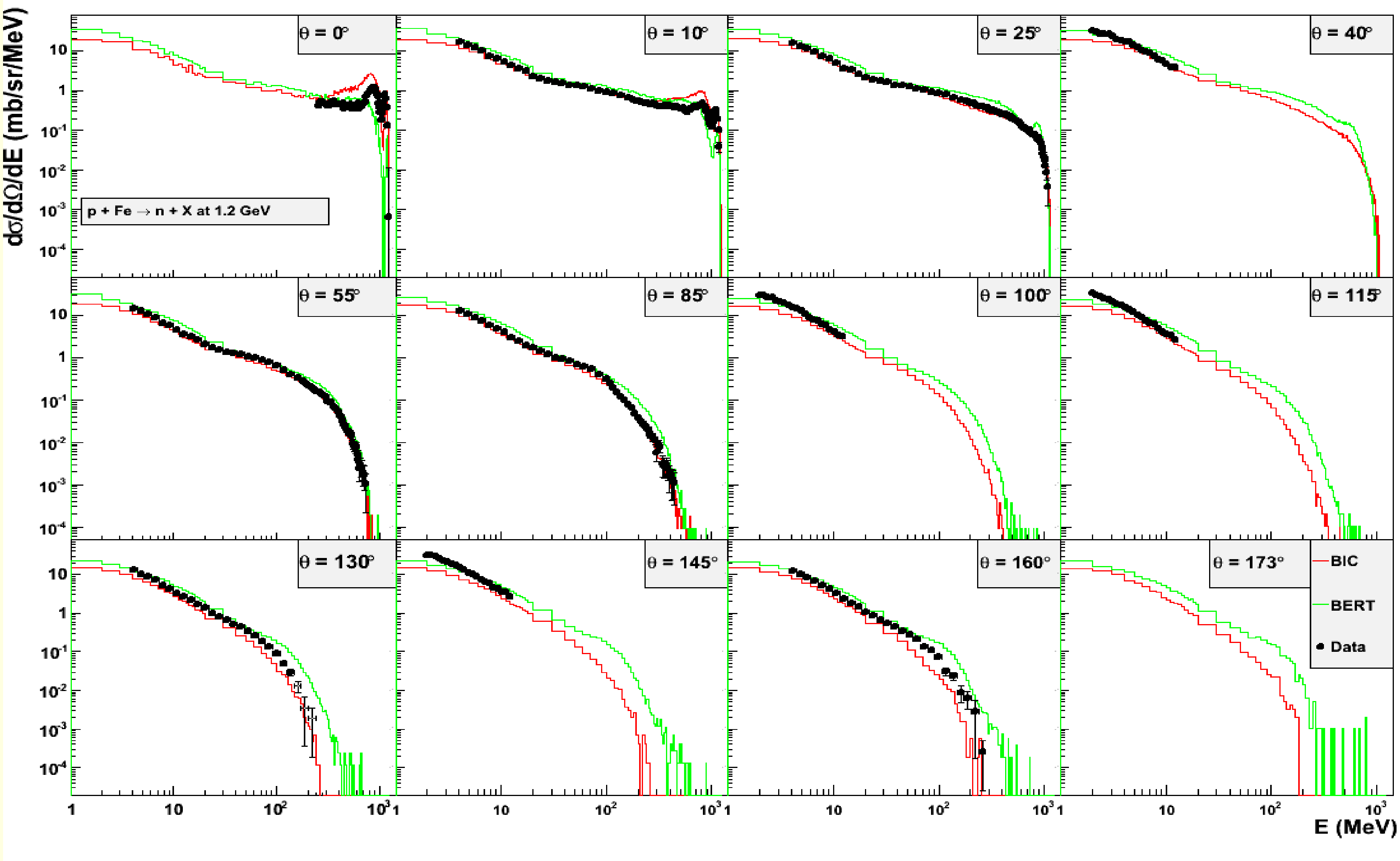
RESULTS

(Geant4 official release 9.2 patch p01)

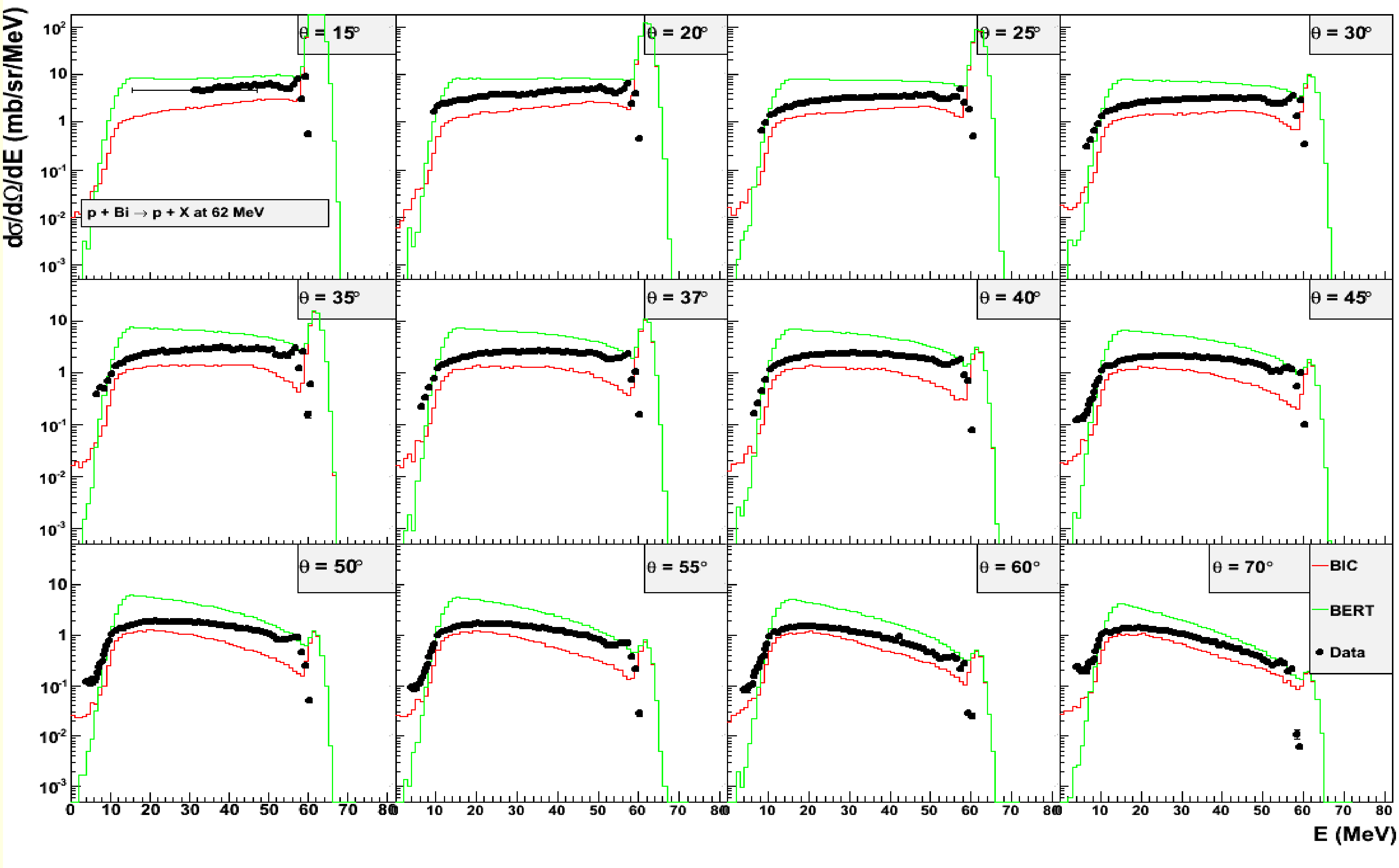
Neutron production at 63 MeV



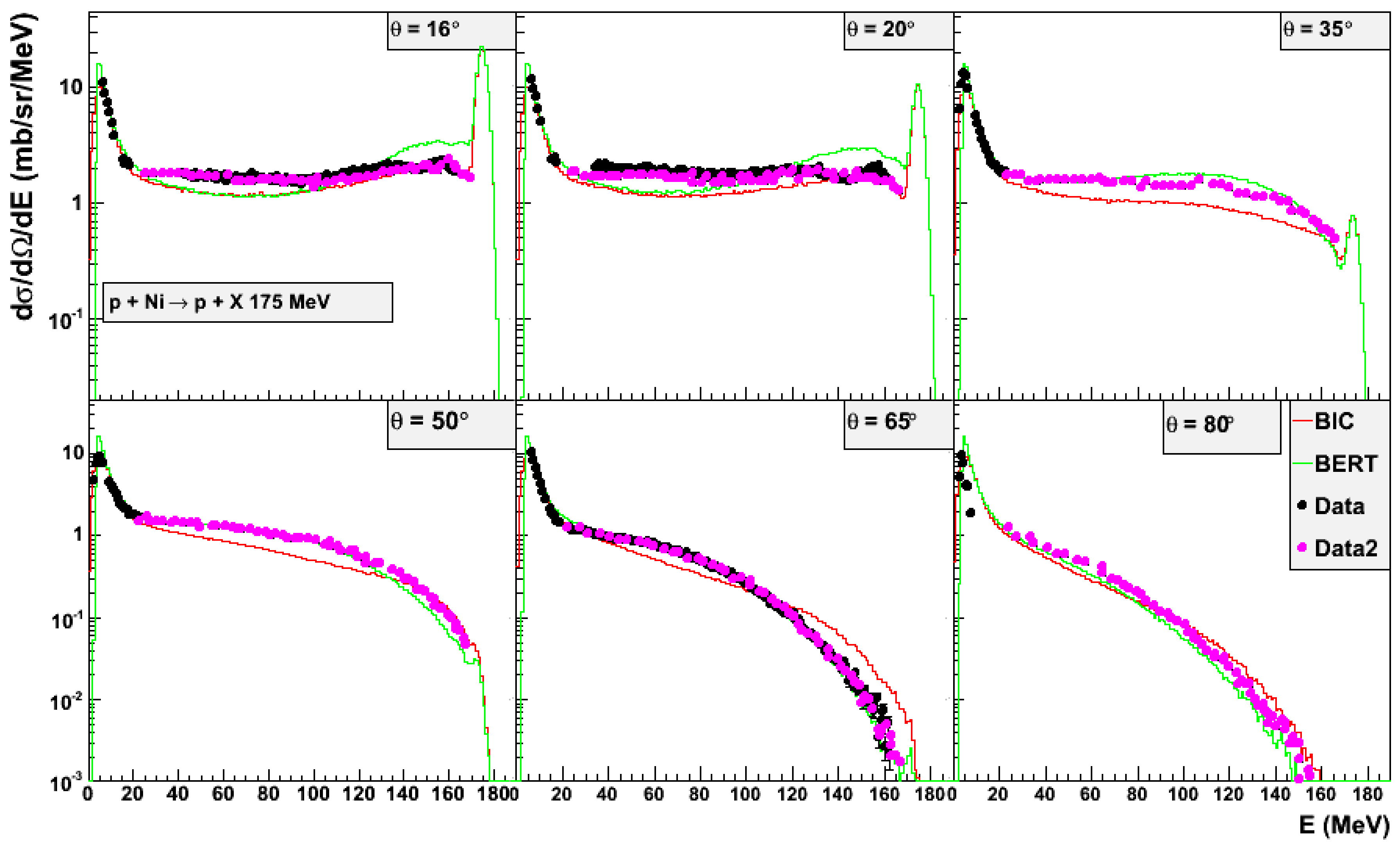
Neutron production at 1200 MeV



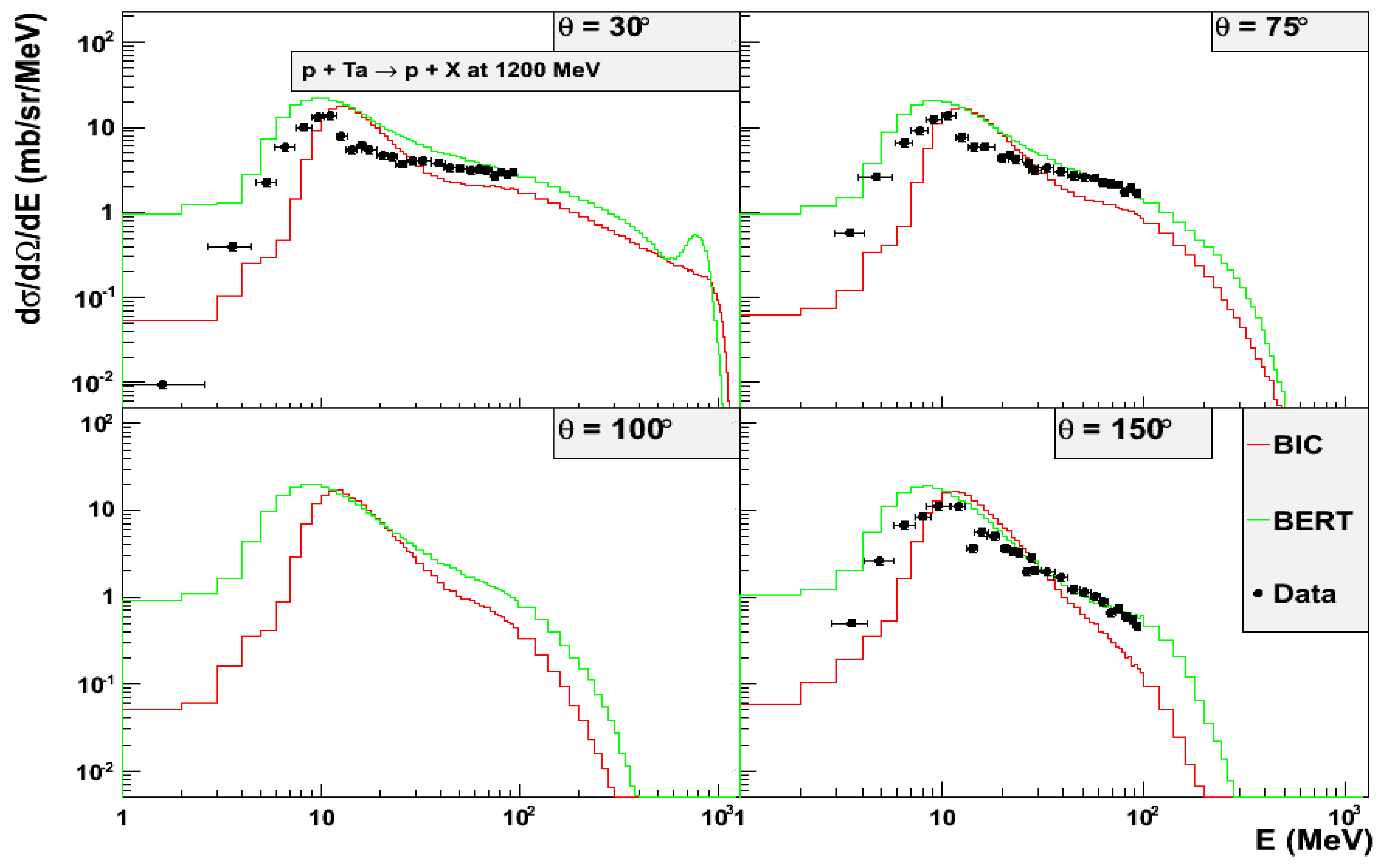
Proton production at 62 MeV



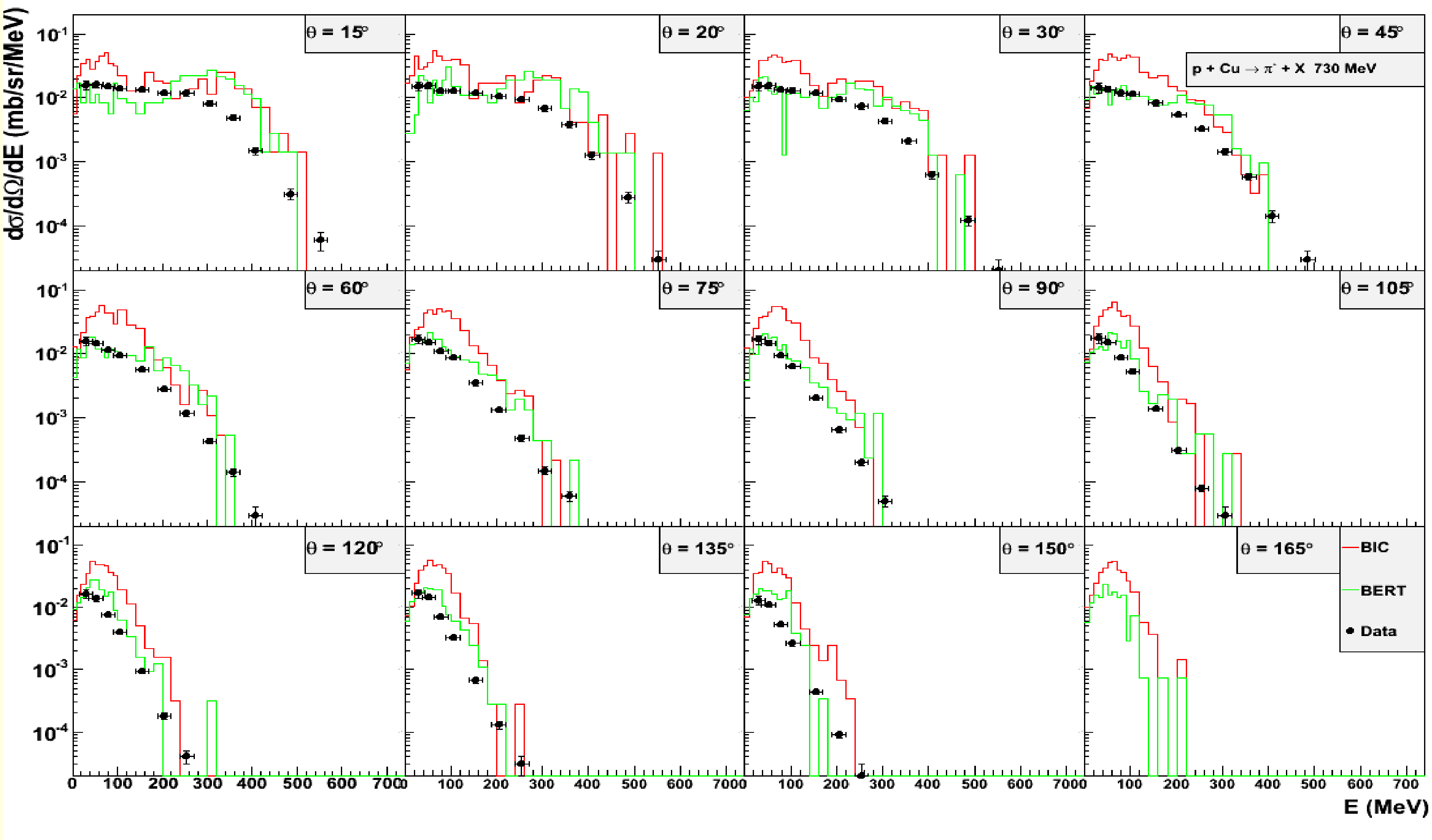
Proton production at 175 MeV



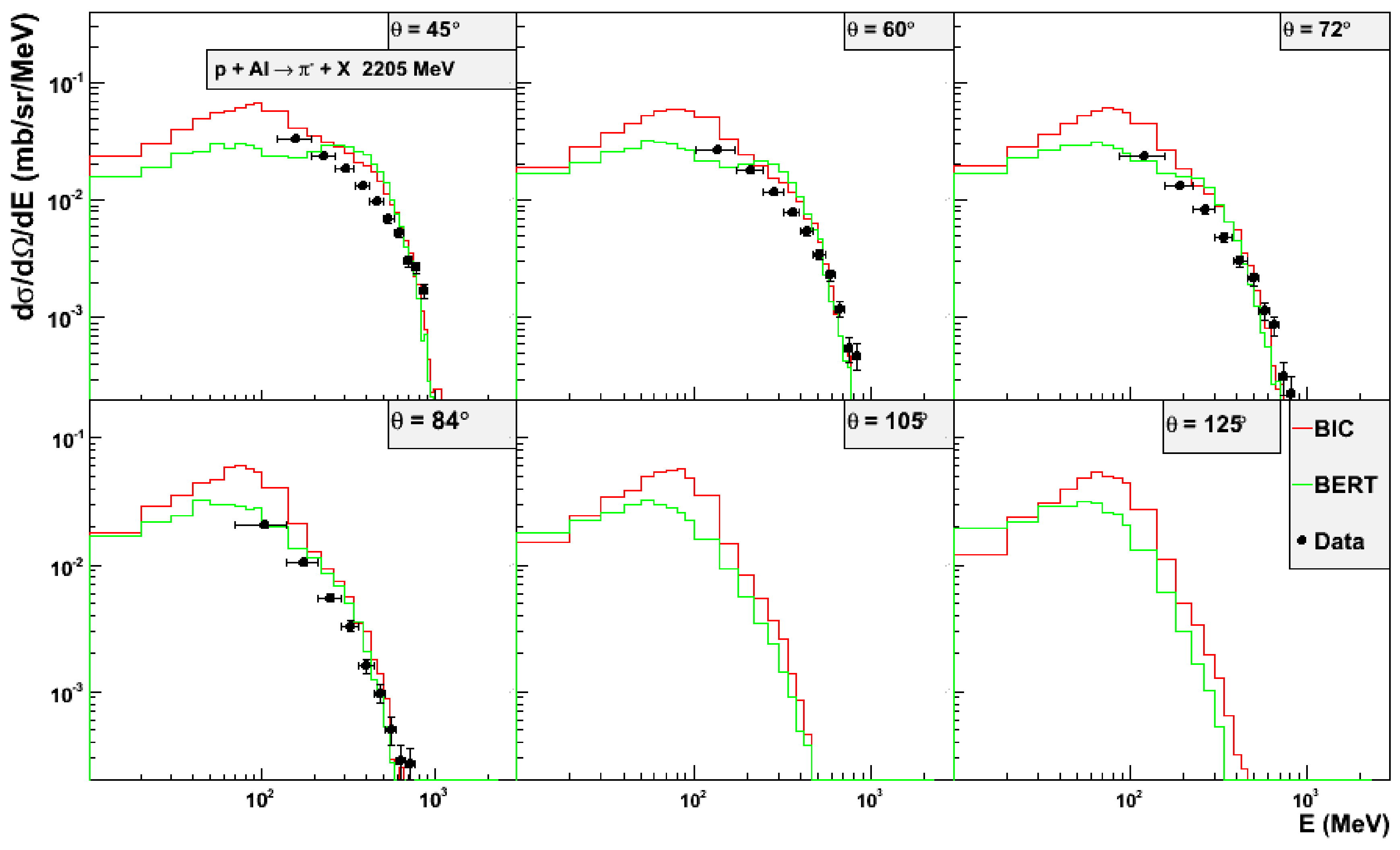
Proton production at 1200 MeV



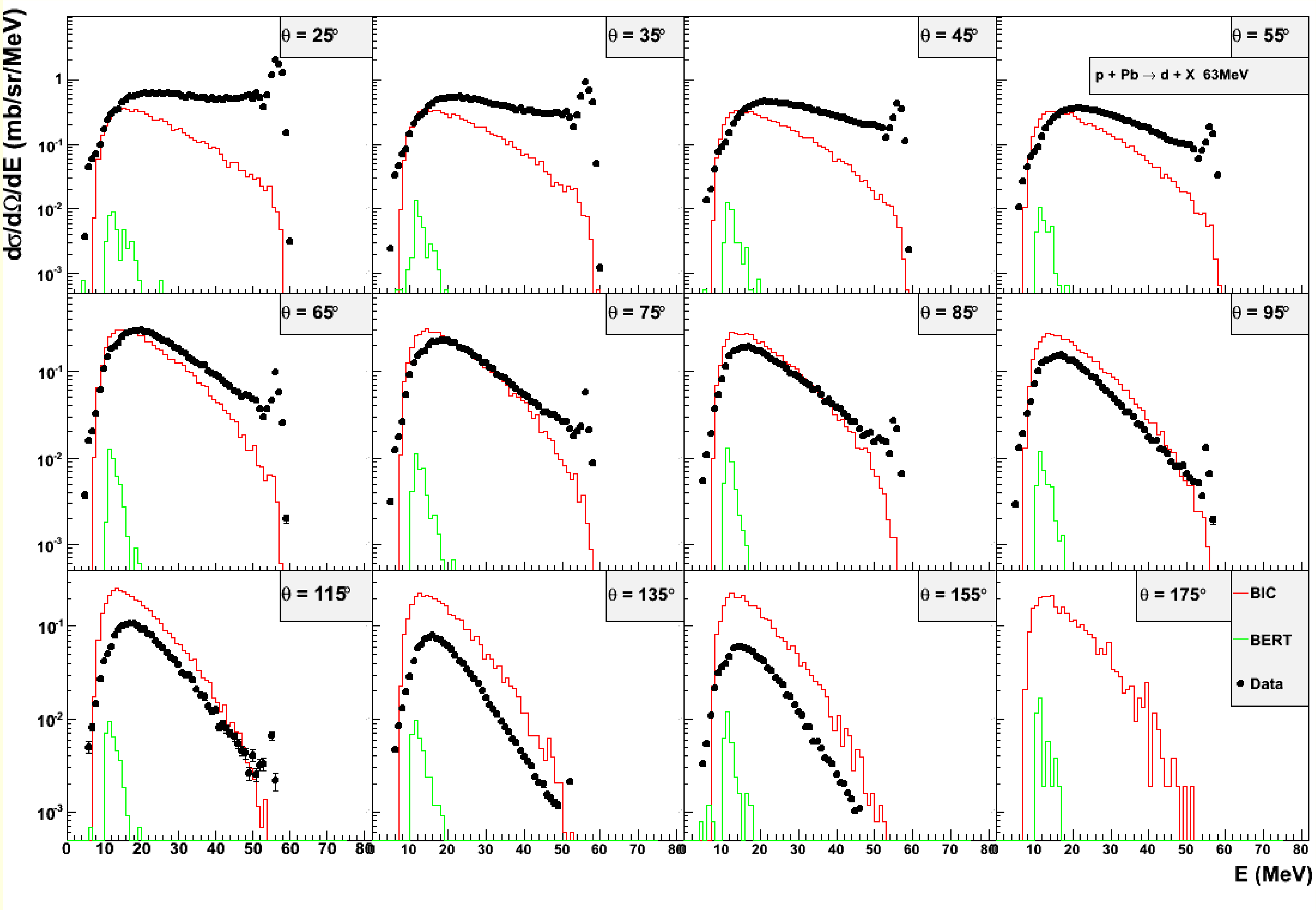
Pion production at 730 MeV



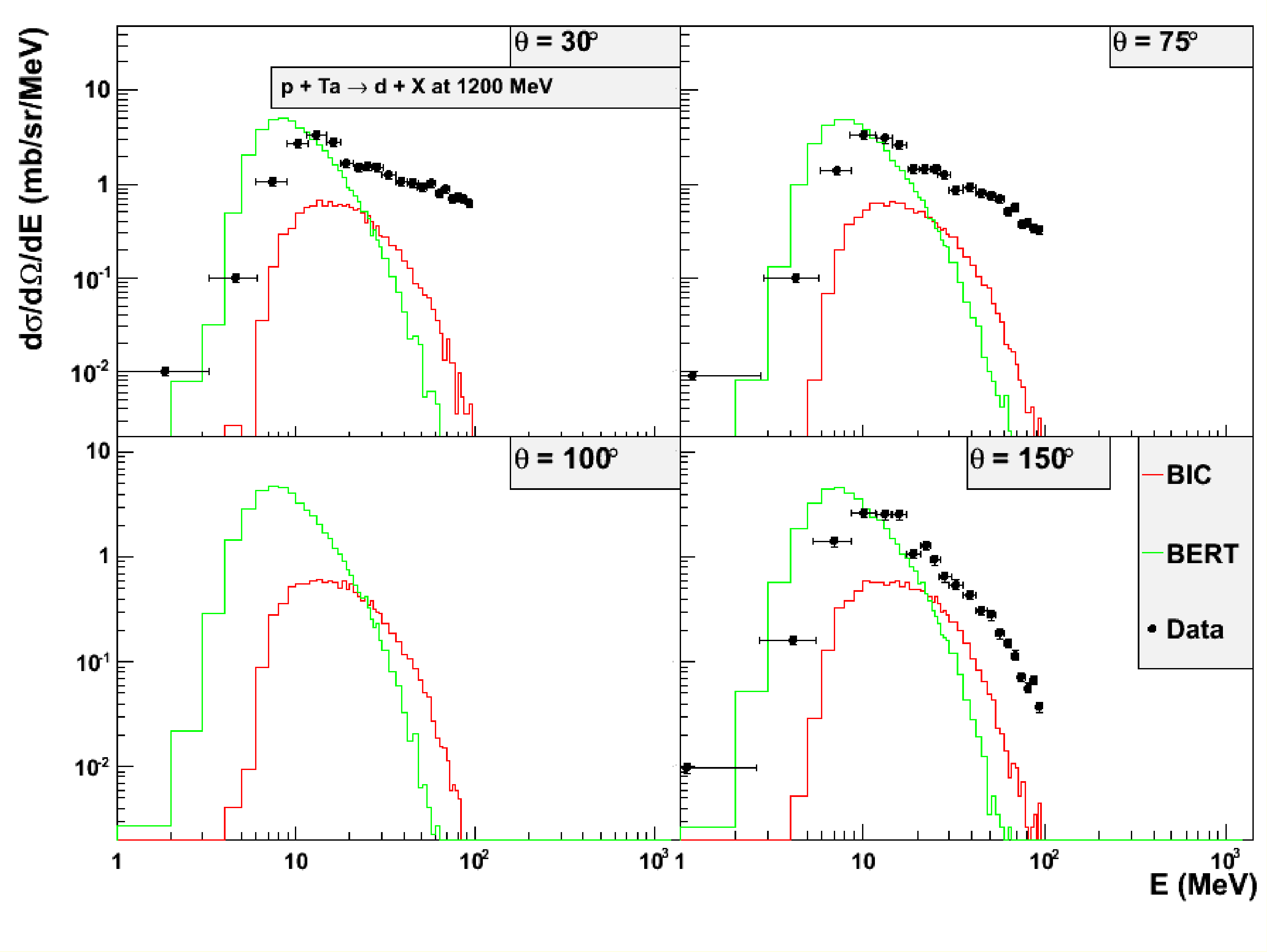
Pion production at 2205 MeV



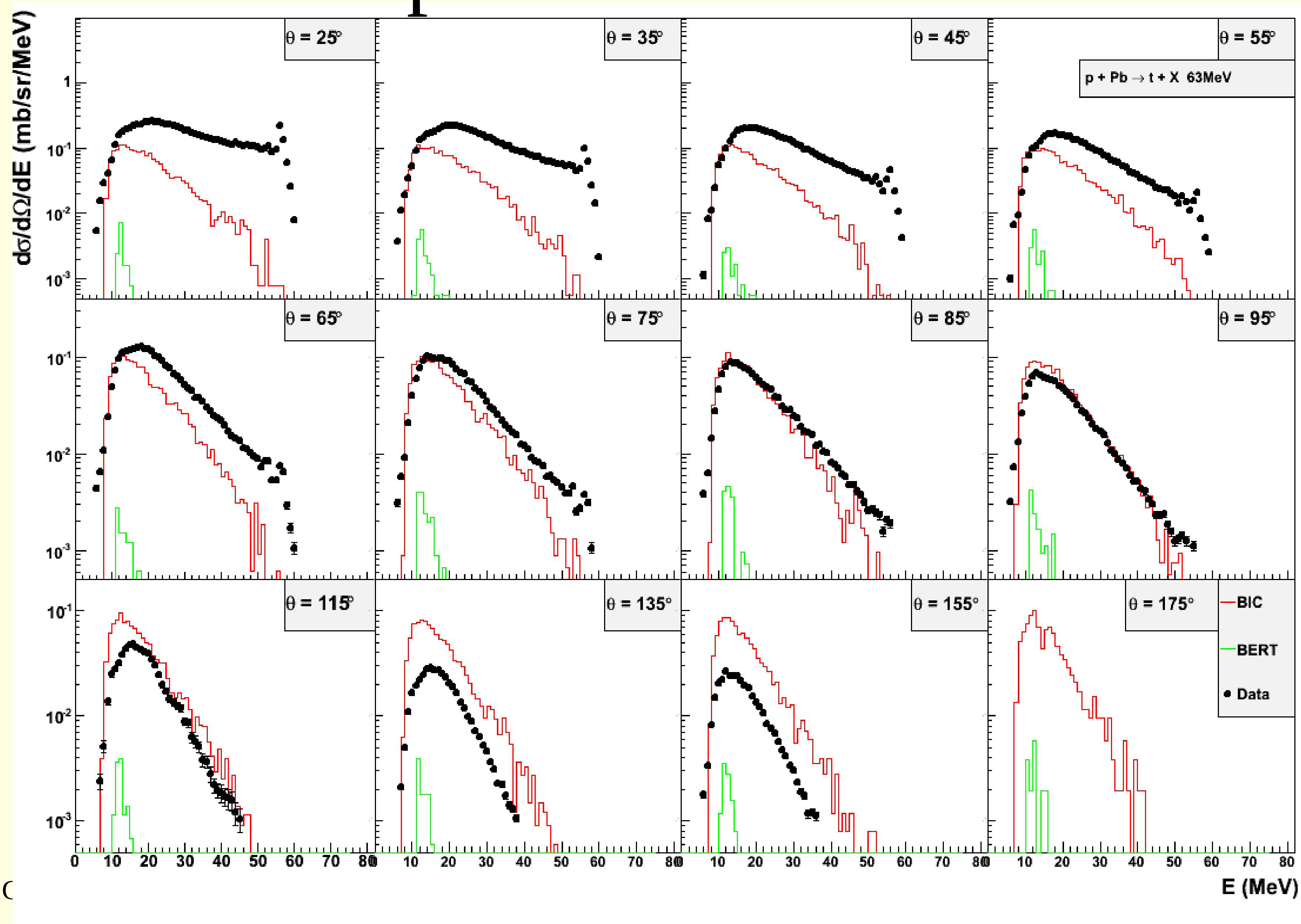
Deuteron production at 63 MeV



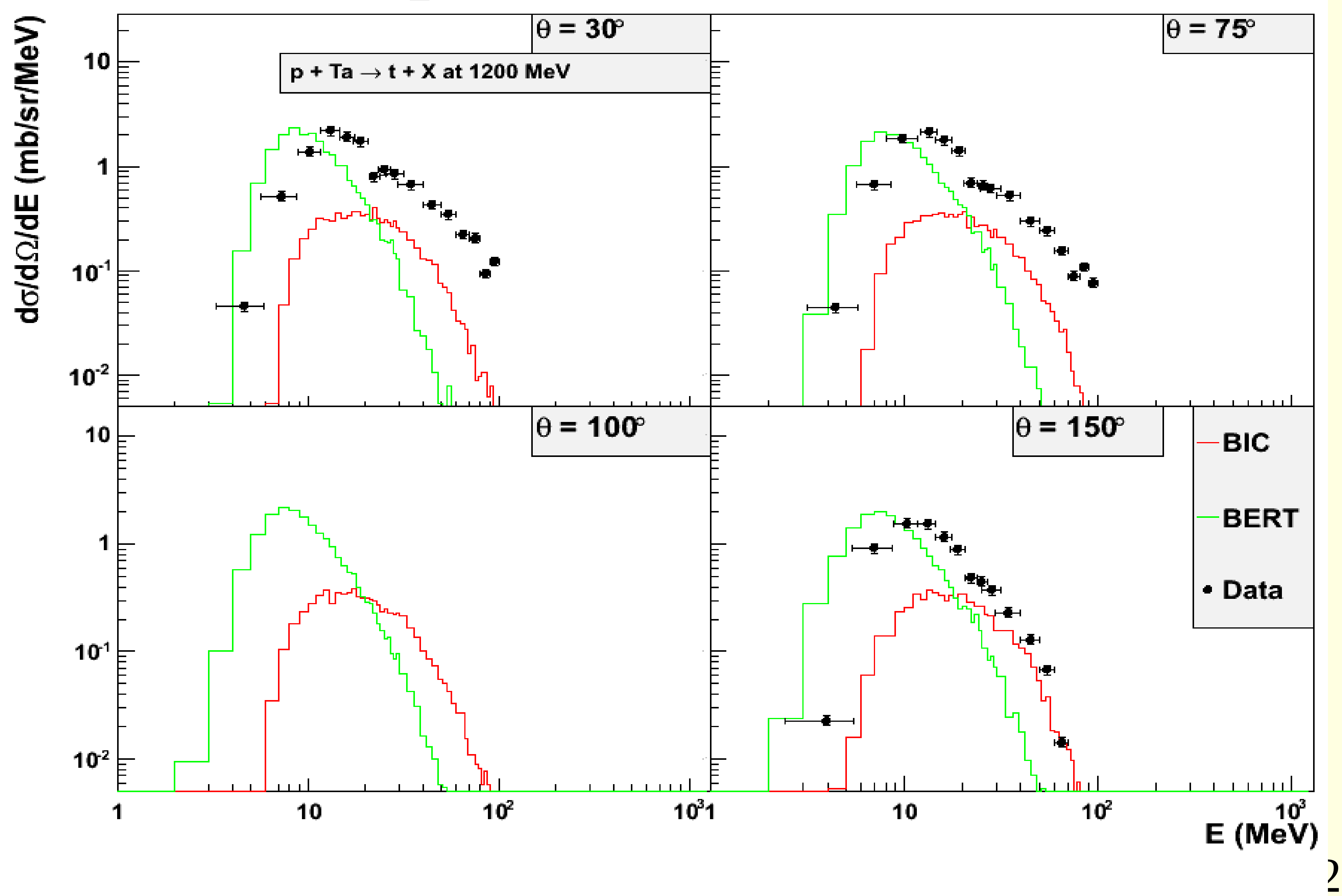
Deuteron production at 1200 MeV



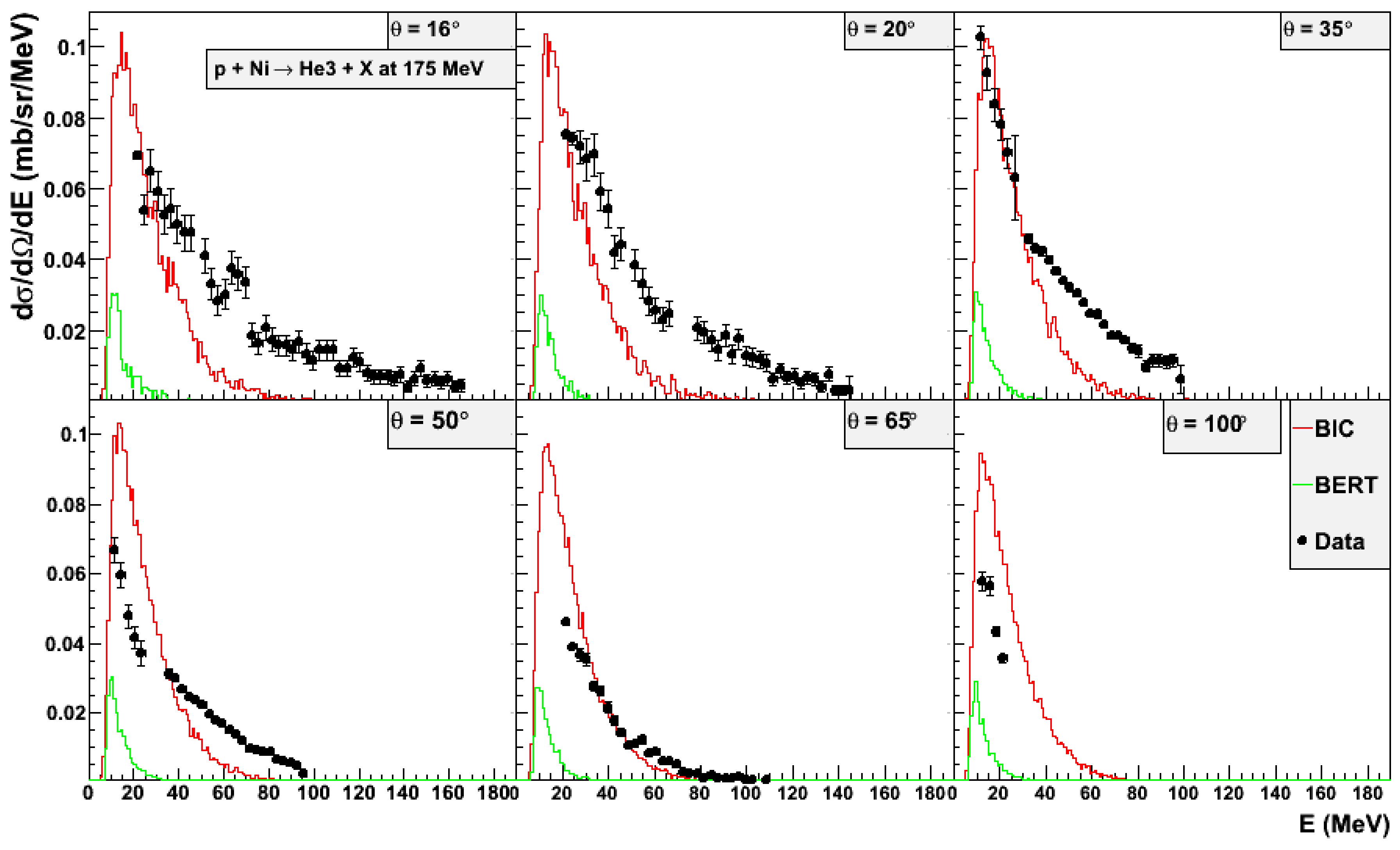
Tritium production at 63 MeV



Tritium production at 1200 MeV



^{3}He production at 175 MeV



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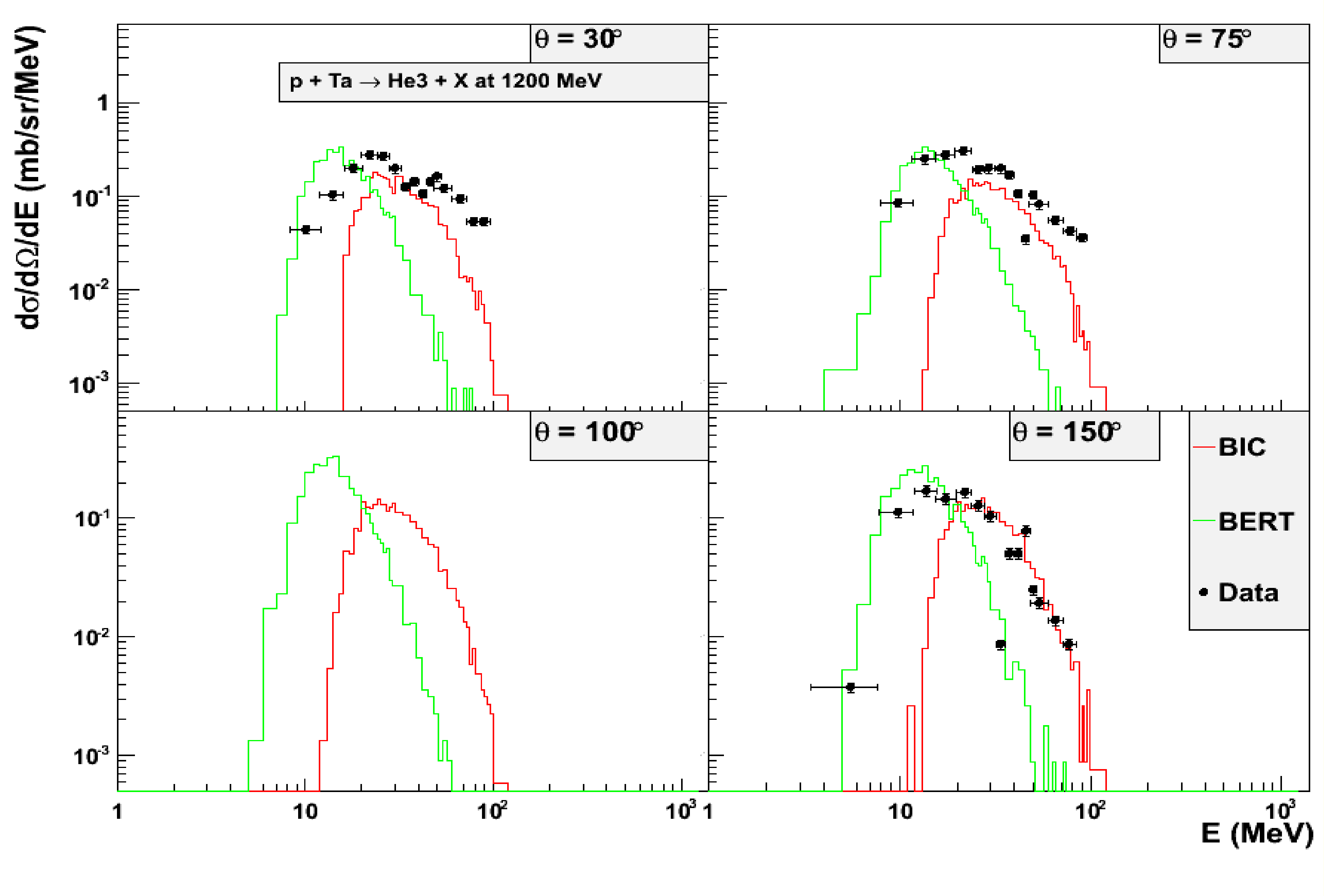
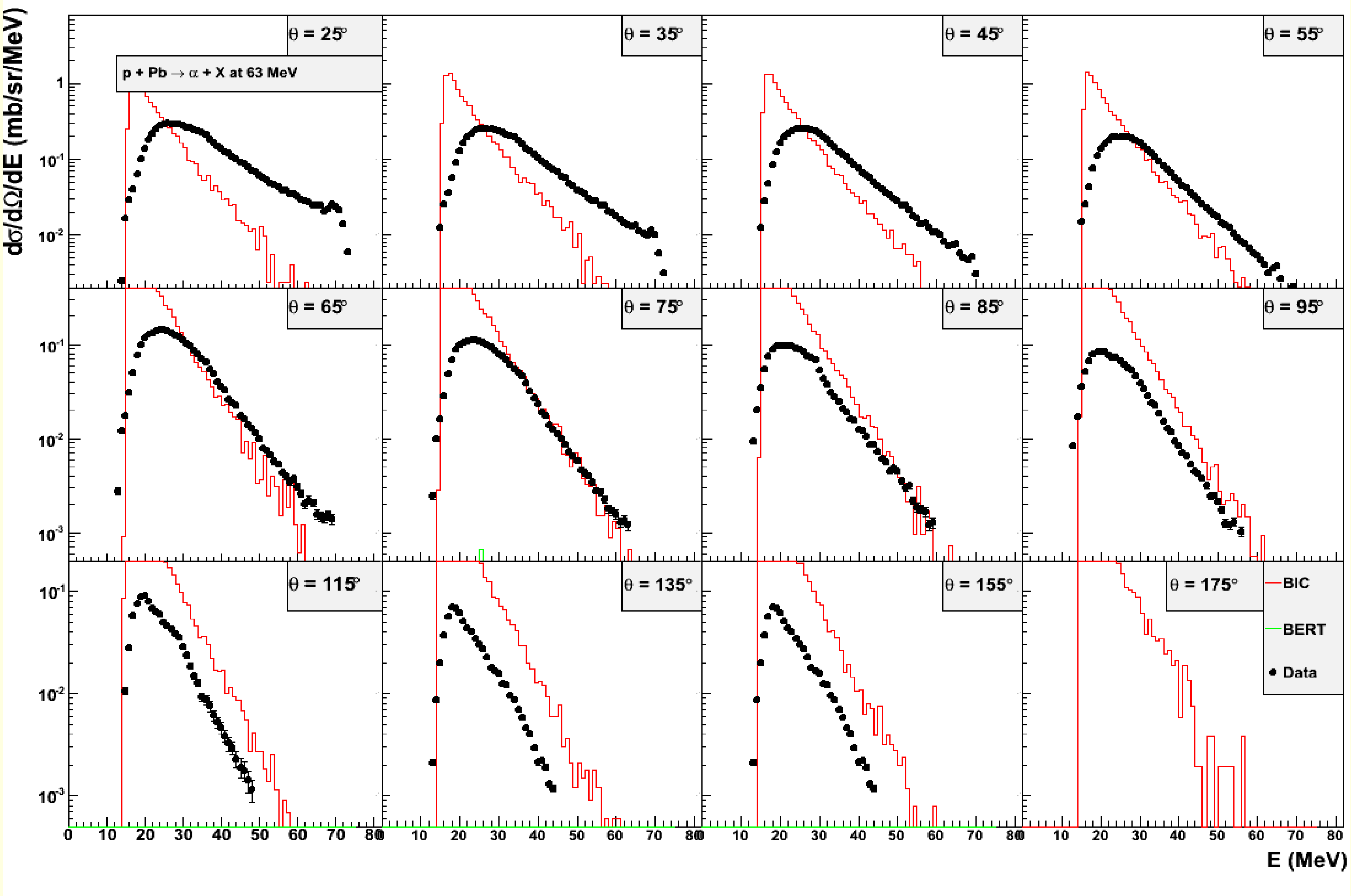
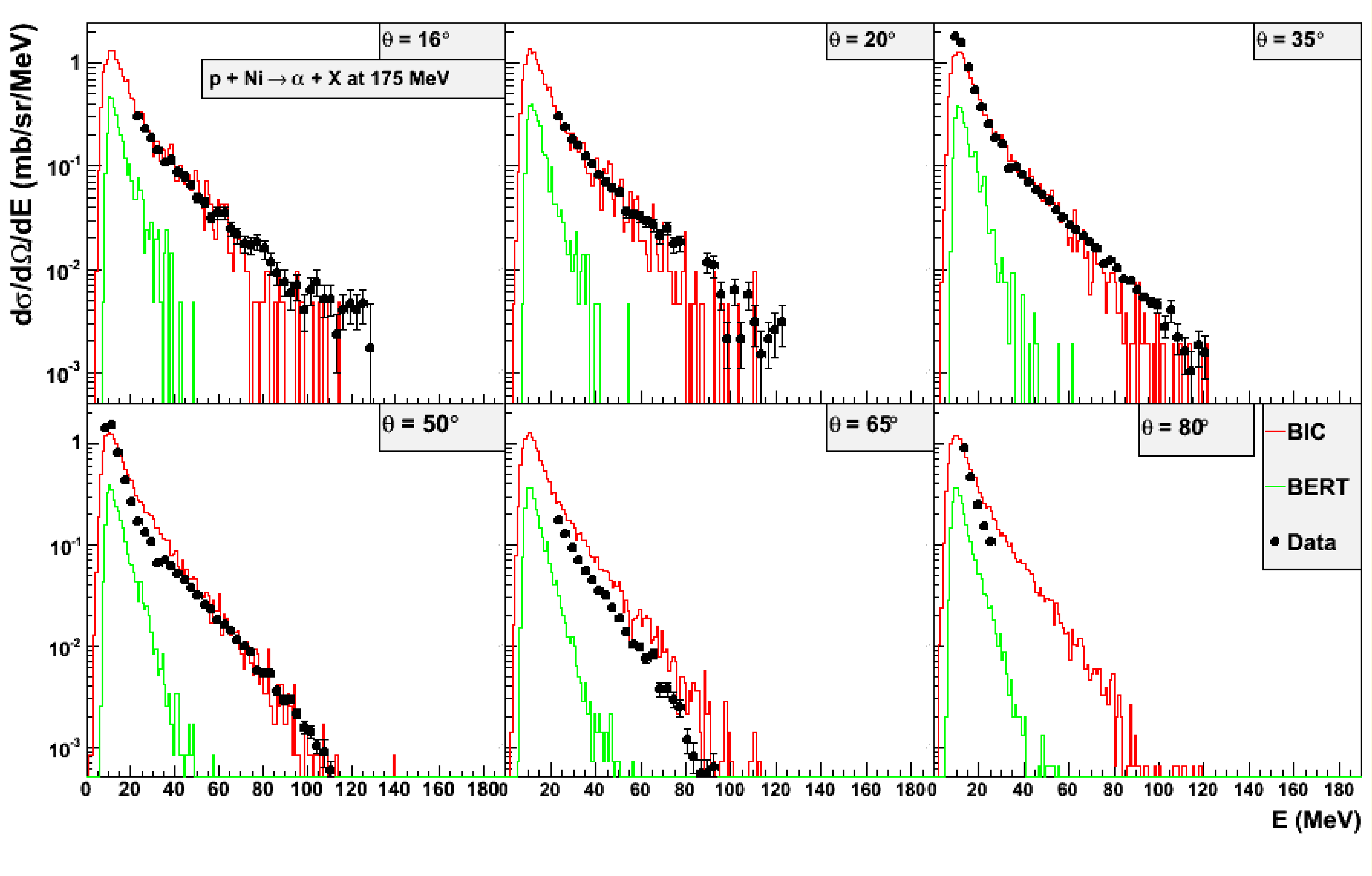


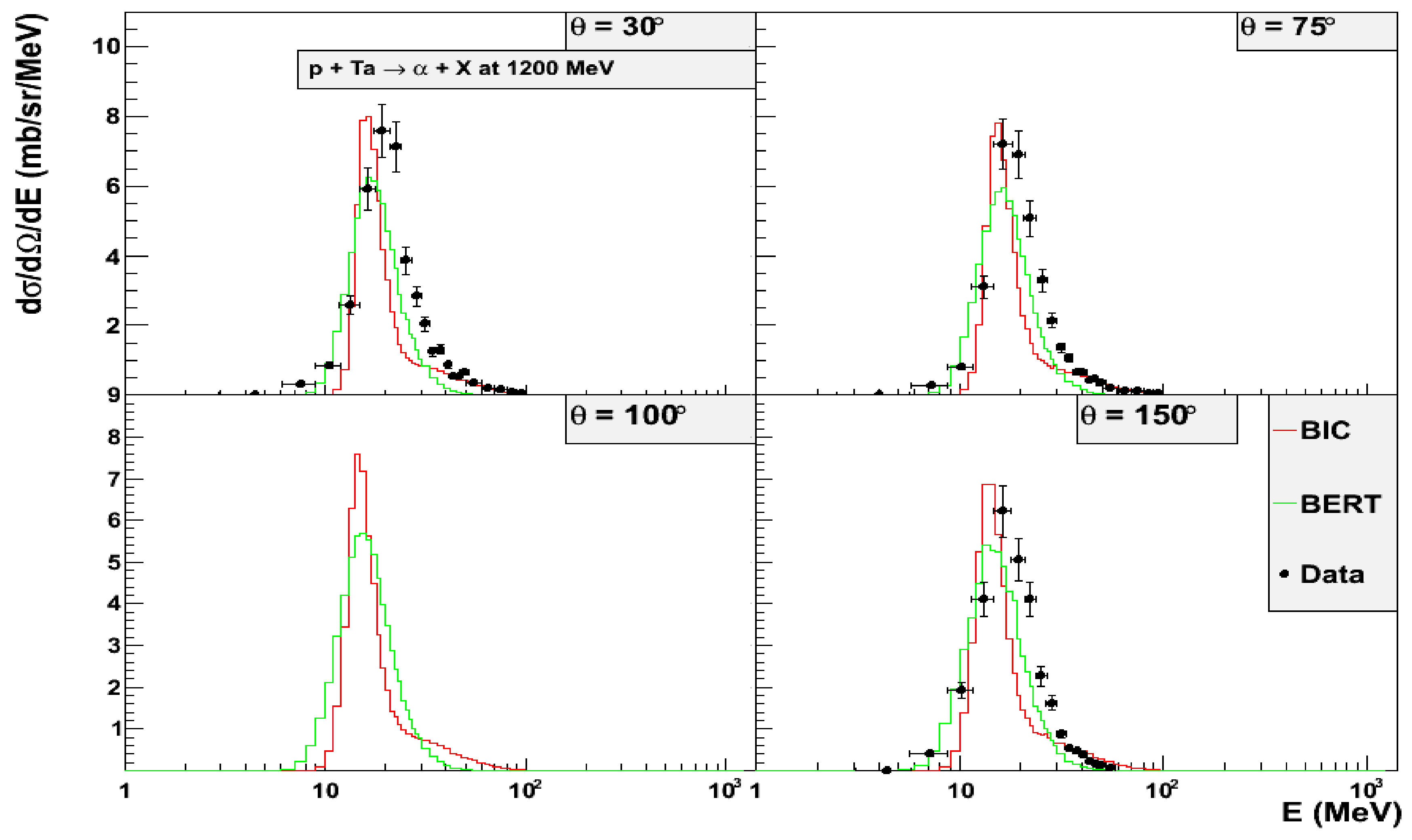
Alpha production at 63 MeV



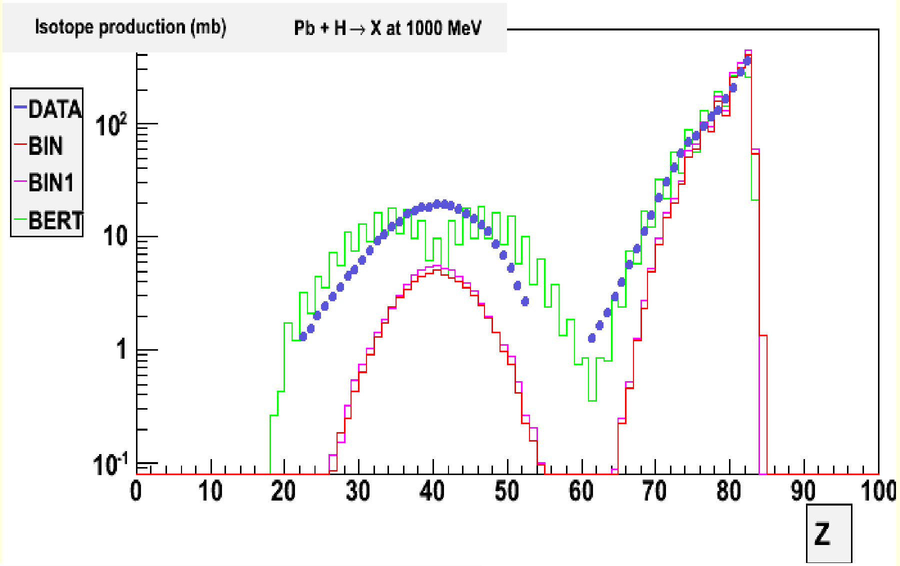
Alpha production at 175 MeV

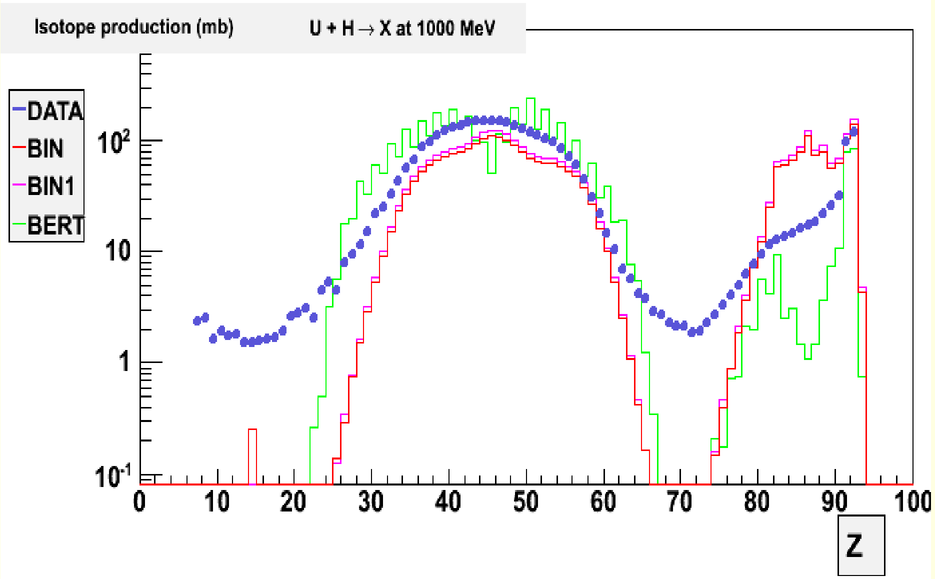


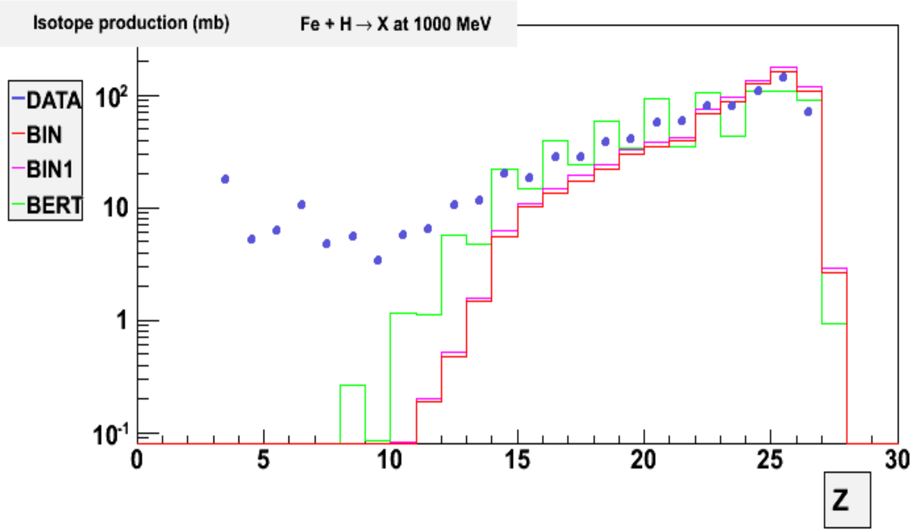
Alpha production at 1200 MeV

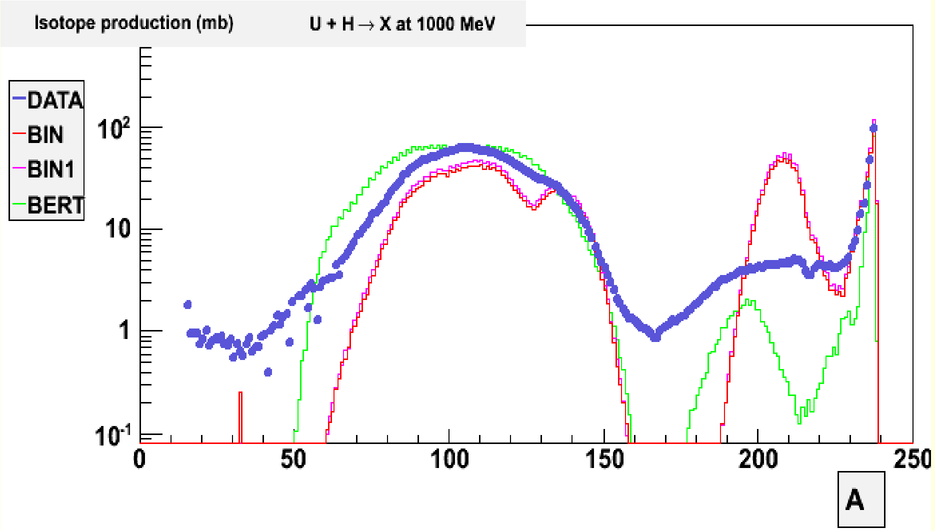


Fission at 1000 MeV









Conclusions (1)

- Bertini agrees better with data for:
  - protons (high energy)
  - pions (high and low energy)
  - fission
- Binary agrees better with data for:
  - low and medium energy protons
  - almost all light ion production, although agreement is not good in either case
- Many cases where neither model is better overall
  - one model may be better for forward angles, the other for backward angles

Conclusions (2)

- 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
- This benchmark study demonstrated areas where improvement is needed. As a result:
  - recently made improvements to precompound
  - plan to add coalescence models for cascade stage
  - improvements to fission are possible

Thanks for your attention

Backup slides

Geant4 Collaboration

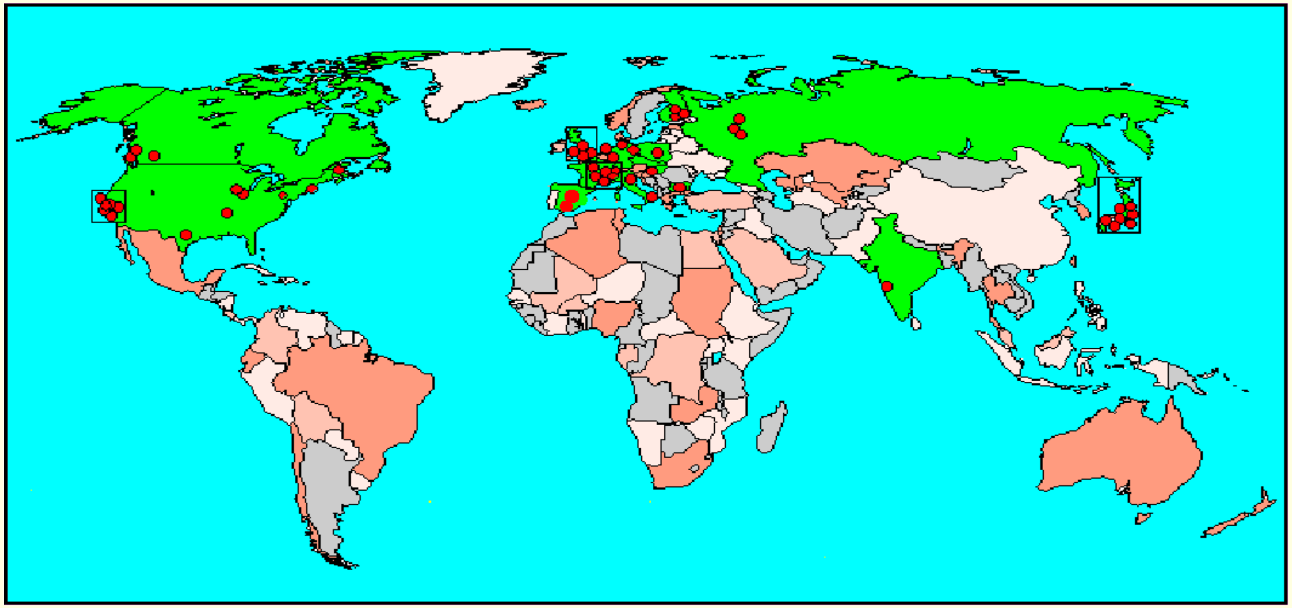
Applications for Physics & Infrastructure
CERN
IT/API

esa

INFN
ISTITUTO NAZIONALE DI FISICA NUCLEARE

大学共同利用機関法人
KEK
高エネルギー加速器研究機構

Stanford
Linear
Accelerator
Center



LIP

Jefferson Lab
Thomas Jefferson National Accelerator Facility

TRIUMF

Российская Академия Наук
Физический Институт
имени
П.Н.Лебедева
Ф И А Н

Lebedev

KAROLINSKA MEDICO CHIRURGISKA INSTITUTET
KONGL. ✱

J.W.Goethe Universität

IN2P3

HELSINKI INSTITUTE OF PHYSICS

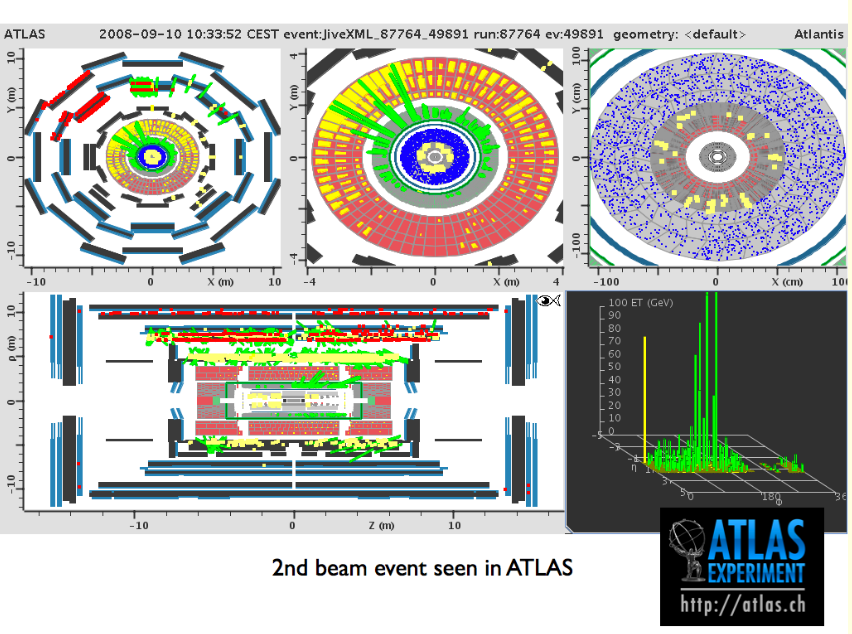
PPARC

UNIVERSITAT DE BARCELONA

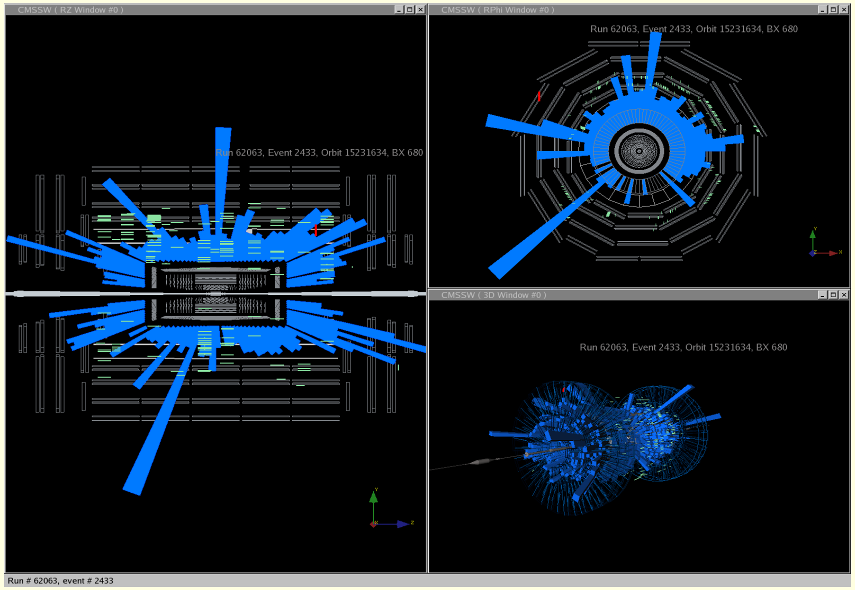
Collaborators also from non-member institutions, including
Budker Inst. of Physics
IHEP Protvino
MEPHI Moscow
Pittsburg University
University of Sevilla
CIEMAT

Brief History

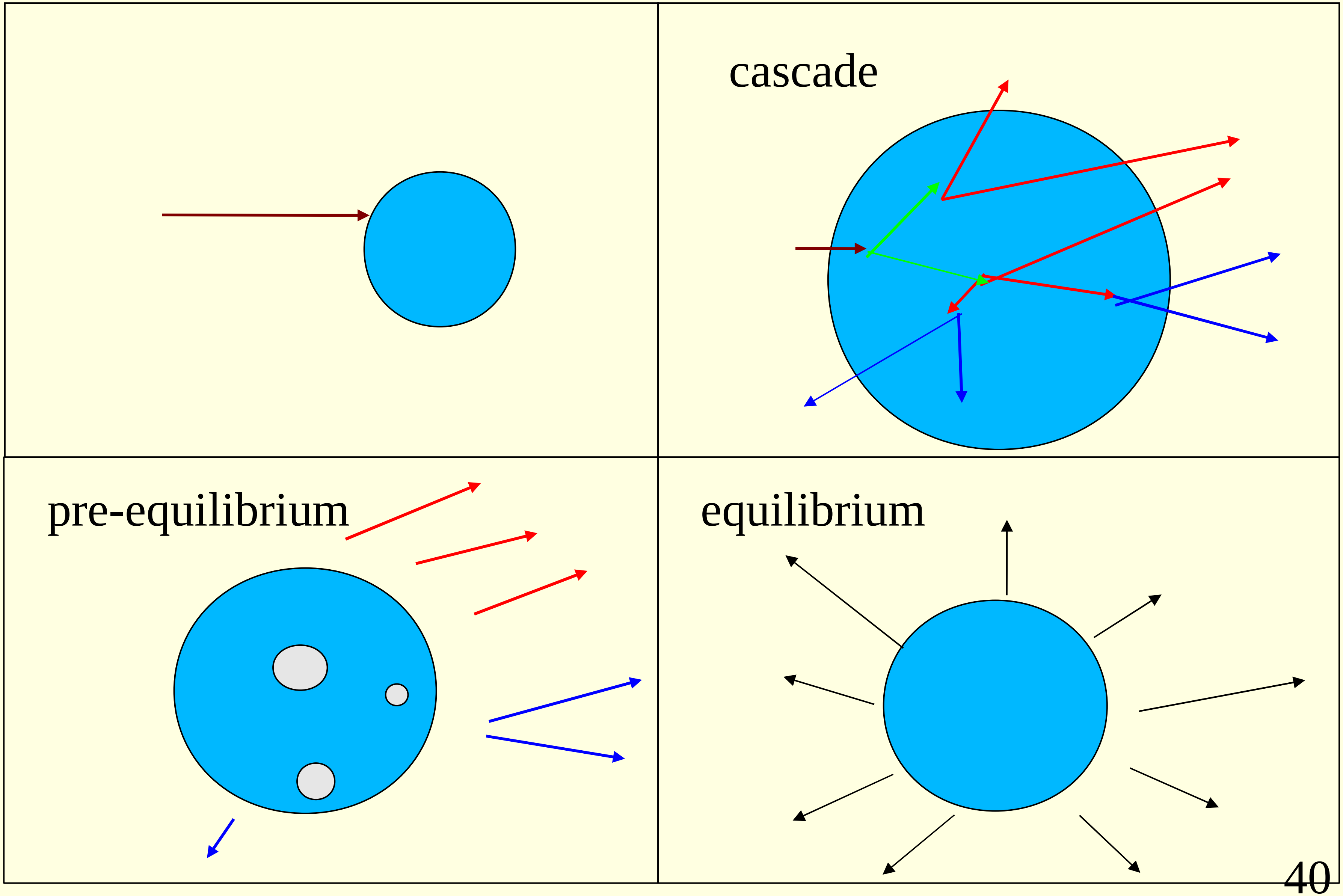
- Dec'94 : Project started
- Dec'98: First public release
- Geant4 was used by BaBar experiment at SLAC since 2000
- Geant4 is used for Monte Carlo simulation of particle transport for ATLAS, CMS, LHCb since 2004
- Hadronic physics packages are an important part of Geant4 for LHC
  - Signal acceptance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



2nd beam event seen in ATLAS



Cascade Modeling Concept



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 6-body final state partial cross sections for pi+p, pi-p, pp, pn from the CERN compilations (V. Flaminio et al., 1983 and 1984). K+, K- partial cross sections also from Flaminio (1983).
    - pi+n, pi-n, nn cross sections are obtained through isospin arguments
  - 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 Modeling 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 Modeling 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 recently
- 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 Modeling 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 fully phenomenological way

Binary Cascade Modeling (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

Binary Cascade Modeling (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 Modeling (3)

- Nucleon-nucleon elastic scattering angular distributions taken from Arndt phase shift analysis of experimental data
- Pauli blocking implemented in its classical form
  - final state nucleons occupy only states above Fermi momentum
- True pion absorption is modeled as s-wave absorption on quasi-deuterons
- Coulomb barrier taken into account for charged hadrons

Binary Cascade Modeling (4)

- If primary below 45 MeV, no cascade, just precompound
- Cascade stops when mean energy of all scattered particles is below A-dependent cut
  - varies from 18 to 9 MeV
- When cascade stops, the properties of the residual exciton system and nucleus are evaluated, and passed to pre-equilibrium de-excitation class (G4PreCompoundModel)

Binary Cascade Modeling (5): pre-equilibrium

- Geant4 precompound model is an extension of the binary cascade for lower energies
- It is a variant of the exciton model used in CEM (Gudima et al, 1983)
- This stage lasts until the nuclear system reaches equilibrium.
- Transition to equilibrium is considered consistently, i.e. the physical condition $\lambda^{t}_{\Delta n=+2}=\lambda^{t}_{\Delta n=-2}$ is applied.
- No need of the rough estimation: $n_{eq}=\sqrt{2gU}$
- No need for enhancement of equilibrium by means of a *soft transtion* to equilibrium

Binary Cascade Modelling (6) : equilibrium

After pre-equilibrium the properties of the residual nucleus are evaluated, and passed to the equilibrium de-excitation handler (G4ExcitationHandler)

Three processes are considered:

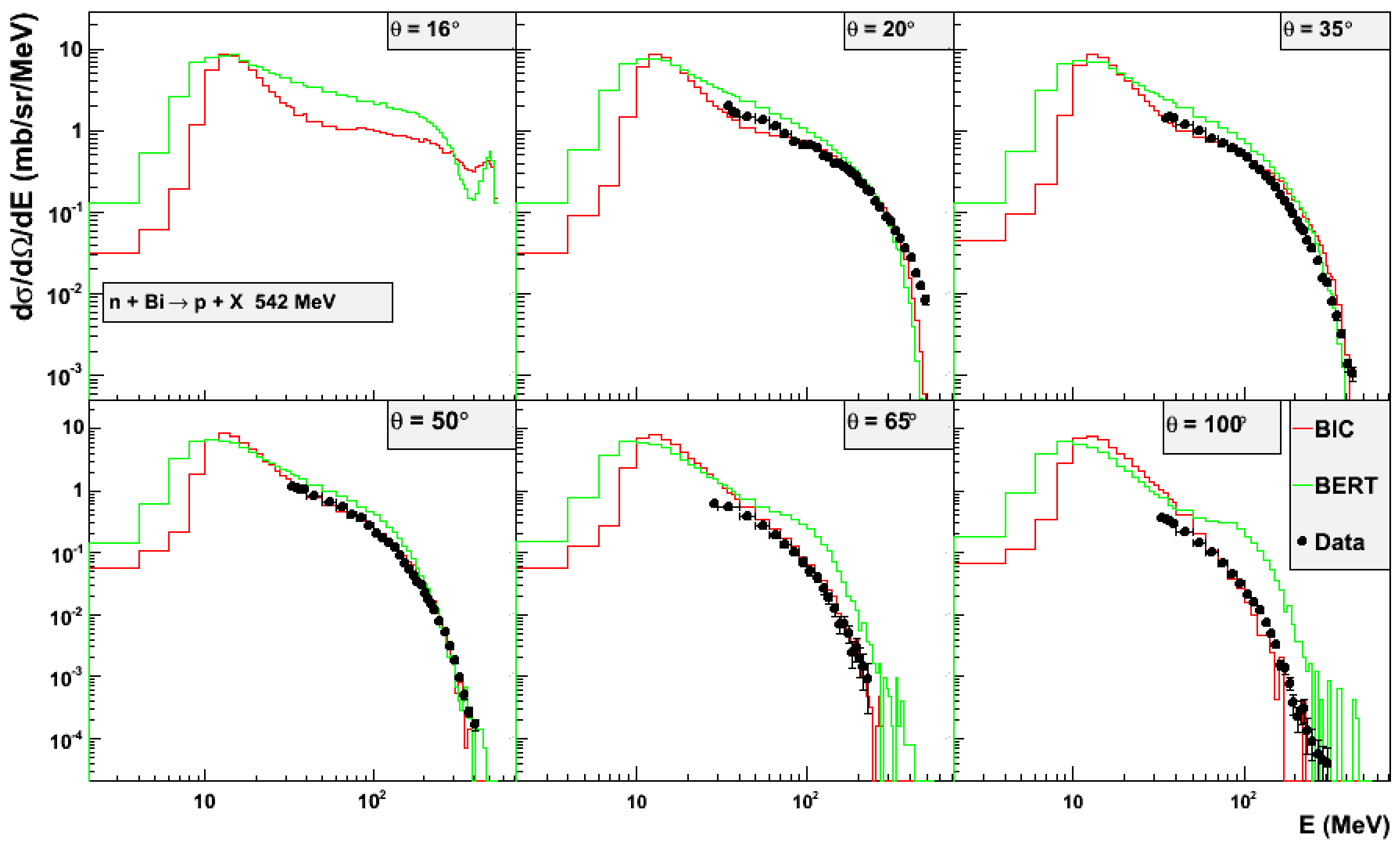
1. Statistical multifragmentation (Botvina *et al*) (for E*/A > 3 MeV).

Competitors:

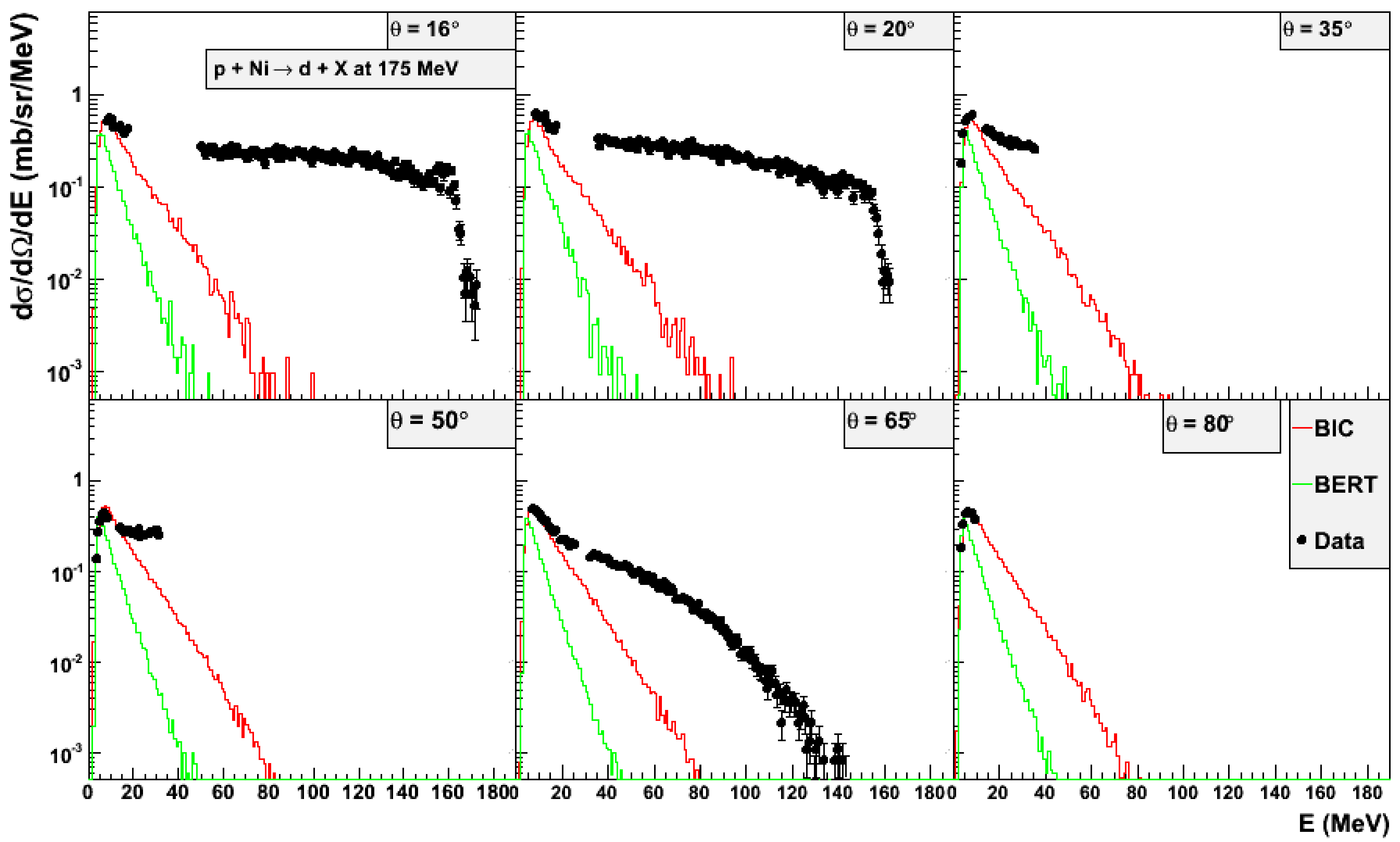
1. Fission (Bohr-Wheeler model + Amelin prescript.)
2. Particle evaporation (Weisskopf-Erwin).

additional
RESULTS
(Geant4 official release 9.2 patch p01)

Proton production at 542 MeV



Deuteron production at 175 MeV



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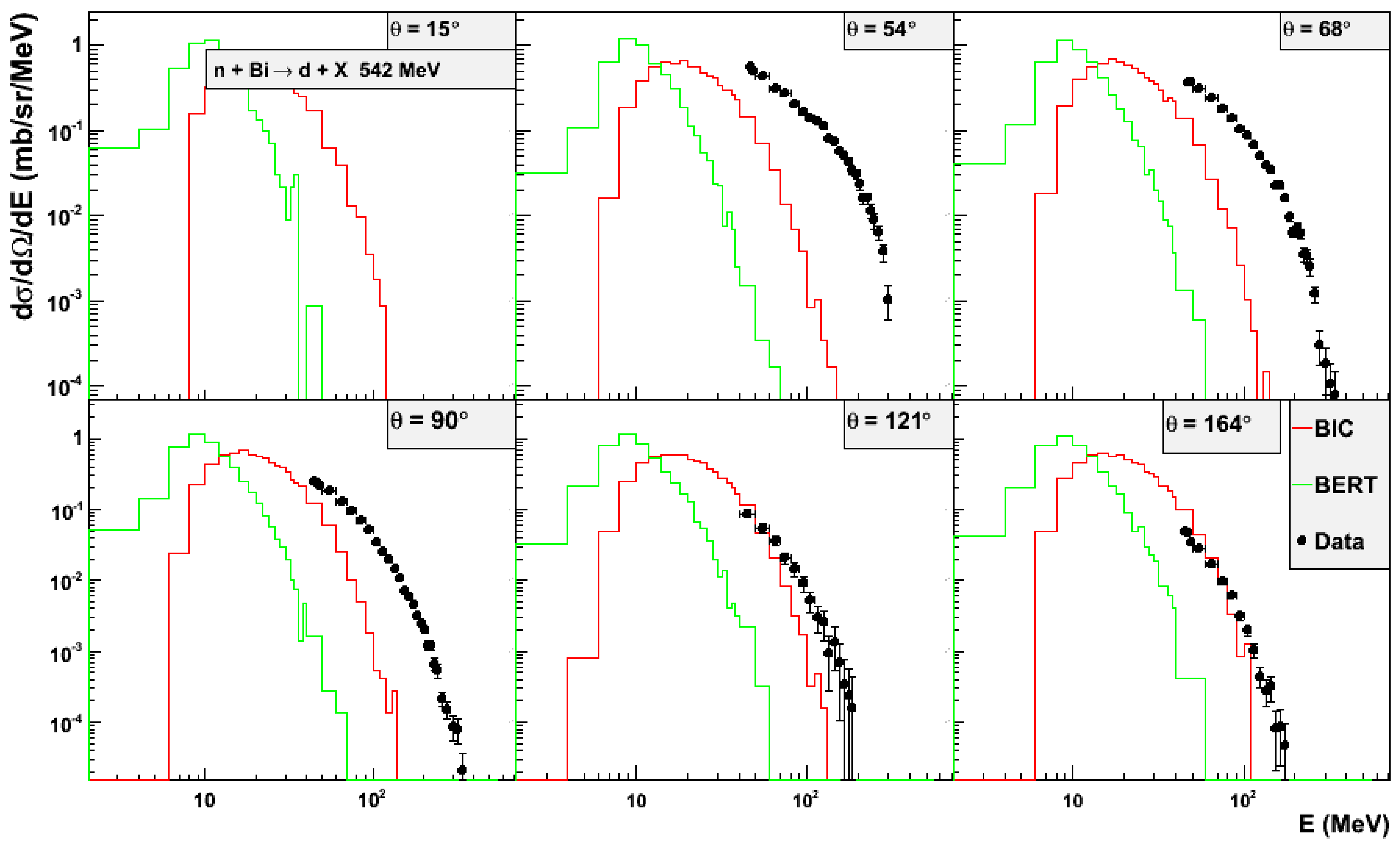

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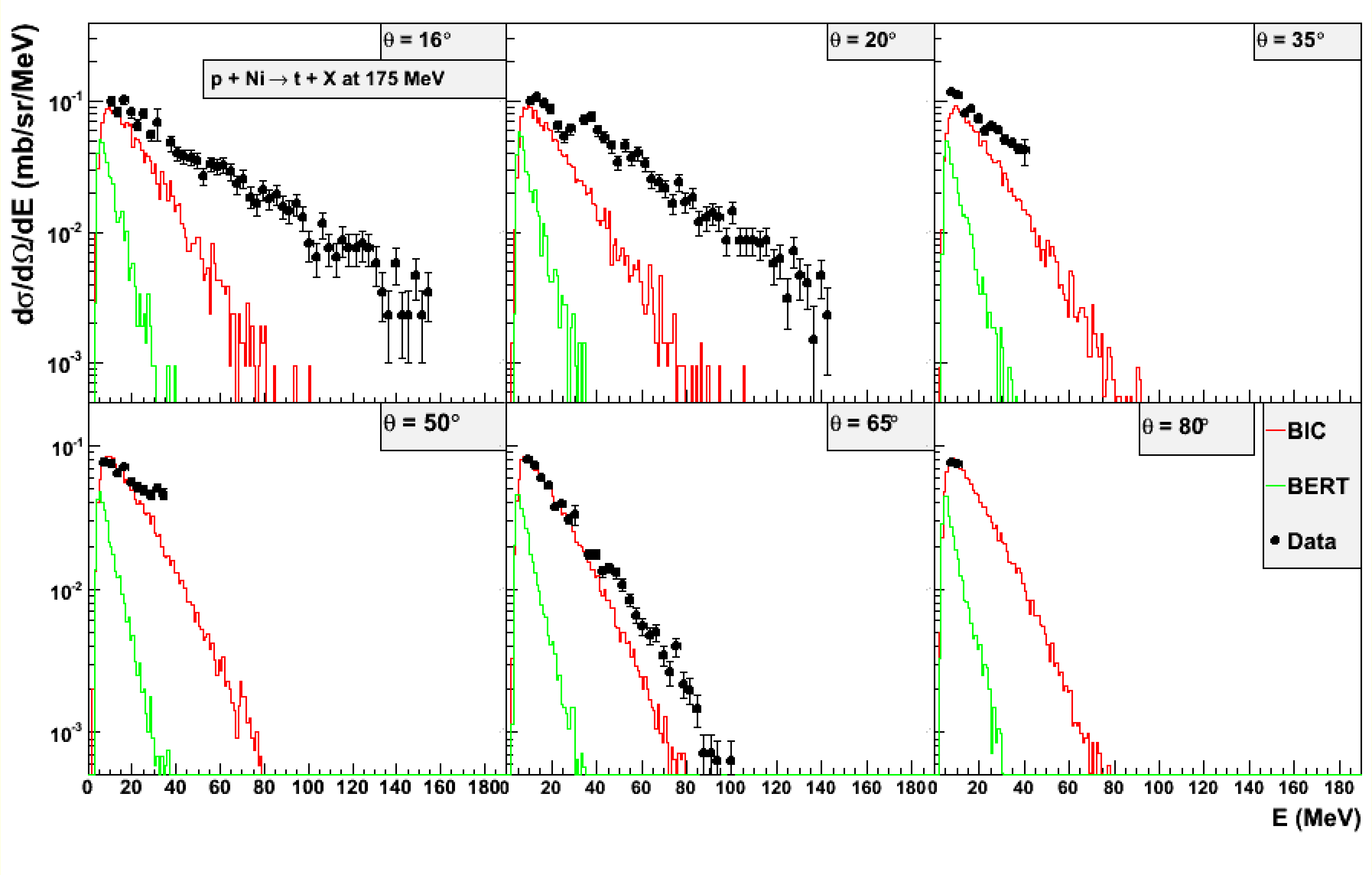

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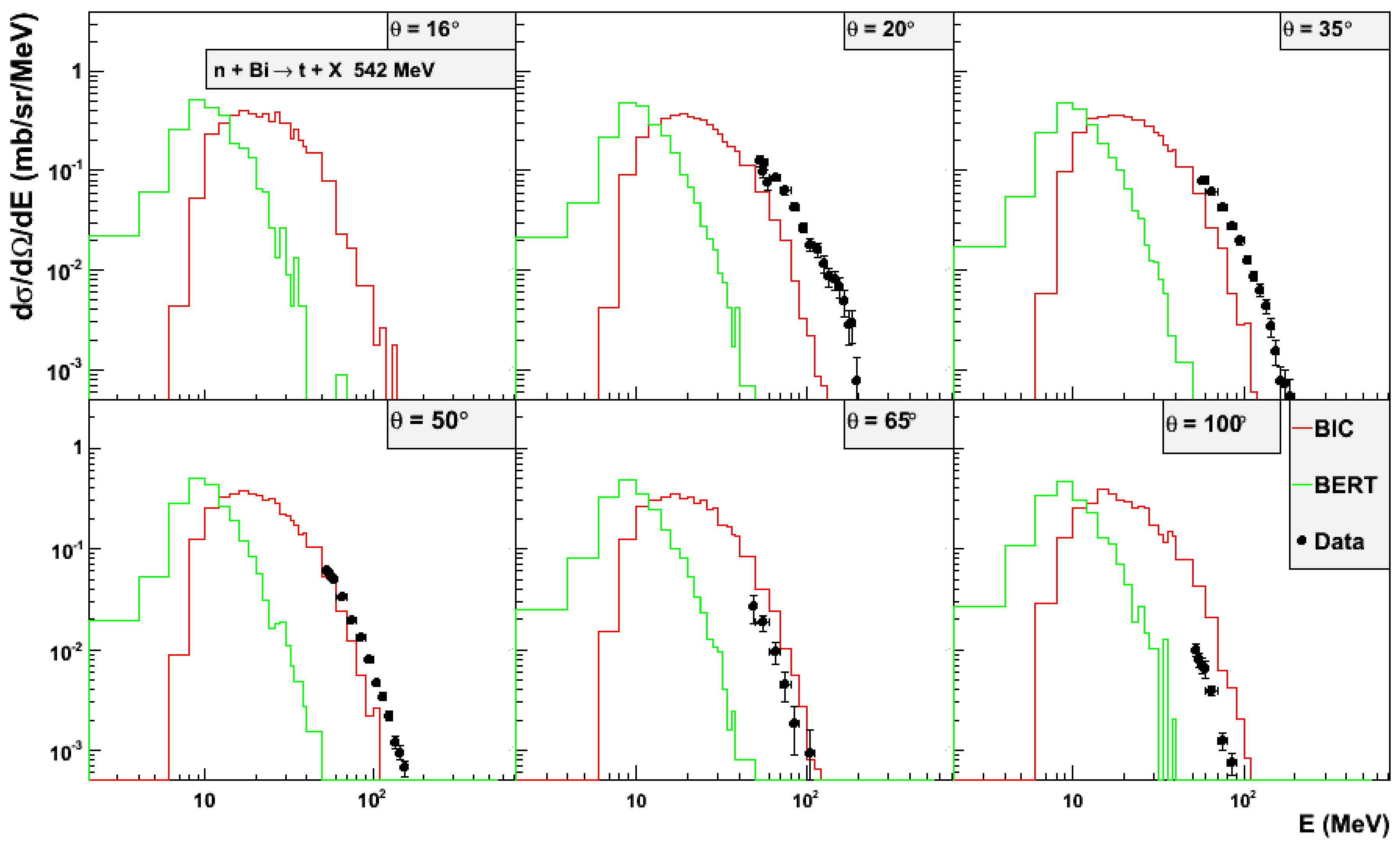
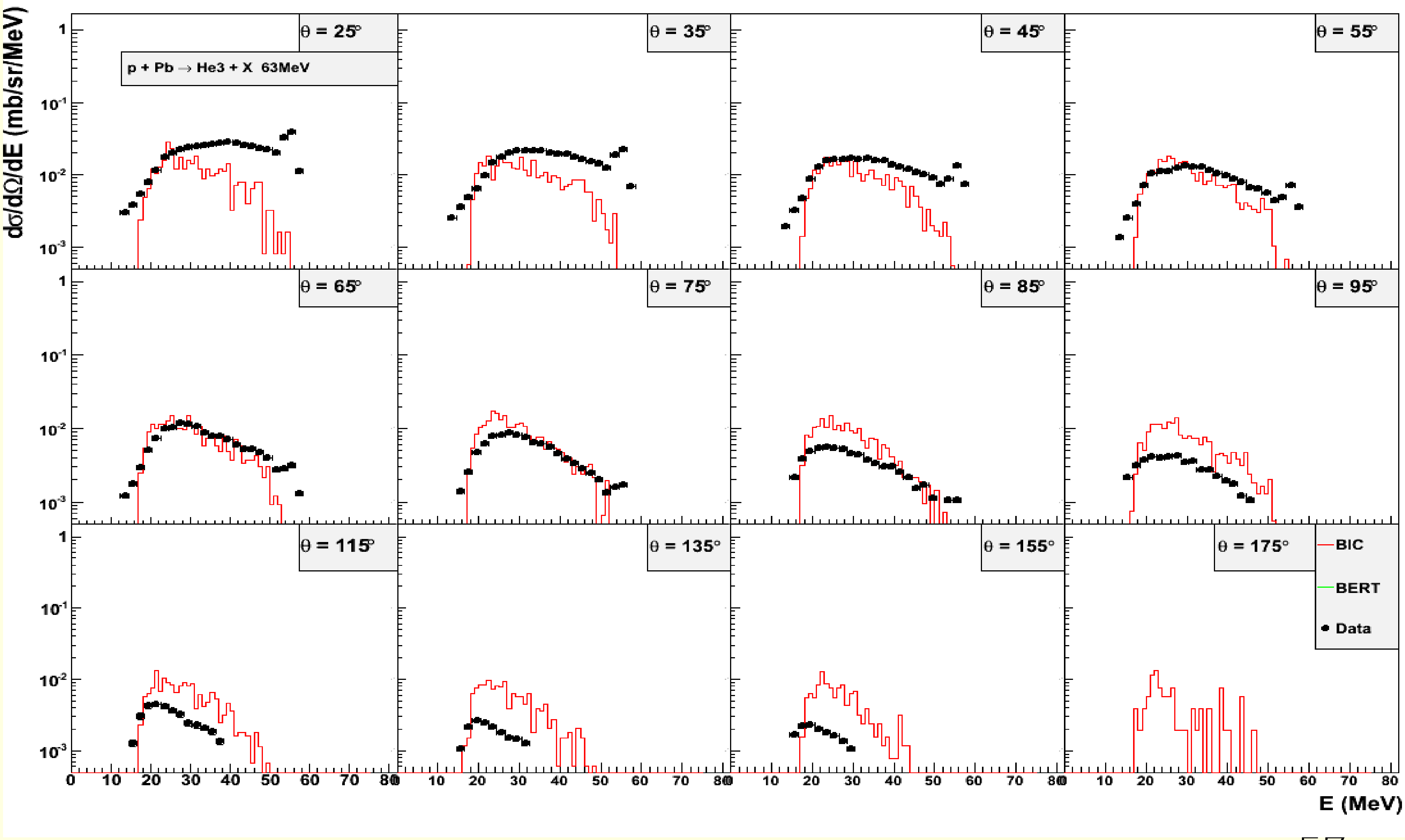
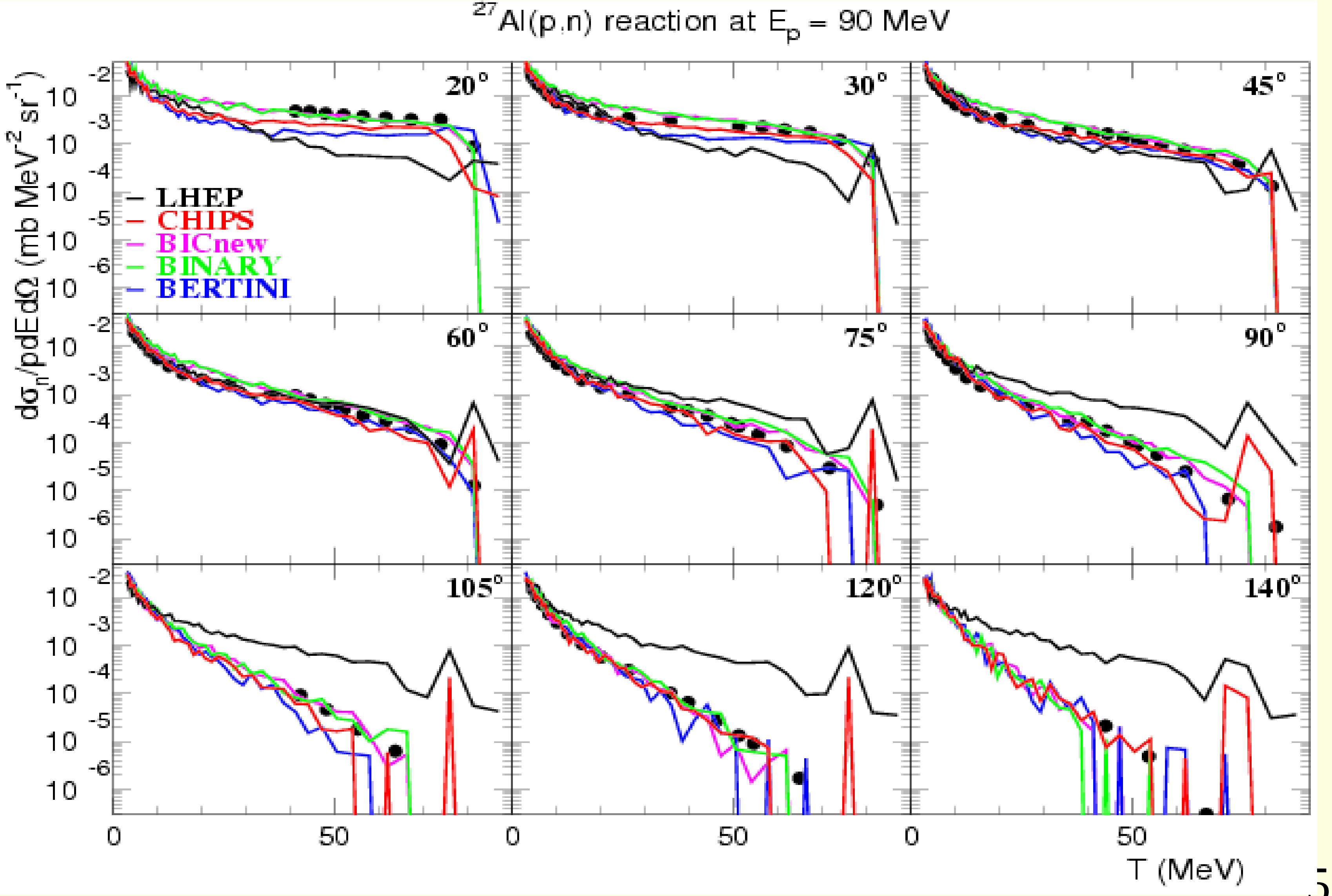


^{3}He production at 63 MeV



Ongoing development effort:
CHIPS

CHIPS:model intercomparison



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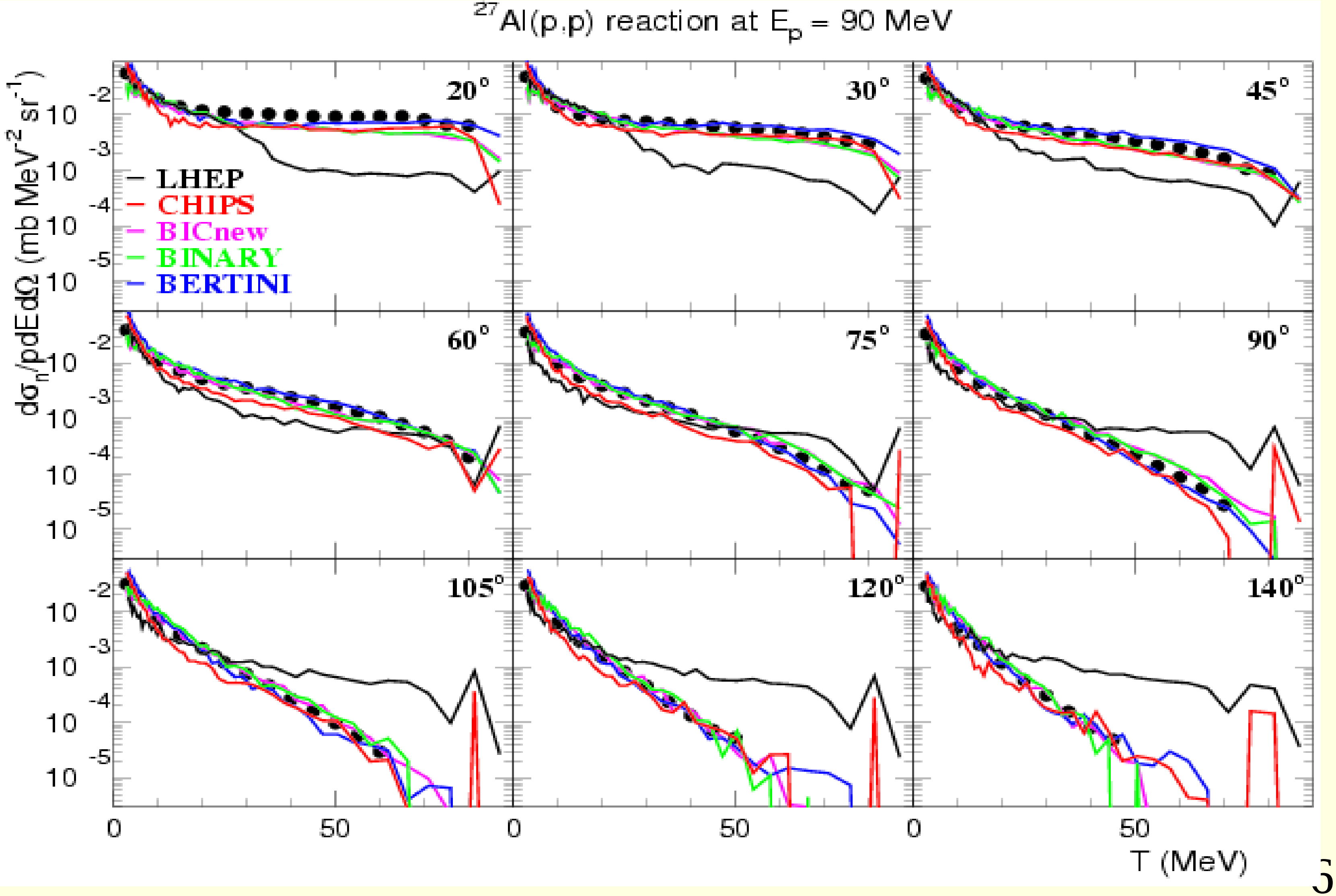

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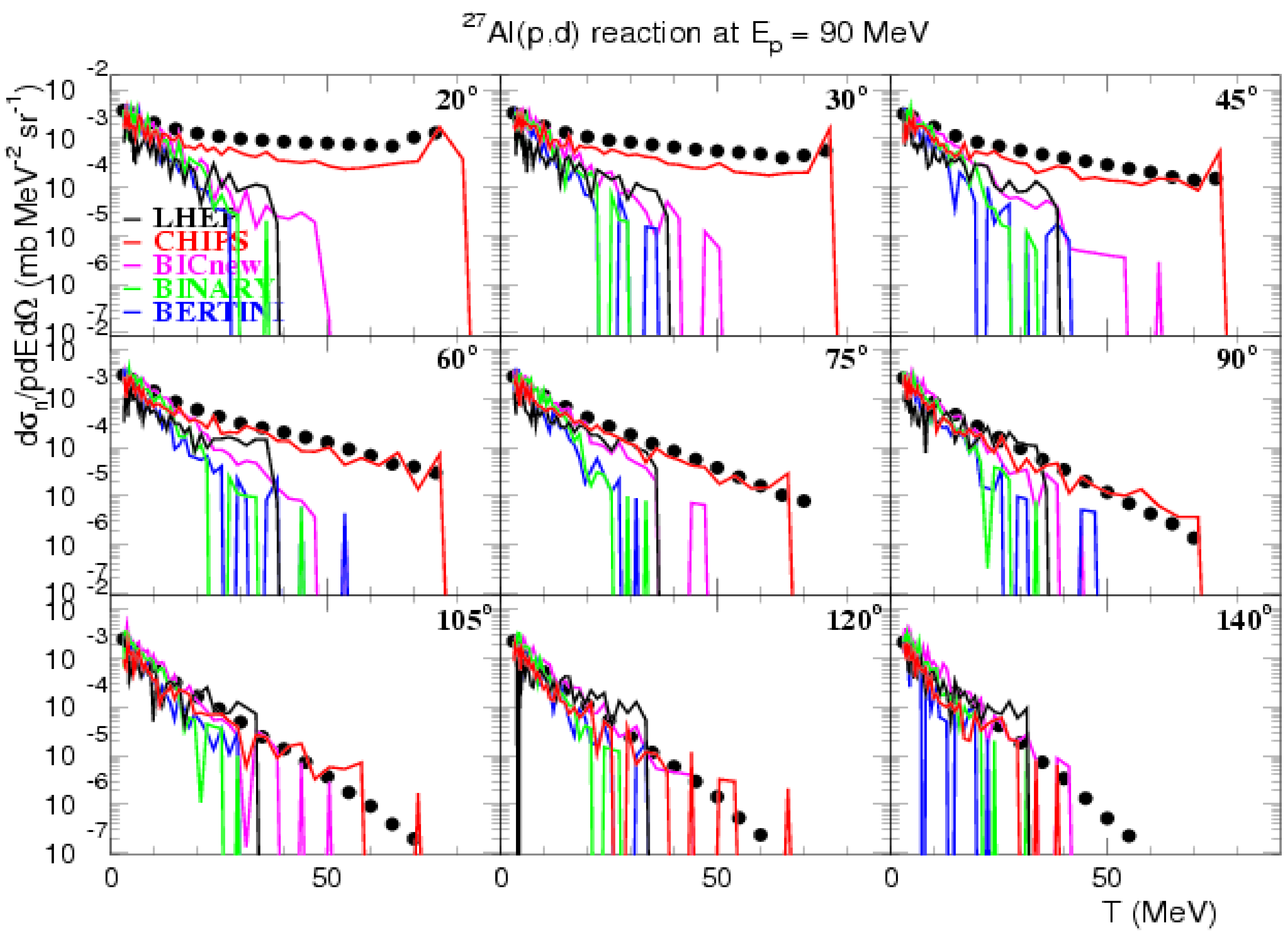

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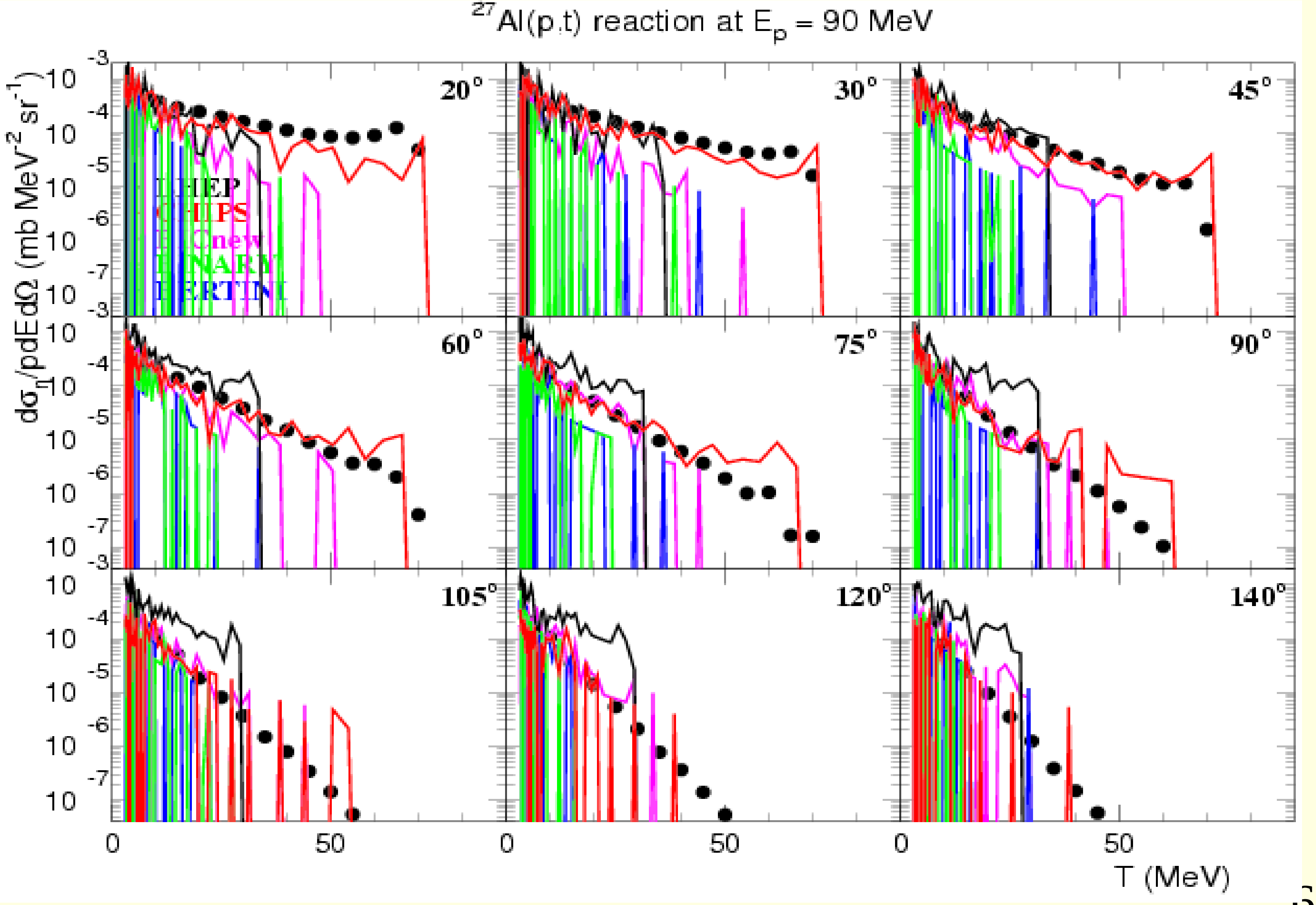

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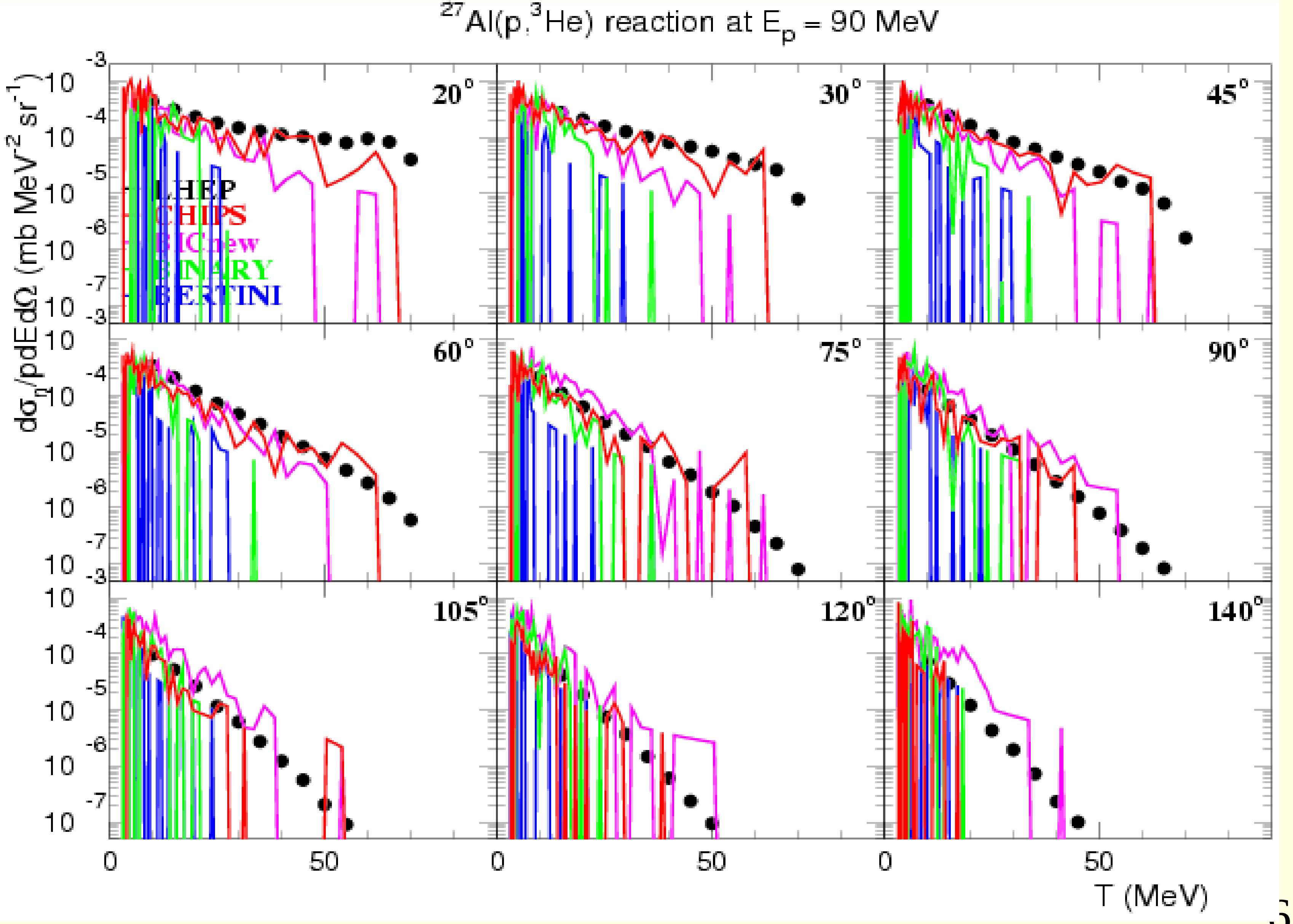

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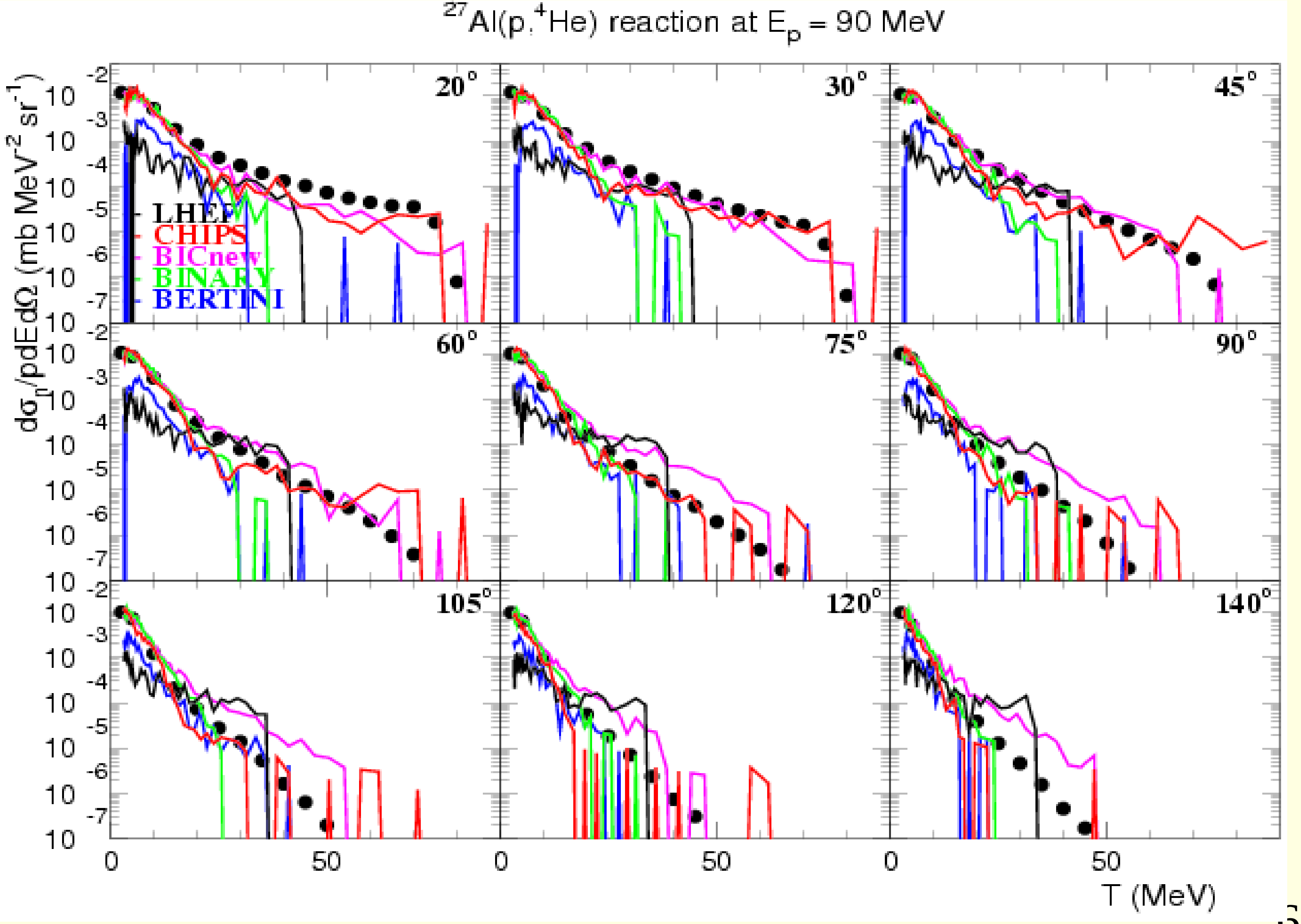

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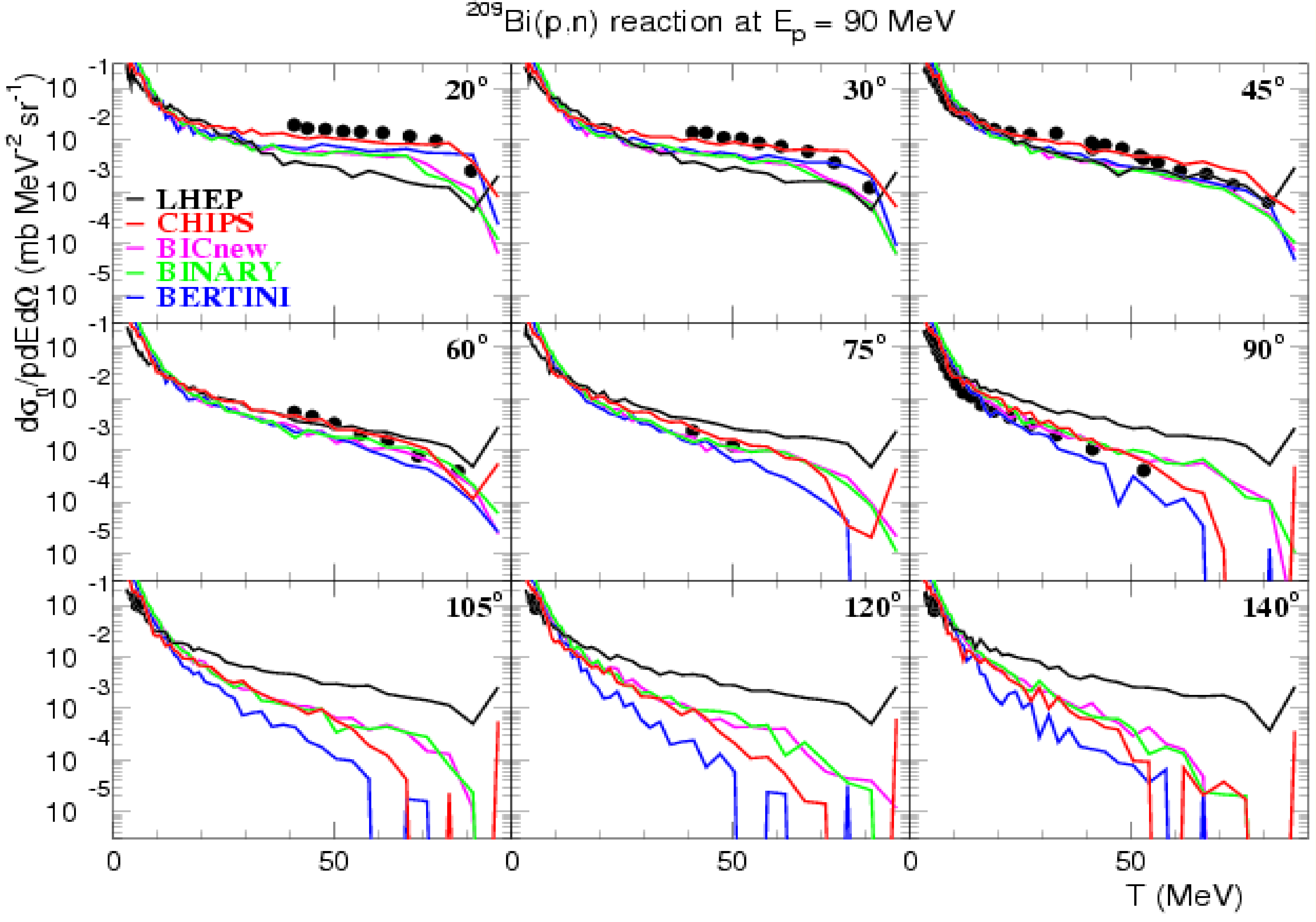

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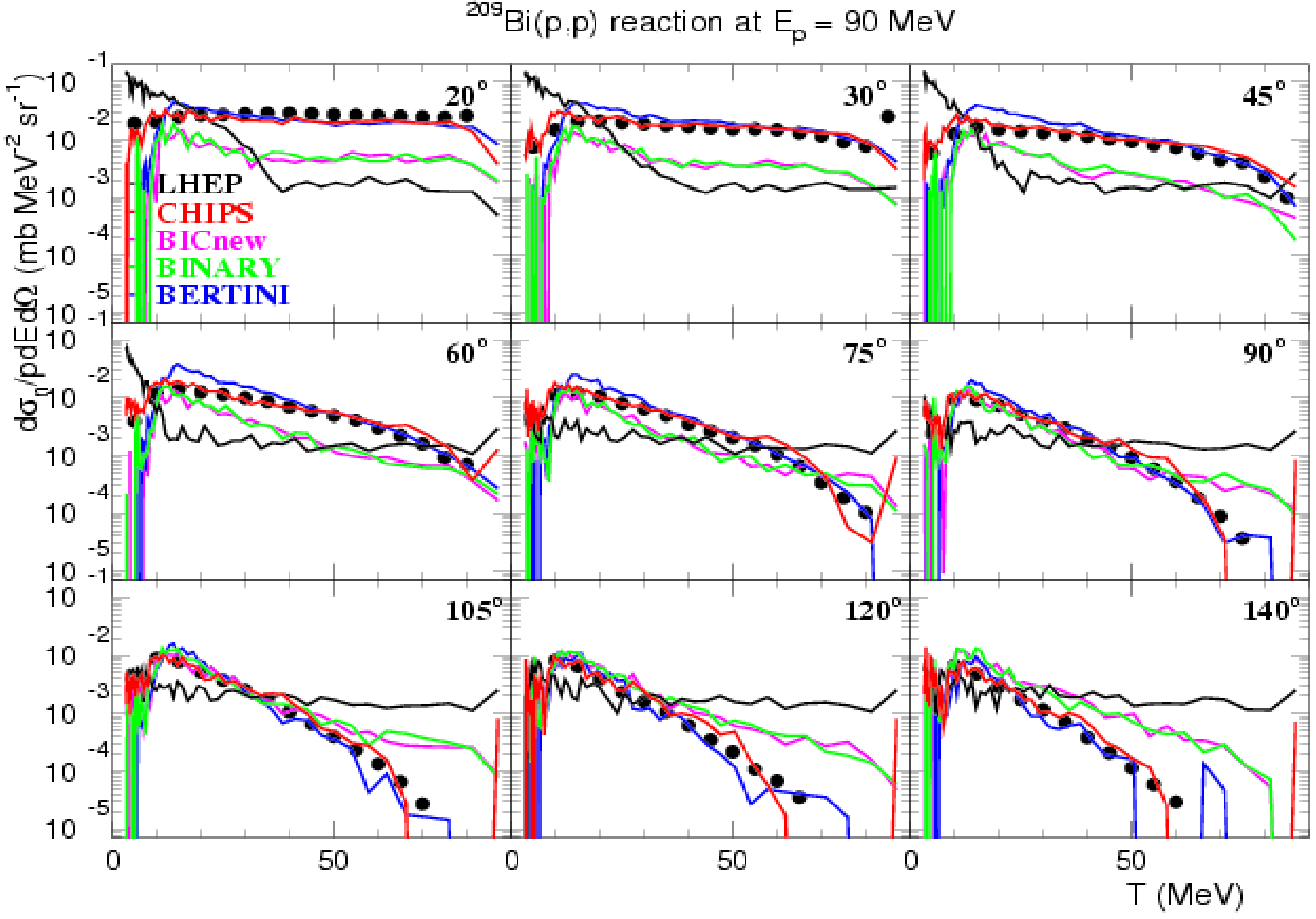

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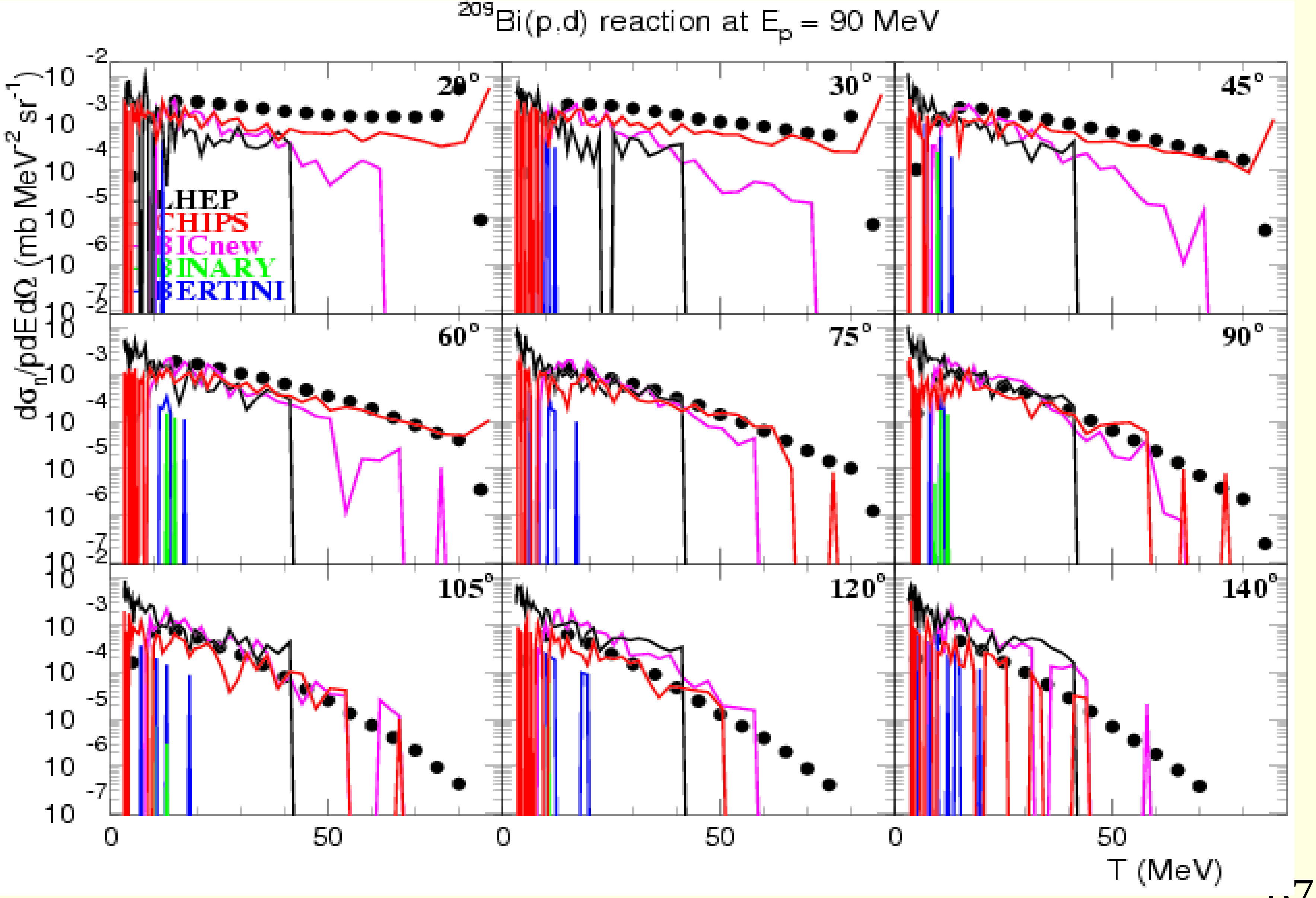

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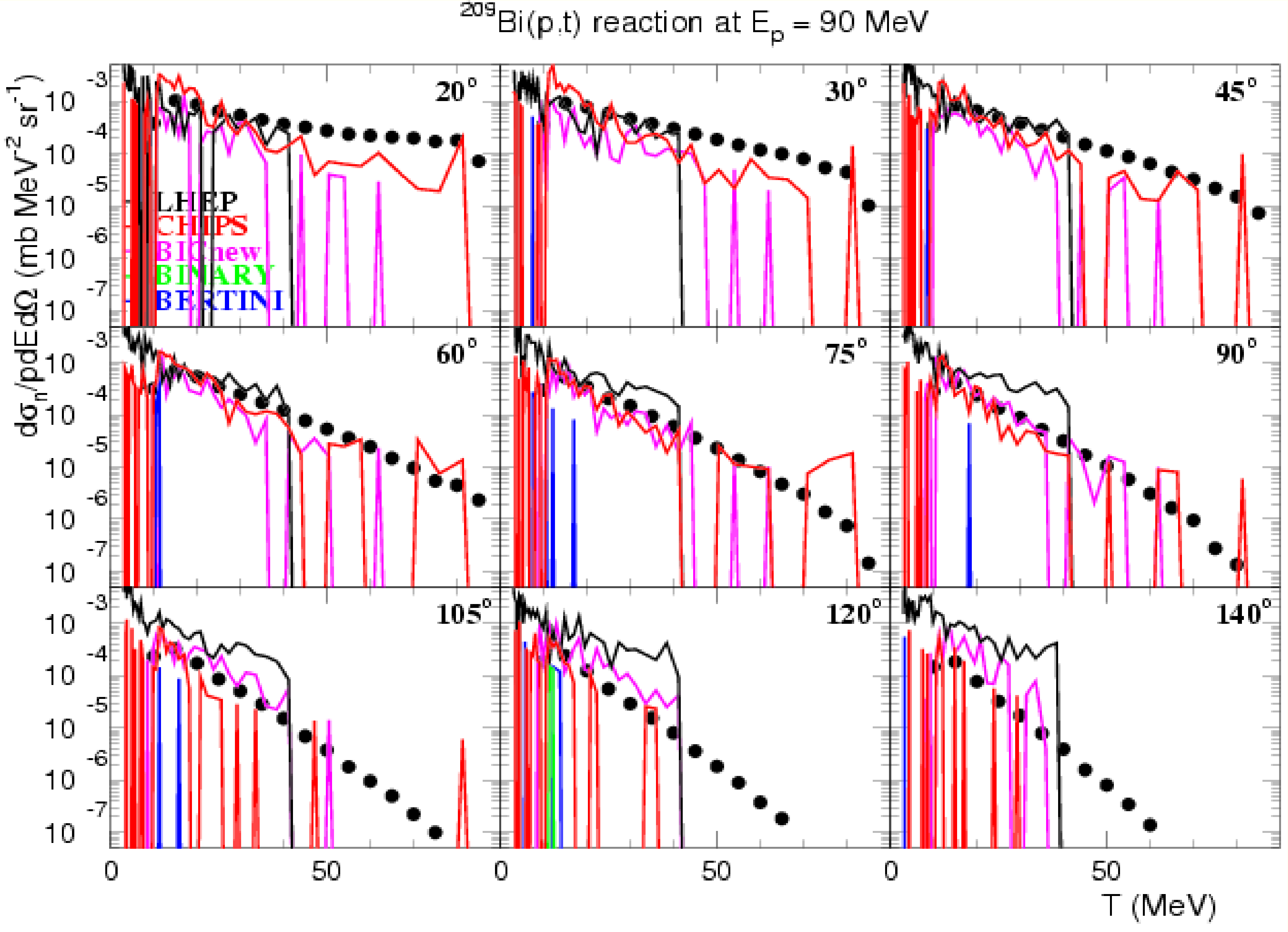

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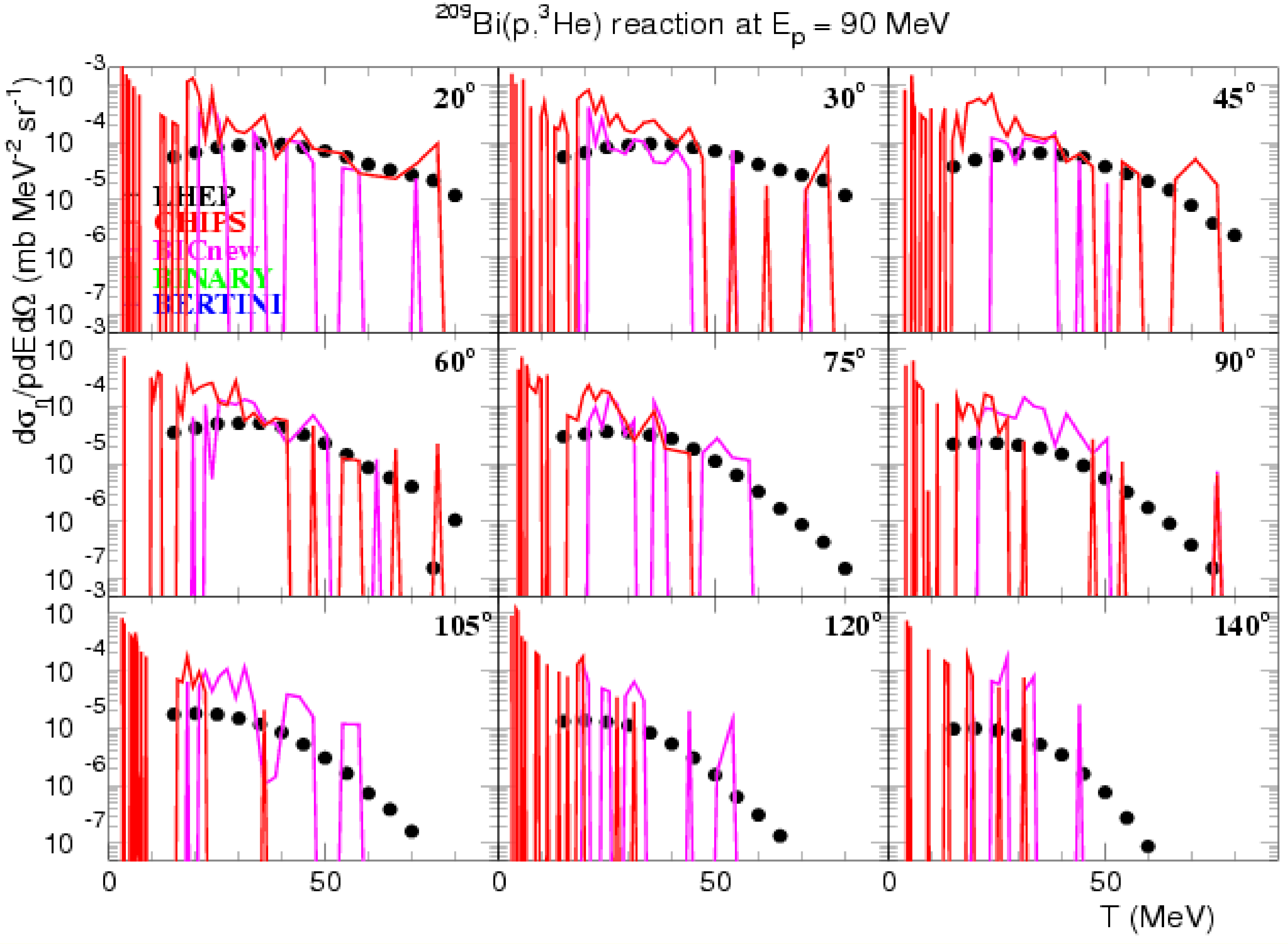

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