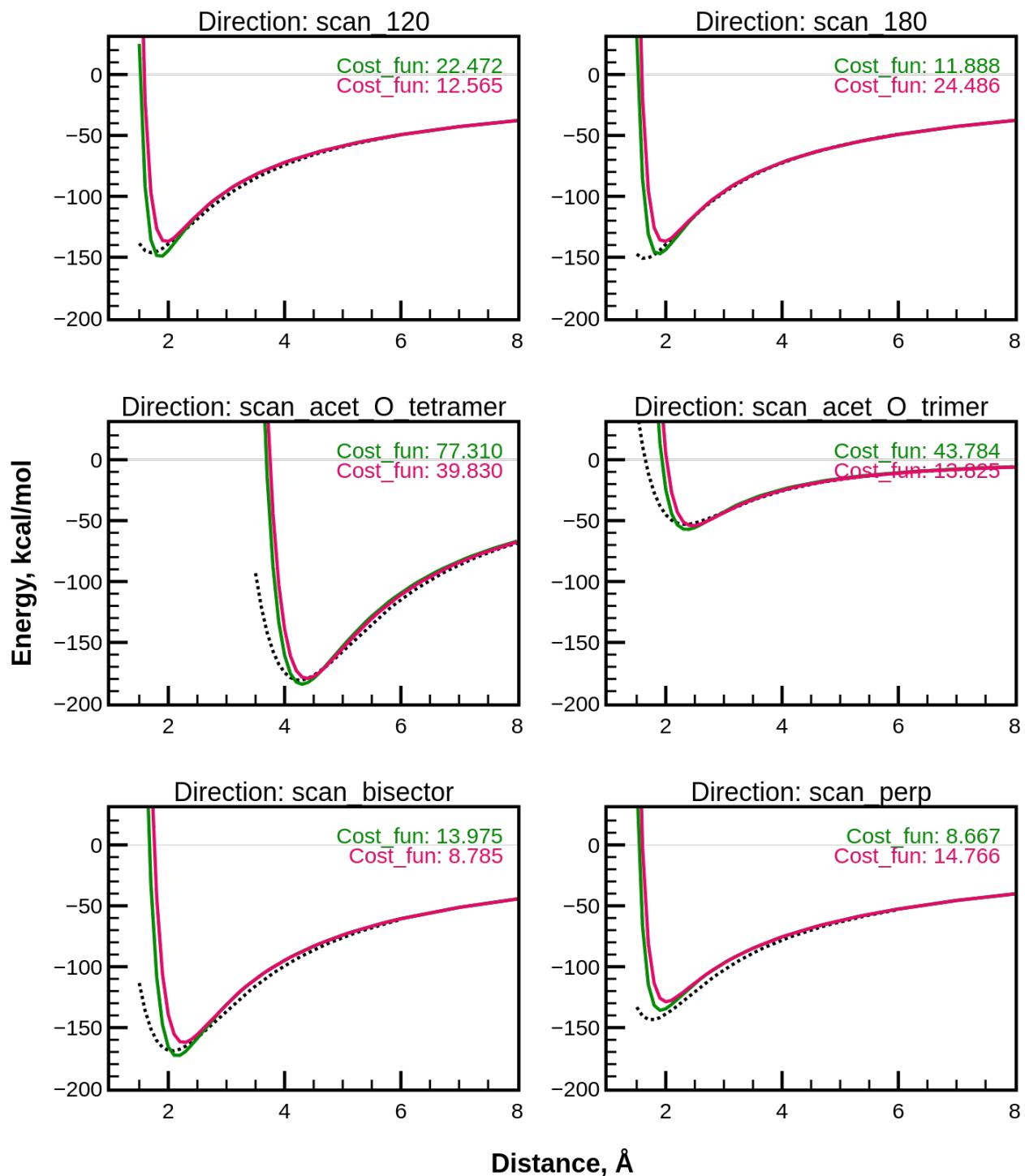


Potential Energy Surfaces (PESs) of Ion-Model Compounds

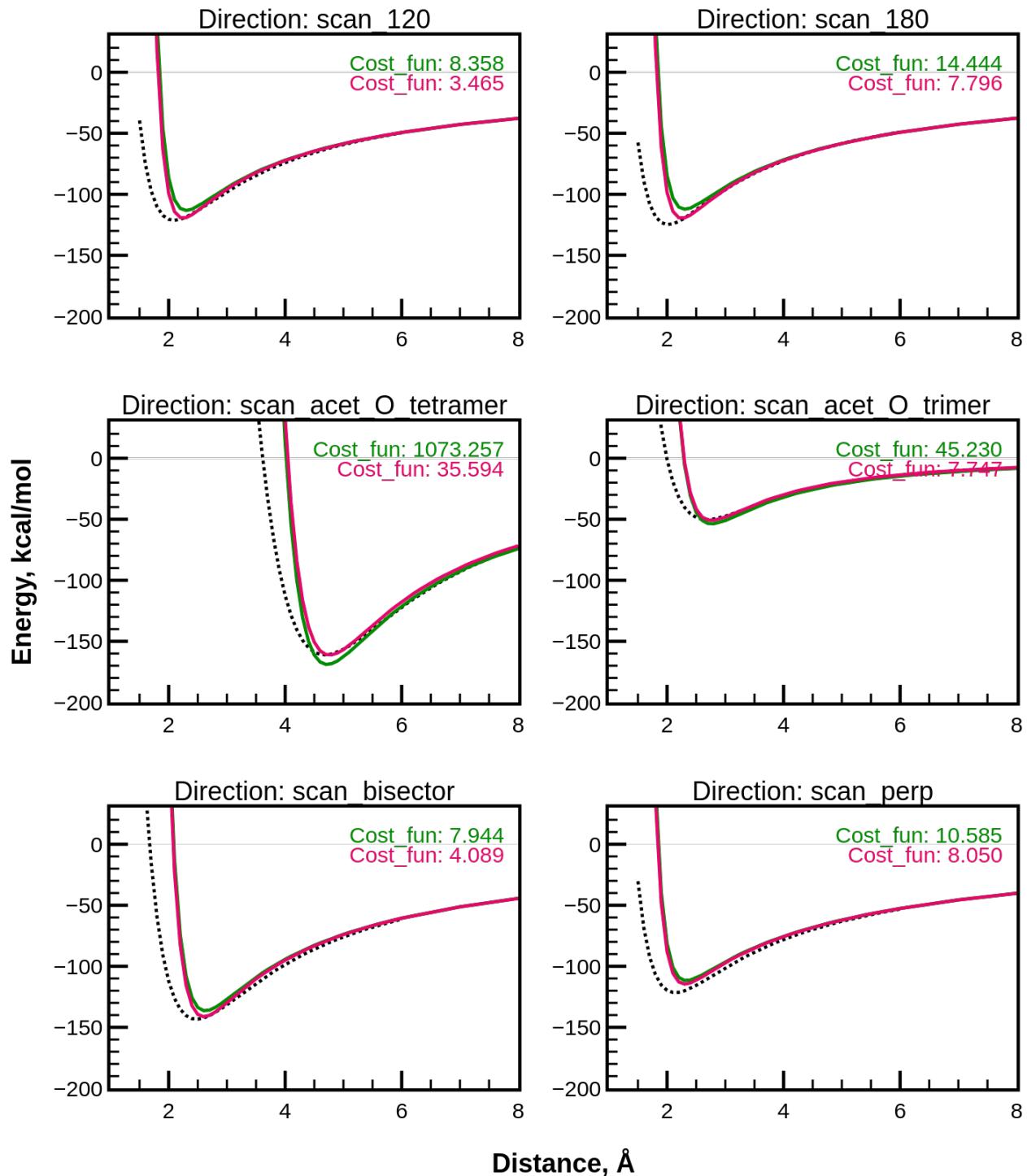
This file contains potential energy surfaces (PES) of the ion-model compounds analyzed in the manuscript titled "*Balancing Group 1 Monoatomic Ion-Polar Compound Interactions in the Polarizable Drude Force Field: Applications in Protein and Nucleic Acid Systems.*"

The dotted lines represent quantum mechanical (QM) results obtained using MP2/cc-pVQZ-X2C model chemistry for K⁺, Rb⁺, and Cs⁺, and MP2/cc-pVQZ model chemistry for all other elements. Green and pink lines correspond to the molecular mechanical (MM) PESs from the original and new parameters, respectively. The cost function values are annotated and color-coded in each subplot, indicating the optimization performance of the force field parameters against the QM reference.

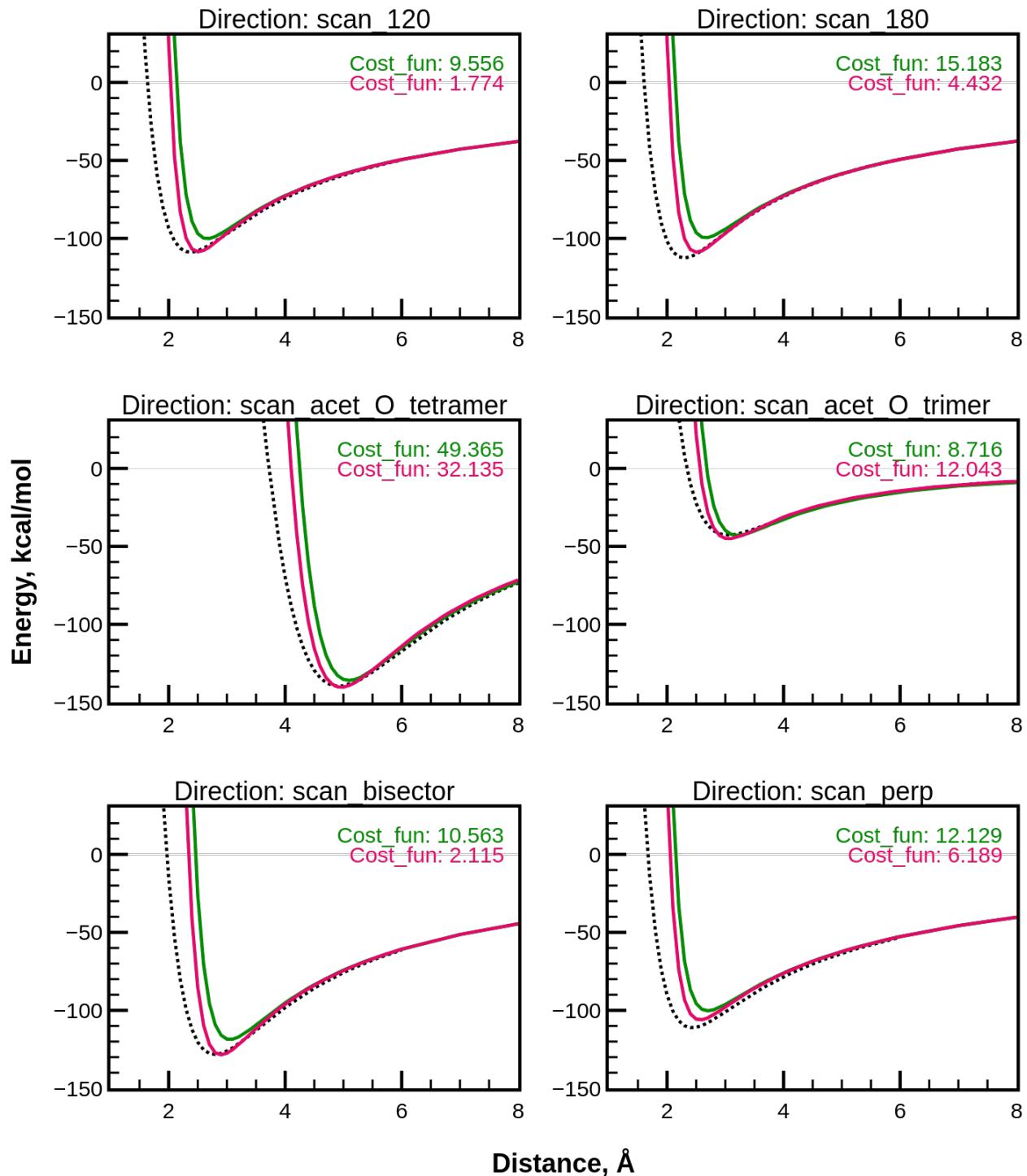
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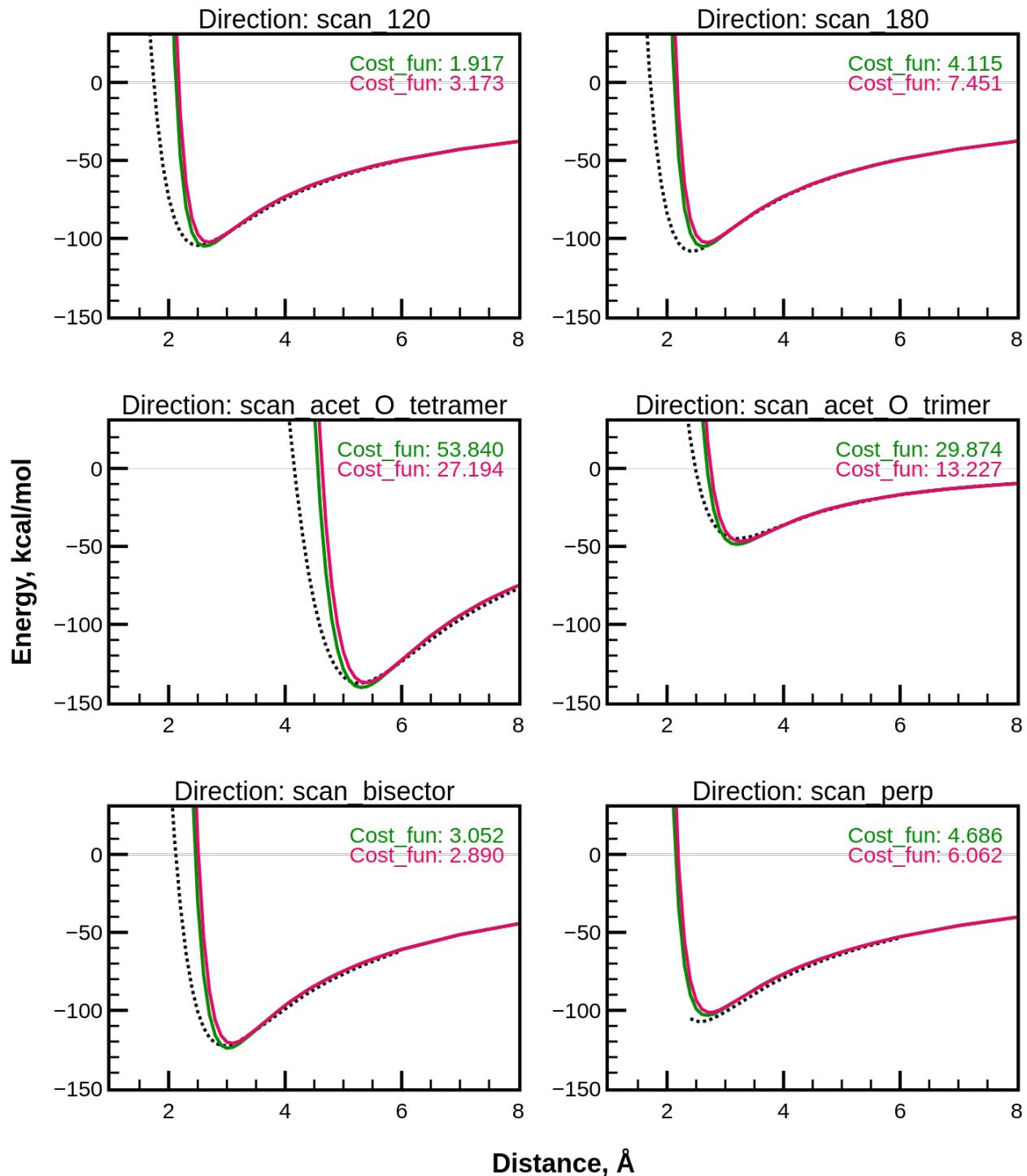
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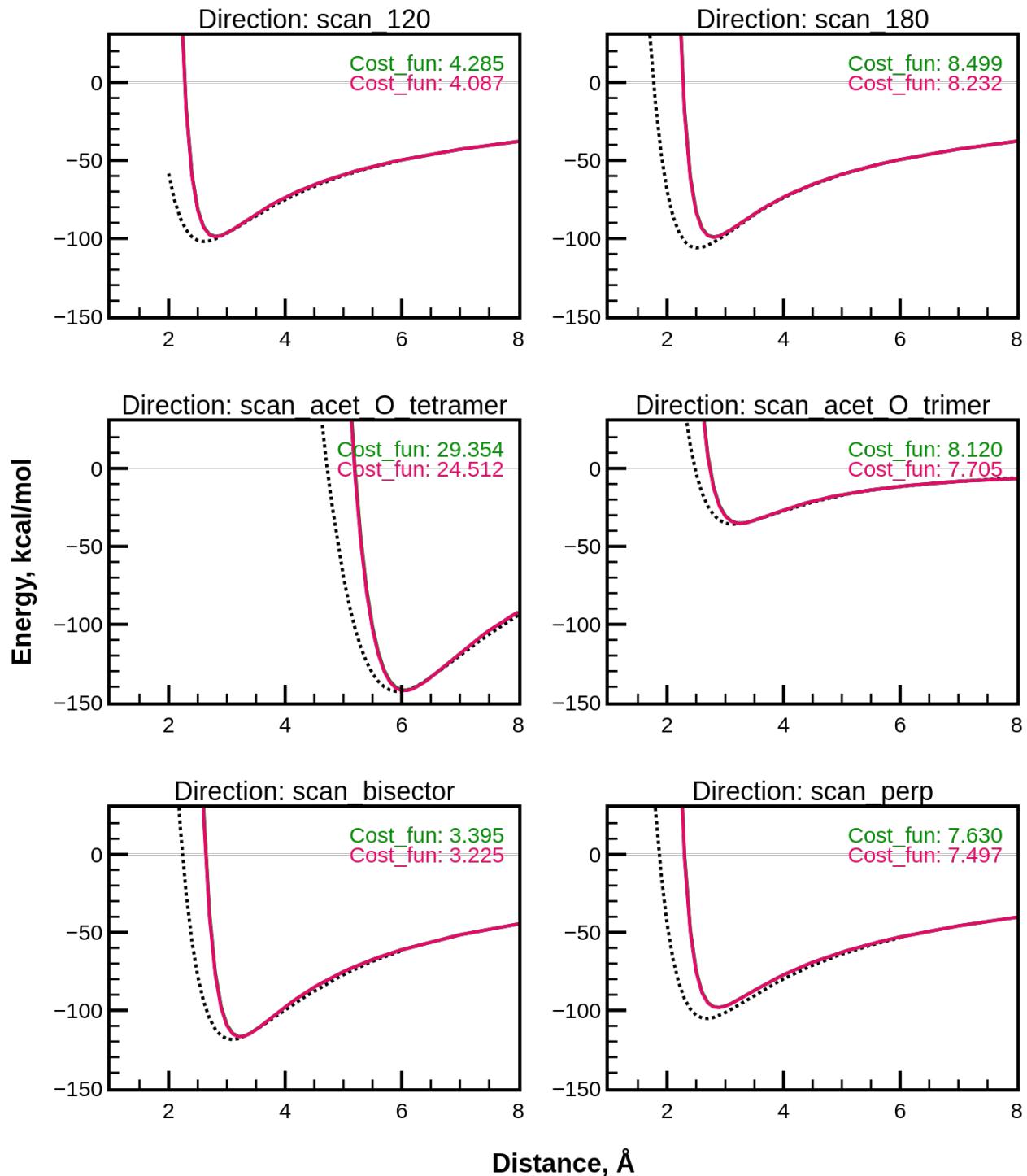
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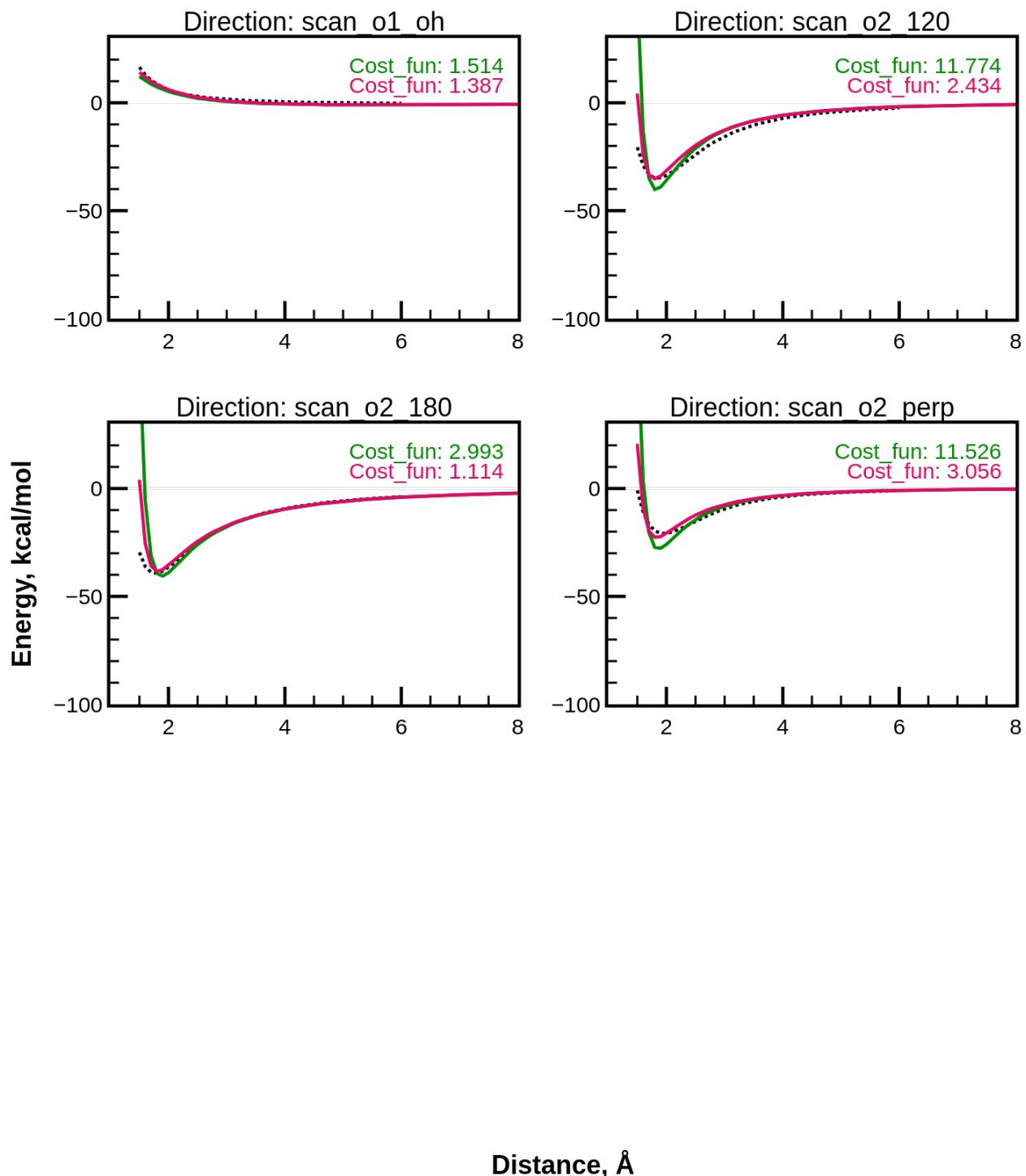
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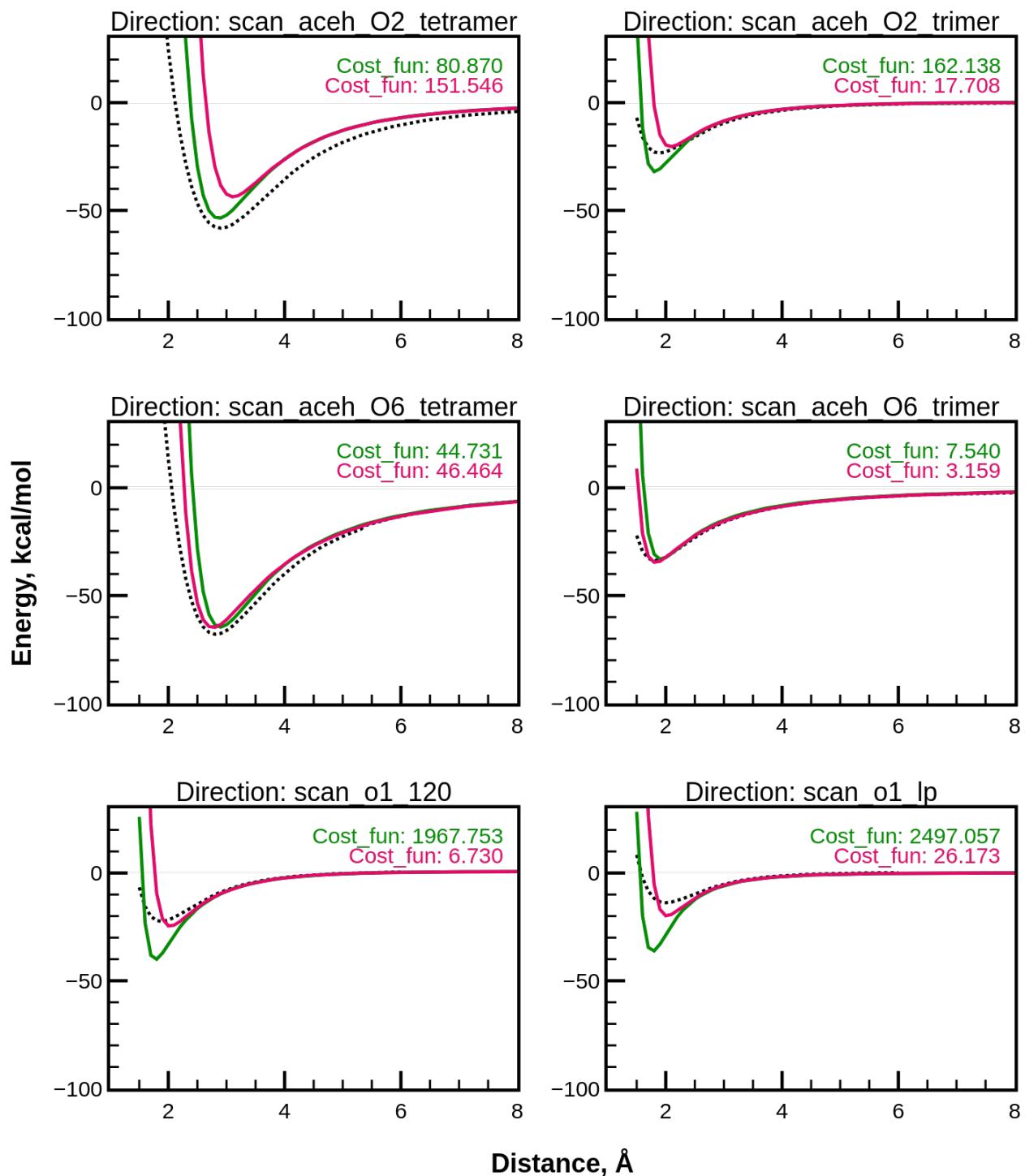
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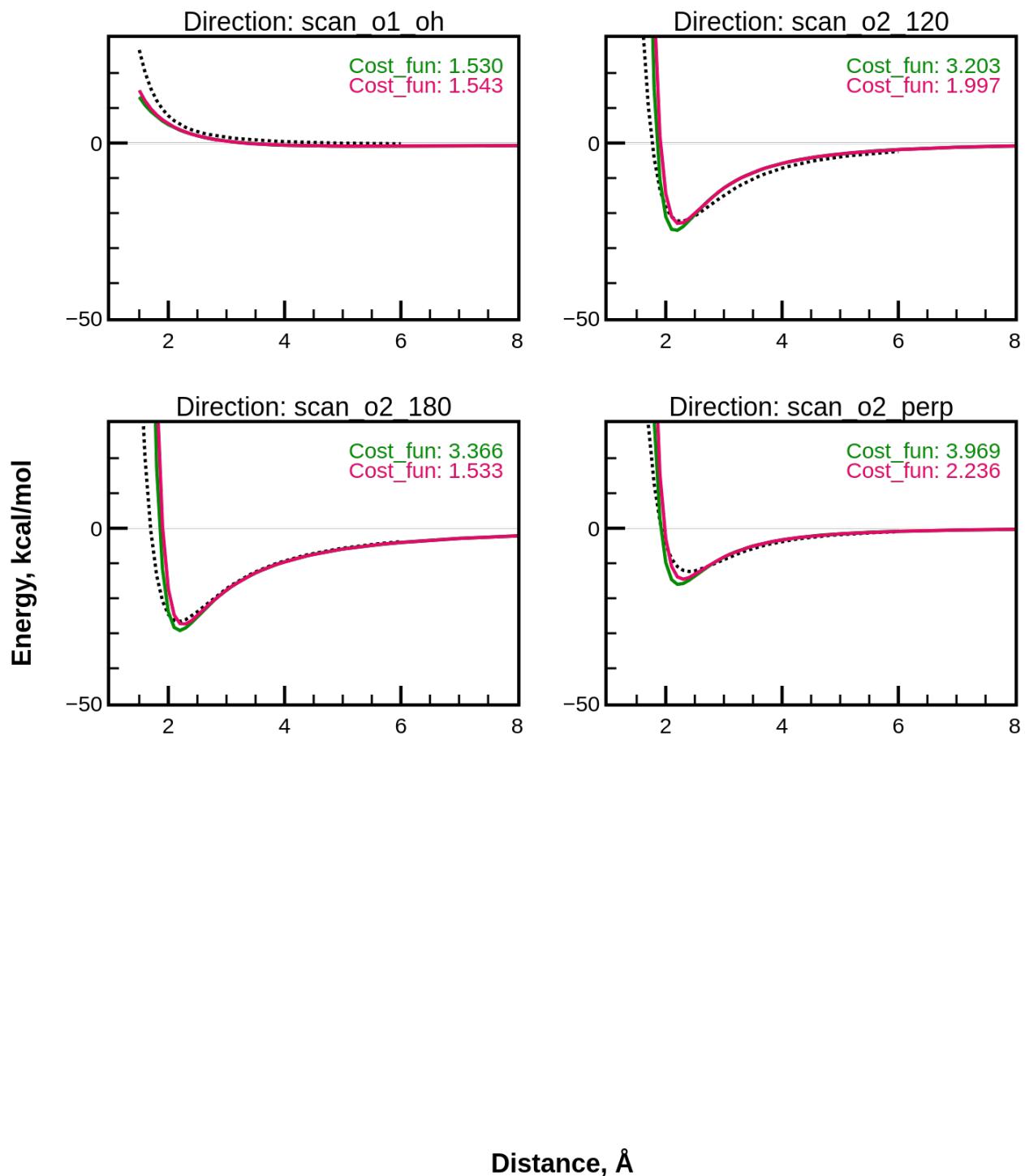
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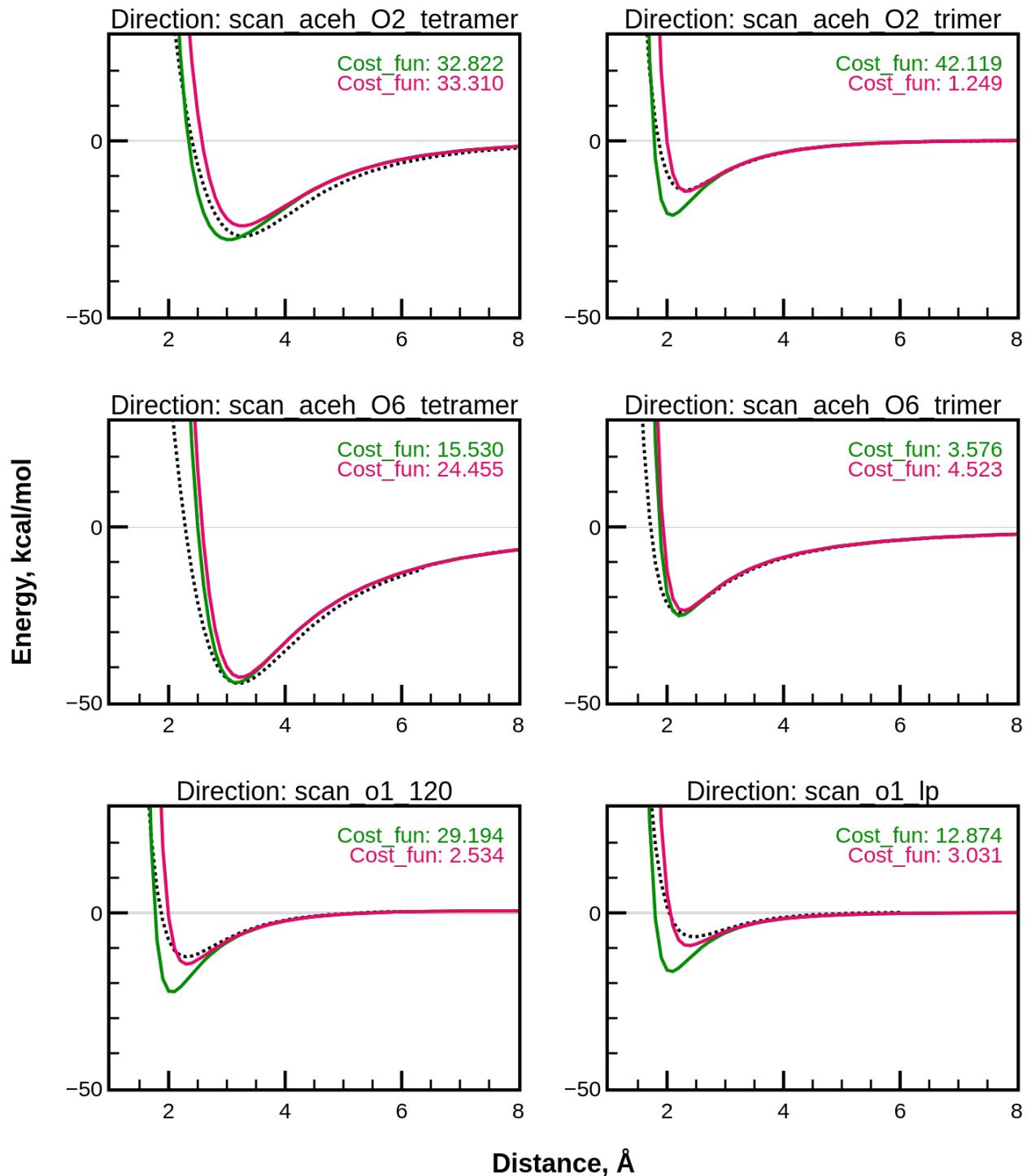
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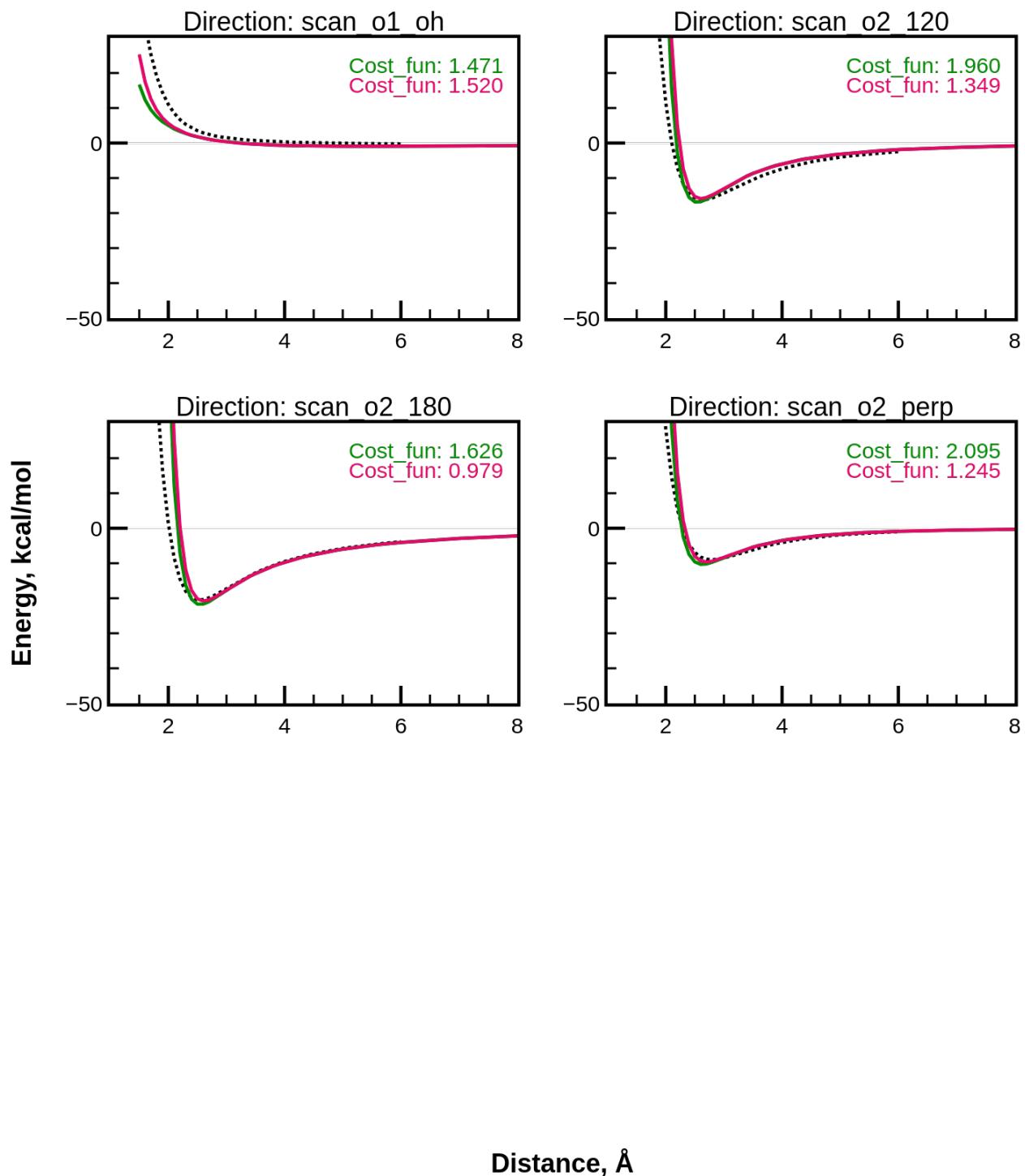
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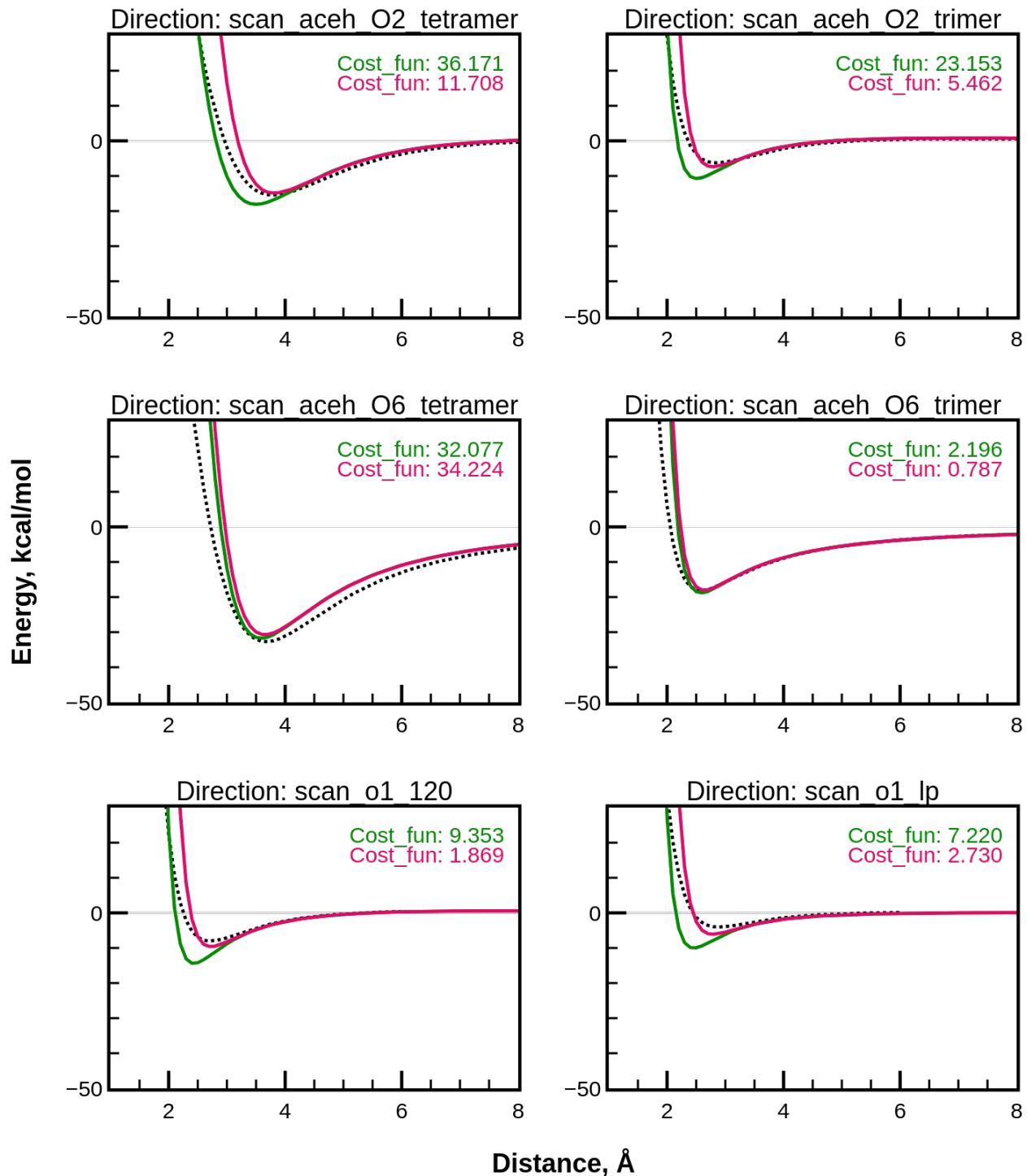
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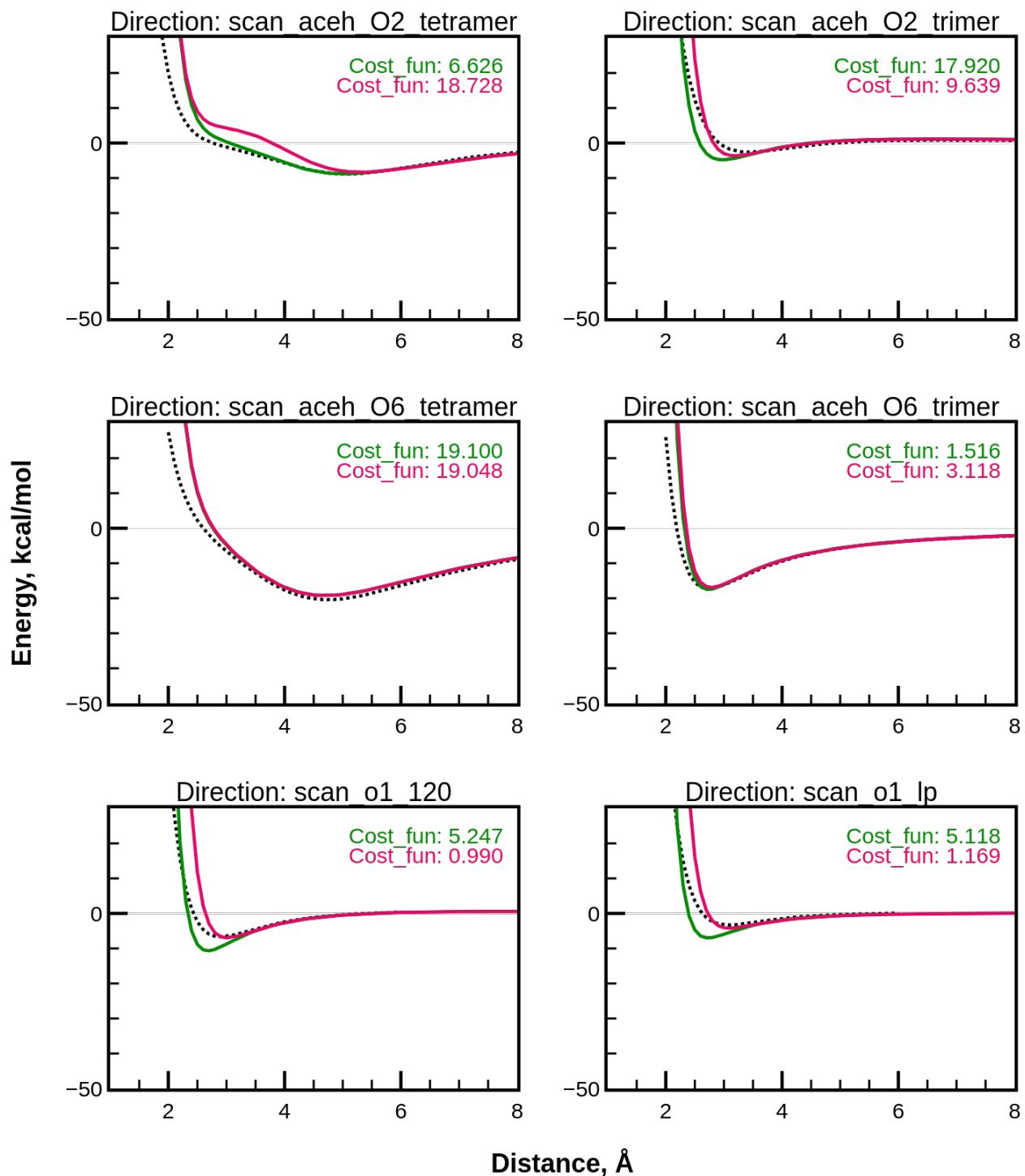
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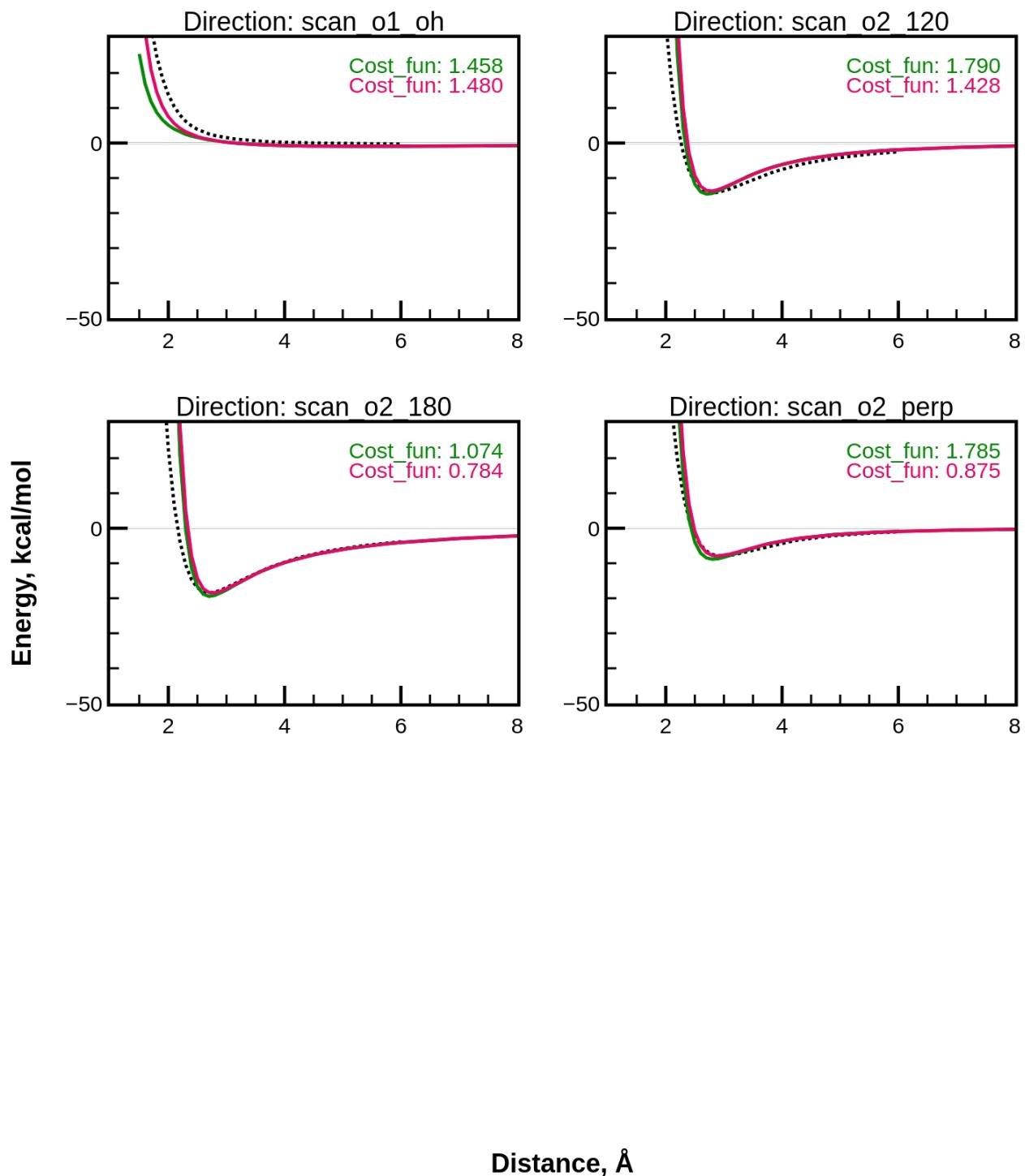
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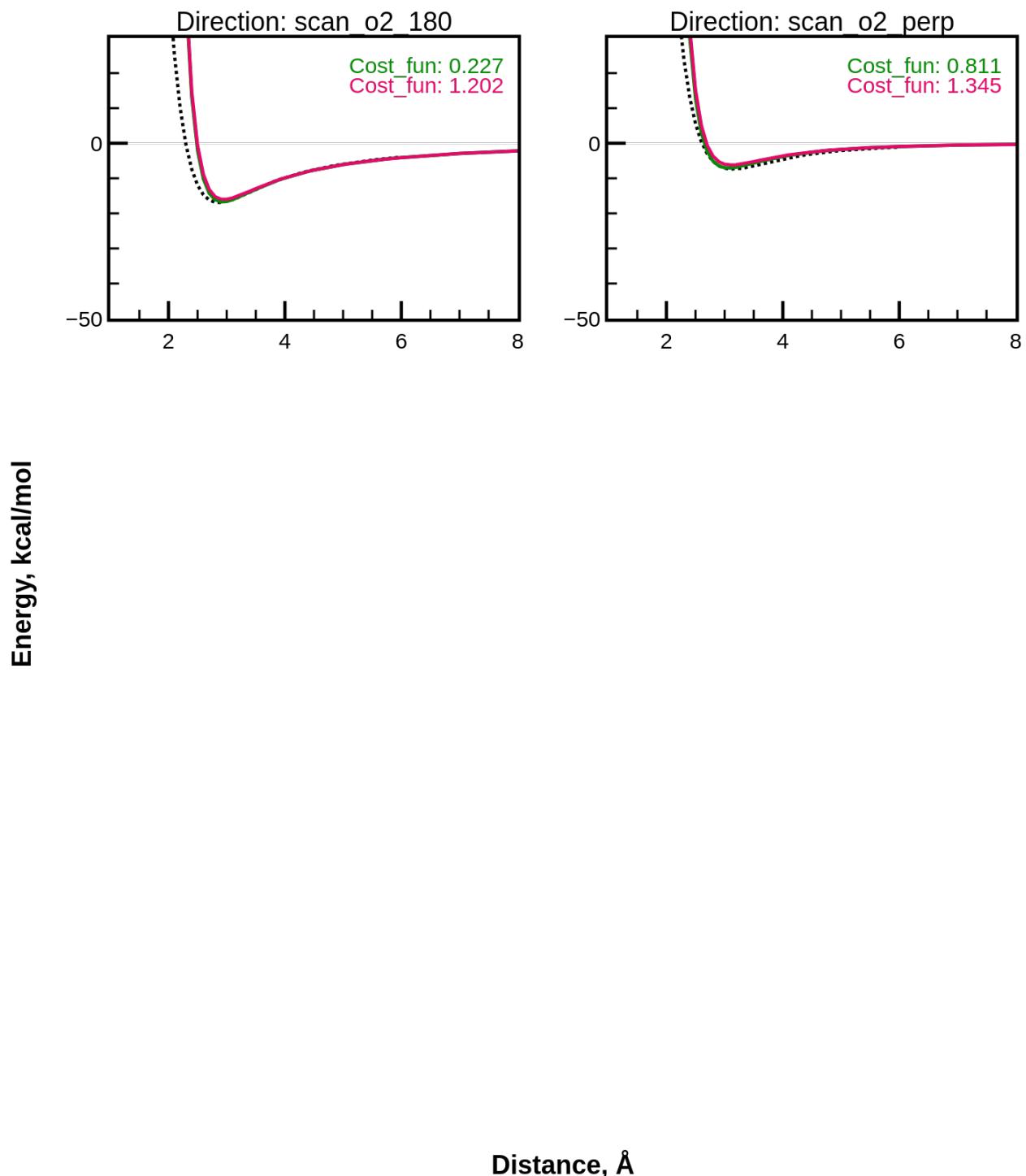
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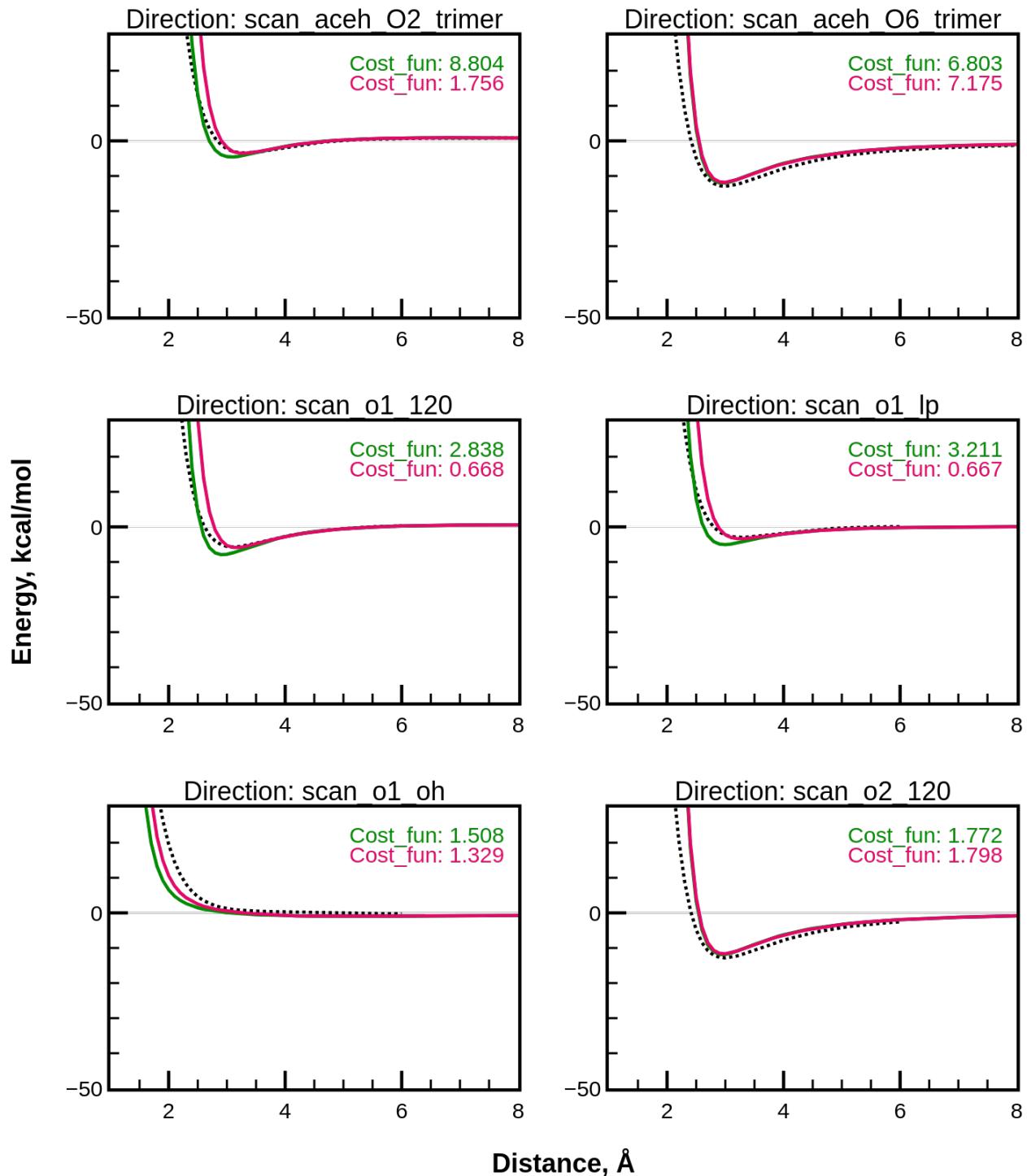
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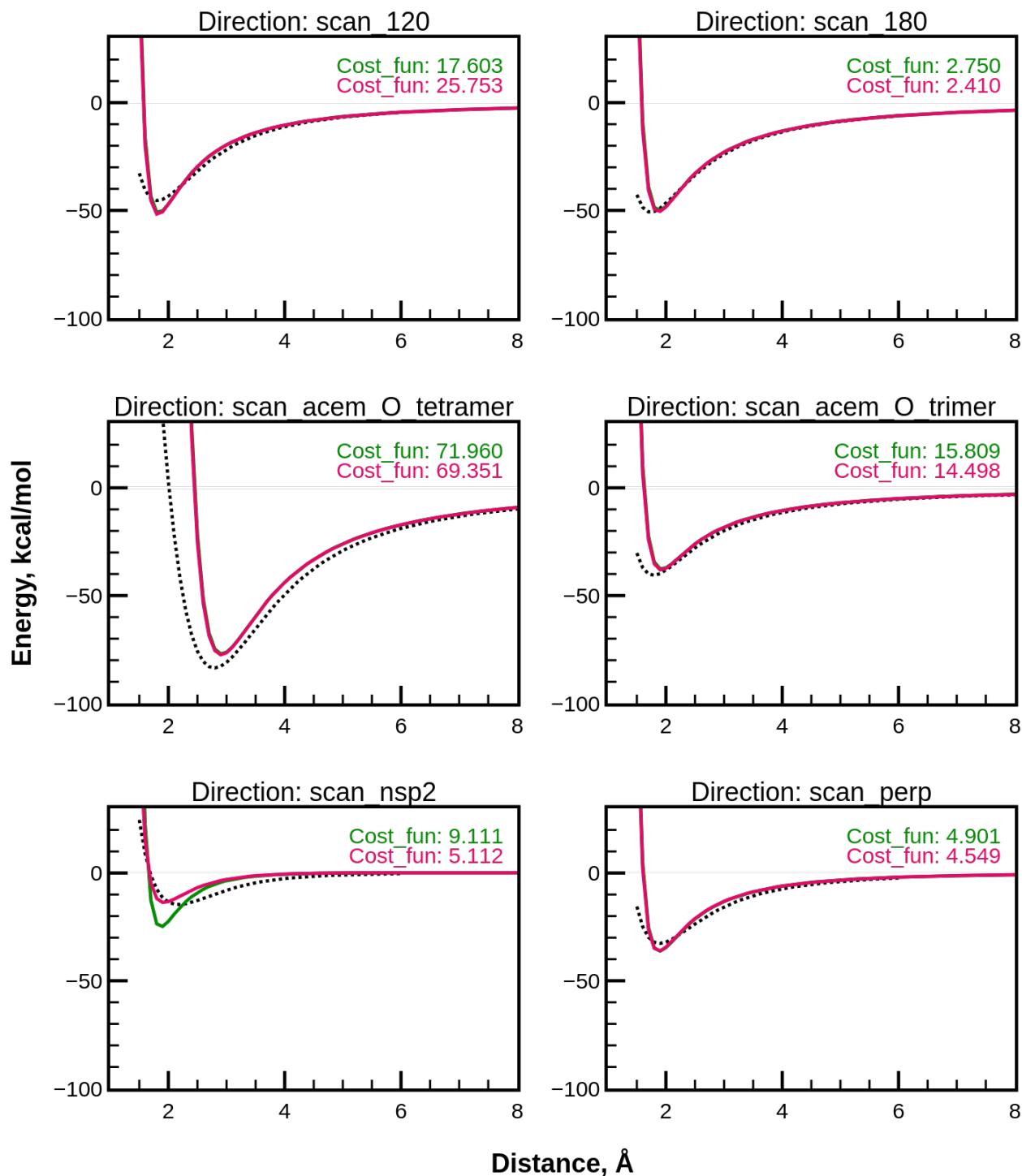
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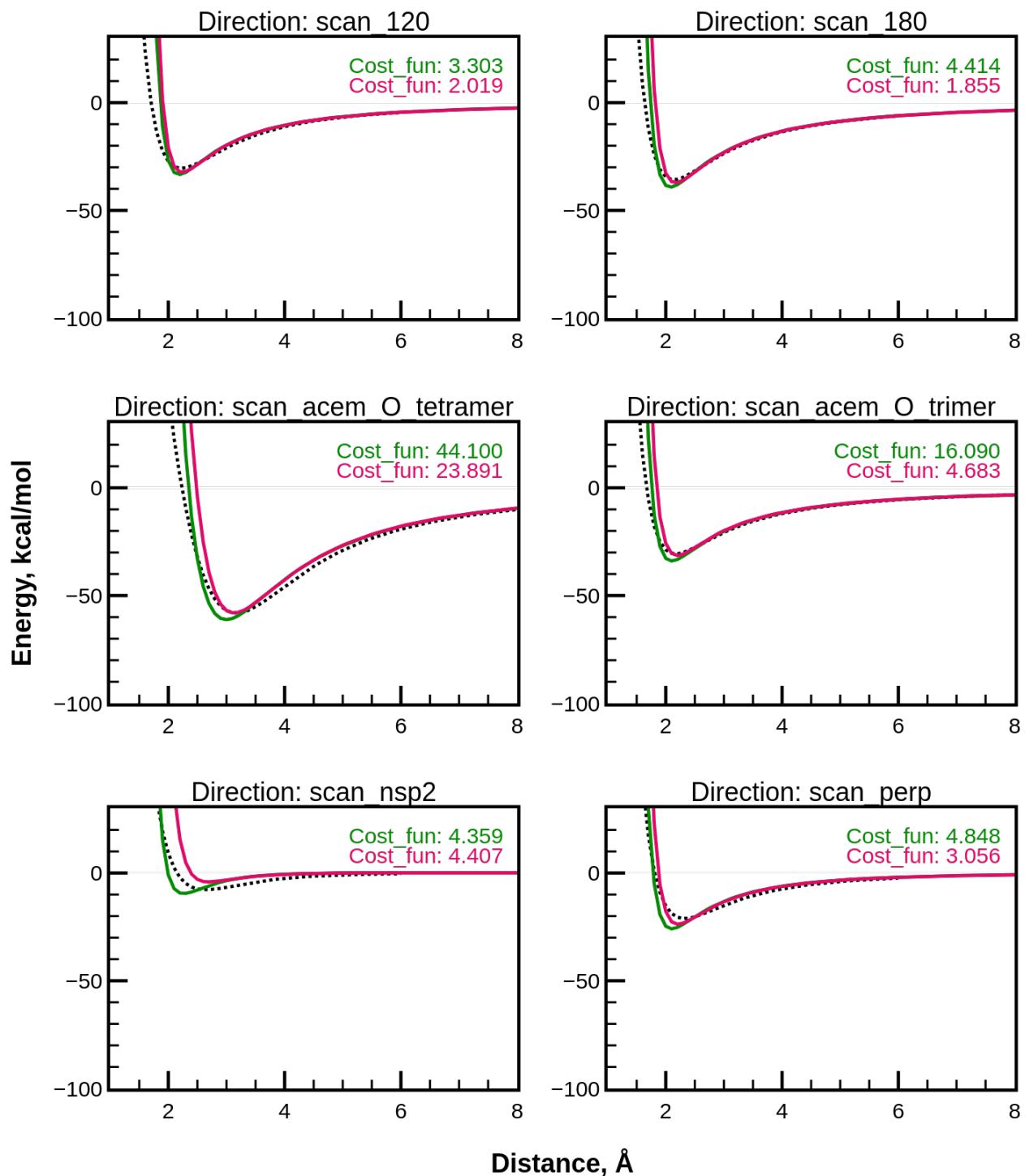
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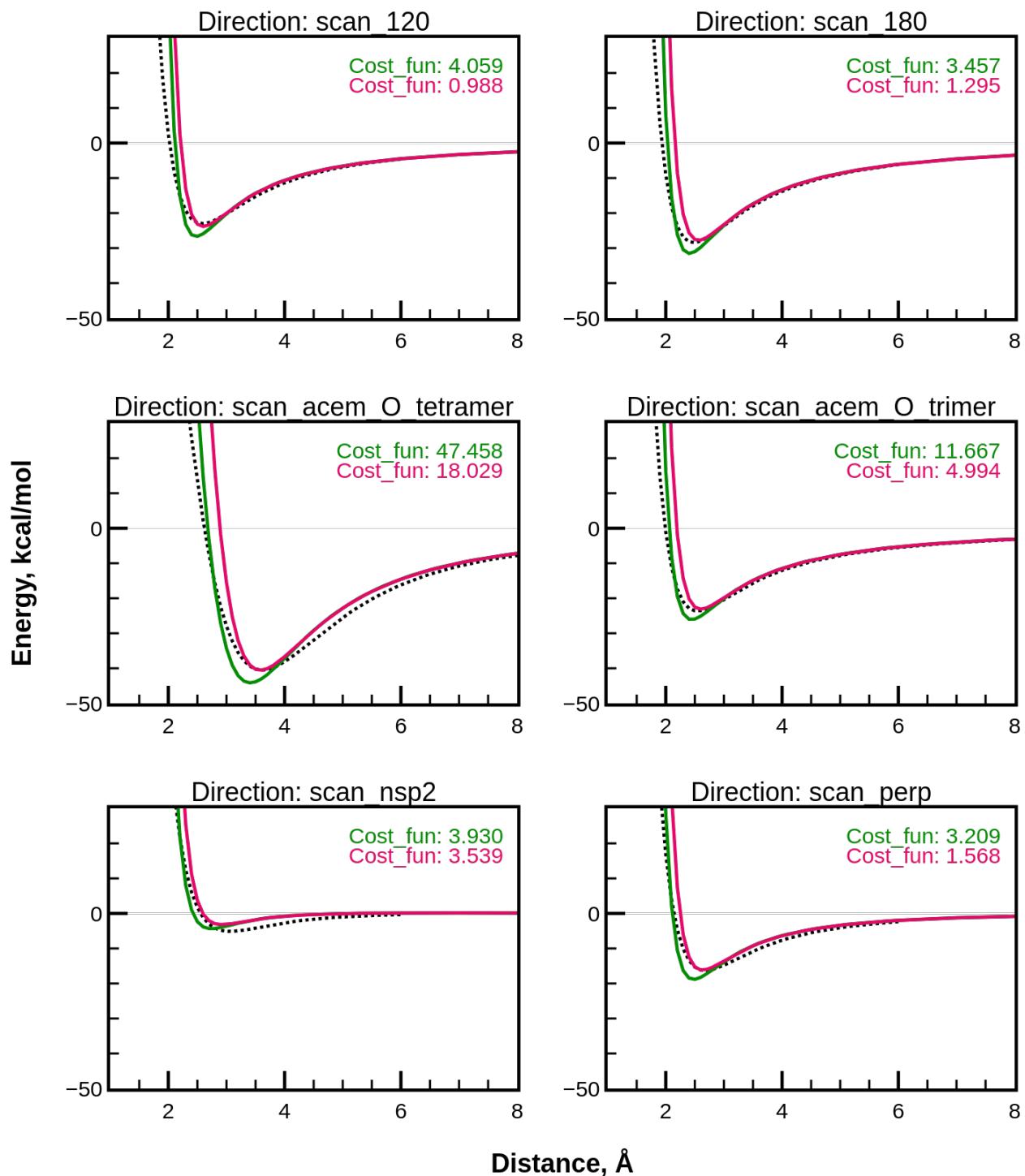
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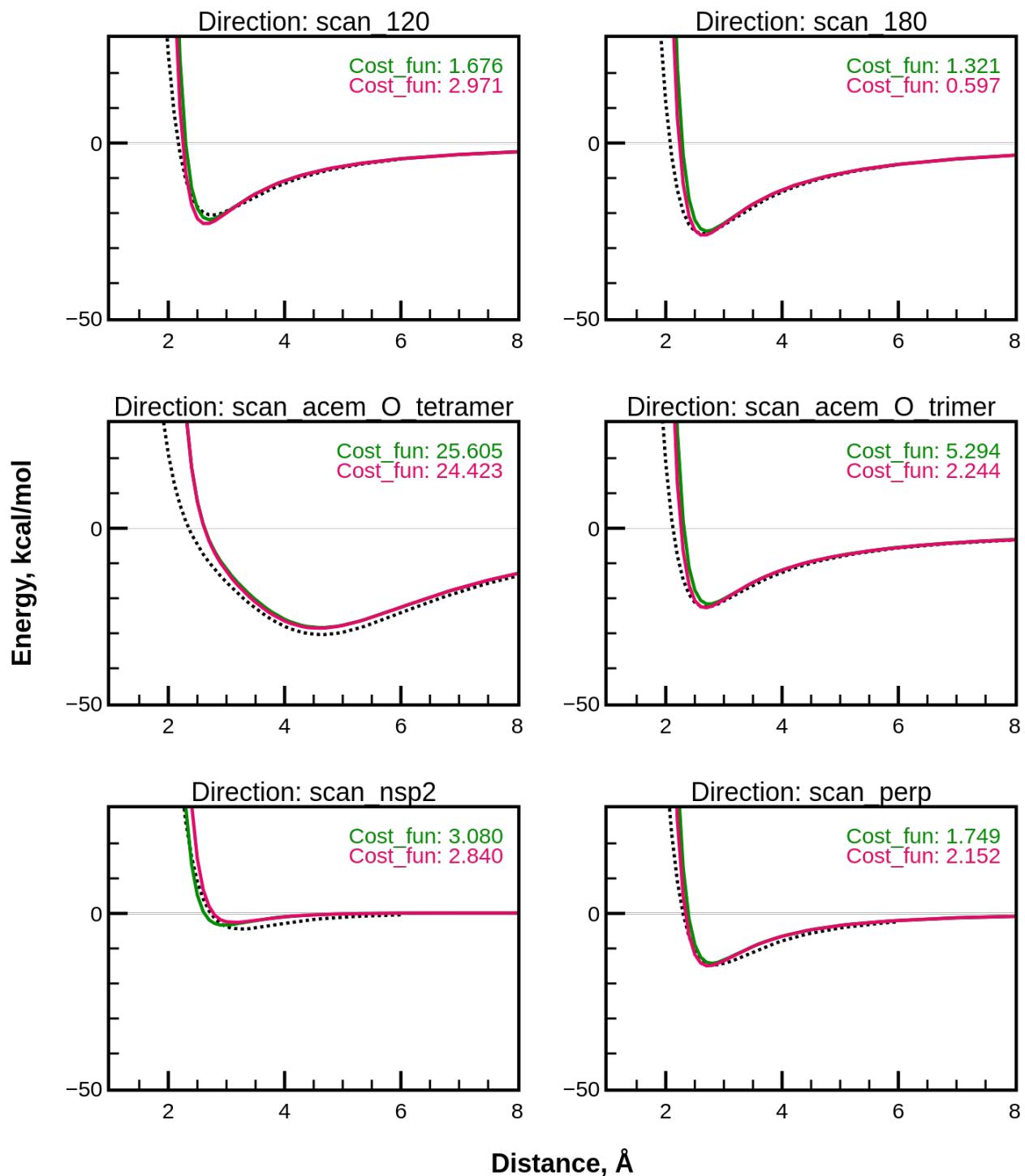
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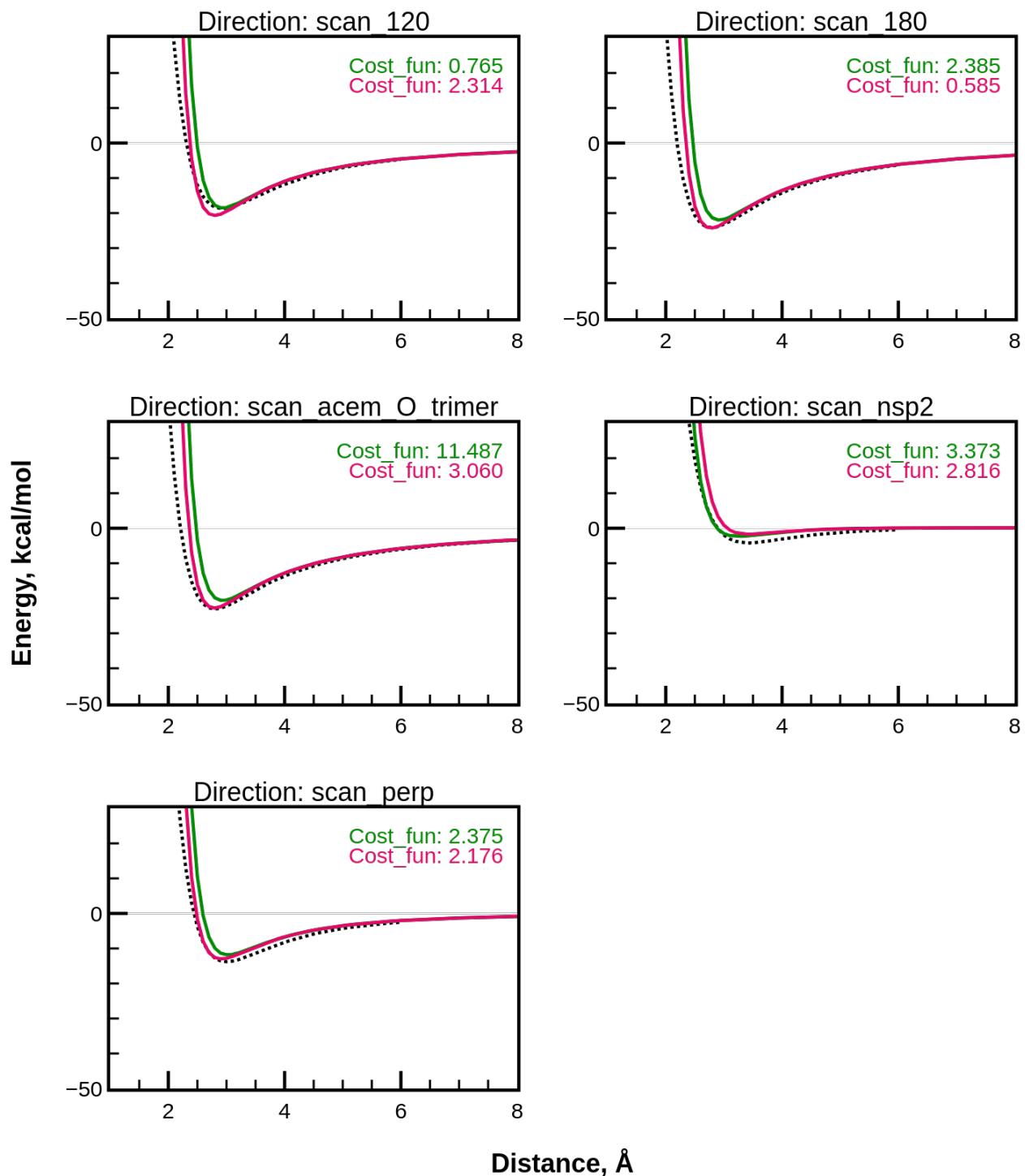
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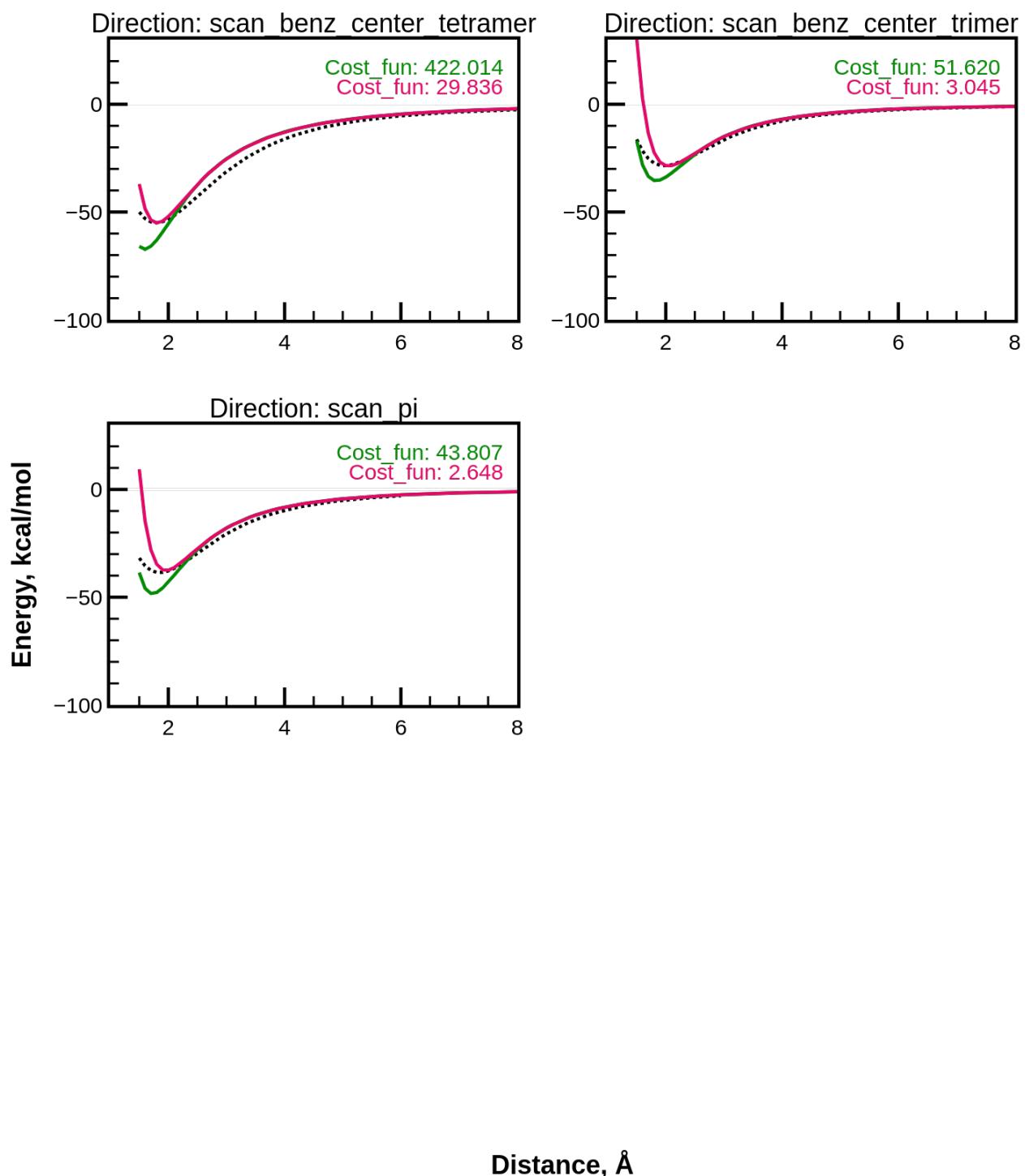
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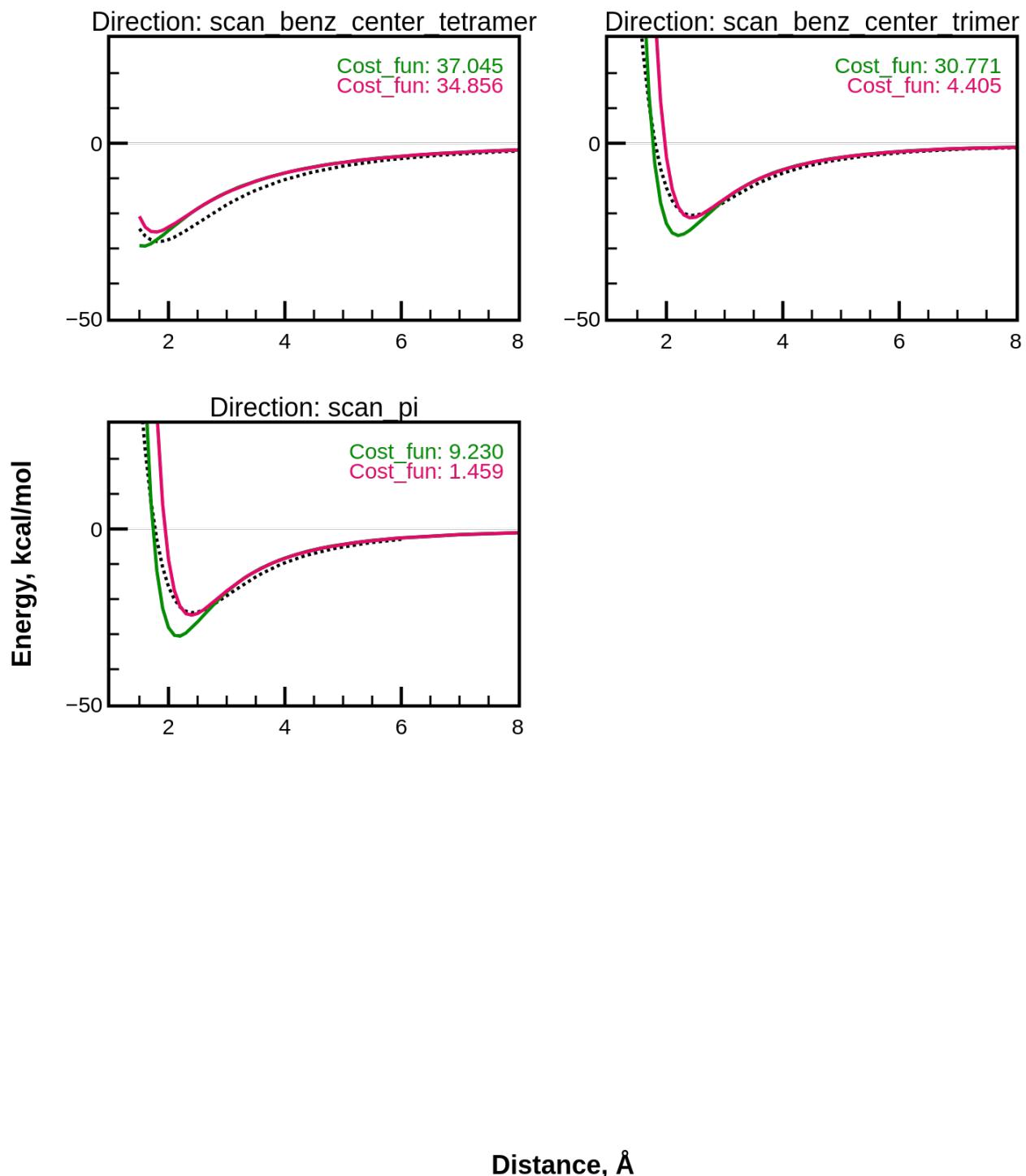
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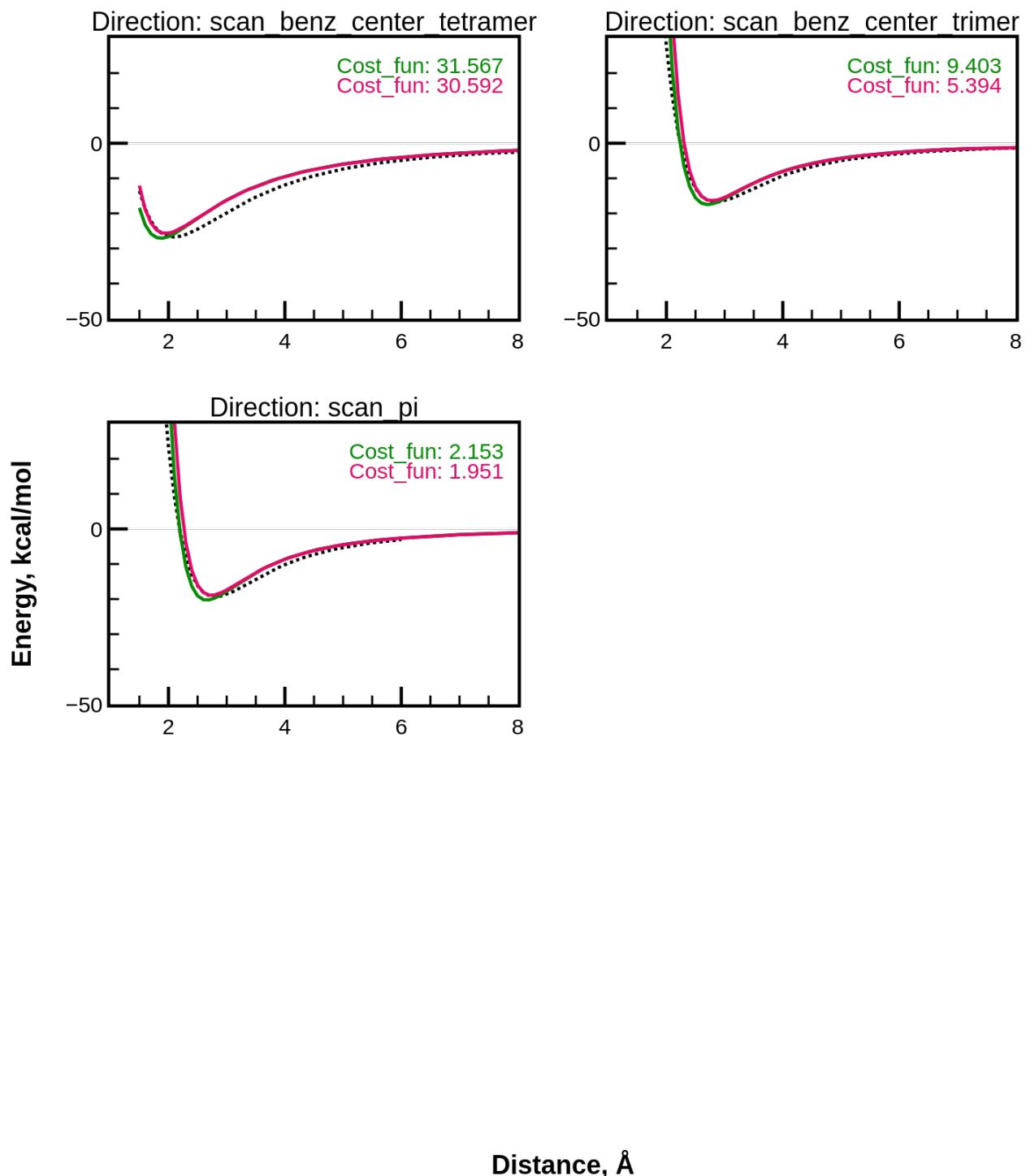
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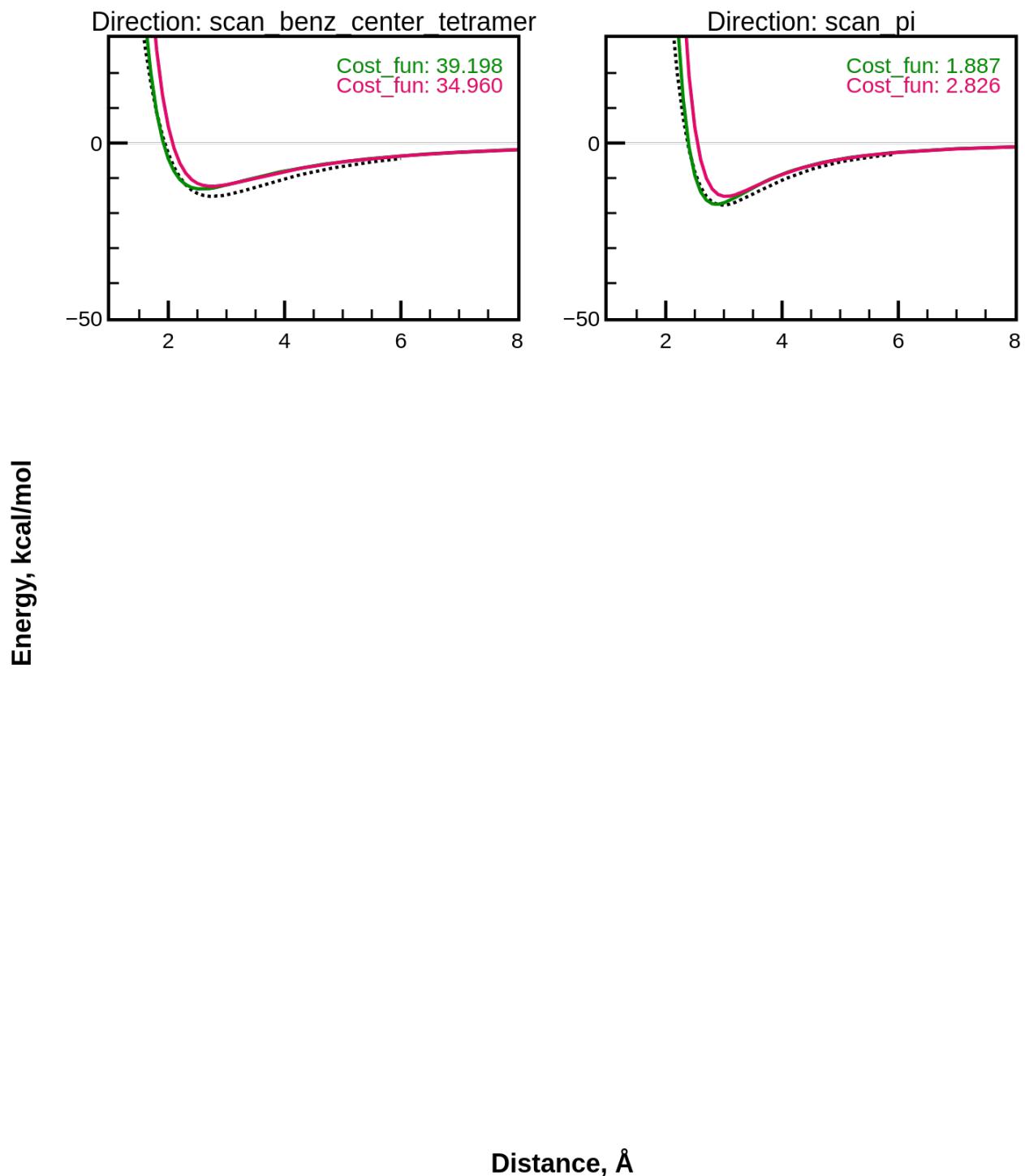
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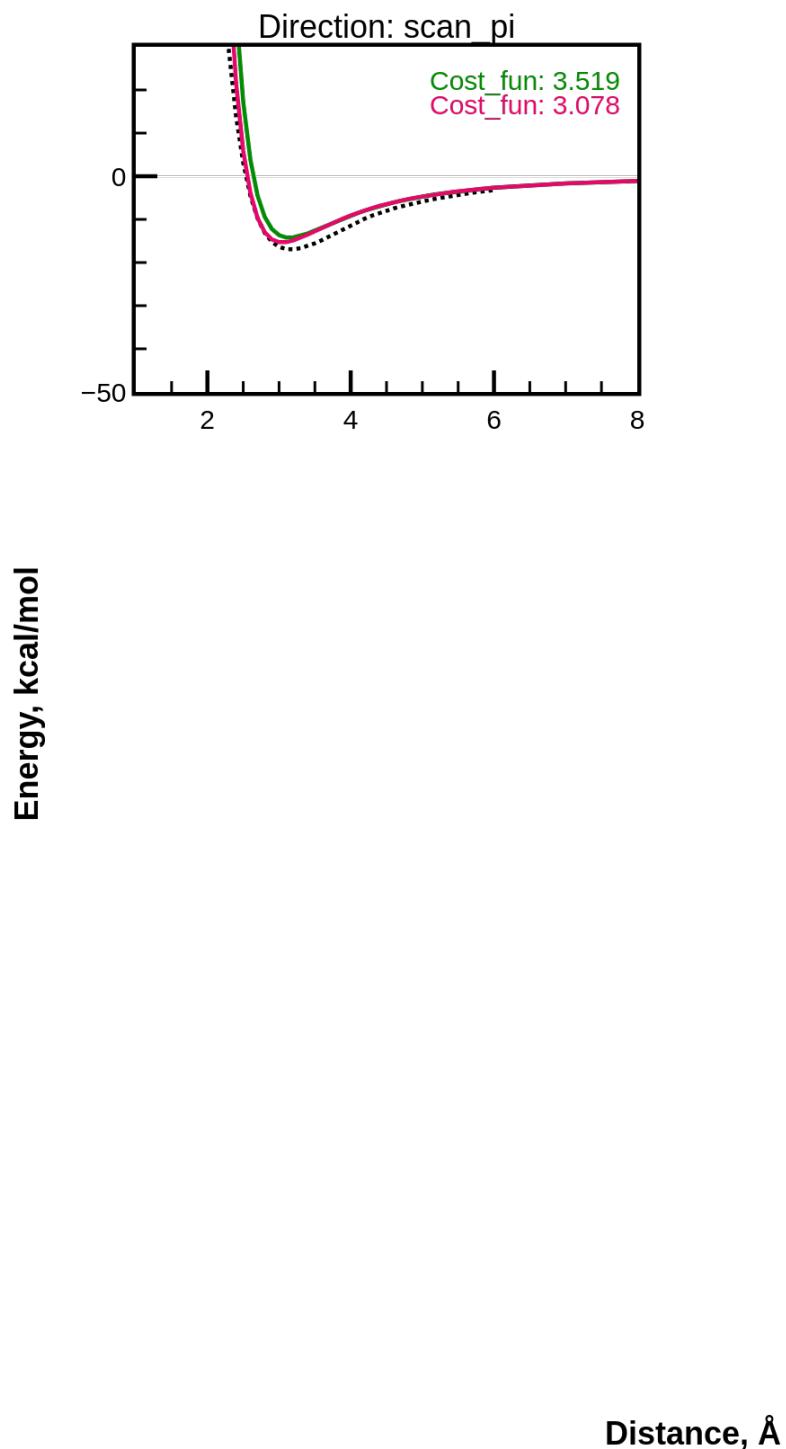
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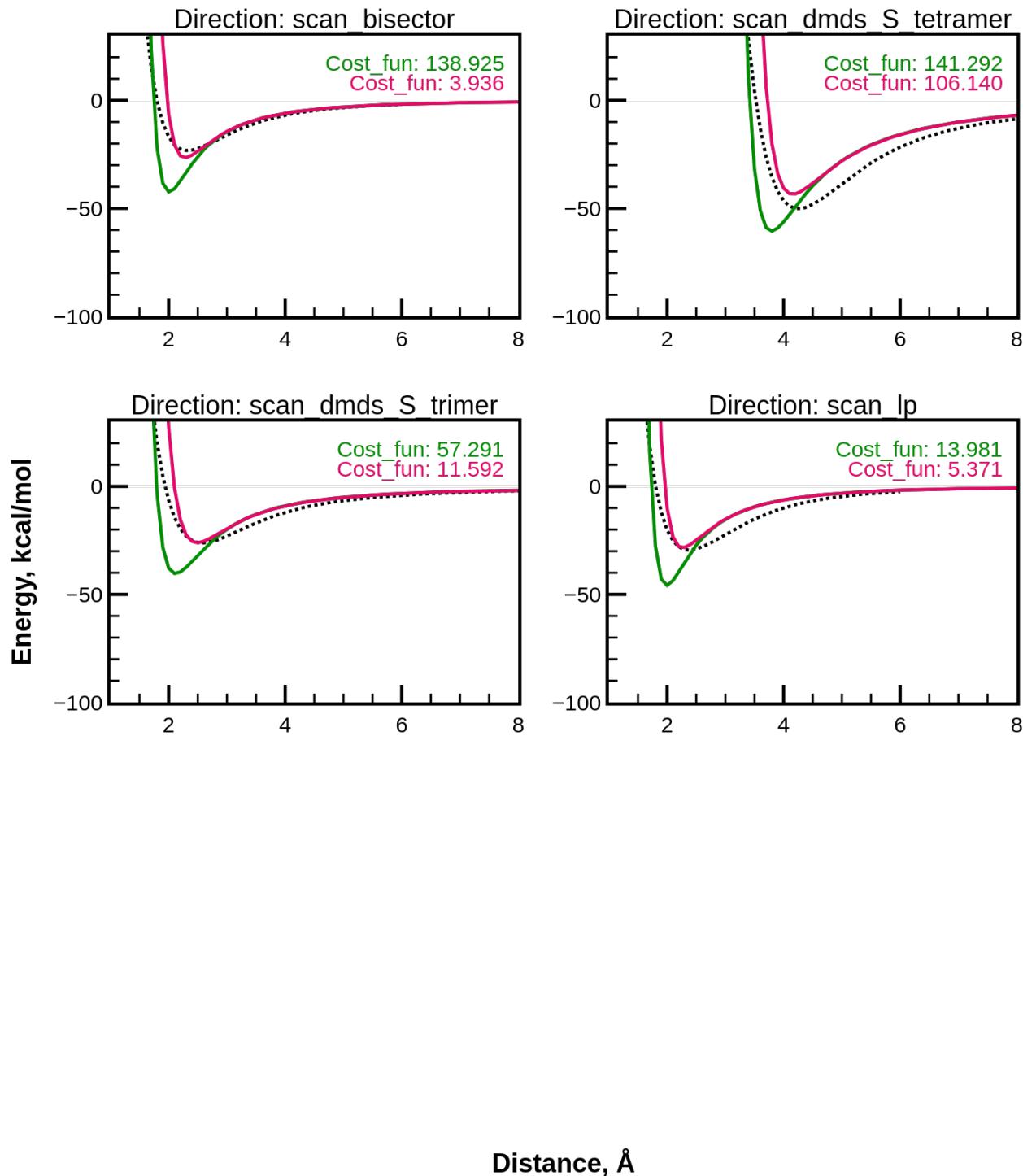
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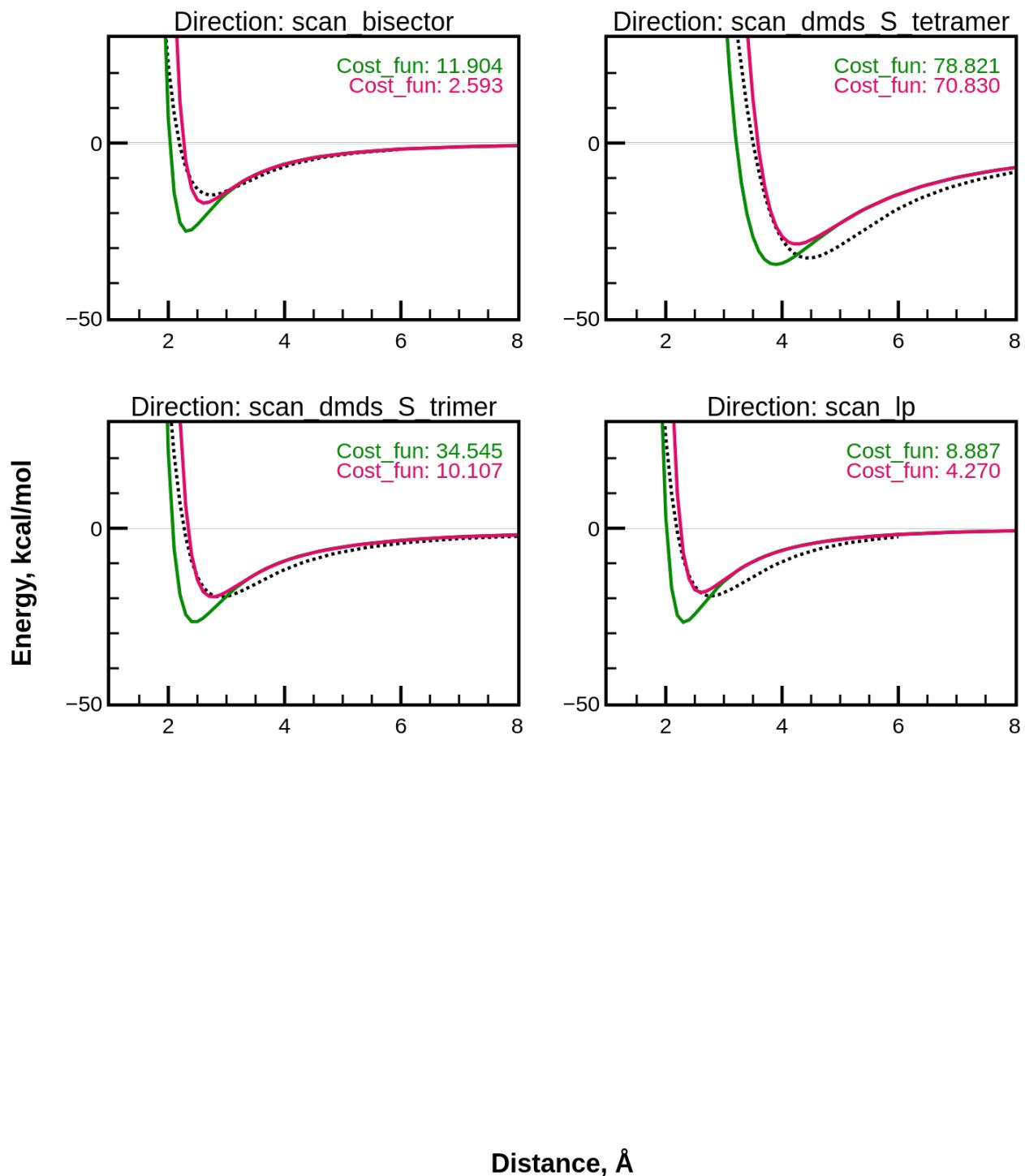
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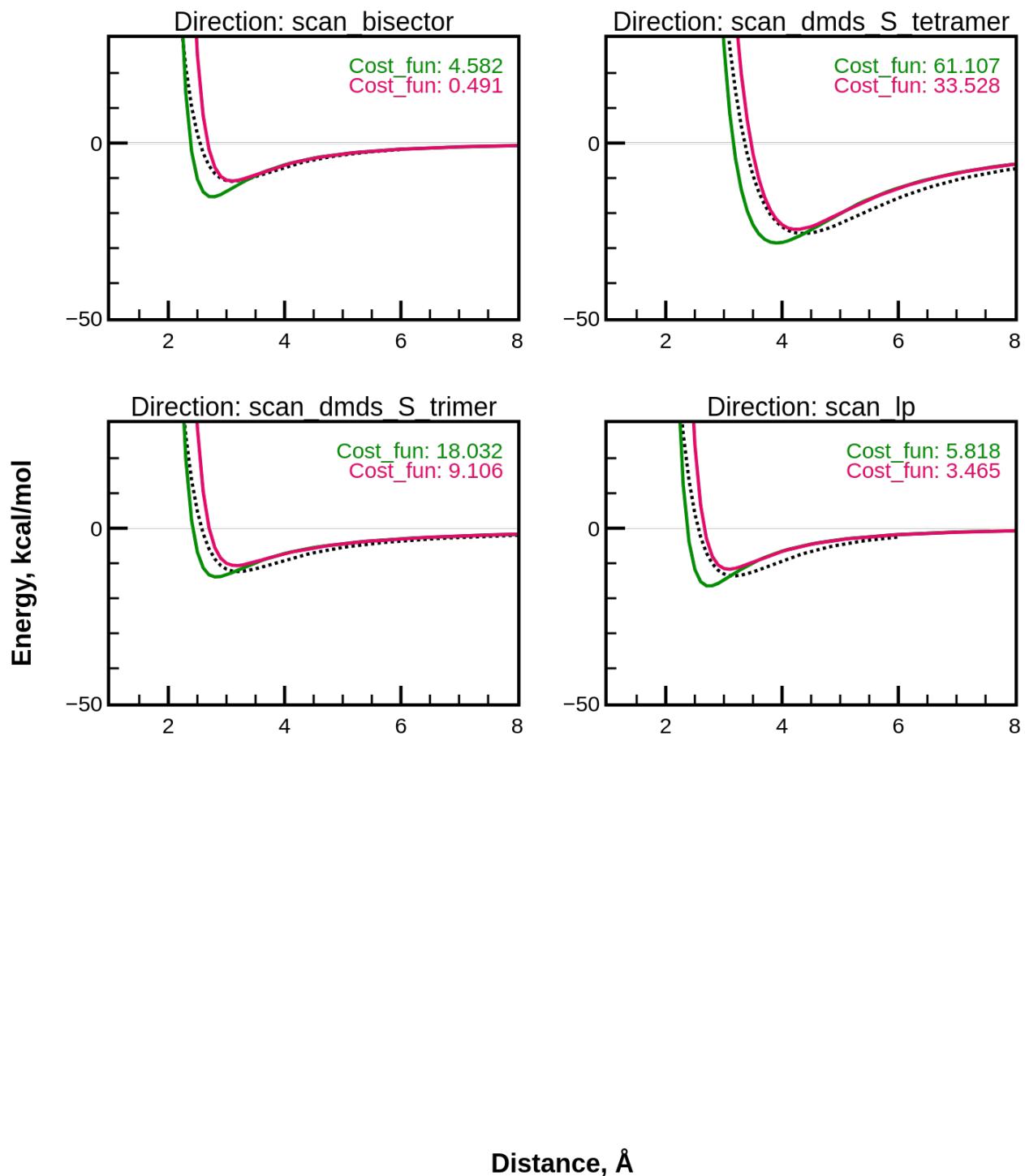
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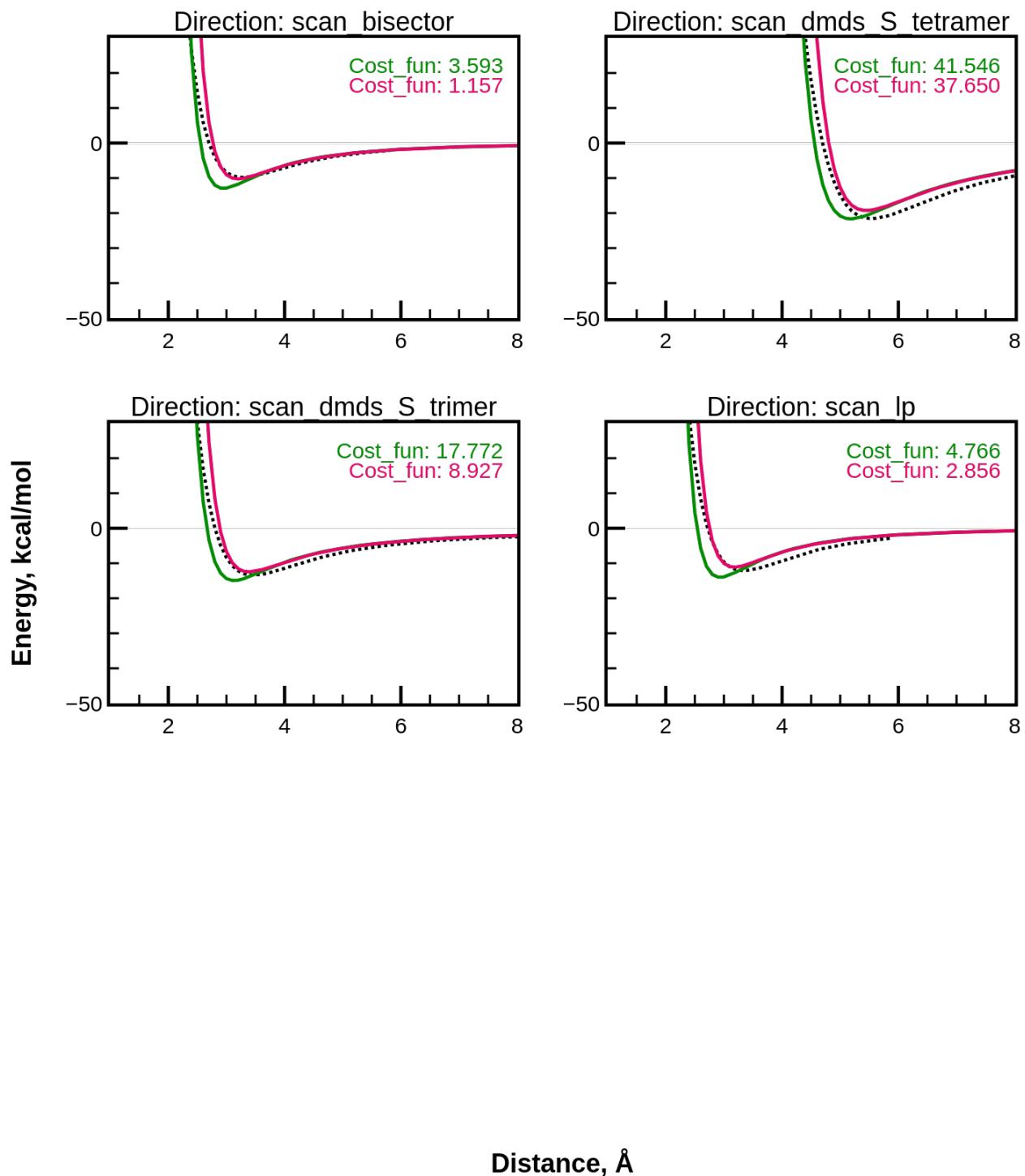
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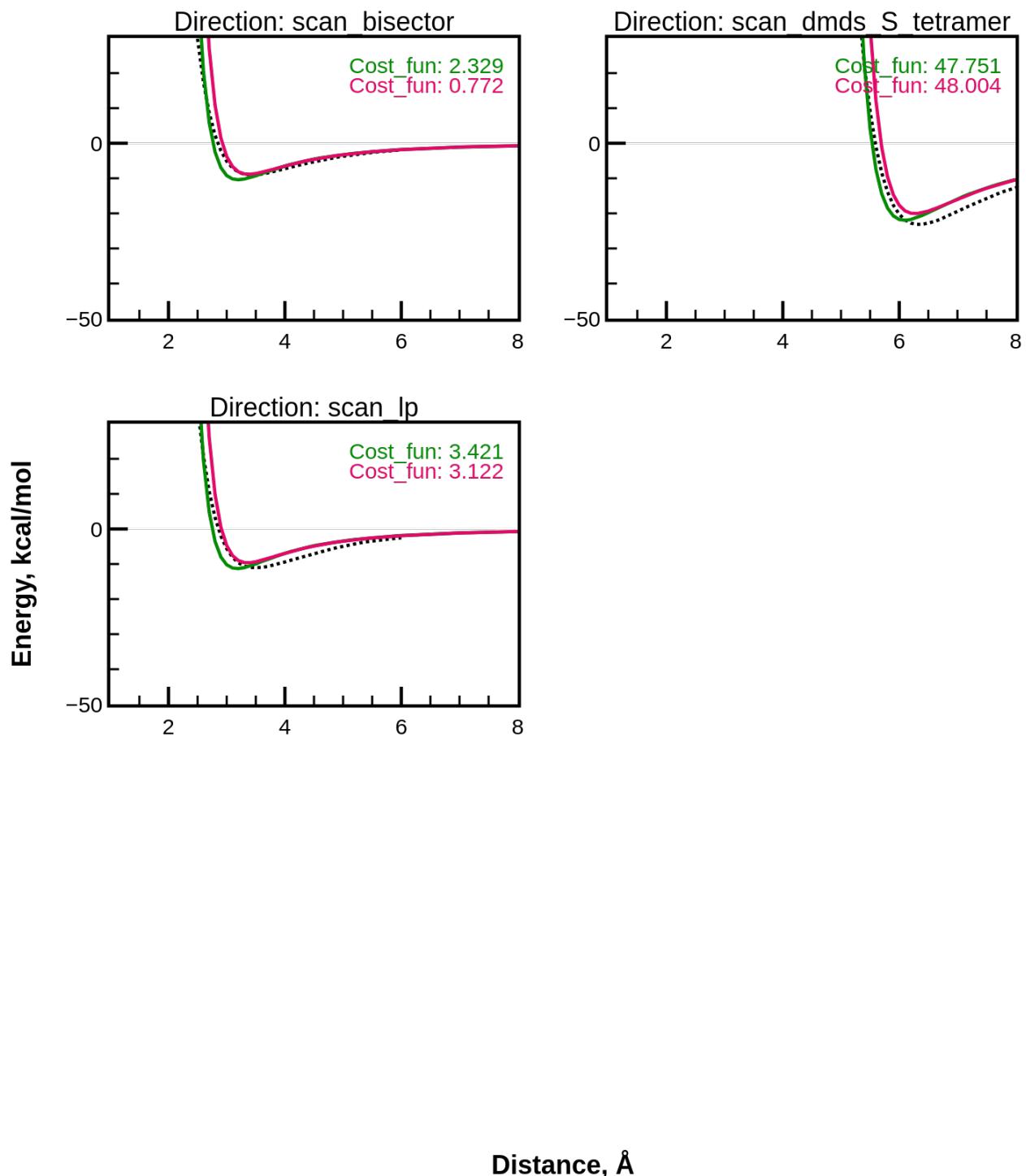
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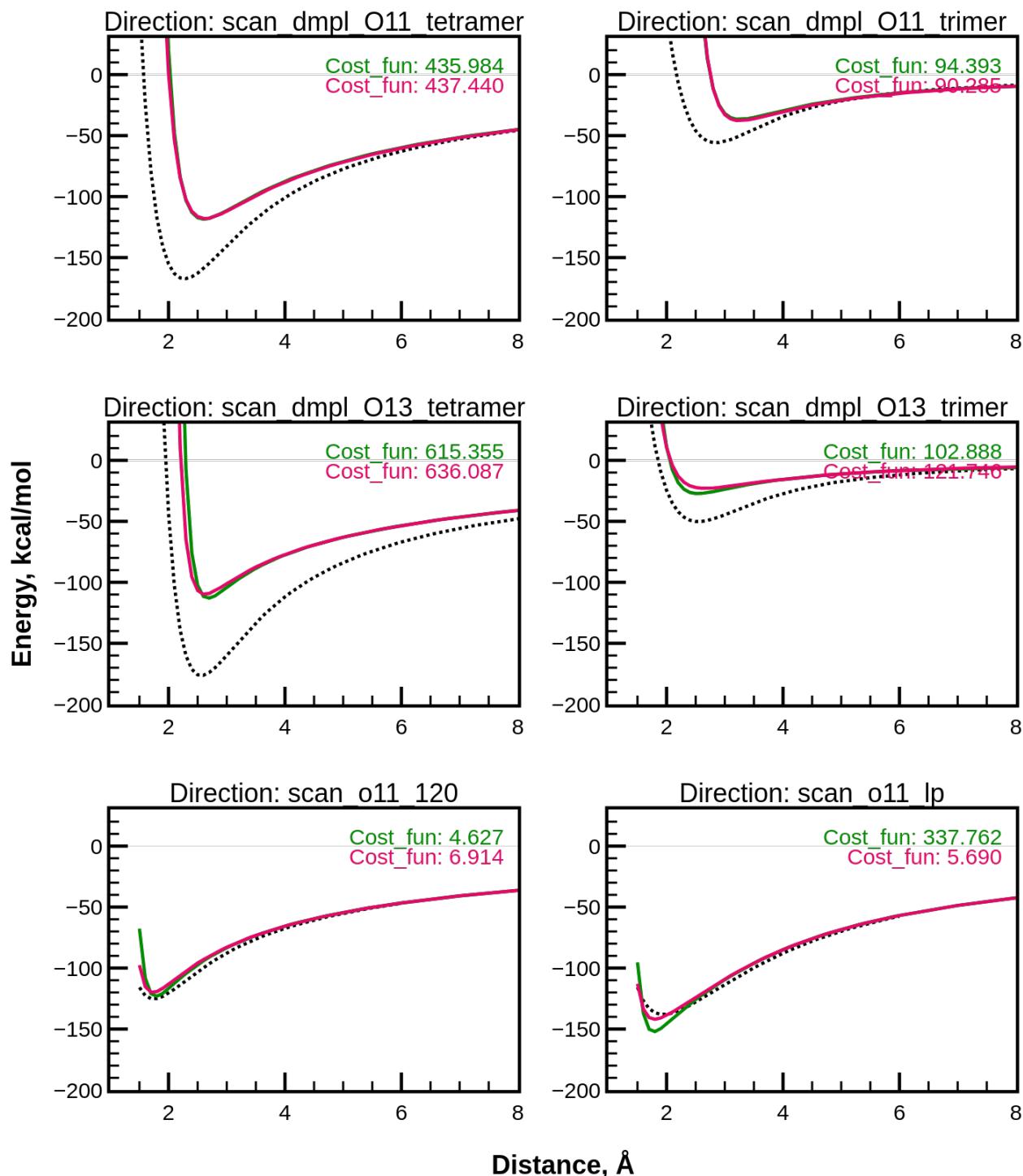
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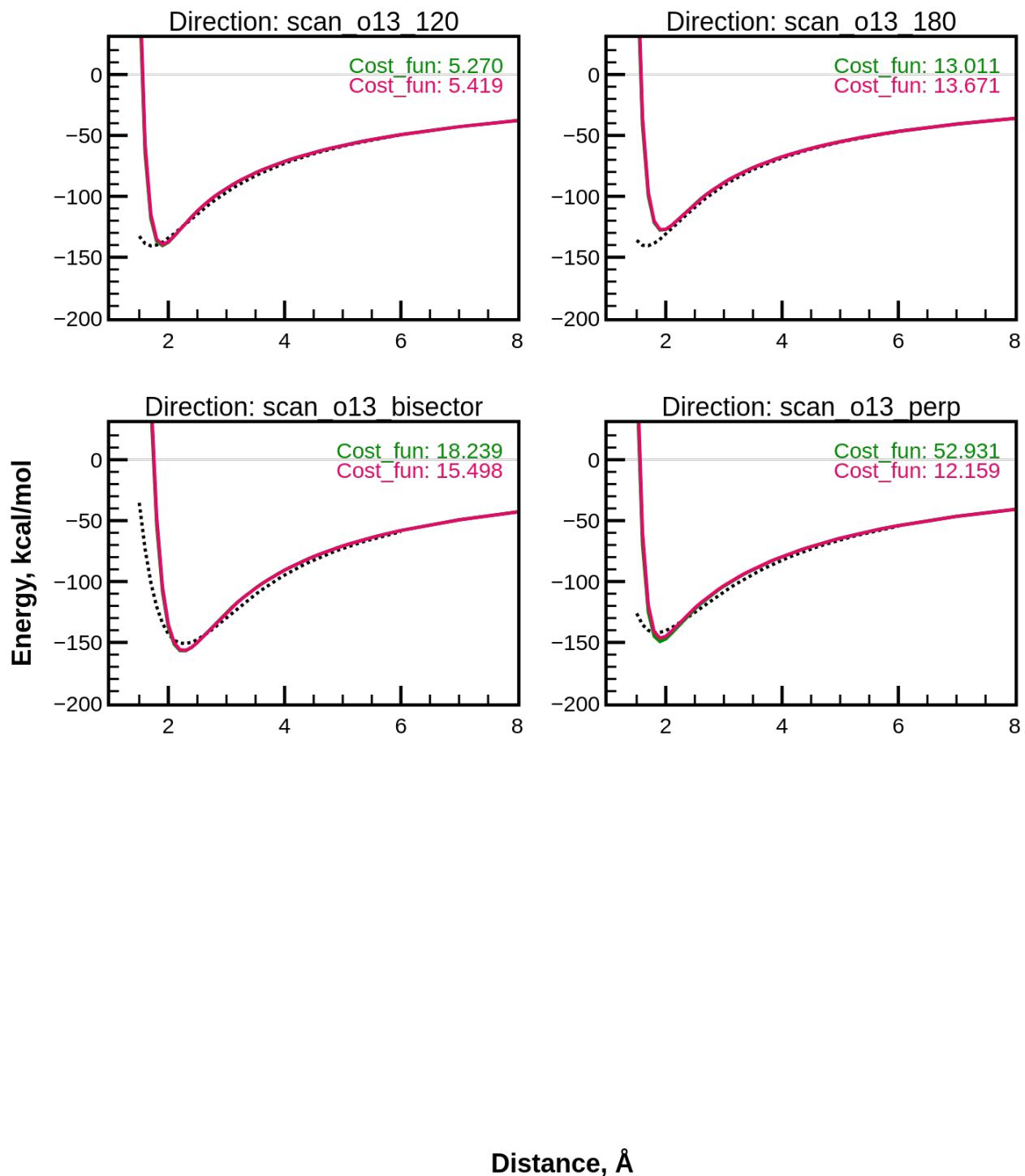
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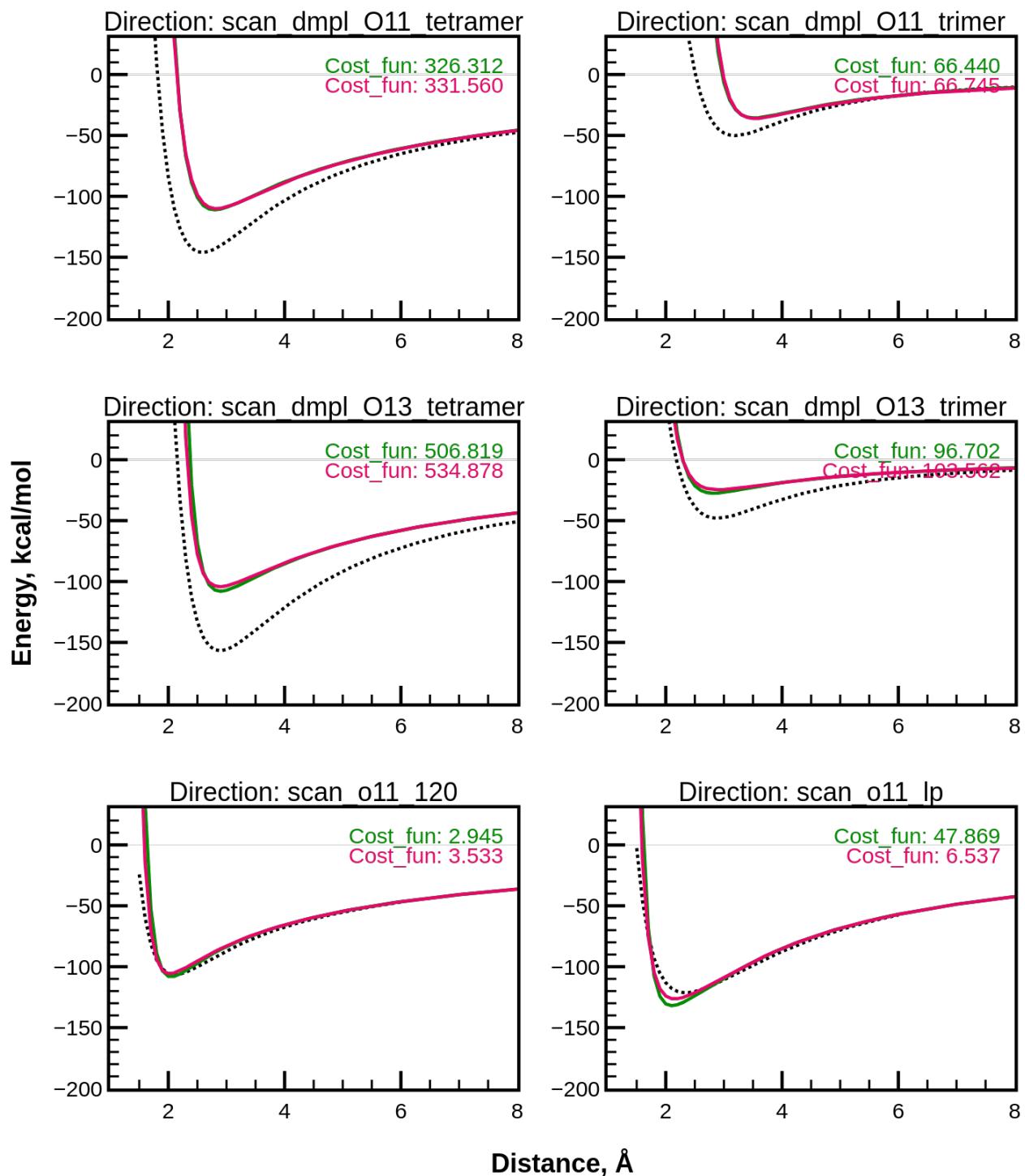
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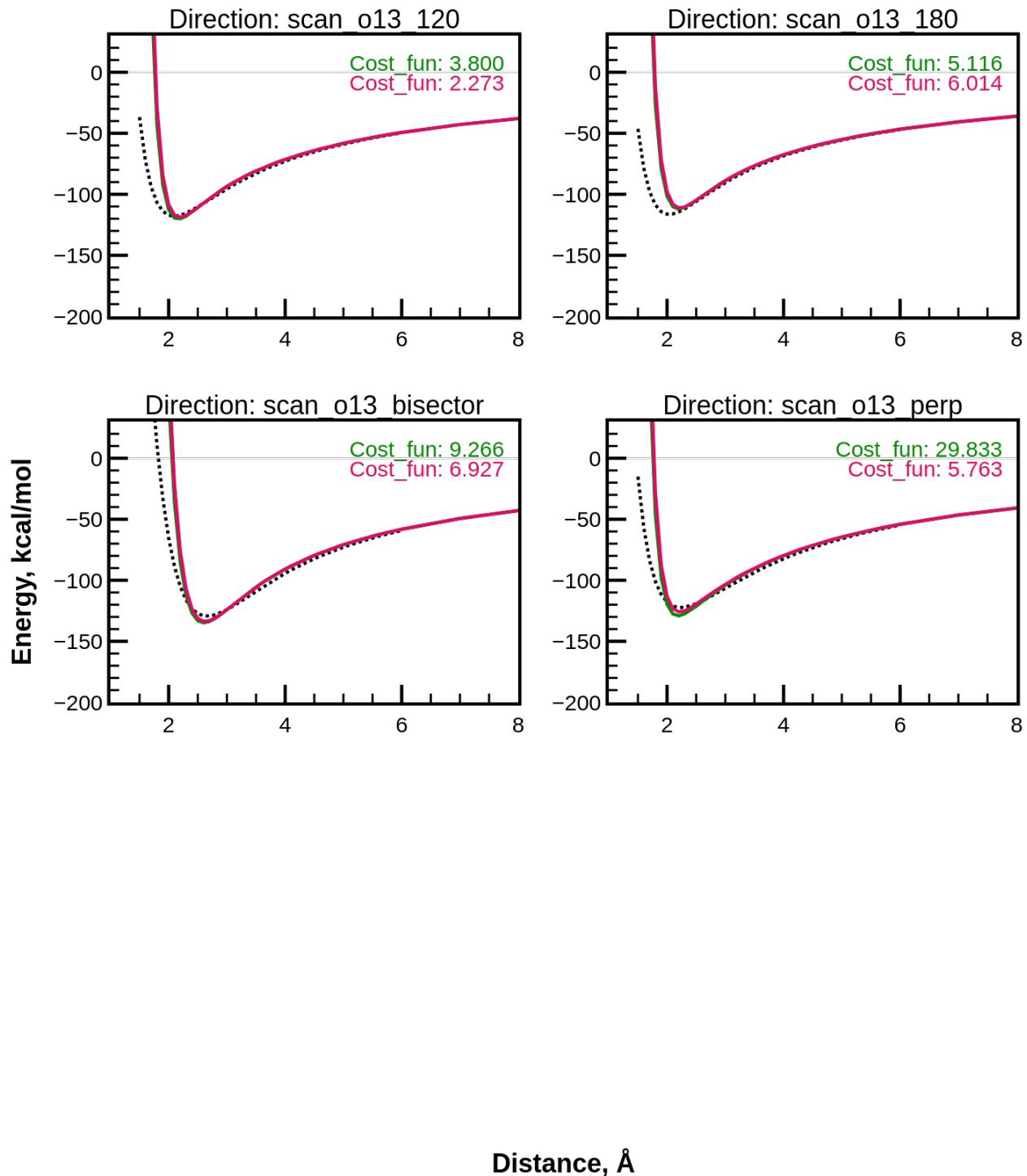
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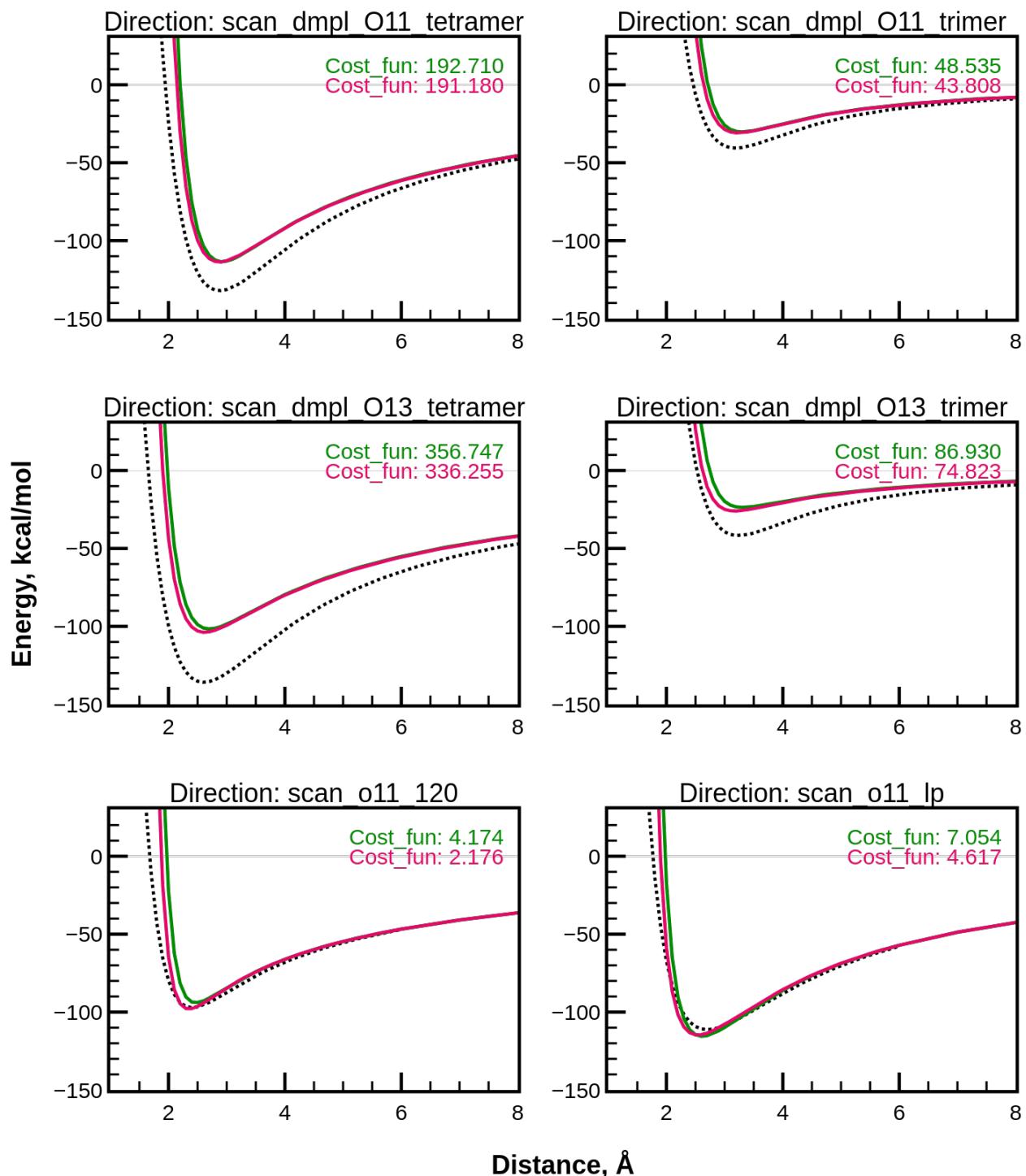
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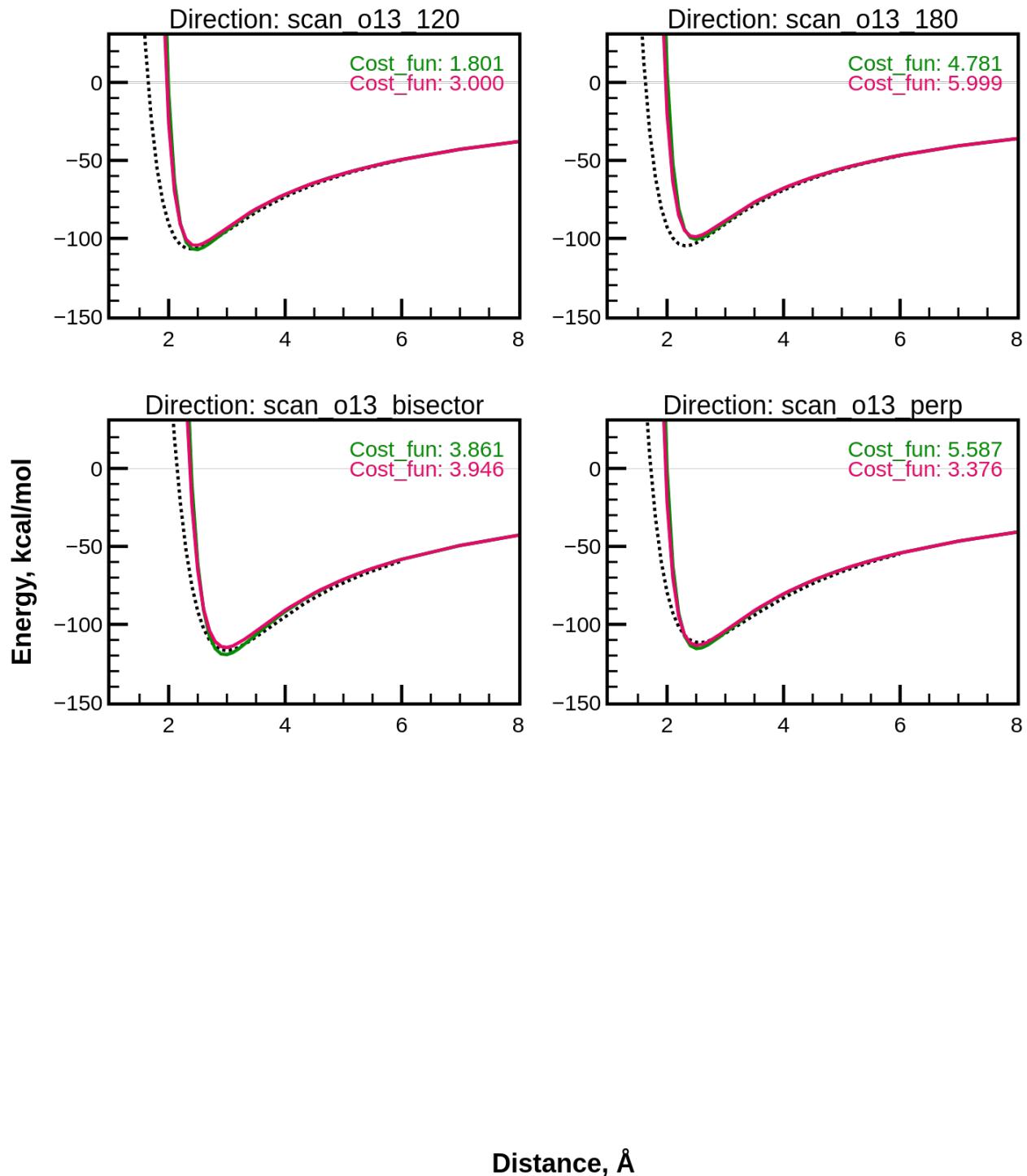
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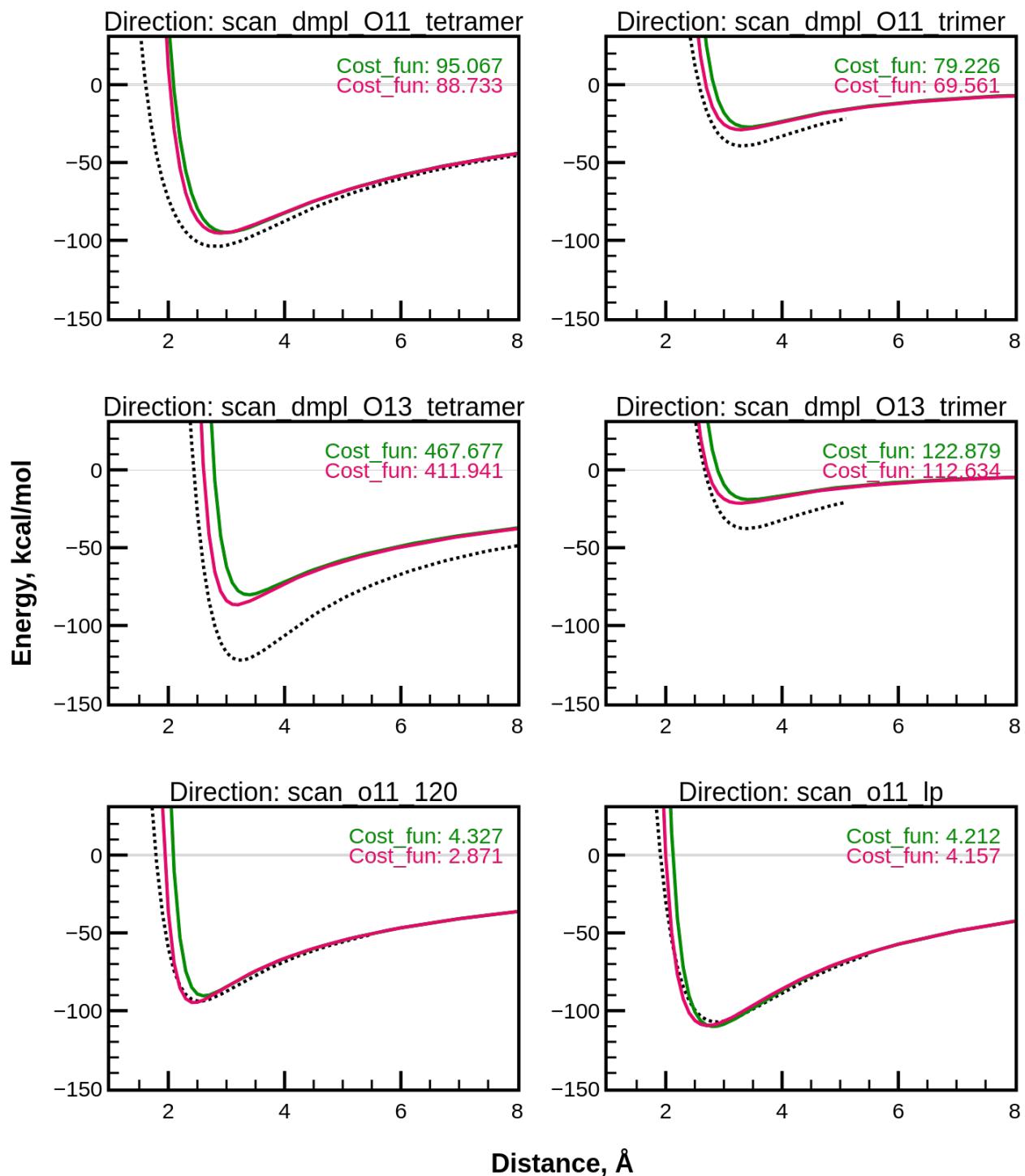
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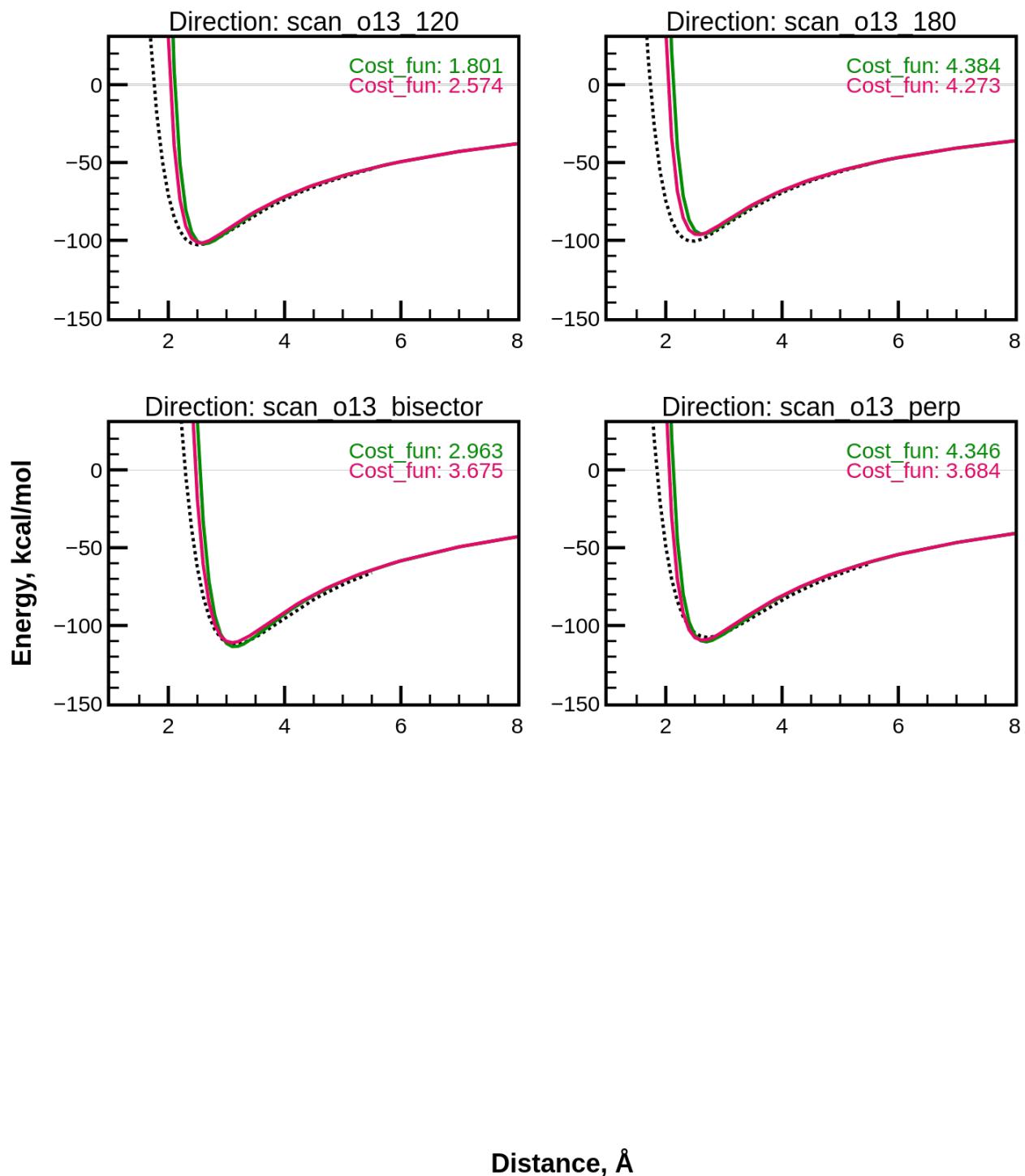
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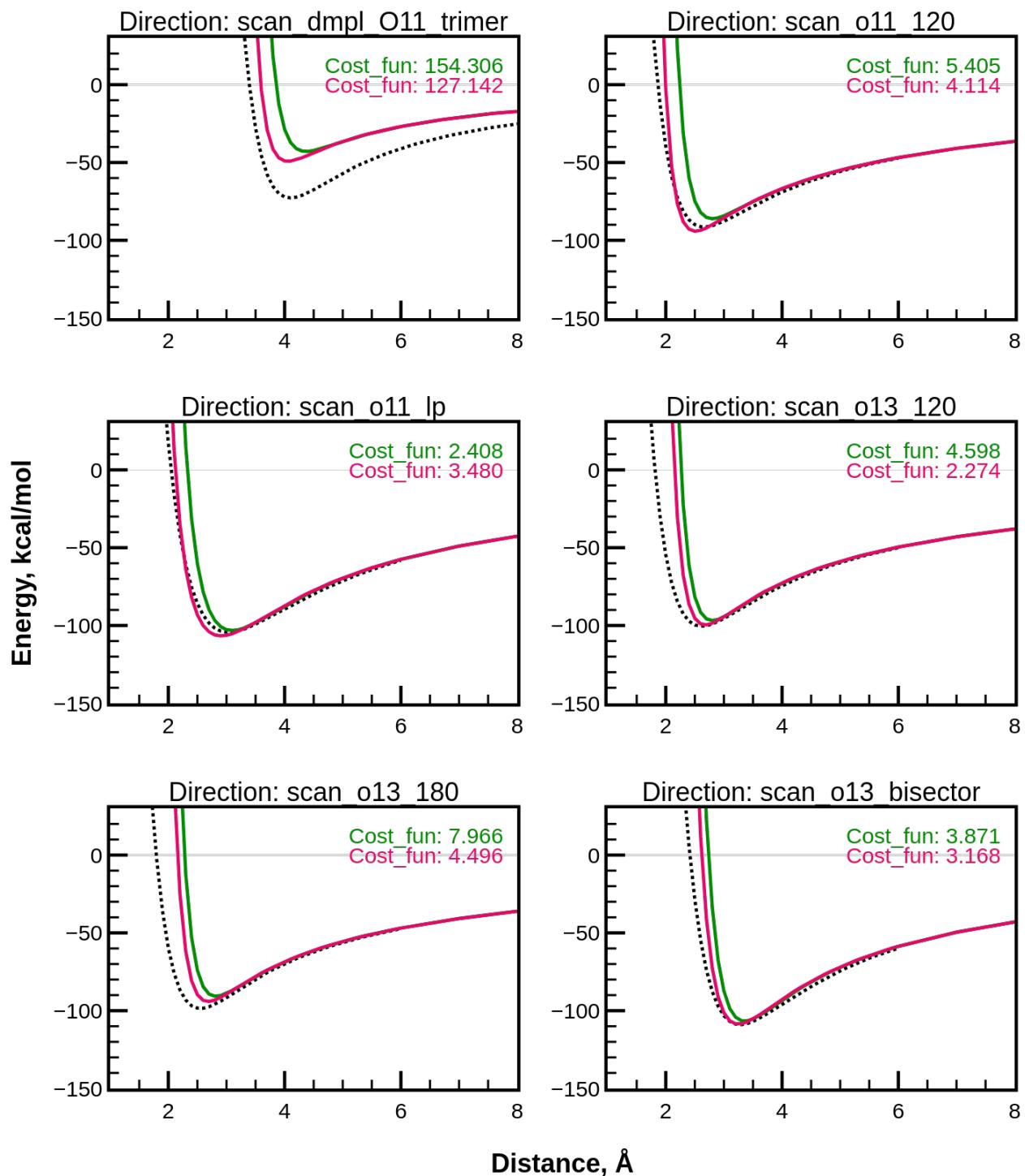
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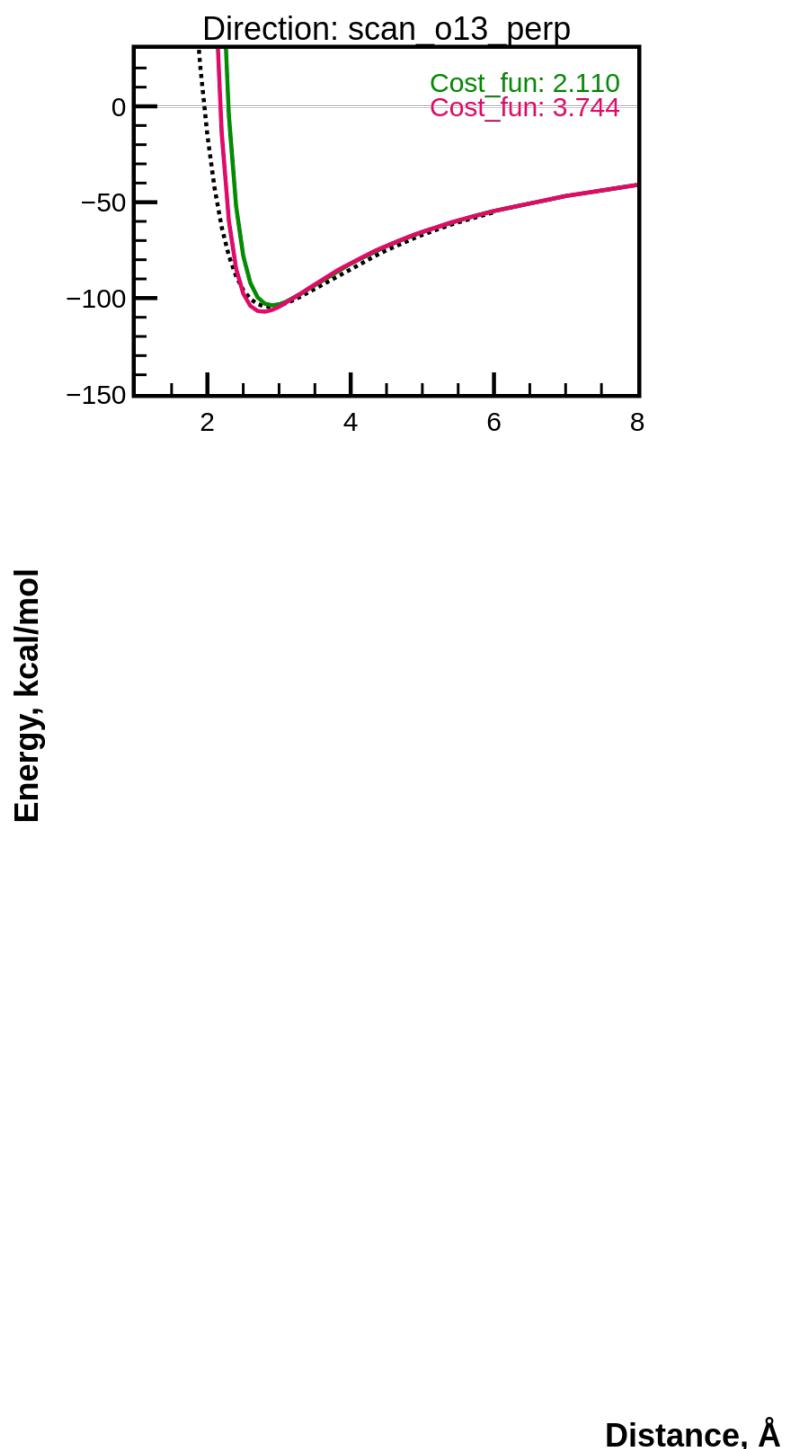
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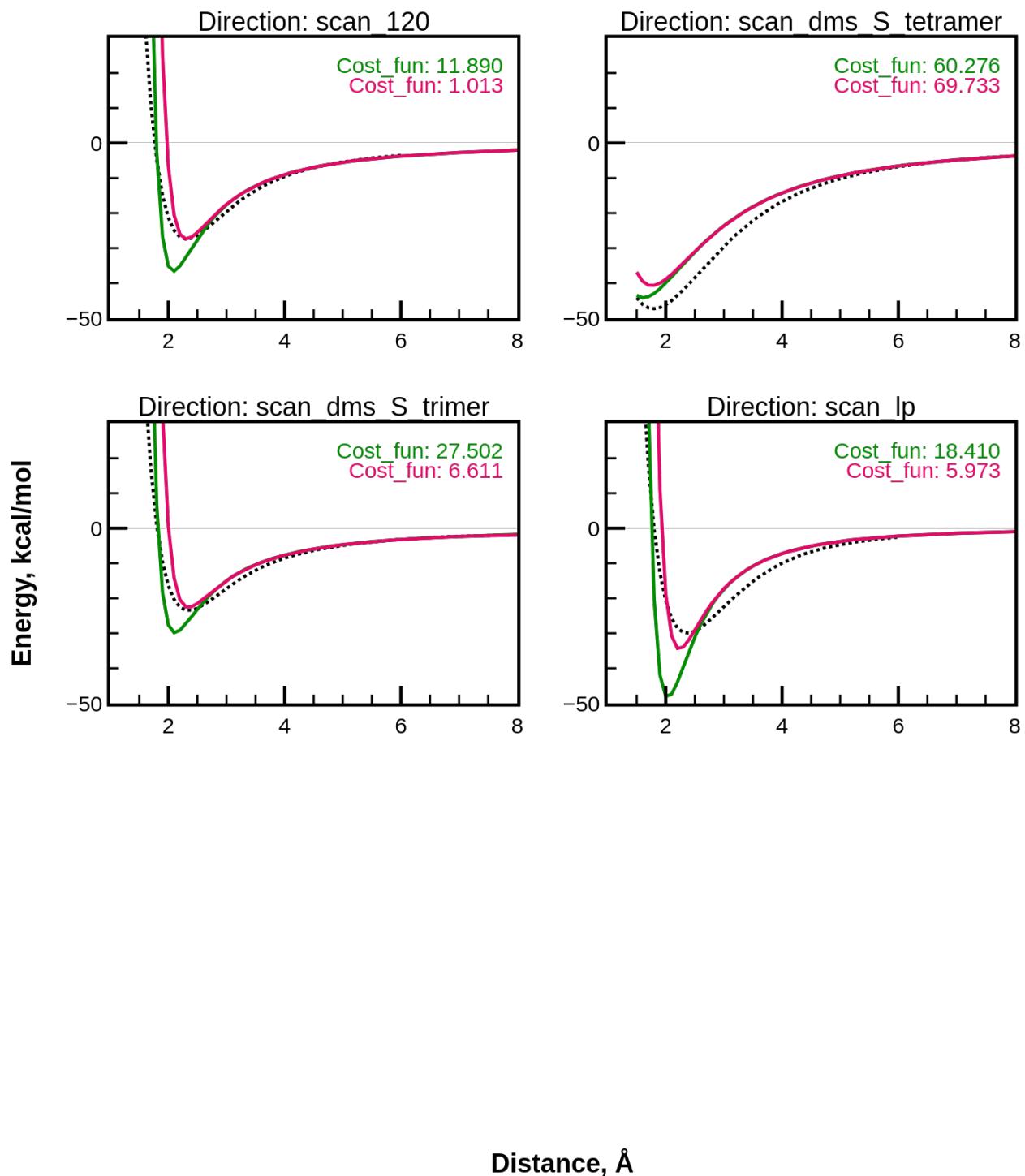
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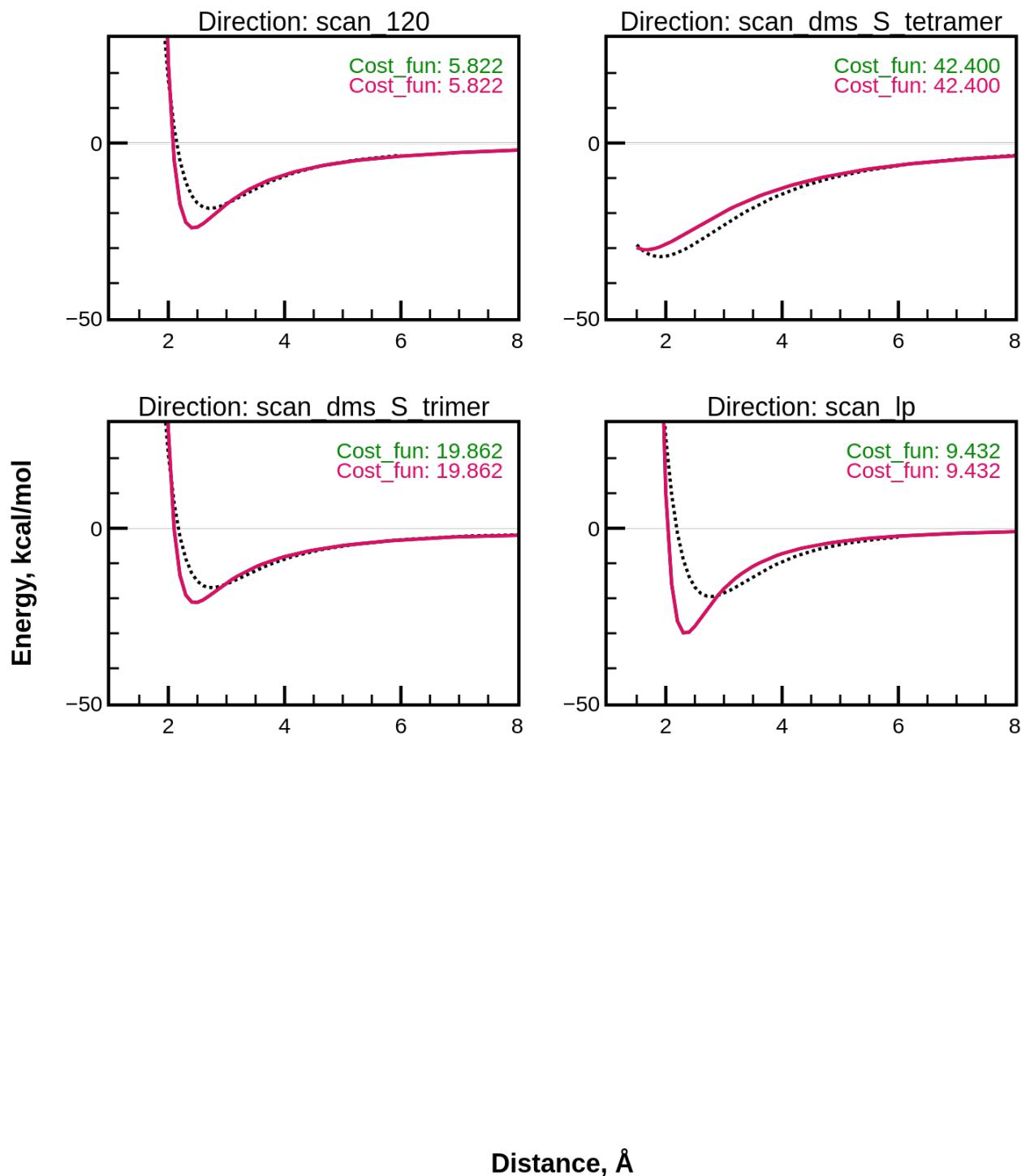
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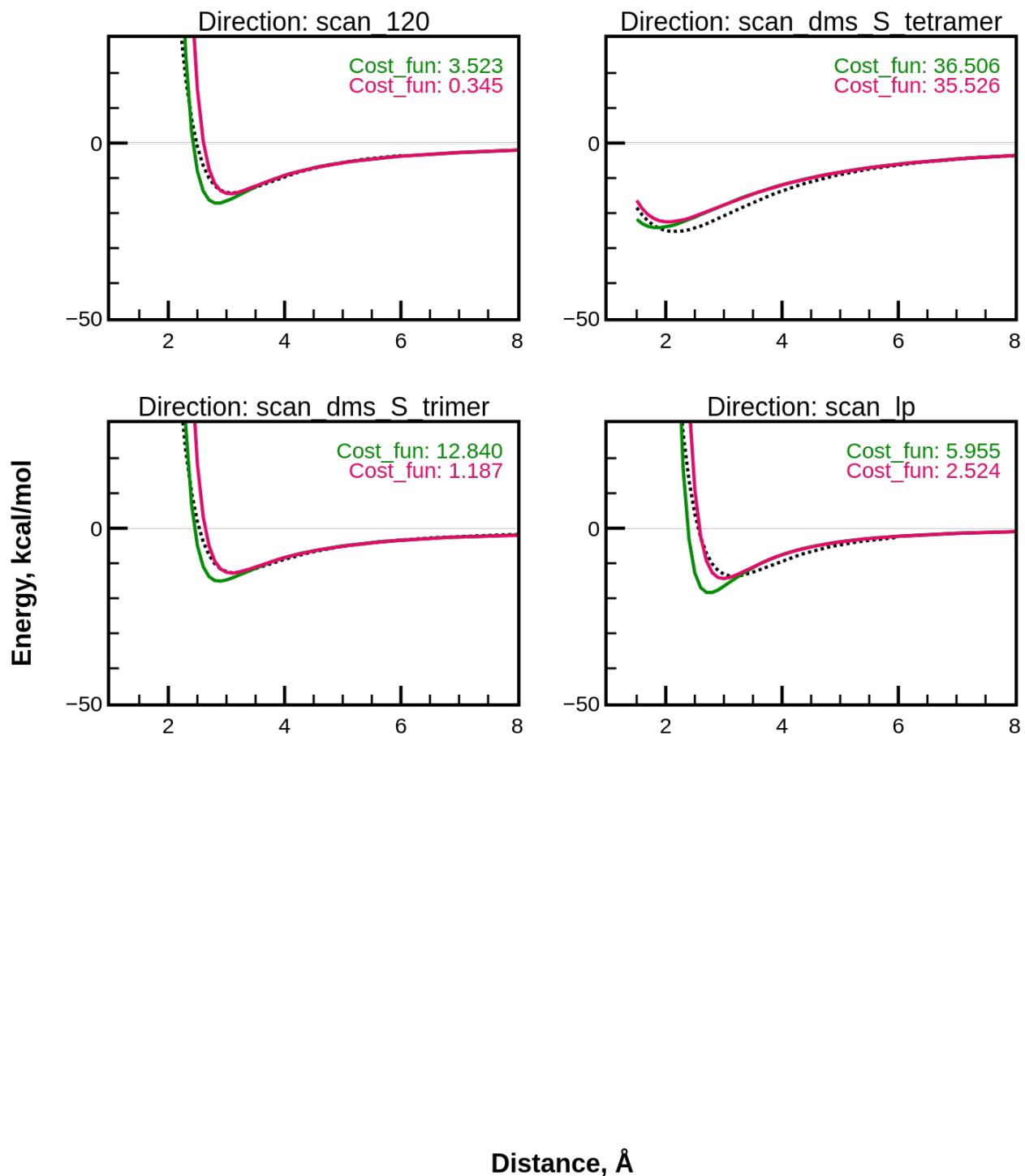
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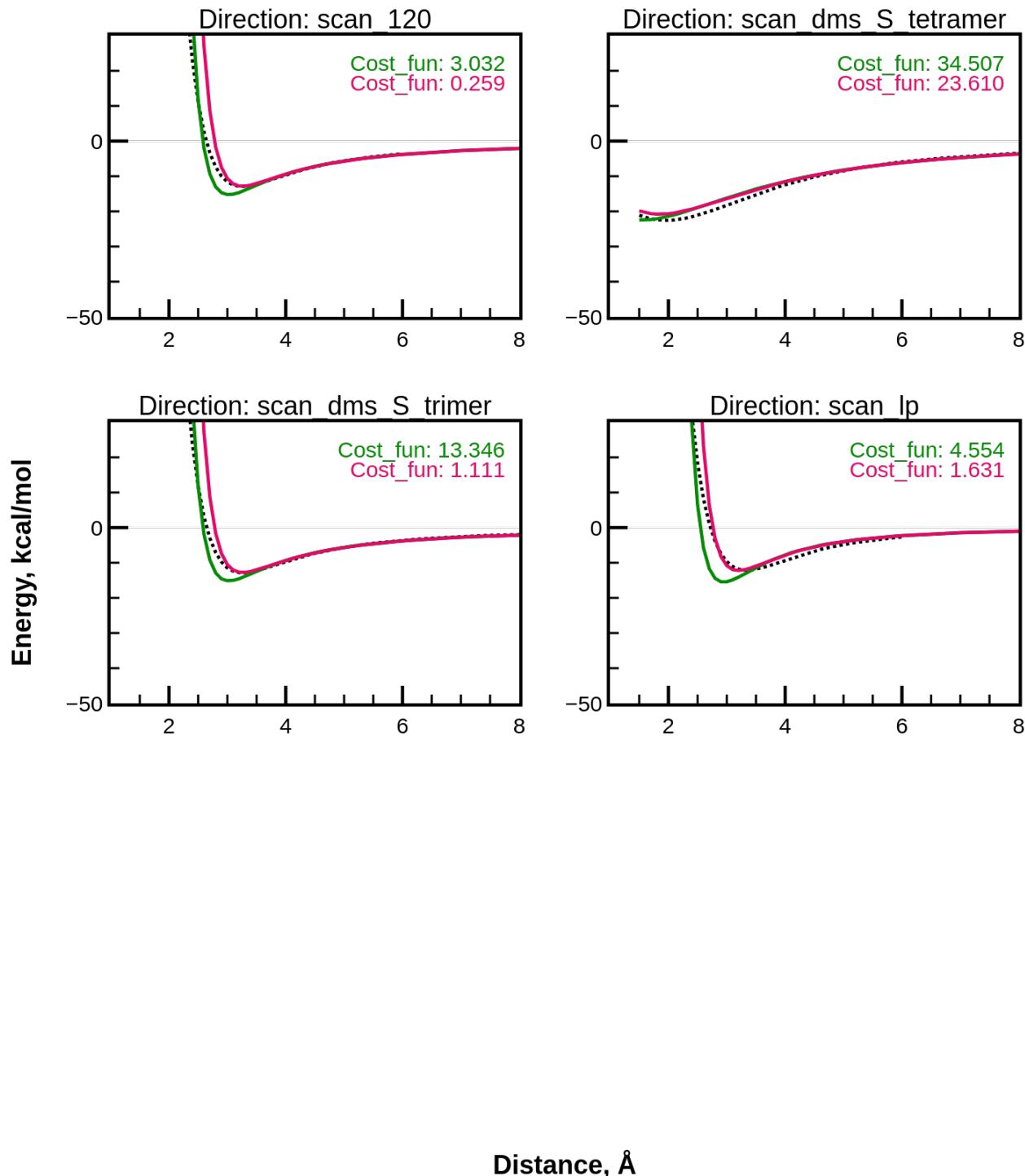
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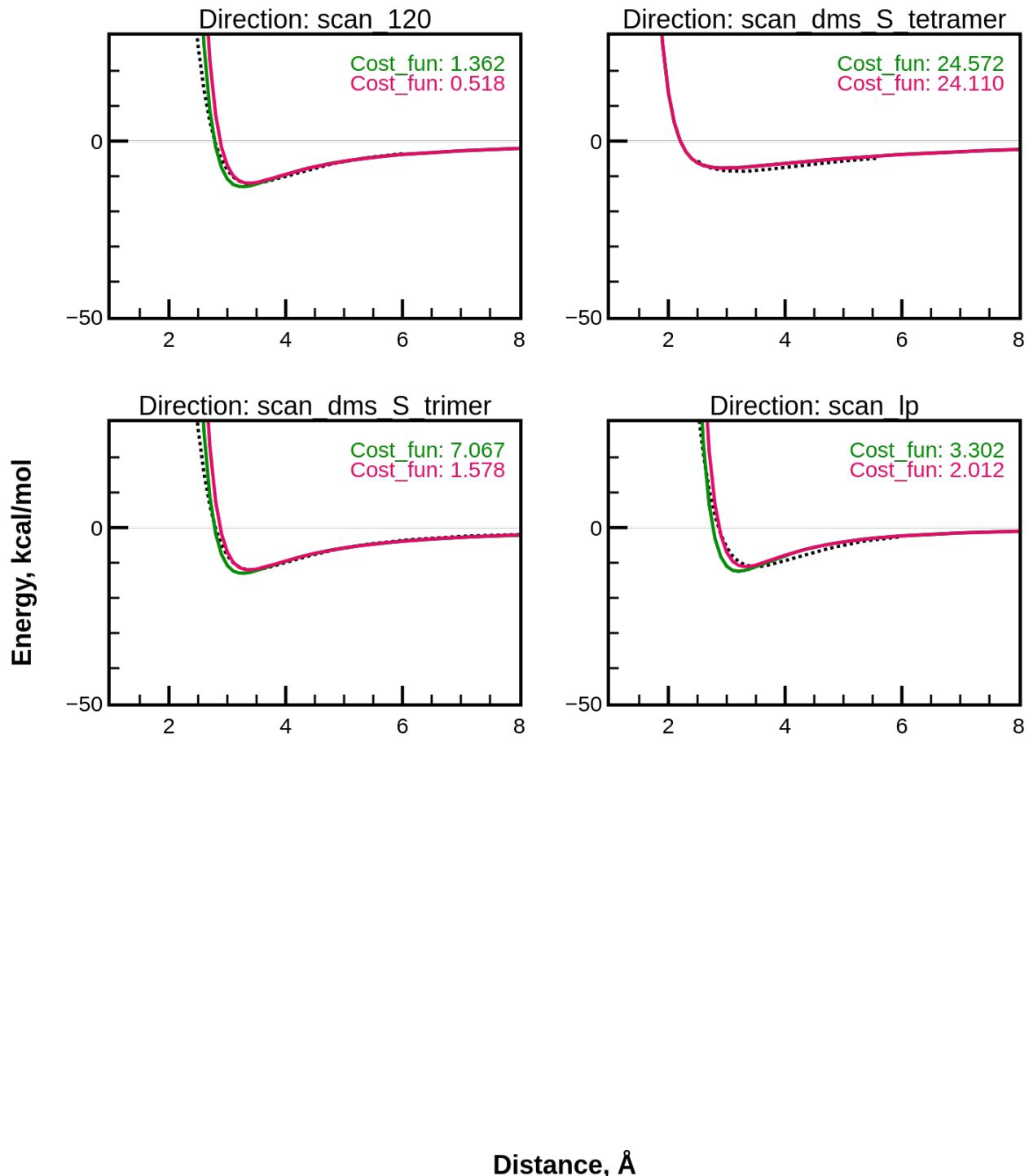
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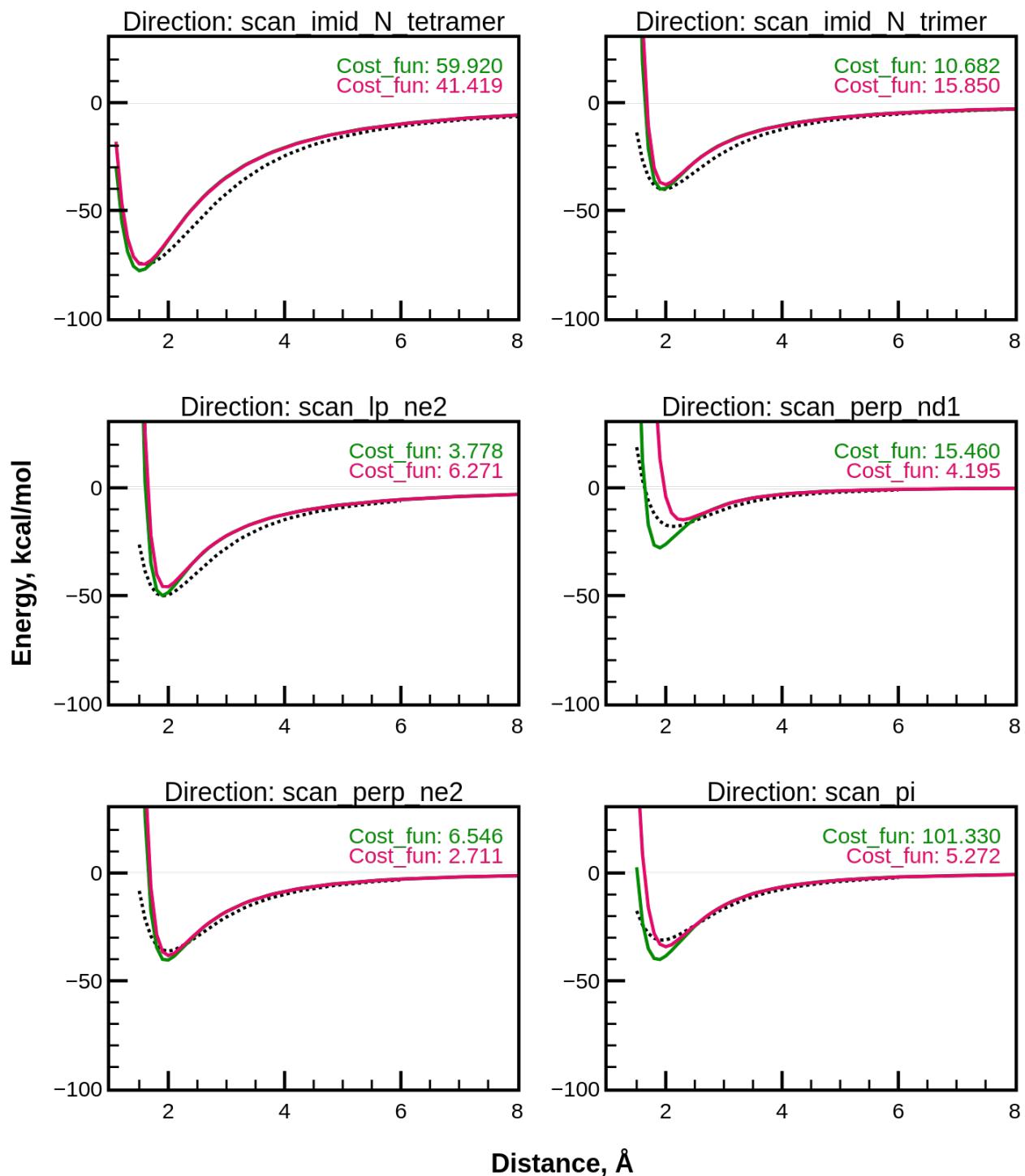
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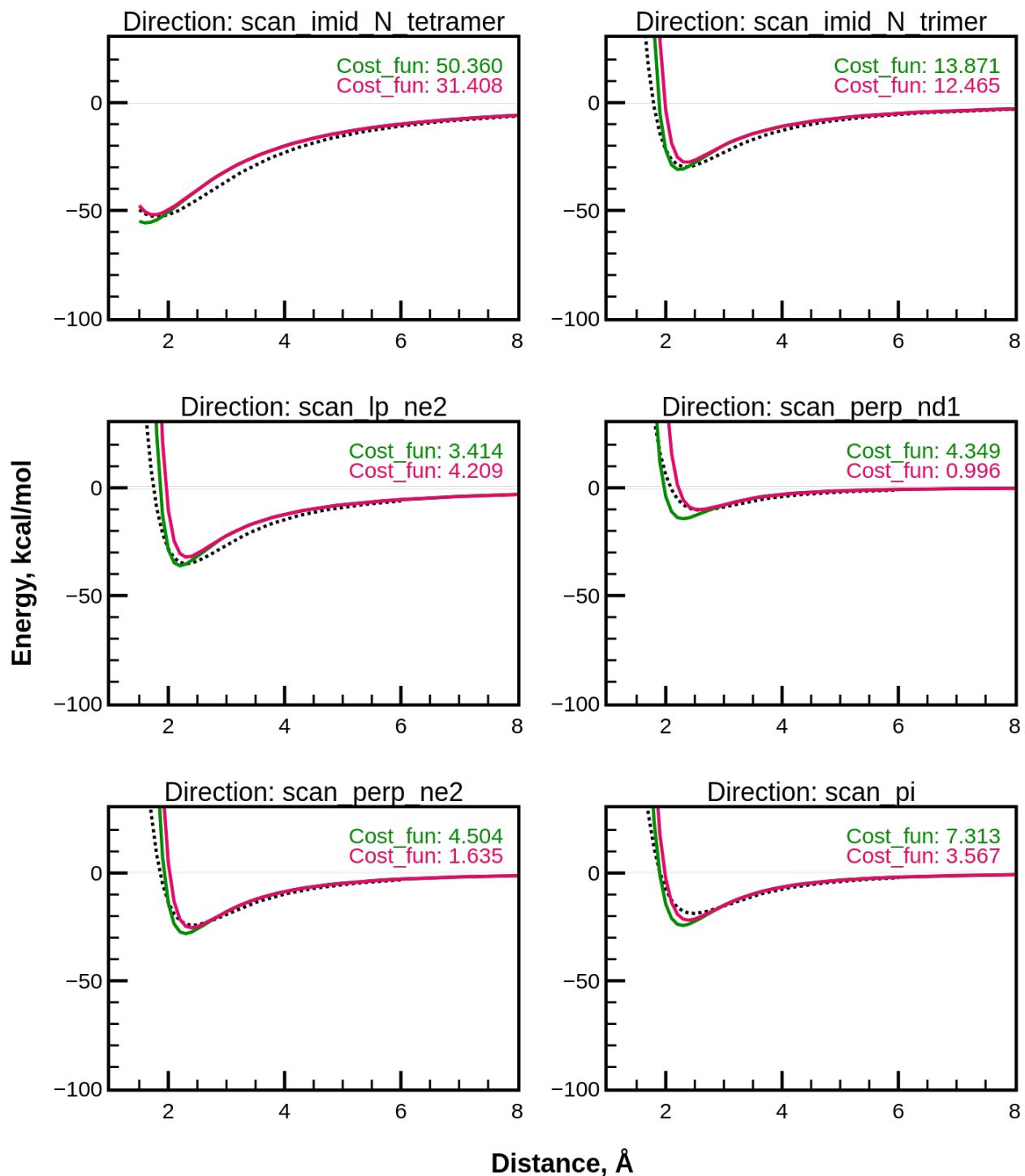
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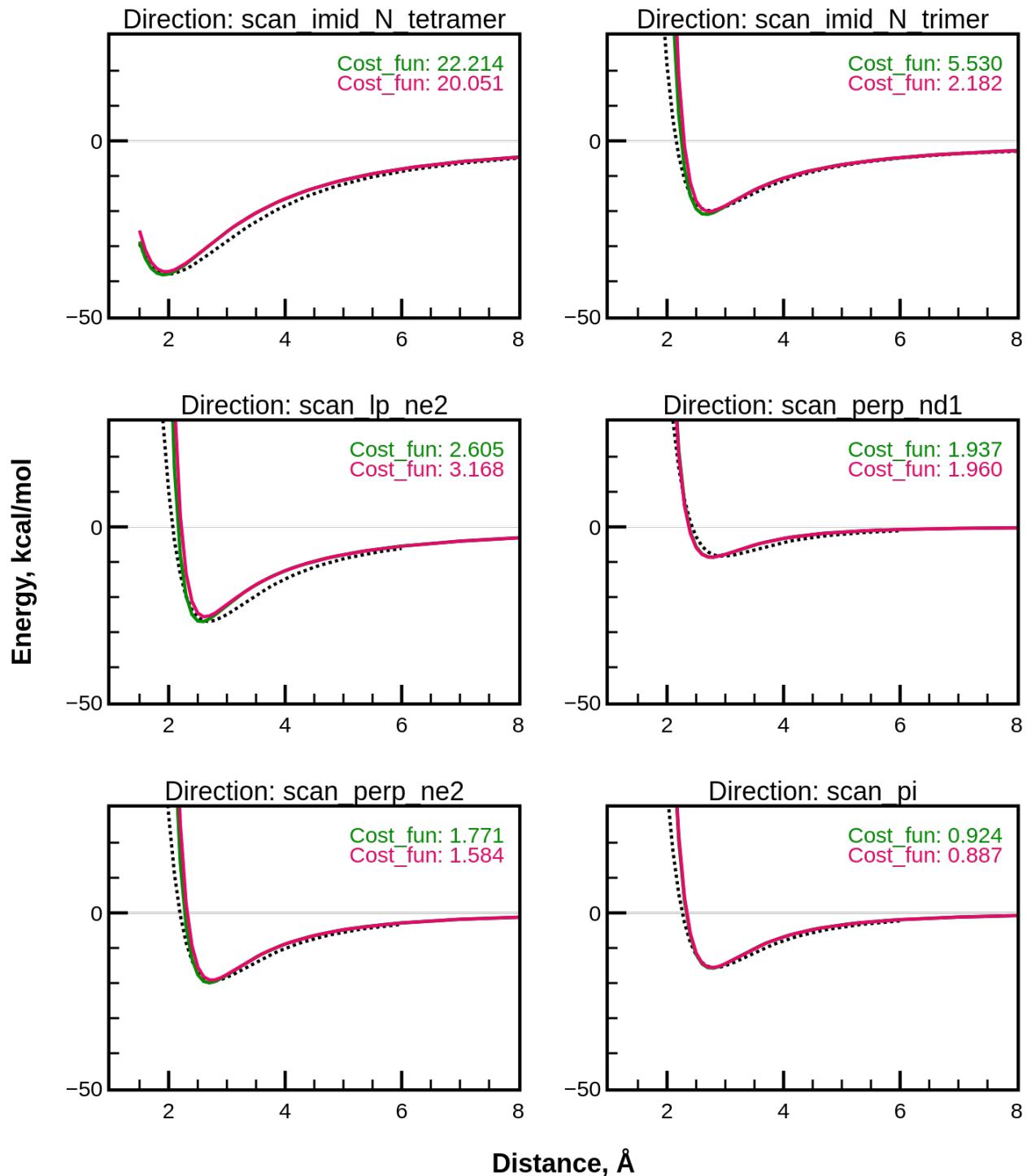
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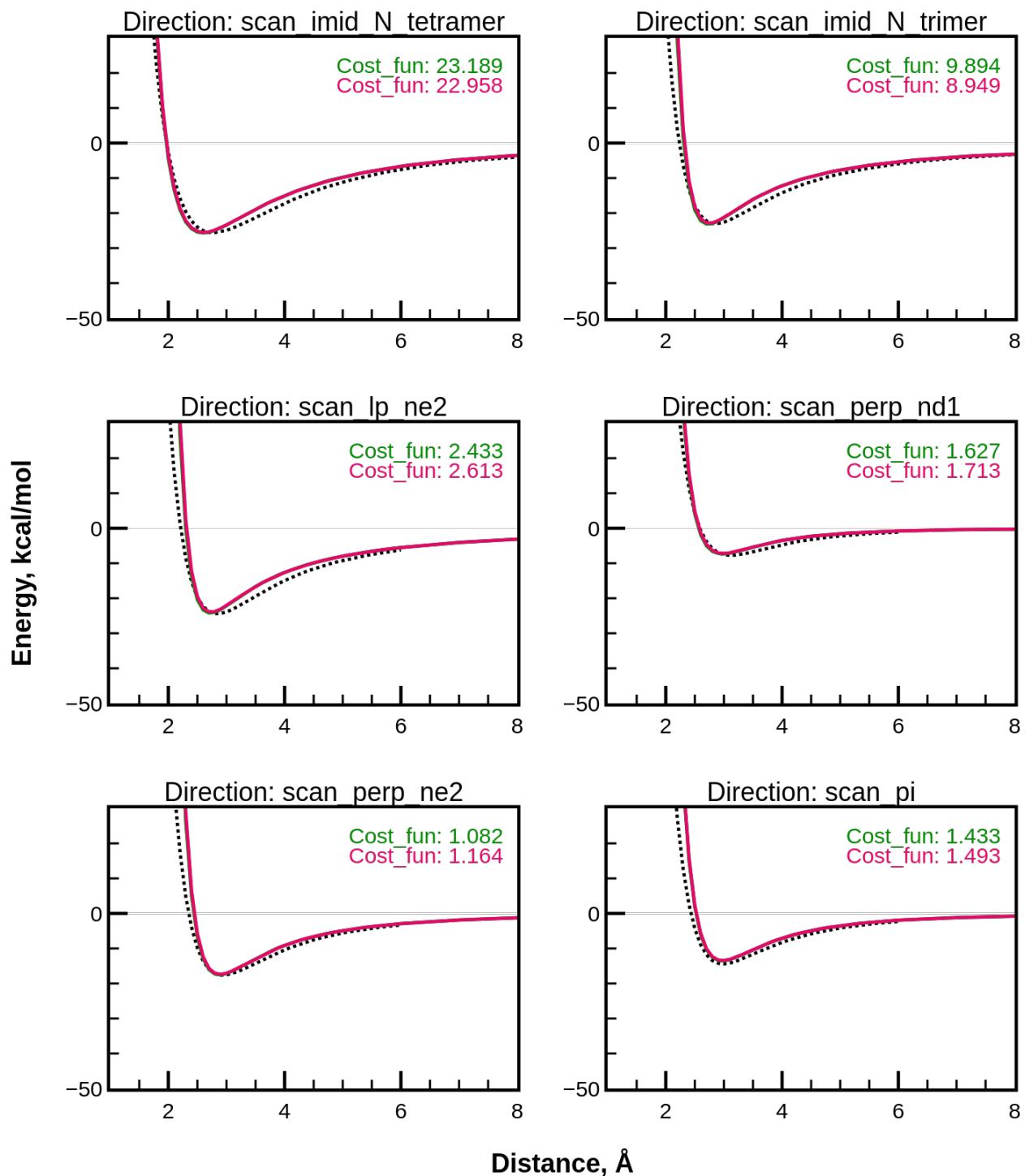
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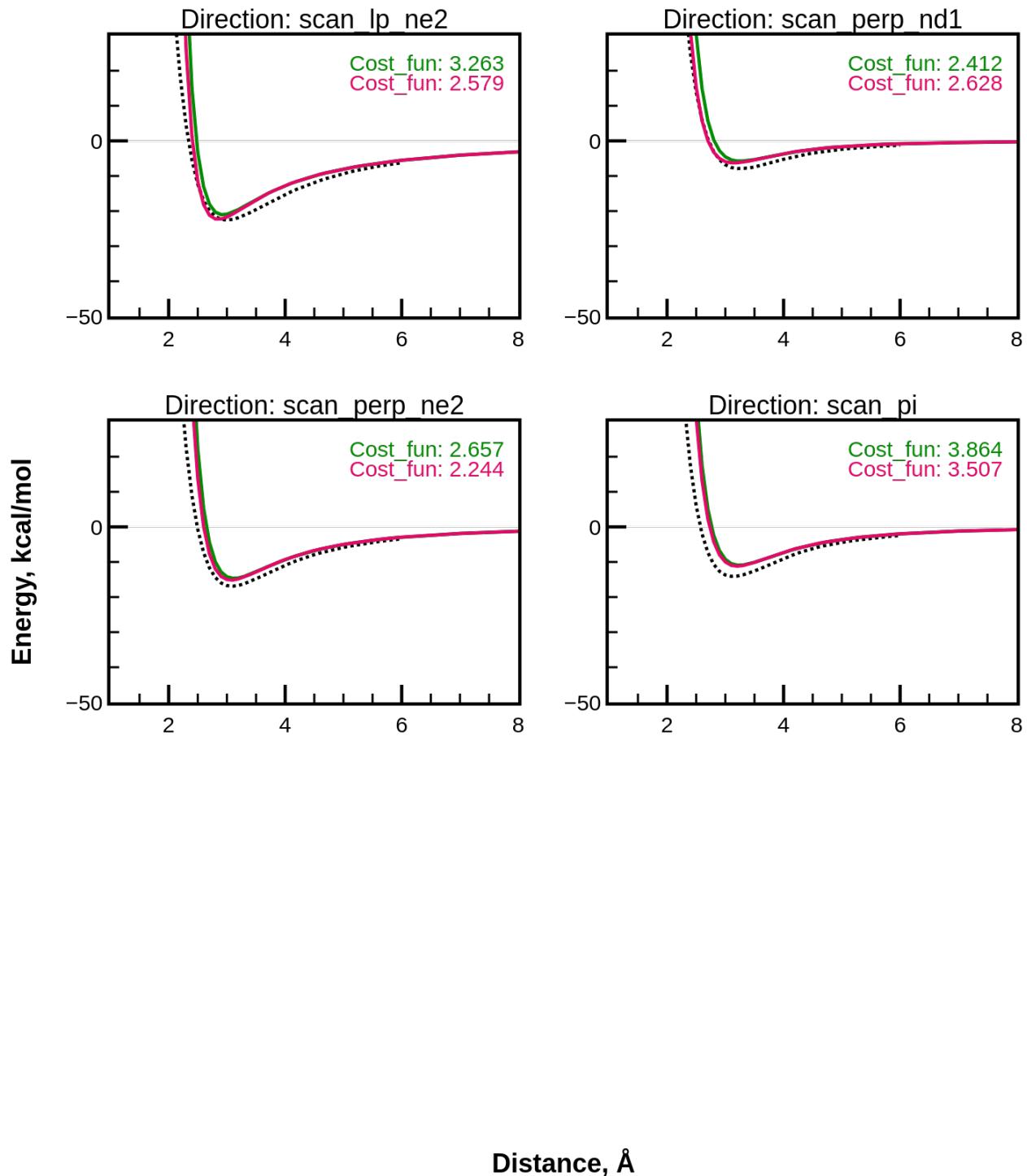
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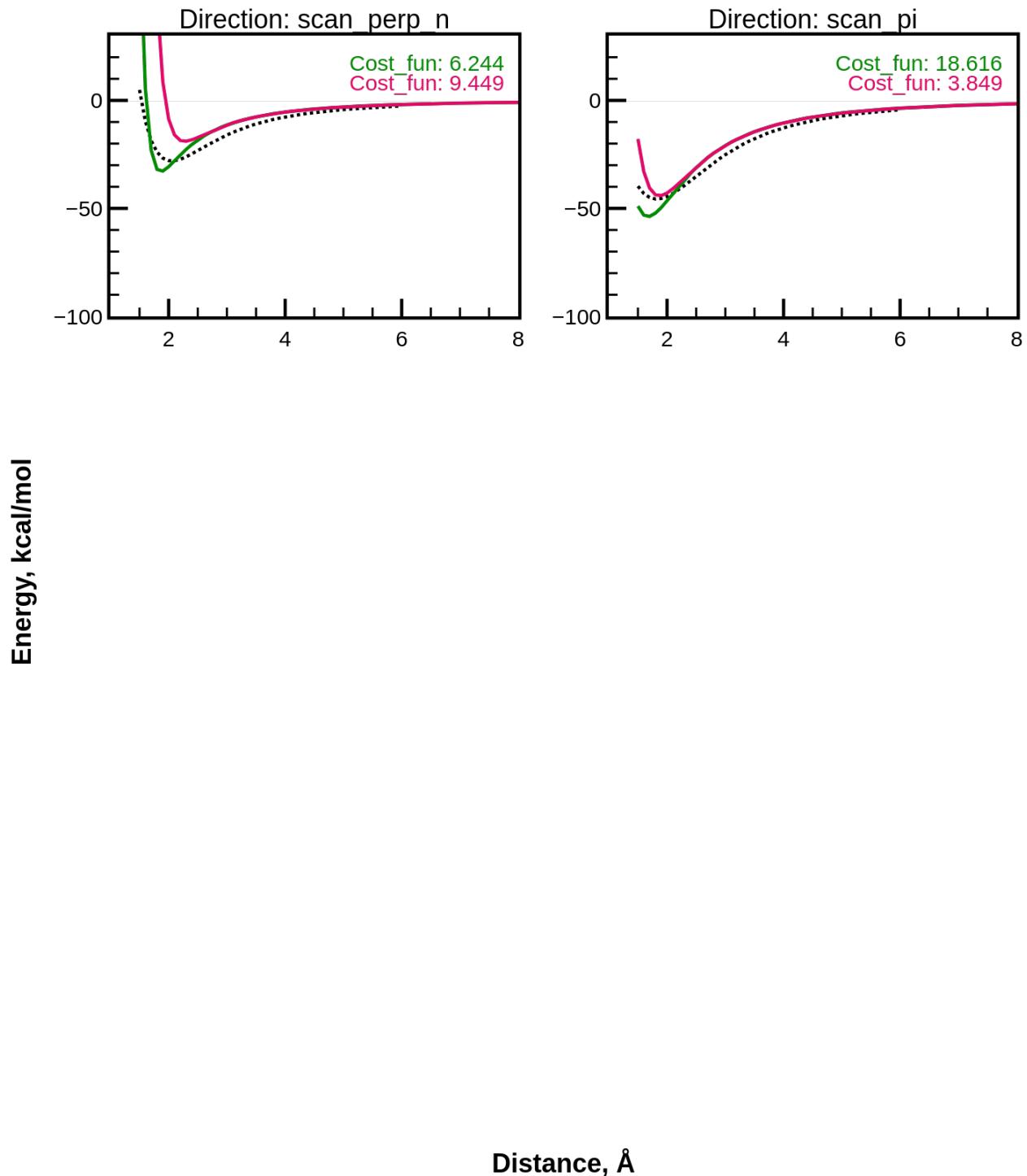
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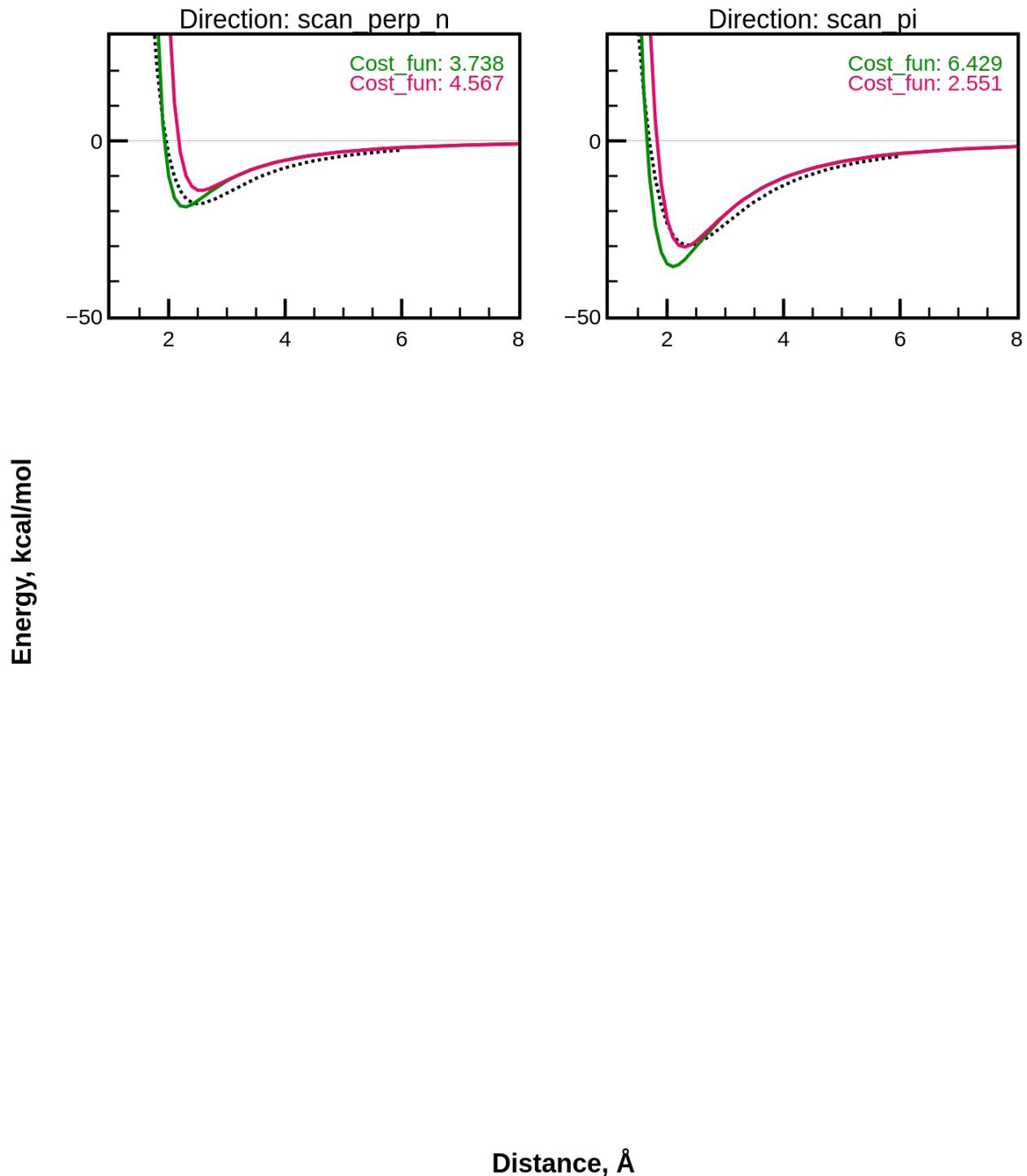
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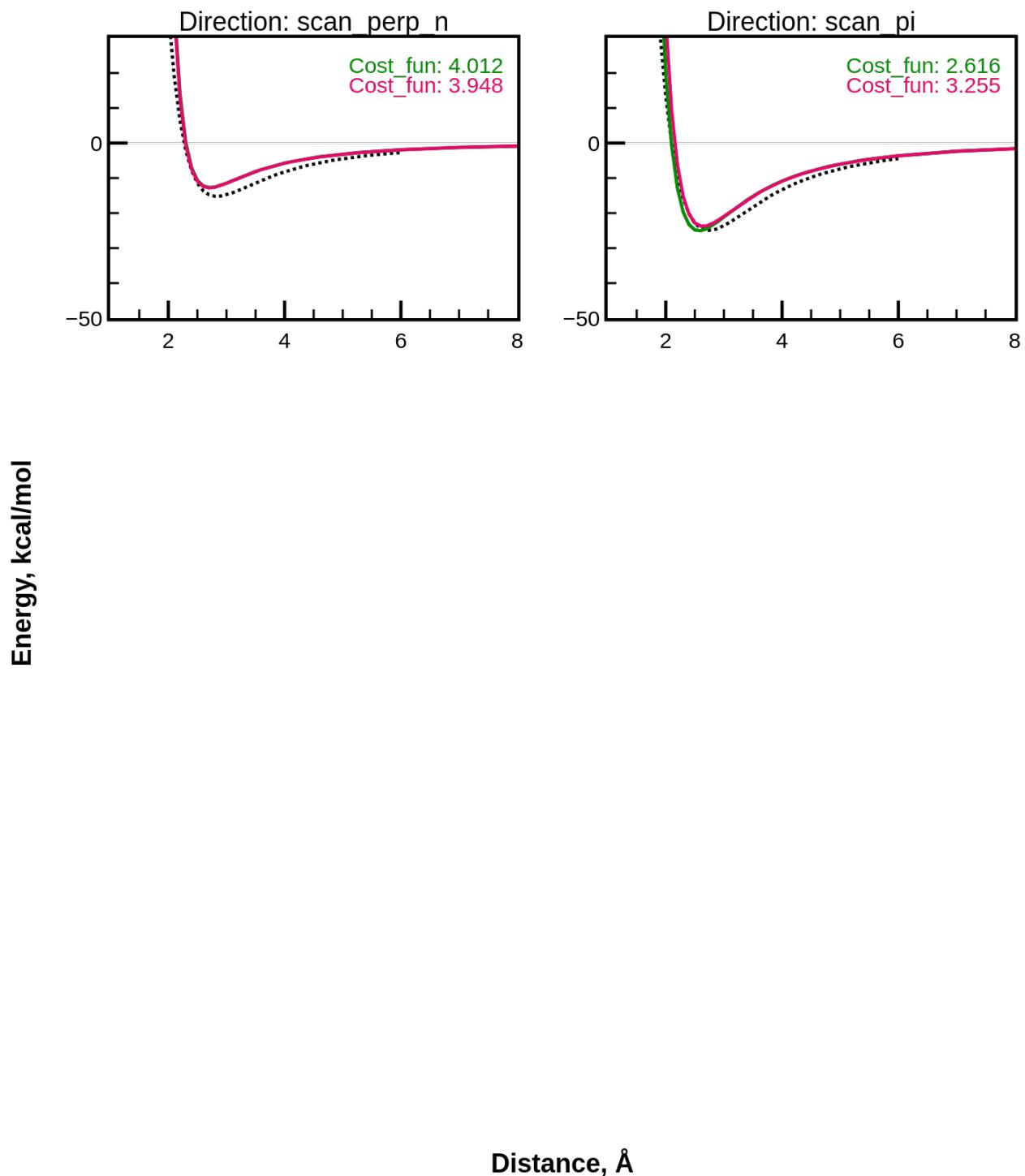
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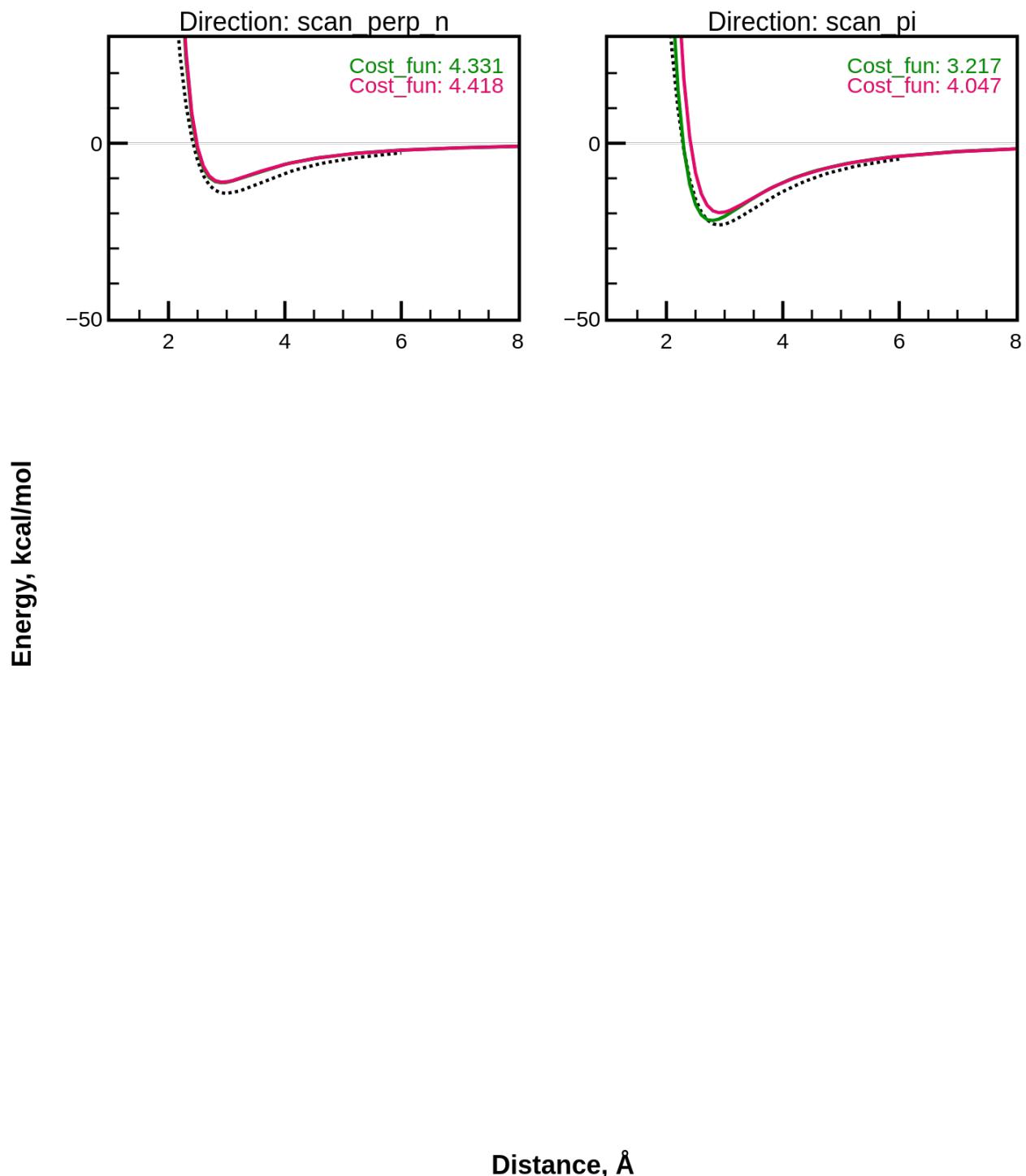
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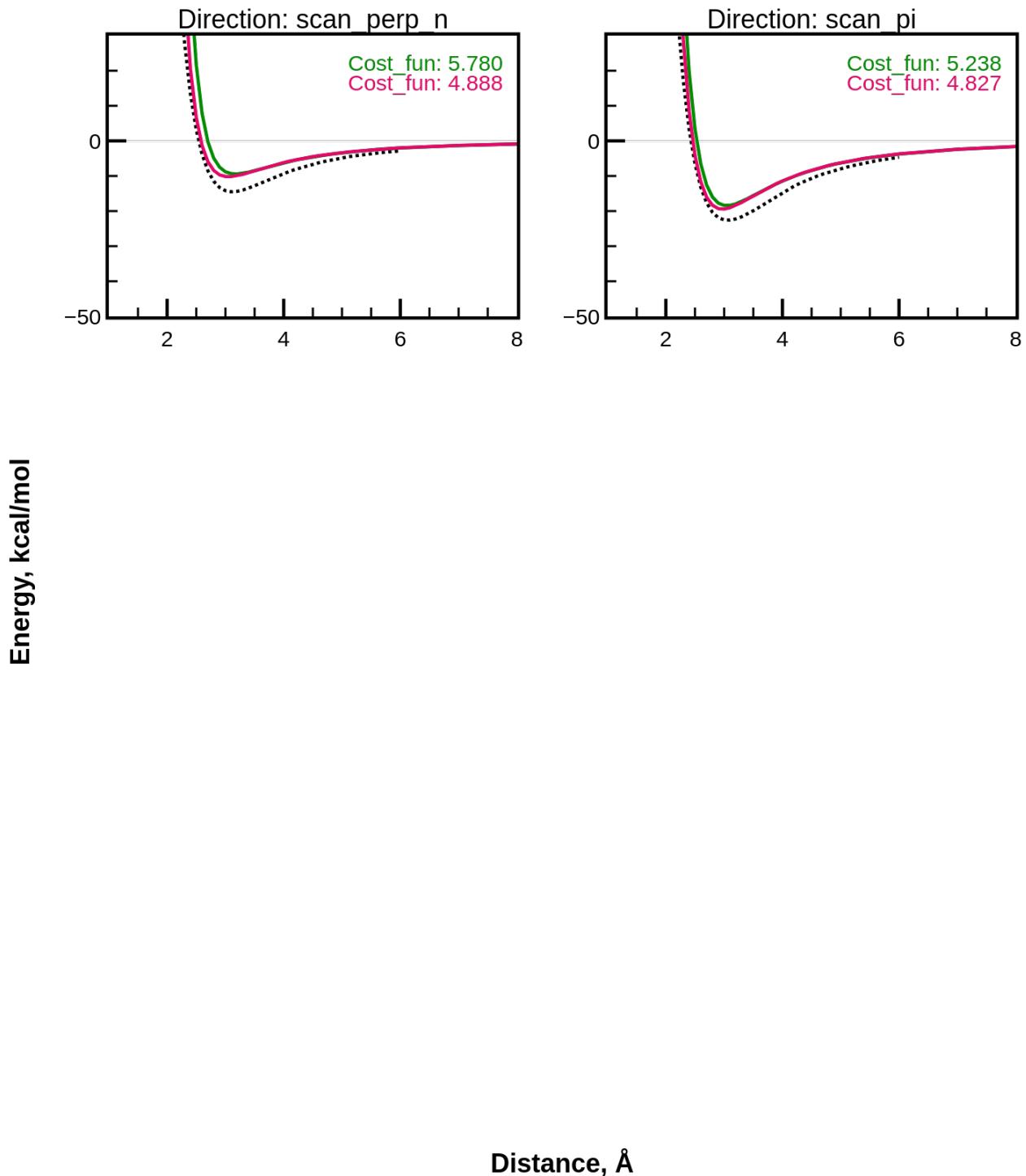
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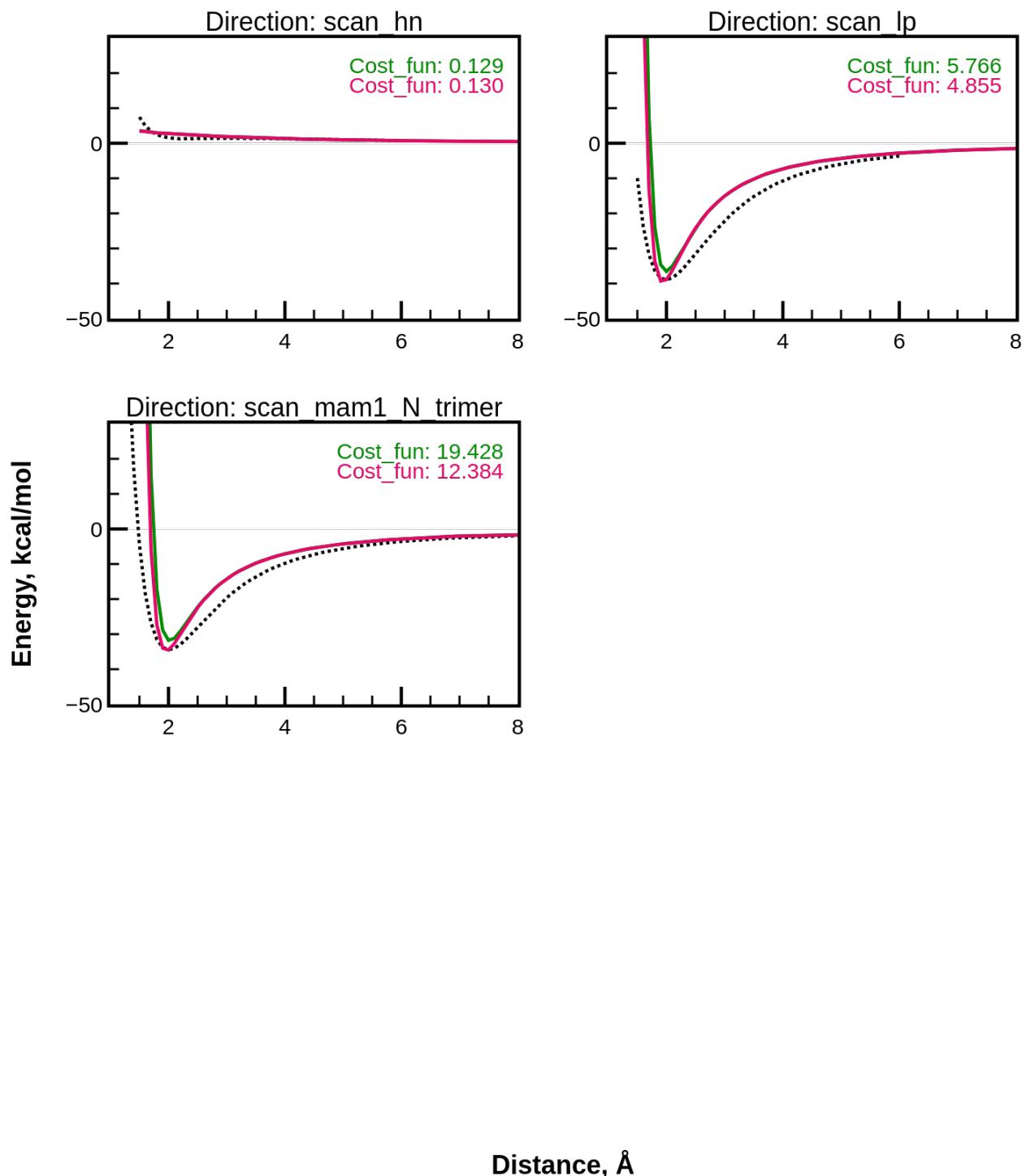
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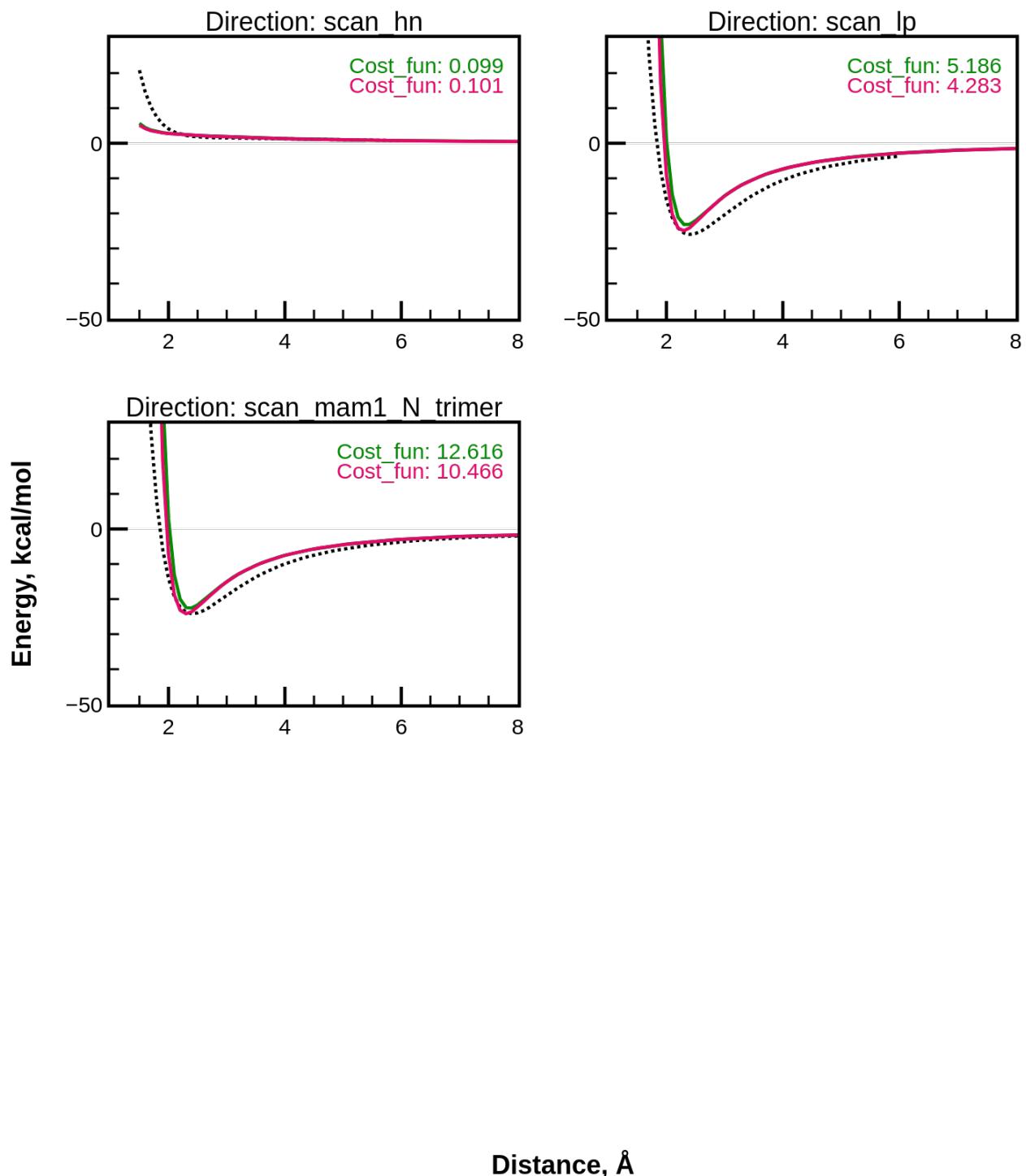
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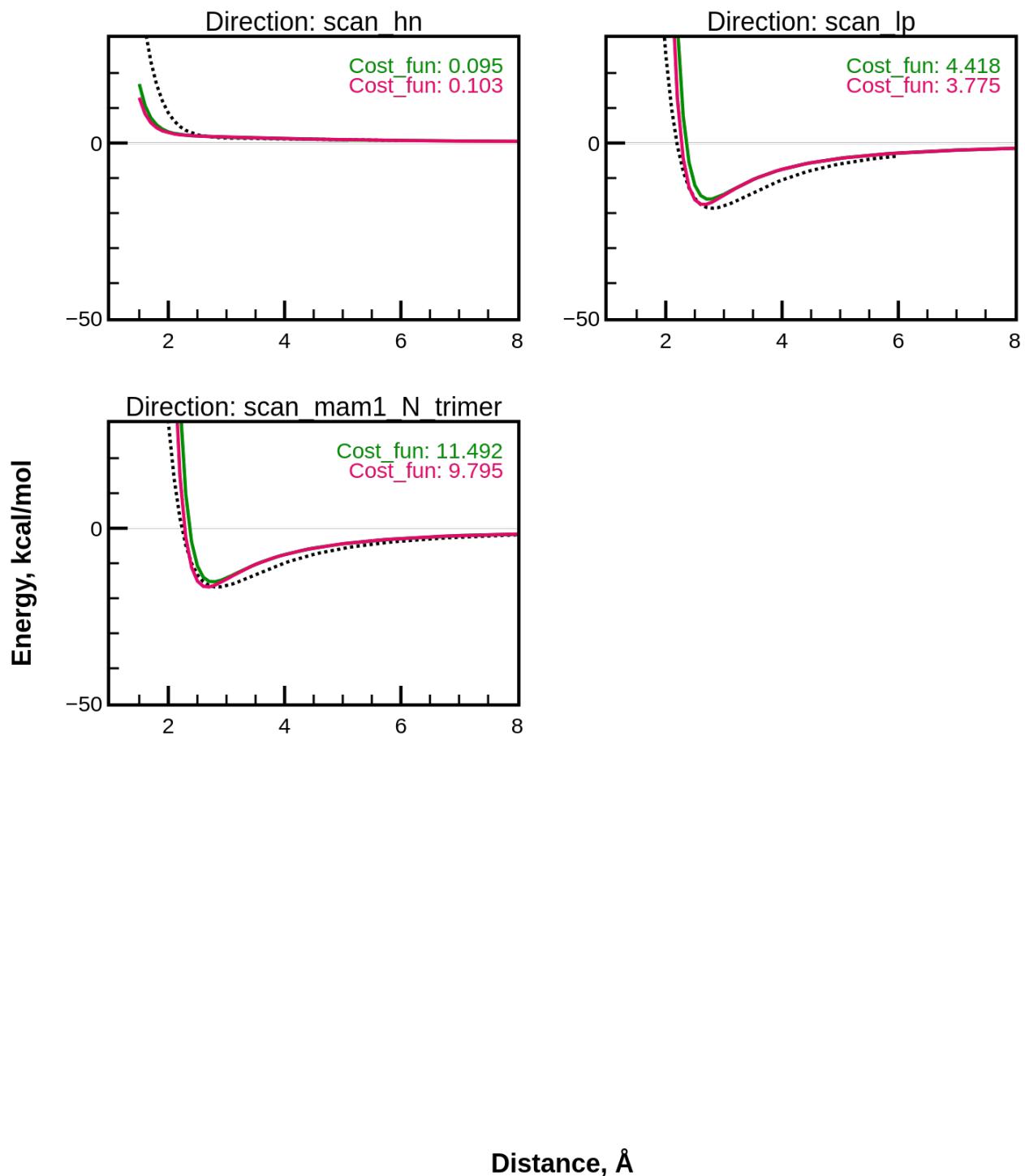
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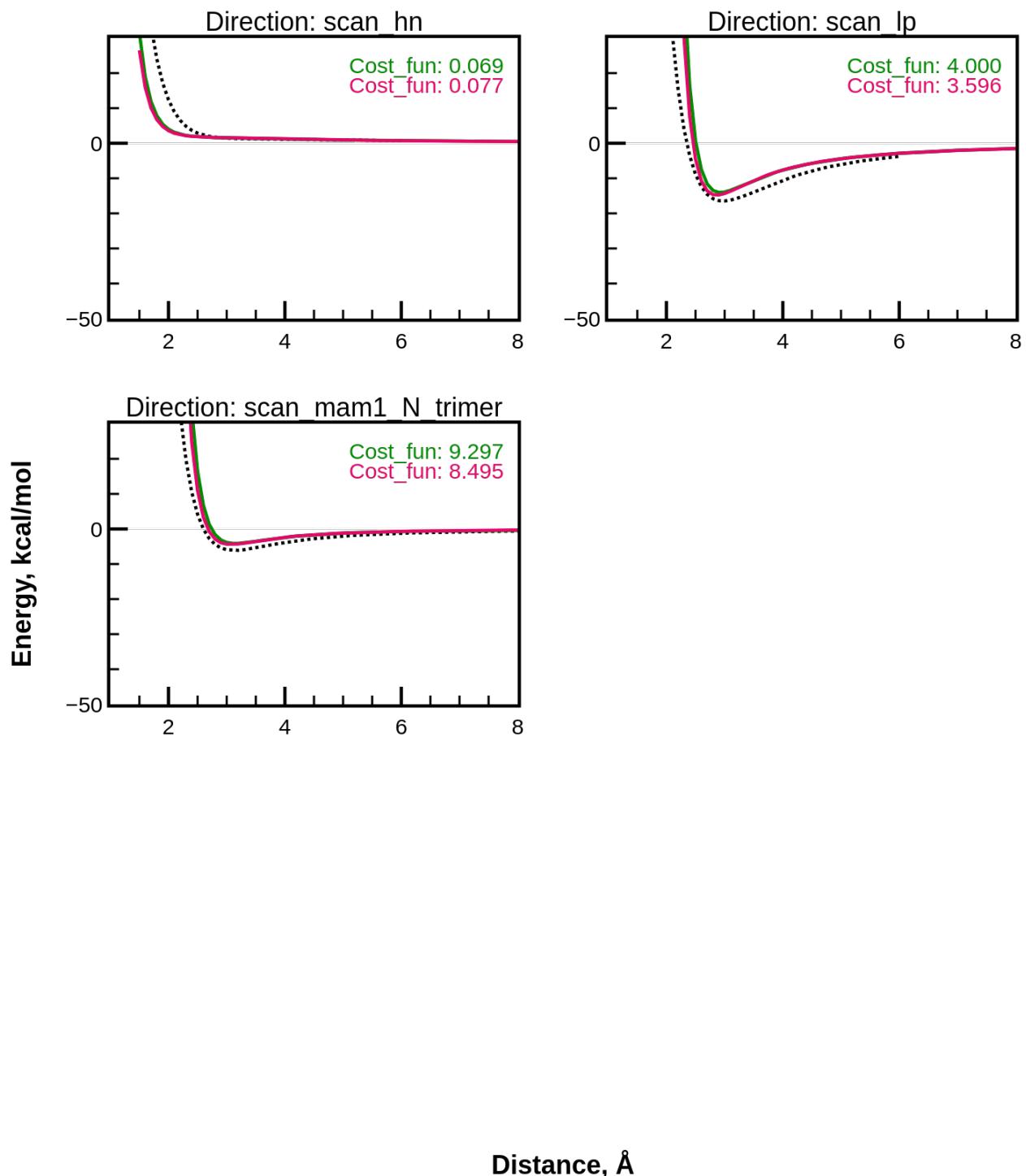
MAM1 SOD 1/1



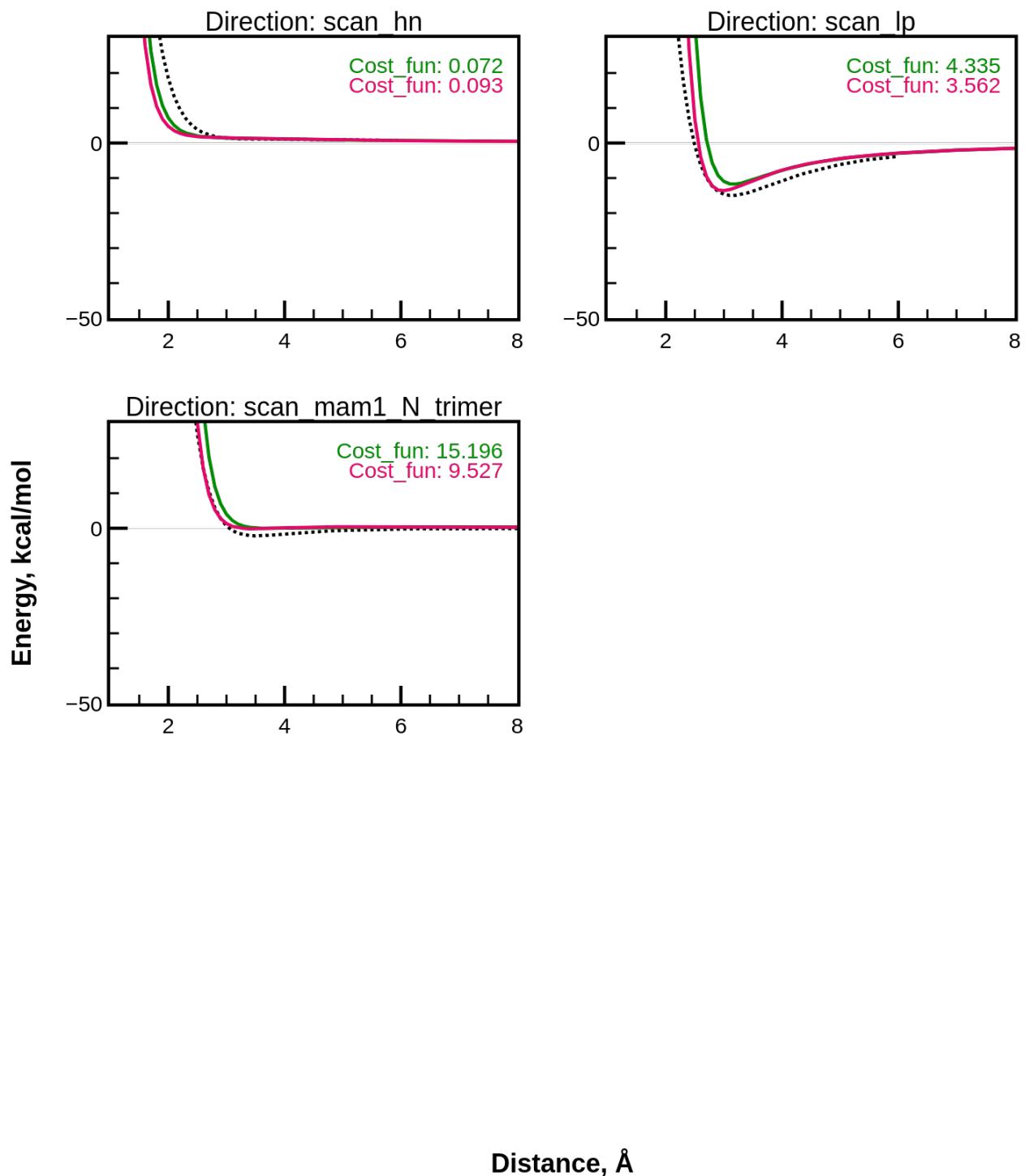
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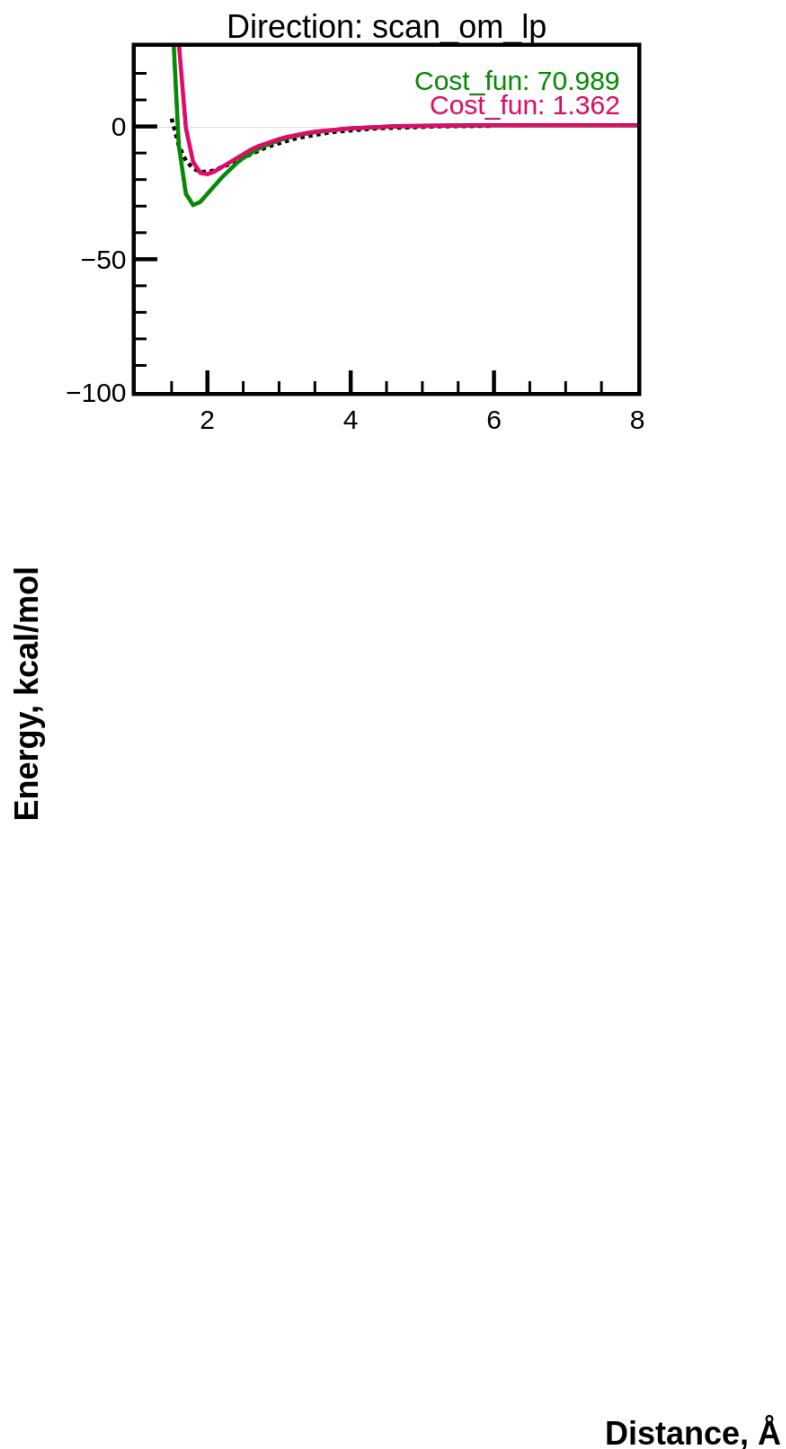
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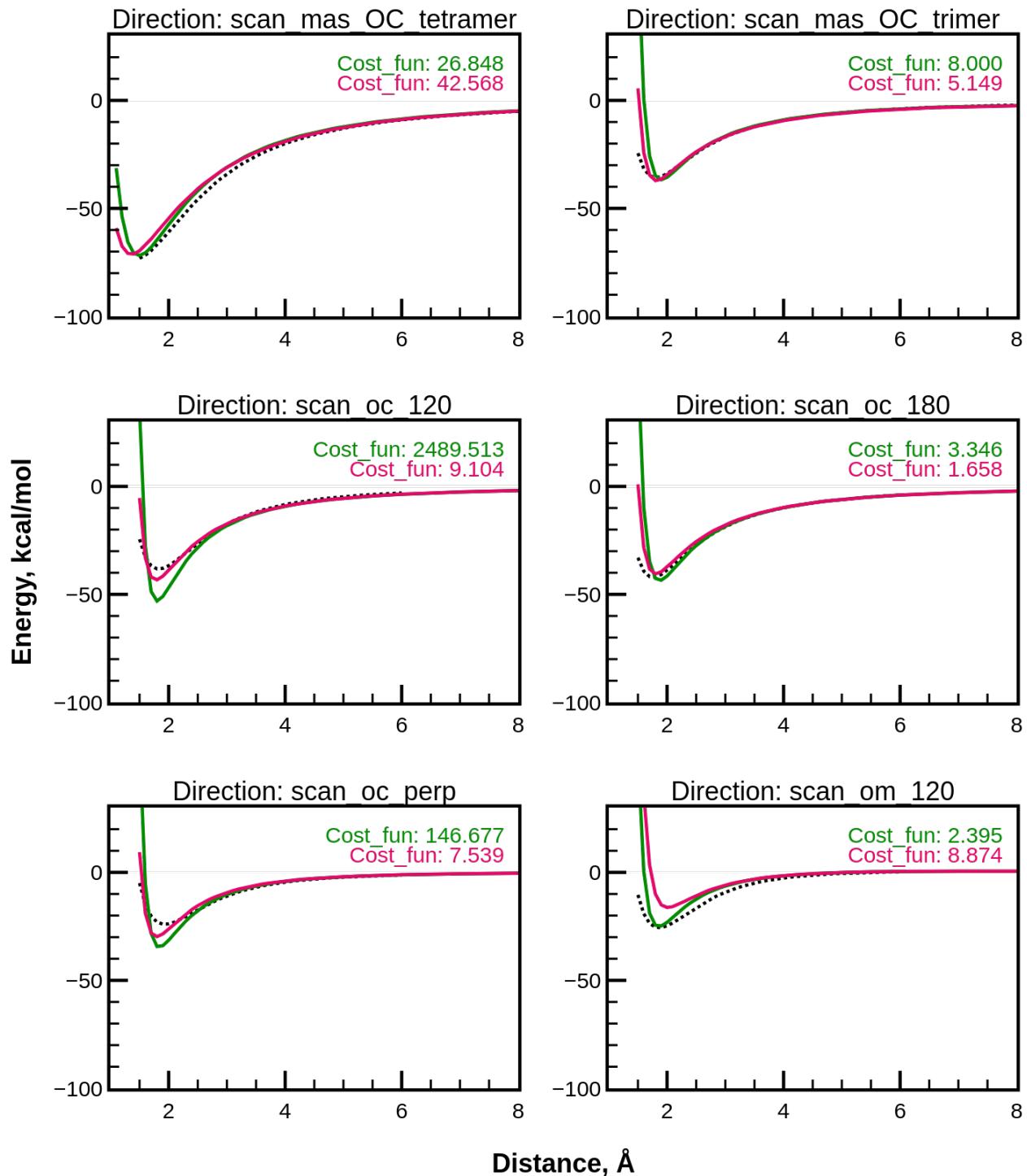
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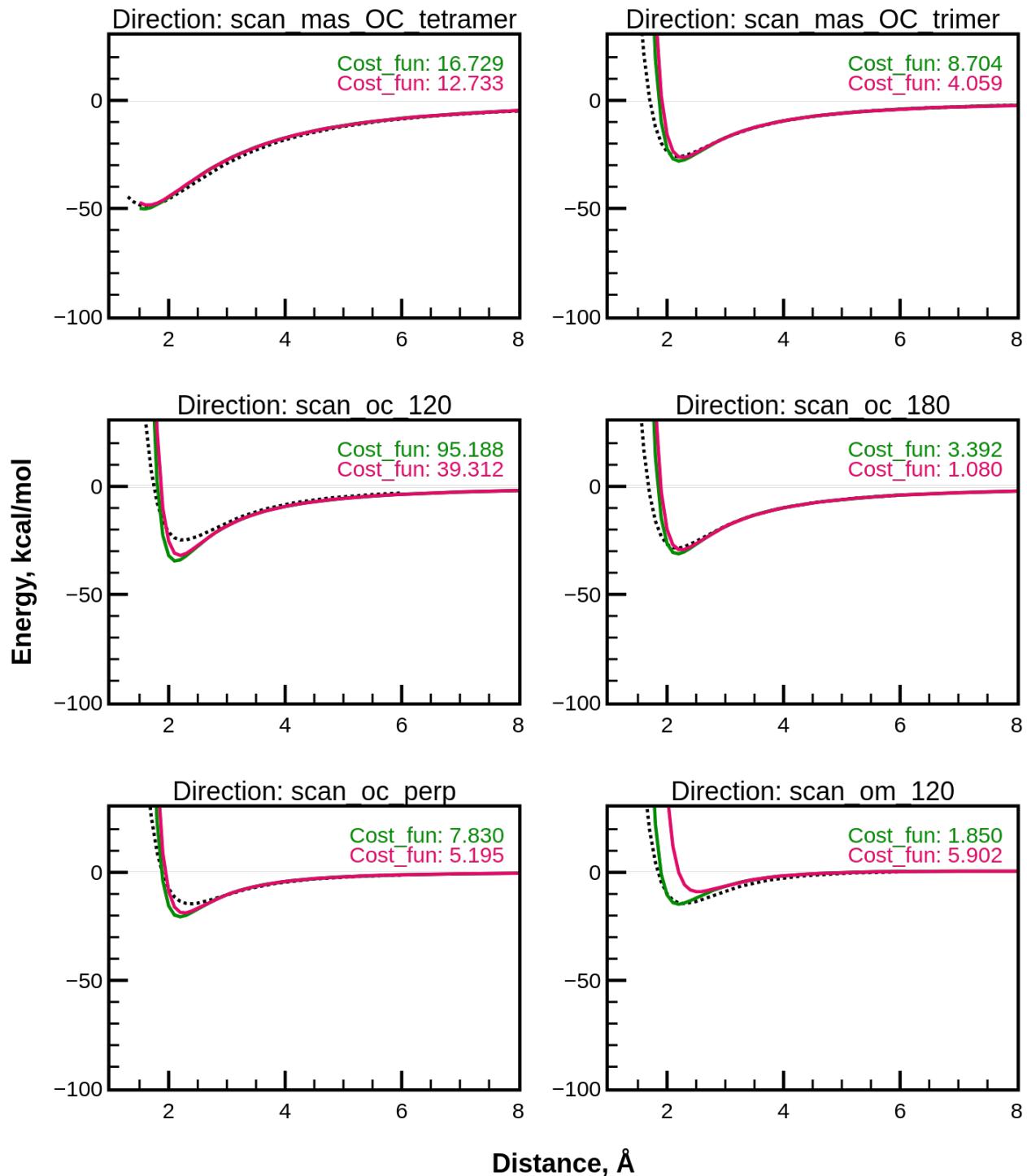
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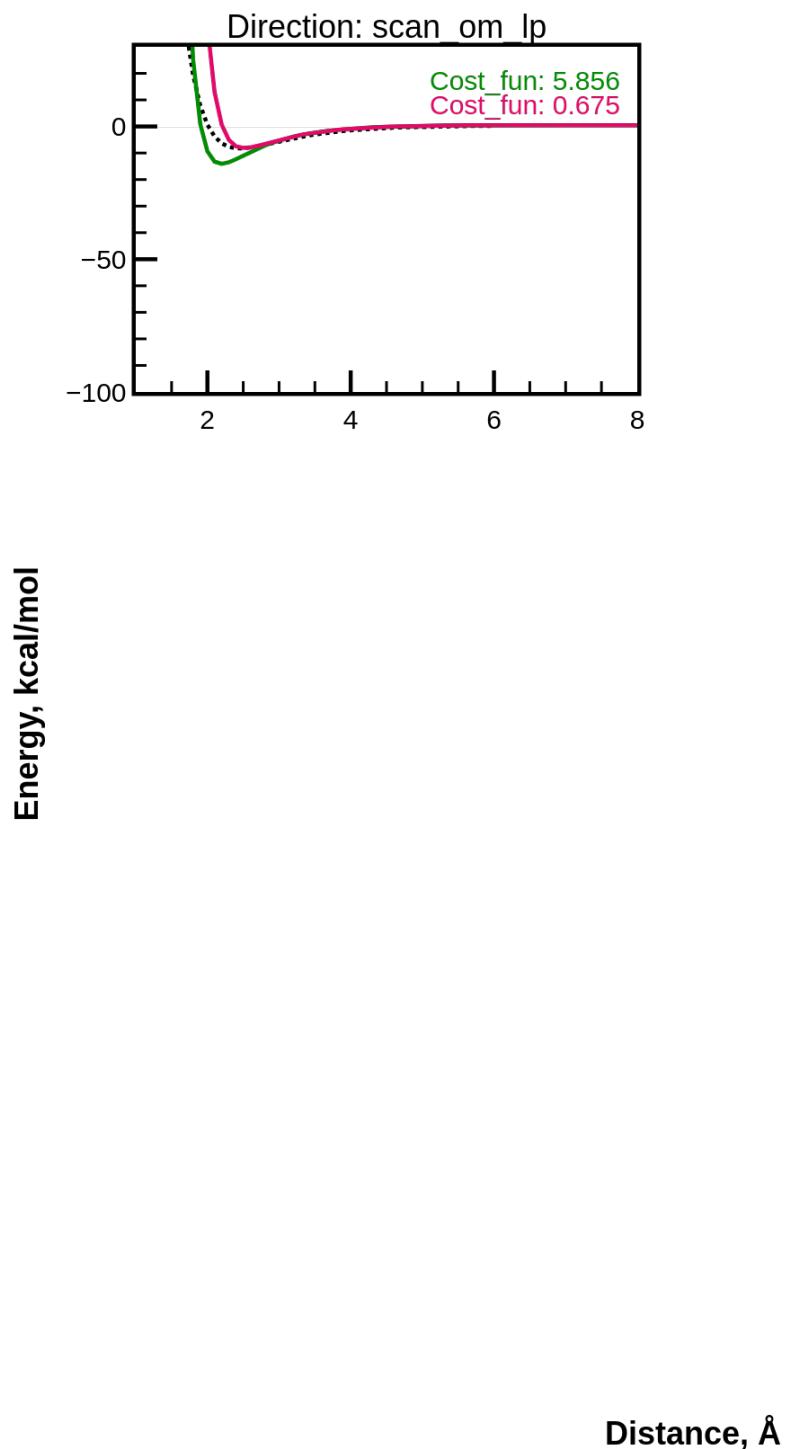
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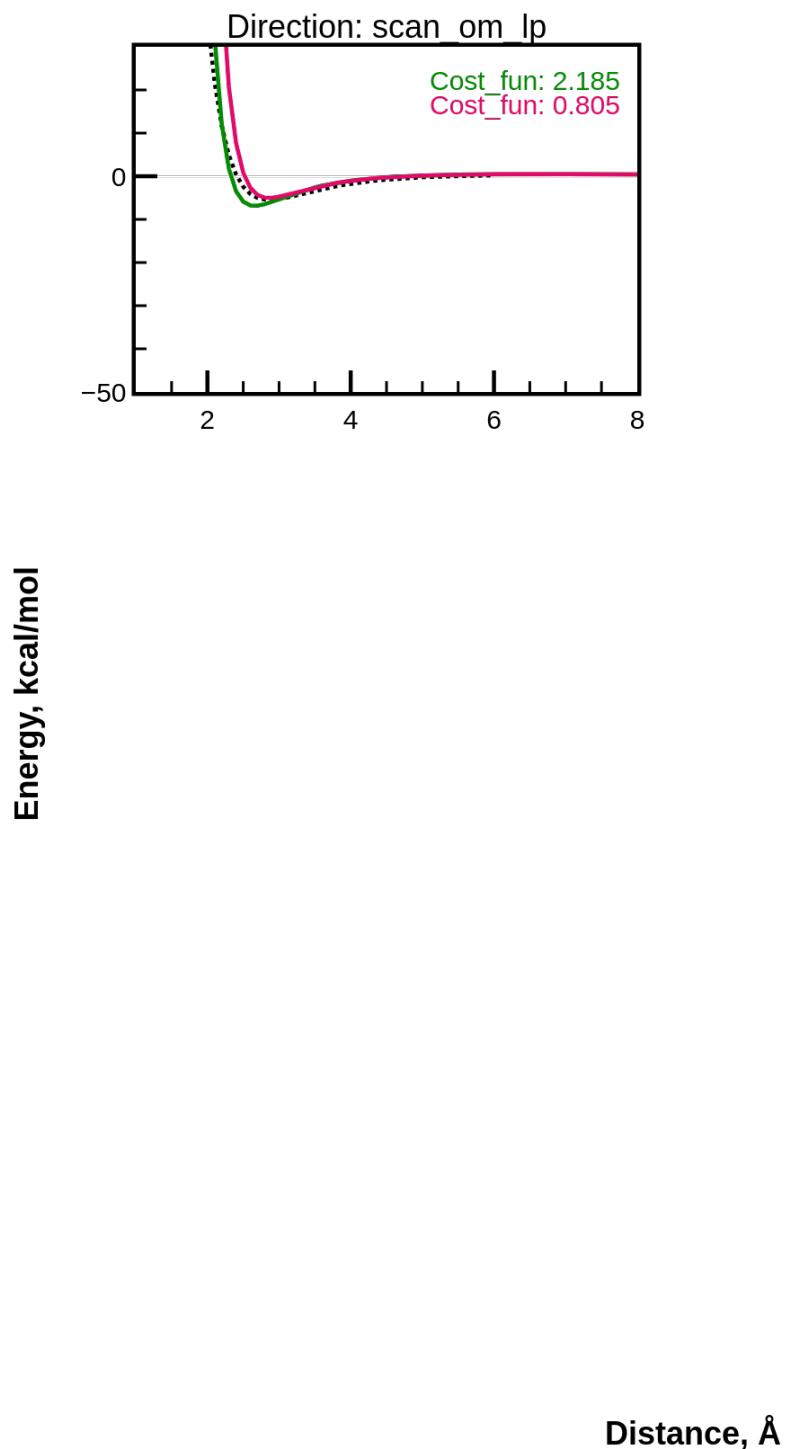
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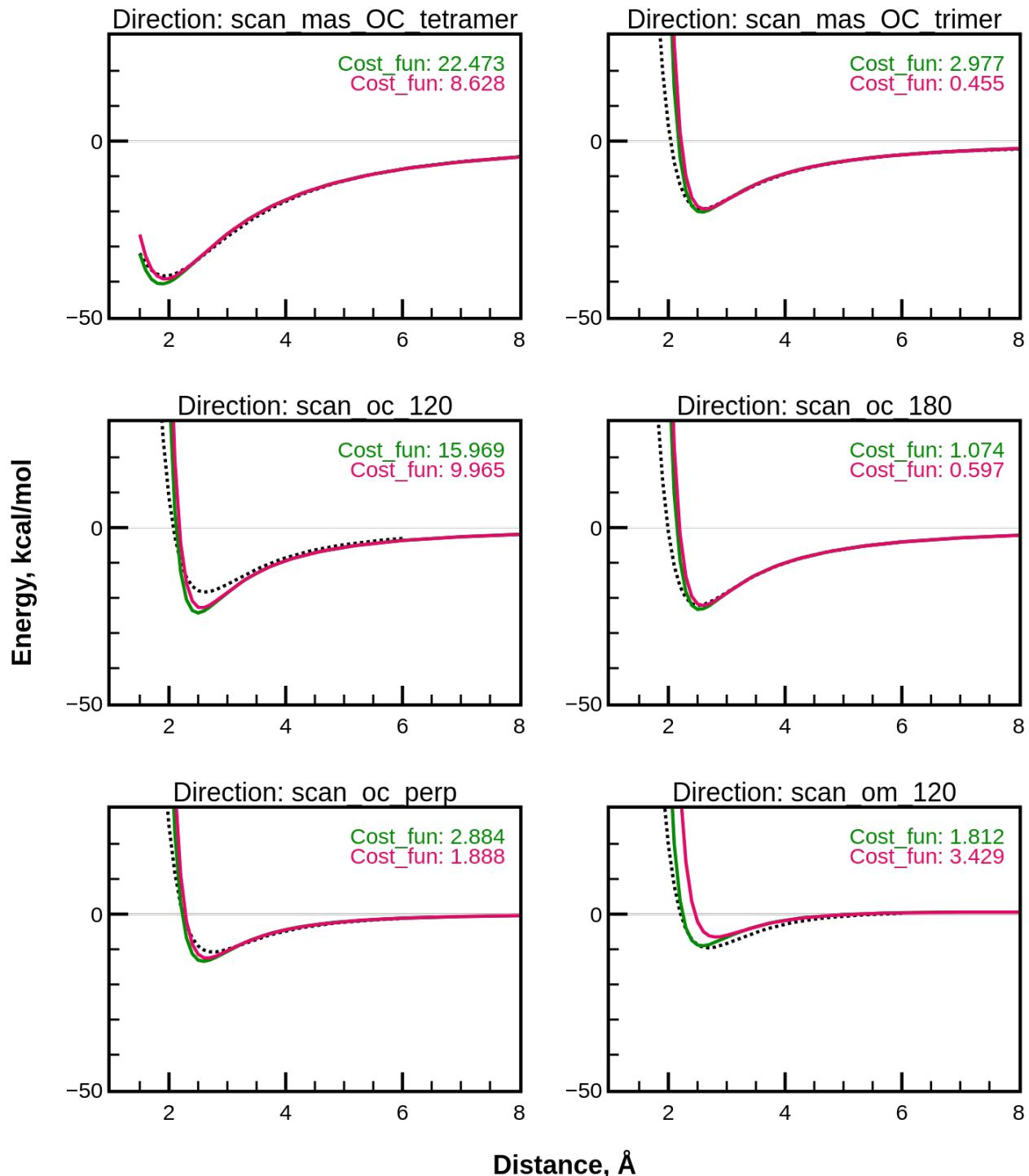
MAS SOD 2/2



MAS POT 2/2

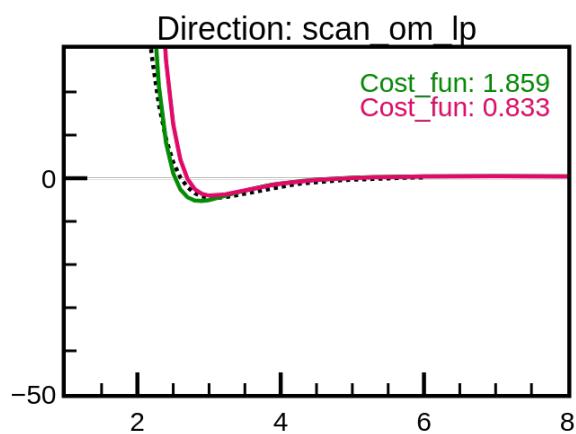


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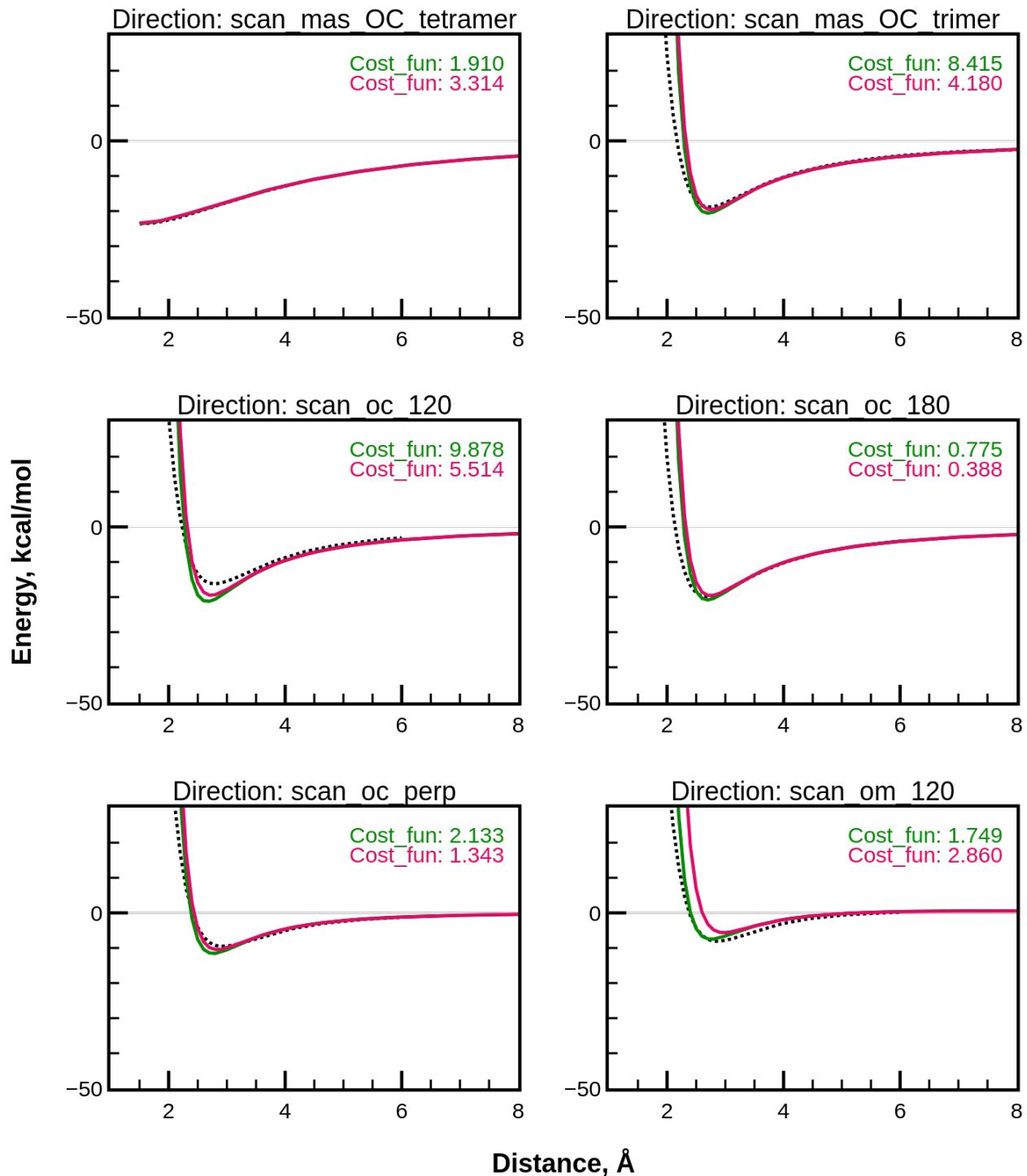
MAS RUB 2/2

Energy, kcal/mol

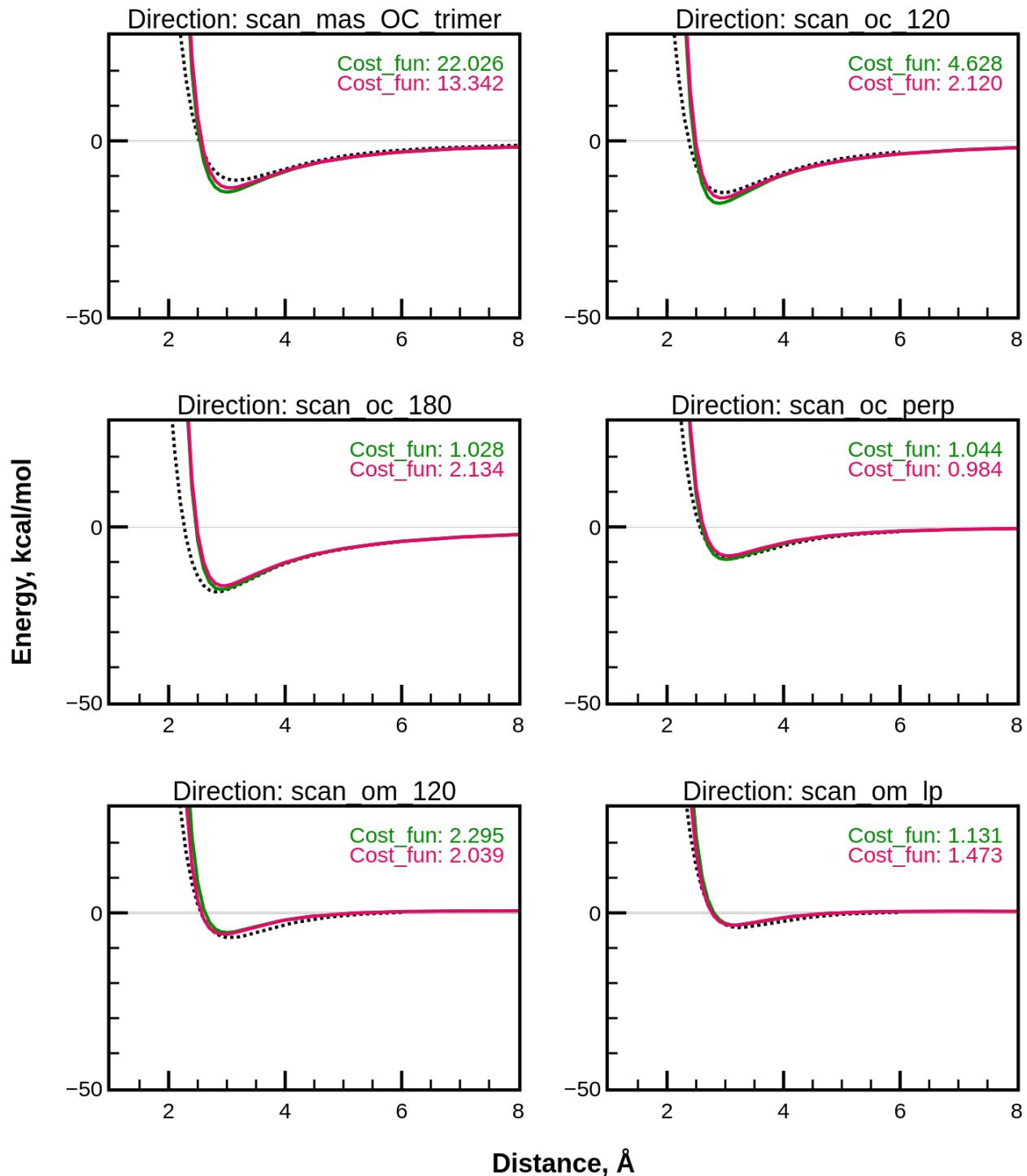


Distance, Å

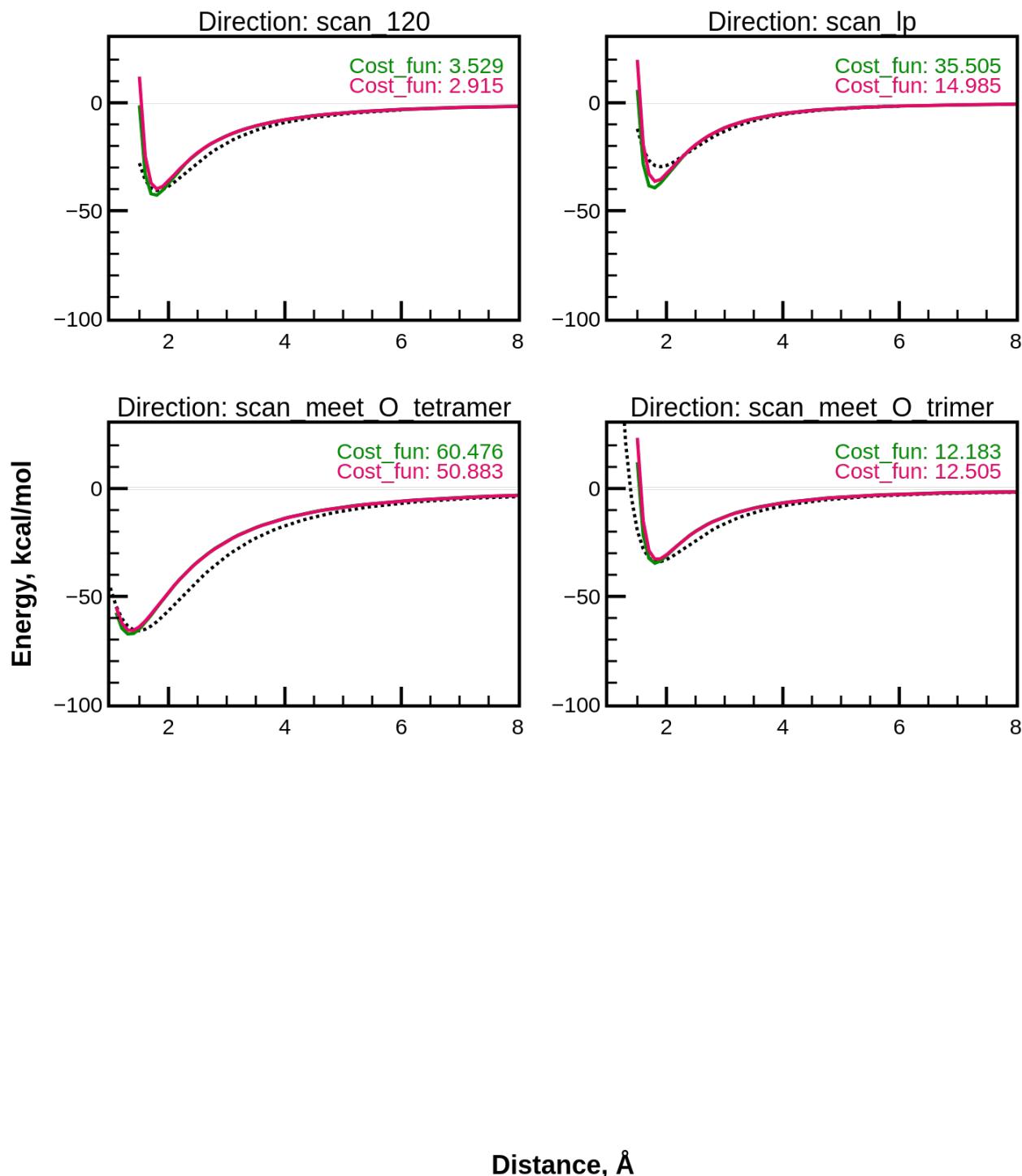
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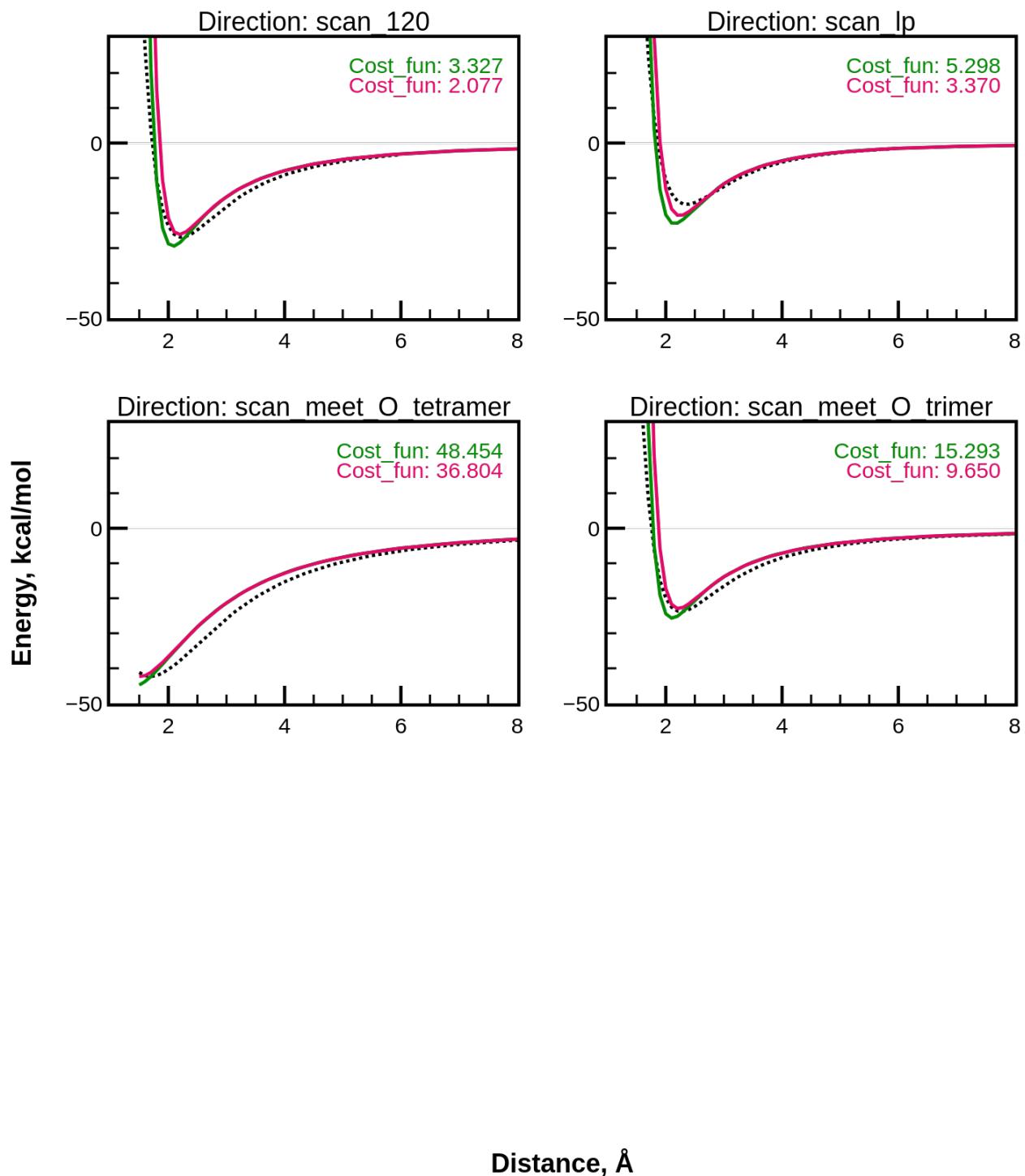
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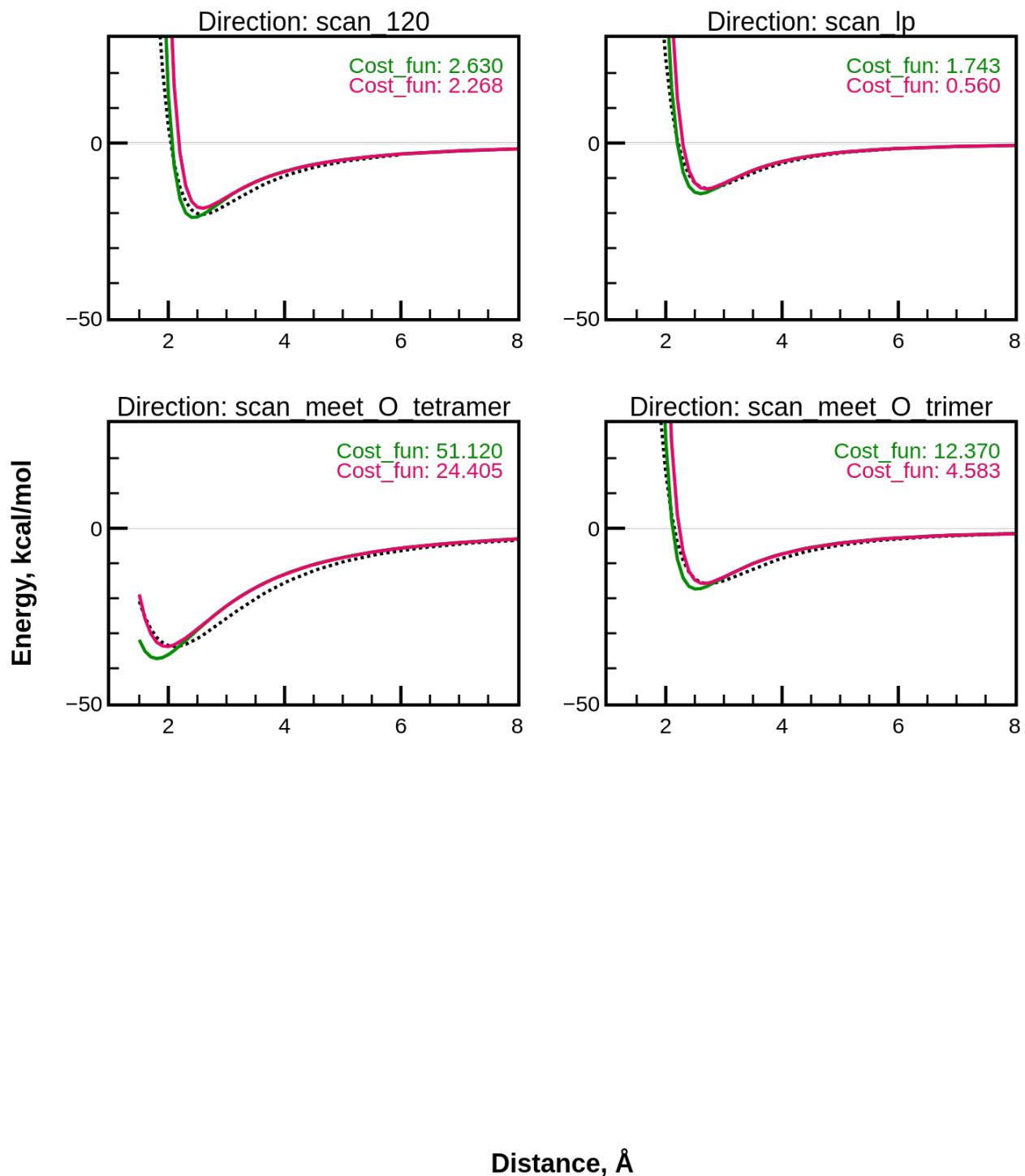
MEET LIT 1/1



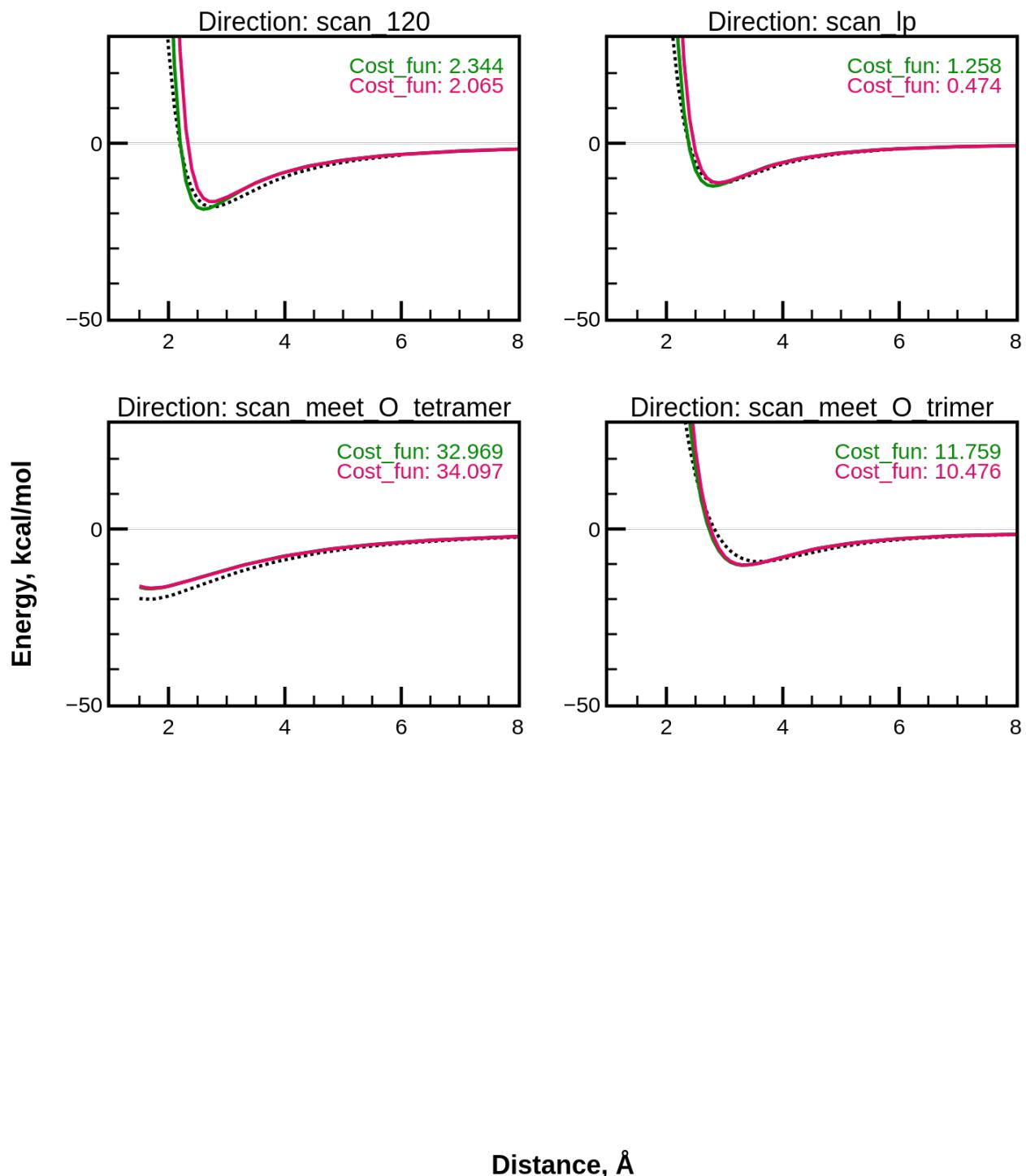
MEET SOD 1/1



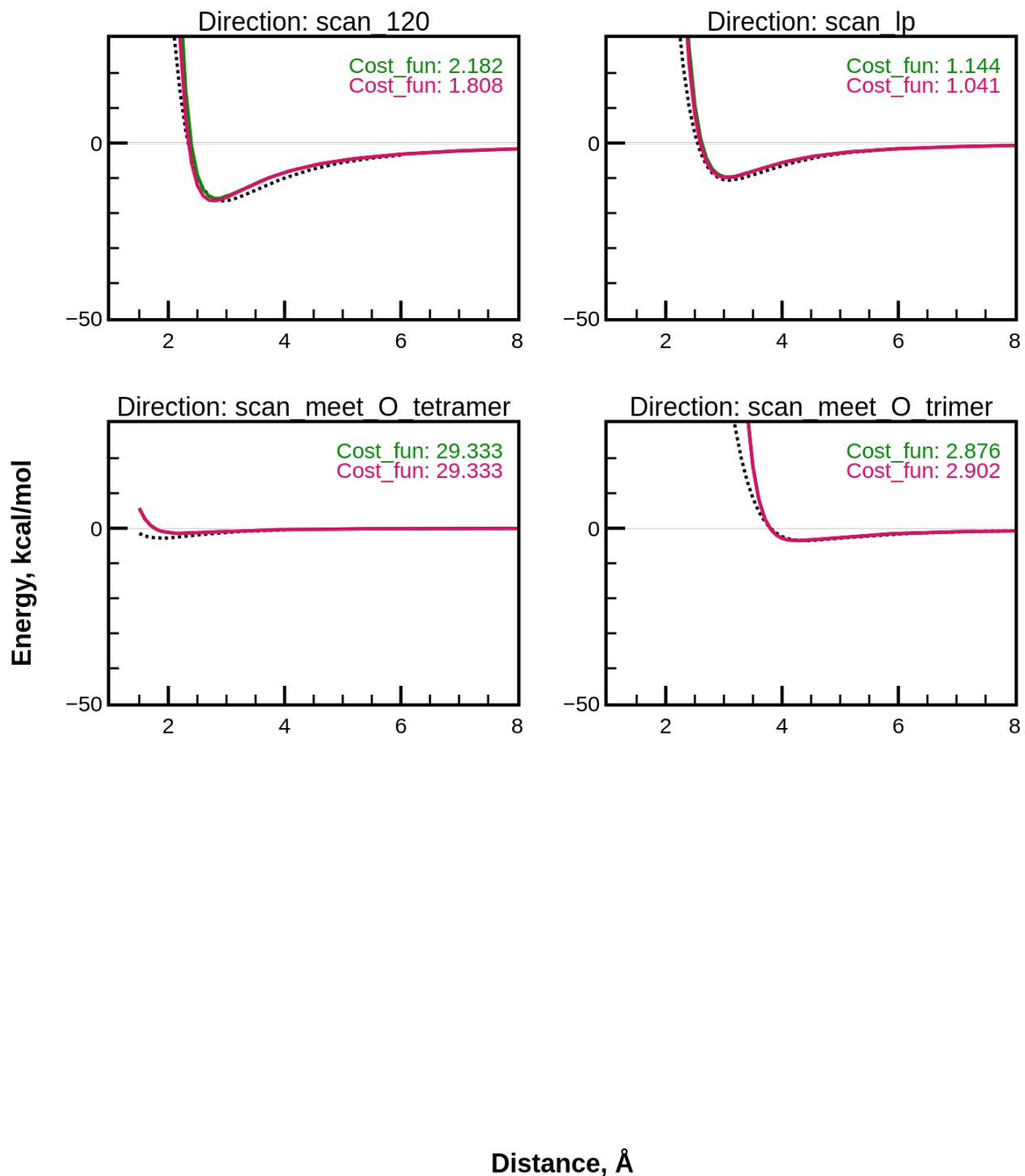
MEET POT 1/1



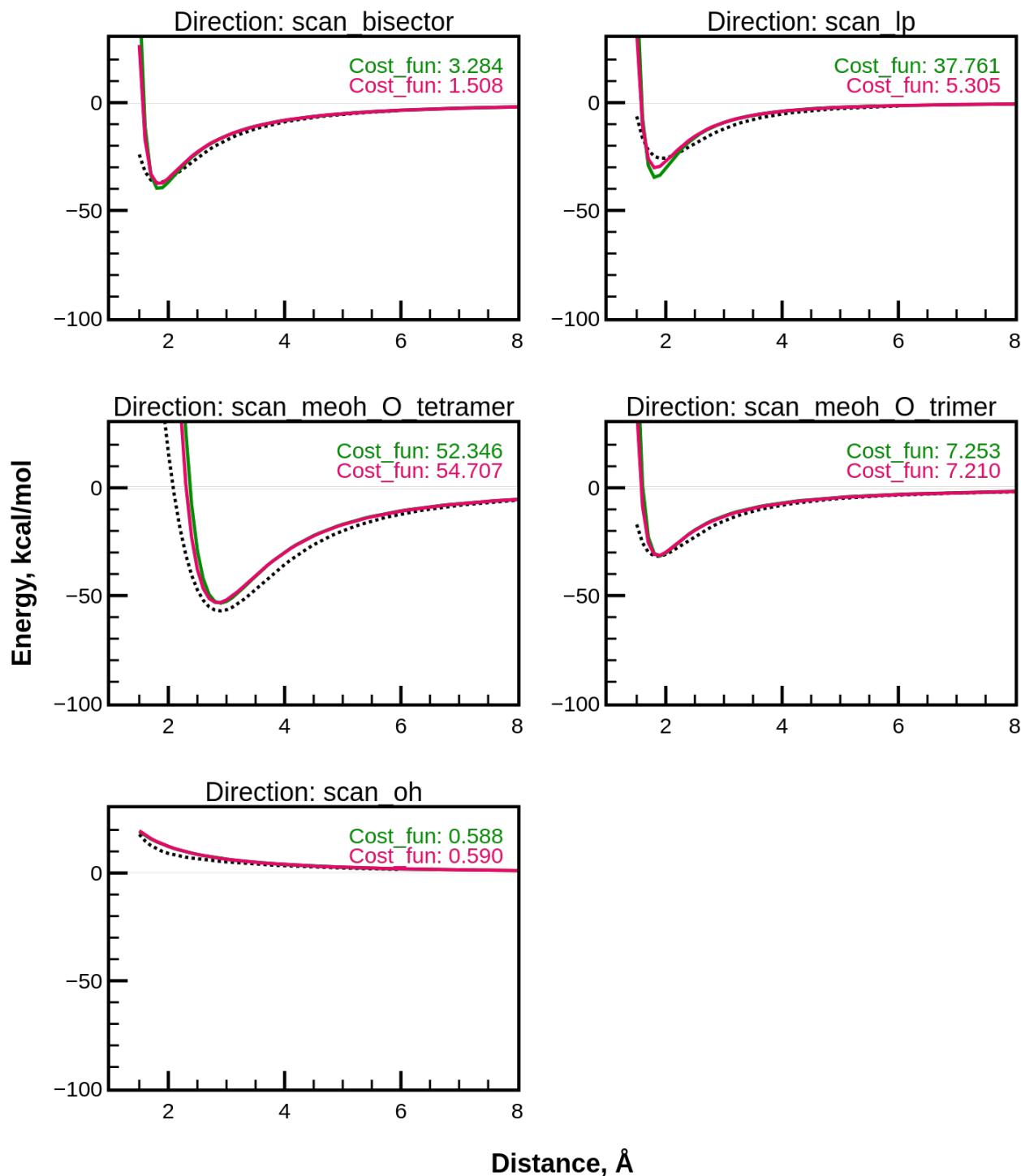
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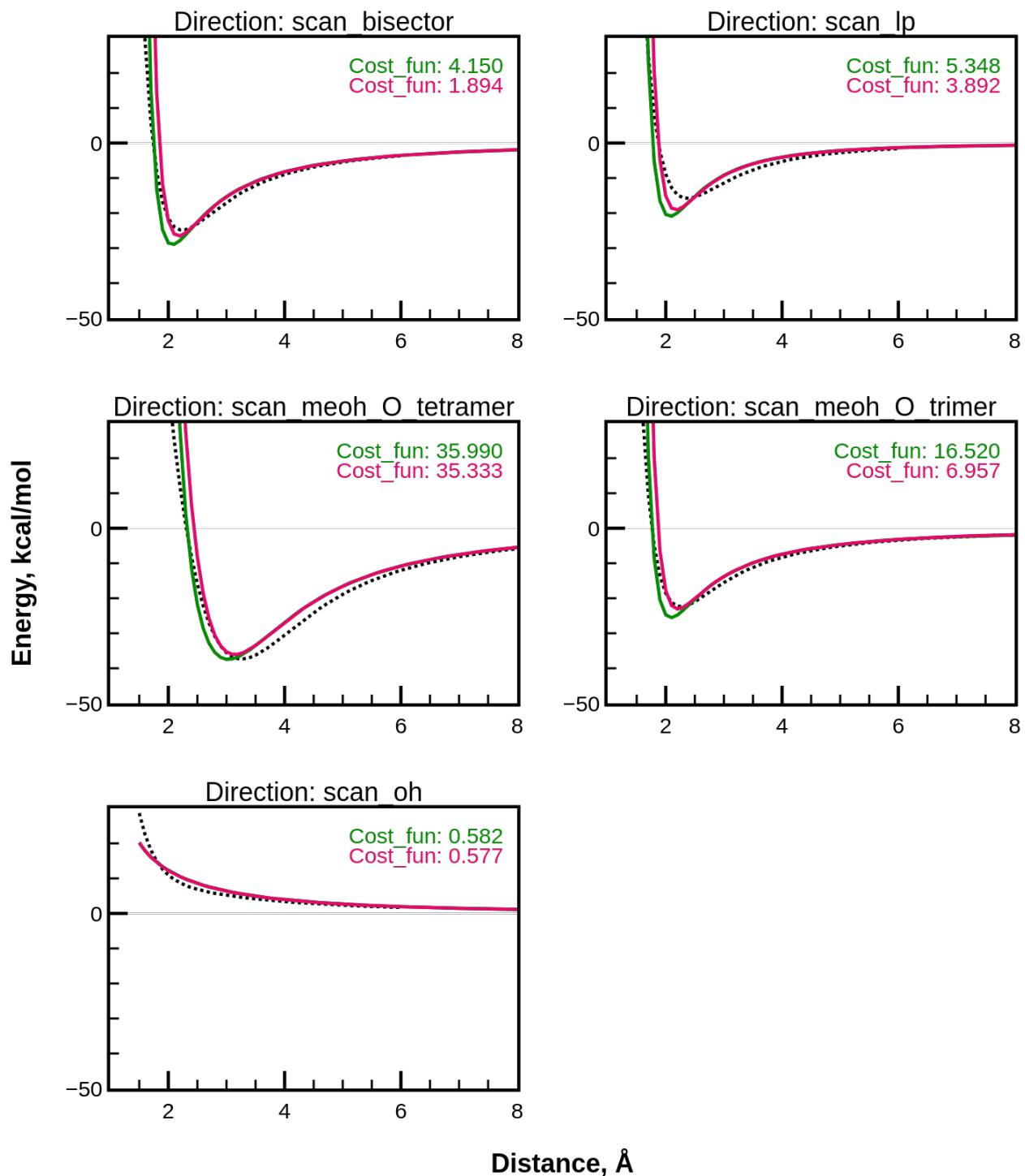
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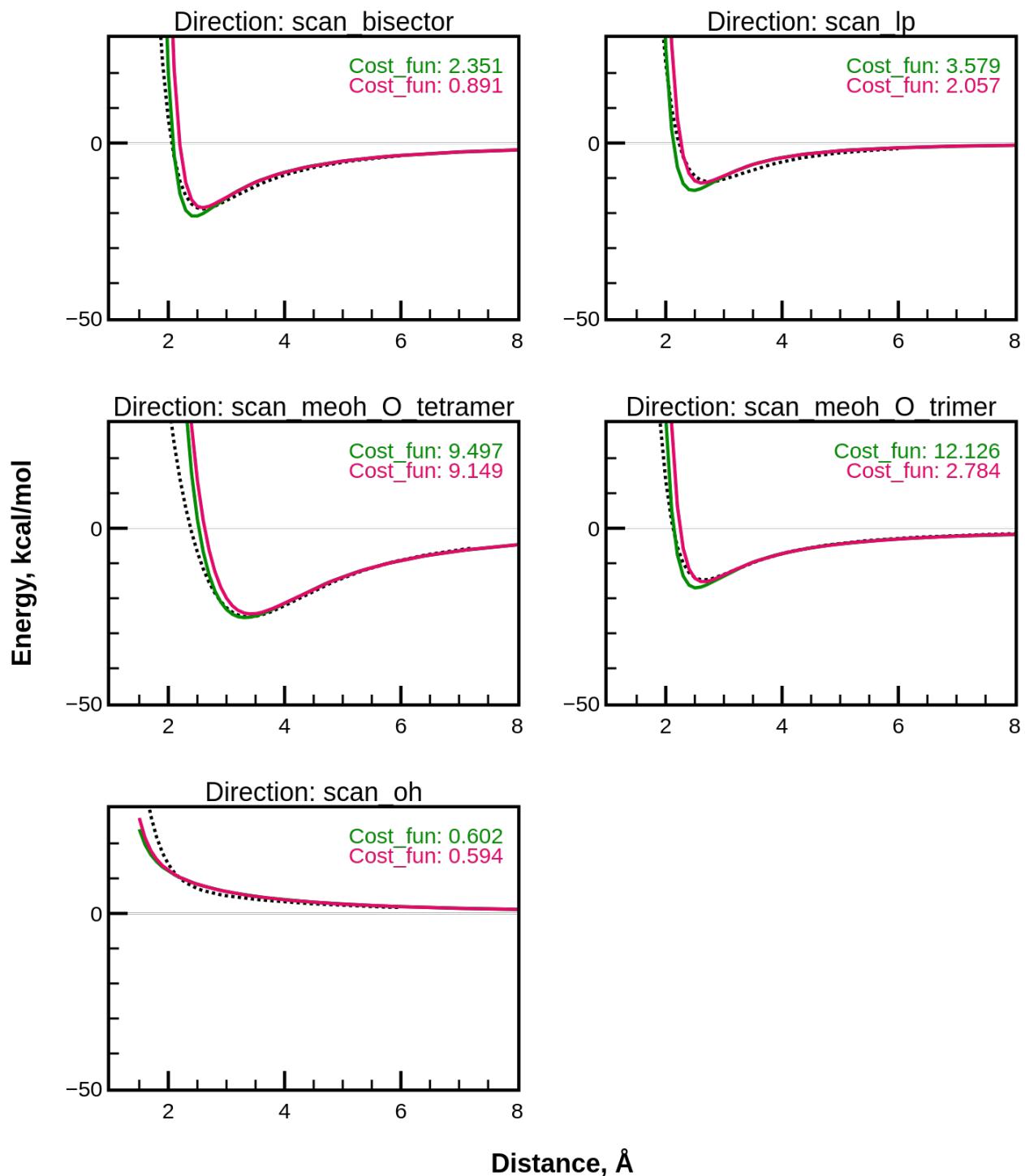
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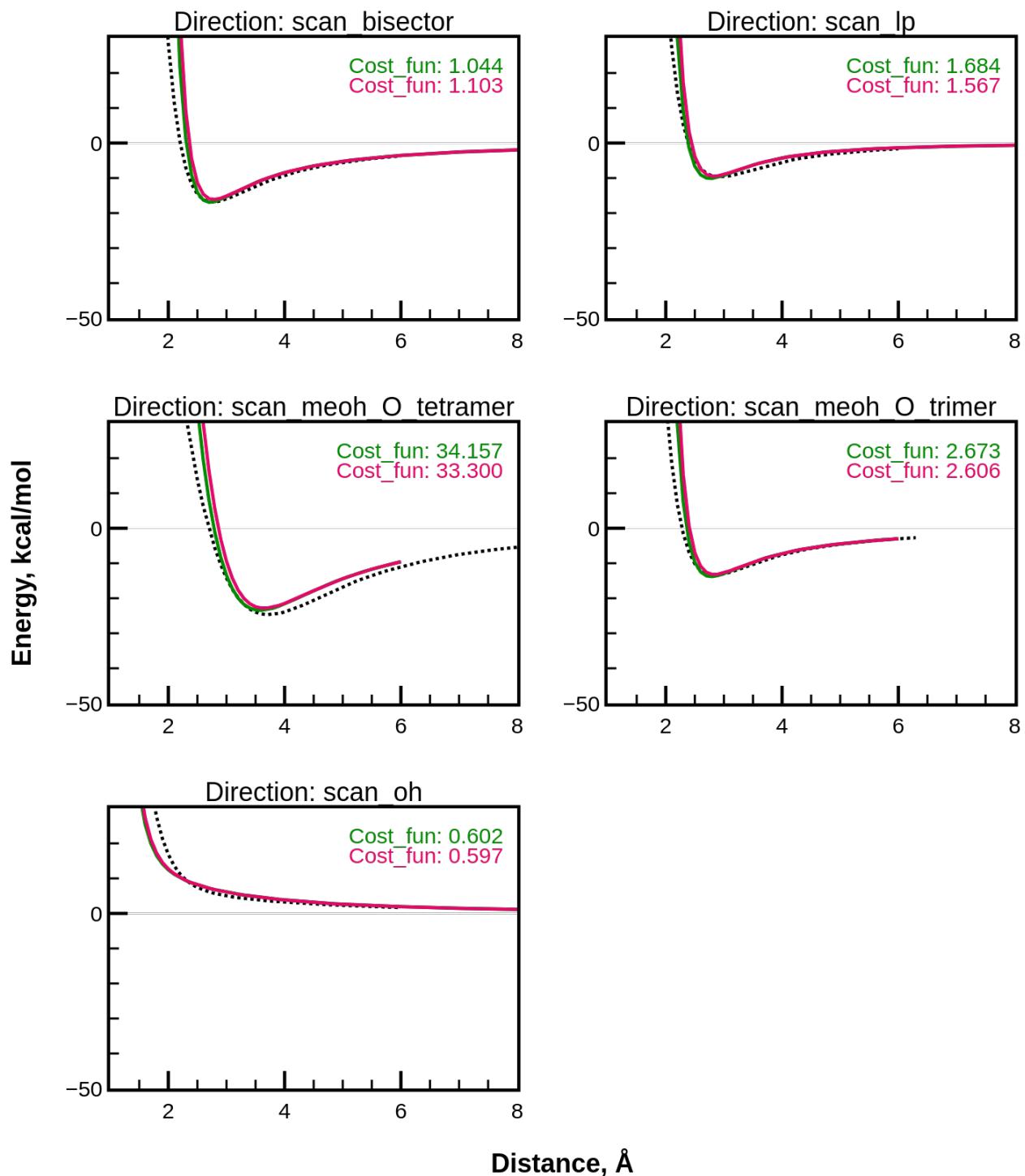
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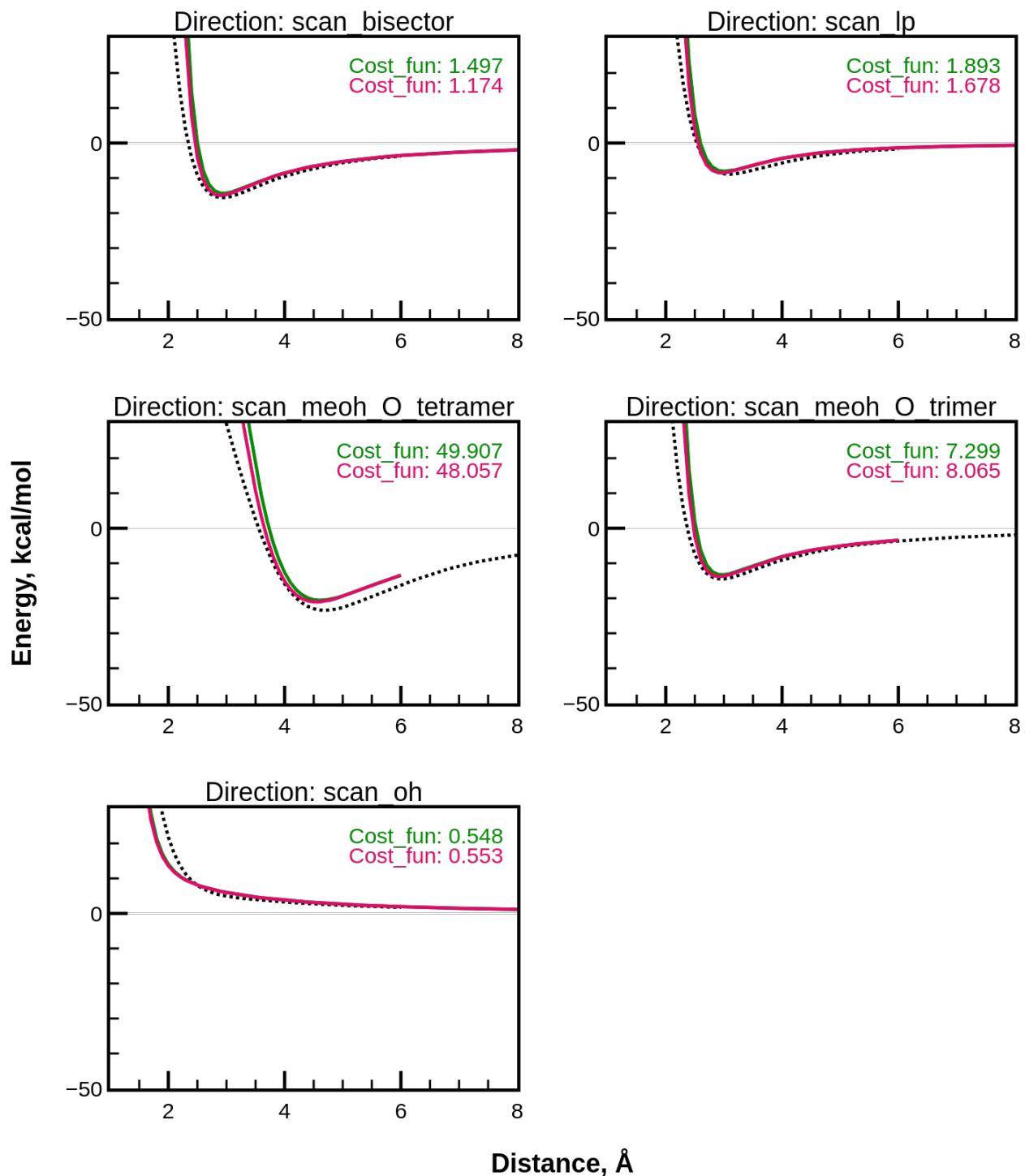
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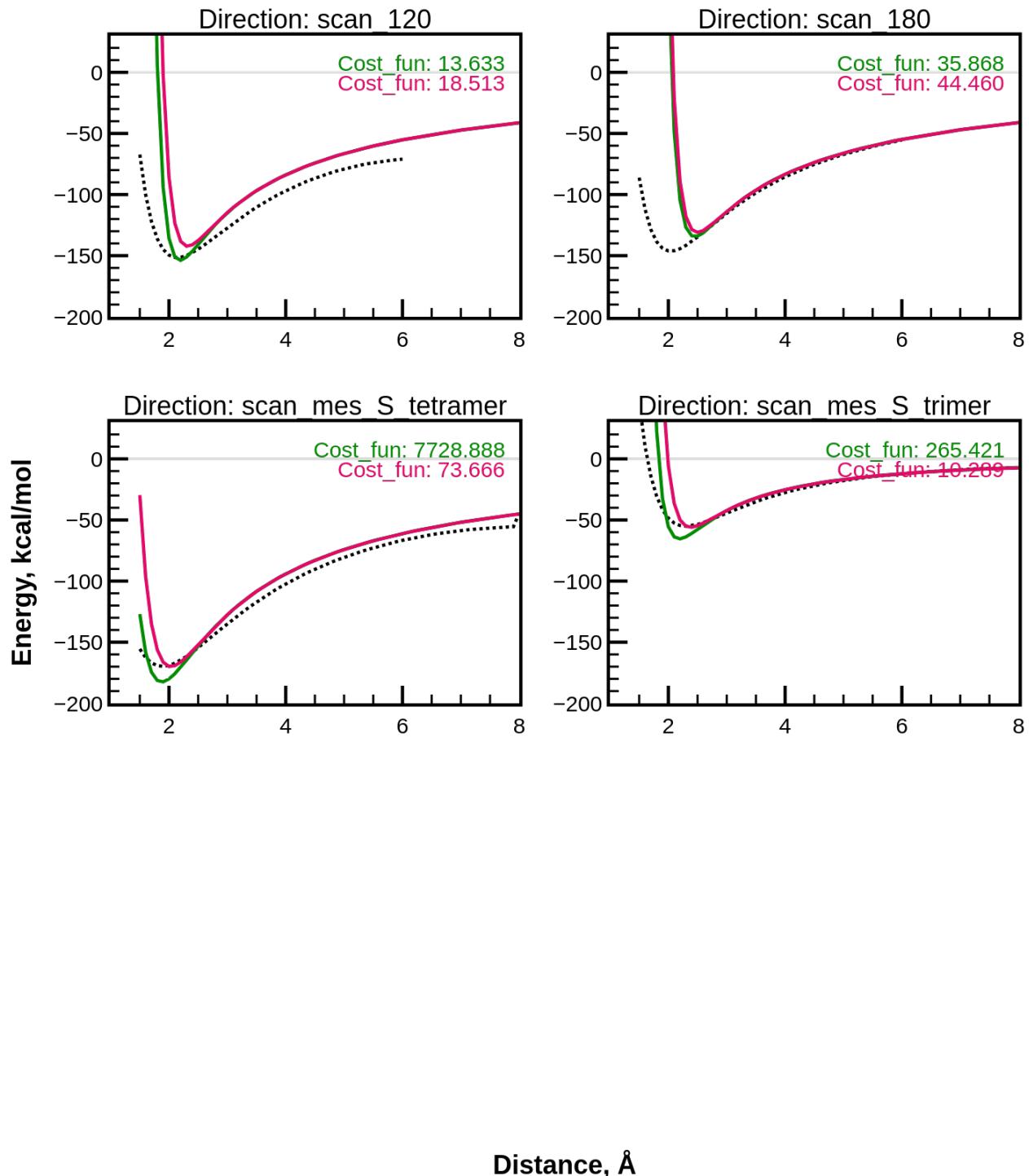
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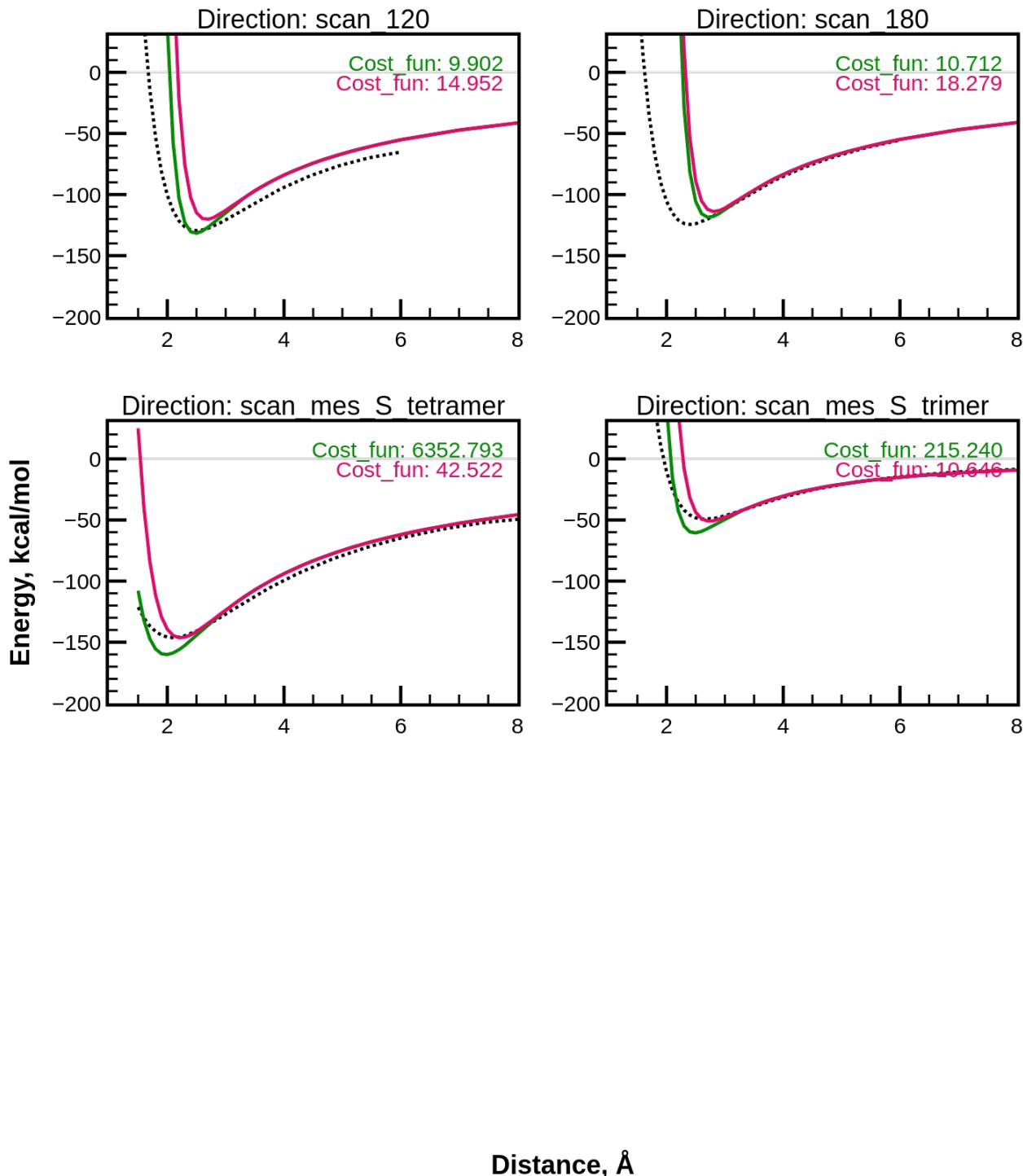
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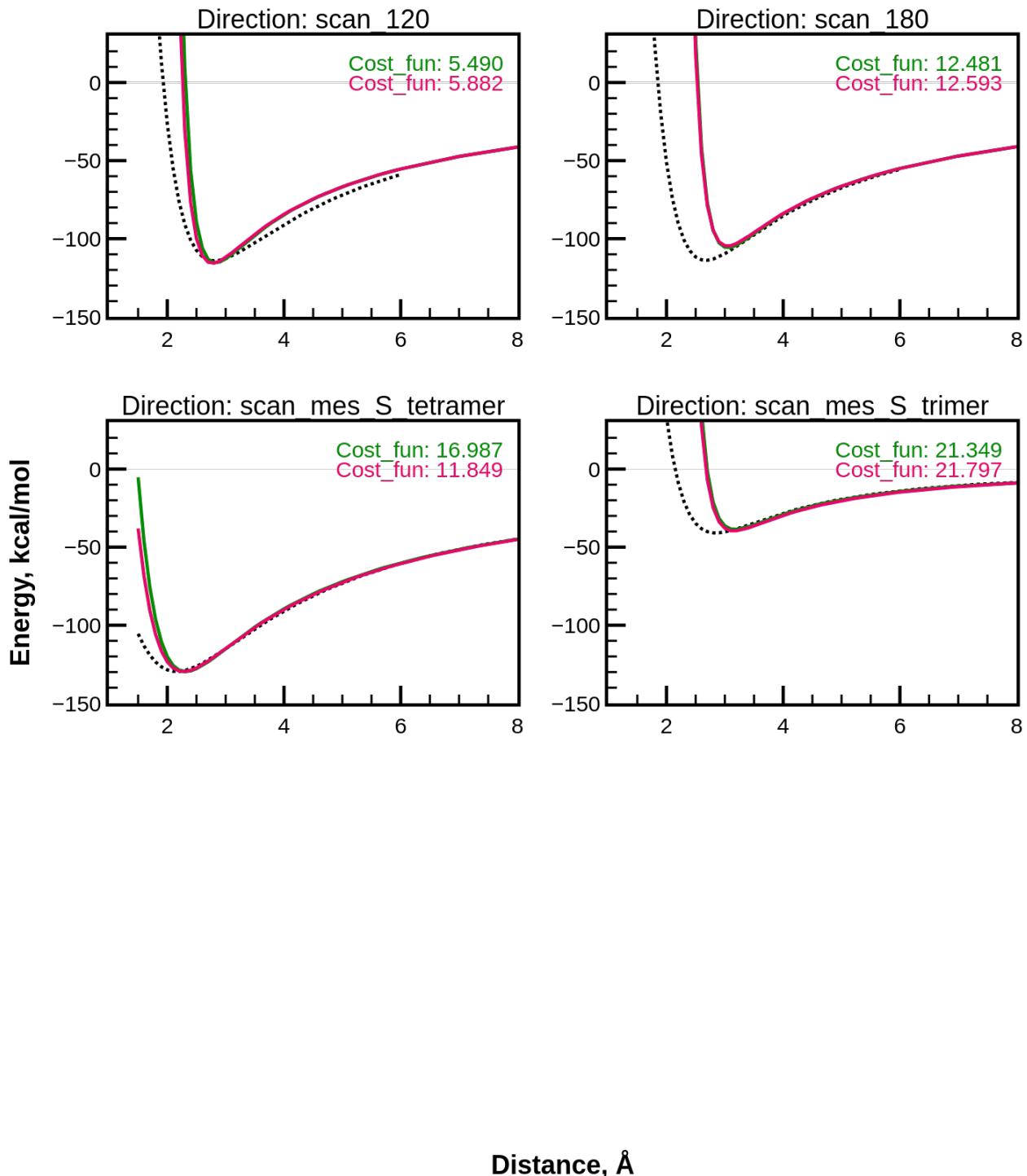
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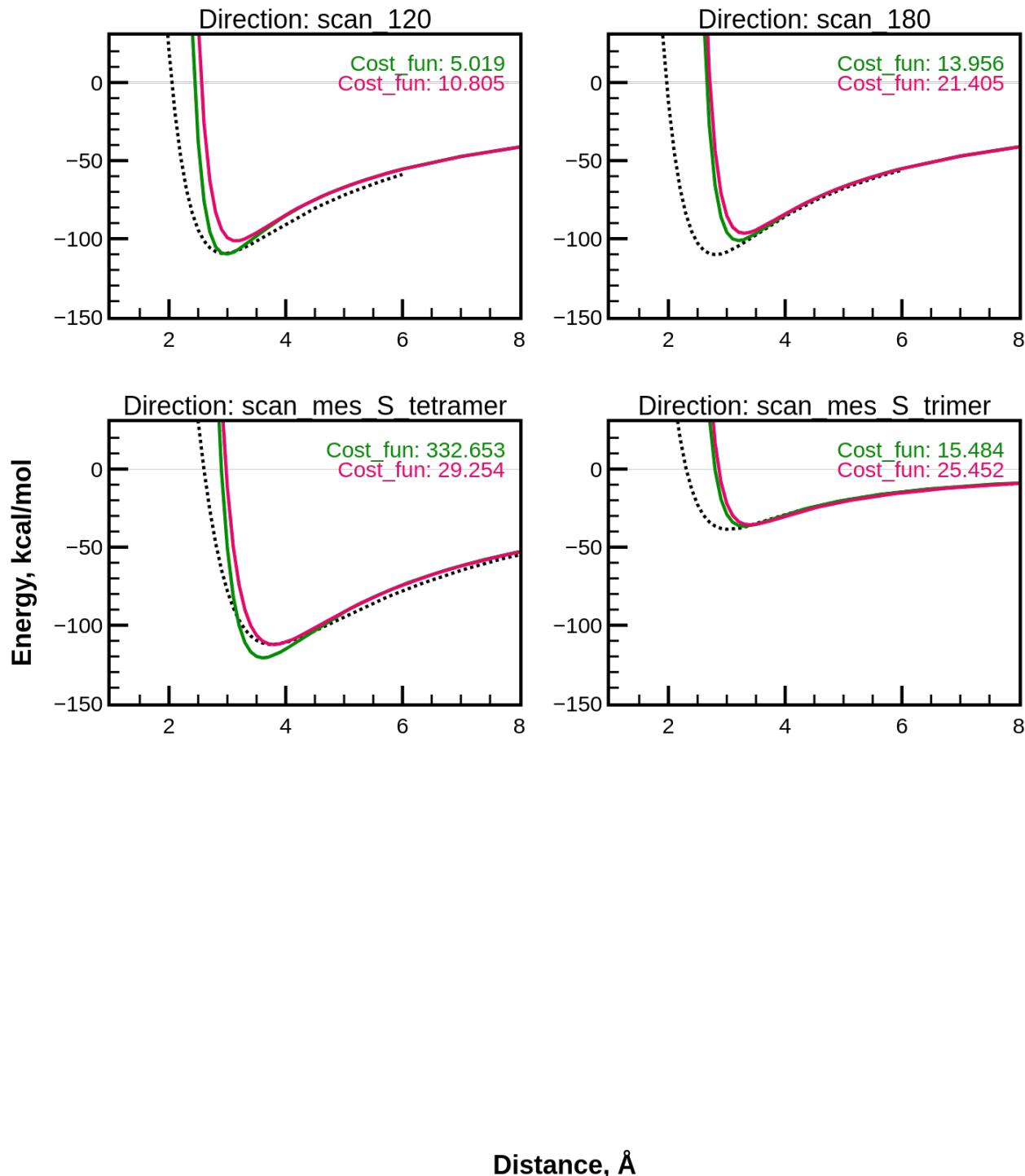
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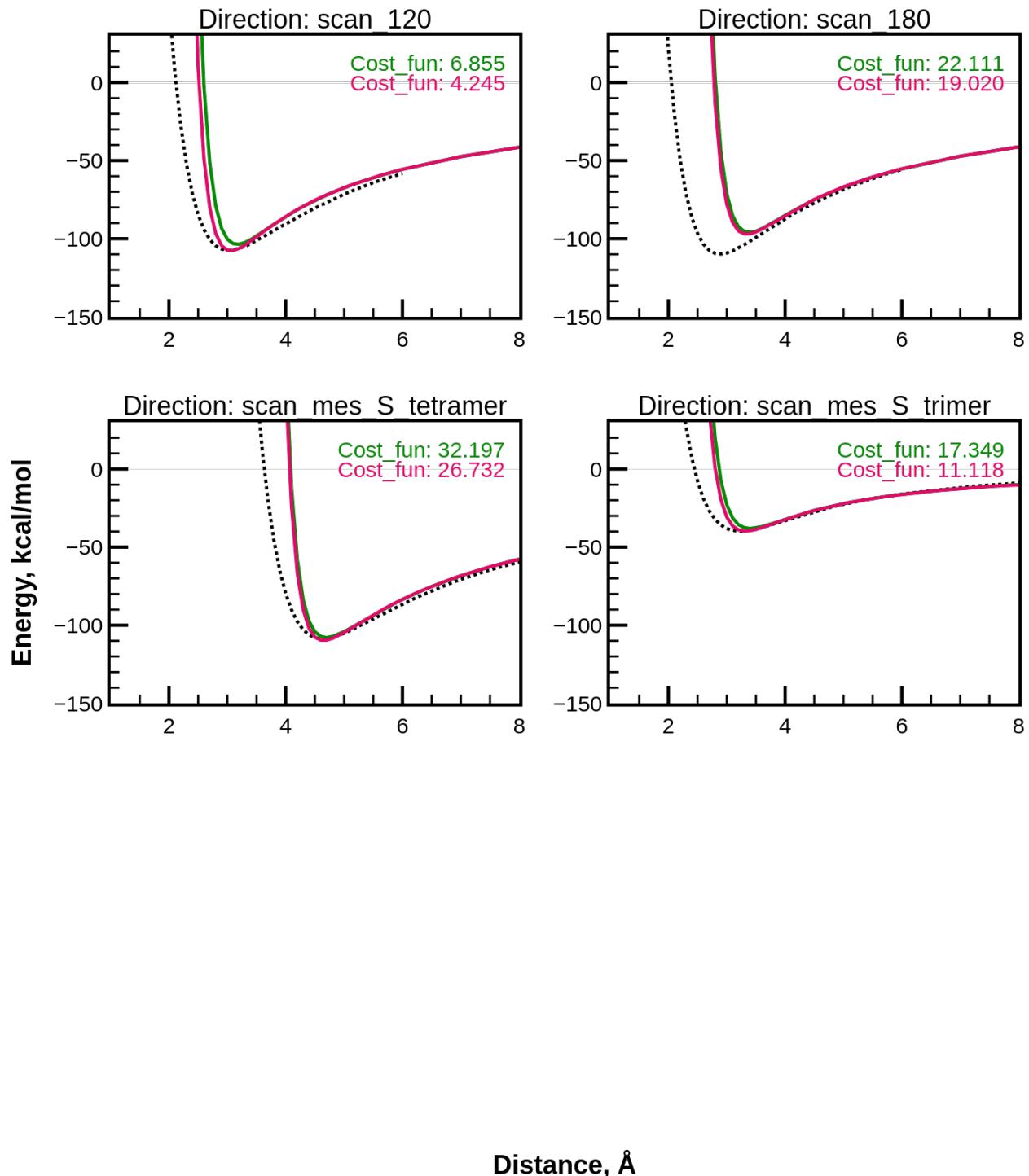
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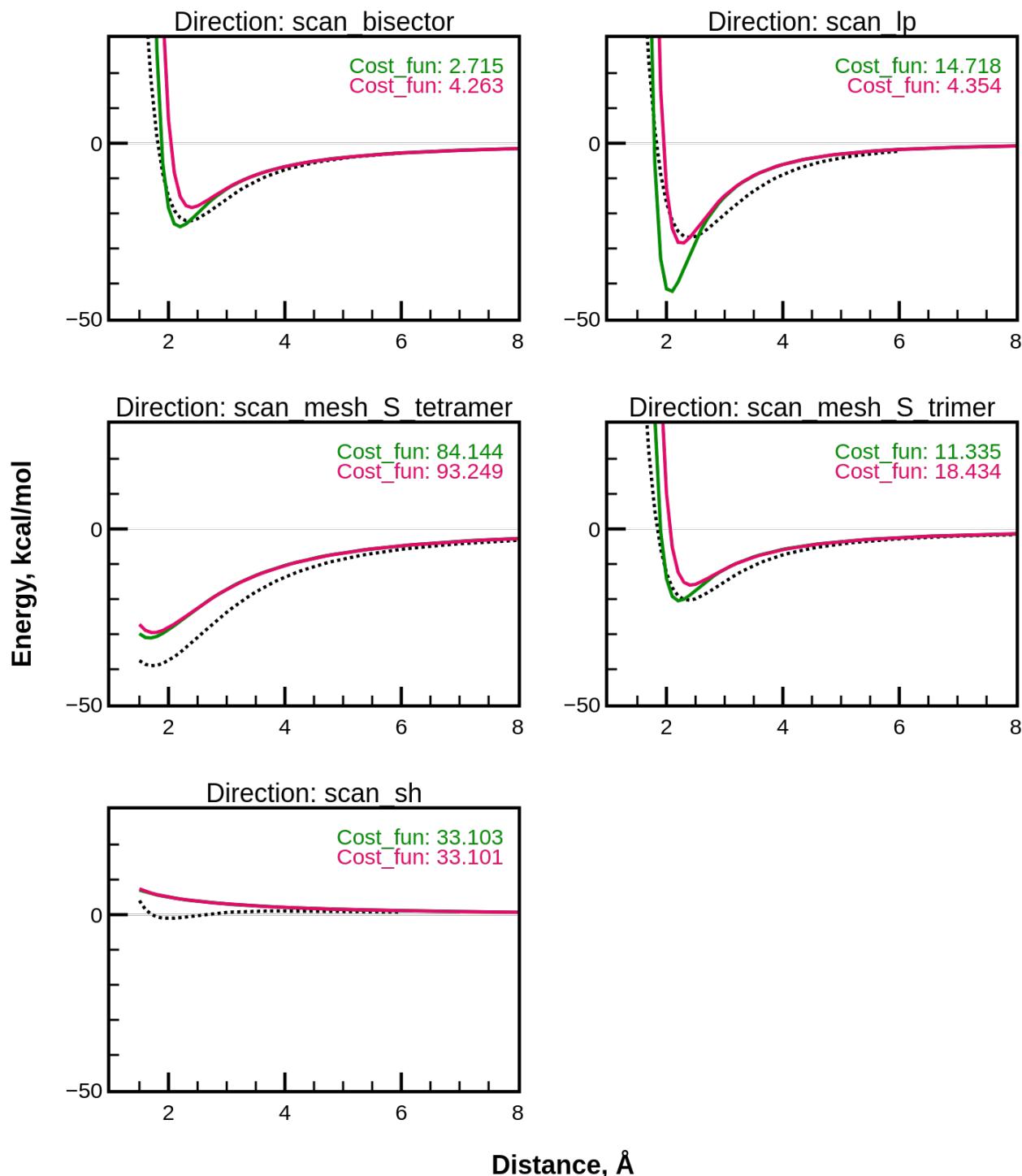
MES RUB 1/1



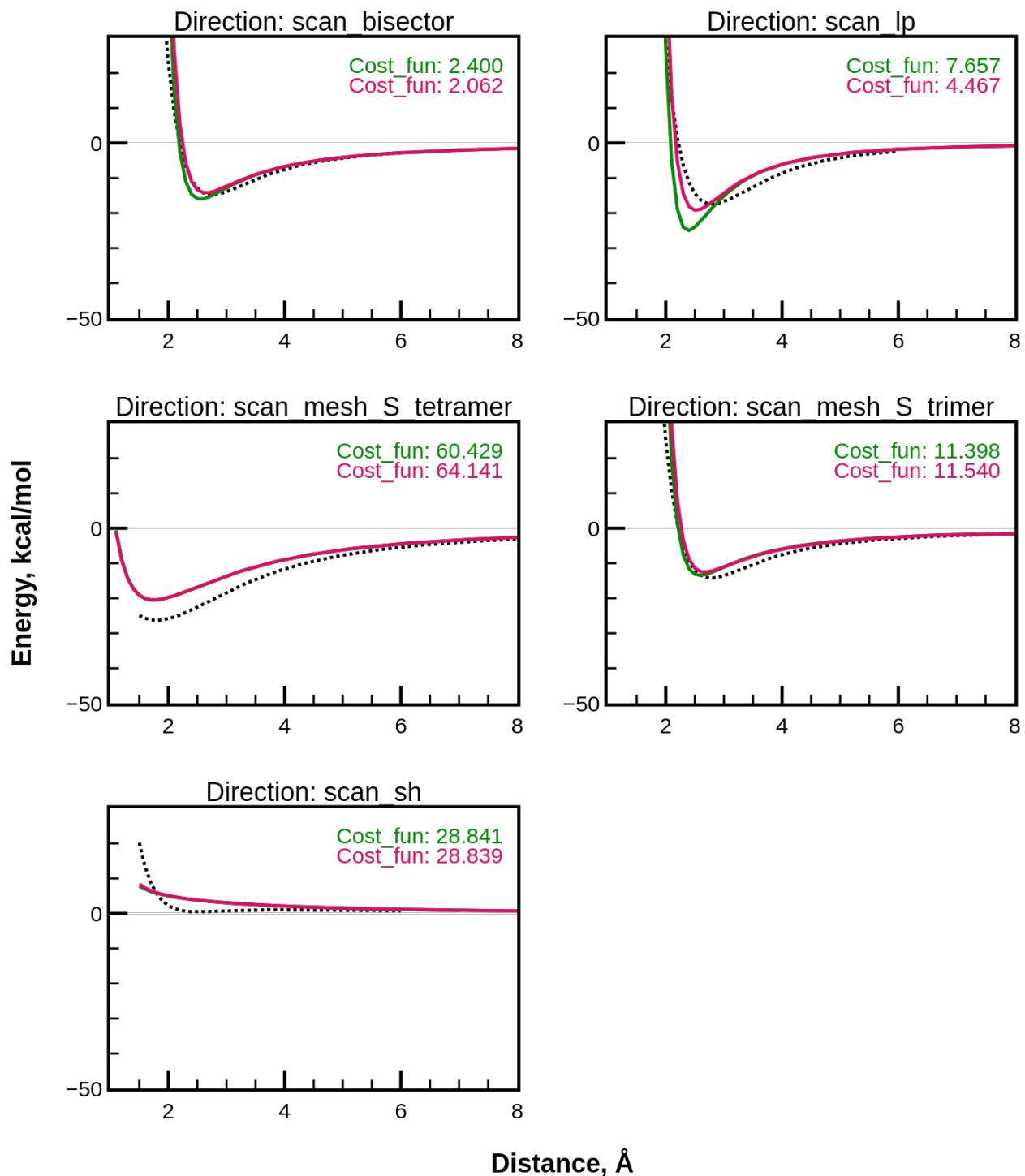
MES CES 1/1



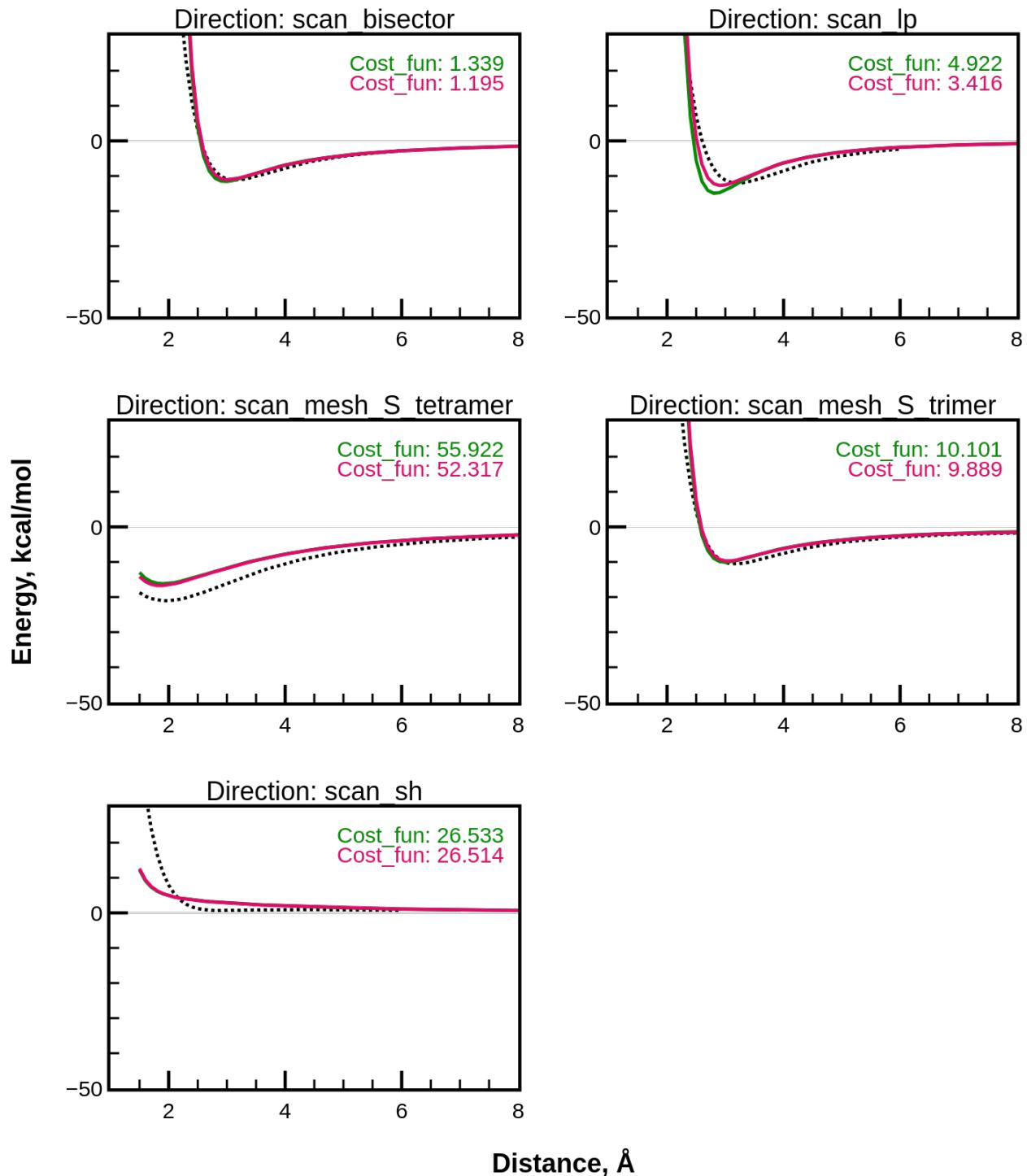
MESH LIT 1/1



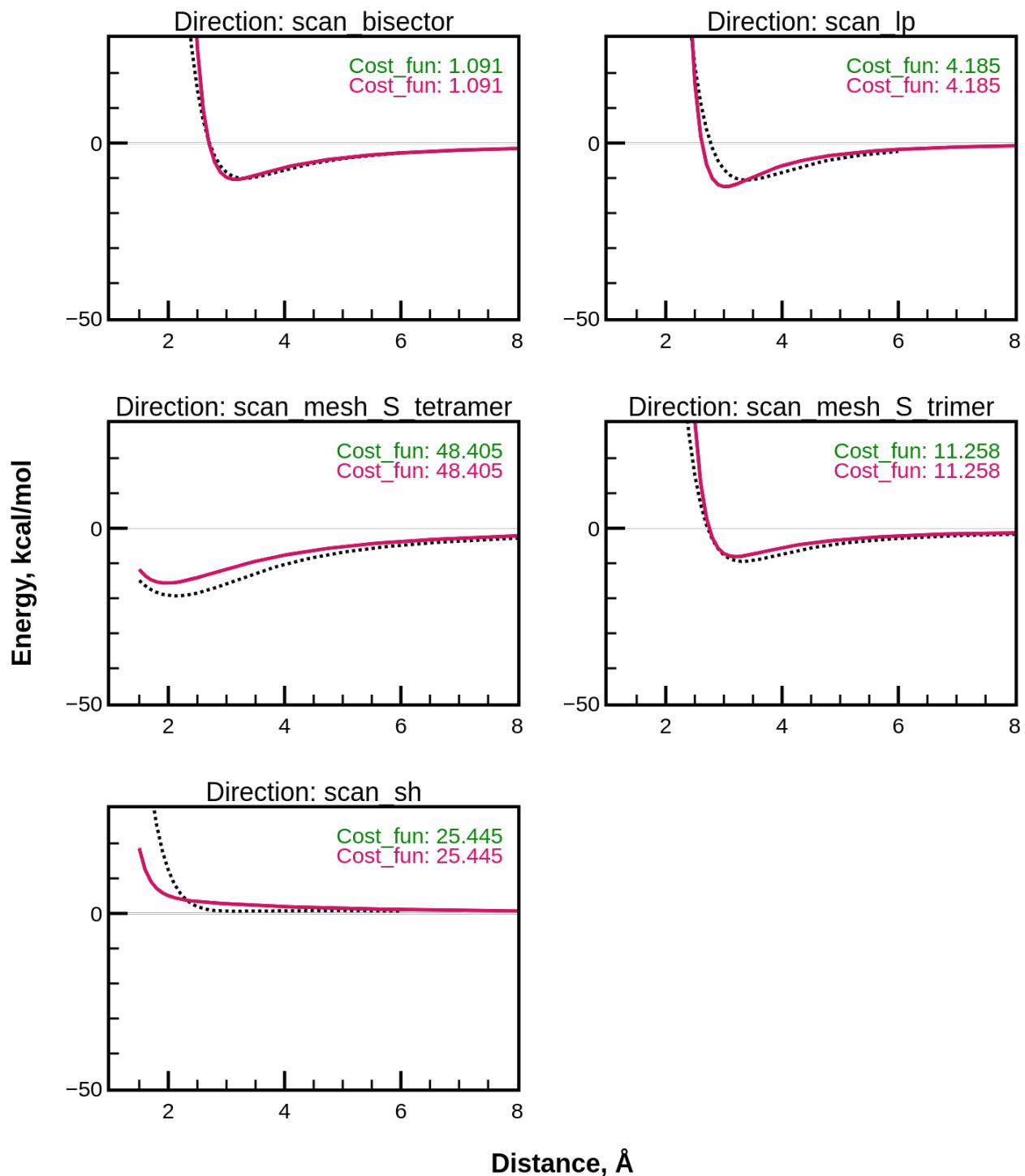
MESH SOD 1/1



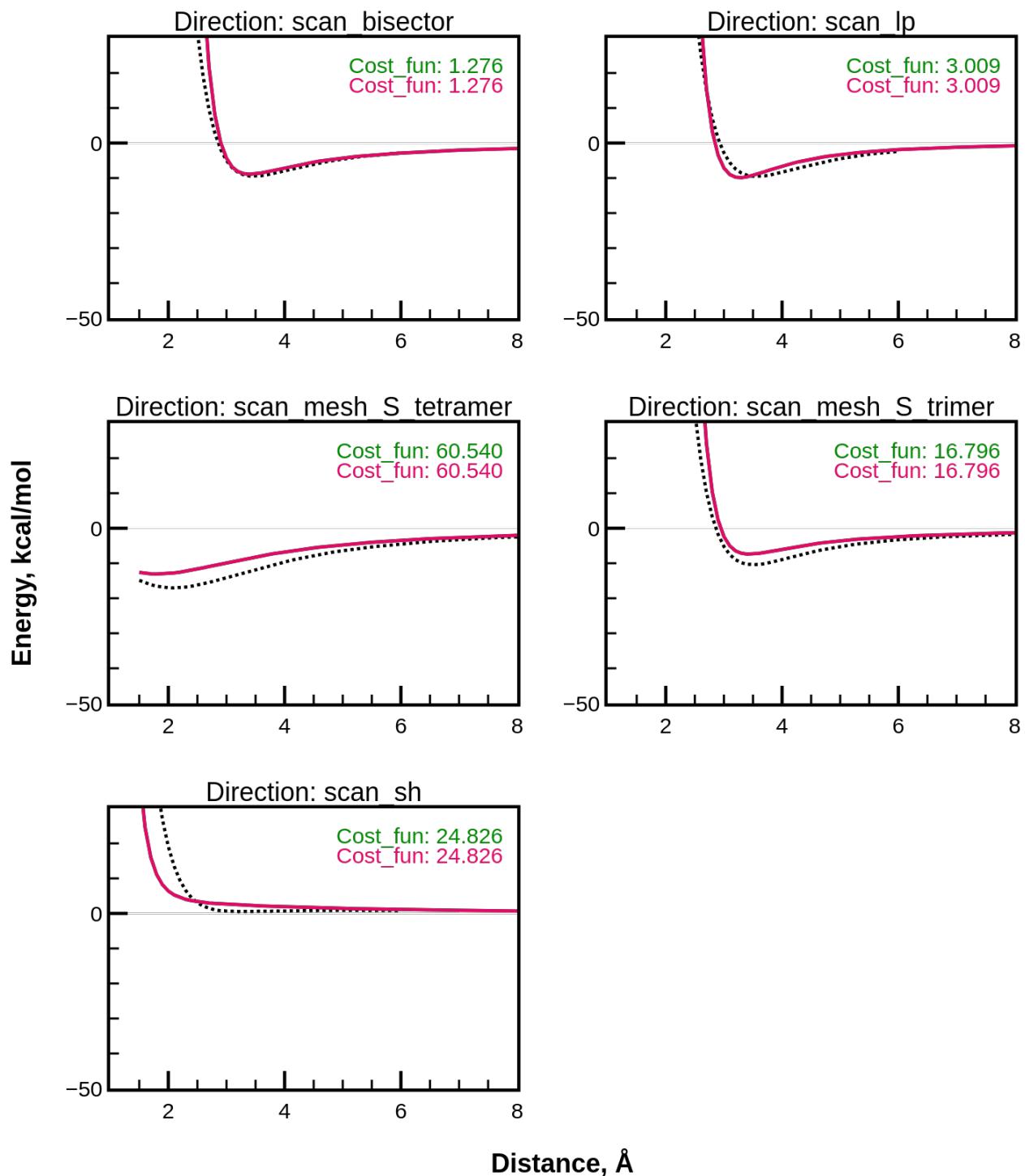
MESH POT 1/1



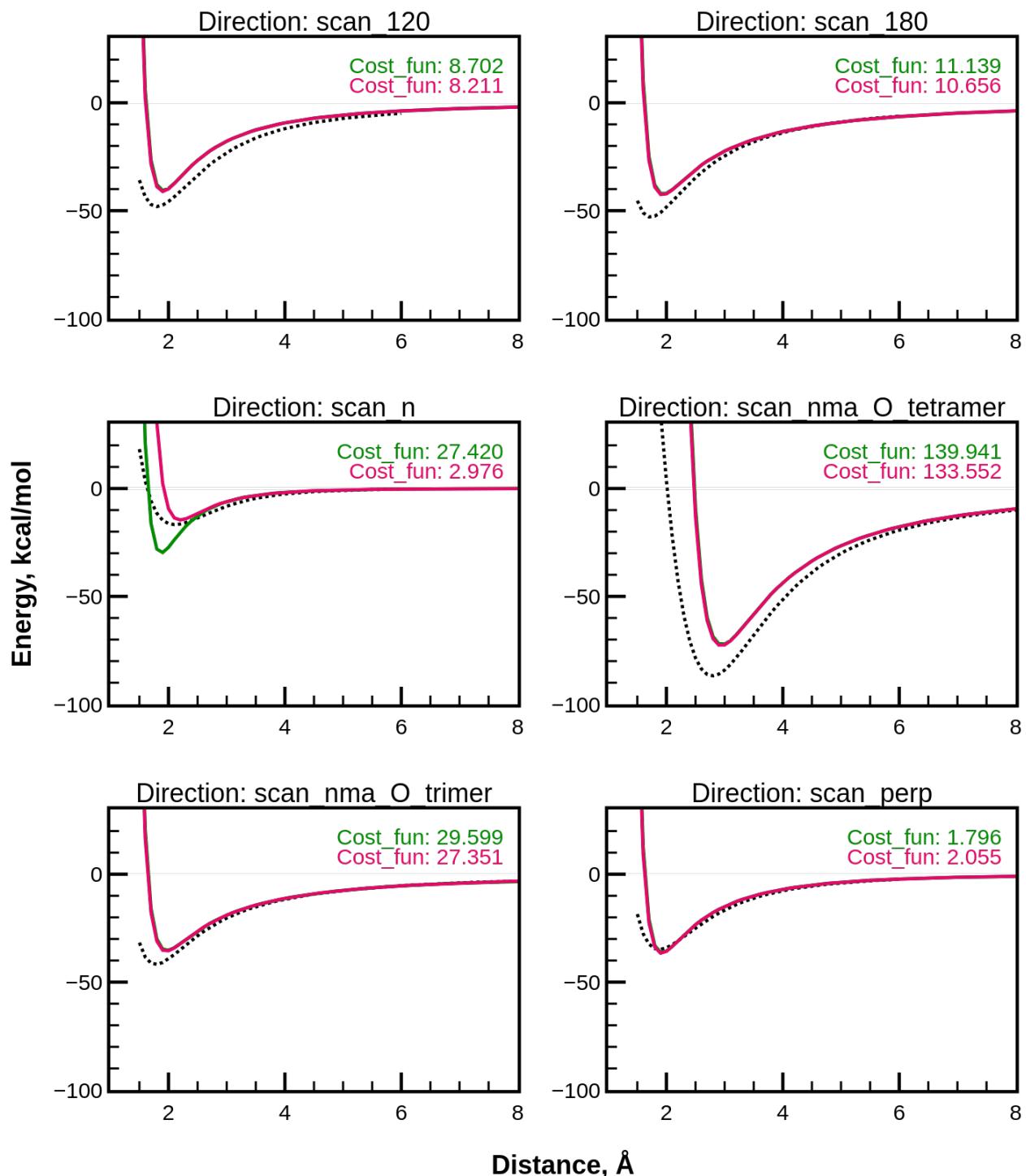
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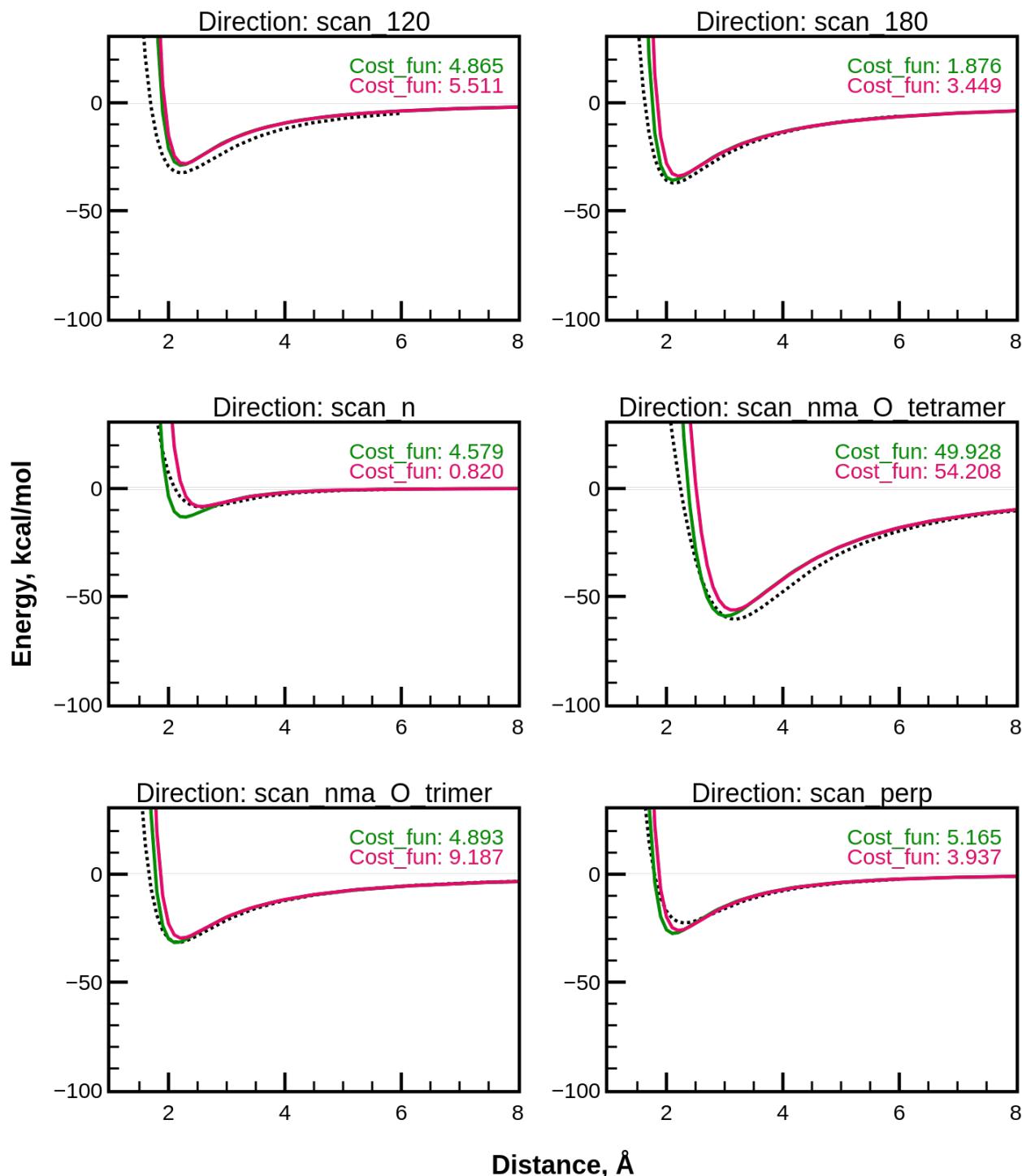
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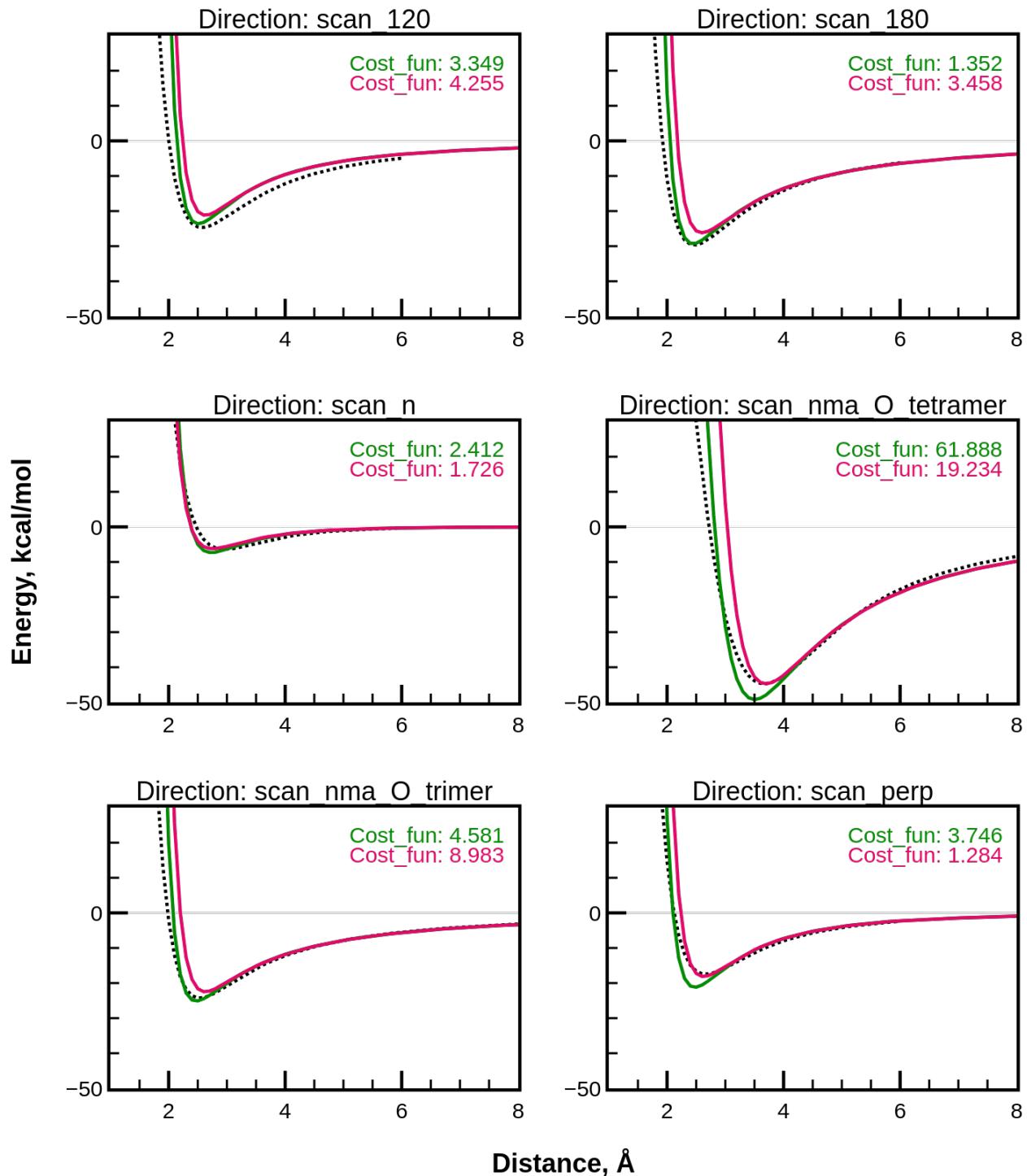
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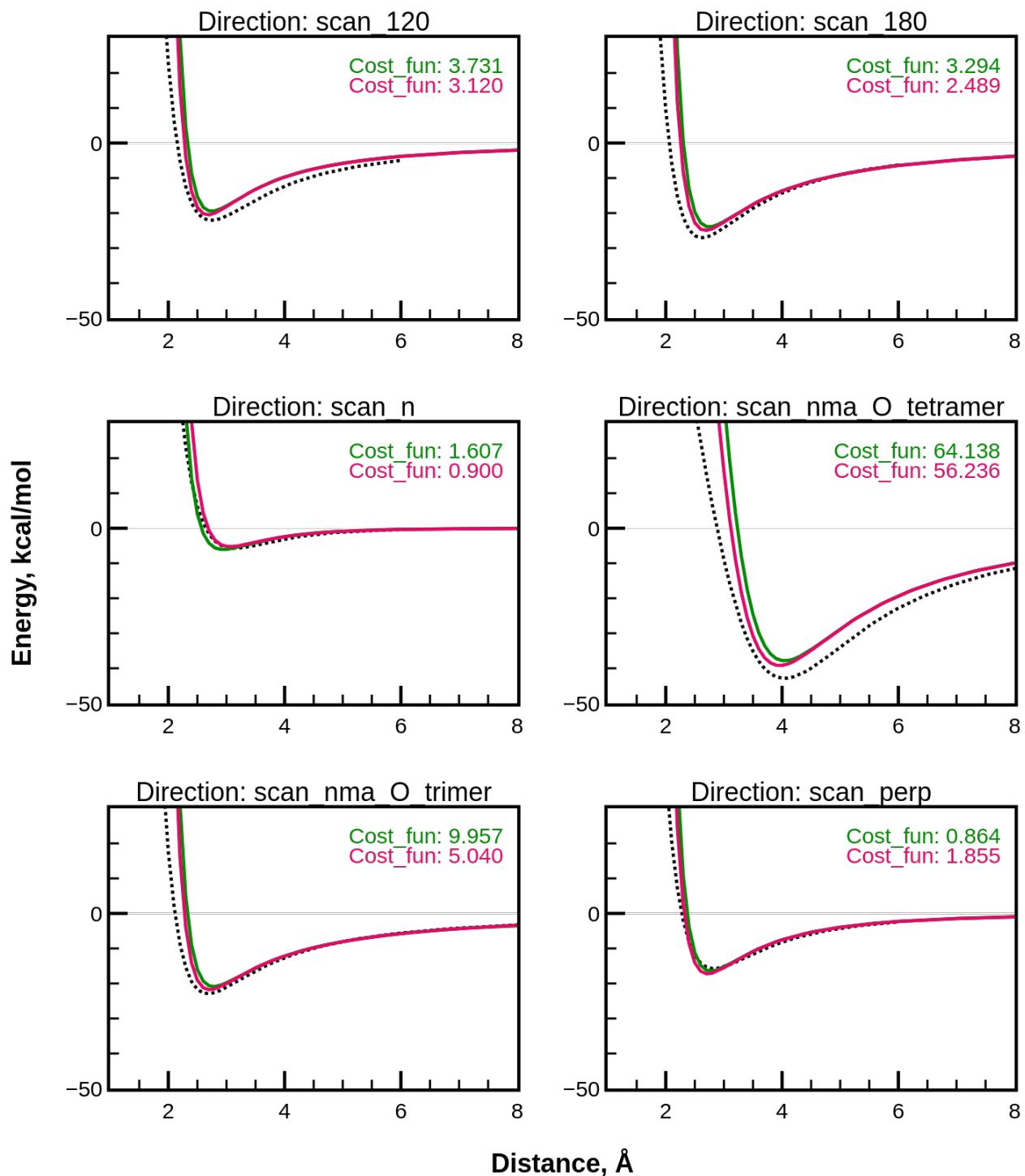
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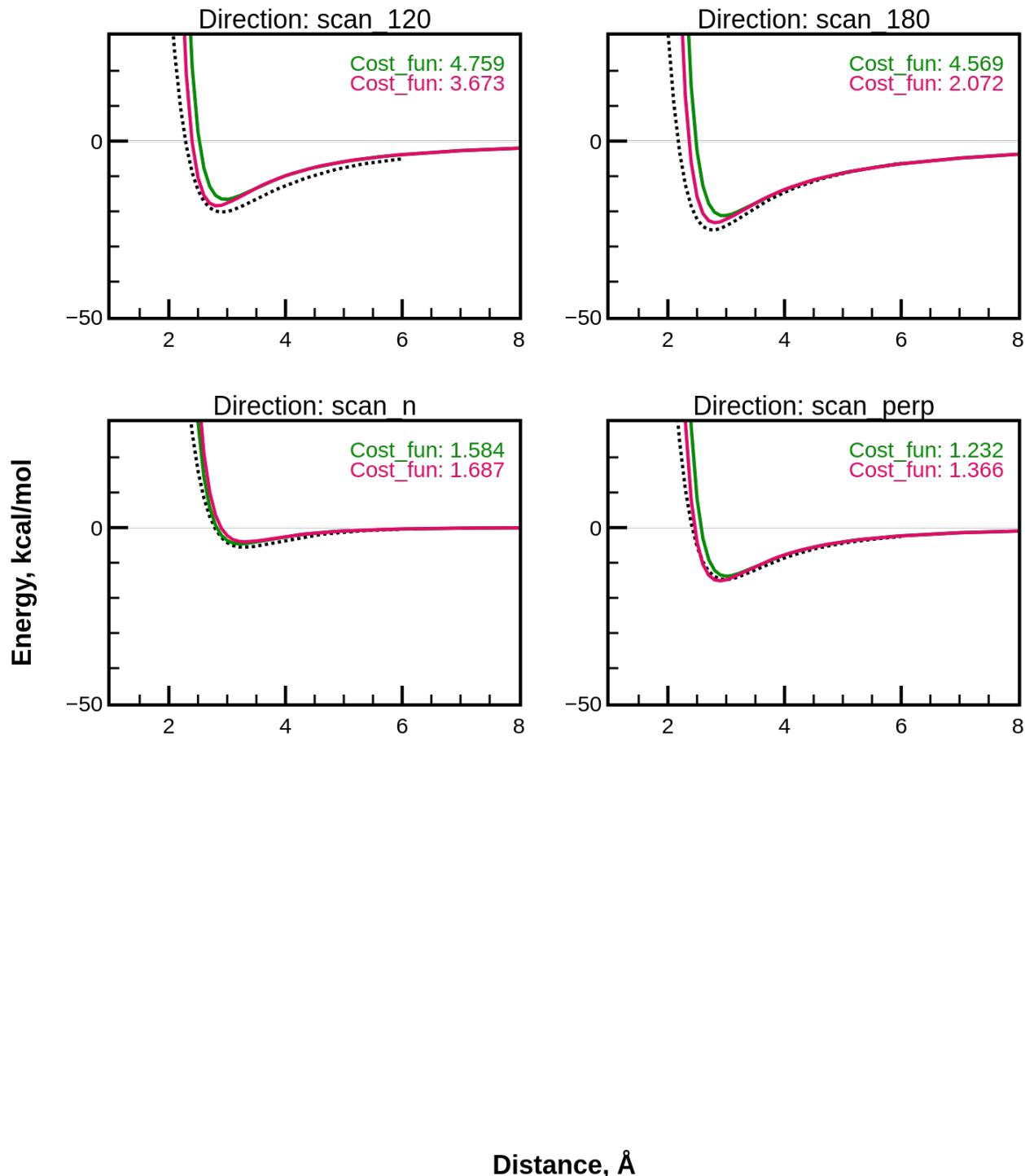
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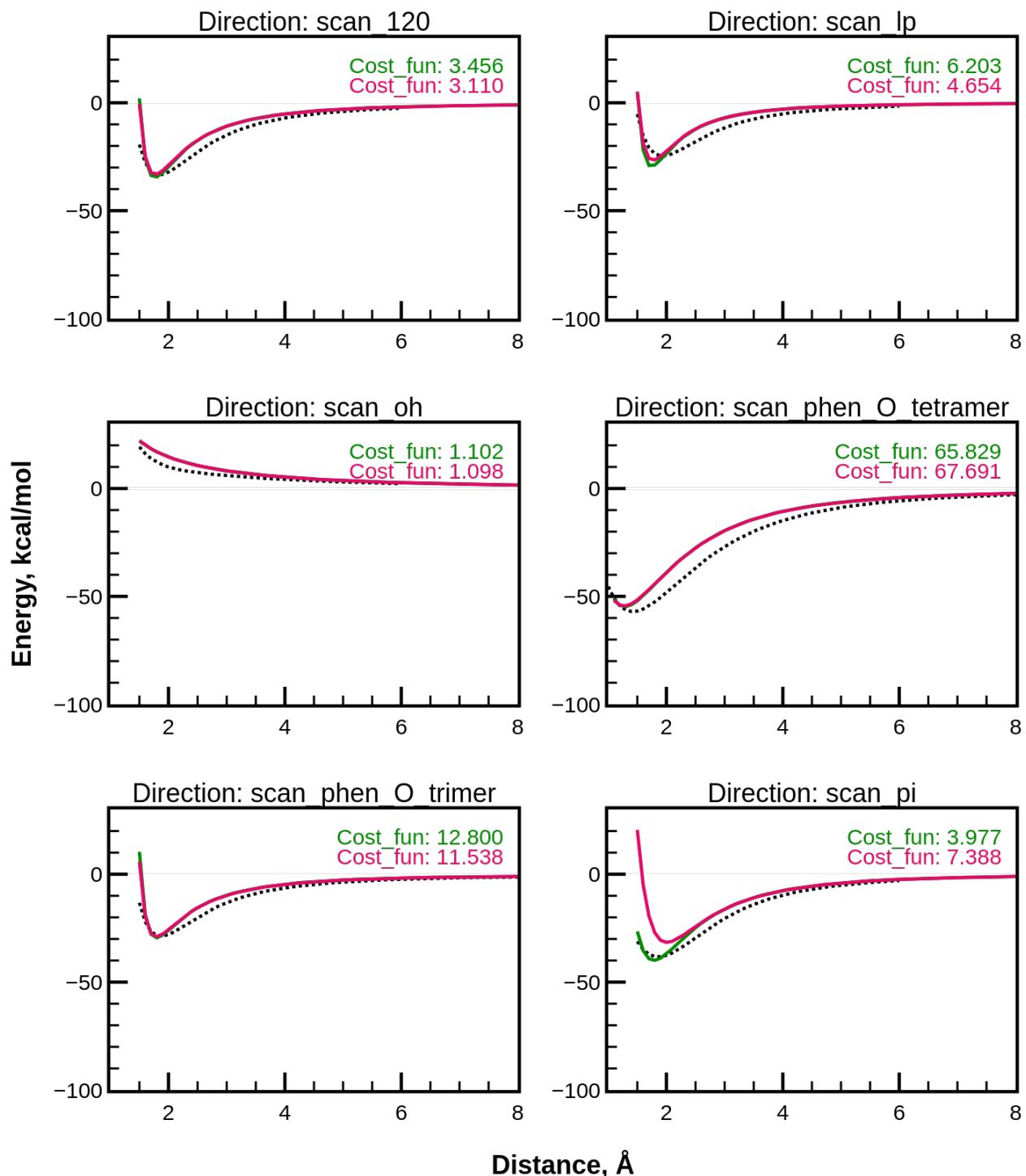
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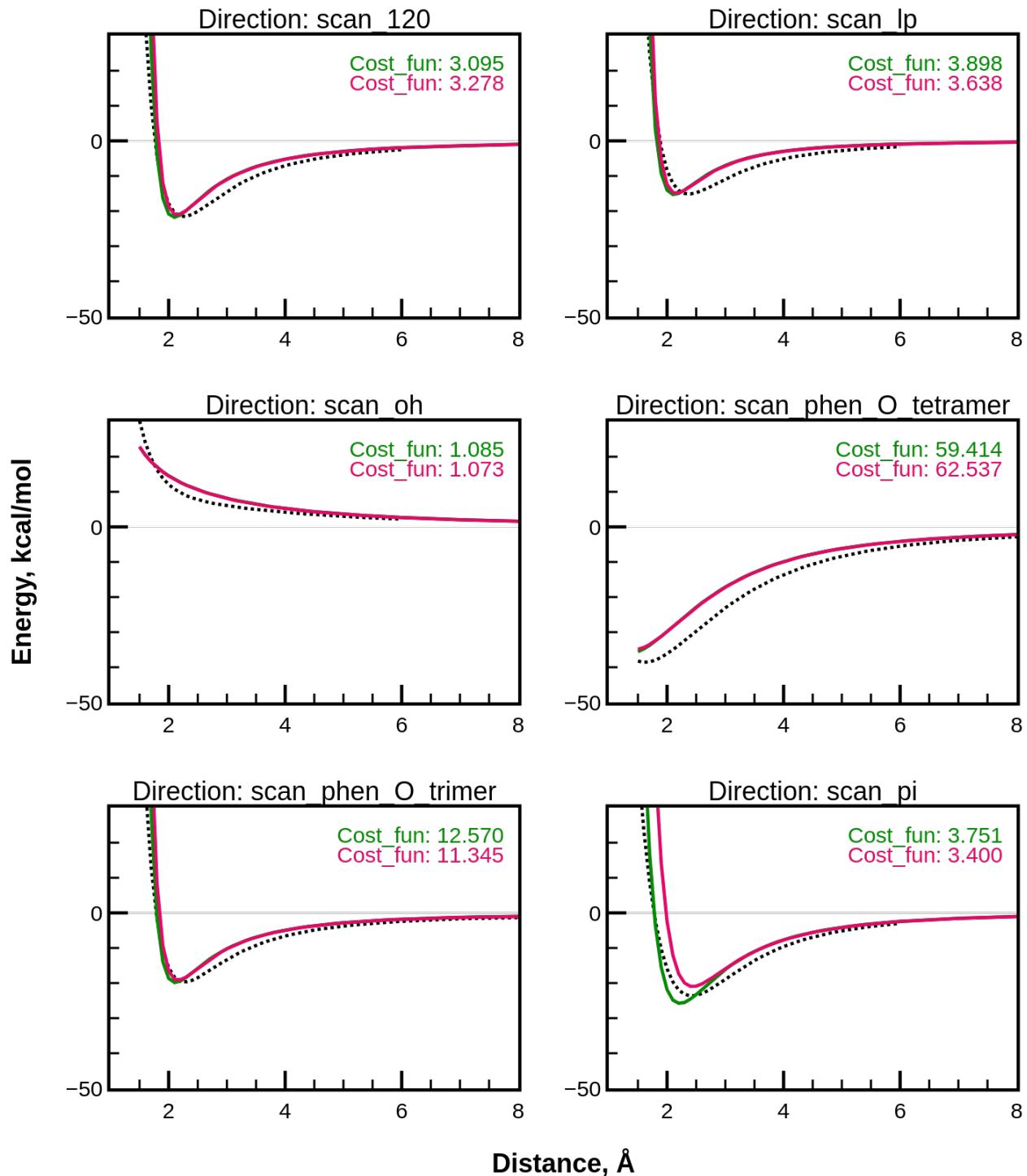
NMA CES 1/1



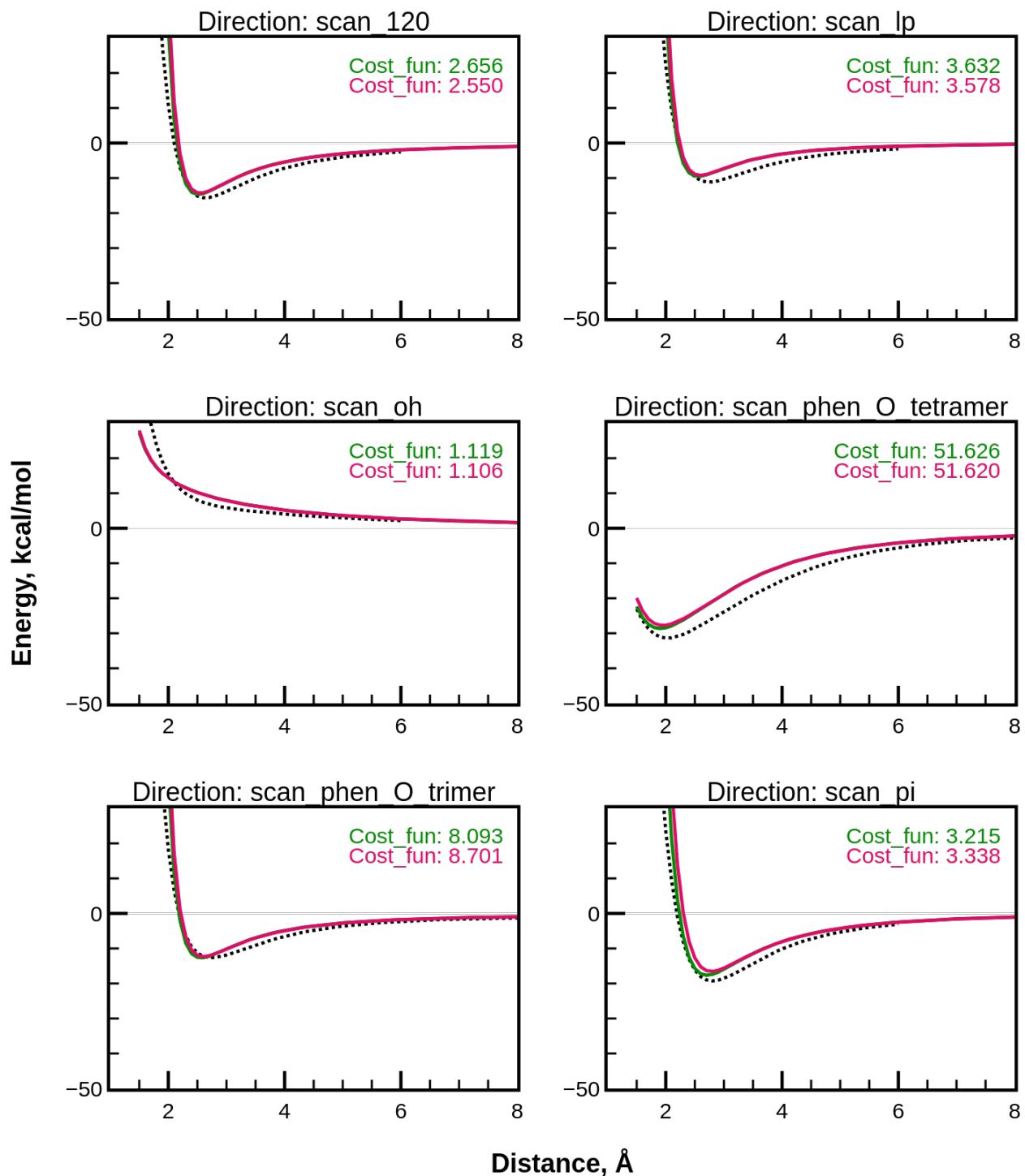
PHEN LIT 1/1



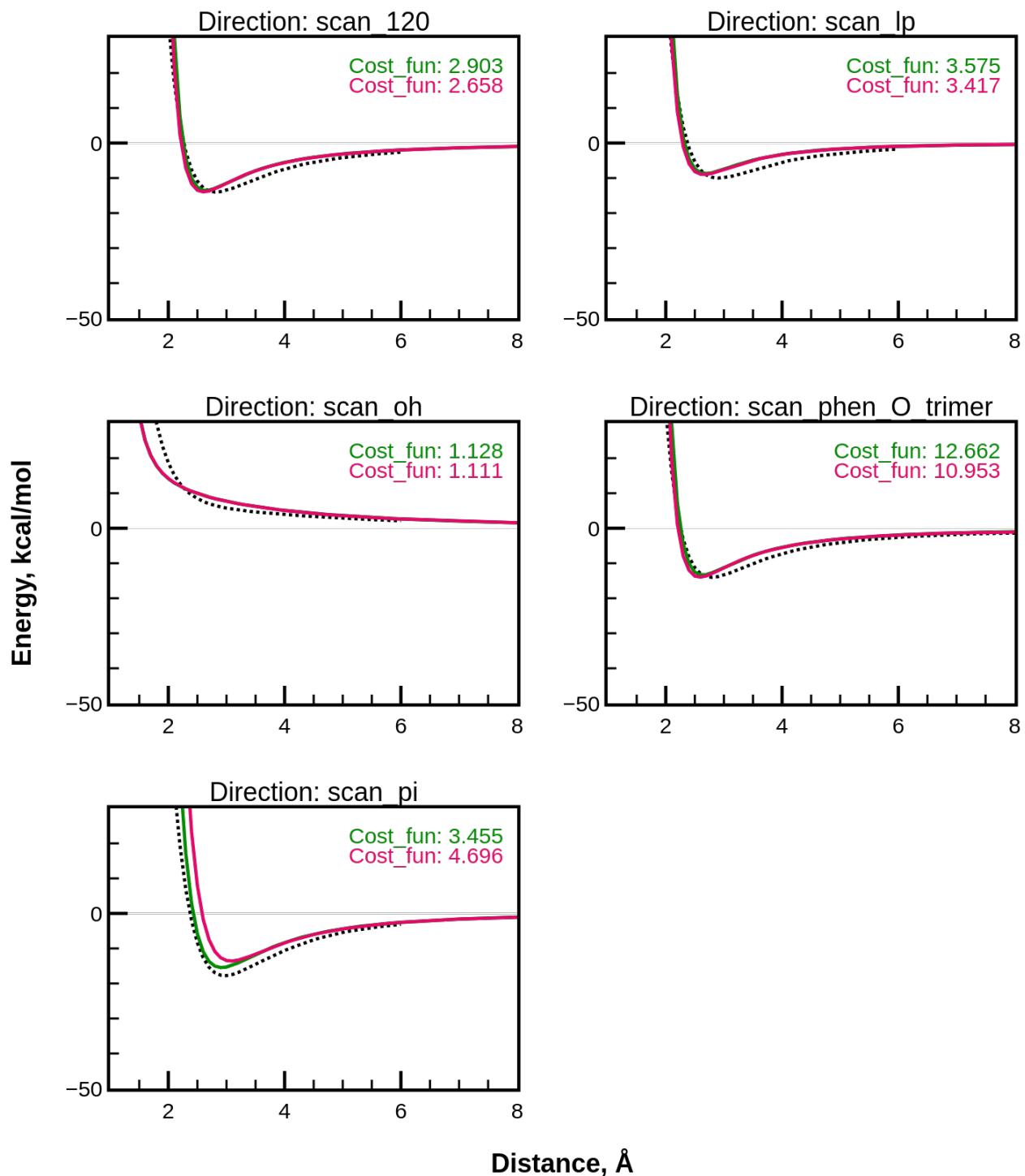
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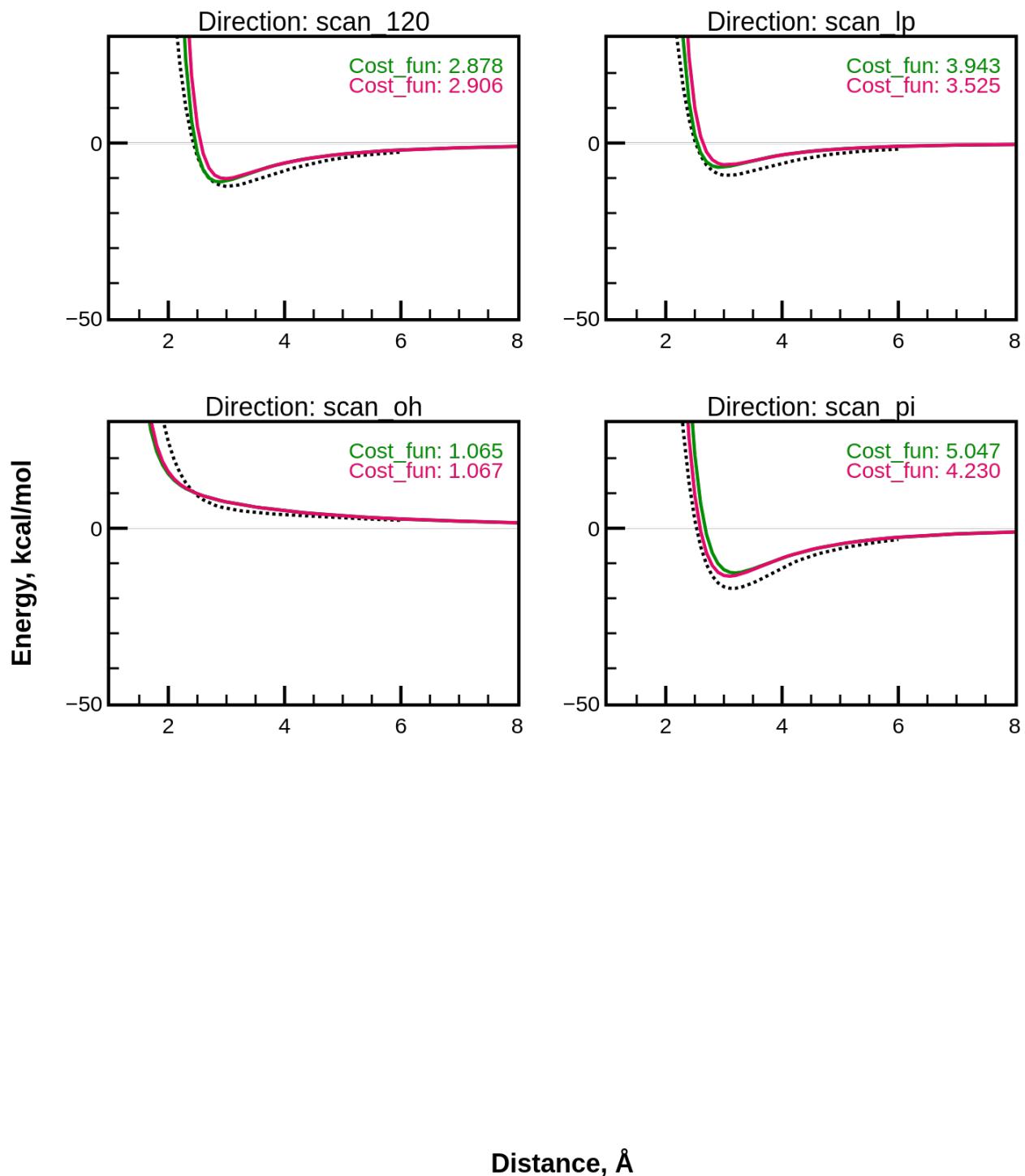
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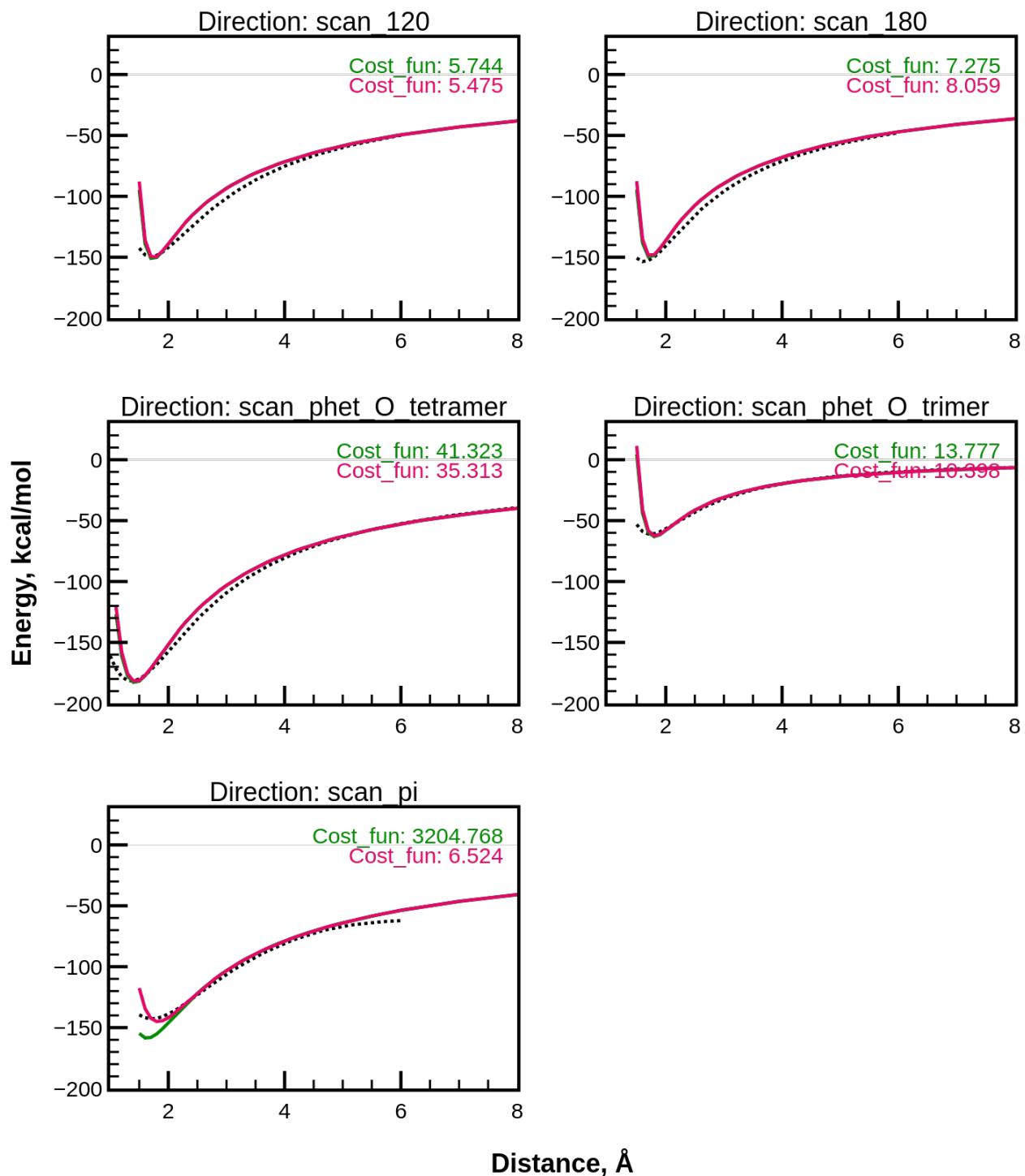
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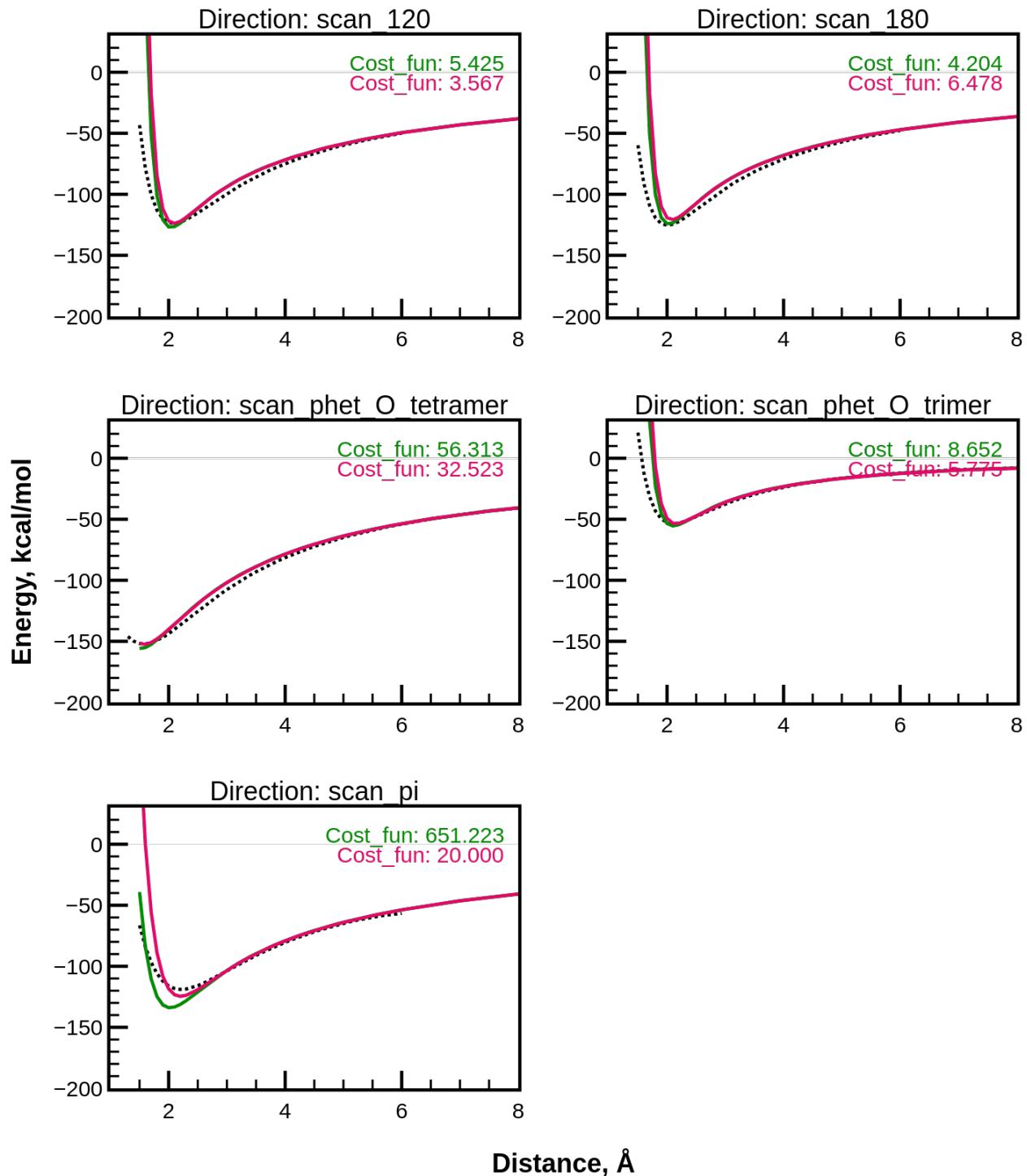
PHEN CES 1/1



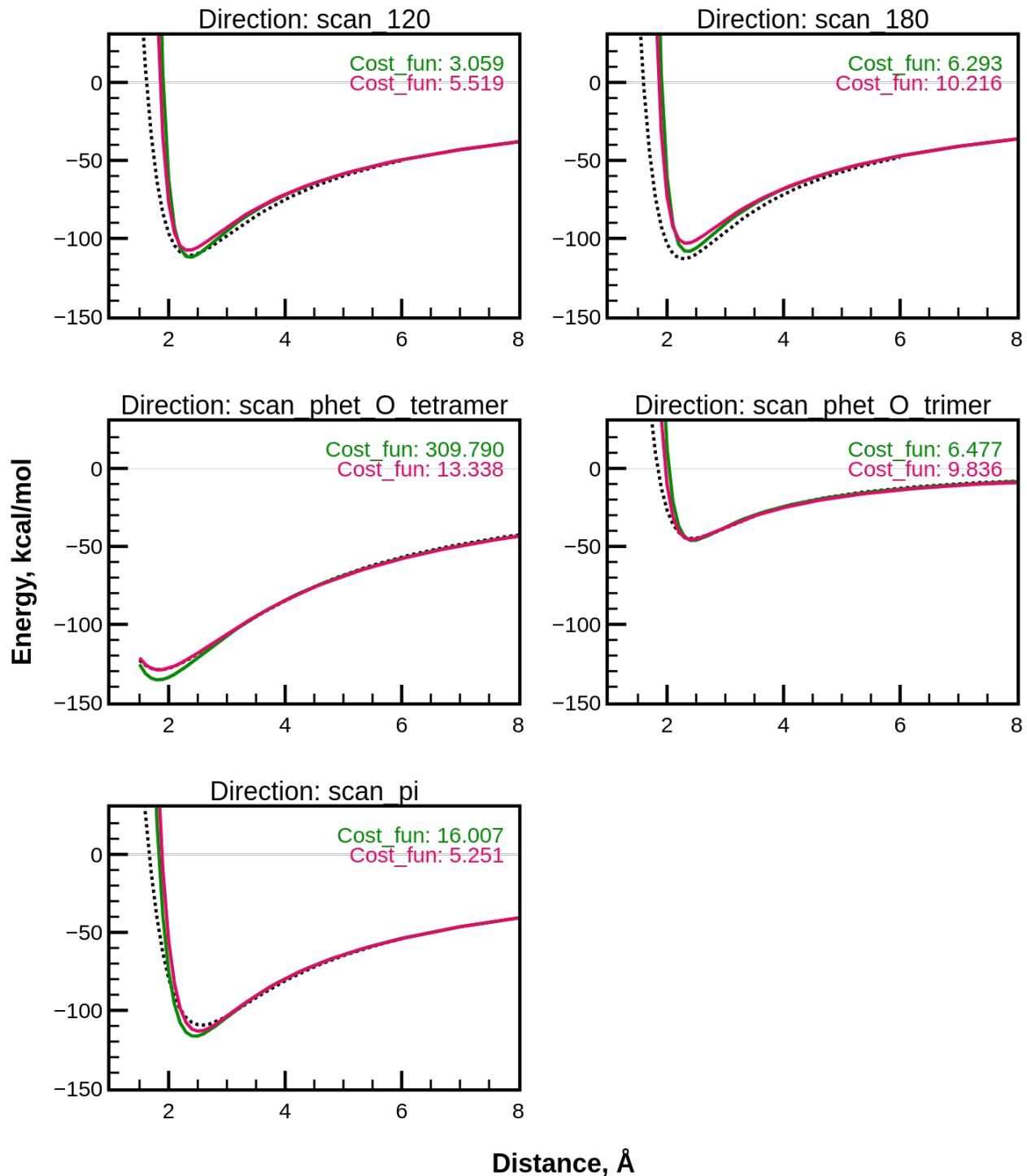
PHET LIT 1/1



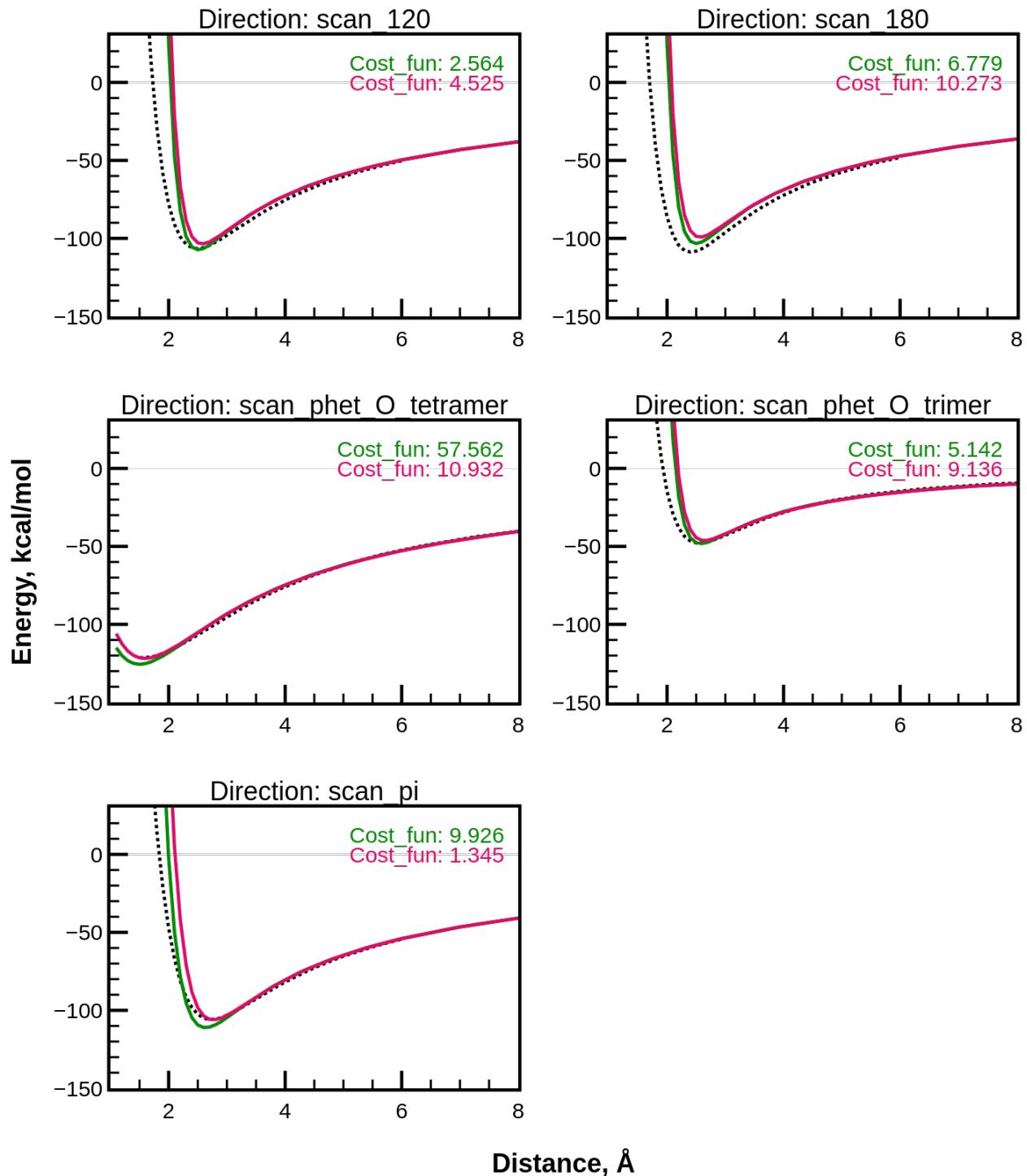
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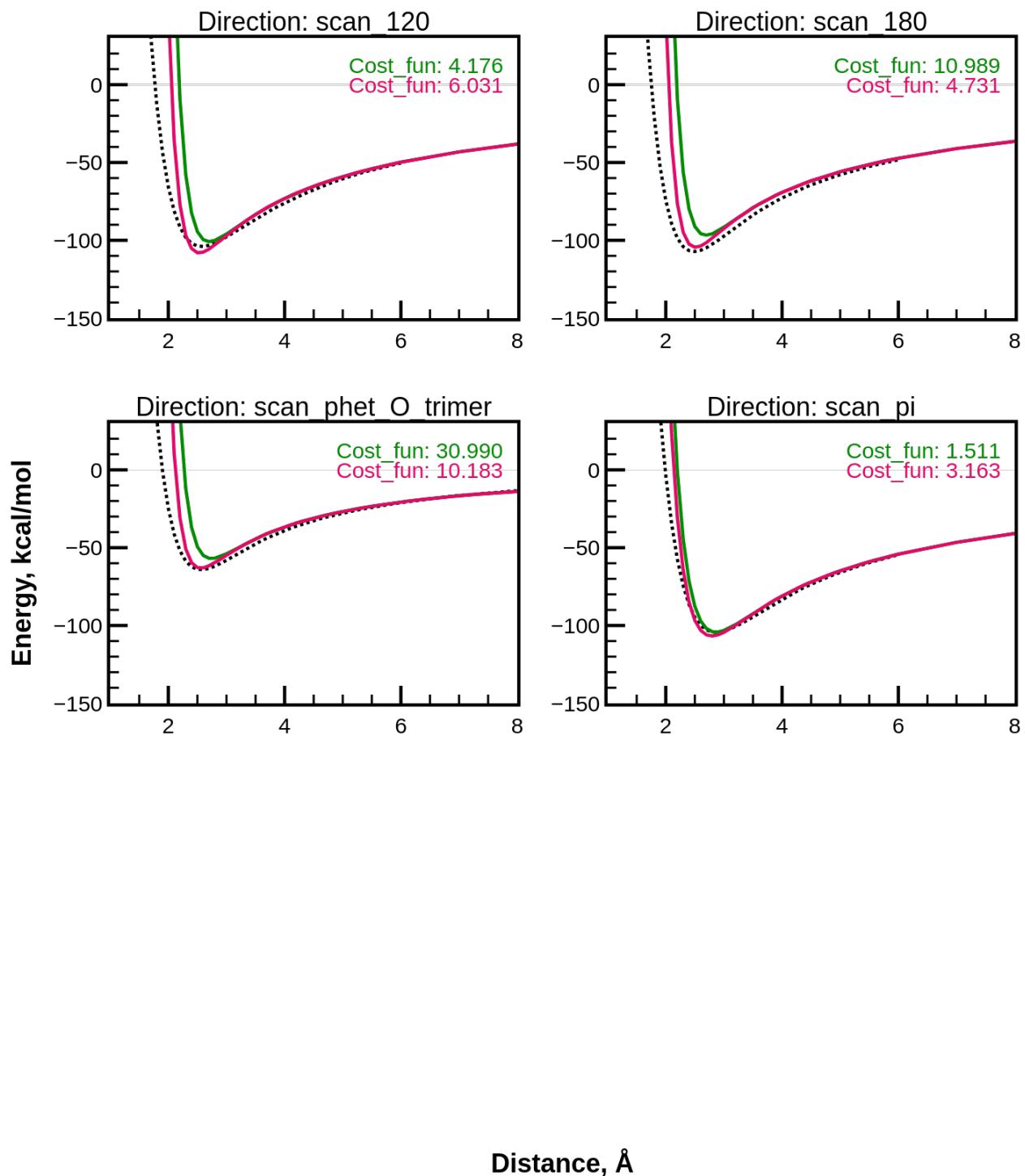
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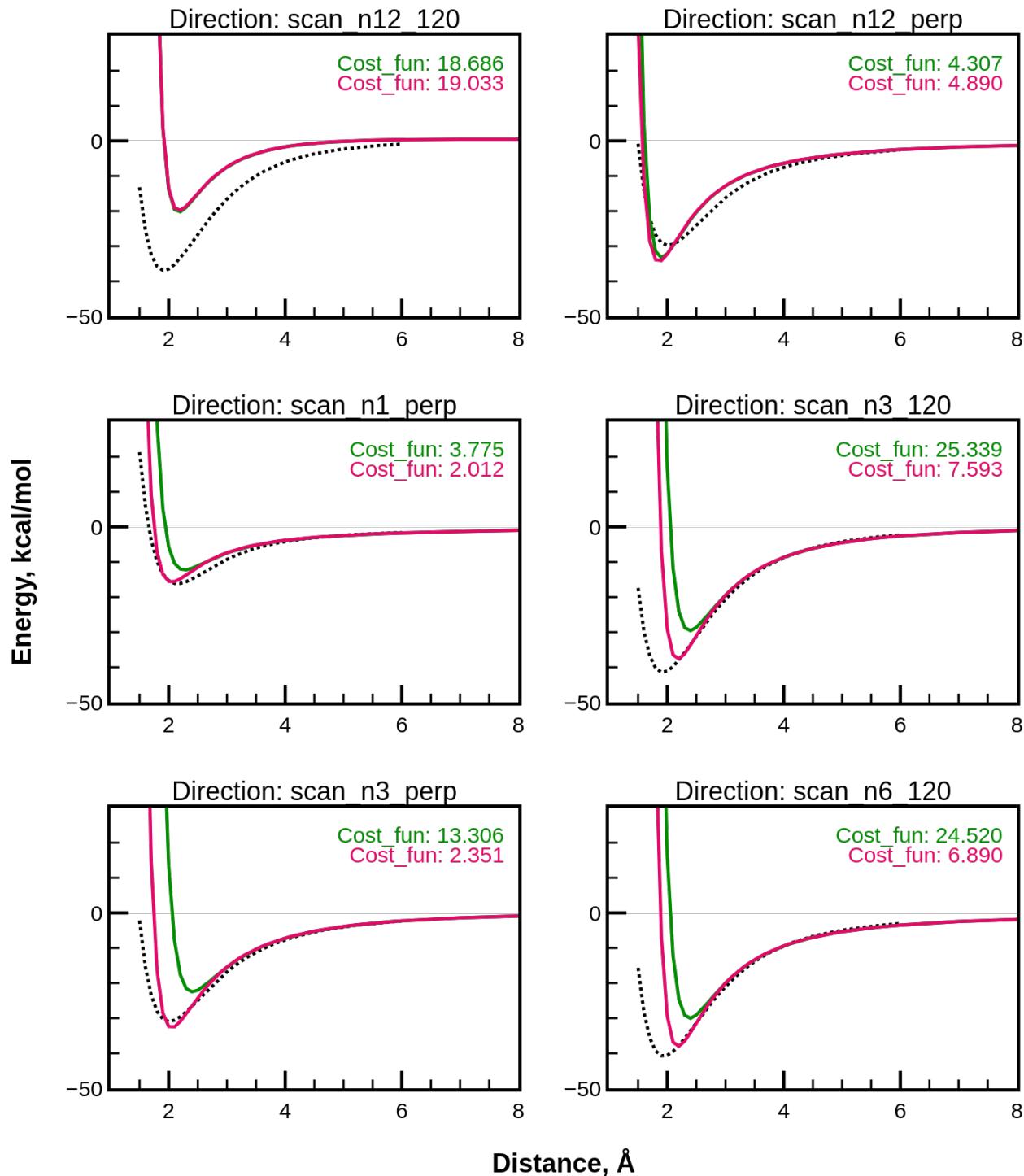
PHET RUB 1/1



PHET CES 1/1

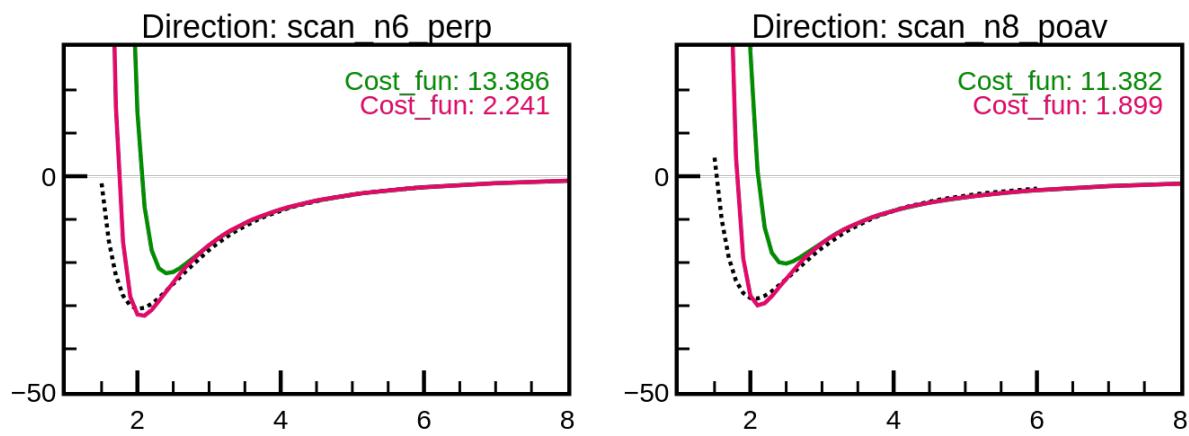


ADEB LIT 1/2

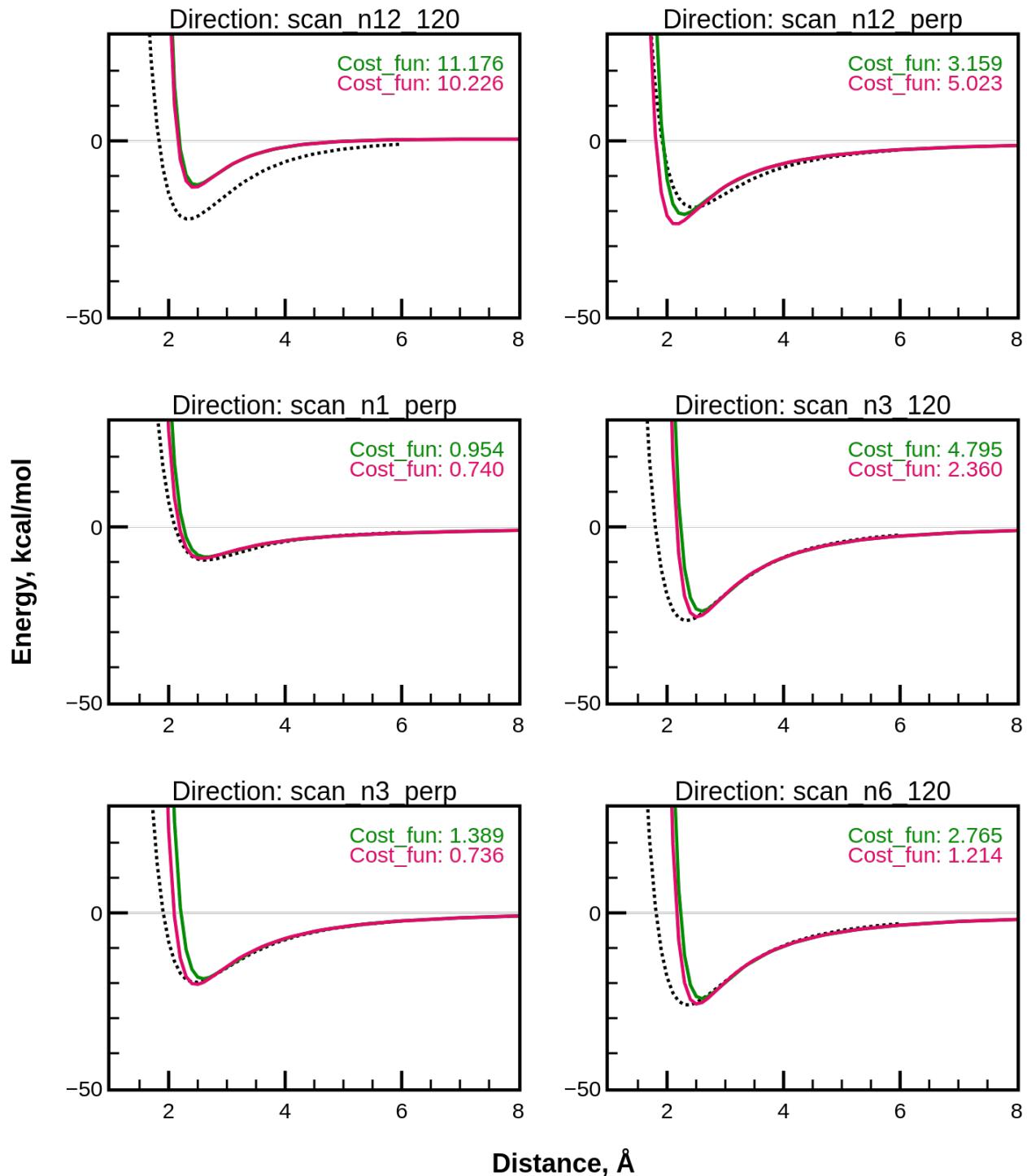


ADEB LIT 2/2

Energy, kcal/mol

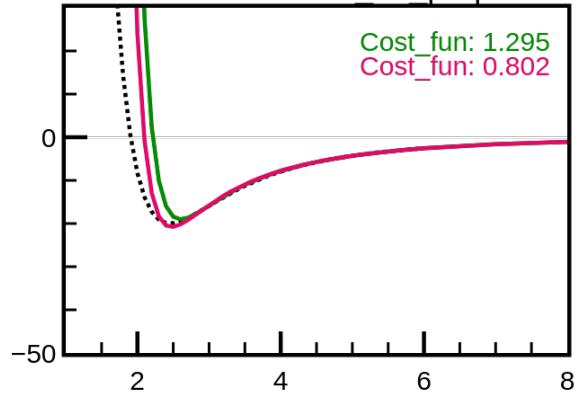


ADEB SOD 1/2

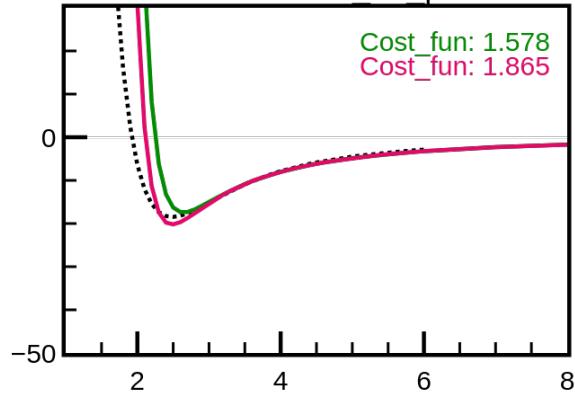


ADEB SOD 2/2

Direction: scan_n6_perp



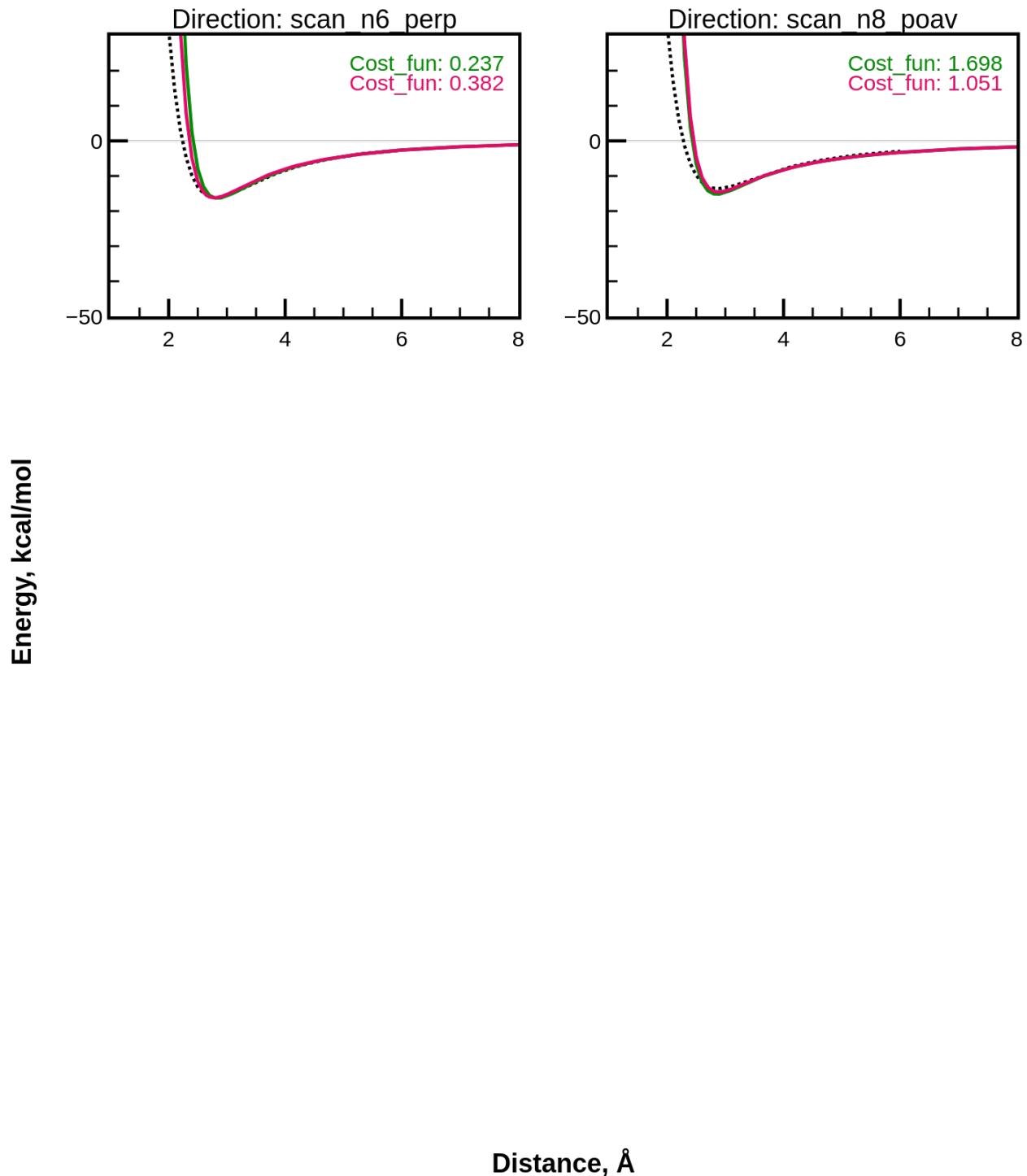
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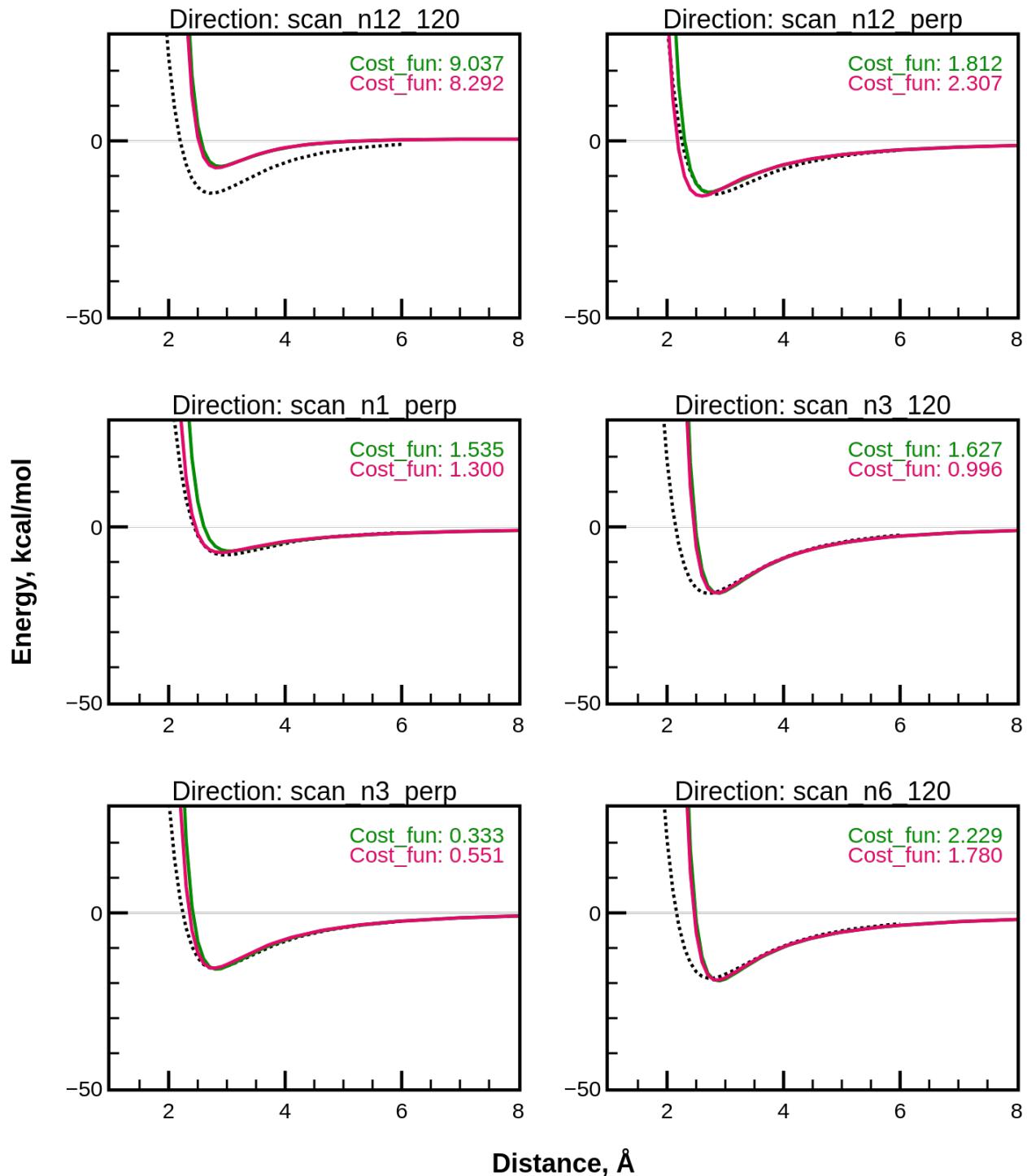
Energy, kcal/mol

Distance, Å

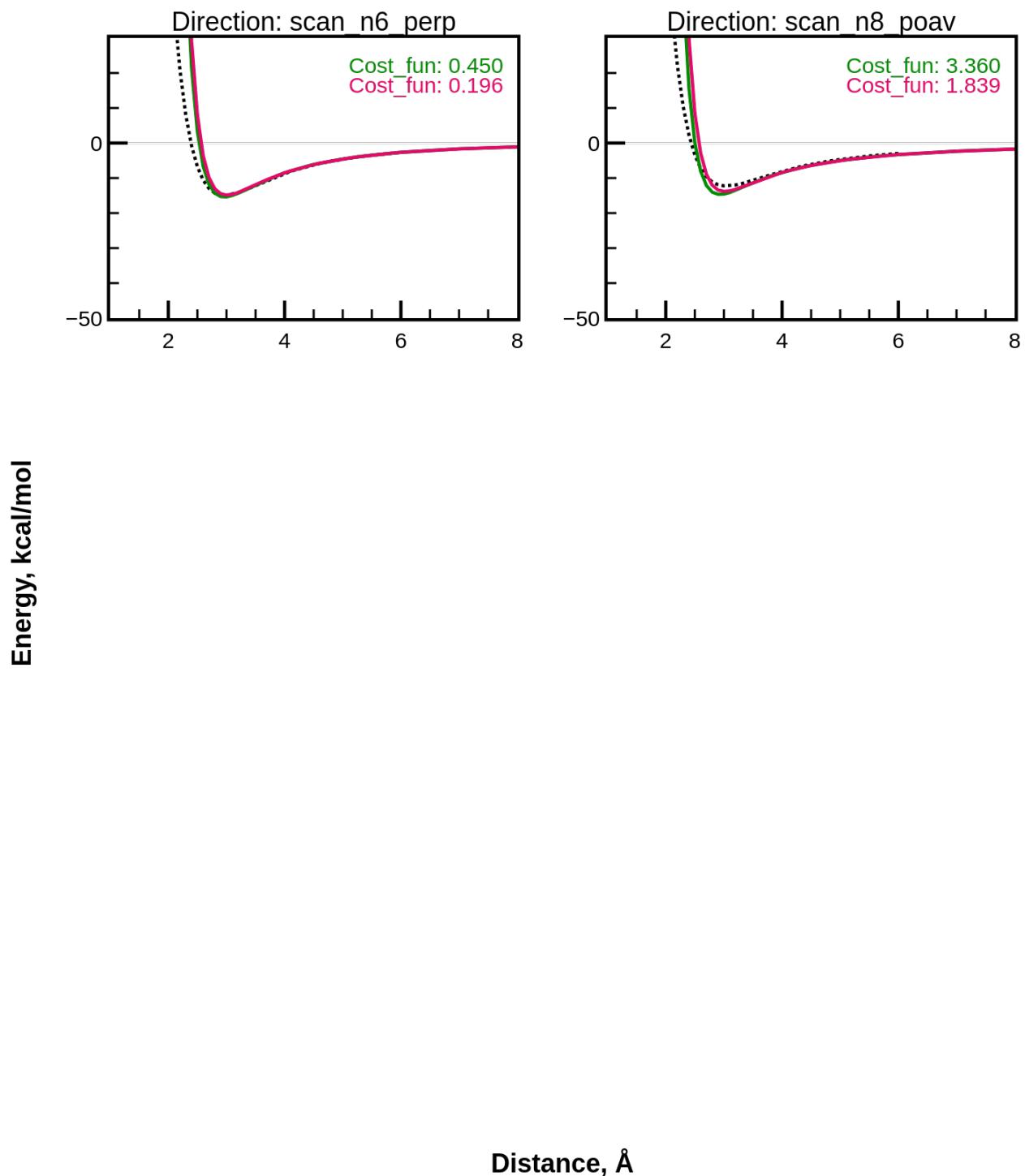
ADEB POT 2/2



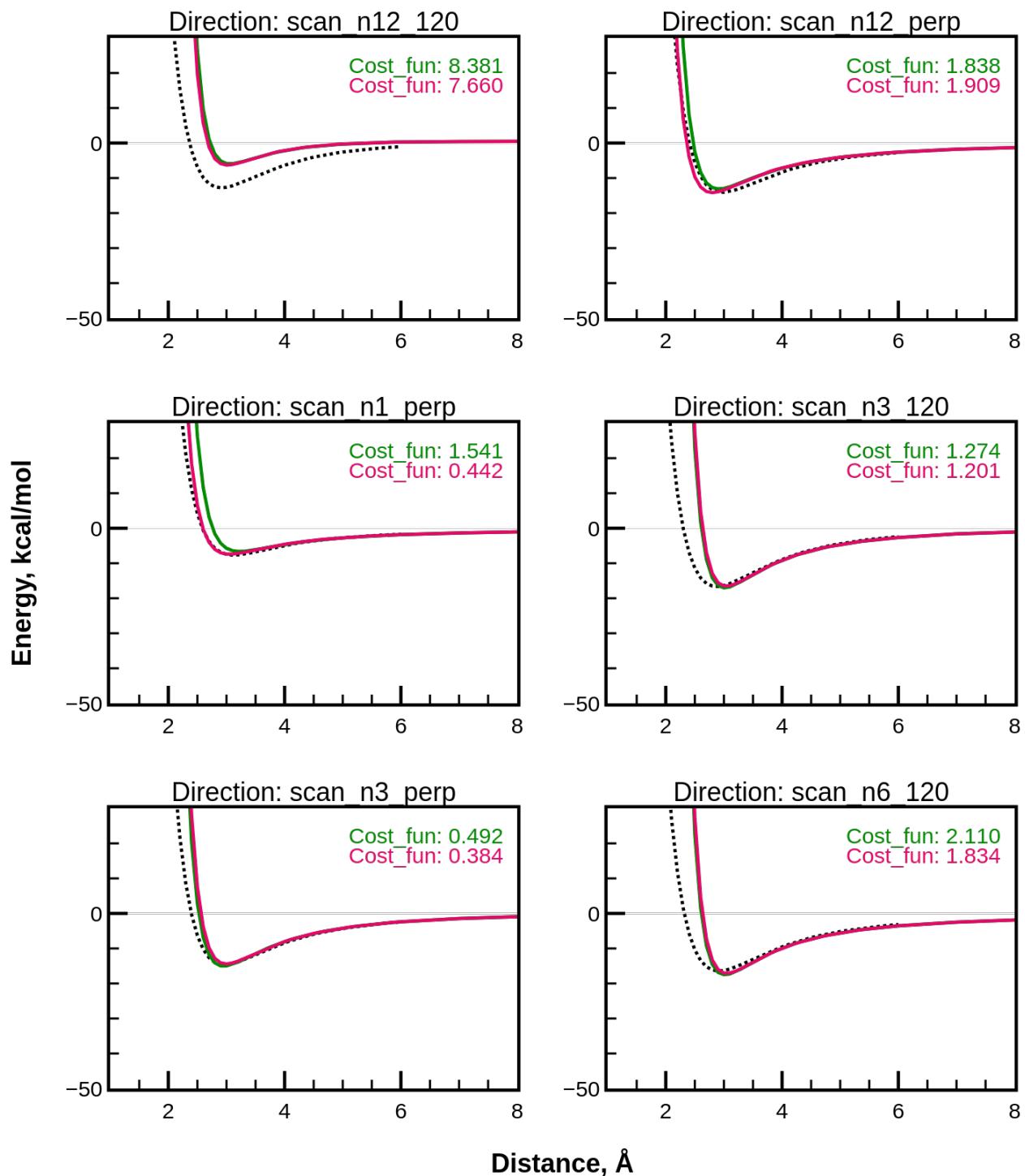
ADEB POT 1/2



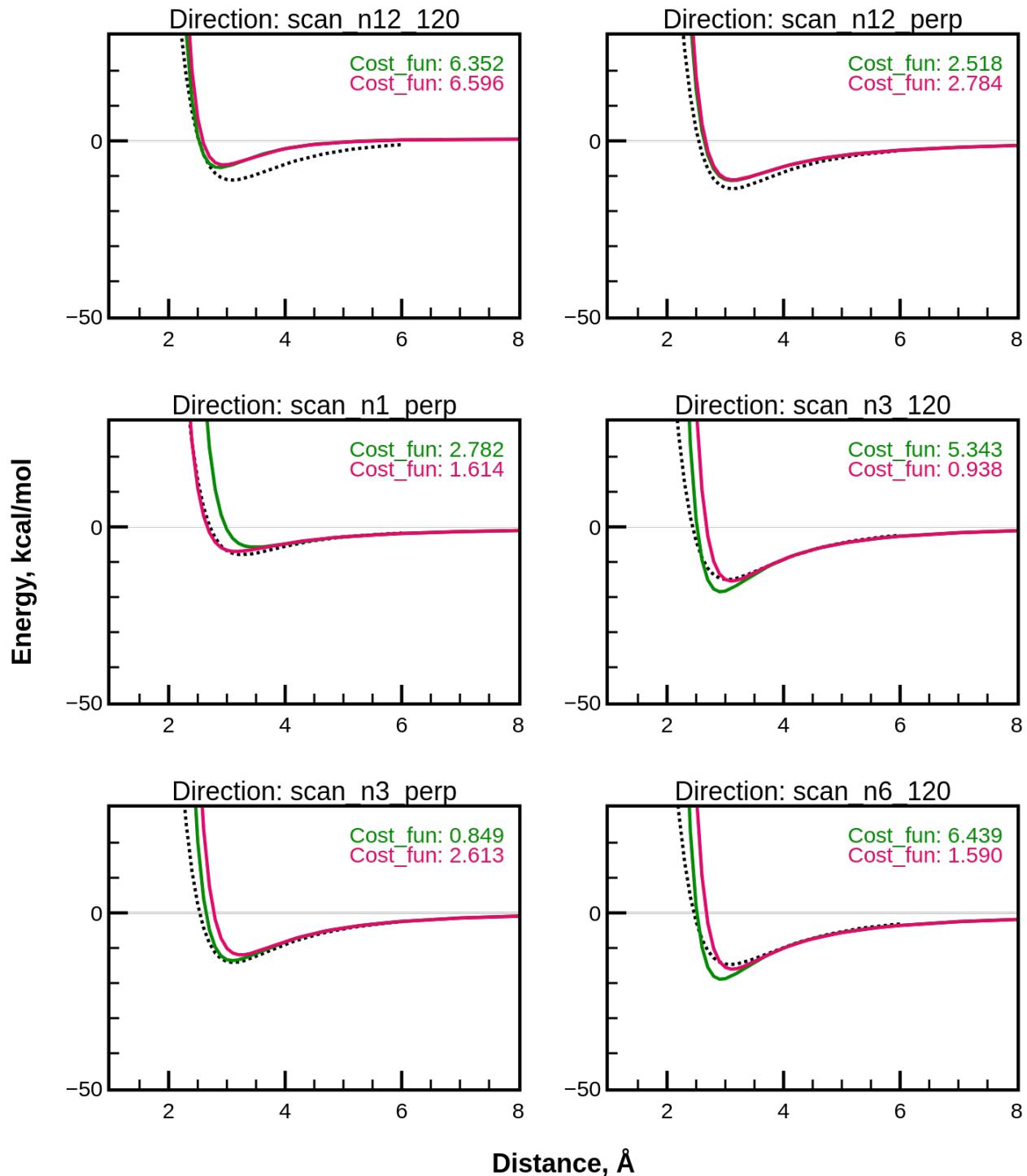
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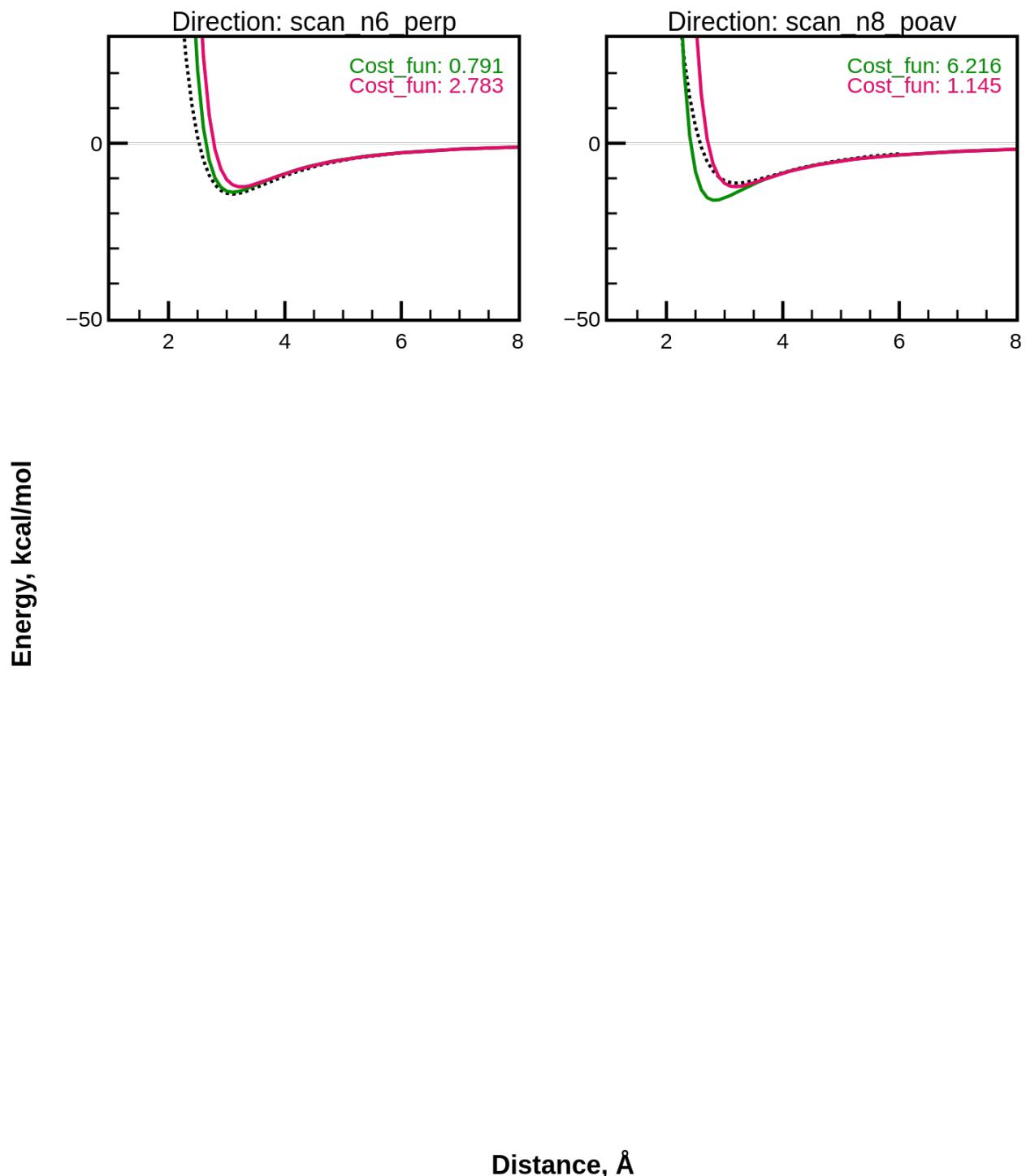
ADEB RUB 1/2



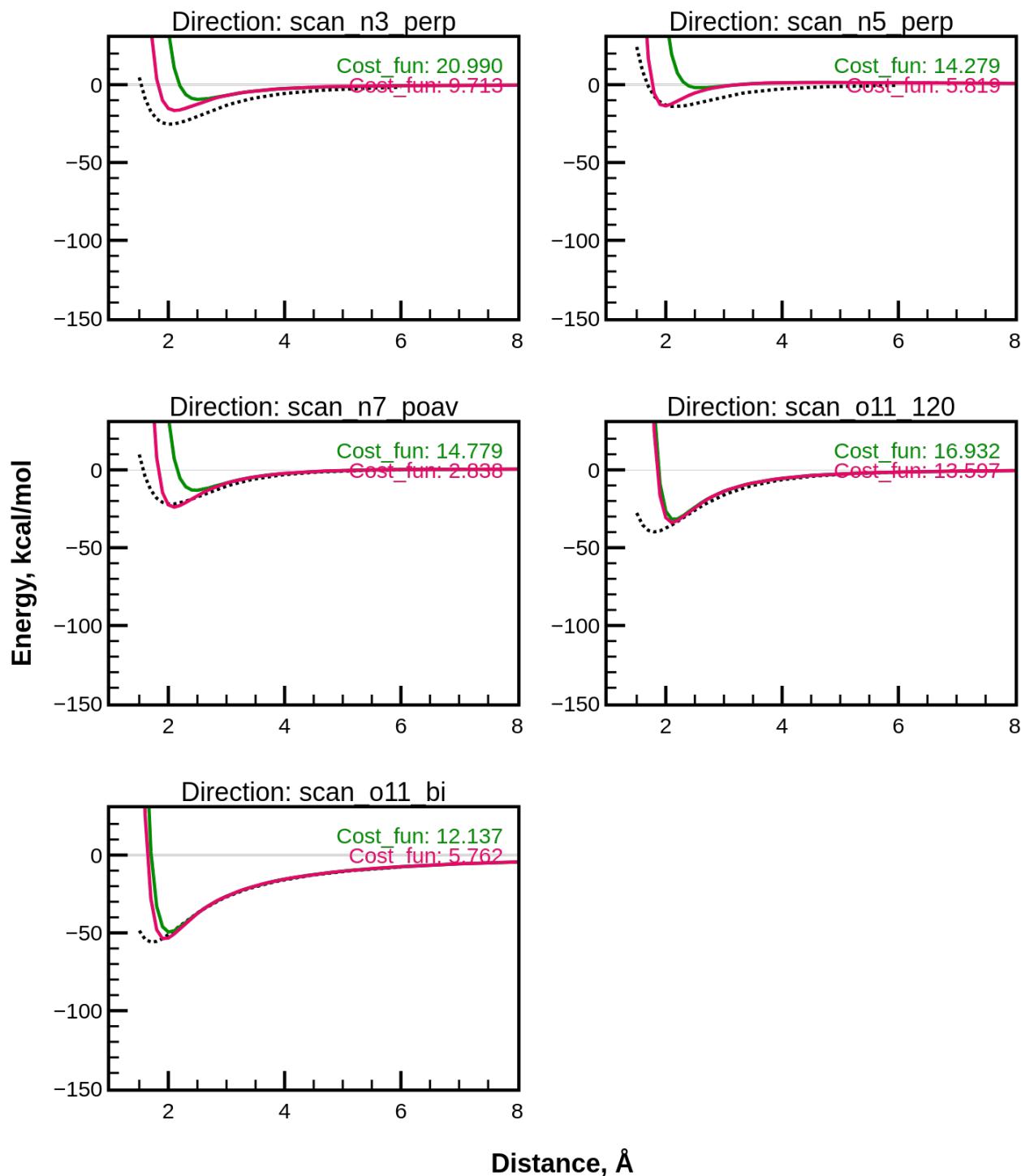
ADEB CES 1/2



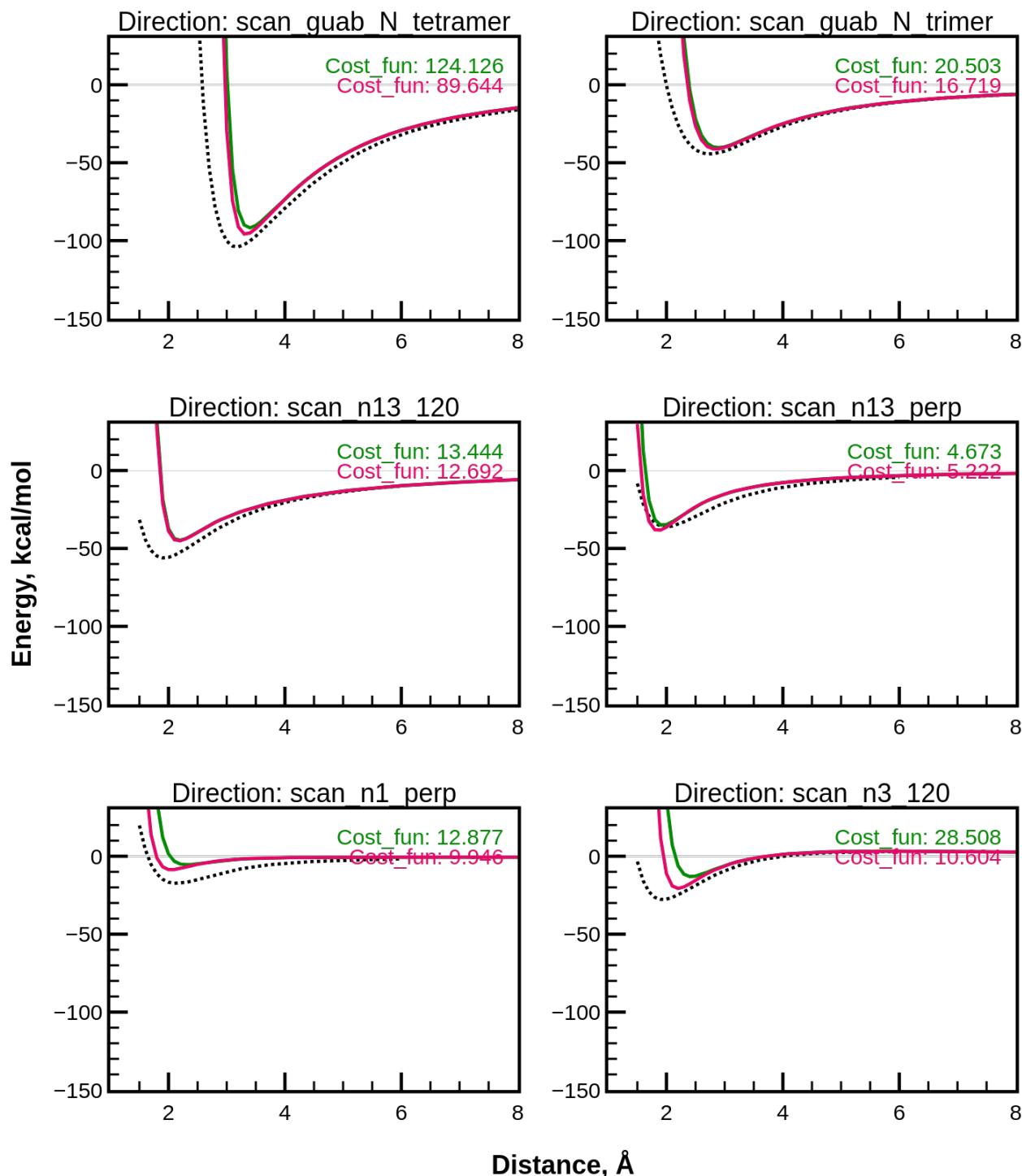
ADEB CES 2/2



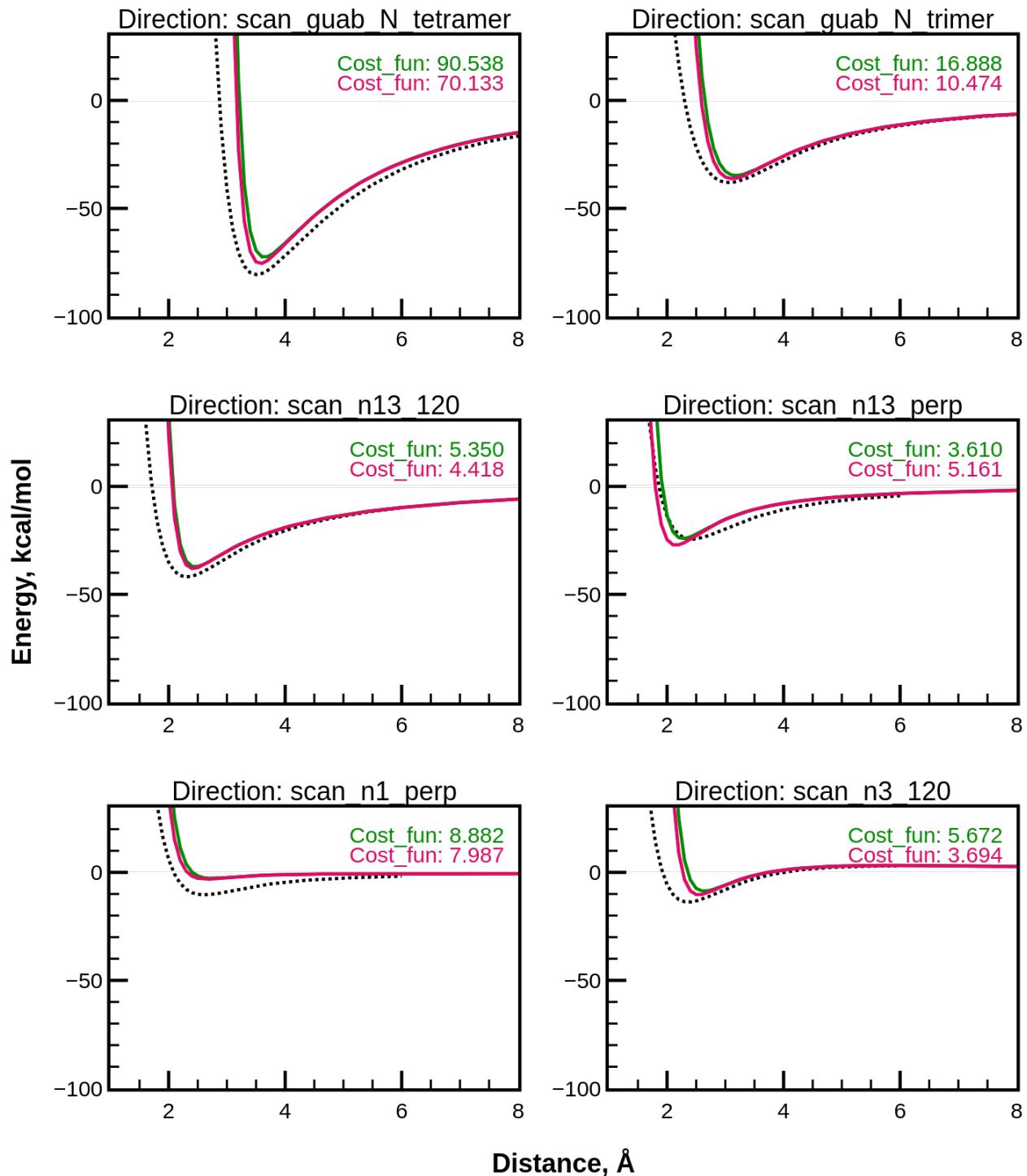
GUAB LIT 2/2



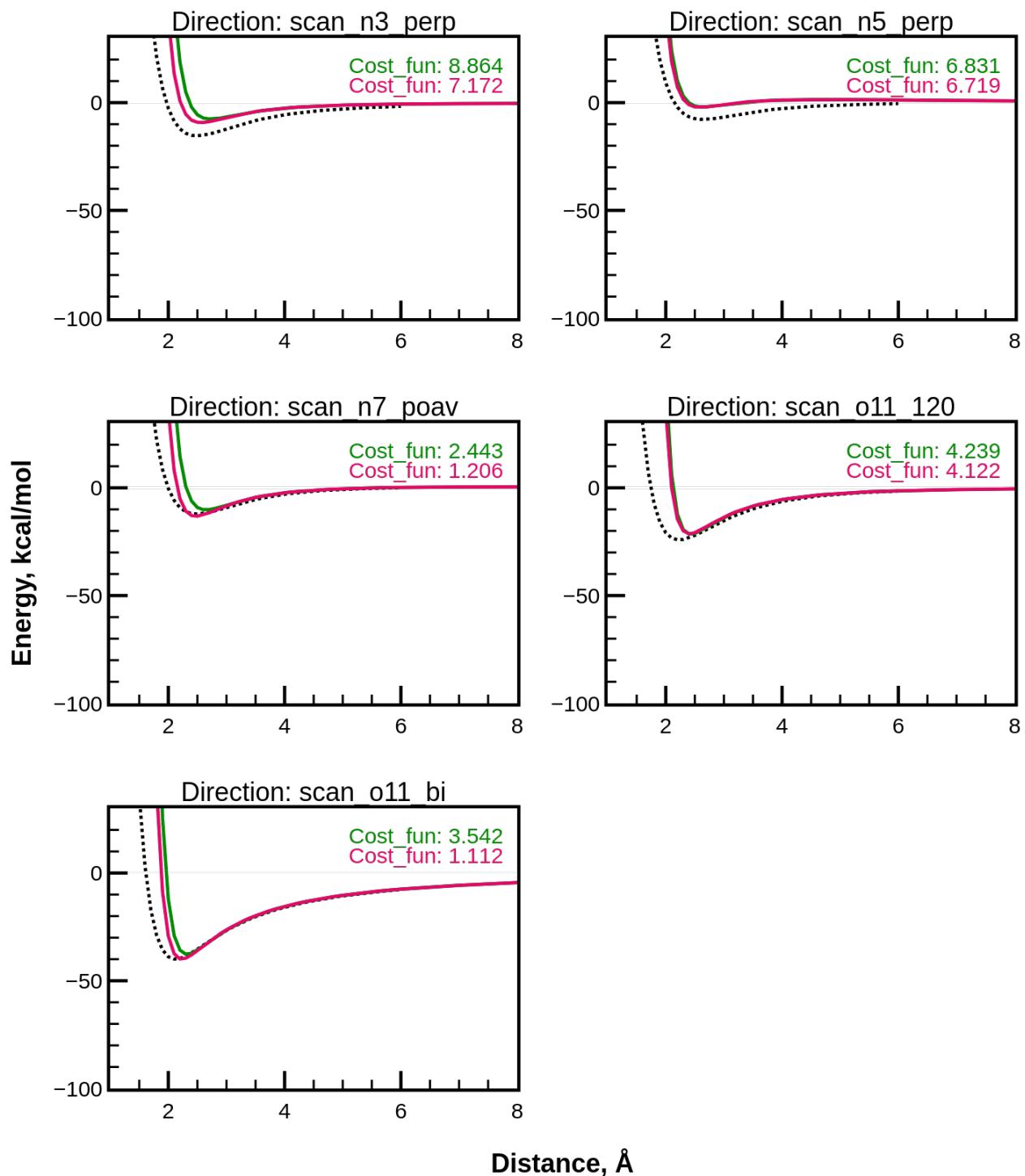
GUAB LIT 1/2



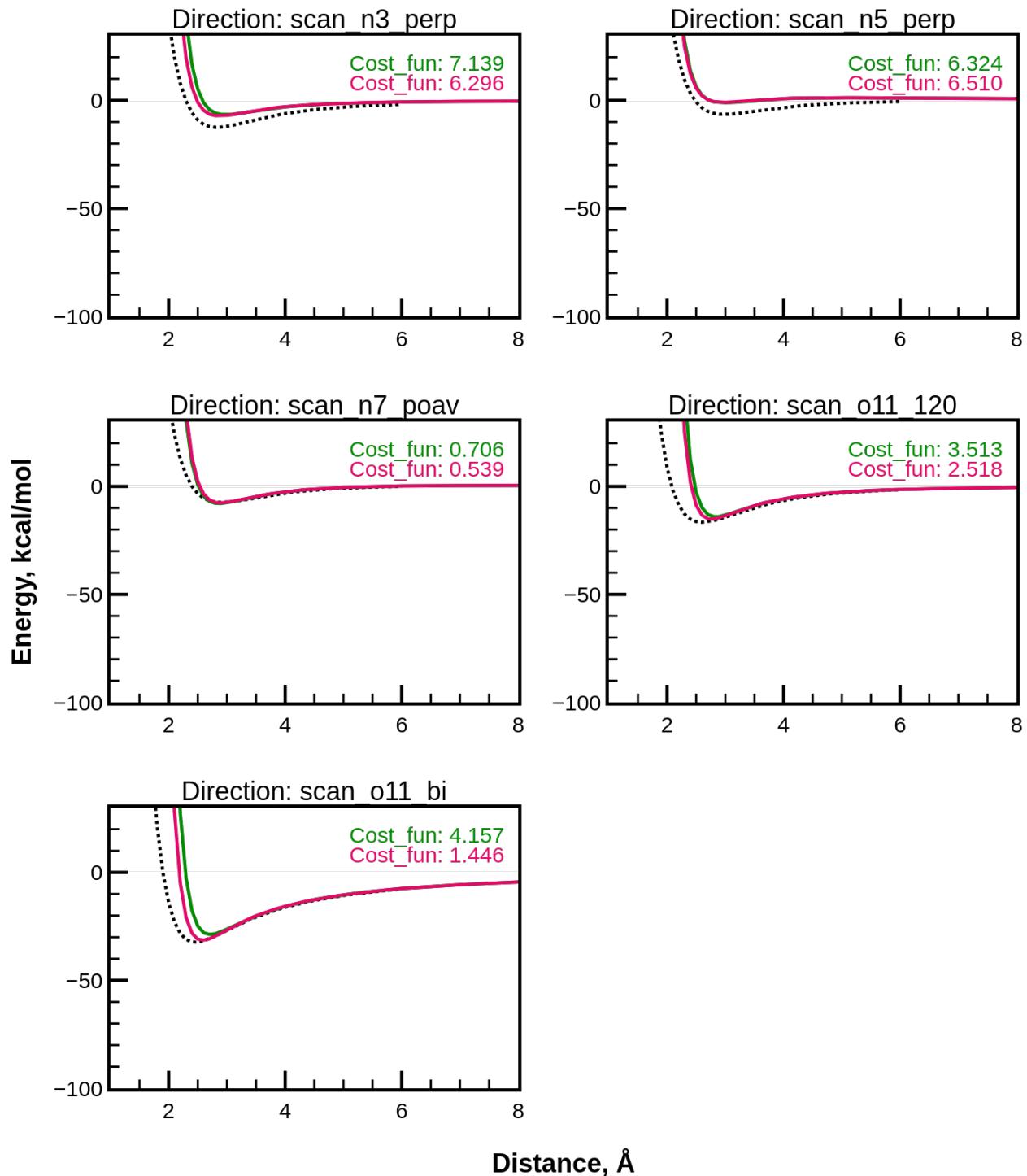
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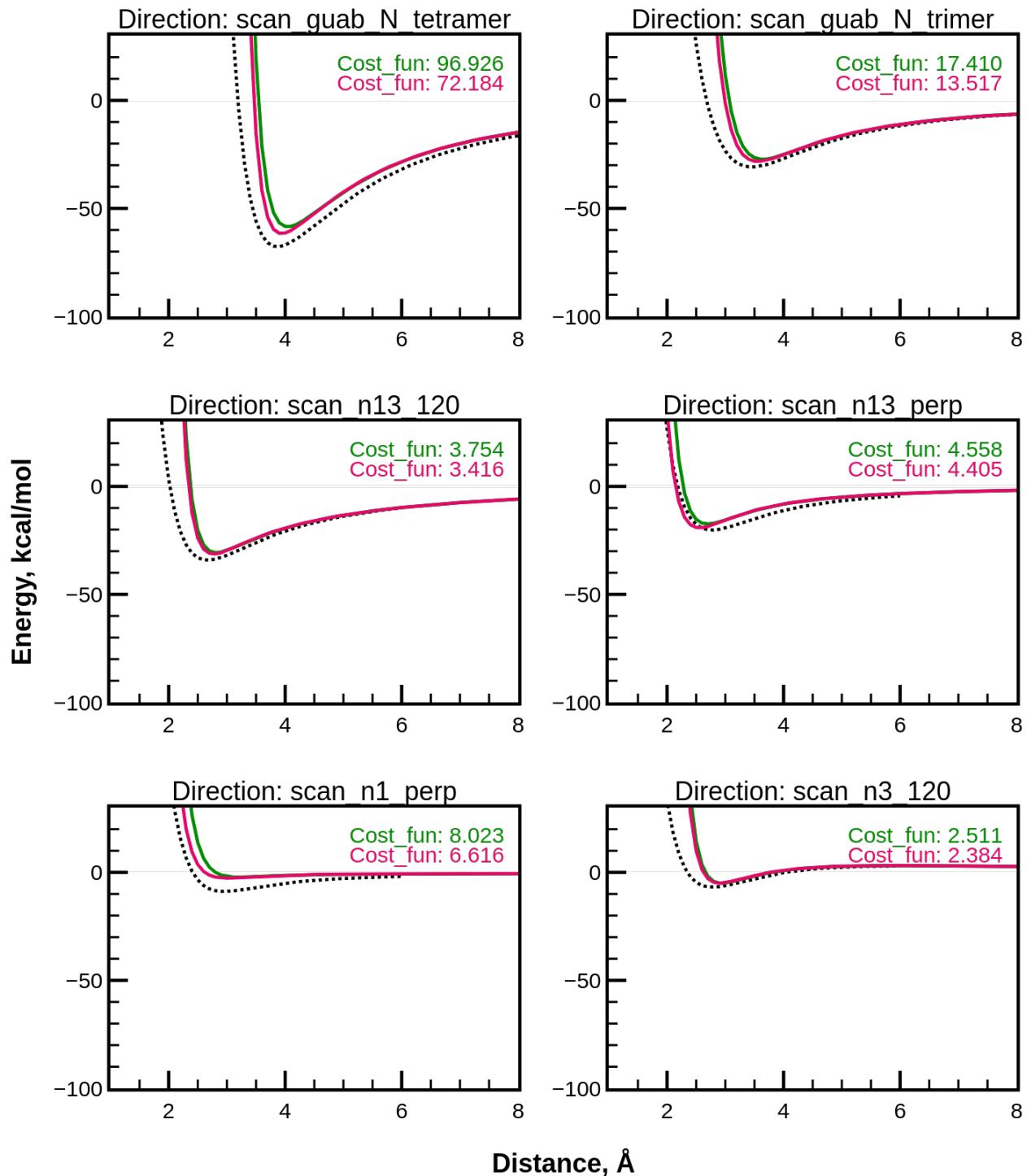
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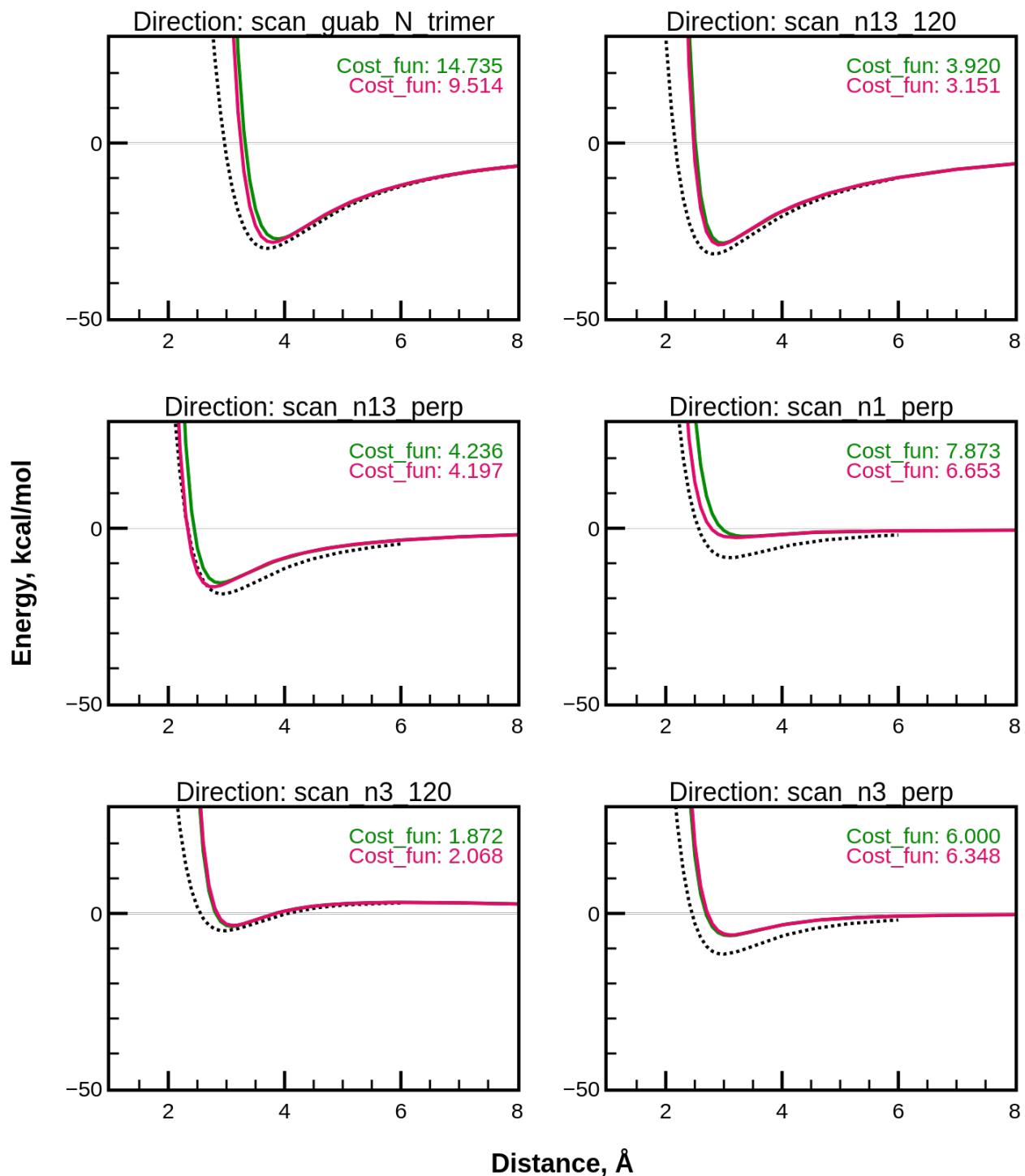
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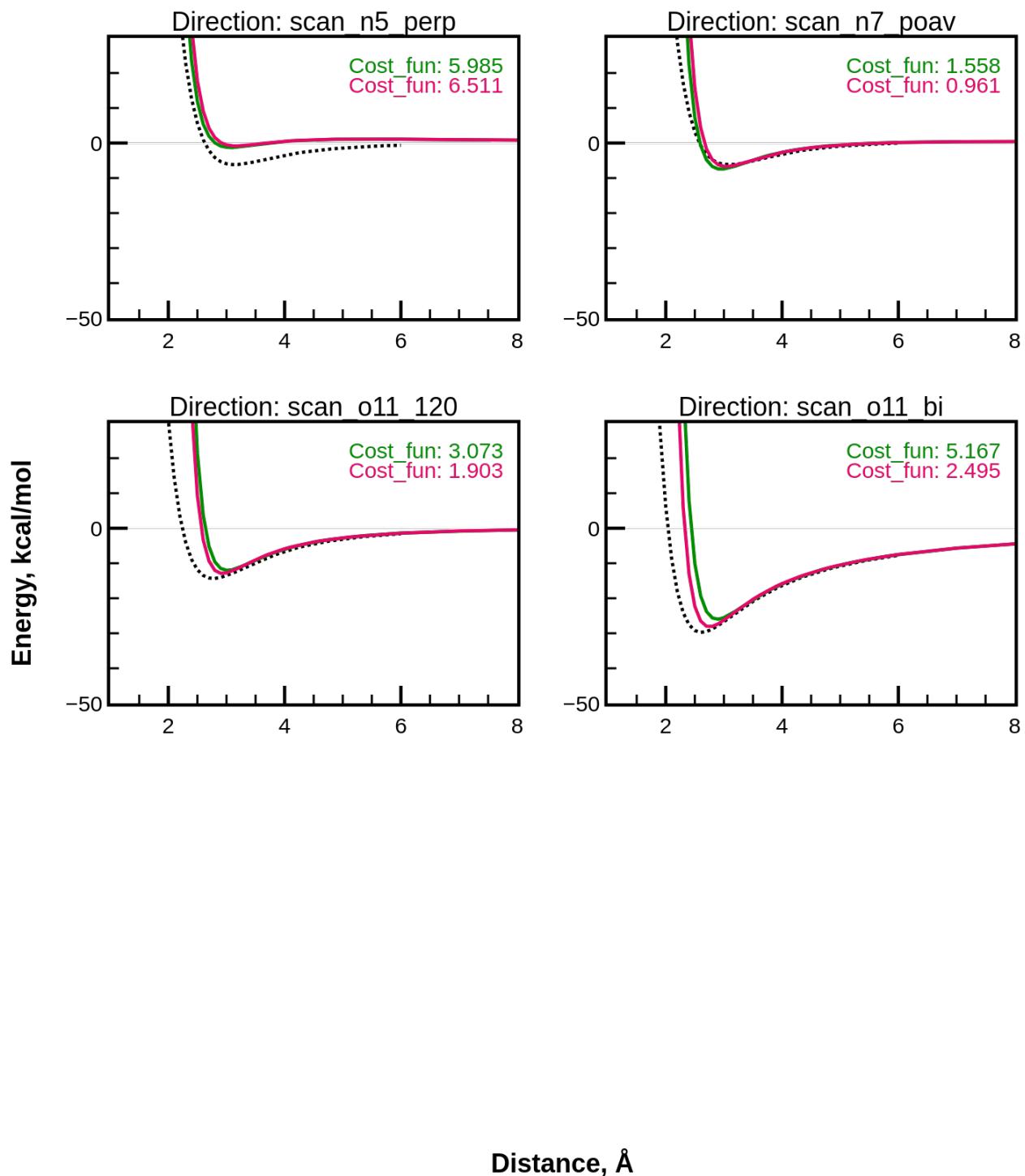
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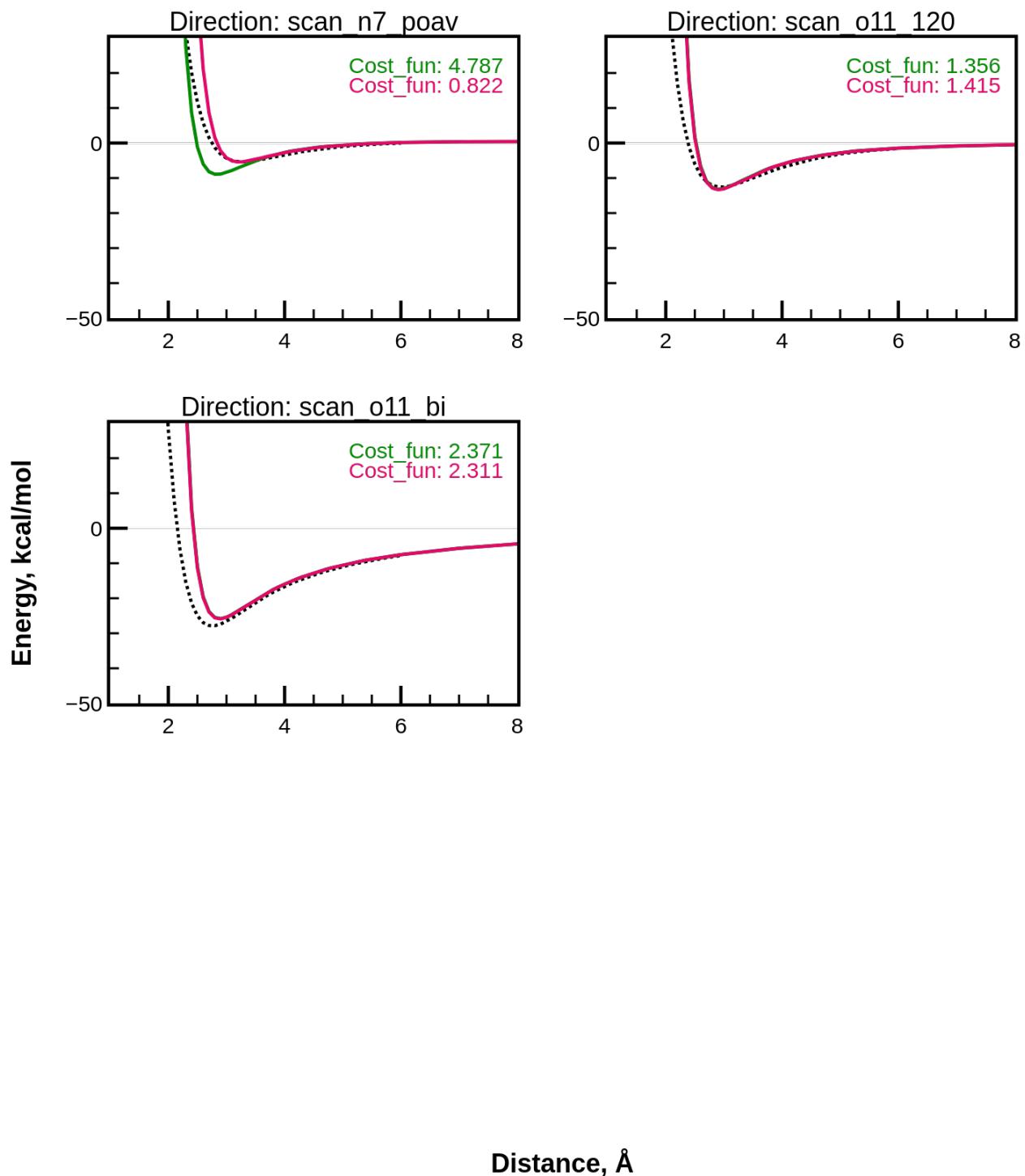
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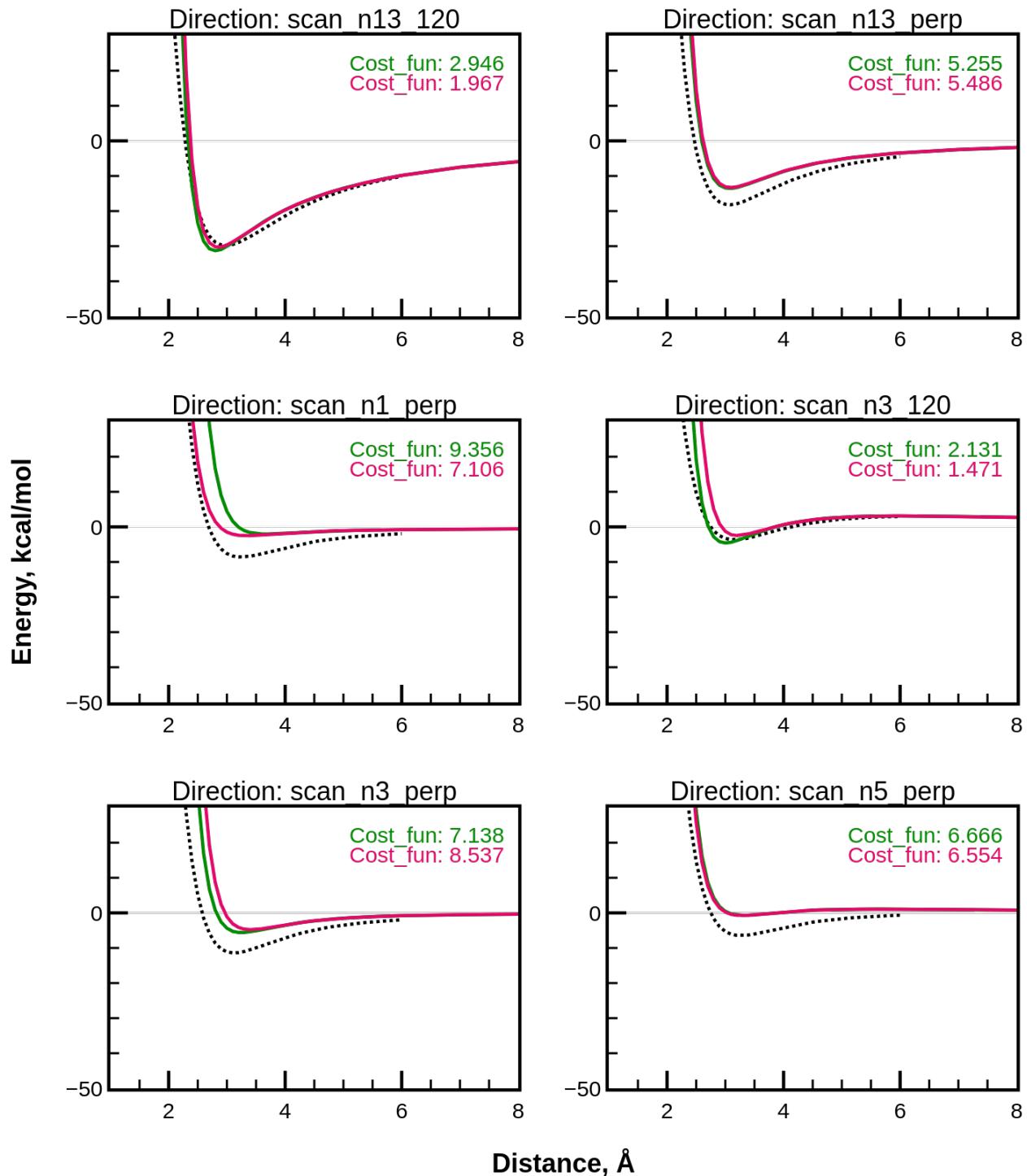
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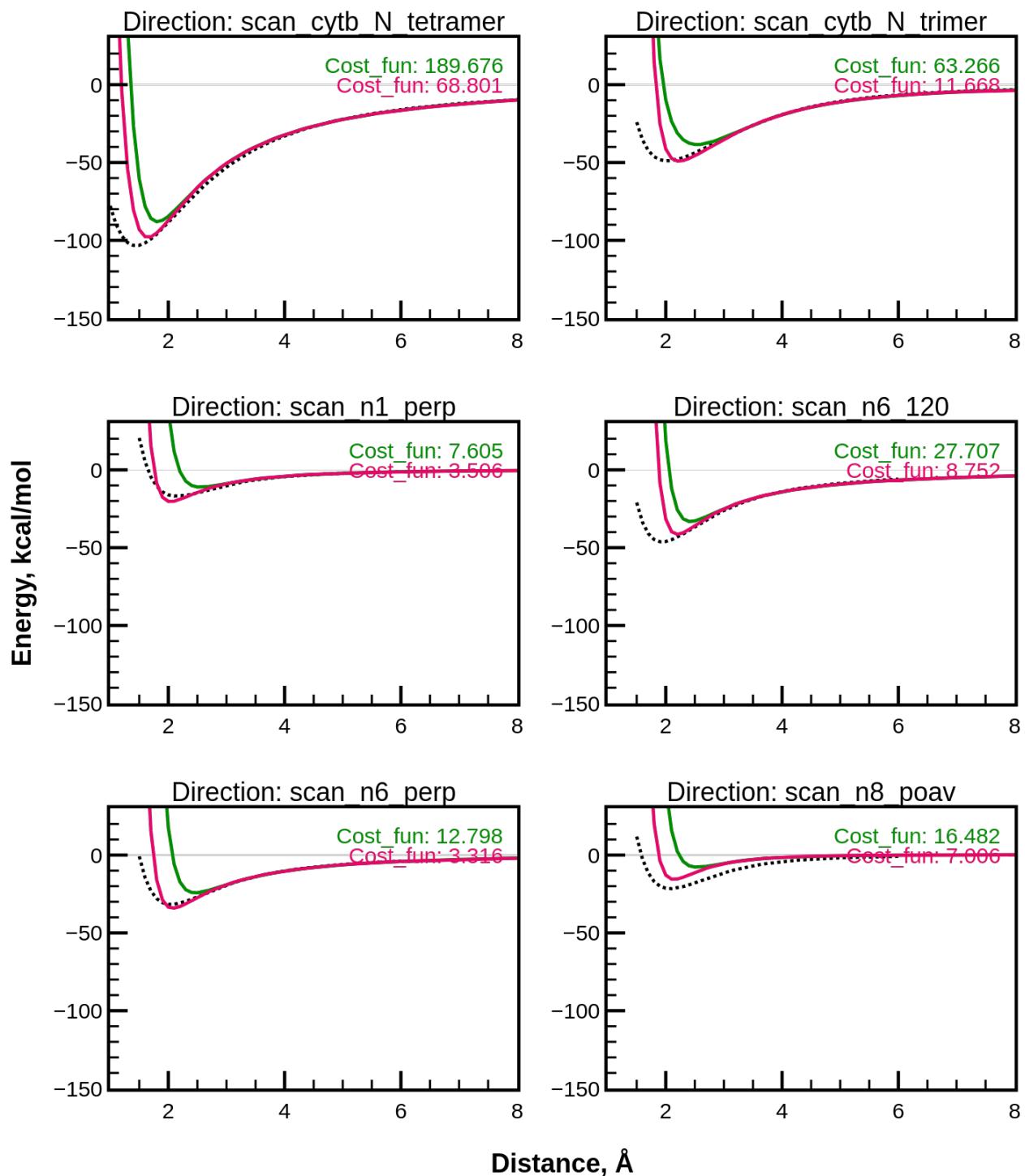
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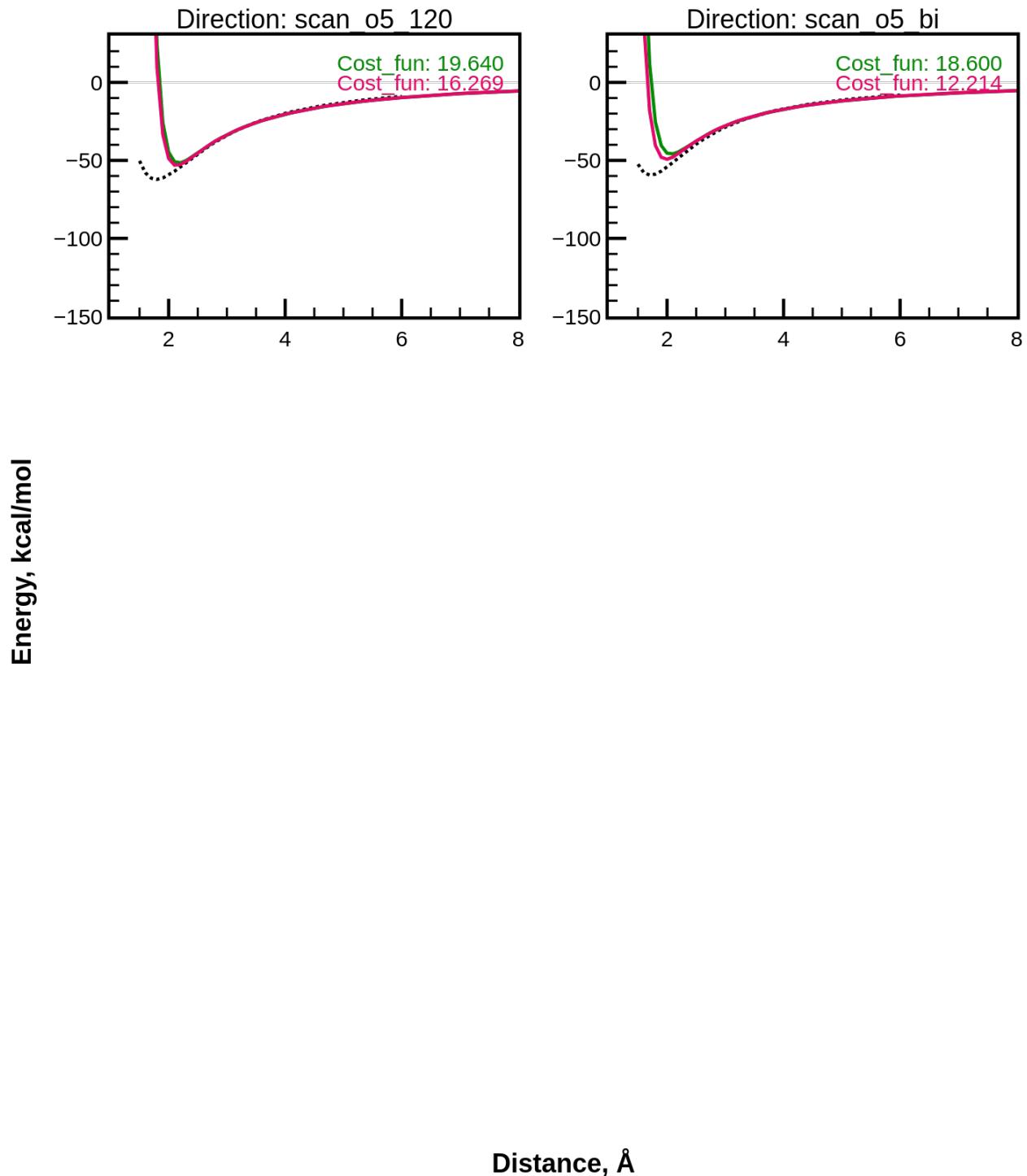
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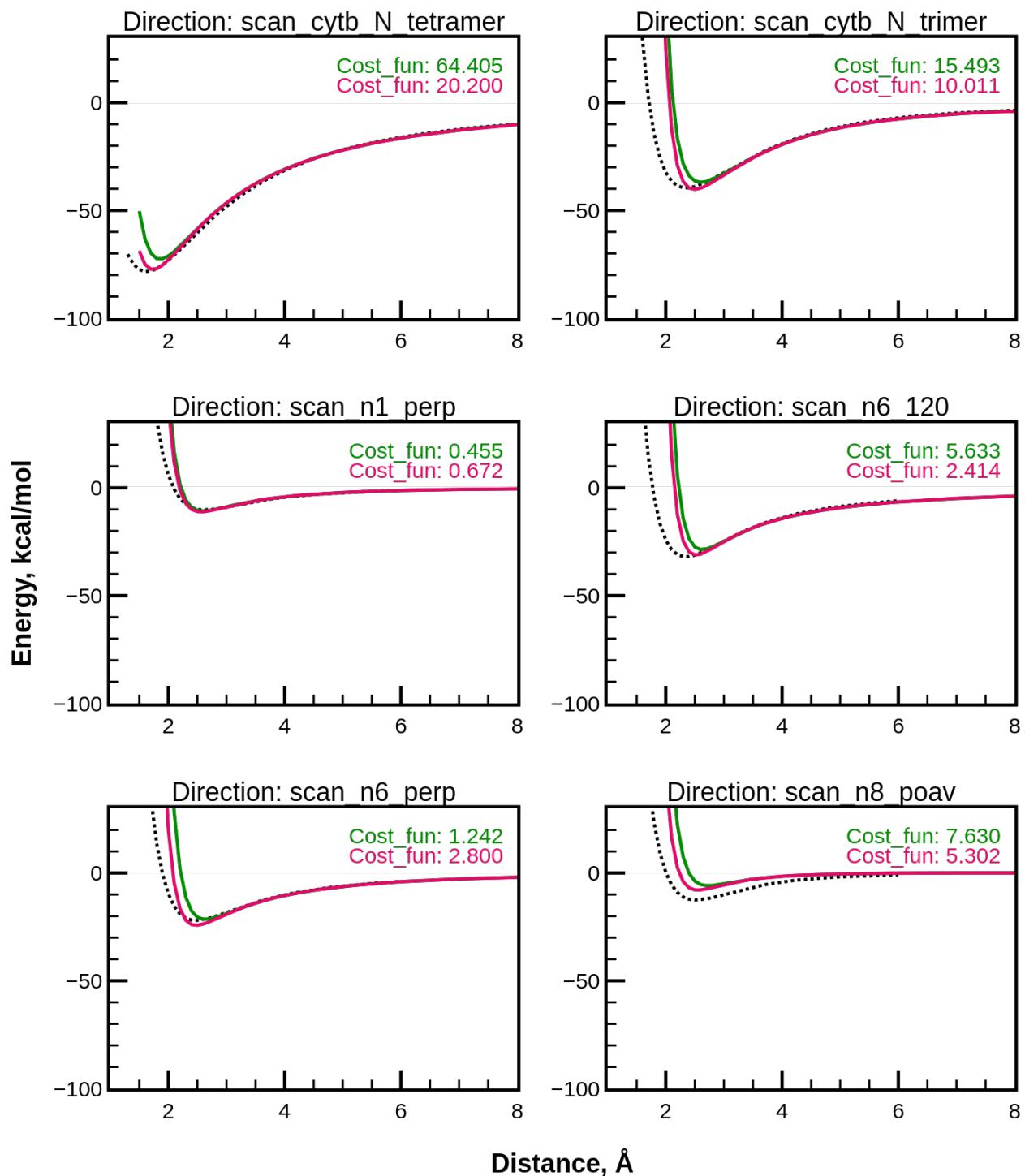
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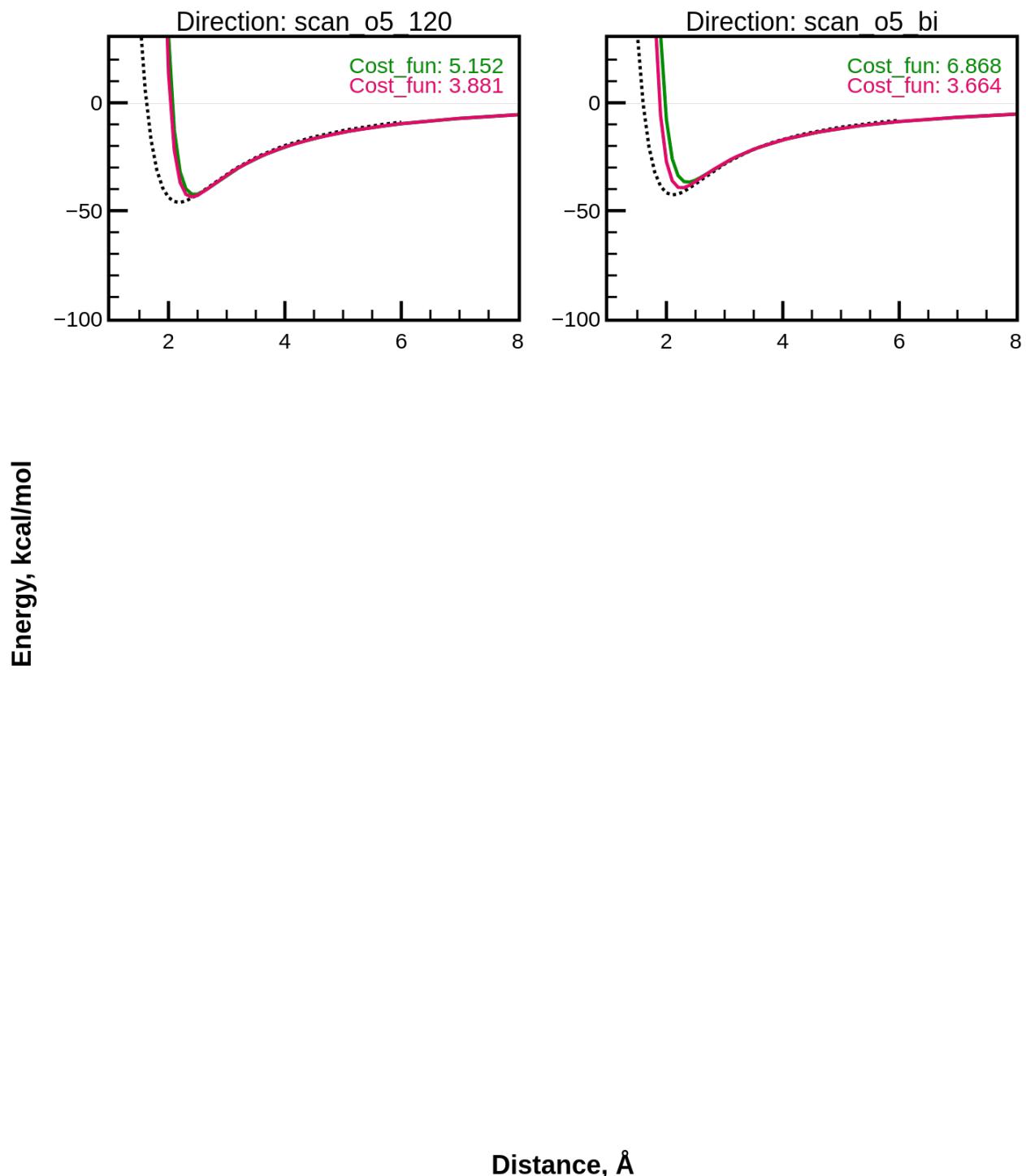
CYTB LIT 2/2



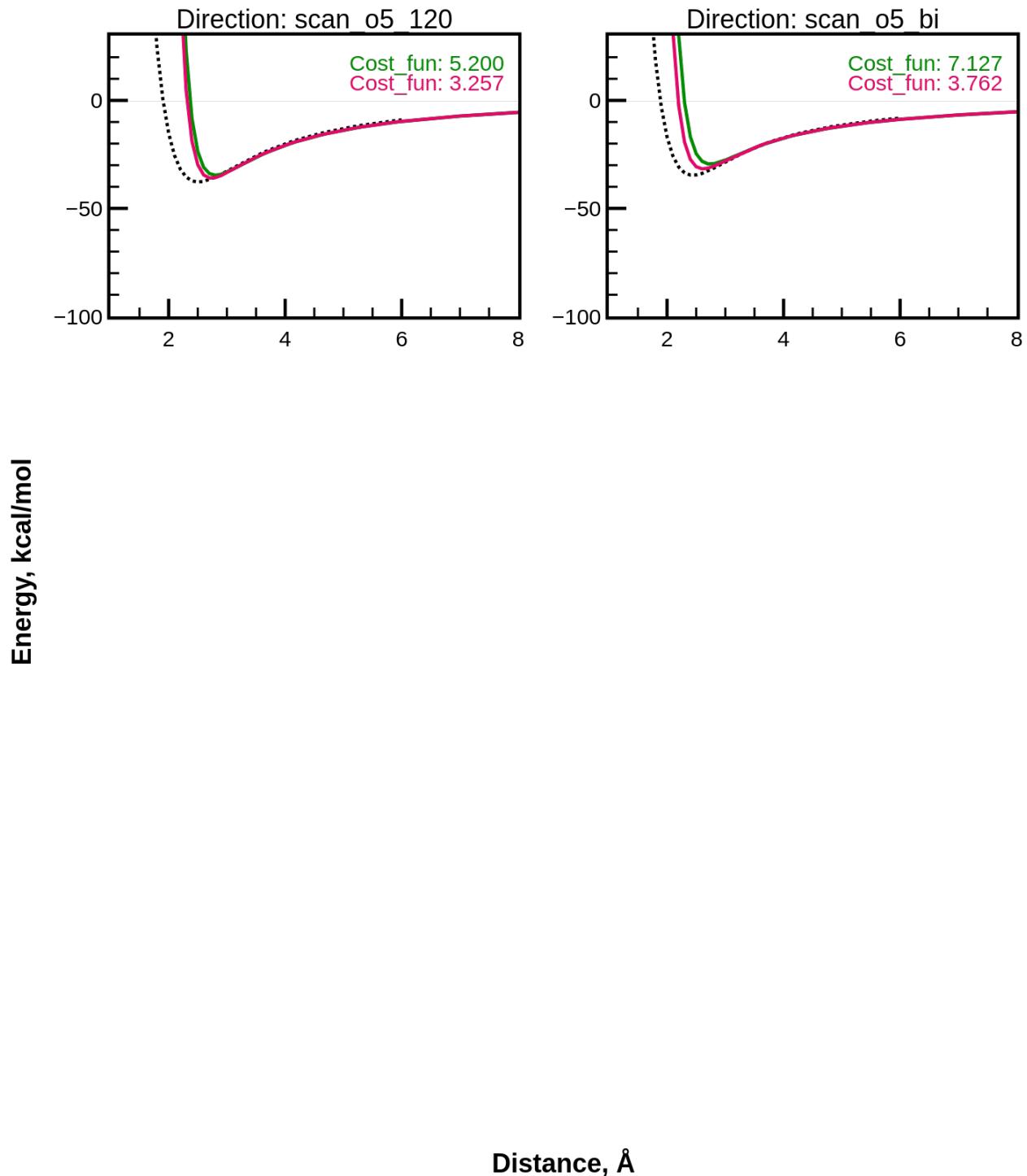
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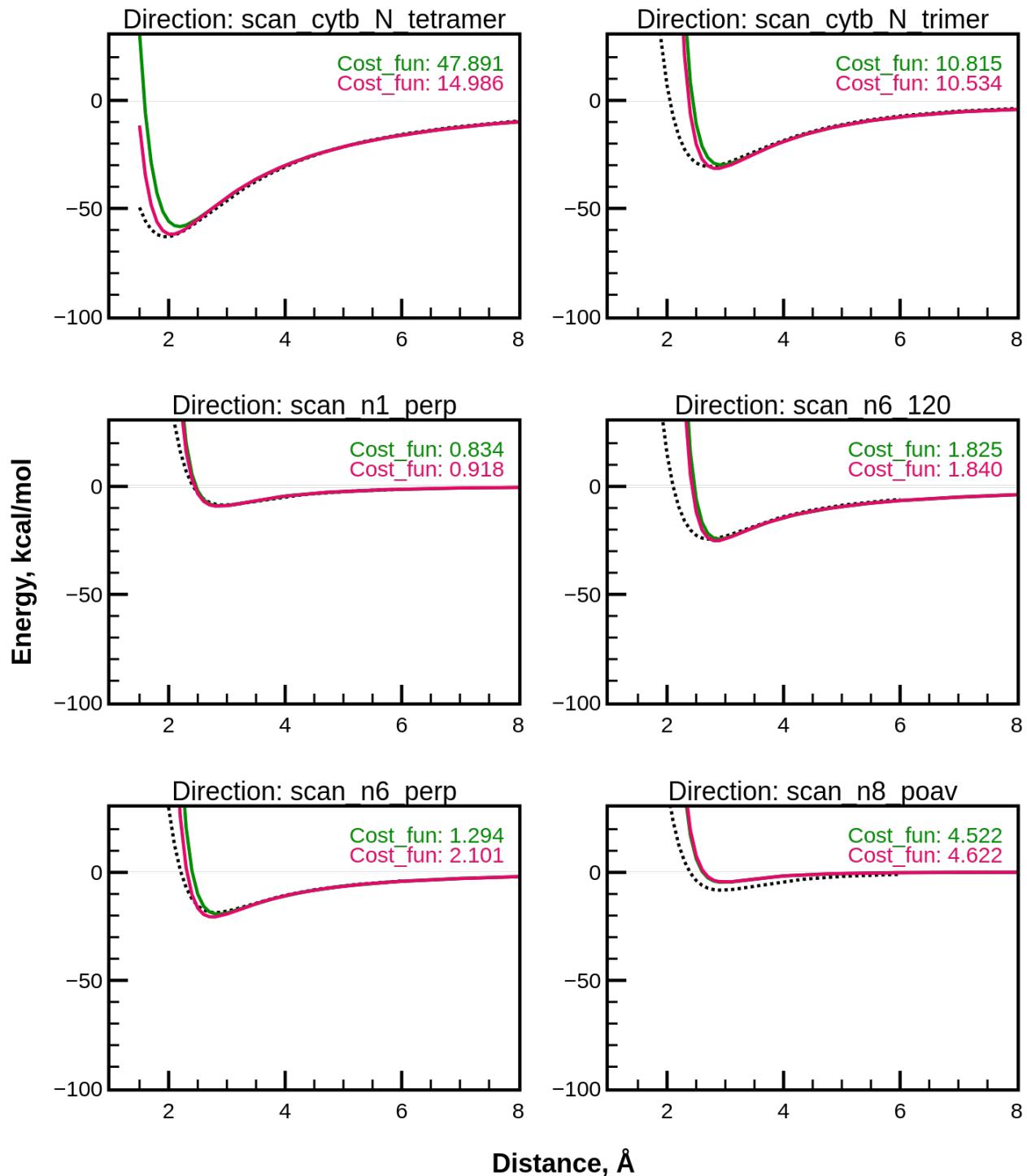
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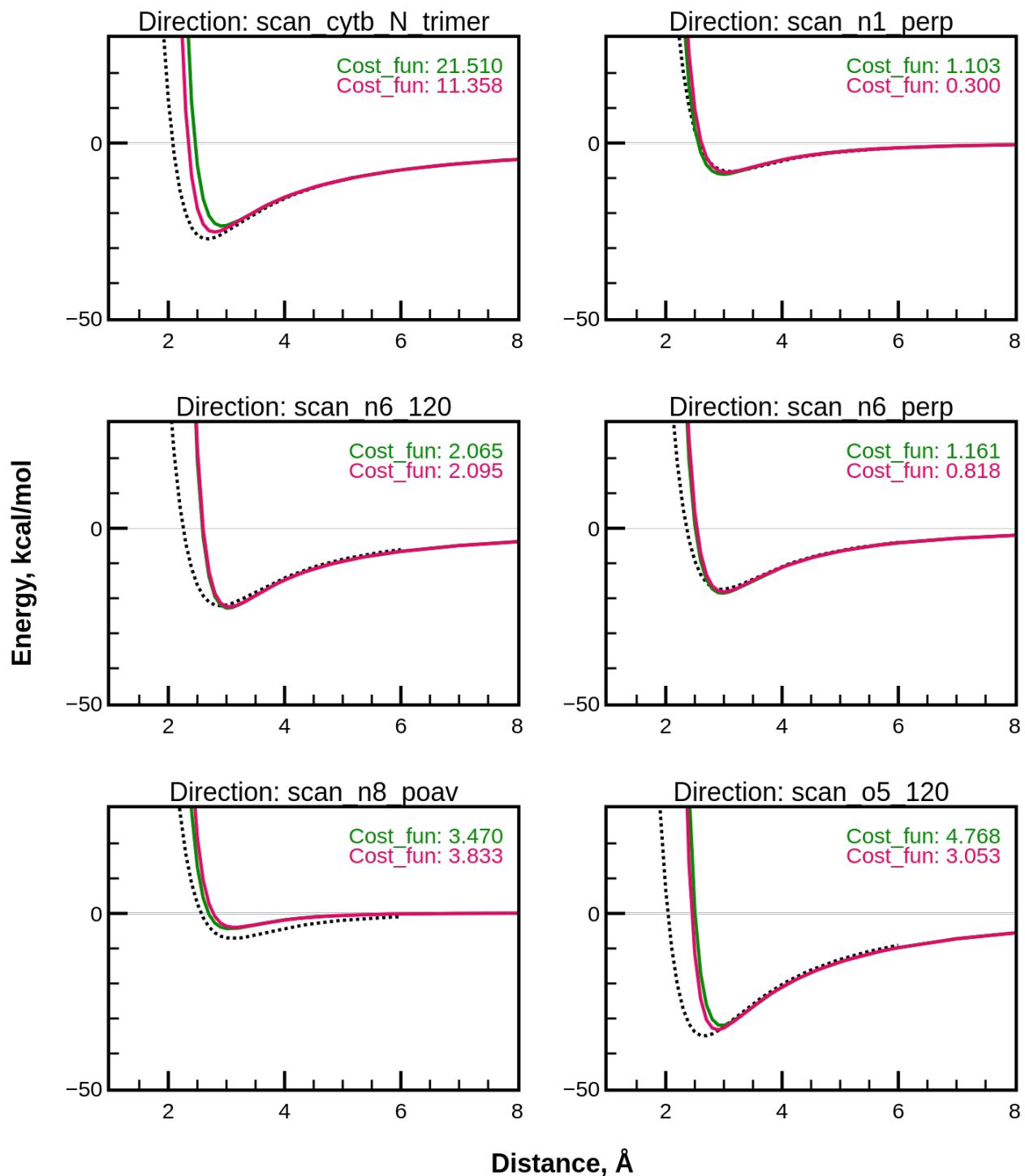
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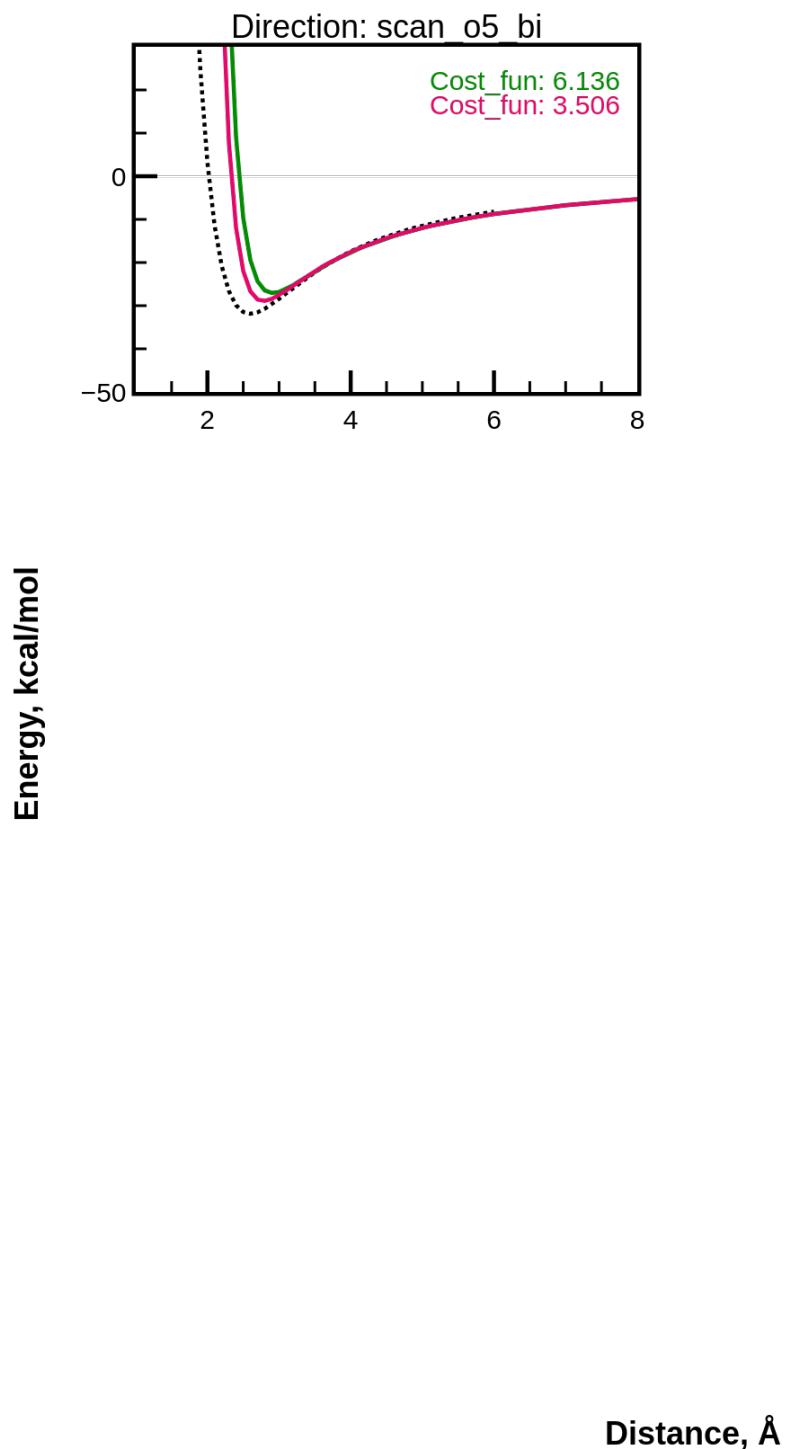
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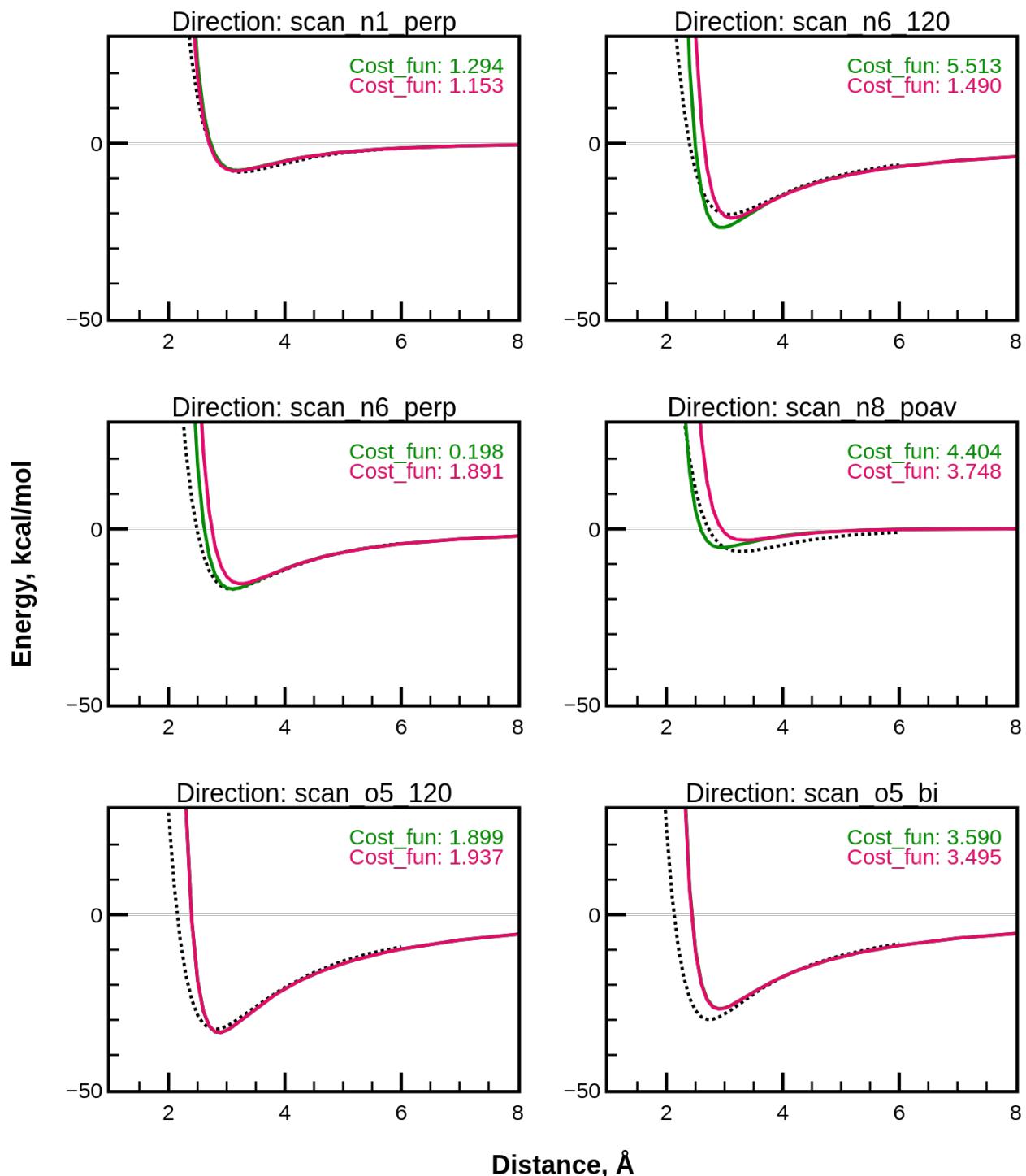
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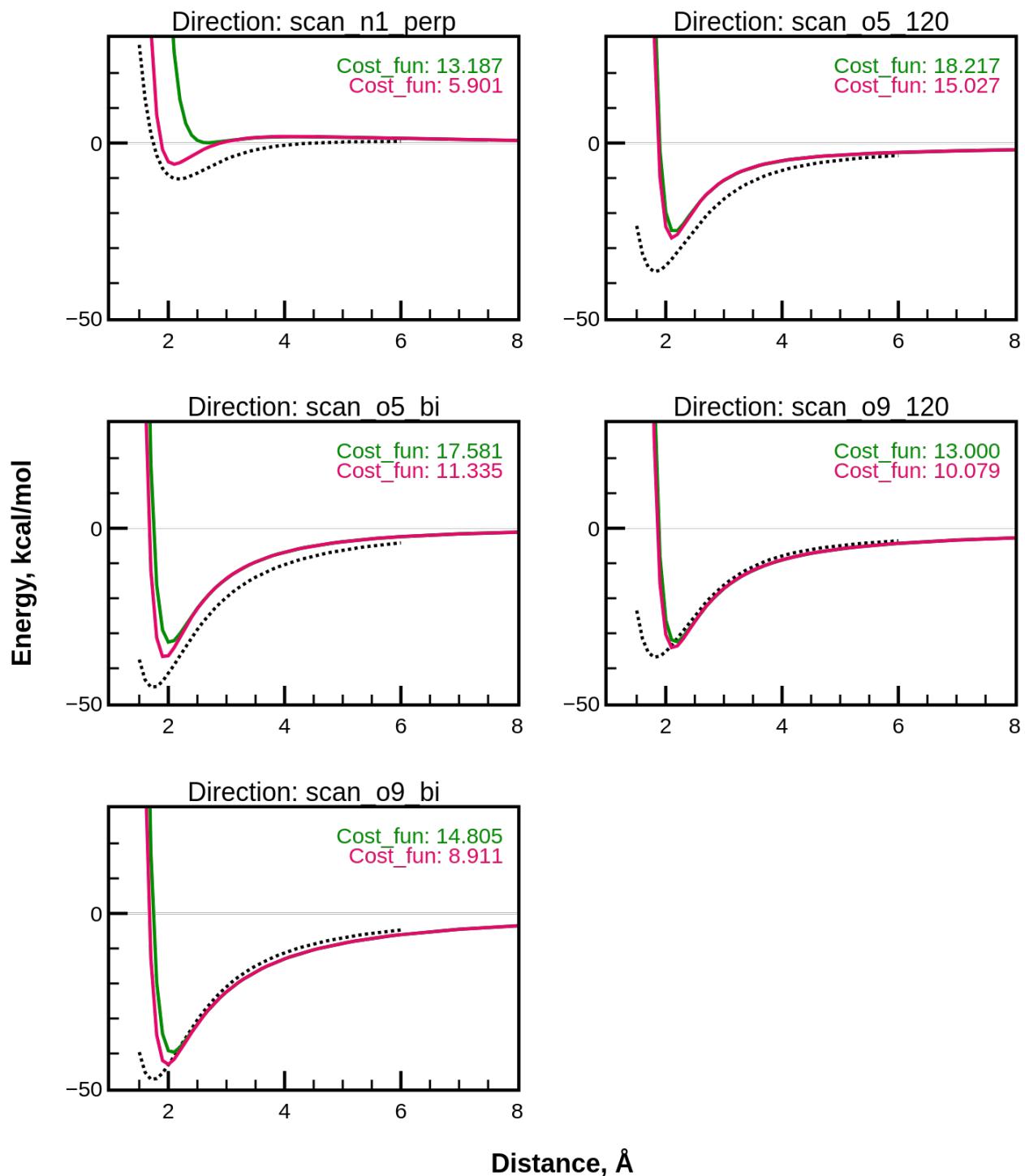
CYTB RUB 2/2



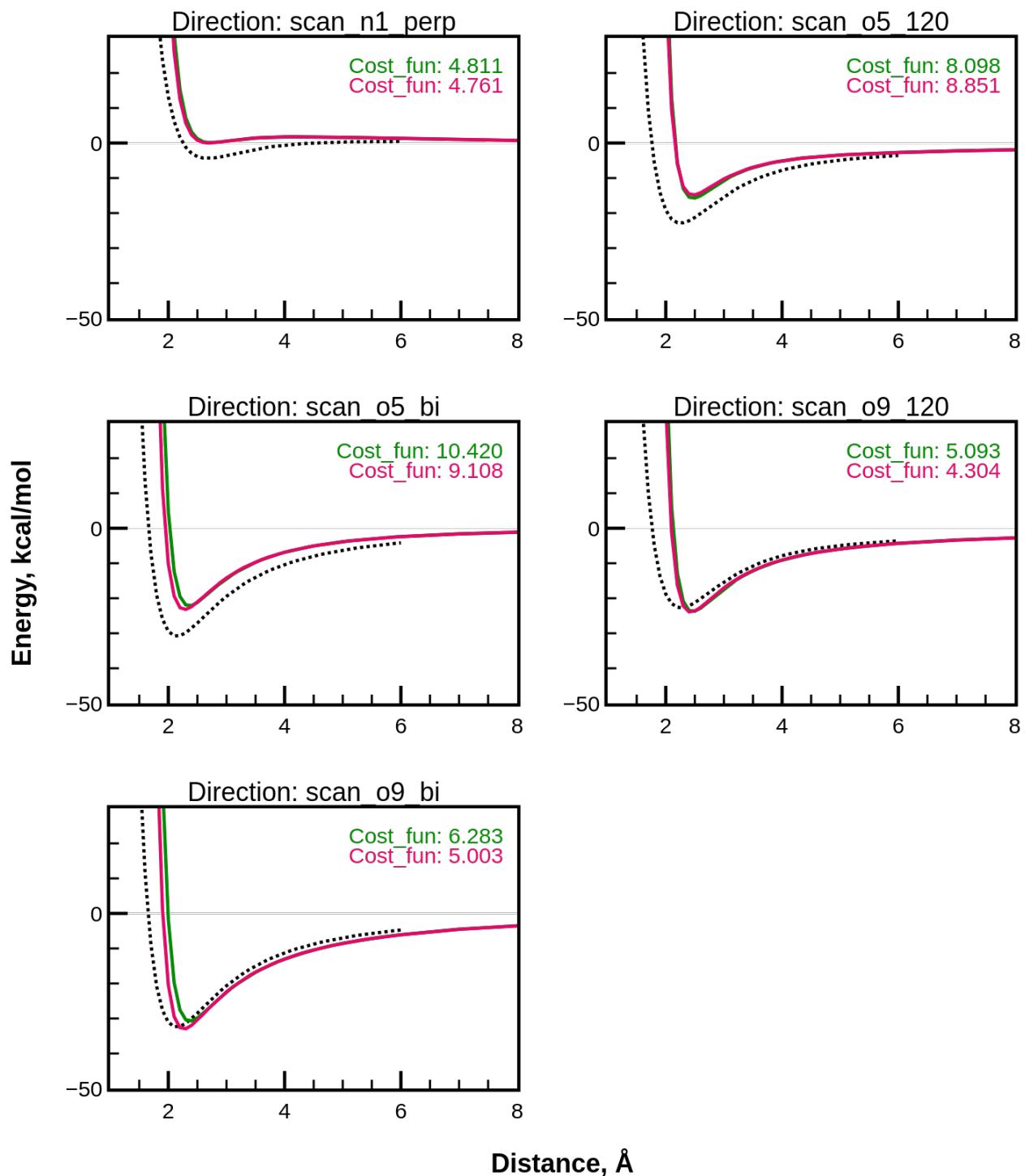
CYTB CES 1/1



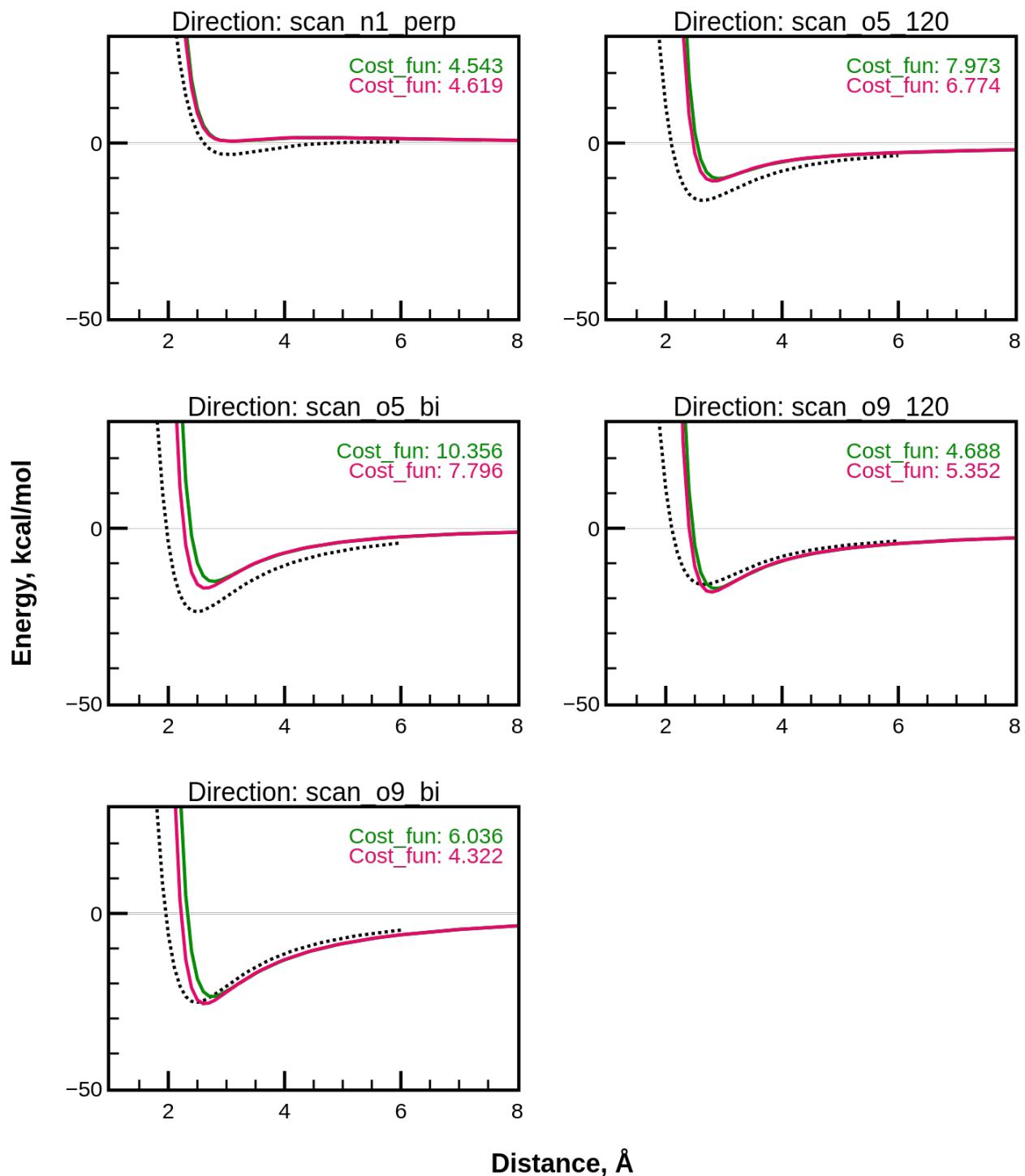
THYB LIT 1/1



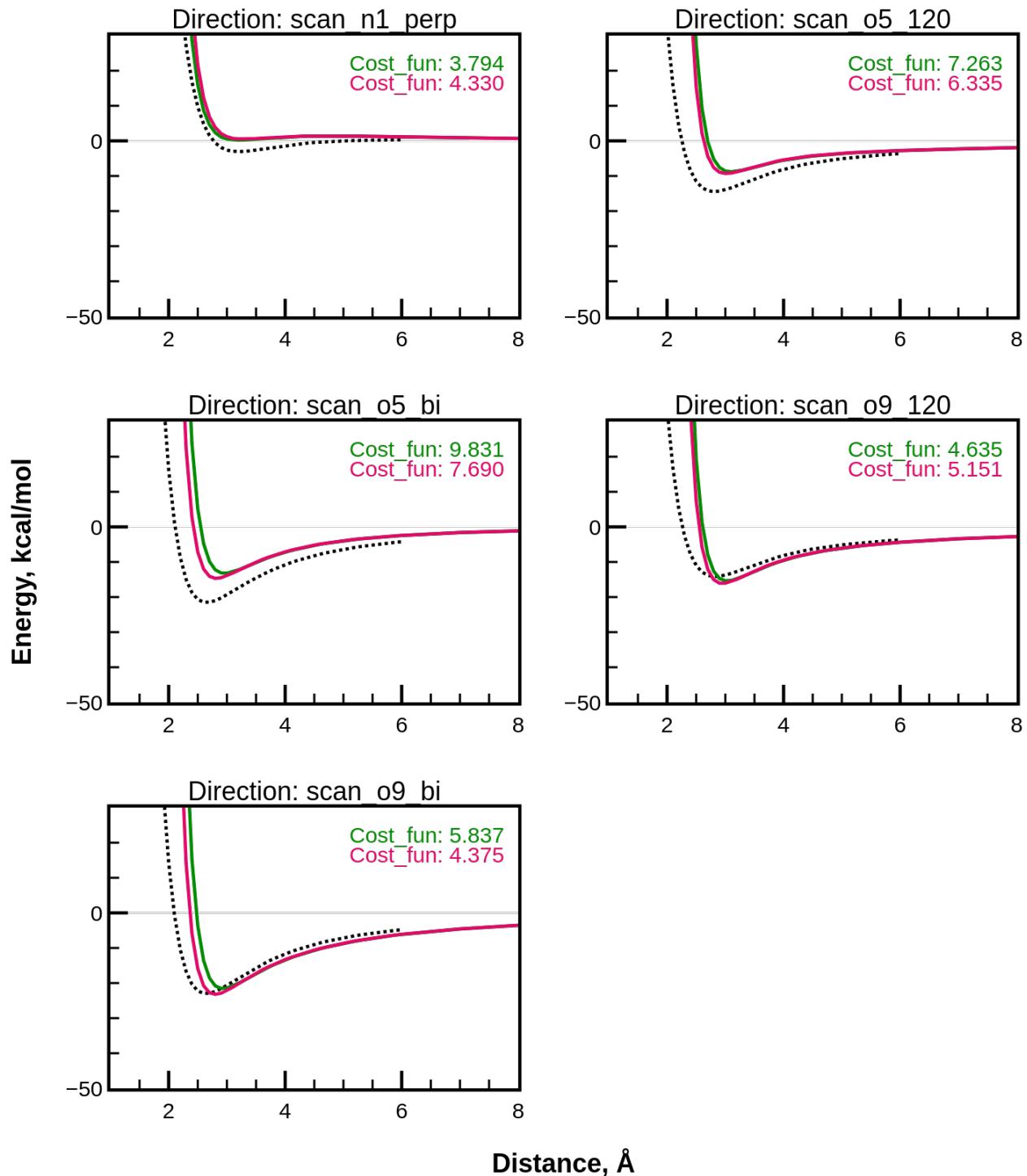
THYB SOD 1/1



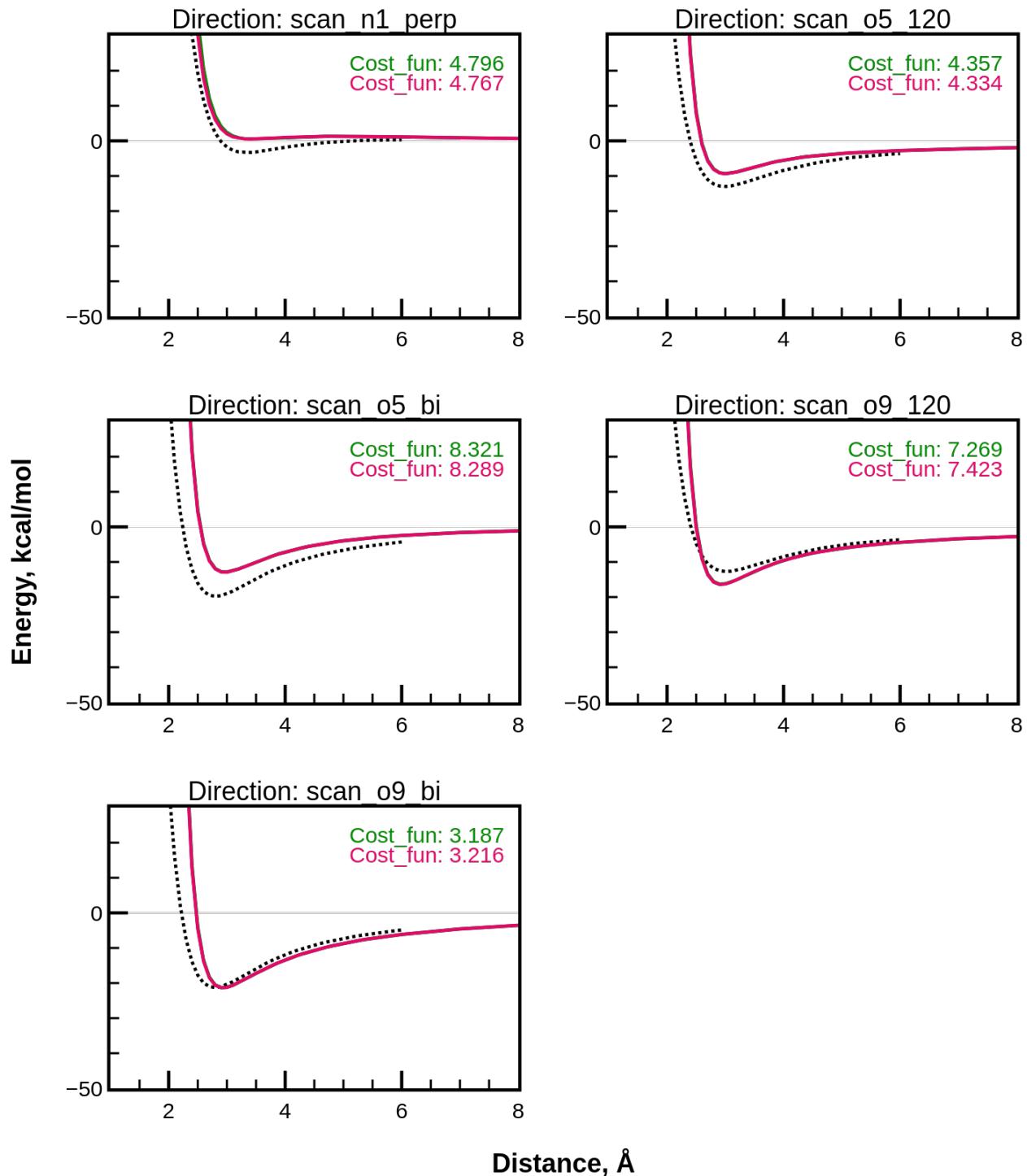
THYB POT 1/1



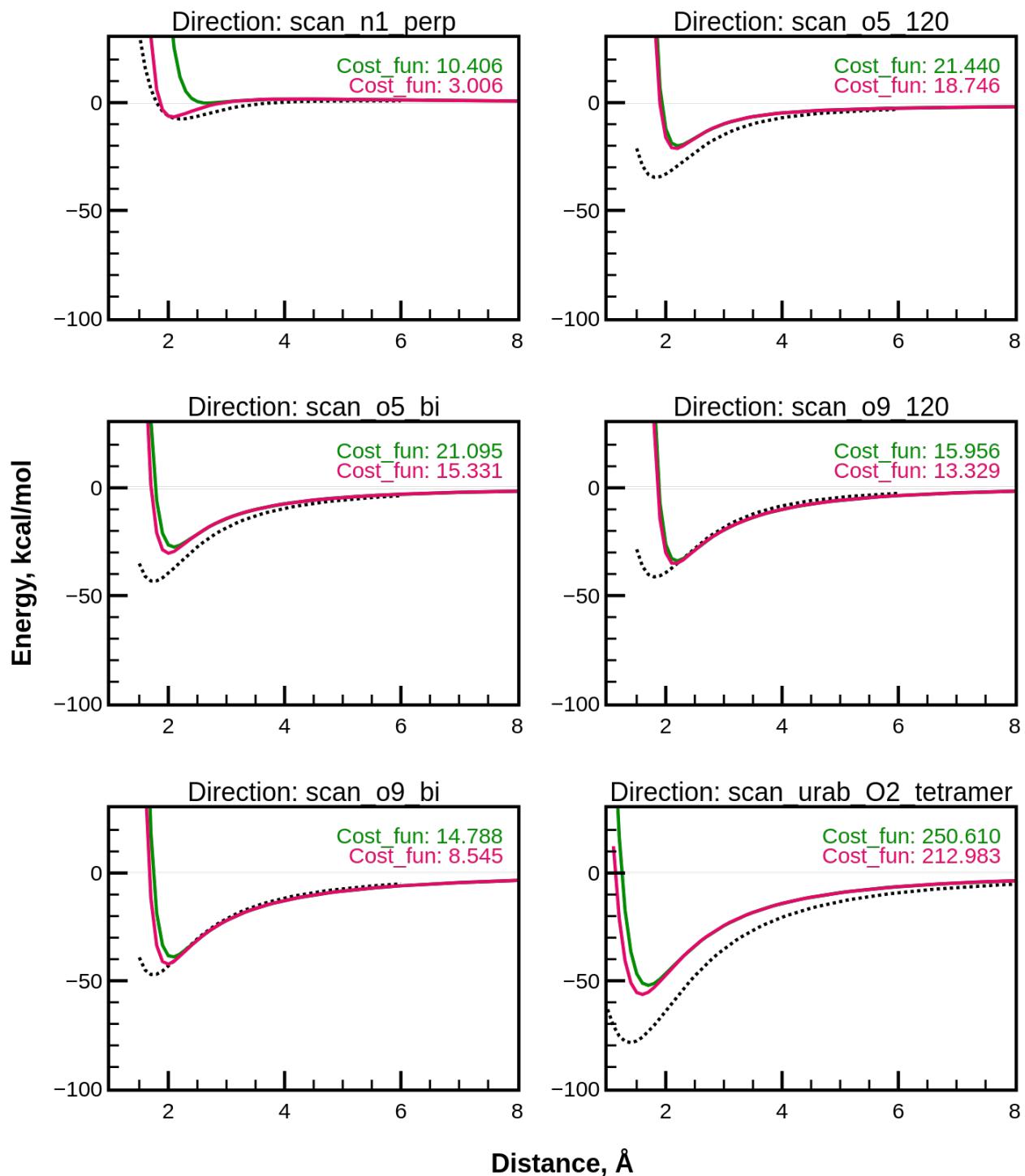
THYB RUB 1/1



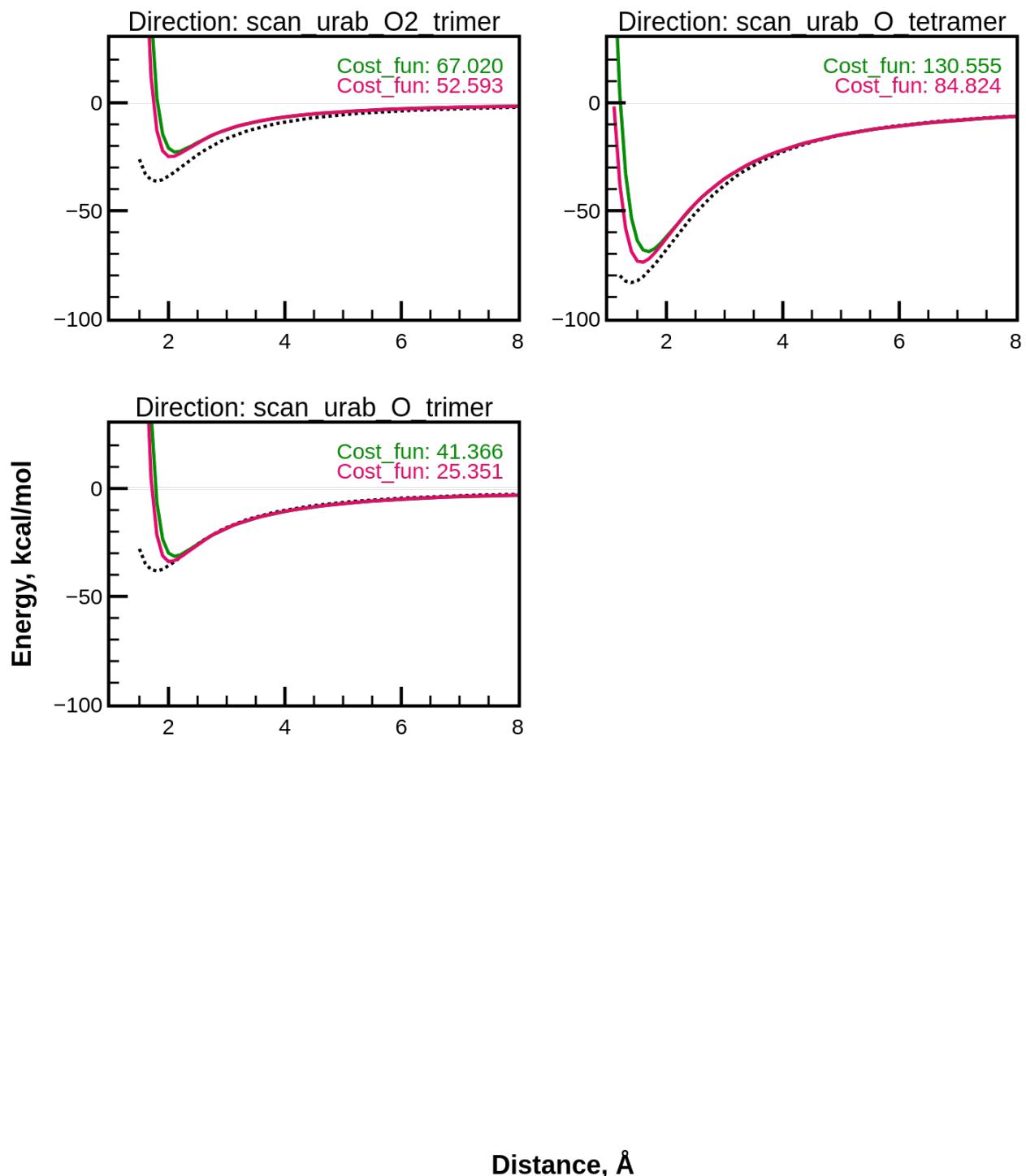
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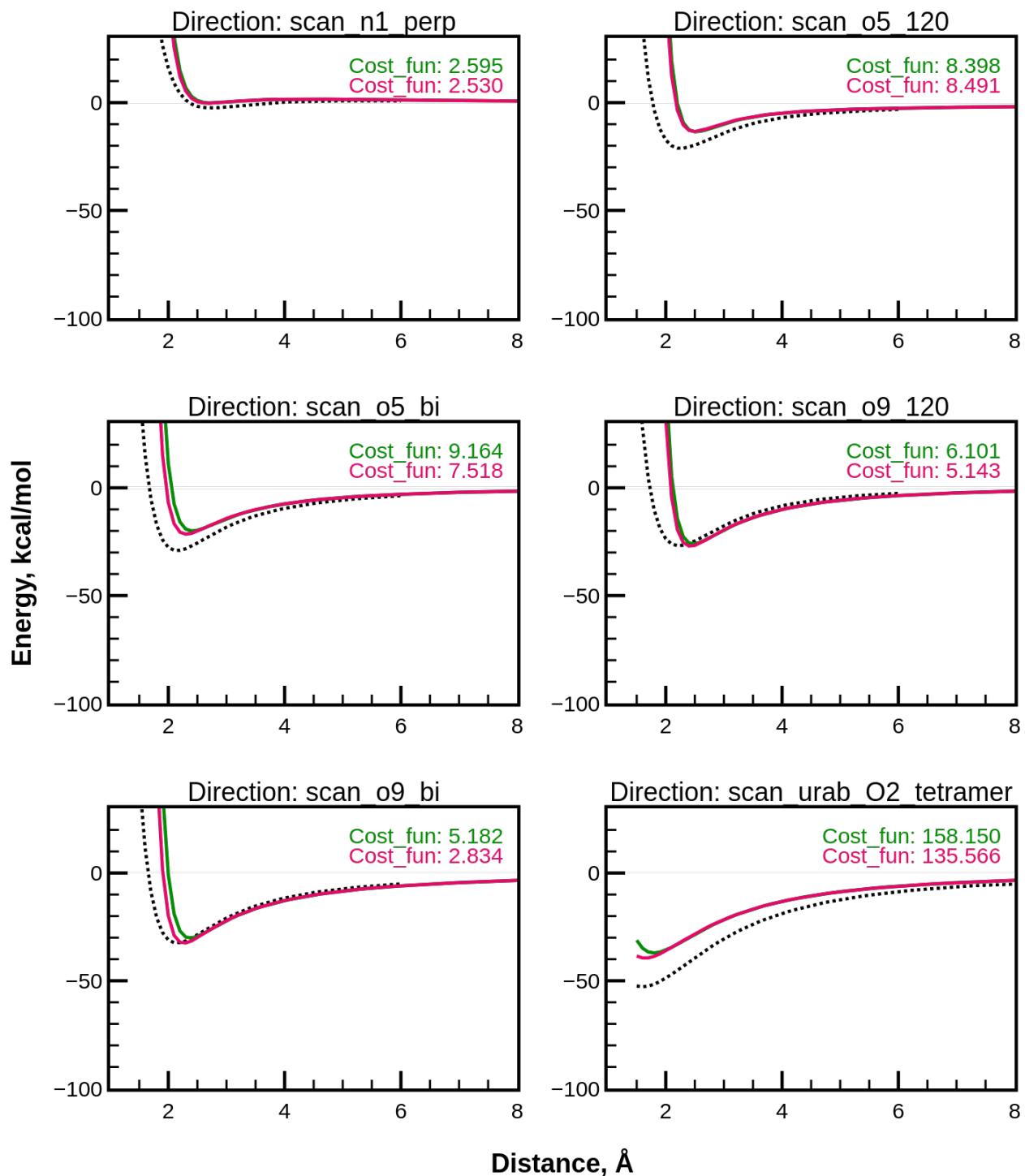
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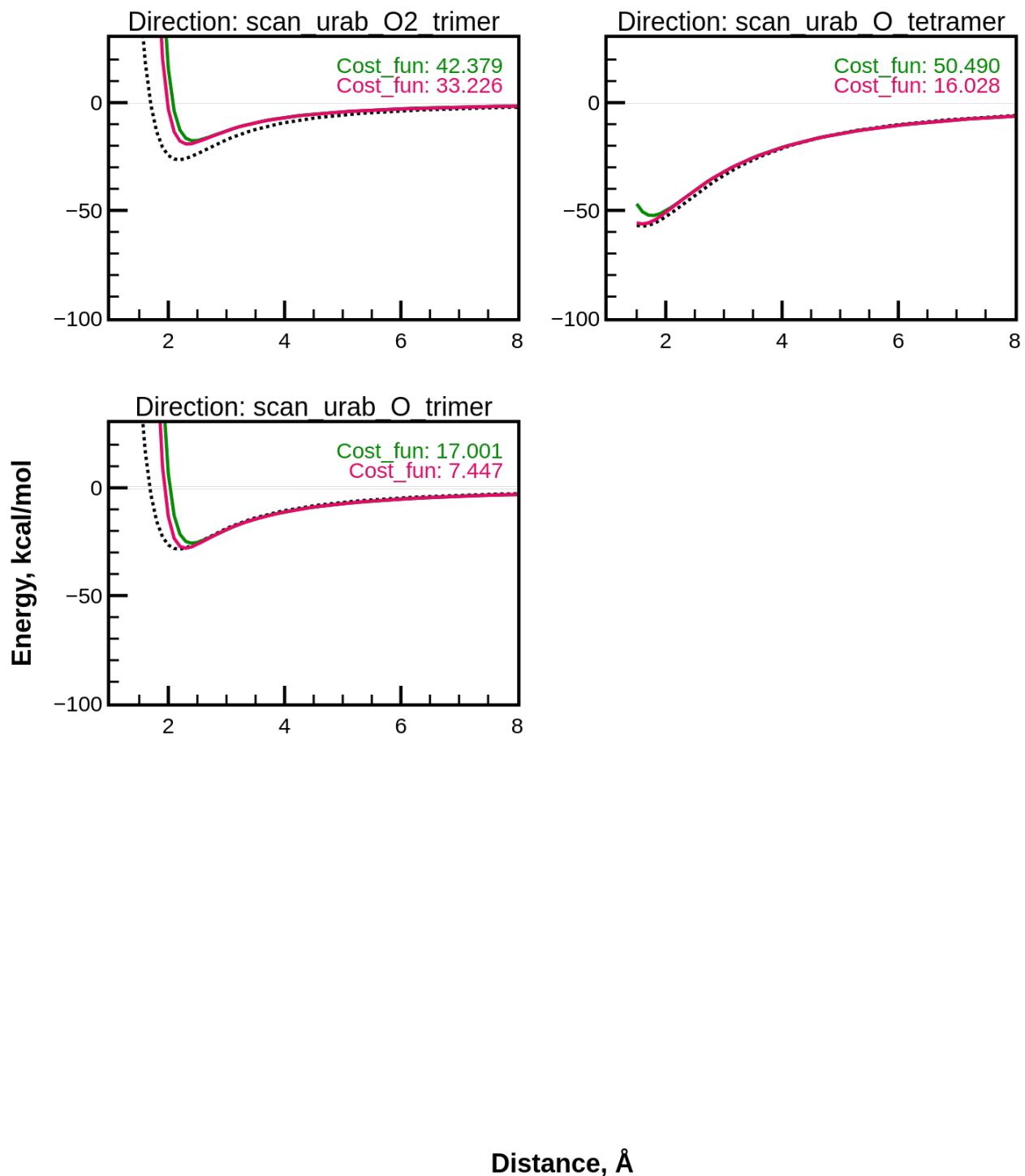
URAB LIT 2/2



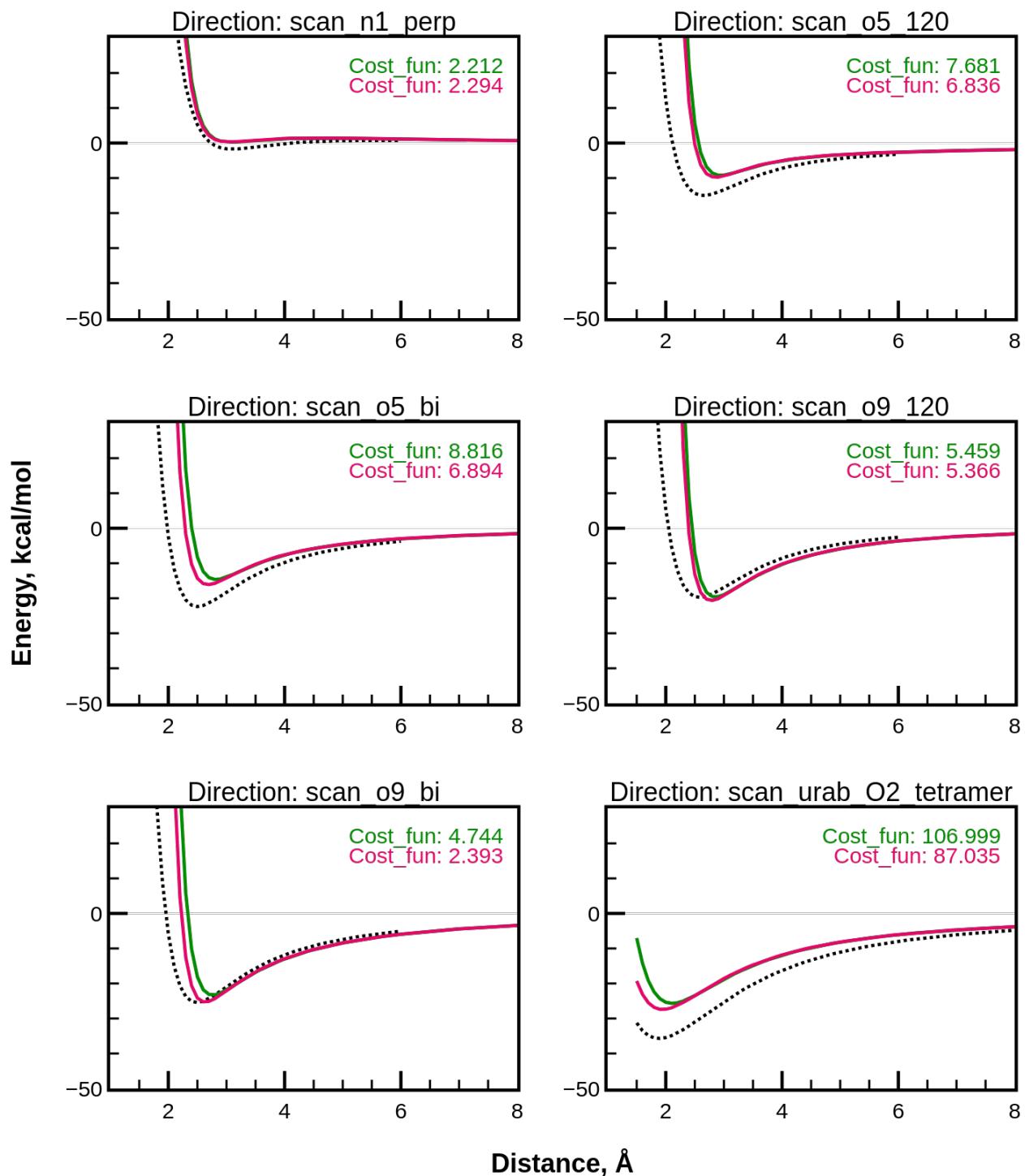
URAB SOD 1/2



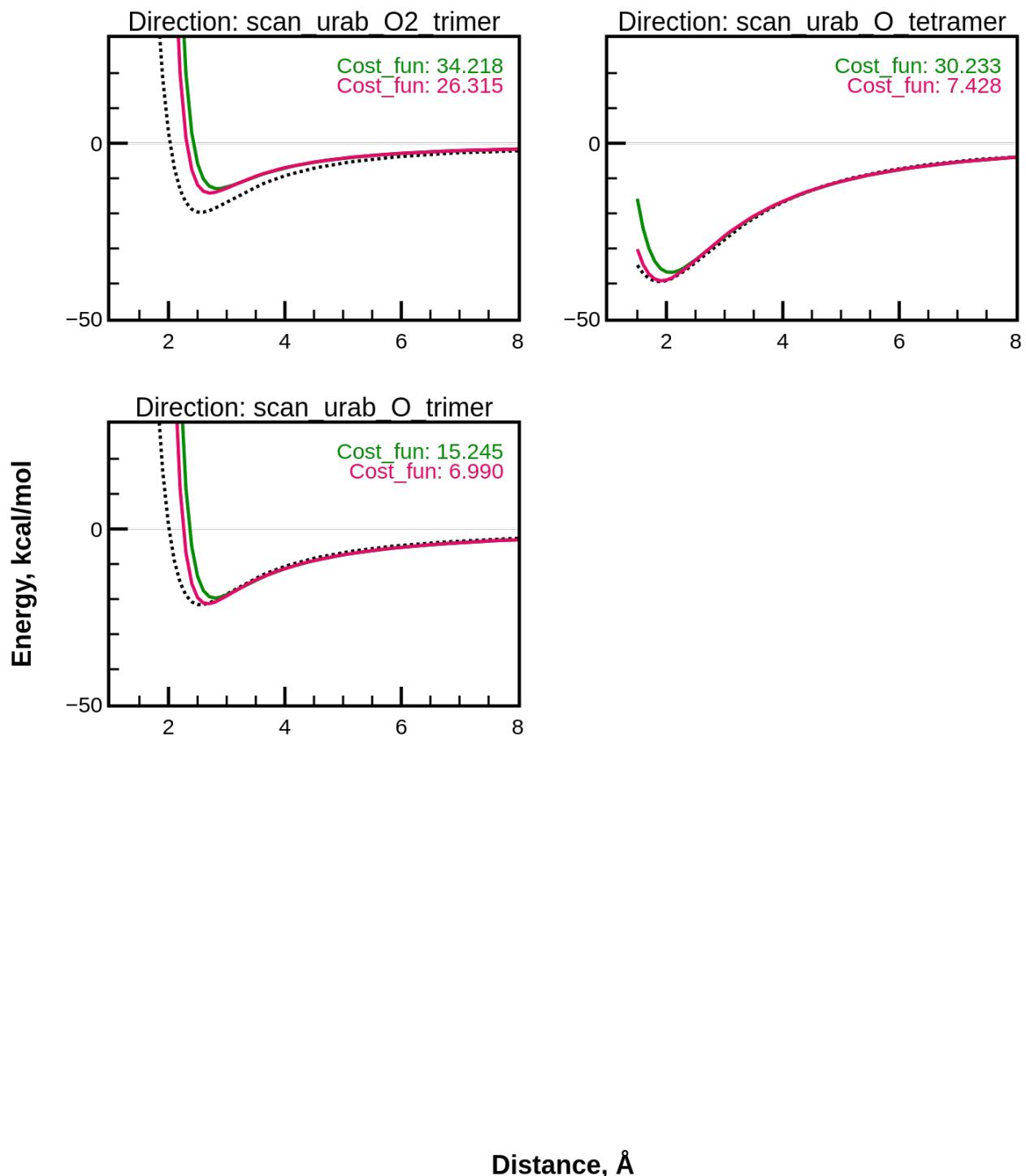
URAB SOD 2/2



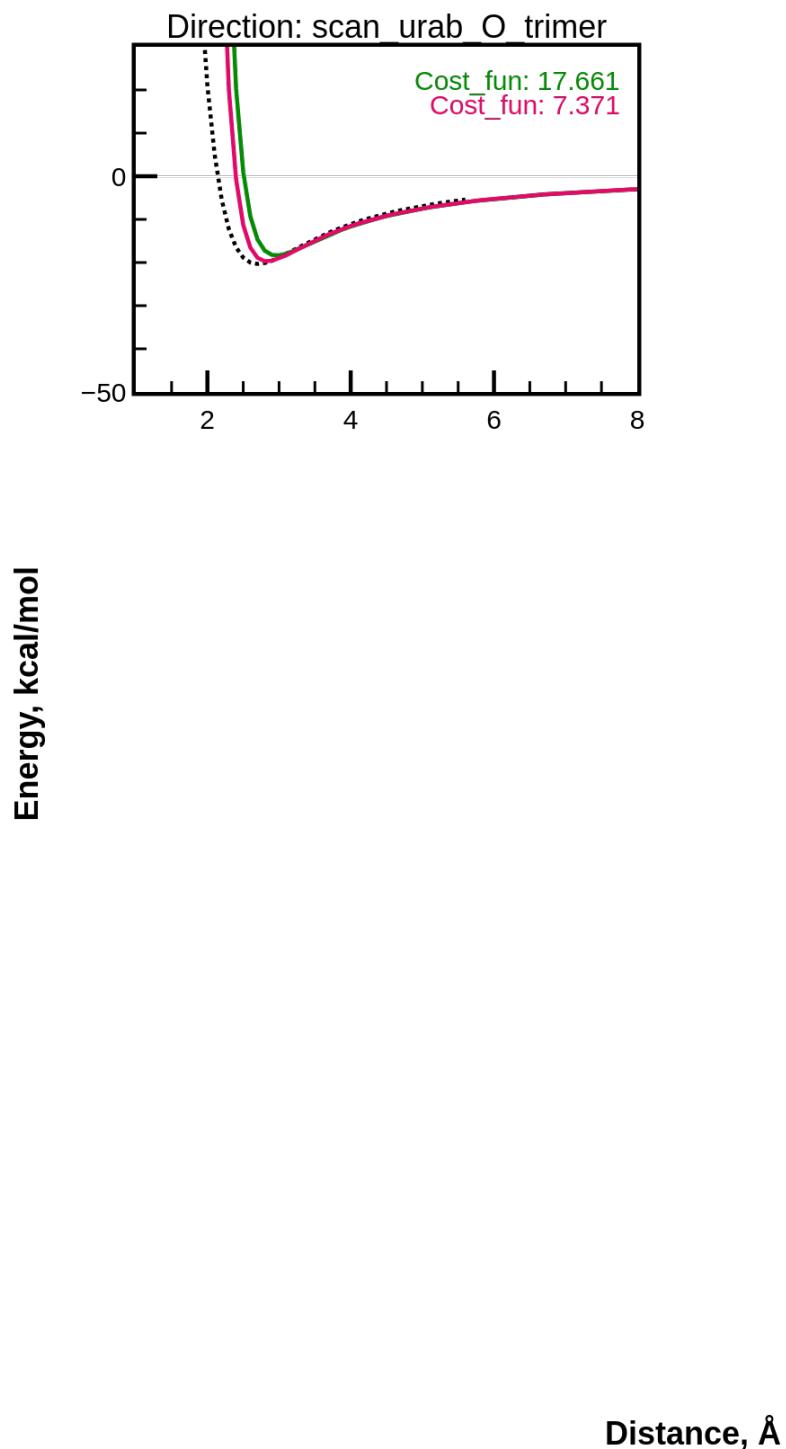
URAB POT 1/2



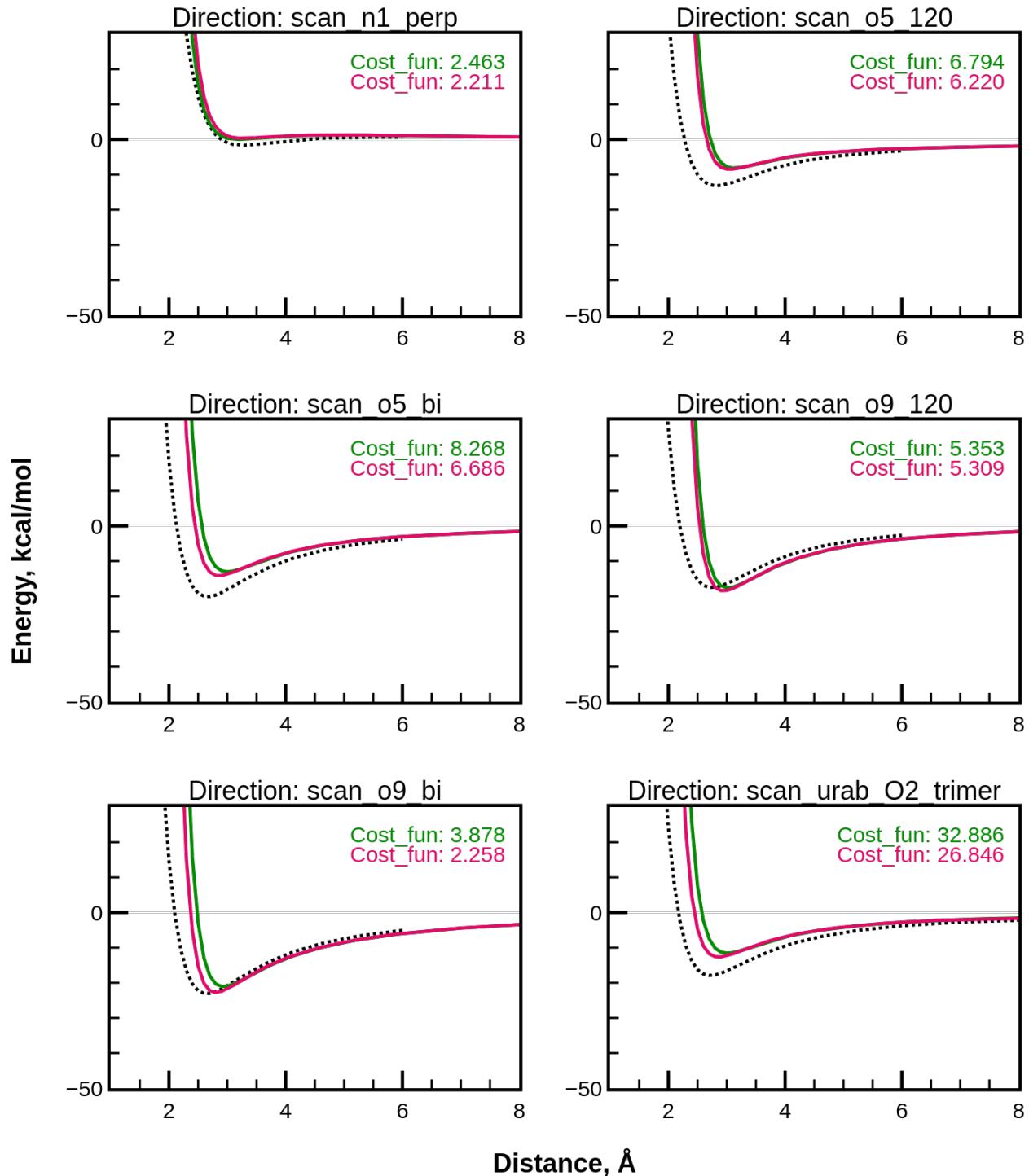
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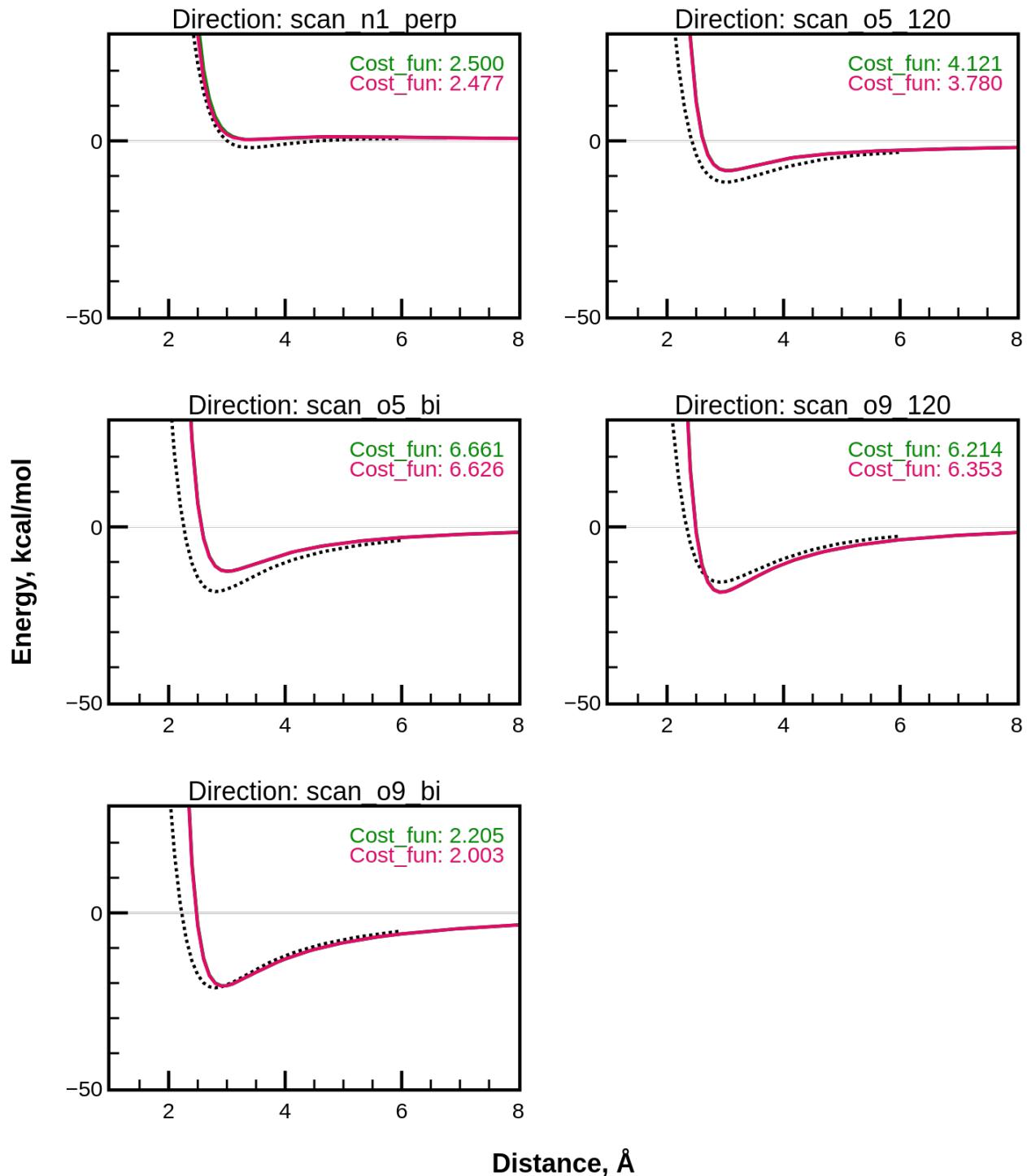
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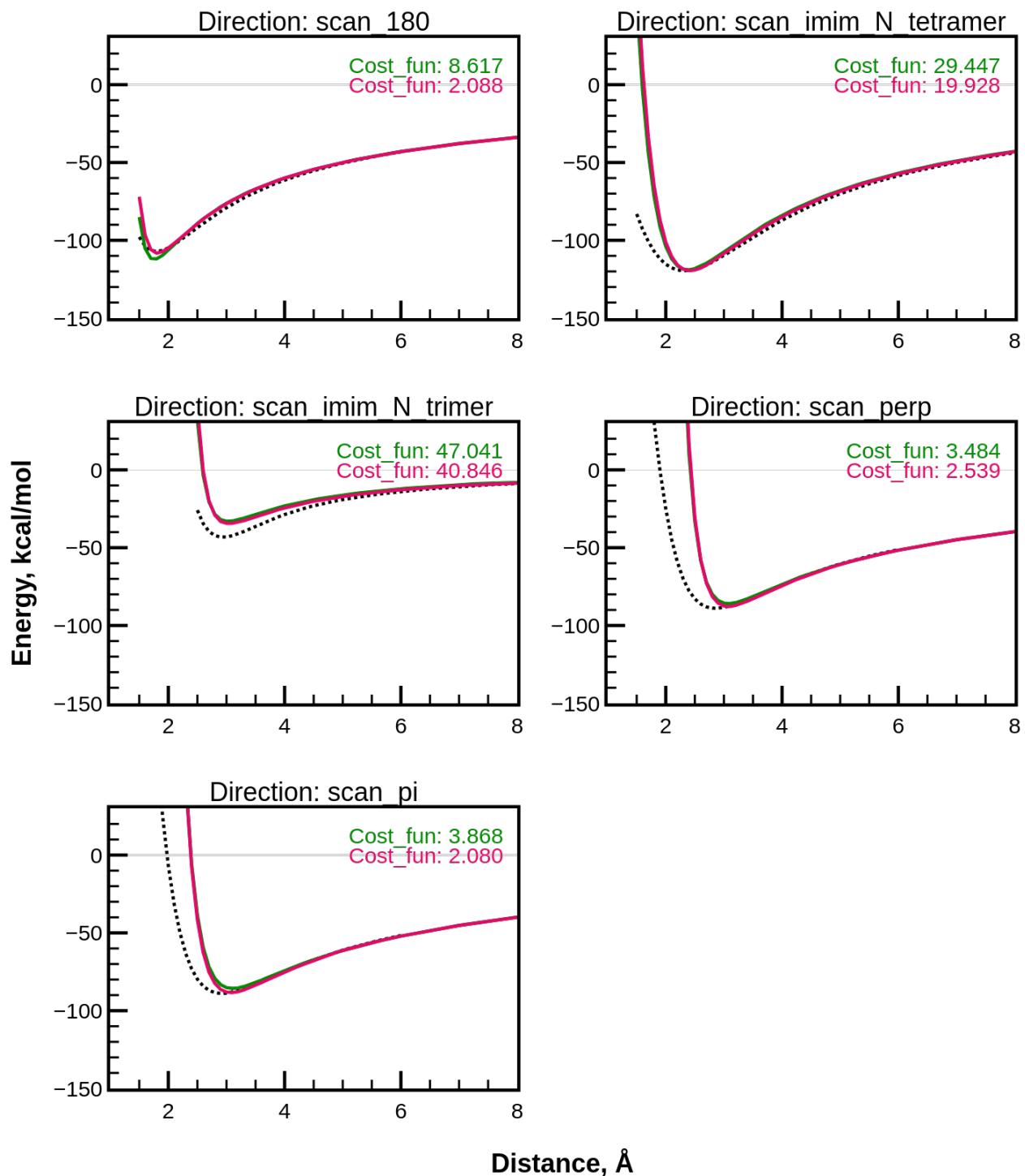
URAB RUB 1/2



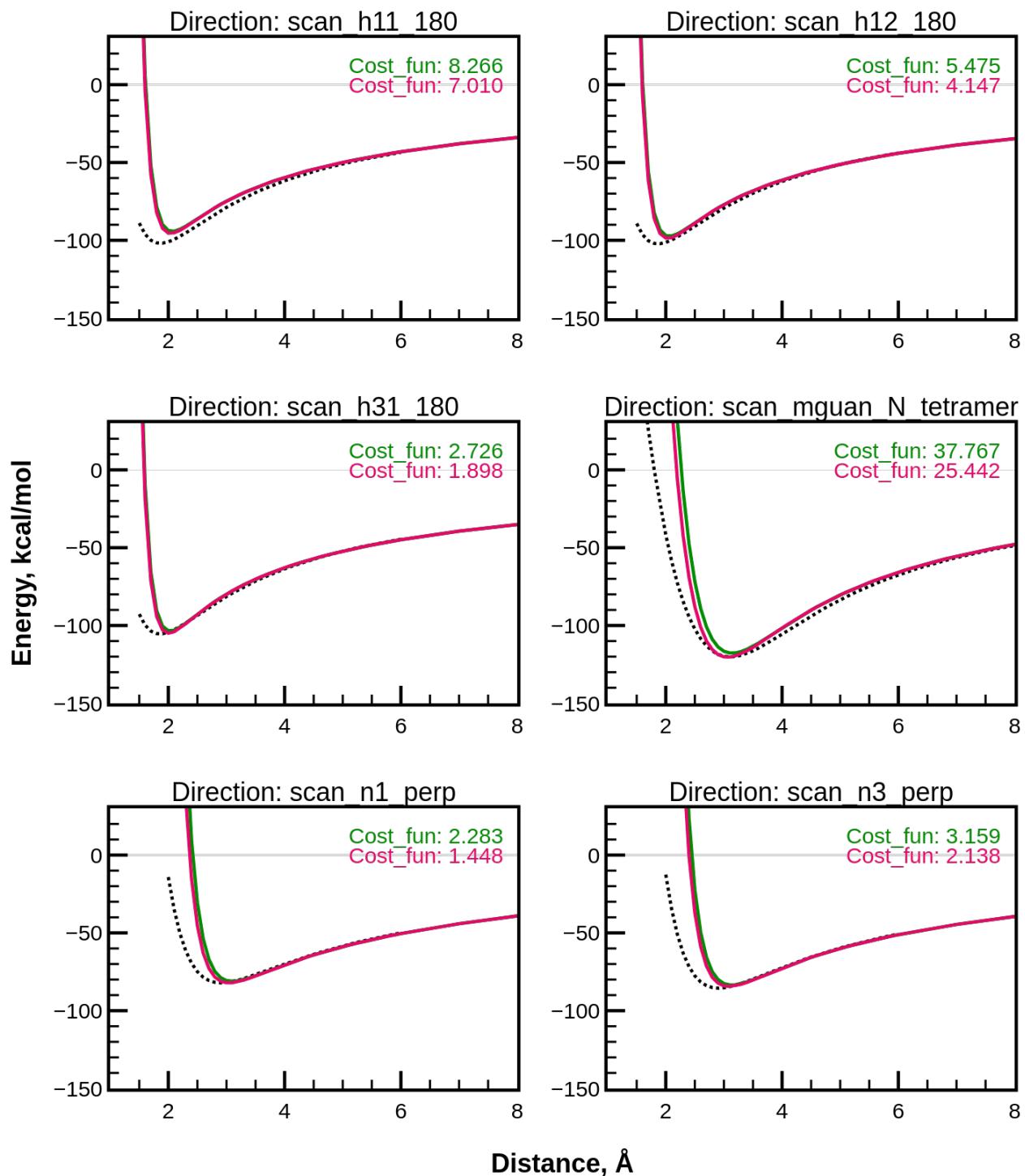
URAB CES 1/1



IMIM CLA 1/1



MGUAN CLA 1/1



NC1 CLA 1/1

