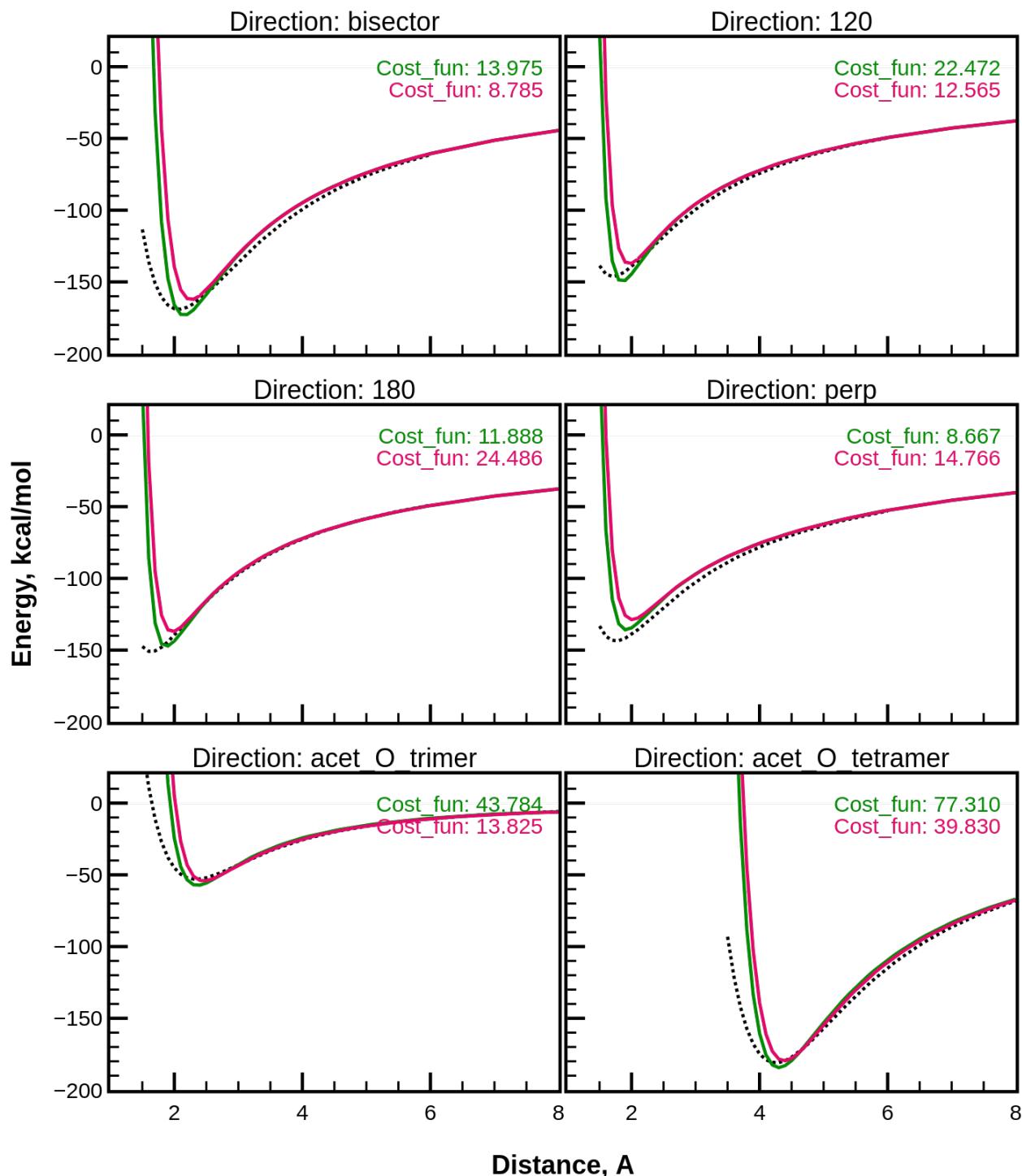


## Potential Energy Surfaces (PESs) of Ion-Model Compounds

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

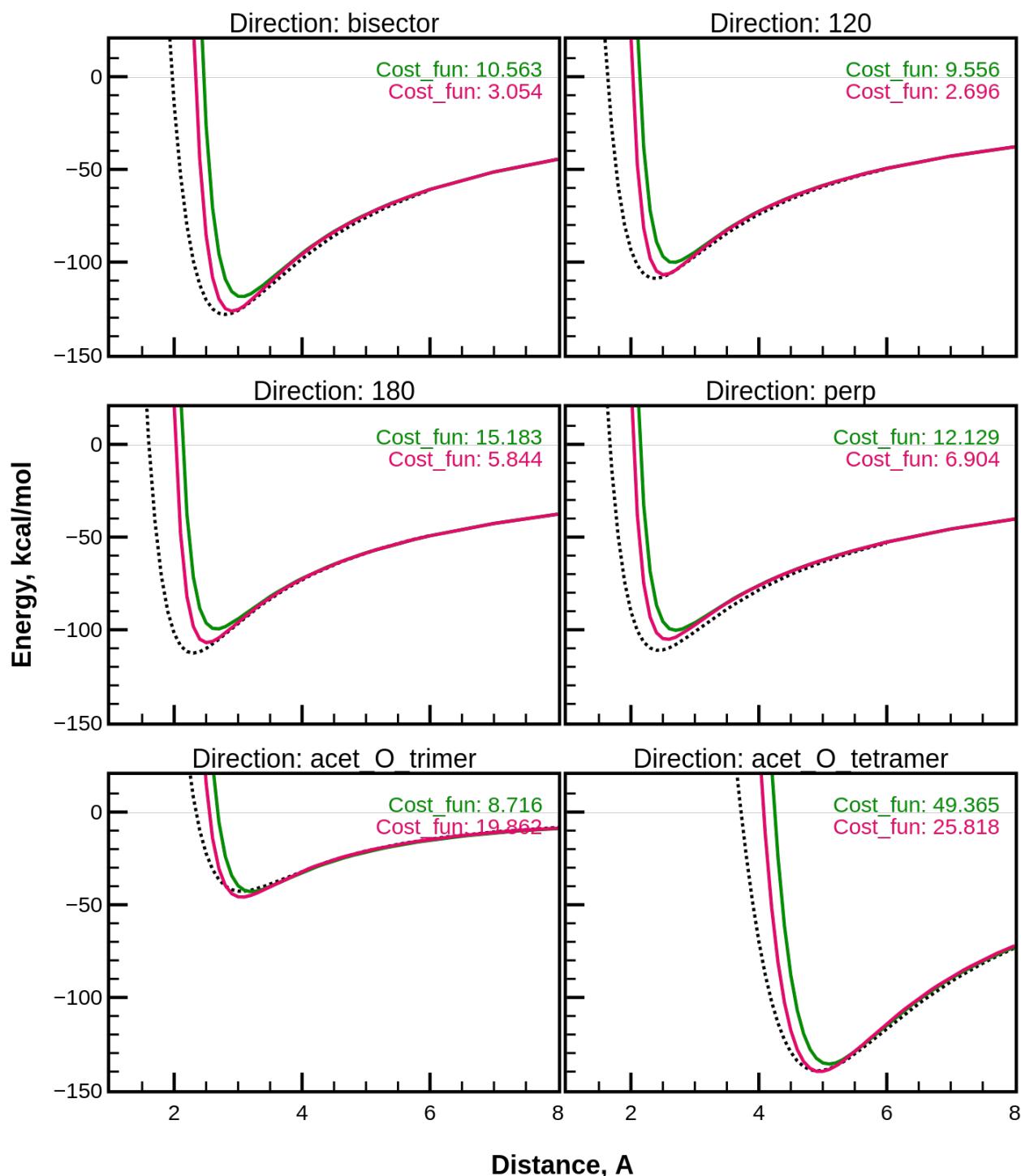
The dotted lines represent quantum mechanical (QM) results obtained using MP2/cc-pVQZ-X2C model chemistry for K<sup>+</sup>, Rb<sup>+</sup>, and Cs<sup>+</sup>, and MP2/cc-pVQZ model chemistry for all other elements. Green and pink lines correspond to the molecular mechanical (MM) PESs from the original 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.



**ACET LIT 1/1**2.92000\_0.09487\_9.99999  
3.00493\_0.09487\_1.26652

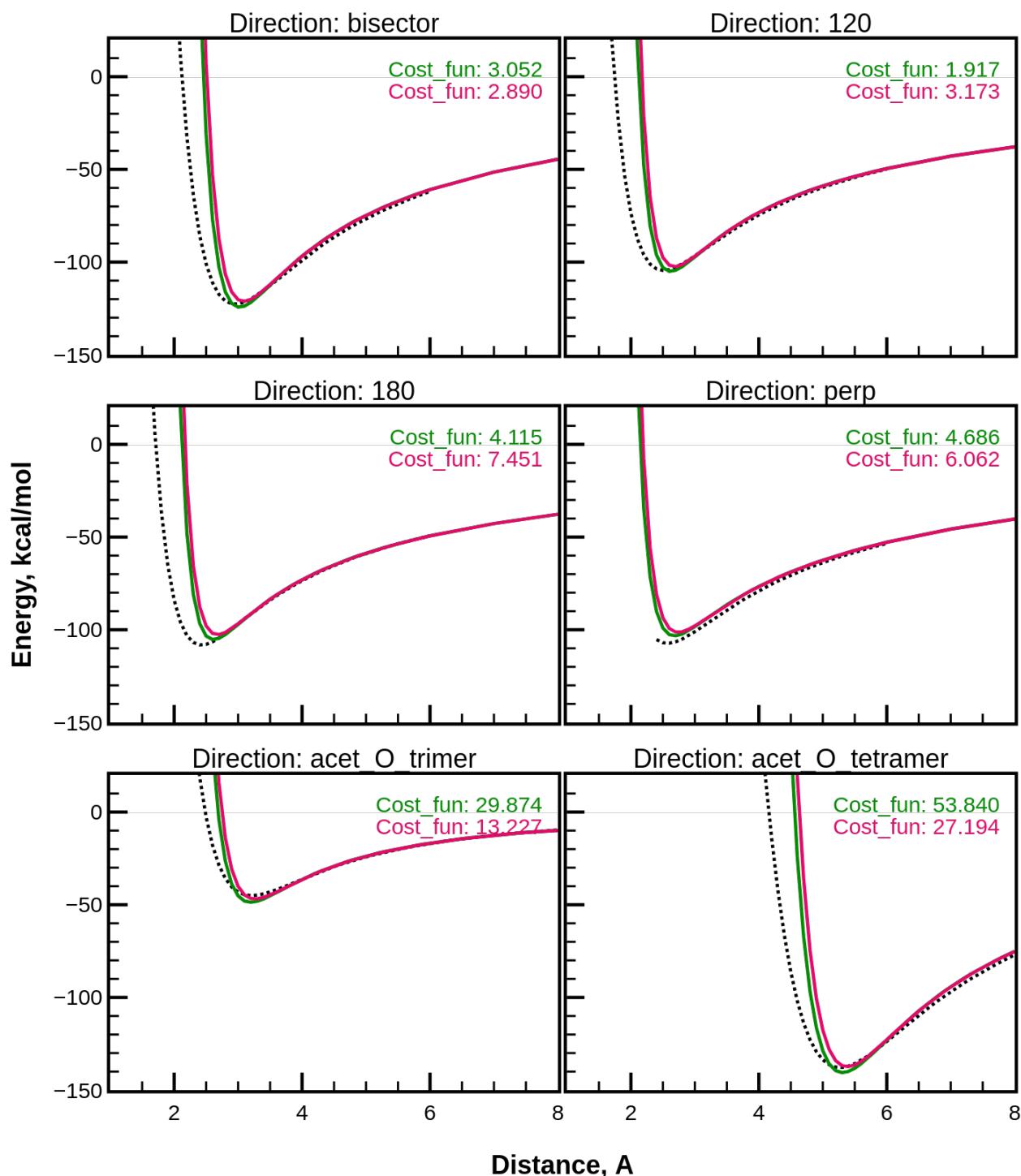
# ACET POT 1/1

3.75000\_0.16850\_0.75000  
3.57951\_0.16850\_1.36307



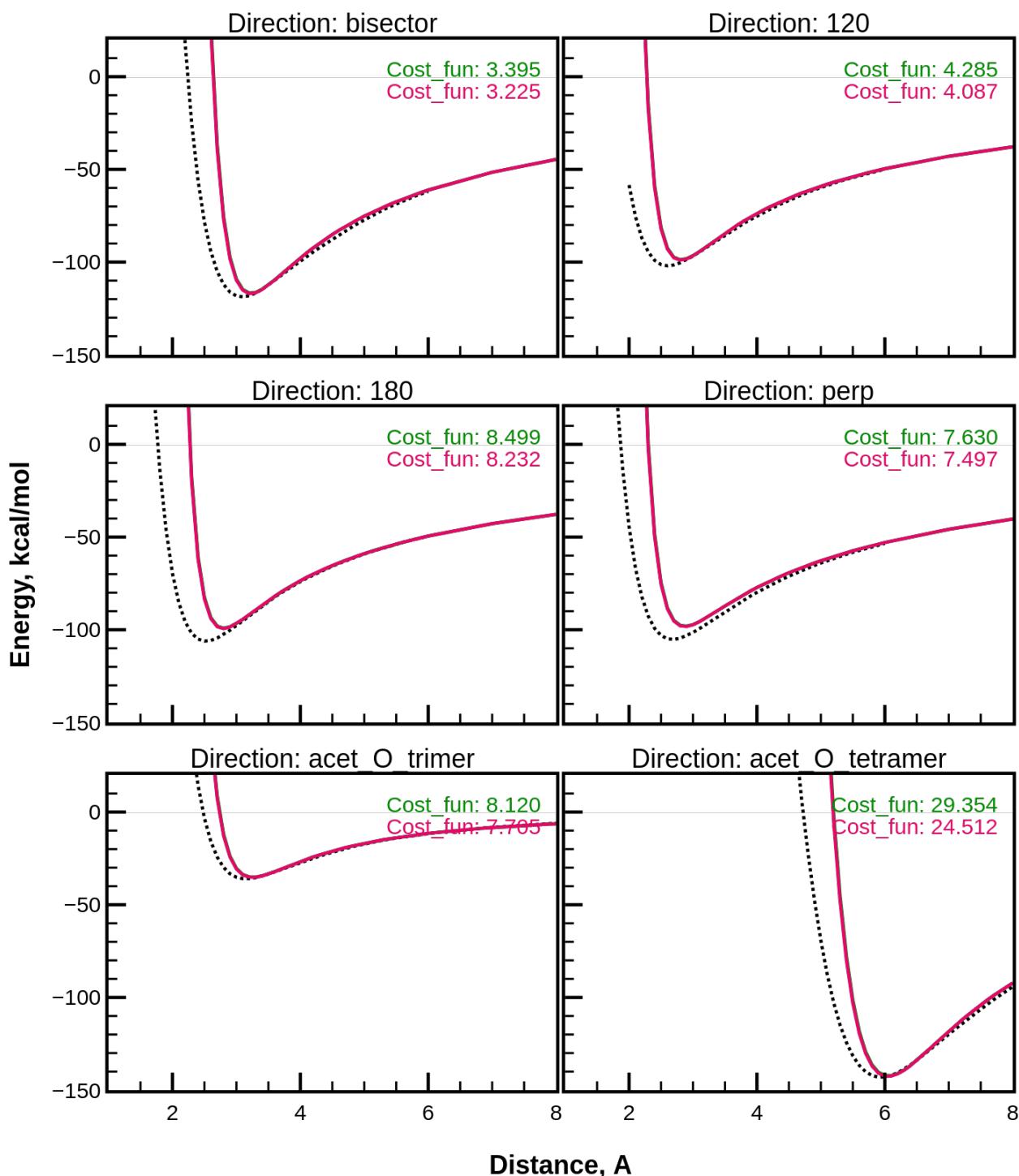
# ACET RUB 1/1

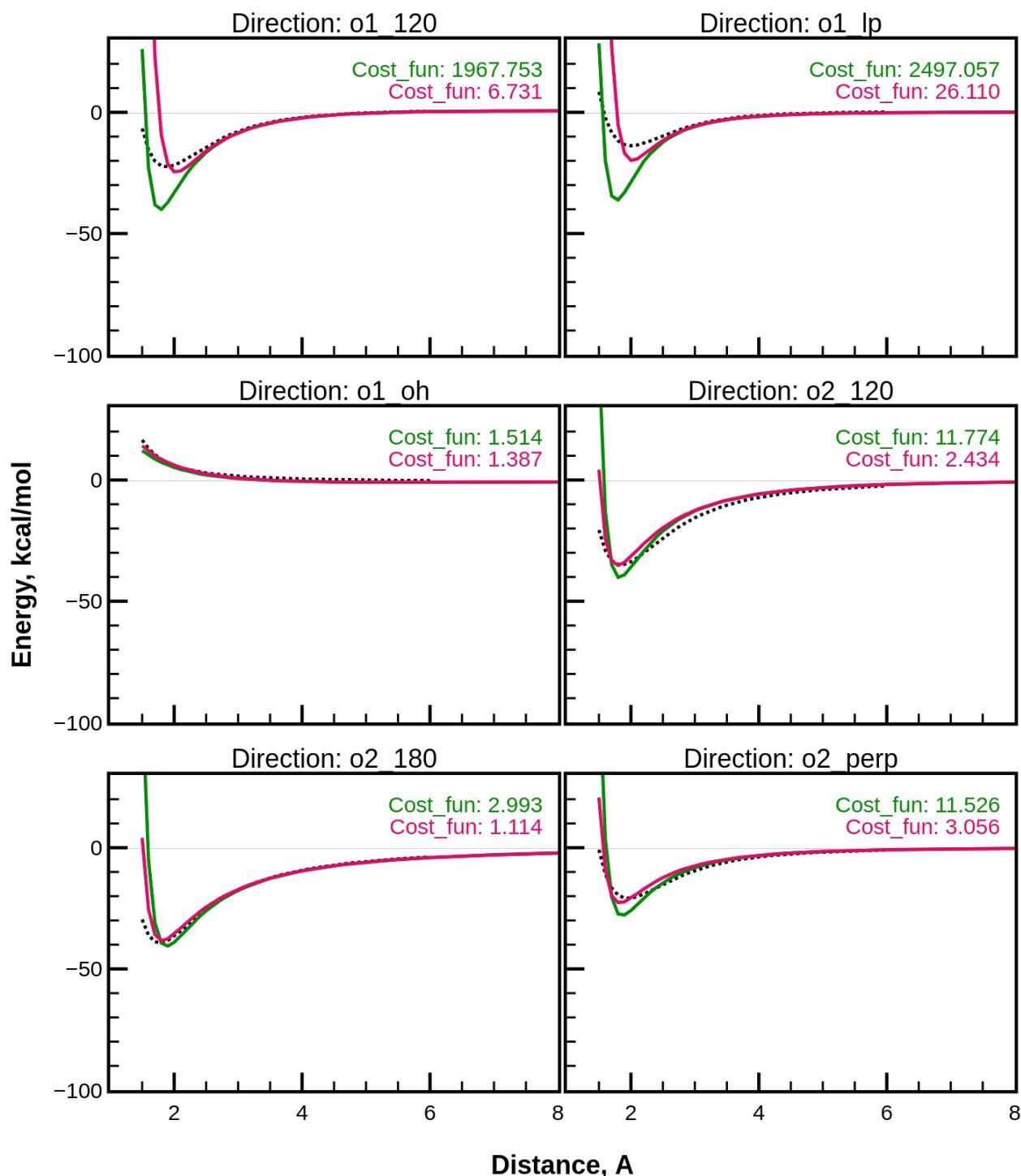
3.60551\_0.28622\_9.99999  
3.67610\_0.28622\_4.45401



# ACET CES 1/1

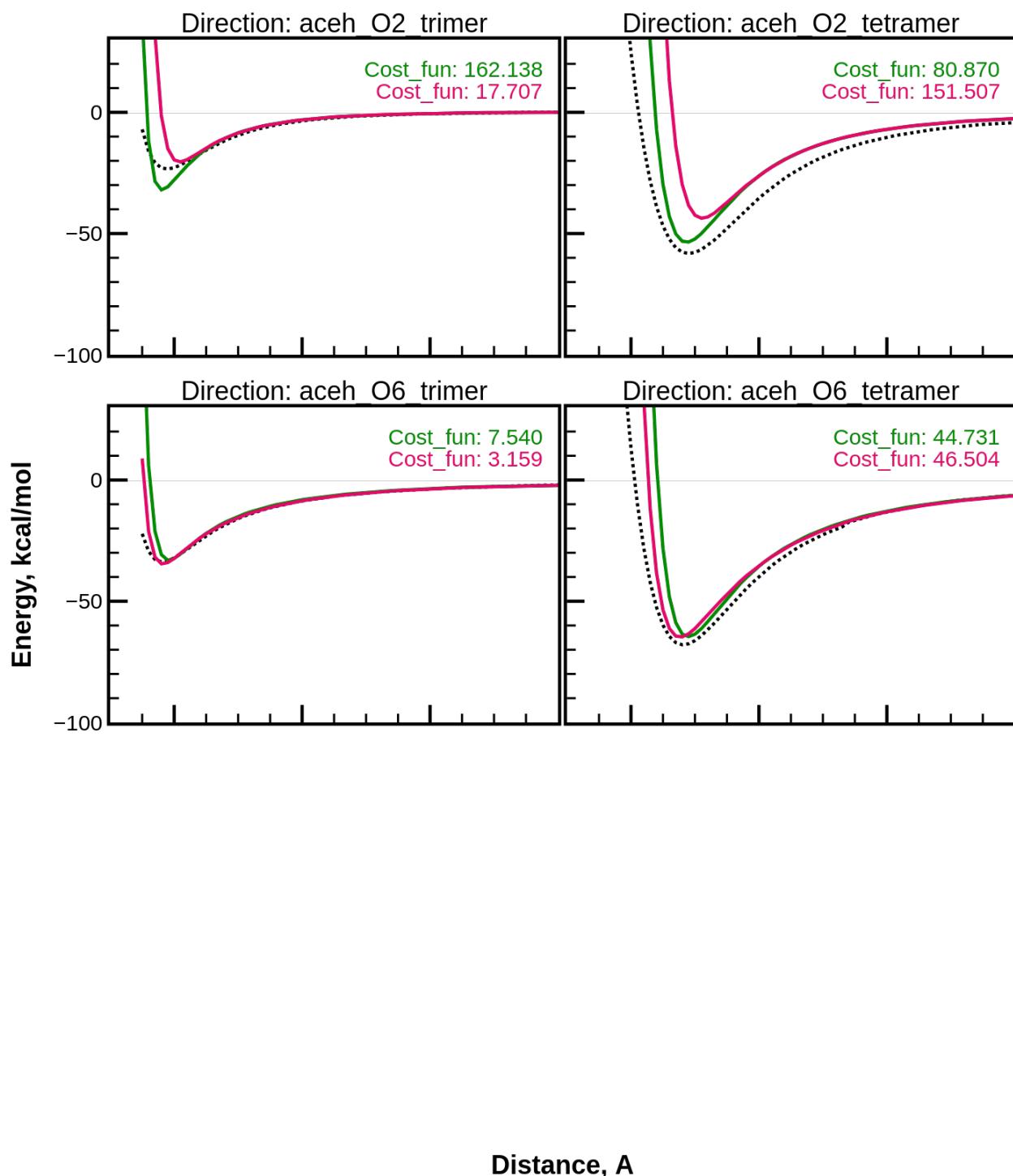
3.84382\_0.28806\_9.99999  
3.83656\_0.28806\_4.06696



**ACEH LIT 1/2**2.85000\_0.07348\_9.99999  
2.65664\_0.07348\_0.64546

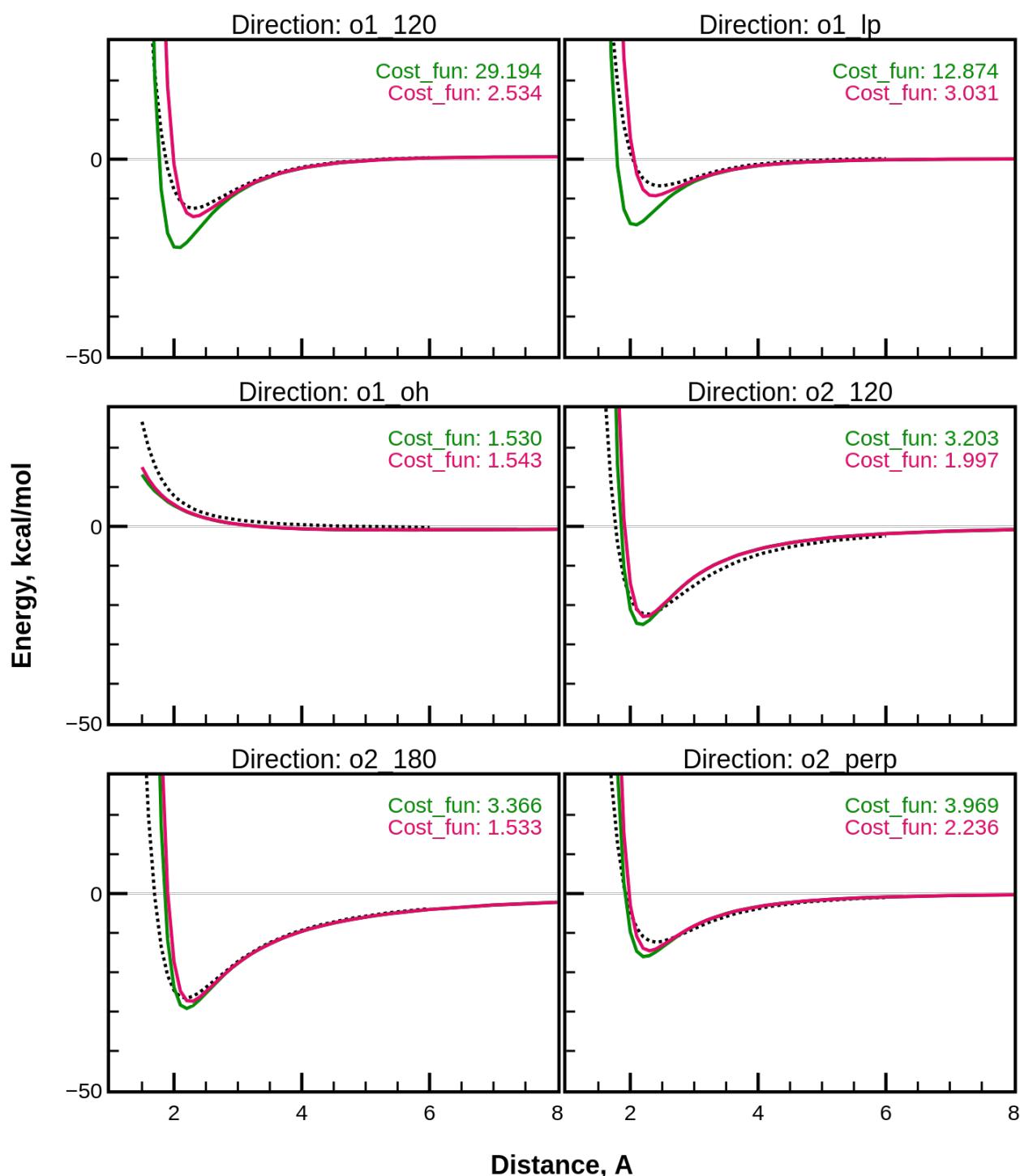
## ACEH LIT 2/2

2.85000\_0.07348\_9.99999  
2.65664\_0.07348\_0.64546



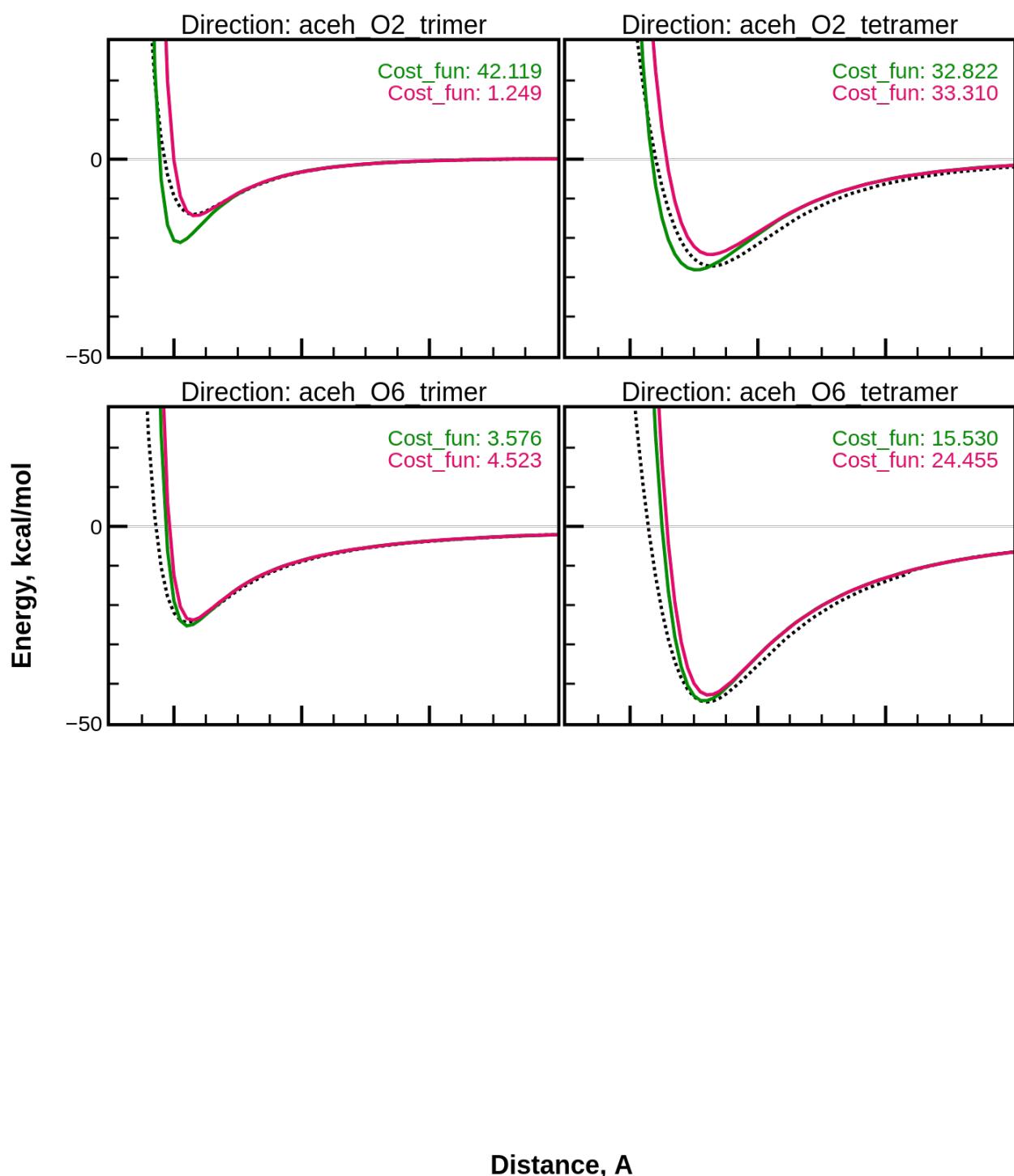
# ACEH SOD 1/2

3.21168\_0.07531\_9.99999  
3.28395\_0.07531\_3.34812



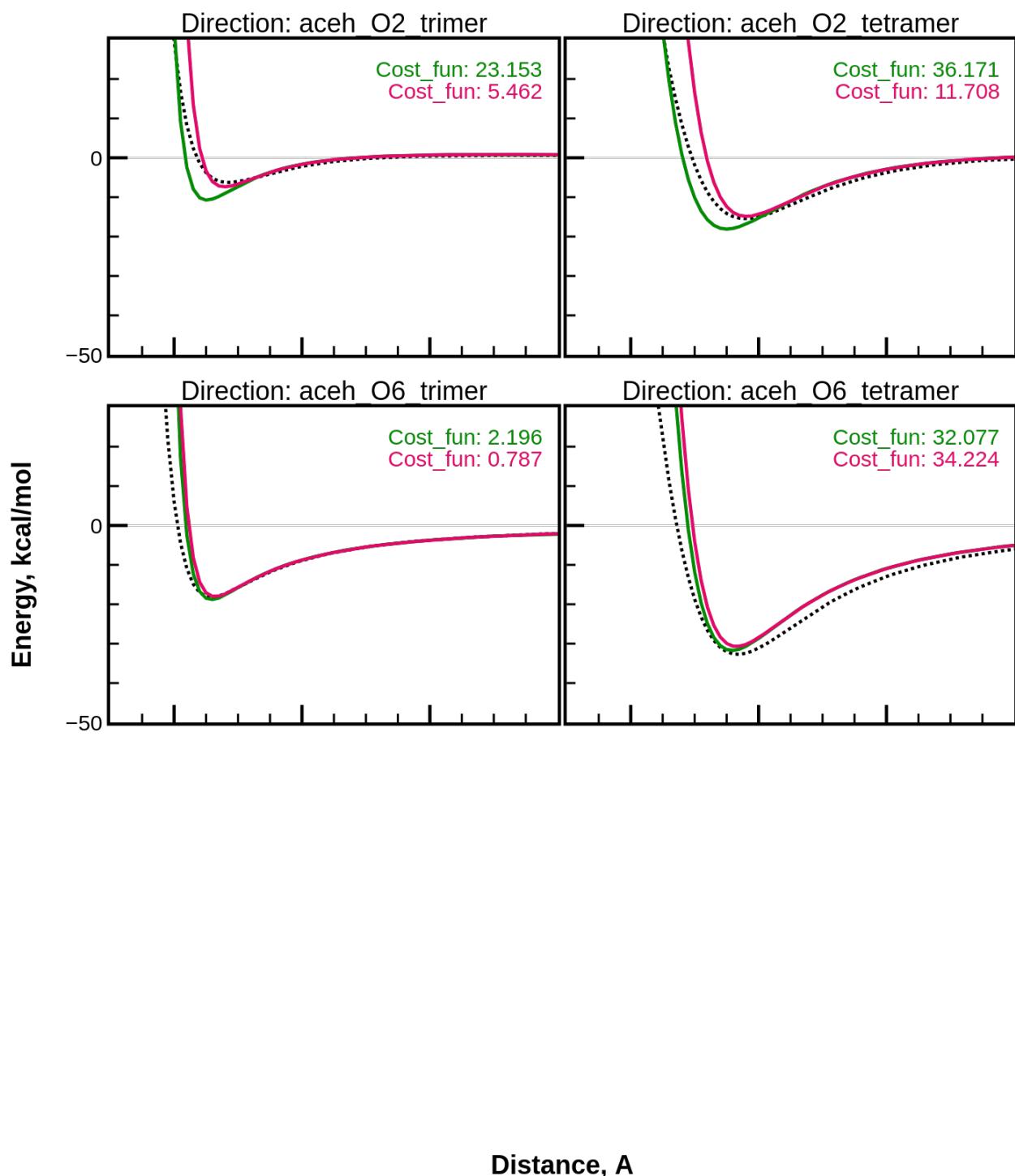
# ACEH SOD 2/2

3.21168\_0.07531\_9.99999  
3.28395\_0.07531\_3.34812



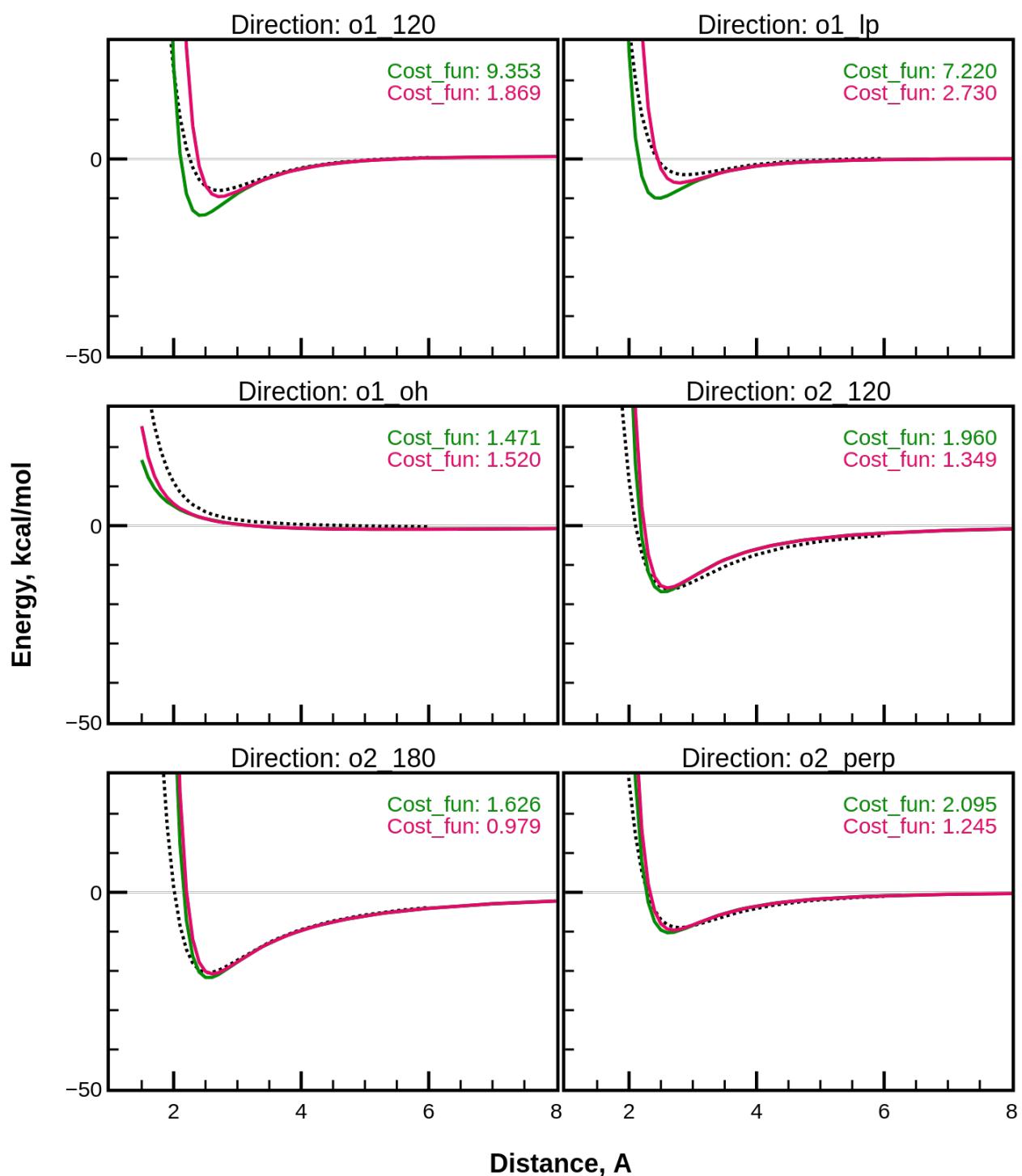
# ACEH POT 2/2

3.43665\_0.15983\_9.99999  
3.49368\_0.15983\_2.83217



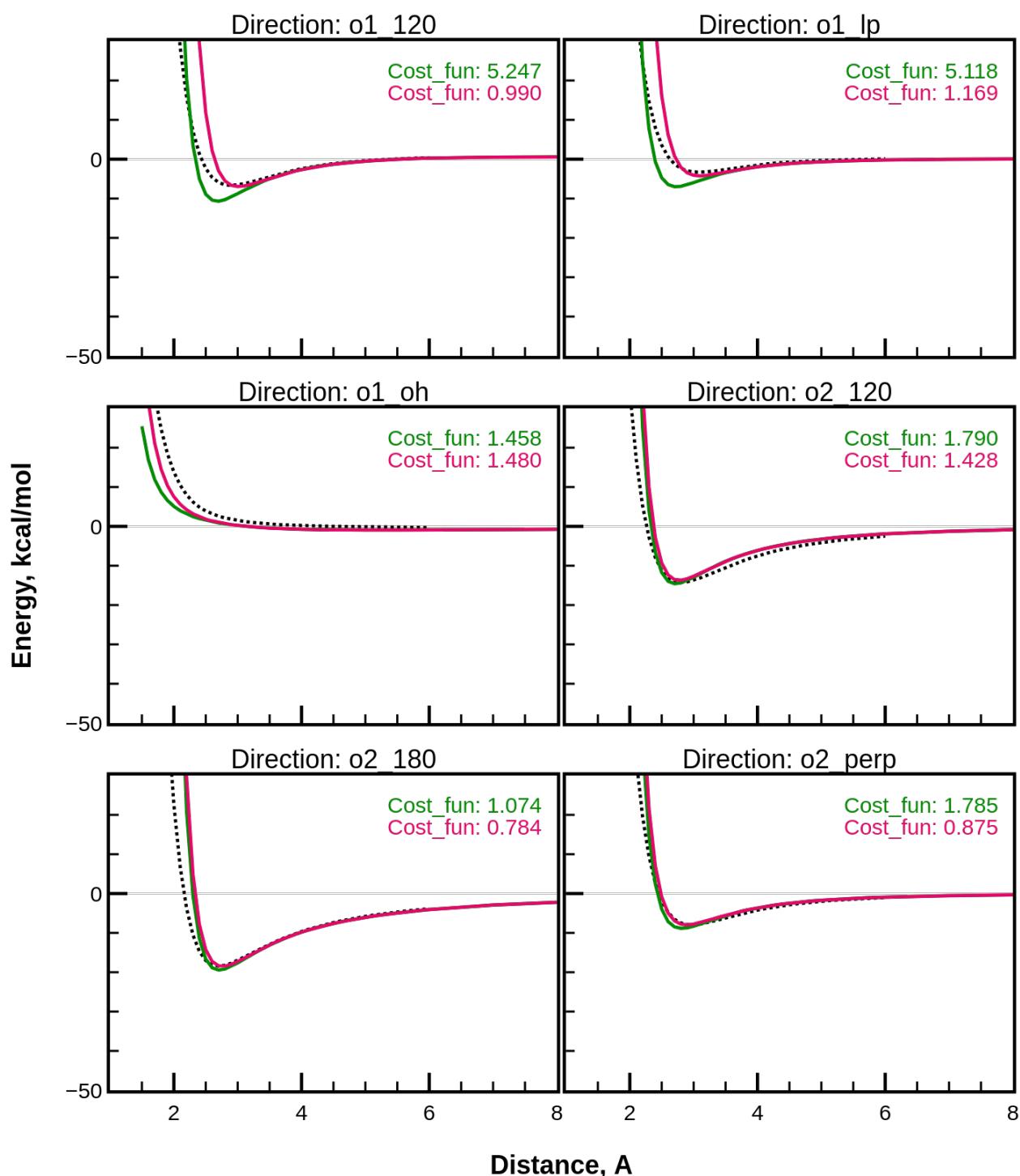
# ACEH POT 1/2

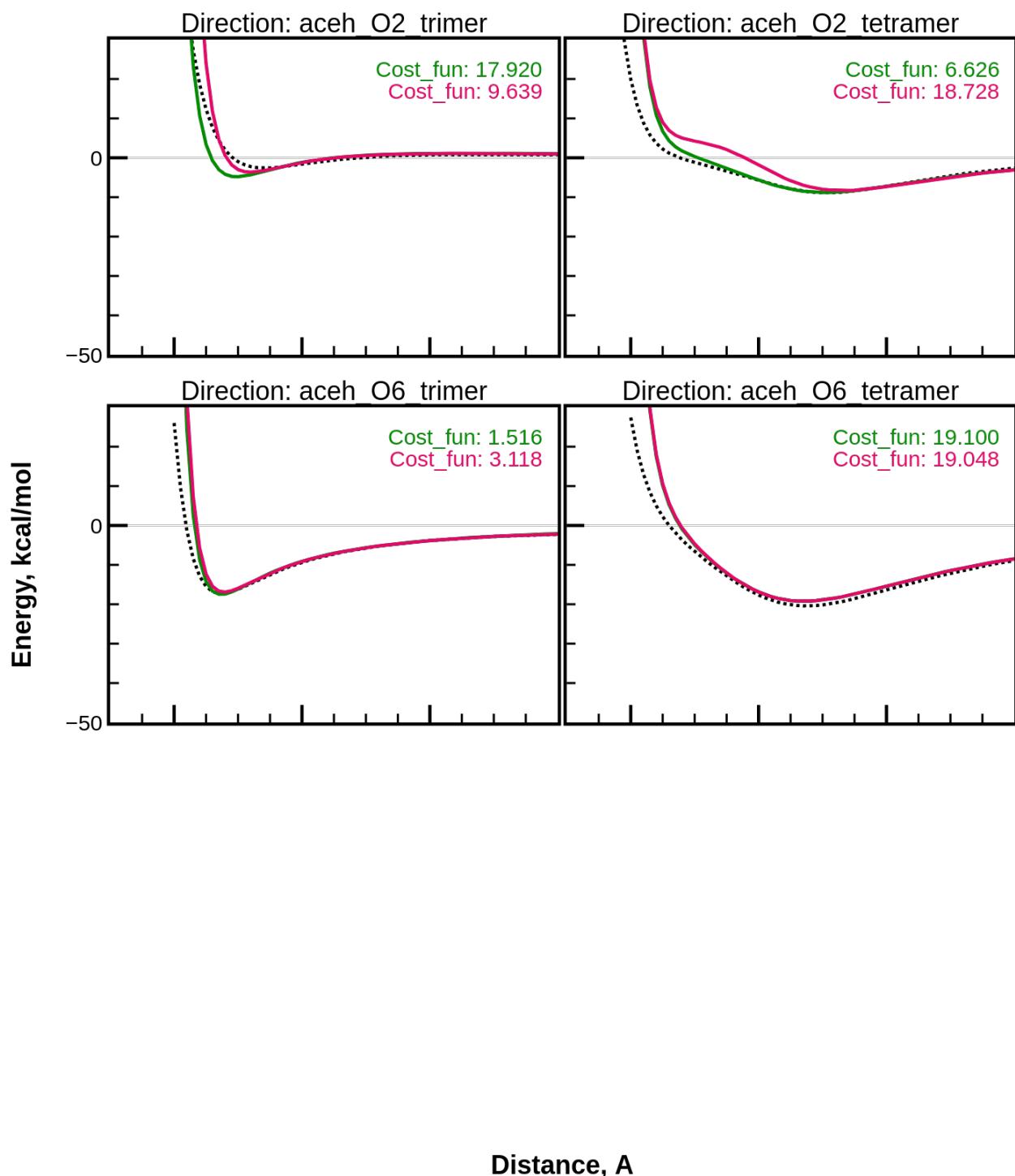
3.43665\_0.15983\_9.99999  
3.49368\_0.15983\_2.83217



# ACEH RUB 1/2

3.53551\_0.22170\_9.99999  
3.55885\_0.22170\_1.61222

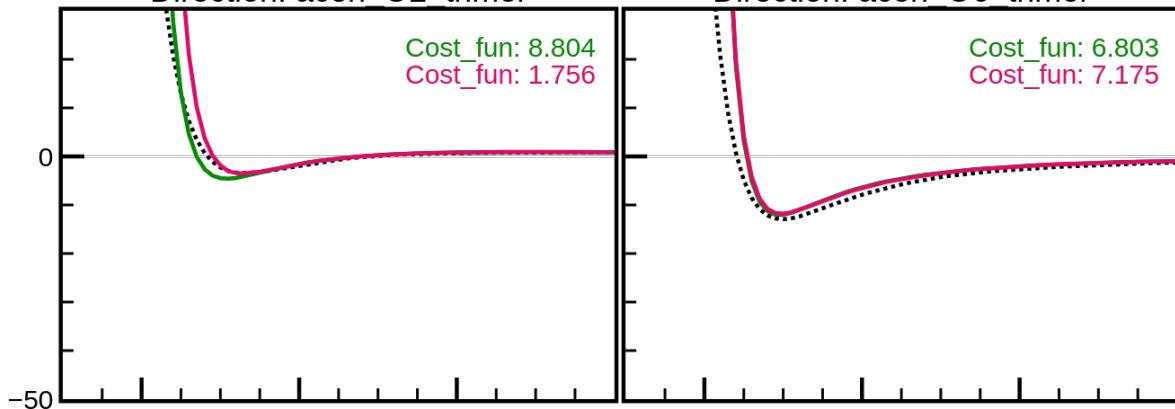


**ACEH RUB 2/2**3.53551\_0.22170\_9.99999  
3.55885\_0.22170\_1.61222

**ACEH CES 2/2**3.77382\_0.22313\_9.99999  
3.76247\_0.22313\_1.03679

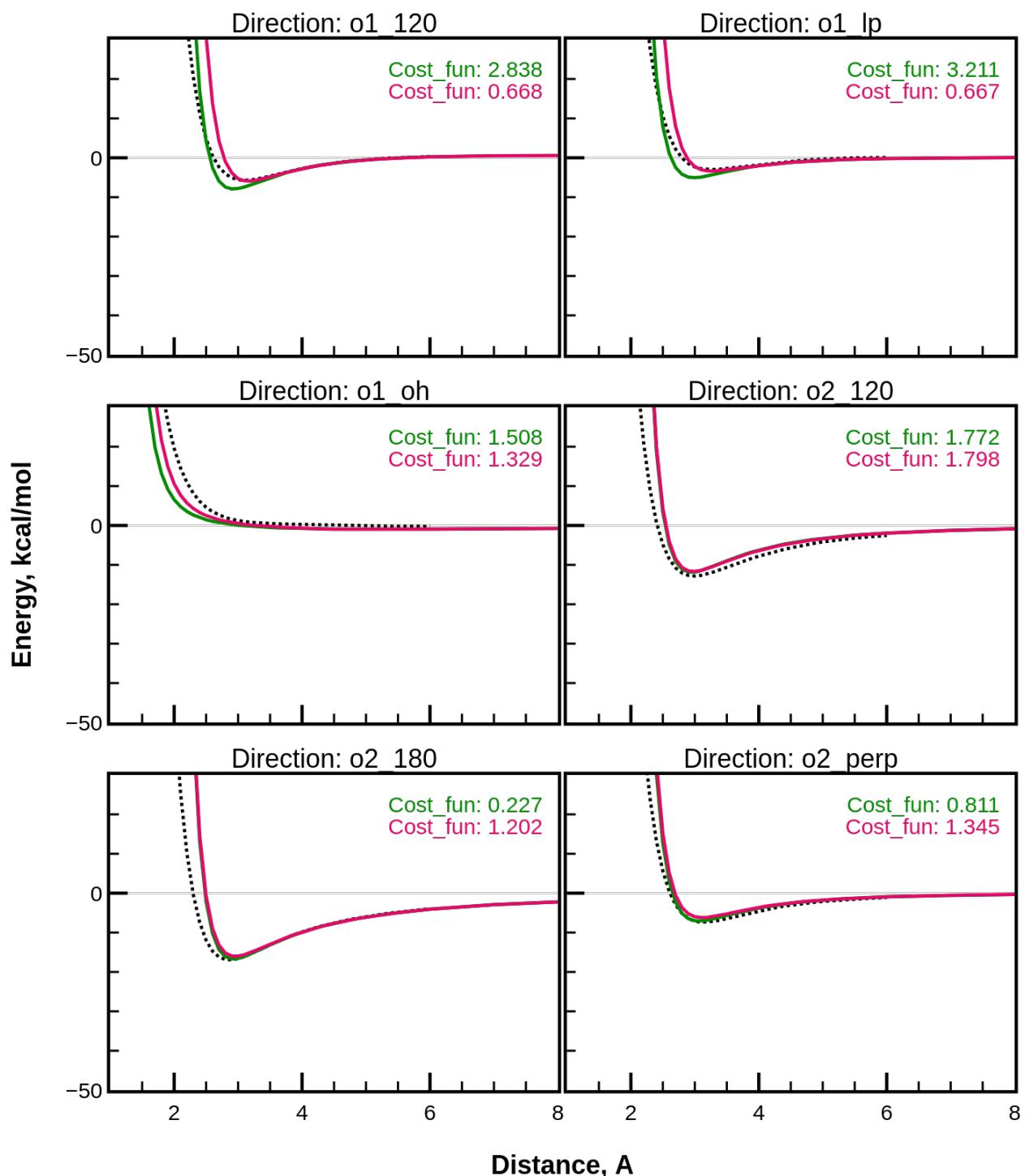
Direction: aceh\_O2\_trimer

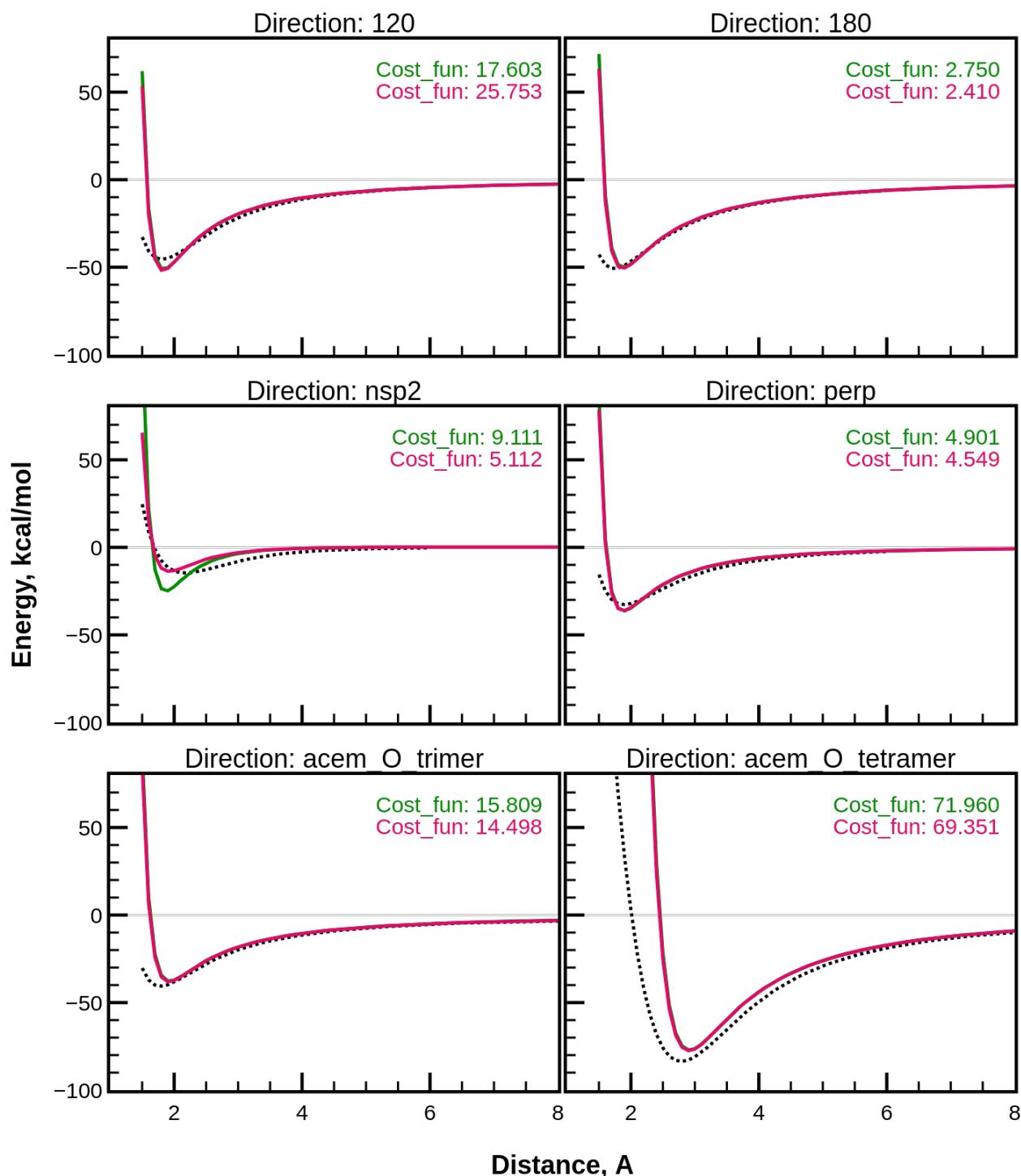
Direction: aceh\_O6\_trimer

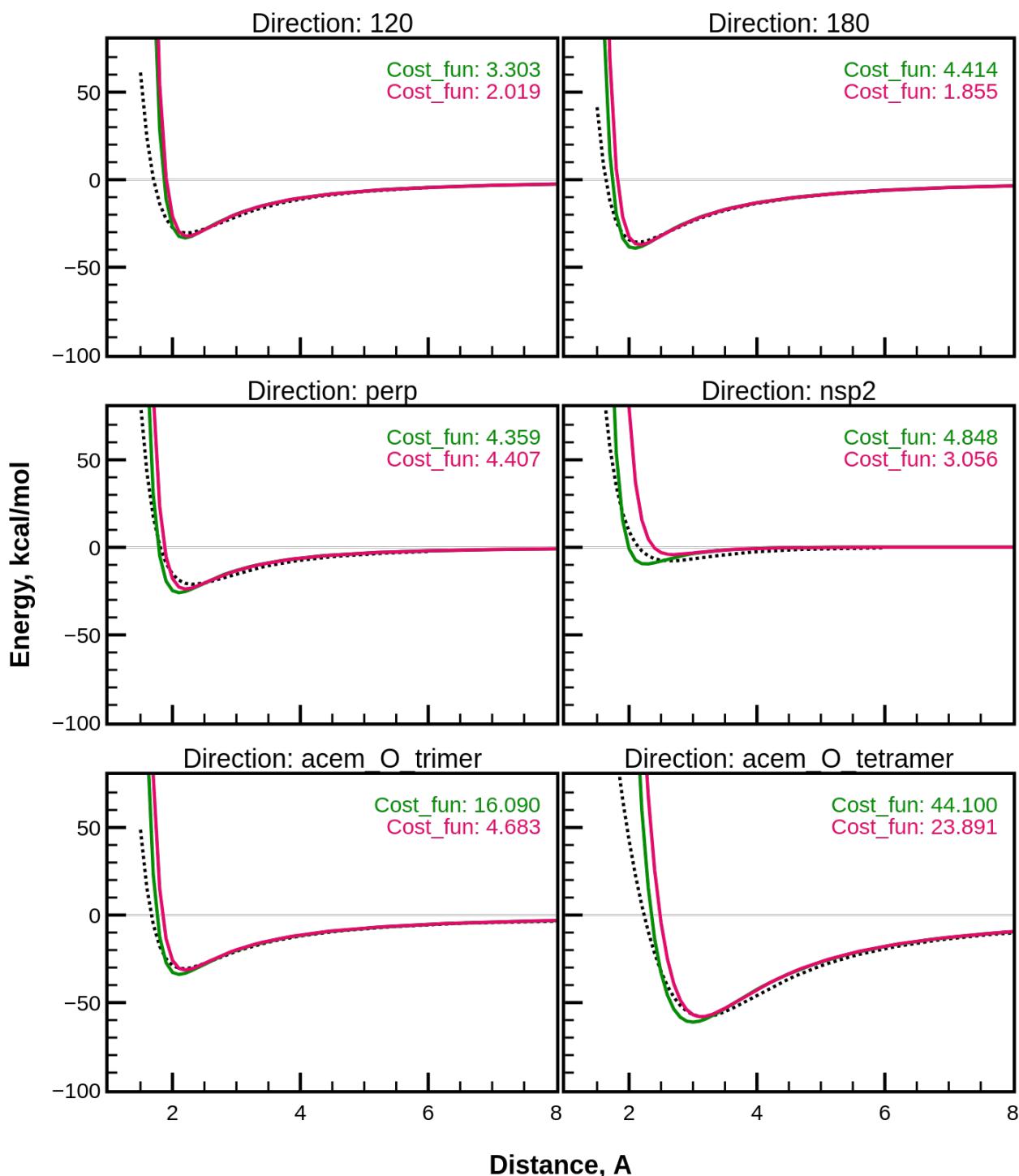
**Distance, A**

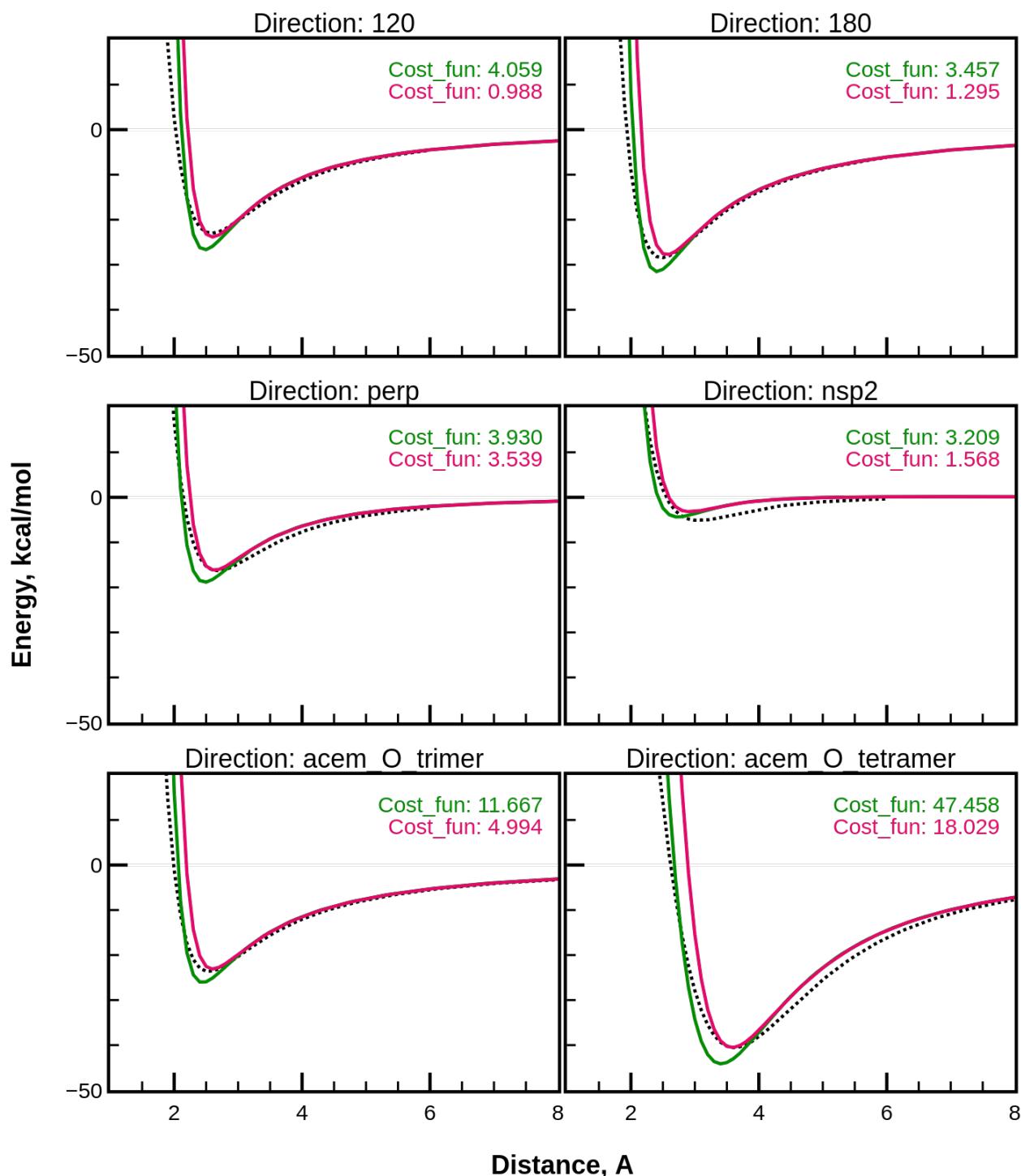
# ACEH CES 1/2

3.77382\_0.22313\_9.99999  
3.76247\_0.22313\_1.03679



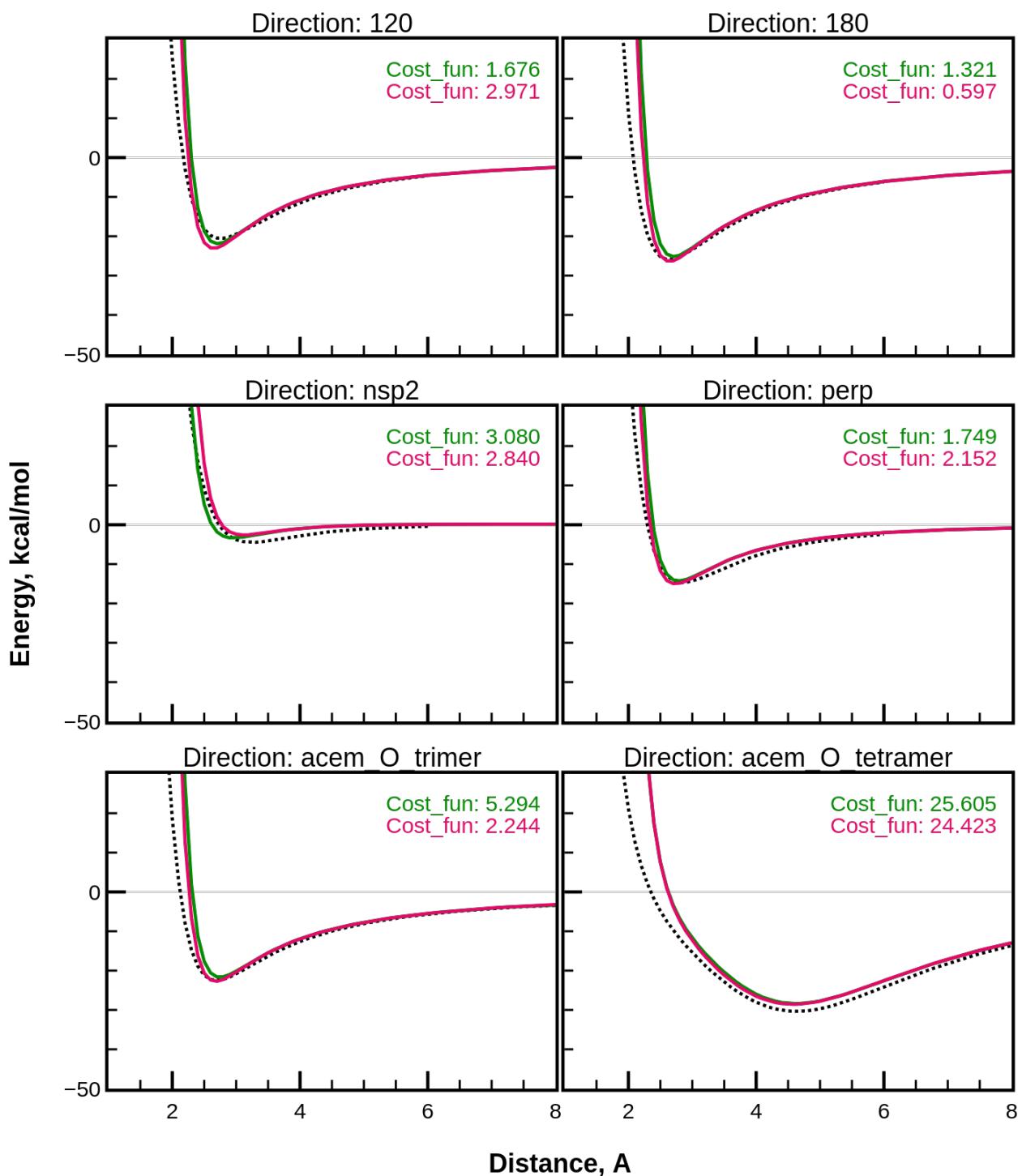
**ACEM LIT 1/1**2.88000\_0.07746\_9.99999  
2.86833\_0.07746\_4.93098

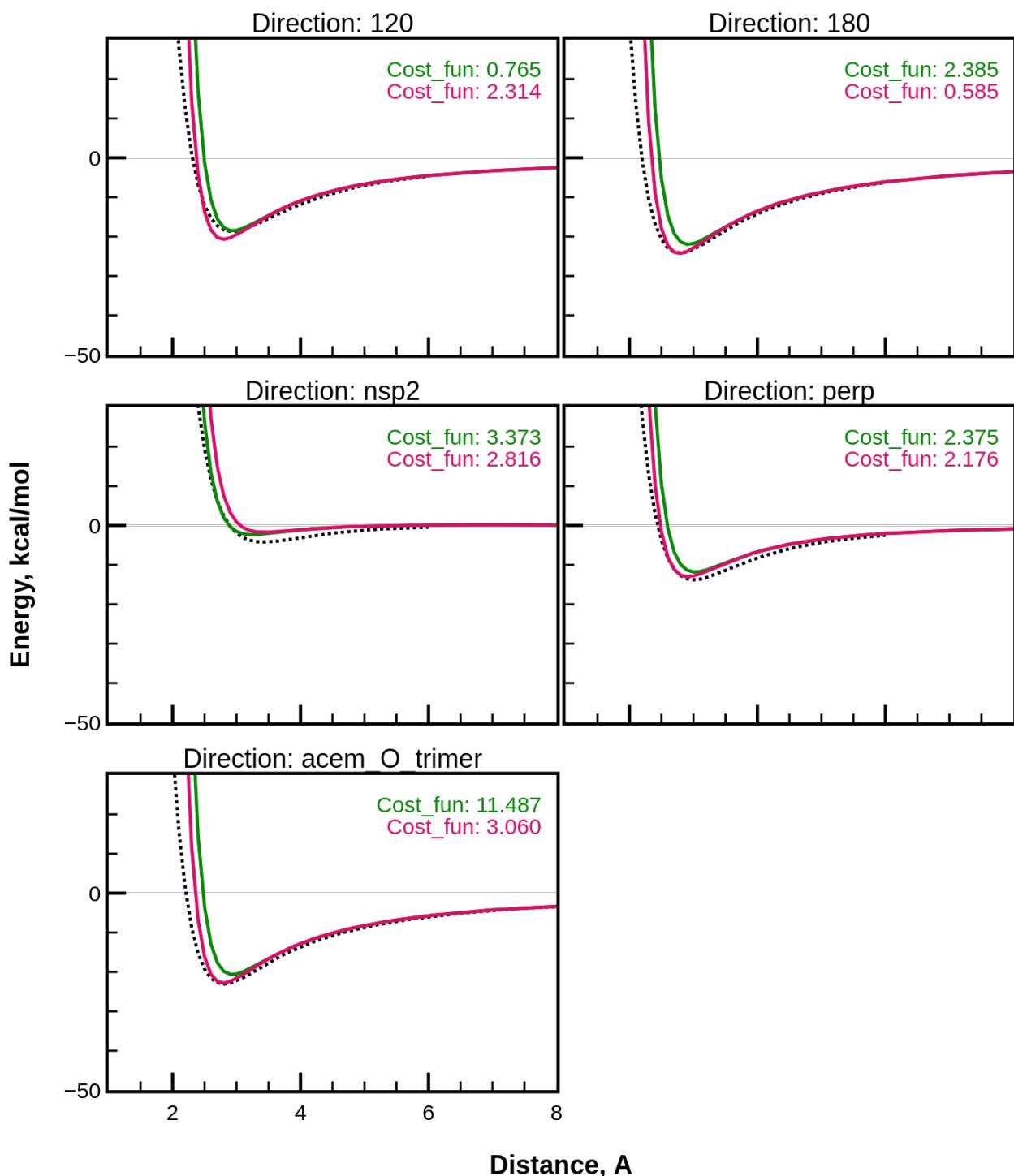
**ACEM SOD 1/1**2.88000\_0.09000\_1.04000  
3.11051\_0.07939\_1.54864

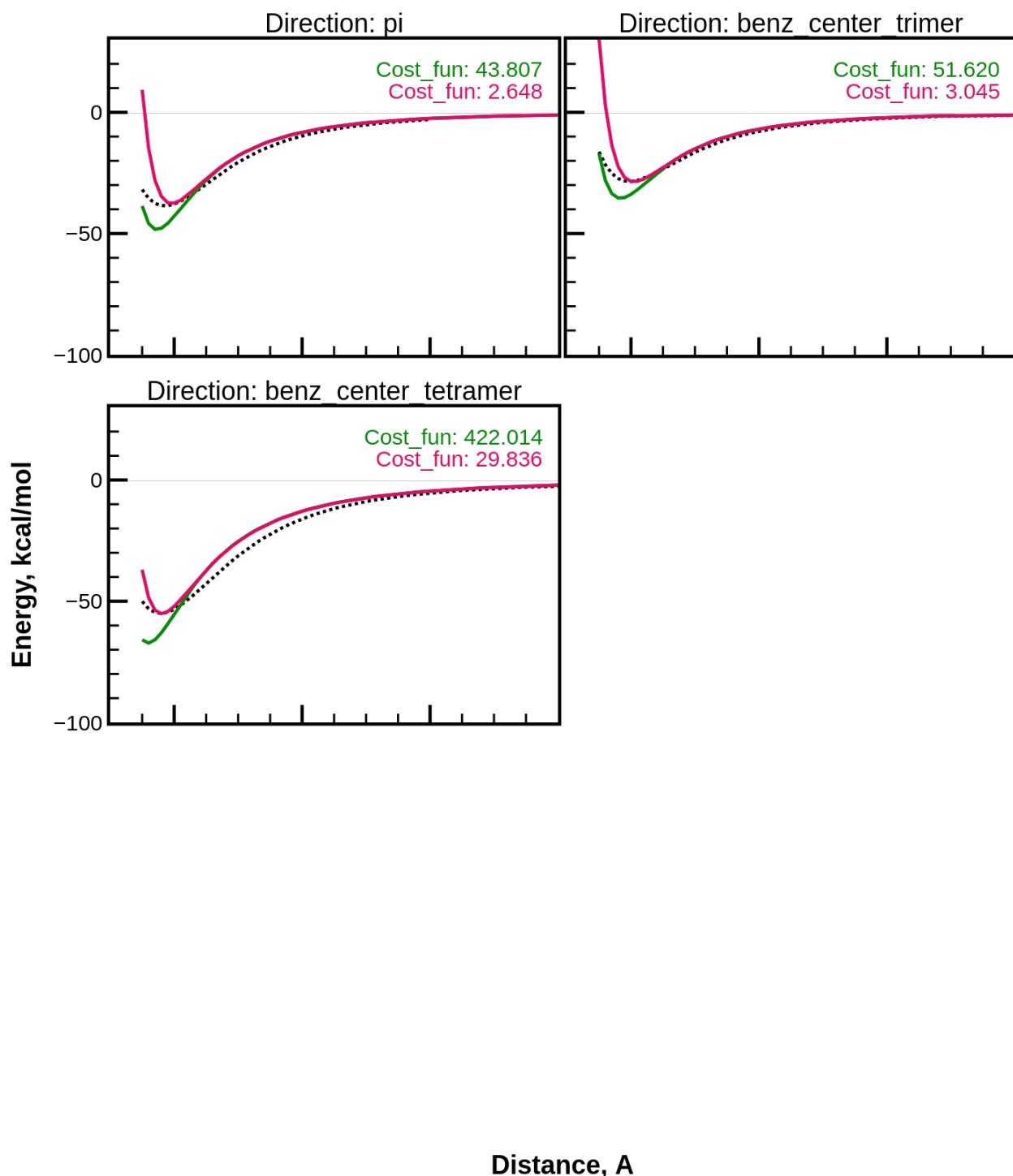
**ACEM POT 1/1**3.21000\_0.18000\_2.19000  
3.43708\_0.16848\_2.09141

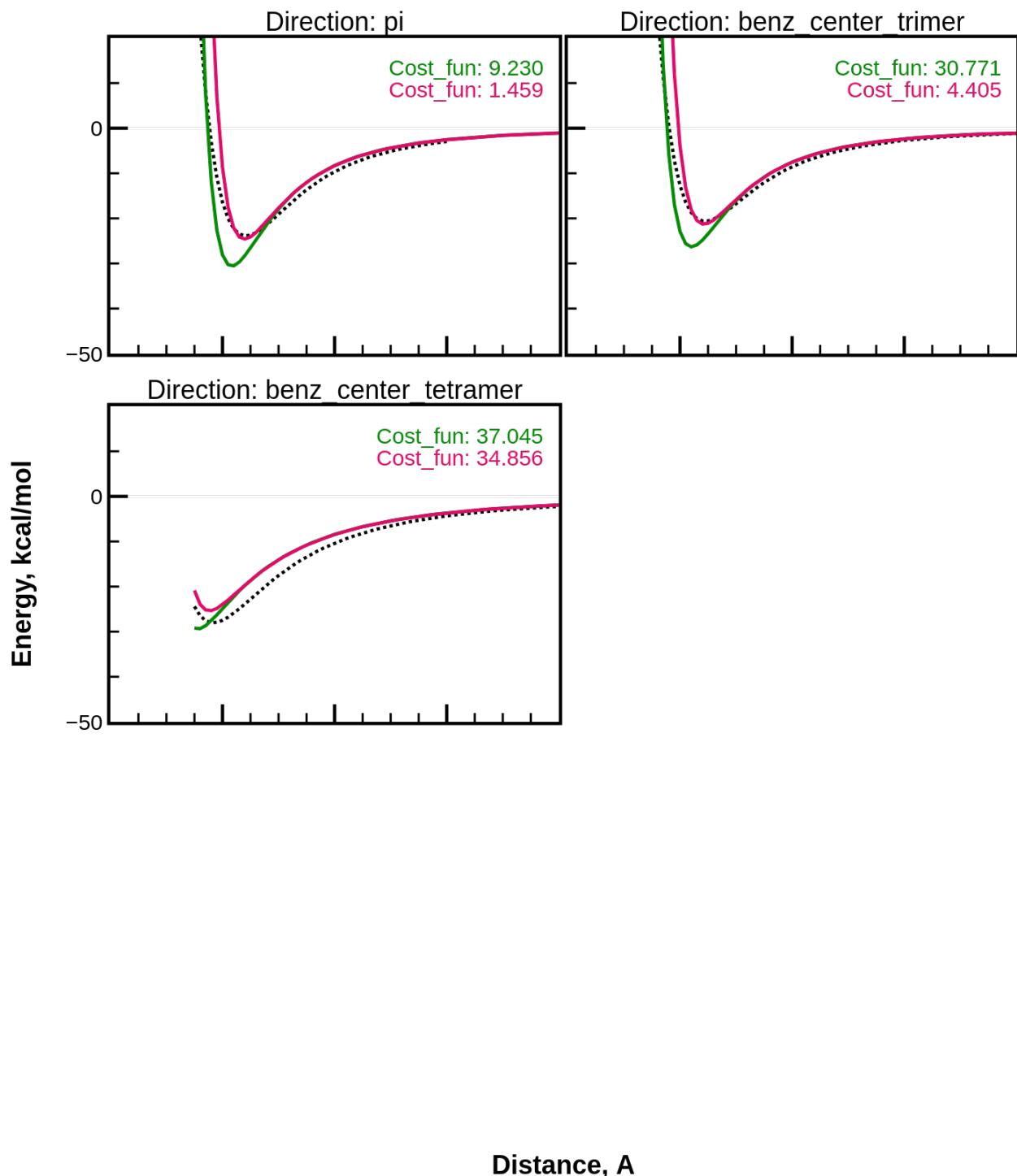
# ACEM RUB 1/1

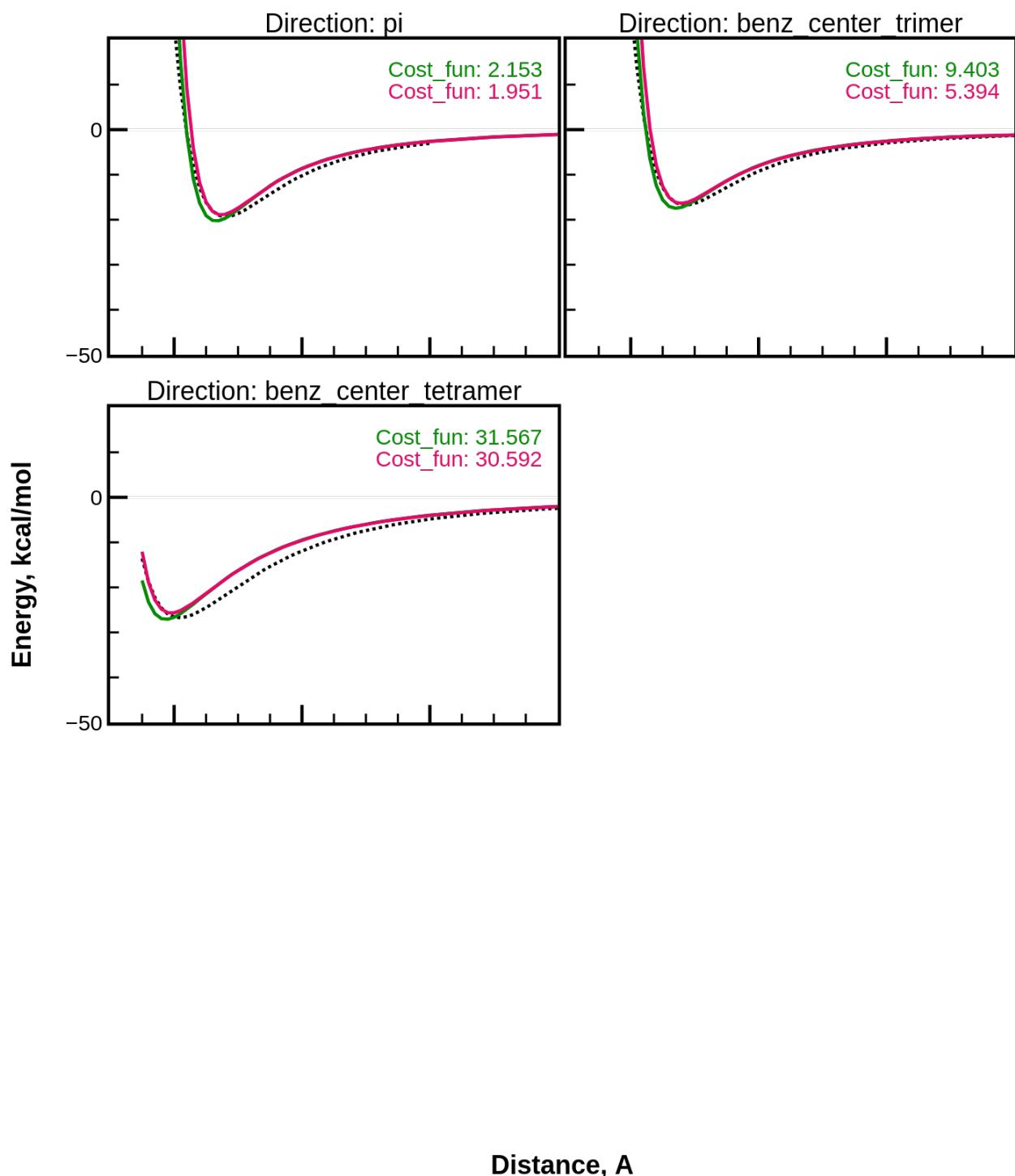
3.56551\_0.23370\_9.99999  
3.49474\_0.23370\_2.99829



**ACEM CES 1/1**3.80382\_0.23520\_9.99999  
3.64357\_0.23520\_2.58963

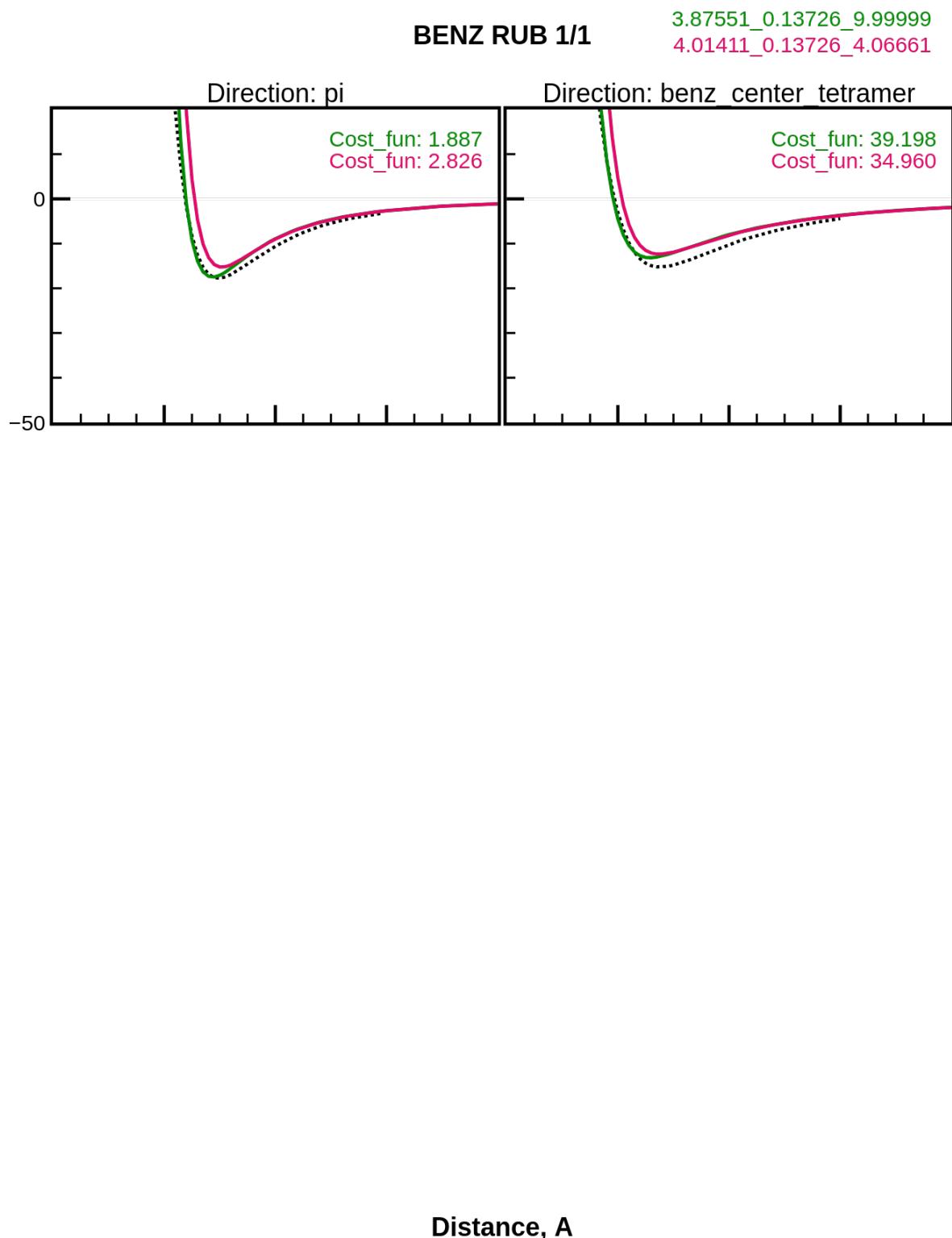
**BENZ LIT 1/1**3.19000\_0.04550\_9.99999  
3.36536\_0.04550\_2.13767

**BENZ SOD 1/1**3.55168\_0.04663\_9.99999  
3.74147\_0.04663\_4.93763

**BENZ POT 1/1**3.77665\_0.09896\_9.99999  
3.84110\_0.09896\_3.83779

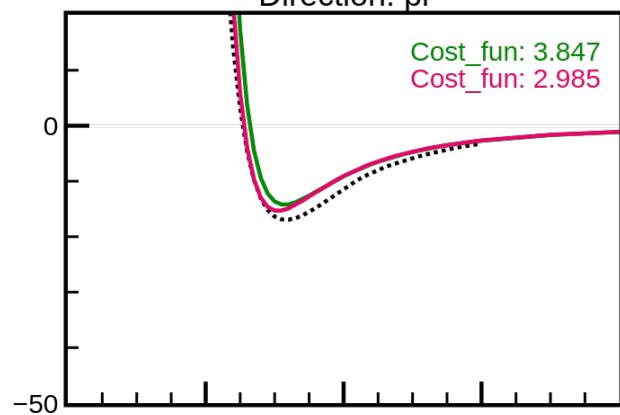
**BENZ RUB 1/1**3.87551\_0.13726\_9.99999  
4.01411\_0.13726\_4.06661

Energy, kcal/mol



**BENZ CES 1/1**4.11382\_0.13815\_9.99999  
4.03106\_0.13815\_3.72515

Direction: pi

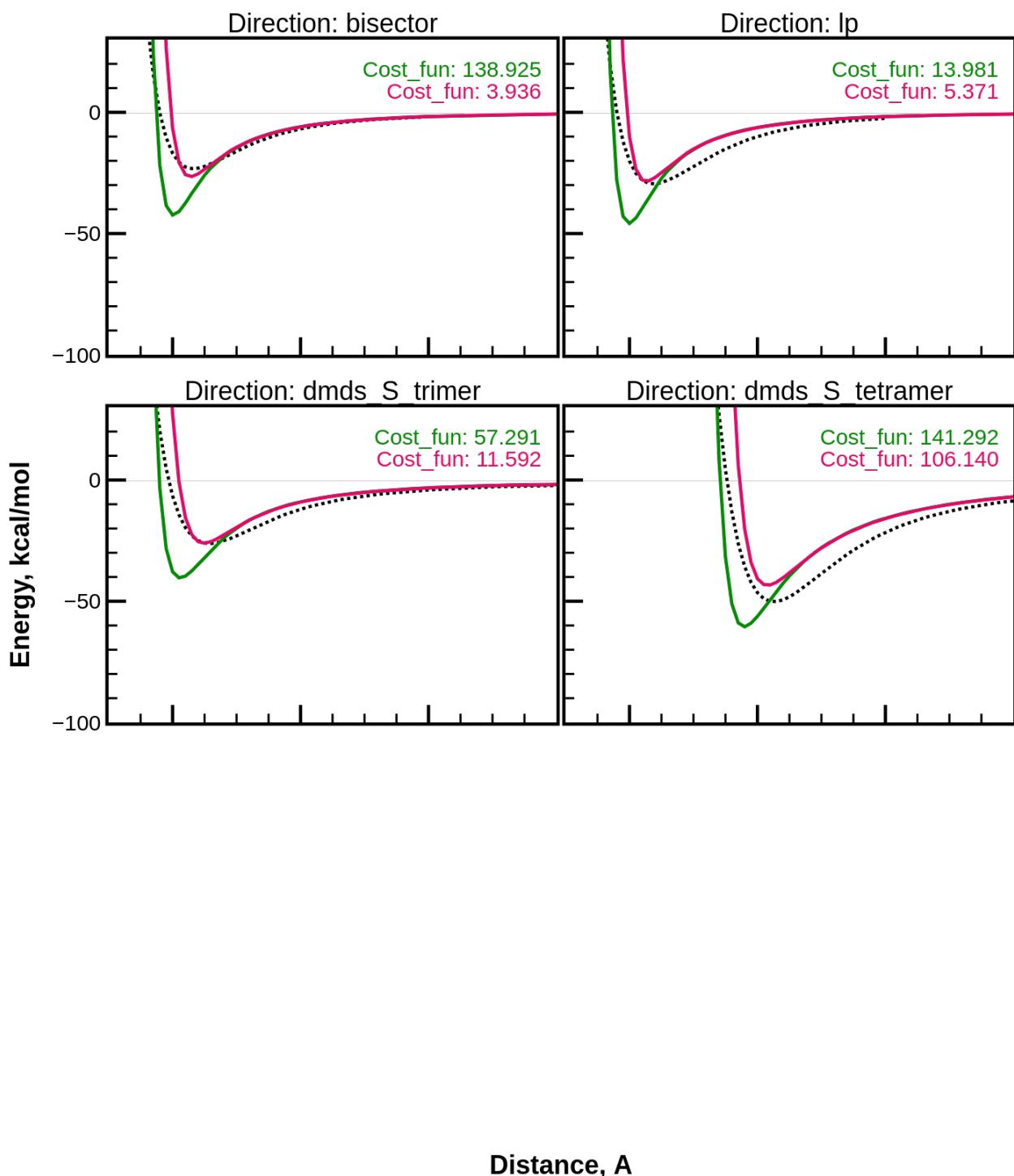


Energy, kcal/mol

Distance, Å

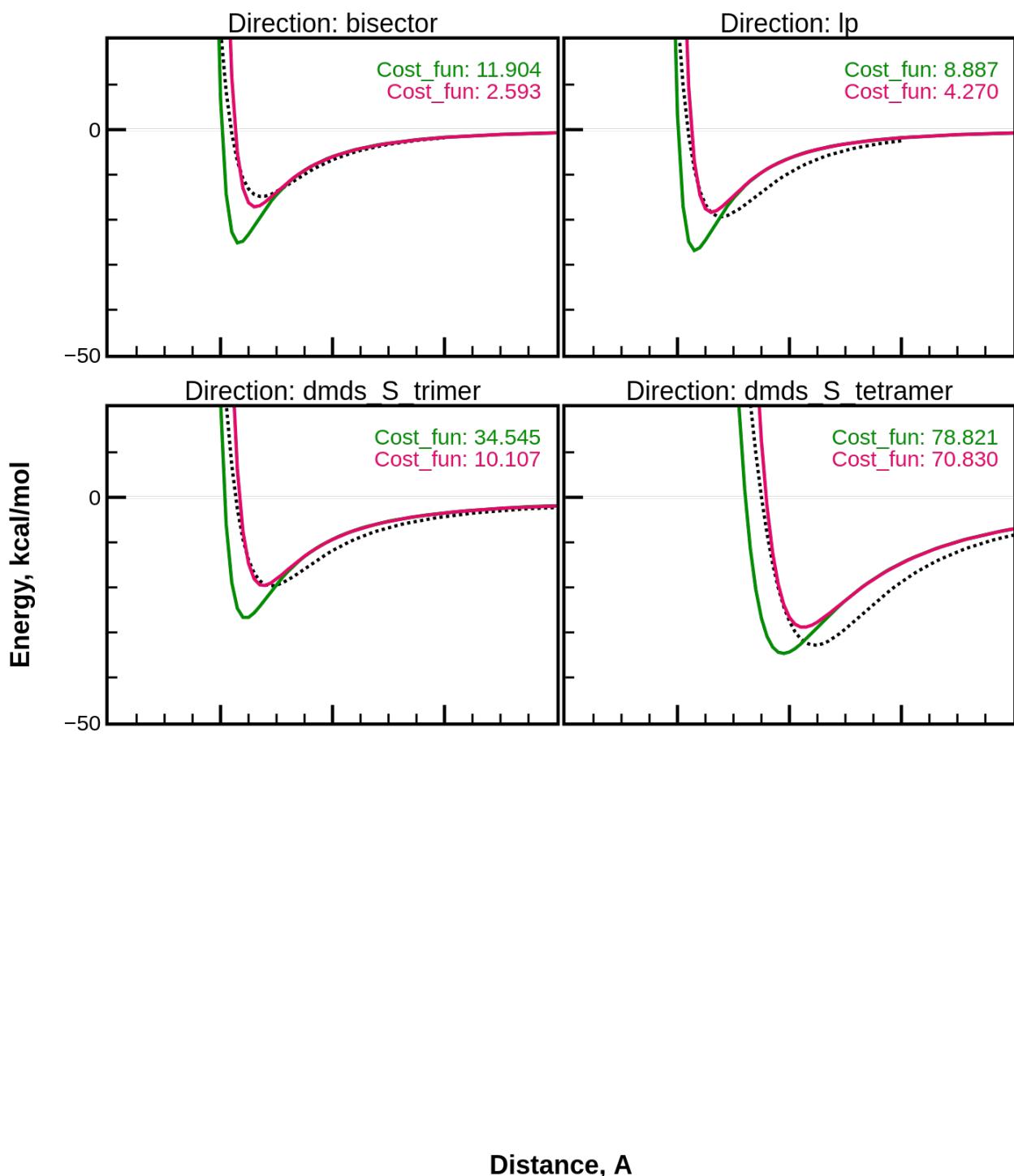
# DMDS LIT 1/1

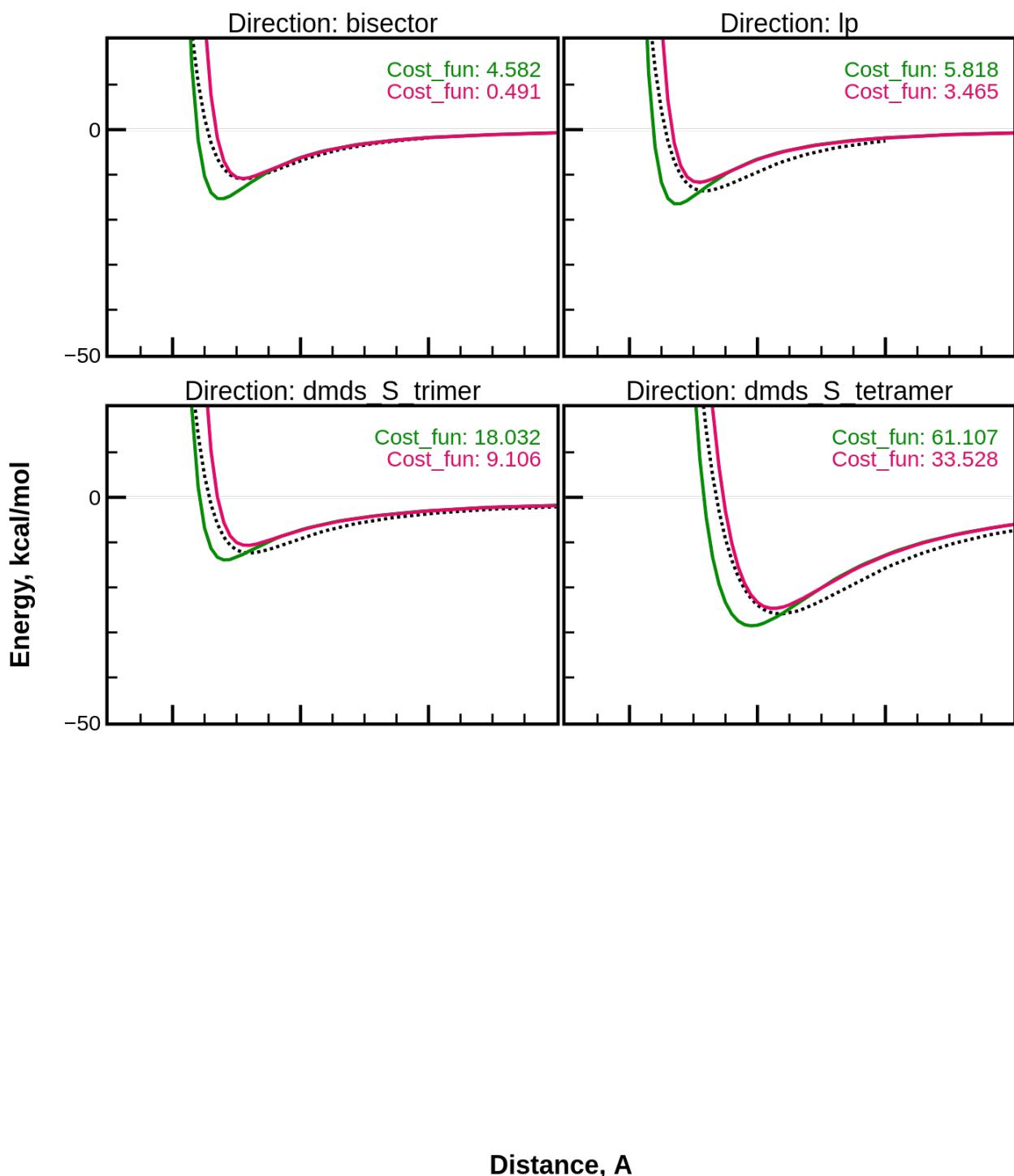
3.10000\_0.09798\_9.99999  
3.36842\_0.09798\_2.07090



# DMDS SOD 1/1

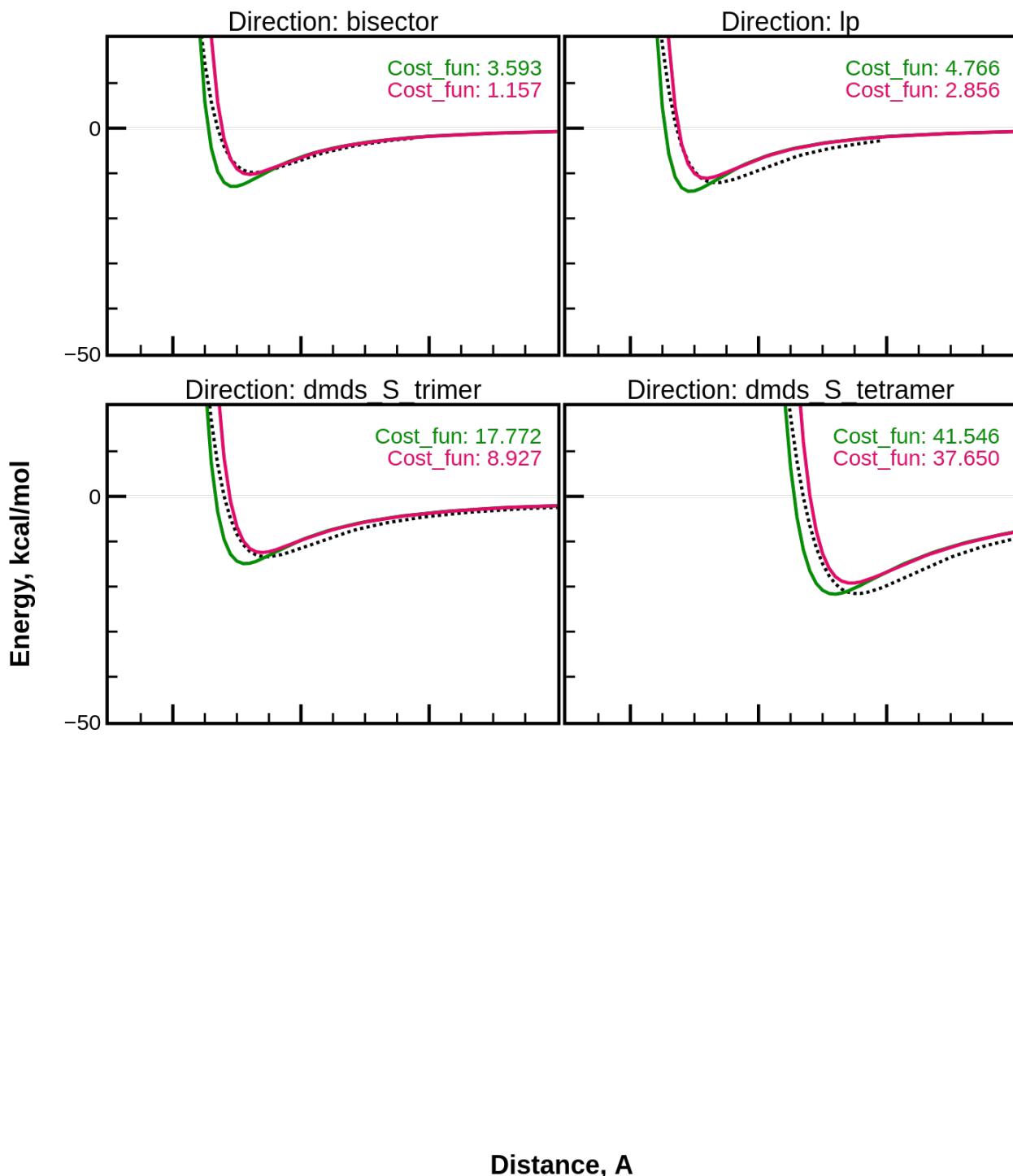
3.46168\_0.10042\_9.99999  
3.73661\_0.10042\_3.02249



**DMDS POT 1/1**3.68665\_0.21311\_9.99999  
4.00448\_0.21311\_4.63005

# DMDS RUB 1/1

3.78551\_0.29560\_9.99999  
4.01139\_0.29560\_4.37659

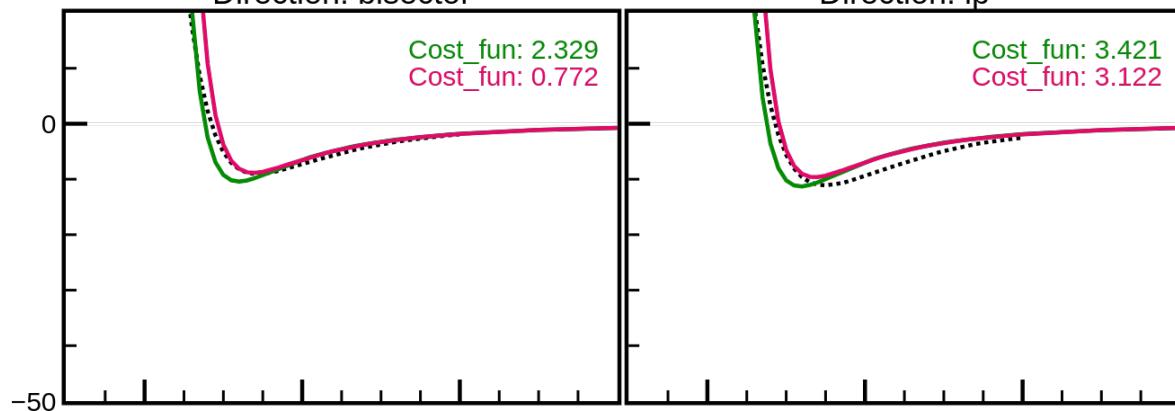


# DMDS CES 1/1

4.02382\_0.29751\_9.99999  
4.19082\_0.29751\_4.26380

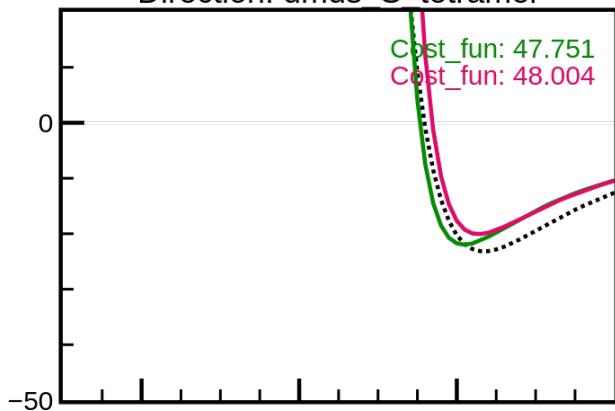
Direction: bisector

Direction: lp

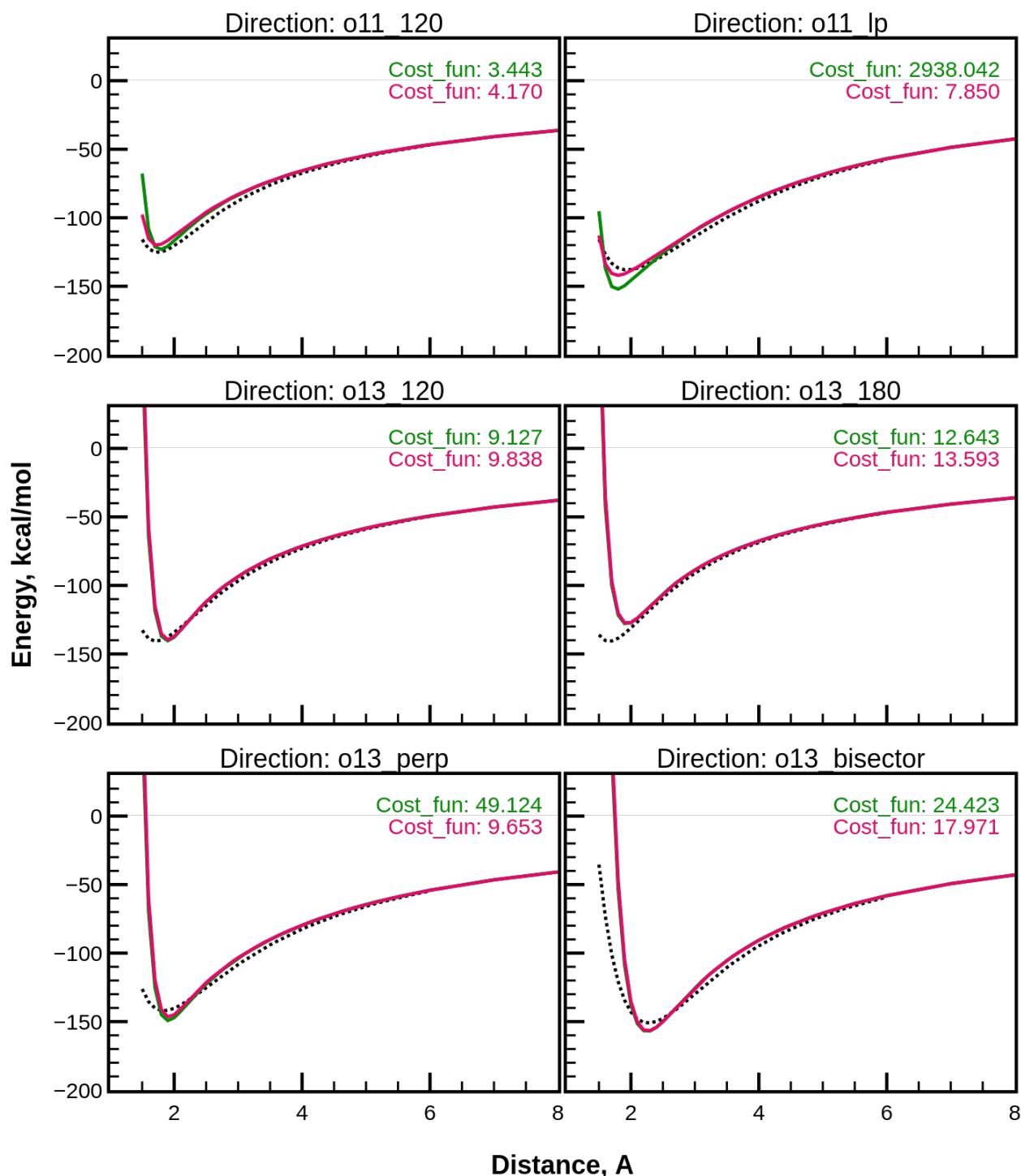


Direction: dmds S tetramer

Energy, kcal/mol

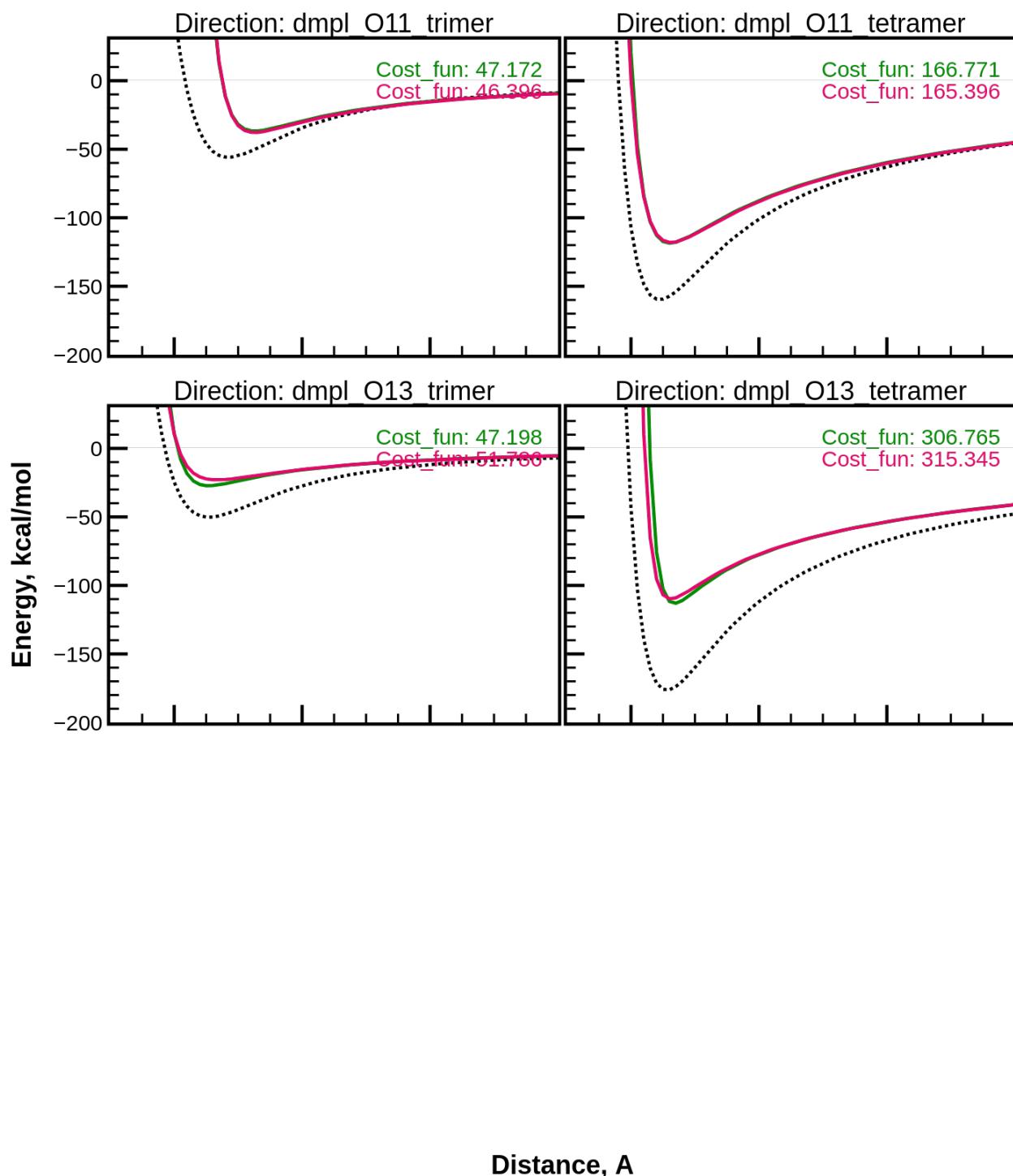


Distance, Å

**DMPL LIT 1/2**3.13500\_0.04582\_9.99999  
3.02241\_0.07550\_4.98471

# DMPL LIT 2/2

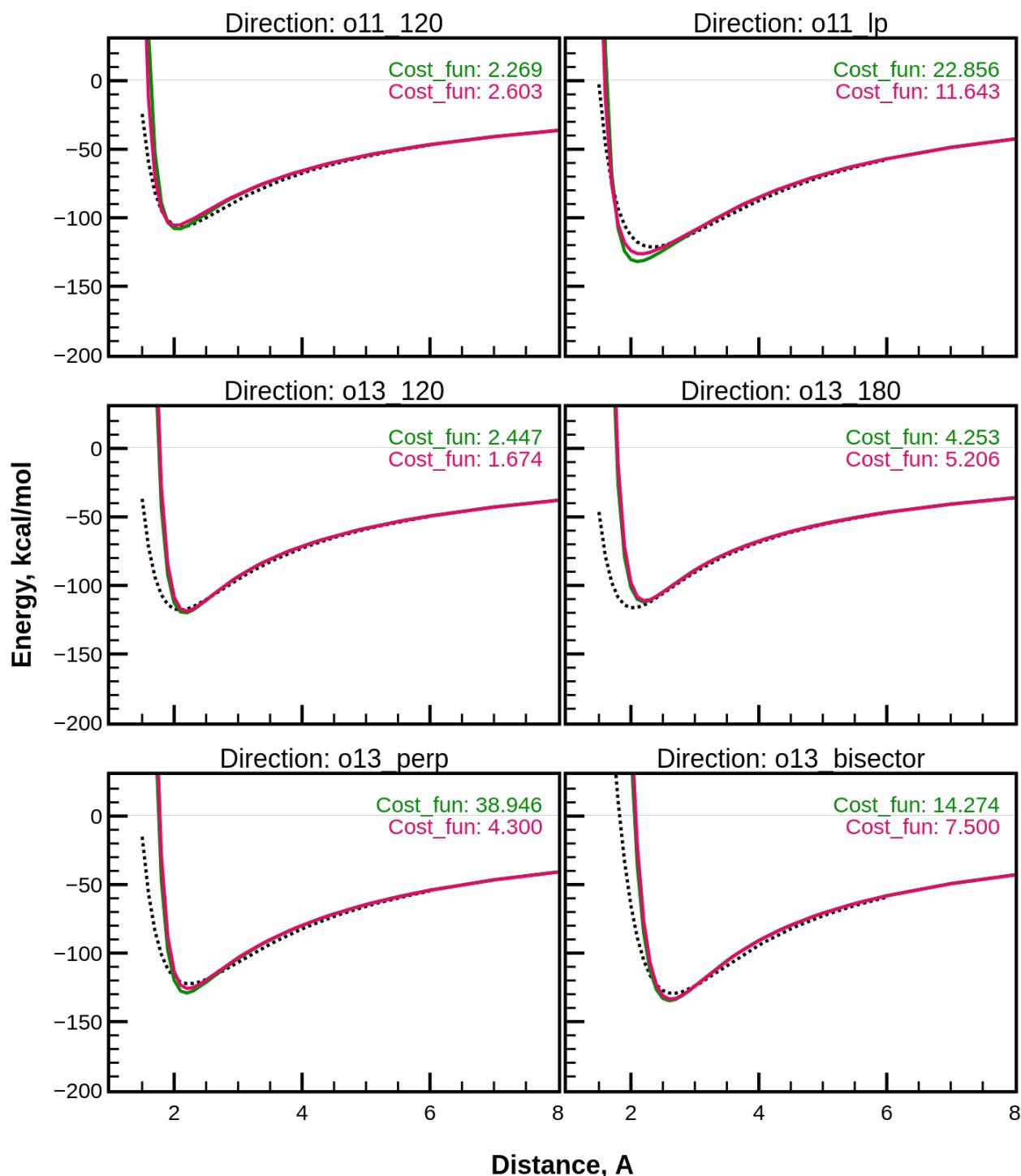
3.13500\_0.04582\_9.99999  
3.02241\_0.07550\_4.98471

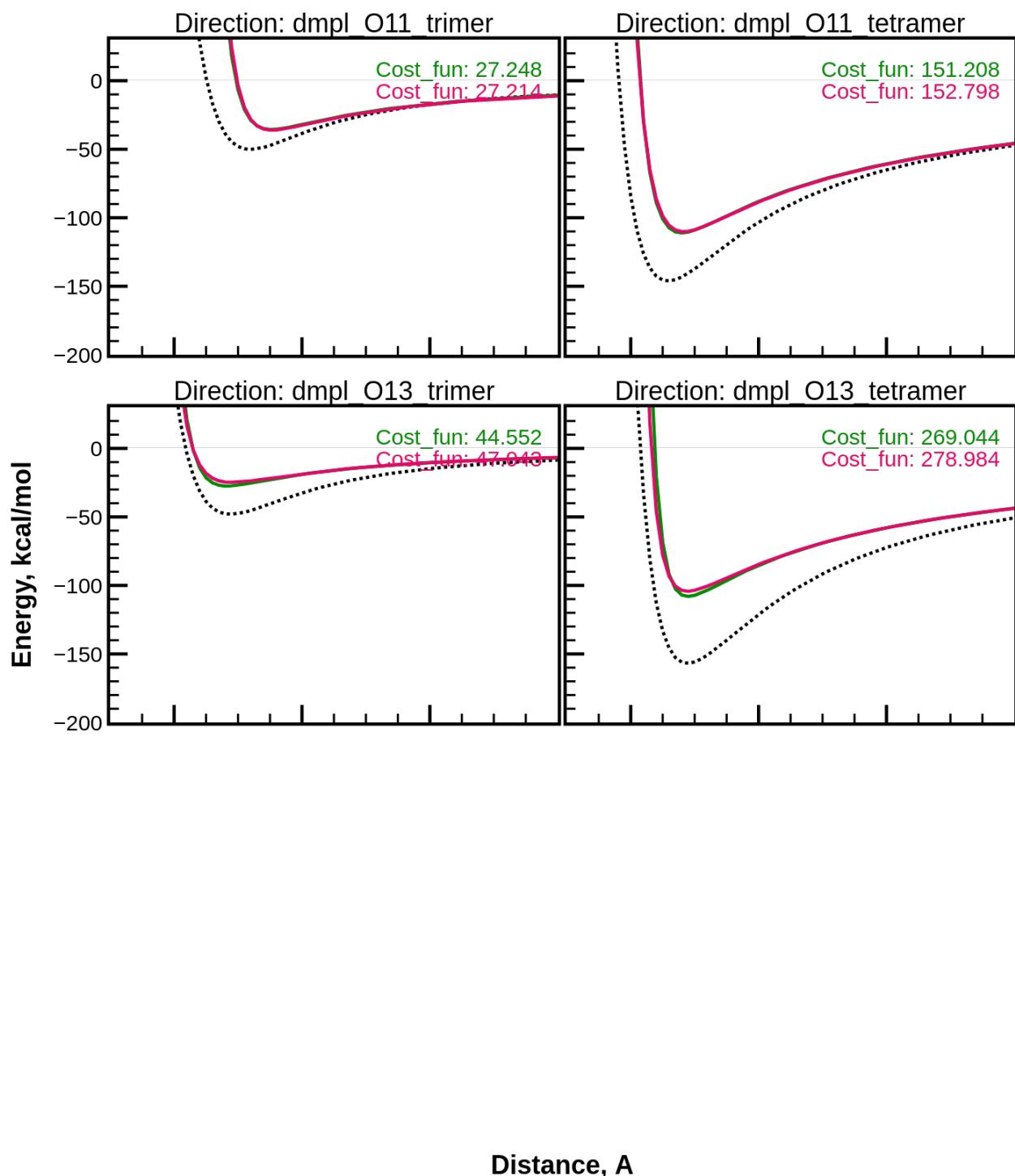


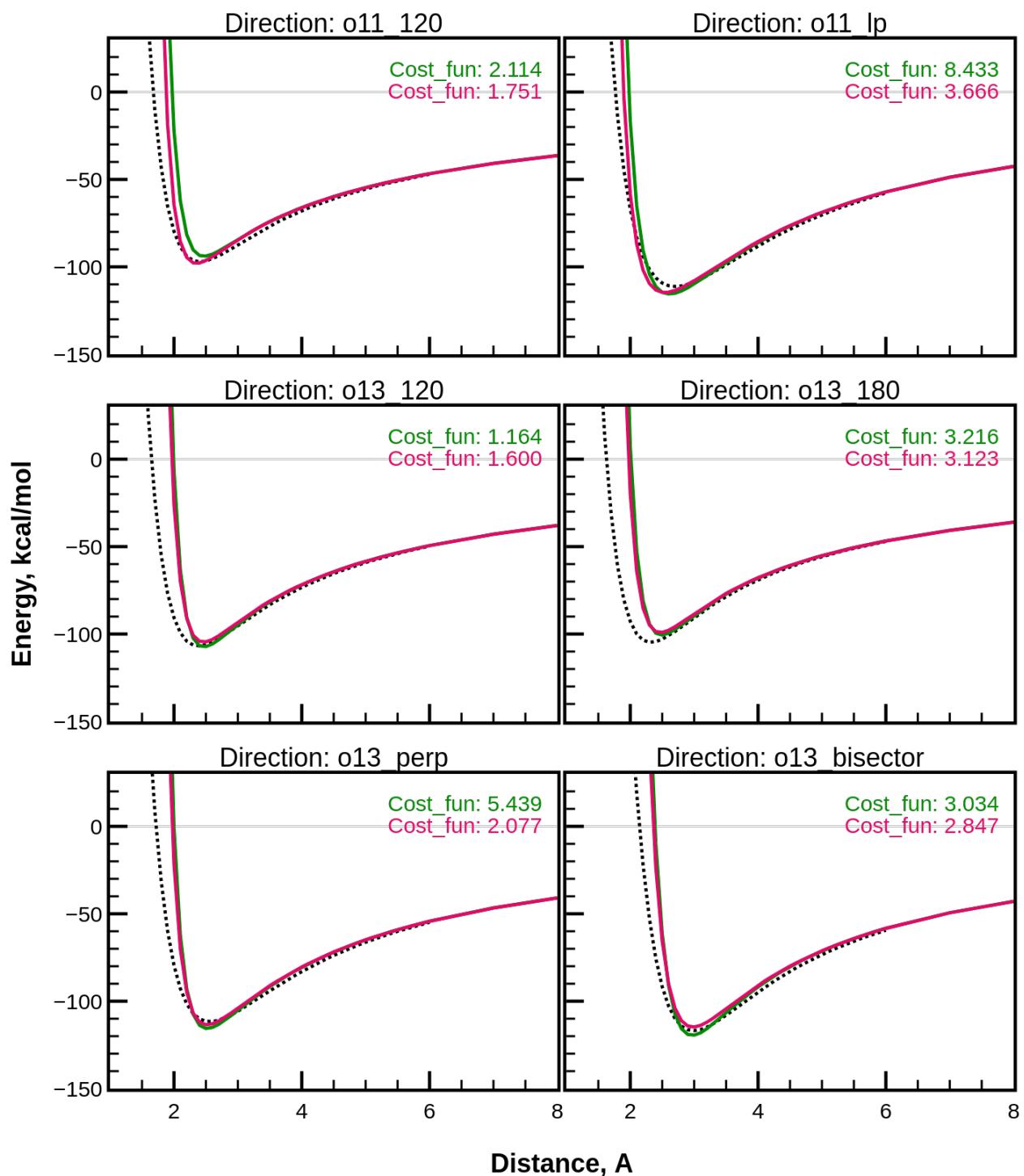
**DMPL SOD 1/2**

3.49668\_0.04696\_9.99999

3.38658\_0.07738\_5.01299

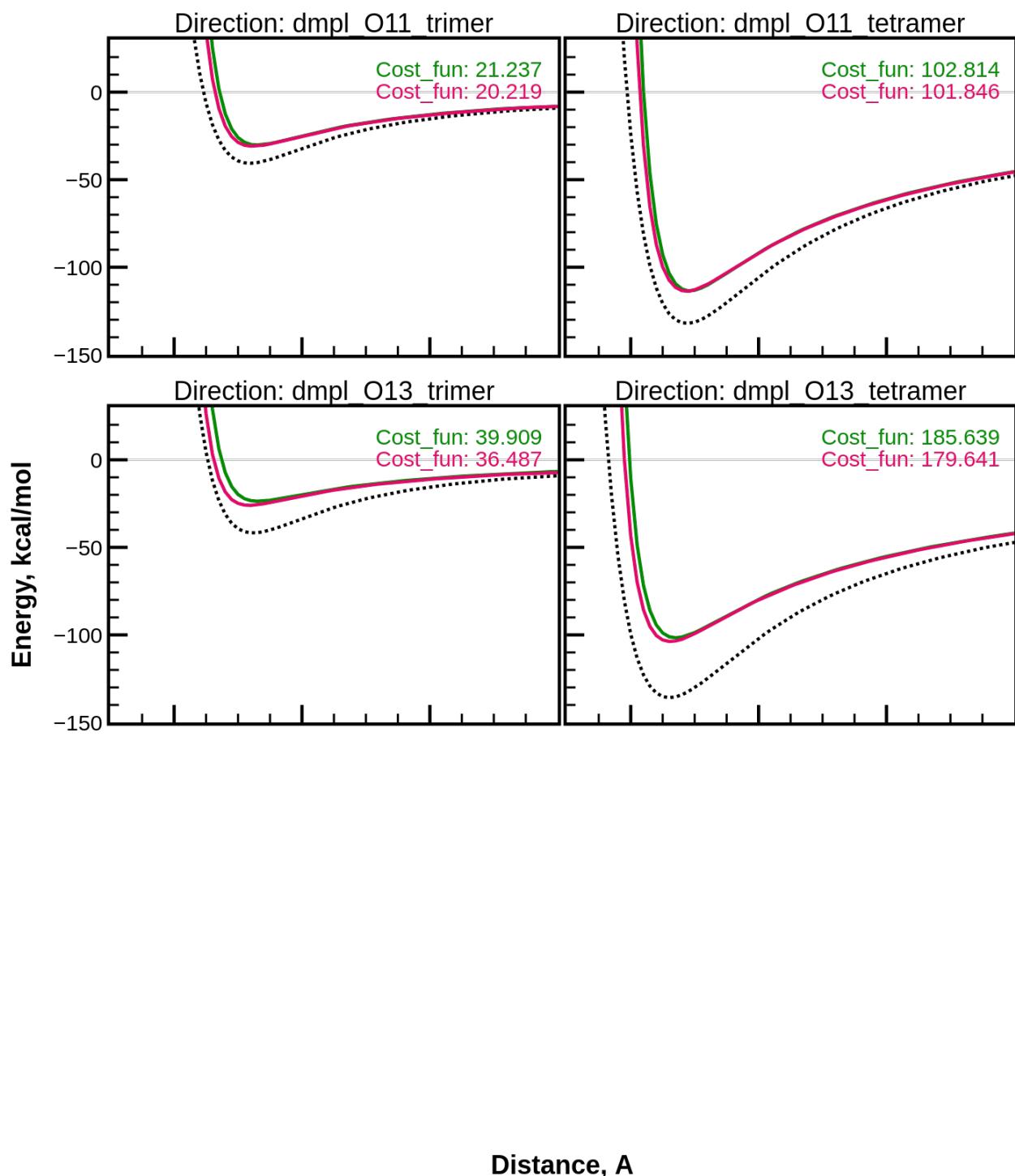


**DMPL SOD 2/2**3.49668\_0.04696\_9.99999  
3.38658\_0.07738\_5.01299

**DMPL POT 1/2**3.55165\_0.16421\_9.99999  
3.45707\_0.16421\_1.88686

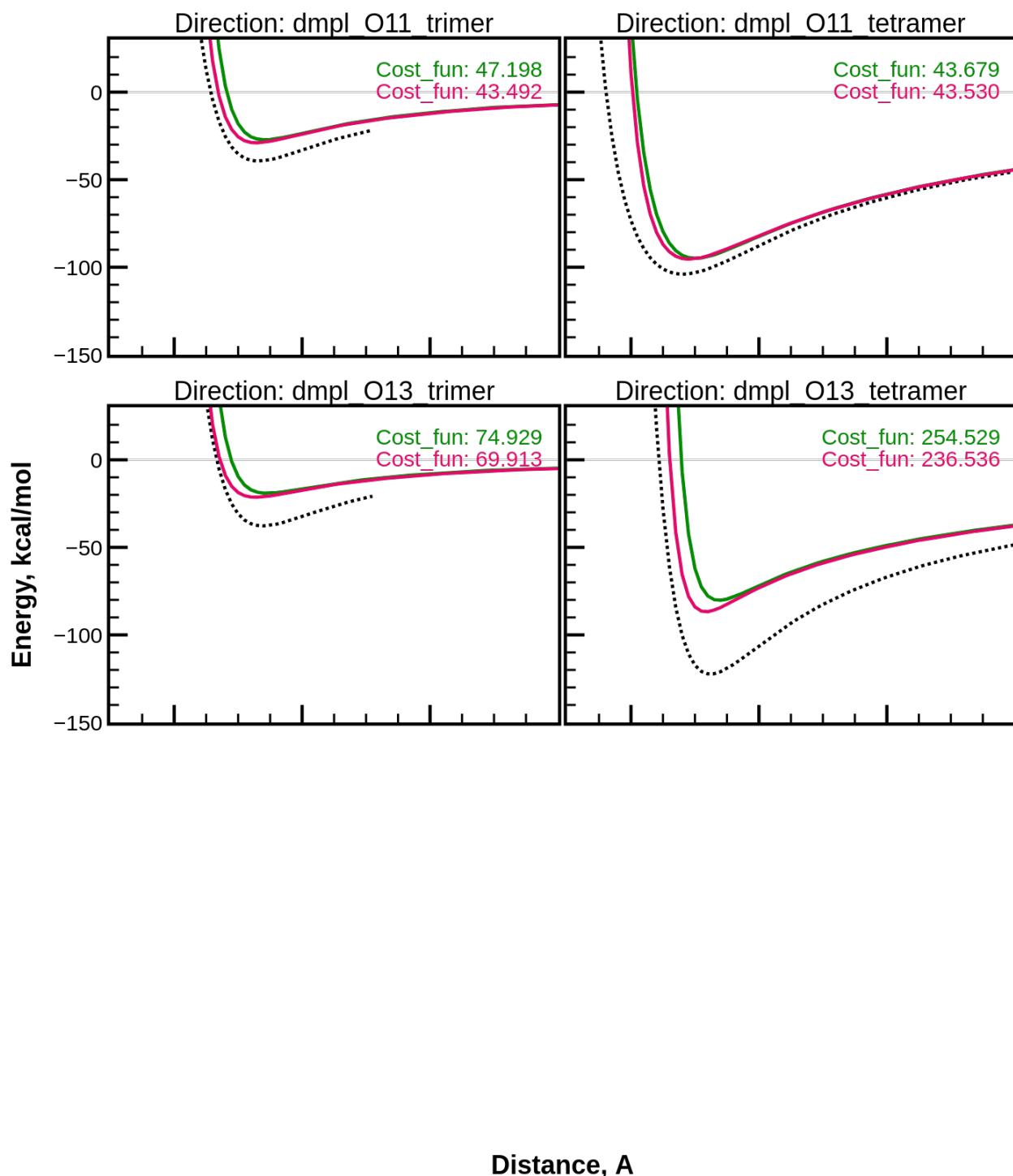
## DMPL POT 2/2

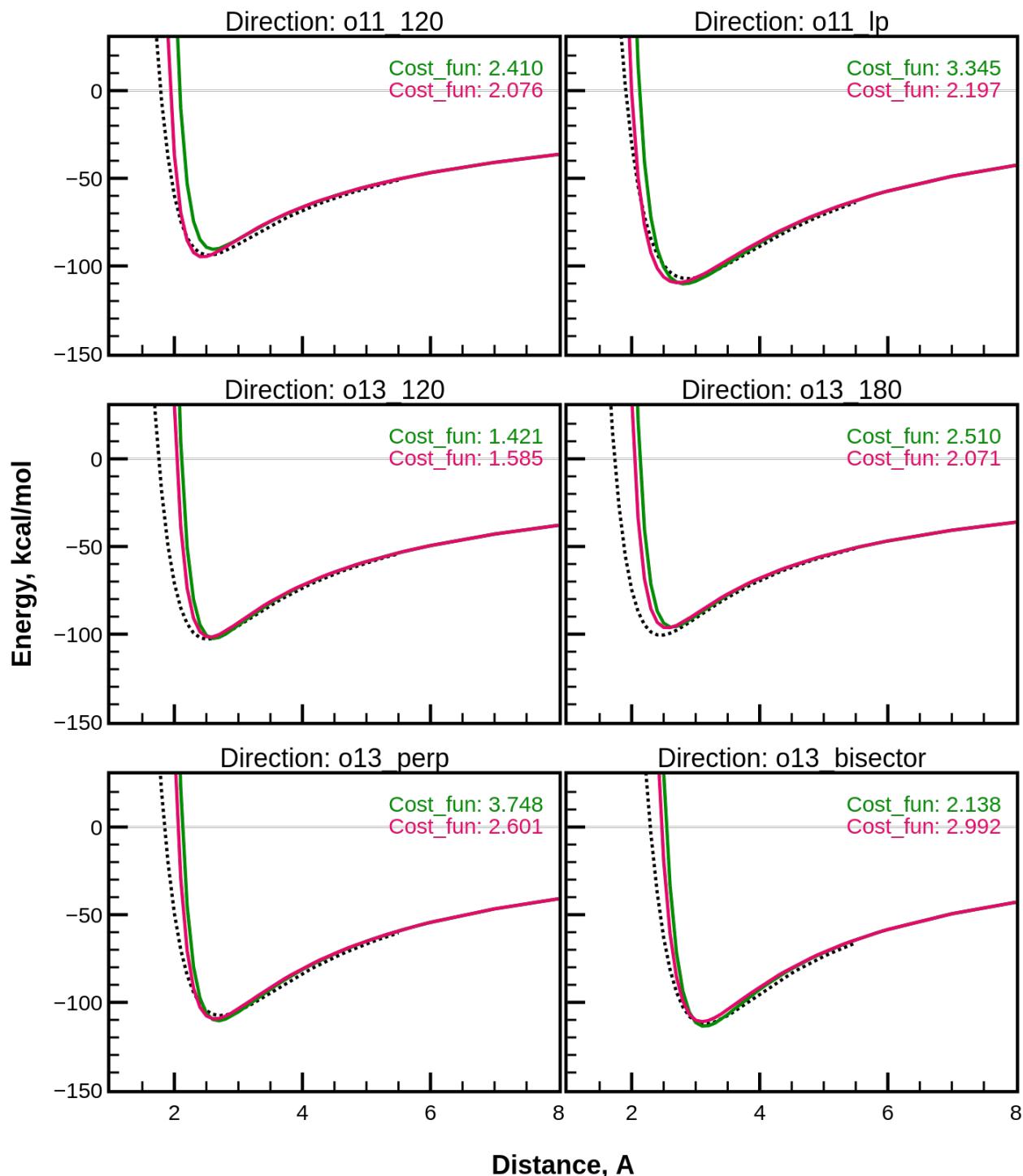
3.55165\_0.16421\_9.99999  
3.45707\_0.16421\_1.88686



# DMPL RUB 2/2

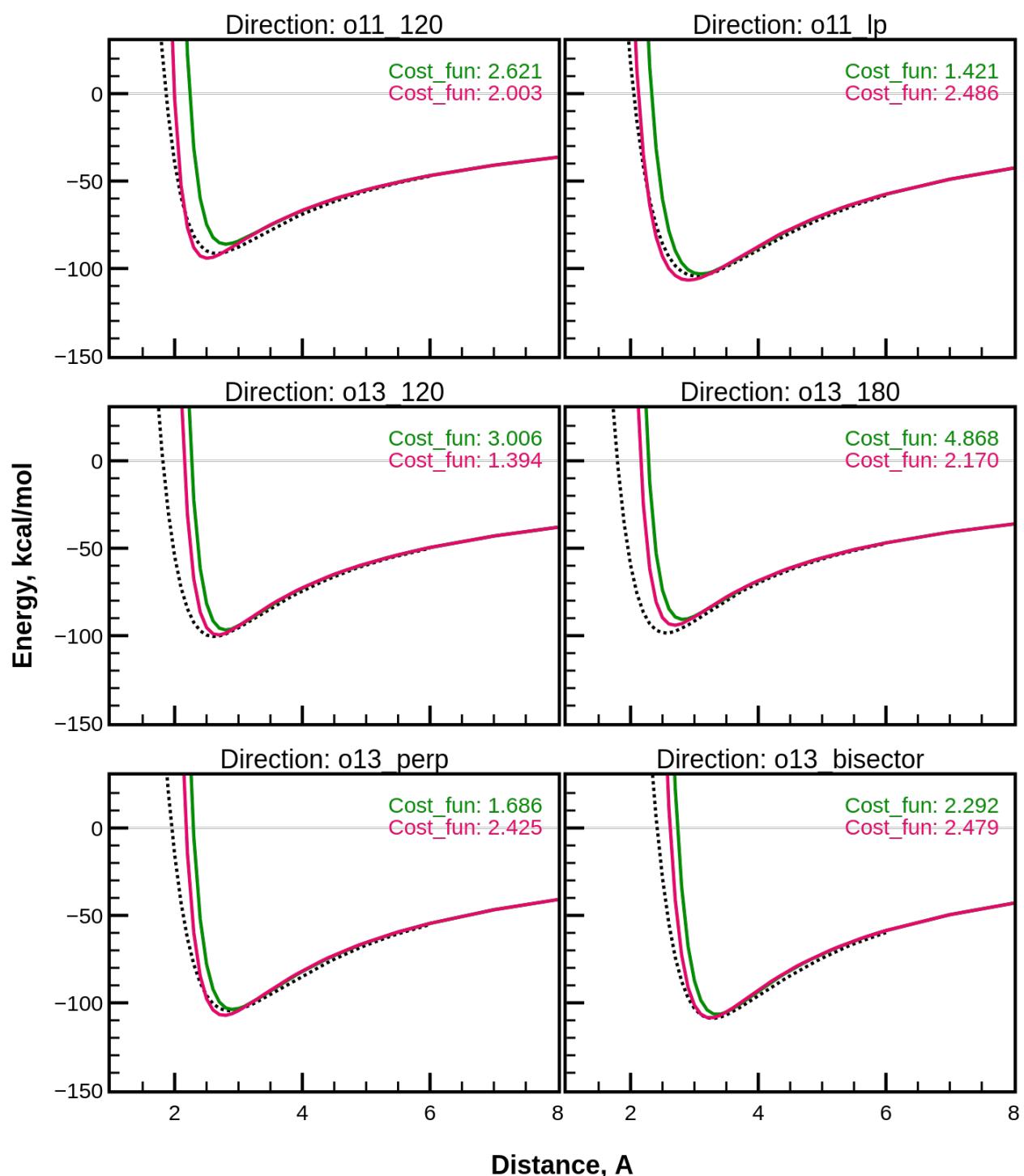
3.65051\_0.22778\_9.99999  
3.48176\_0.22778\_1.94273



**DMPL RUB 1/2**3.65051\_0.22778\_9.99999  
3.48176\_0.22778\_1.94273

# DMPL CES 1/2

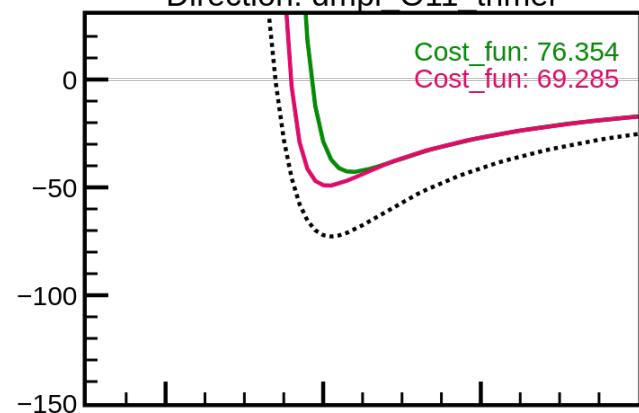
3.88882\_0.22925\_9.99999  
3.67501\_0.22925\_2.30625



**DMPL CES 2/2**

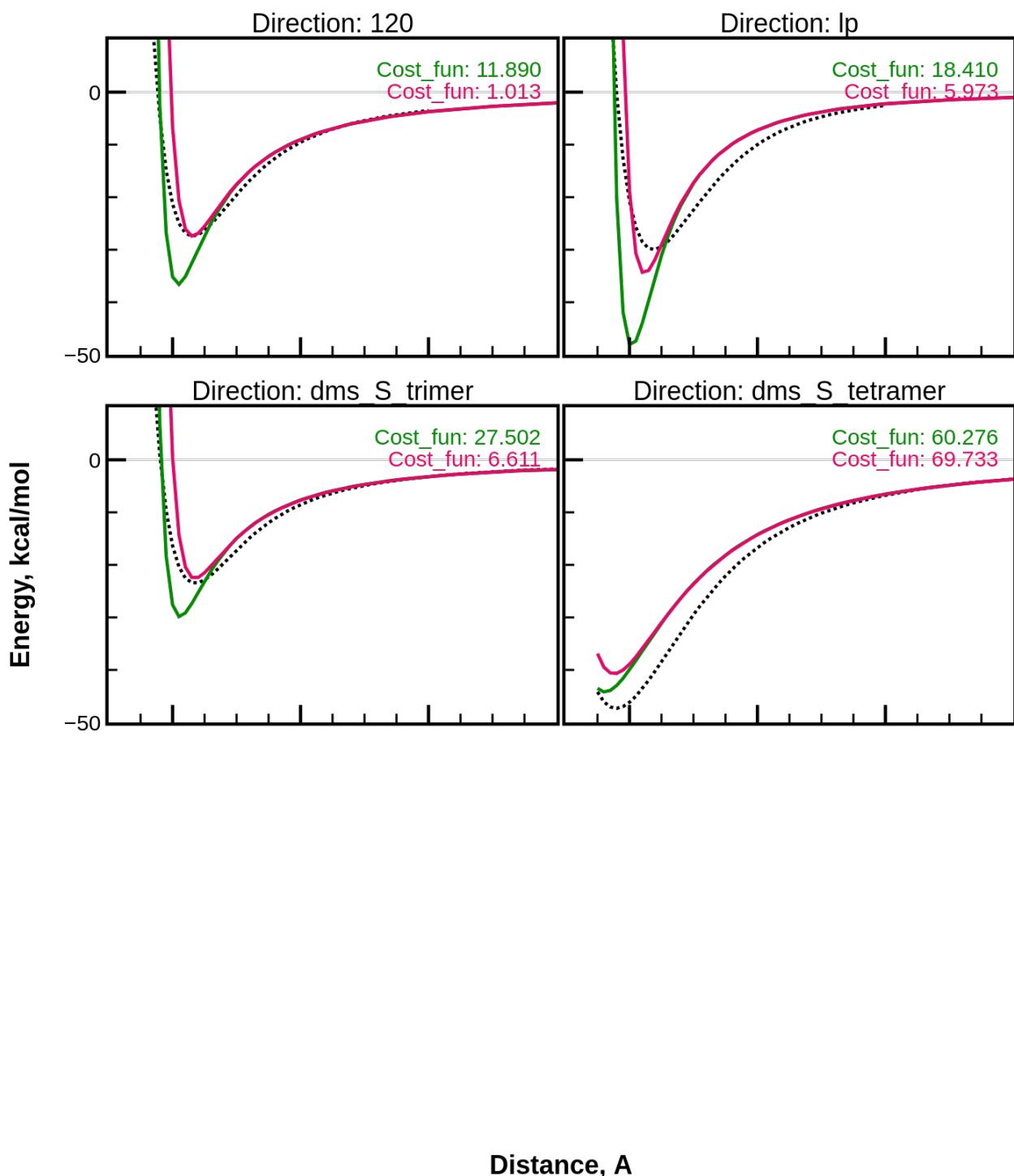
3.88882\_0.22925\_9.99999  
3.67501\_0.22925\_2.30625

Direction: dmpl\_O11\_trimer



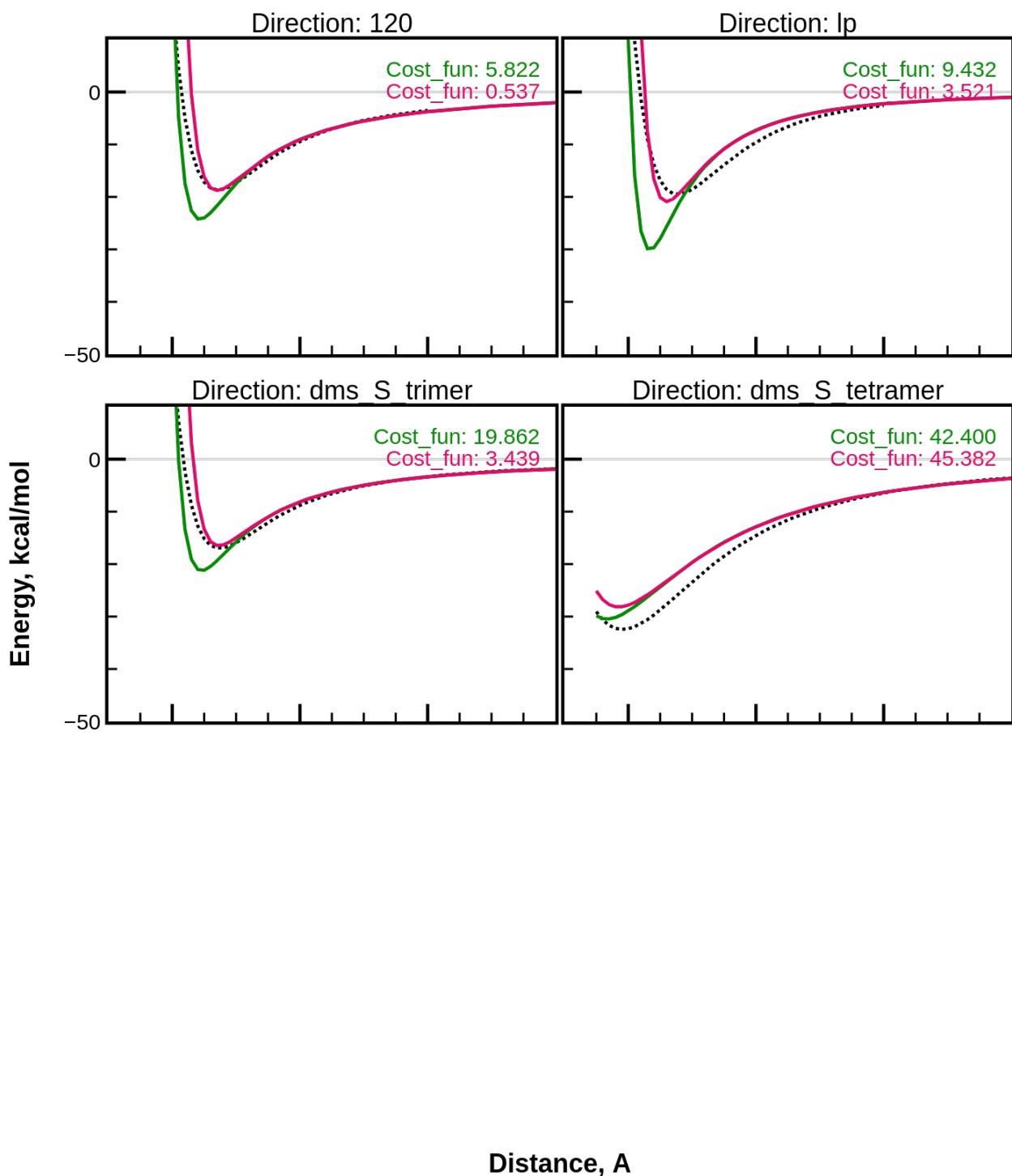
Energy, kcal/mol

Distance, Å

**DMS LIT 1/1**3.15000\_0.09644\_9.99999  
3.35945\_0.09644\_2.02916

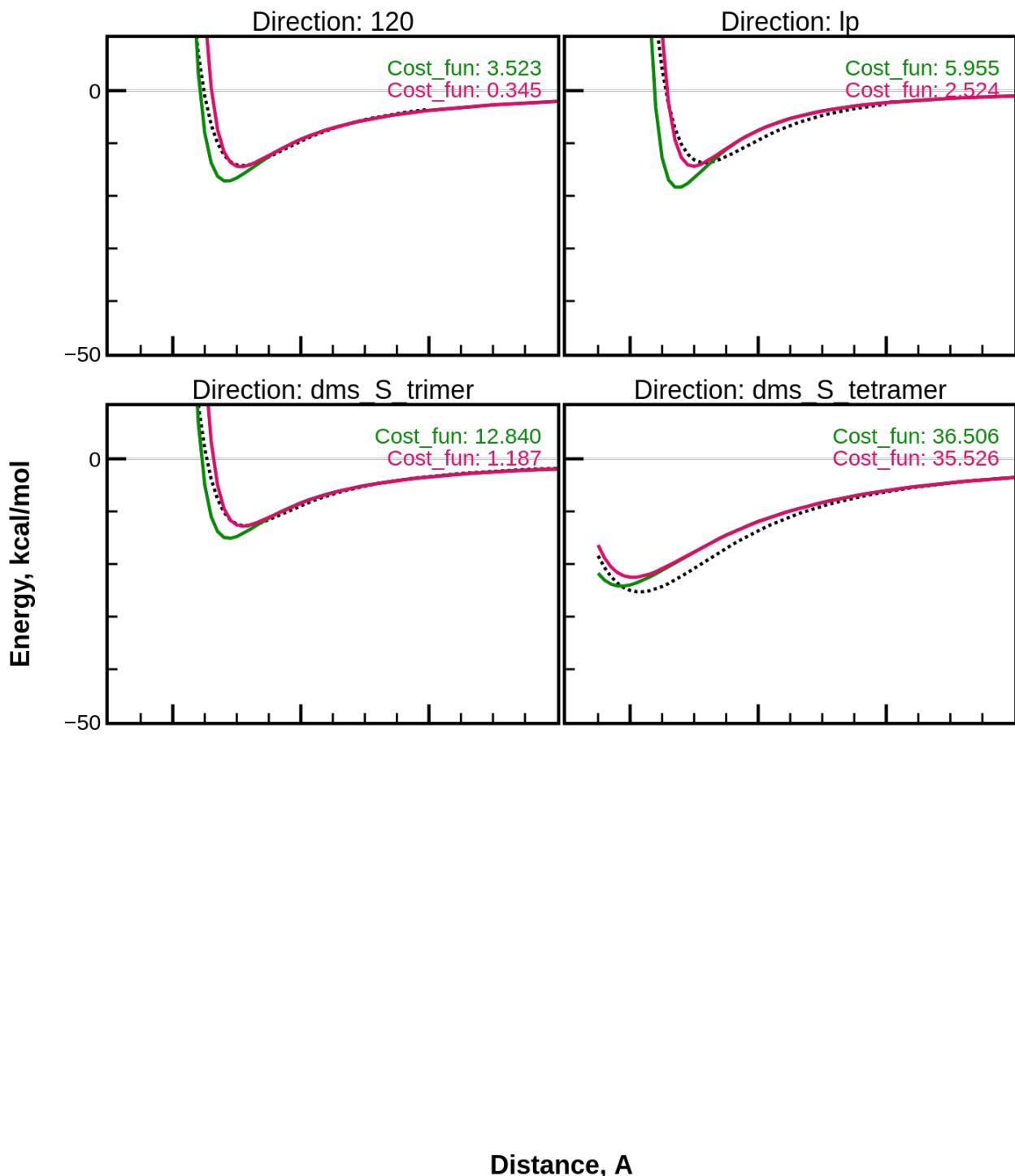
# DMS SOD 1/1

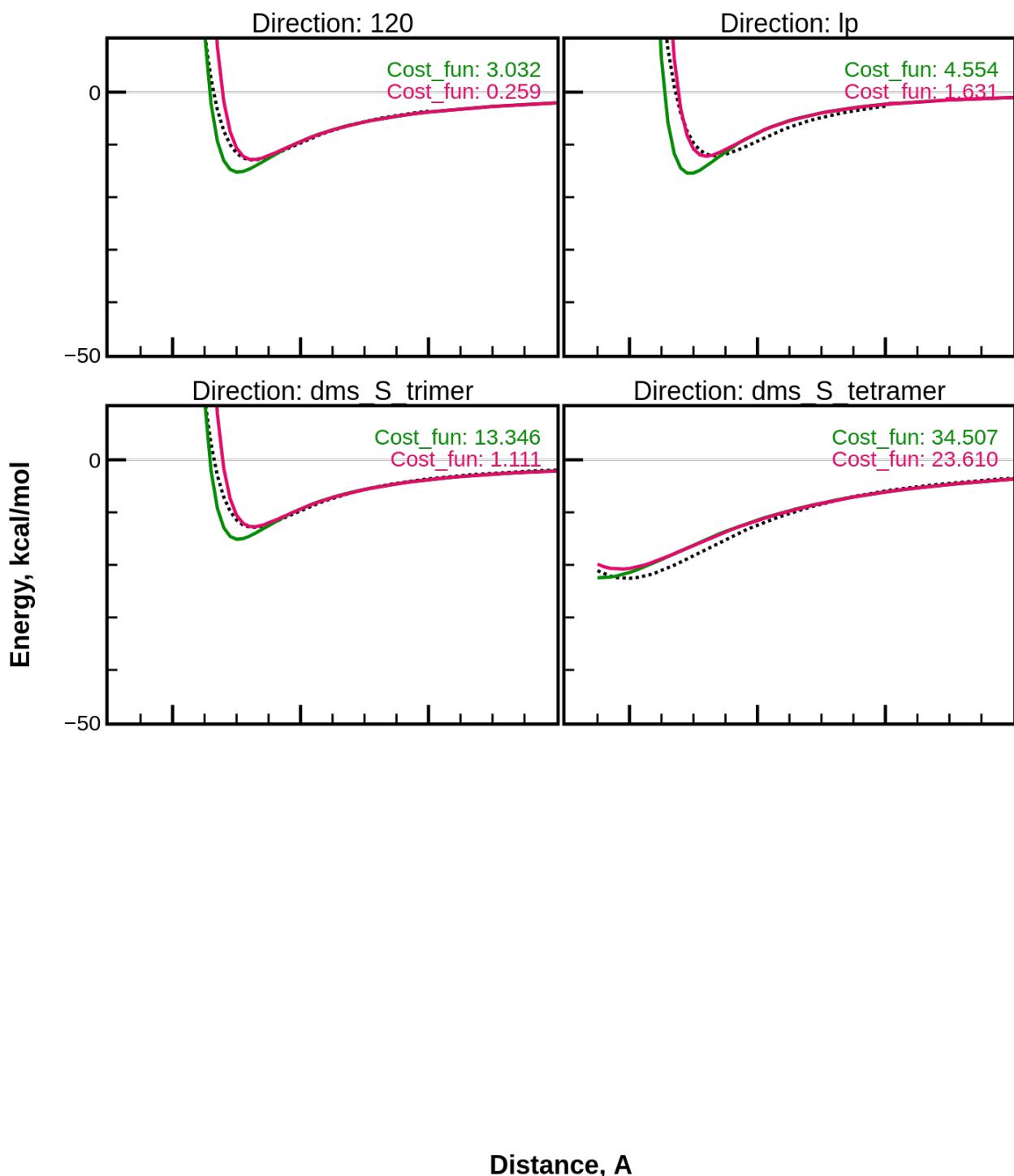
3.51168\_0.09883\_9.99999  
3.78891\_0.09883\_3.72287

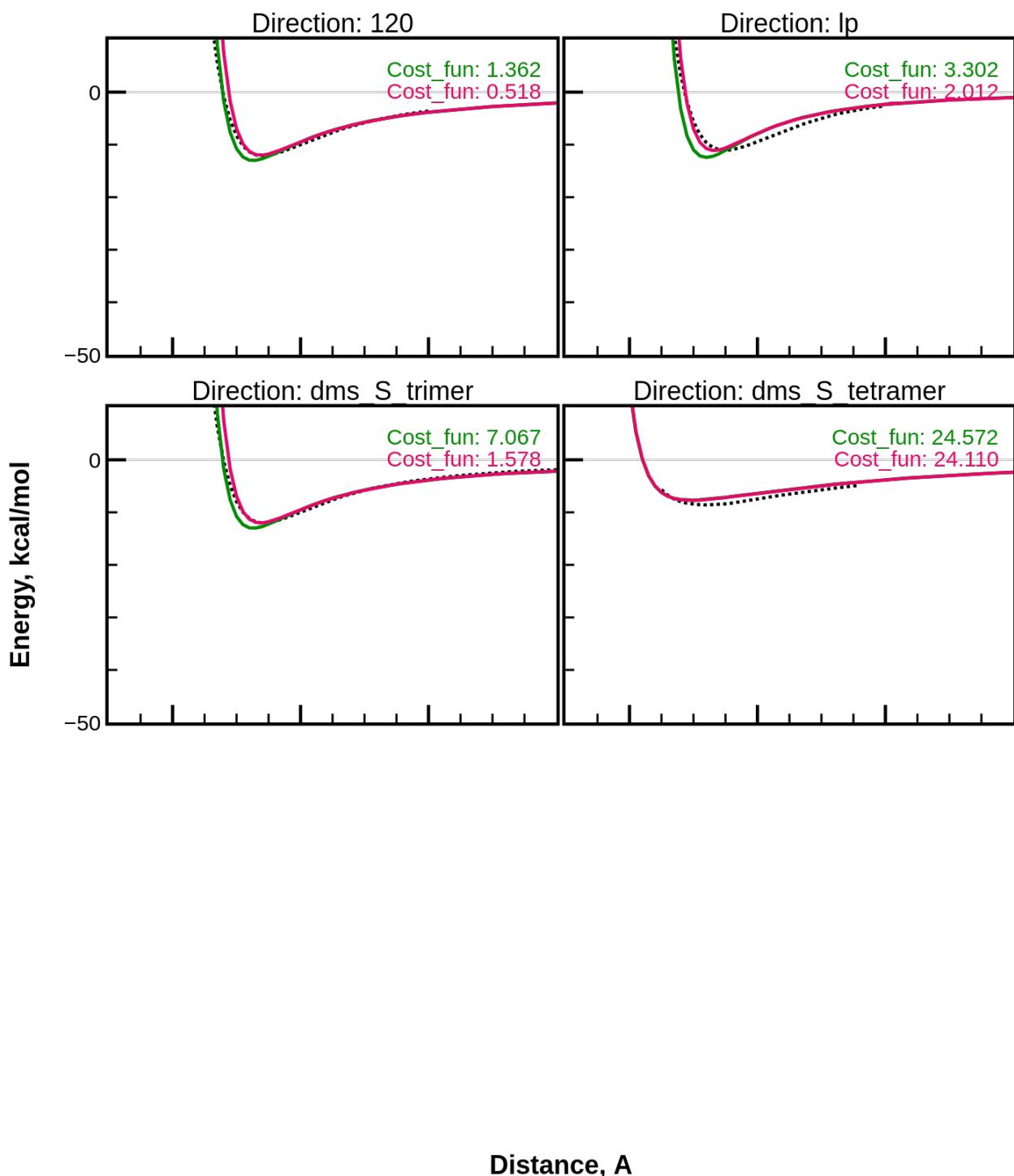


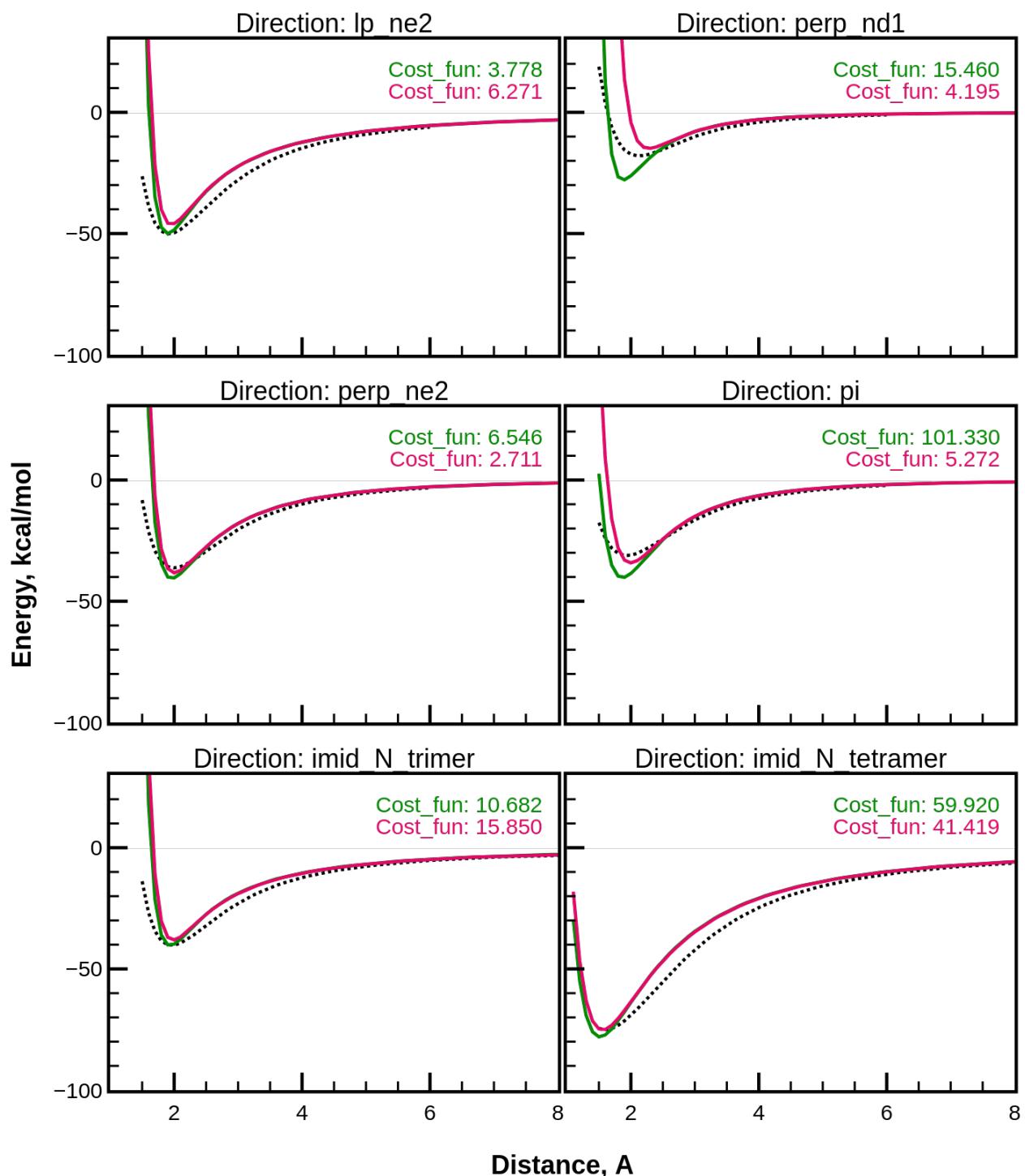
# DMS POT 1/1

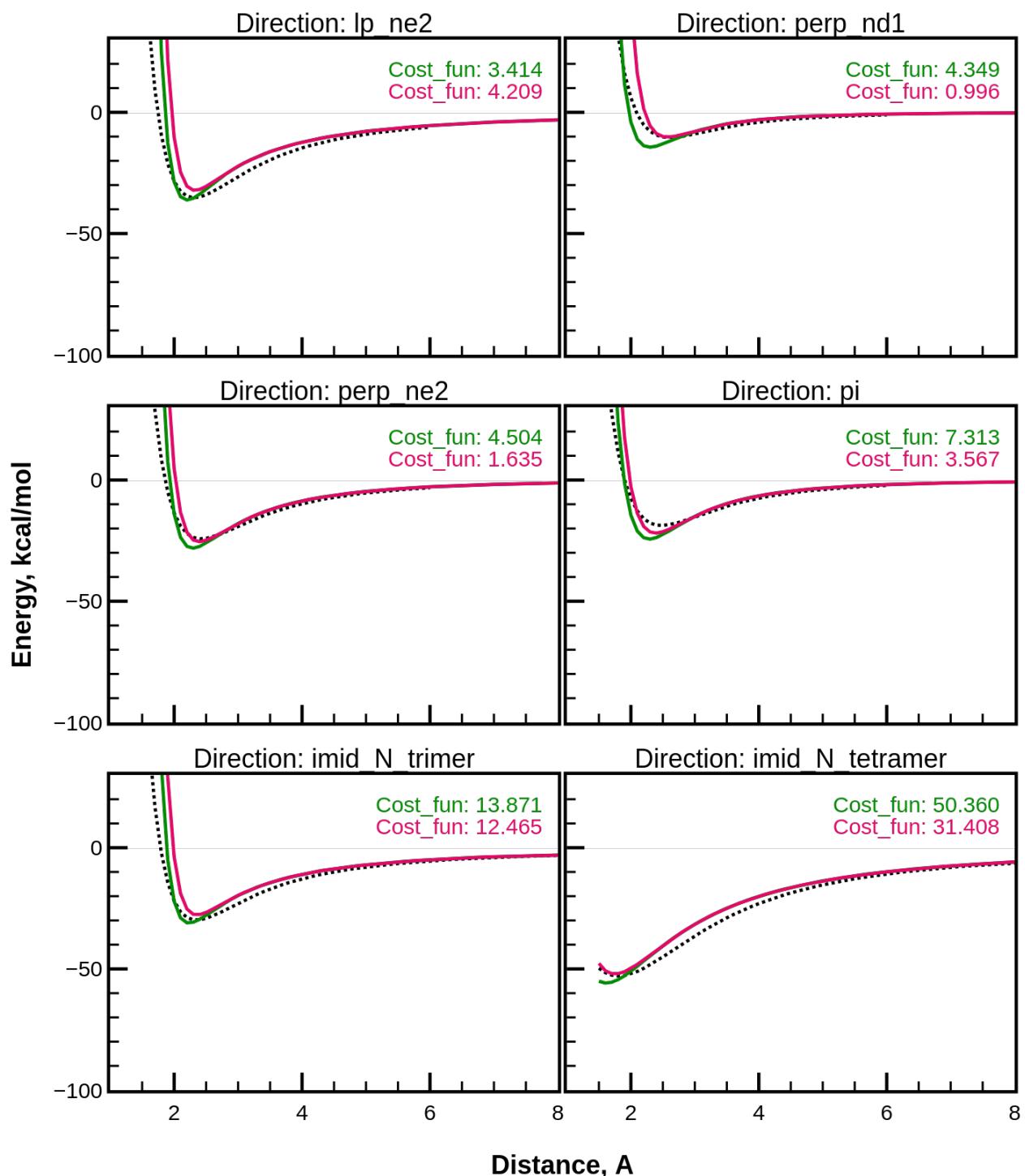
3.73665\_0.20976\_9.99999  
3.95002\_0.20976\_3.43827

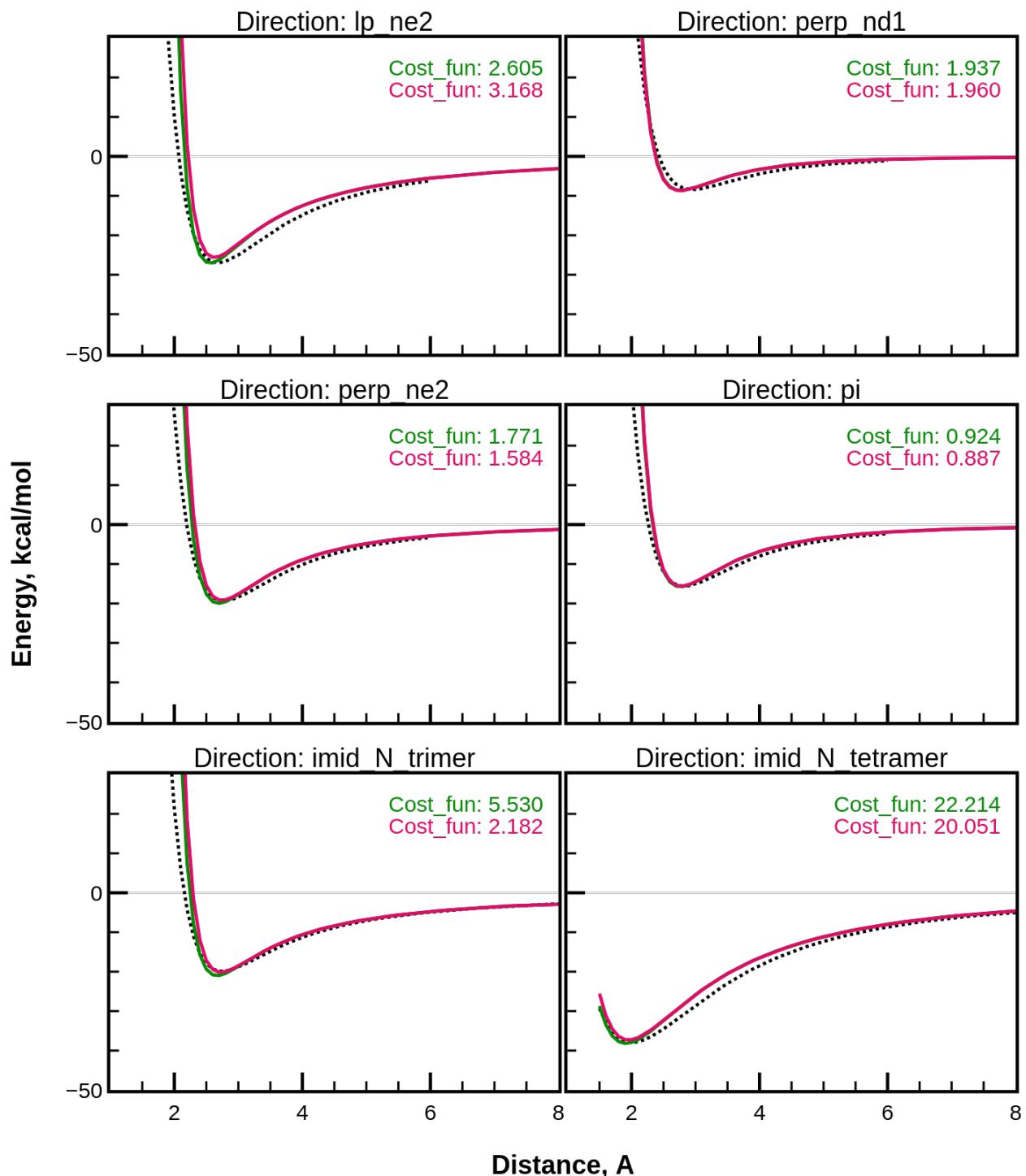


**DMS RUB 1/1**3.83551\_0.29095\_9.99999  
4.06564\_0.29095\_4.25802

**DMS CES 1/1**4.07382\_0.29283\_9.99999  
4.17814\_0.29283\_3.17830

**IMID LIT 1/1**2.96100\_0.05109\_9.99999  
3.39327\_0.05109\_4.39296

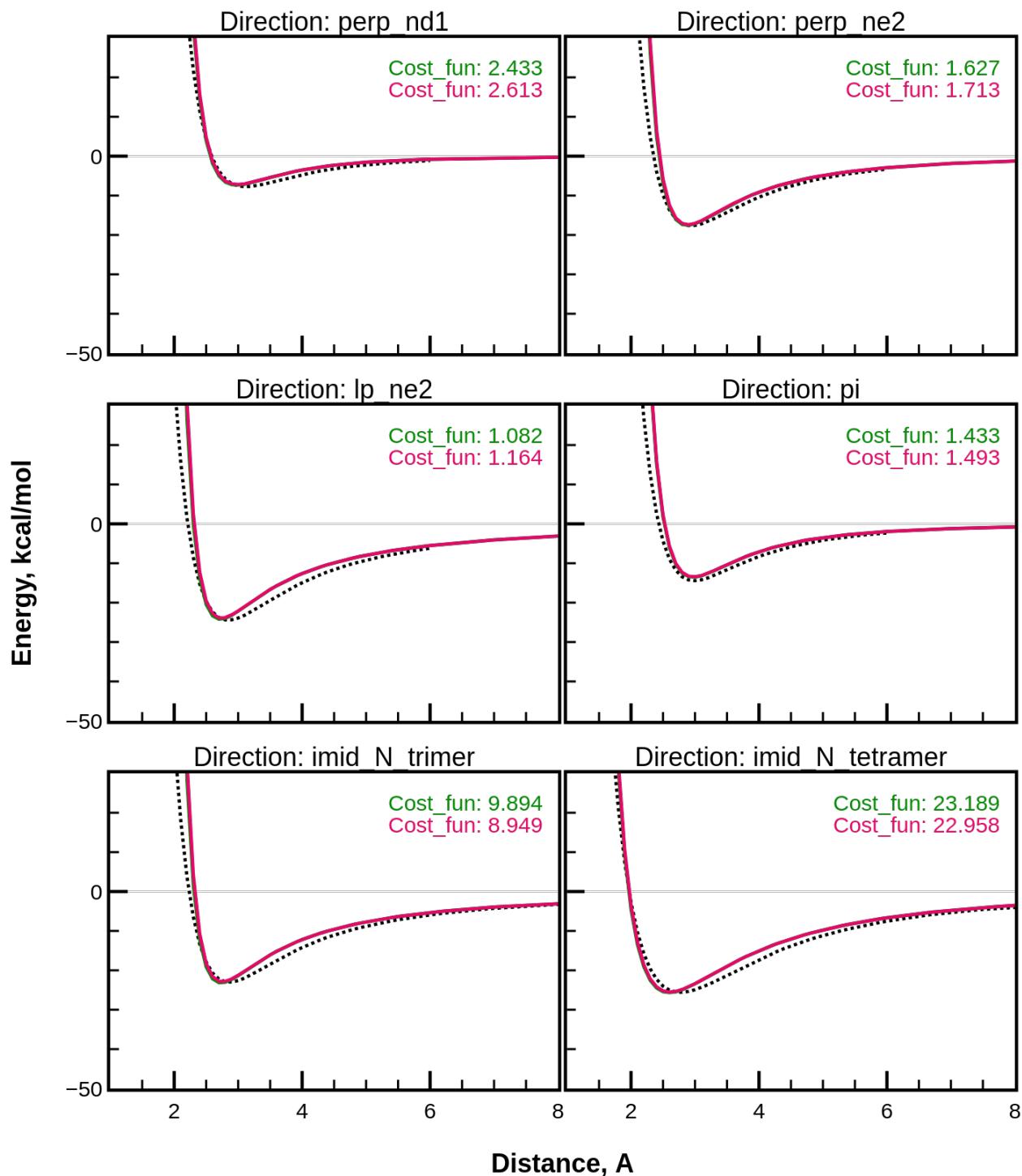
**IMID SOD 1/1**3.32268\_0.05236\_9.99999  
3.66106\_0.05236\_4.83751

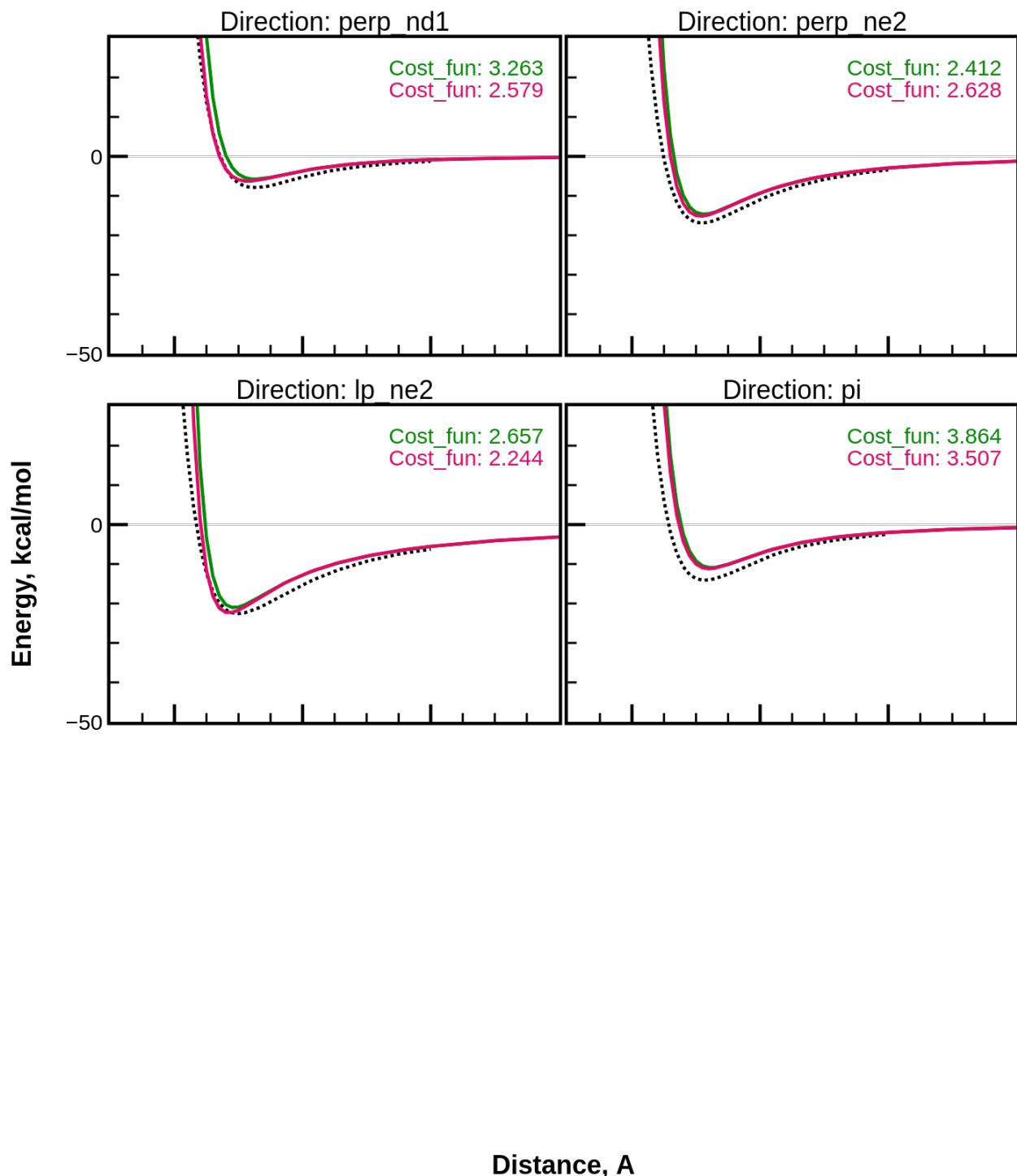
**IMID POT 1/1**3.54765\_0.11112\_9.99999  
3.52615\_0.11112\_3.46580

**IMID RUB 1/1**

3.64651\_0.15413\_9.99999

3.64509\_0.15413\_2.83449

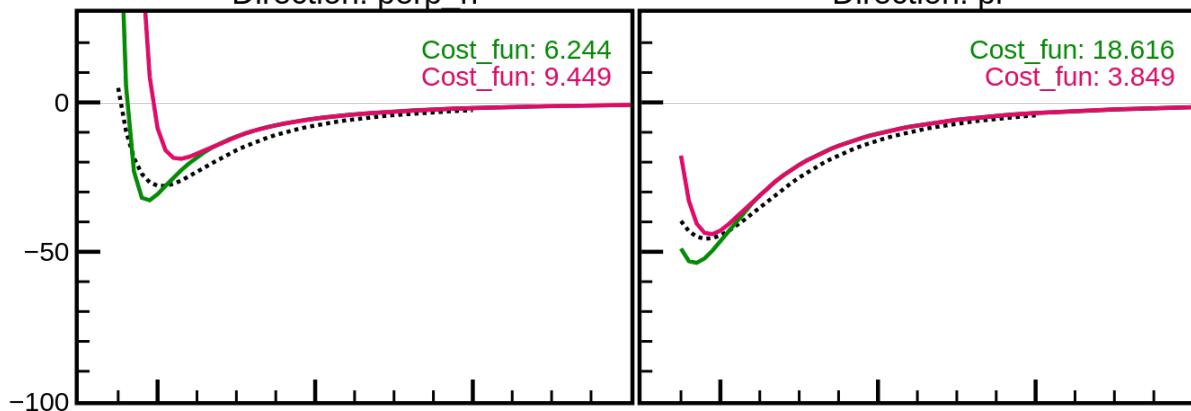


**IMID CES 1/1**3.88482\_0.15513\_9.99999  
3.64608\_0.15513\_4.63164

**INDO LIT 1/1**2.96100\_0.05109\_9.99999  
3.39327\_0.05109\_4.39296

Direction: perp\_n

Direction: pi



Energy, kcal/mol

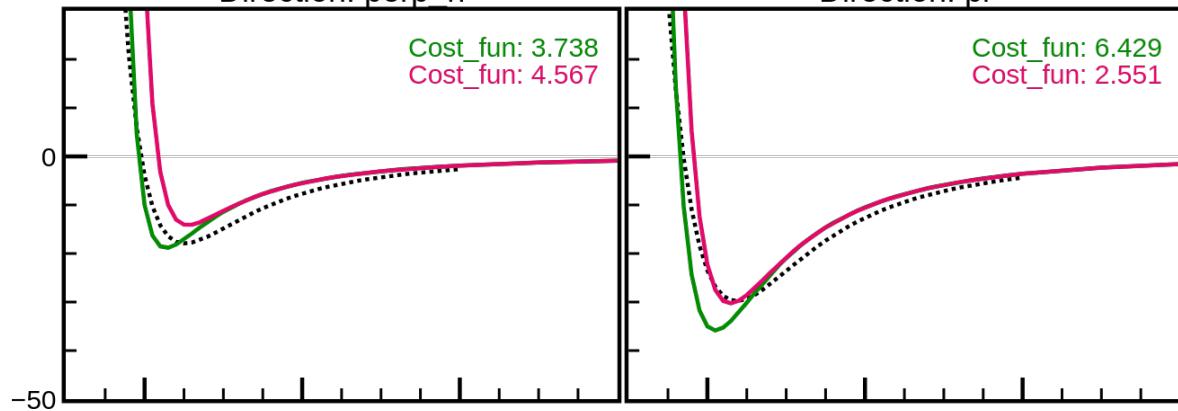
Distance, A

# INDO SOD 1/1

3.32268\_0.05236\_9.99999  
3.66106\_0.05236\_4.83751

Direction: perp\_n

Direction: pi



Energy, kcal/mol

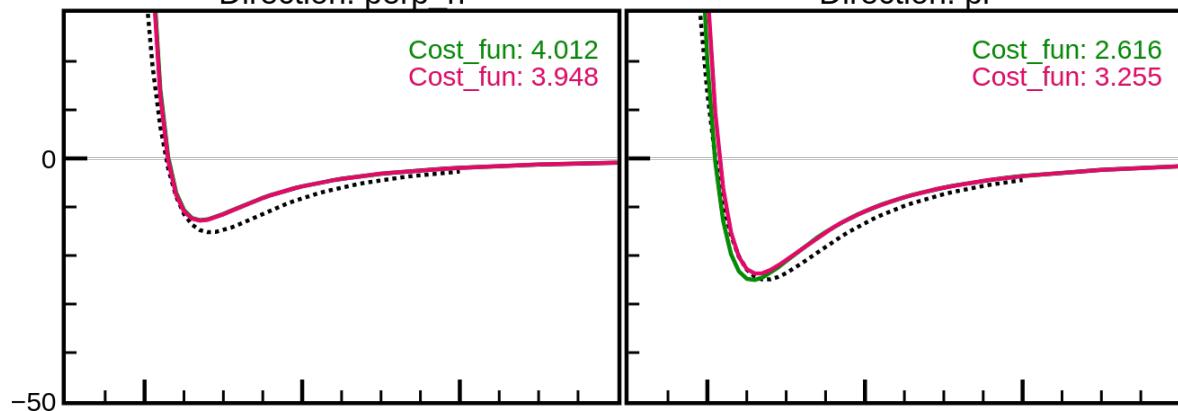
Distance, A

# INDO POT 1/1

3.54765\_0.11112\_9.99999  
3.52615\_0.11112\_3.46580

Direction: perp\_n

Direction: pi



Energy, kcal/mol

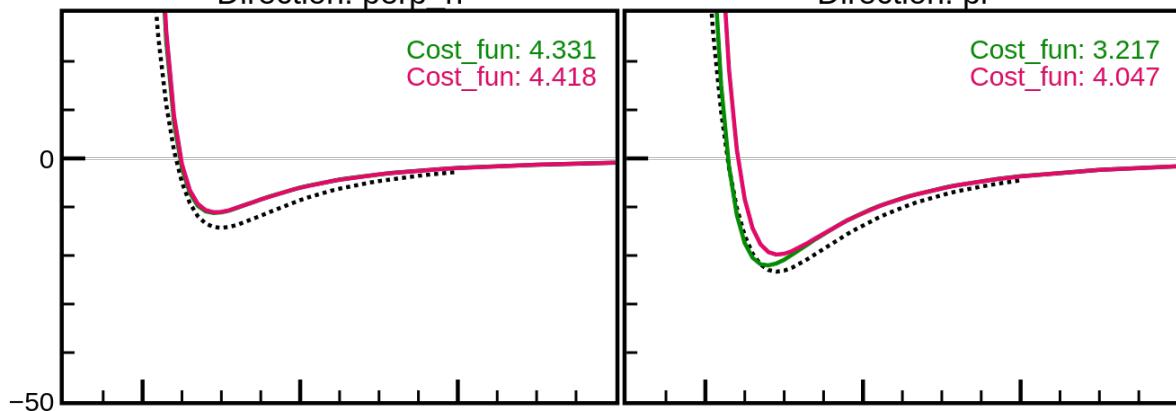
Distance, Å

# INDO RUB 1/1

3.64651\_0.15413\_9.99999  
3.64509\_0.15413\_2.83449

Direction: perp\_n

Direction: pi



Energy, kcal/mol

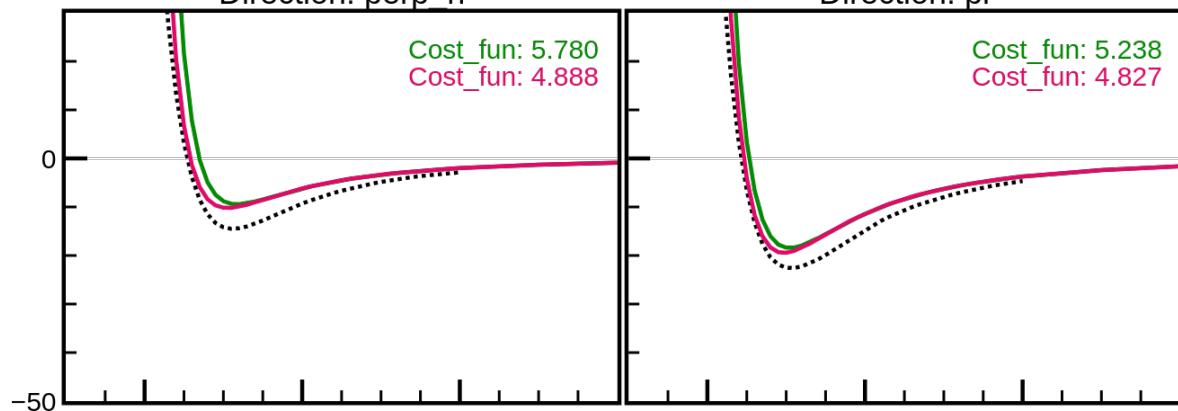
Distance, A

# INDO CES 1/1

3.88482\_0.15513\_9.99999  
3.64608\_0.15513\_4.63164

Direction: perp\_n

Direction: pi

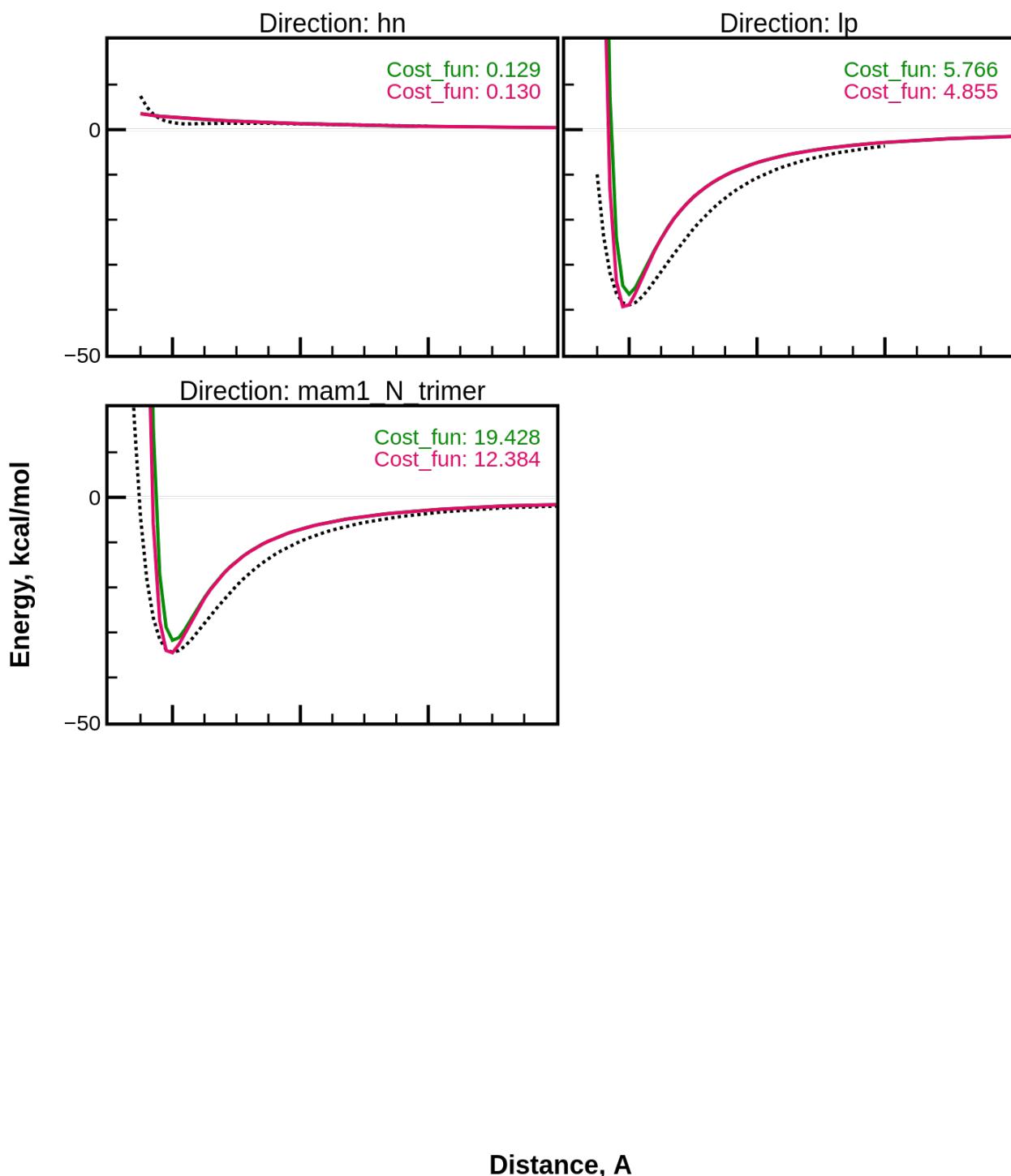


Energy, kcal/mol

Distance, A

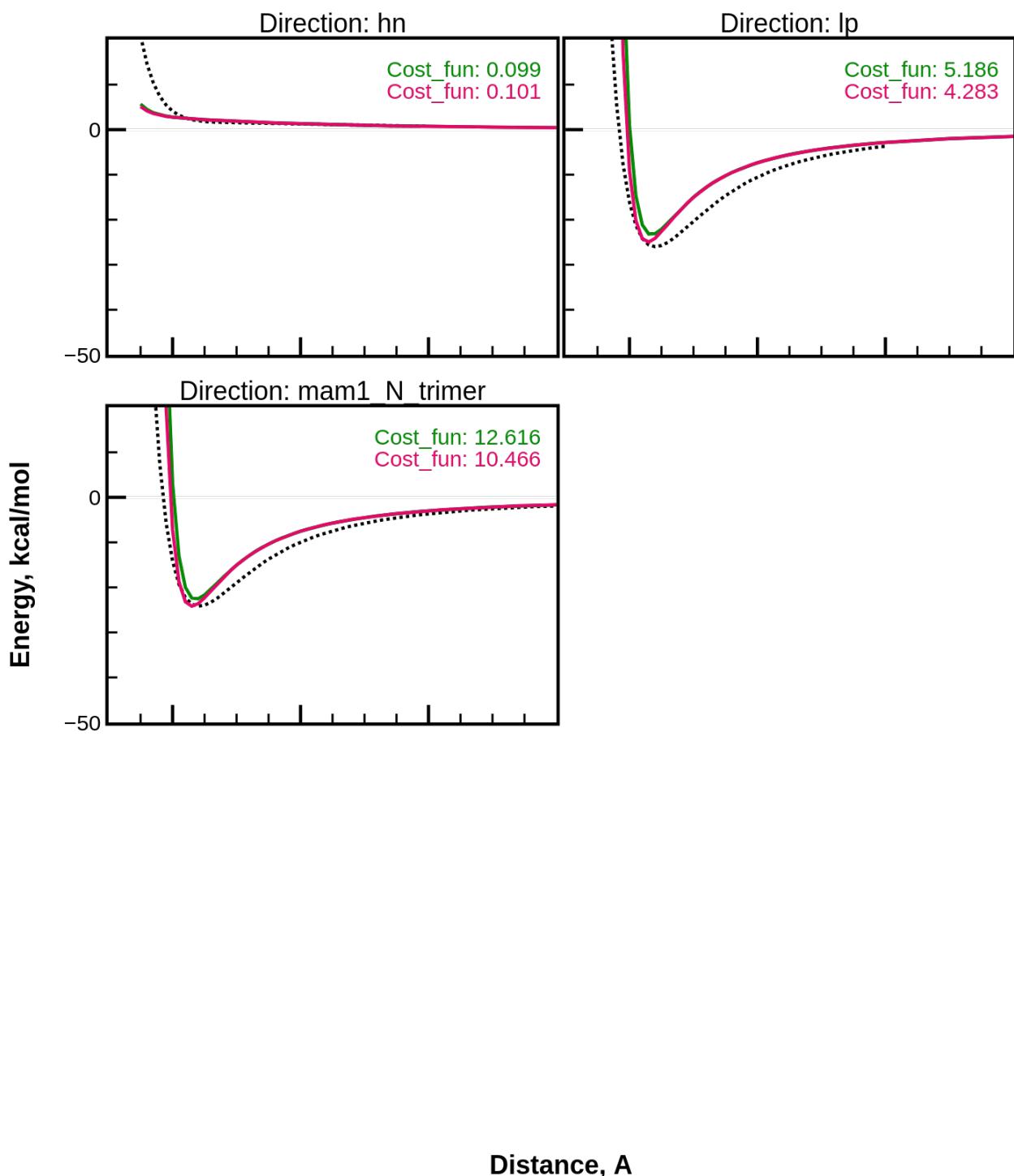
# MAM1 LIT 1/1

3.00000\_0.10507\_9.99999  
2.91762\_0.10507\_2.28851



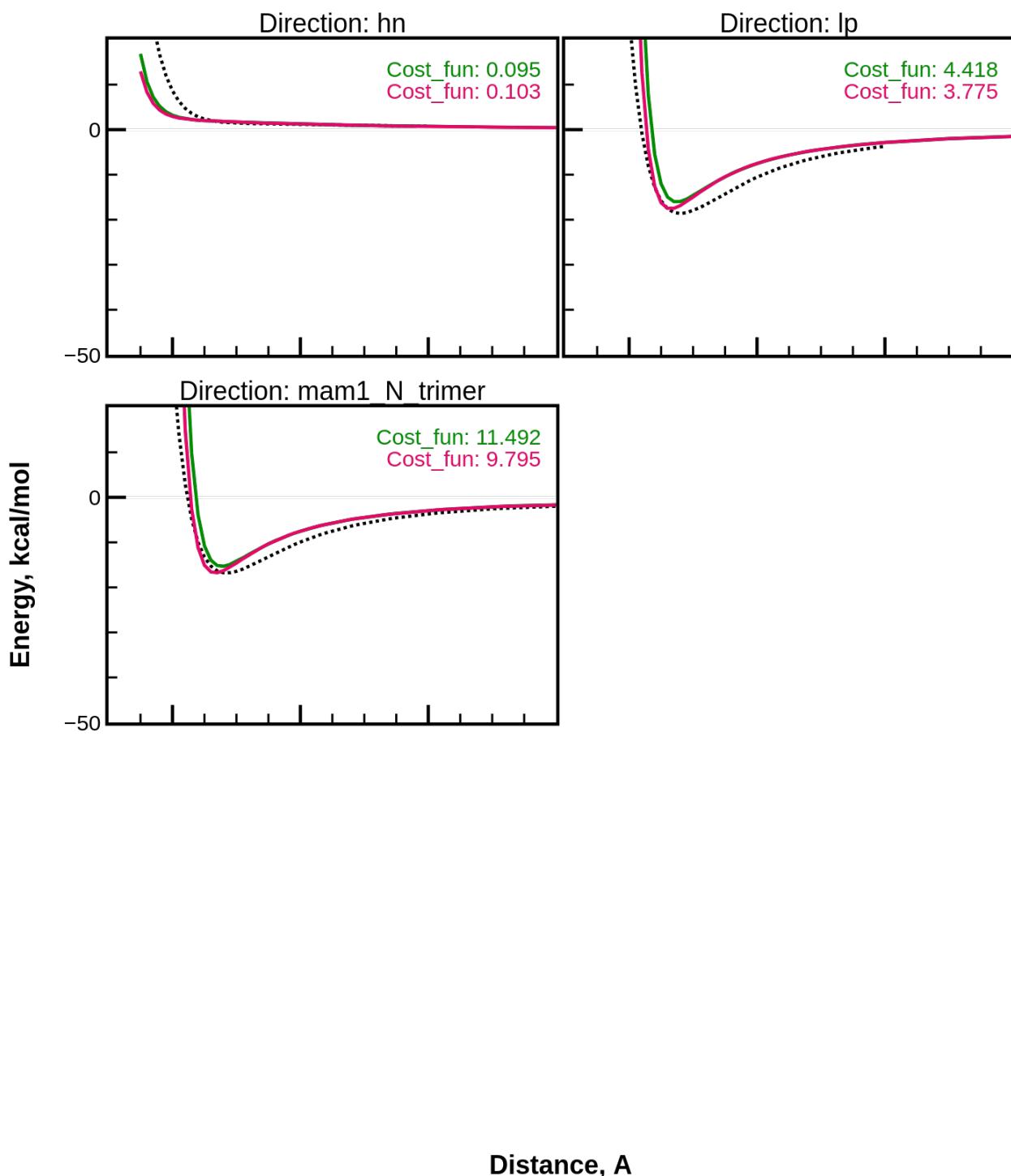
# MAM1 SOD 1/1

3.36168\_0.10768\_9.99999  
3.29369\_0.10768\_3.02188



# MAM1 POT 1/1

3.58665\_0.22854\_9.99999  
3.48076\_0.22854\_3.11158

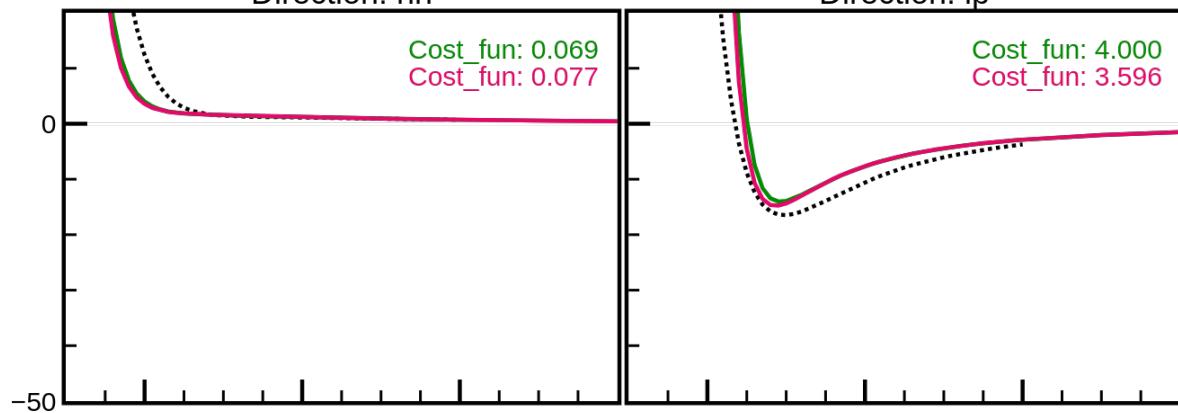


# MAM1 RUB 1/1

3.68551\_0.31700\_9.99999  
3.62004\_0.31700\_3.35747

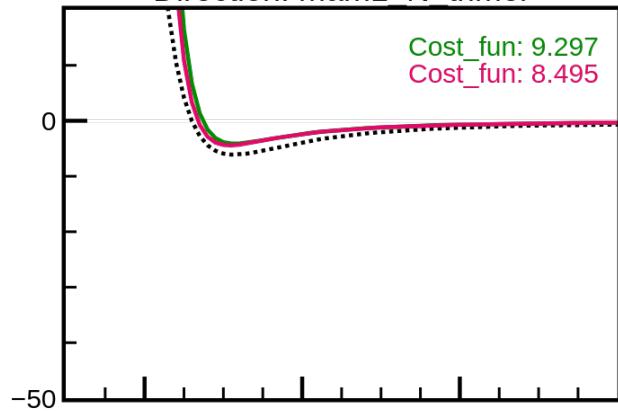
Direction: hn

Direction: lp



Direction: mam1\_N\_trimer

Energy, kcal/mol



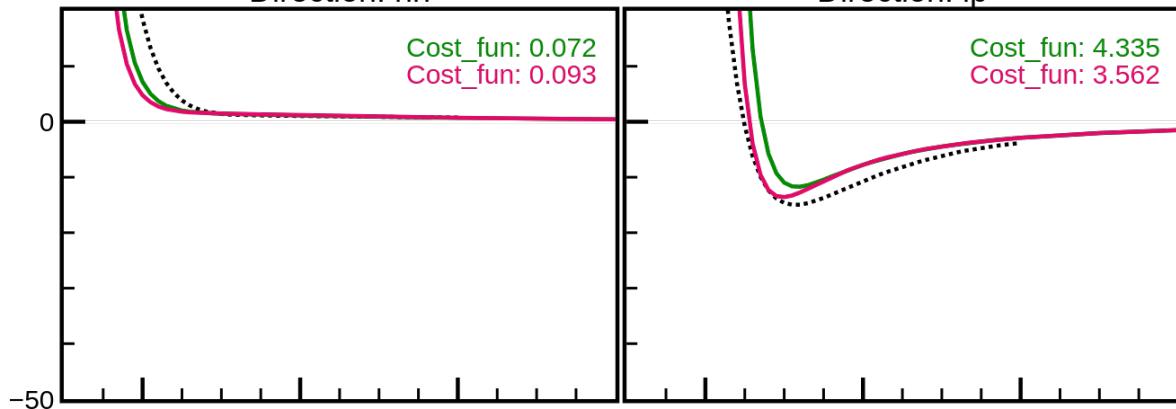
Distance, Å

# MAM1 CES 1/1

3.92382\_0.31905\_9.99999  
3.74421\_0.31905\_3.75857

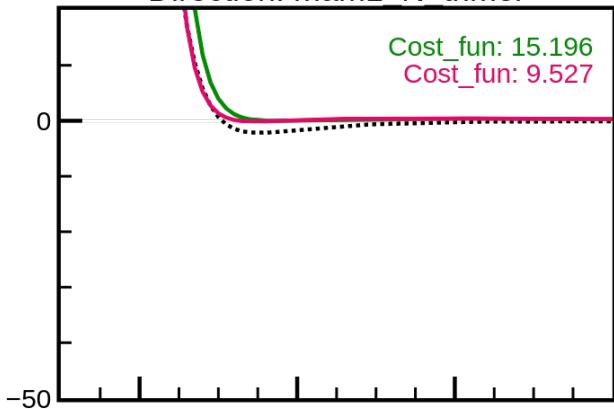
Direction: hn

Direction: lp

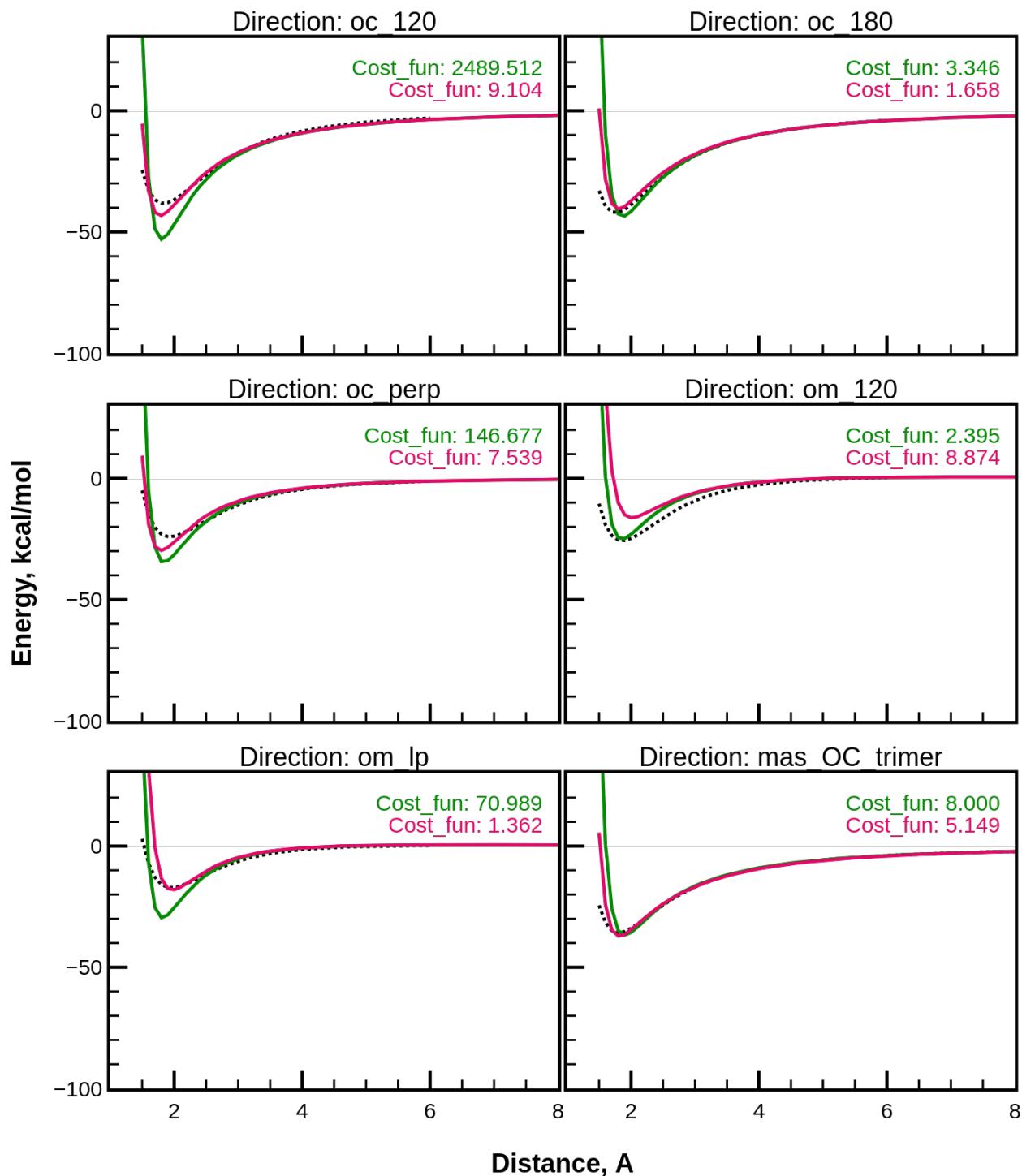


Direction: mam1\_N\_trimer

Energy, kcal/mol

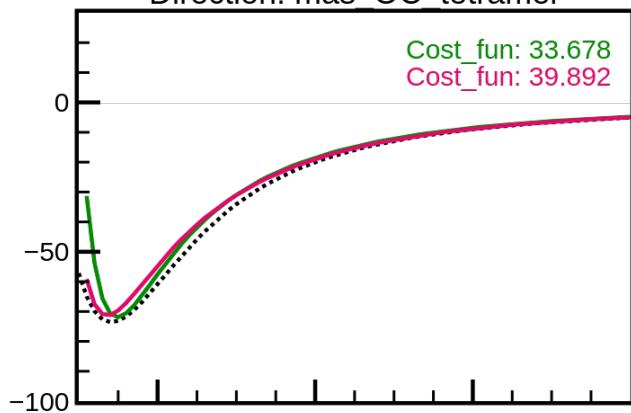


Distance, Å

**MAS LIT 1/2**2.85000\_0.07348\_9.99999  
2.65664\_0.07348\_0.64546

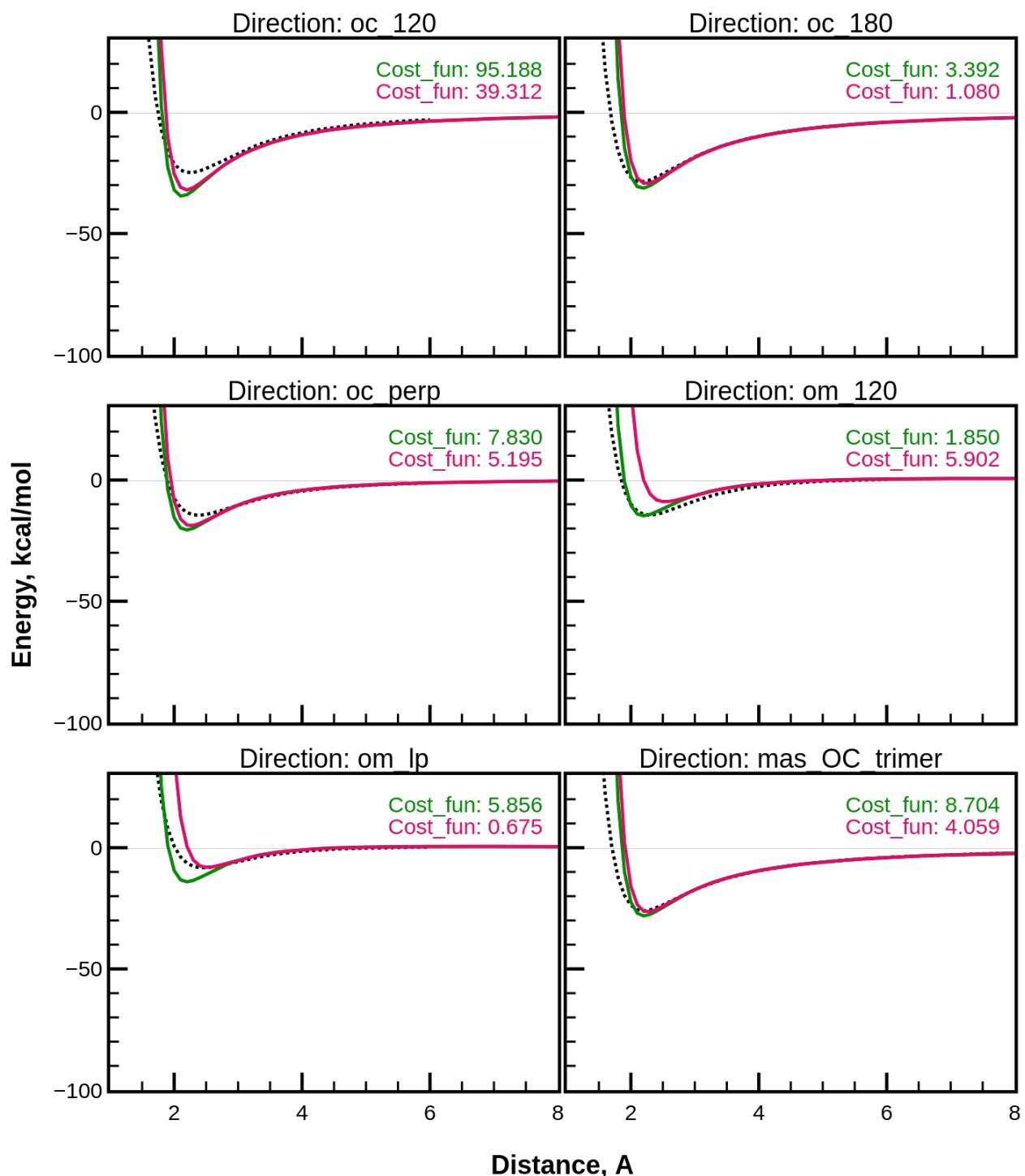
**MAS LIT 2/2**2.85000\_0.07348\_9.99999  
2.65664\_0.07348\_0.64546

Direction: mas OC tetramer



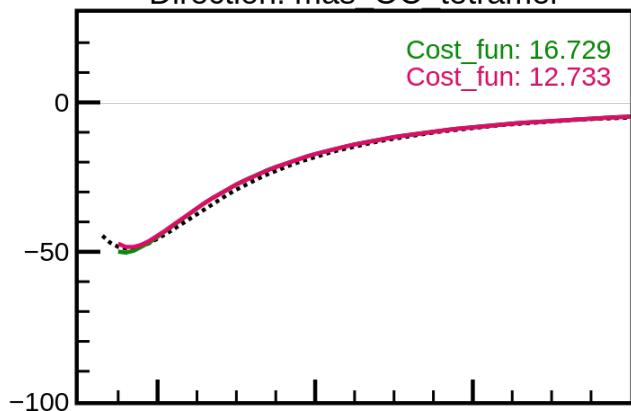
Energy, kcal/mol

Distance, Å

**MAS SOD 1/2**3.21168\_0.07531\_9.99999  
3.28395\_0.07531\_3.34812

**MAS SOD 2/2**3.21168\_0.07531\_9.99999  
3.28395\_0.07531\_3.34812

Direction: mas OC tetramer

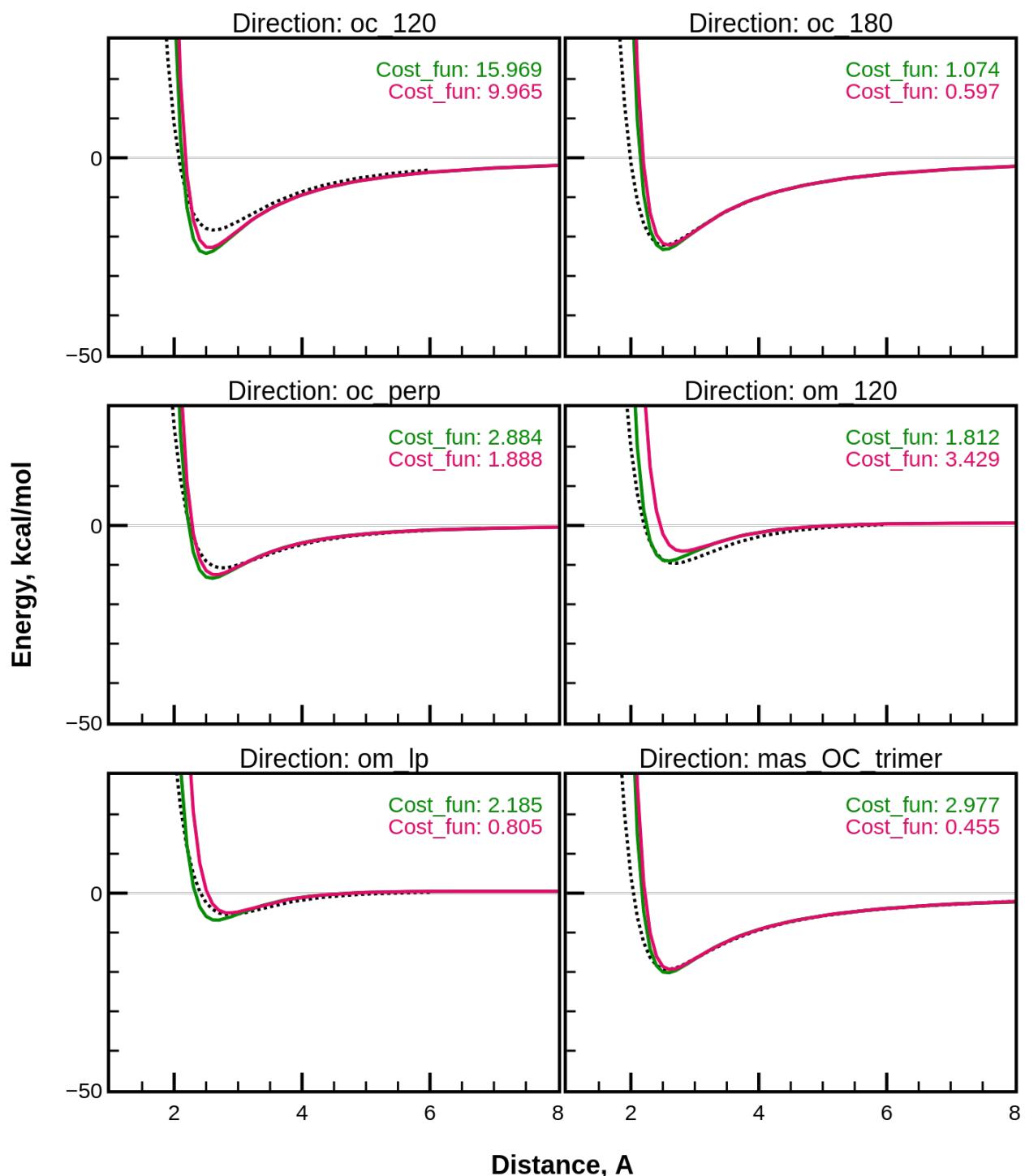


Energy, kcal/mol

Distance, Å

# MAS POT 1/2

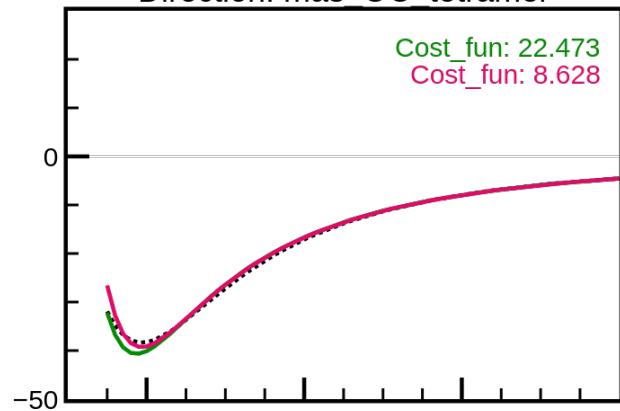
3.43665\_0.15983\_9.99999  
3.49368\_0.15983\_2.83217

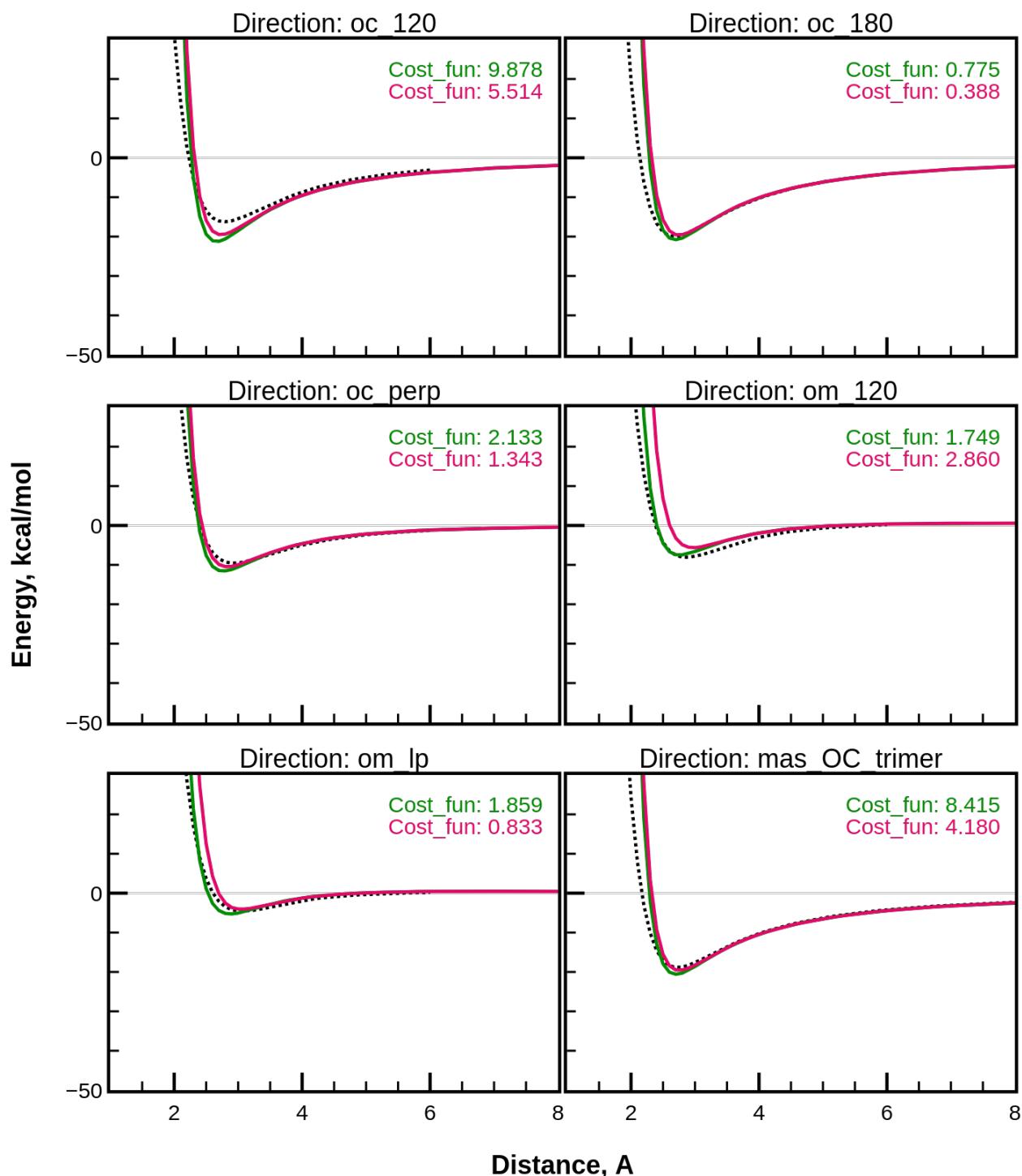


## MAS POT 2/2

3.43665\_0.15983\_9.99999  
3.49368\_0.15983\_2.83217

Direction: mas OC tetramer

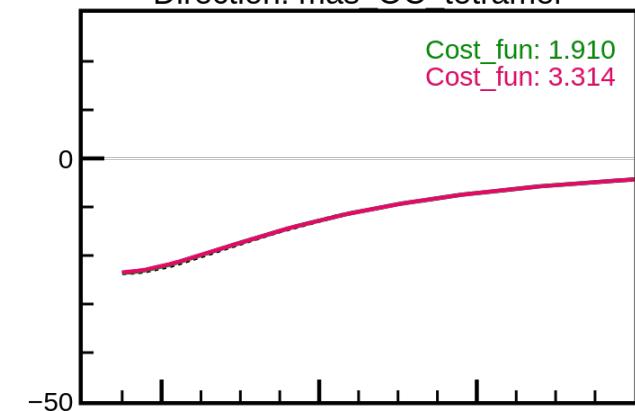


**MAS RUB 1/2**3.53551\_0.22170\_9.99999  
3.55885\_0.22170\_1.61222

**MAS RUB 2/2**

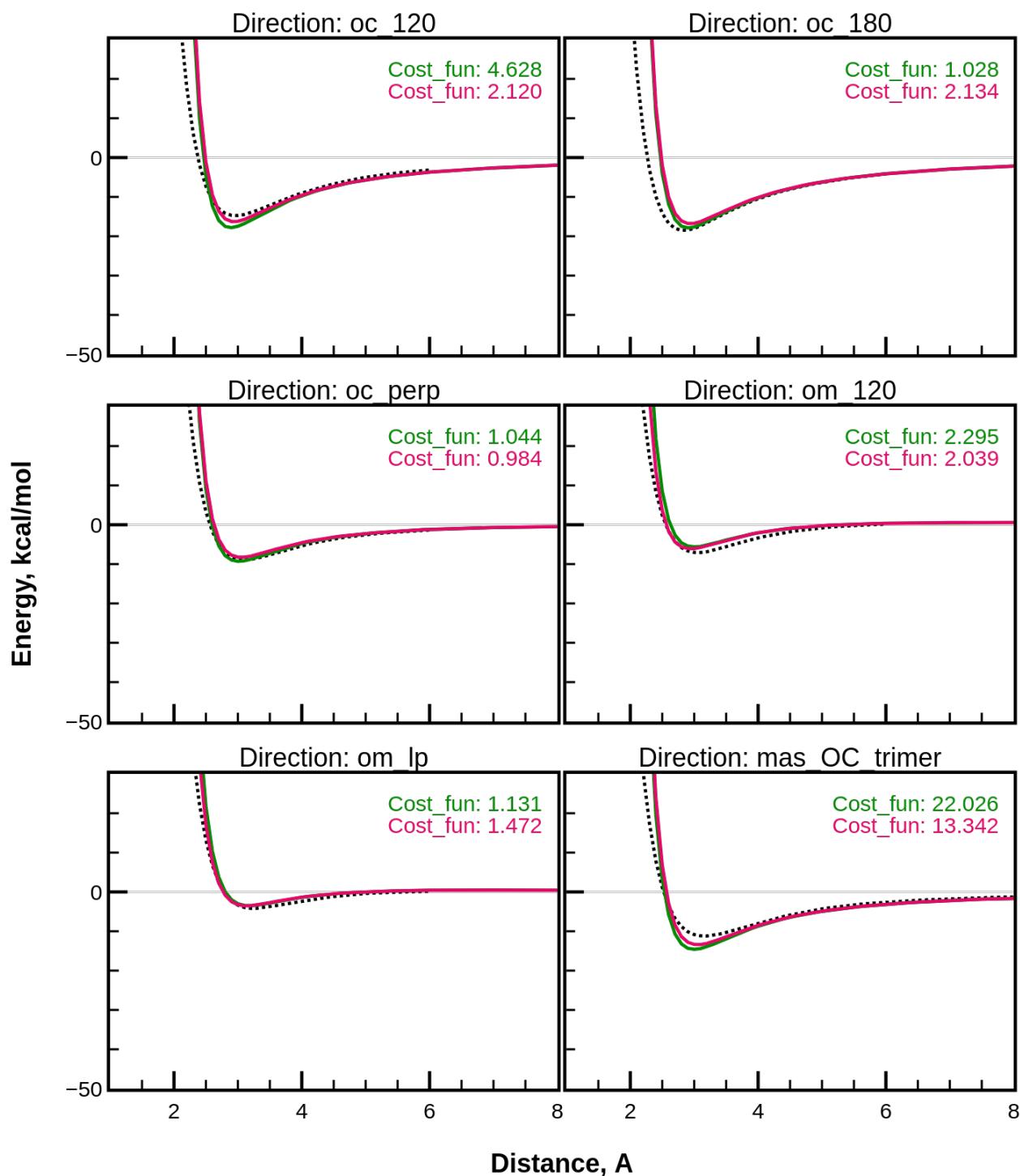
3.53551\_0.22170\_9.99999  
3.55885\_0.22170\_1.61222

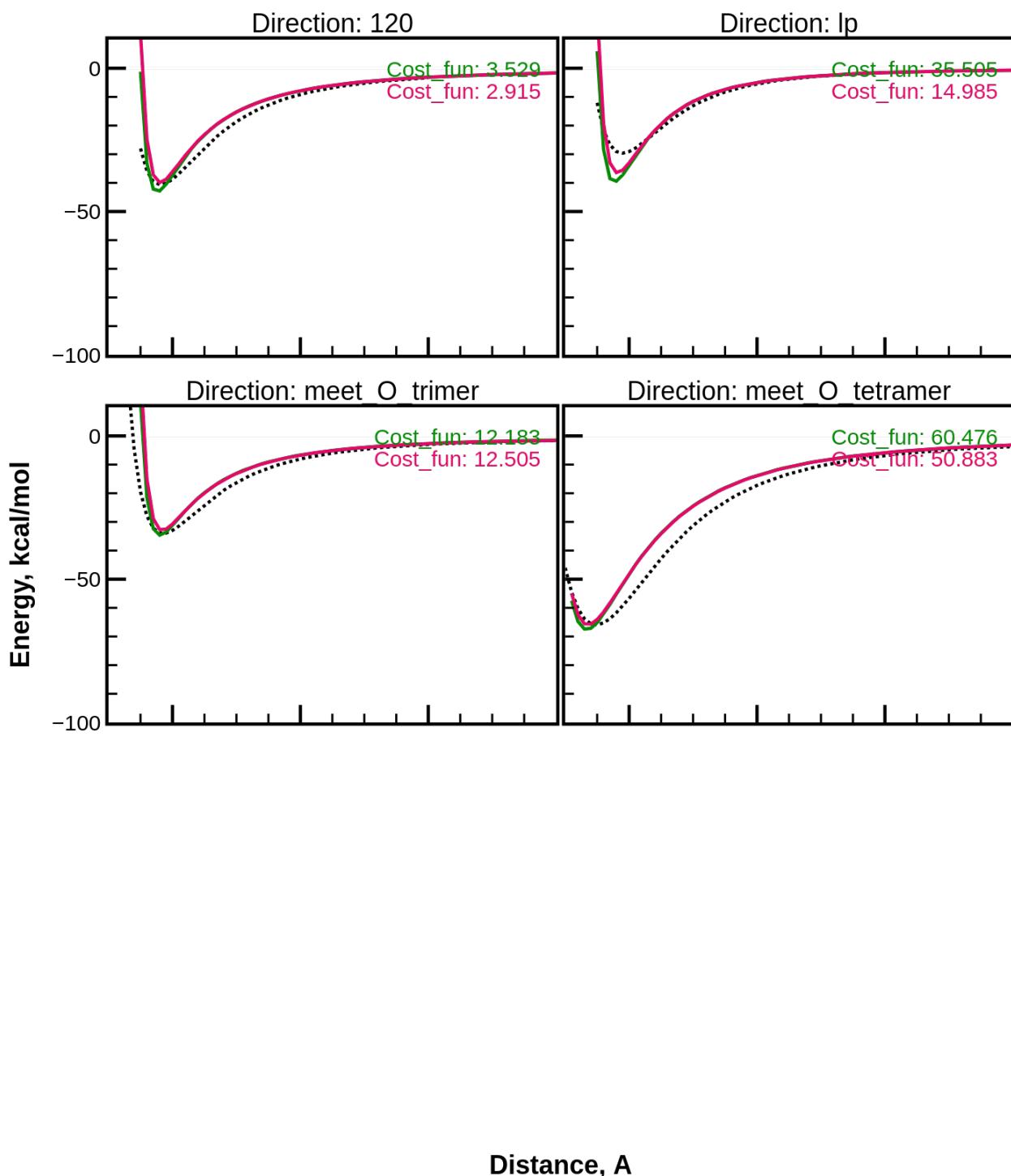
Direction: mas OC tetramer



**Distance, Å**

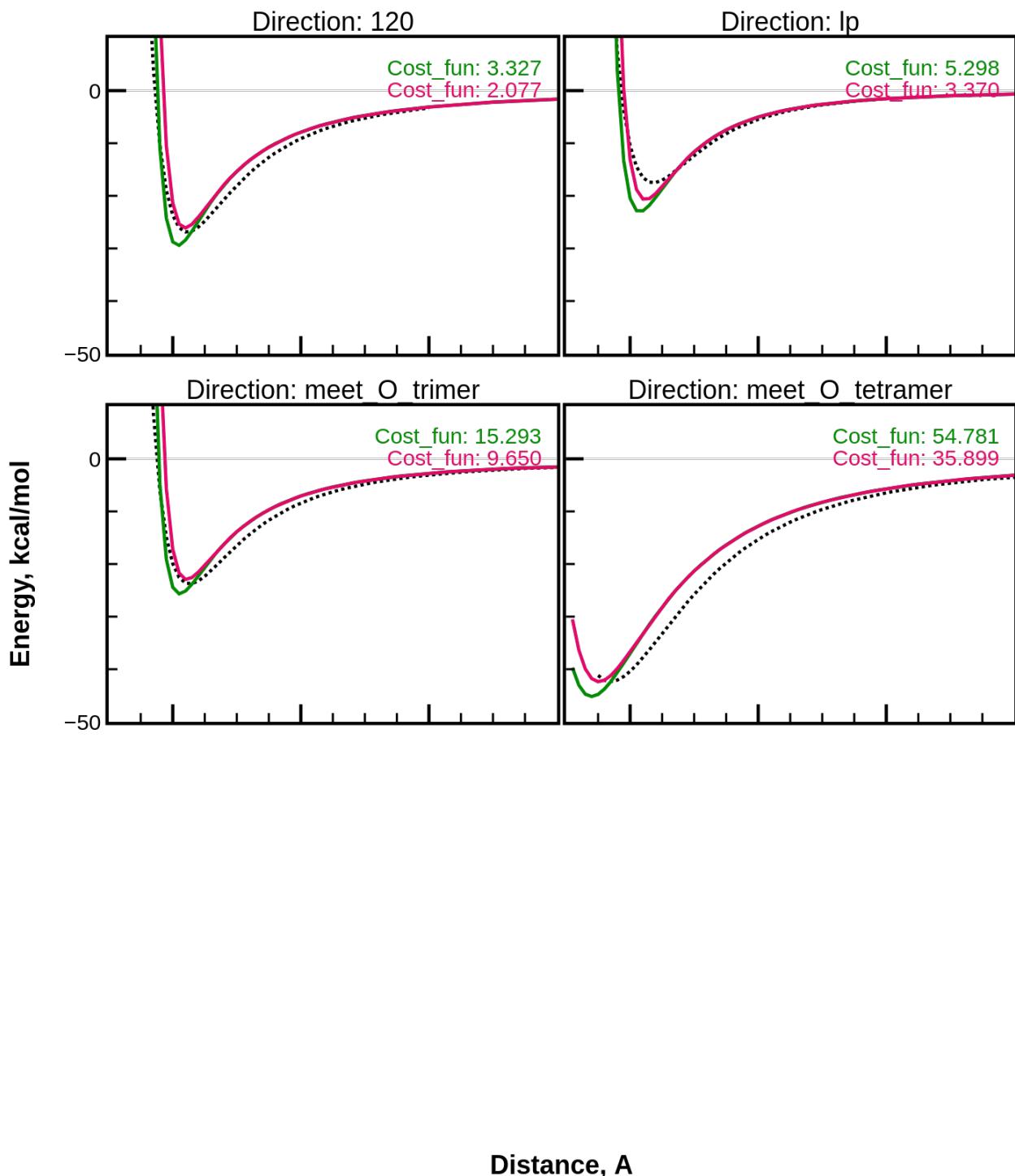
Energy, kcal/mol

**MAS CES 1/1**3.77382\_0.22313\_9.99999  
3.76247\_0.22313\_1.03679

**MEET LIT 1/1**2.84000\_0.04243\_9.99999  
2.83896\_0.04243\_1.67374

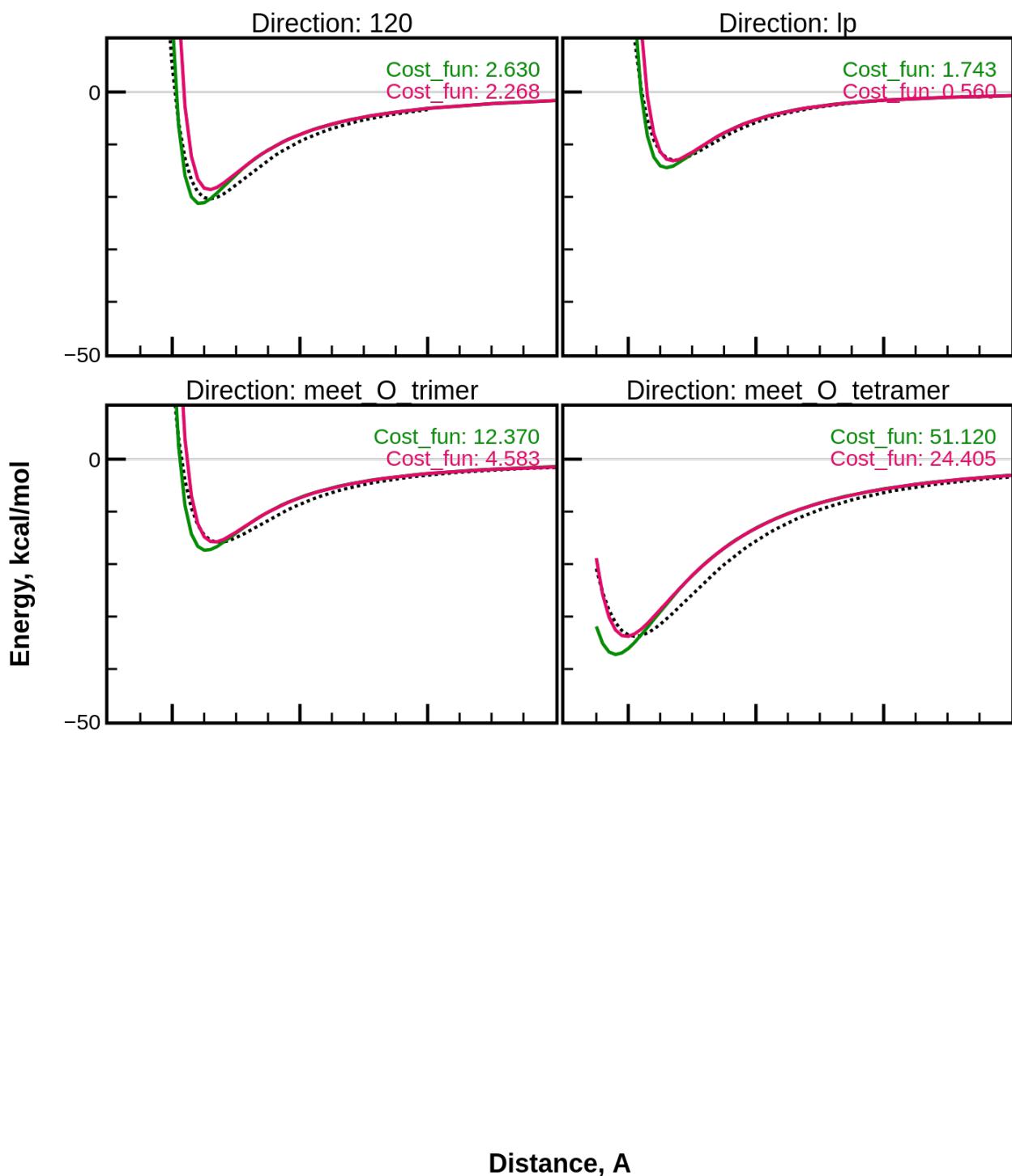
# MEET SOD 1/1

3.20168\_0.04348\_9.99999  
3.32356\_0.04348\_2.38138



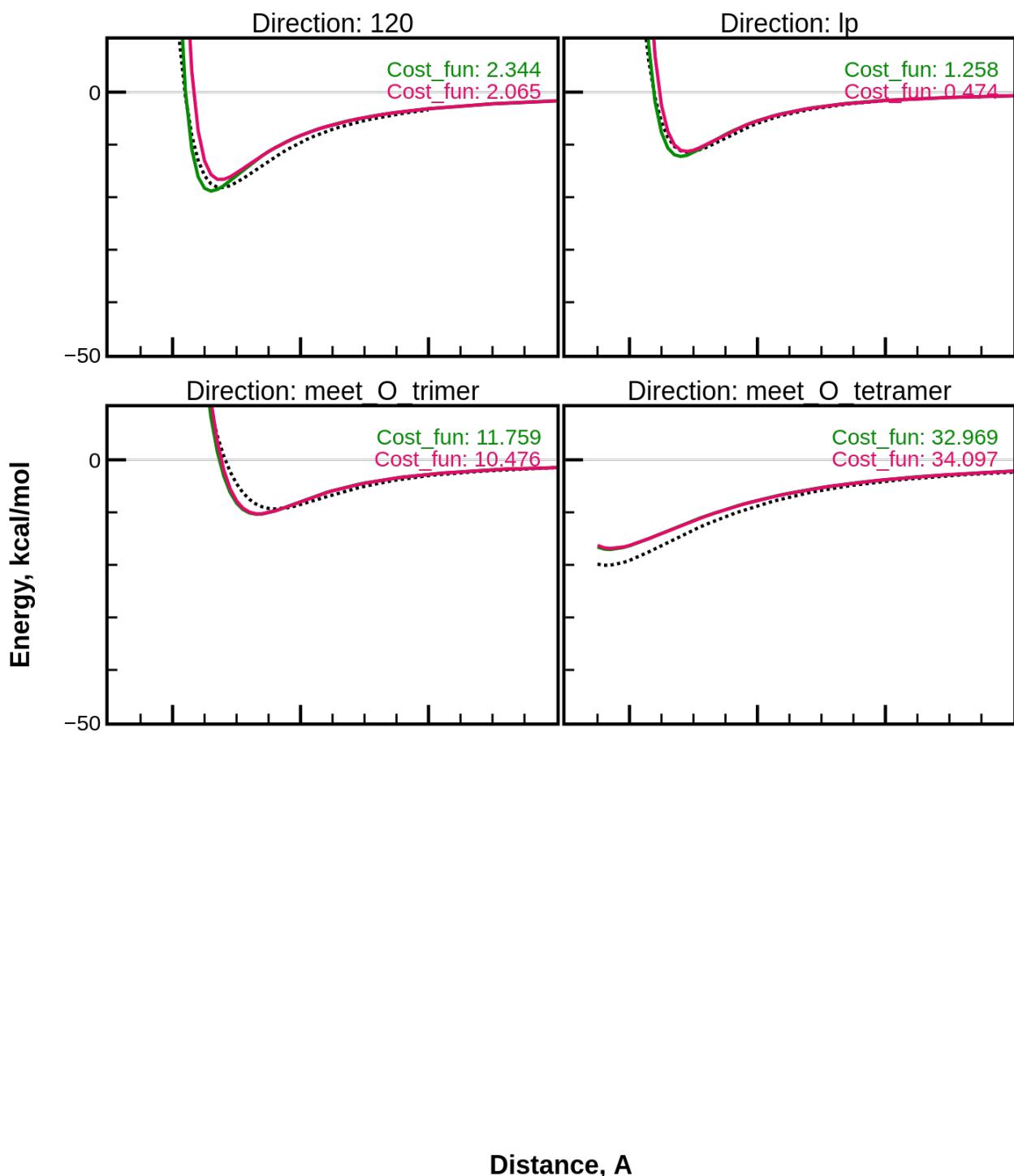
# MEET POT 1/1

3.42665\_0.09228\_9.99999  
3.57463\_0.09228\_2.23398



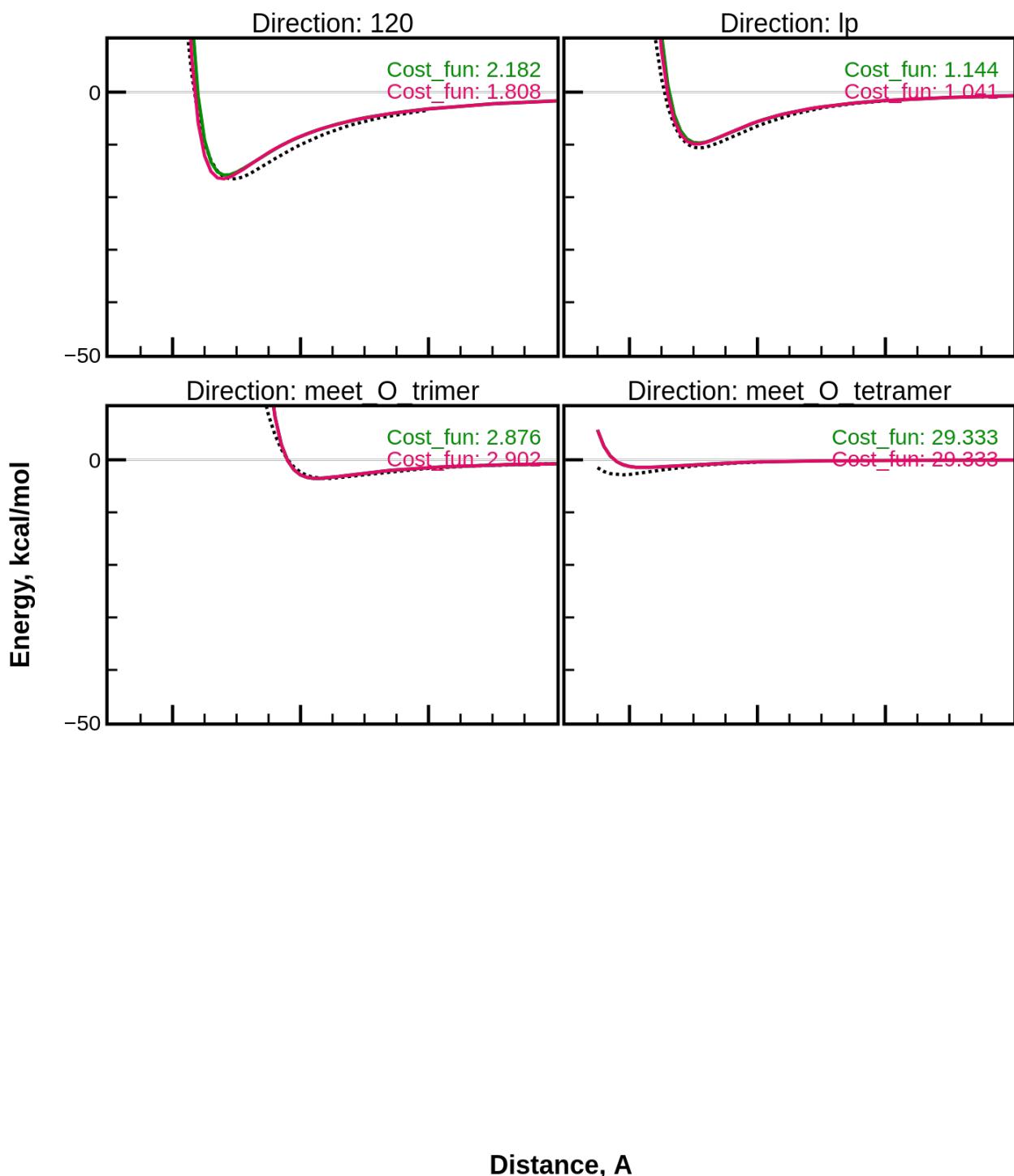
# MEET RUB 1/1

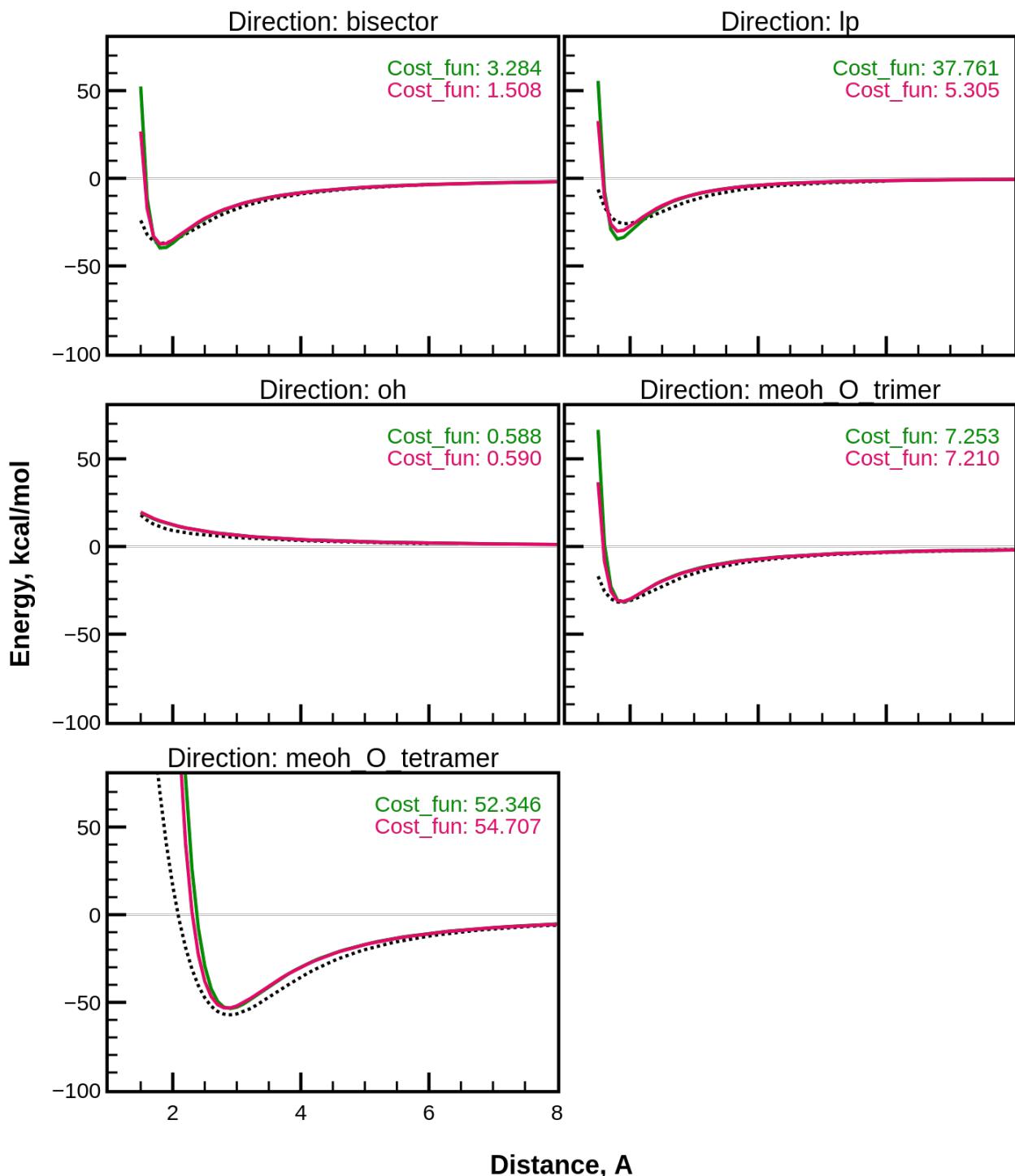
3.52551\_0.12800\_9.99999  
3.69056\_0.12800\_3.56696

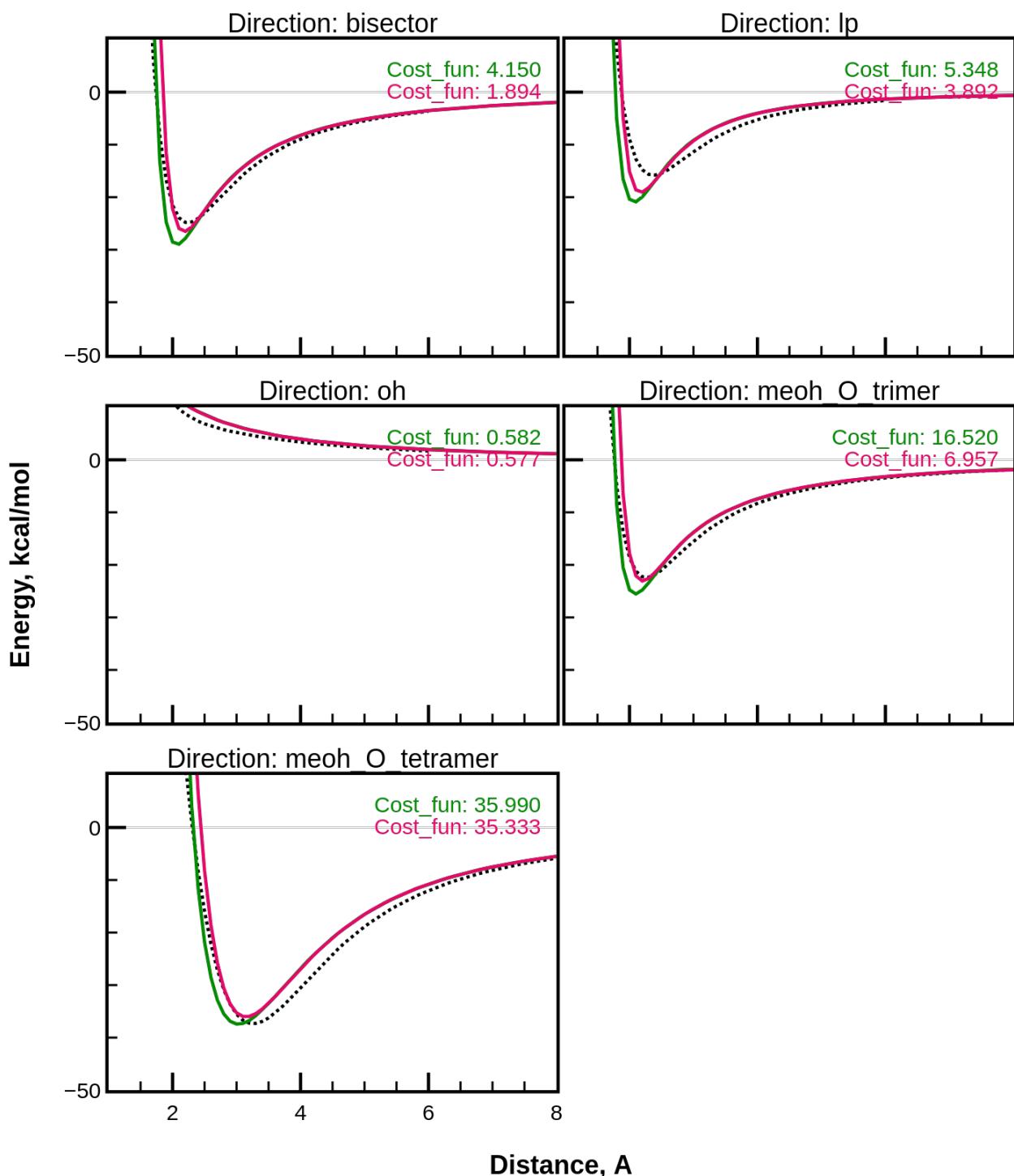


# MEET CES 1/1

3.76382\_0.12883\_9.99999  
3.69778\_0.12883\_4.23998

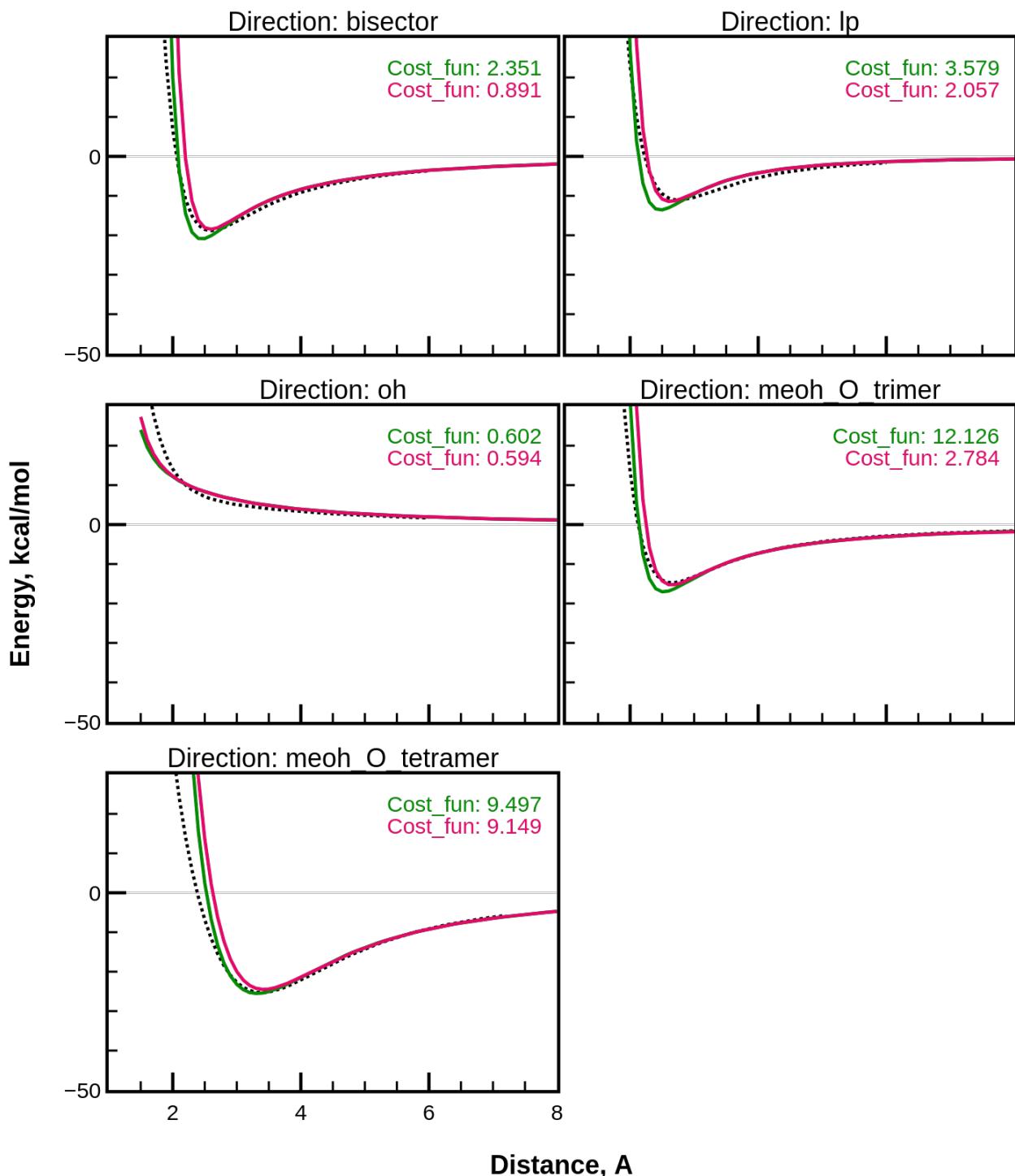


**MEOH LIT 1/1**2.86500\_0.06708\_9.99999  
2.76202\_0.06708\_1.45978

**MEOH SOD 1/1**3.07000\_0.06000\_1.82000  
3.21654\_0.06780\_2.59341

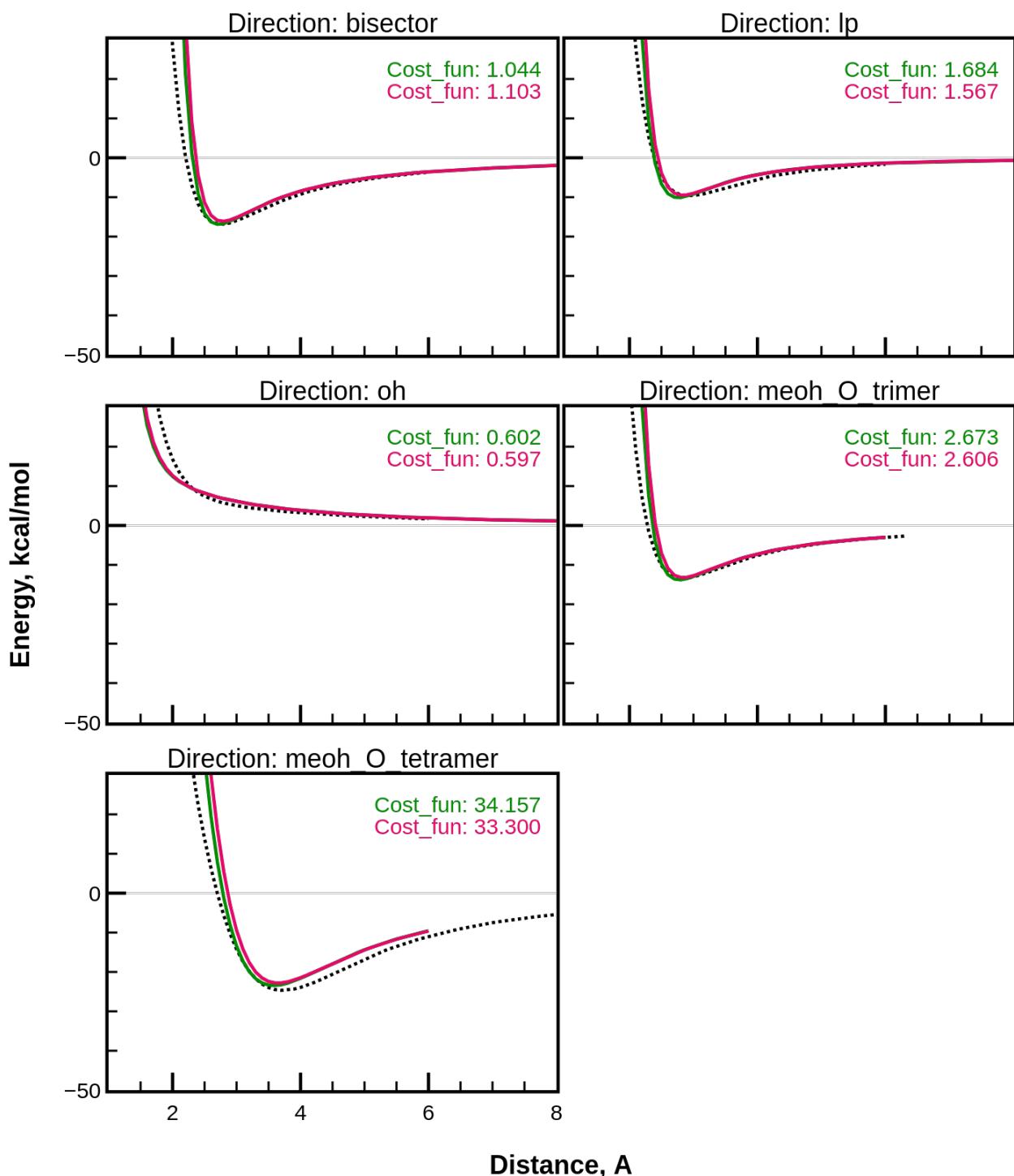
# MEOH POT 1/1

3.34000\_0.15000\_9.99999  
3.49152\_0.14591\_4.59270



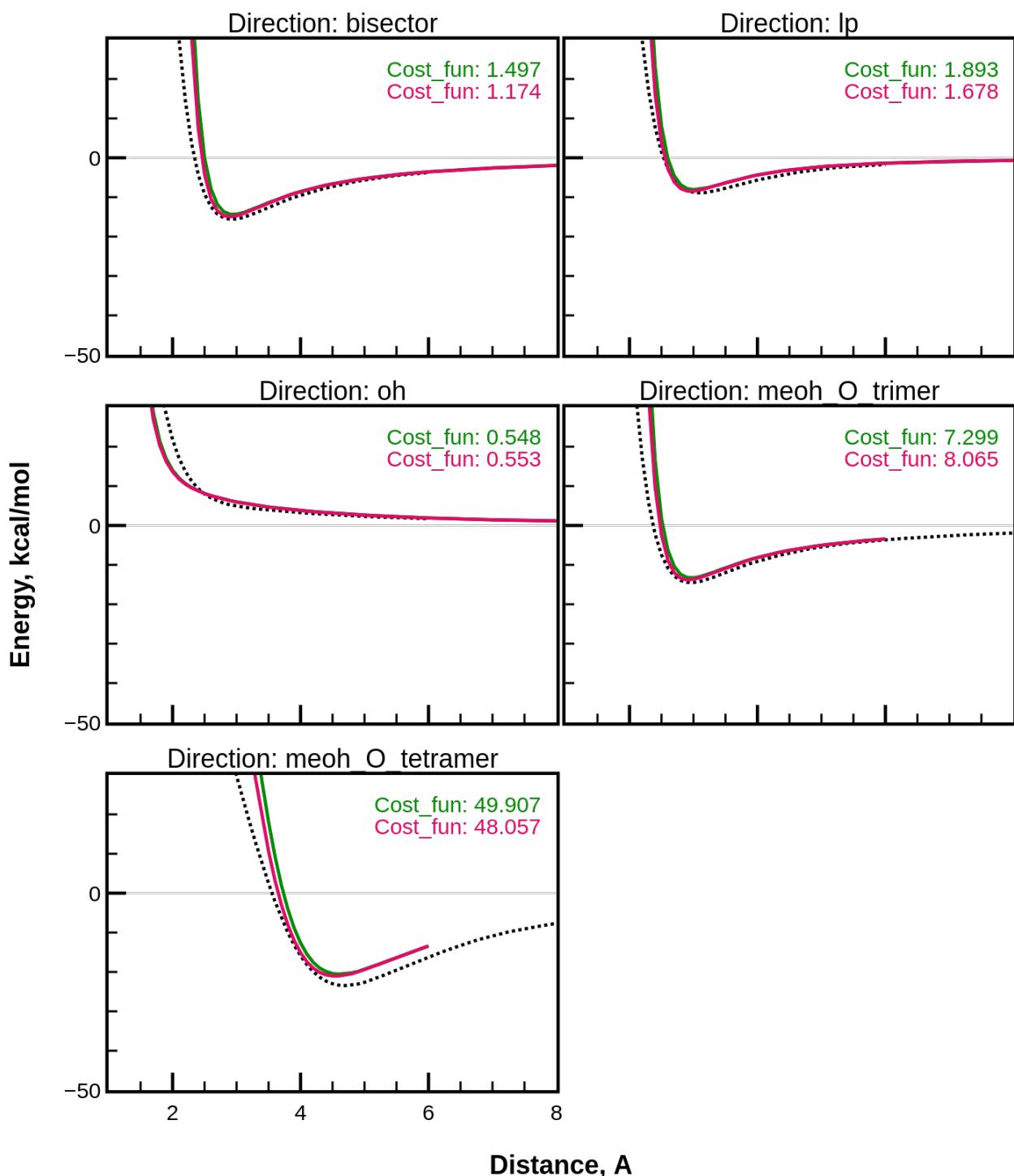
# MEOH RUB 1/1

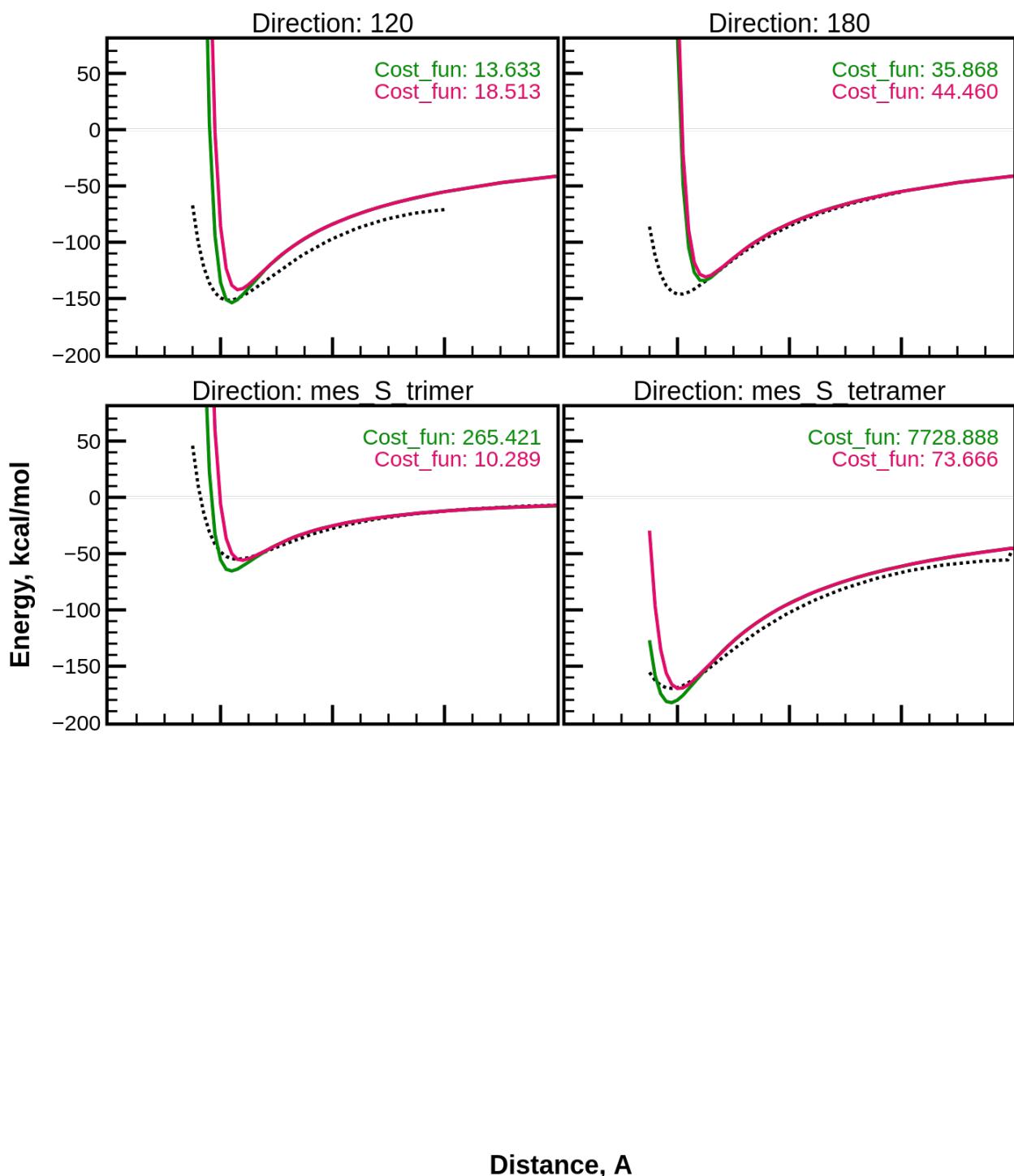
3.55051\_0.20239\_9.99999  
3.61044\_0.20239\_3.86775



# MEOH CES 1/1

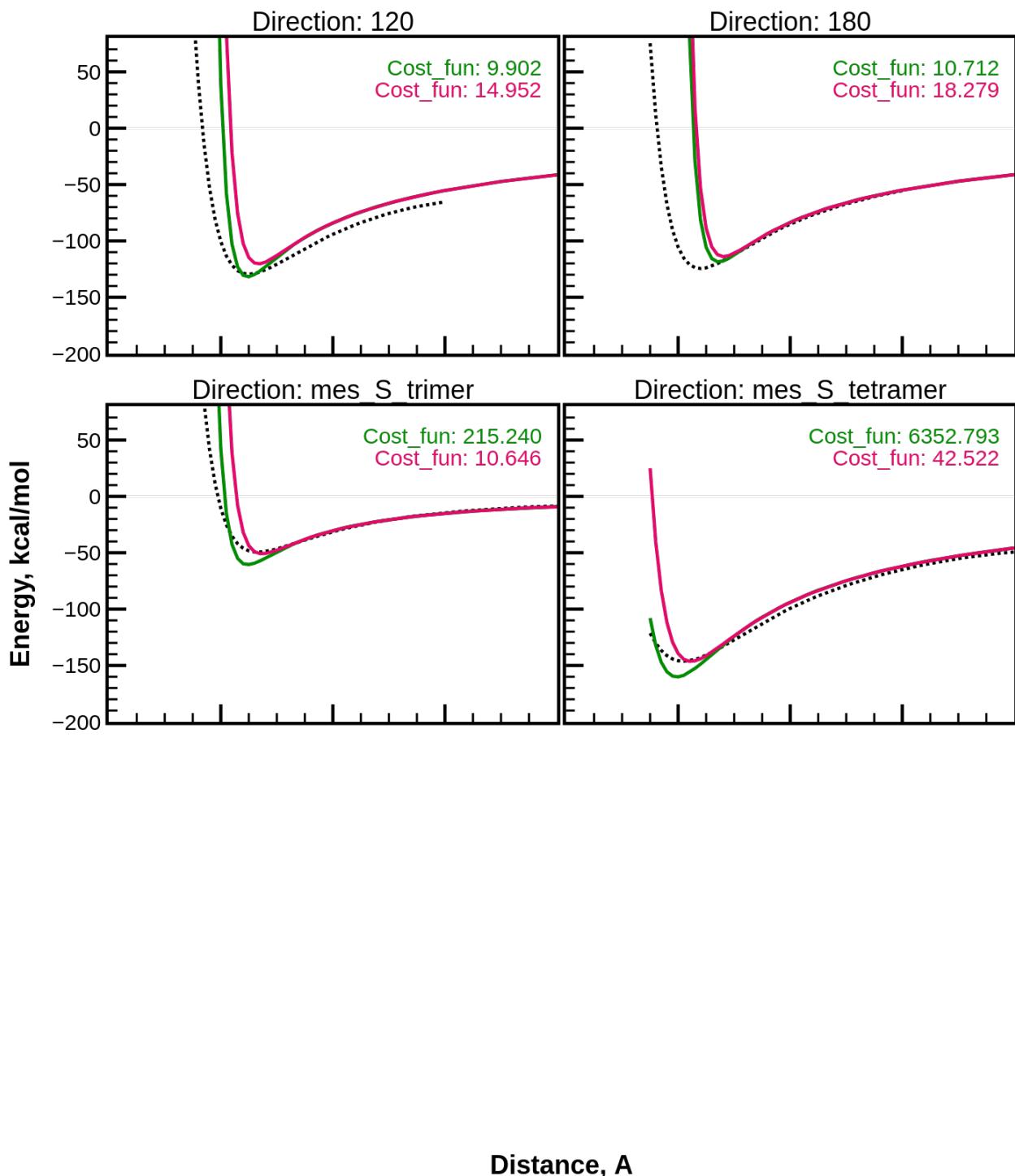
3.78882\_0.20369\_9.99999  
3.73546\_0.20369\_4.77880



**MES LIT 1/1**3.27000\_0.07746\_9.99999  
3.56646\_0.07746\_3.08189

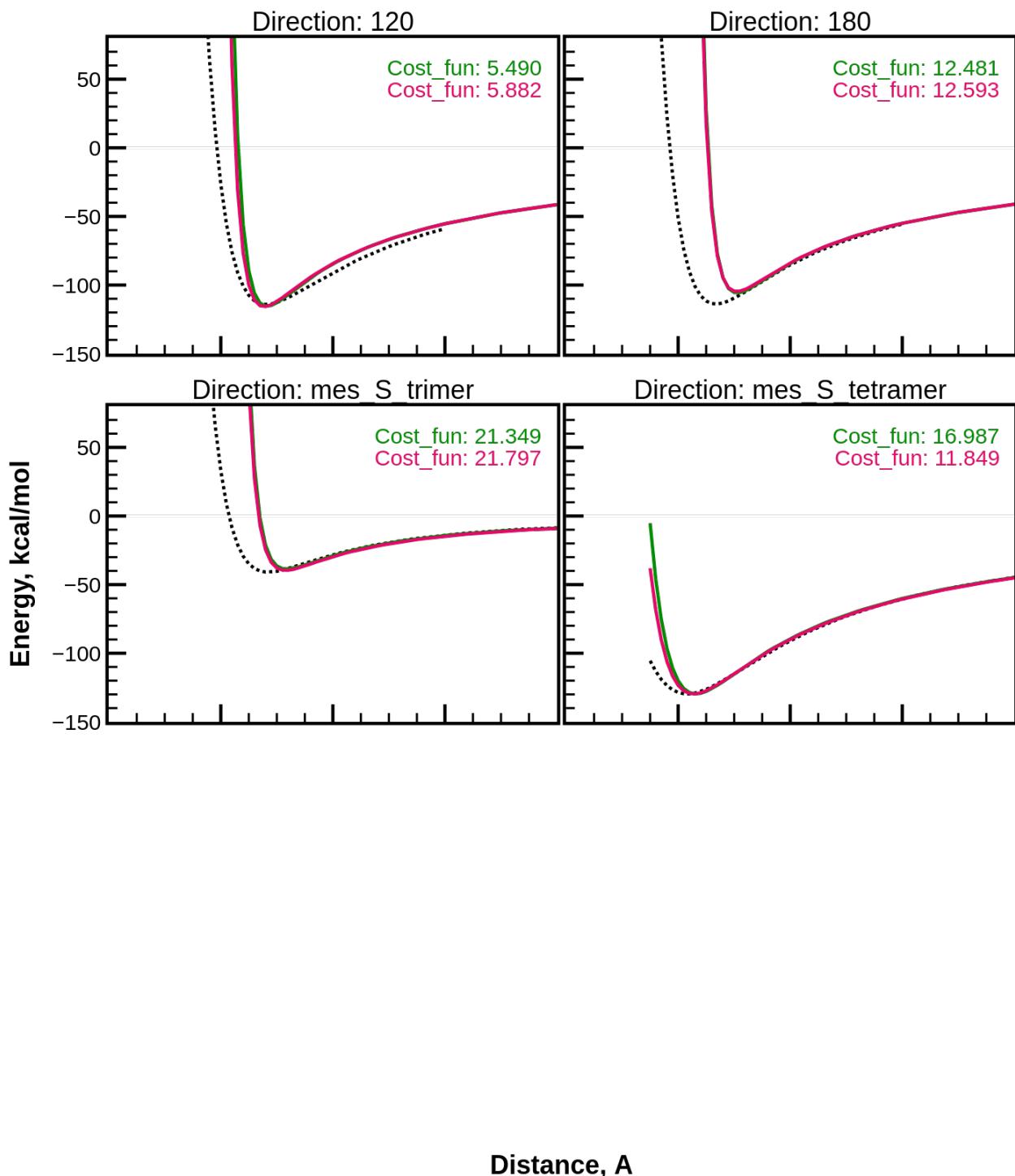
# MES SOD 1/1

3.63168\_0.07939\_9.99999  
4.03799\_0.07939\_3.25689



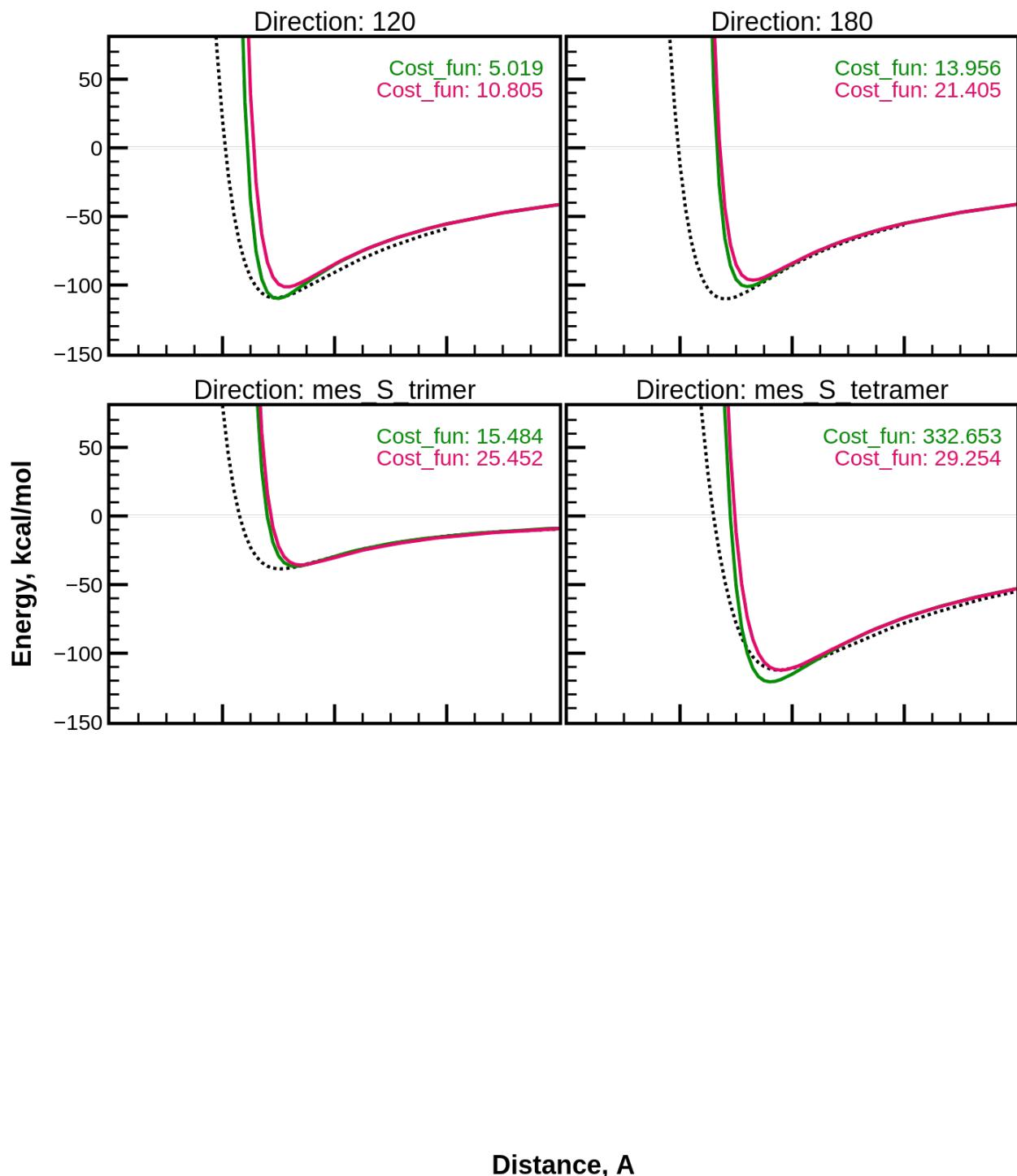
# MES POT 1/1

3.85665\_0.16848\_9.99999  
3.44105\_0.16848\_2.11686



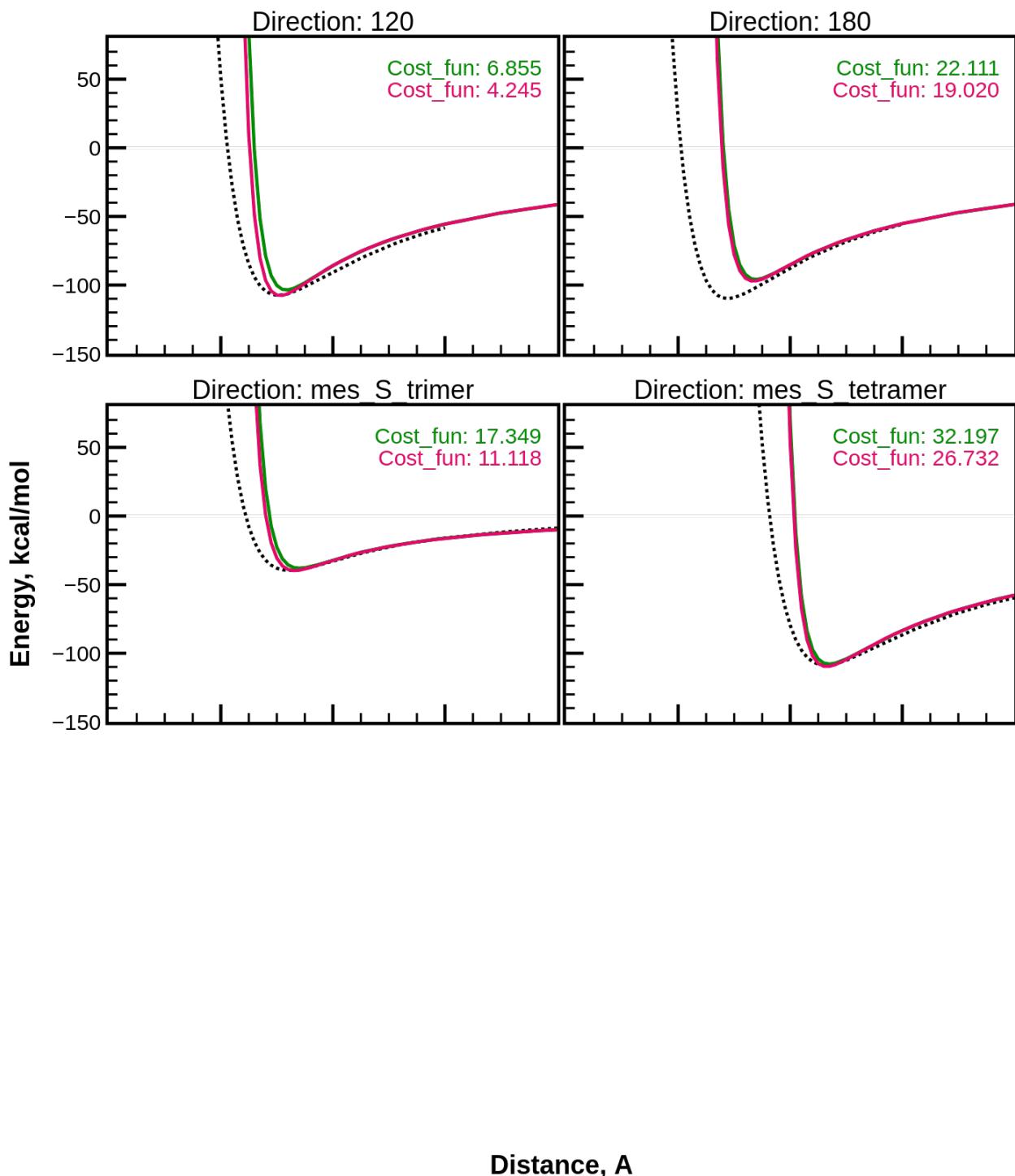
# MES RUB 1/1

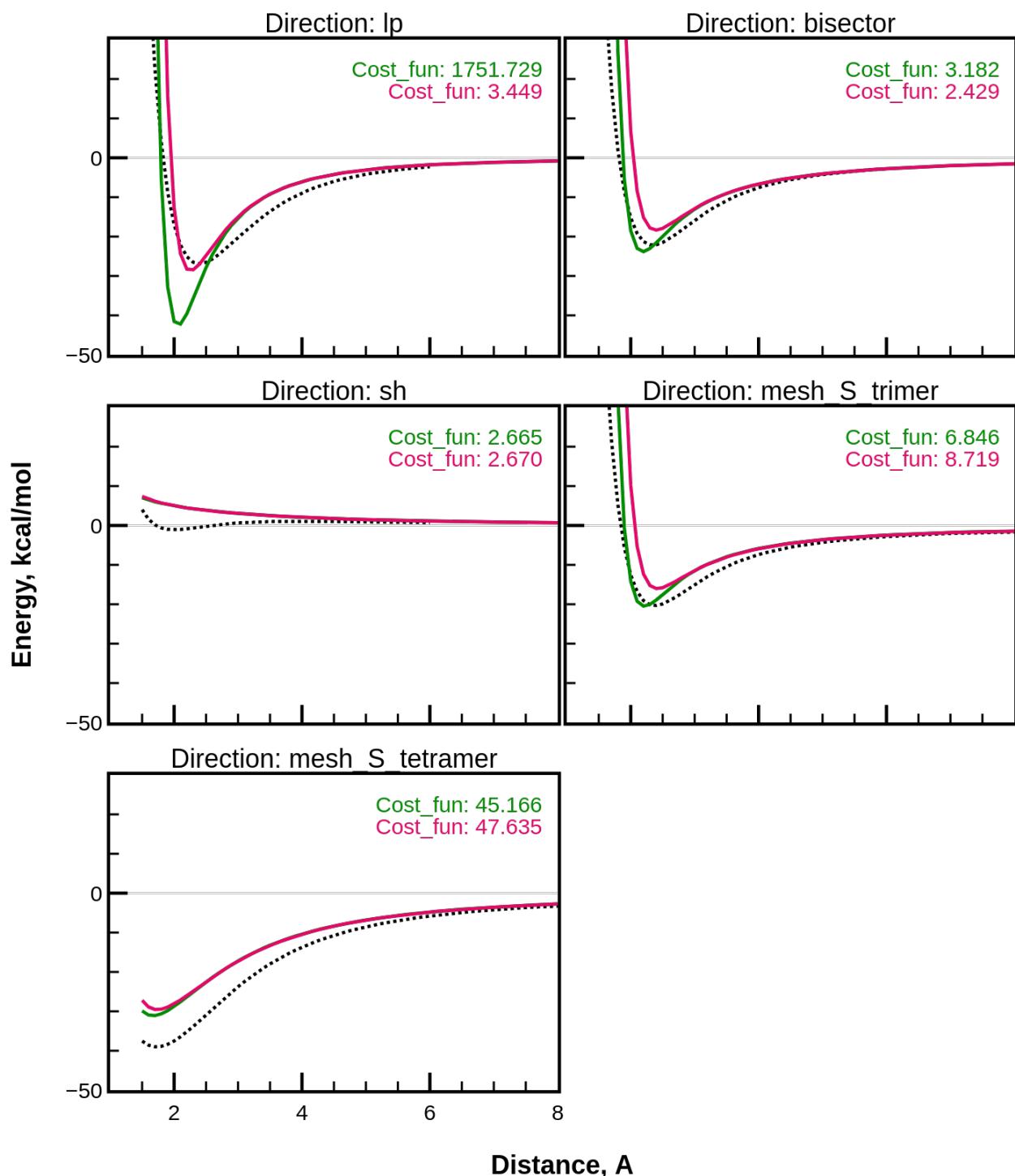
3.95551\_0.23370\_9.99999  
4.21446\_0.23370\_2.09814

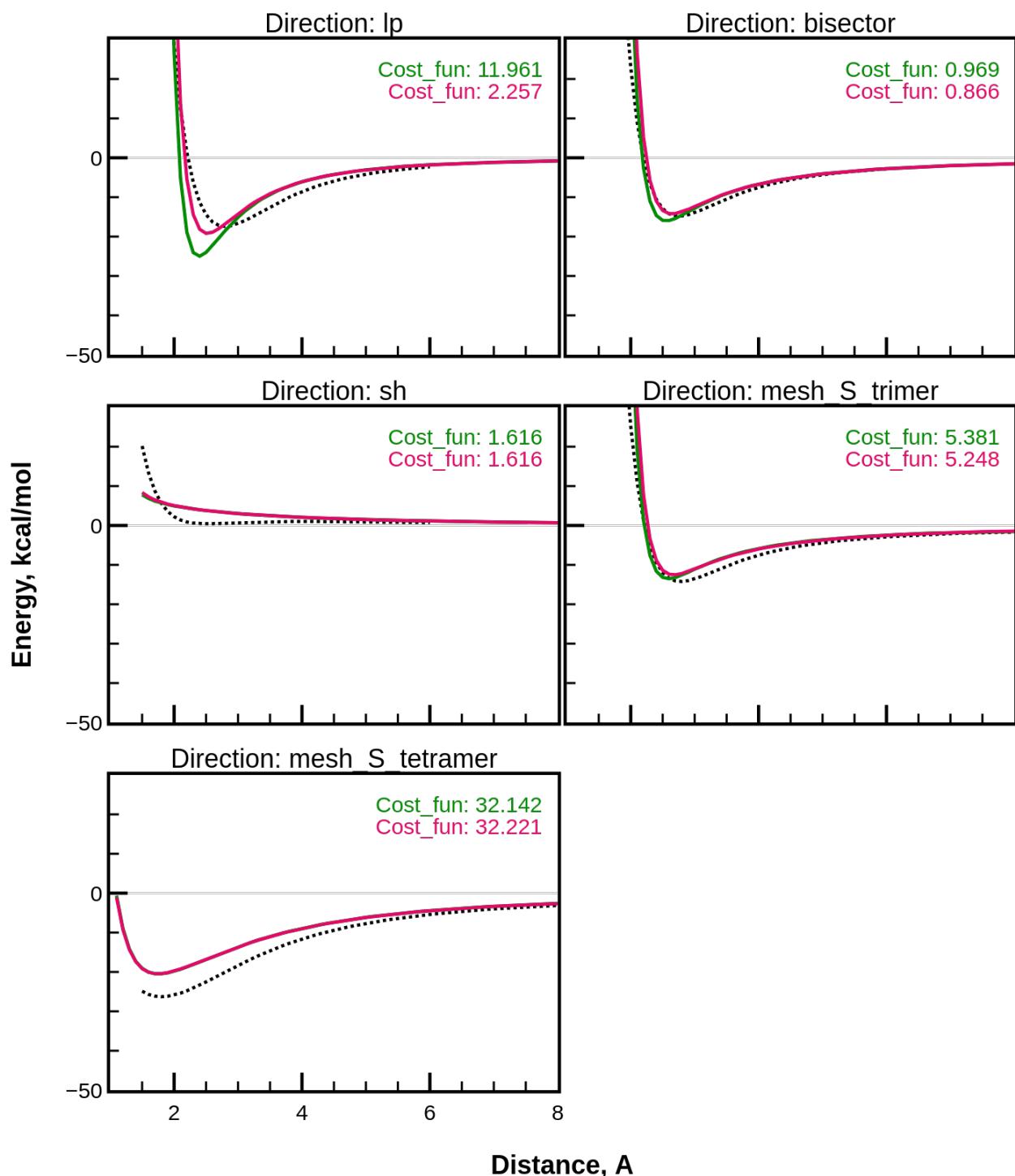


# MES CES 1/1

4.19382\_0.23520\_9.99999  
3.70638\_0.23520\_3.13433

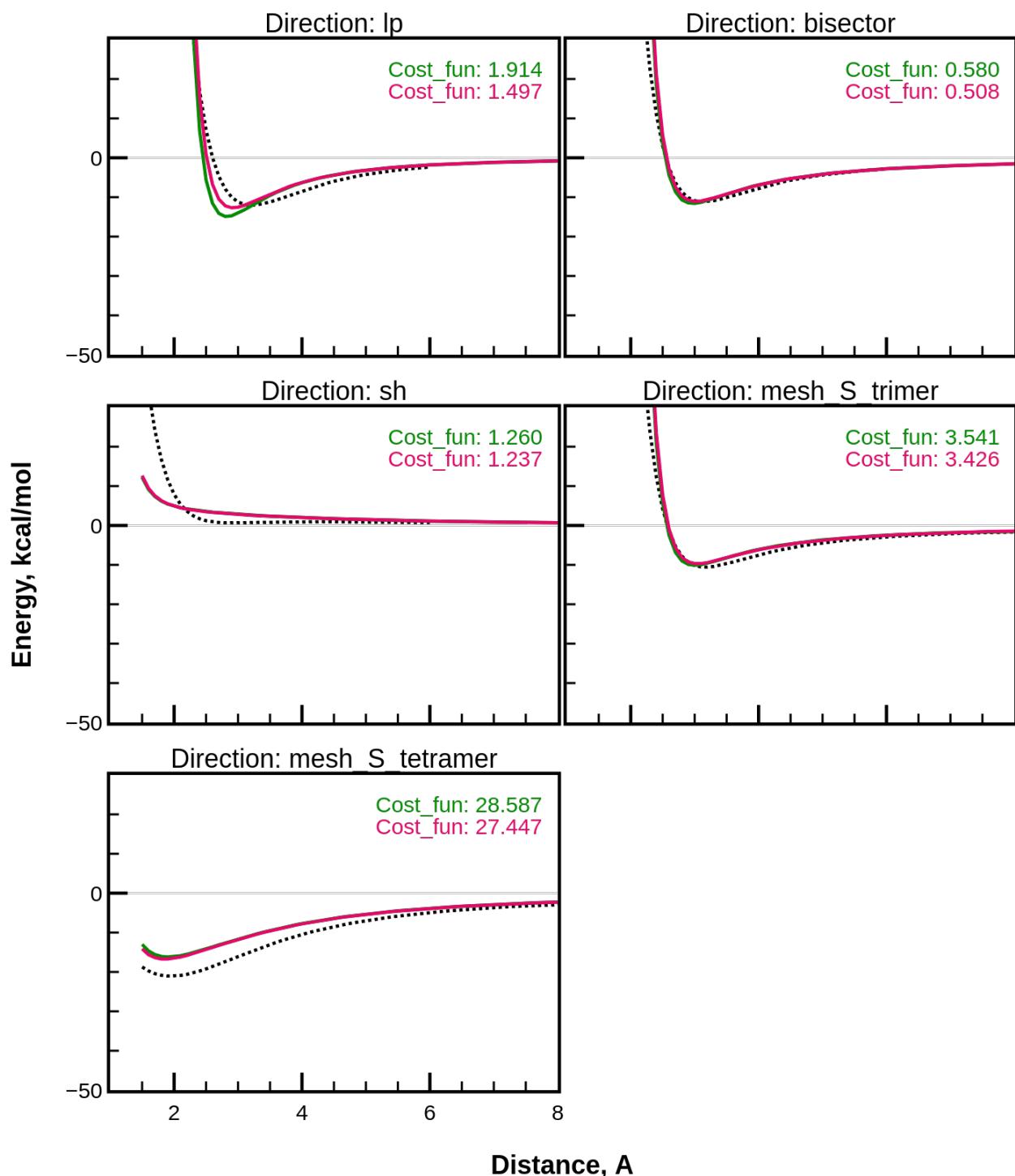


**MESH LIT 1/1**3.15000\_0.11358\_9.99999  
3.29425\_0.11358\_1.52517

**MESH SOD 1/1**3.51168\_0.11640\_9.99999  
3.52978\_0.11640\_1.51323

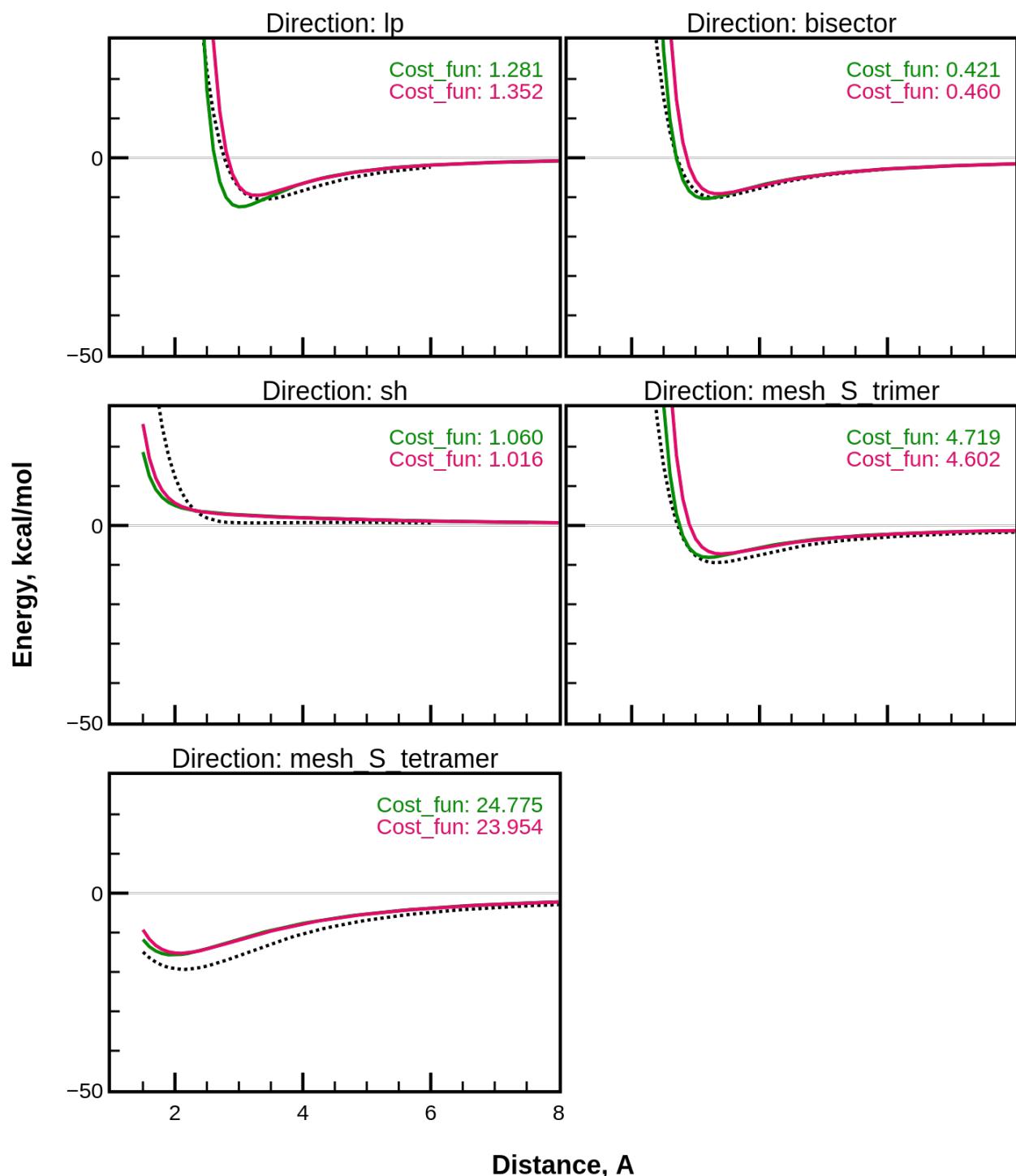
# MESH POT 1/1

3.73665\_0.24704\_9.99999  
3.72316\_0.24704\_1.50040



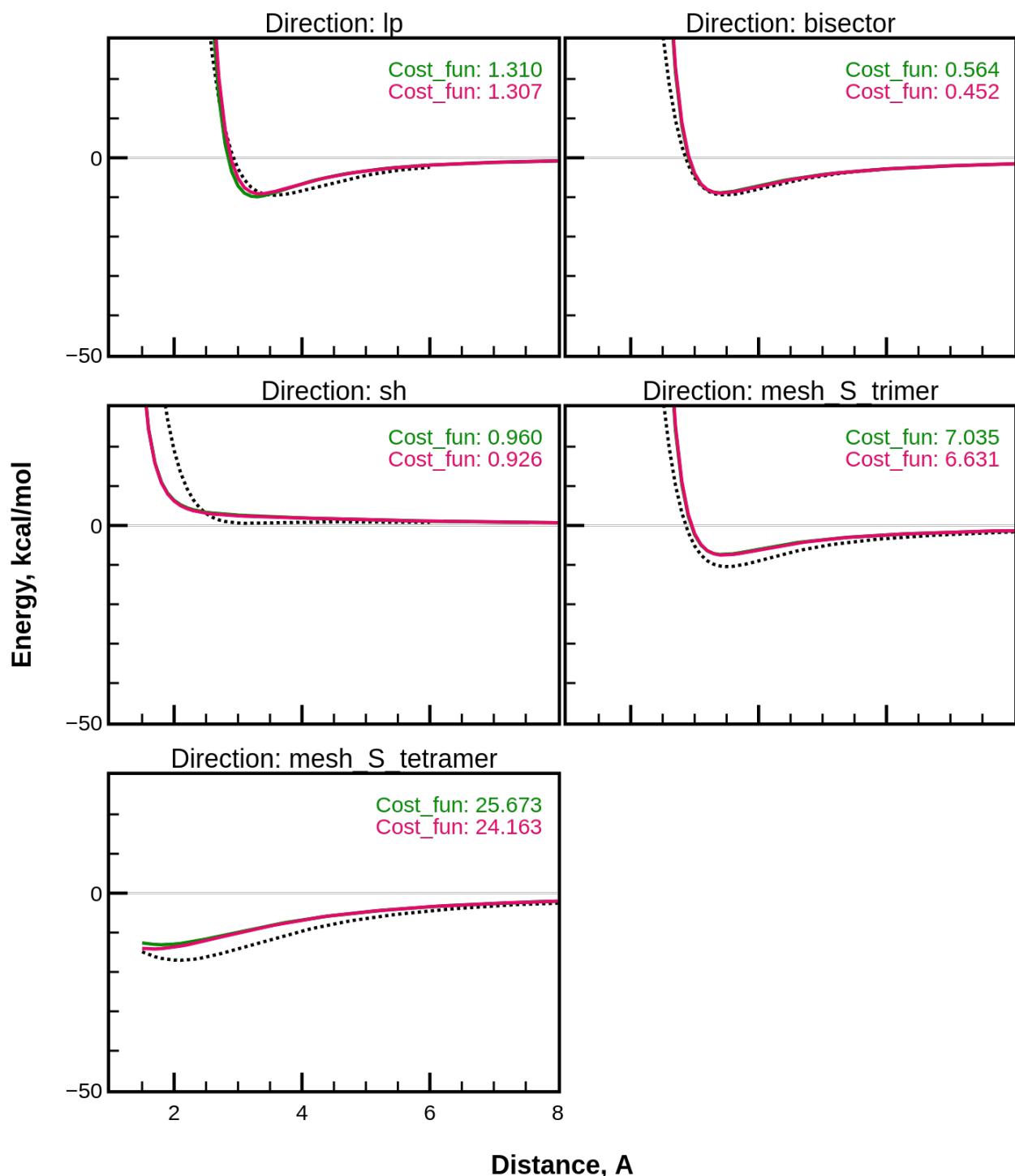
# MESH RUB 1/1

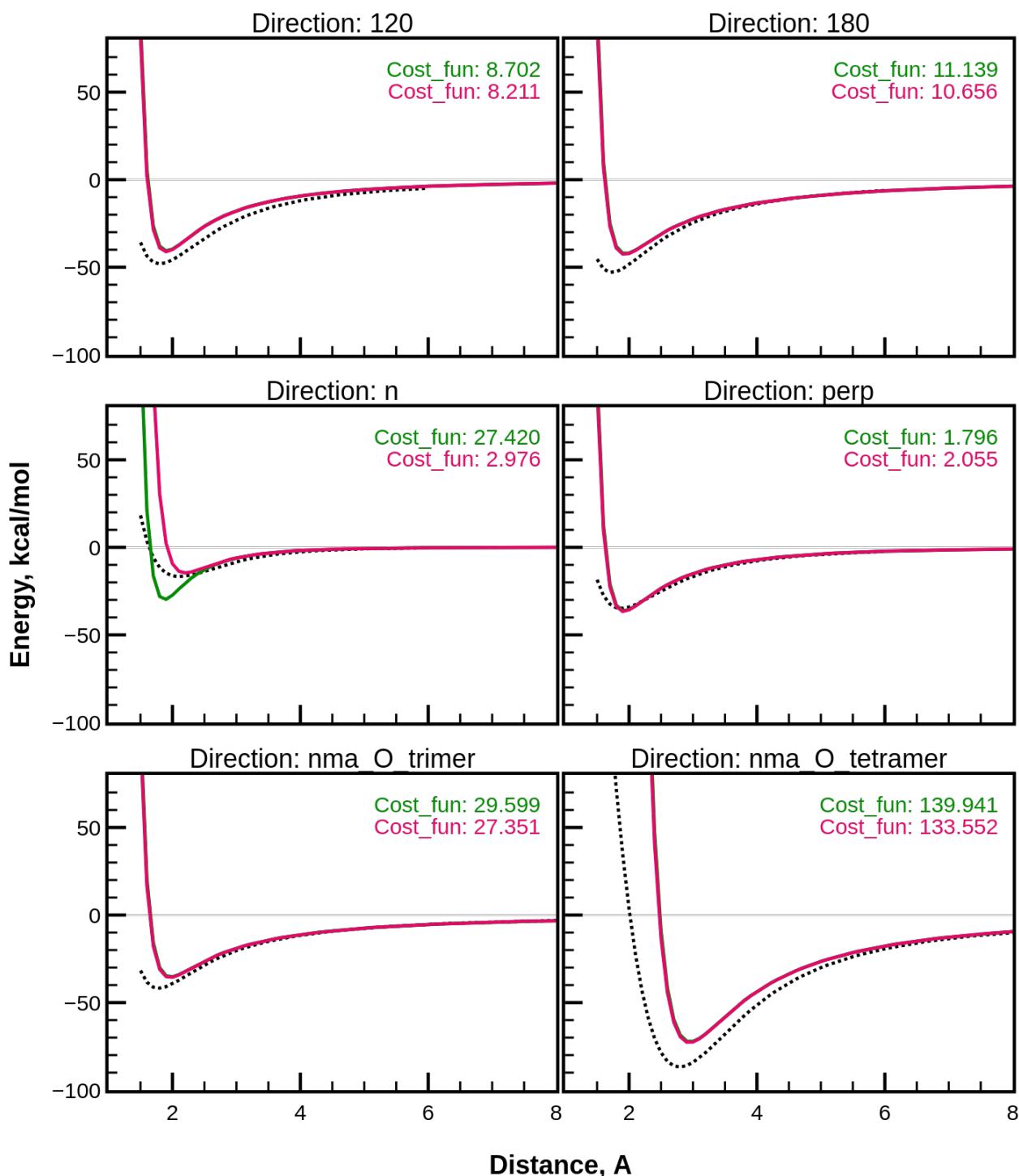
3.83551\_0.34266\_9.99999  
3.99694\_0.34266\_1.51324

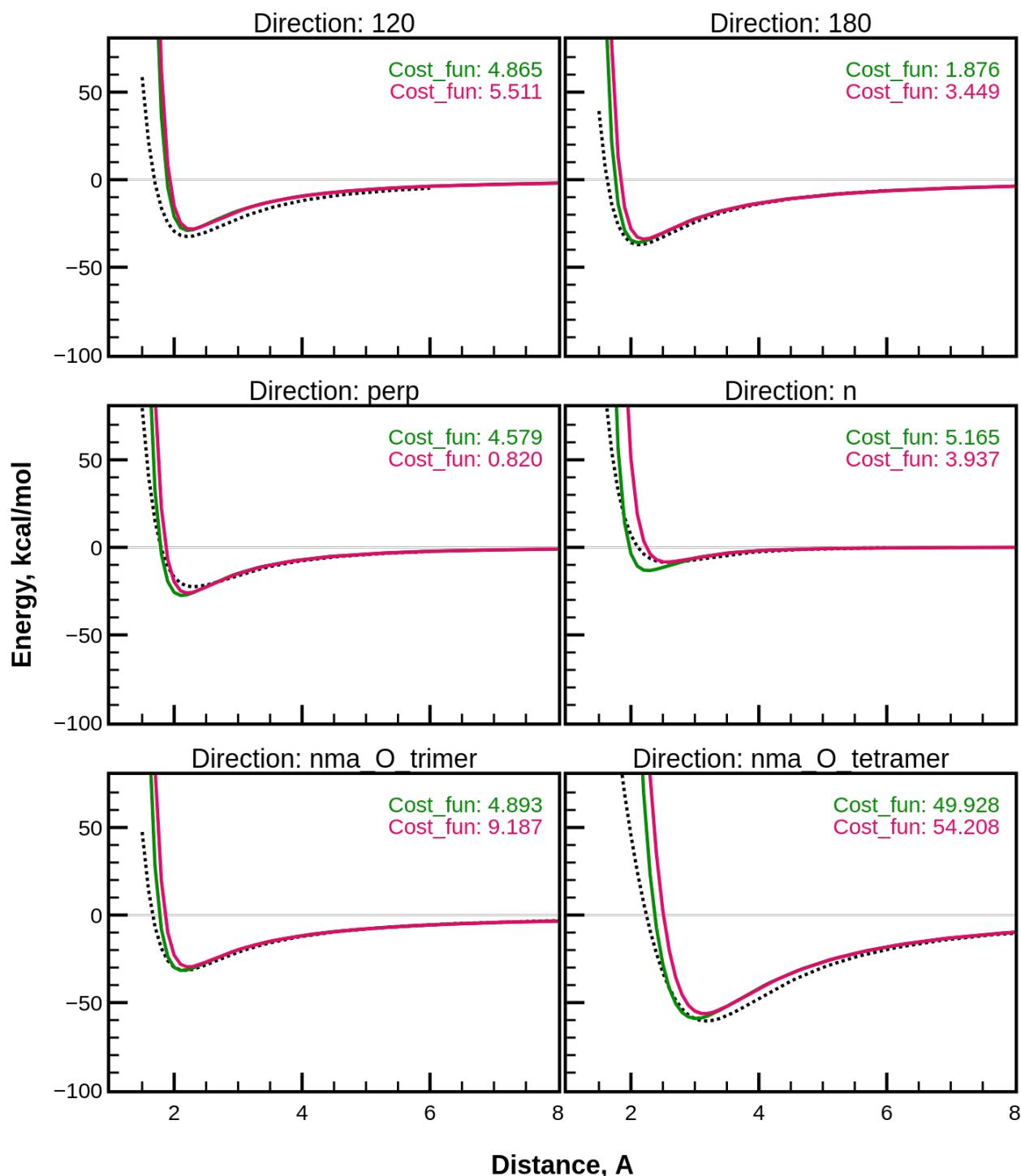


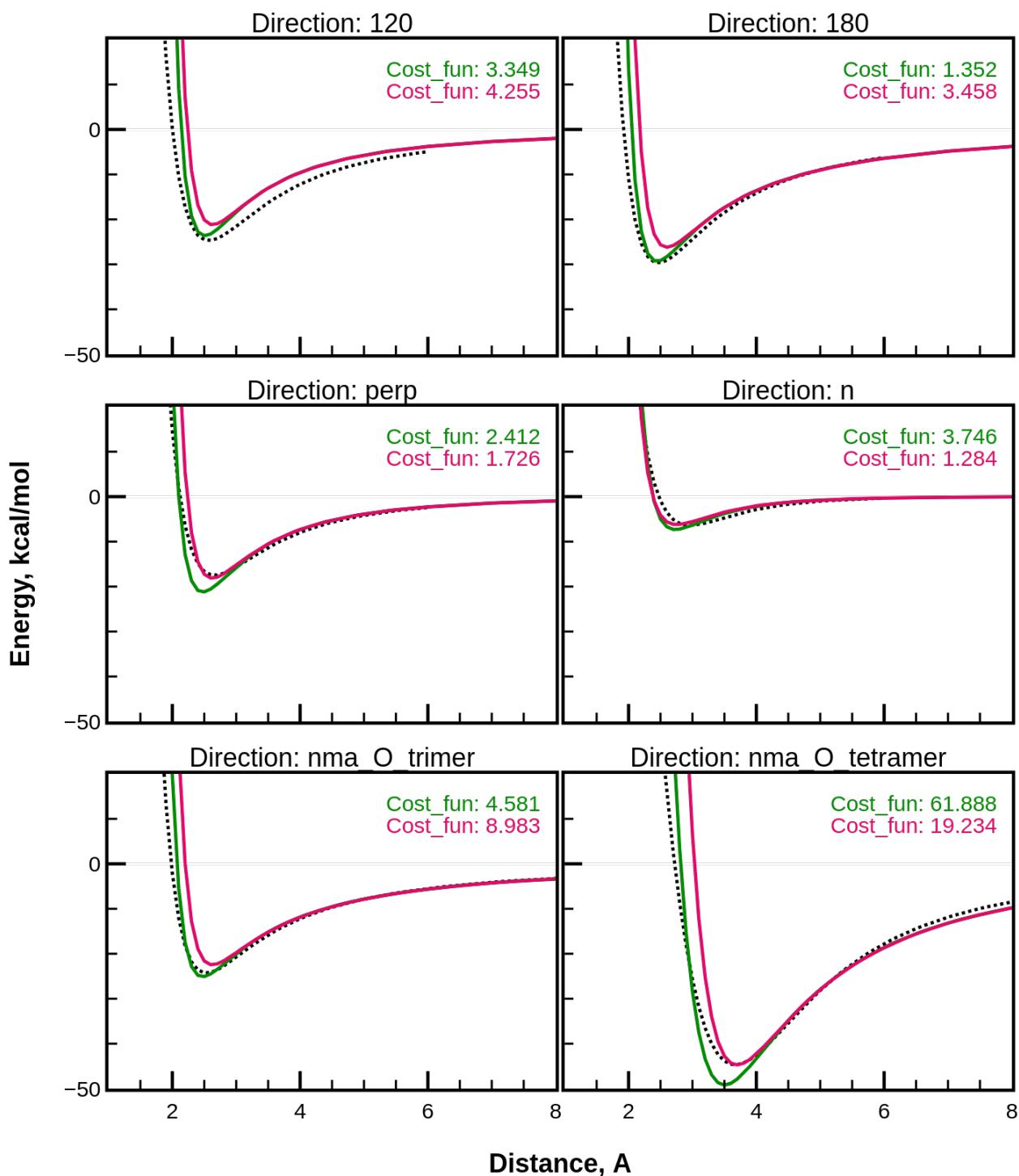
# MESH CES 1/1

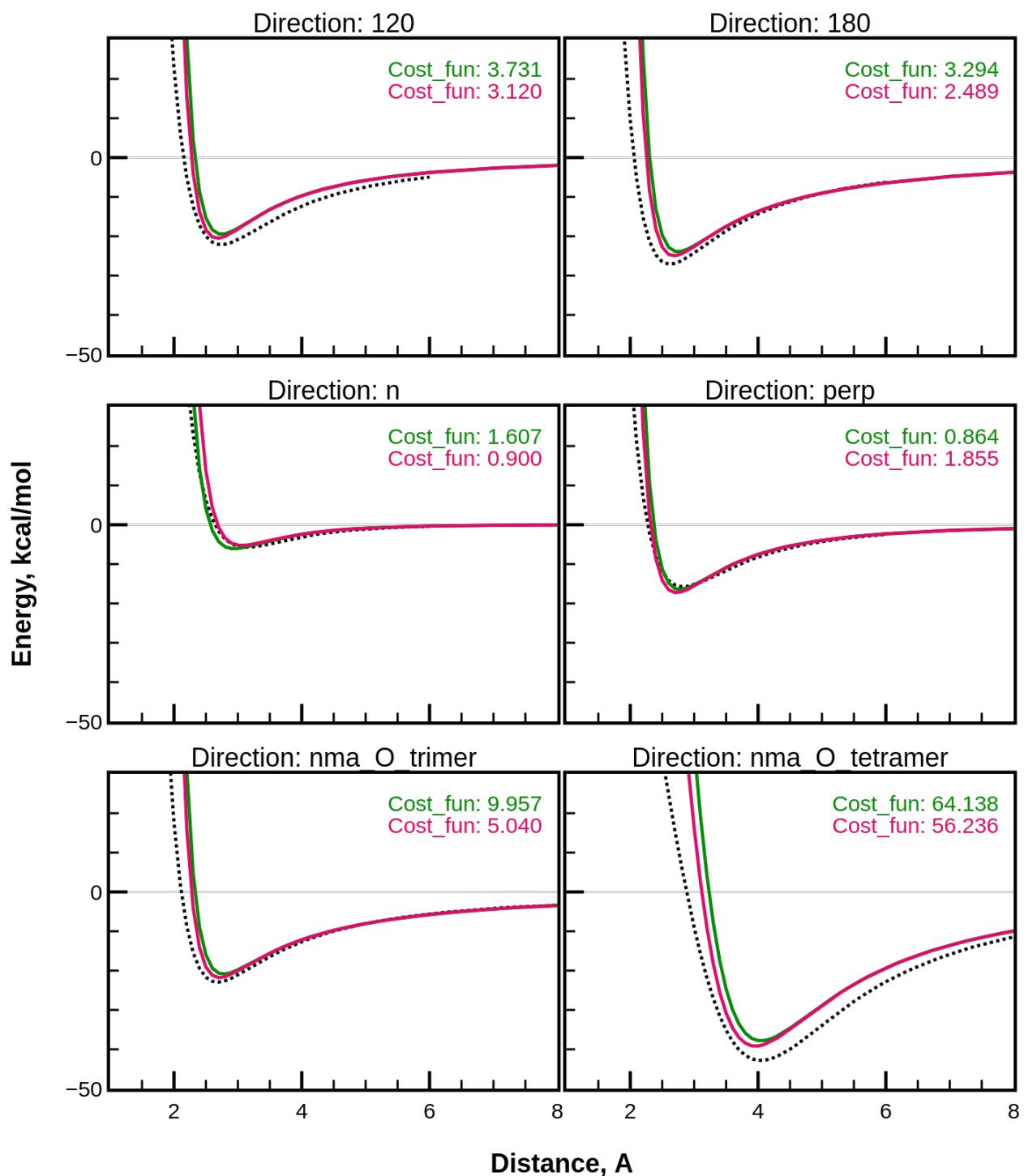
4.07382\_0.34488\_9.99999  
4.06835\_0.34488\_1.50014

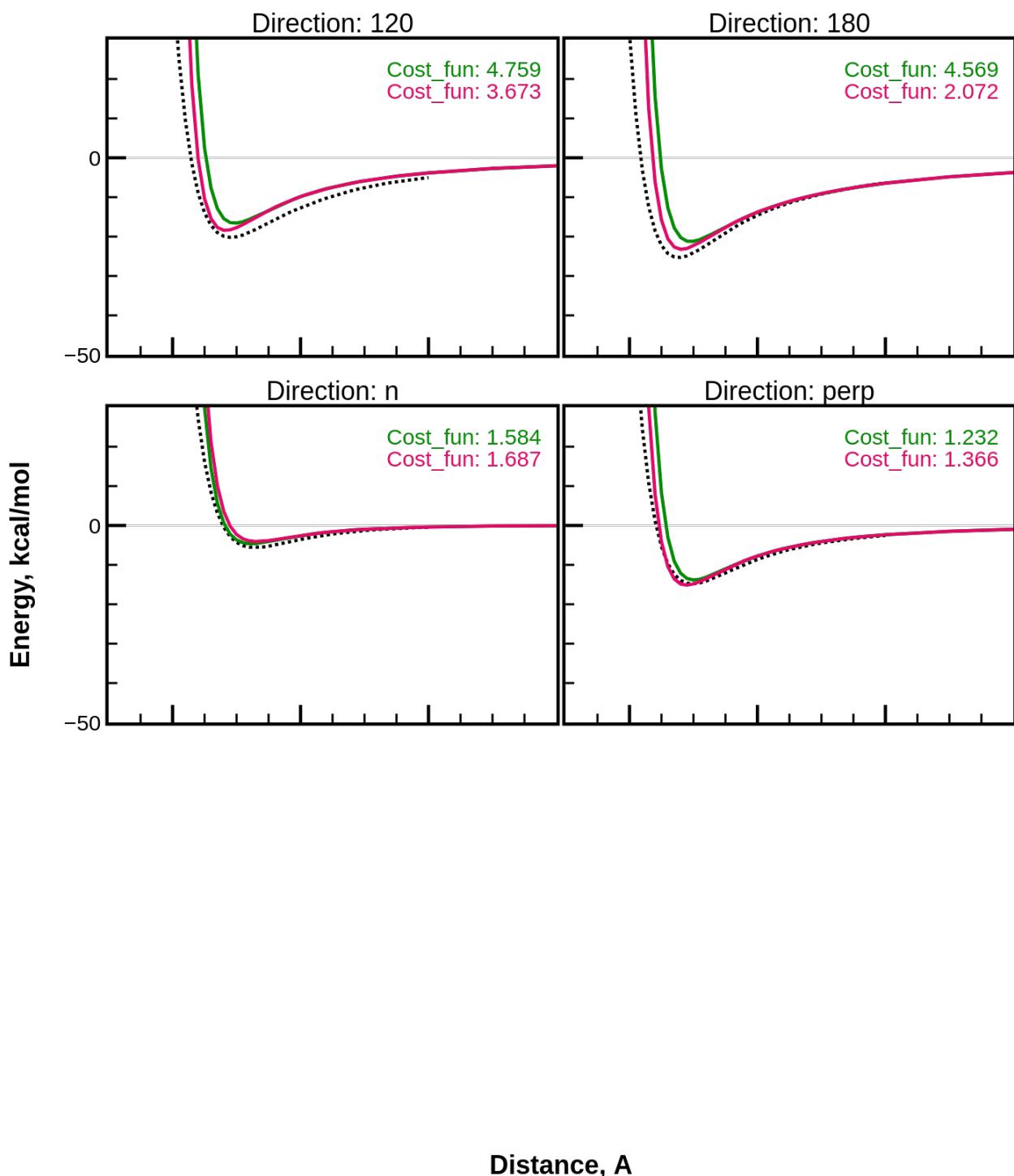


**NMA LIT 1/1**2.88000\_0.07746\_9.99999  
2.86833\_0.07746\_4.93098

**NMA SOD 1/1**2.88000\_0.09000\_1.04000  
3.11051\_0.07939\_1.54864

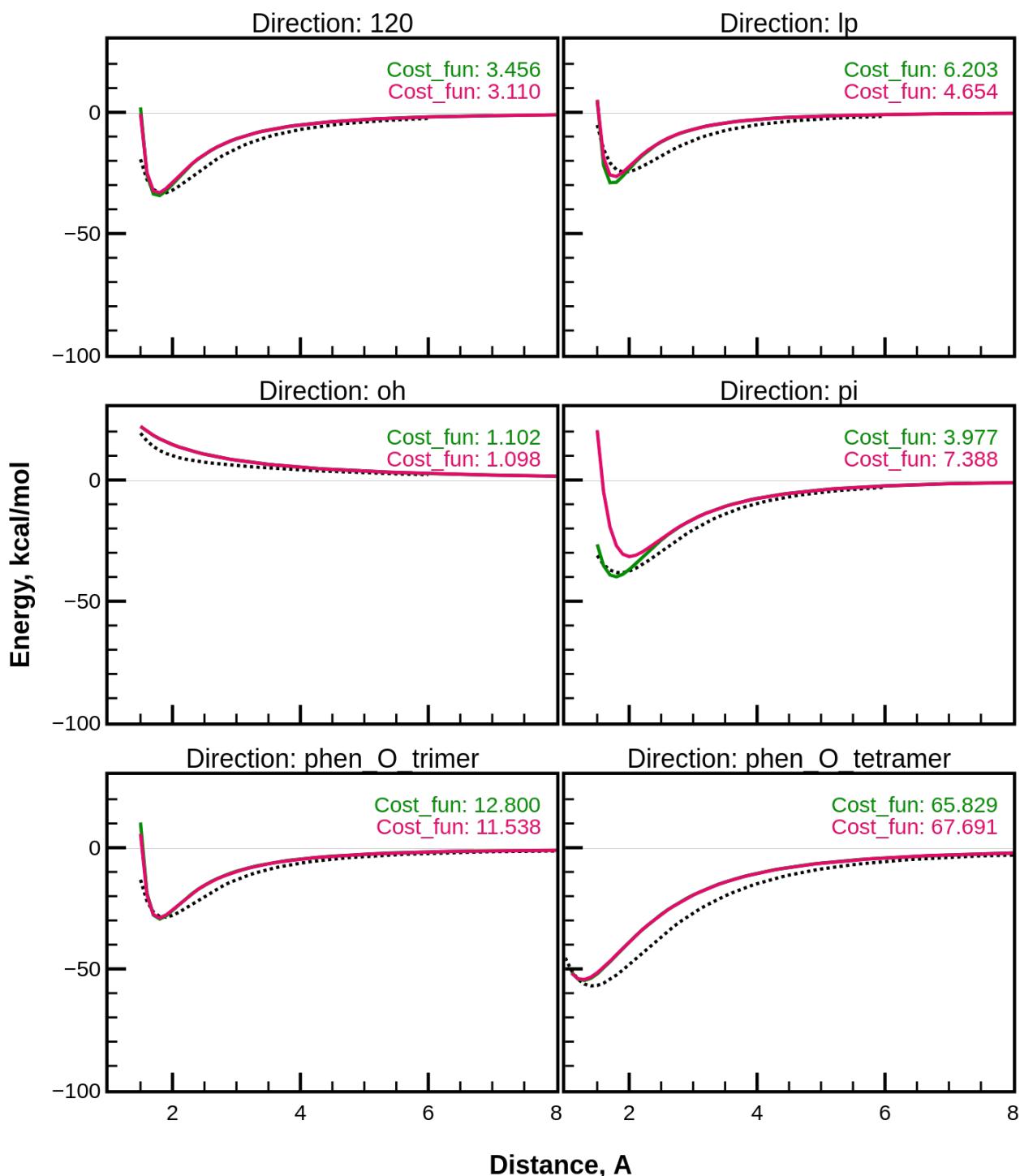
**NMA POT 1/1**3.21000\_0.18000\_2.19000  
3.43708\_0.16848\_2.09141

**NMA RUB 1/1**3.56551\_0.23370\_9.99999  
3.49474\_0.23370\_2.99829

**NMA CES 1/1**3.80382\_0.23520\_9.99999  
3.64357\_0.23520\_2.58963

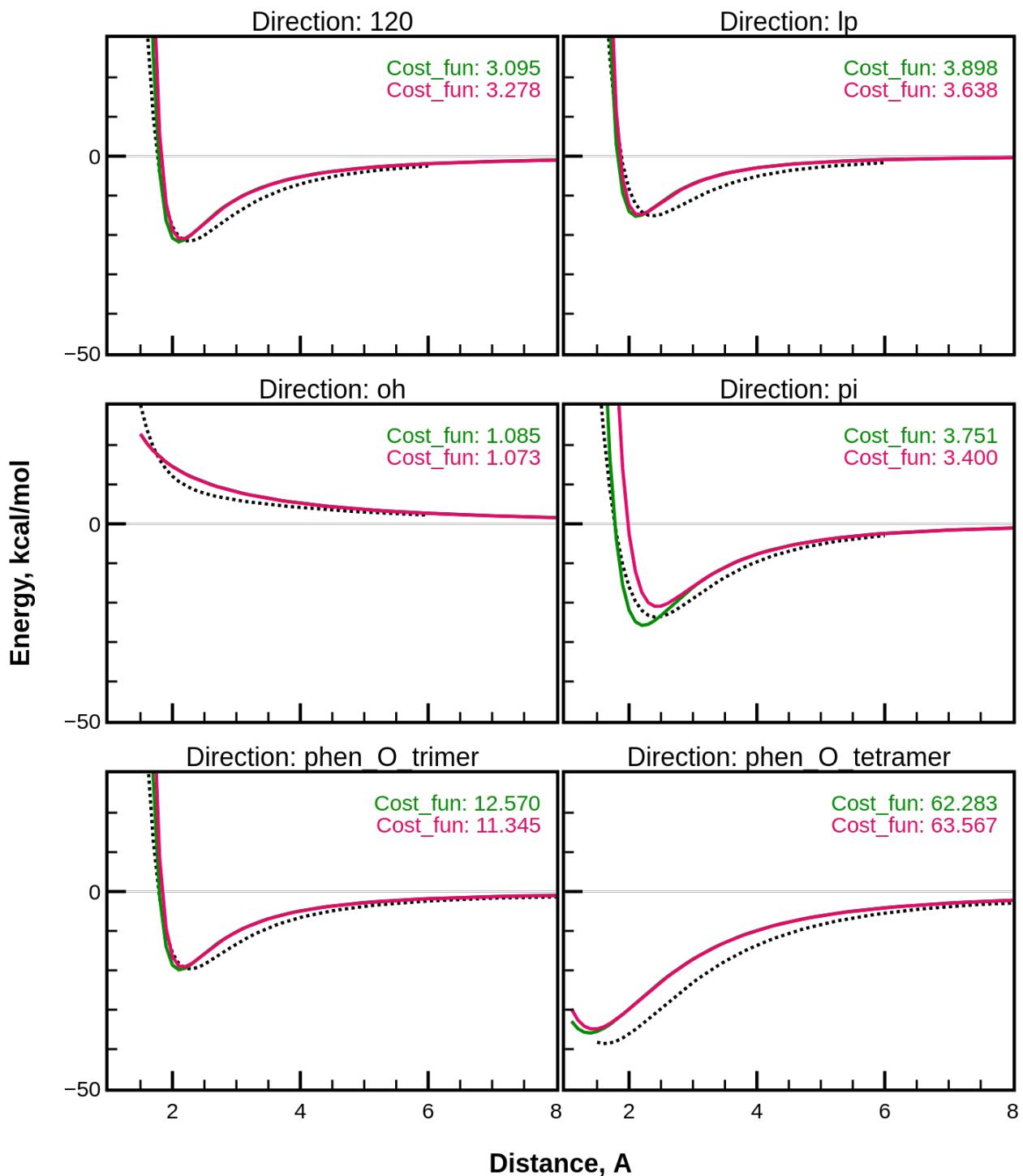
# PHEN LIT 1/1

2.65000\_0.08660\_9.99999  
2.59700\_0.08660\_1.58033



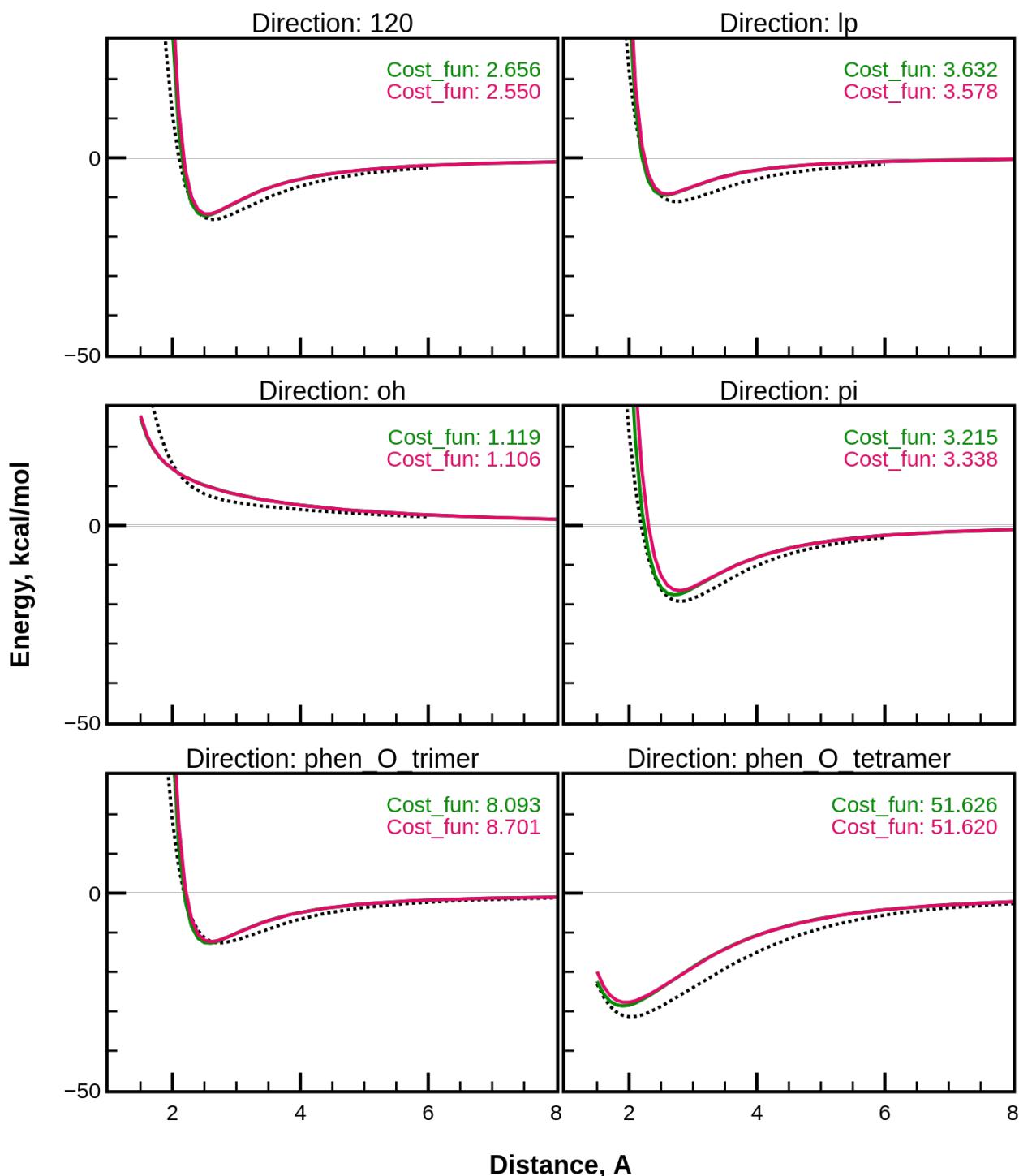
# PHEN SOD 1/1

3.07000\_0.06000\_1.82000  
3.05370\_0.08876\_4.41661



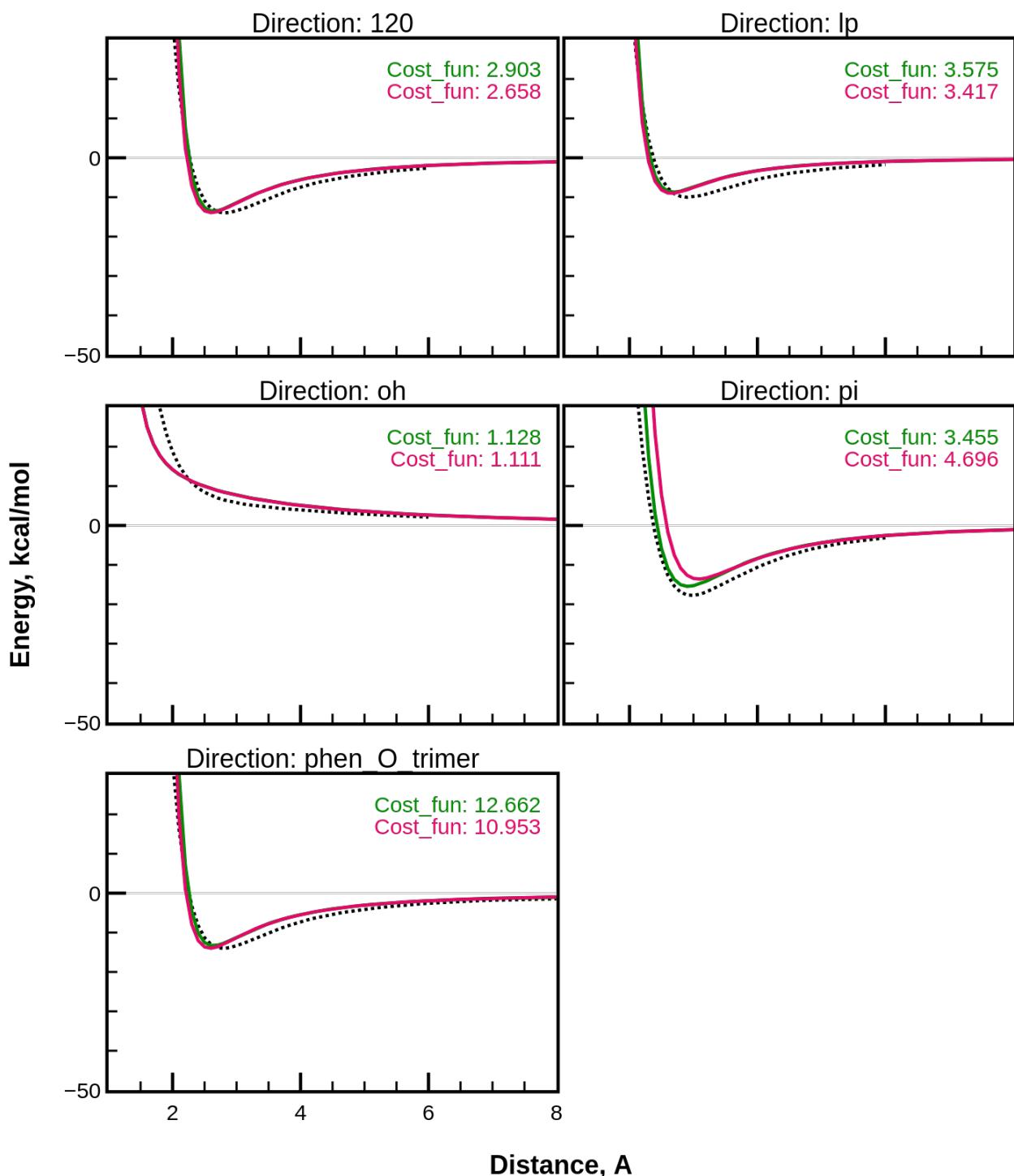
# PHEN POT 1/1

3.34000\_0.15000\_9.99999  
3.30998\_0.18837\_2.77881



# PHEN RUB 1/1

3.33551\_0.26128\_9.99999  
3.27395\_0.26128\_2.94201

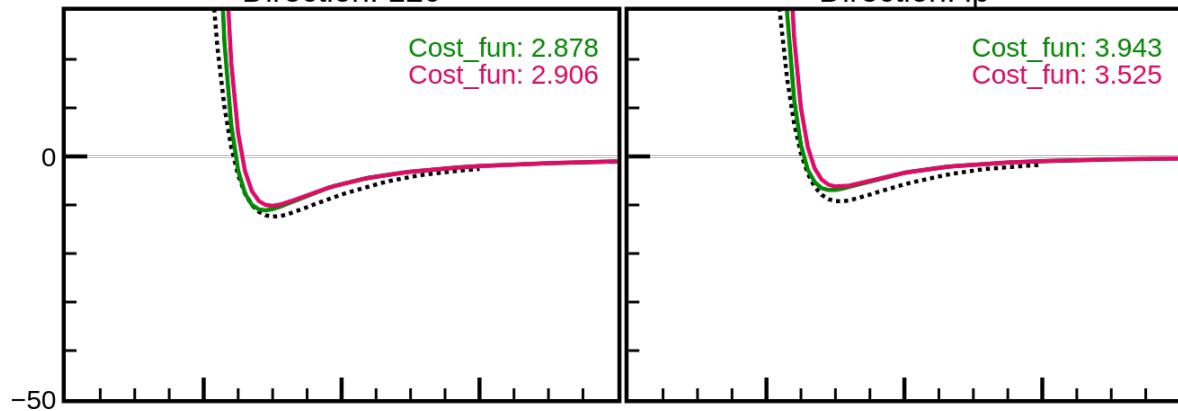


# PHEN CES 1/1

3.57382\_0.26297\_9.99999  
3.68851\_0.26297\_3.48395

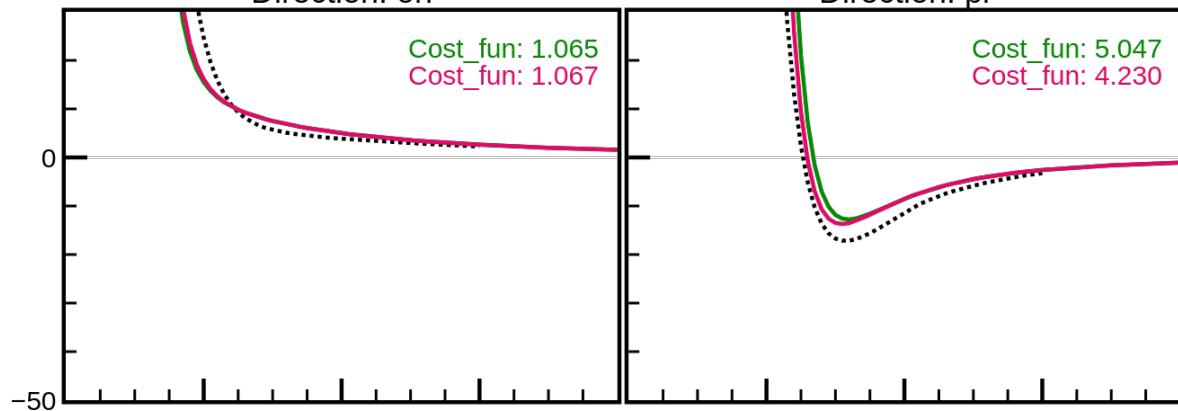
Direction: 120

Direction: lp



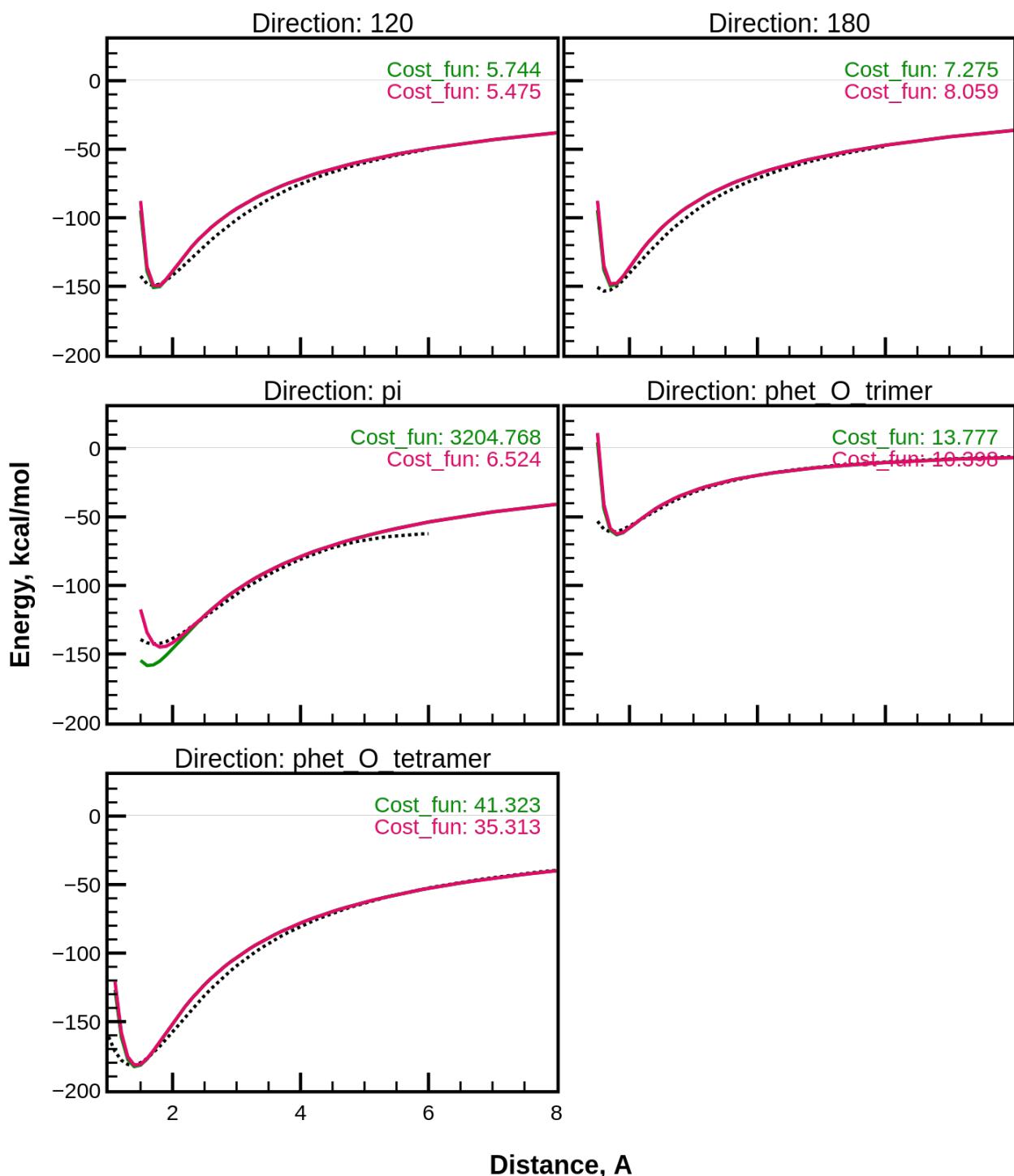
Direction: oh

Direction: pi



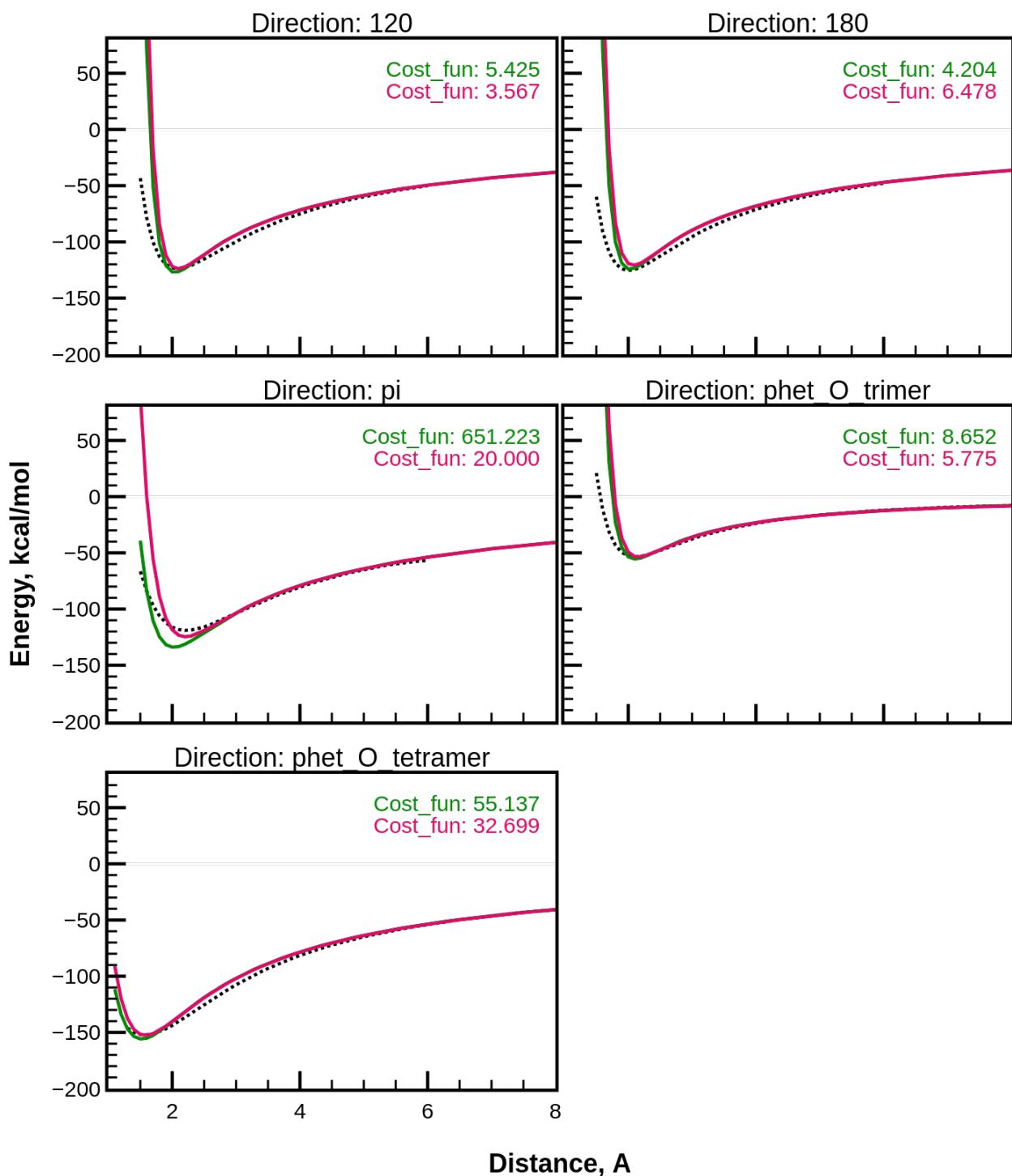
Energy, kcal/mol

Distance, Å

**PHET LIT 1/1**2.62000\_0.15780\_9.99999  
2.63213\_0.15780\_4.78169

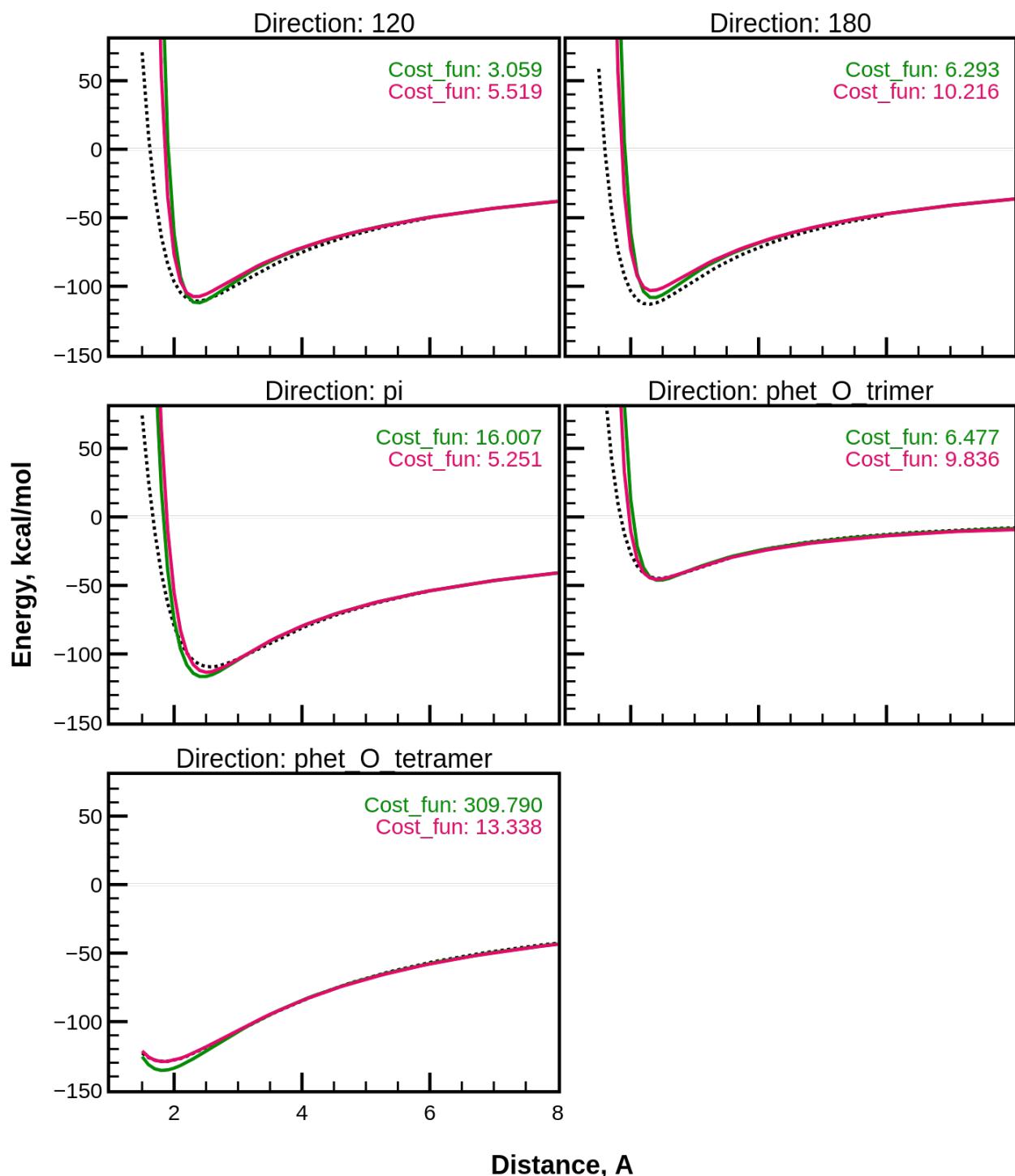
# PHET SOD 1/1

2.98168\_0.16172\_9.99999  
3.03166\_0.16172\_2.70081



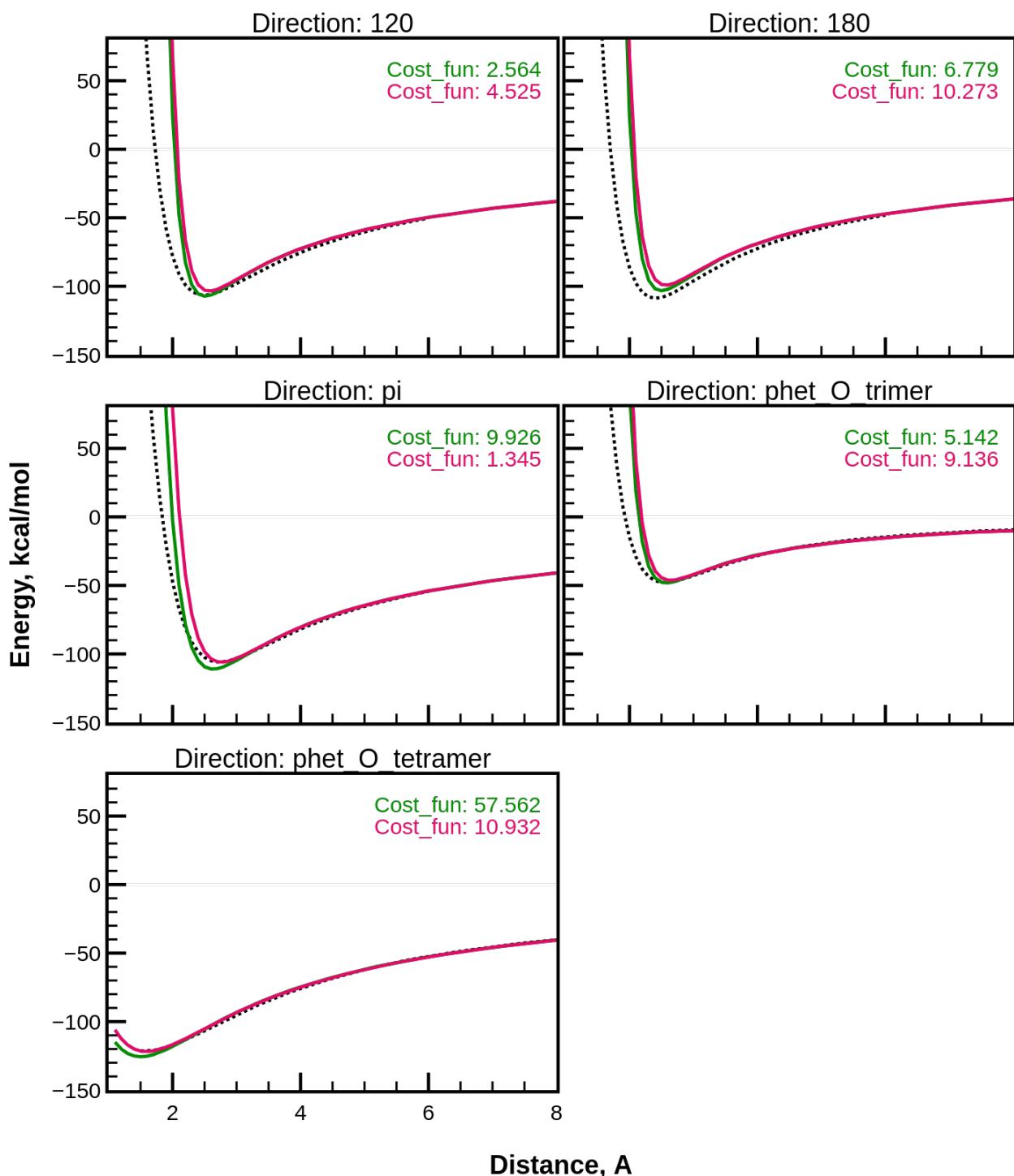
# PHET POT 1/1

3.20665\_0.34322\_9.99999  
3.07056\_0.34322\_1.53325



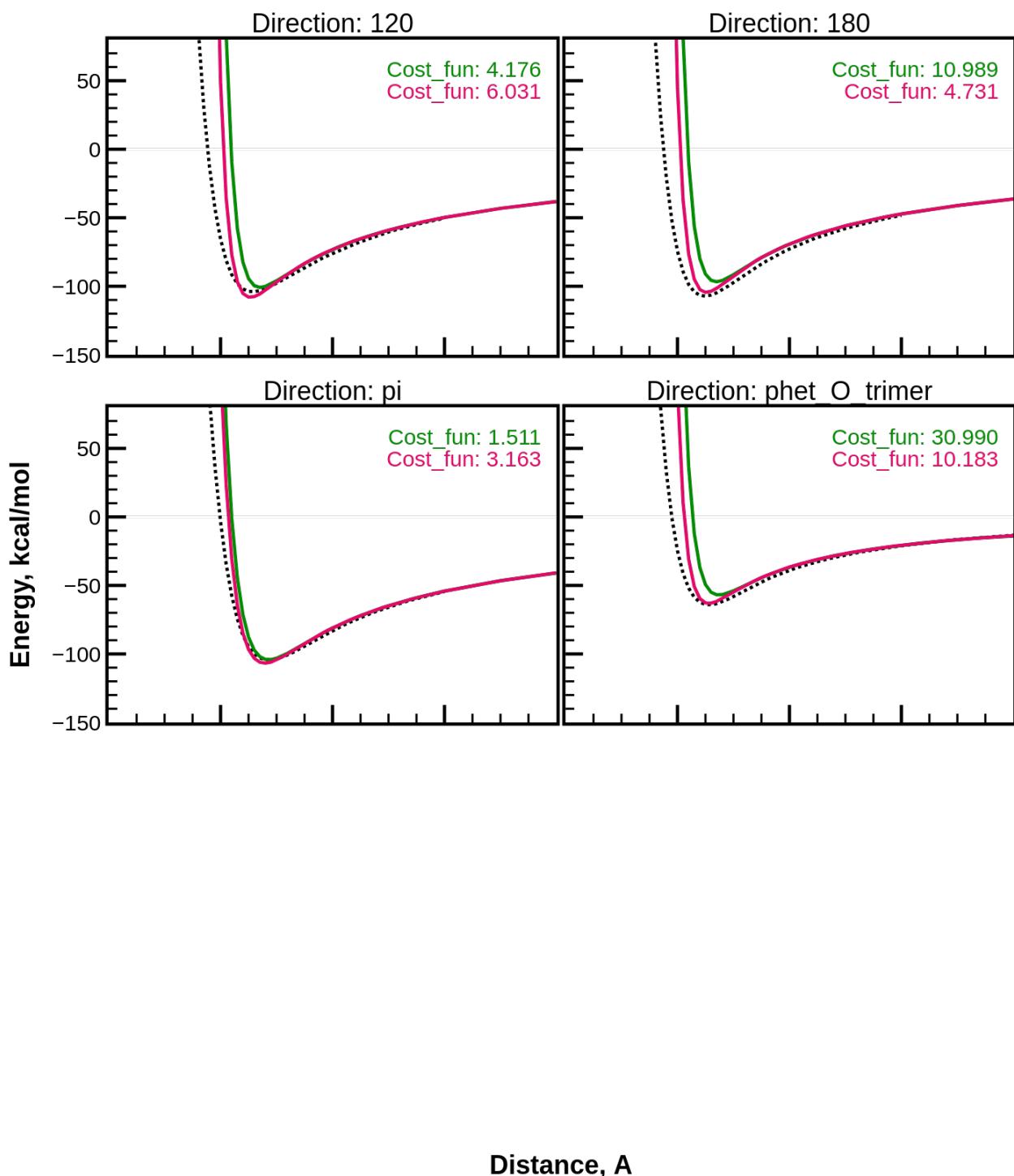
# PHET RUB 1/1

3.30551\_0.47607\_9.99999  
3.34533\_0.47607\_2.24767



**PHET CES 1/1**

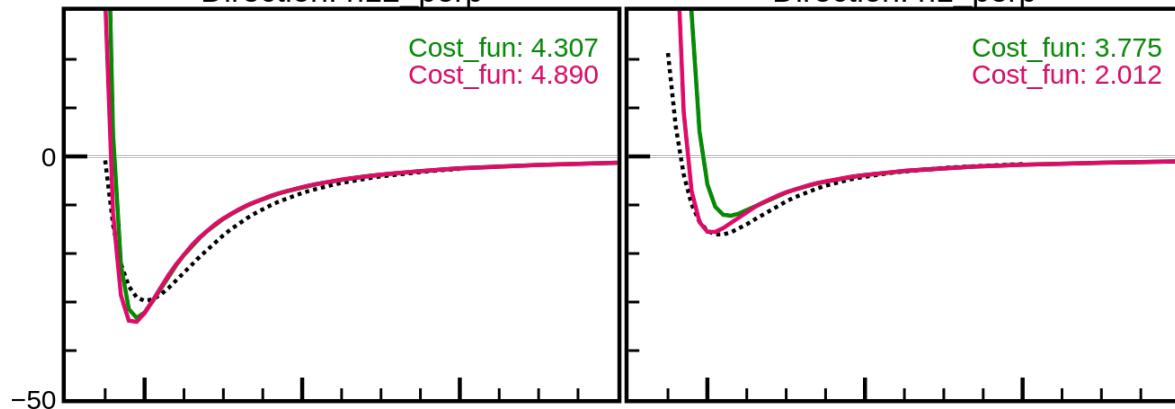
3.54382\_0.47915\_9.99999  
3.34382\_0.47915\_4.19384



**ADEB LIT 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

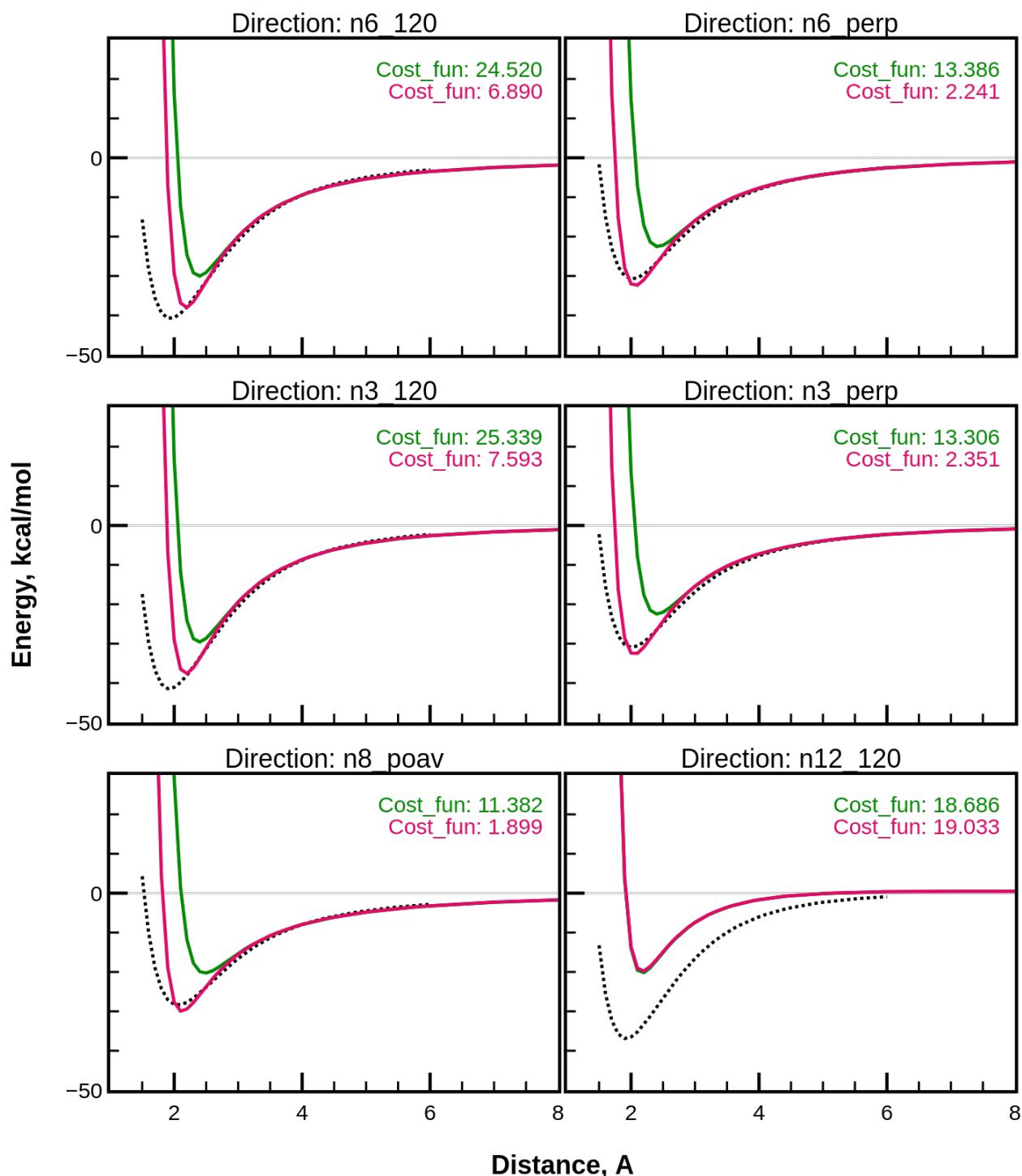
Direction: n12\_perp

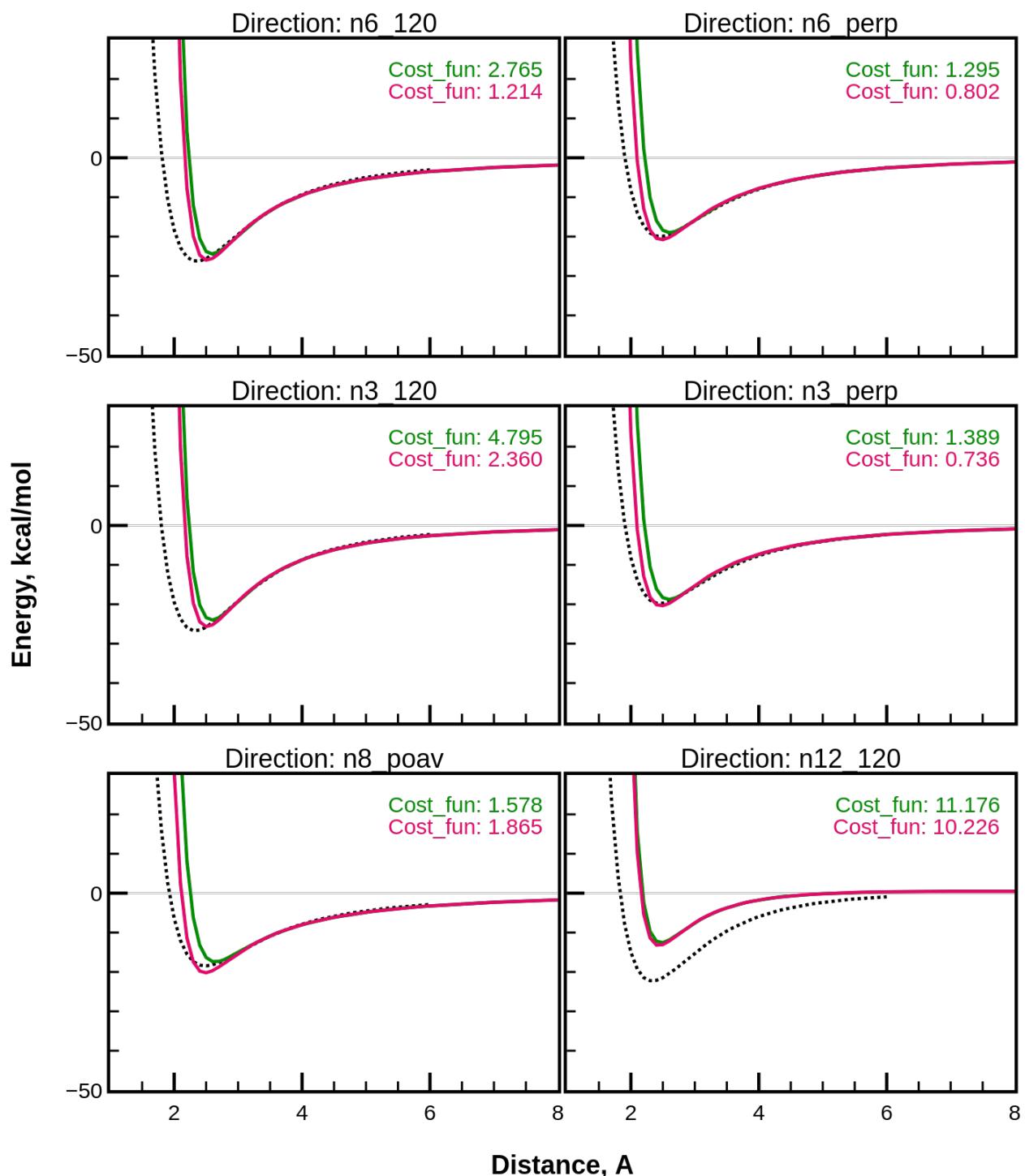
Direction: n1\_perp



Energy, kcal/mol

Distance, A

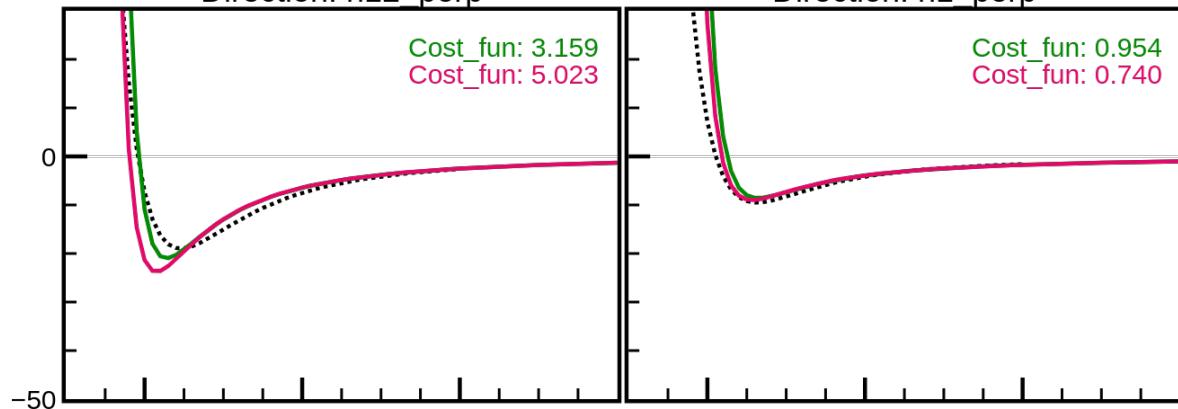
**ADEB LIT 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**ADEB SOD 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**ADEB SOD 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

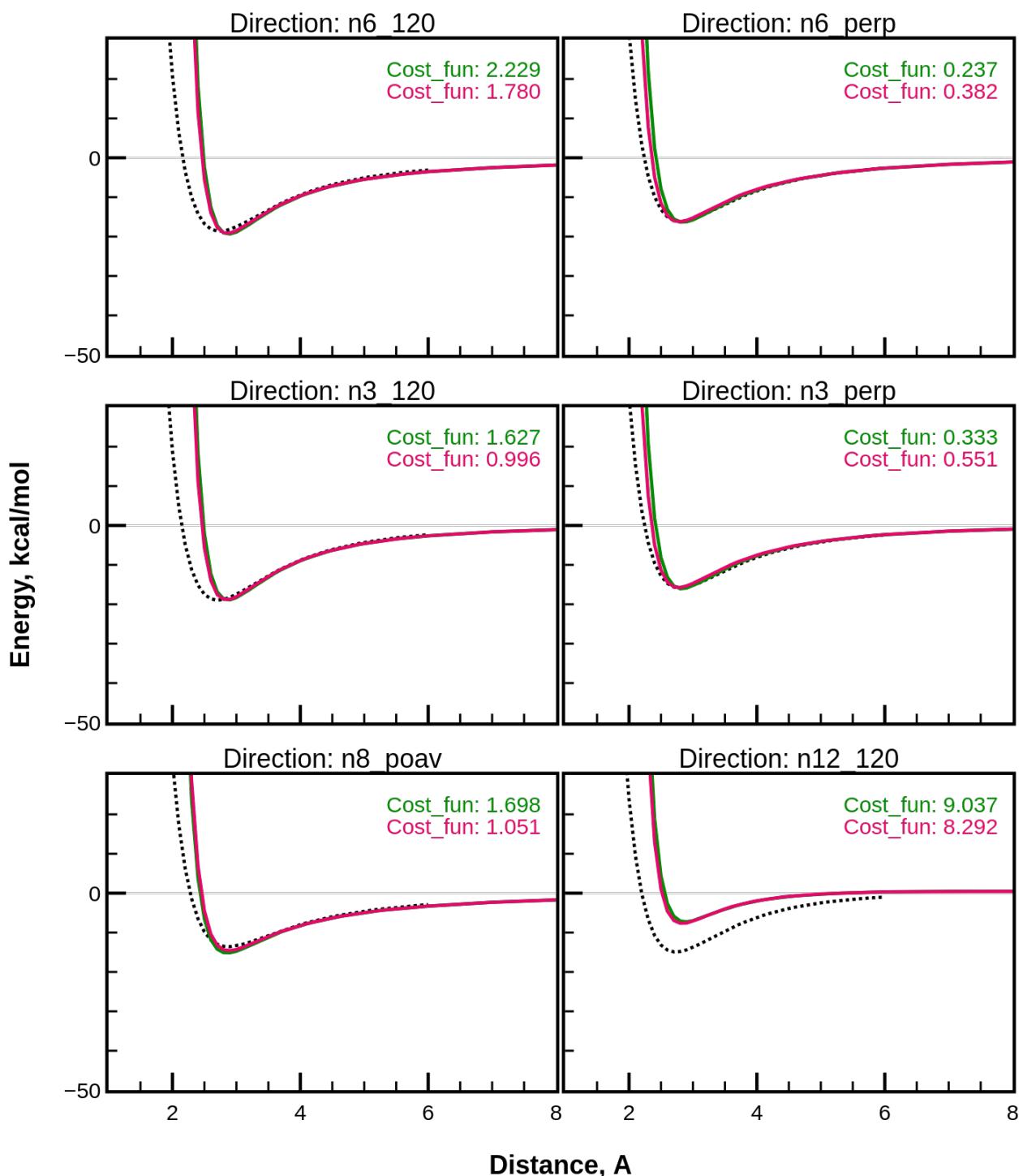
Direction: n12\_perp

Direction: n1\_perp



Energy, kcal/mol

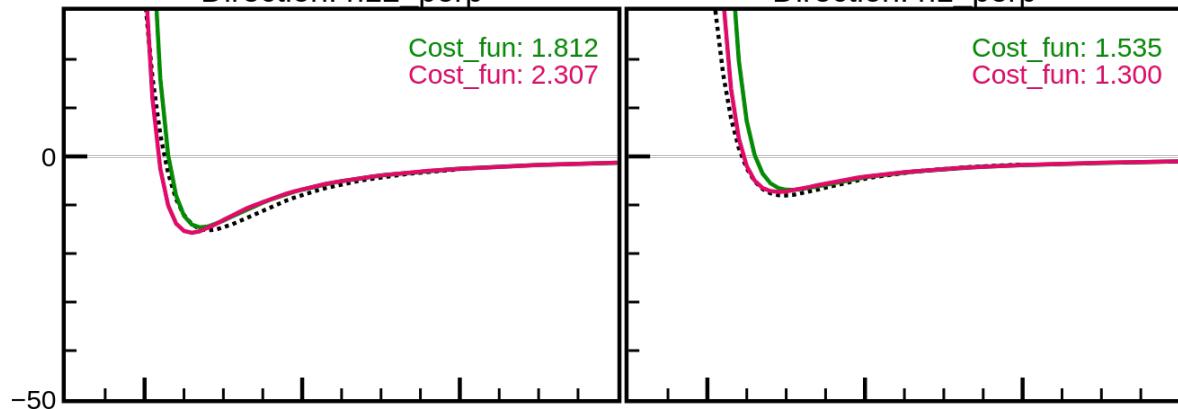
Distance, Å

**ADEB POT 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**ADEB POT 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

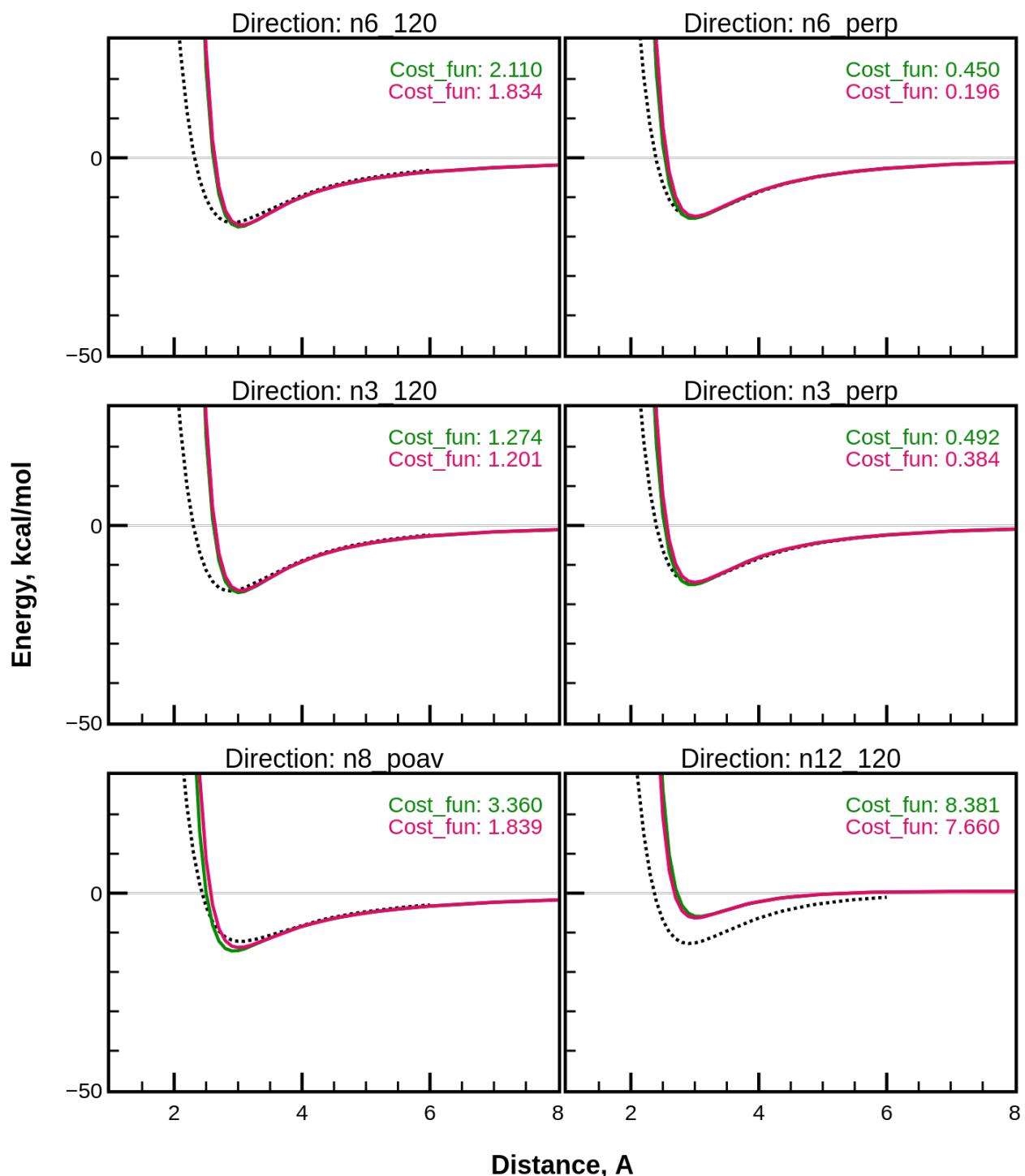
Direction: n12\_perp

Direction: n1\_perp



Energy, kcal/mol

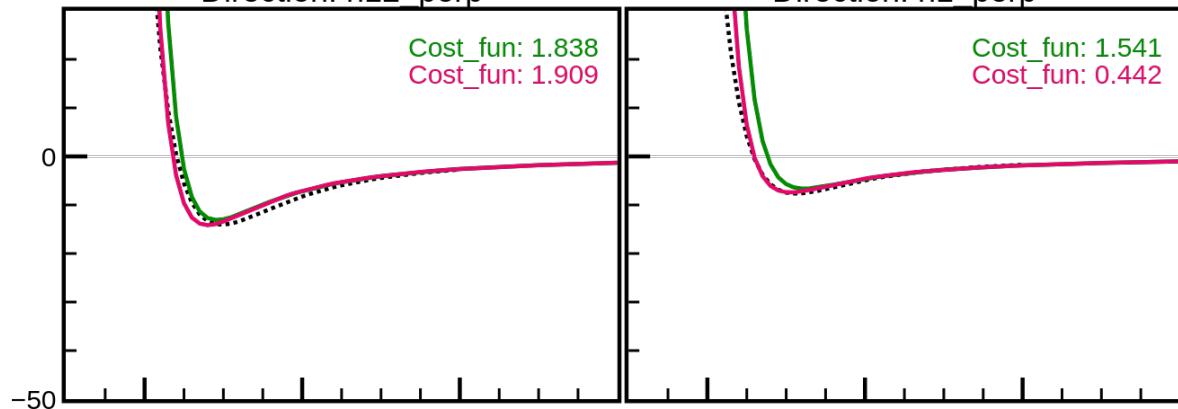
Distance, Å

**ADEB RUB 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**ADEB RUB 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

Direction: n12\_perp

Direction: n1\_perp



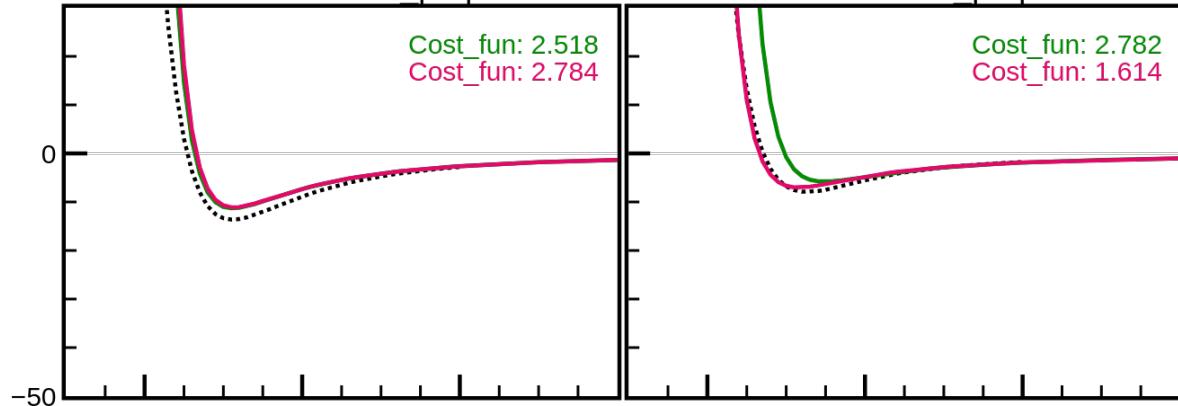
Energy, kcal/mol

Distance, Å

**ADEB CES 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

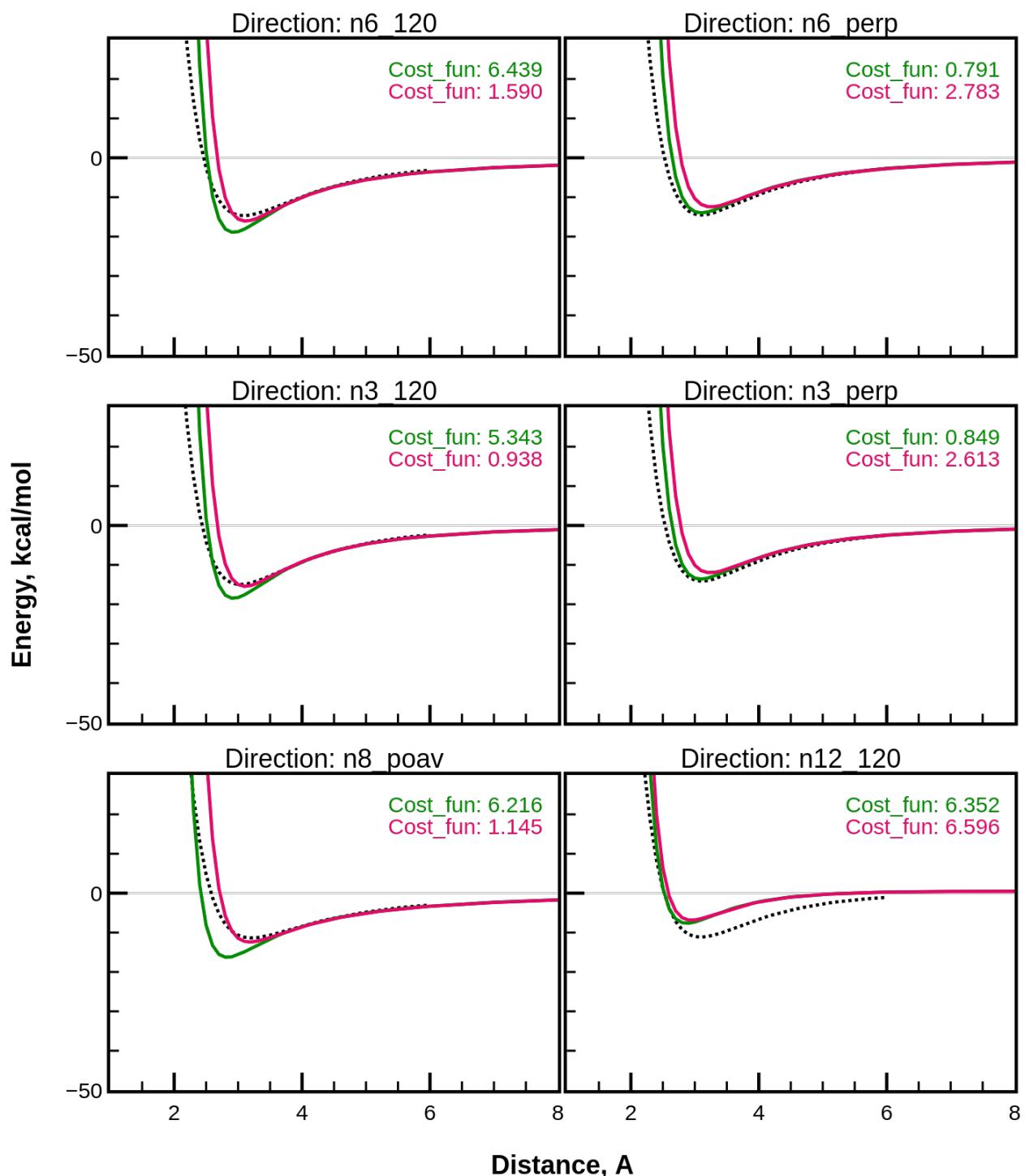
Direction: n12\_perp

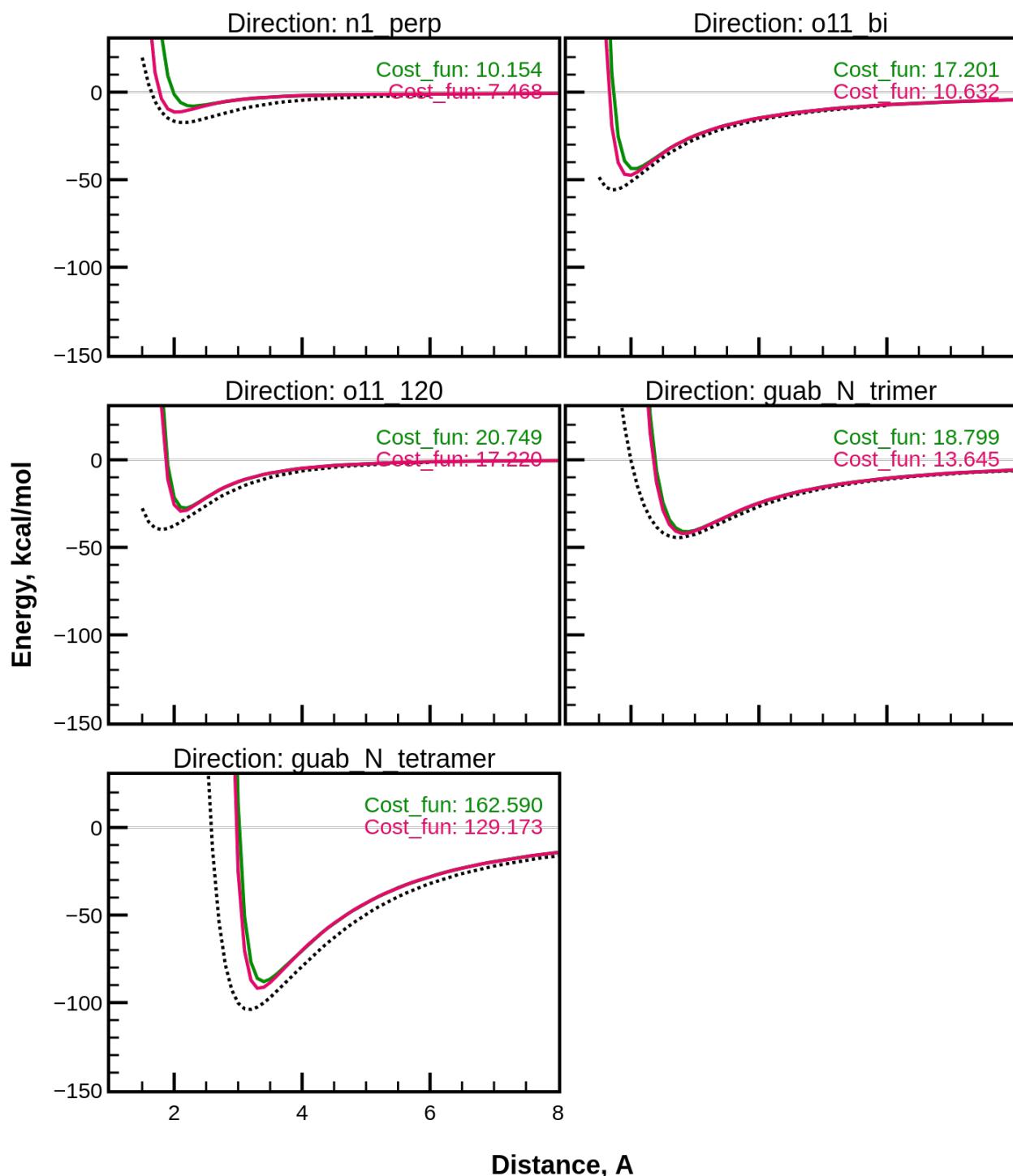
Direction: n1\_perp

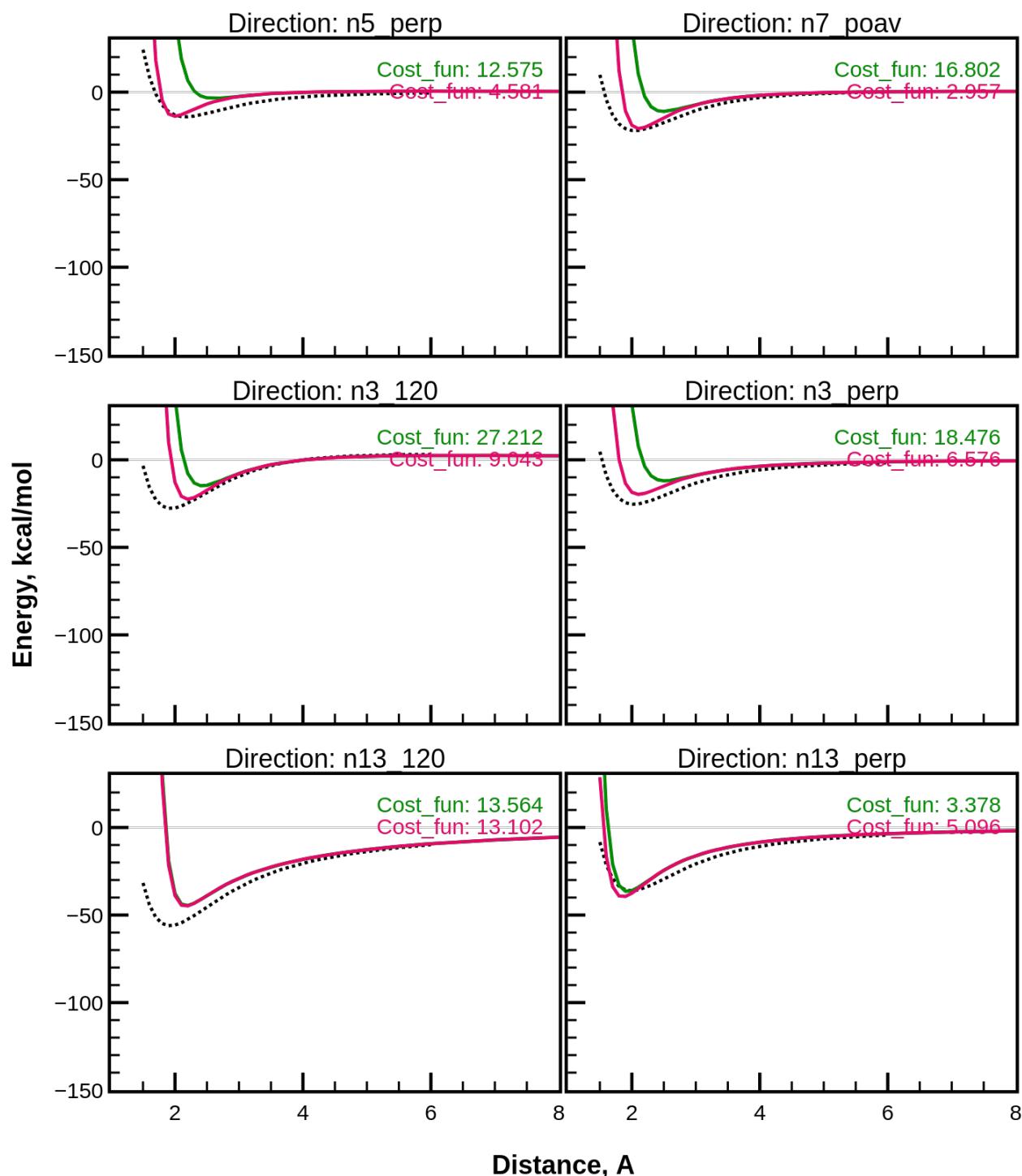


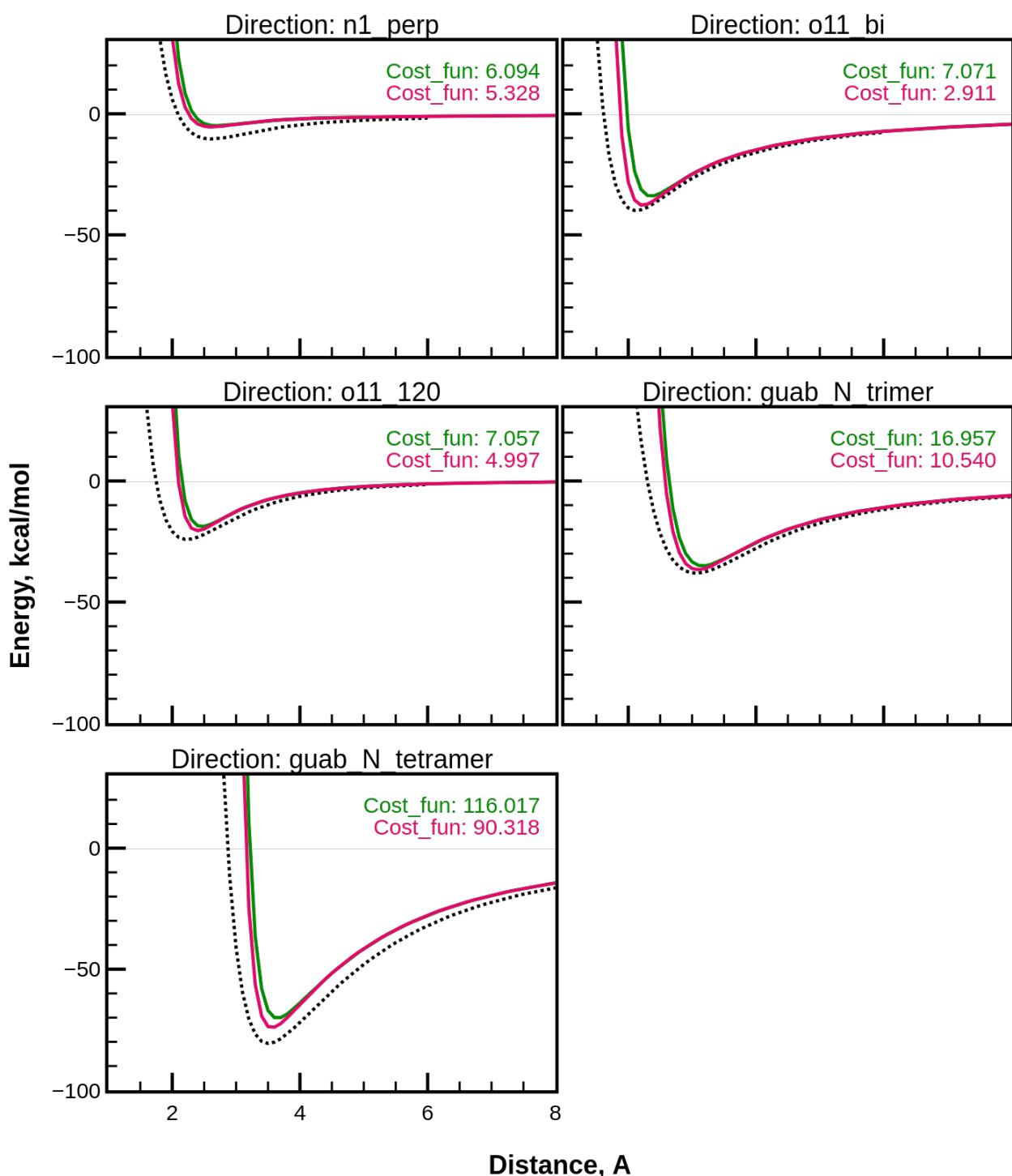
Energy, kcal/mol

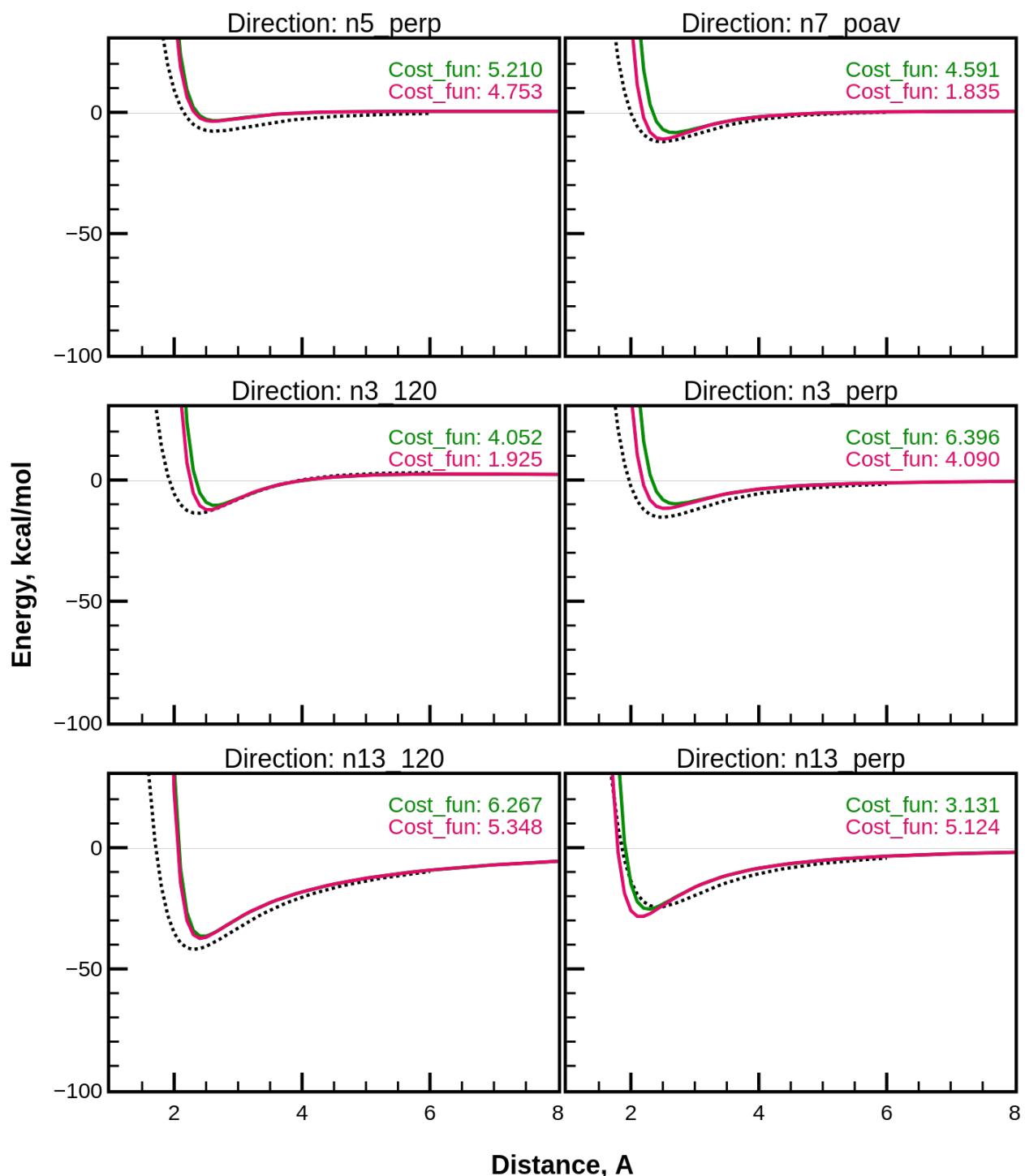
Distance, A

**ADEB CES 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**GUAB LIT 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

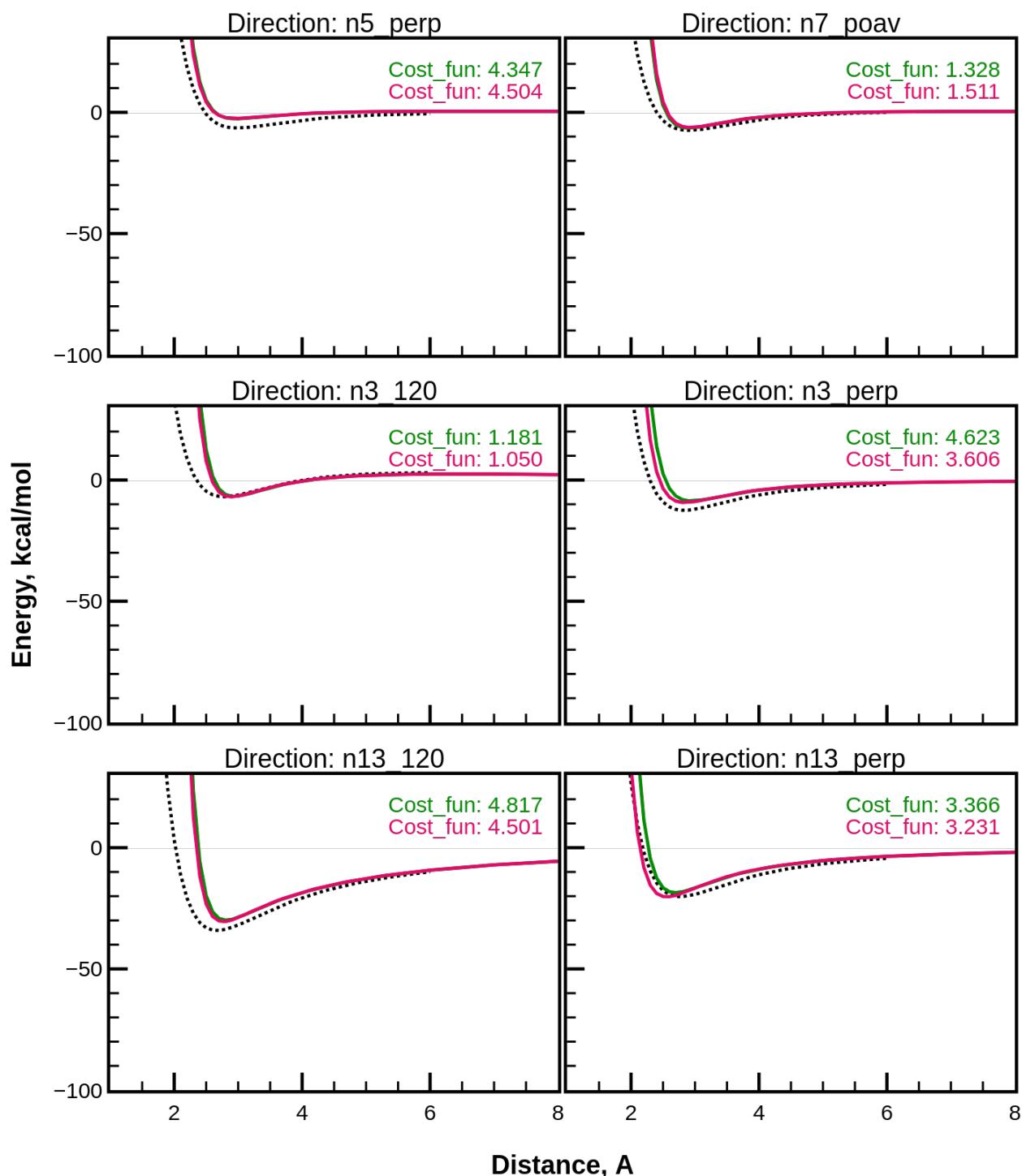
**GUAB LIT 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**GUAB SOD 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**GUAB SOD 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

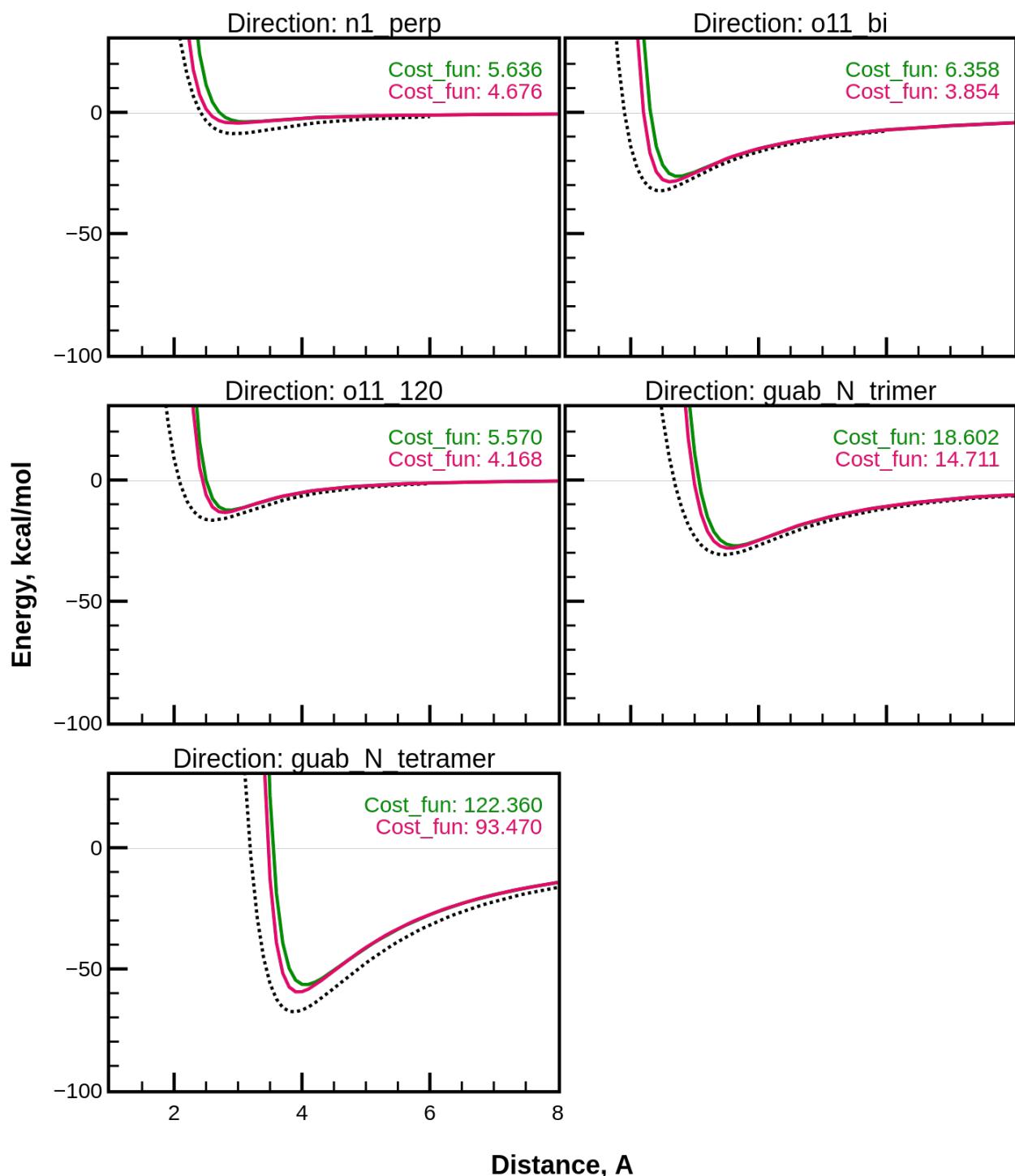
## GUAB POT 1/2

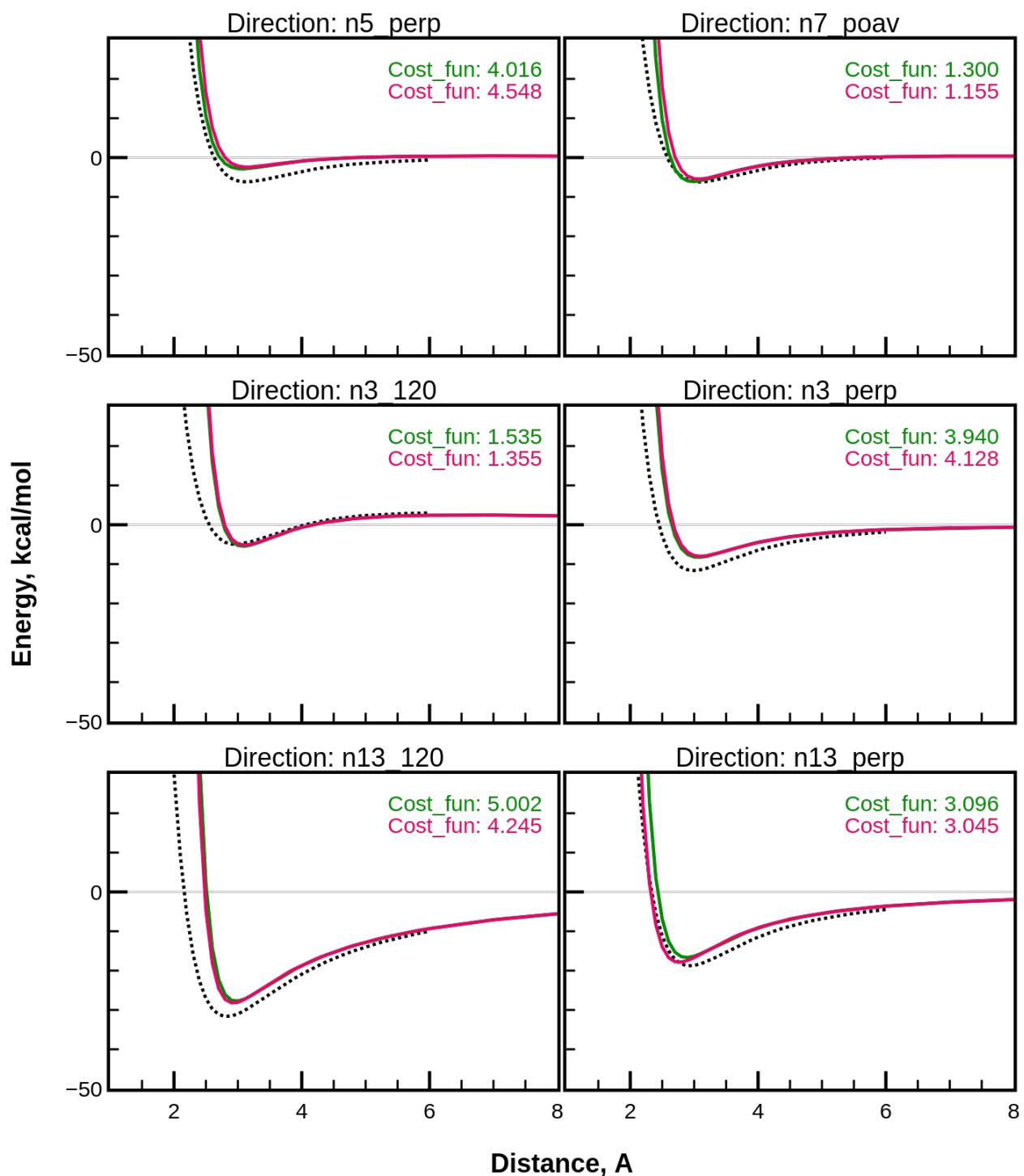
9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

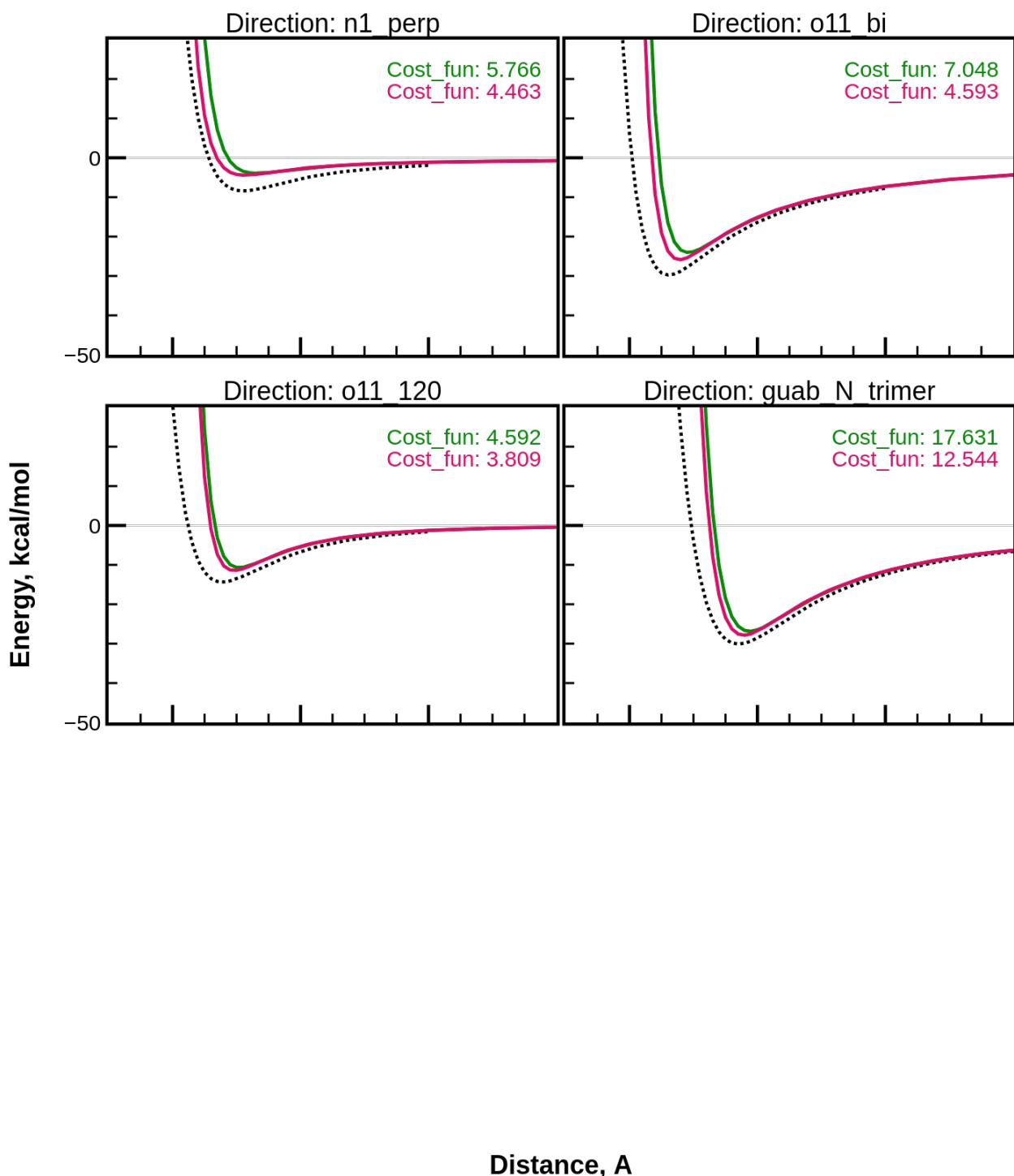


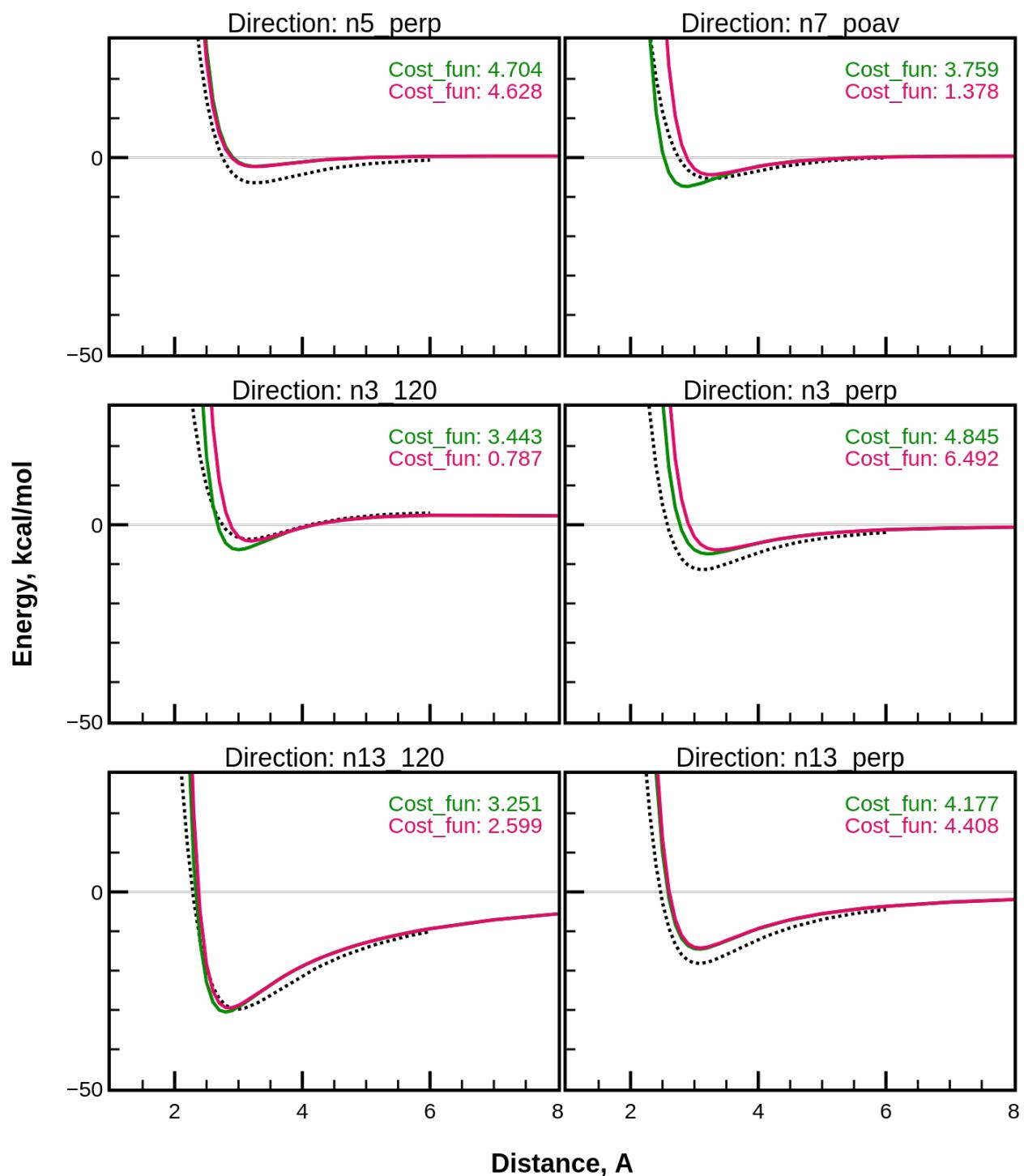
## GUAB POT 2/2

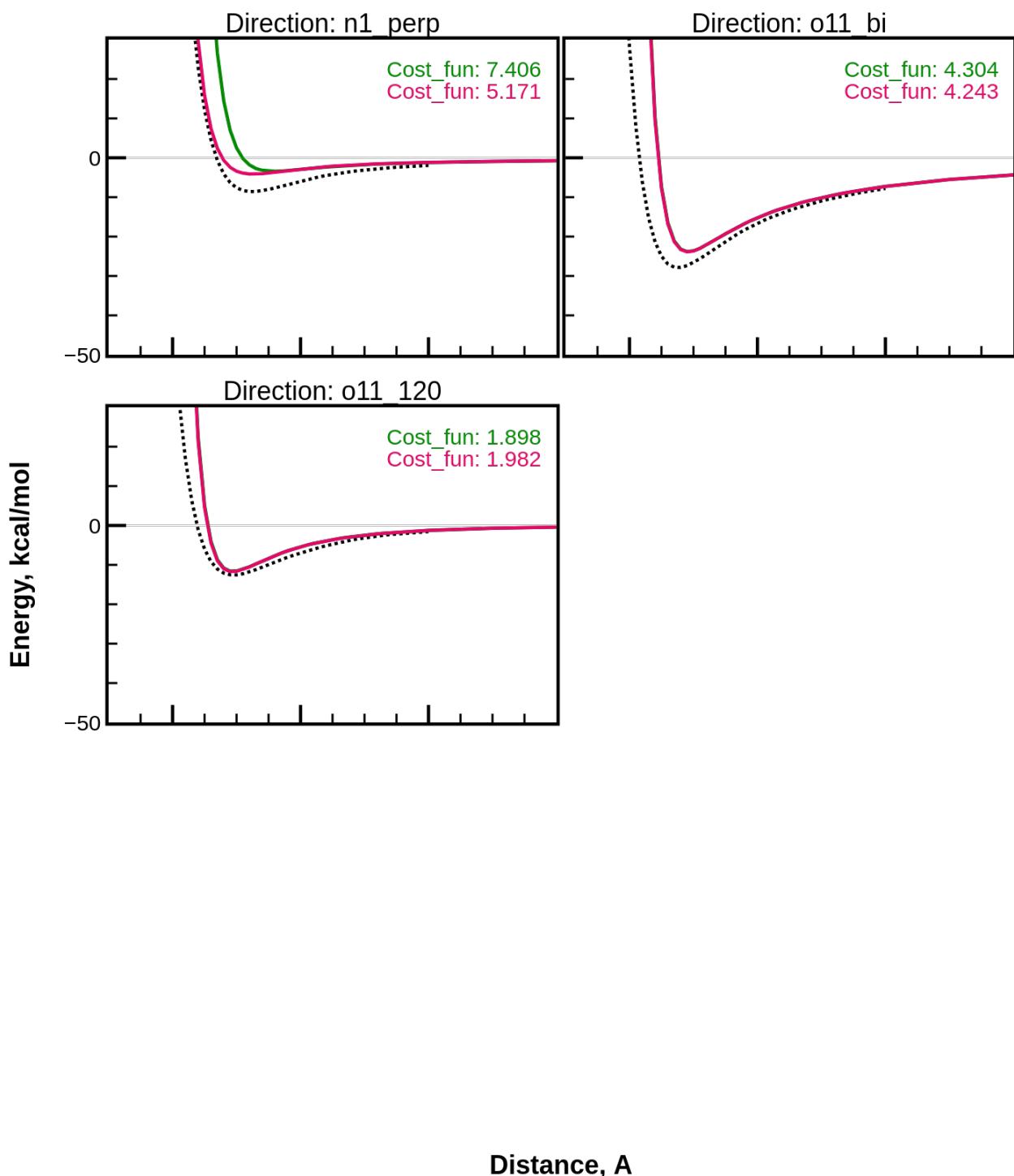
9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

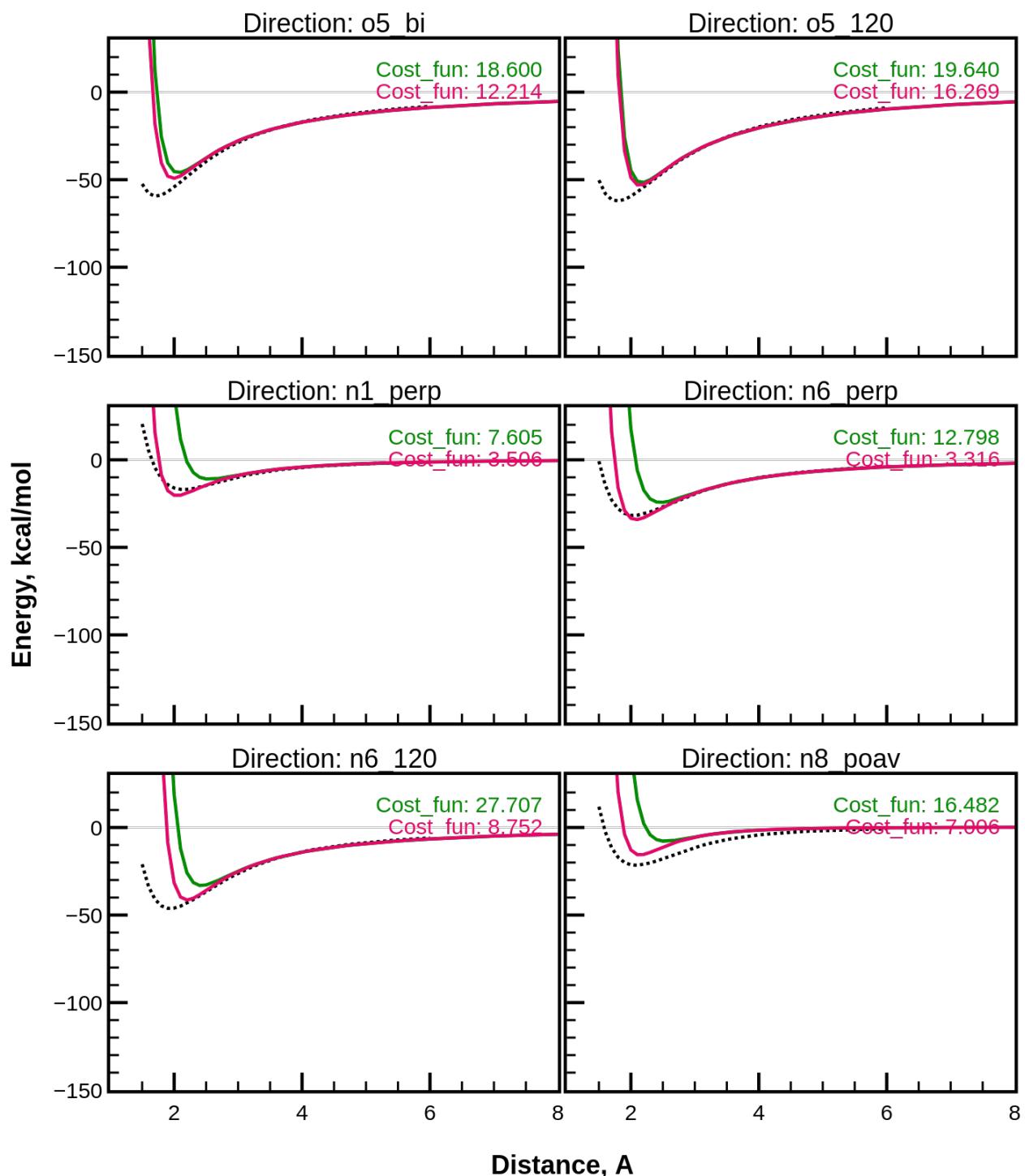


**GUAB RUB 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**GUAB RUB 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**GUAB CES 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**GUAB CES 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

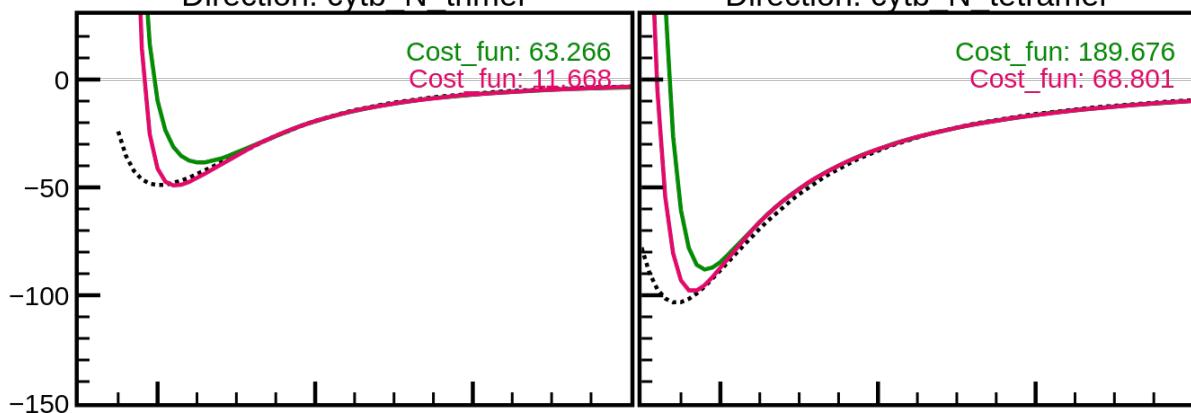
**CYTB LIT 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

# CYTB LIT 2/2

9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

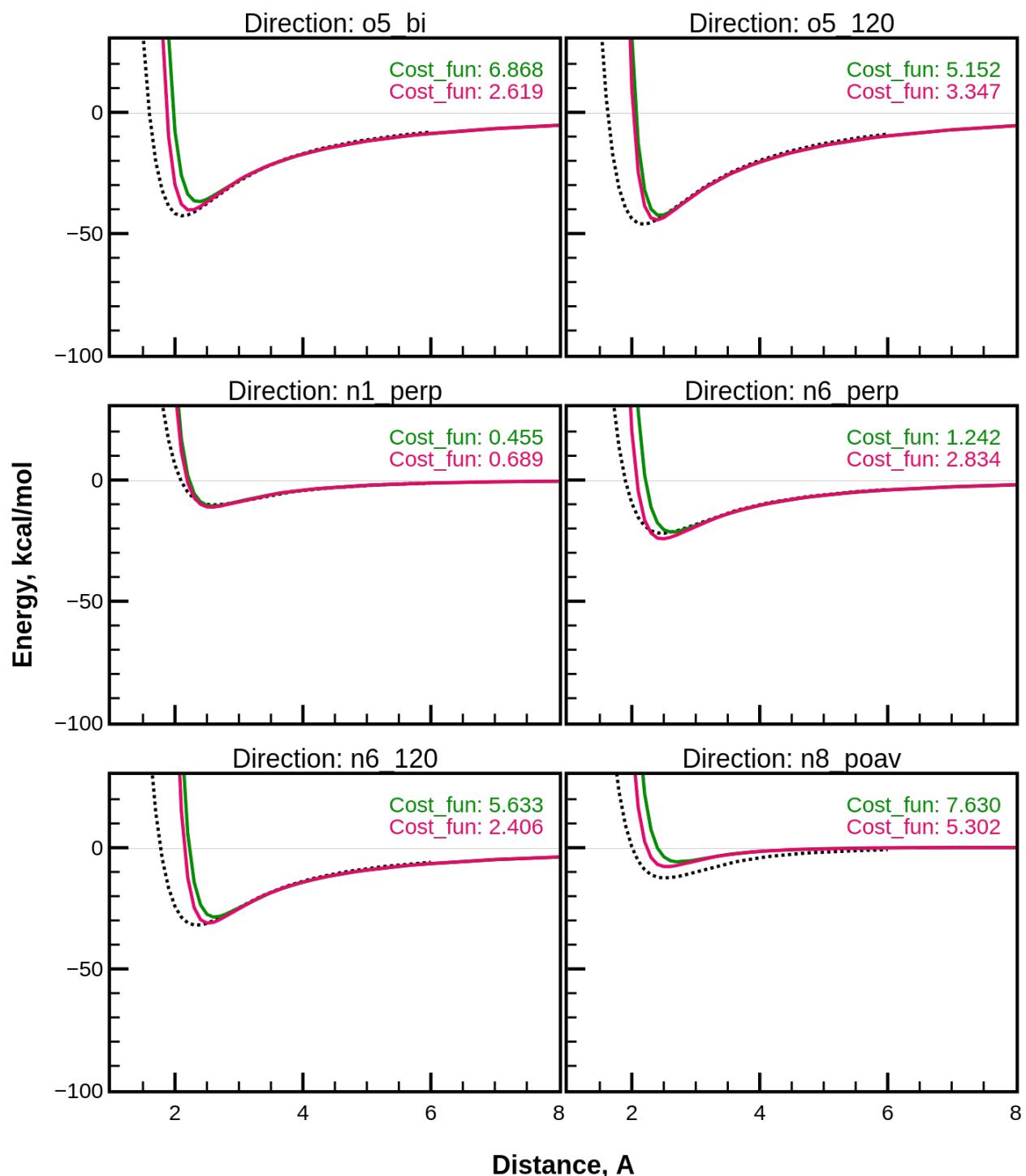
Direction: cytb N trimer

Direction: cytb N tetramer



Energy, kcal/mol

Distance, A

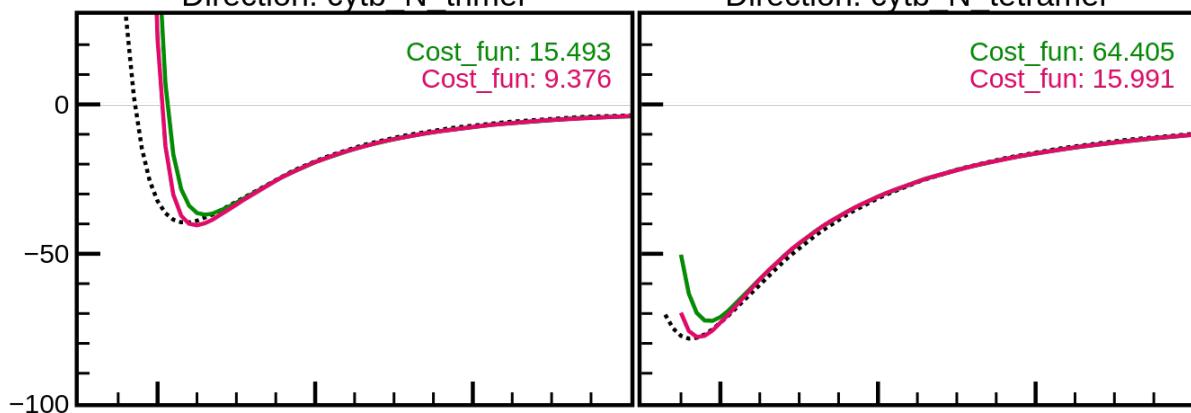
**CYTB SOD 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

# CYTB SOD 2/2

9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

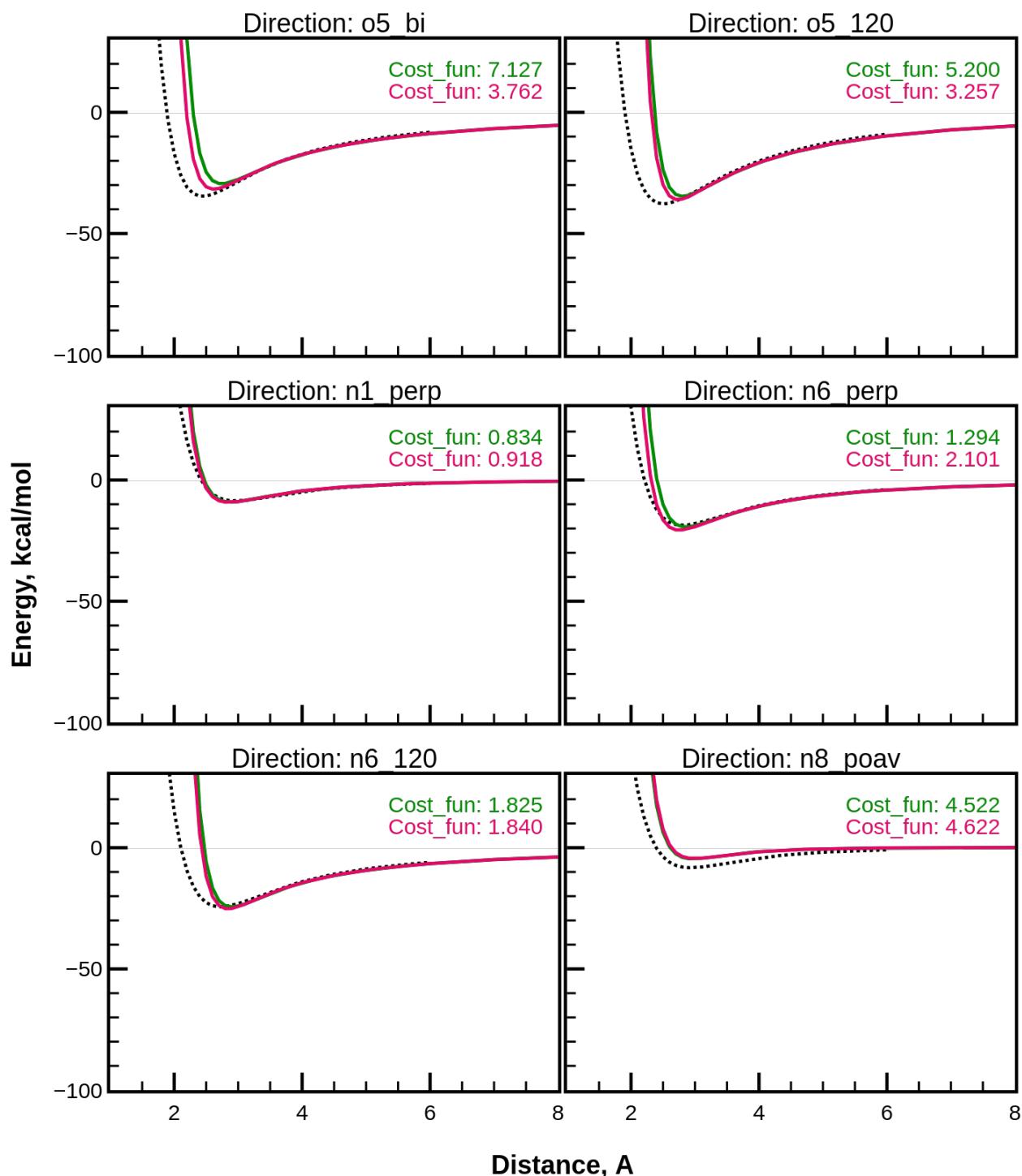
Direction: cyt b N trimer

Direction: cyt b N tetramer



Energy, kcal/mol

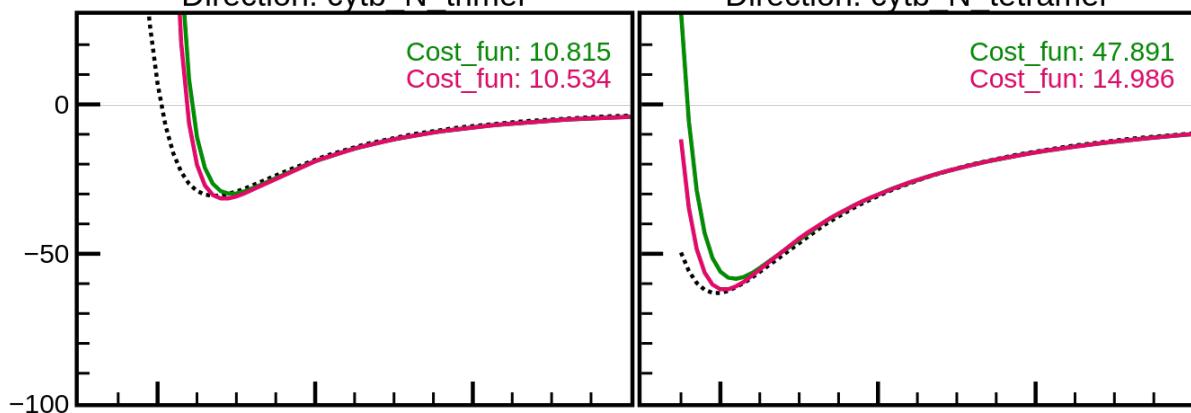
Distance, A

**CYTB POT 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**CYTB POT 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

Direction: cytb N trimer

Direction: cytb N tetramer



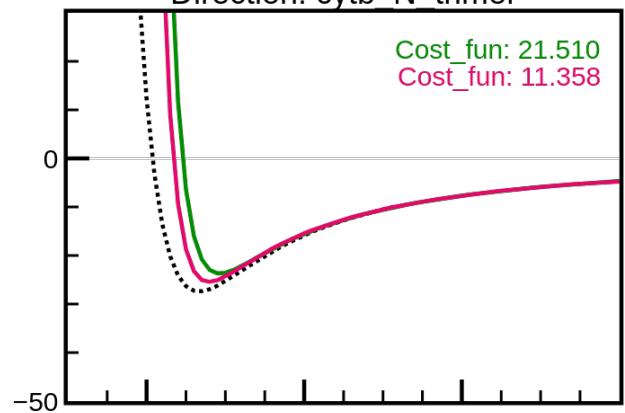
Energy, kcal/mol

Distance, A

# CYTB RUB 2/2

9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

Direction: cytb N trimer

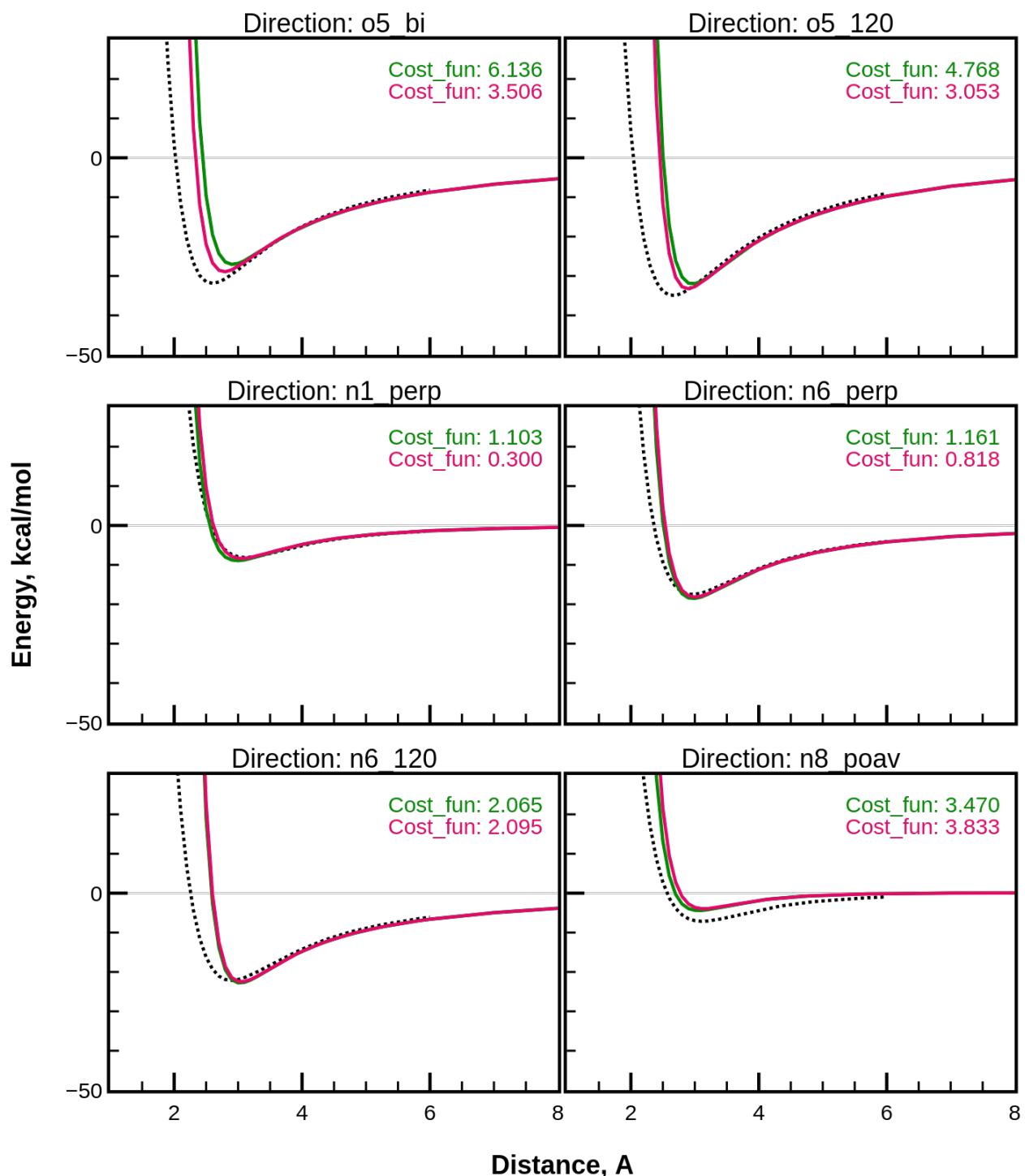


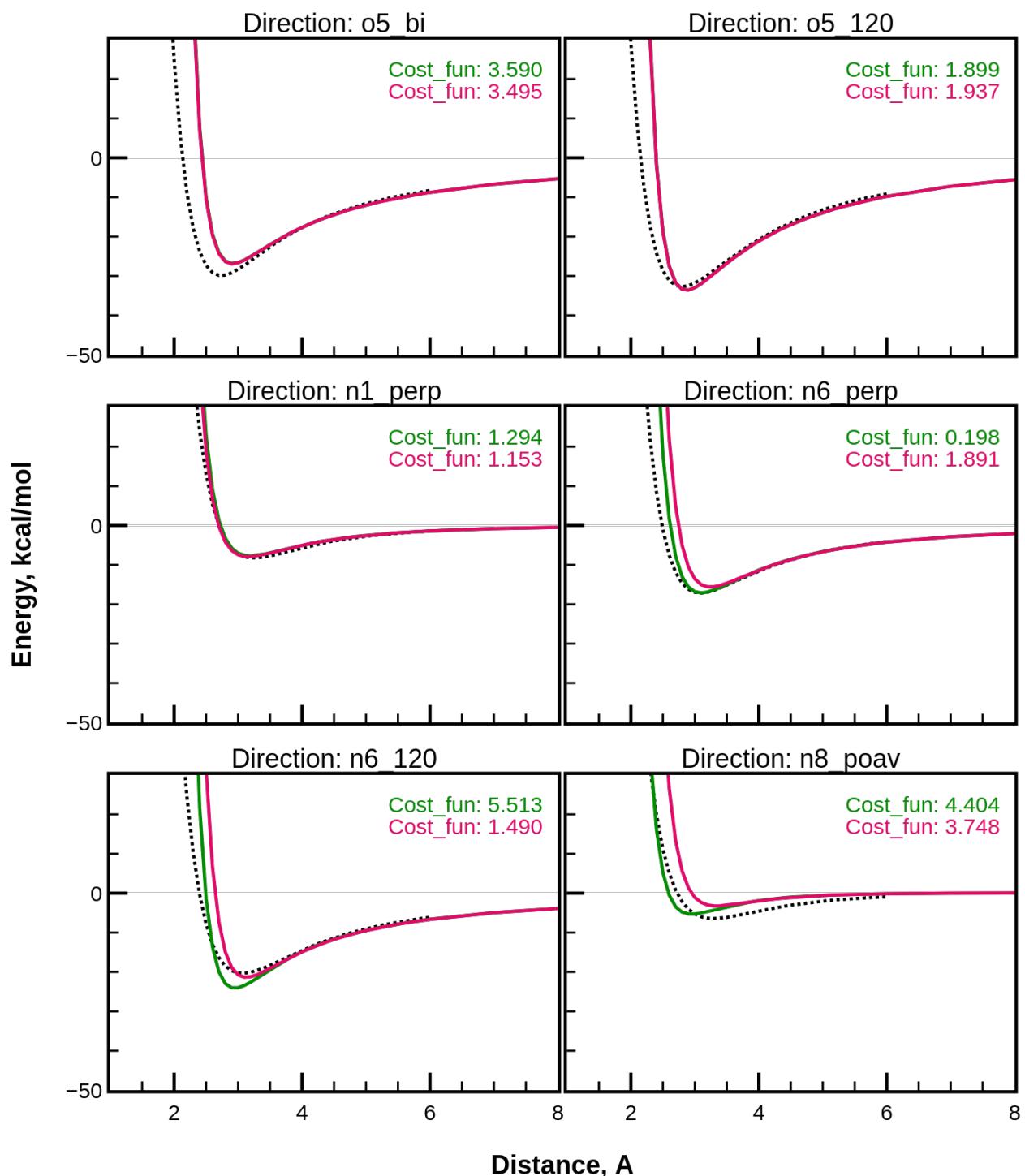
Energy, kcal/mol

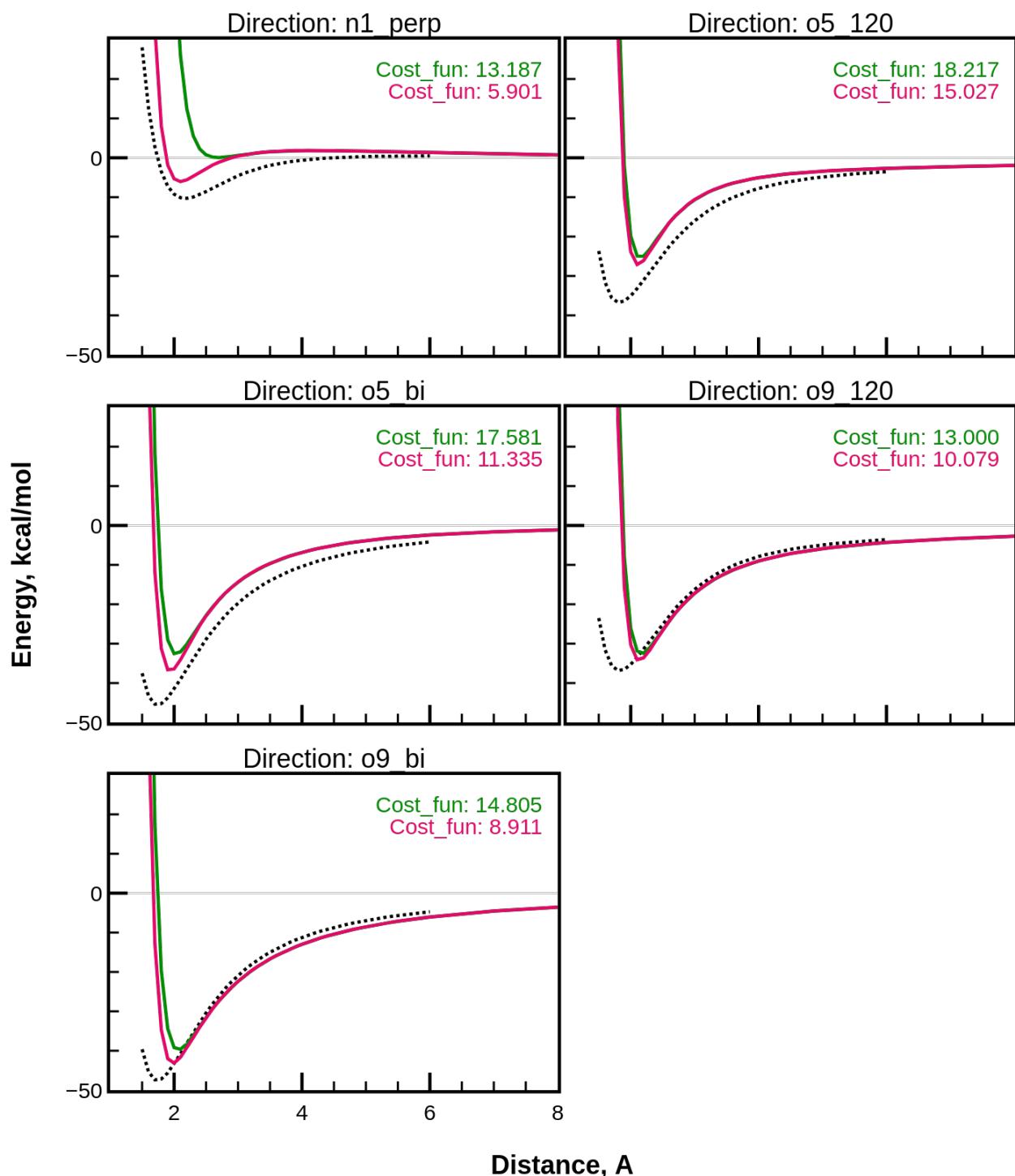
Distance, Å

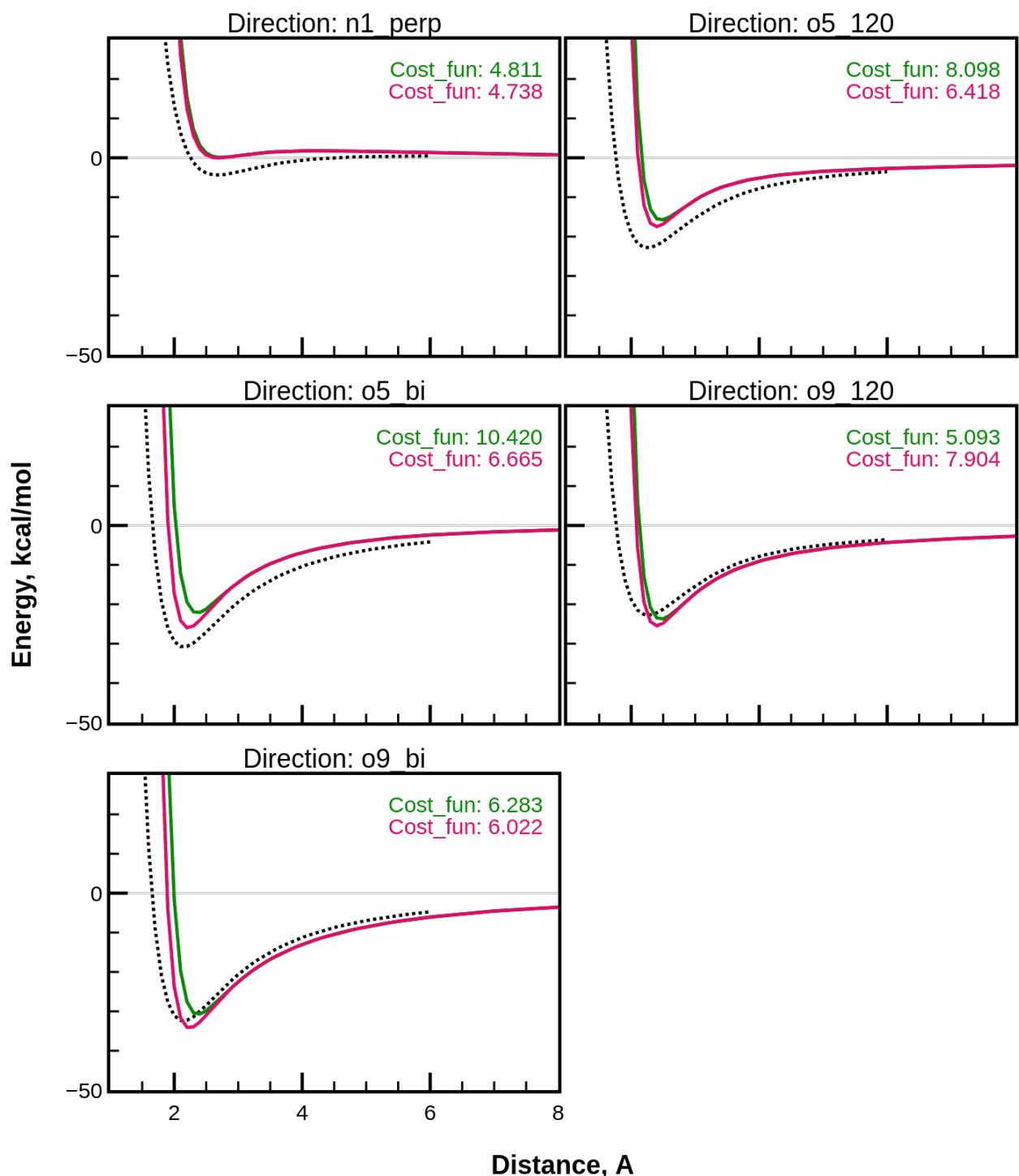
# CYTB RUB 1/2

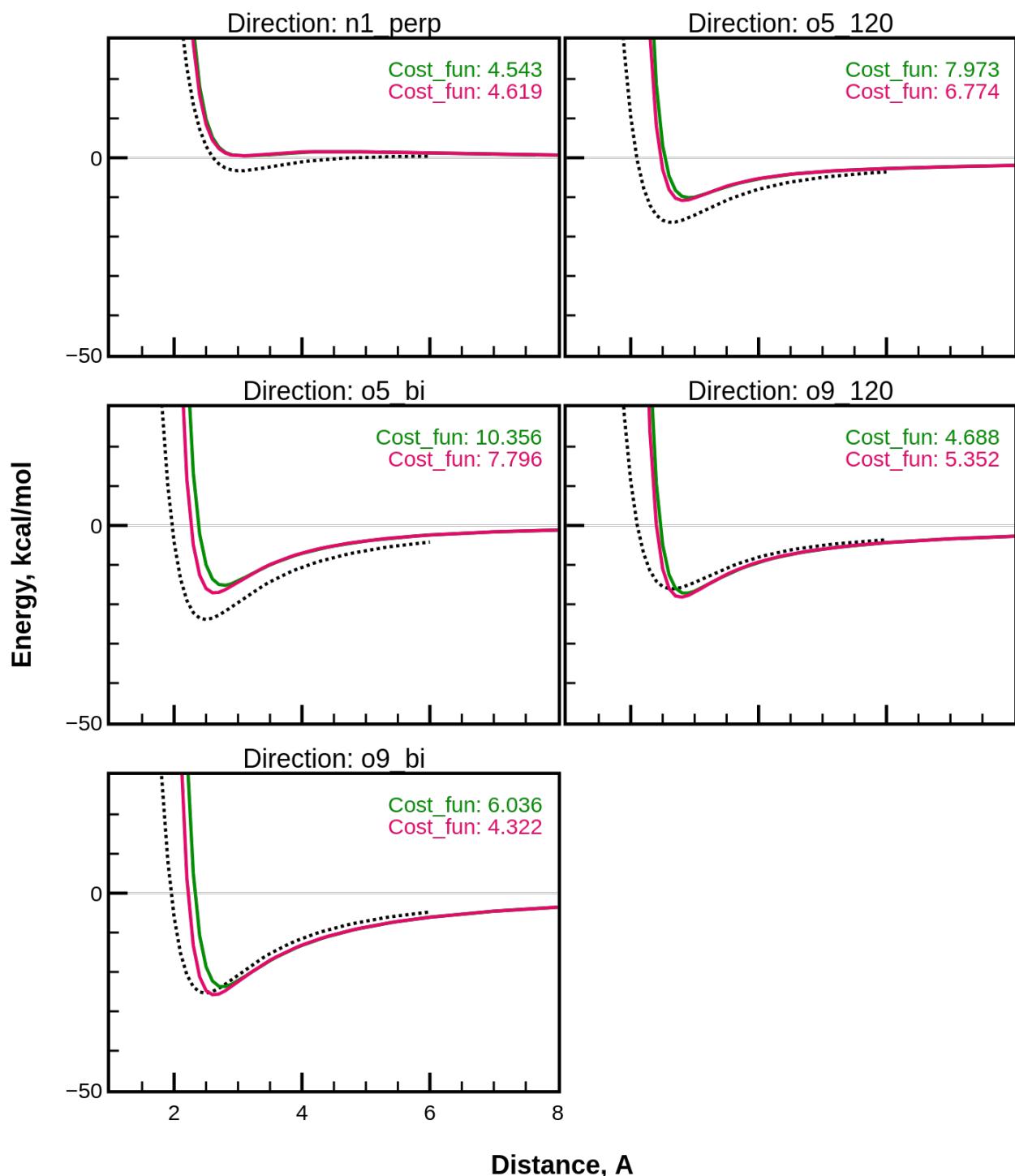
9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

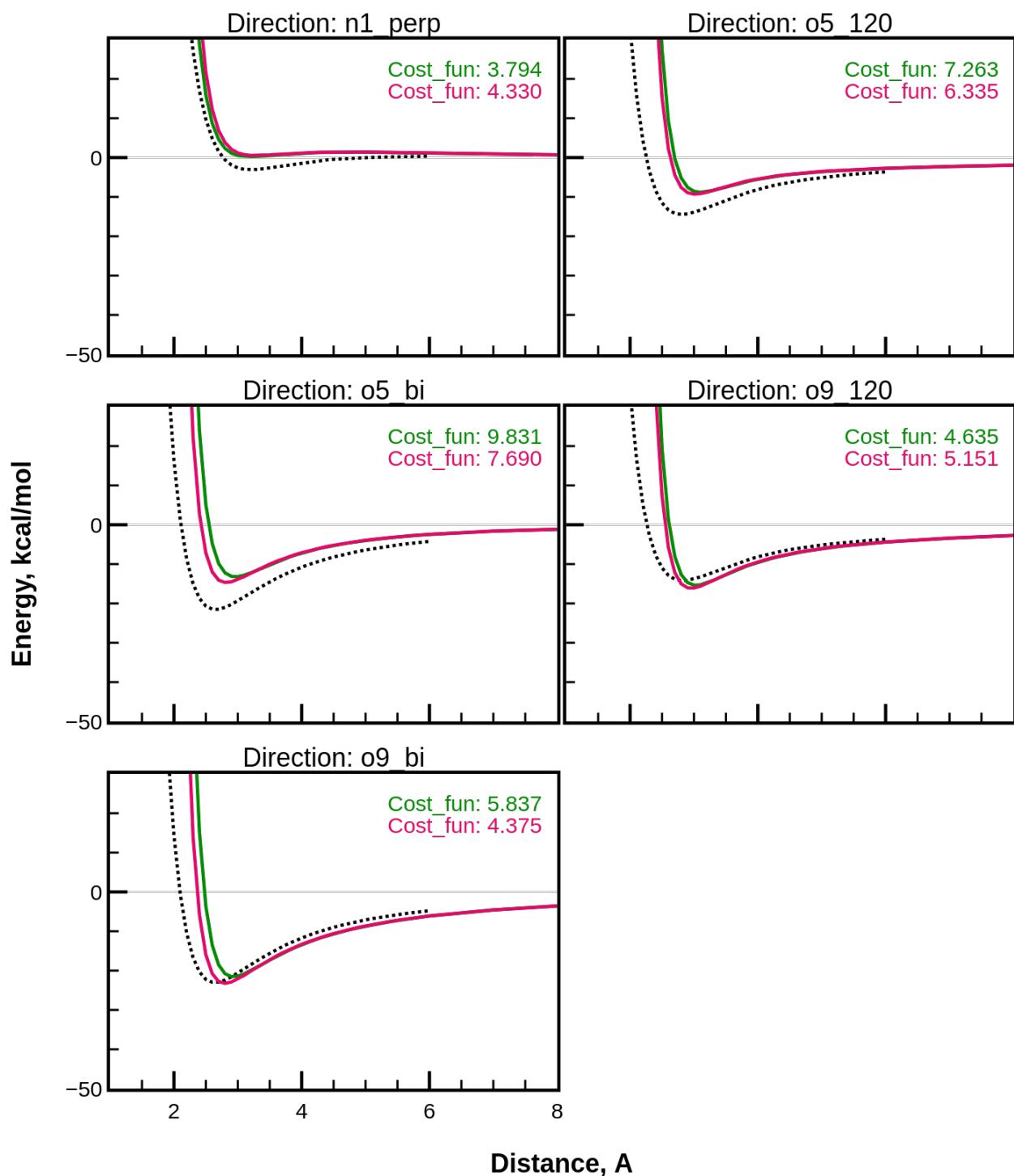


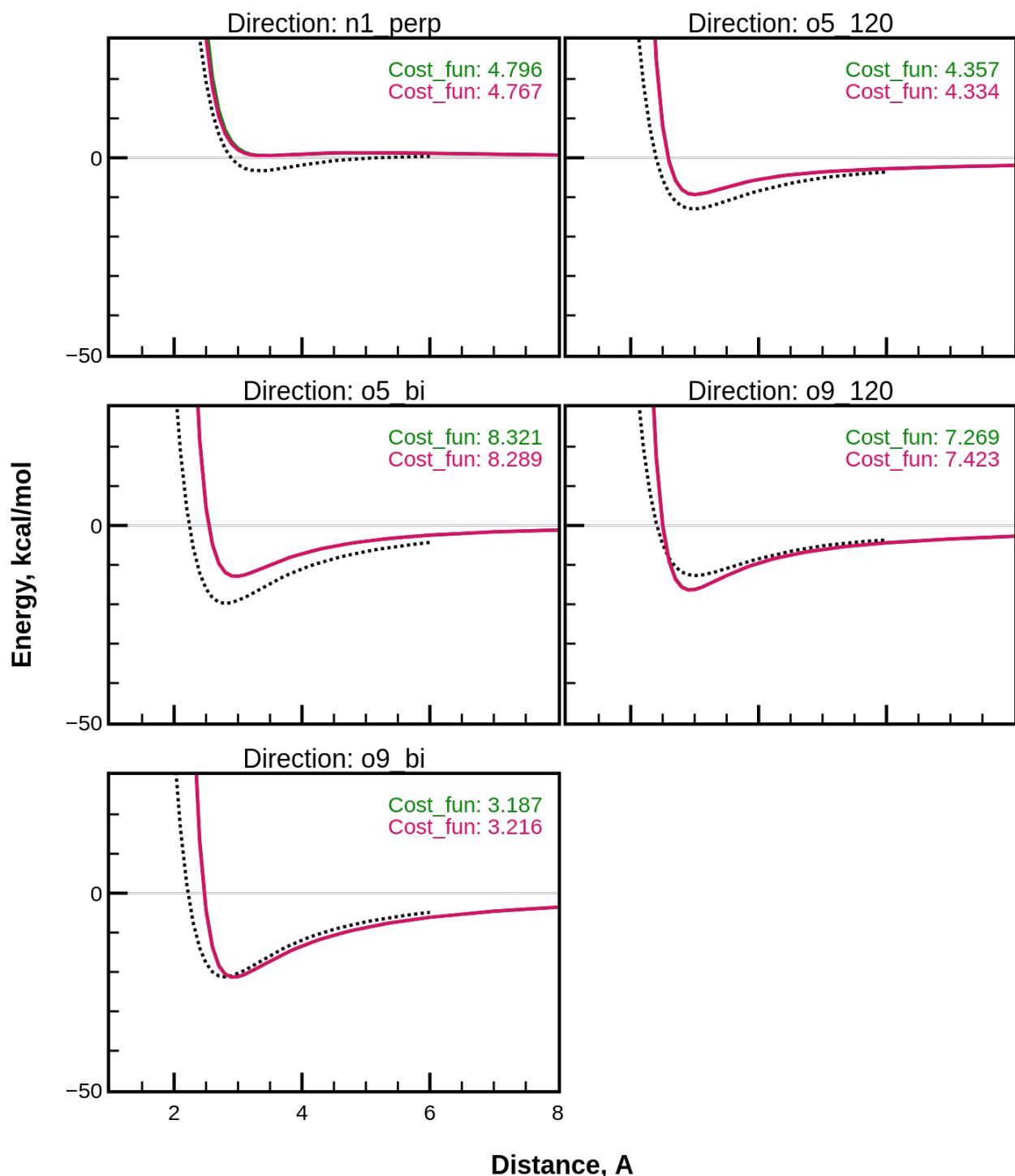
**CYTB CES 1/1**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

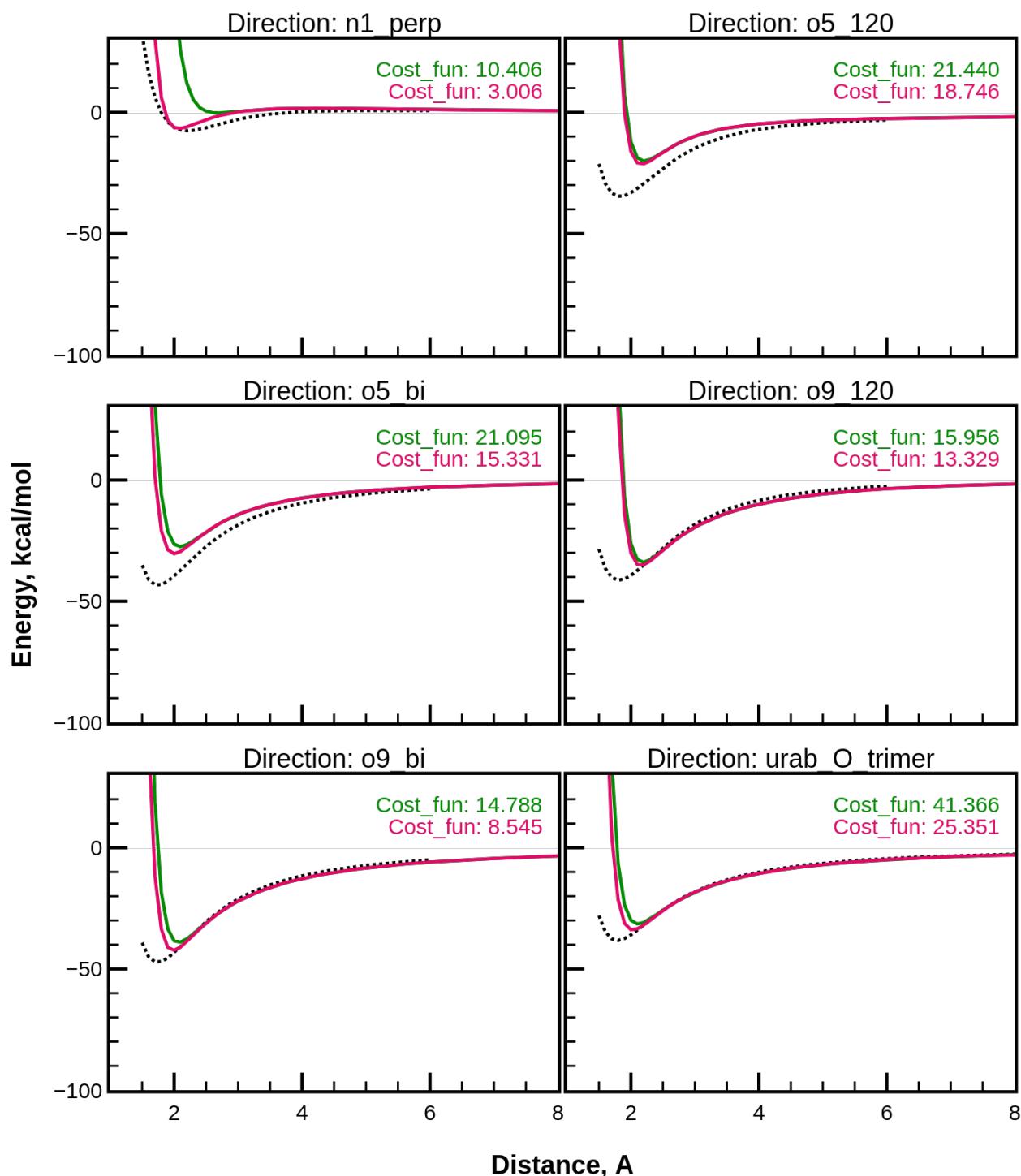
**THYB LIT 1/1**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

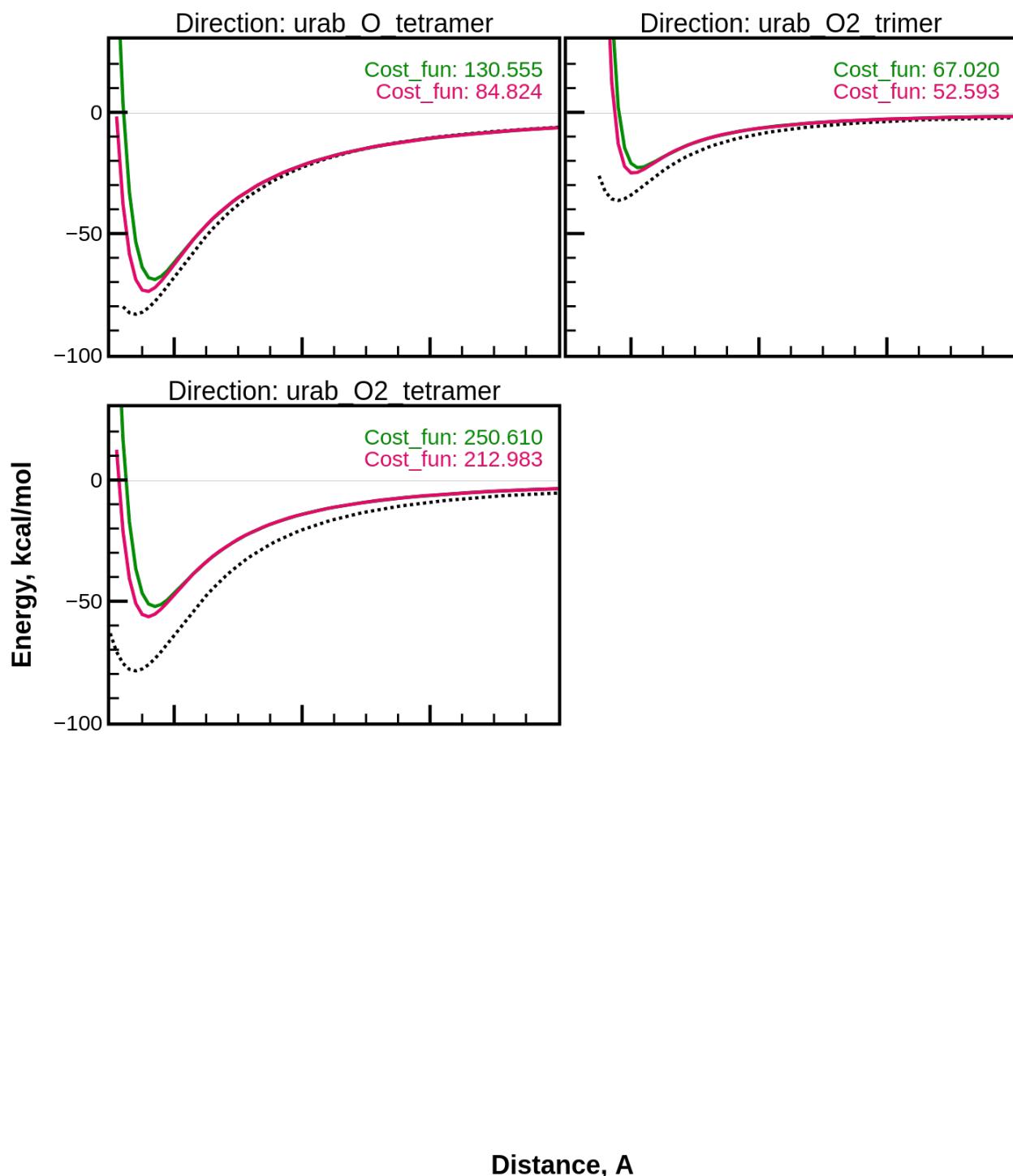
**THYB SOD 1/1**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

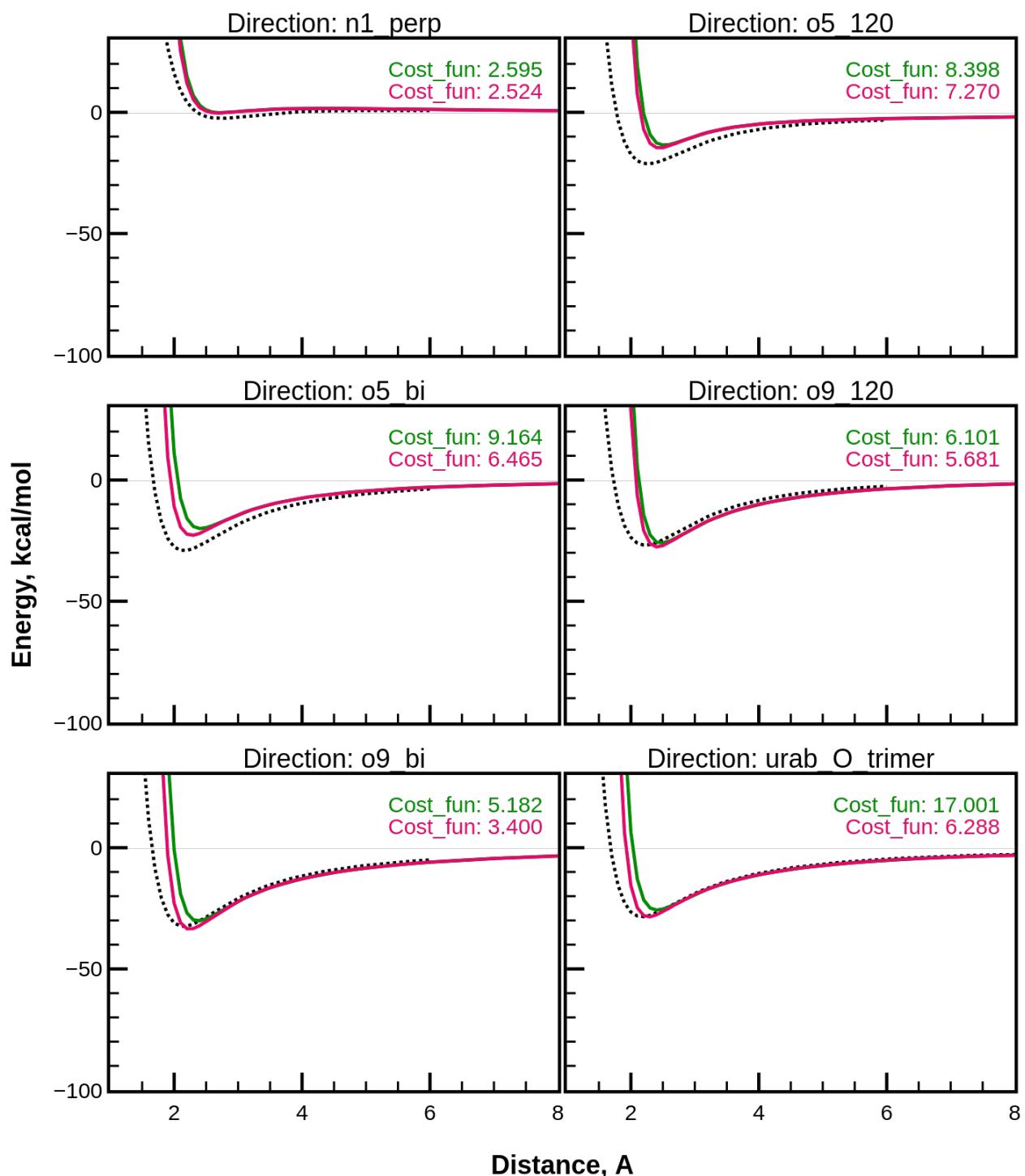
**THYB POT 1/1**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**THYB RUB 1/1**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**THYB CES 1/1**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

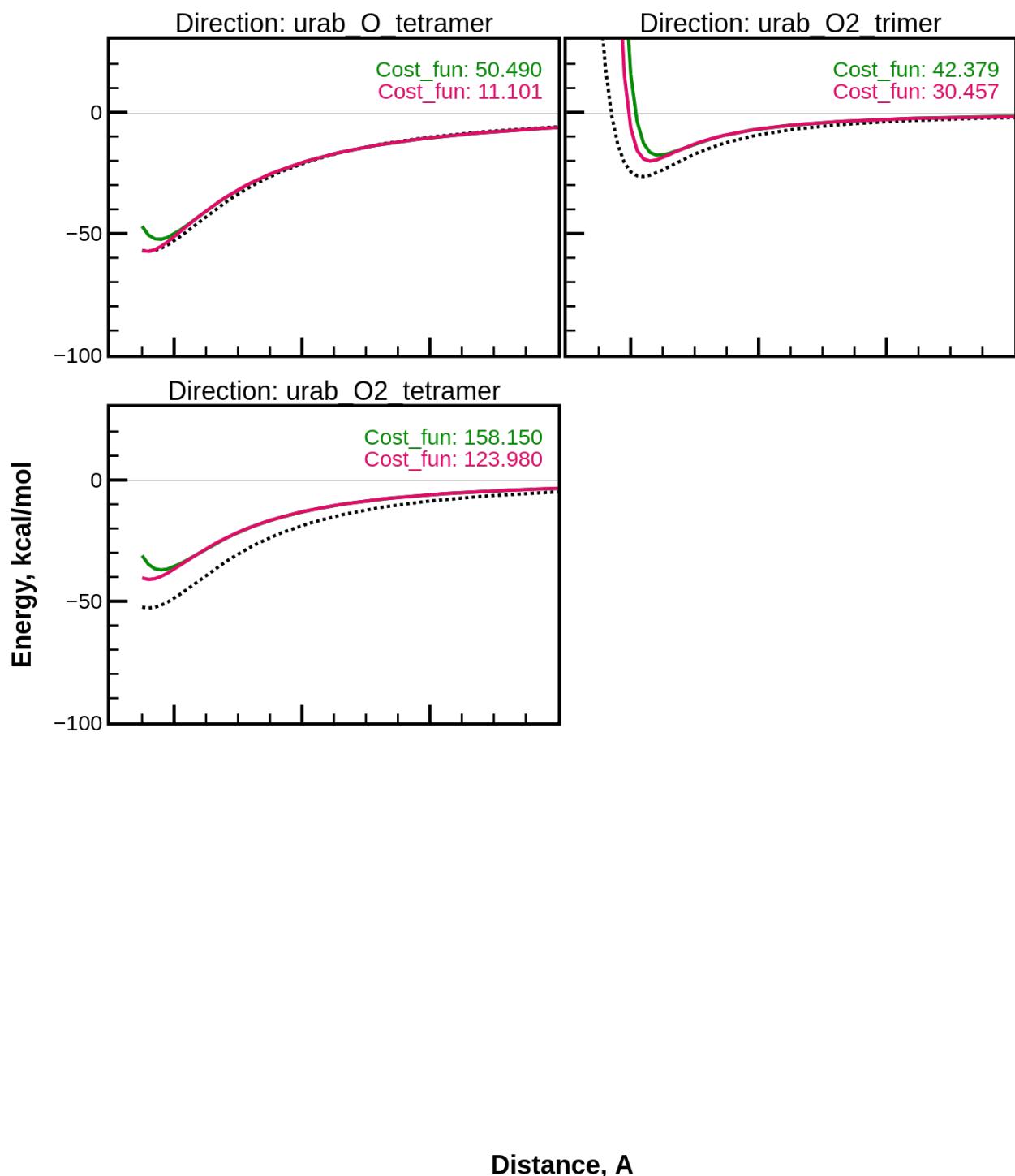
**URAB LIT 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**URAB LIT 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**URAB SOD 1/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

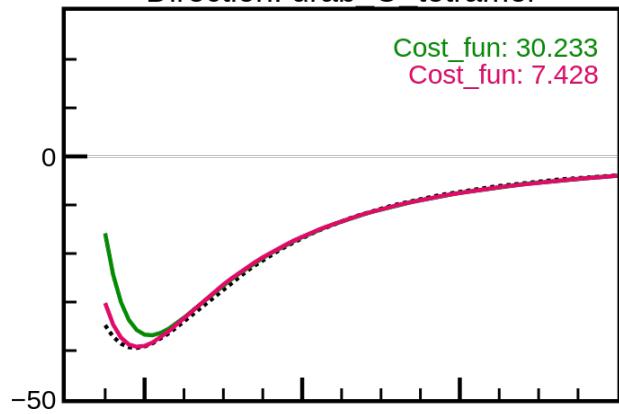
# URAB SOD 2/2

9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

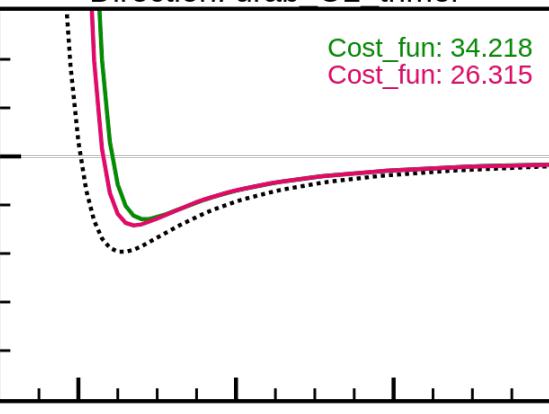


**URAB POT 2/2**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

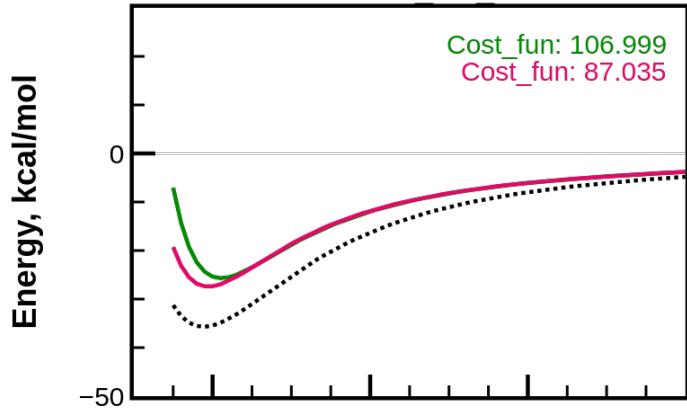
Direction: urab\_O\_tetramer



Direction: urab\_O2\_trimer



Direction: urab\_O2\_tetramer

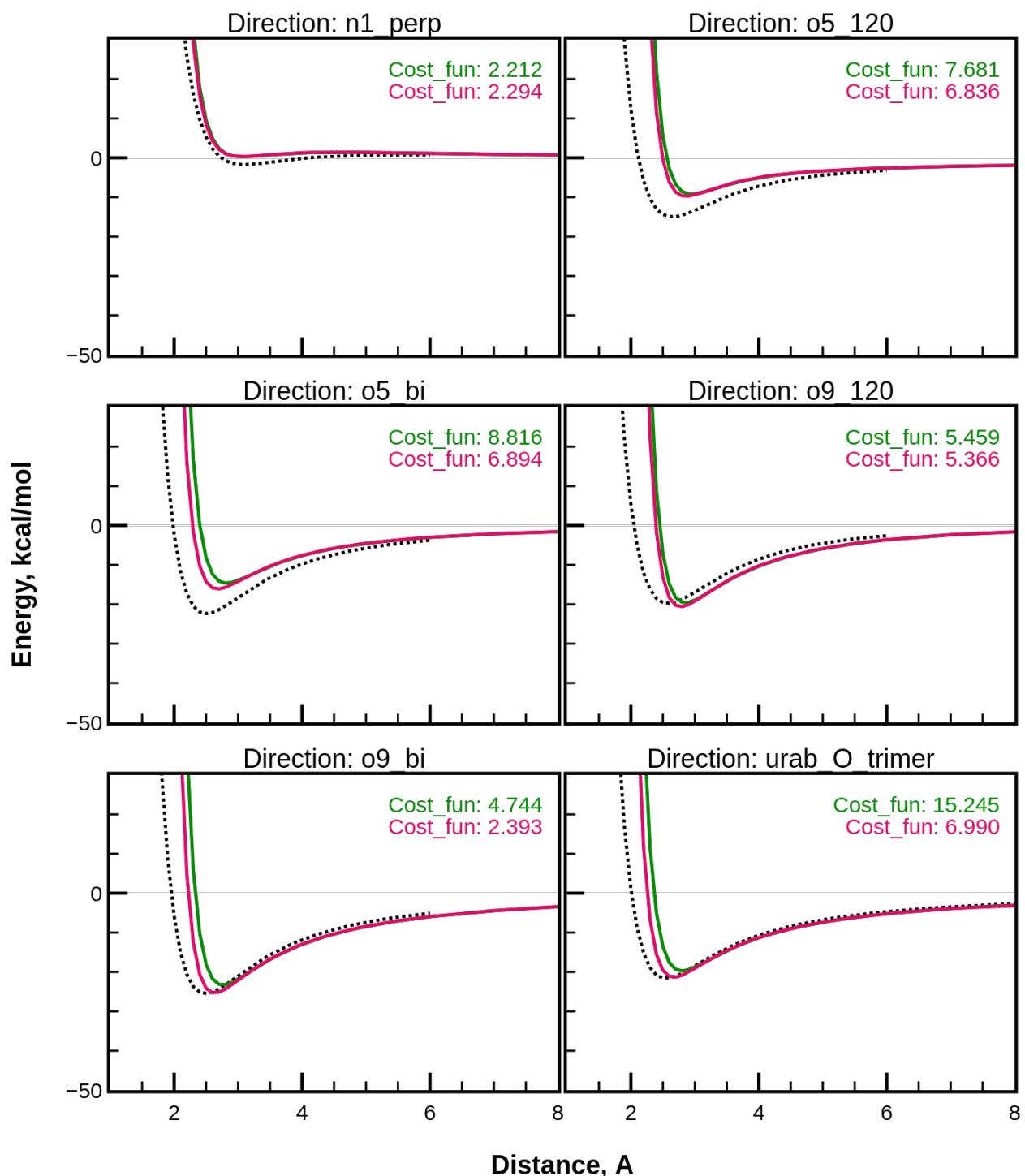


Distance, Å

Energy, kcal/mol

# URAB POT 1/2

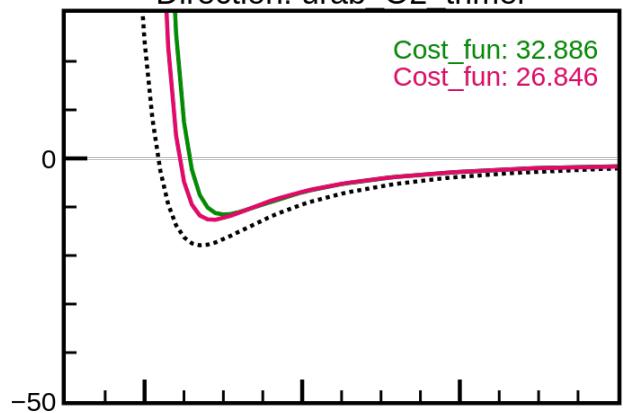
9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111



# URAB RUB 2/2

9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

Direction: urab\_O2\_trimer

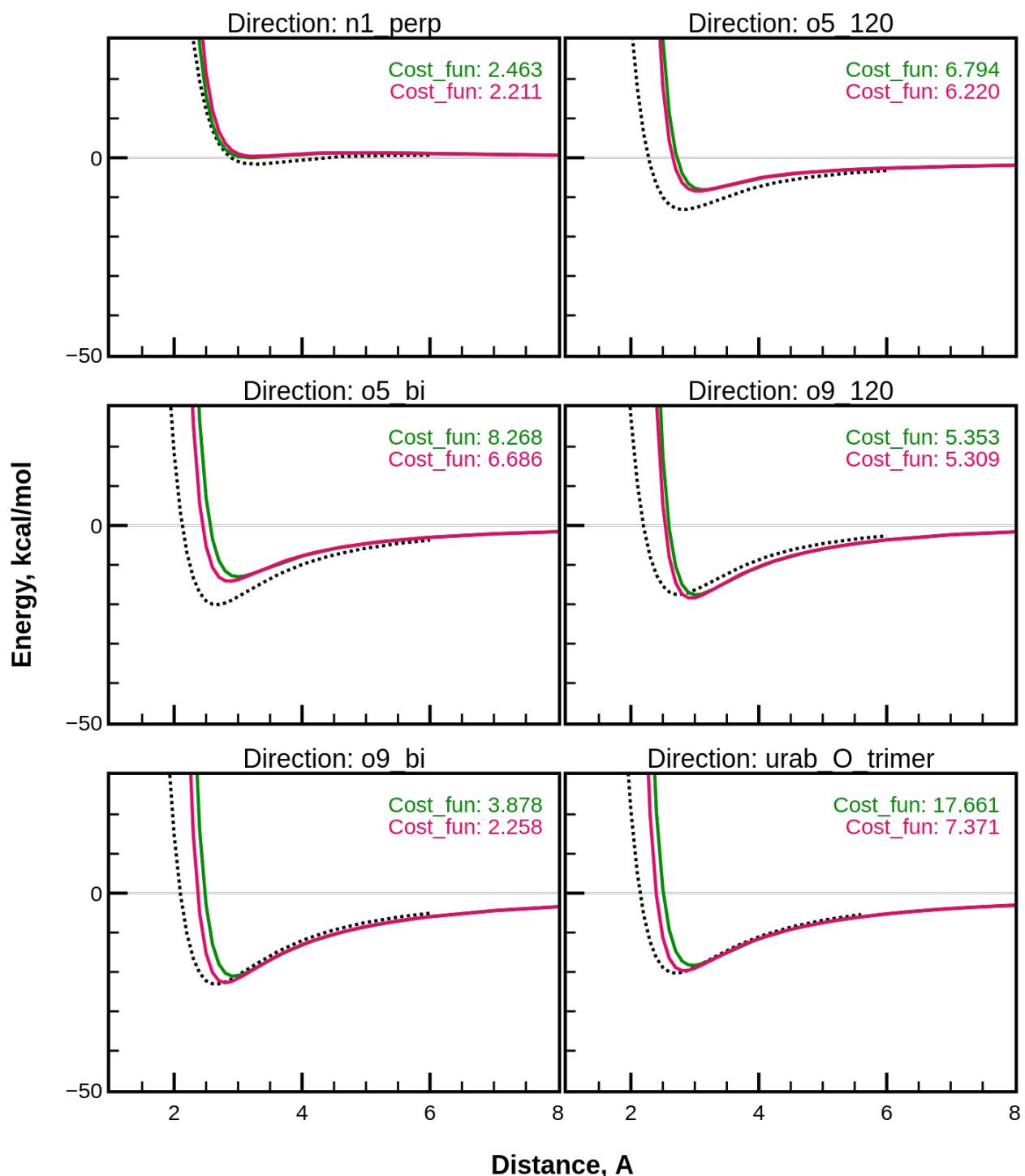


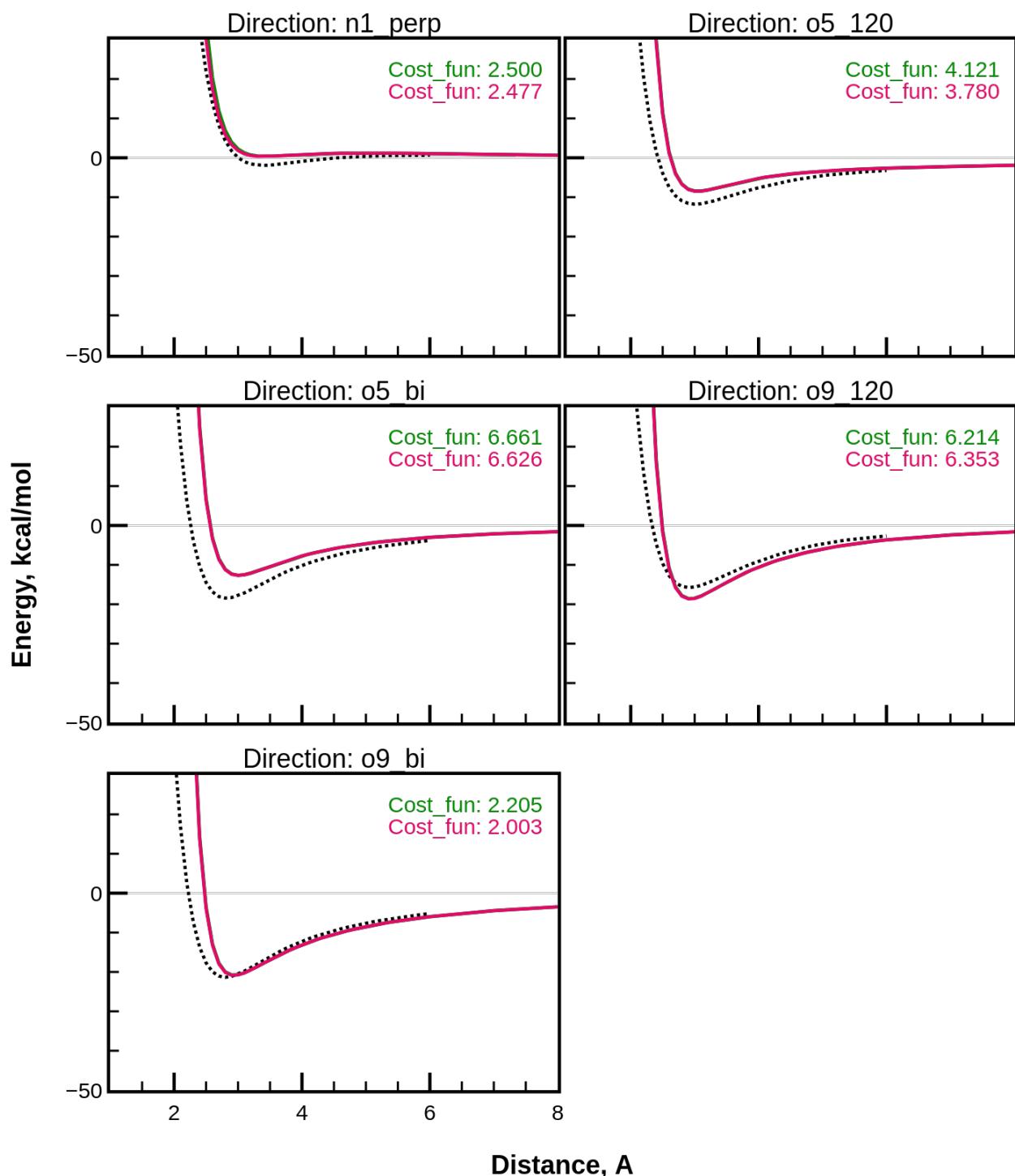
Energy, kcal/mol

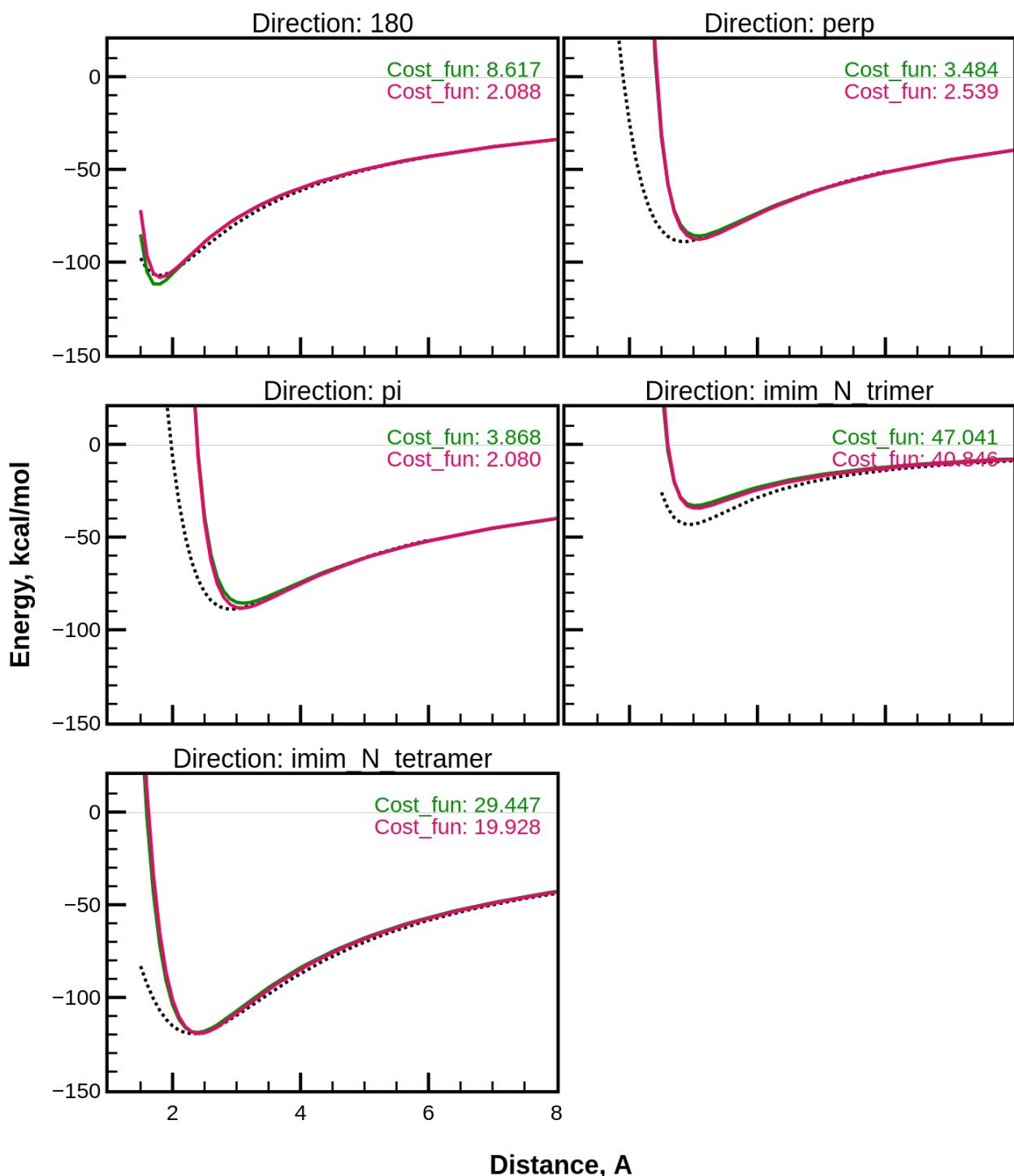
Distance, Å

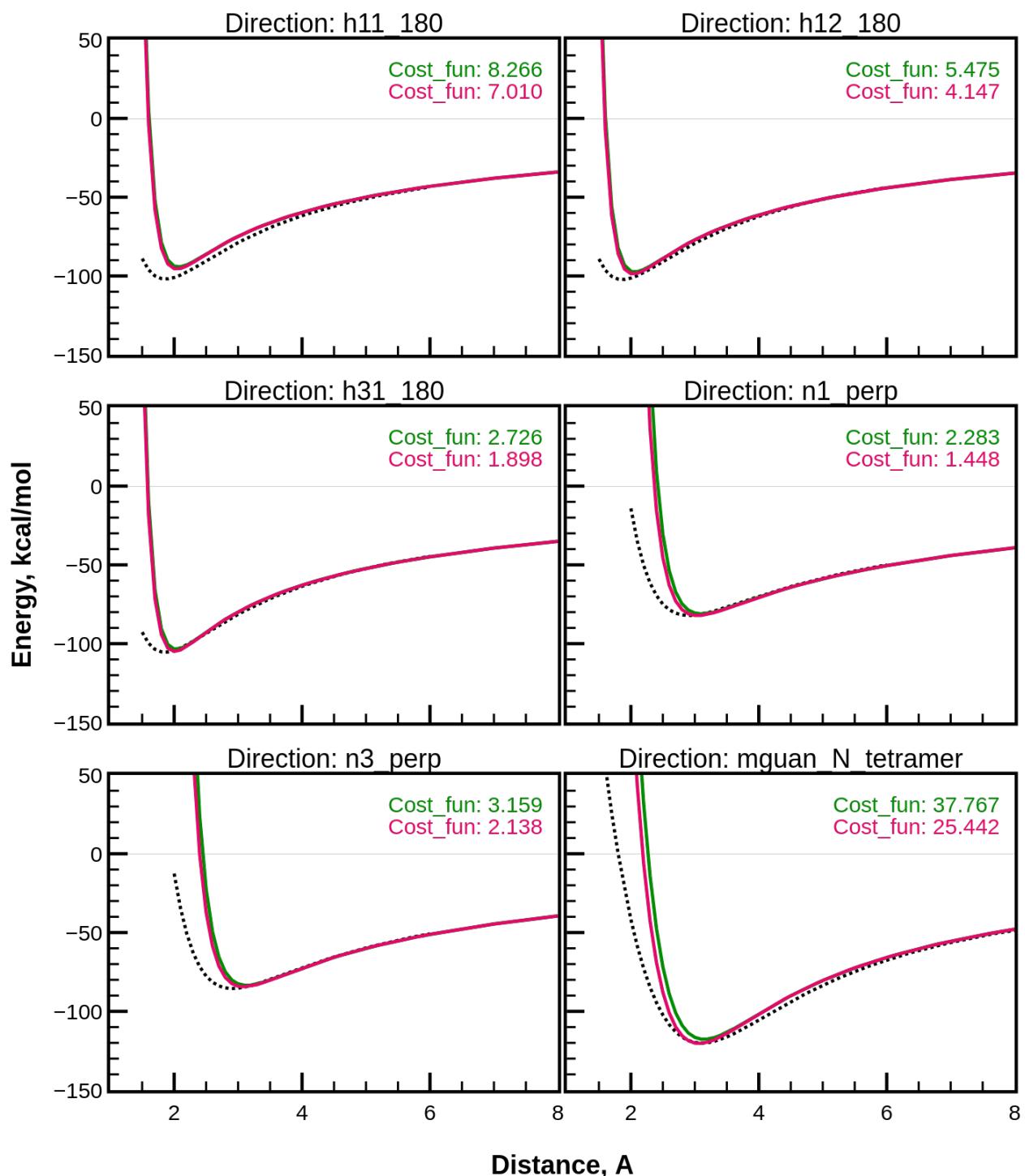
# URAB RUB 1/2

9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111



**URAB CES 1/1**9.99999\_9.99999\_9.99999  
1.11111\_1.11111\_1.11111

**IMIM CLA 1/1**4.33111\_0.08693\_9.99999  
4.36326\_0.08693\_1.41768

**MGUAN CLA 1/1**4.28111\_0.08269\_9.99999  
4.14635\_0.08269\_4.10351

**NC1 CLA 1/1**4.03111\_0.04242\_9.99999  
4.62234\_0.04242\_1.59027