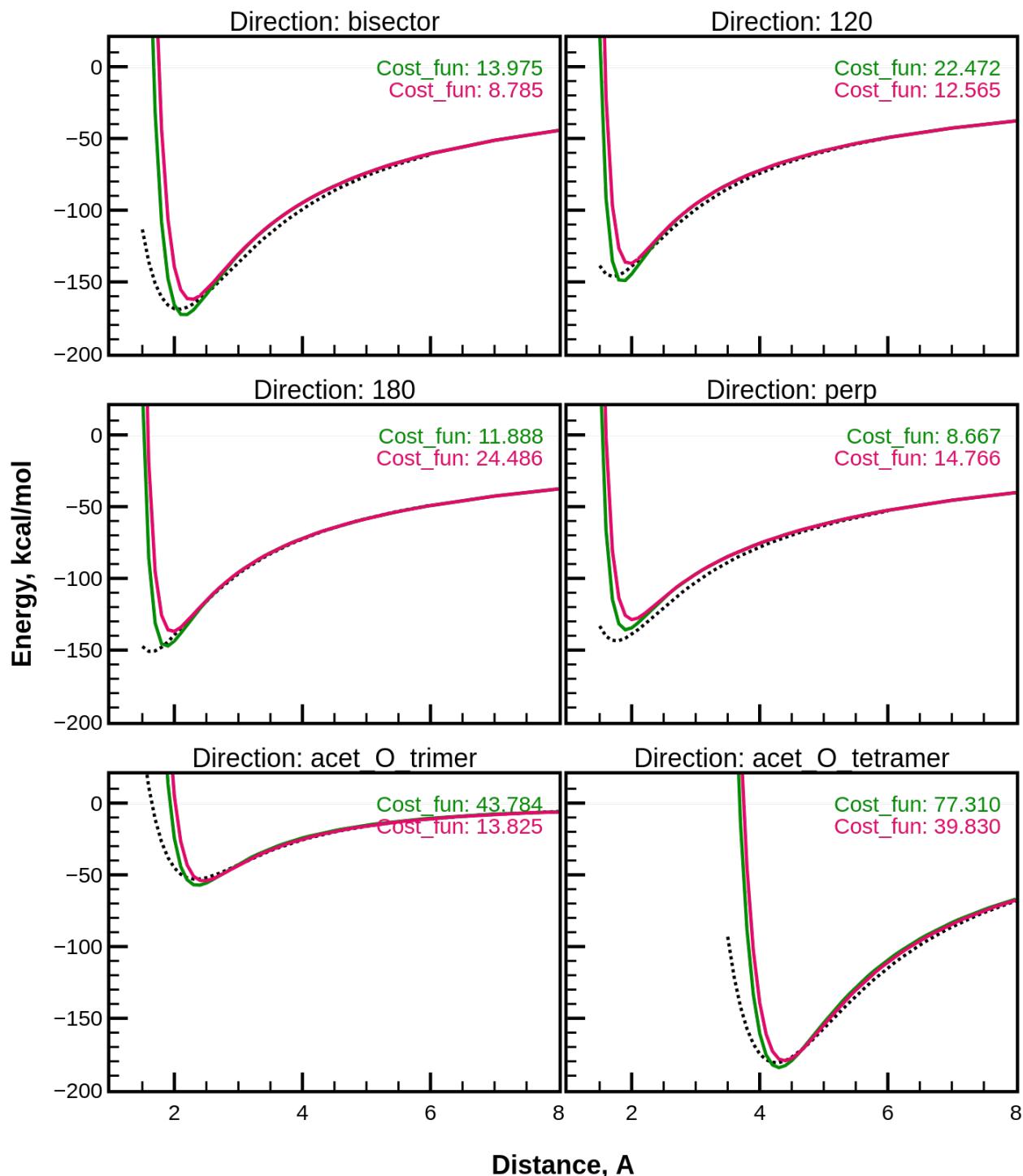
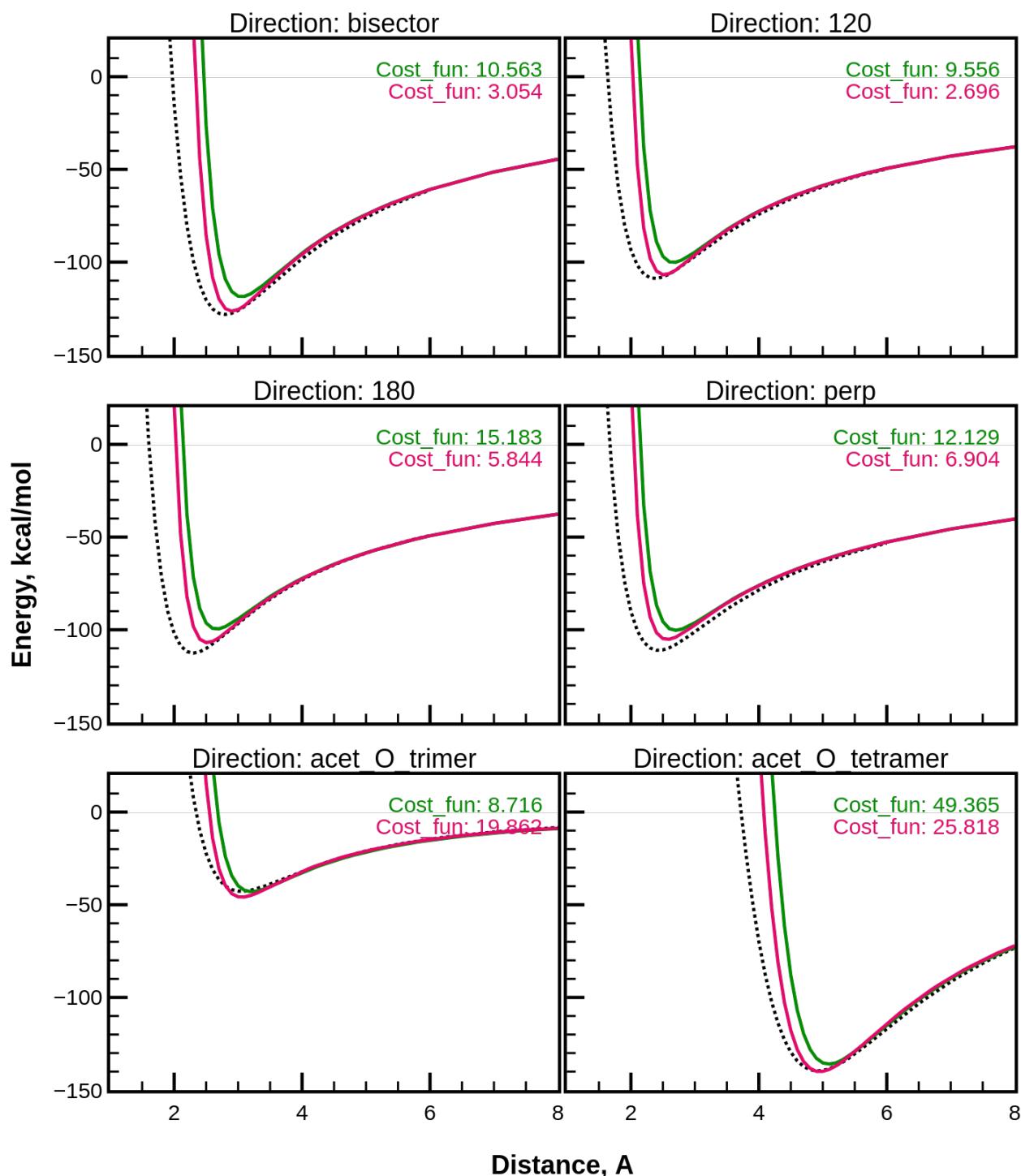


ACET LIT 1/12.92000_0.09487_9.99999
3.00493_0.09487_1.26652

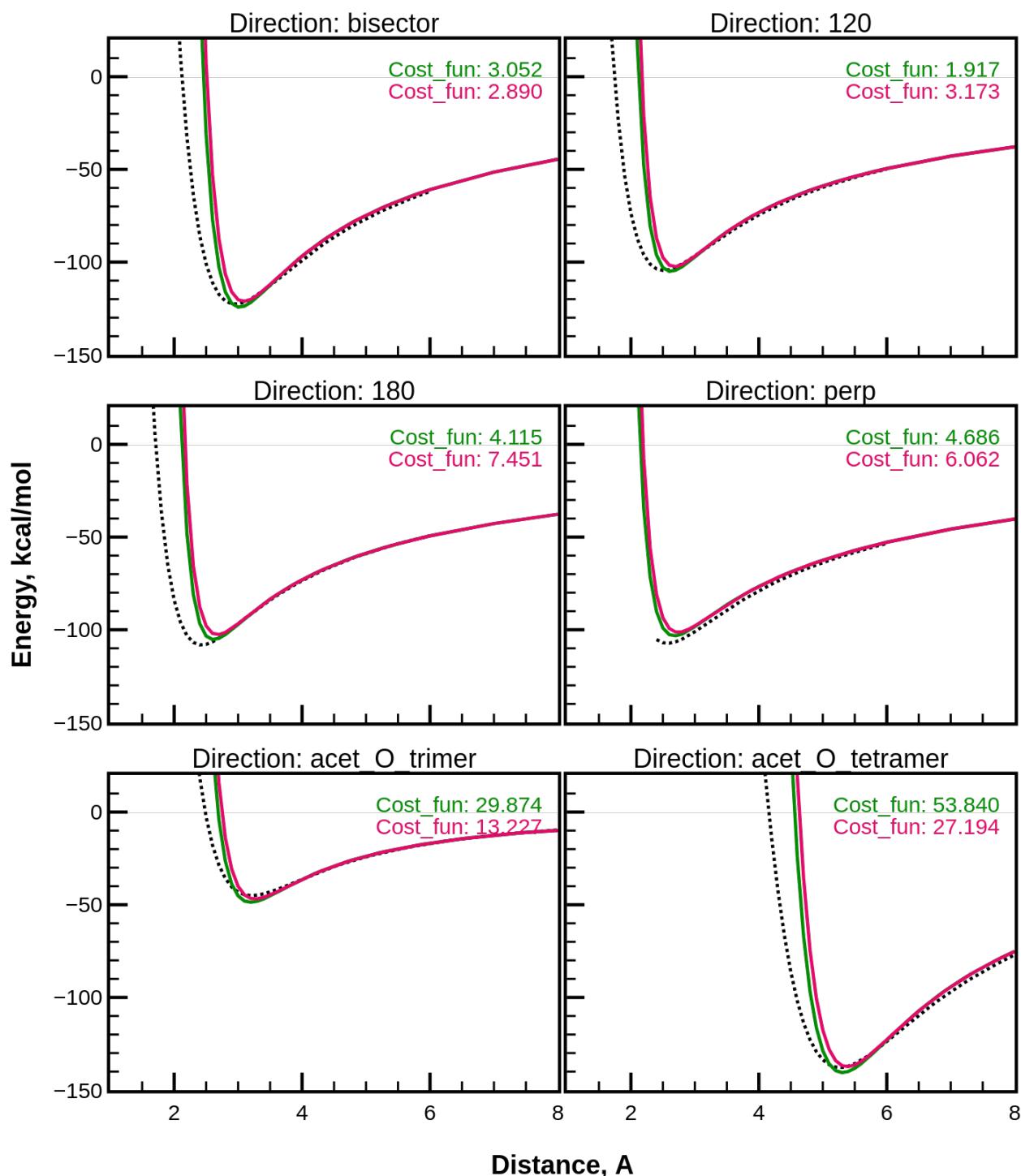
ACET POT 1/1

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



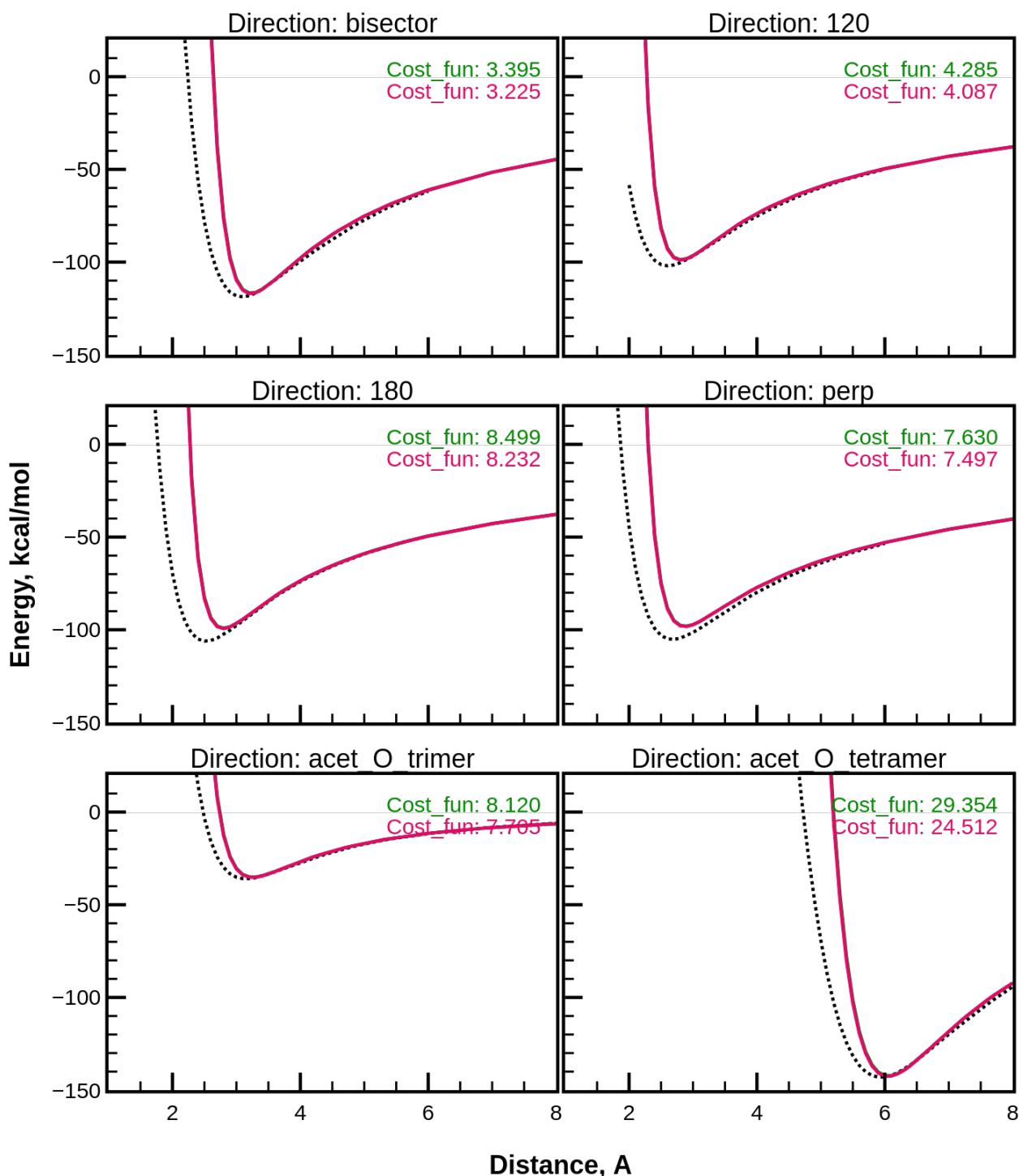
ACET RUB 1/1

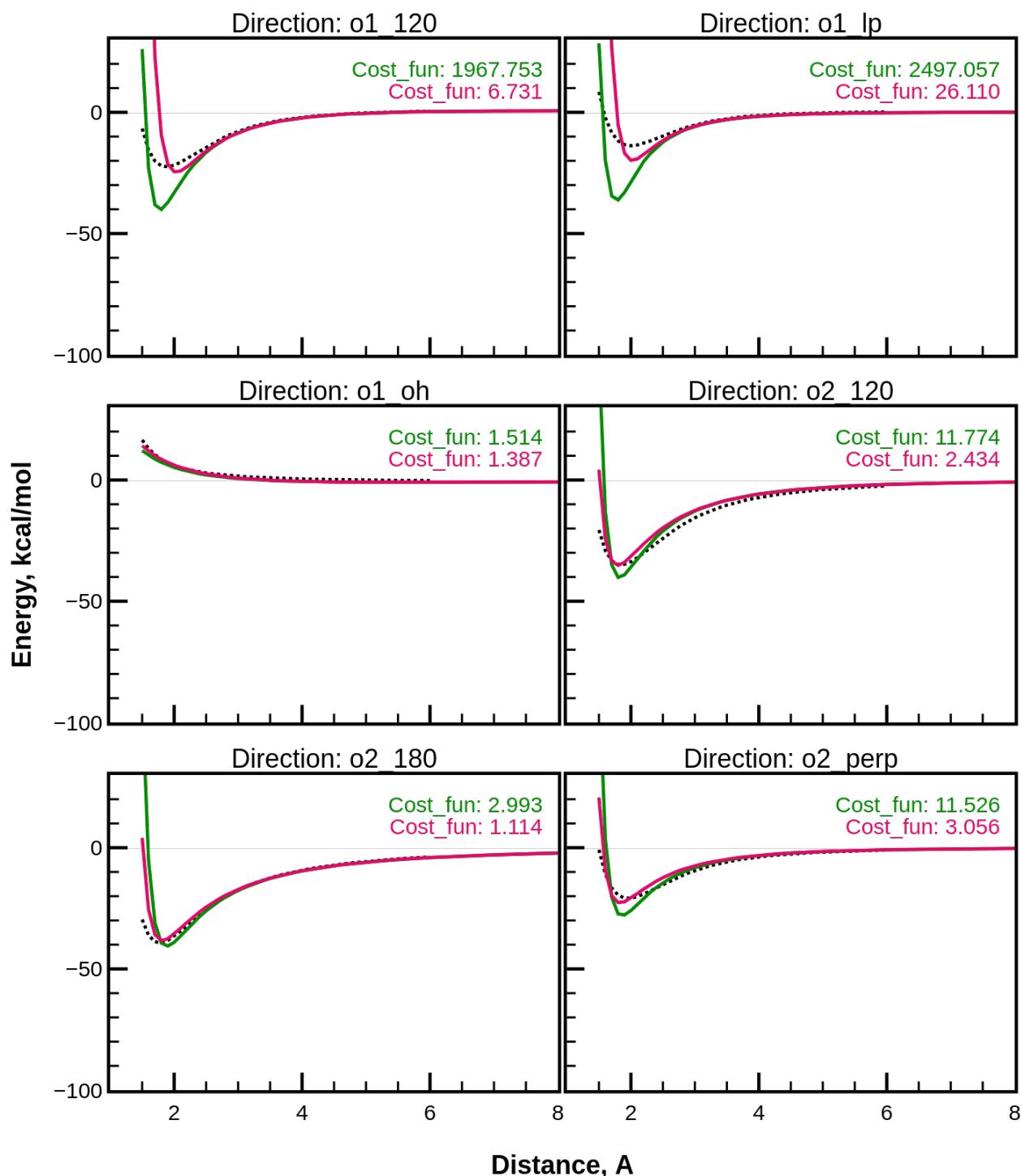
3.60551_0.28622_9.99999
3.67610_0.28622_4.45401



ACET CES 1/1

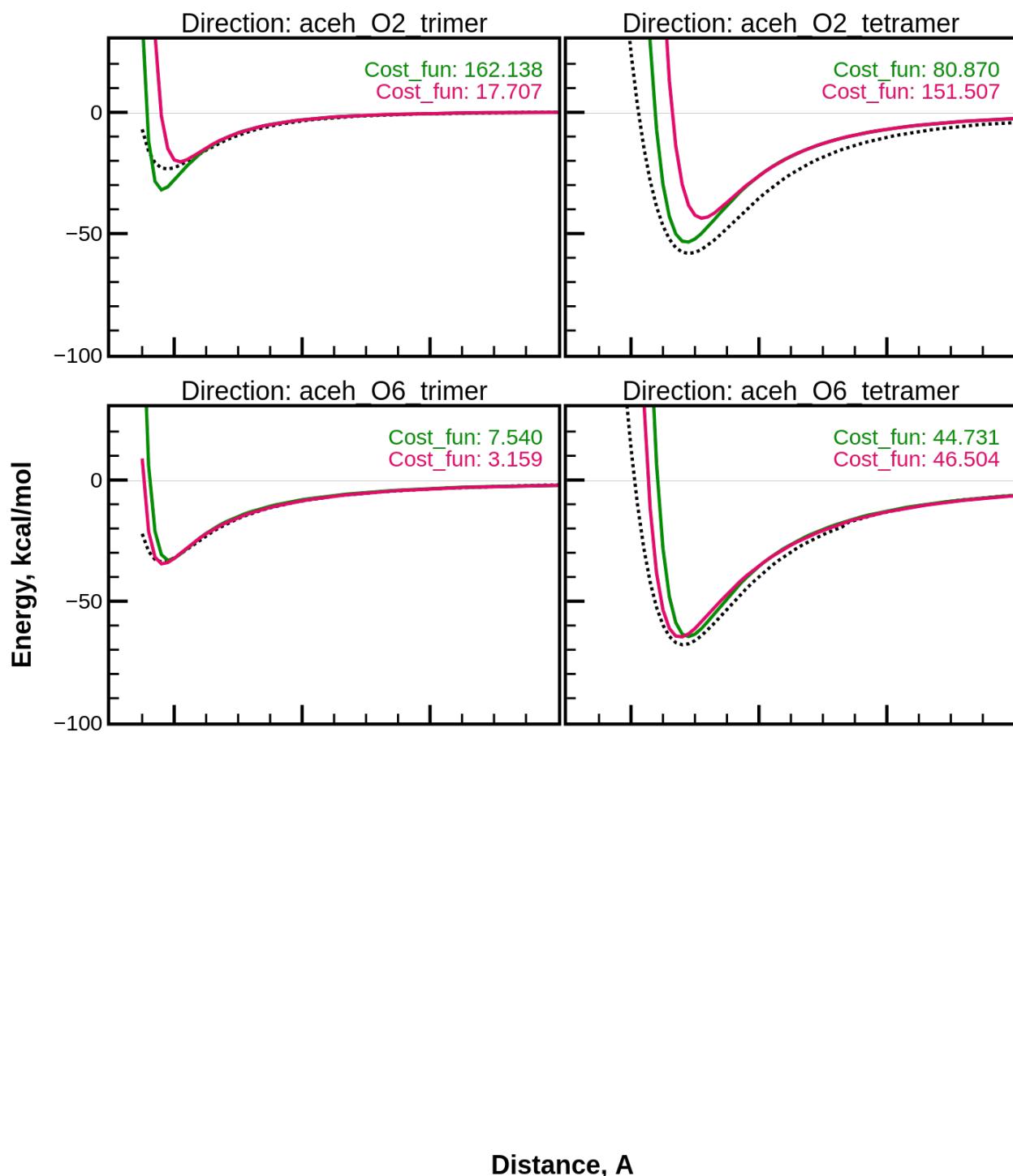
3.84382_0.28806_9.99999
3.83656_0.28806_4.06696



ACEH LIT 1/22.85000_0.07348_9.99999
2.65664_0.07348_0.64546

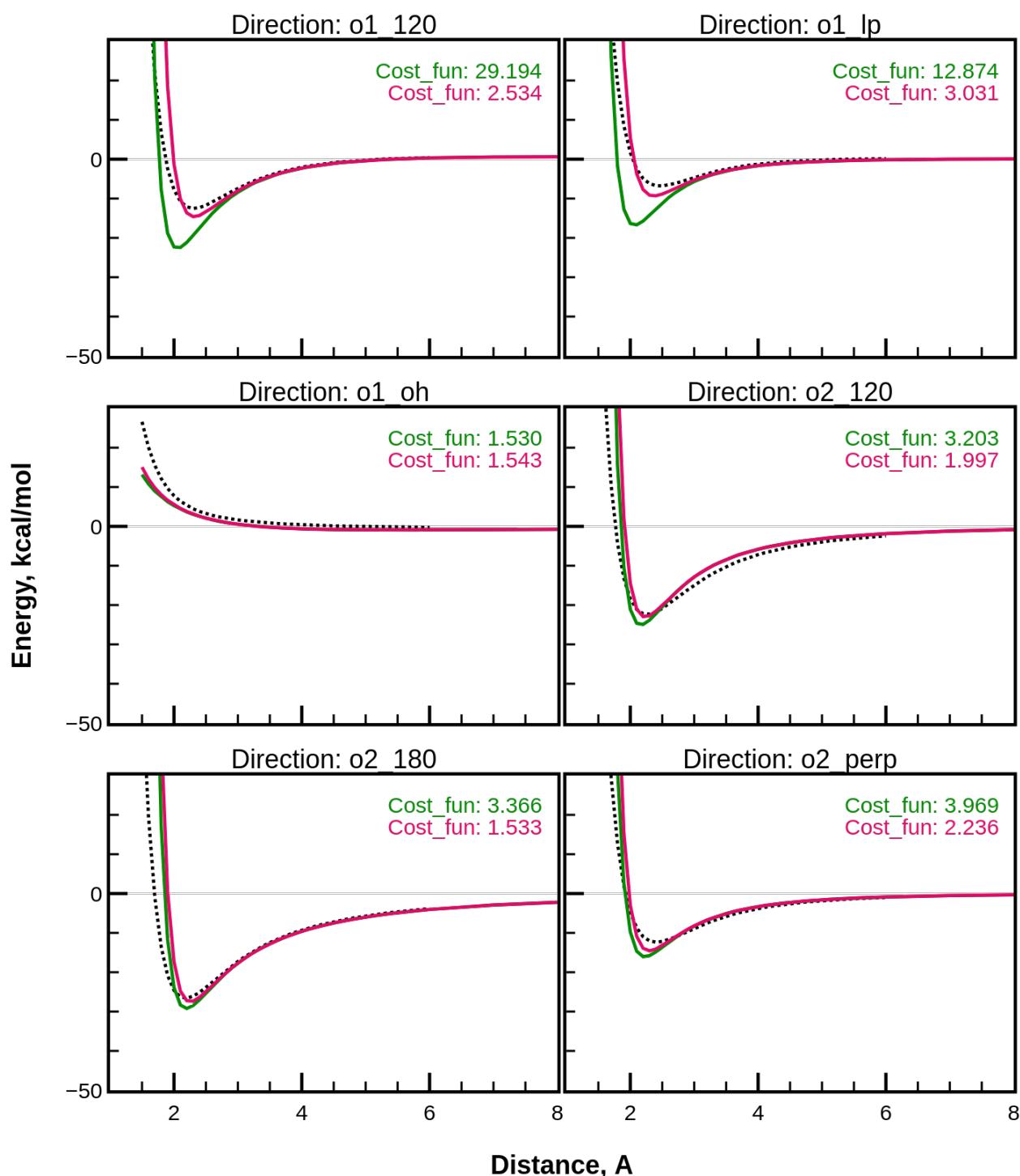
ACEH LIT 2/2

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



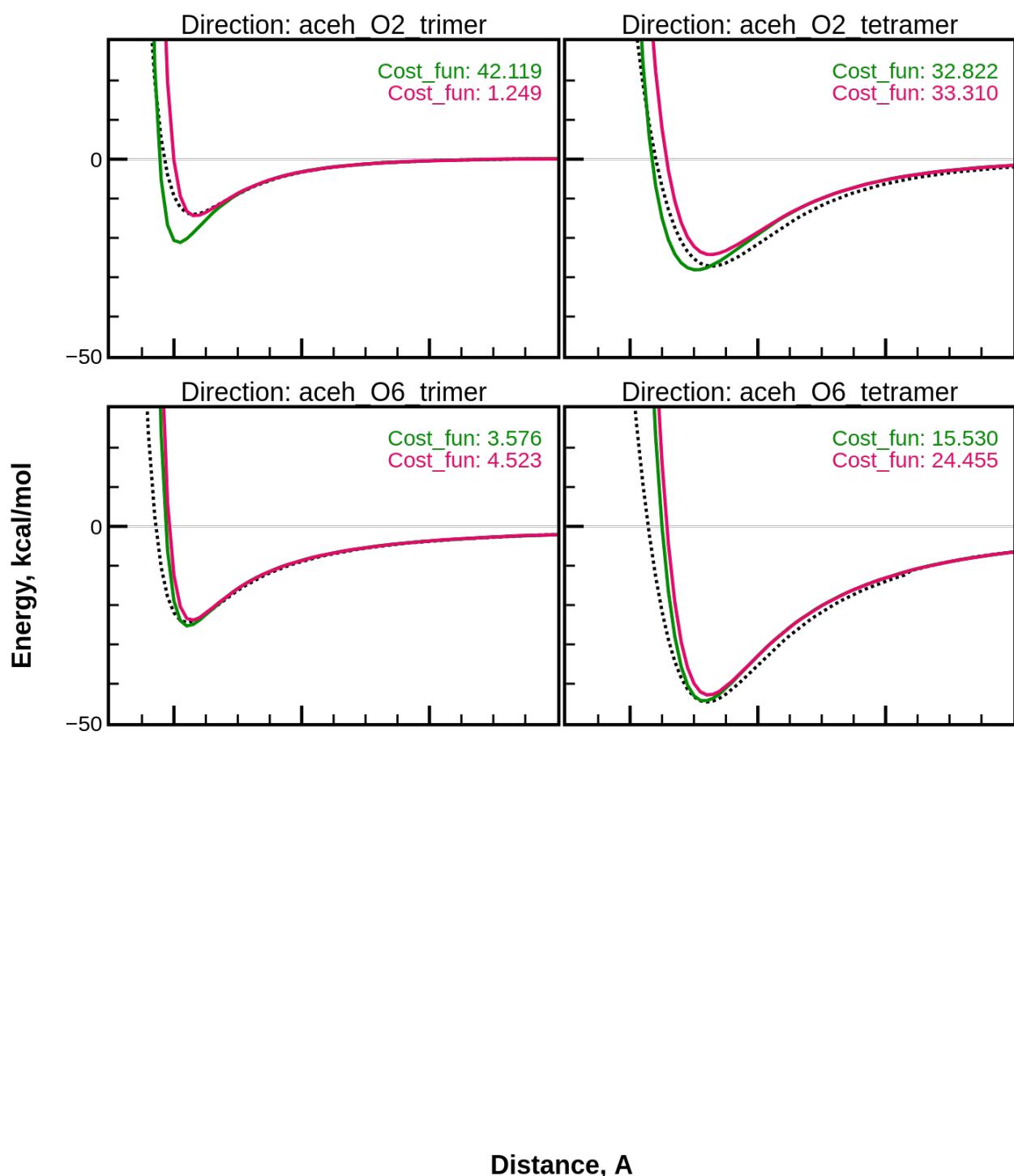
ACEH SOD 1/2

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



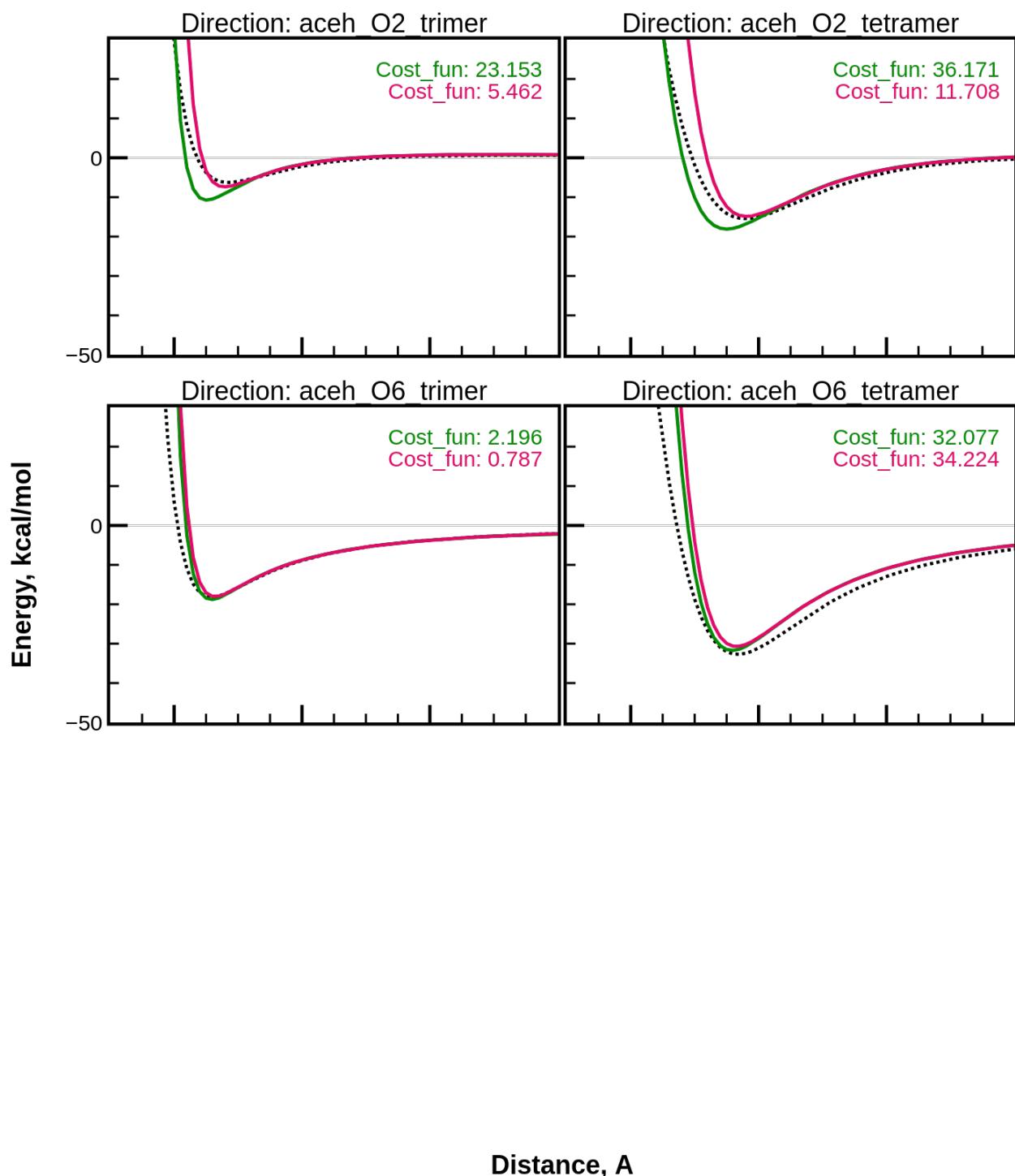
ACEH SOD 2/2

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



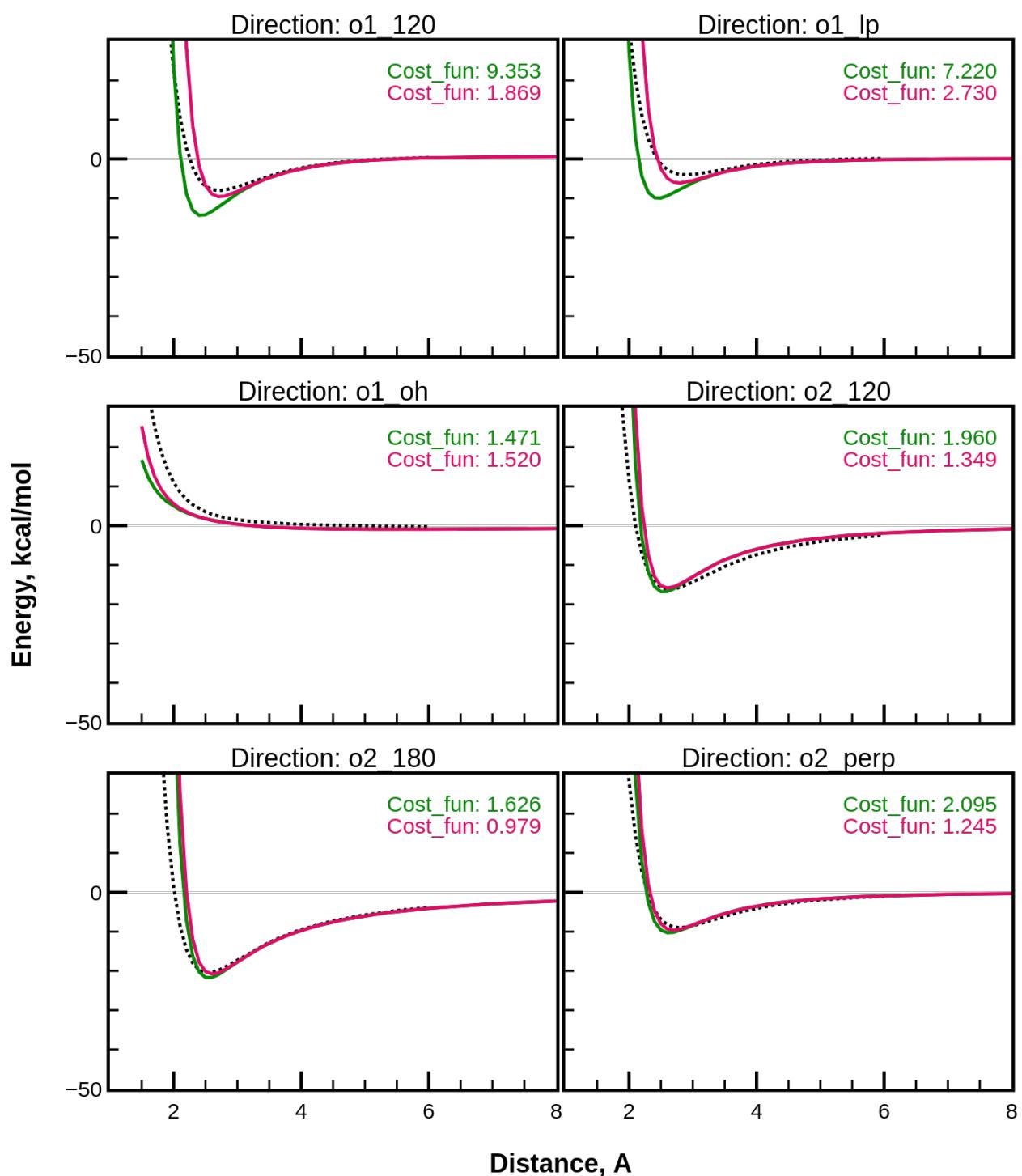
ACEH POT 2/2

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



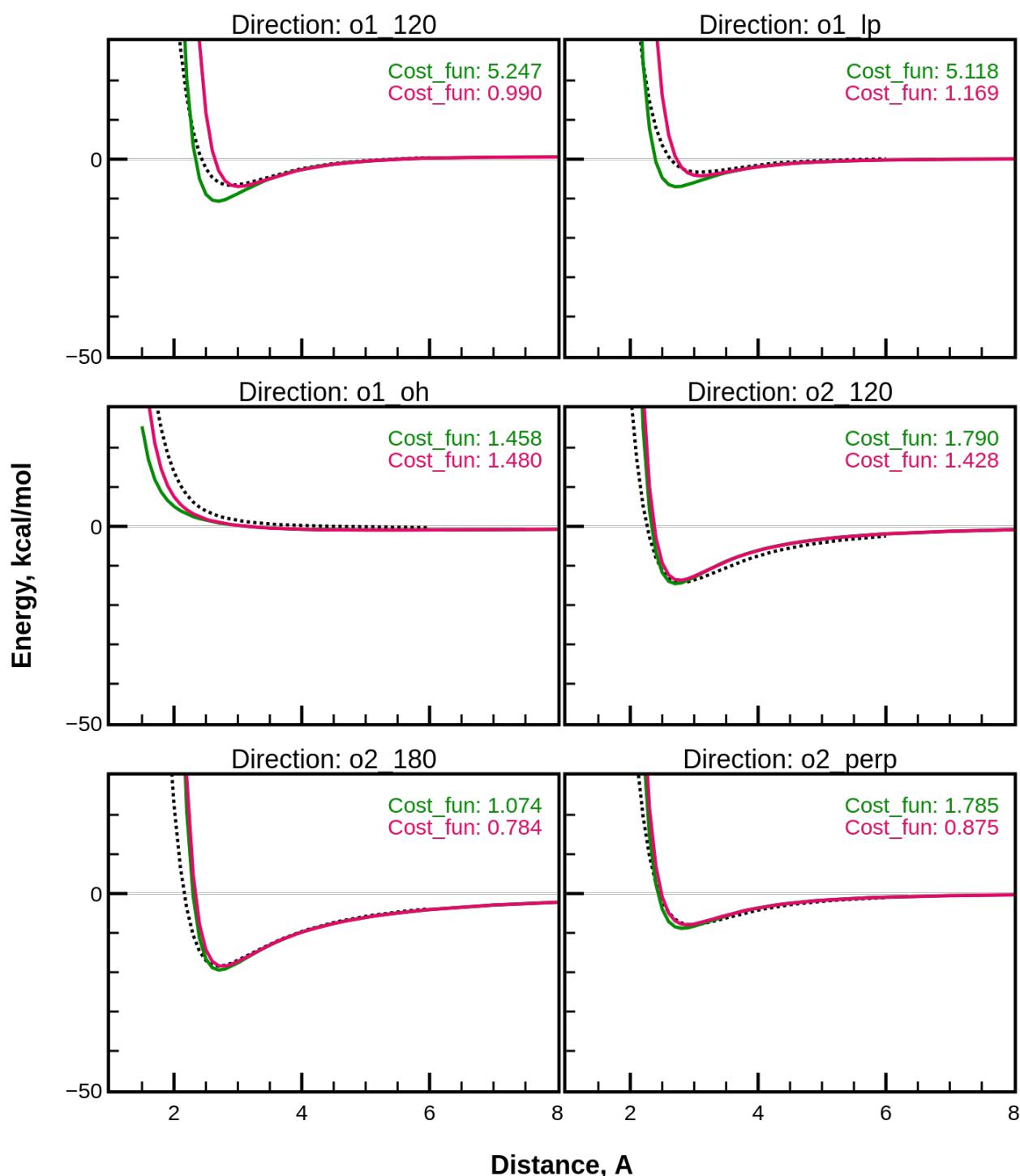
ACEH POT 1/2

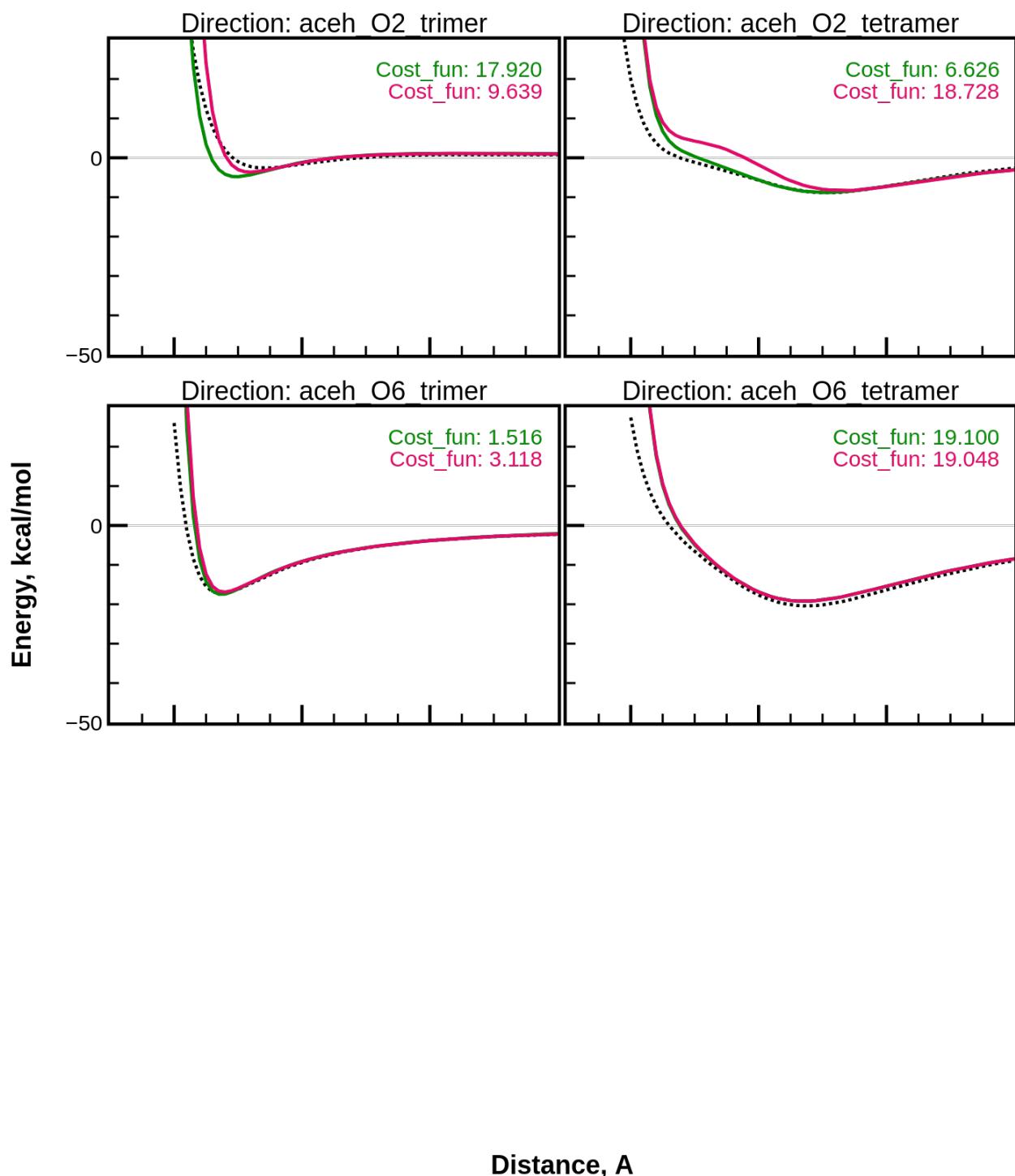
3.43665_0.15983_9.99999
3.49368_0.15983_2.83217



ACEH RUB 1/2

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

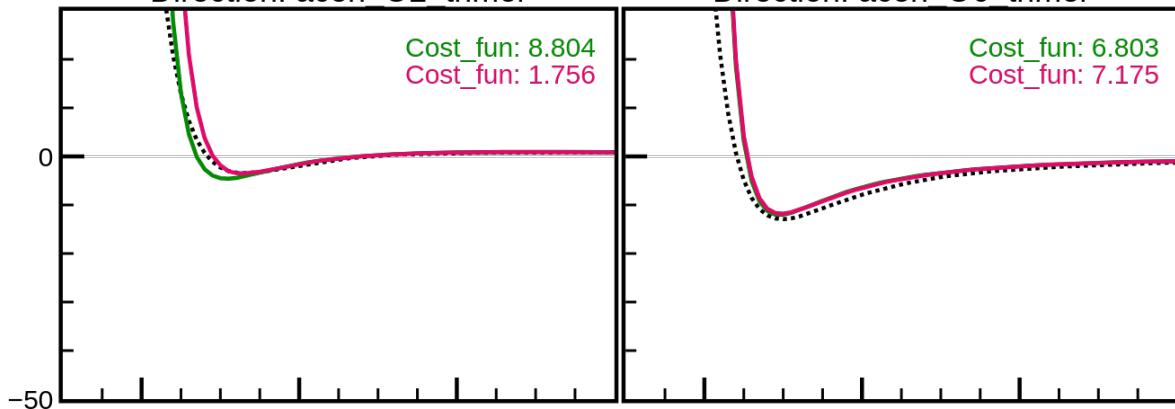


ACEH RUB 2/23.53551_0.22170_9.99999
3.55885_0.22170_1.61222

ACEH CES 2/23.77382_0.22313_9.99999
3.76247_0.22313_1.03679

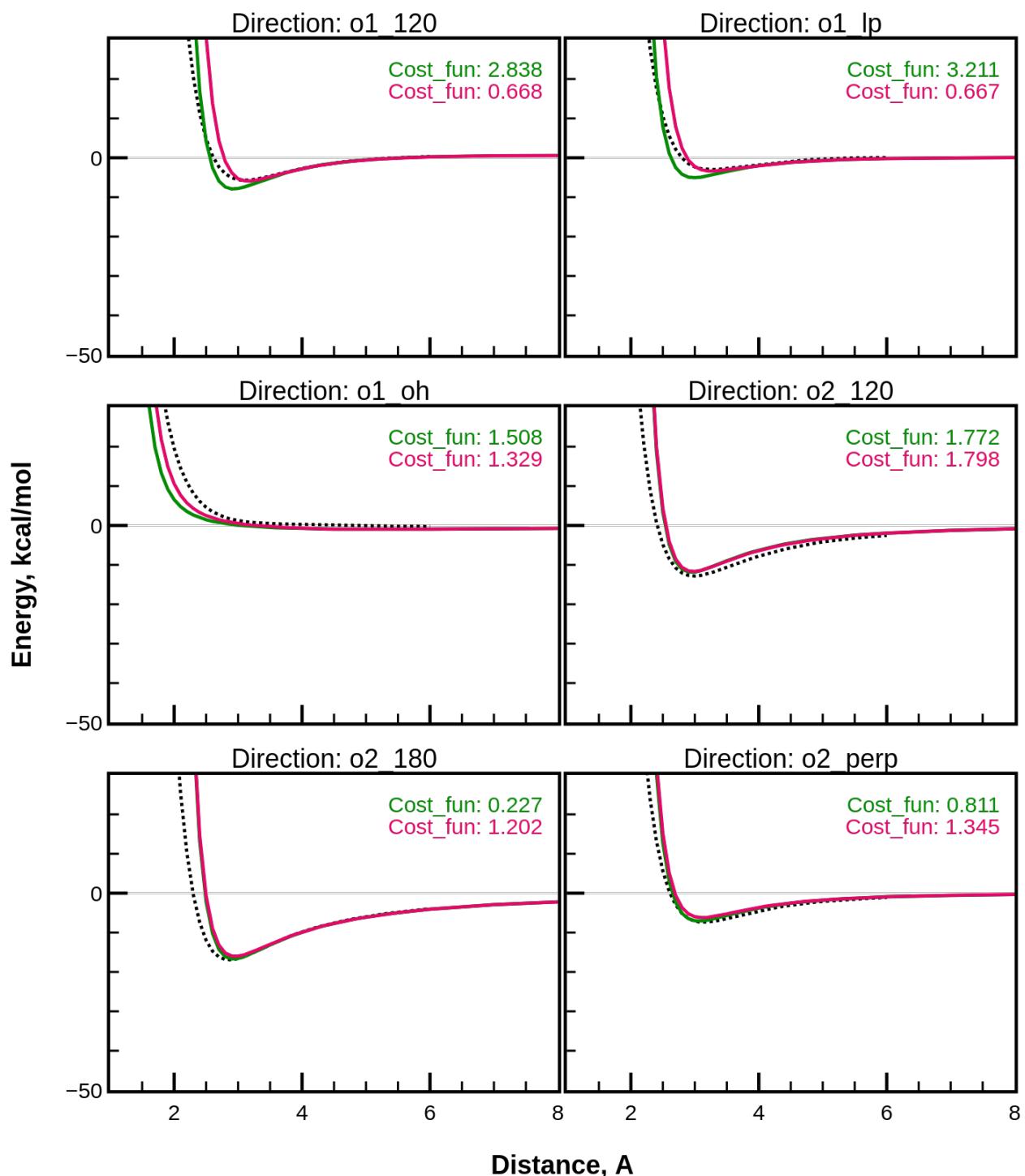
Direction: aceh_O2_trimer

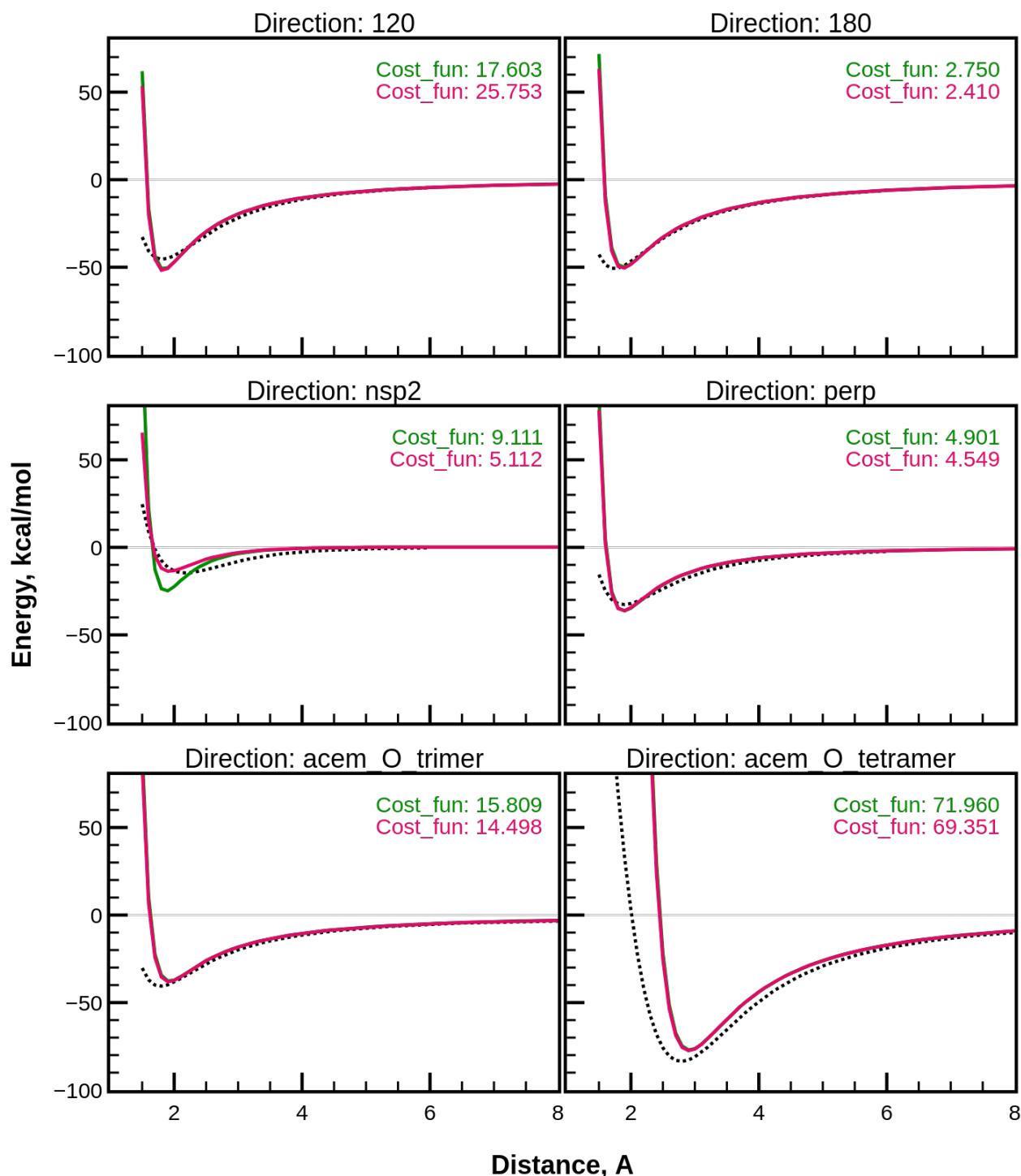
Direction: aceh_O6_trimer

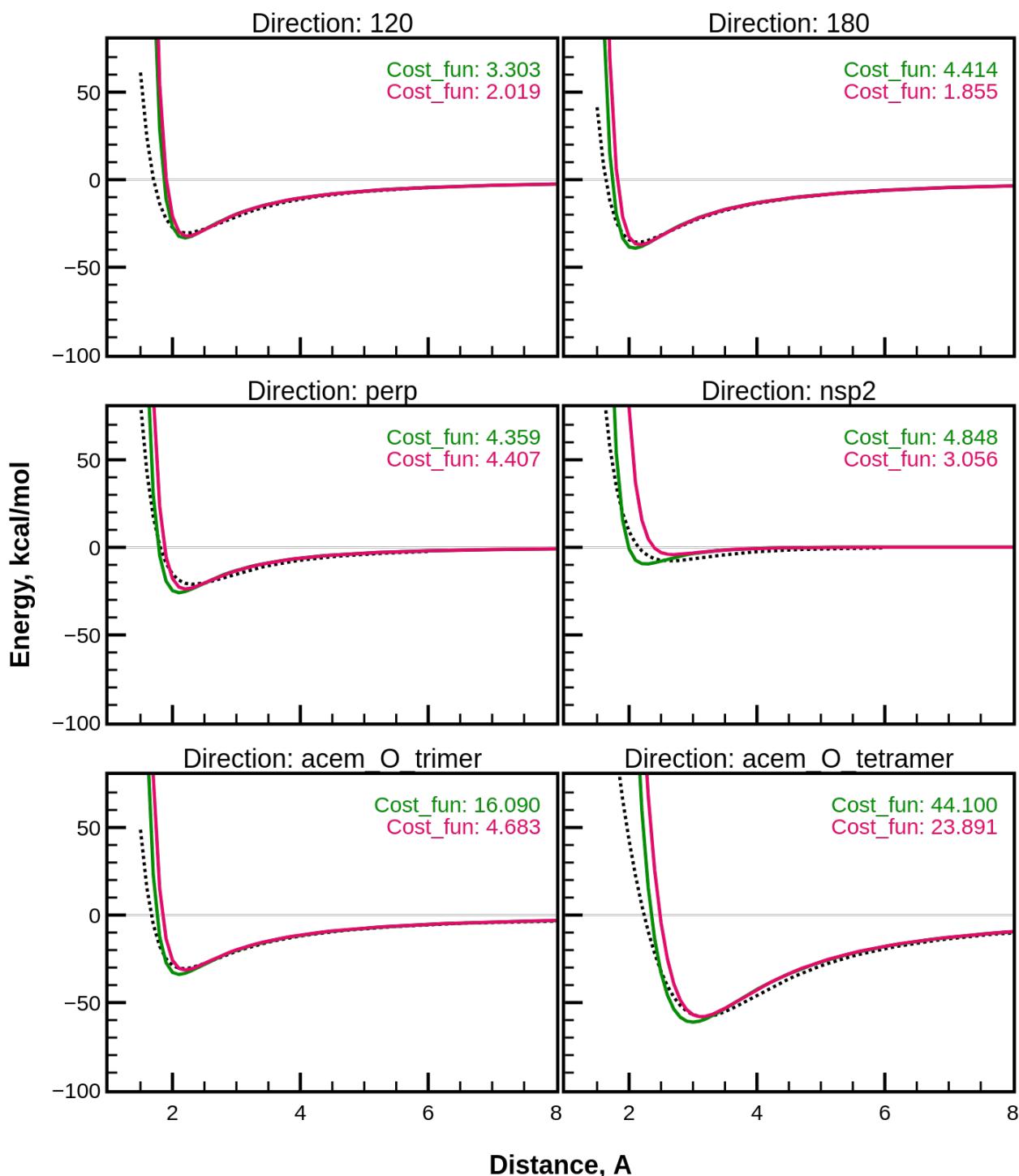
**Distance, A**

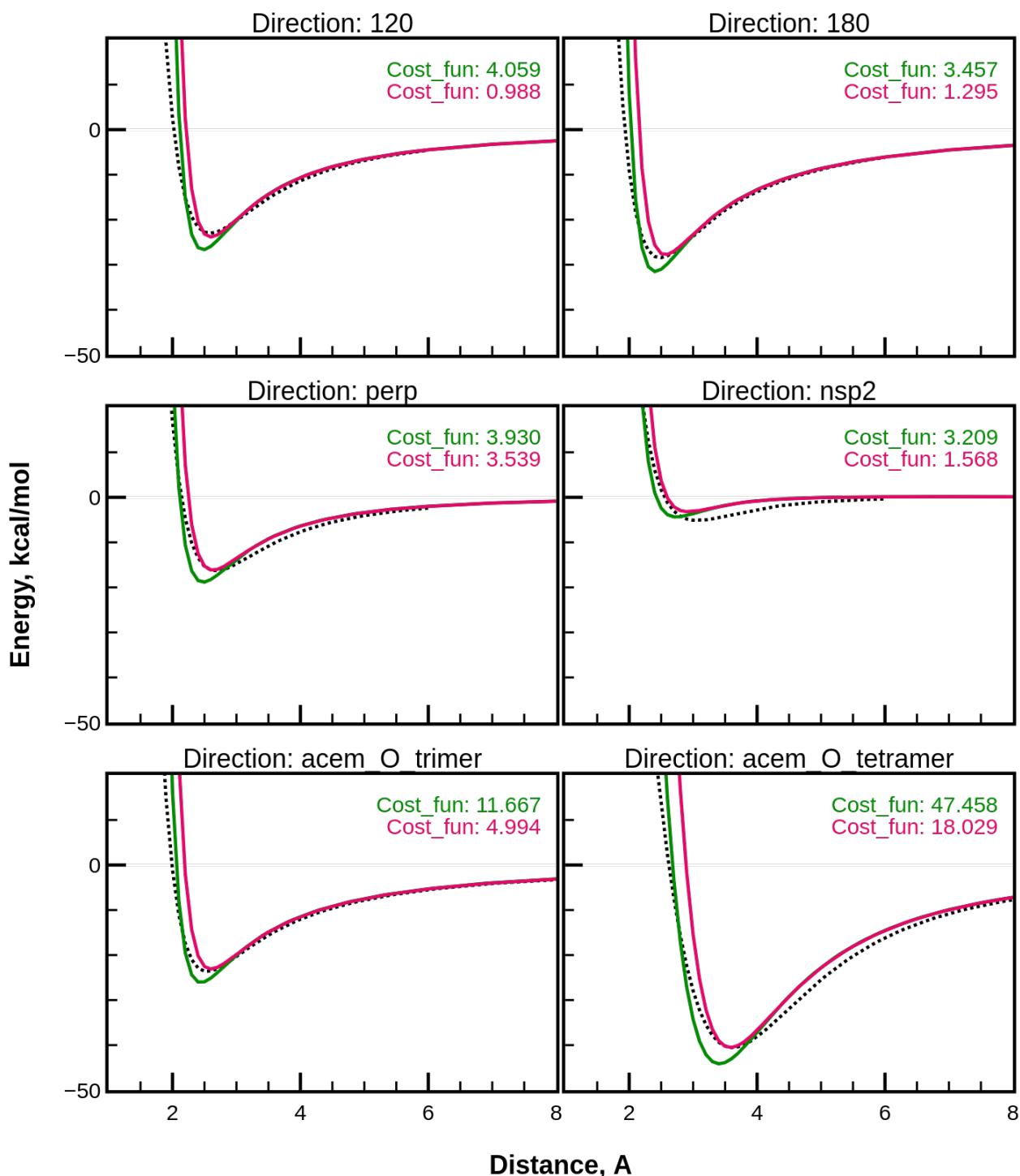
ACEH CES 1/2

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



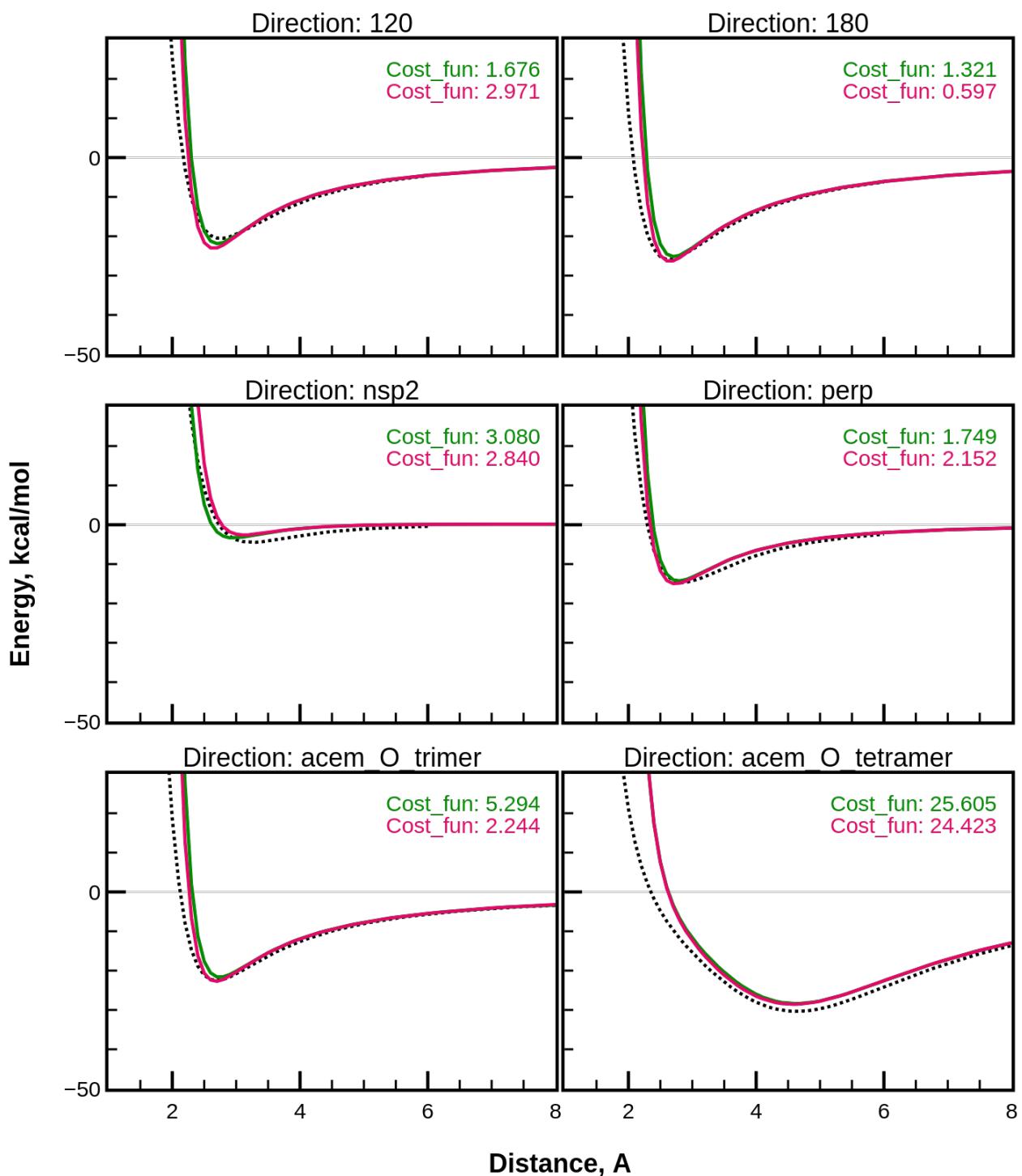
ACEM LIT 1/12.88000_0.07746_9.99999
2.86833_0.07746_4.93098

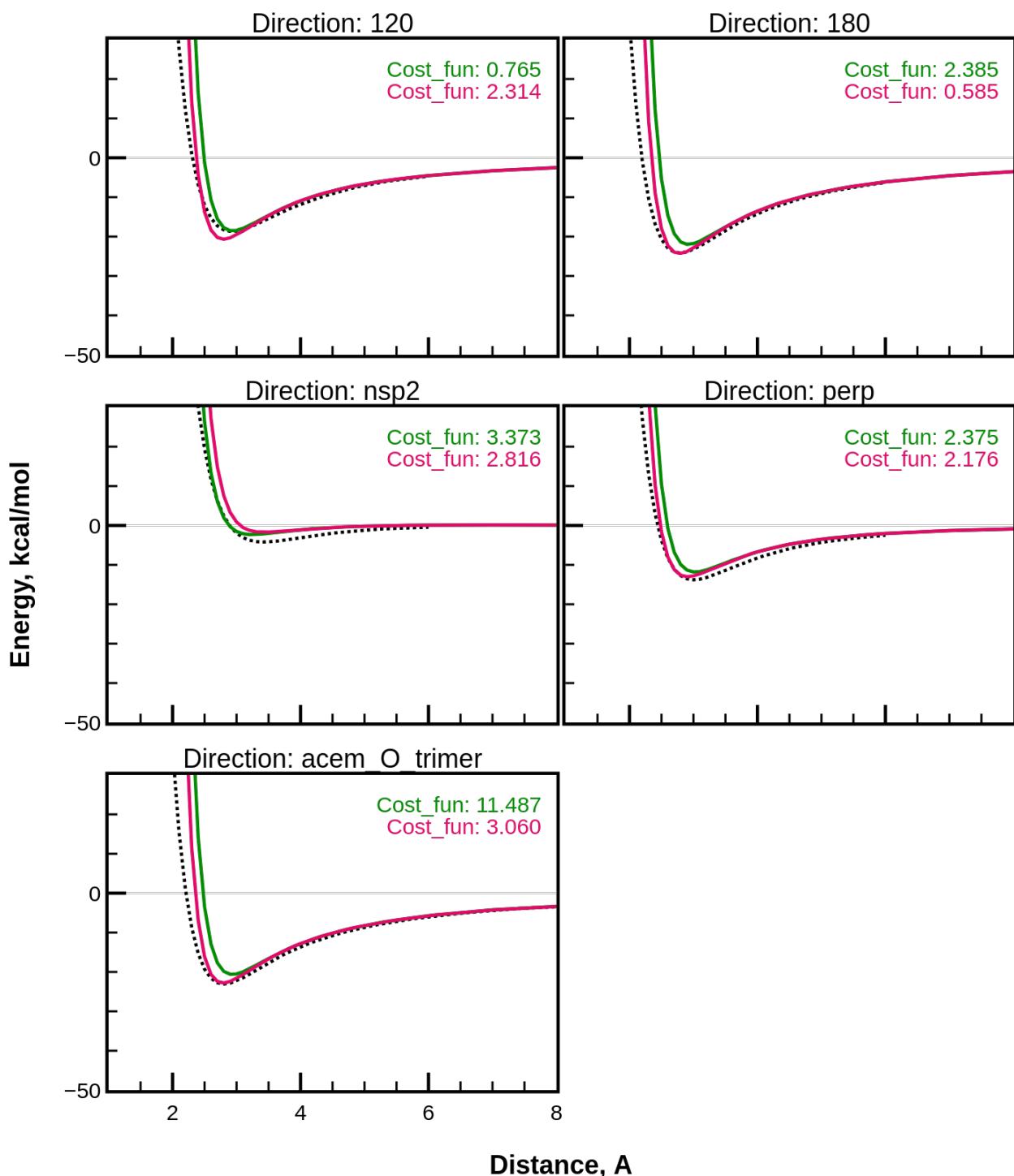
ACEM SOD 1/12.88000_0.09000_1.04000
3.11051_0.07939_1.54864

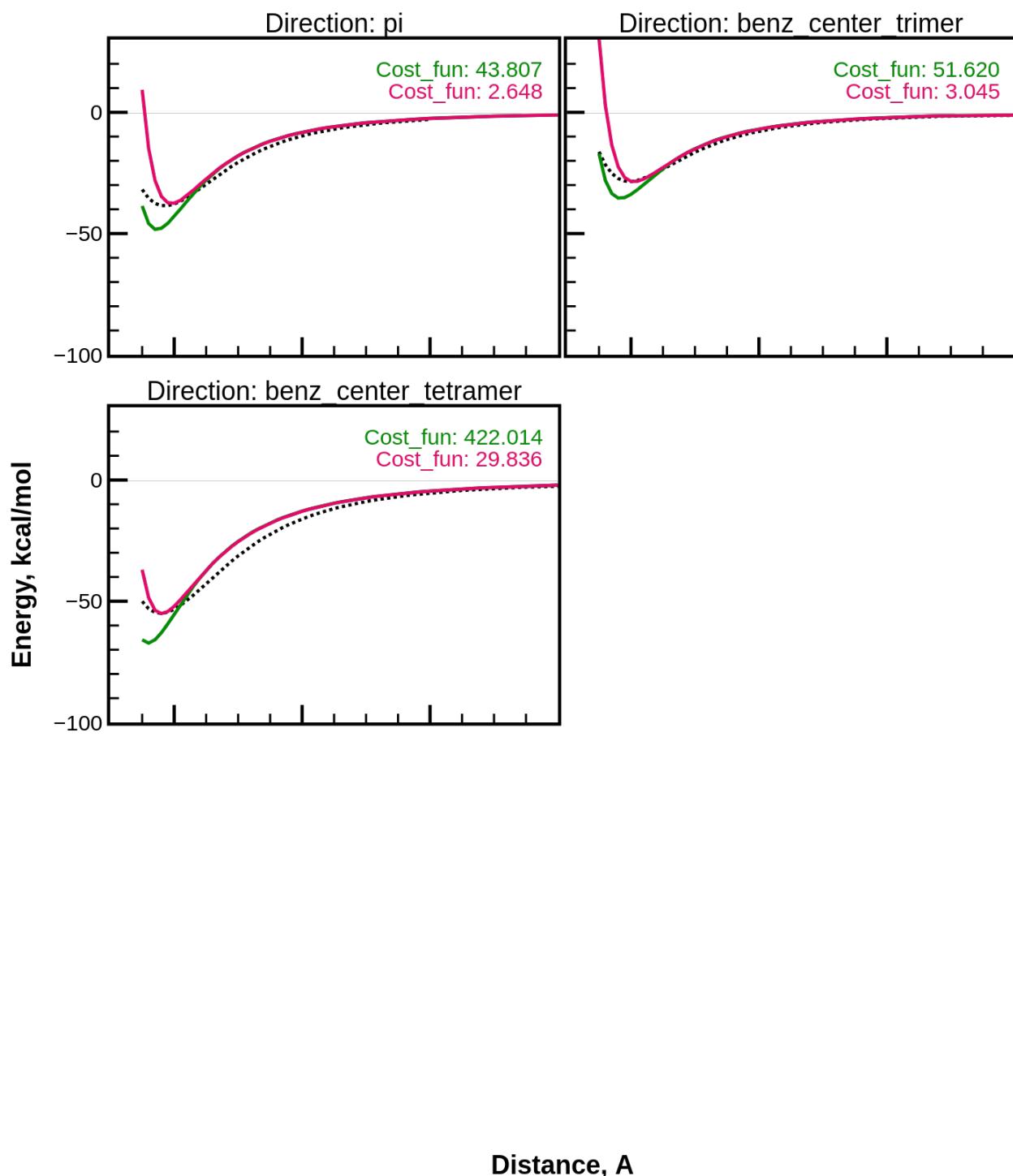
ACEM POT 1/13.21000_0.18000_2.19000
3.43708_0.16848_2.09141

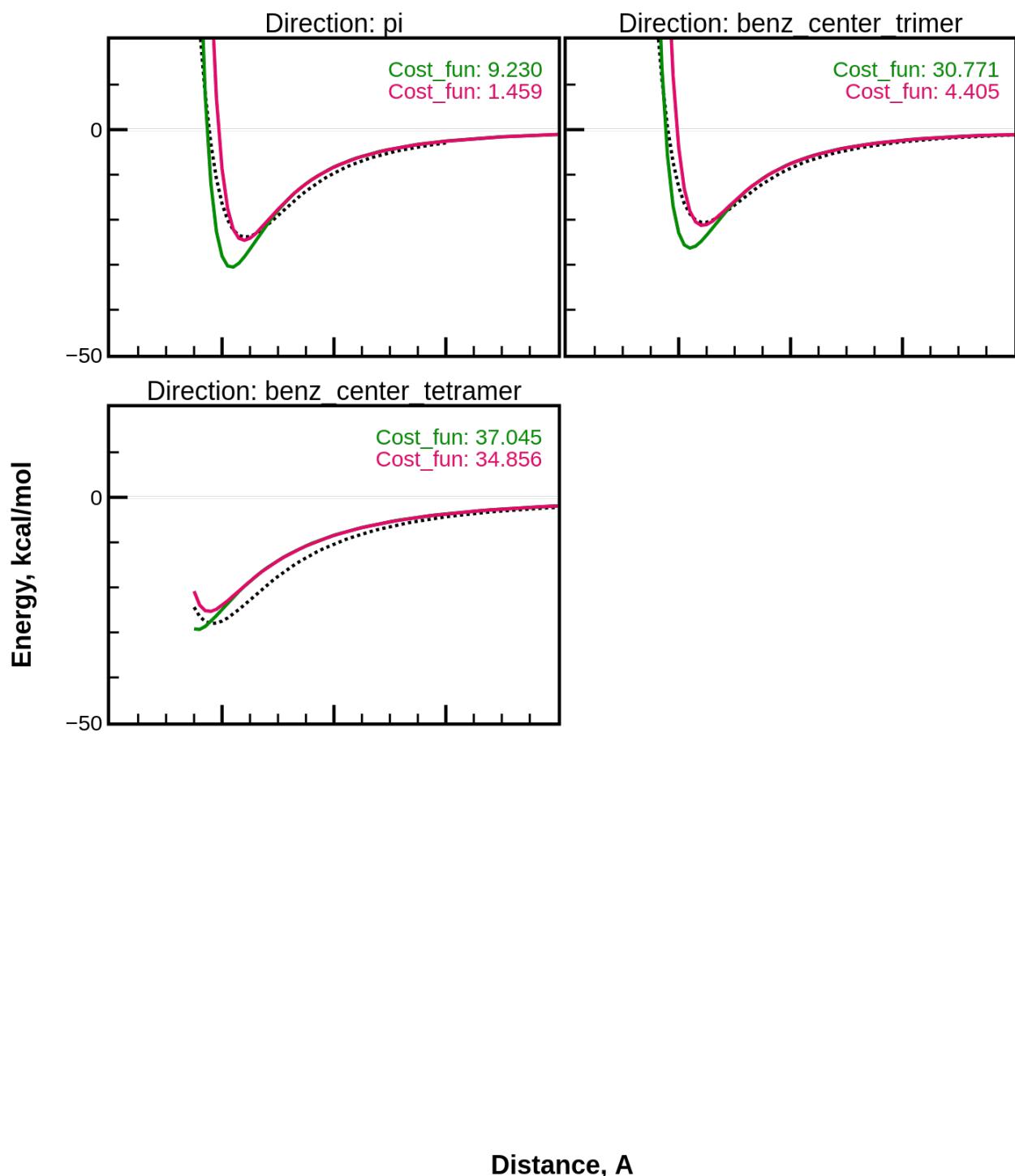
ACEM RUB 1/1

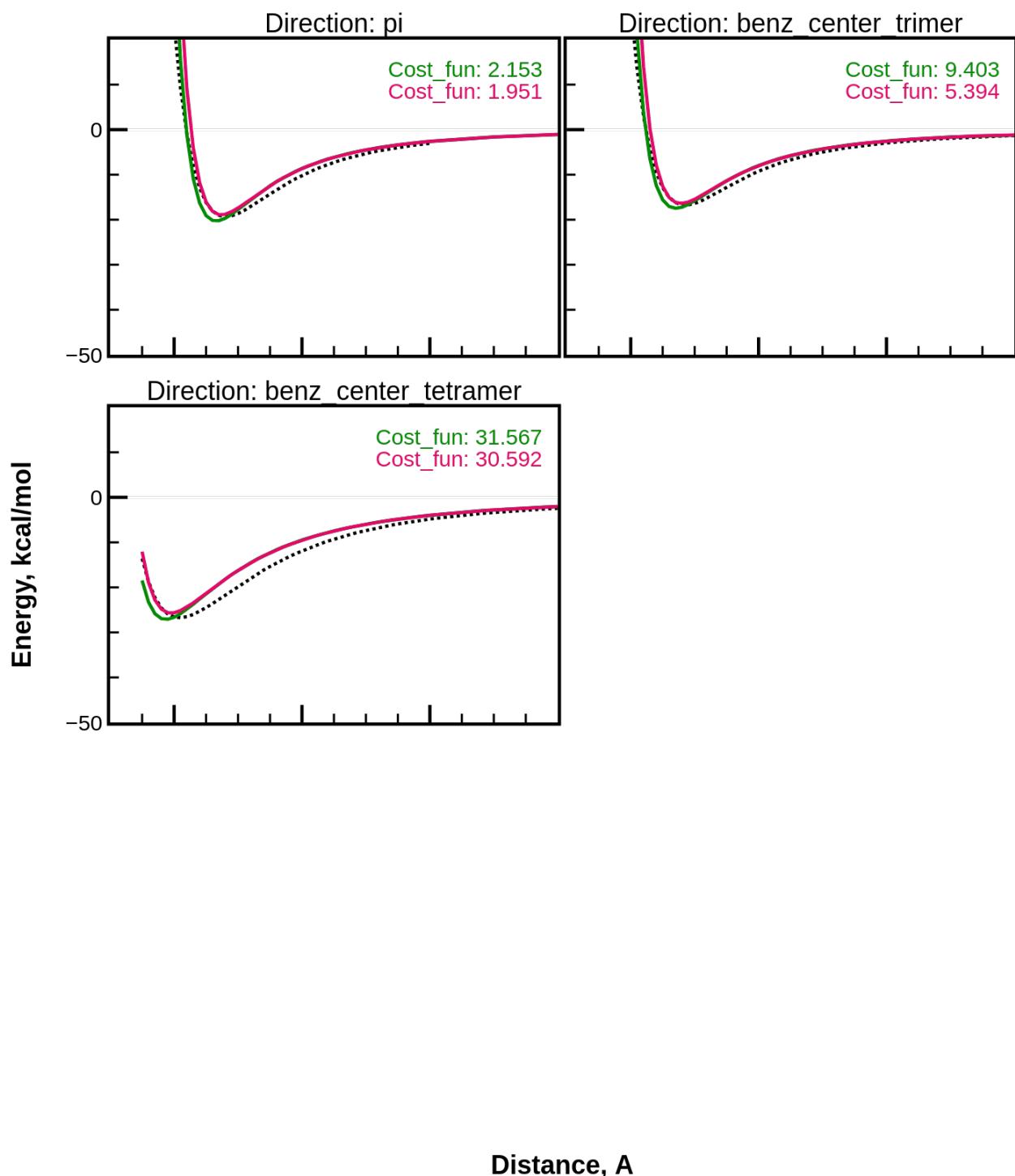
3.56551_0.23370_9.99999
3.49474_0.23370_2.99829



ACEM CES 1/13.80382_0.23520_9.99999
3.64357_0.23520_2.58963

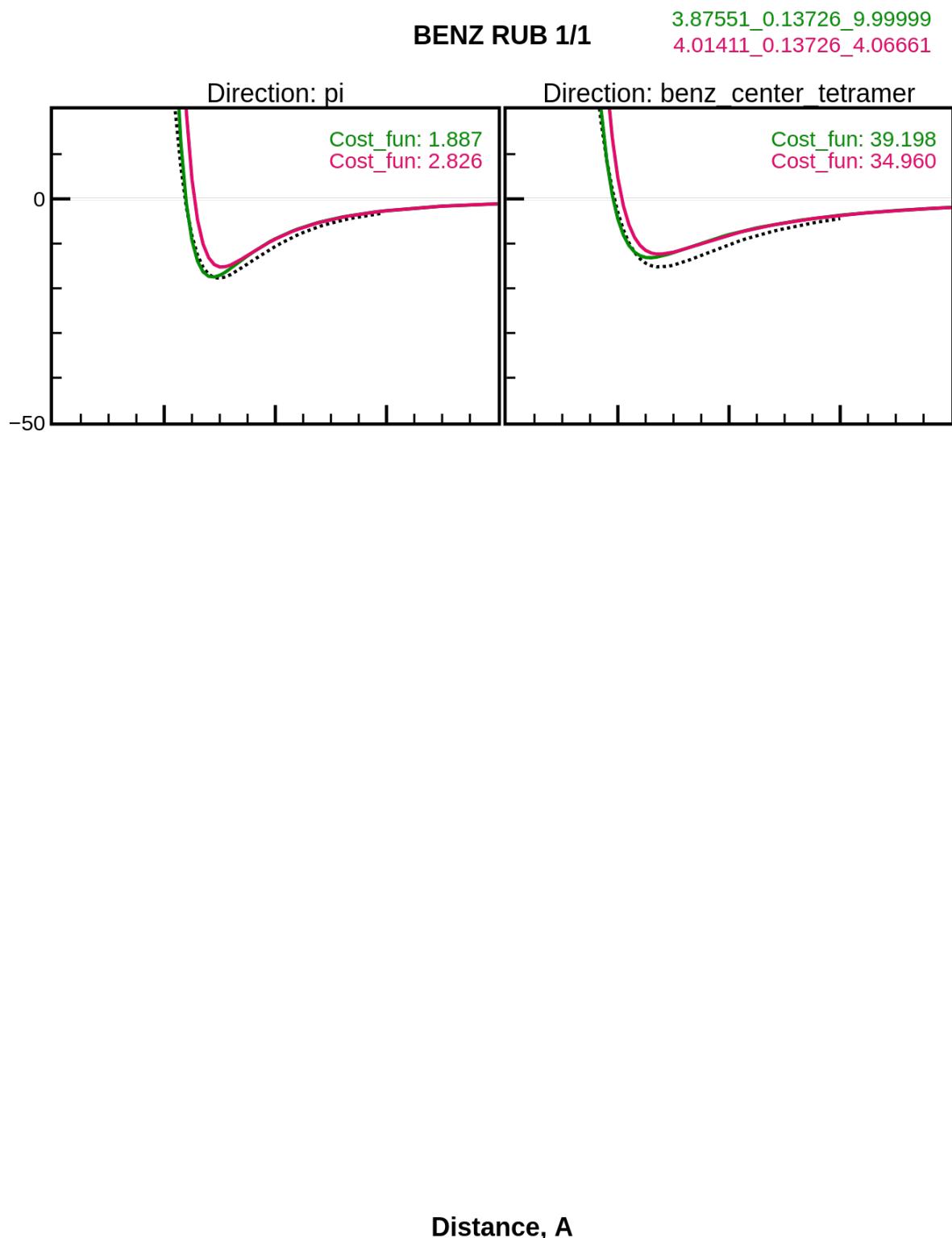
BENZ LIT 1/13.19000_0.04550_9.99999
3.36536_0.04550_2.13767

BENZ SOD 1/13.55168_0.04663_9.99999
3.74147_0.04663_4.93763

BENZ POT 1/13.77665_0.09896_9.99999
3.84110_0.09896_3.83779

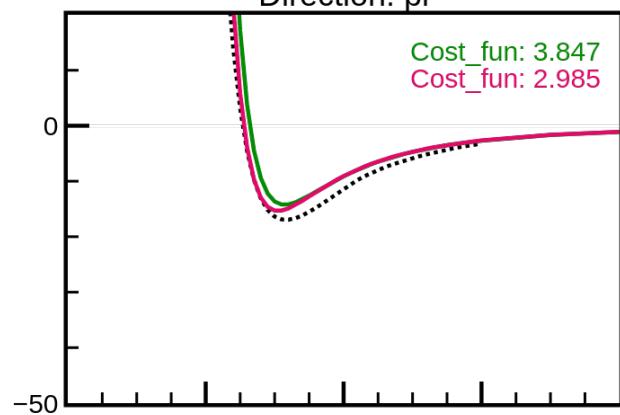
BENZ RUB 1/13.87551_0.13726_9.99999
4.01411_0.13726_4.06661

Energy, kcal/mol



BENZ CES 1/14.11382_0.13815_9.99999
4.03106_0.13815_3.72515

Direction: pi

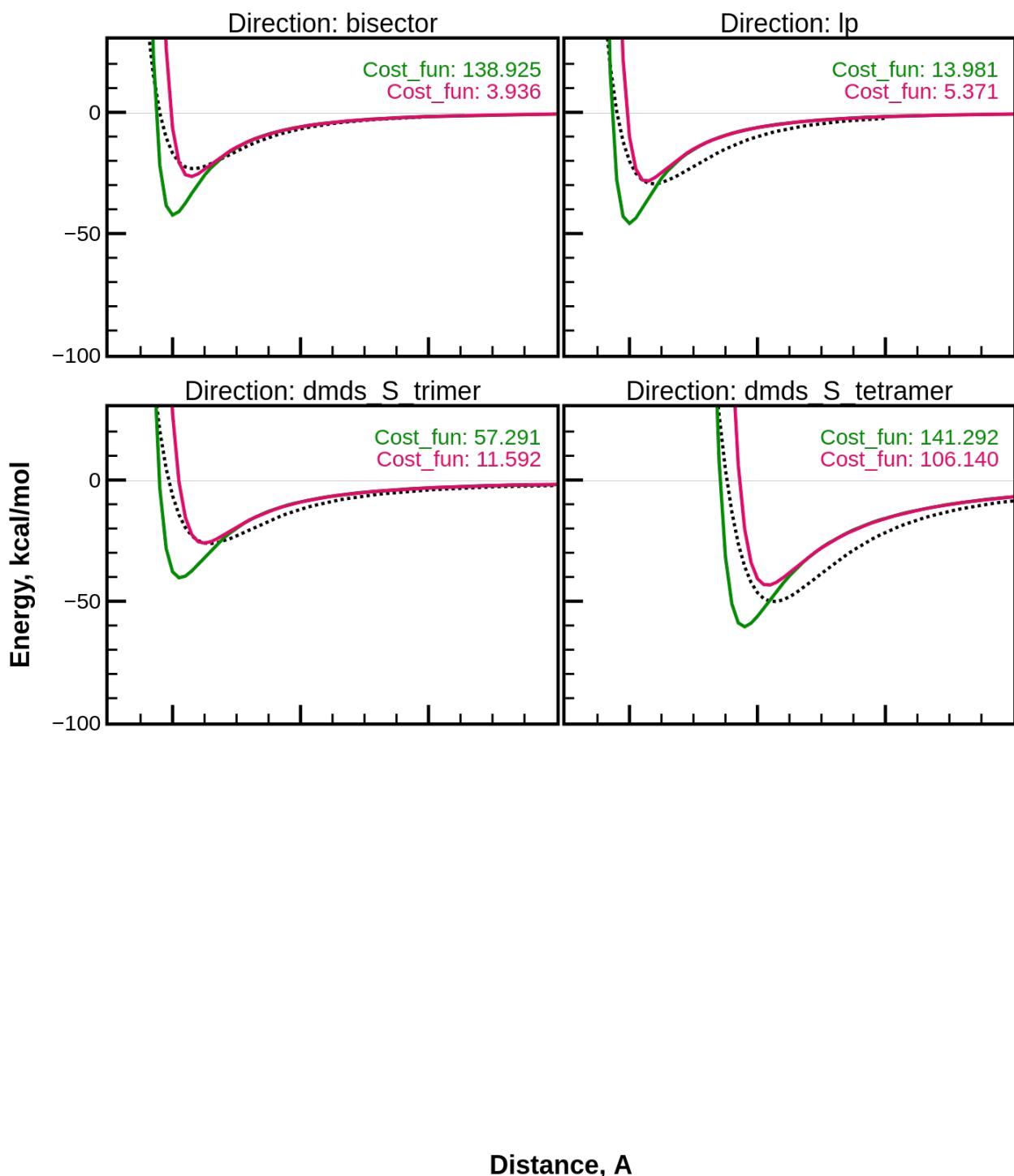


Energy, kcal/mol

Distance, Å

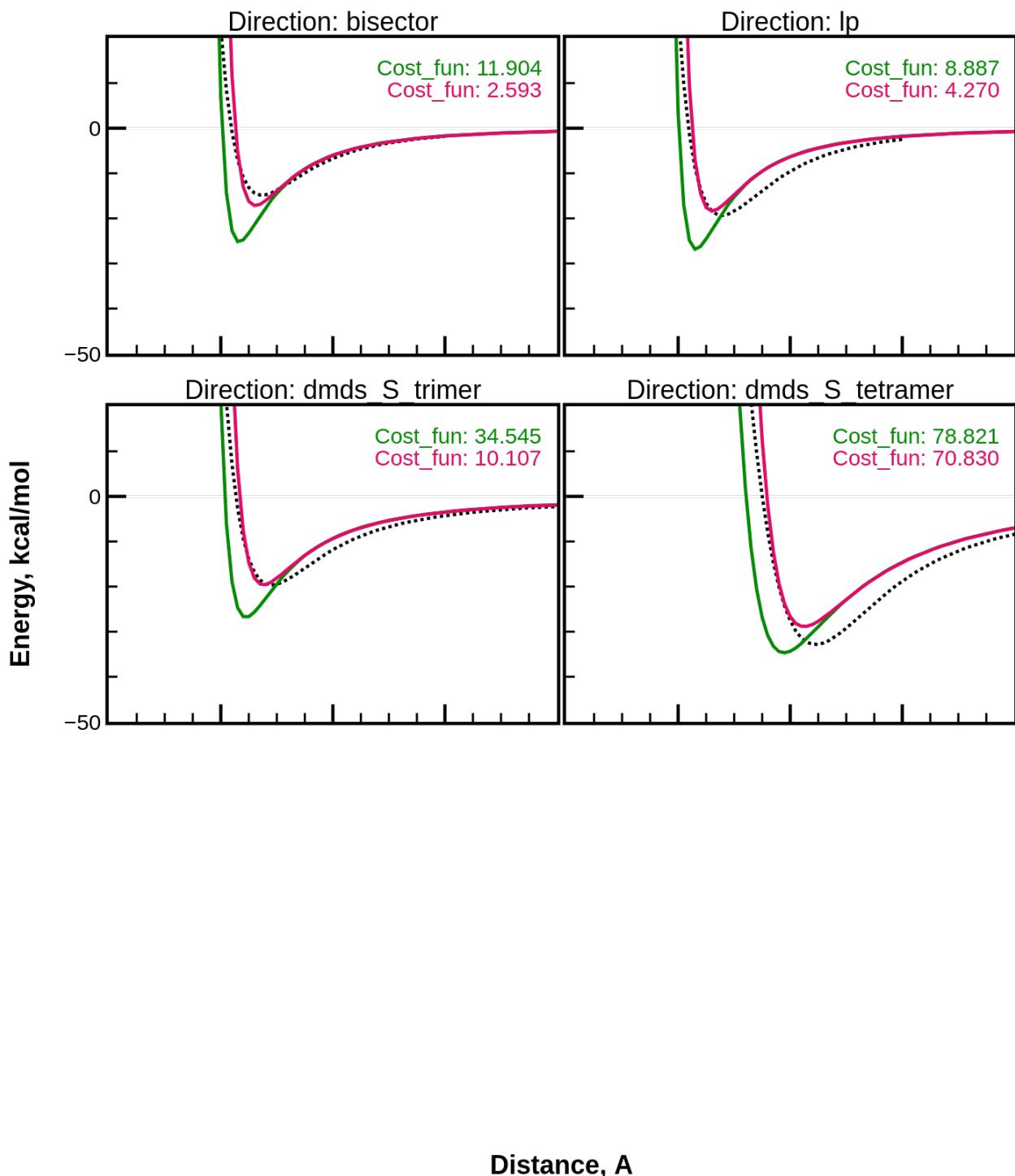
DMDS LIT 1/1

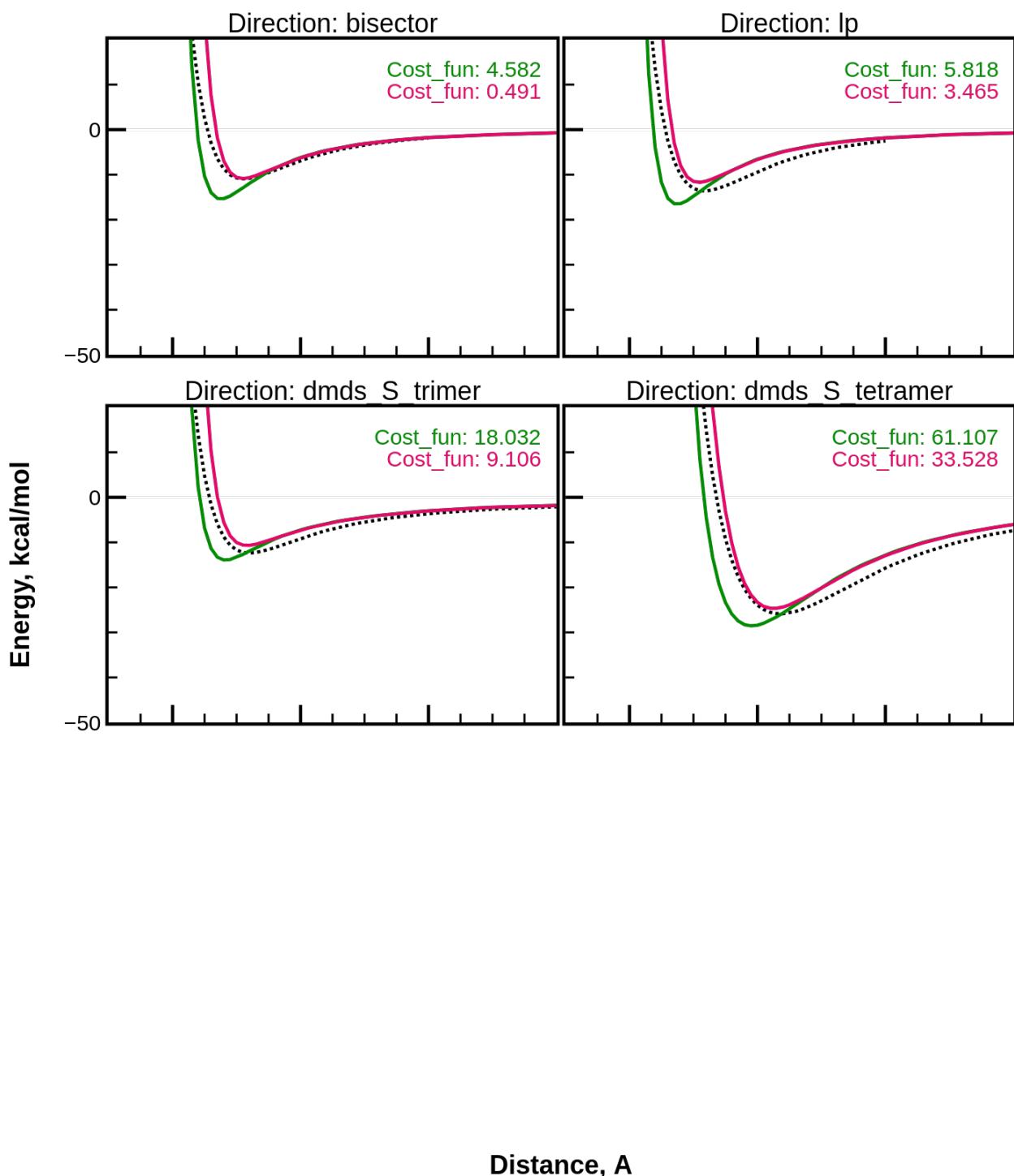
3.10000_0.09798_9.99999
3.36842_0.09798_2.07090



DMDS SOD 1/1

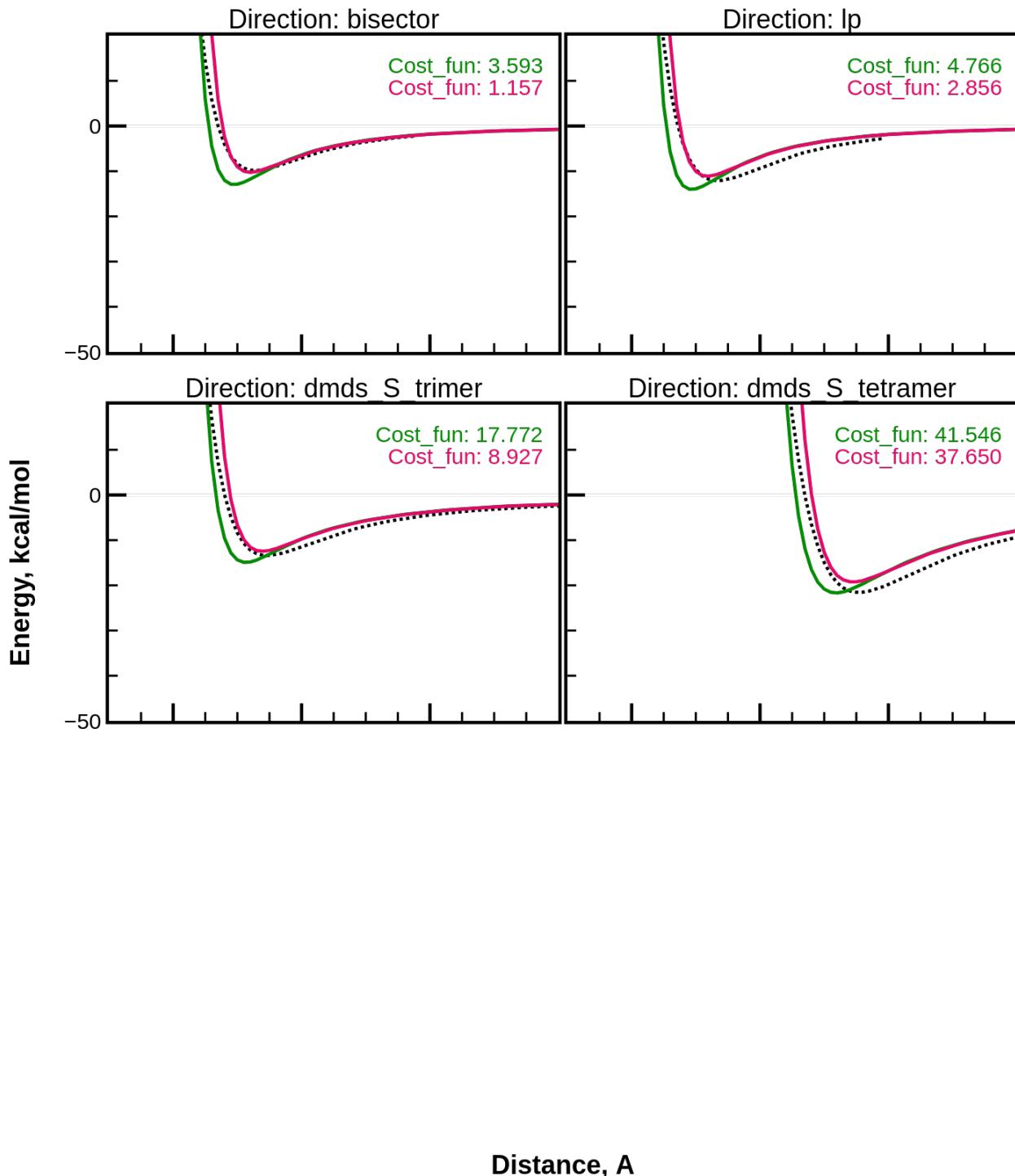
3.46168_0.10042_9.9999
3.73661_0.10042_3.02249



DMDS POT 1/13.68665_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

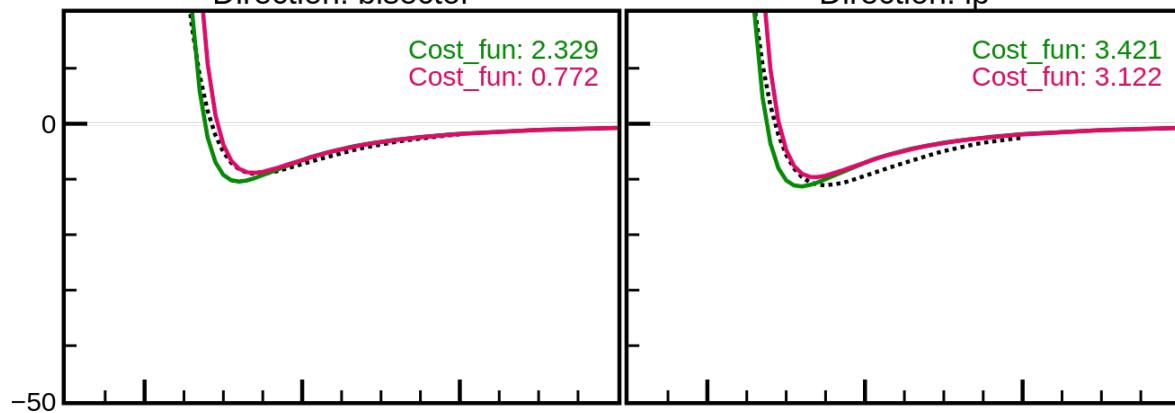


DMDS CES 1/1

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

Direction: bisector

Direction: lp

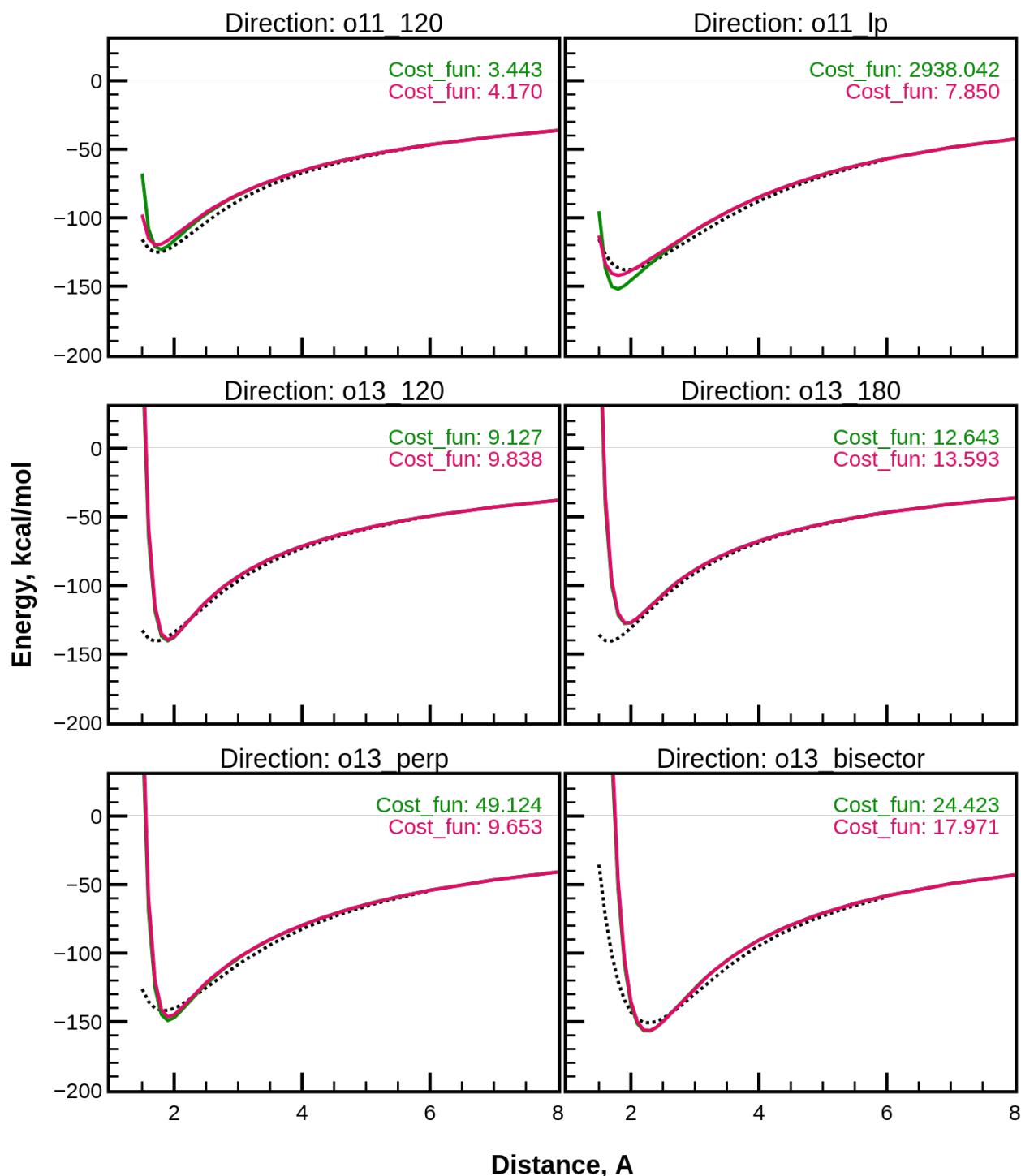


Direction: dmds S tetramer

Energy, kcal/mol

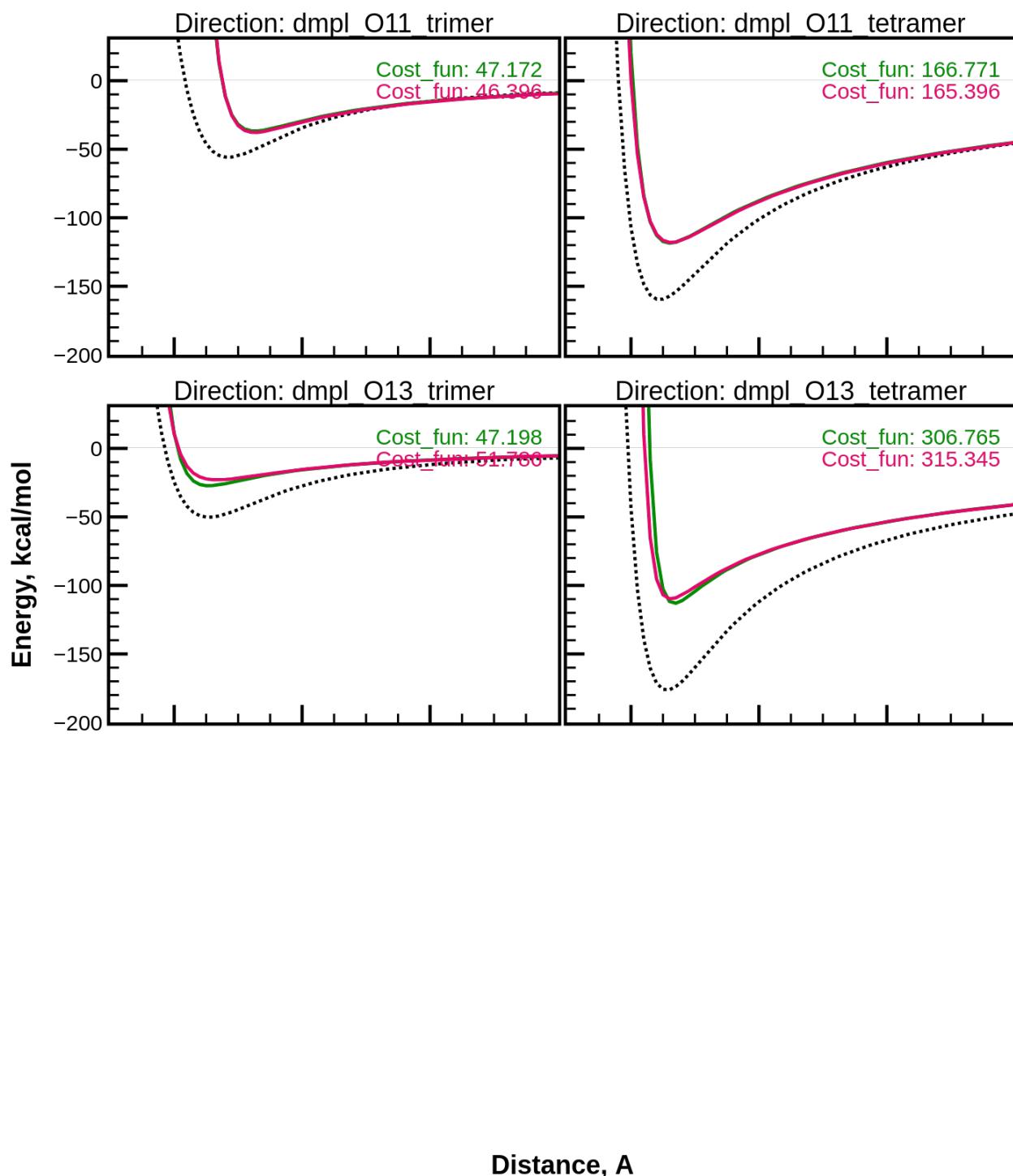
Cost_fun: 47.751
Cost_fun: 48.004

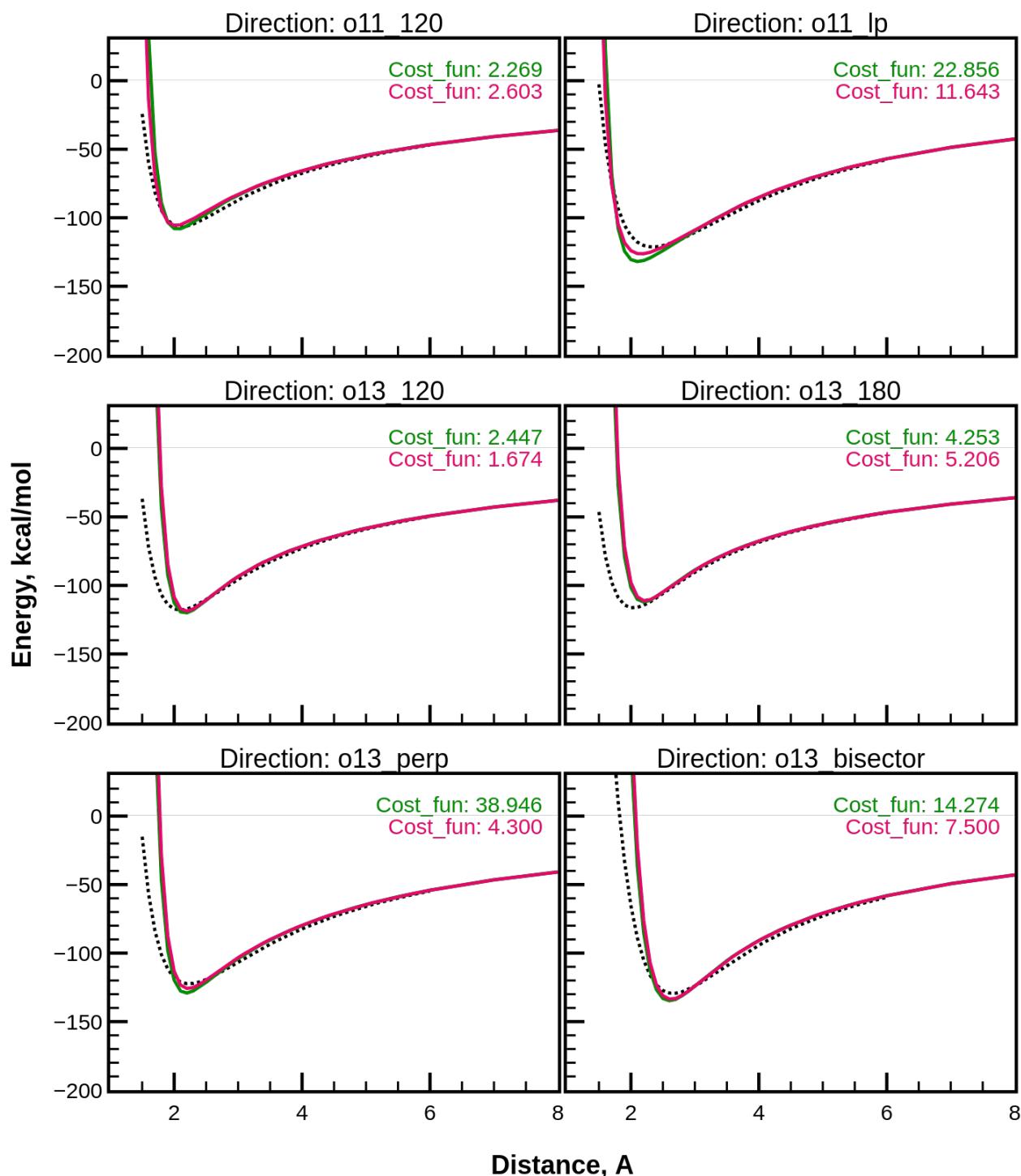
Distance, Å

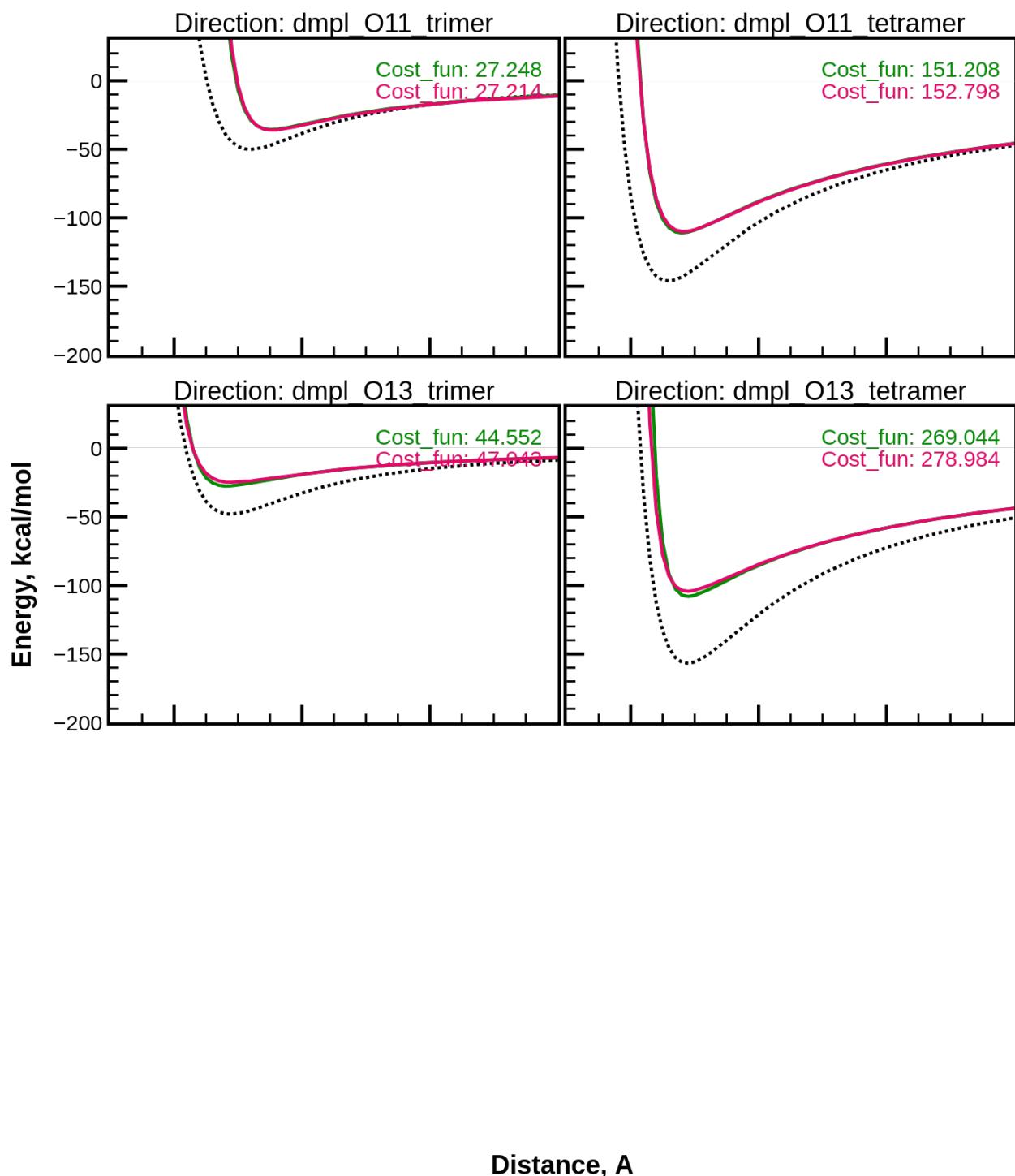
DMPL LIT 1/23.13500_0.04582_9.99999
3.02241_0.07550_4.98471

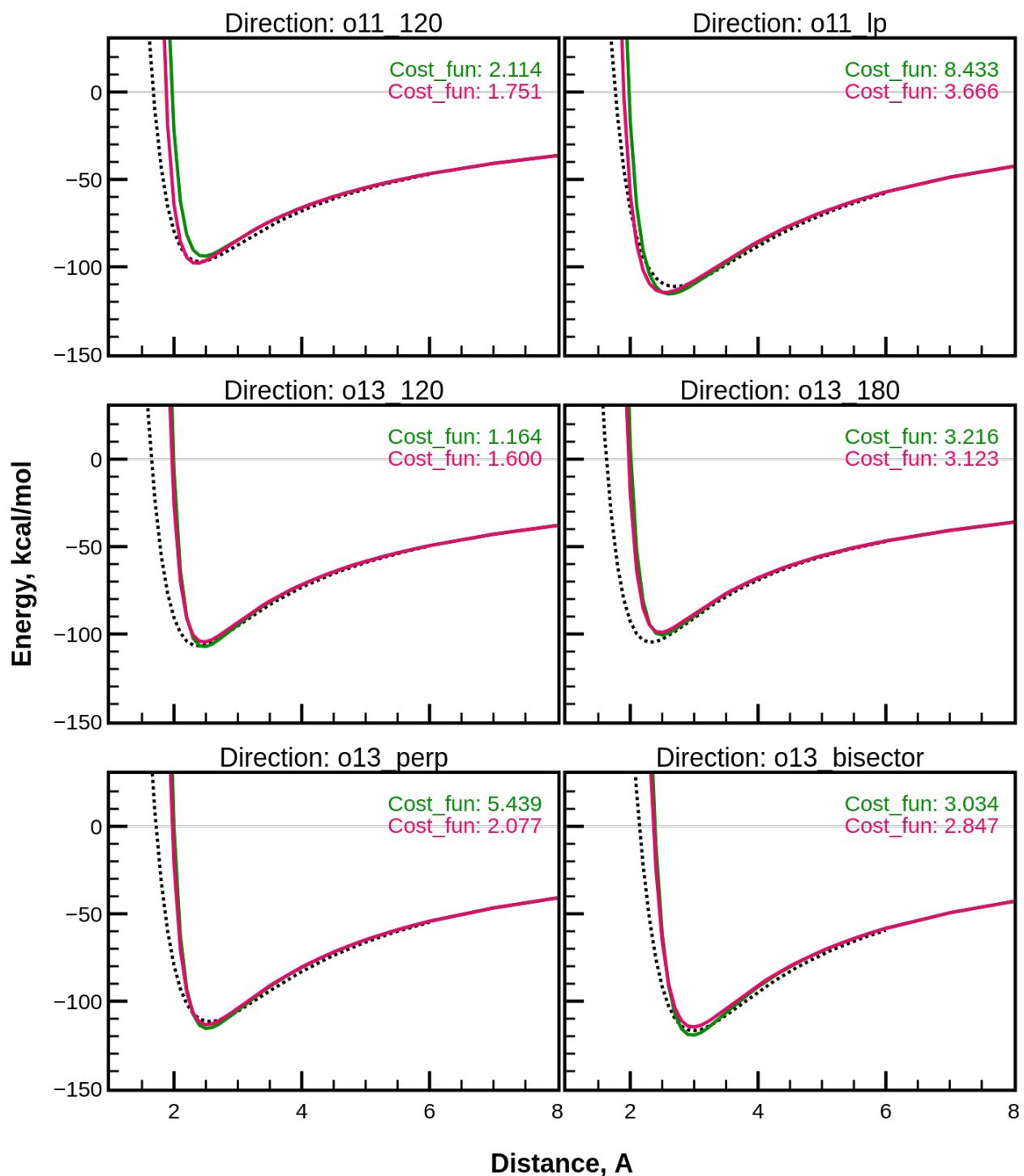
DMPL LIT 2/2

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



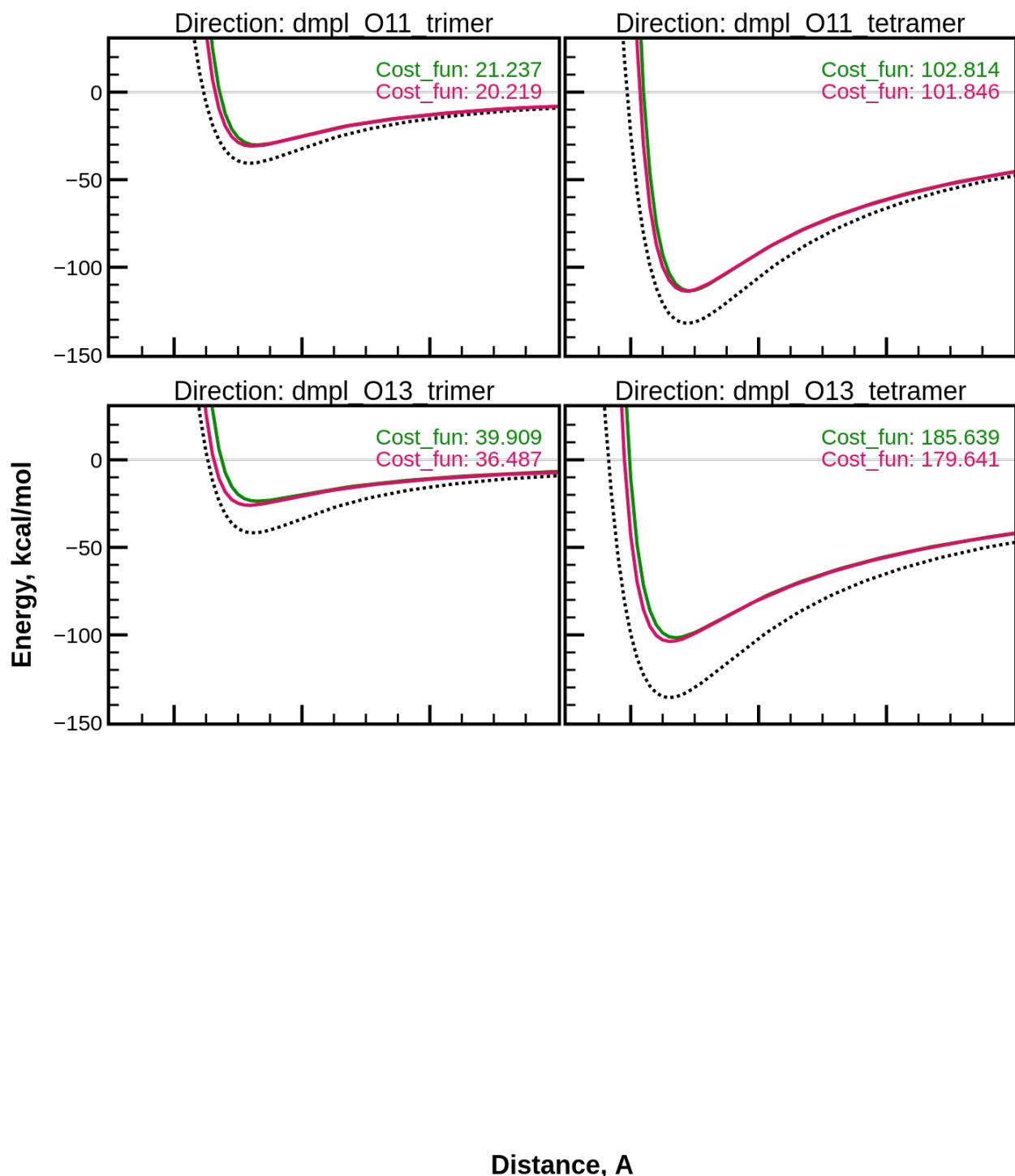
DMPL SOD 1/23.49668_0.04696_9.99999
3.38658_0.07738_5.01299

DMPL SOD 2/23.49668_0.04696_9.99999
3.38658_0.07738_5.01299

DMPL POT 1/23.55165_0.16421_9.99999
3.45707_0.16421_1.88686

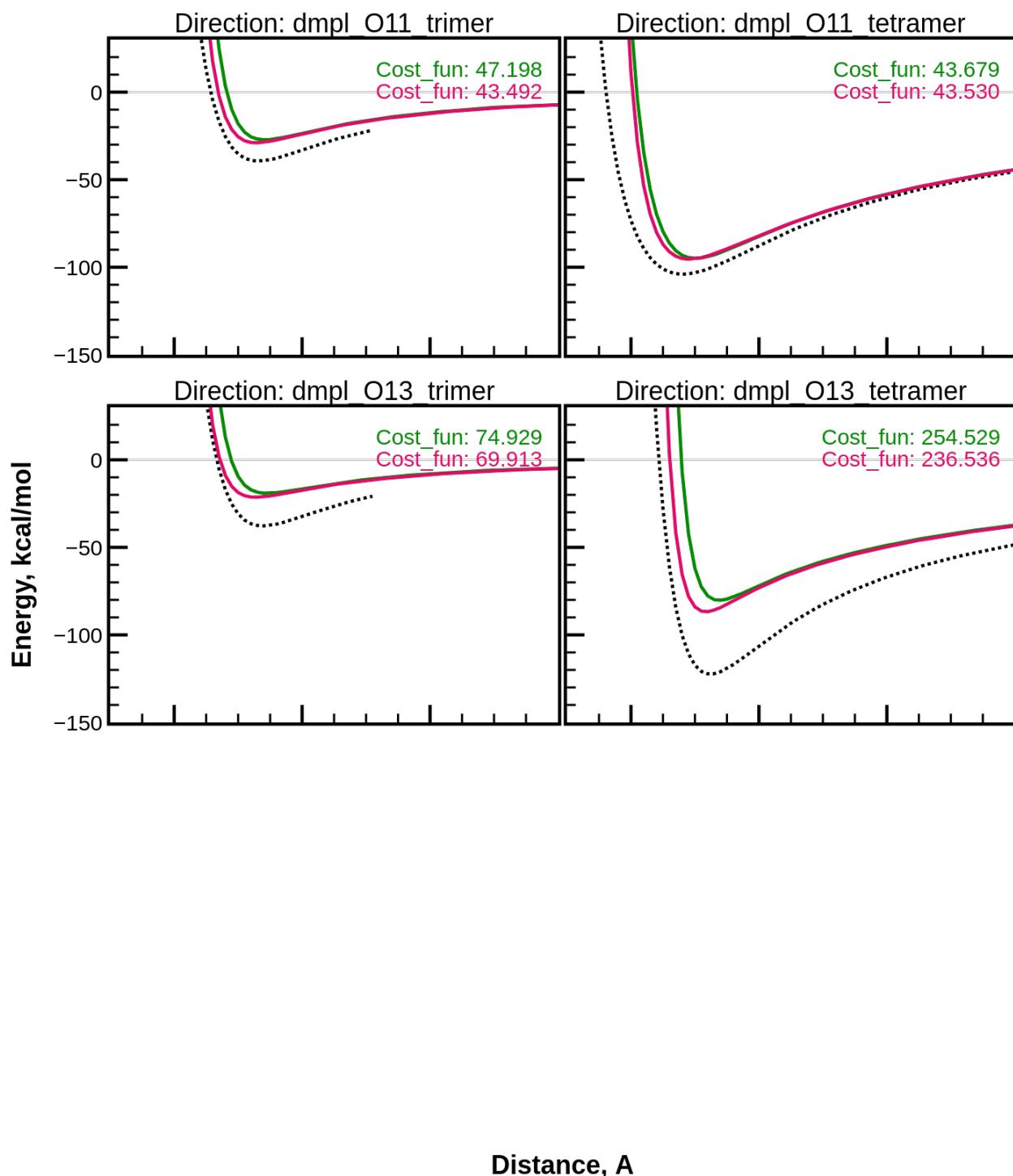
DMPL POT 2/2

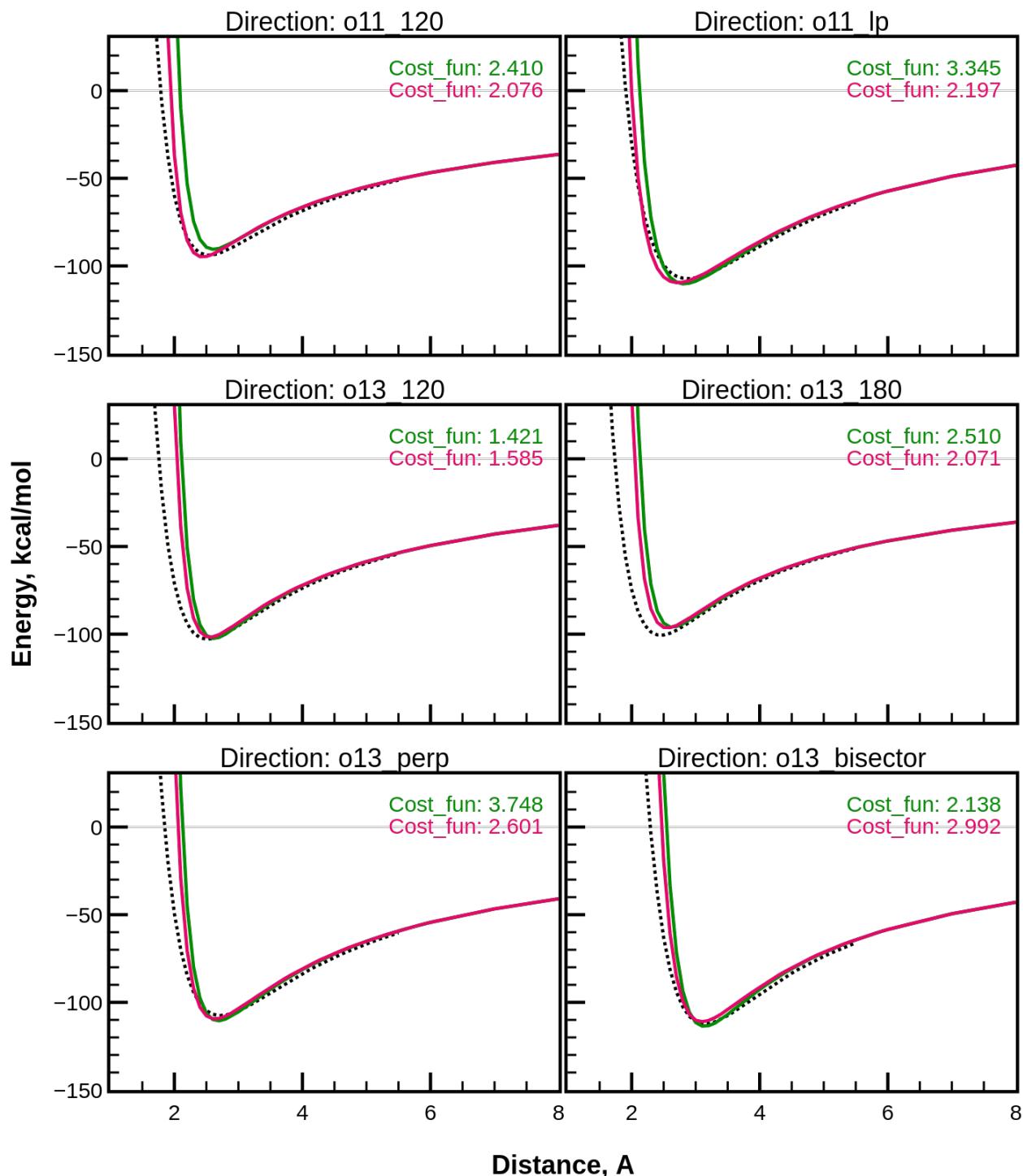
3.55165_0.16421_9.99999
3.45707_0.16421_1.88686



DMPL RUB 2/2

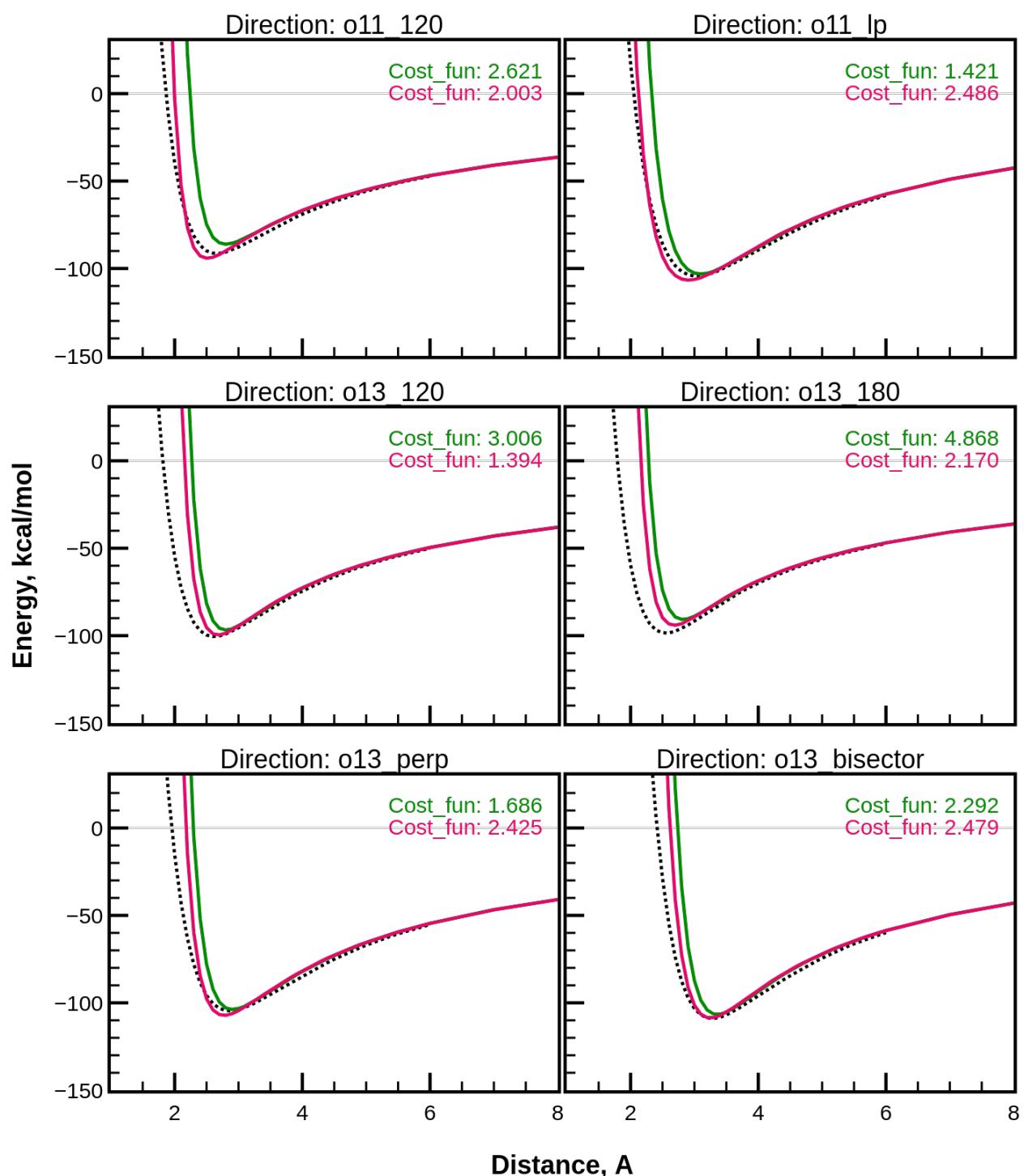
3.65051_0.22778_9.99999
3.48176_0.22778_1.94273



DMPL RUB 1/23.65051_0.22778_9.99999
3.48176_0.22778_1.94273

DMPL CES 1/2

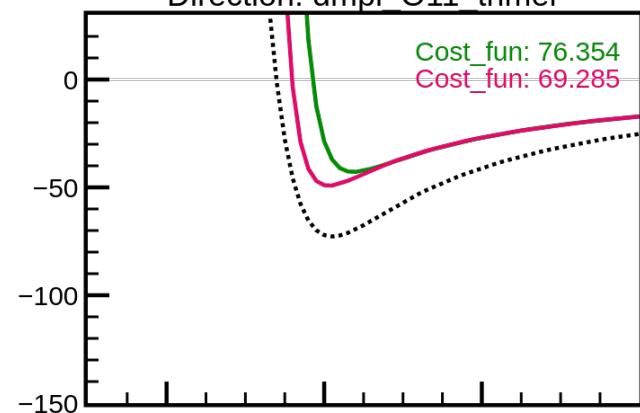
3.88882_0.22925_9.99999
3.67501_0.22925_2.30625



DMPL CES 2/2

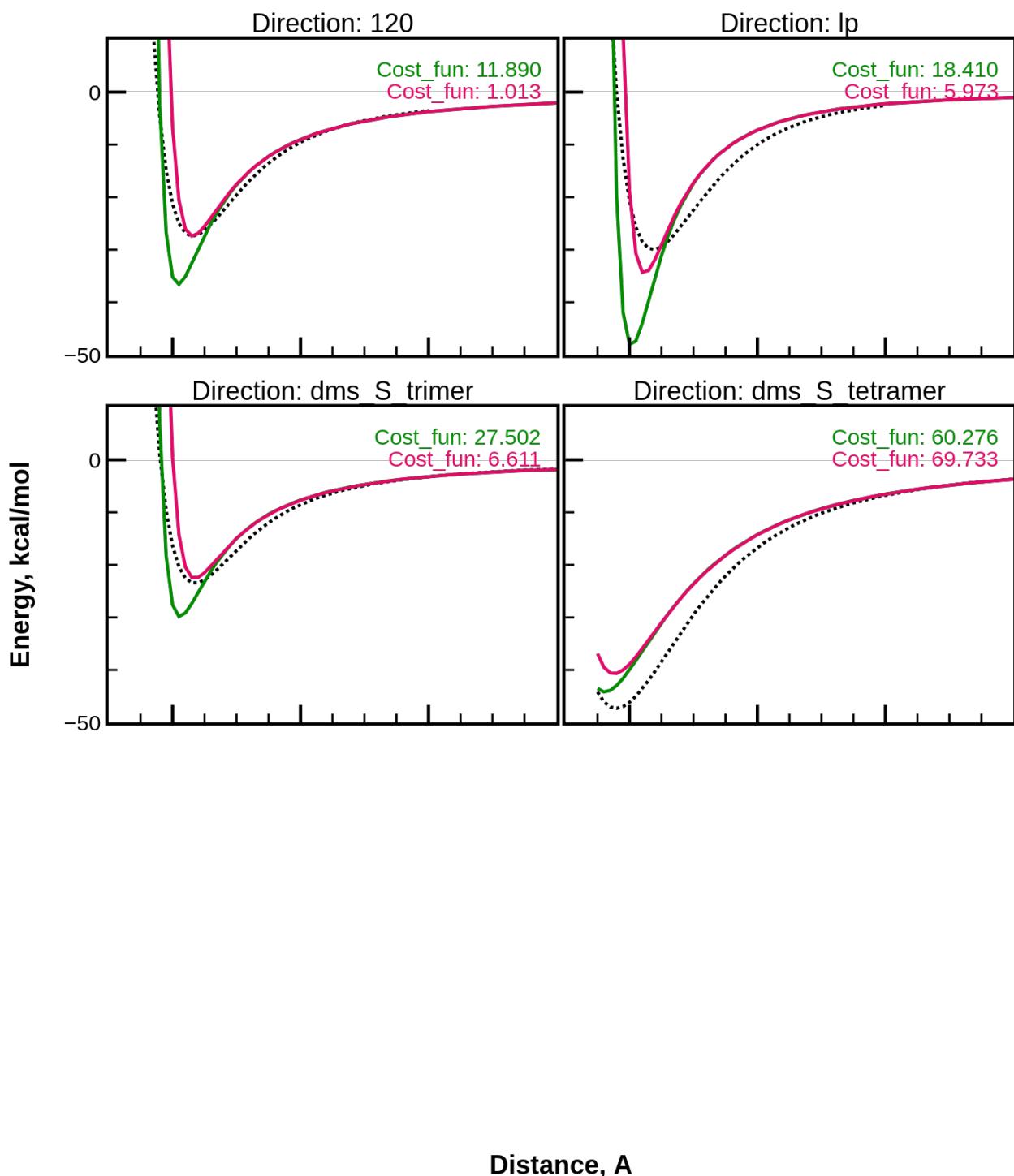
3.88882_0.22925_9.99999
3.67501_0.22925_2.30625

Direction: dmpl_O11_trimer



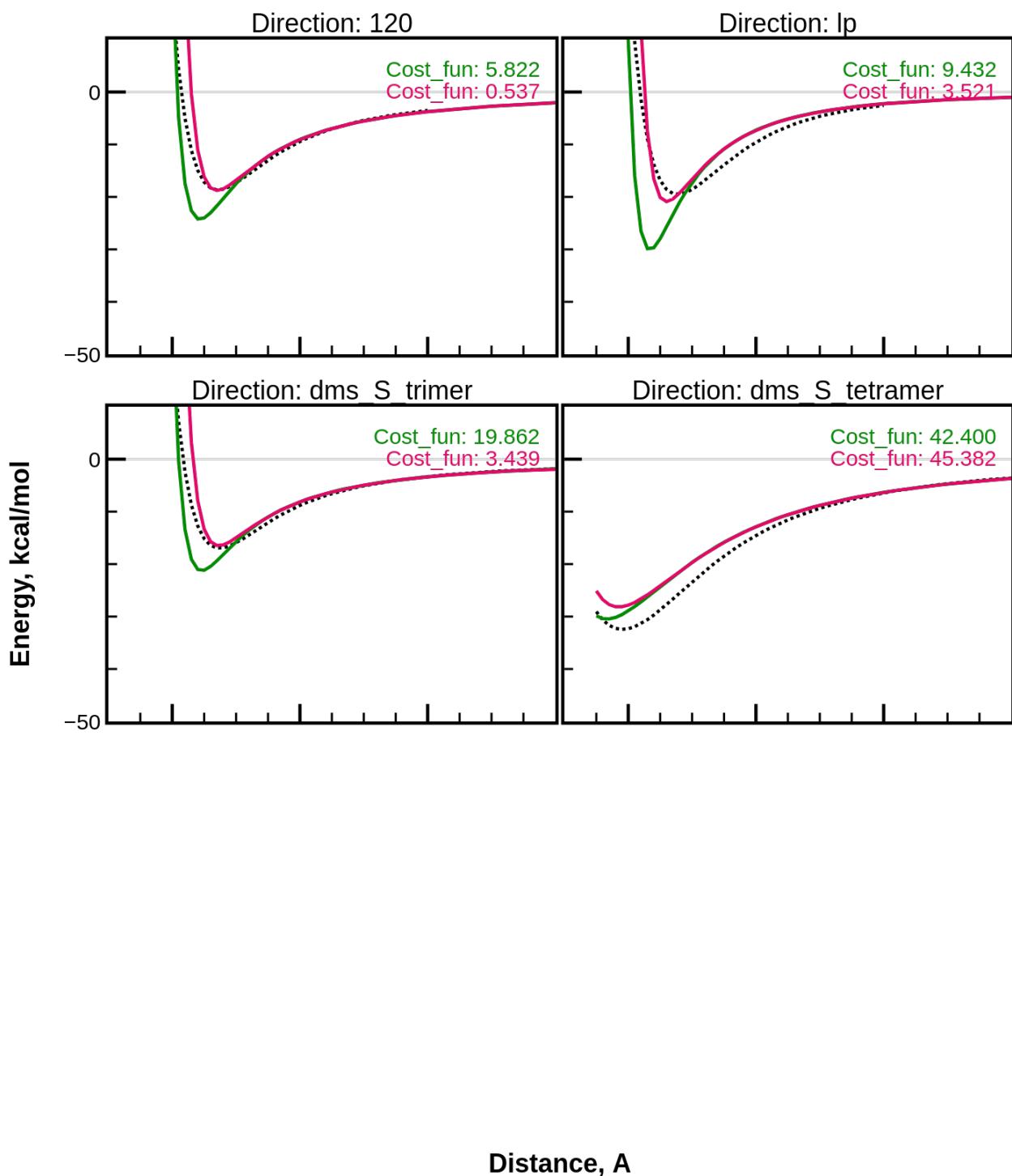
Energy, kcal/mol

Distance, Å

DMS LIT 1/13.15000_0.09644_9.99999
3.35945_0.09644_2.02916

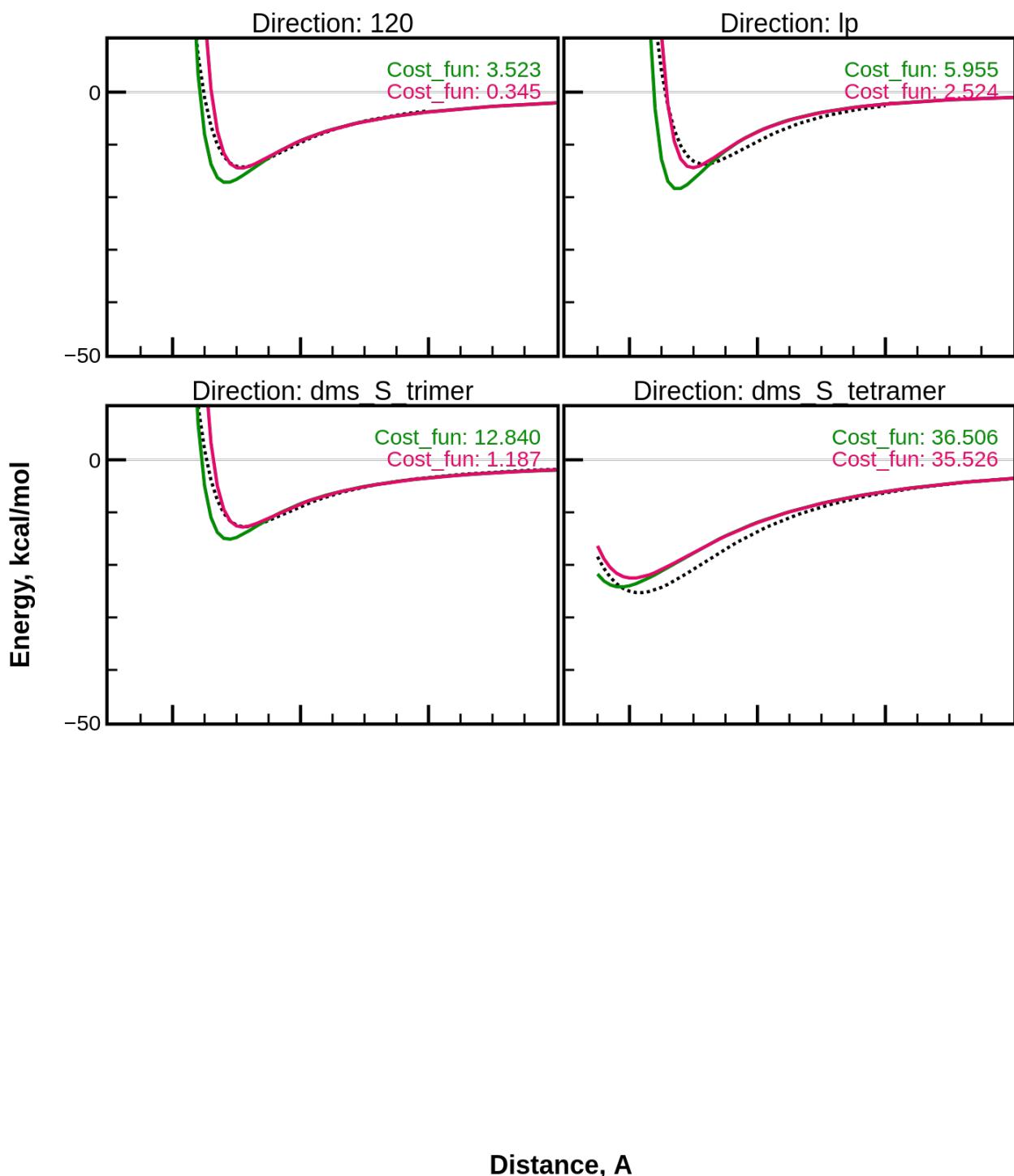
DMS SOD 1/1

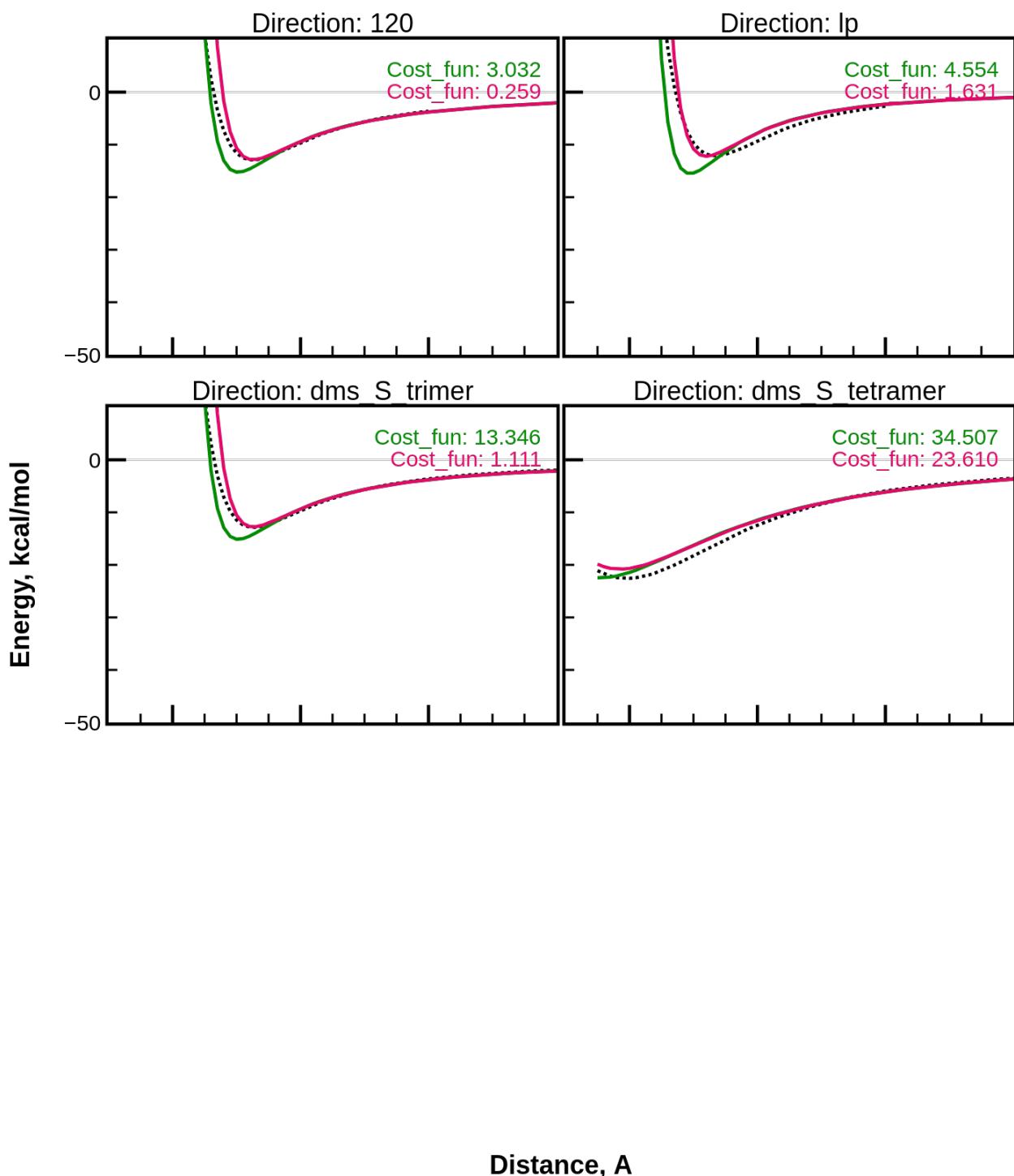
3.51168_0.09883_9.99999
3.78891_0.09883_3.72287

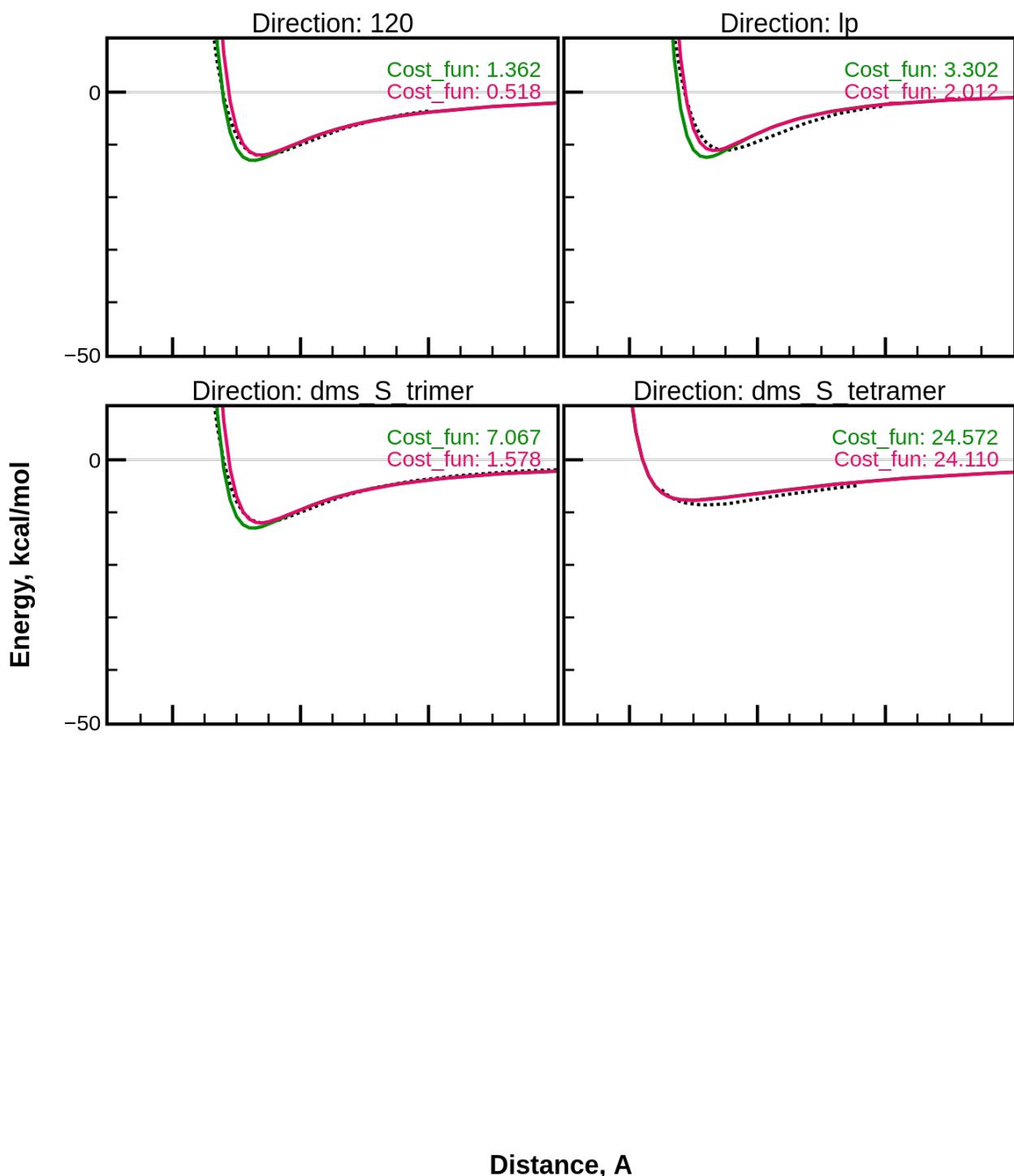


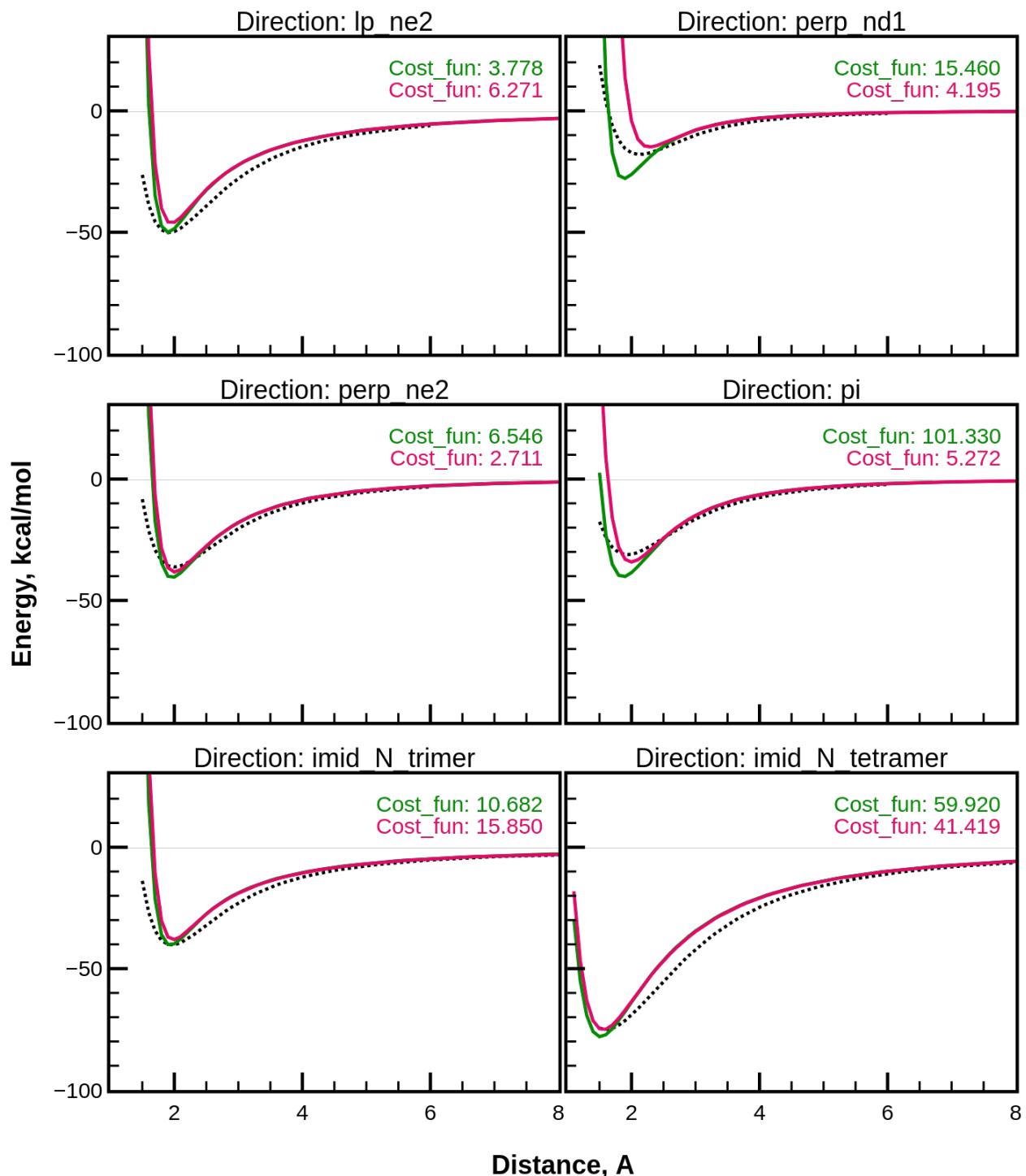
DMS POT 1/1

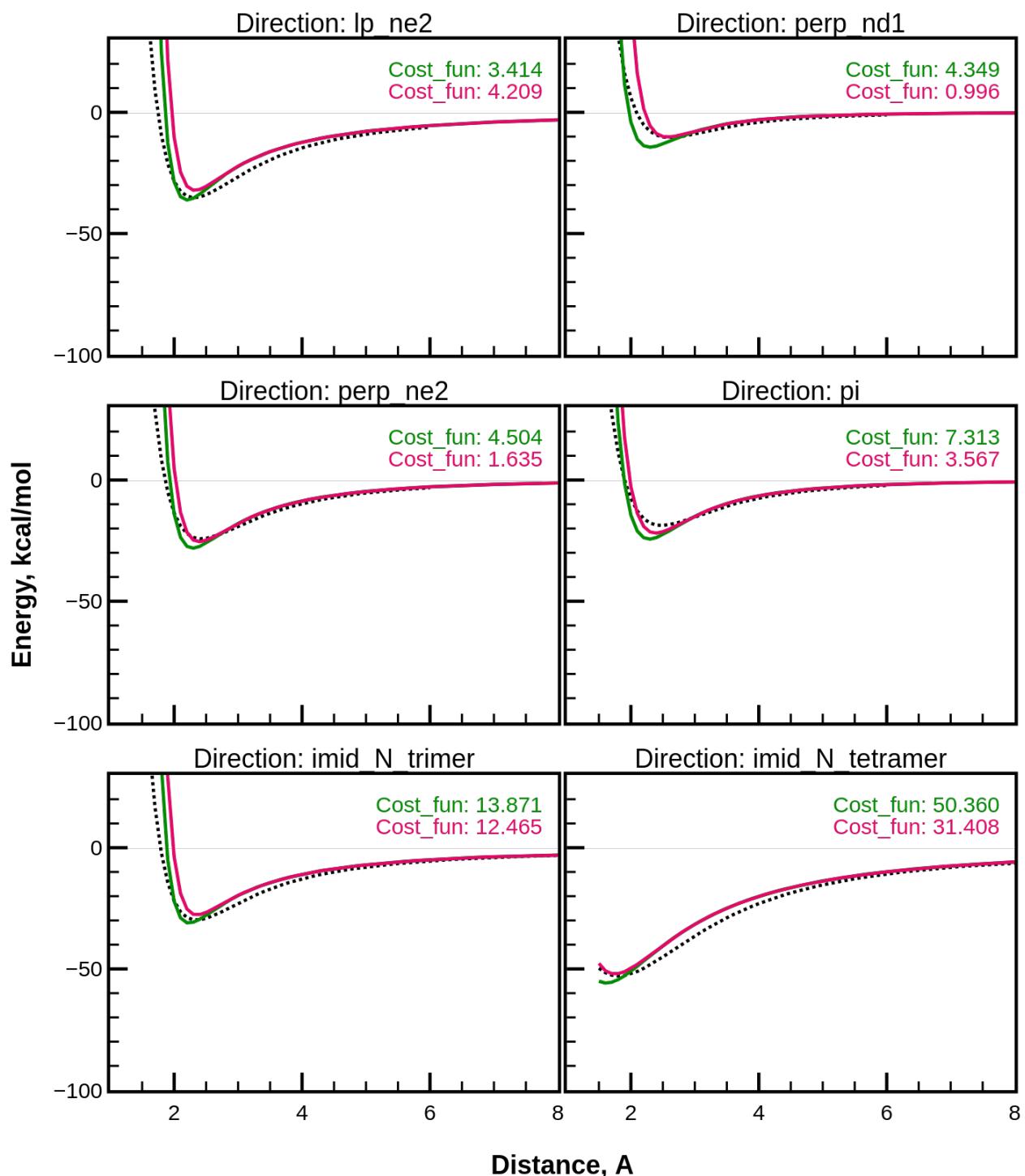
3.73665_0.20976_9.99999
3.95002_0.20976_3.43827

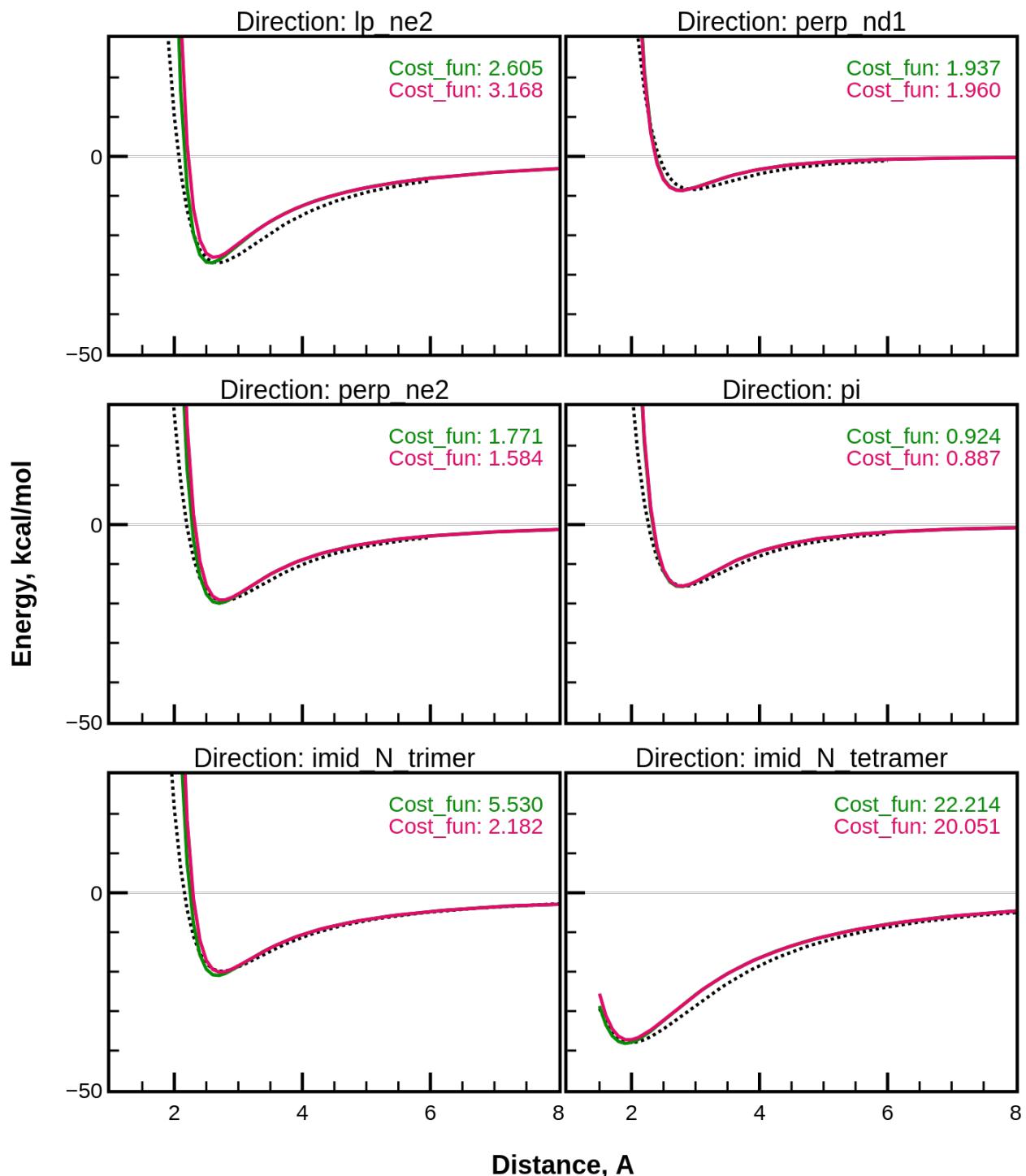


DMS RUB 1/13.83551_0.29095_9.99999
4.06564_0.29095_4.25802

DMS CES 1/14.07382_0.29283_9.99999
4.17814_0.29283_3.17830

IMID LIT 1/12.96100_0.05109_9.99999
3.39327_0.05109_4.39296

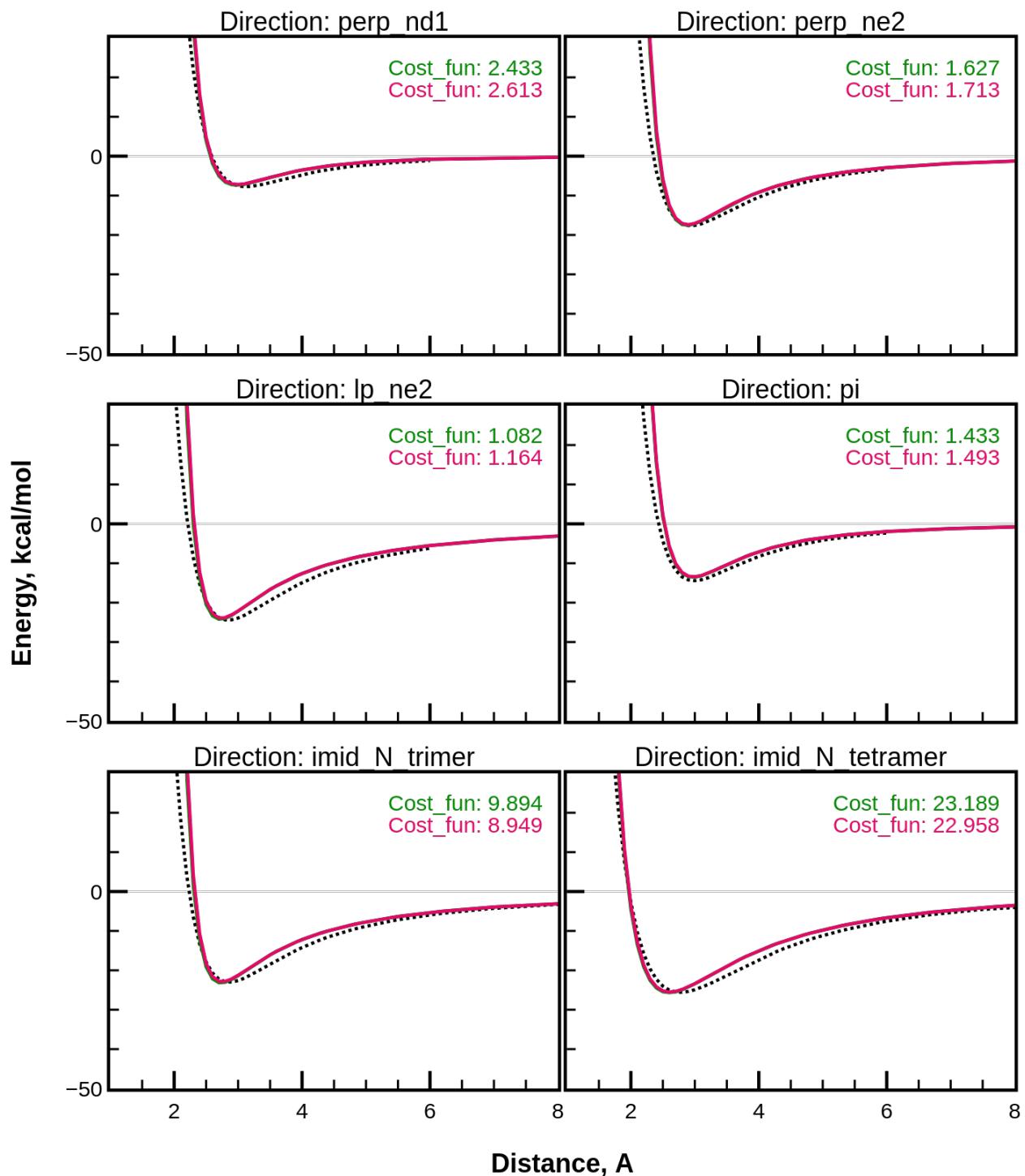
IMID SOD 1/13.32268_0.05236_9.99999
3.66106_0.05236_4.83751

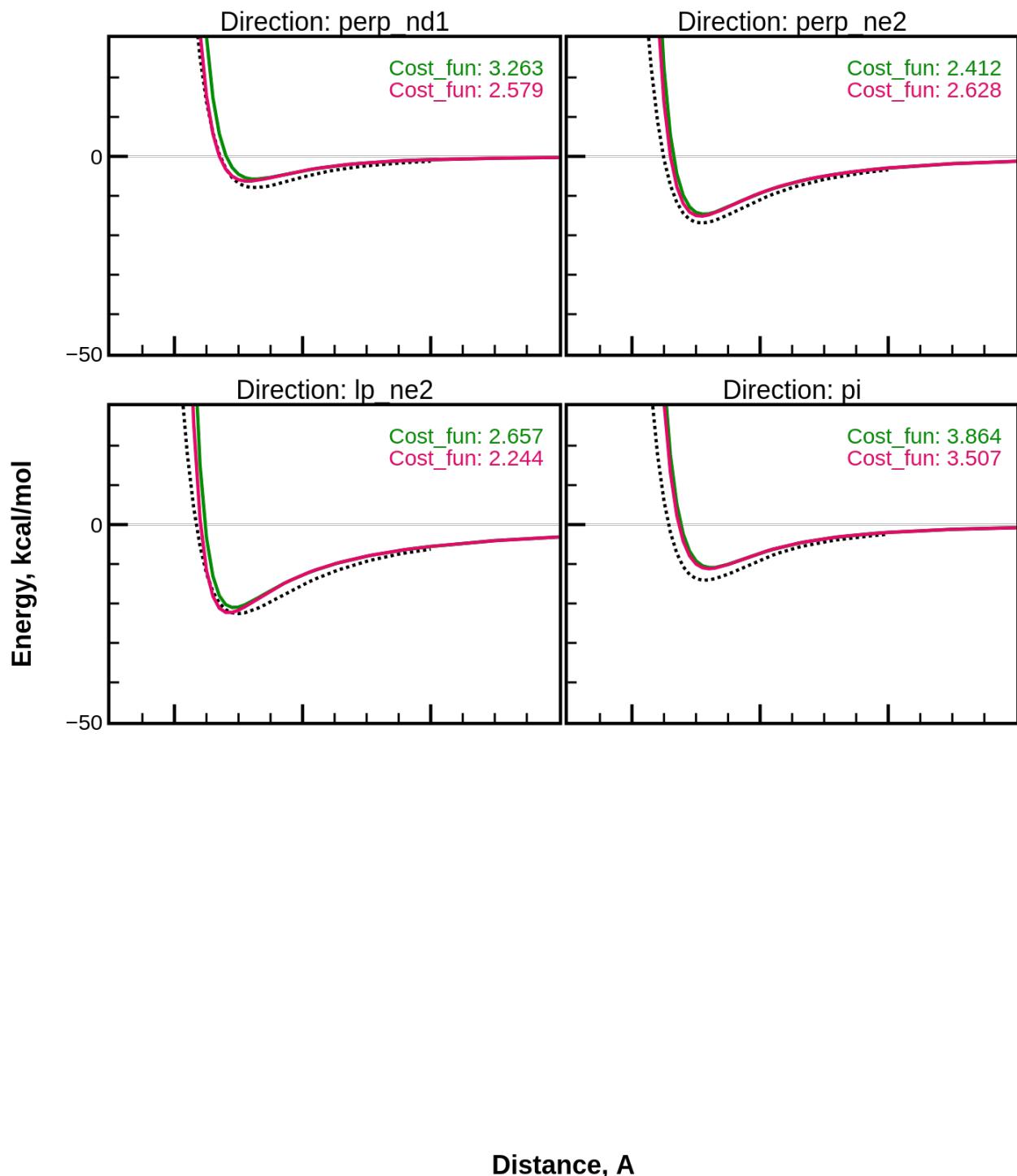
IMID POT 1/13.54765_0.11112_9.99999
3.52615_0.11112_3.46580

IMID RUB 1/1

3.64651_0.15413_9.99999

3.64509_0.15413_2.83449

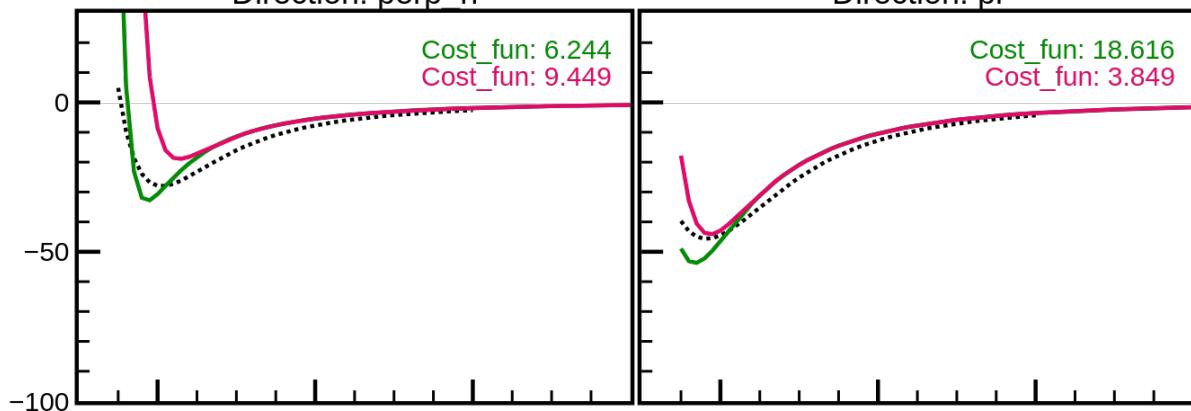


IMID CES 1/13.88482_0.15513_9.99999
3.64608_0.15513_4.63164

INDO LIT 1/12.96100_0.05109_9.99999
3.39327_0.05109_4.39296

Direction: perp_n

Direction: pi



Energy, kcal/mol

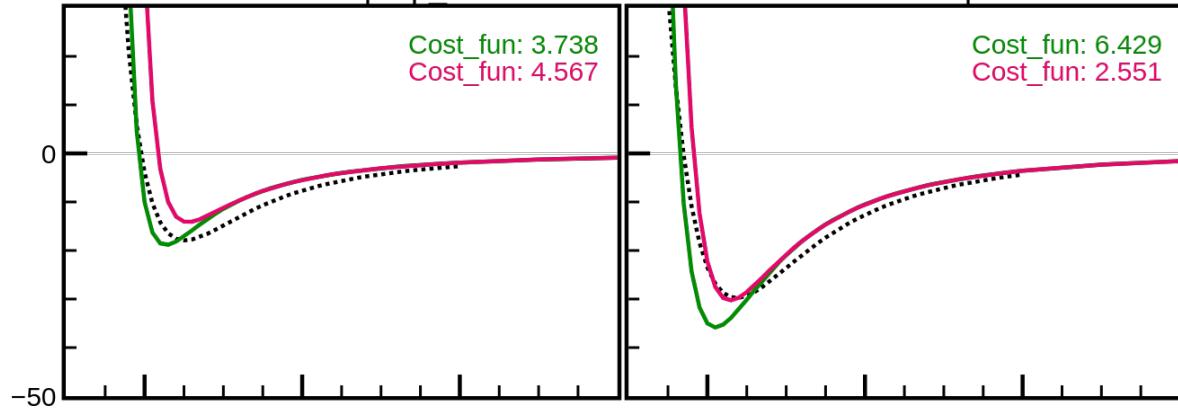
Distance, A

INDO SOD 1/1

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

Direction: perp_n

Direction: pi



Energy, kcal/mol

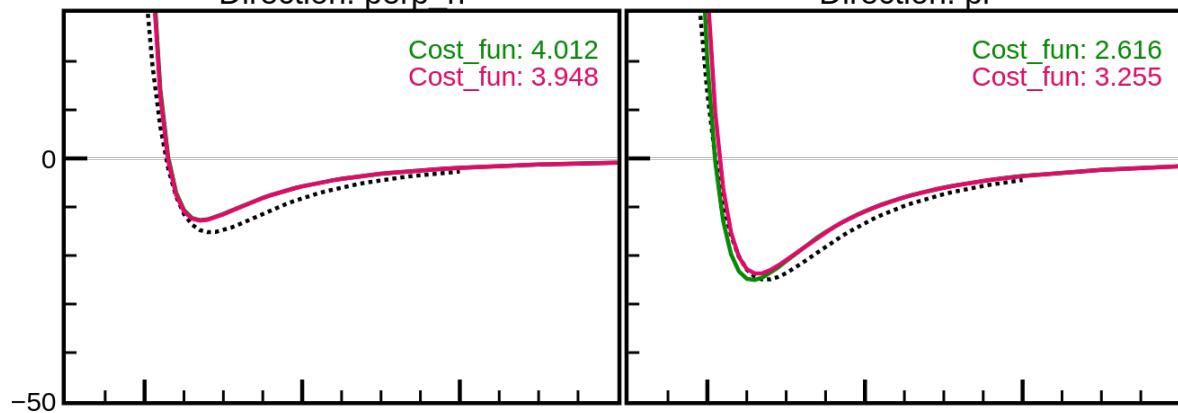
Distance, A

INDO POT 1/1

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

Direction: perp_n

Direction: pi



Energy, kcal/mol

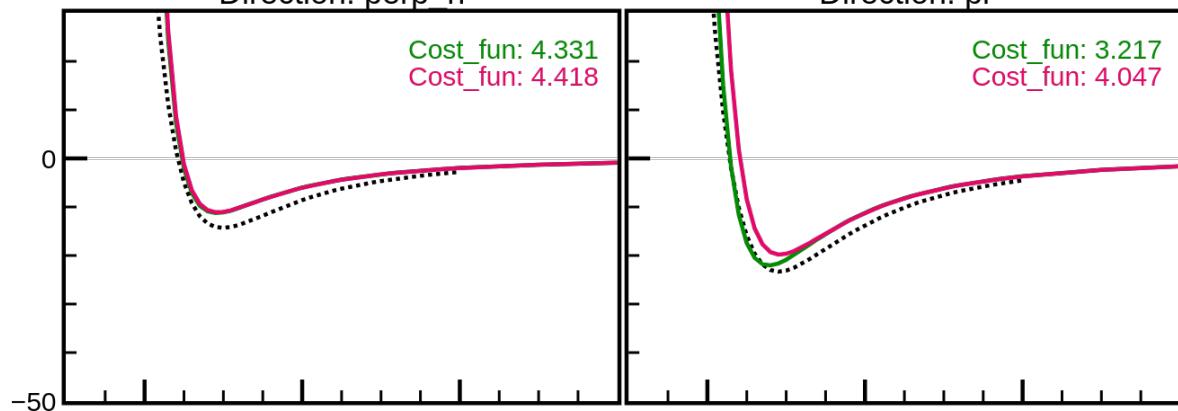
Distance, A

INDO RUB 1/1

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

Direction: perp_n

Direction: pi



Energy, kcal/mol

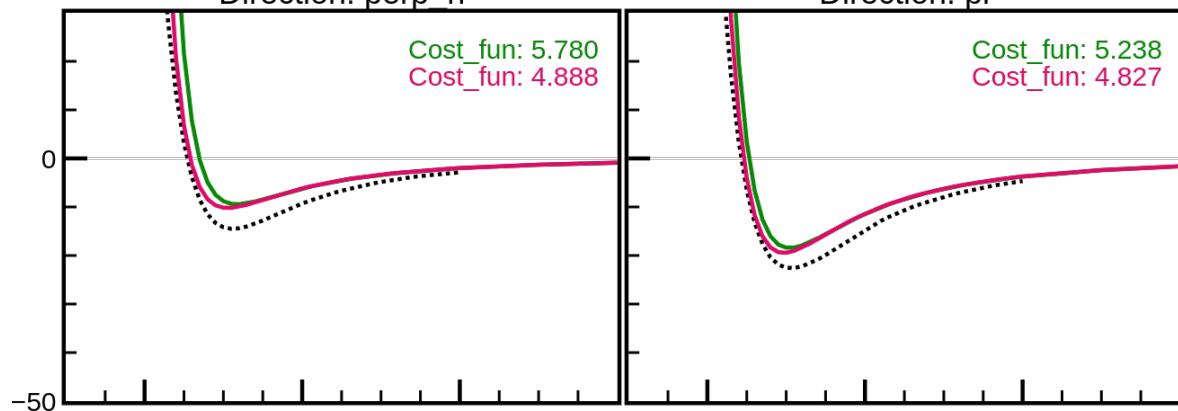
Distance, A

INDO CES 1/1

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

Direction: perp_n

Direction: pi

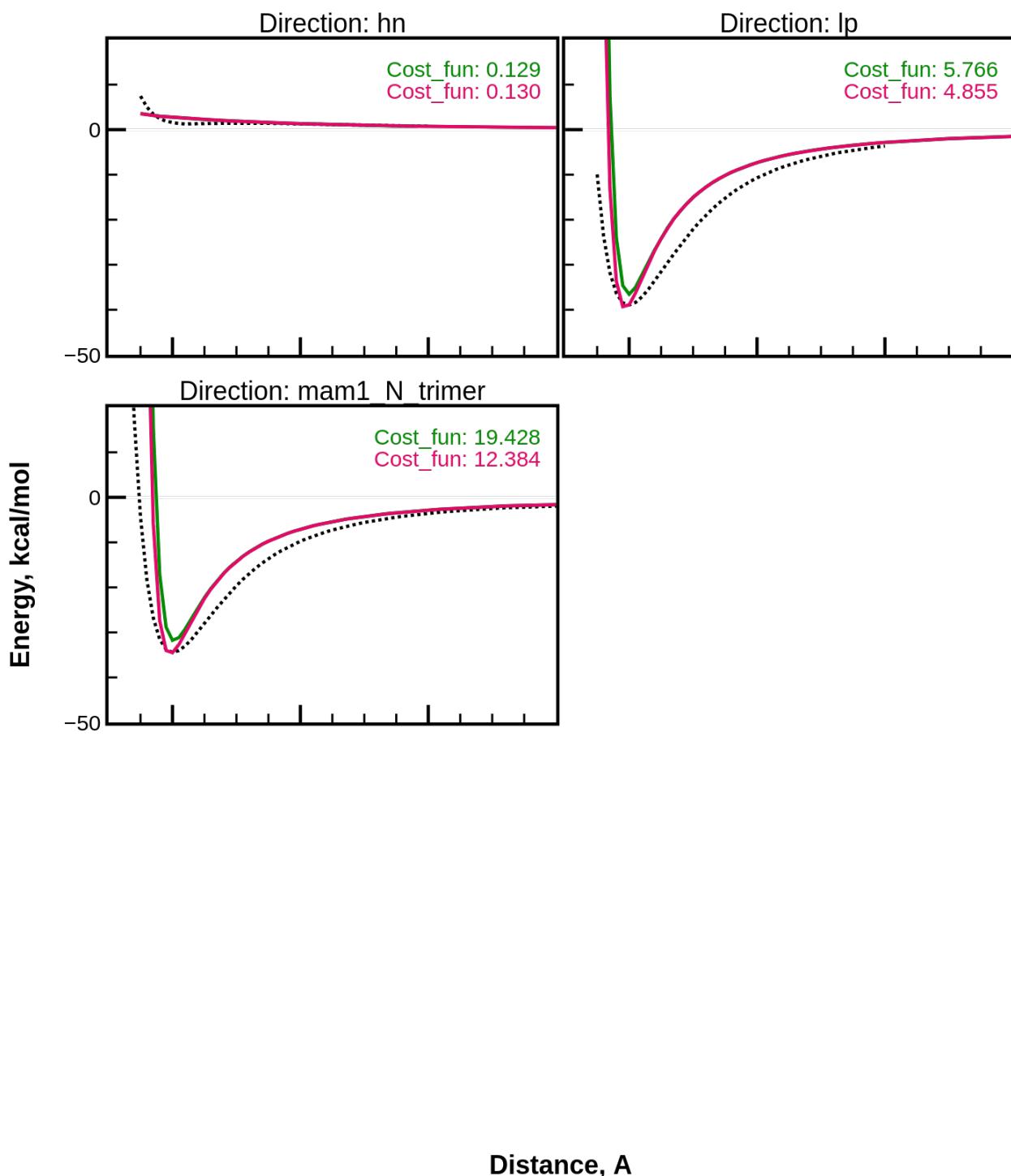


Energy, kcal/mol

Distance, A

MAM1 LIT 1/1

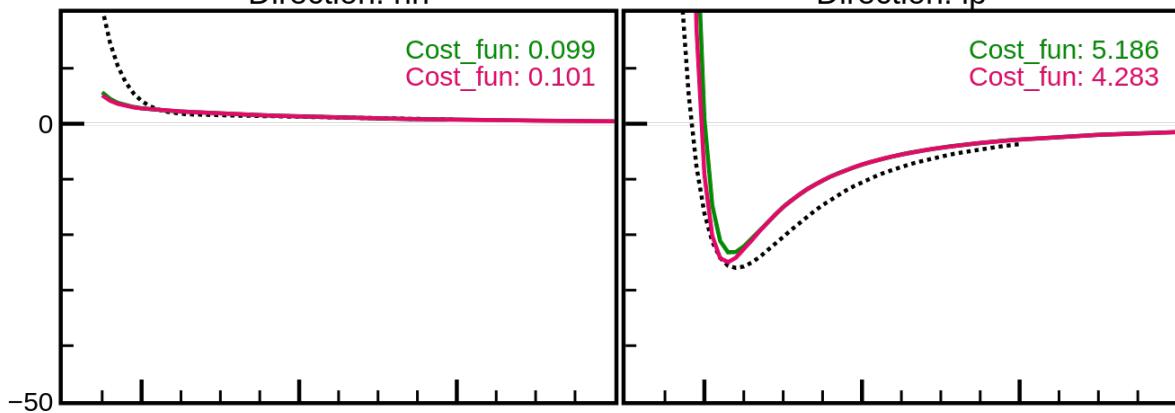
3.00000_0.10507_9.99999
2.91762_0.10507_2.28851



MAM1 SOD 1/1

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

Direction: hn



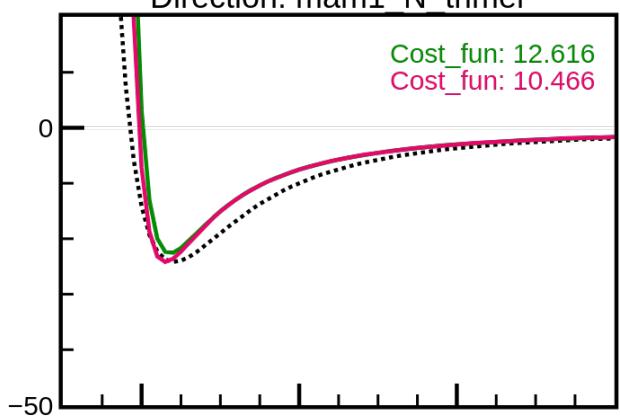
Direction: lp

Cost_fun: 5.186
Cost_fun: 4.283

Direction: mam1_N_trimer

Cost_fun: 12.616
Cost_fun: 10.466

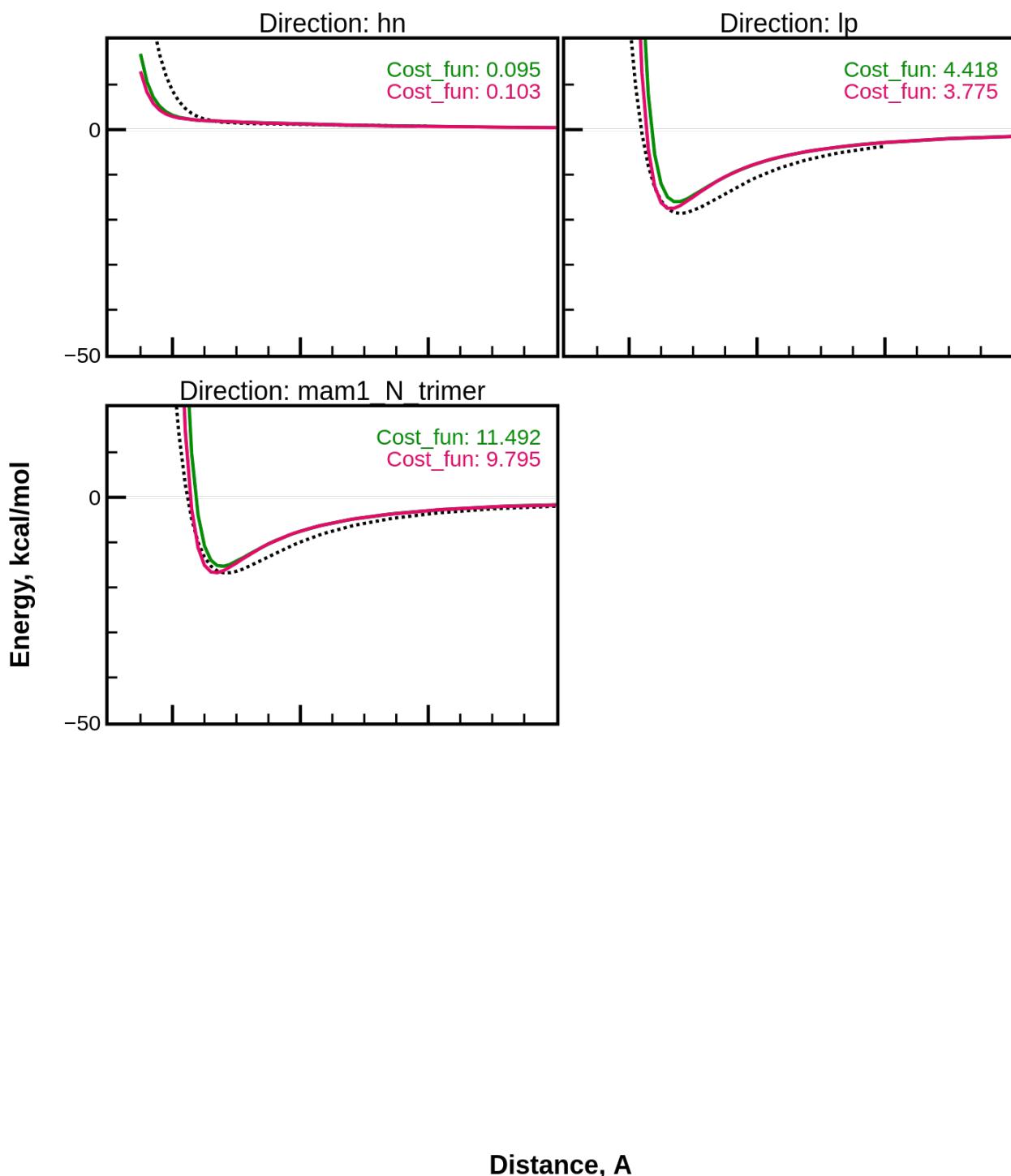
Energy, kcal/mol



Distance, A

MAM1 POT 1/1

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

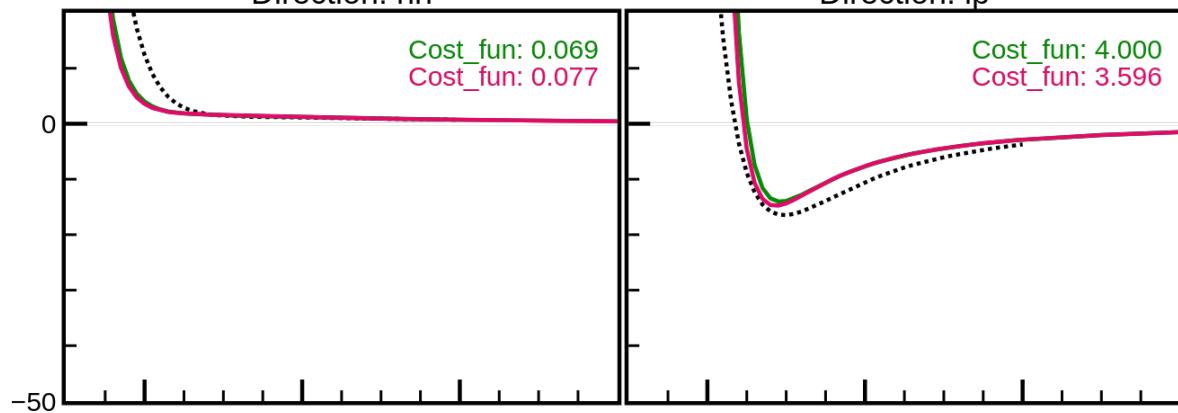


MAM1 RUB 1/1

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

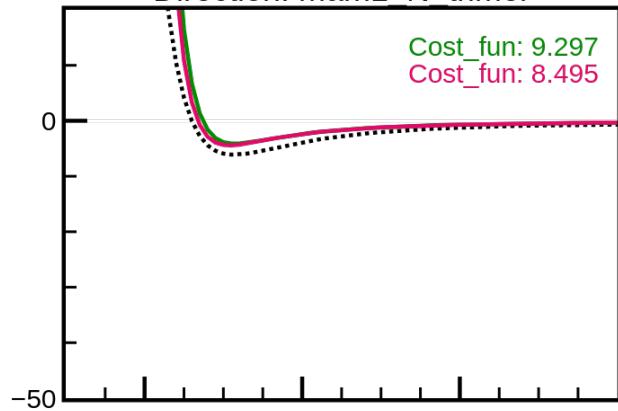
Direction: hn

Direction: lp



Direction: mam1_N_trimer

Energy, kcal/mol



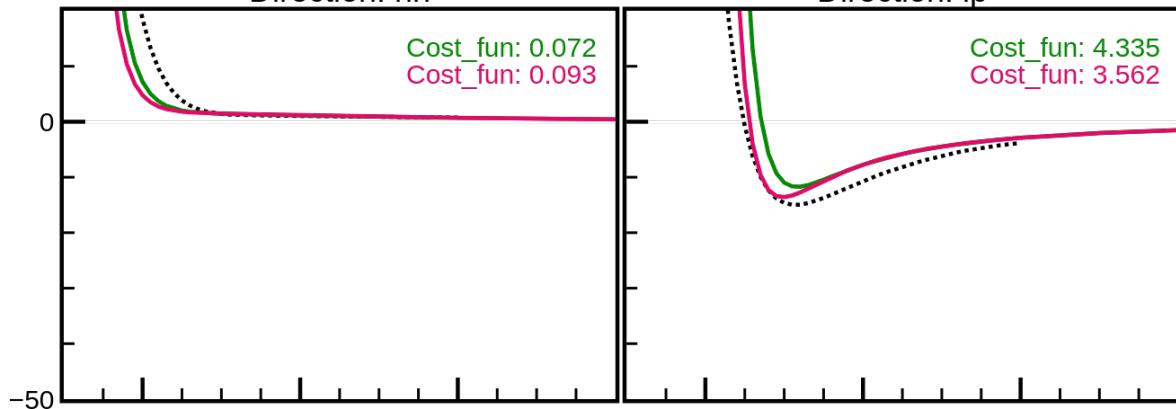
Distance, Å

MAM1 CES 1/1

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

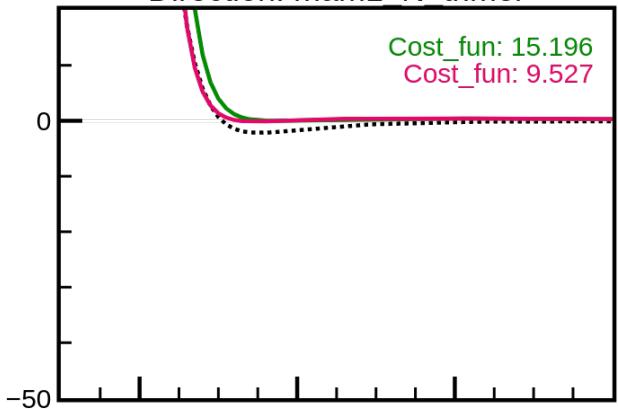
Direction: hn

Direction: lp

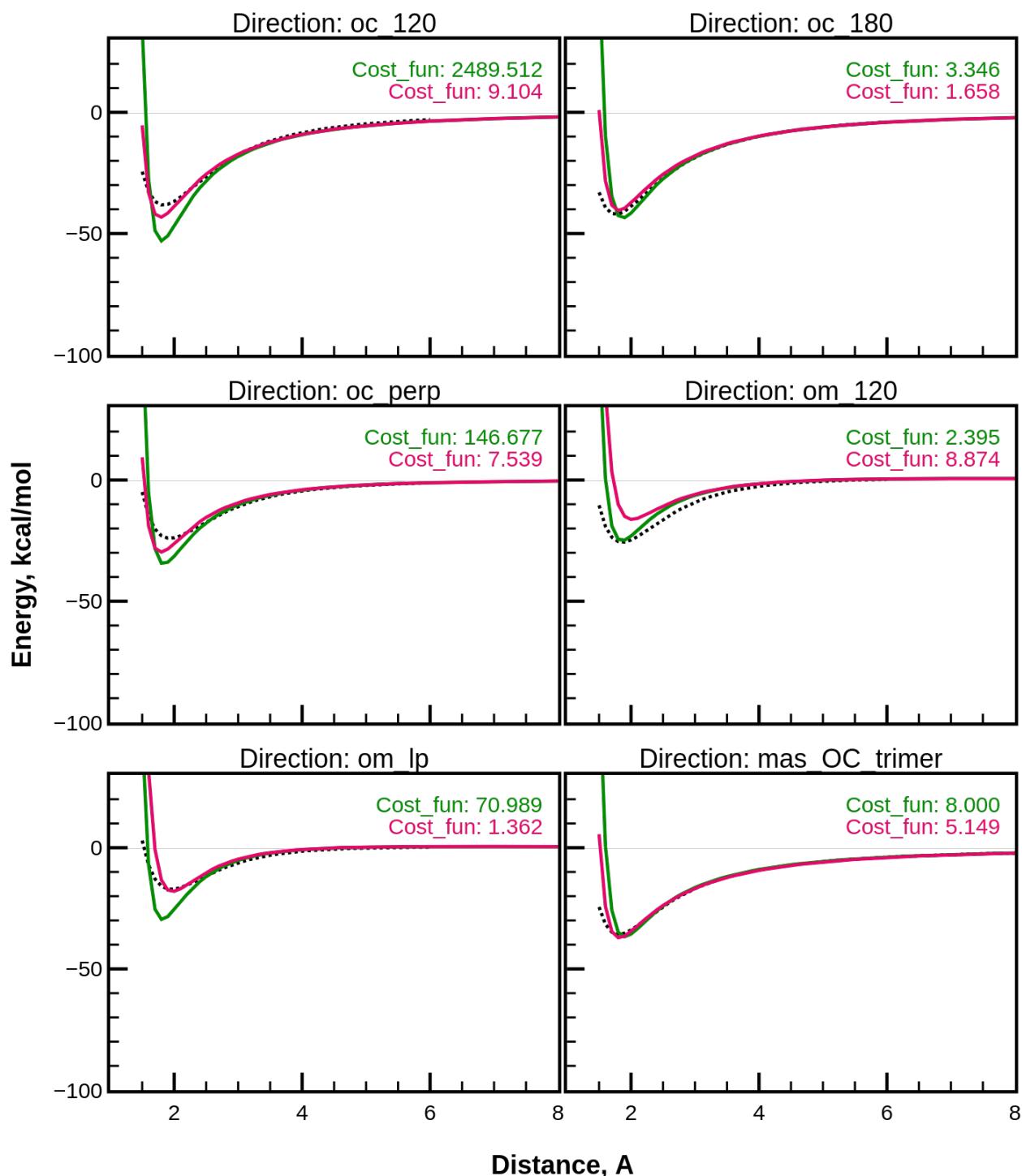


Direction: mam1_N_trimer

Energy, kcal/mol

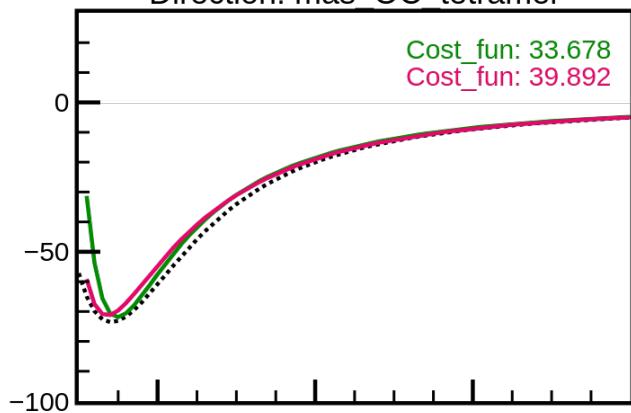


Distance, Å

MAS LIT 1/22.85000_0.07348_9.99999
2.65664_0.07348_0.64546

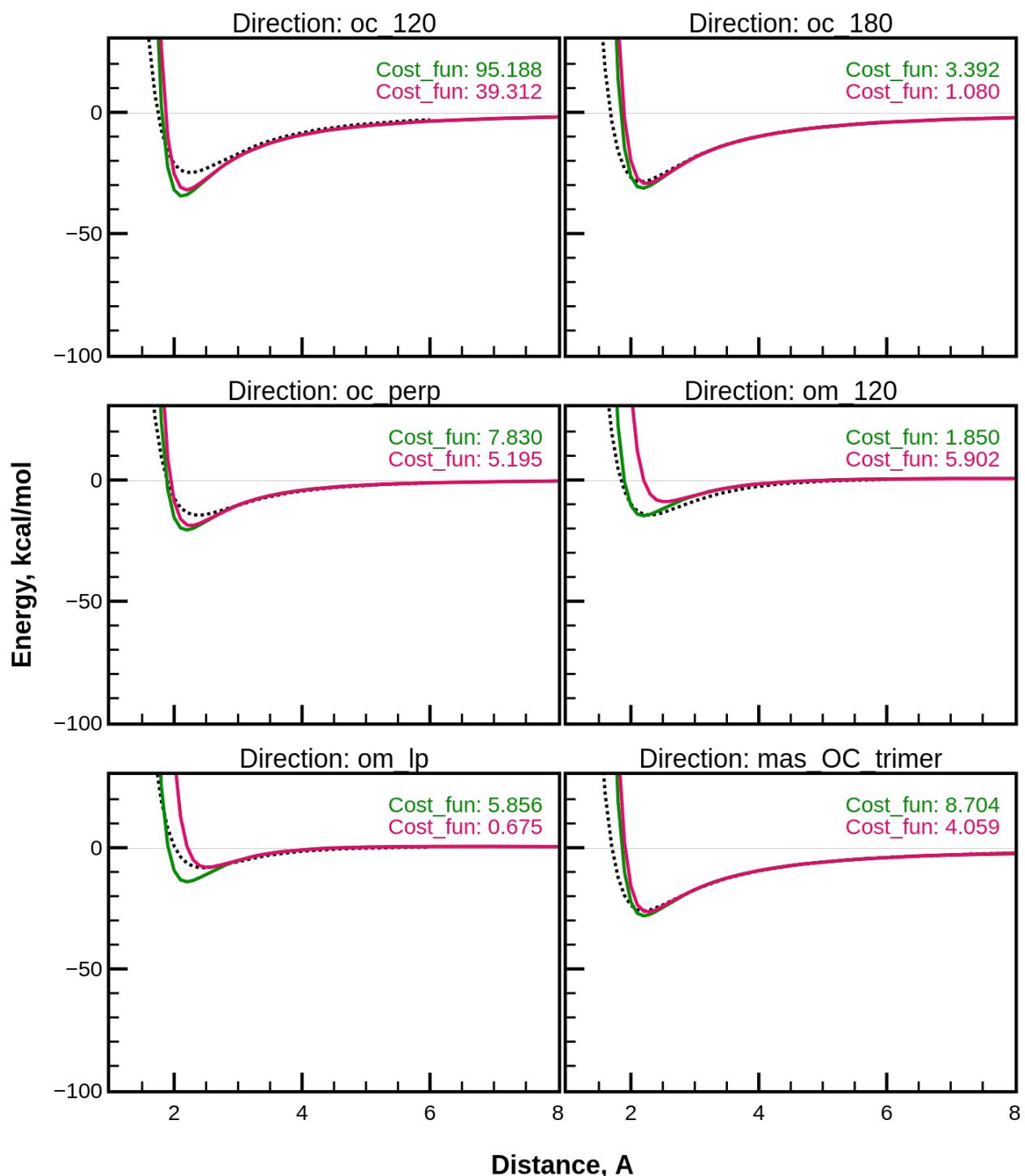
MAS LIT 2/22.85000_0.07348_9.99999
2.65664_0.07348_0.64546

Direction: mas OC tetramer



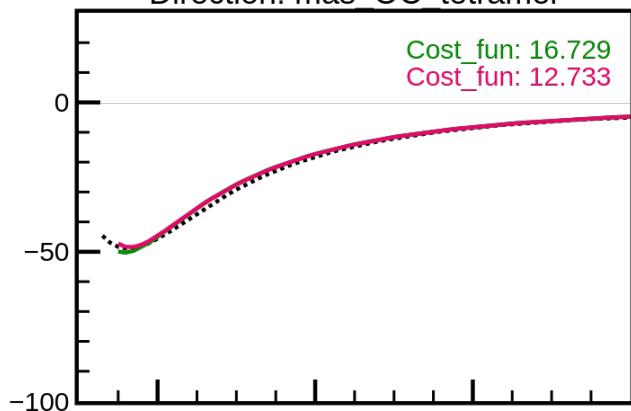
Energy, kcal/mol

Distance, Å

MAS SOD 1/23.21168_0.07531_9.99999
3.28395_0.07531_3.34812

MAS SOD 2/23.21168_0.07531_9.99999
3.28395_0.07531_3.34812

Direction: mas OC tetramer

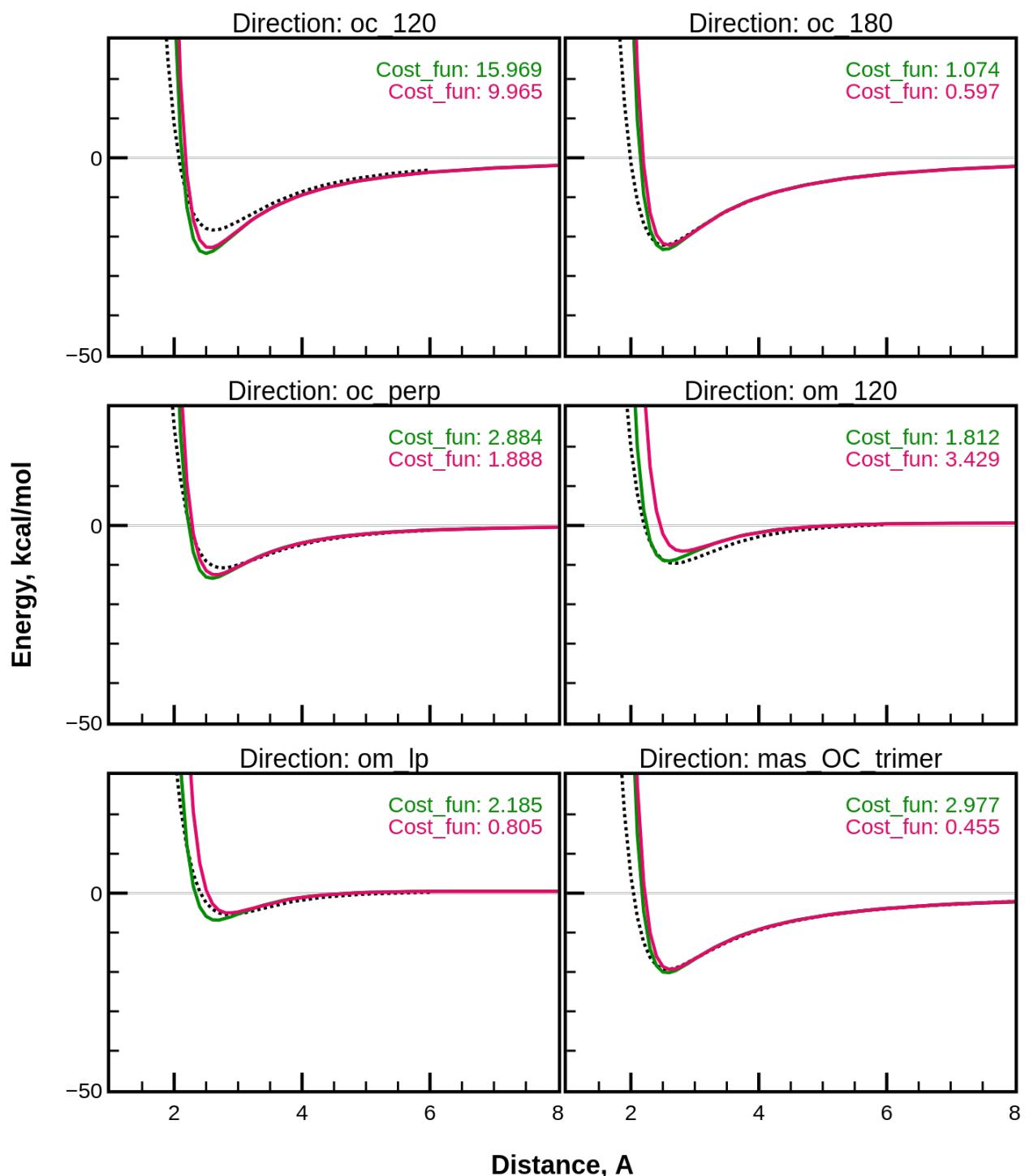


Energy, kcal/mol

Distance, Å

MAS POT 1/2

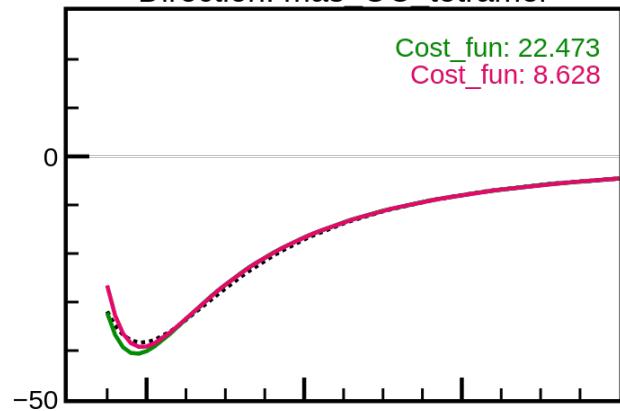
3.43665_0.15983_9.99999
3.49368_0.15983_2.83217

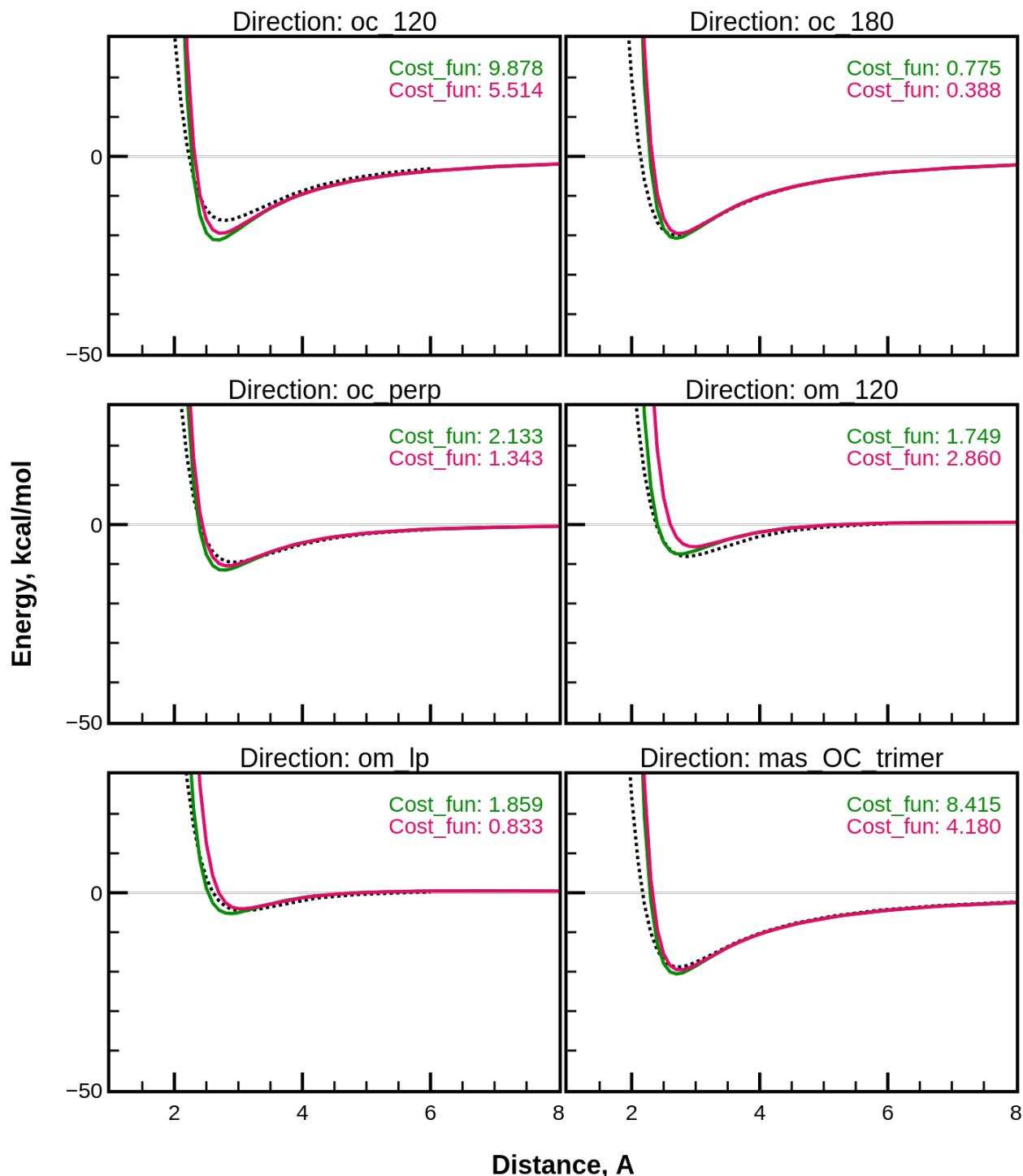


MAS POT 2/2

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

Direction: mas OC tetramer

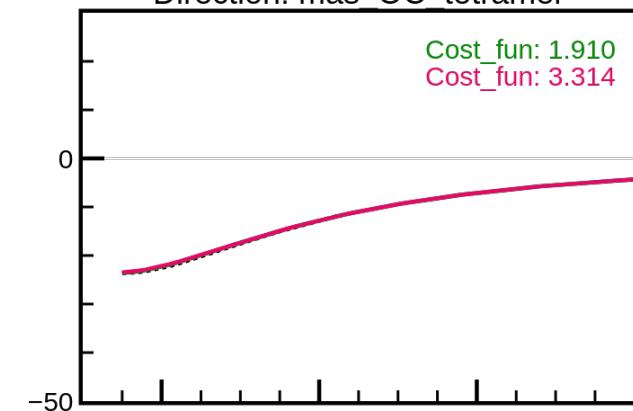


MAS RUB 1/23.53551_0.22170_9.99999
3.55885_0.22170_1.61222

MAS RUB 2/2

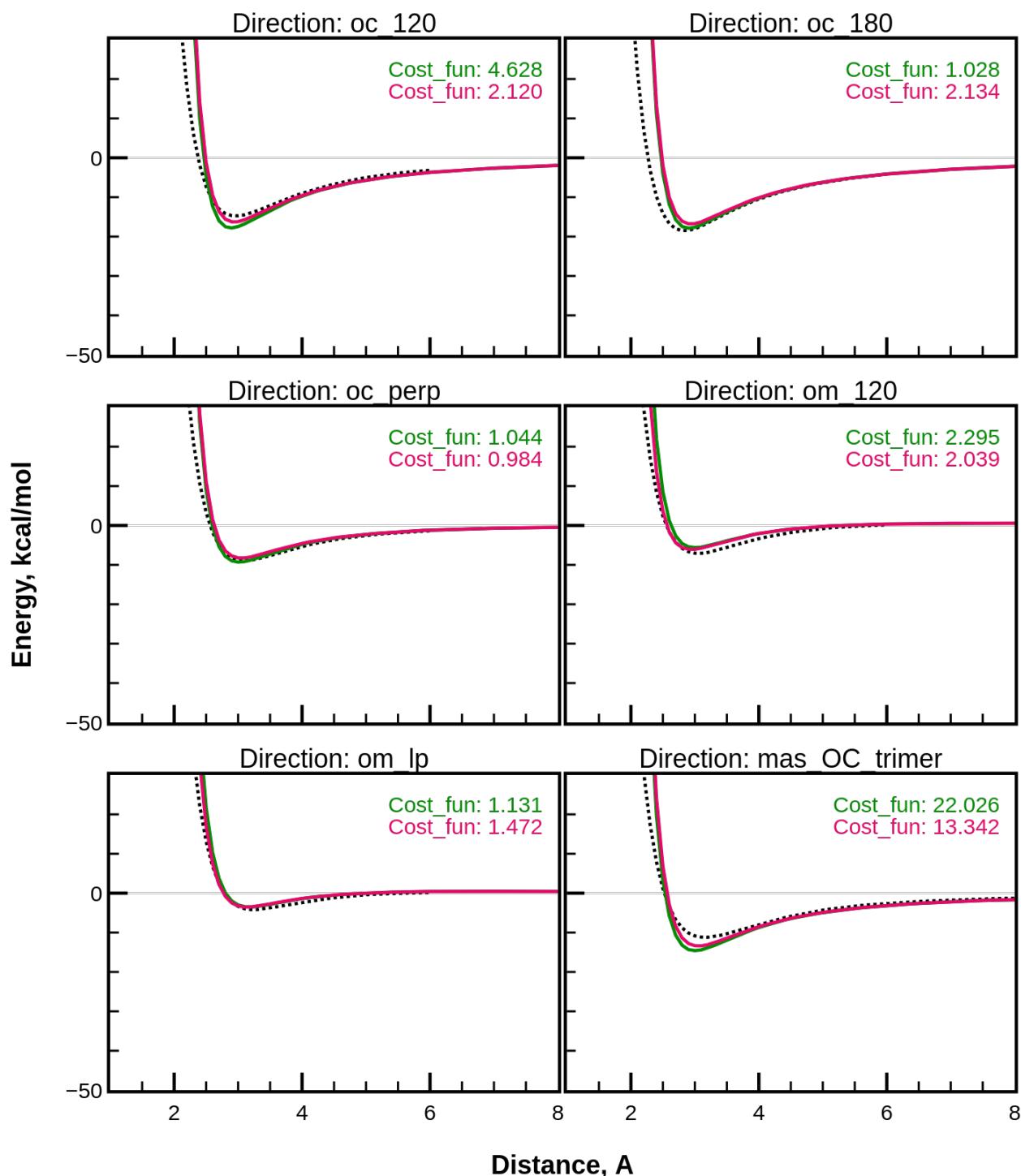
3.53551_0.22170_9.99999
3.55885_0.22170_1.61222

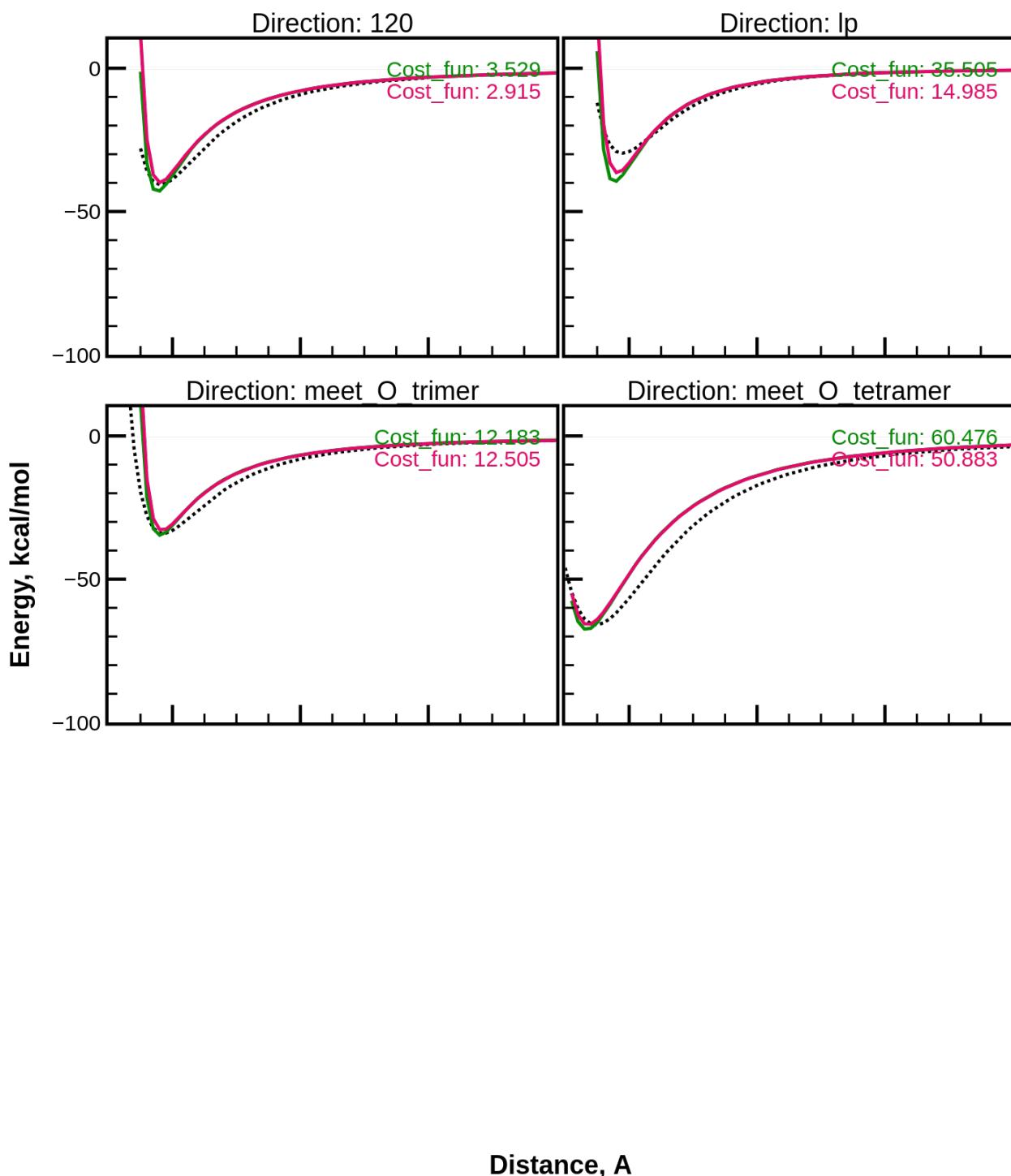
Direction: mas OC tetramer



Distance, Å

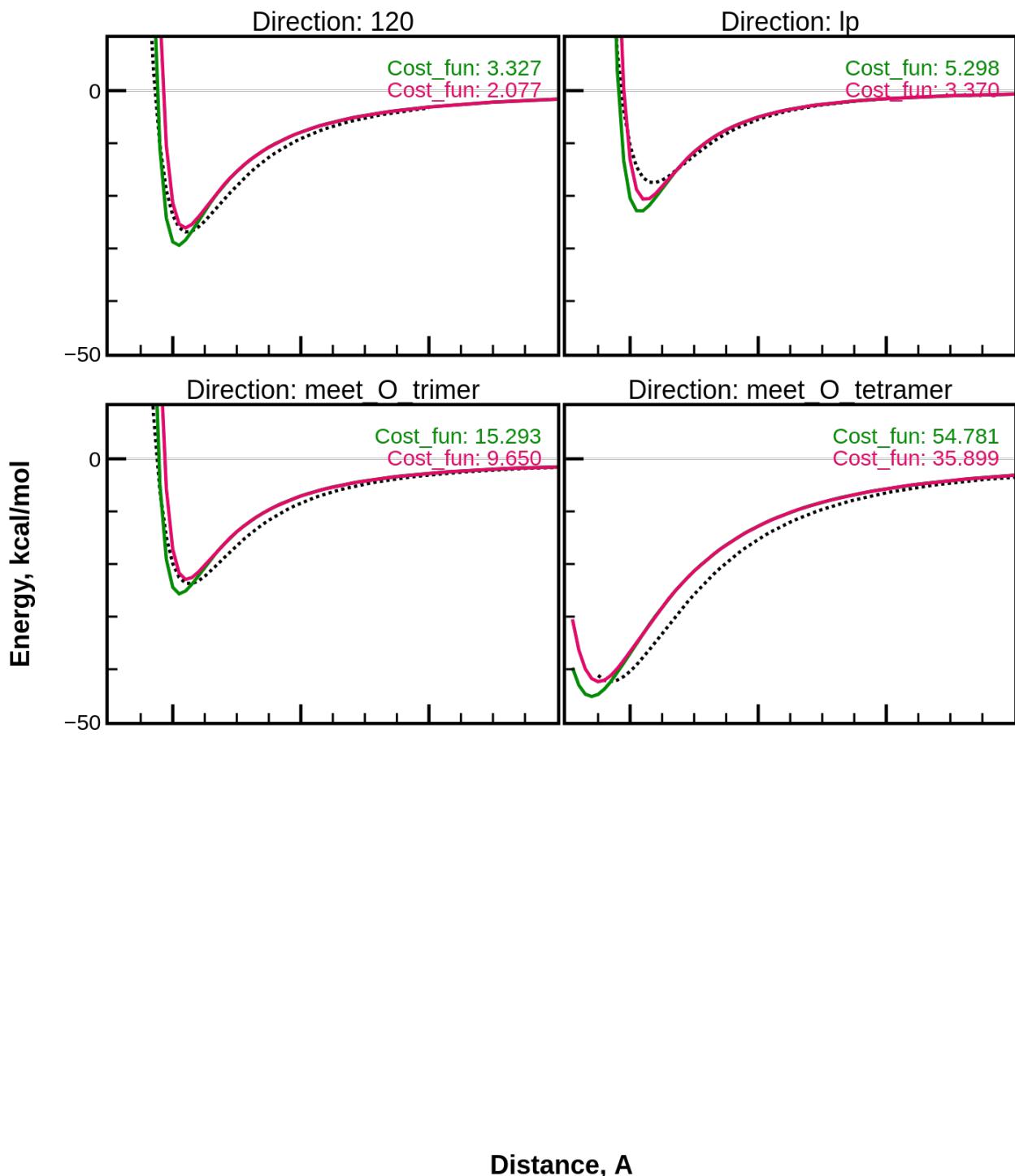
Energy, kcal/mol

MAS CES 1/13.77382_0.22313_9.99999
3.76247_0.22313_1.03679

MEET LIT 1/12.84000_0.04243_9.99999
2.83896_0.04243_1.67374

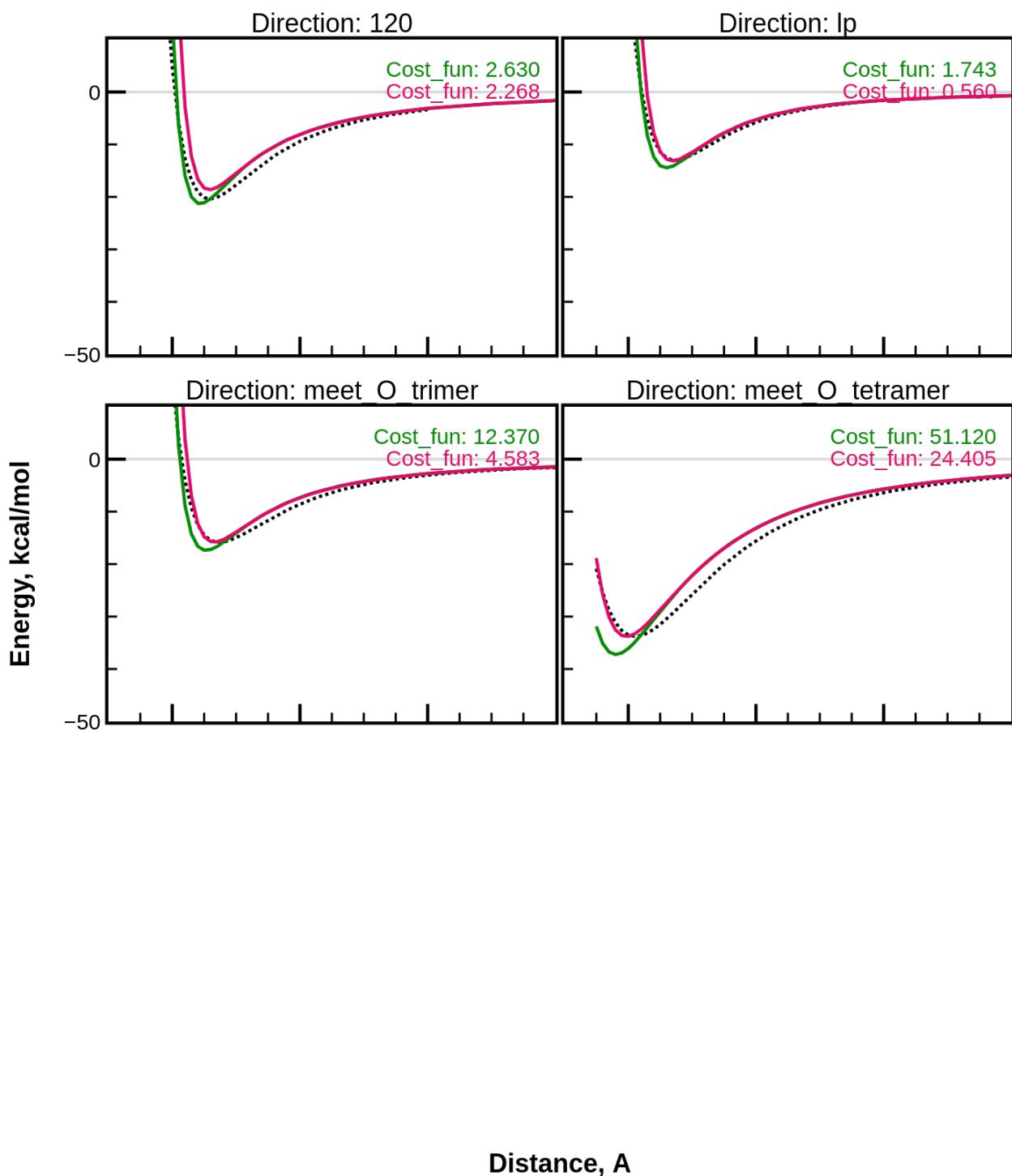
MEET SOD 1/1

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



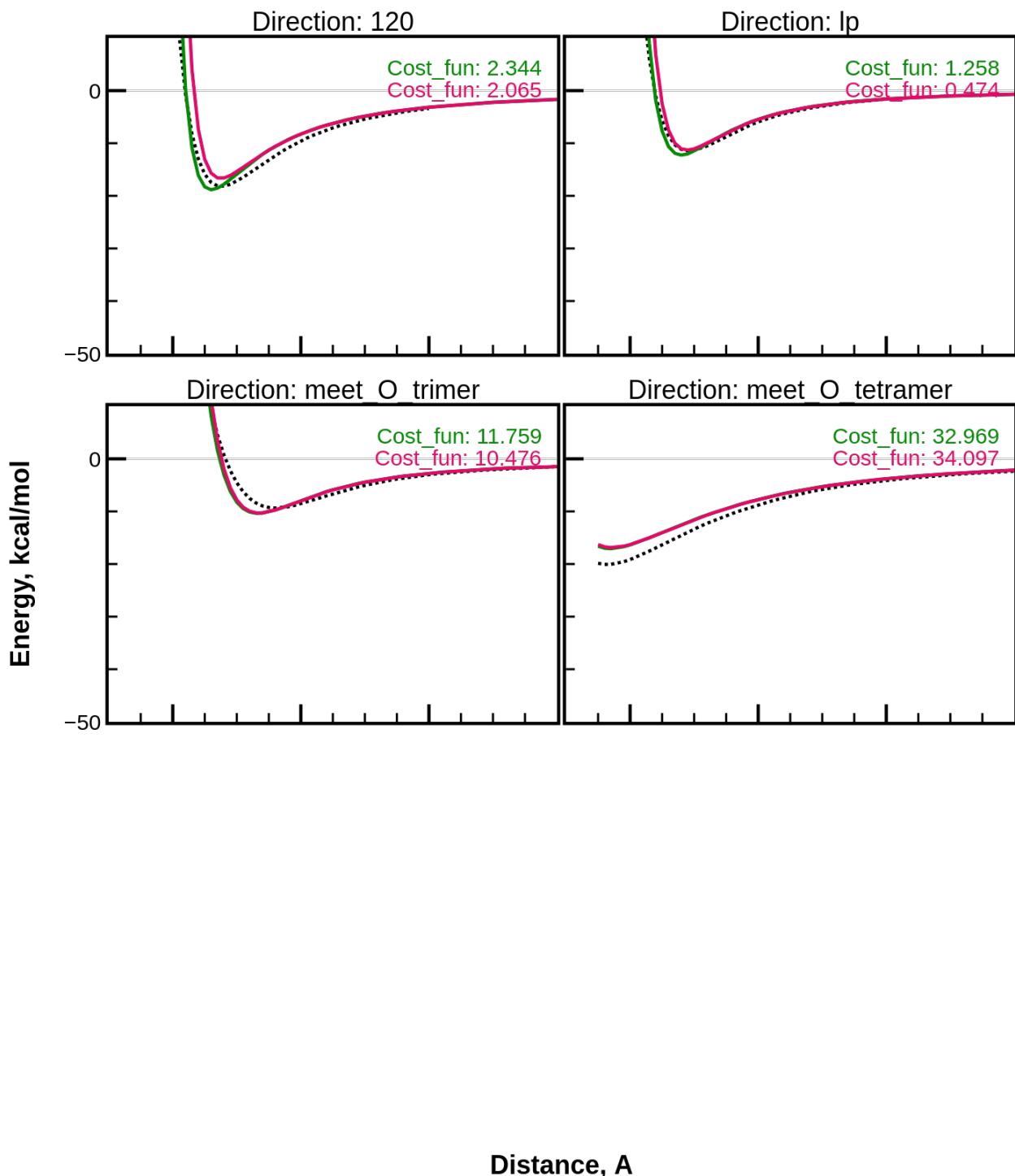
MEET POT 1/1

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



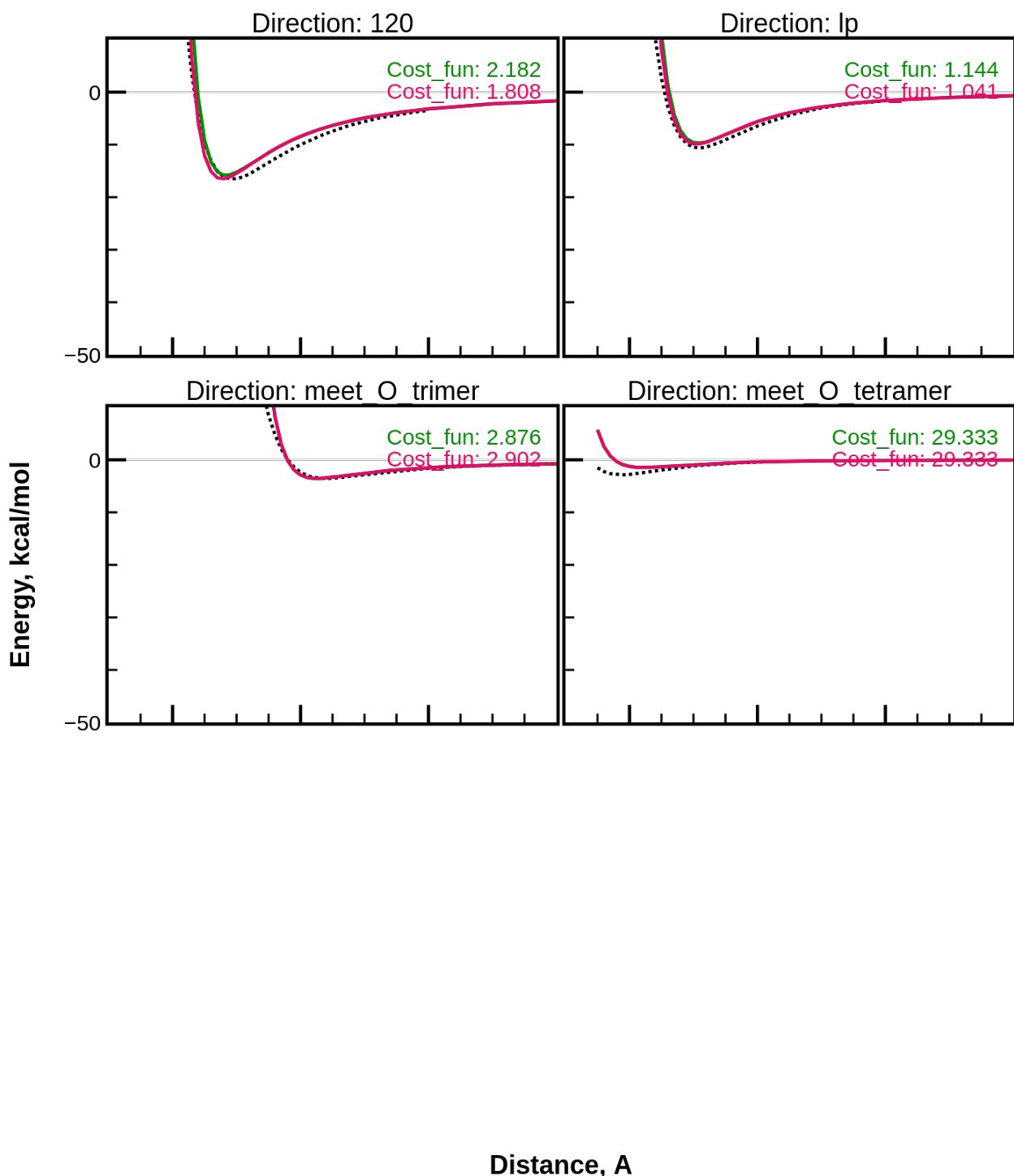
MEET RUB 1/1

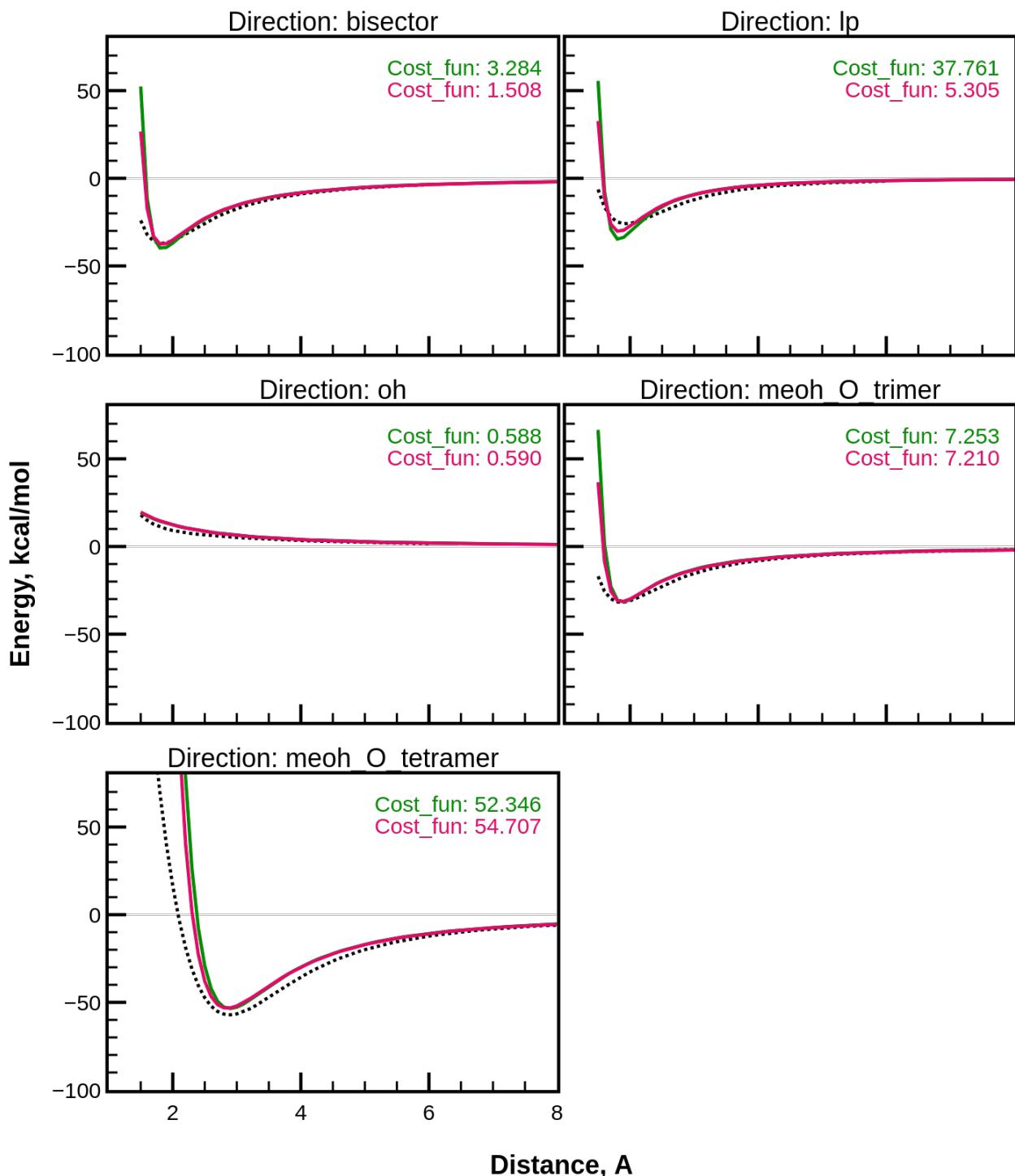
3.52551_0.12800_9.99999
3.69056_0.12800_3.56696

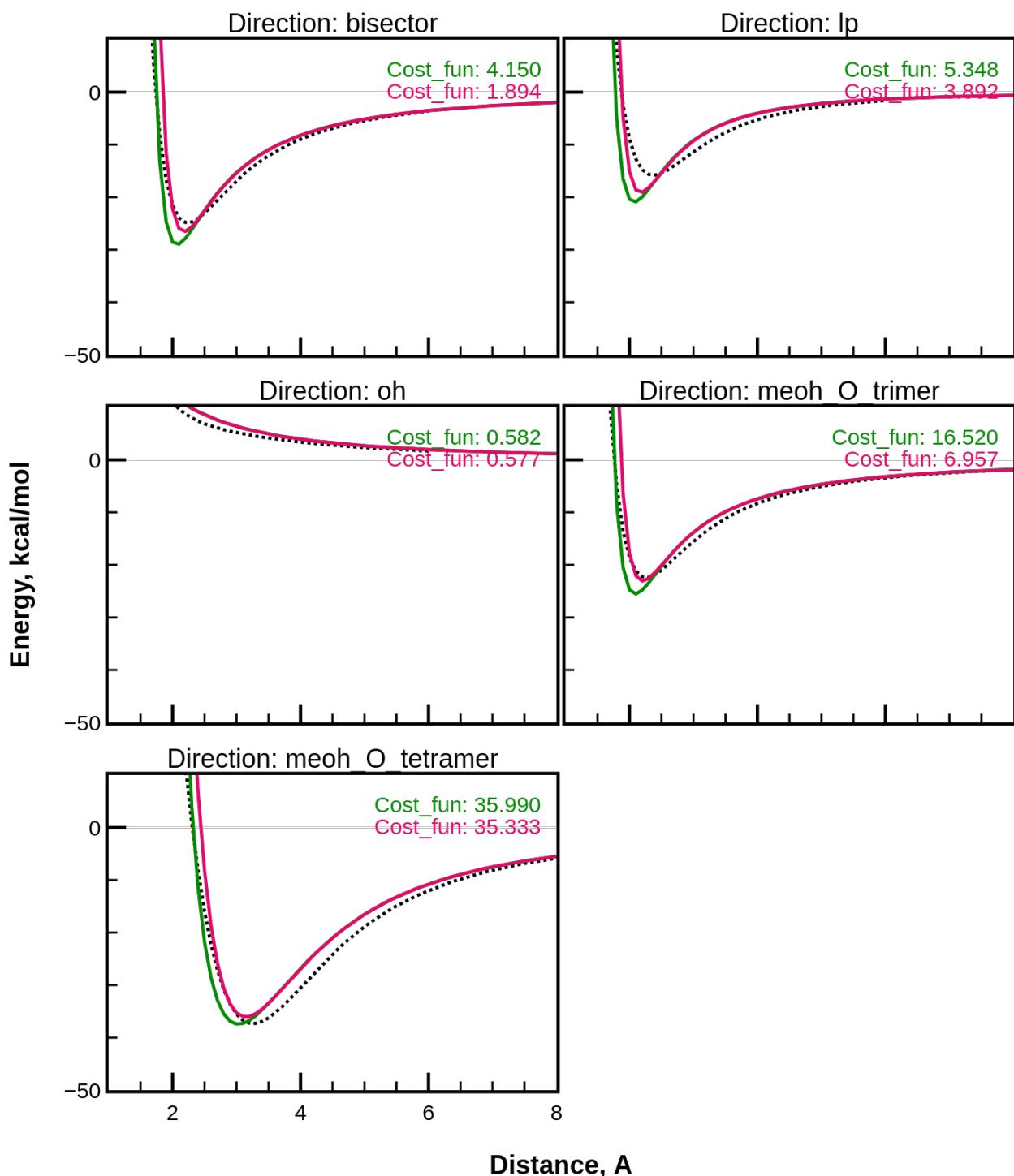


MEET CES 1/1

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

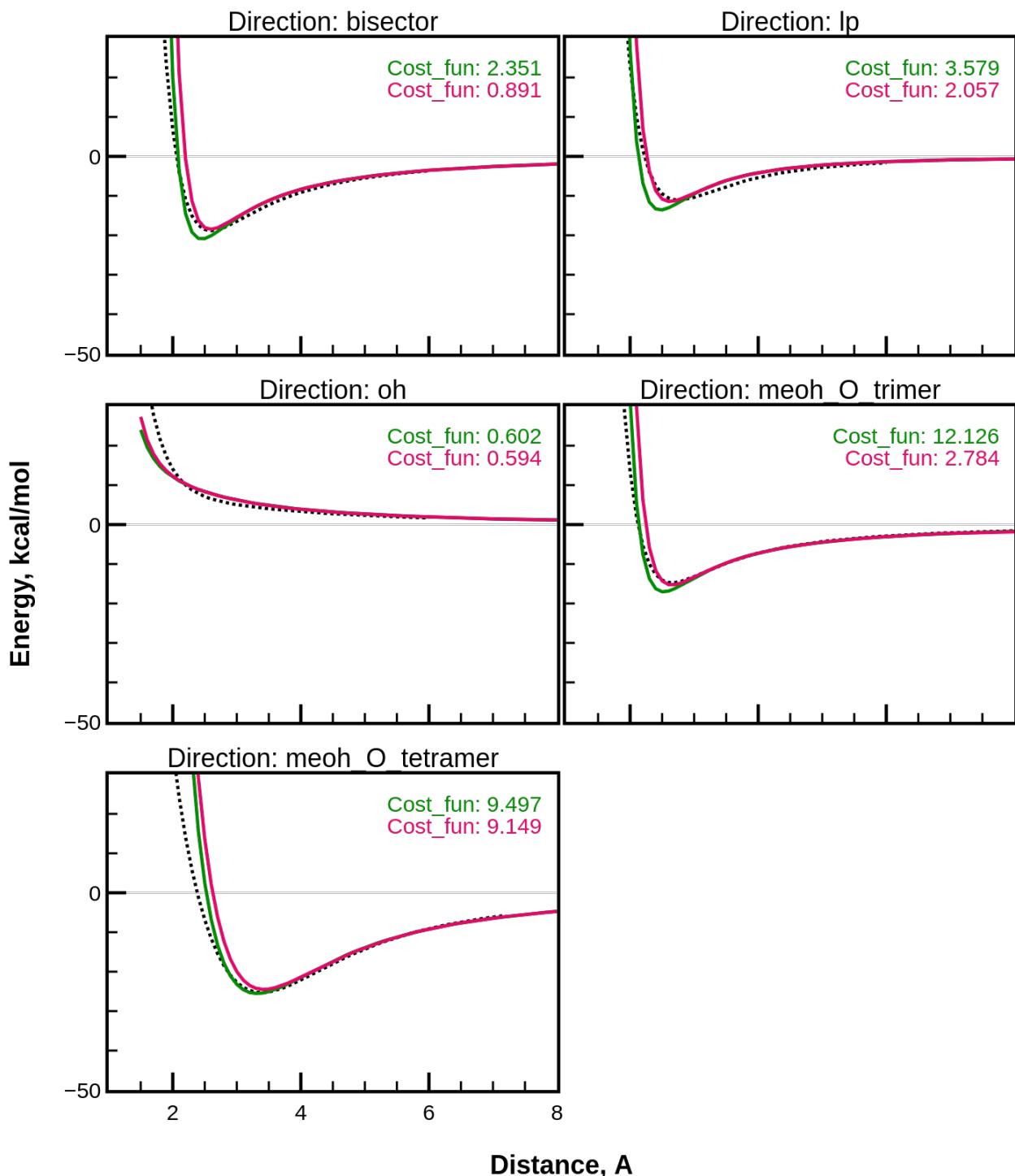


MEOH LIT 1/12.86500_0.06708_9.99999
2.76202_0.06708_1.45978

MEOH SOD 1/13.07000_0.06000_1.82000
3.21654_0.06780_2.59341

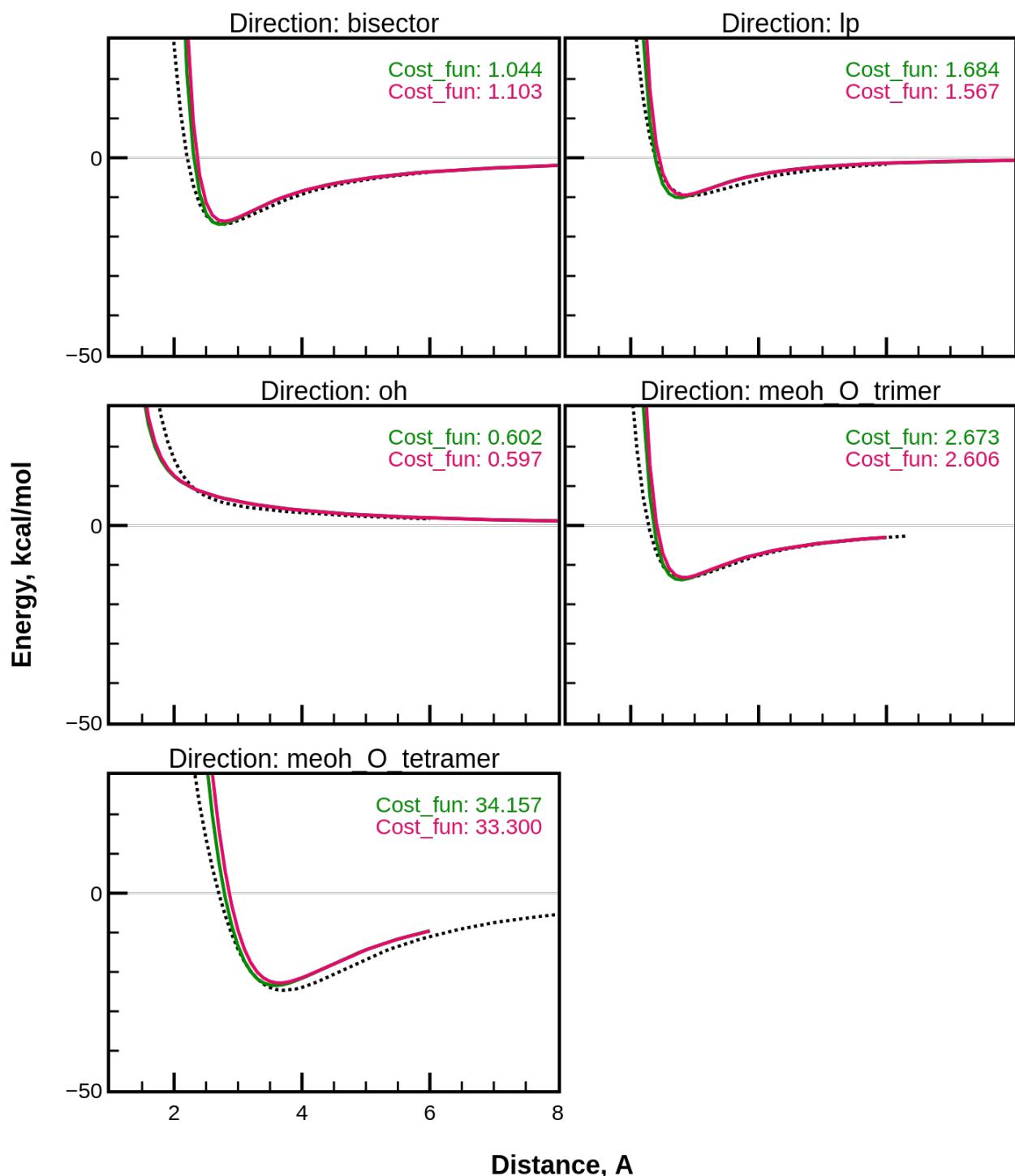
MEOH POT 1/1

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



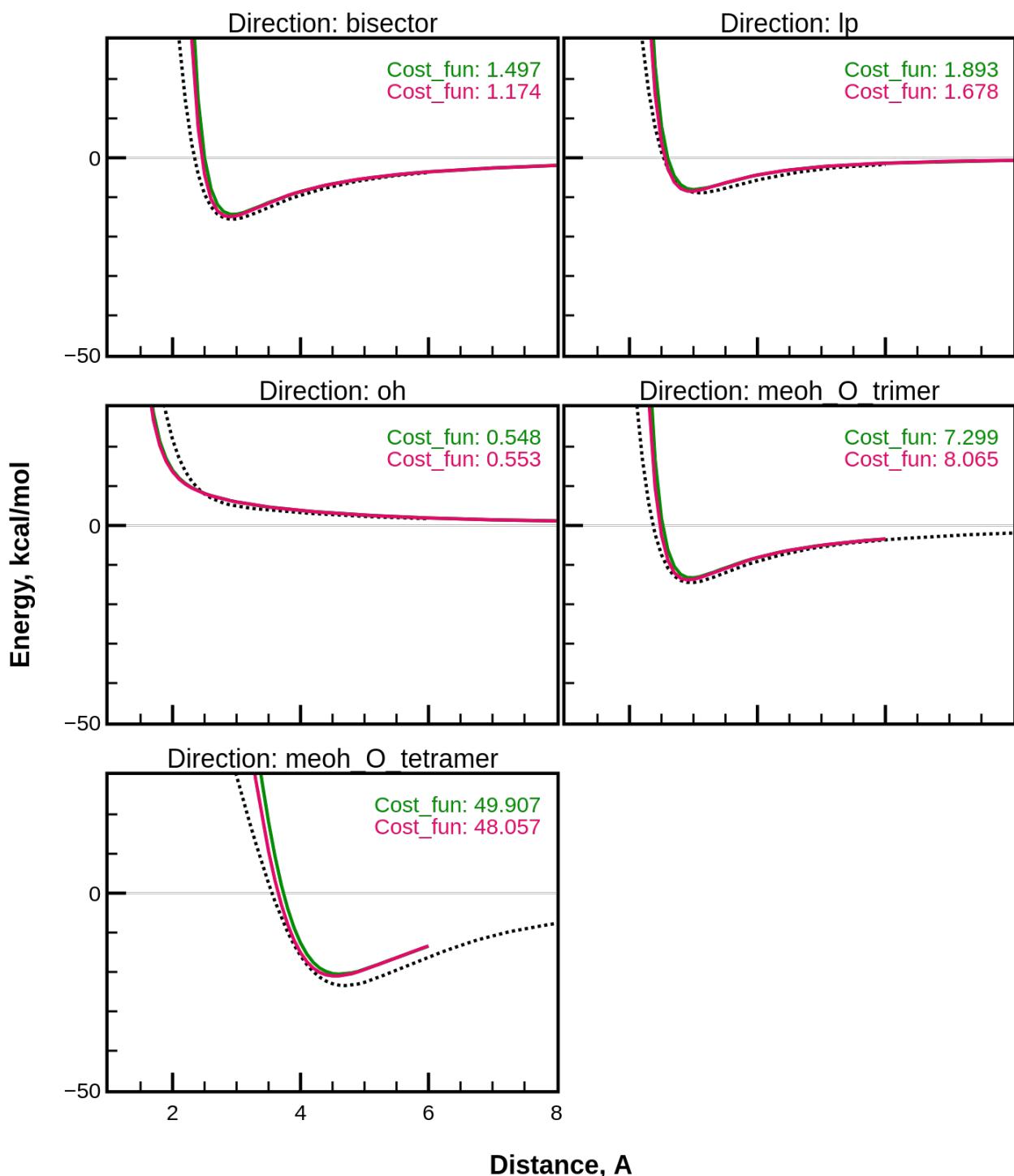
MEOH RUB 1/1

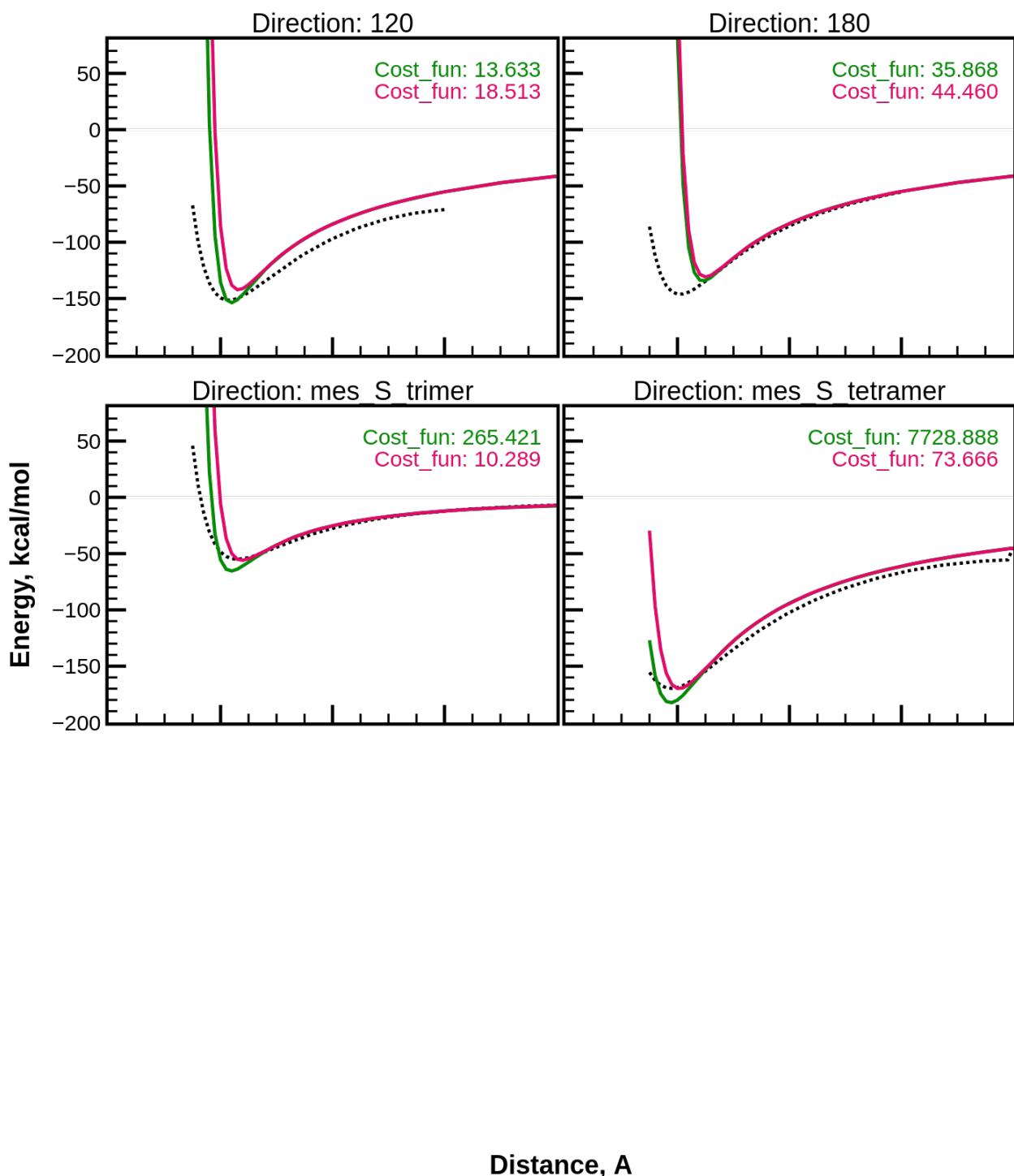
3.55051_0.20239_9.99999
3.61044_0.20239_3.86775



MEOH CES 1/1

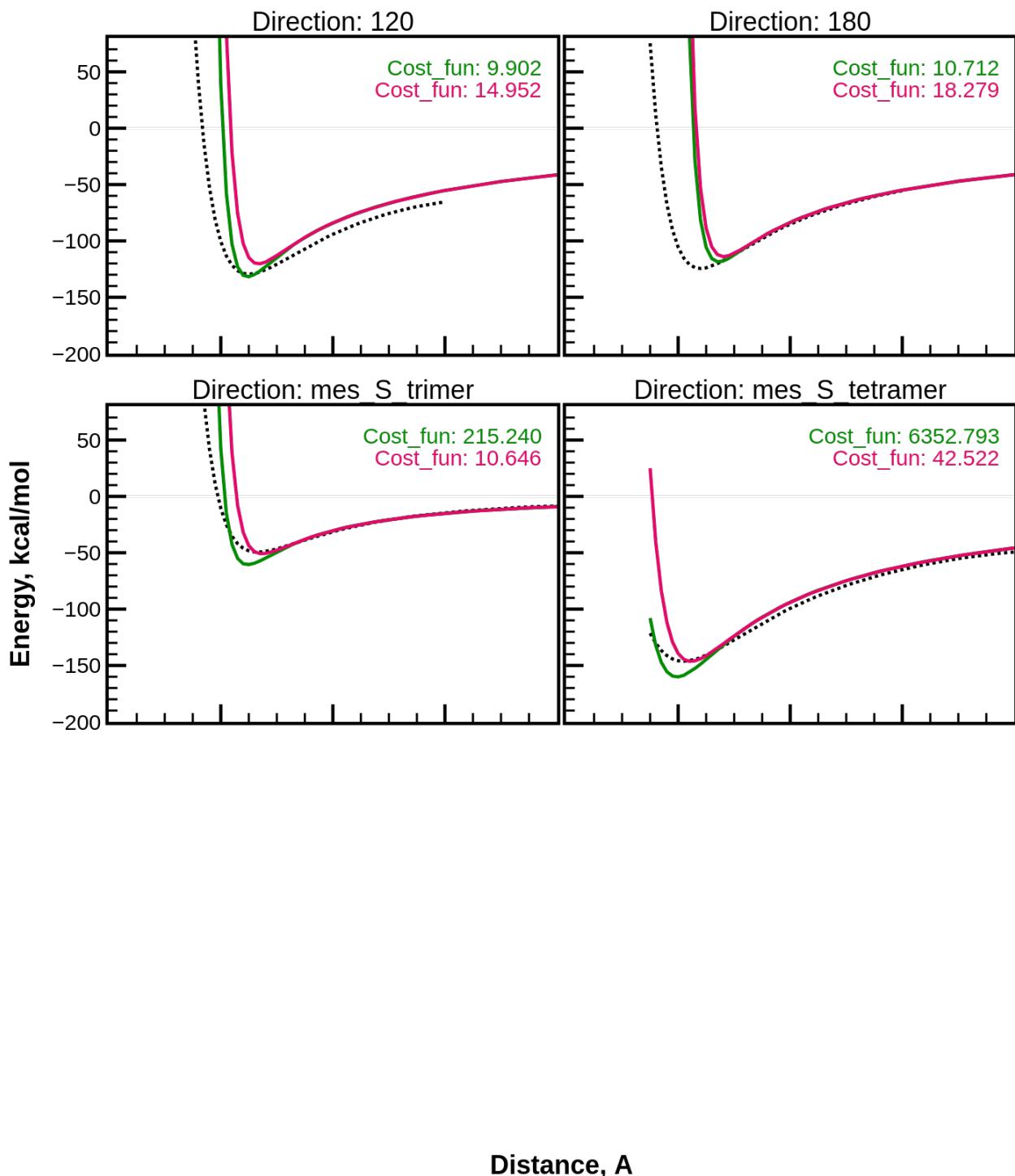
3.78882_0.20369_9.99999
3.73546_0.20369_4.77880



MES LIT 1/13.27000_0.07746_9.99999
3.56646_0.07746_3.08189

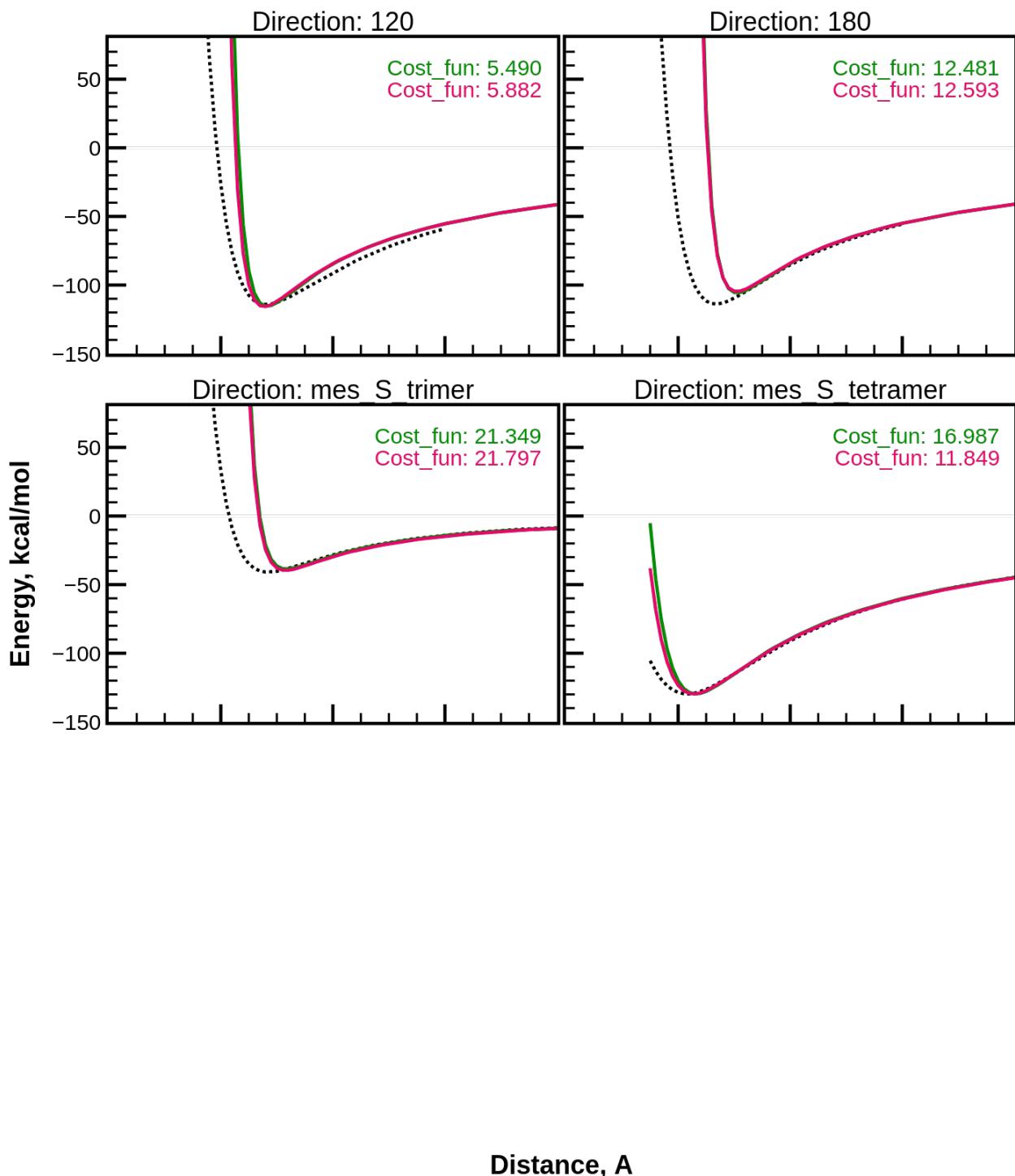
MES SOD 1/1

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



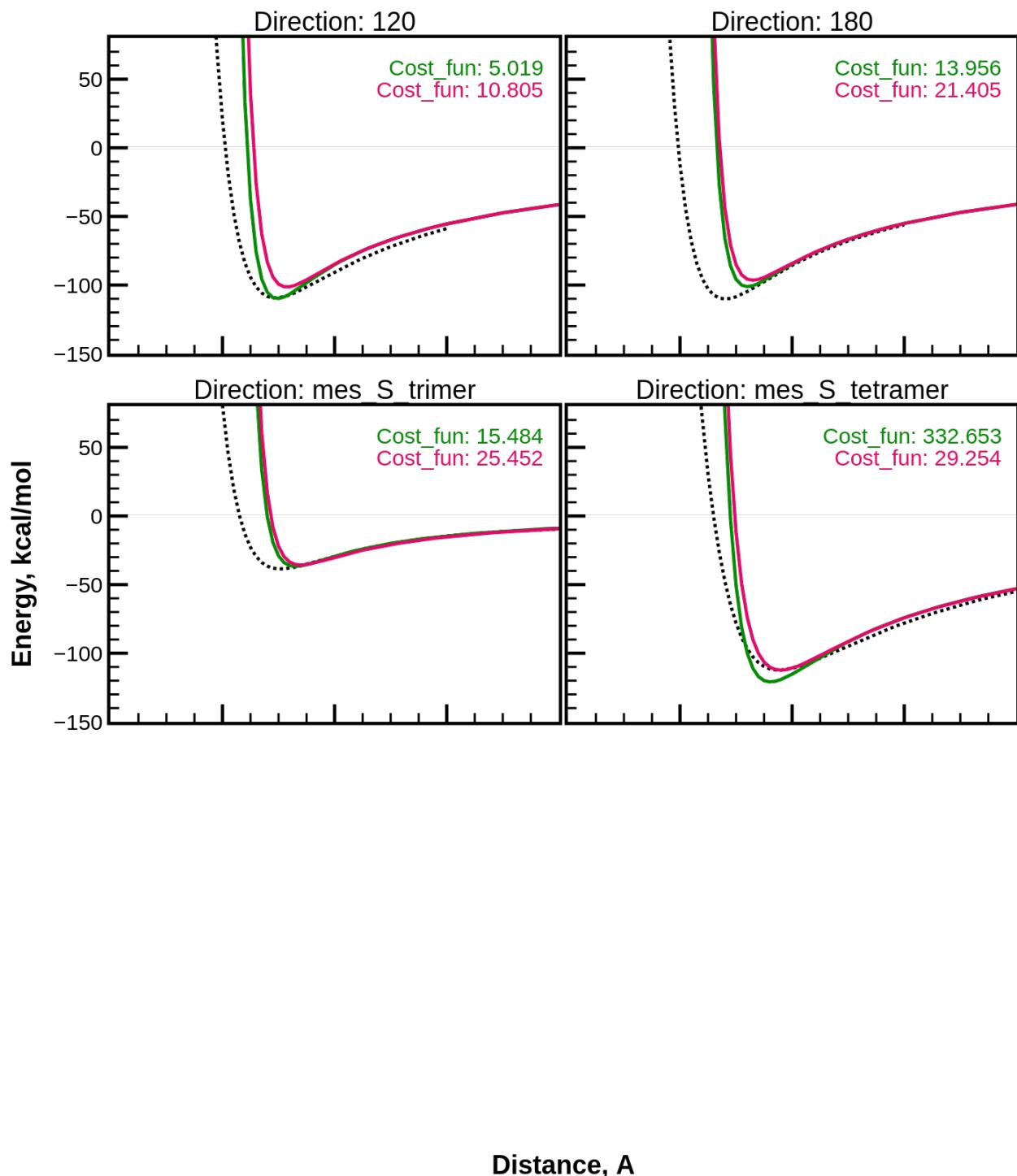
MES POT 1/1

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



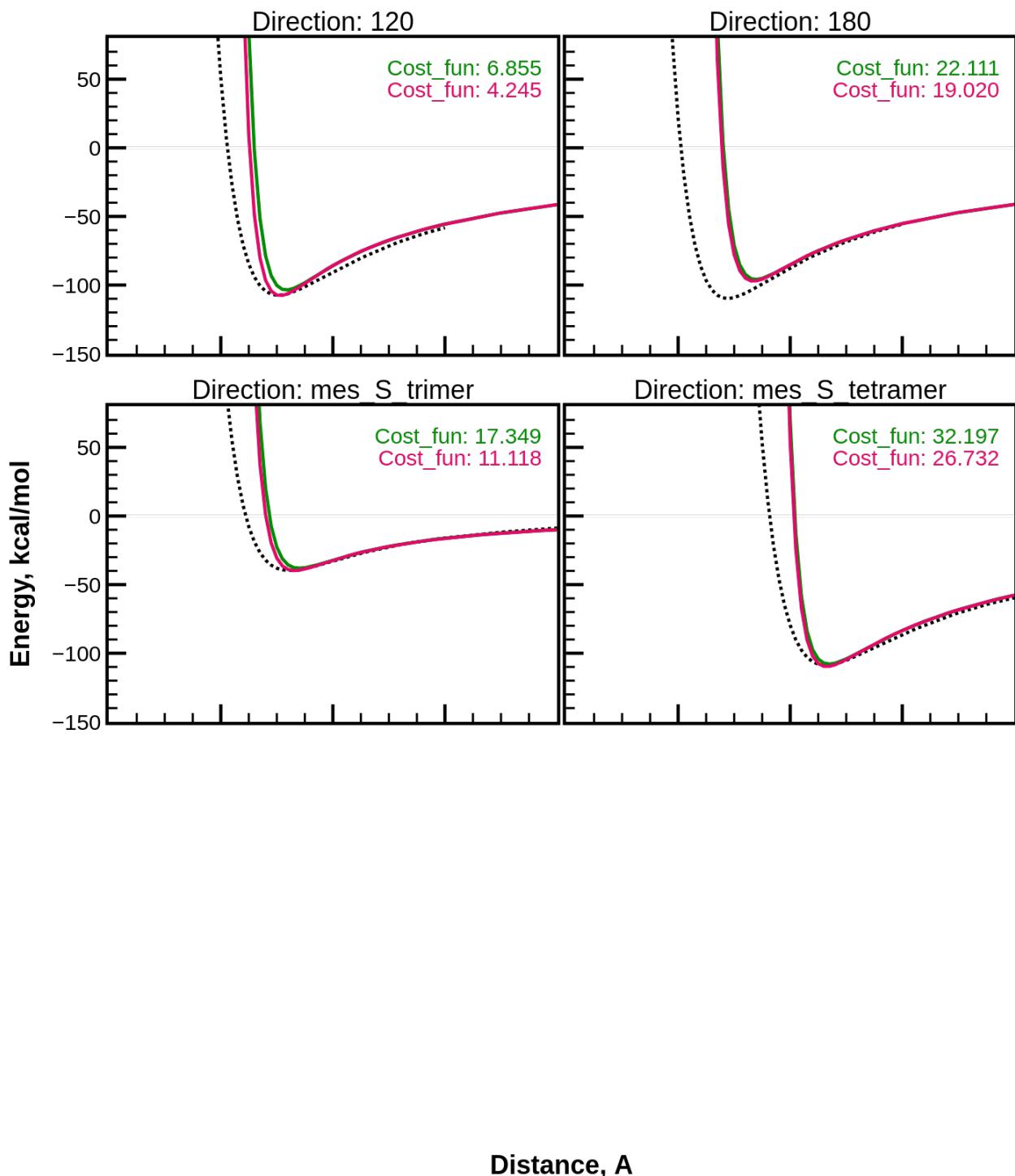
MES RUB 1/1

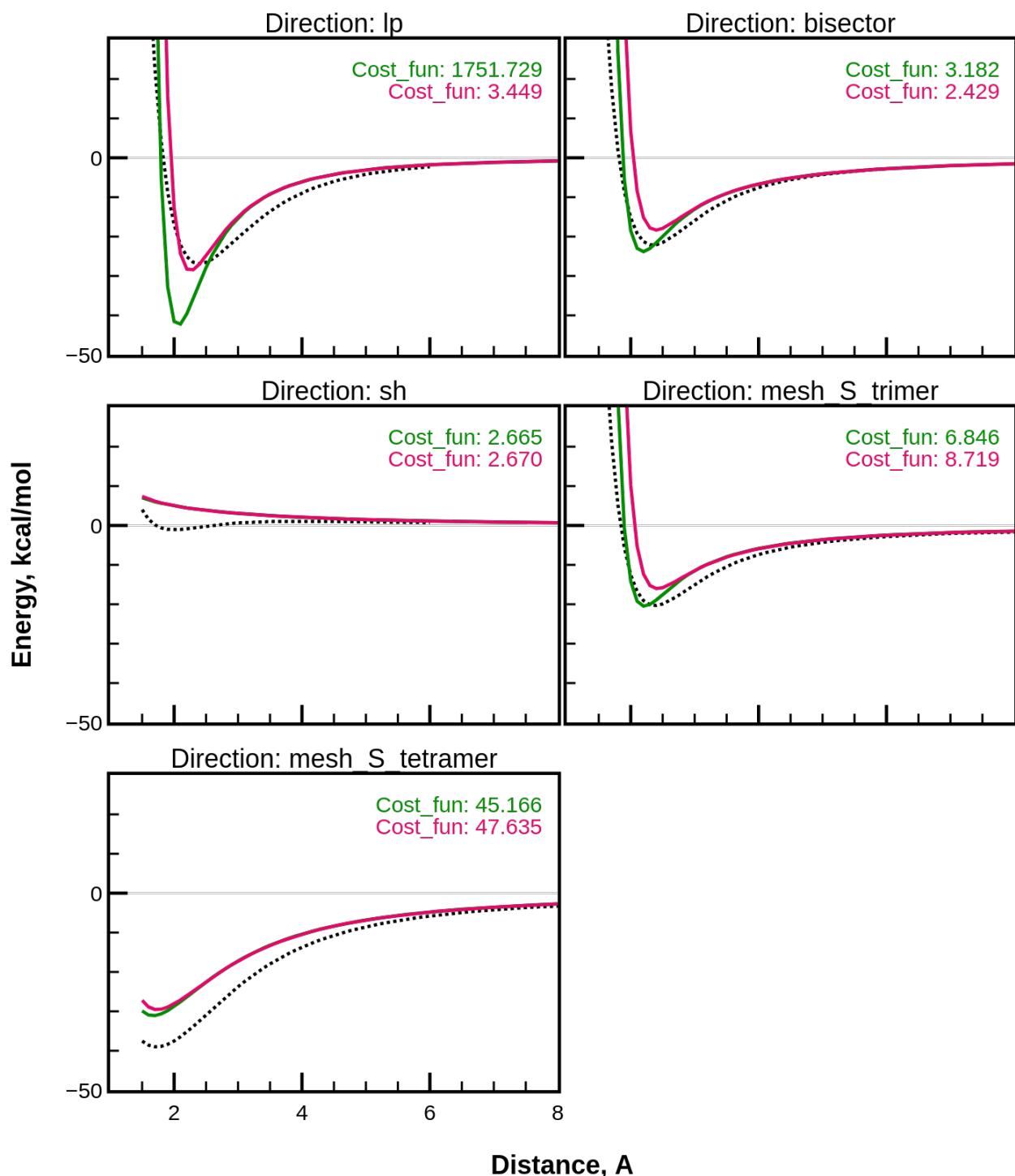
3.95551_0.23370_9.99999
4.21446_0.23370_2.09814

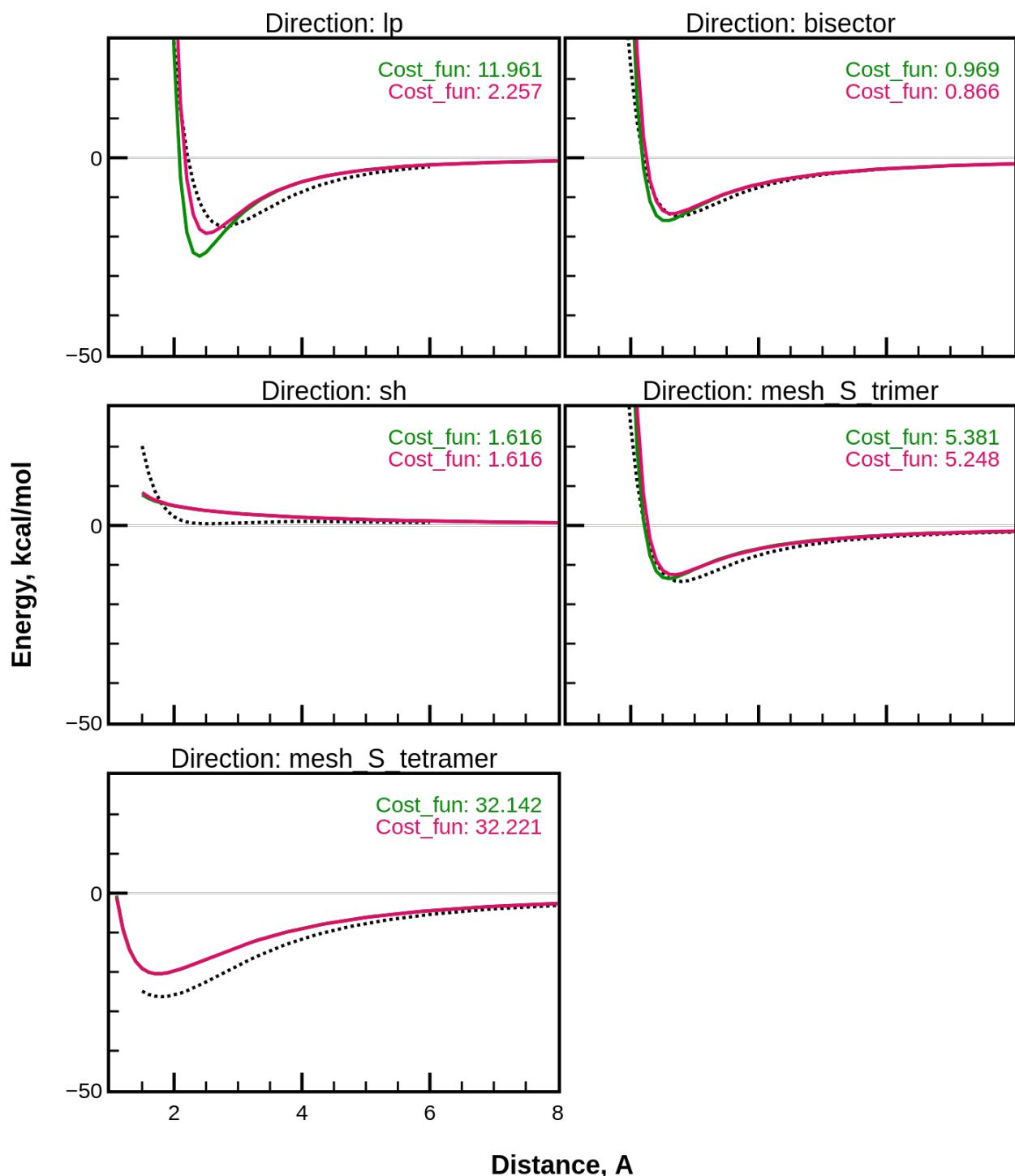


MES CES 1/1

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

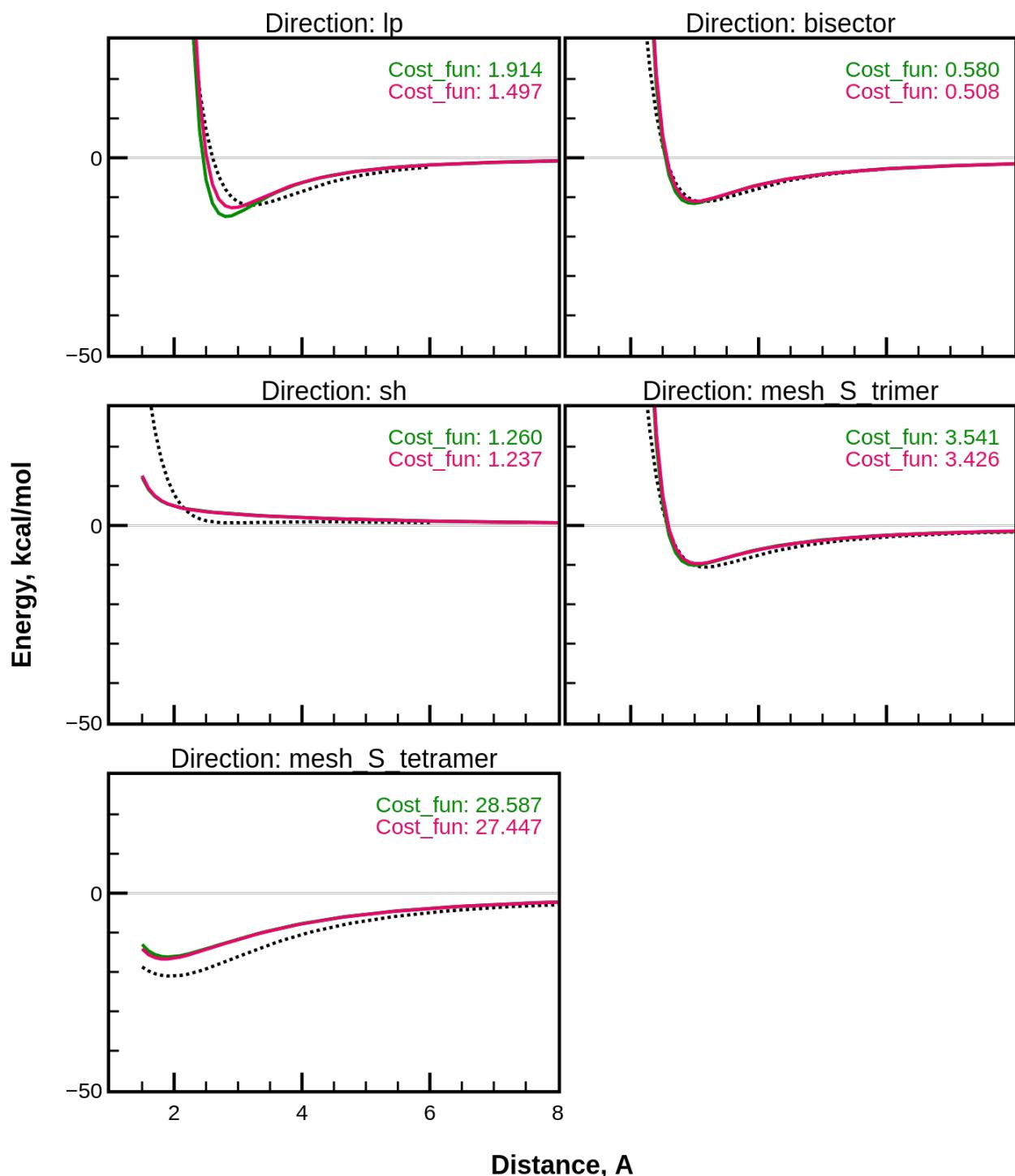


MESH LIT 1/13.15000_0.11358_9.99999
3.29425_0.11358_1.52517

MESH SOD 1/13.51168_0.11640_9.99999
3.52978_0.11640_1.51323

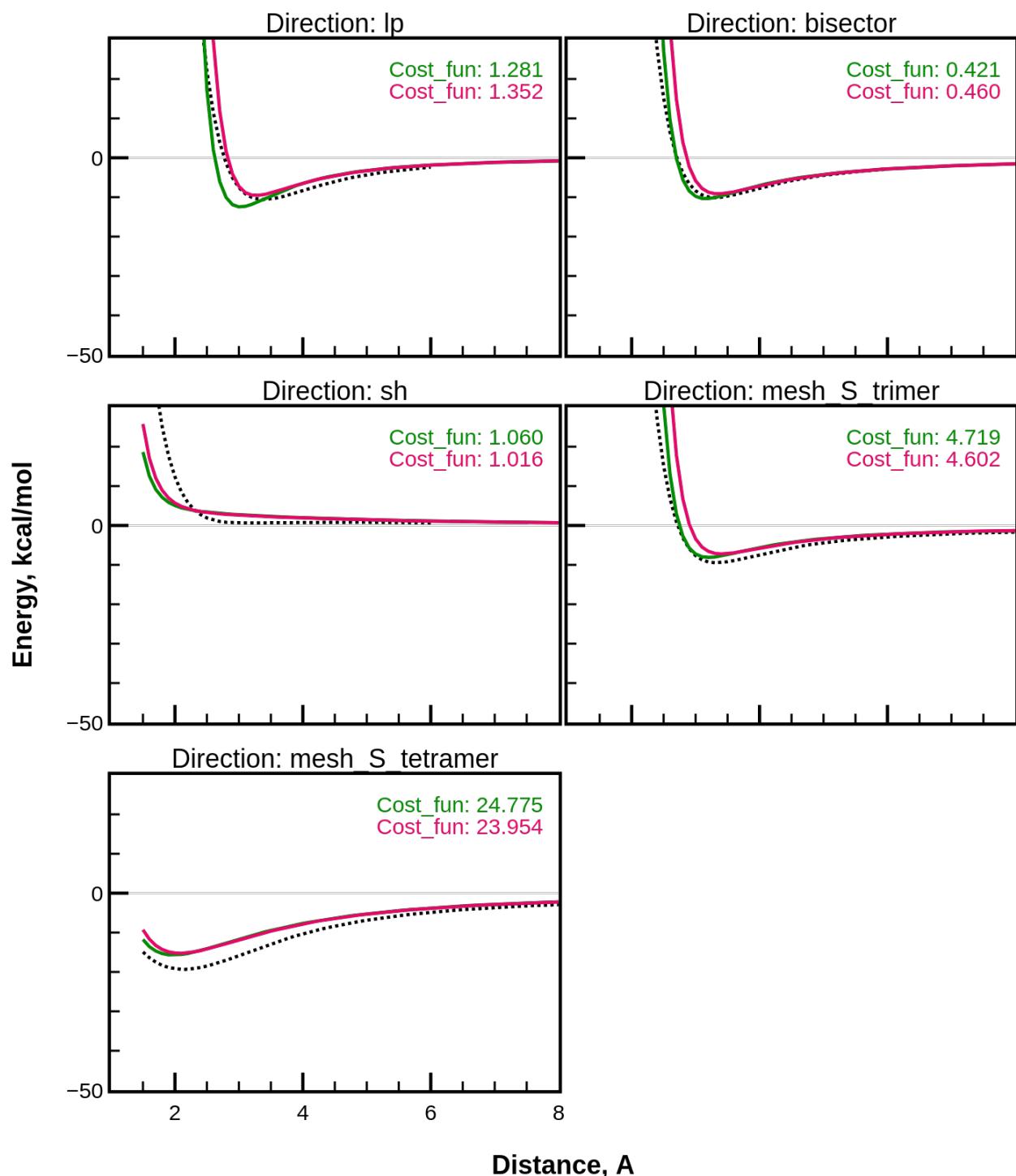
MESH POT 1/1

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



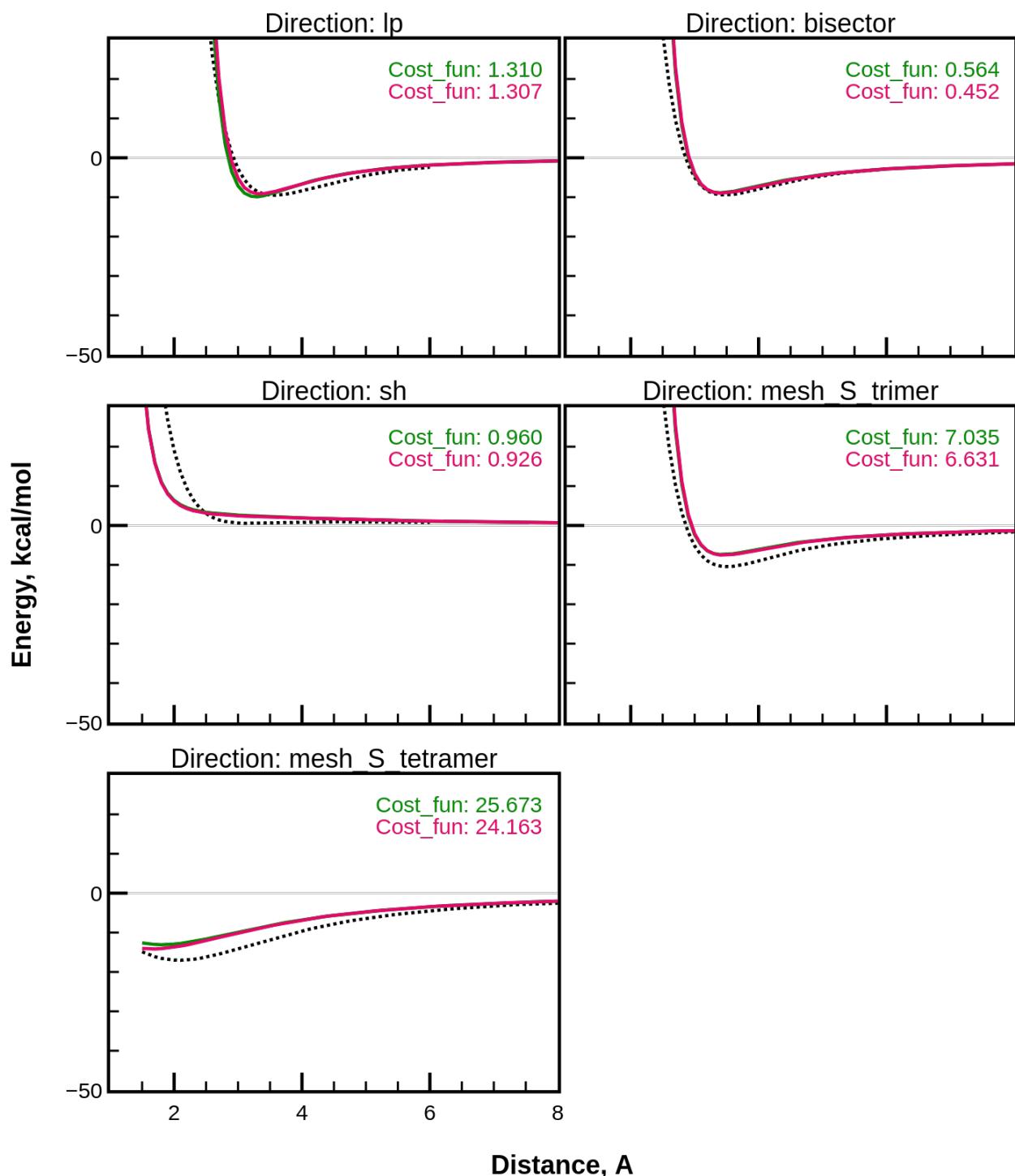
MESH RUB 1/1

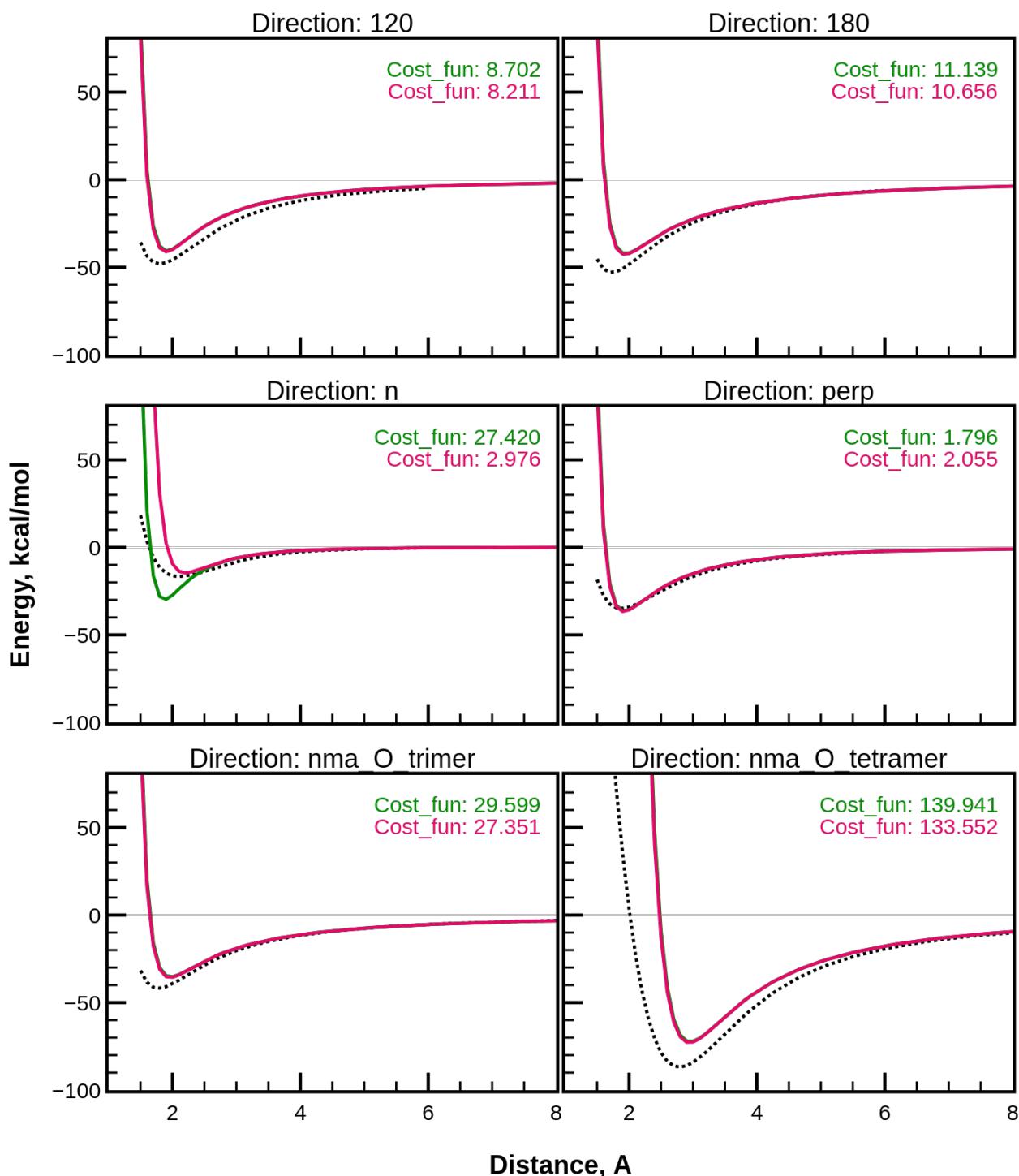
3.83551_0.34266_9.99999
3.99694_0.34266_1.51324

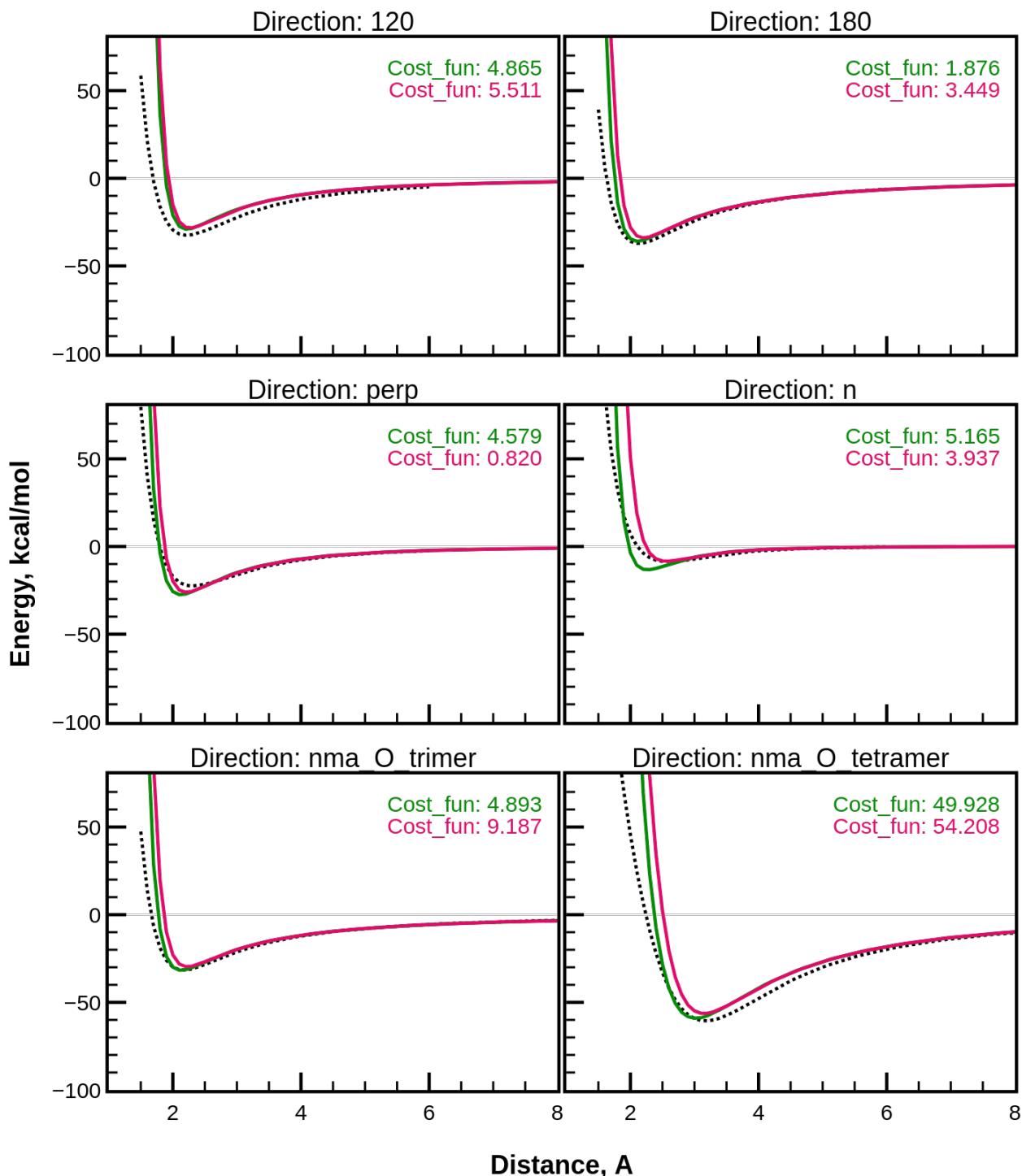


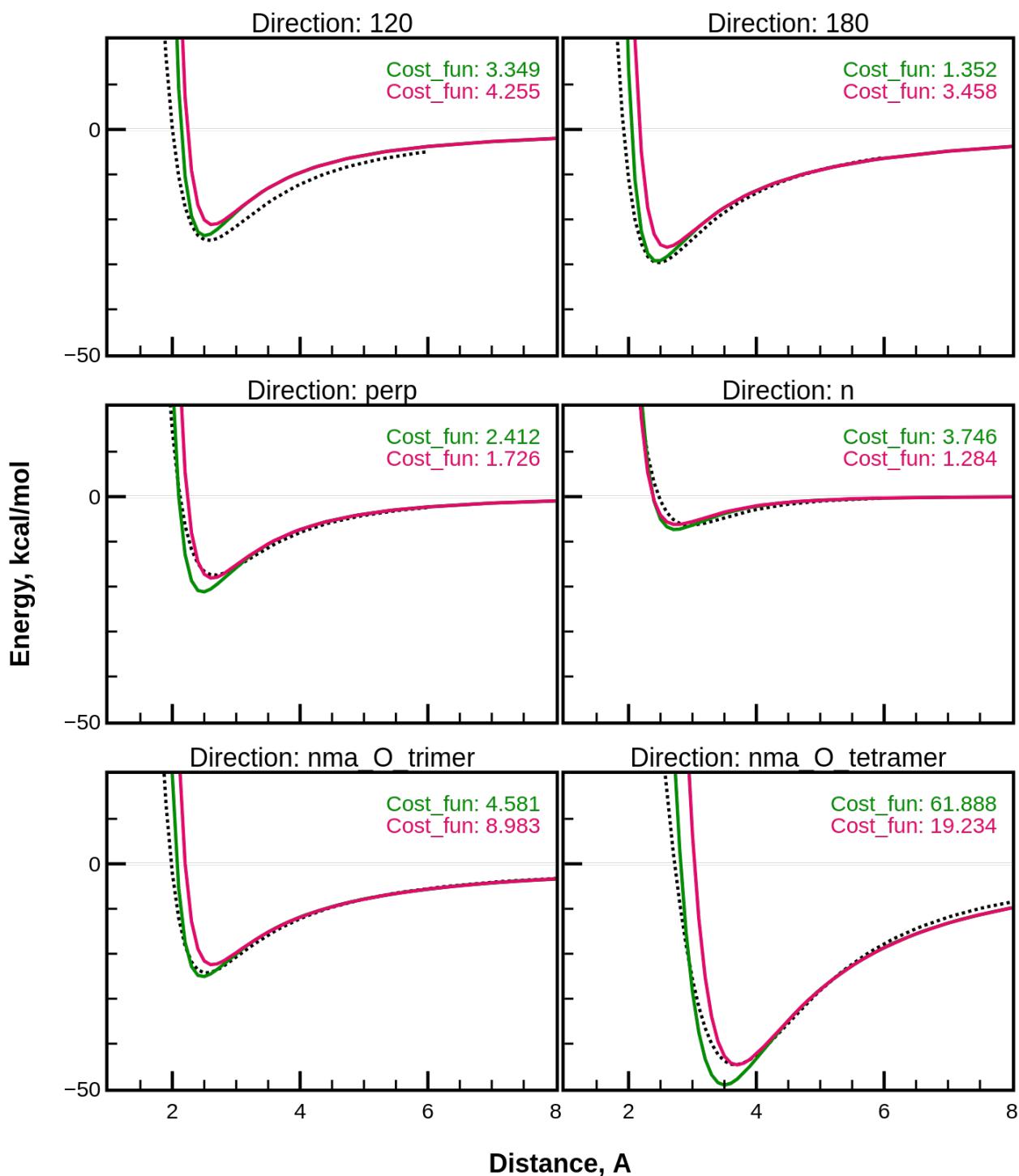
MESH CES 1/1

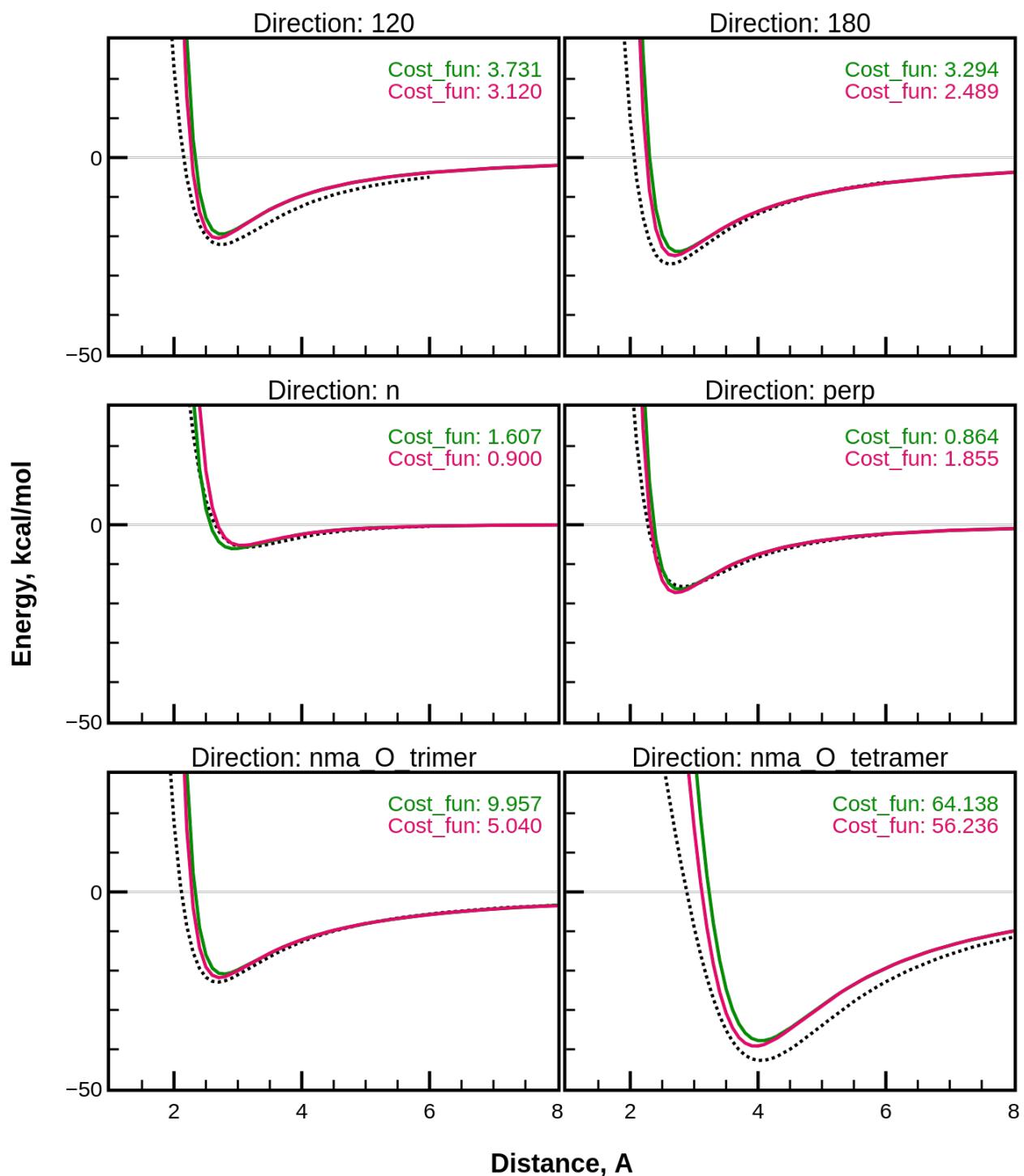
4.07382_0.34488_9.99999
4.06835_0.34488_1.50014

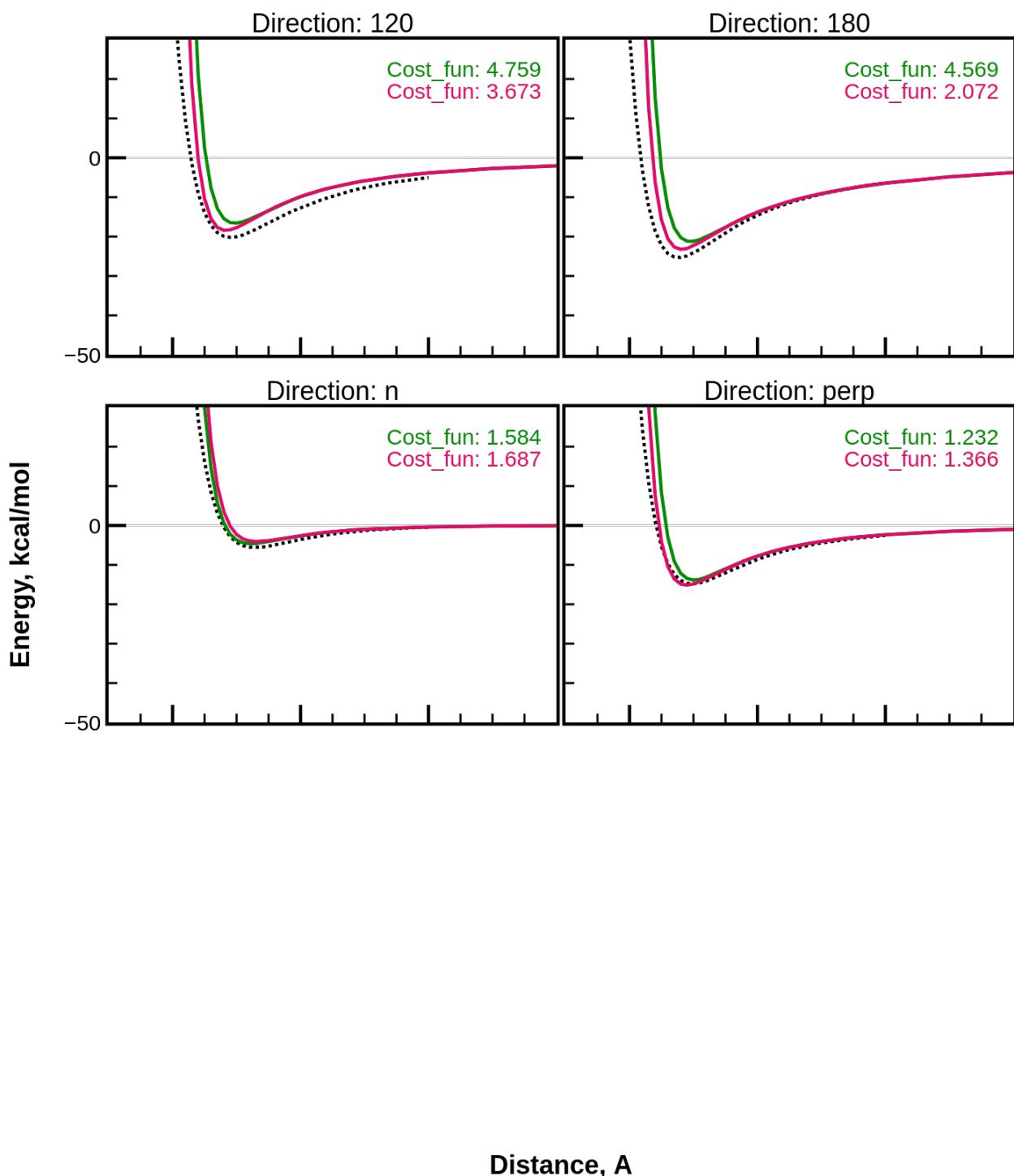


NMA LIT 1/12.88000_0.07746_9.99999
2.86833_0.07746_4.93098

NMA SOD 1/12.88000_0.09000_1.04000
3.11051_0.07939_1.54864

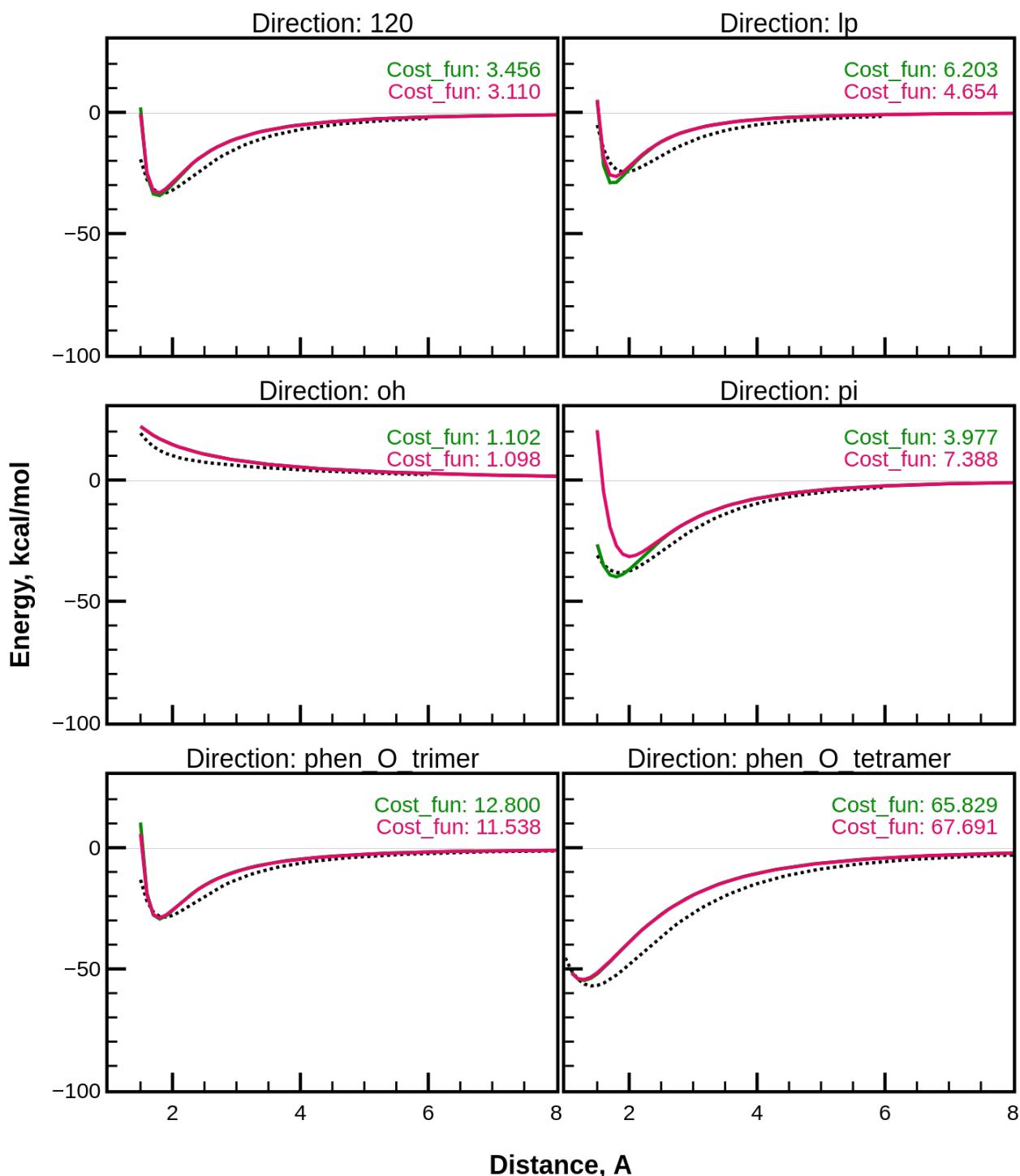
NMA POT 1/13.21000_0.18000_2.19000
3.43708_0.16848_2.09141

NMA RUB 1/13.56551_0.23370_9.99999
3.49474_0.23370_2.99829

NMA CES 1/13.80382_0.23520_9.99999
3.64357_0.23520_2.58963

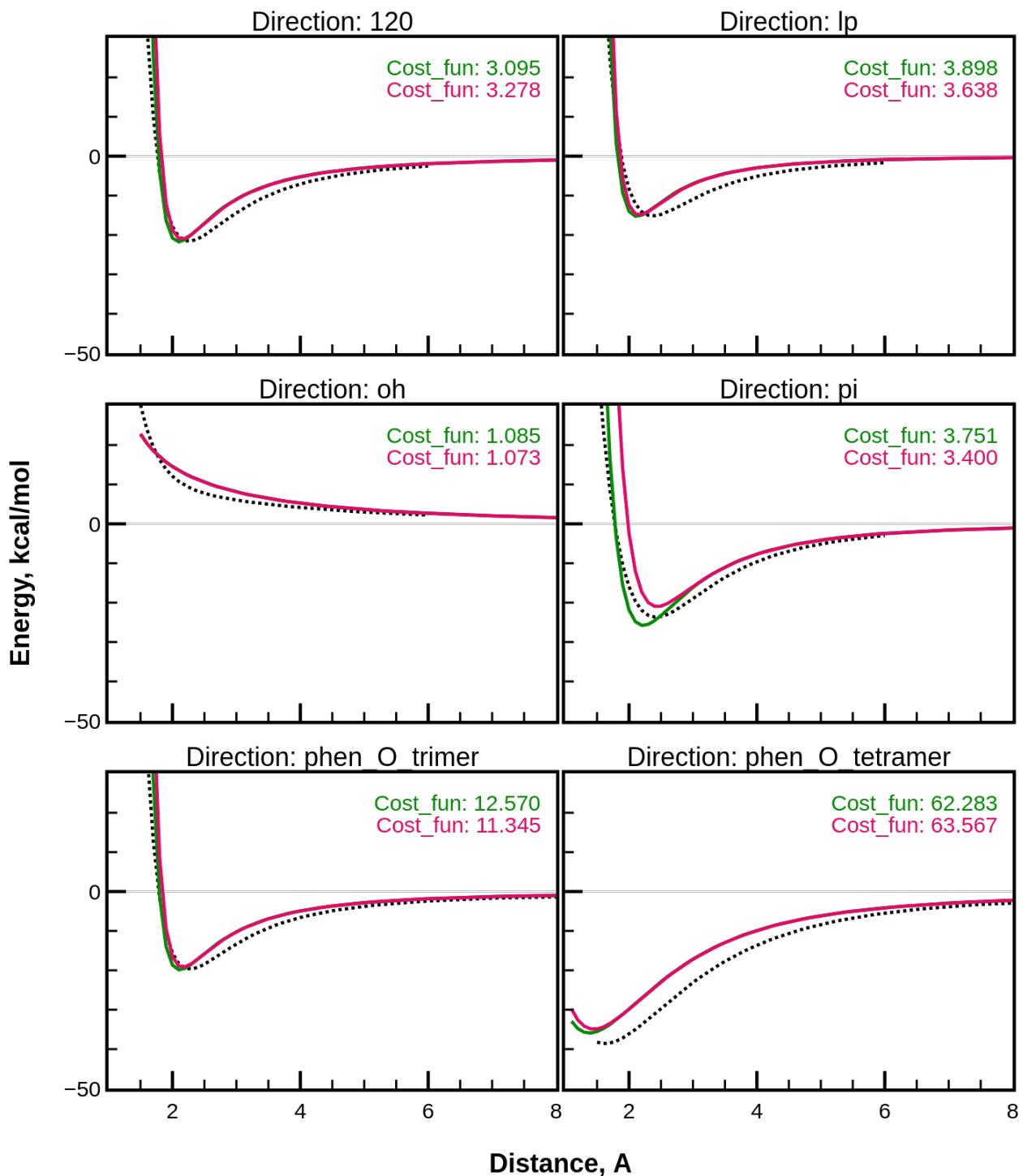
PHEN LIT 1/1

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



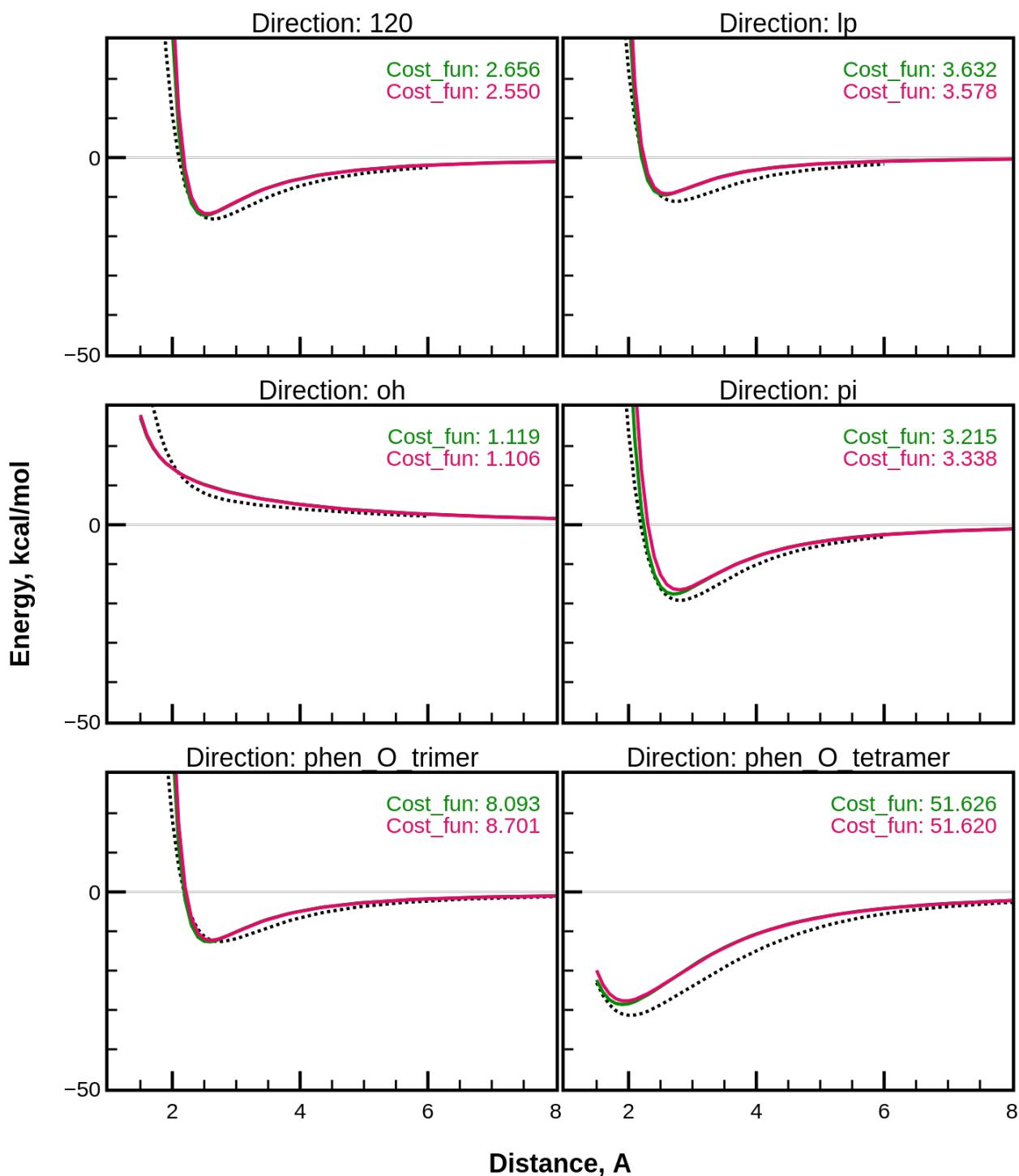
PHEN SOD 1/1

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



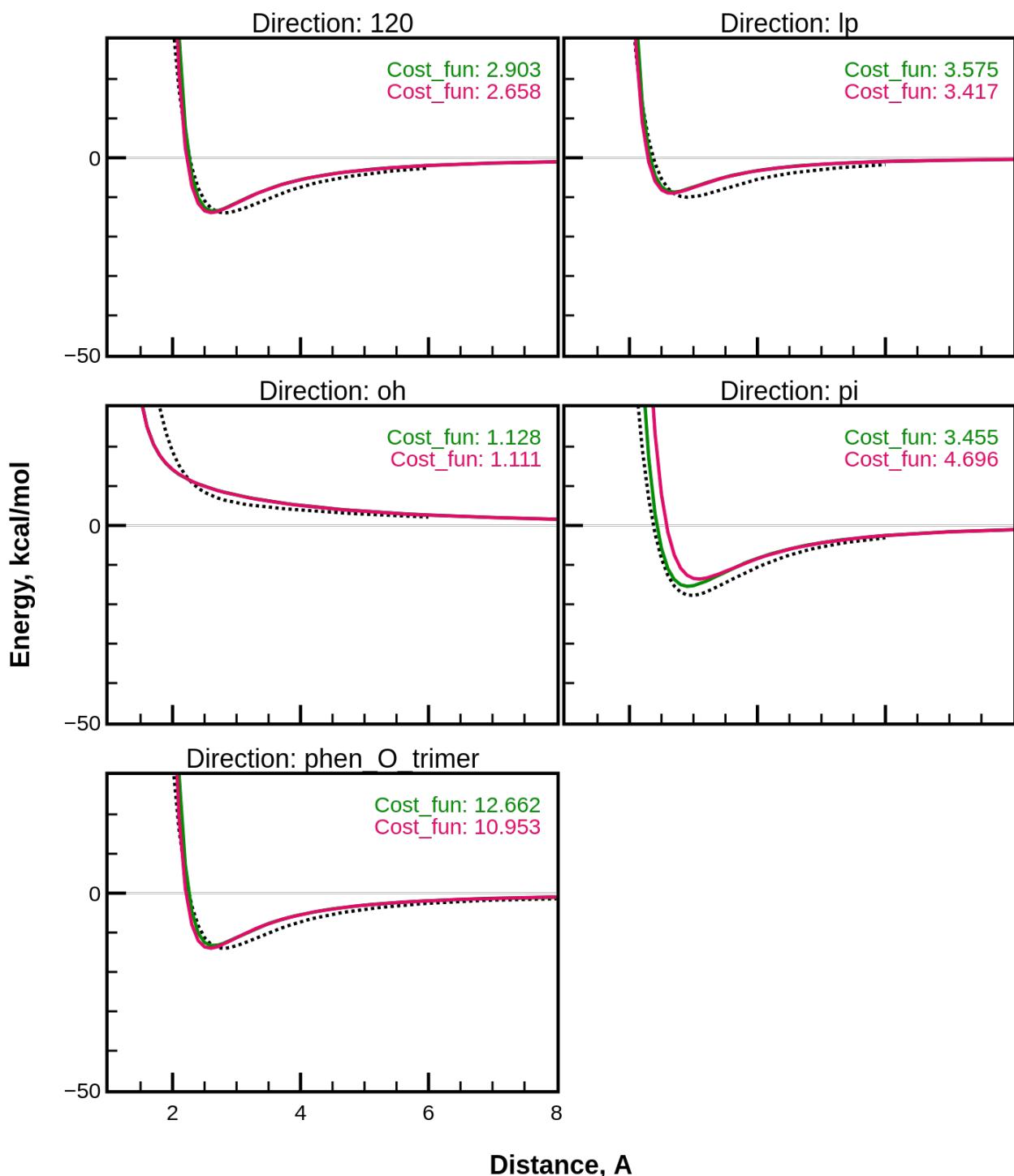
PHEN POT 1/1

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

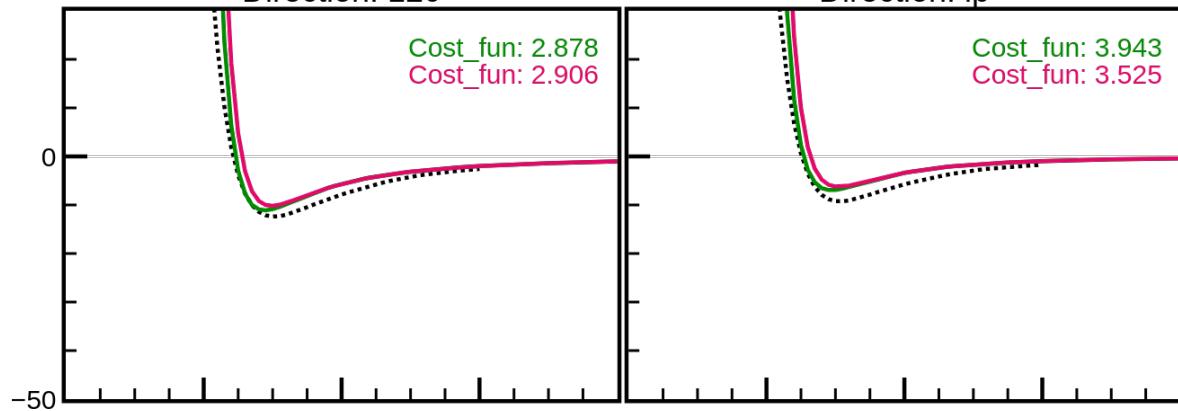


PHEN CES 1/1

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

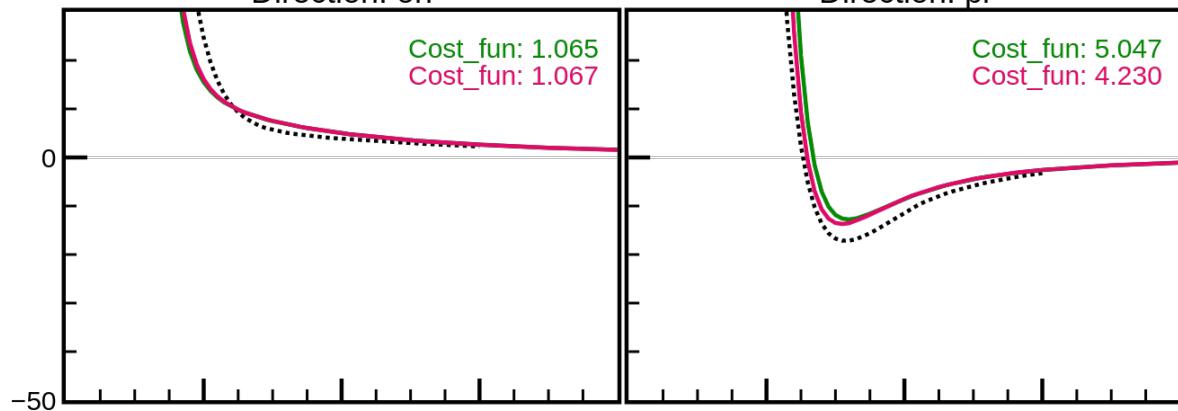
Direction: 120

Direction: lp



Direction: oh

Direction: pi

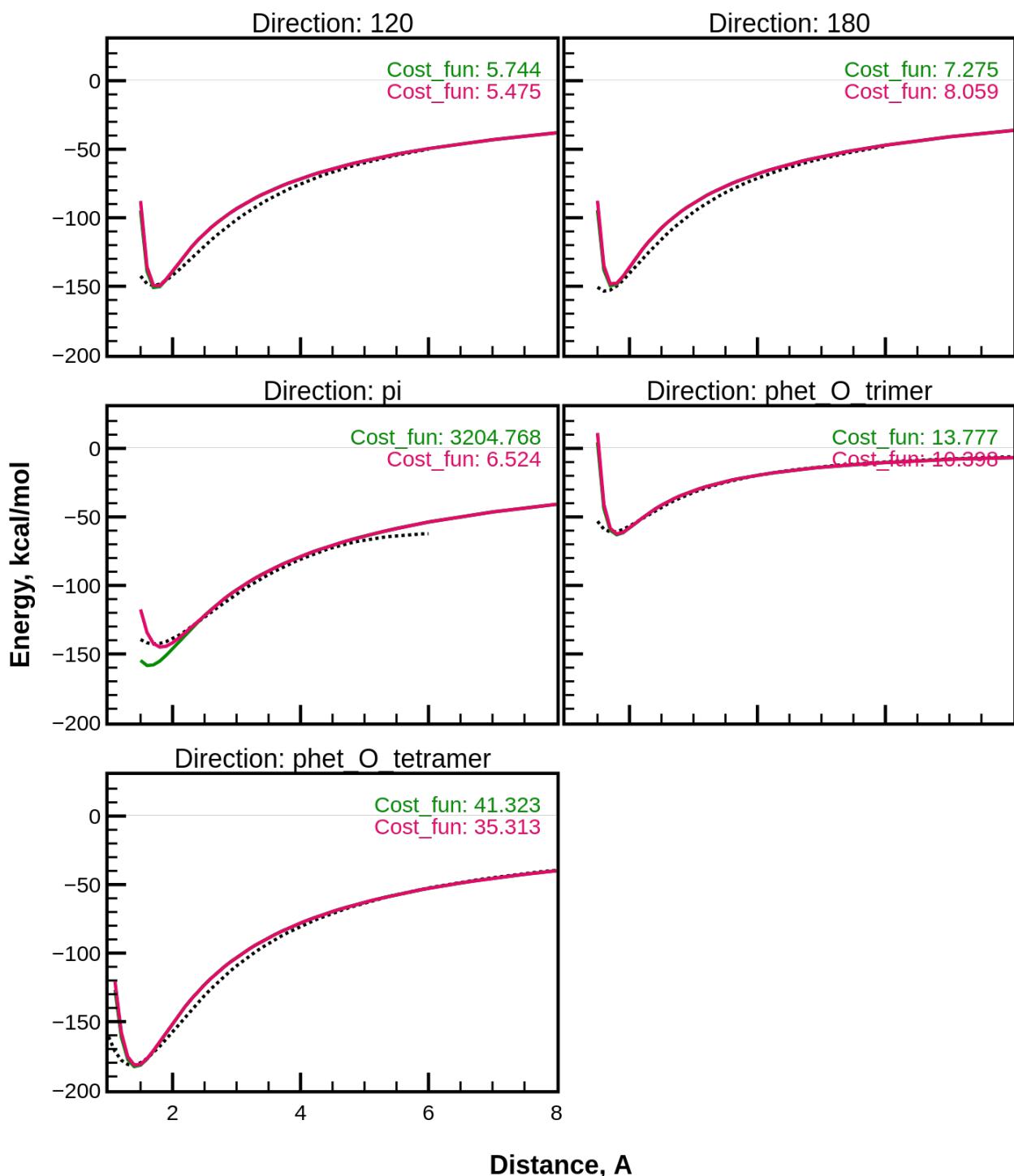


Energy, kcal/mol

Distance, Å

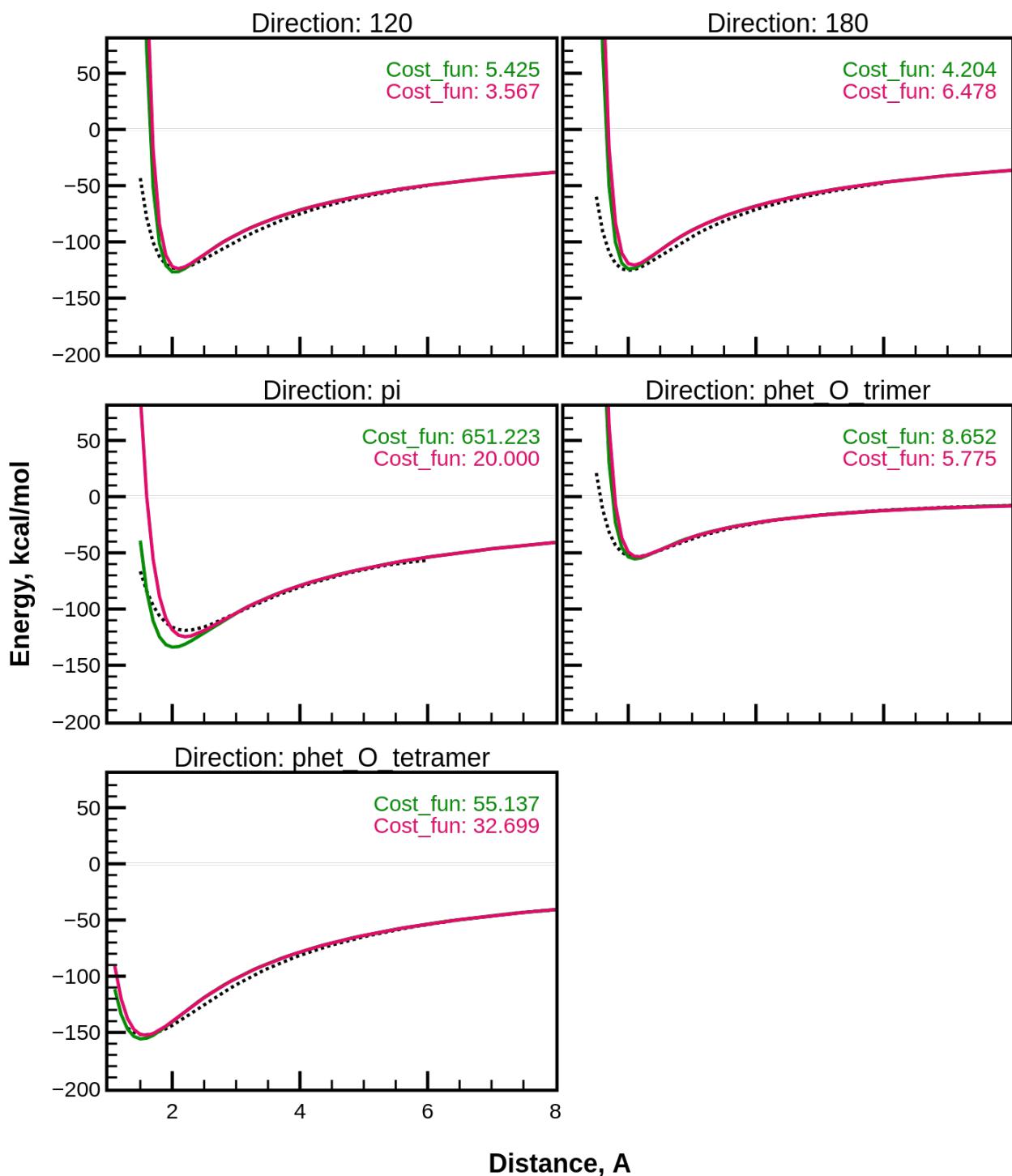
PHET LIT 1/1

2.62000_0.15780_9.99999
2.63213_0.15780_4.78169



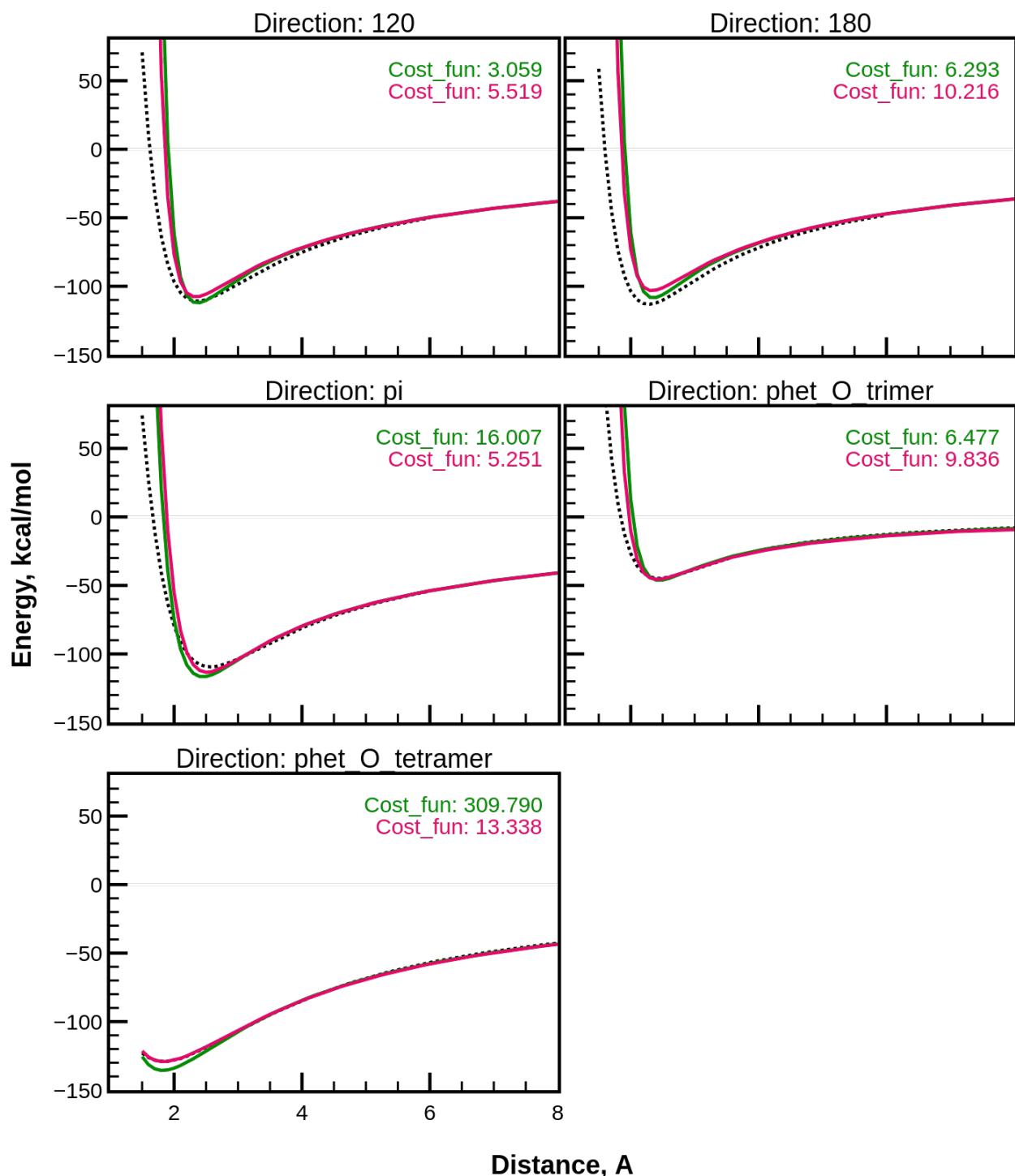
PHET SOD 1/1

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



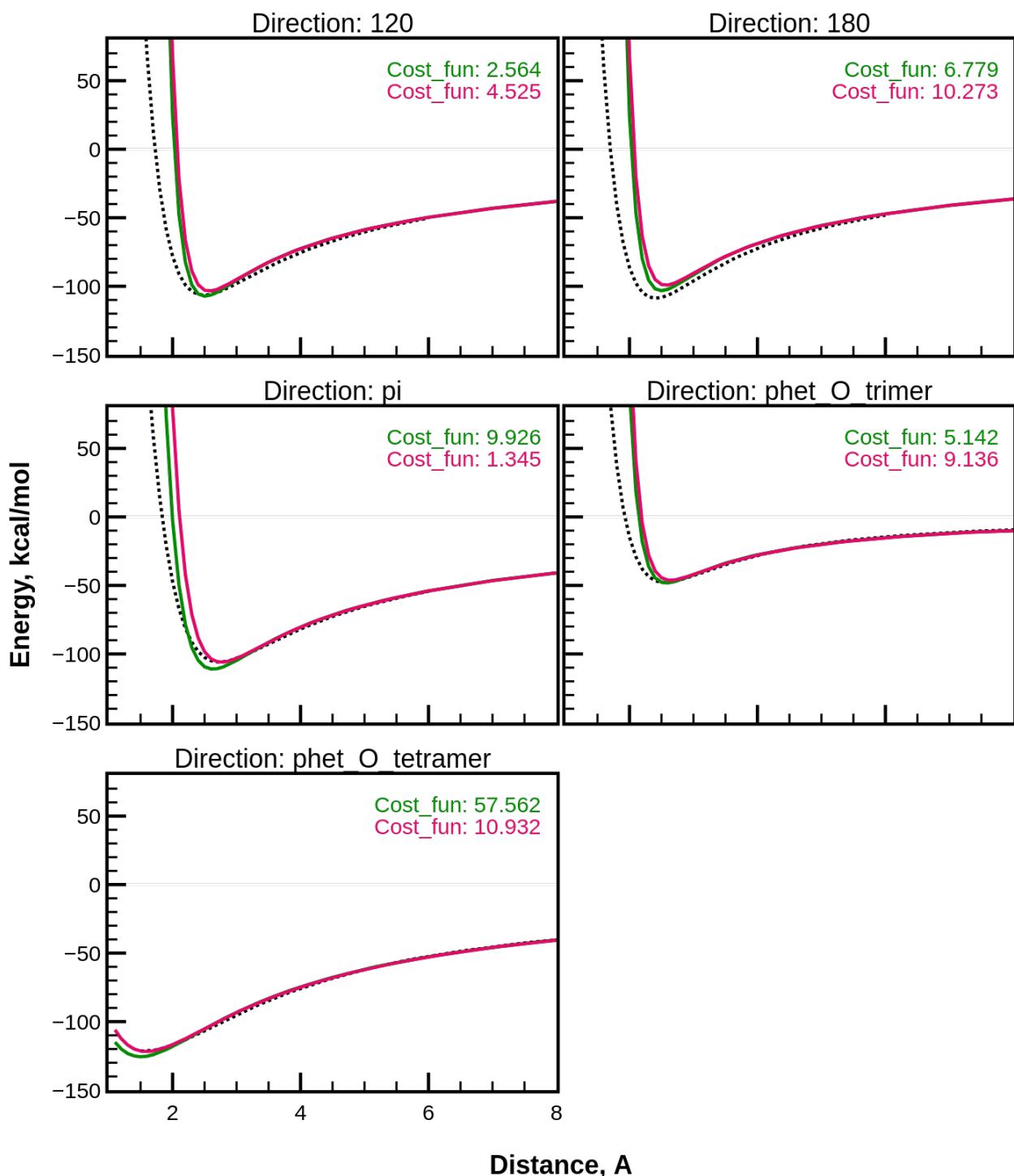
PHET POT 1/1

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



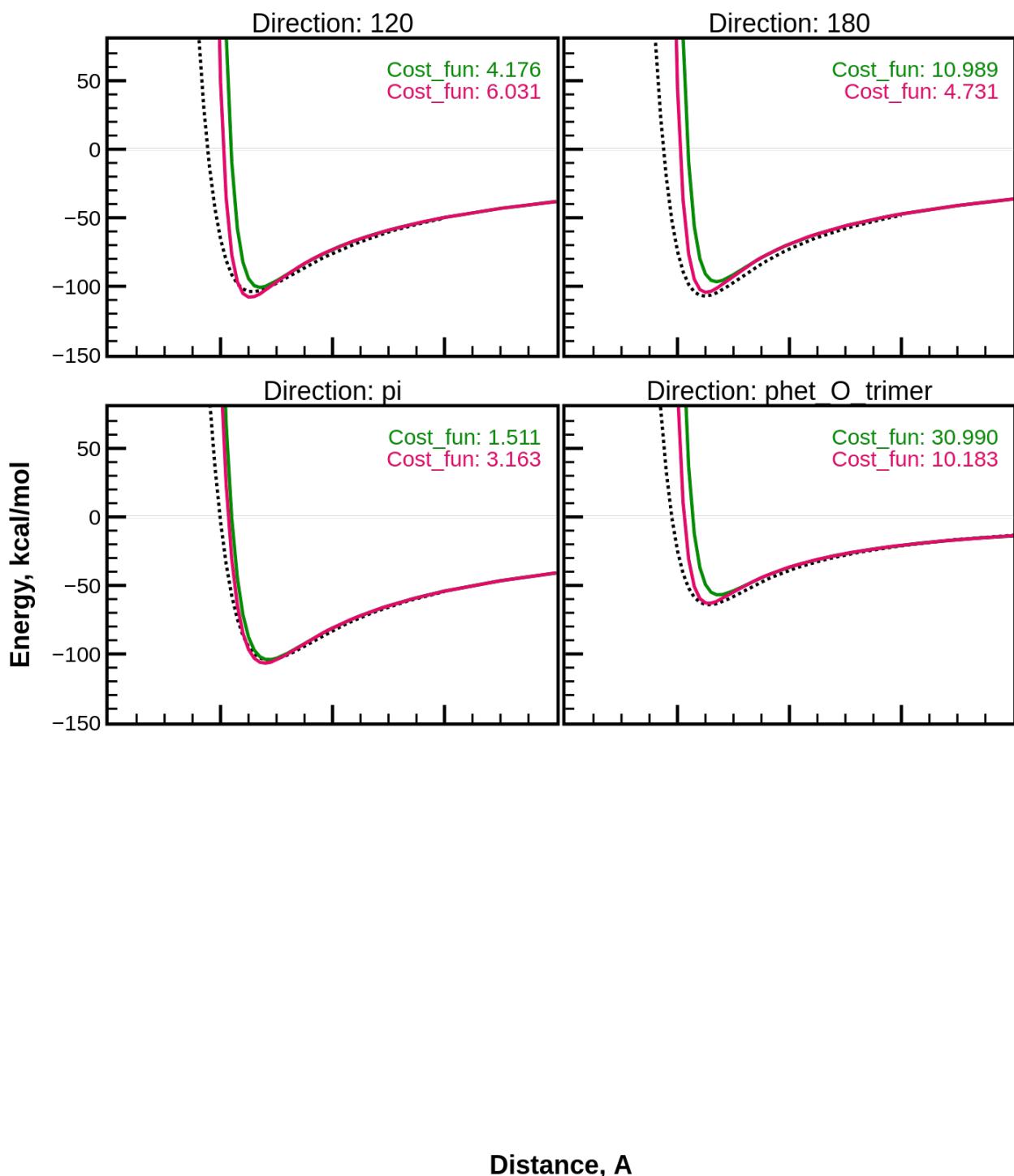
PHET RUB 1/1

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



PHET CES 1/1

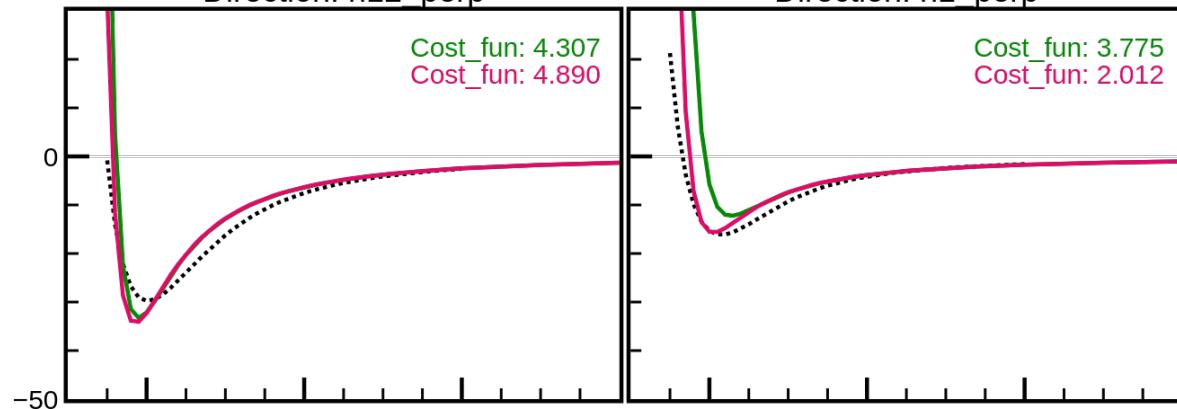
3.54382_0.47915_9.99999
3.34382_0.47915_4.19384



ADEB LIT 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

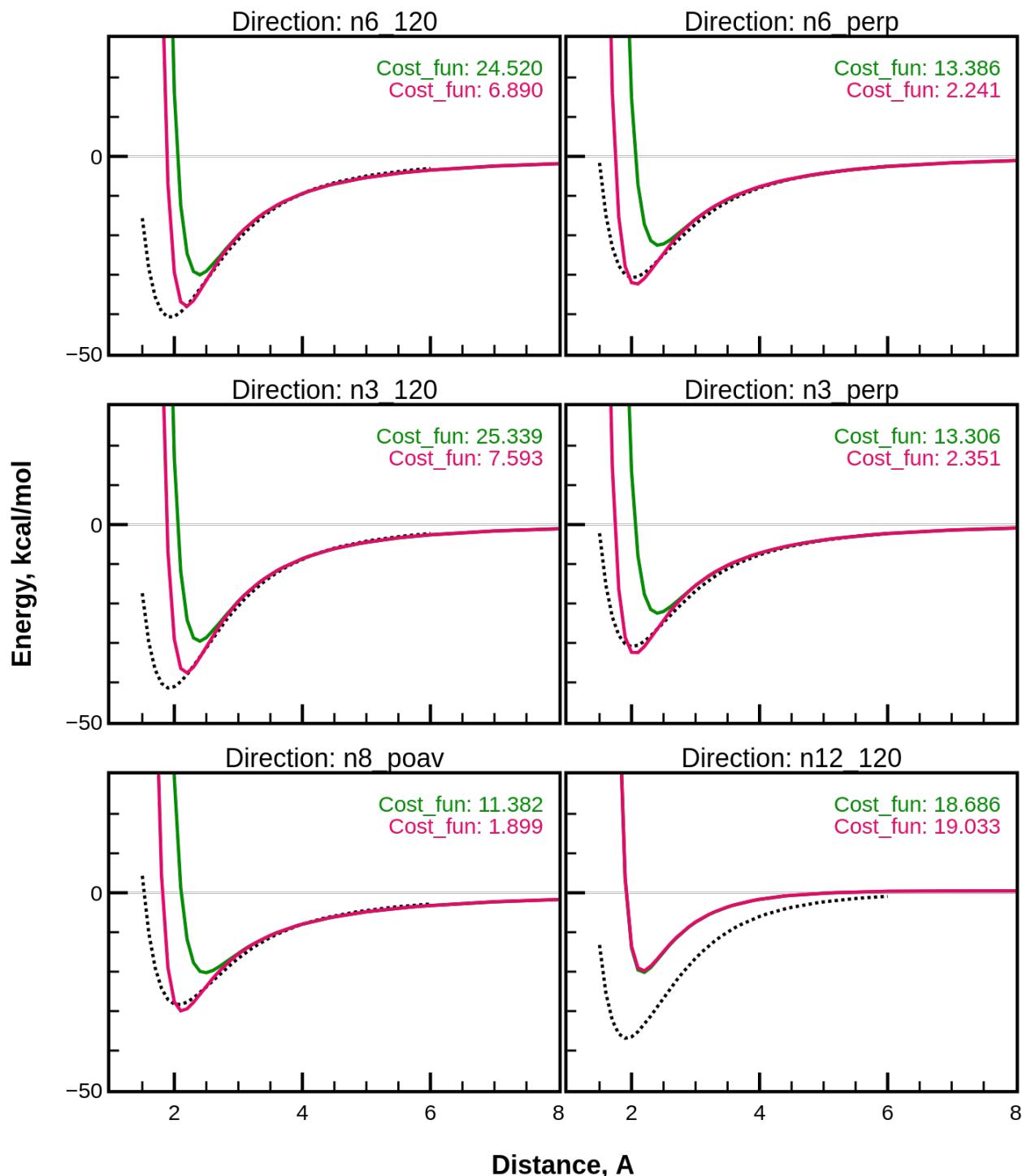
Direction: n12_perp

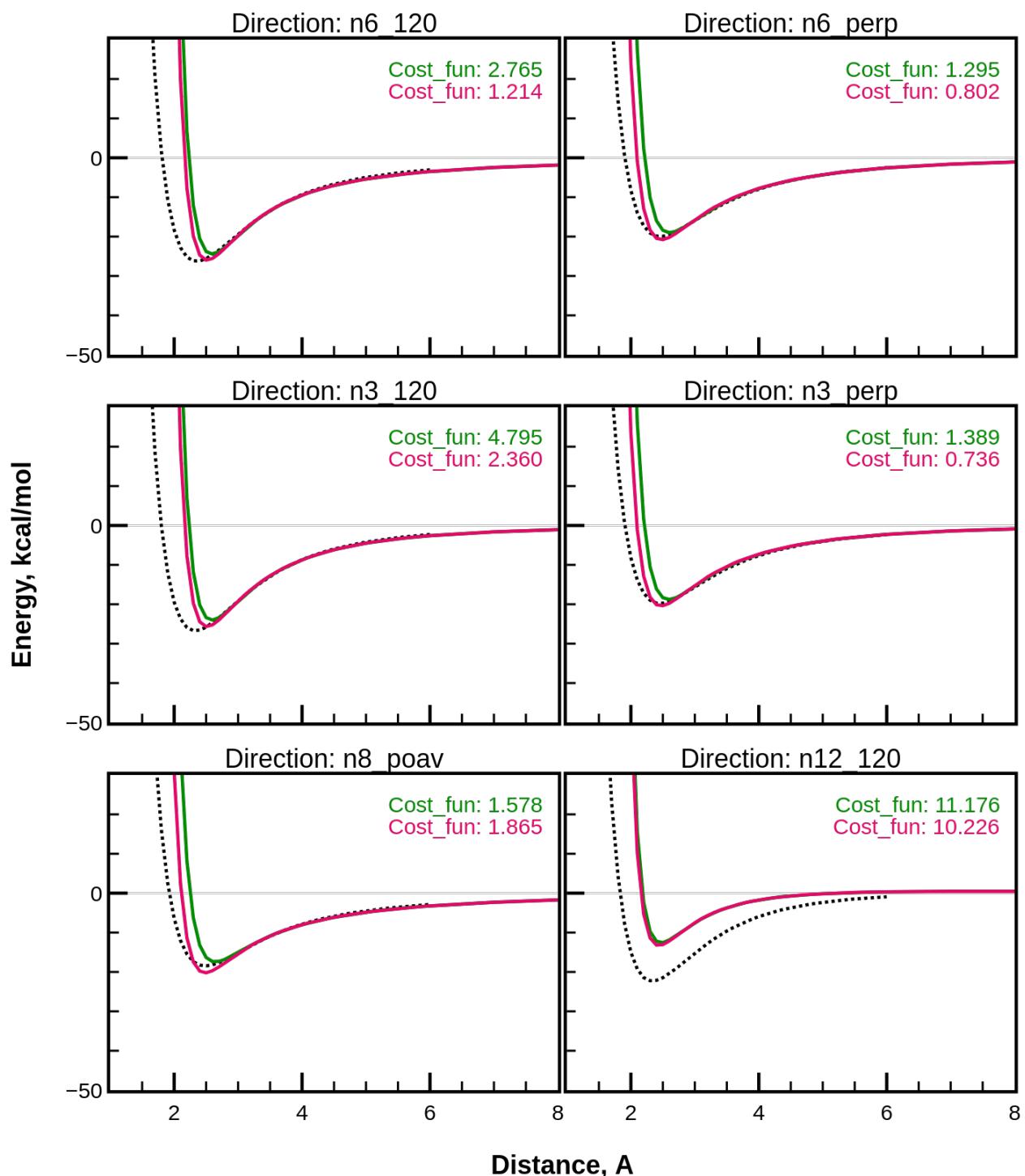
Direction: n1_perp



Energy, kcal/mol

Distance, A

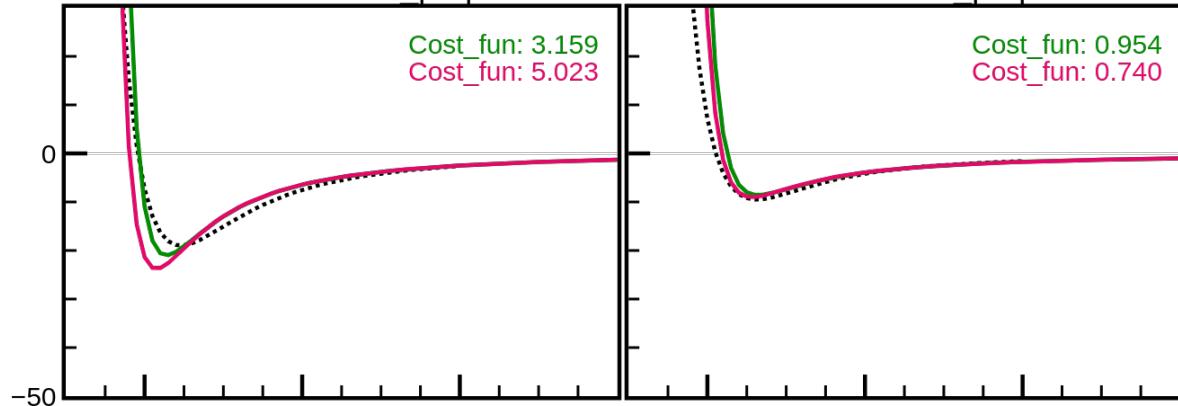
ADEB LIT 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

ADEB SOD 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

ADEB SOD 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

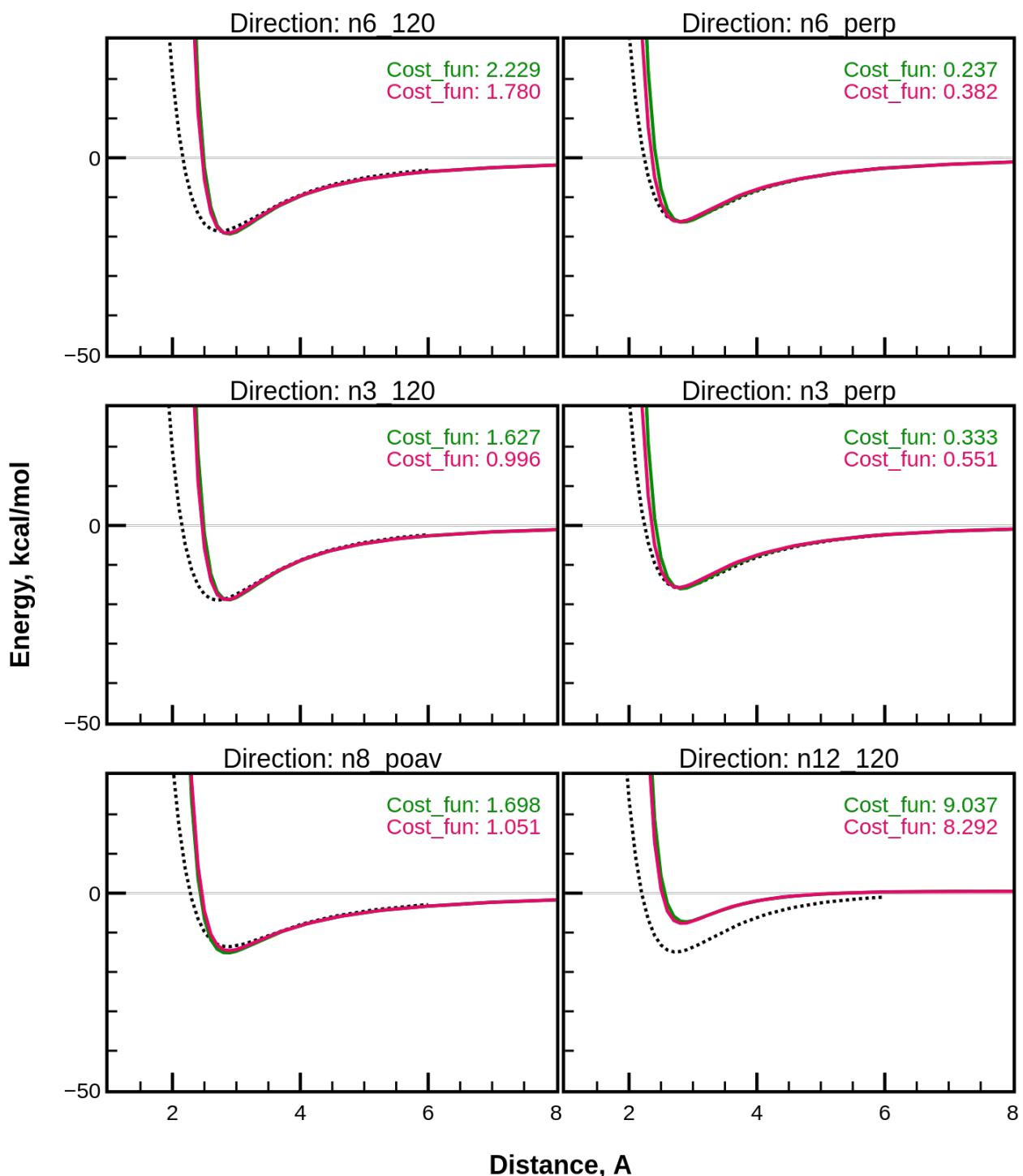
Direction: n12_perp

Direction: n1_perp



Energy, kcal/mol

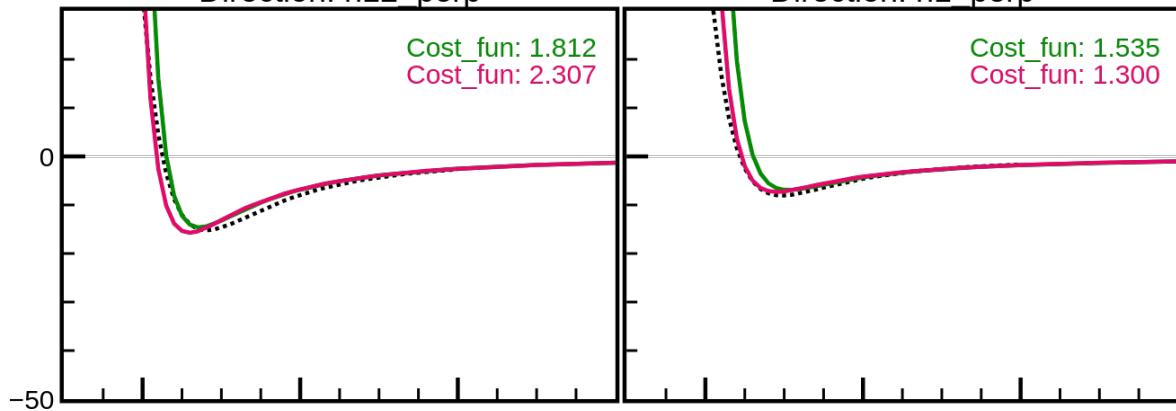
Distance, Å

ADEB POT 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

ADEB POT 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

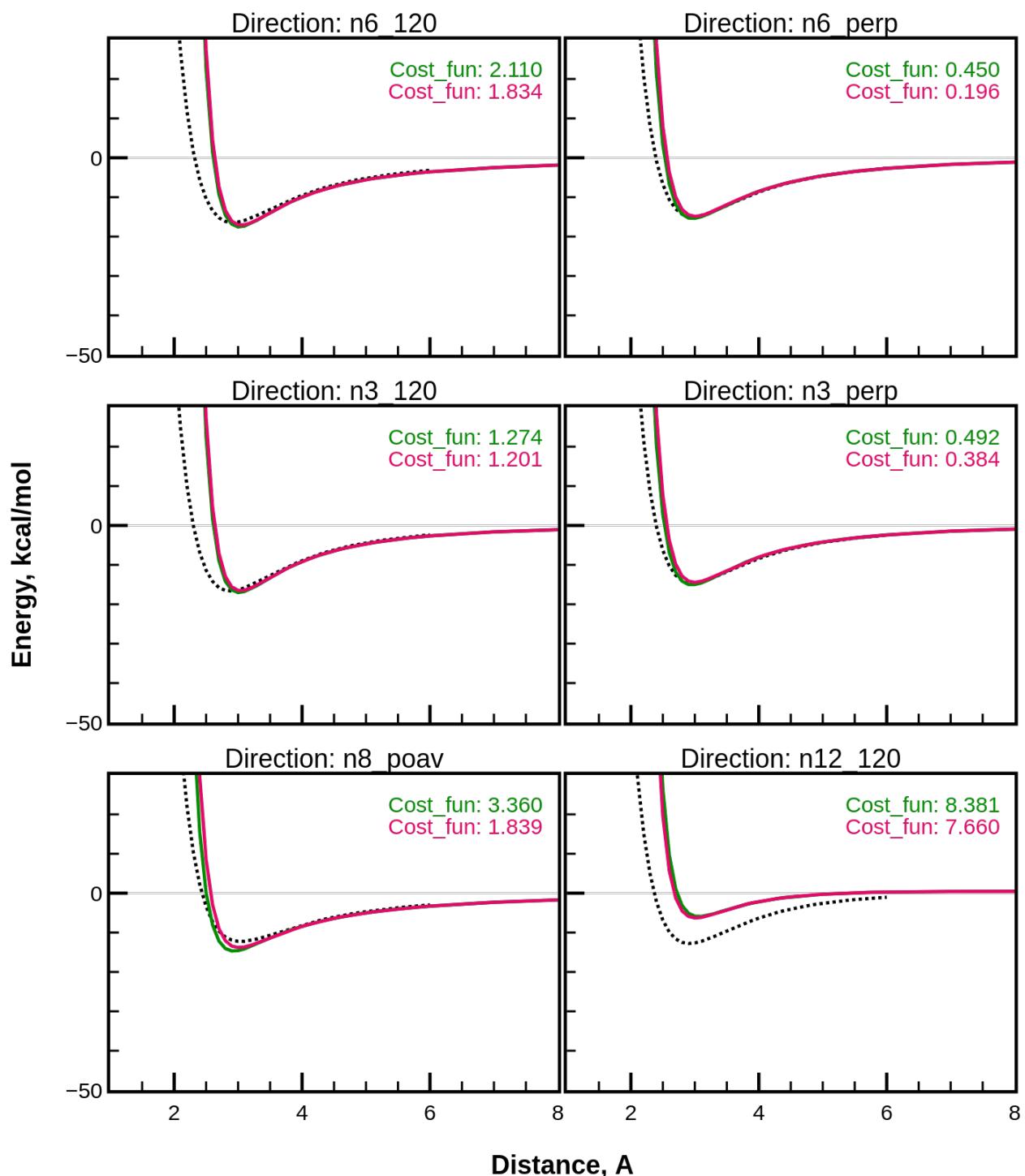
Direction: n12_perp

Direction: n1_perp



Energy, kcal/mol

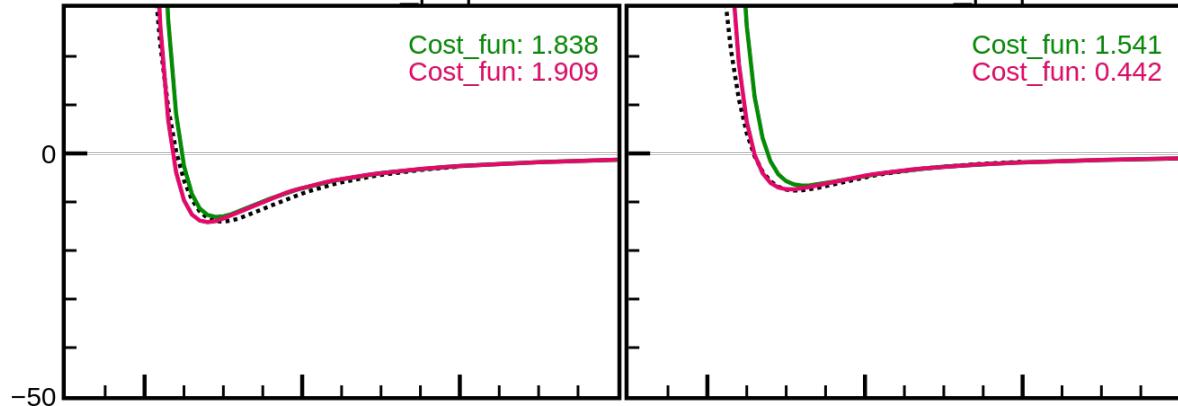
Distance, A

ADEB RUB 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

ADEB RUB 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

Direction: n12_perp

Direction: n1_perp



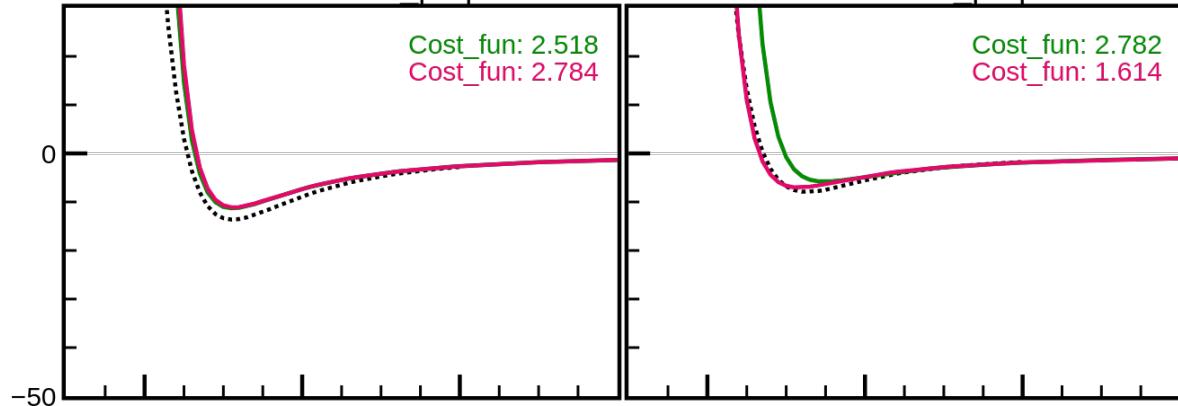
Energy, kcal/mol

Distance, Å

ADEB CES 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

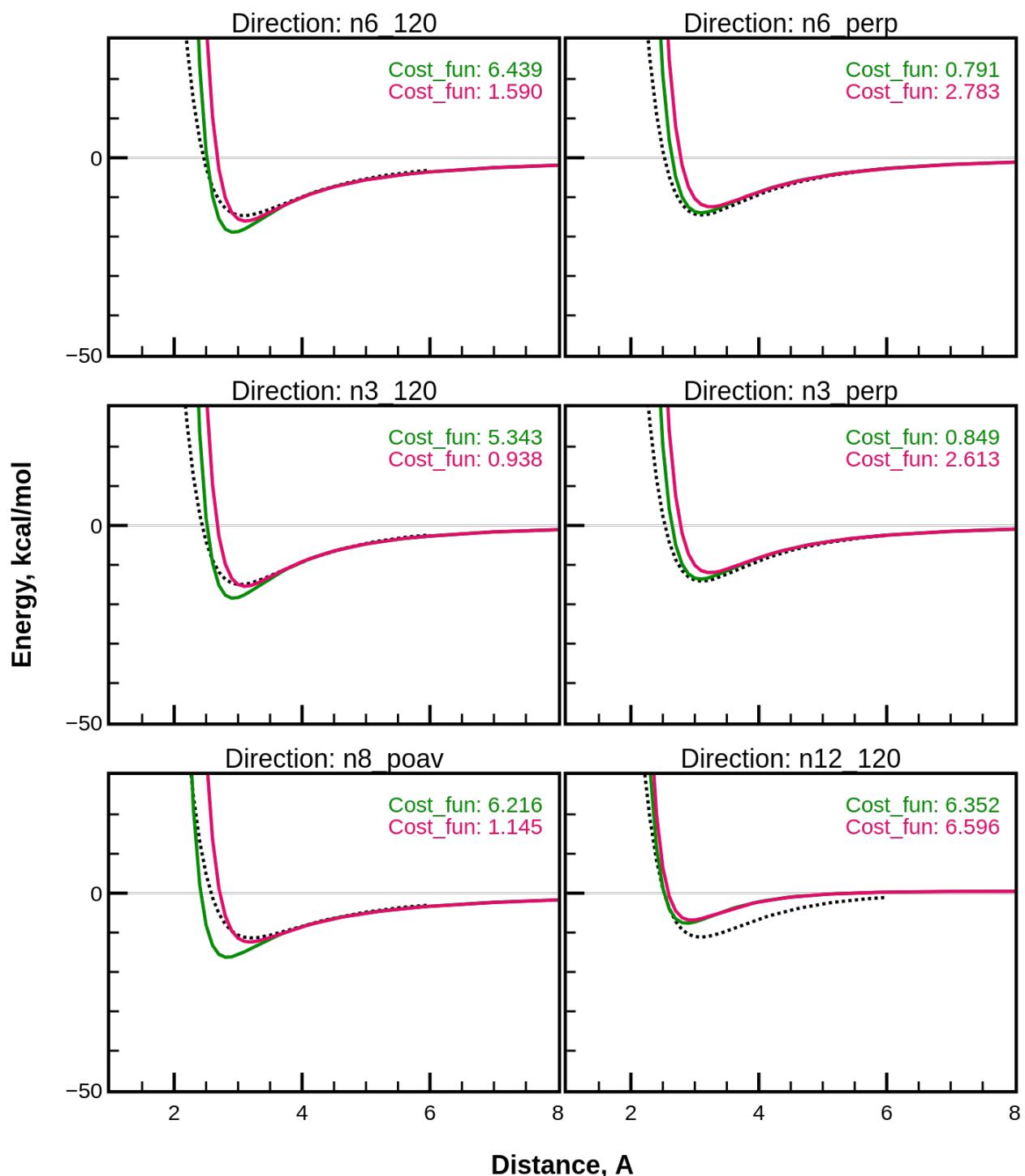
Direction: n12_perp

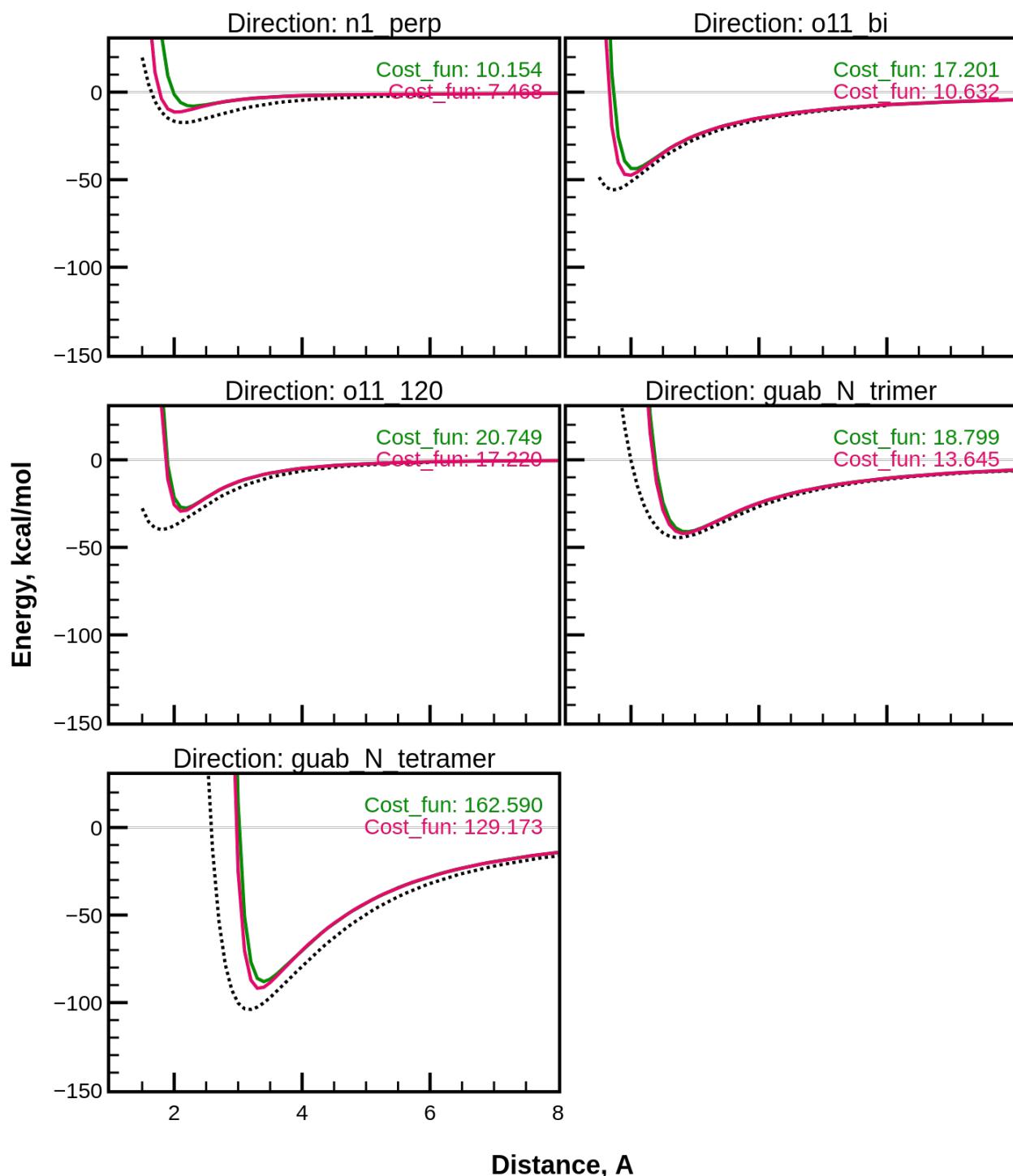
Direction: n1_perp

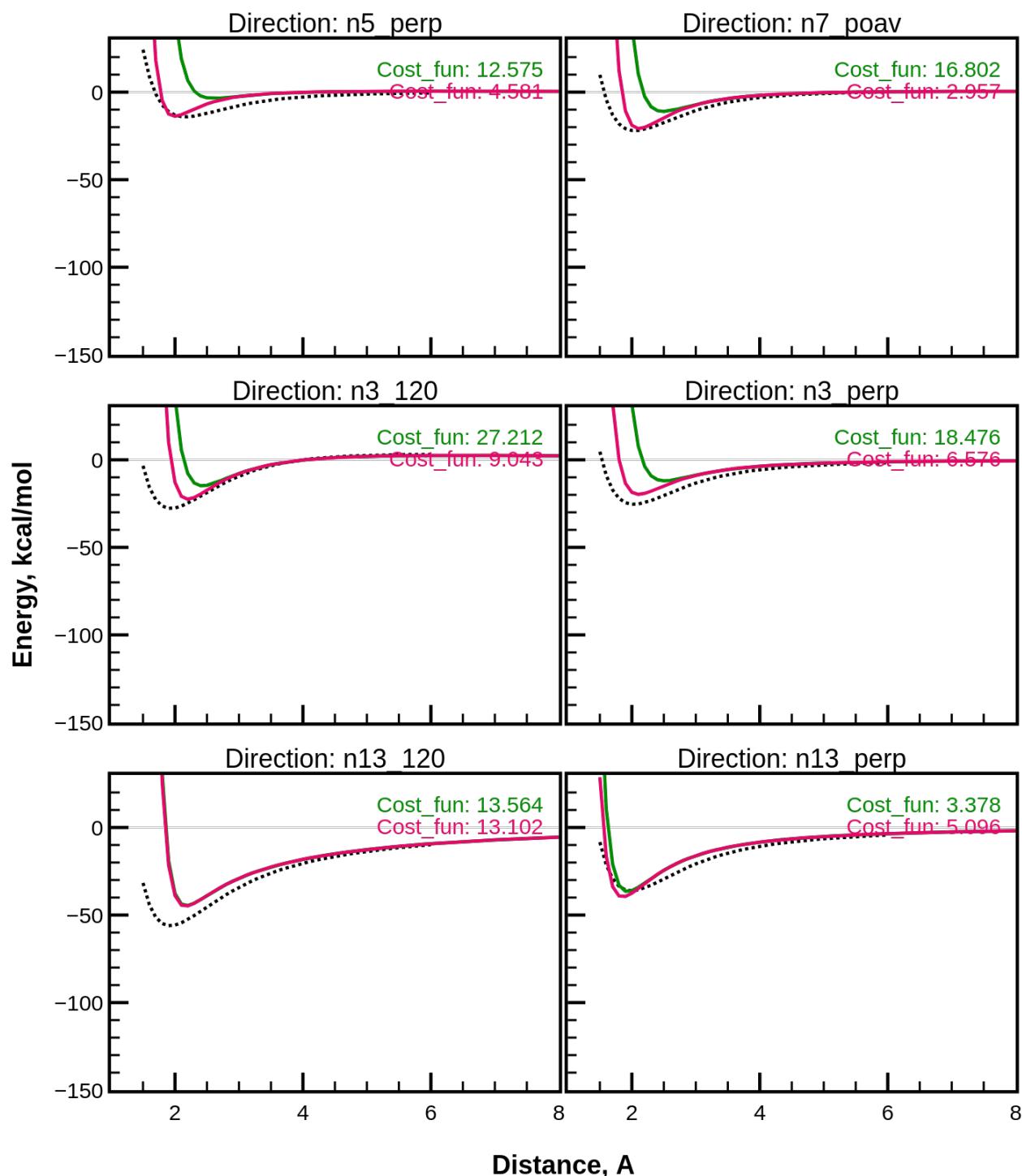


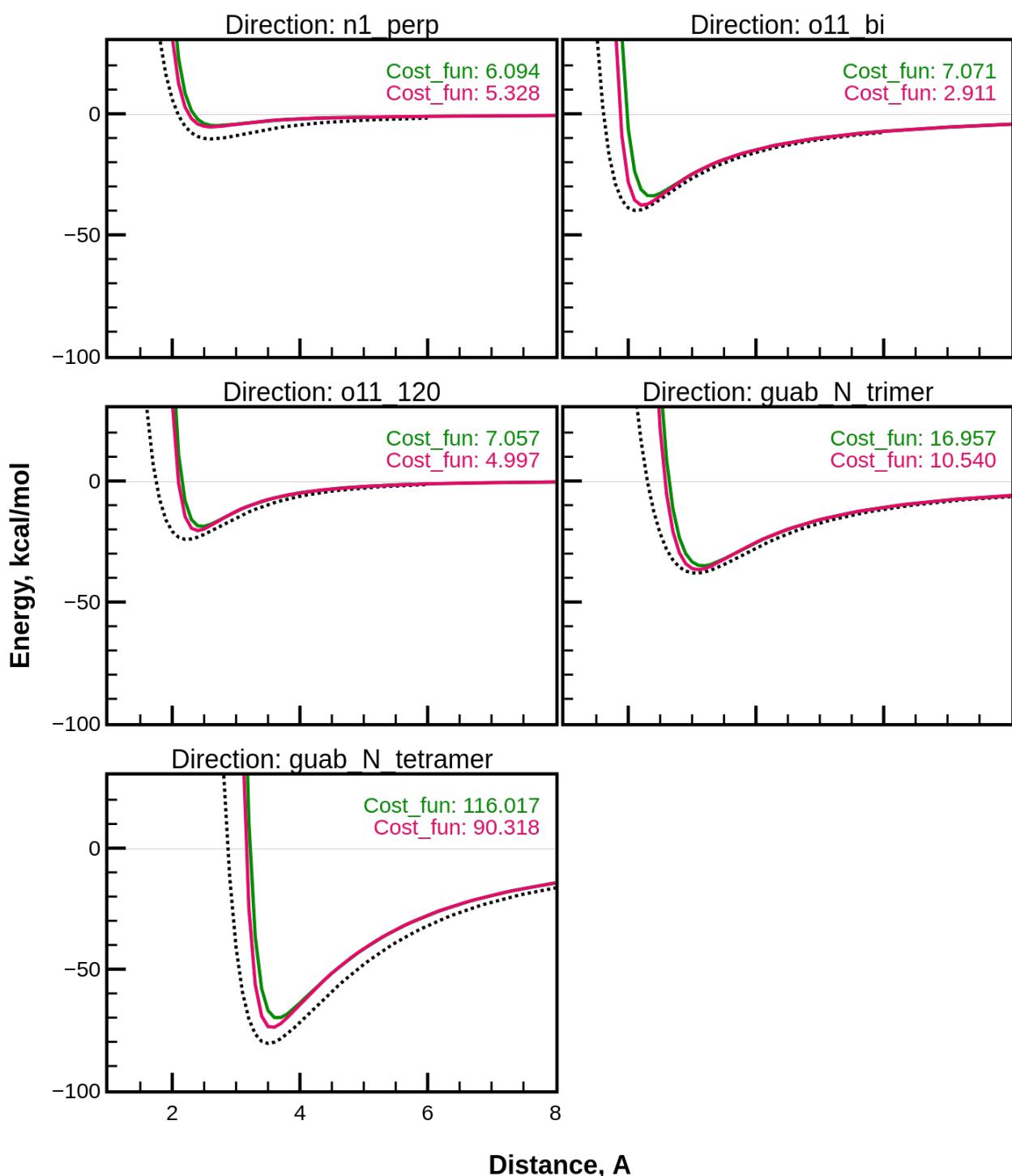
Energy, kcal/mol

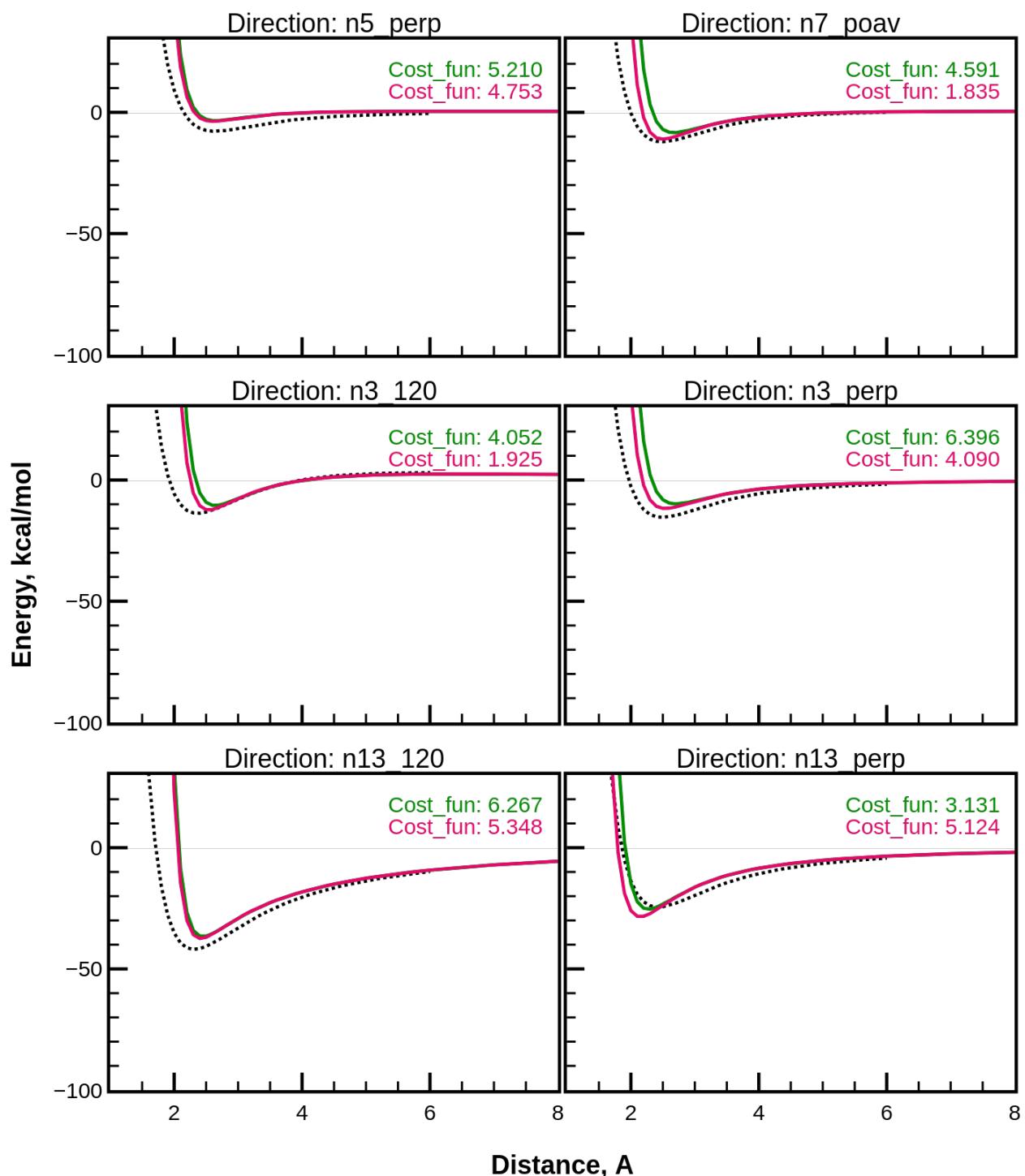
Distance, A

ADEB CES 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

GUAB LIT 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

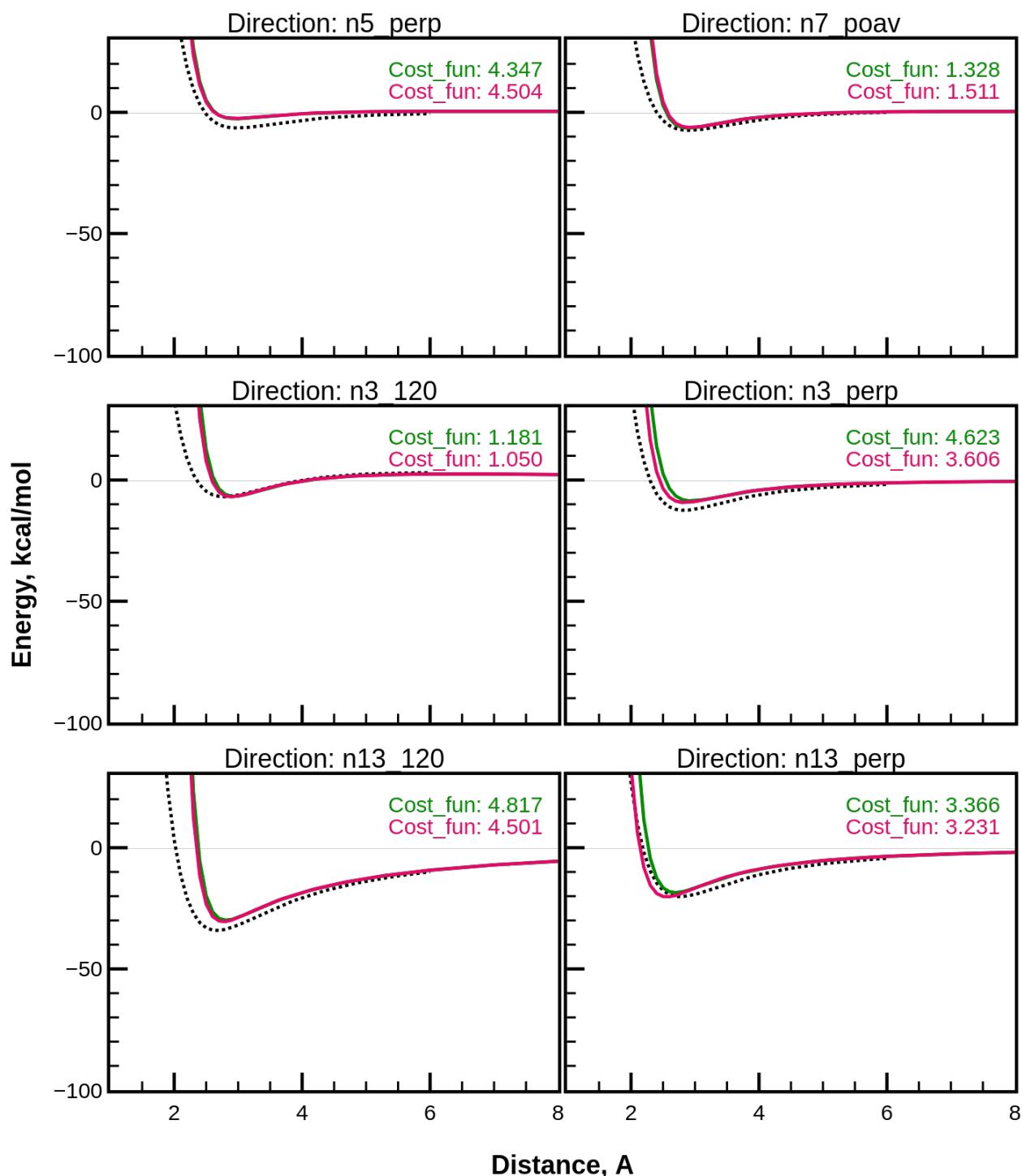
GUAB LIT 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

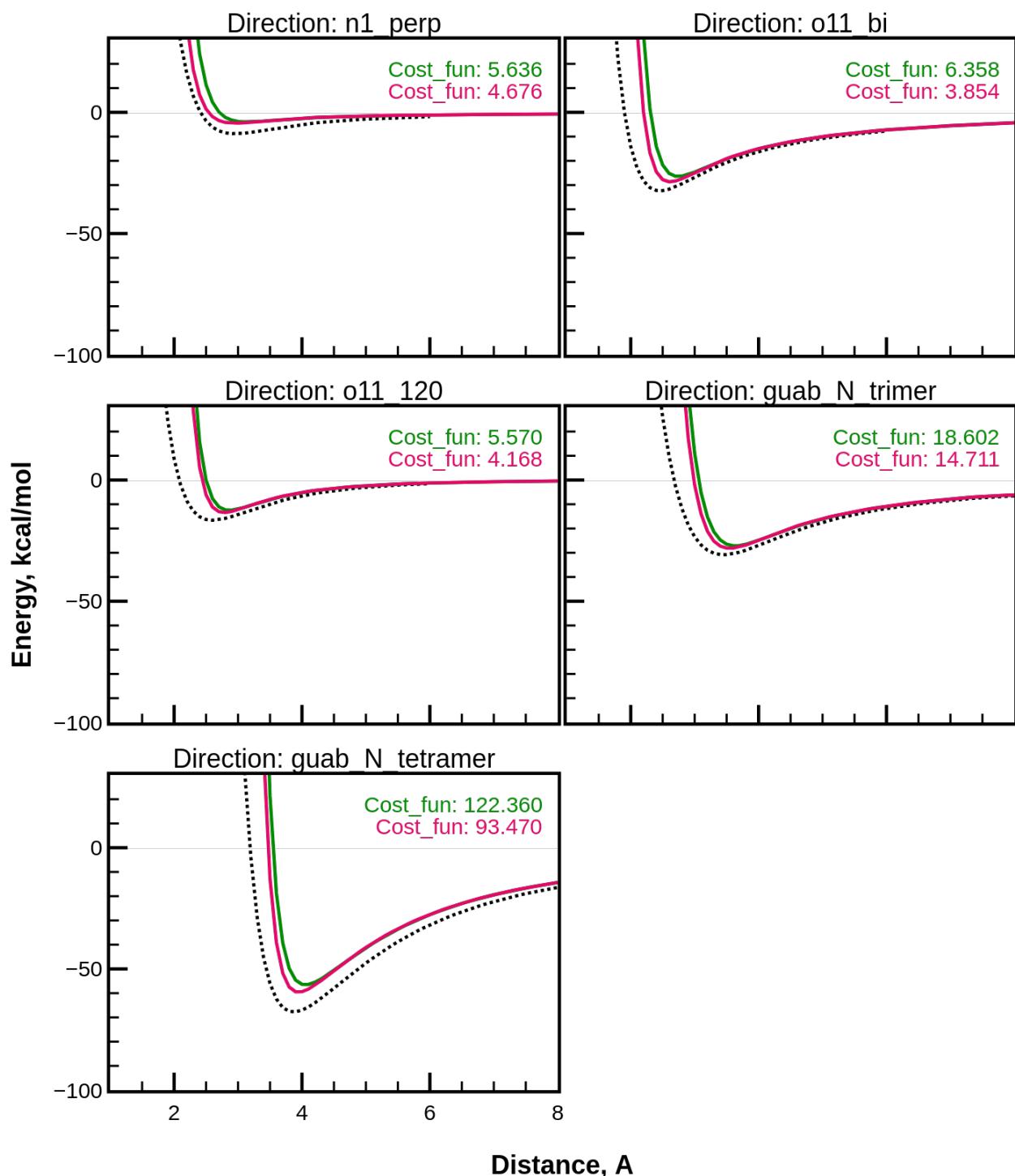
GUAB SOD 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

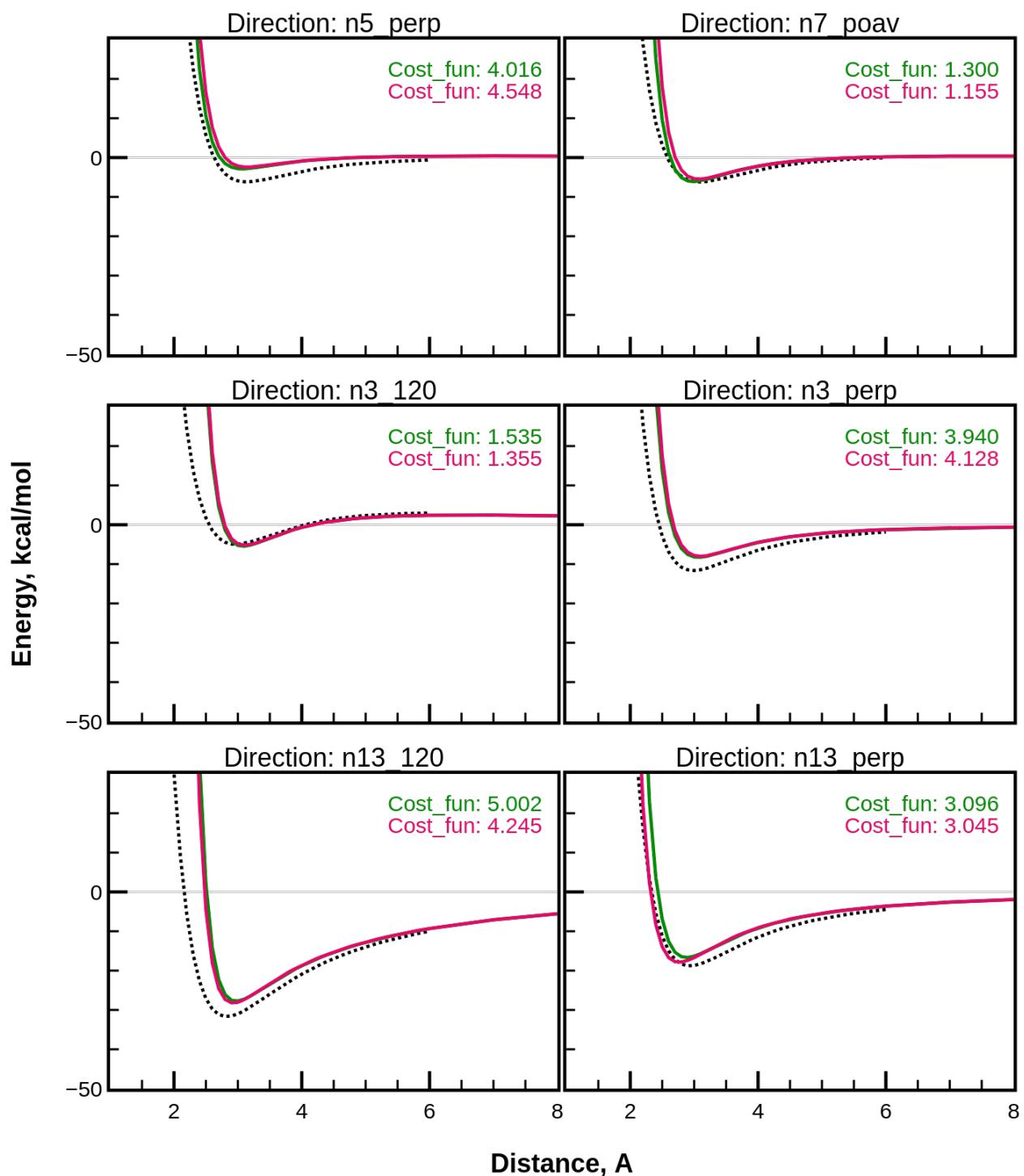
GUAB SOD 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

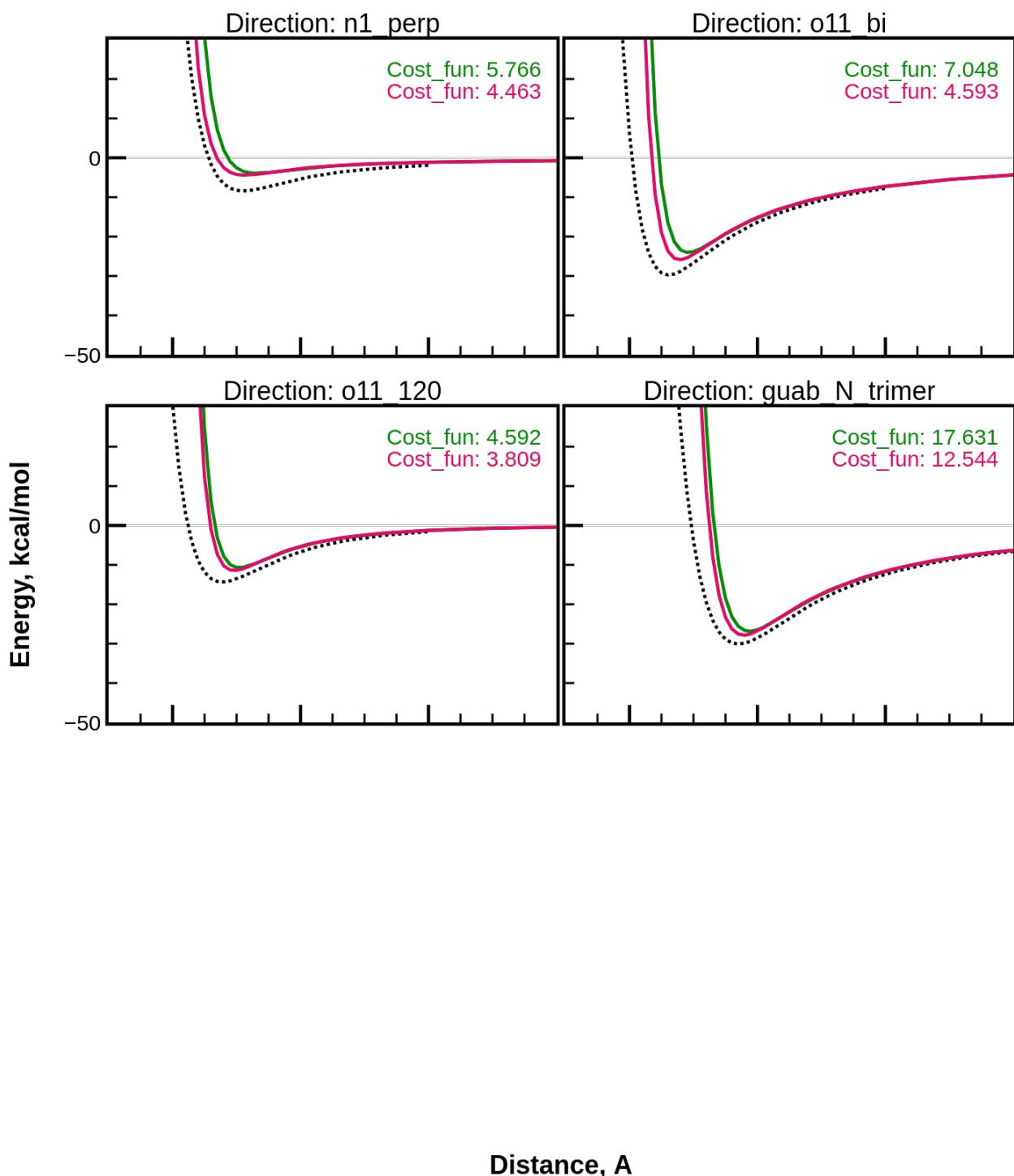
GUAB POT 1/2

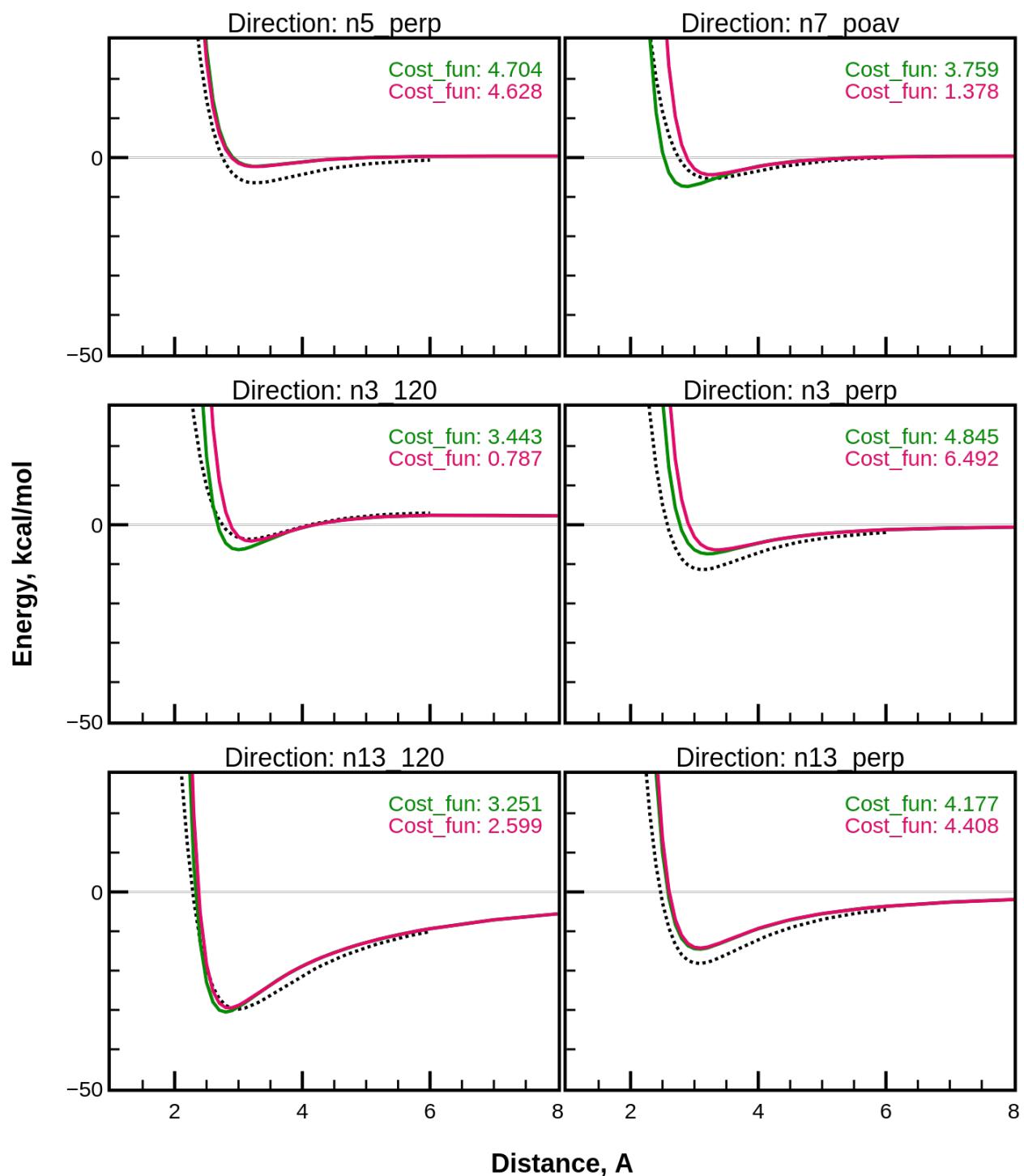
9.99999_9.99999_9.99999
1.11111_1.11111_1.11111

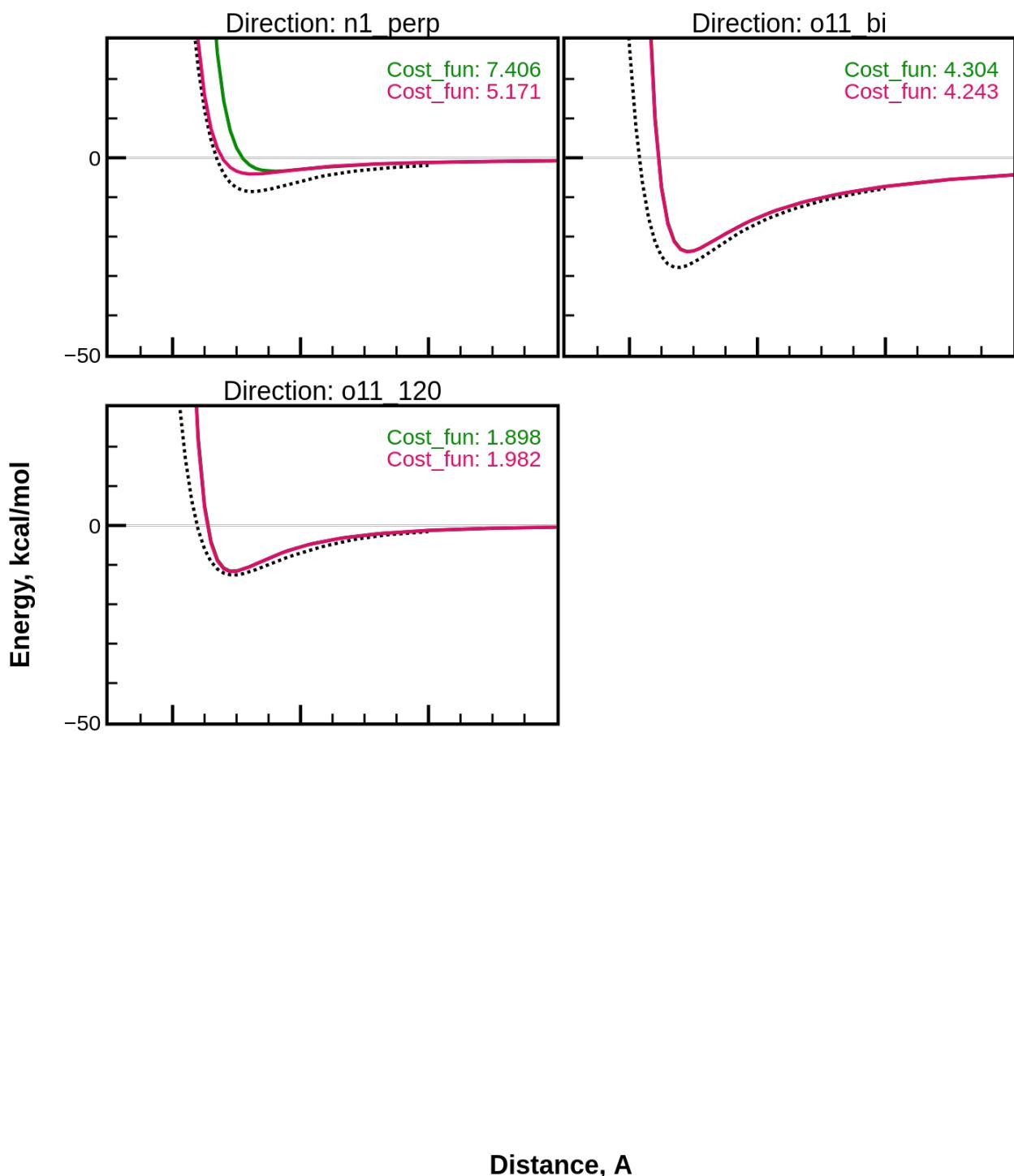


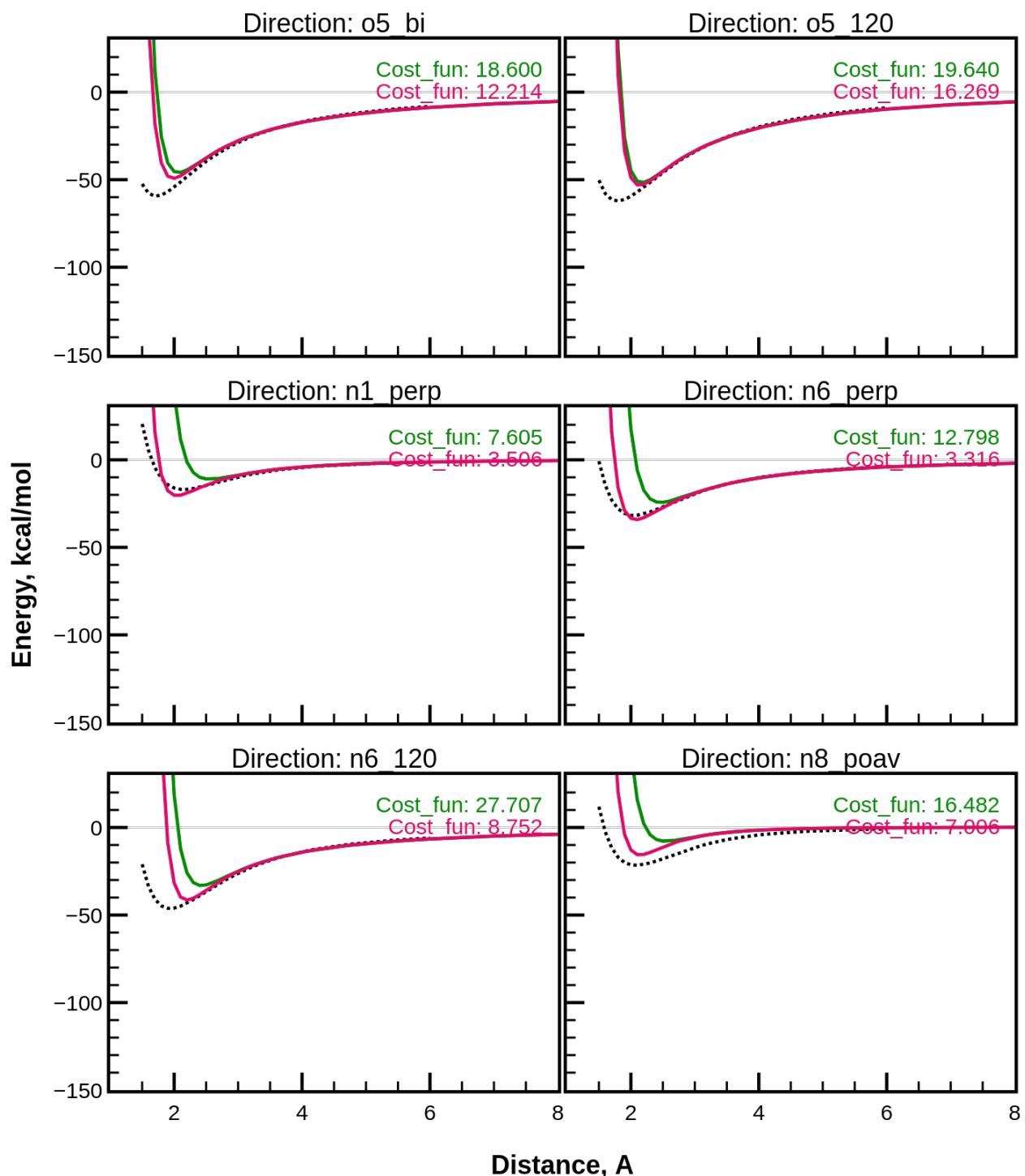
GUAB POT 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

GUAB RUB 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

GUAB RUB 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

GUAB CES 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

GUAB CES 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

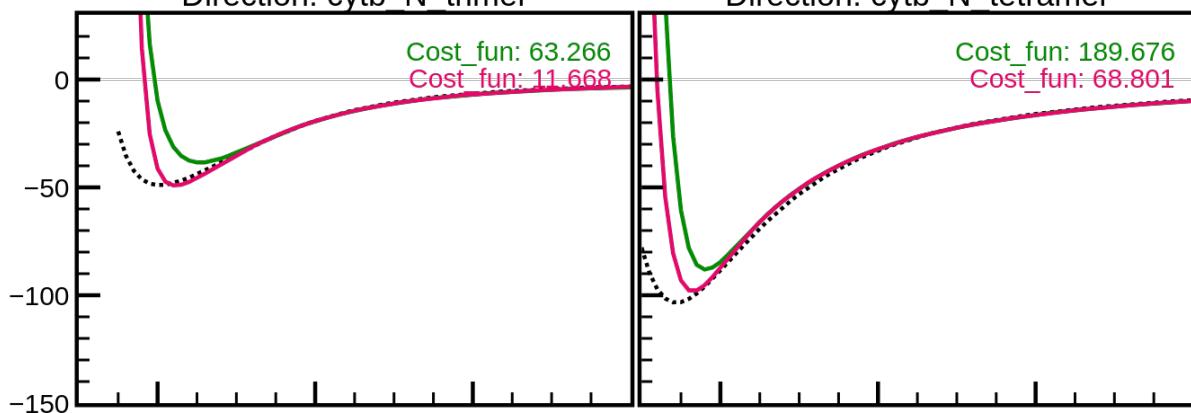
CYTB LIT 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

CYTB LIT 2/2

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

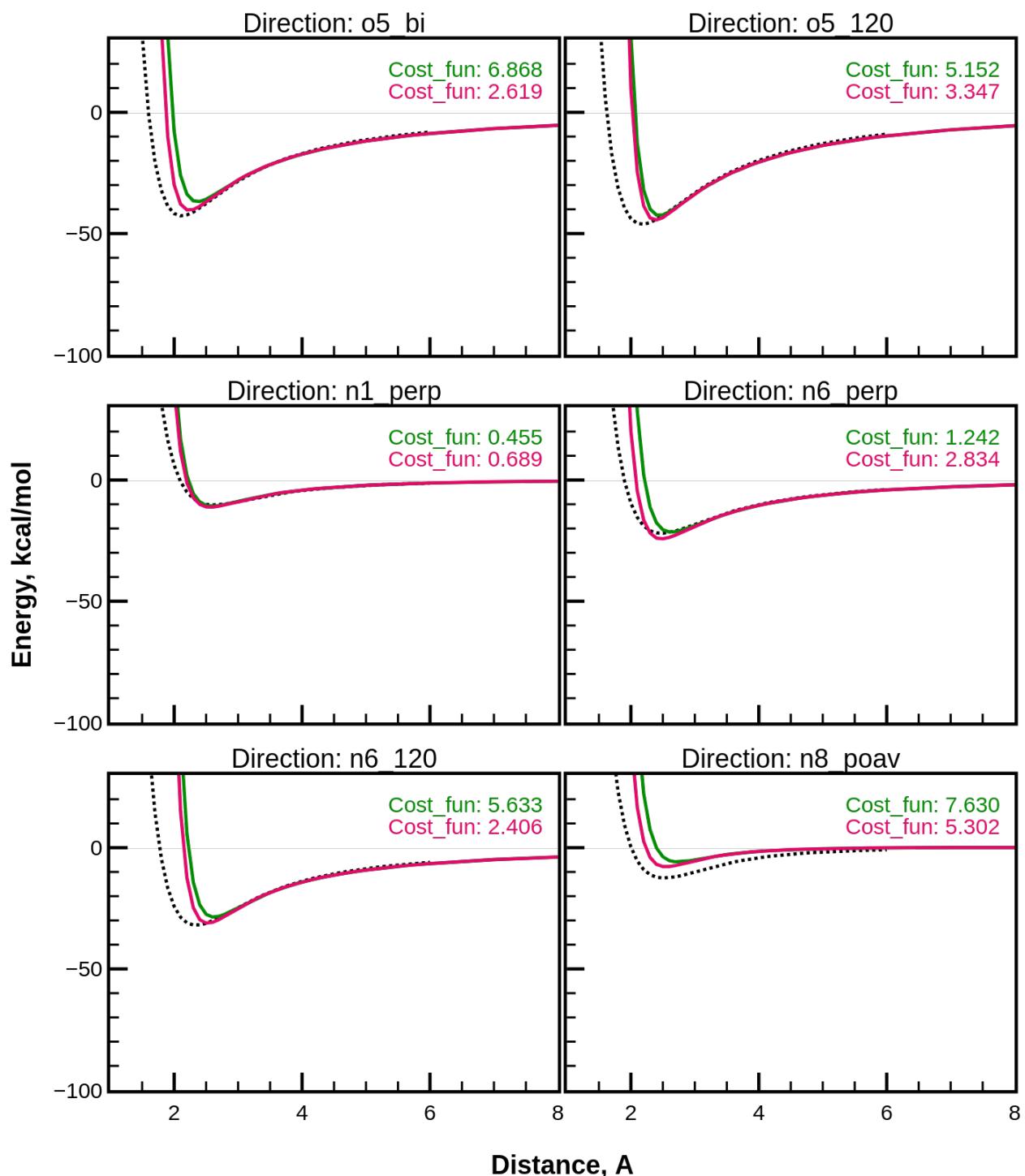
Direction: cytb N trimer

Direction: cytb N tetramer



Energy, kcal/mol

Distance, A

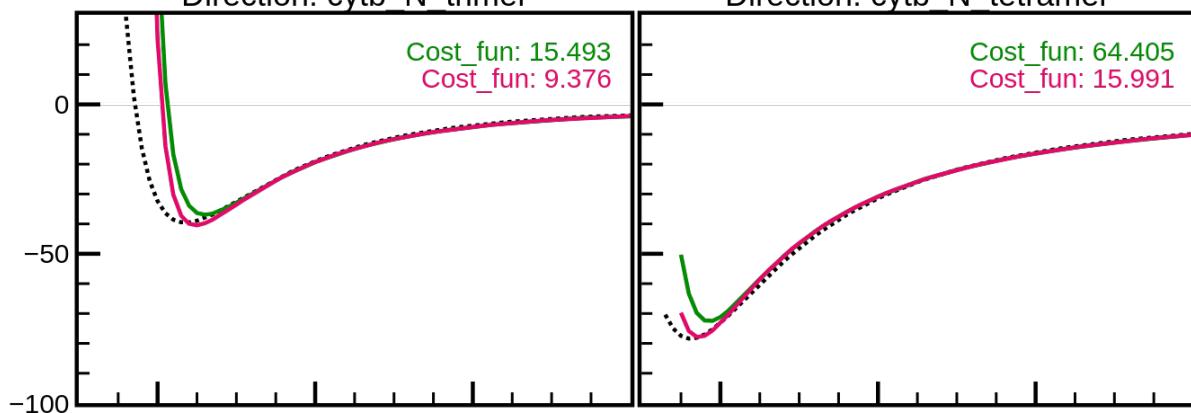
CYTB SOD 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

CYTB SOD 2/2

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

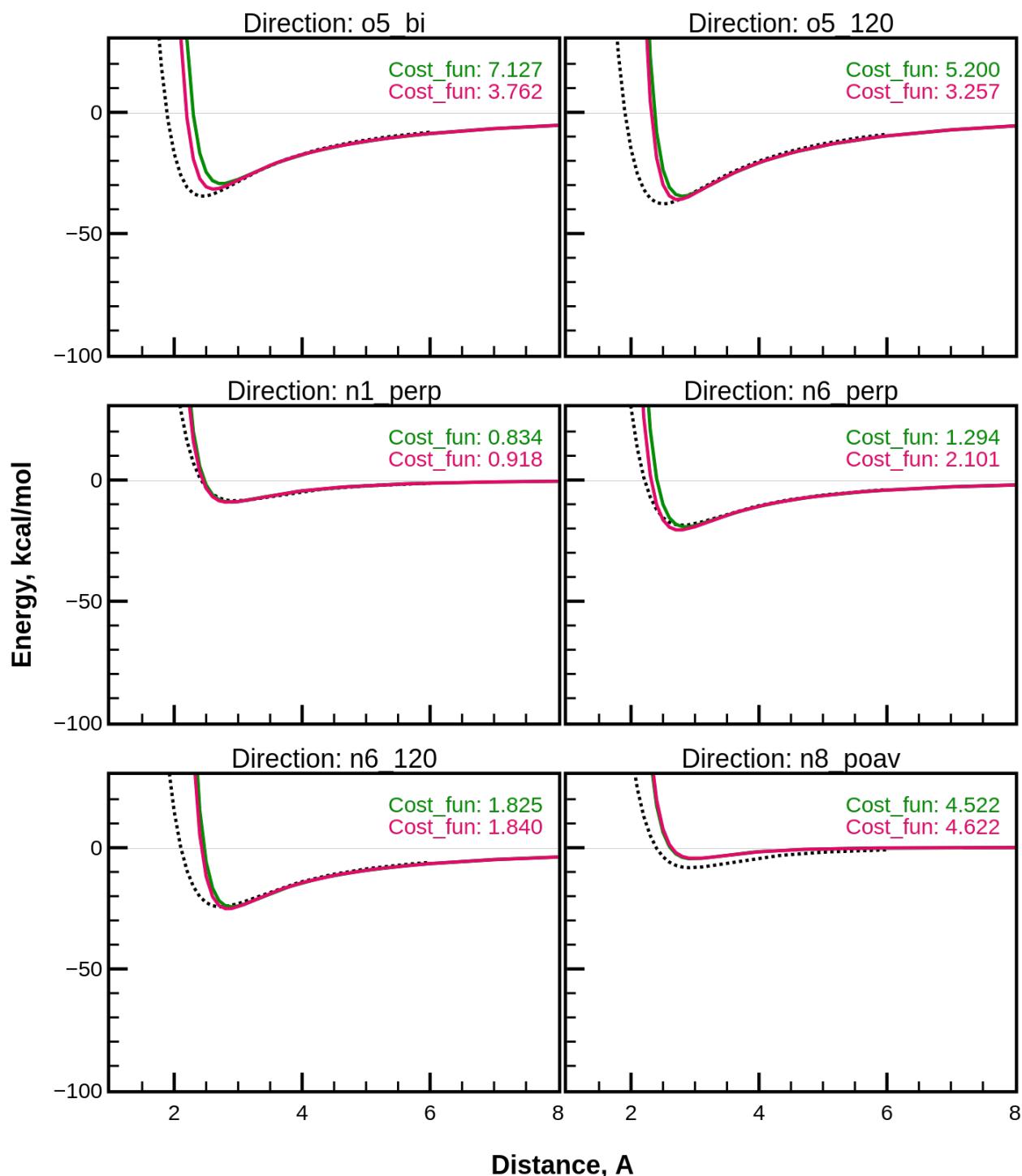
Direction: cyt b N trimer

Direction: cyt b N tetramer



Energy, kcal/mol

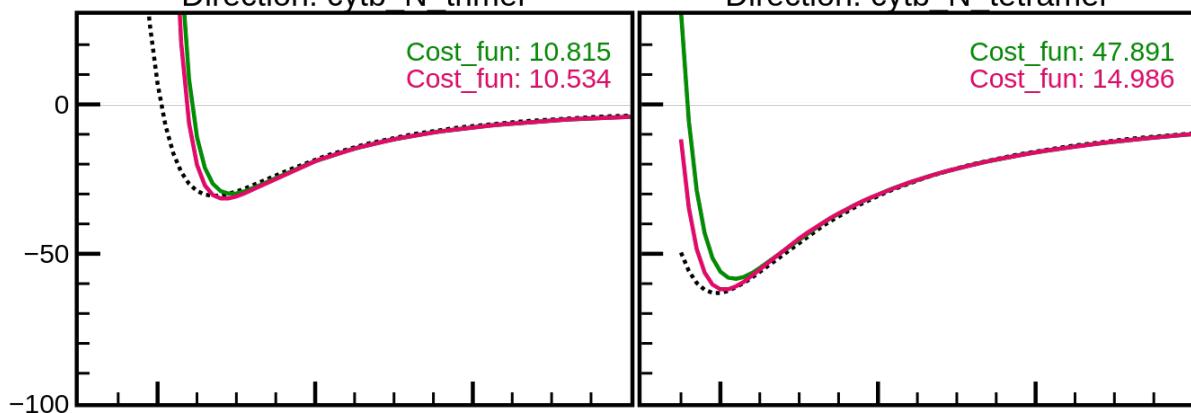
Distance, A

CYTB POT 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

CYTB POT 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

Direction: cytb N trimer

Direction: cytb N tetramer



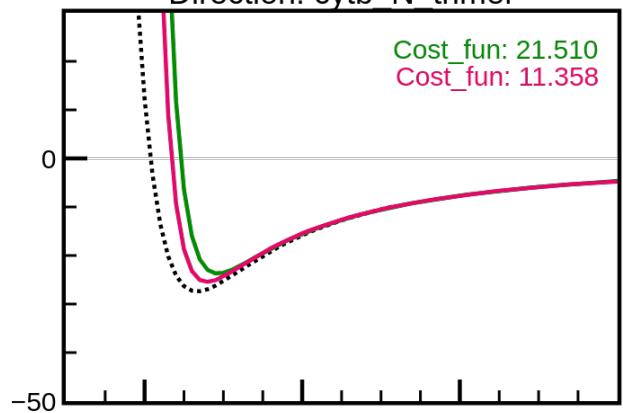
Energy, kcal/mol

Distance, A

CYTB RUB 2/2

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

Direction: cytb N trimer

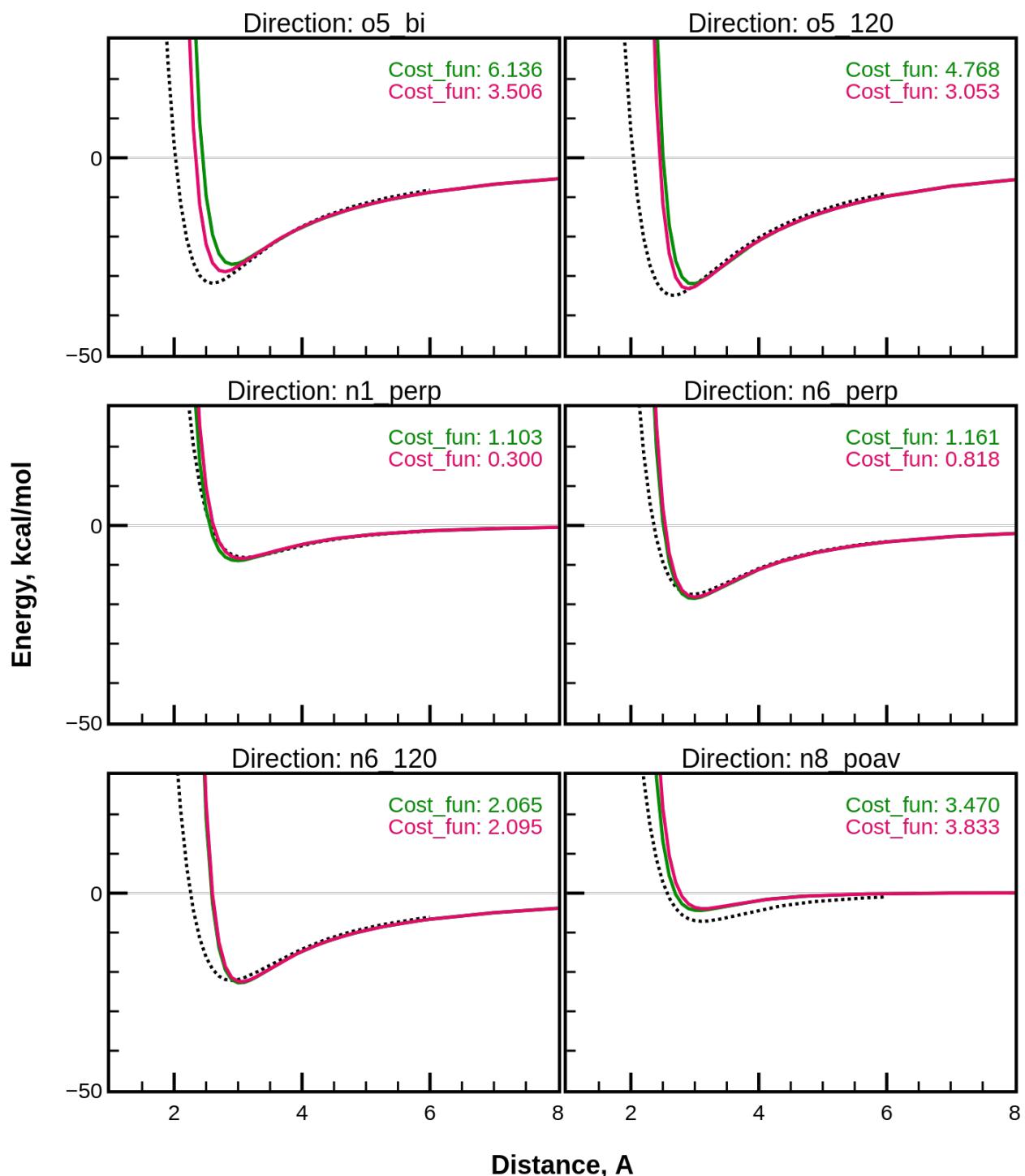


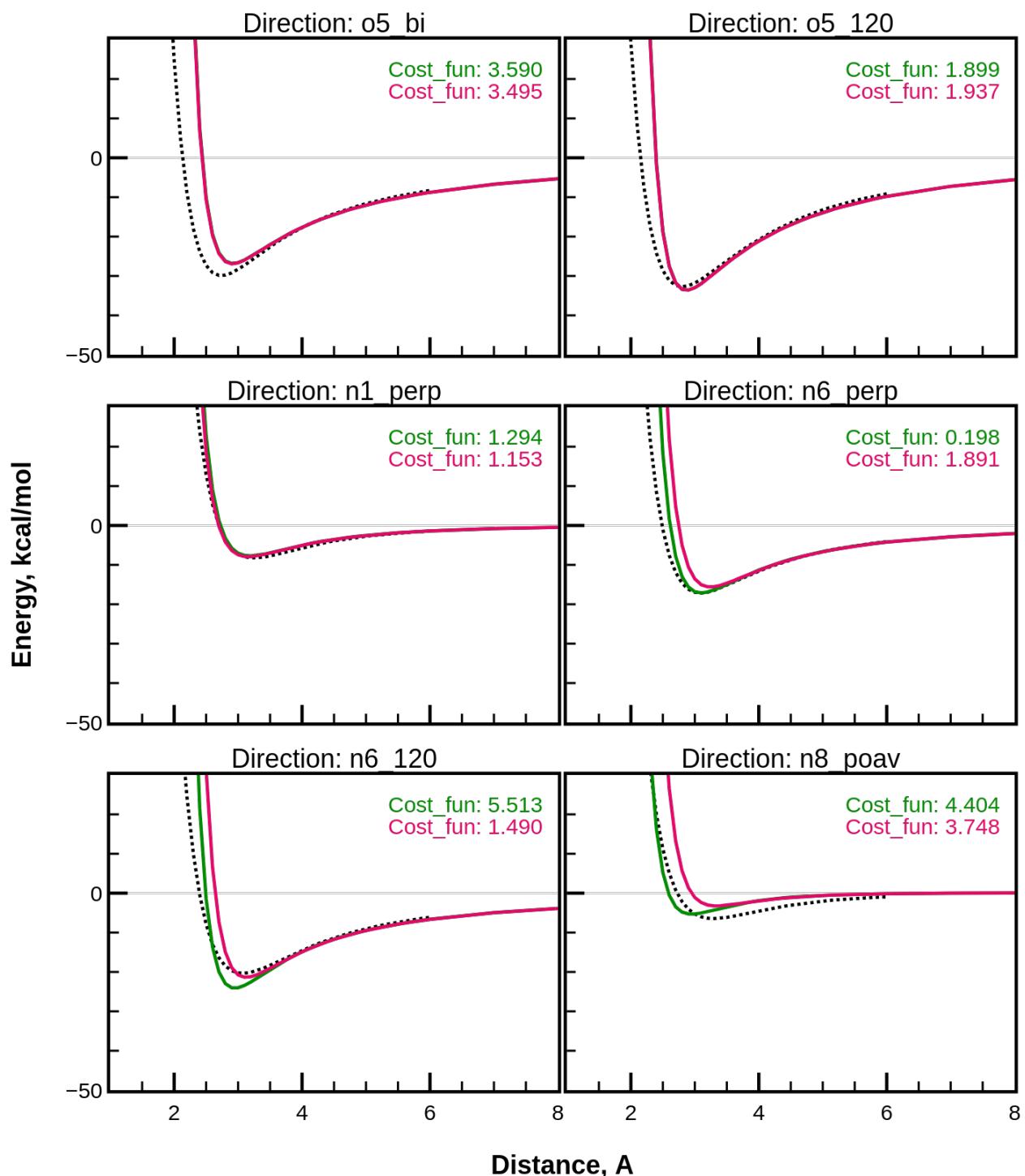
Energy, kcal/mol

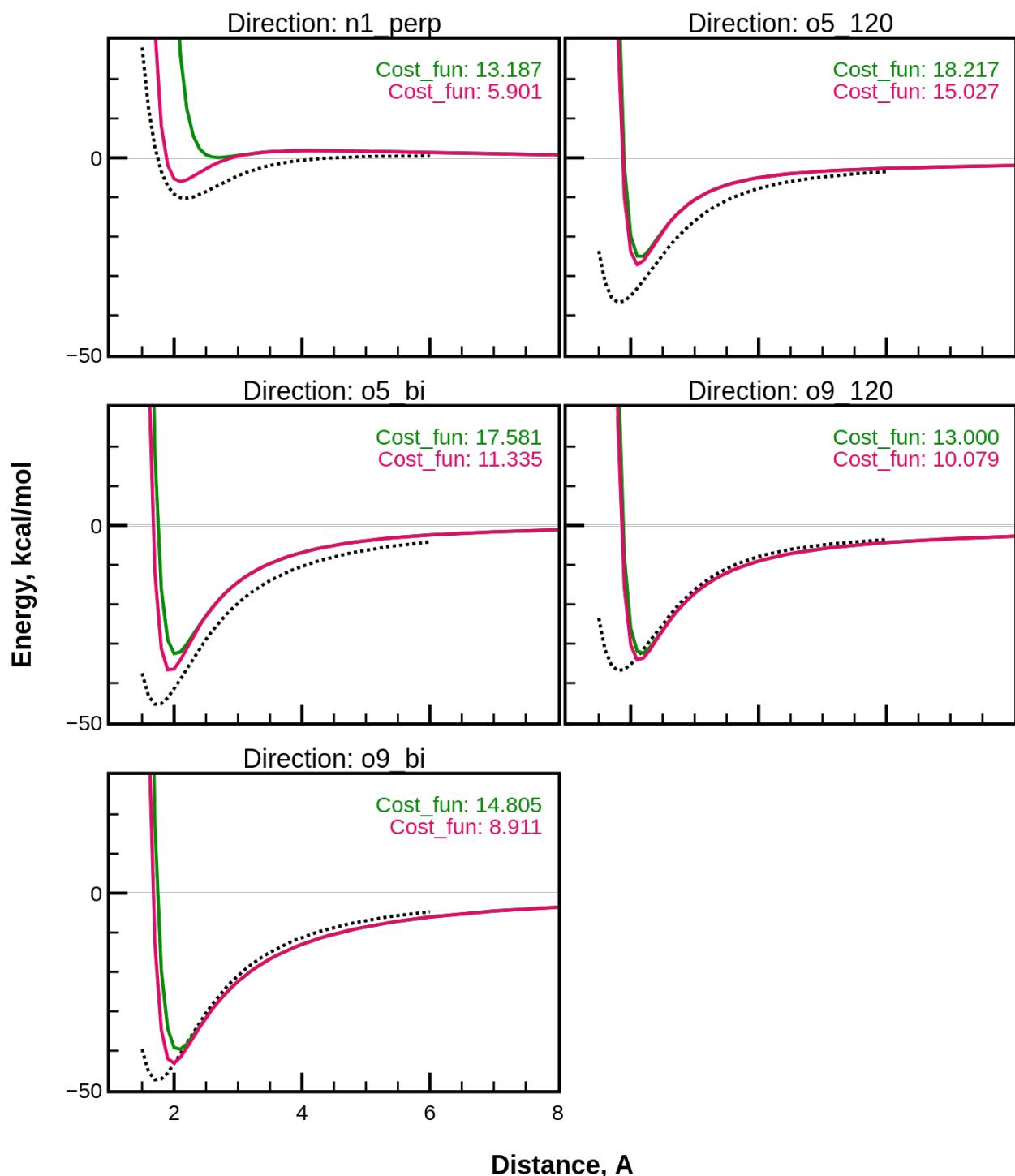
Distance, Å

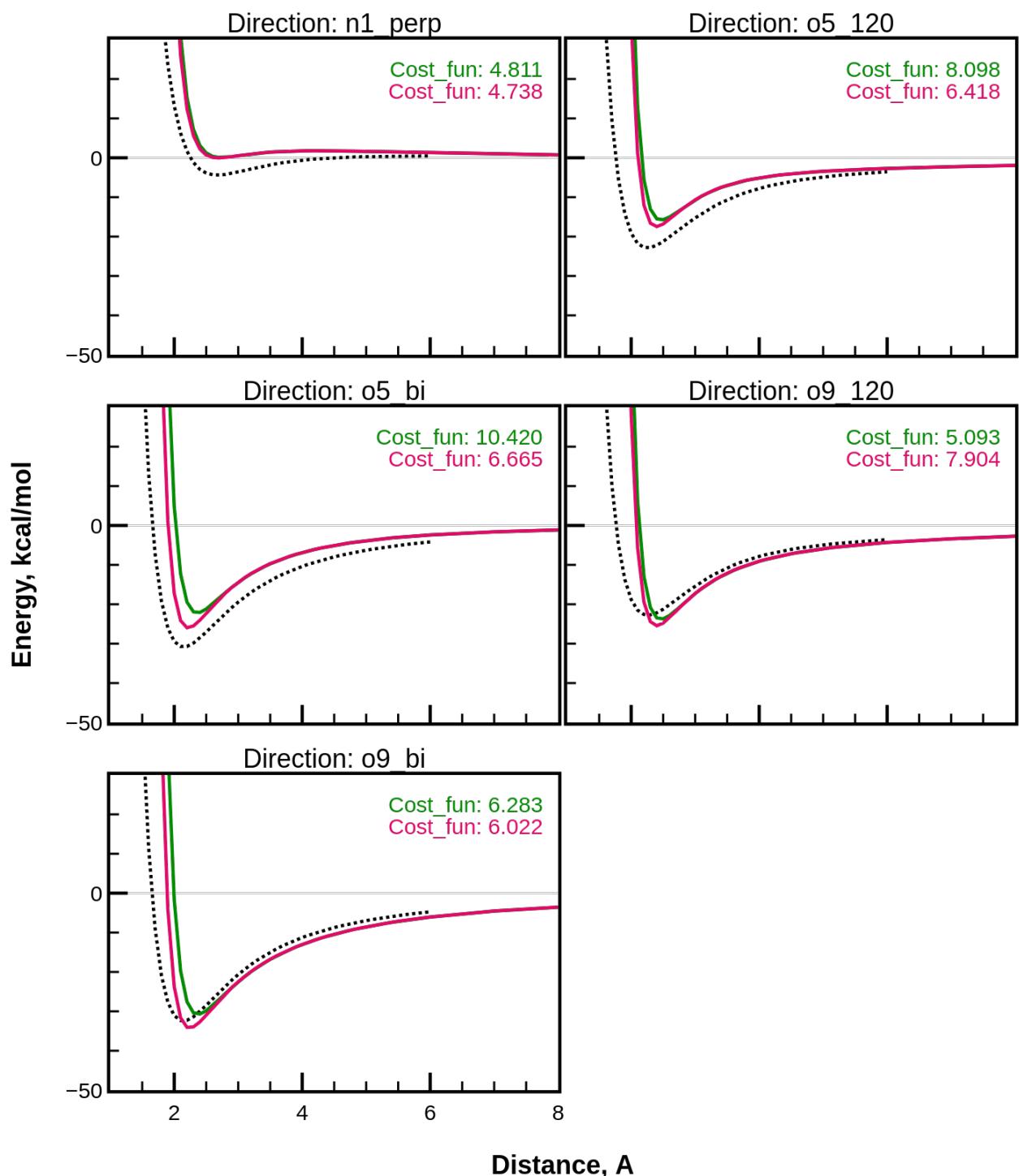
CYTB RUB 1/2

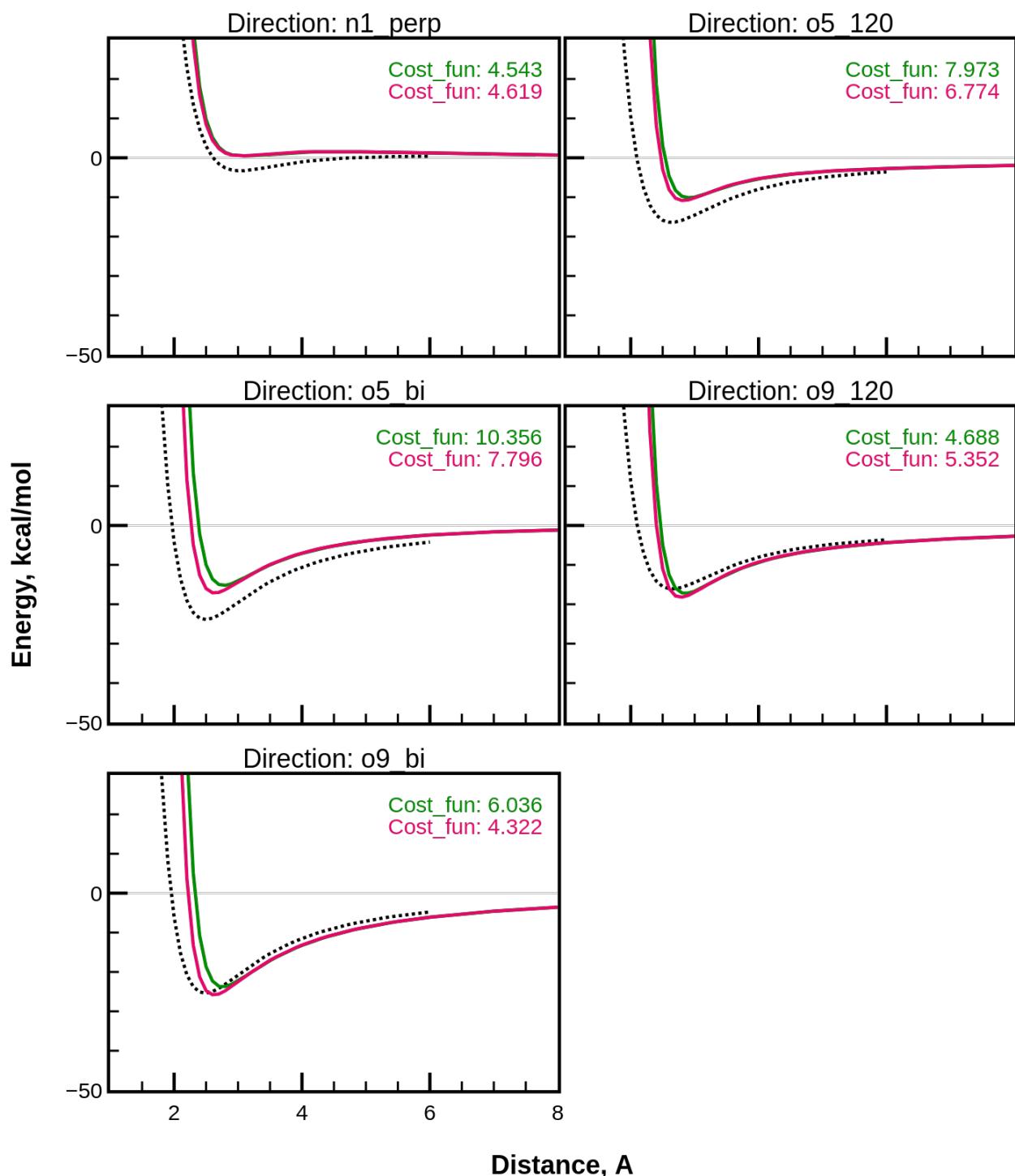
9.99999_9.99999_9.99999
1.11111_1.11111_1.11111

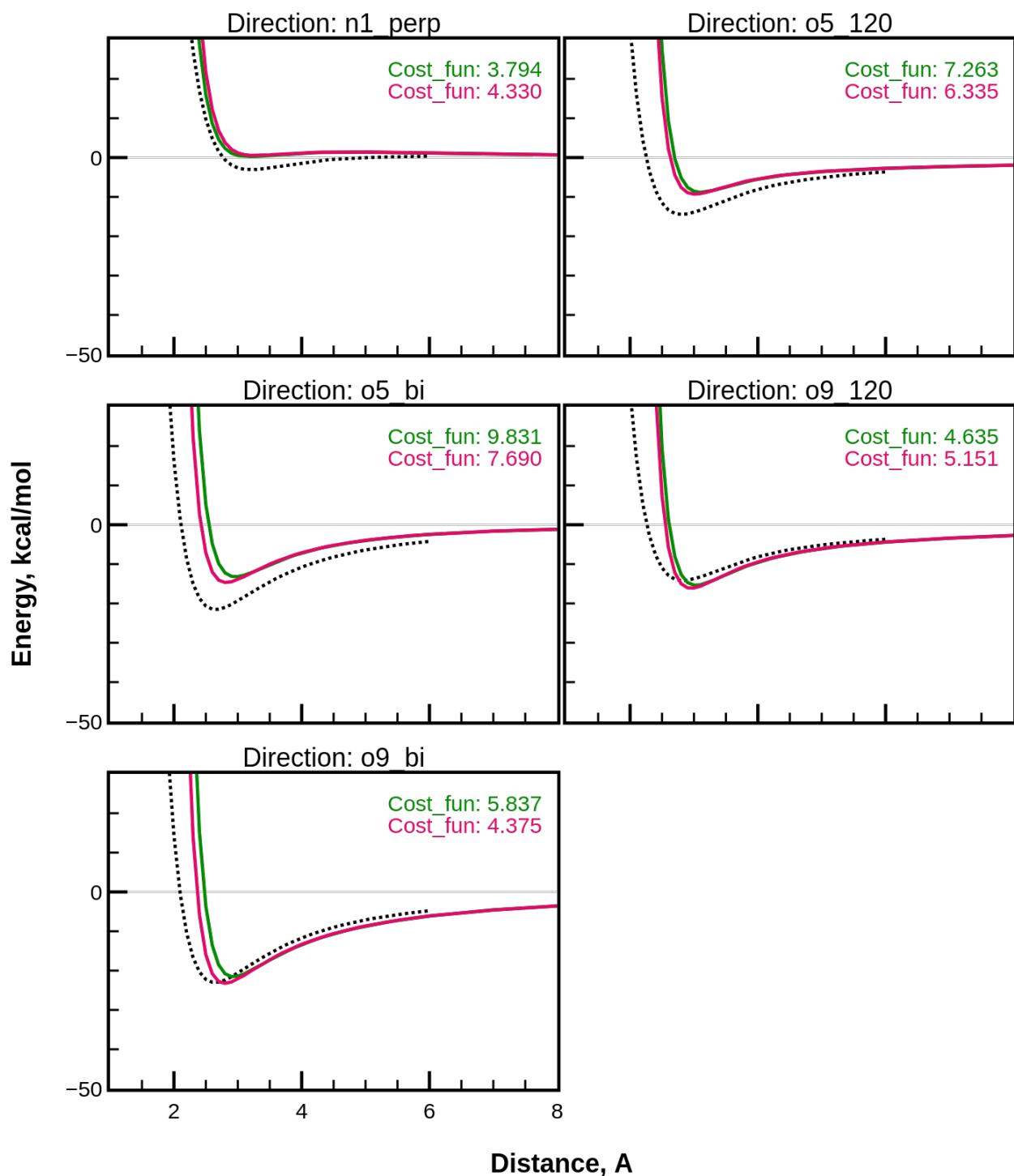


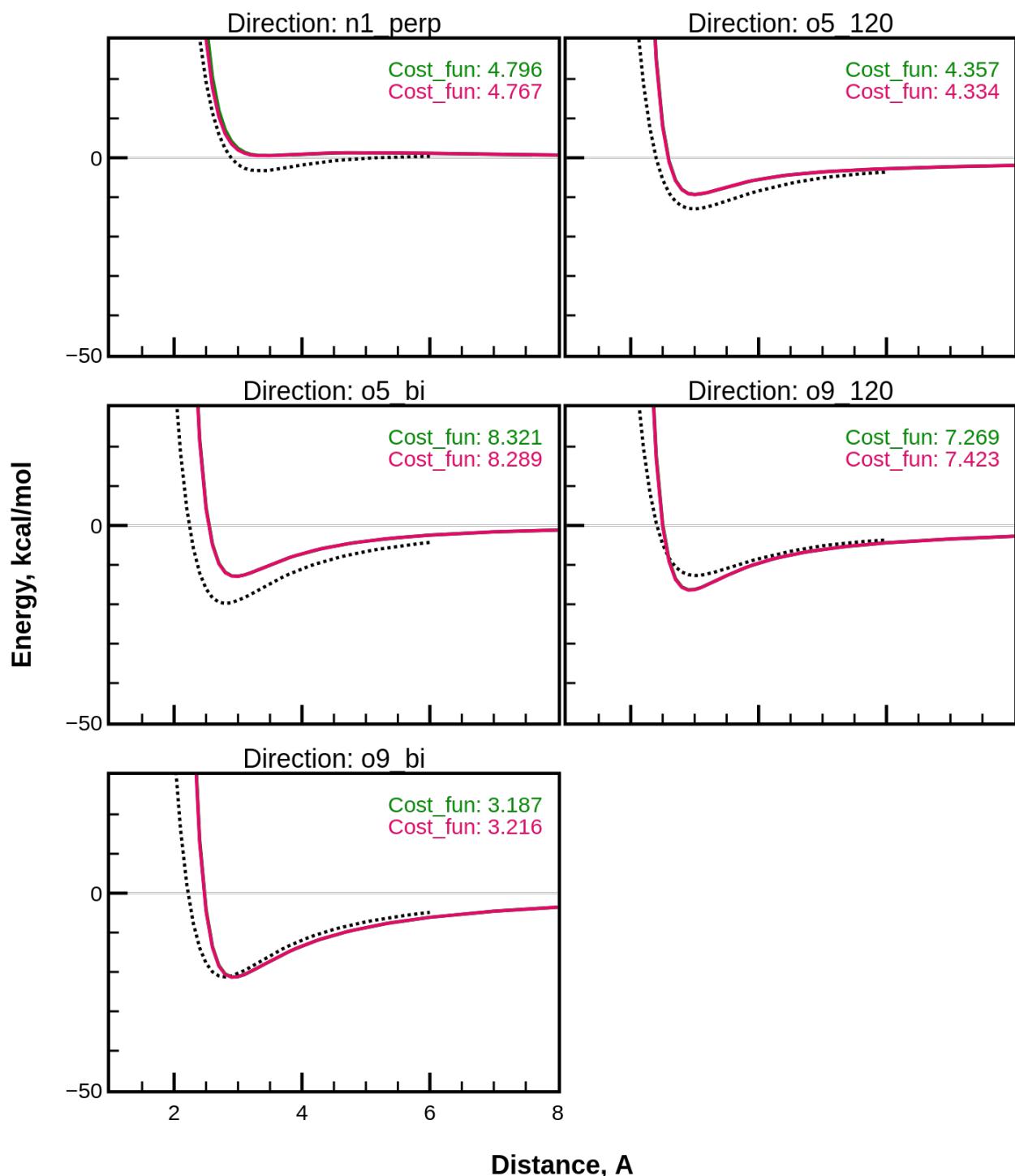
CYTB CES 1/19.99999_9.99999_9.99999
1.11111_1.11111_1.11111

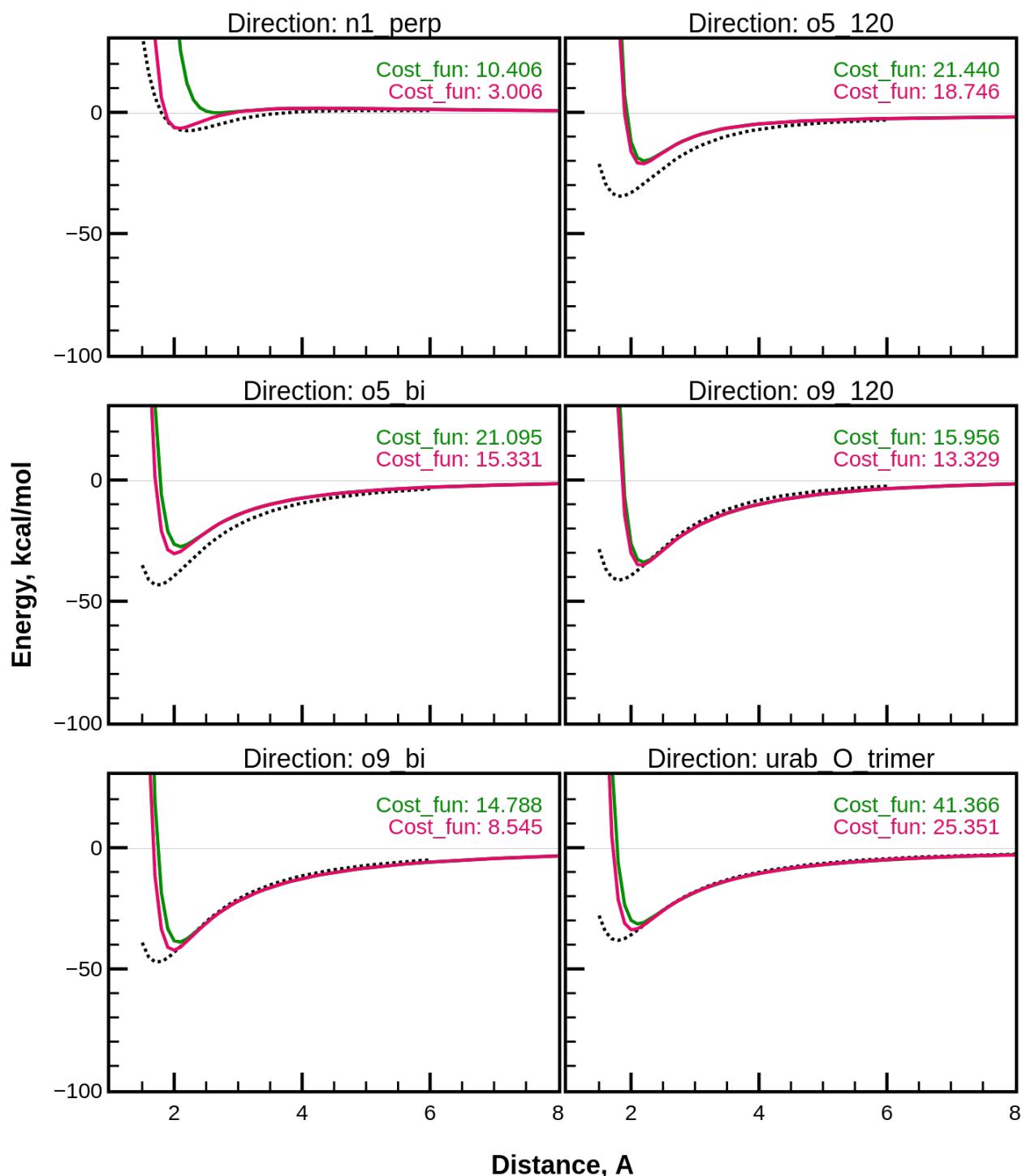
THYB LIT 1/19.99999_9.99999_9.99999
1.11111_1.11111_1.11111

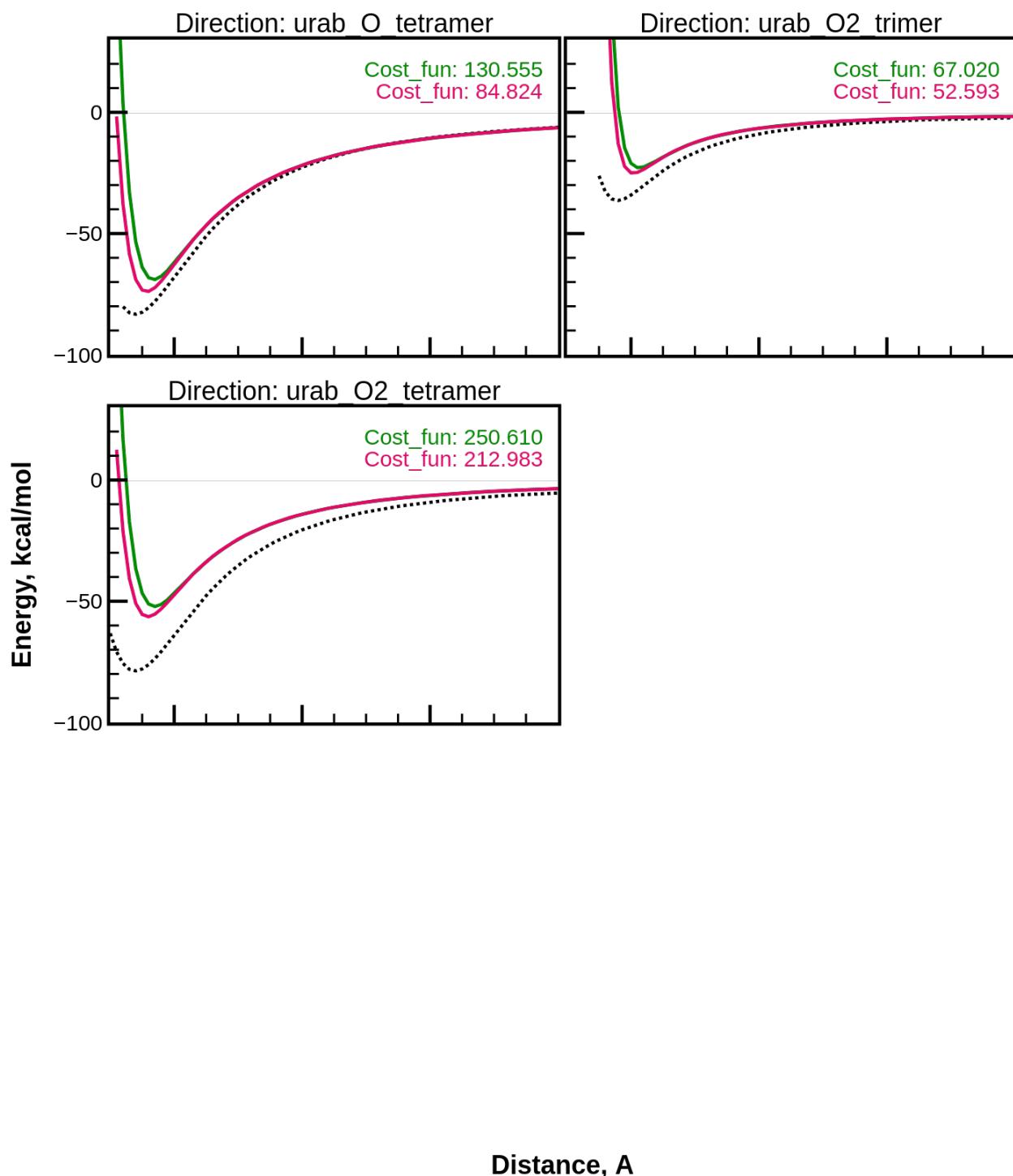
THYB SOD 1/19.99999_9.99999_9.99999
1.11111_1.11111_1.11111

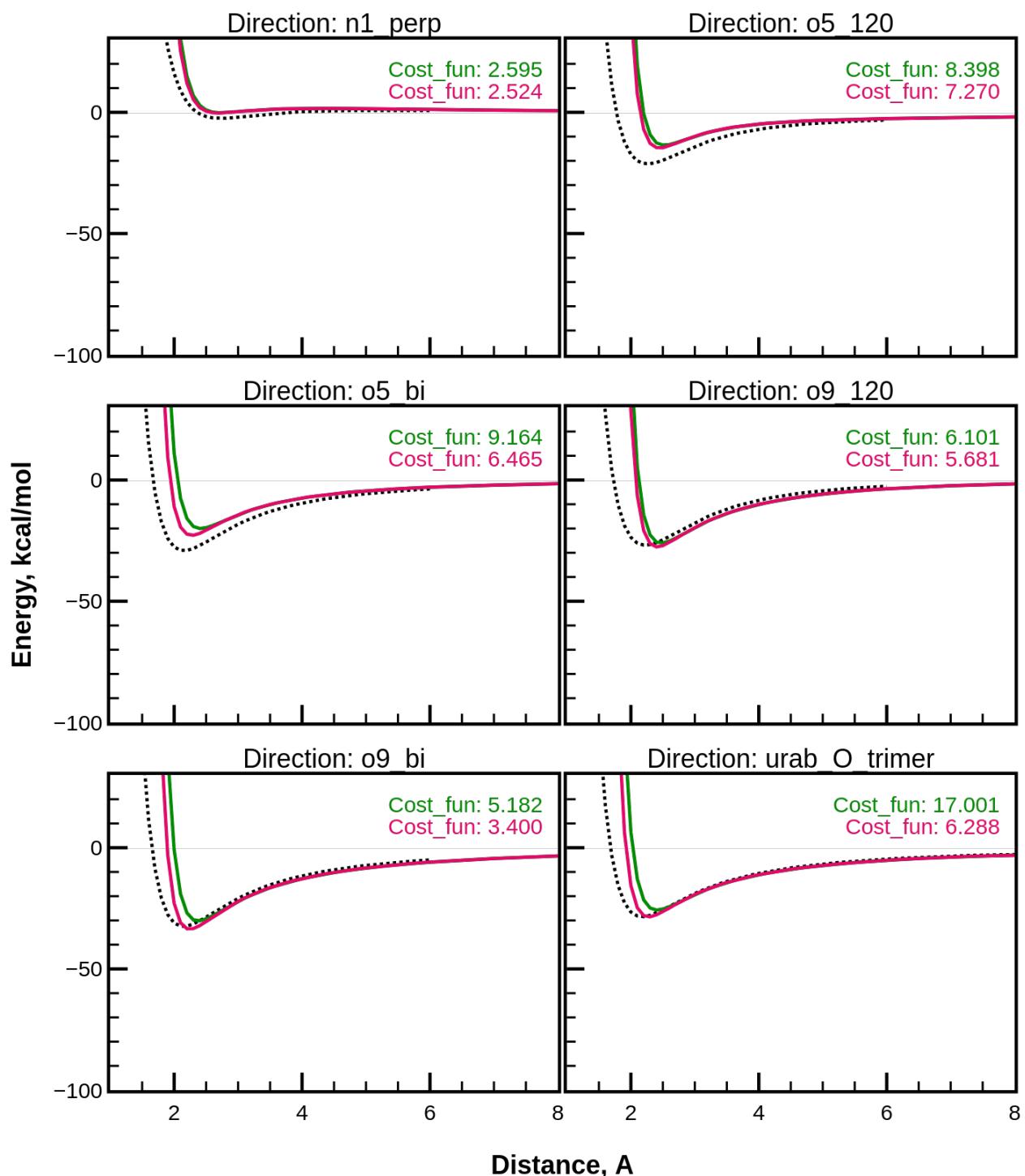
THYB POT 1/19.99999_9.99999_9.99999
1.11111_1.11111_1.11111

THYB RUB 1/19.99999_9.99999_9.99999
1.11111_1.11111_1.11111

THYB CES 1/19.99999_9.99999_9.99999
1.11111_1.11111_1.11111

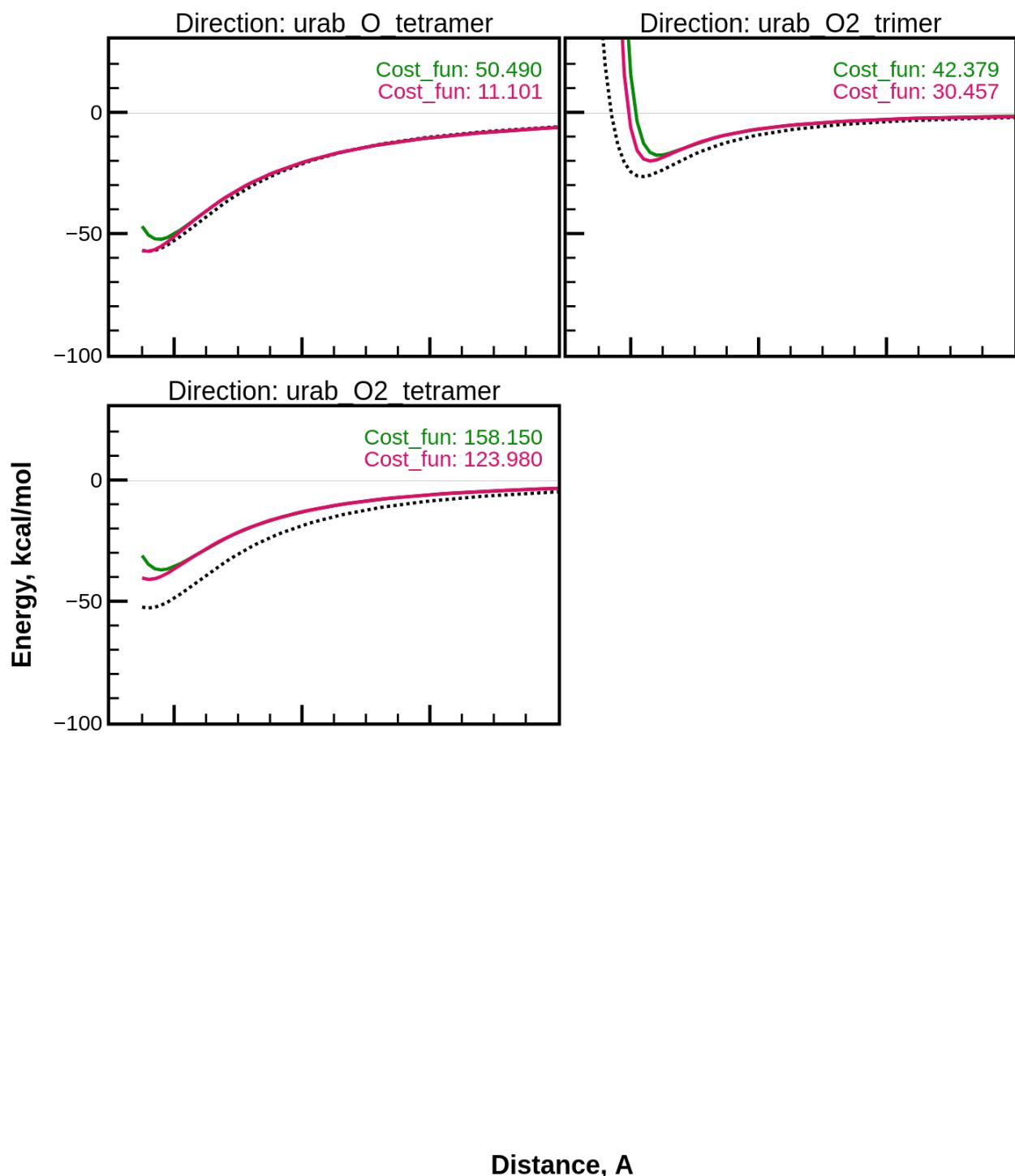
URAB LIT 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

URAB LIT 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

URAB SOD 1/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

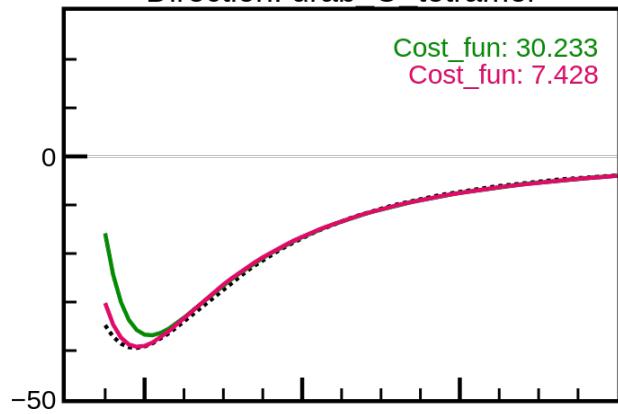
URAB SOD 2/2

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

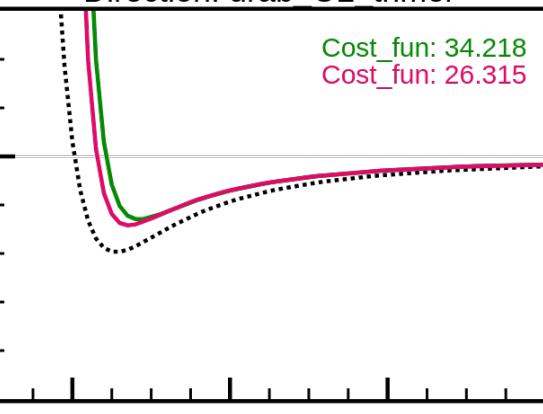


URAB POT 2/29.99999_9.99999_9.99999
1.11111_1.11111_1.11111

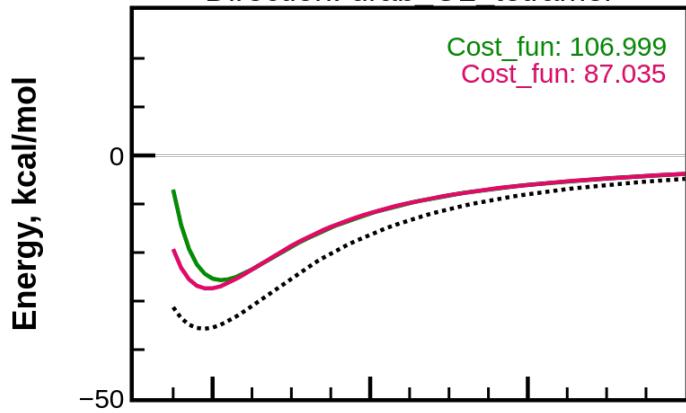
Direction: urab_O_tetramer



Direction: urab_O2_trimer



Direction: urab_O2_tetramer

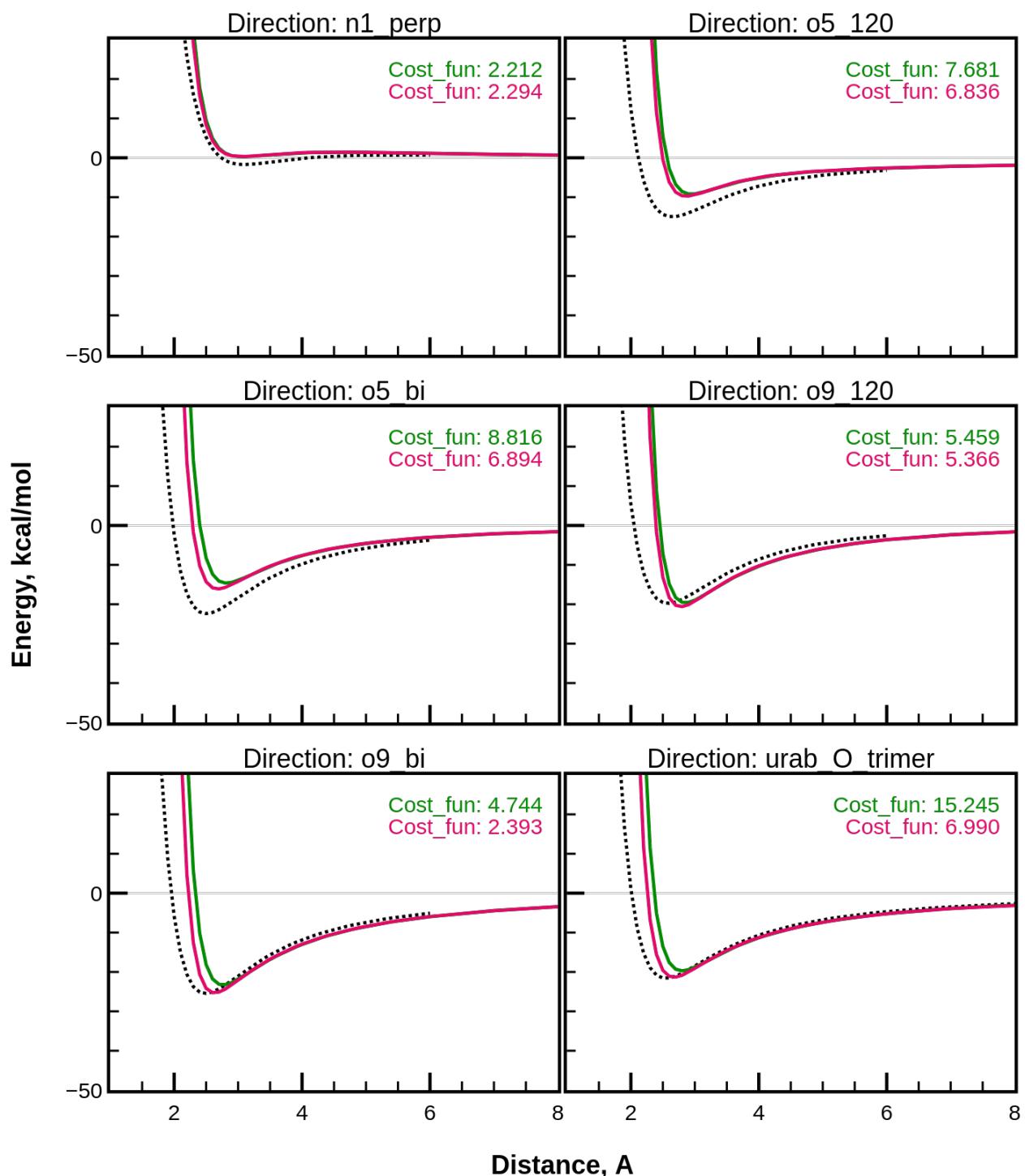


Distance, Å

Energy, kcal/mol

URAB POT 1/2

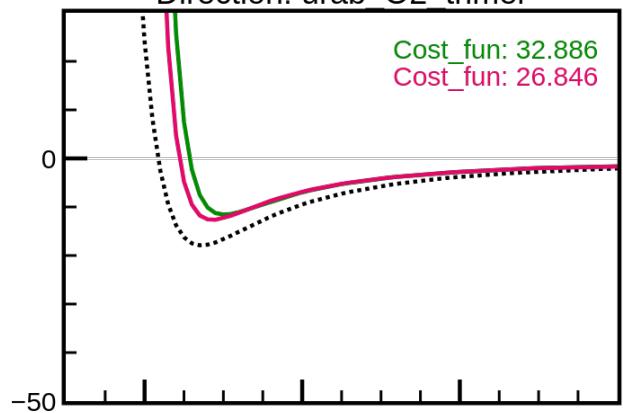
9.99999_9.99999_9.99999
1.11111_1.11111_1.11111



URAB RUB 2/2

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

Direction: urab_O2_trimer

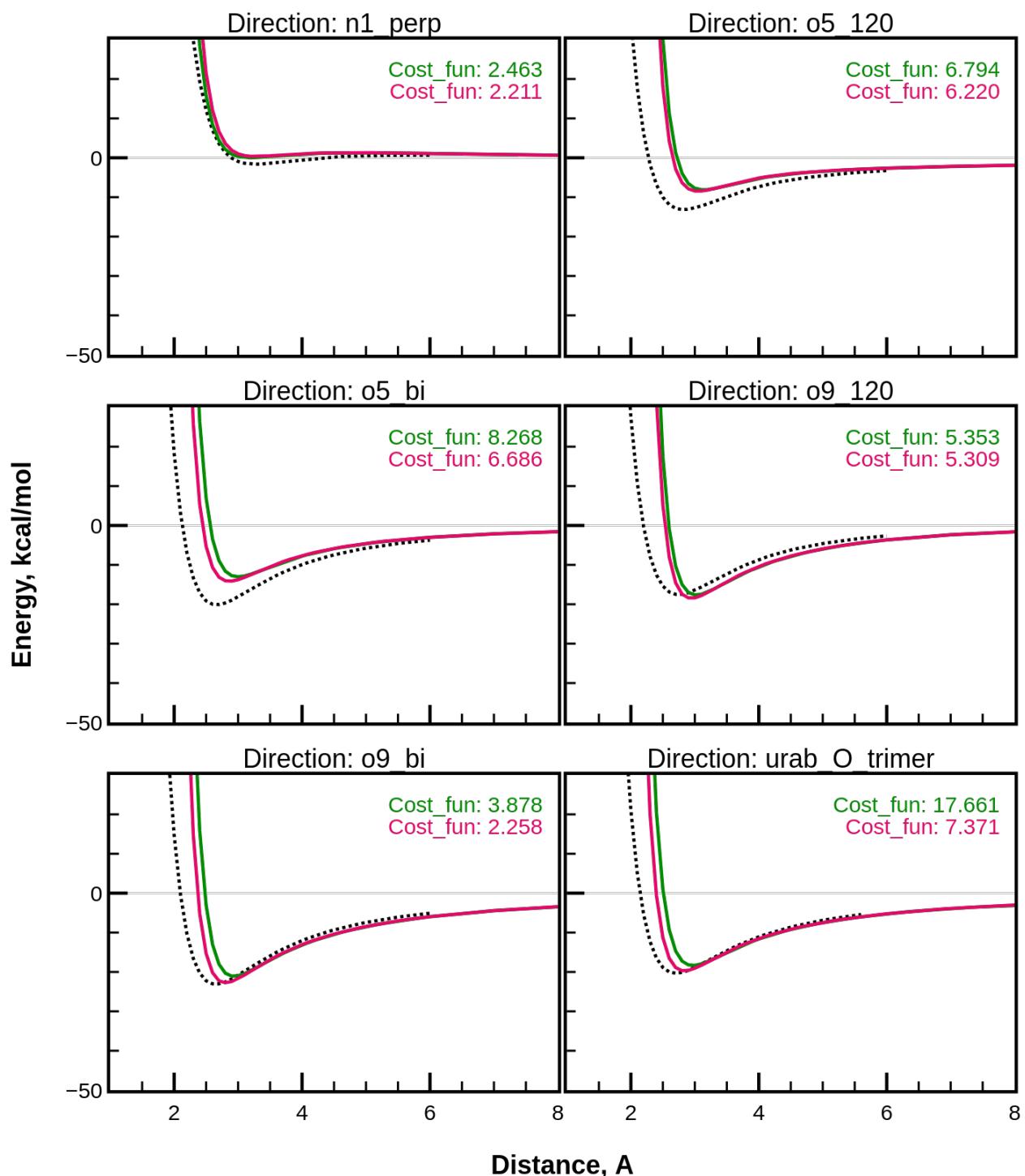


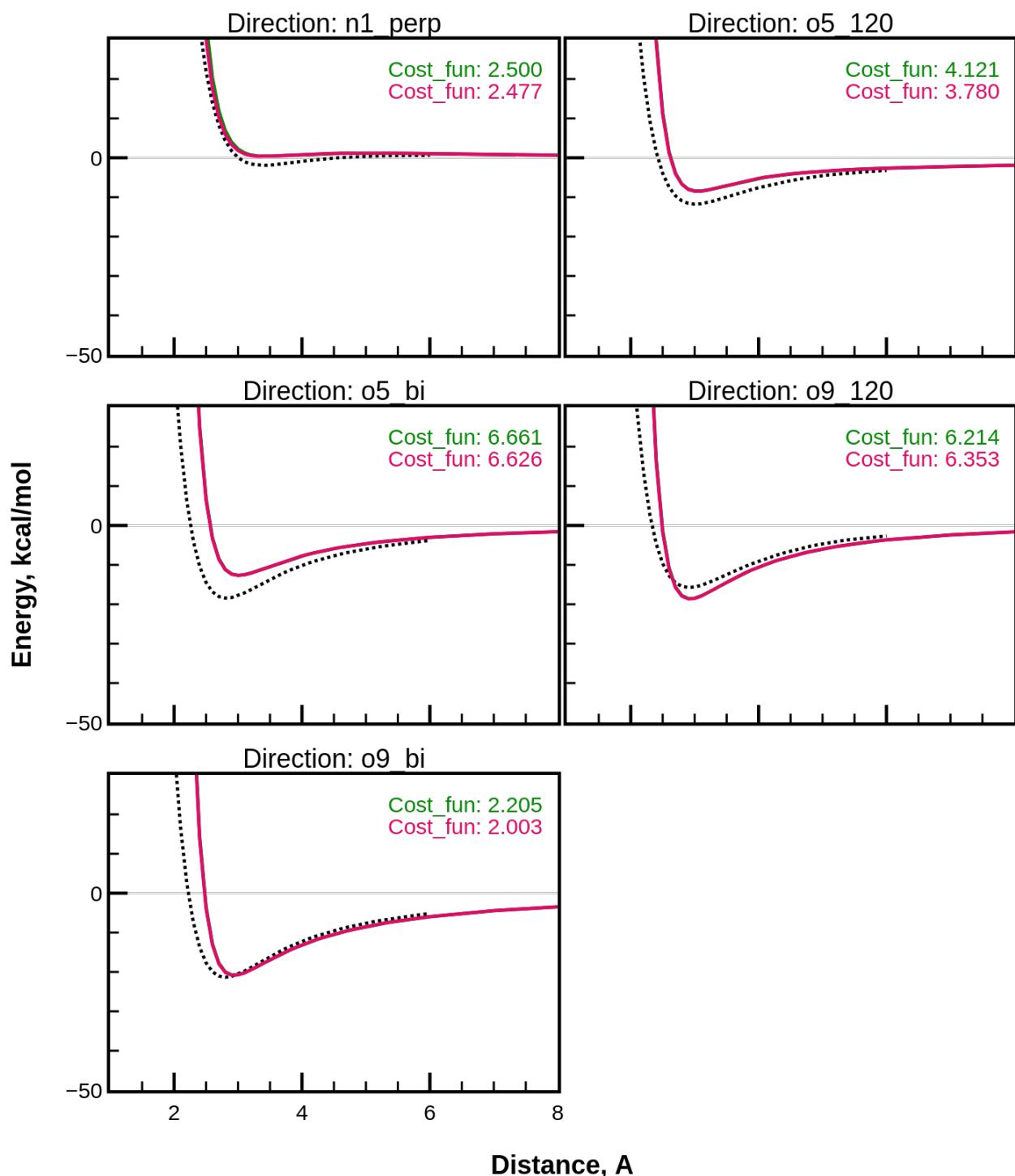
Energy, kcal/mol

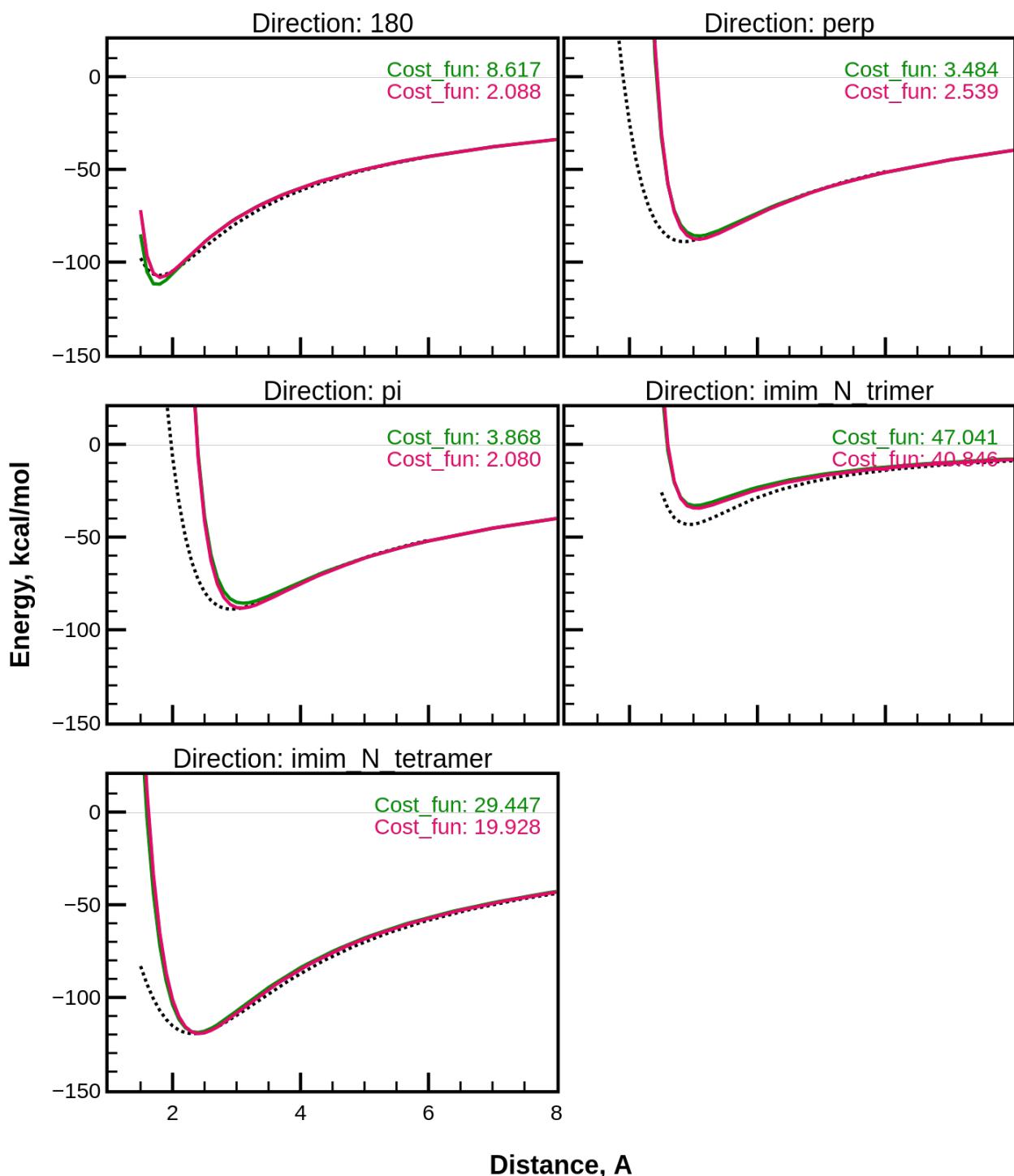
Distance, Å

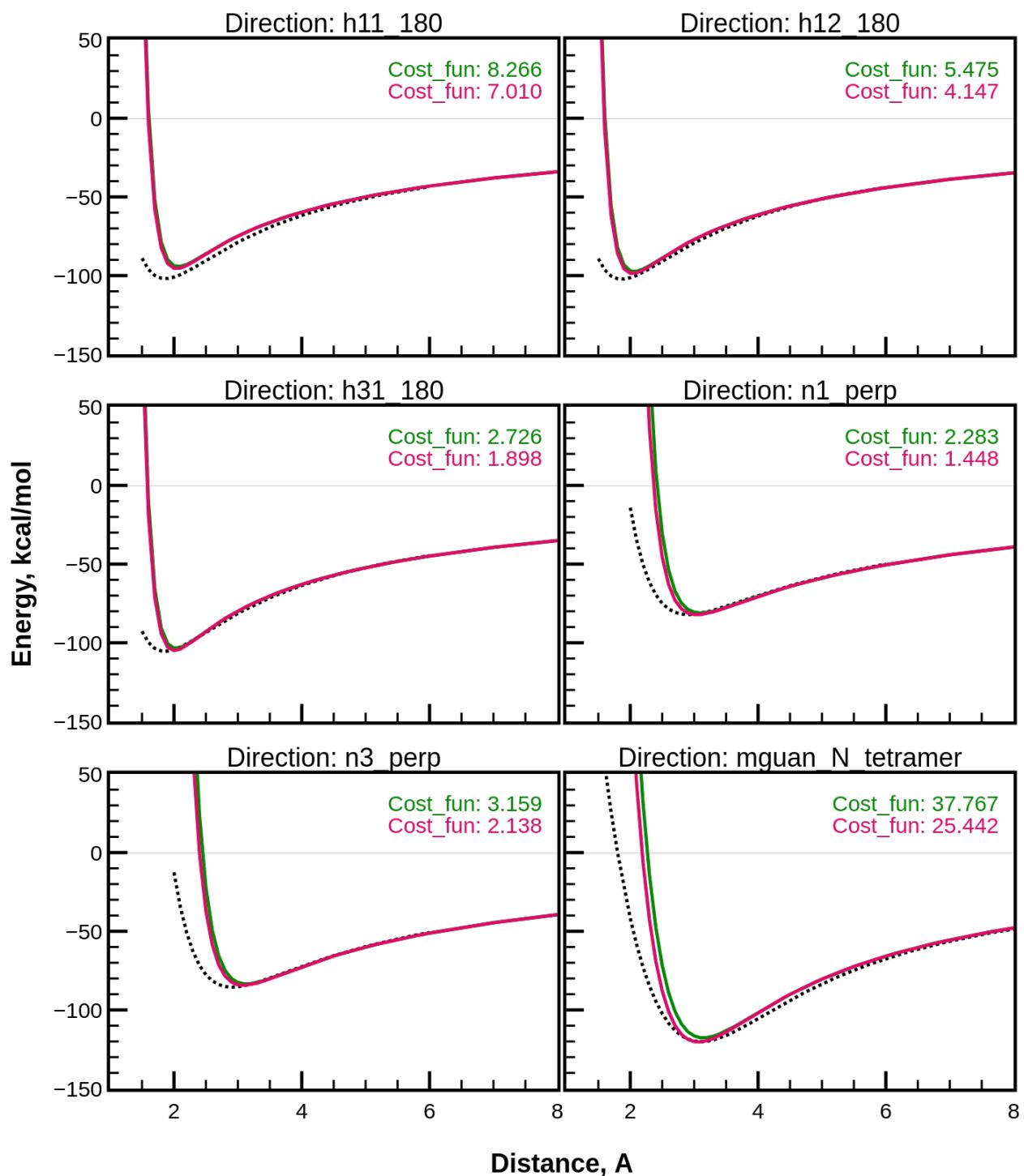
URAB RUB 1/2

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



URAB CES 1/19.99999_9.99999_9.99999
1.11111_1.11111_1.11111

IMIM CLA 1/14.33111_0.08693_9.99999
4.36326_0.08693_1.41768

MGUAN CLA 1/14.28111_0.08269_9.99999
4.14635_0.08269_4.10351

NC1 CLA 1/14.03111_0.04242_9.99999
4.62234_0.04242_1.59027