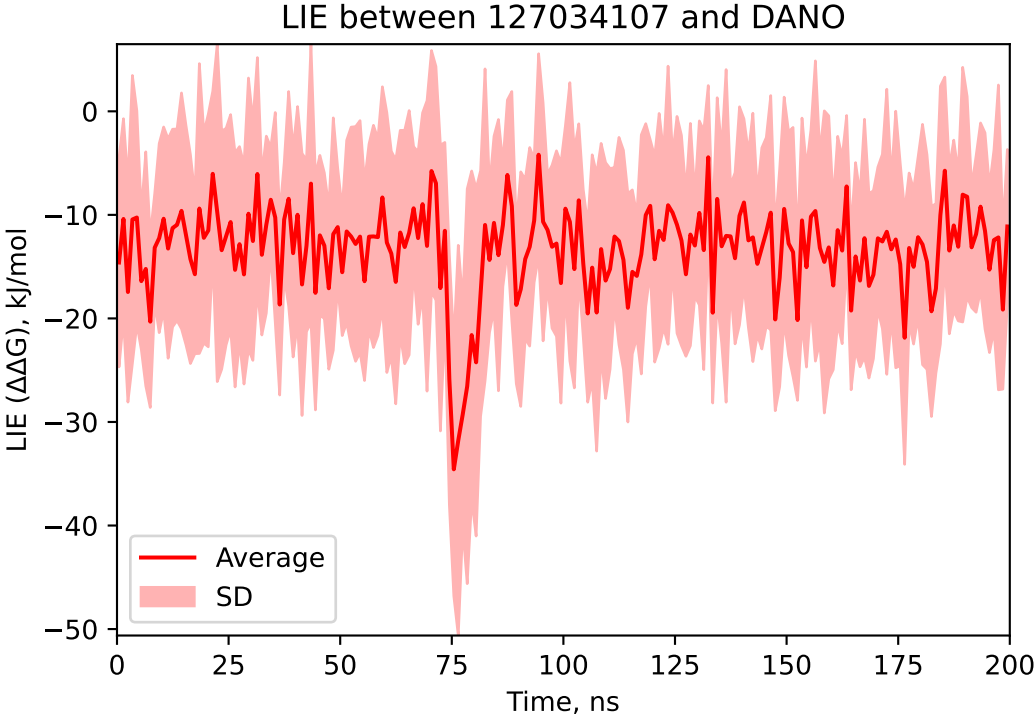
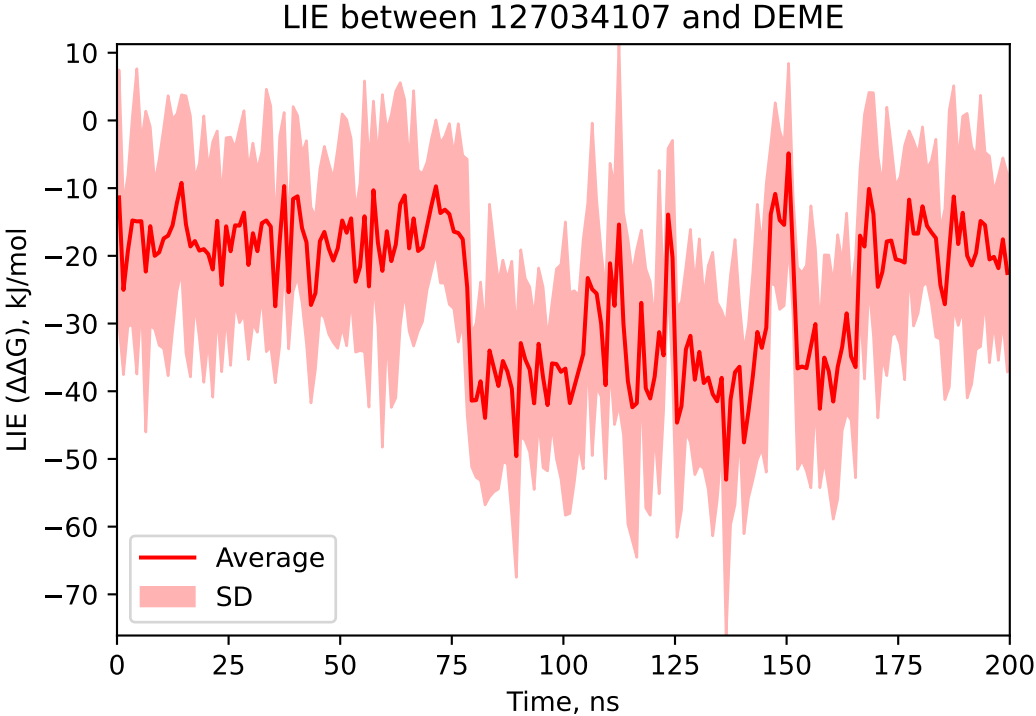
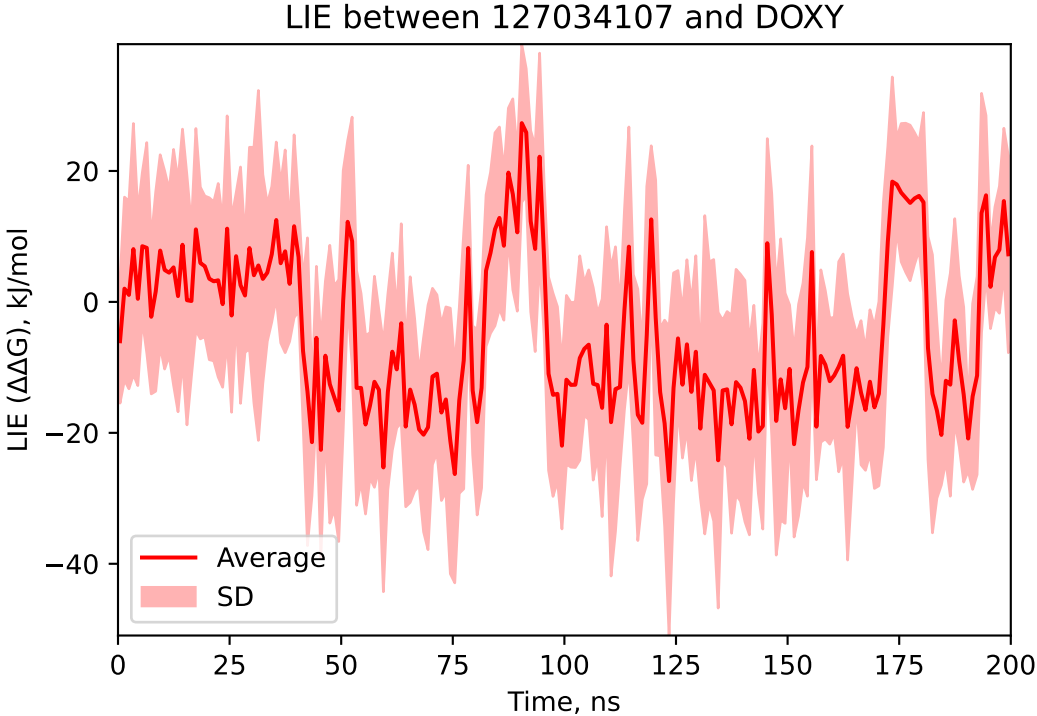
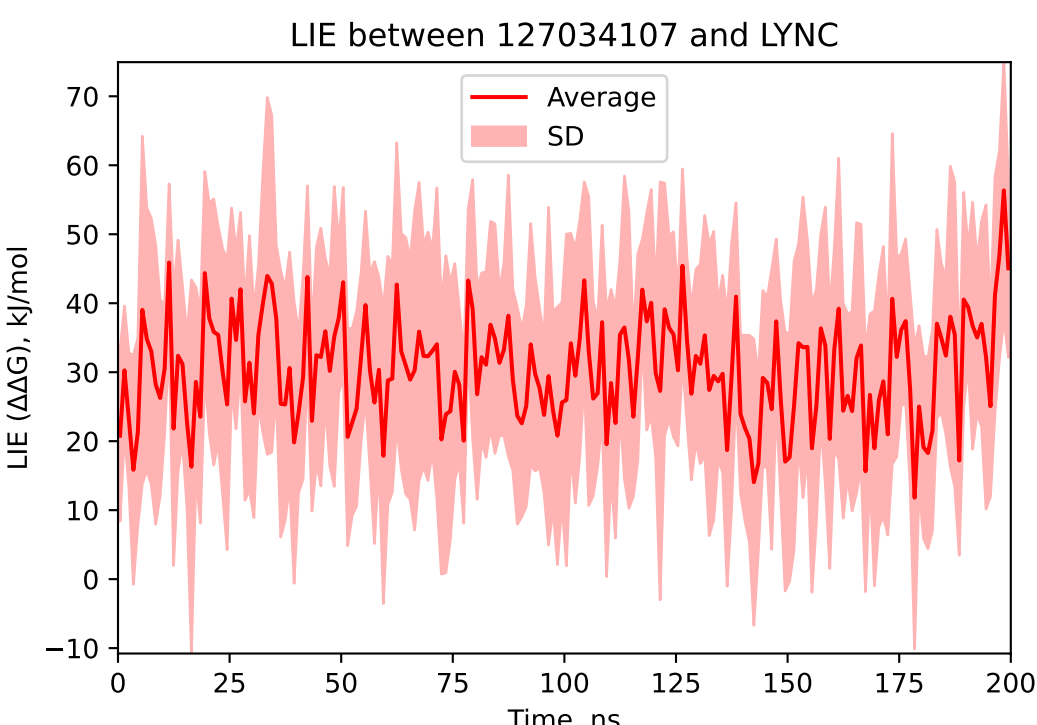
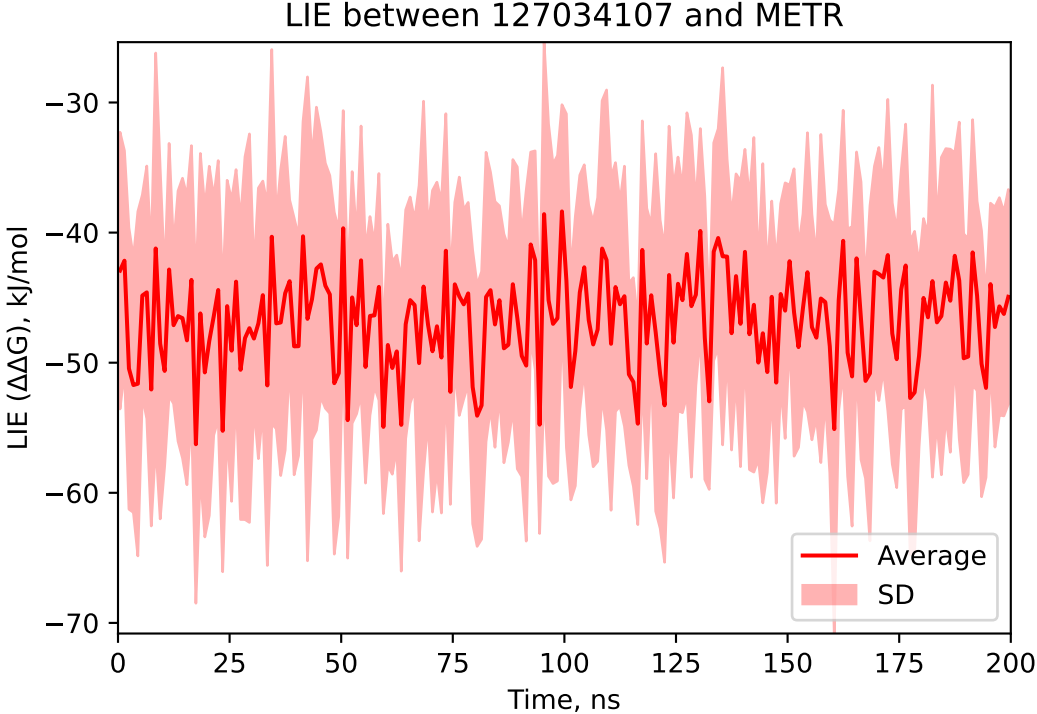
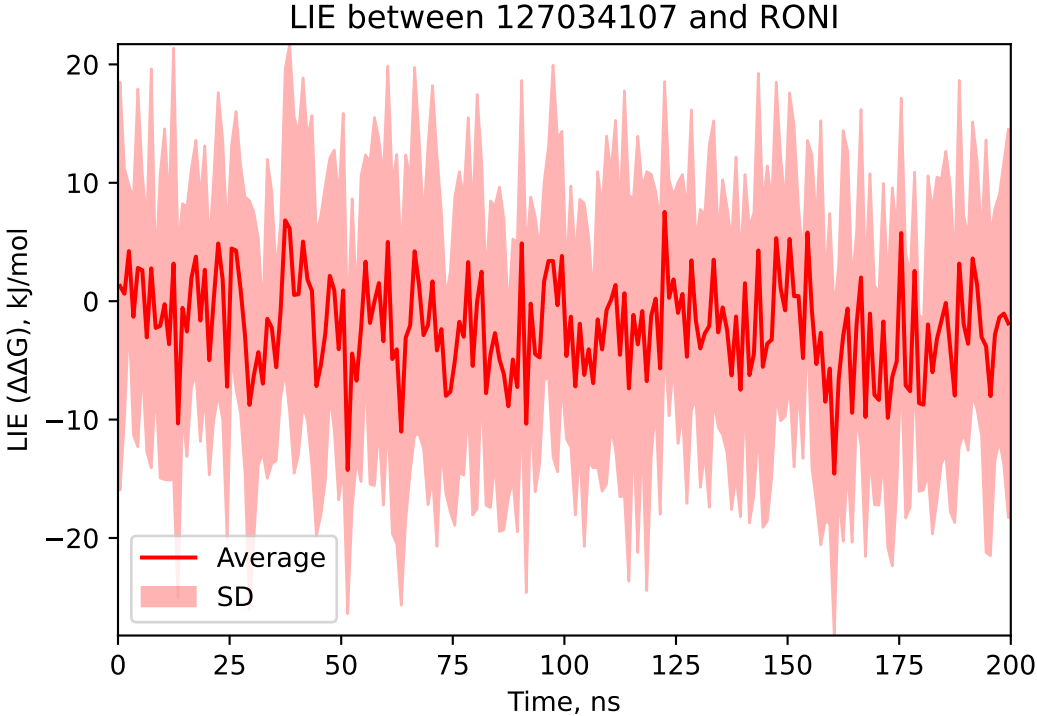

LIE between 127034107 and DANO
LIE (ΔΔG), kJ/mol
0
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

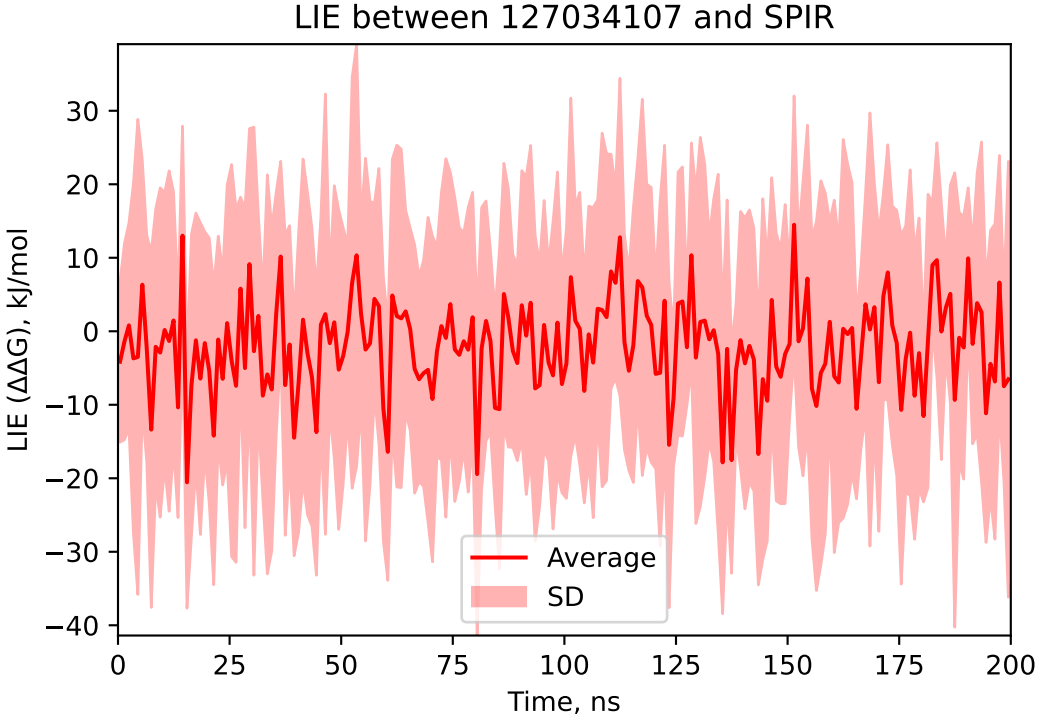

LIE between 127034107 and DEME
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
−40
−50
−60
−70
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

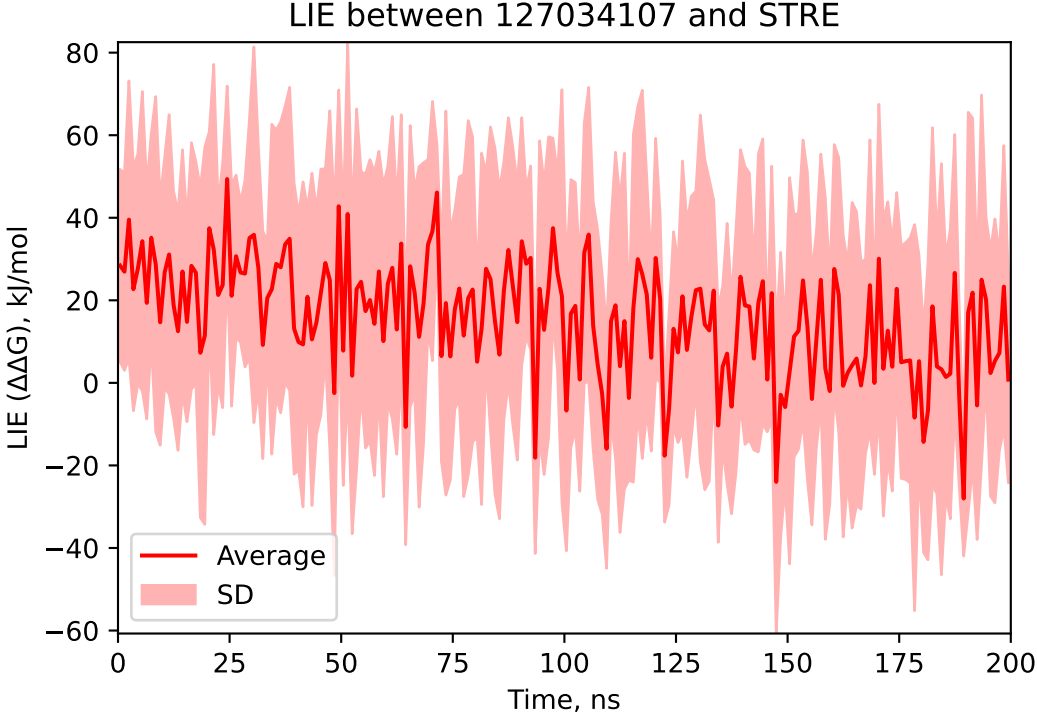

LIE between 127034107 and DOXY
LIE (ΔΔG), kJ/mol
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

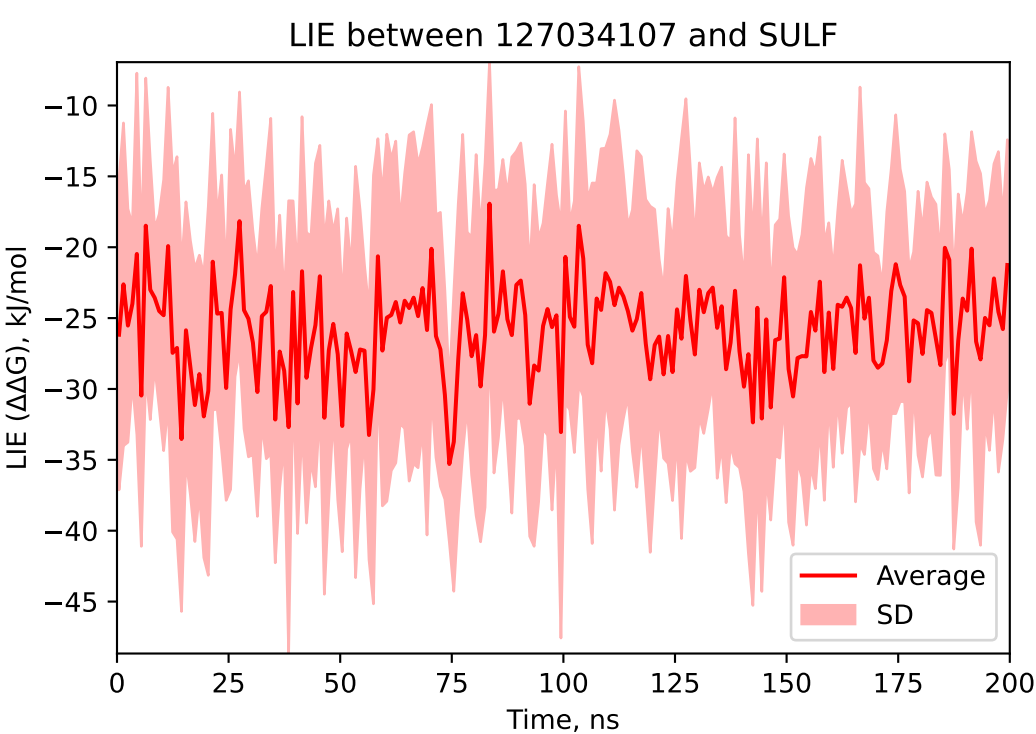

LIE between 127034107 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
70
60
50
40
30
20
10
0
−10
0
25
50
75
100
125
150
175
200
Time, ns

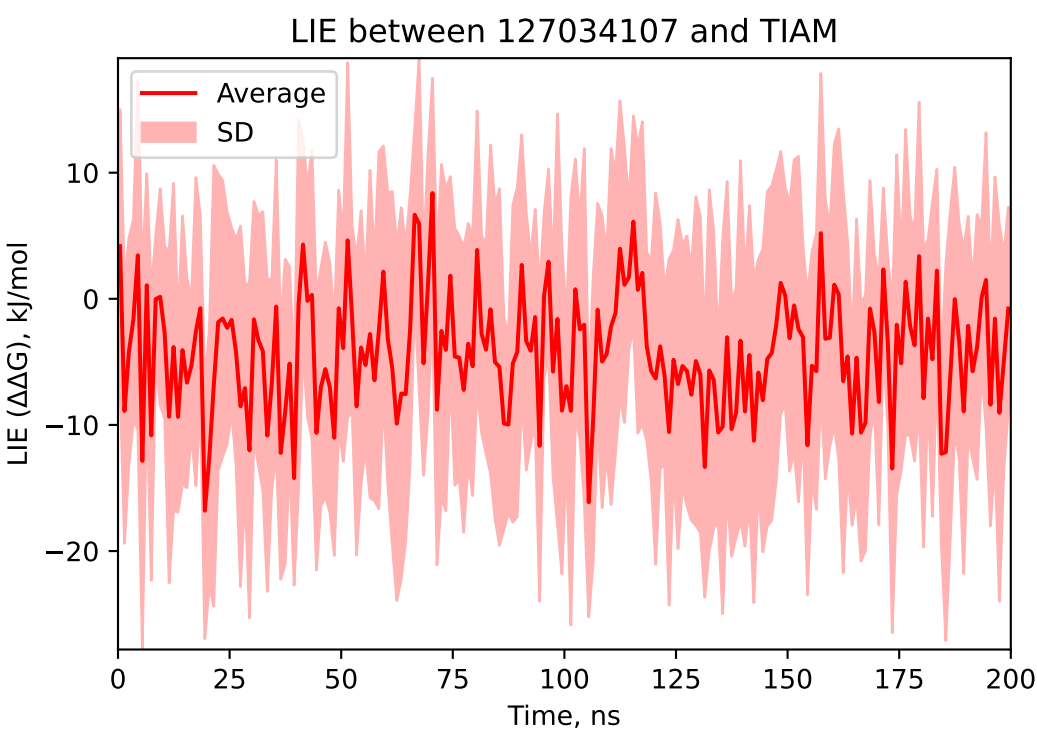

LIE between 127034107 and METR
LIE (ΔΔG), kJ/mol
−30
−40
−50
−60
−70
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

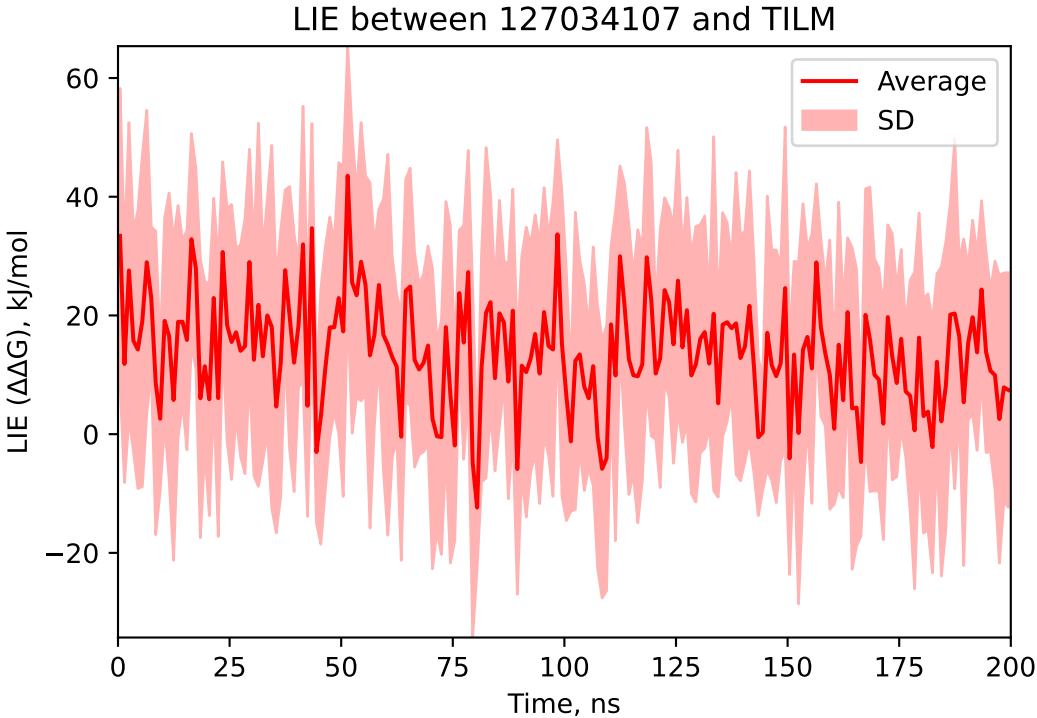

LIE between 127034107 and RONI
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200

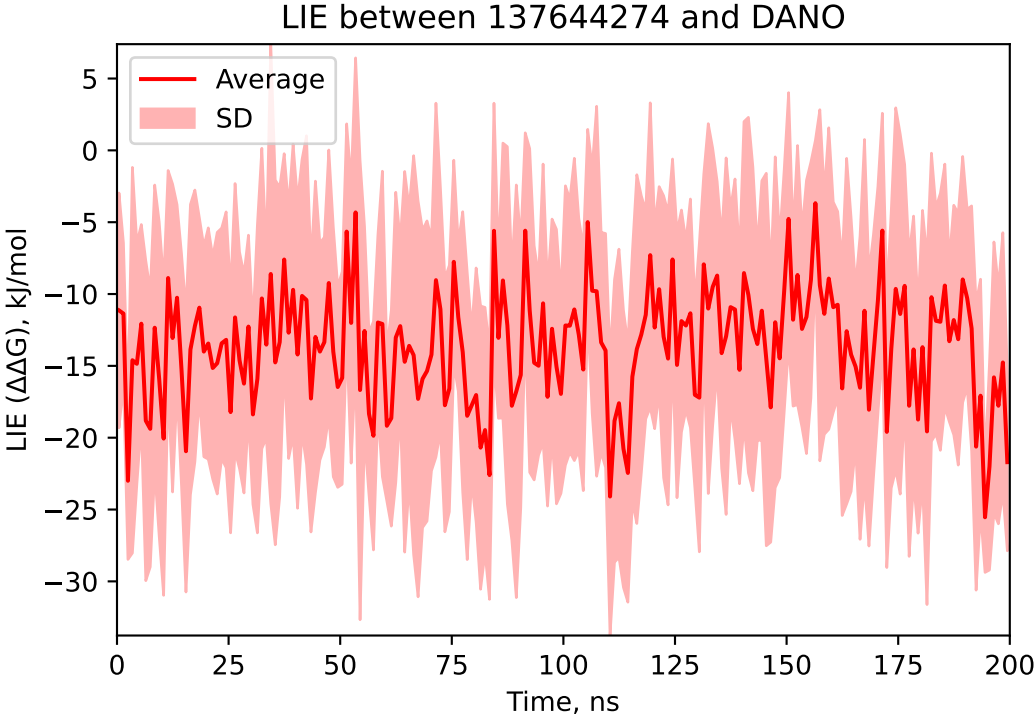

LIE between 127034107 and SPIR
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200

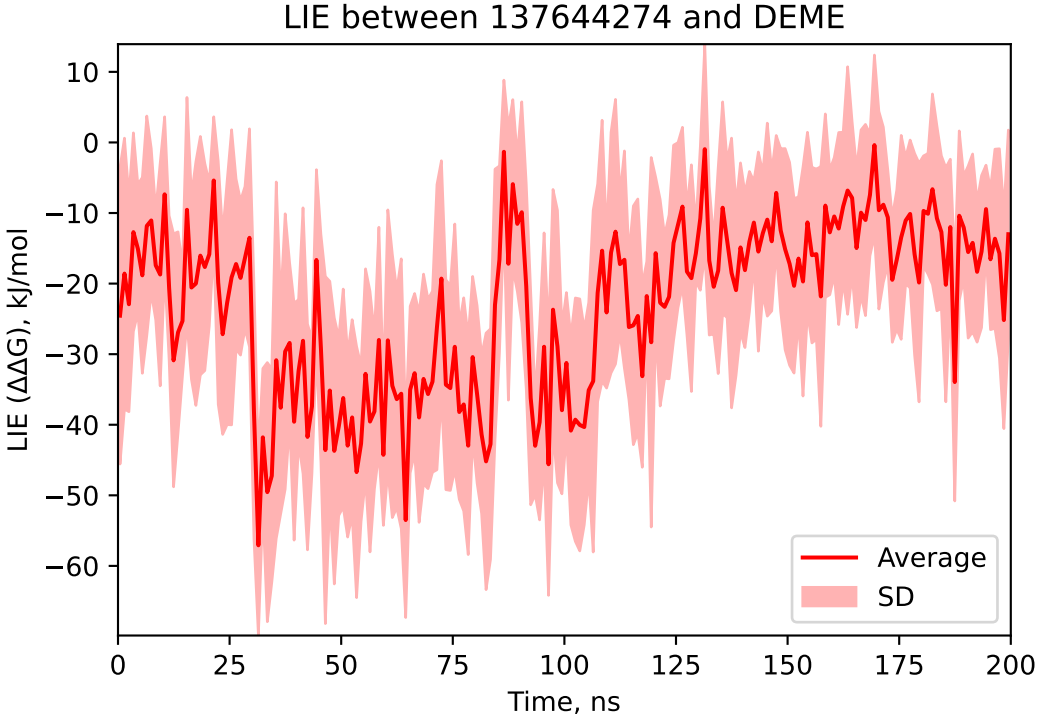

LIE between 127034107 and STRE
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
80
60
40
20
0
−20
−40
−60
0
25
50
75
100
125
150
175
200

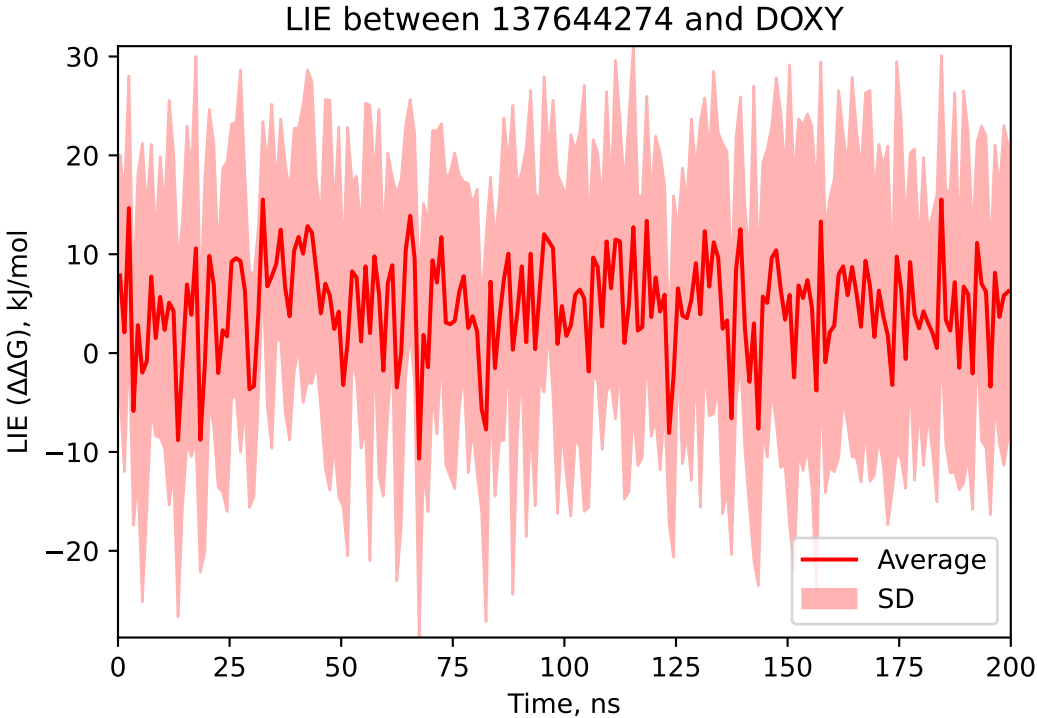

LIE between 127034107 and SULF
LIE (ΔΔG), kJ/mol
−10
−15
−20
−25
−30
−35
−40
−45
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

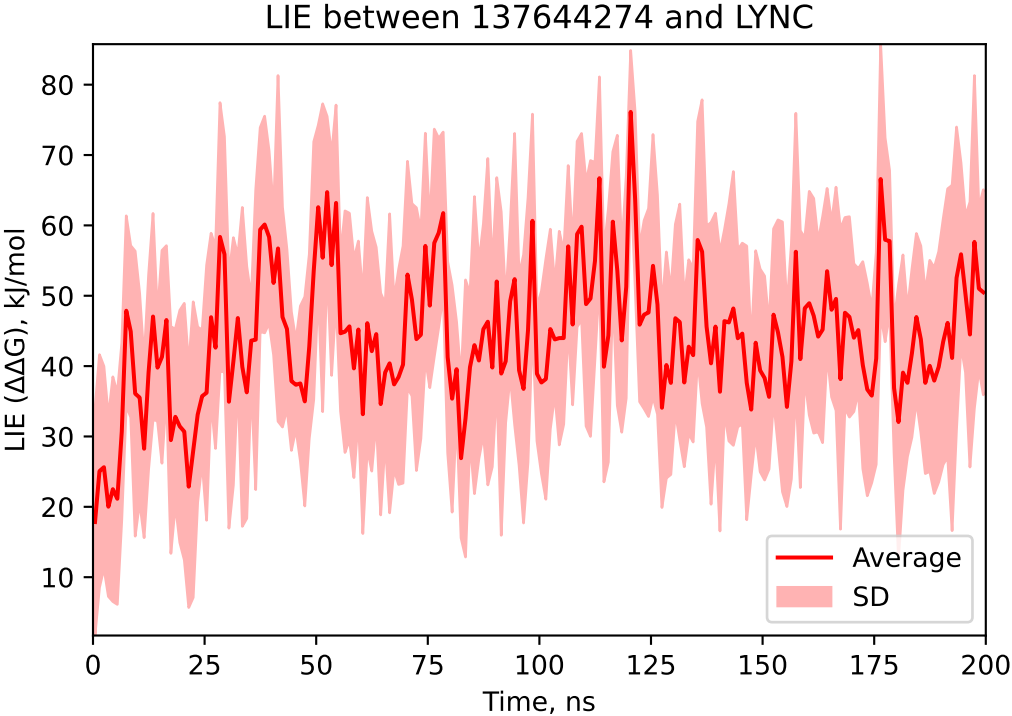

LIE between 127034107 and TIAM
Average
SD
10
0
−10
−20
LIE (ΔΔG), kJ/mol
0
25
50
75
100
125
150
175
200
Time, ns

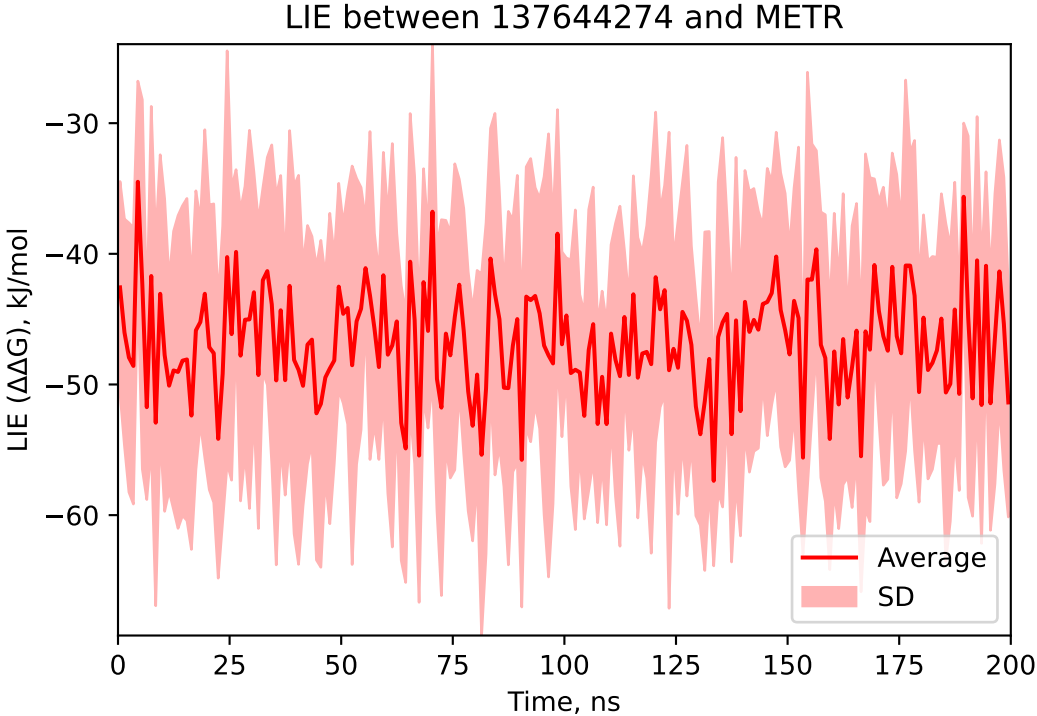

LIE between 127034107 and TILM
Average
SD
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
0
25
50
75
100
125
150
175
200
Time, ns

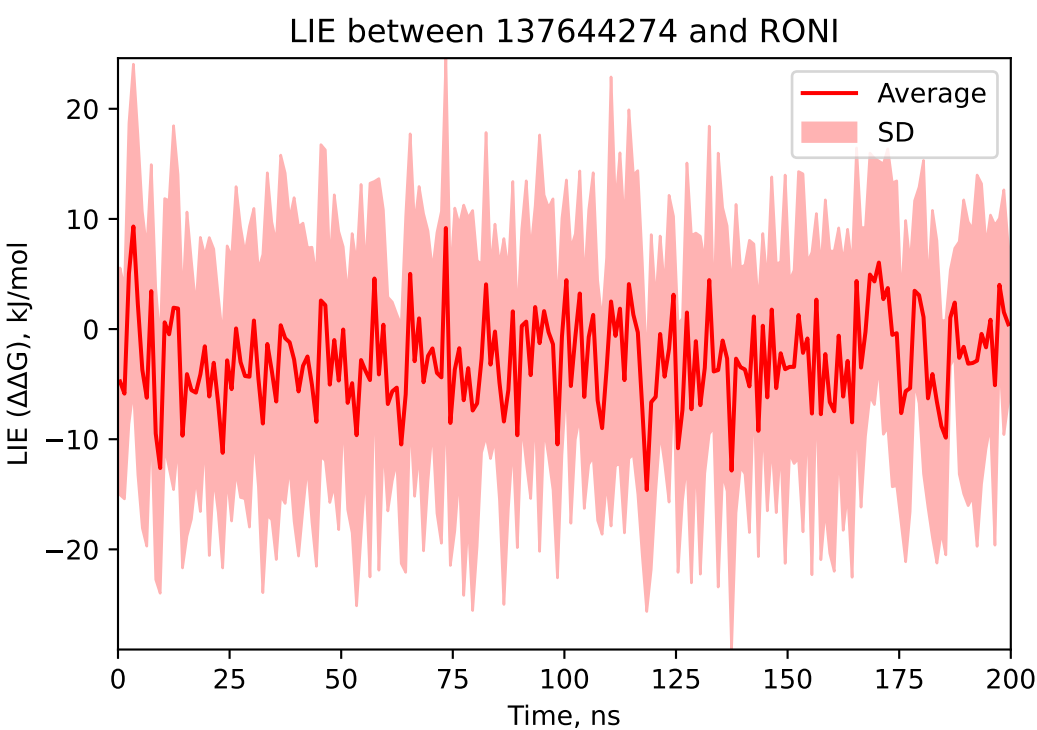

LIE between 137644274 and DANO
Average
SD
LIE (ΔΔG), kJ/mol
5
0
−5
−10
−15
−20
−25
−30
0
25
50
75
100
125
150
175
200
Time, ns

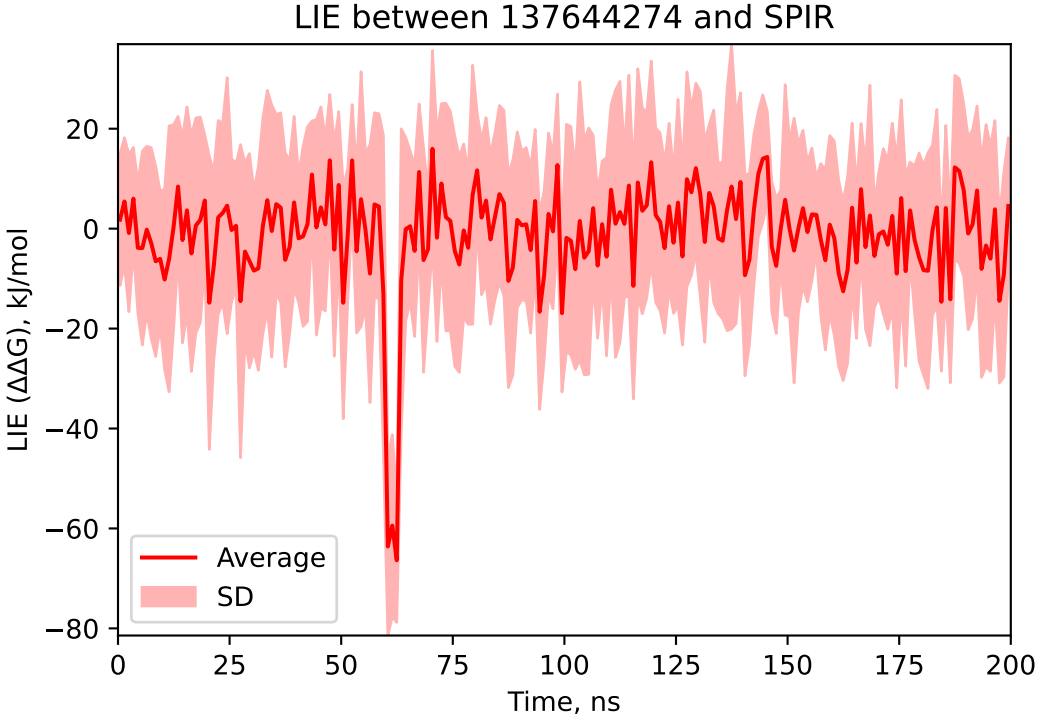

LIE between 137644274 and DEME
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
−40
−50
−60
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

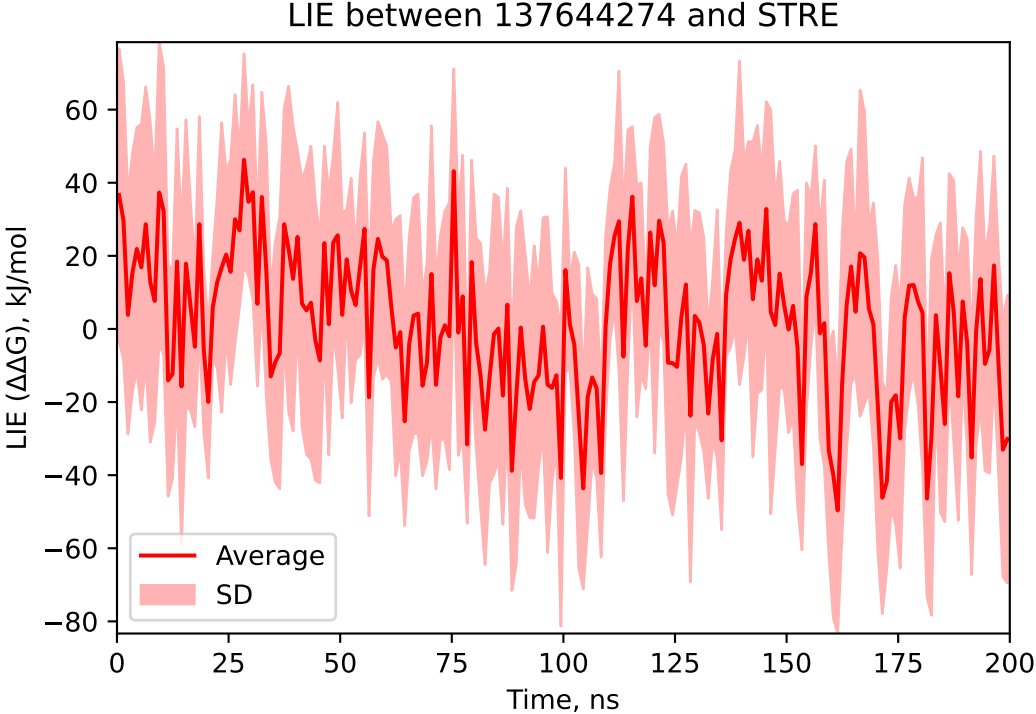

LIE between 137644274 and DOXY
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

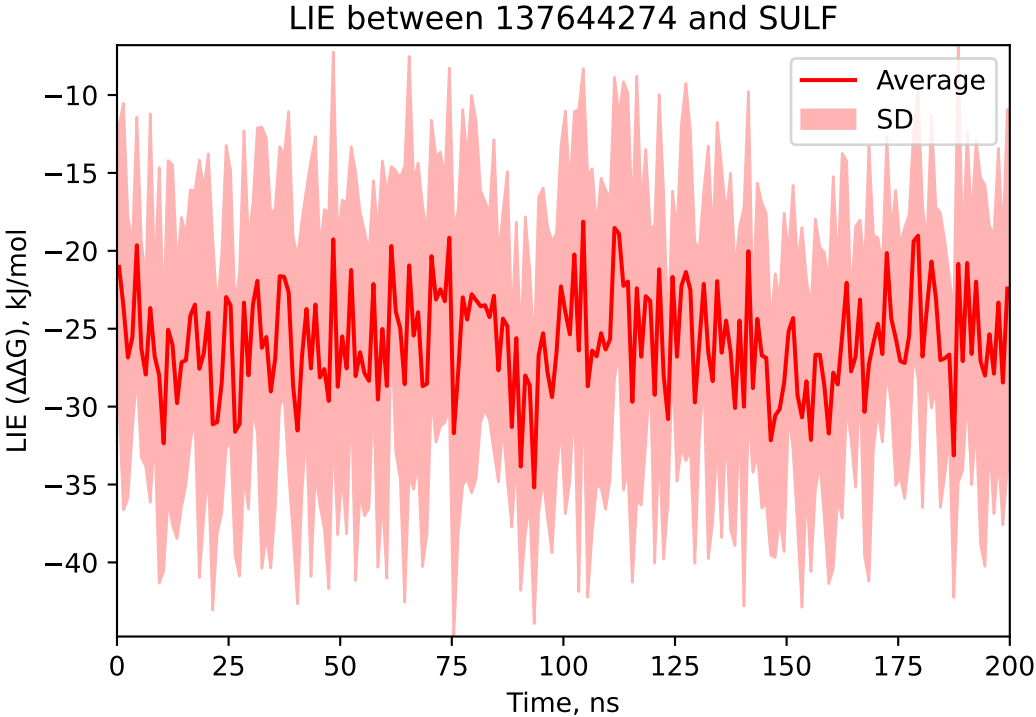

LIE between 137644274 and LYNC
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
10
20
30
40
50
60
70
80
0
25
50
75
100
125
150
175
200

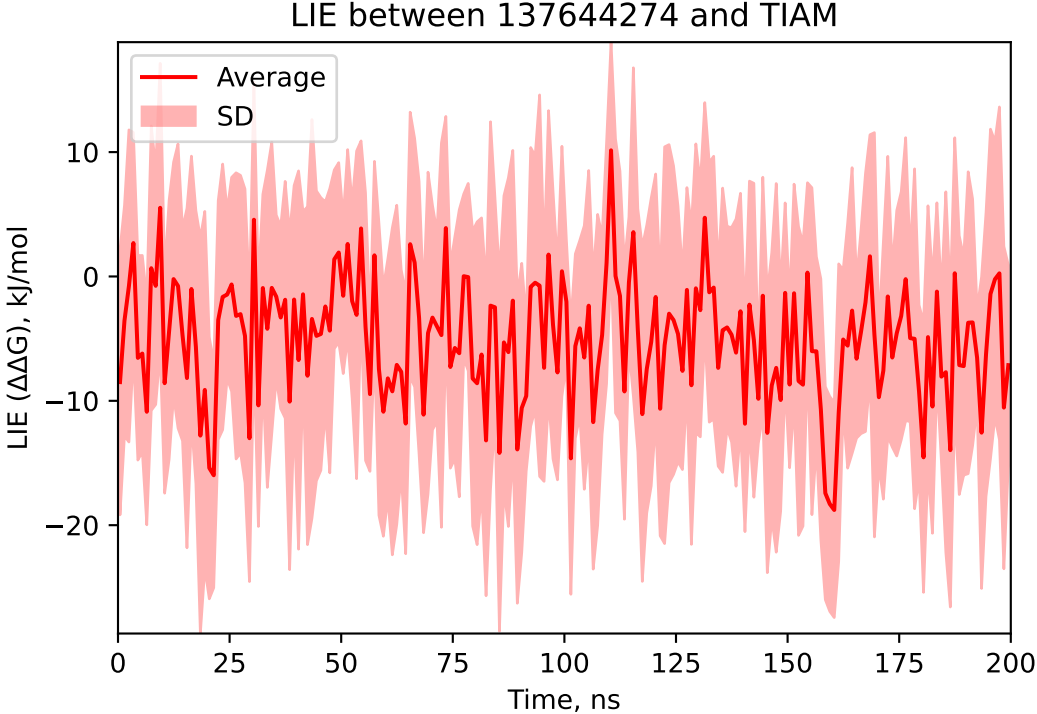

LIE between 137644274 and METR
LIE (ΔΔG), kJ/mol
−30
−40
−50
−60
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

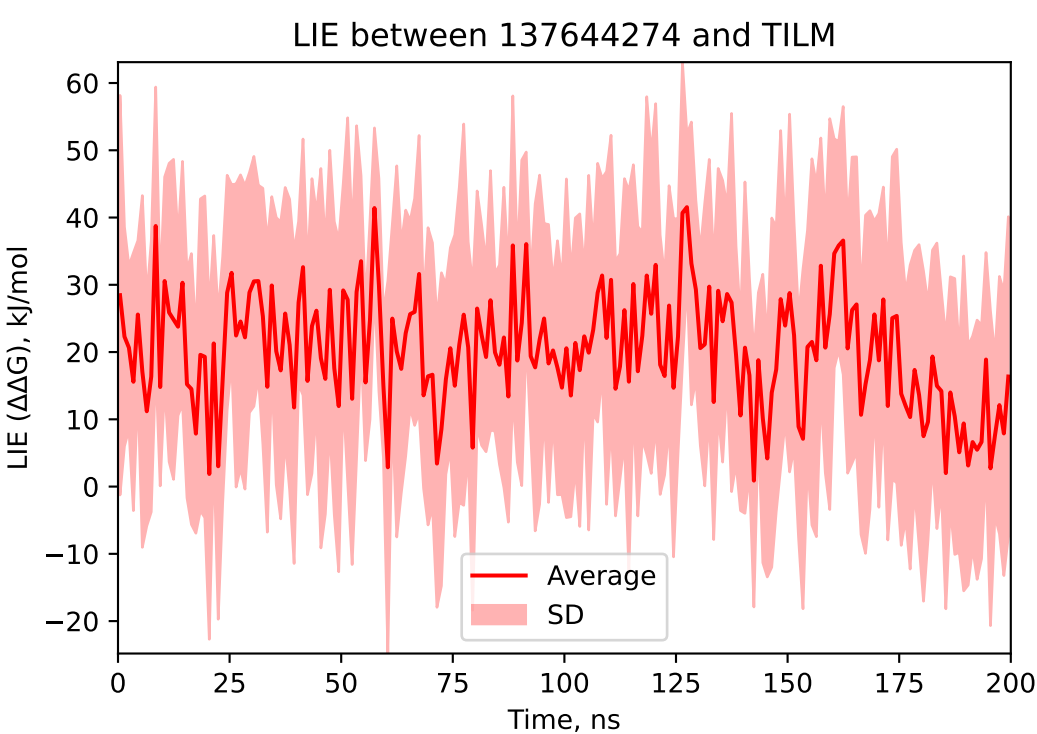

LIE between 137644274 and RONI
Average
SD
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns

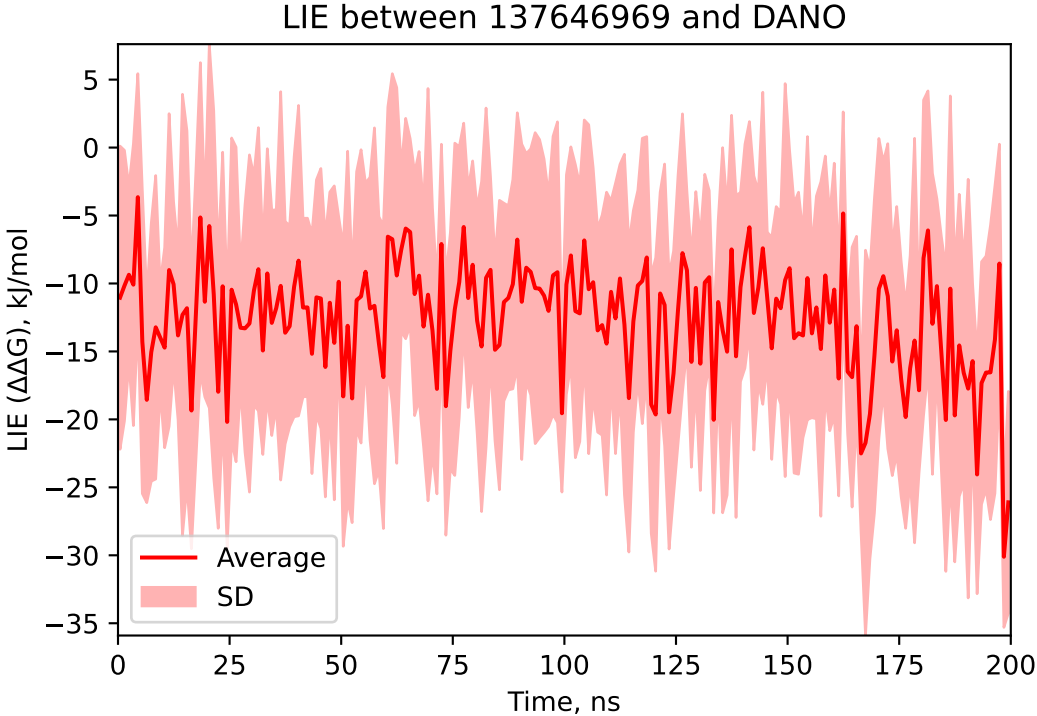

LIE between 137644274 and SPIR
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
20
0
−20
−40
−60
−80
0
25
50
75
100
125
150
175
200

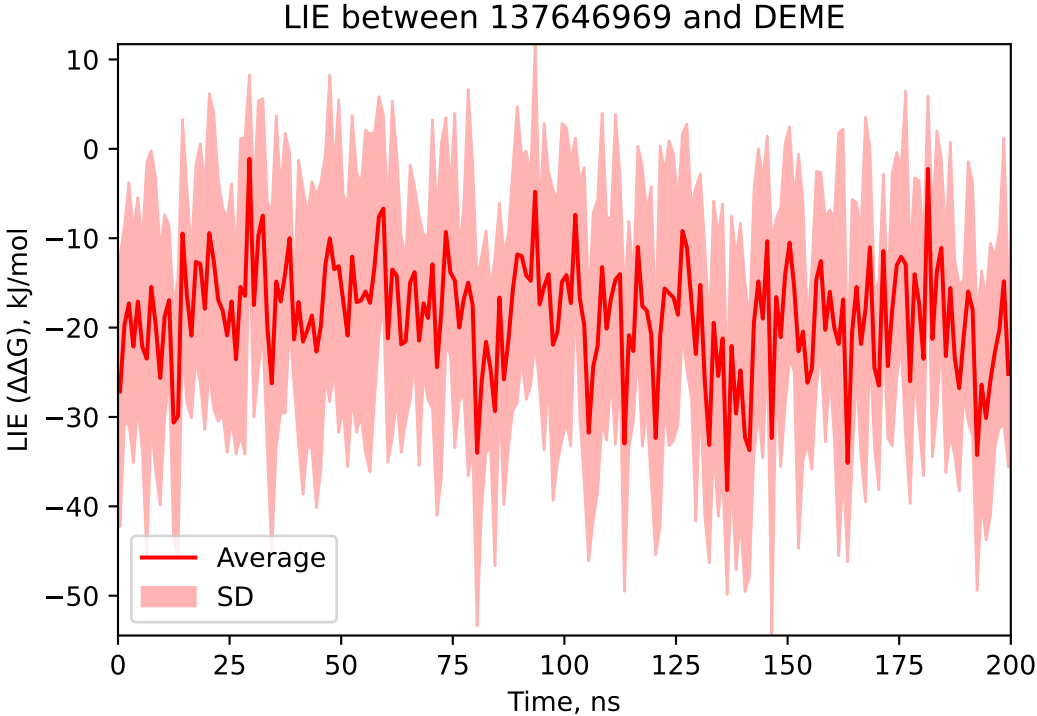

LIE between 137644274 and STRE
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
−40
−60
−80
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

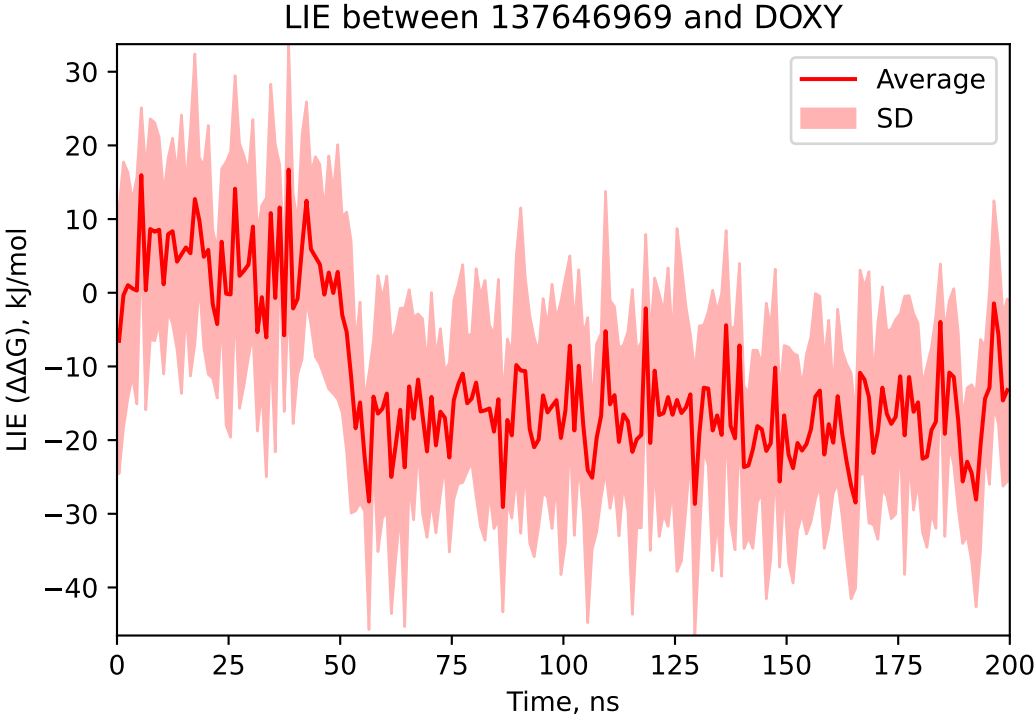

LIE between 137644274 and SULF
Average
SD
LIE (ΔΔG), kJ/mol
−10
−15
−20
−25
−30
−35
−40
0
25
50
75
100
125
150
175
200
Time, ns

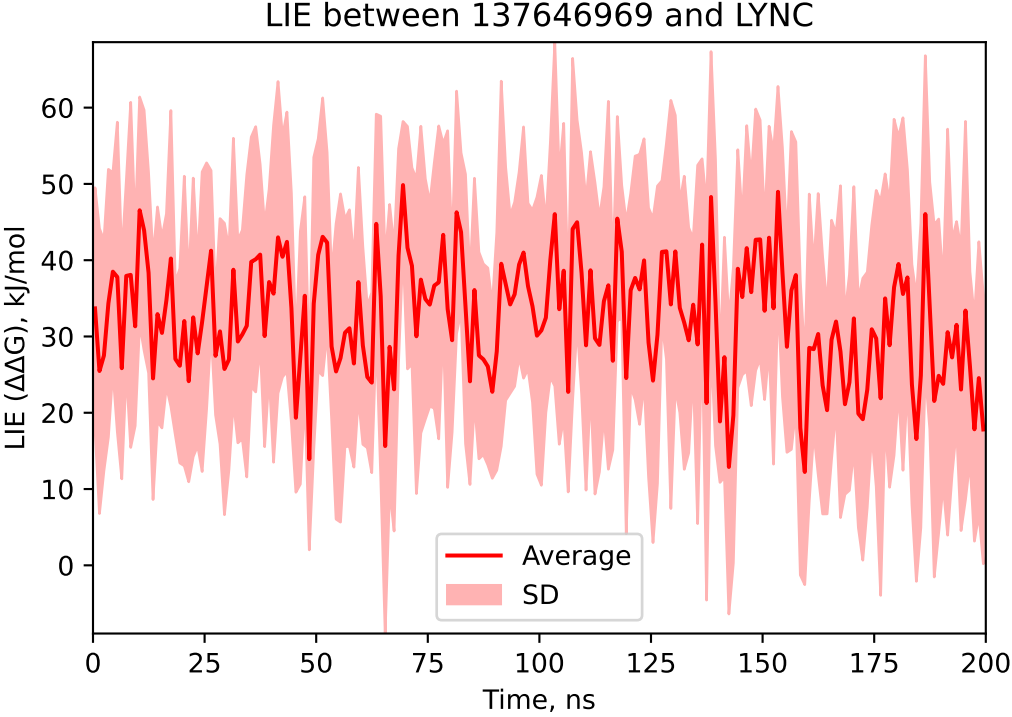

LIE between 137644274 and TIAM
Average
SD
10
0
−10
−20
LIE (ΔΔG), kJ/mol
0
25
50
75
100
125
150
175
200
Time, ns

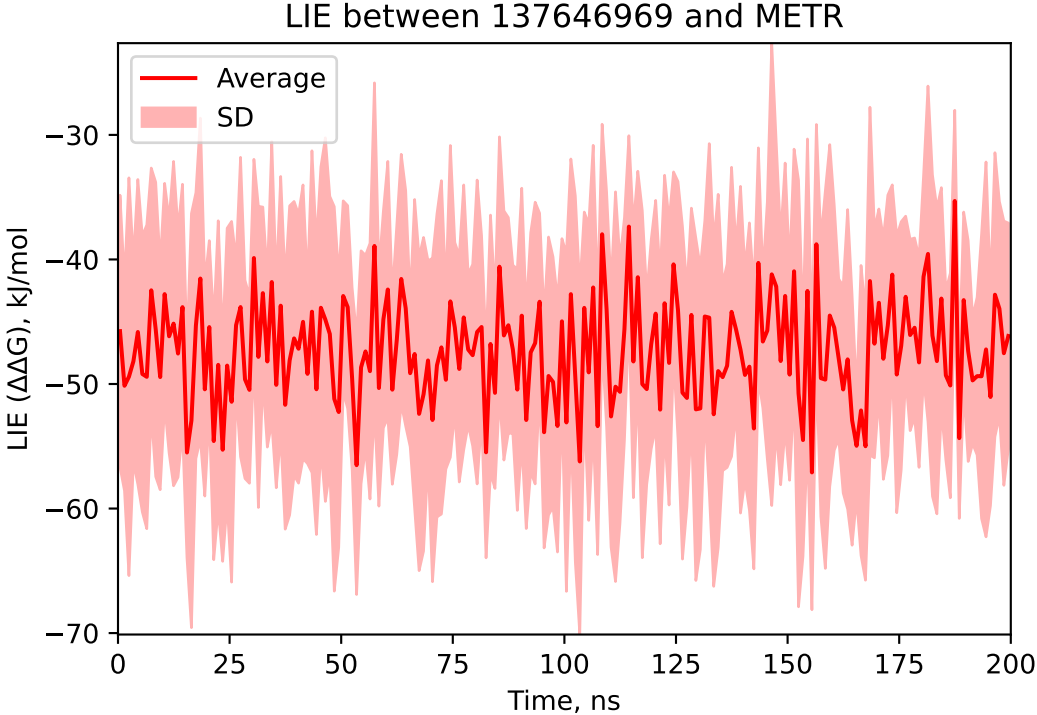

LIE between 137644274 and TILM
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
60
50
40
30
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200

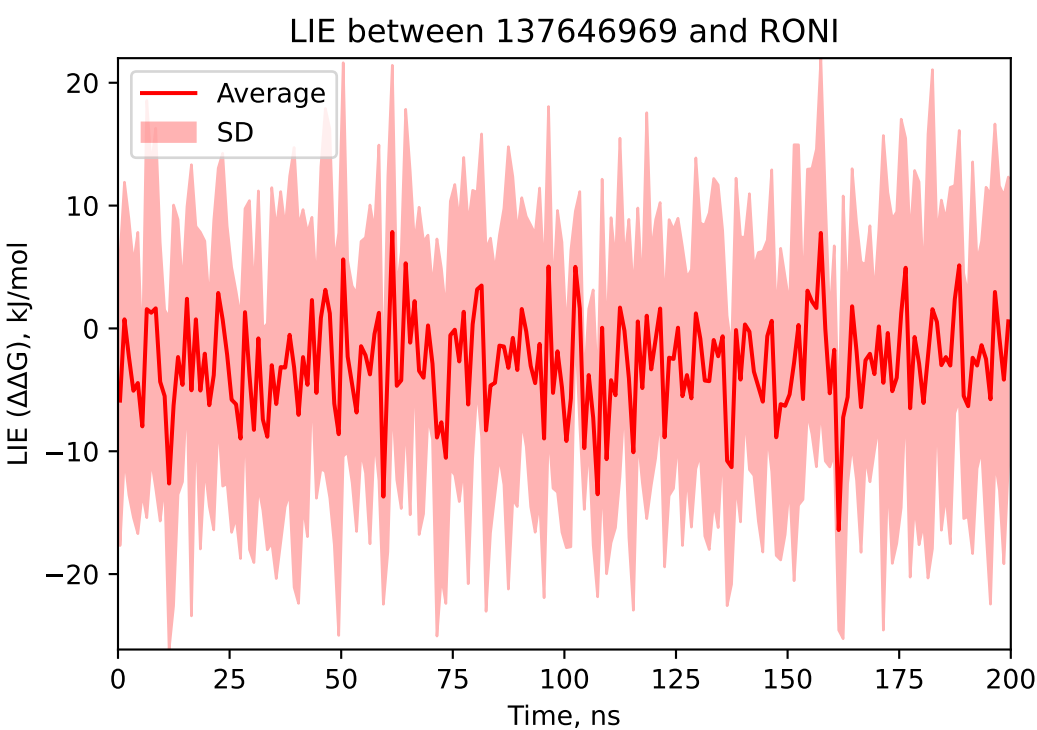

LIE between 137646969 and DANO
LIE (ΔΔG), kJ/mol
5
0
−5
−10
−15
−20
−25
−30
−35
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

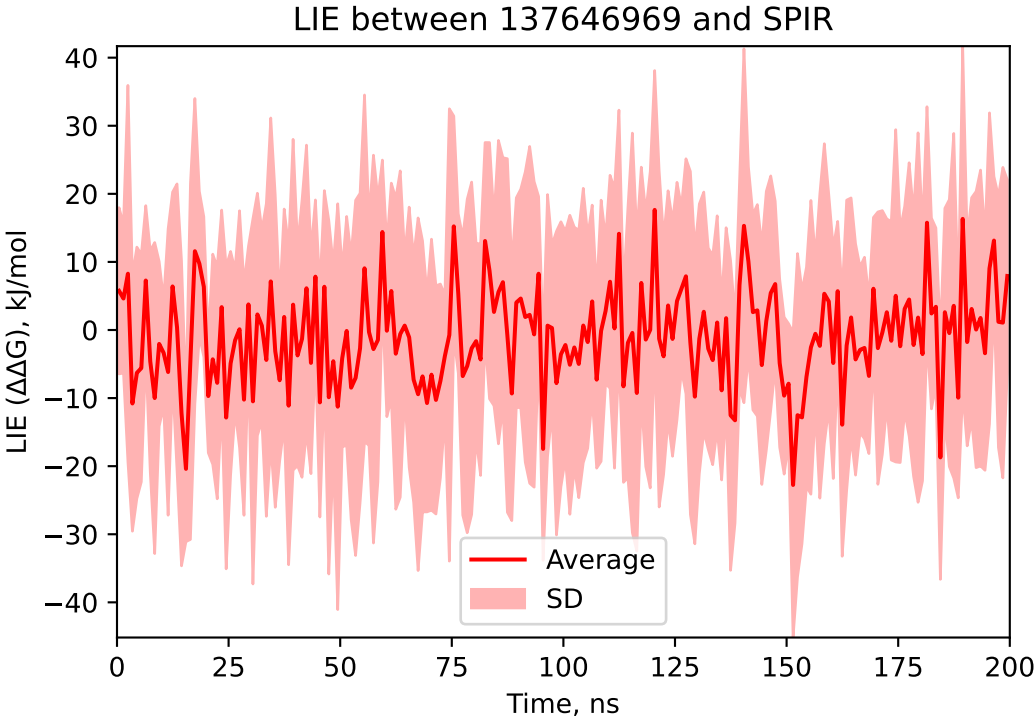

LIE between 137646969 and DEME
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

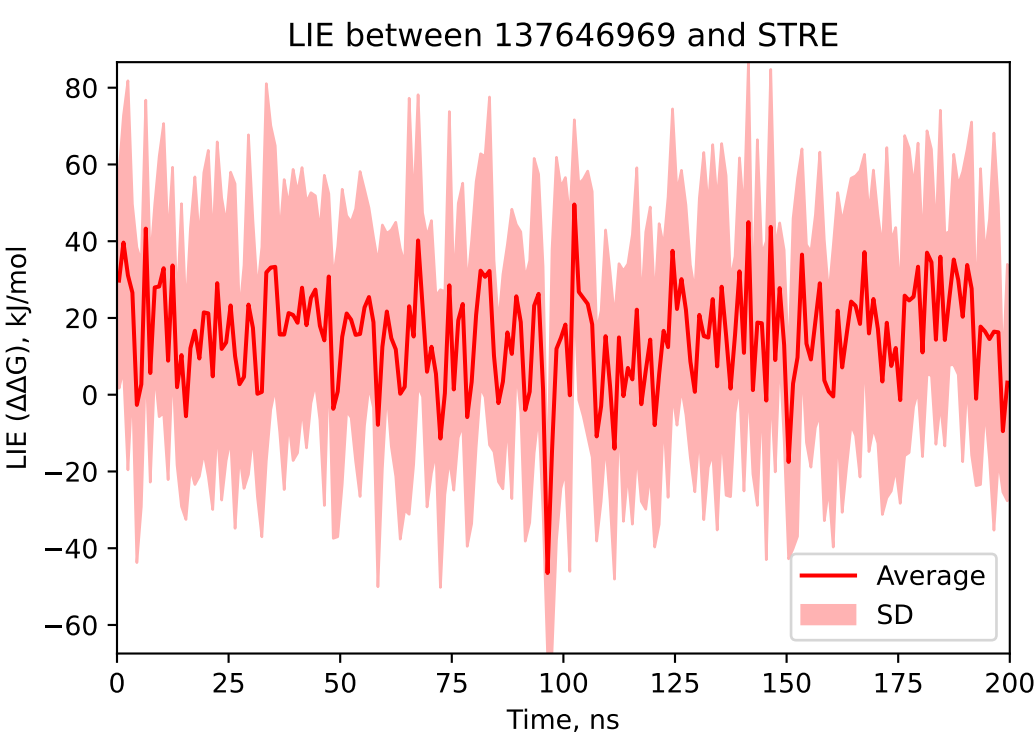

LIE between 137646969 and DOXY
Average
SD
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns

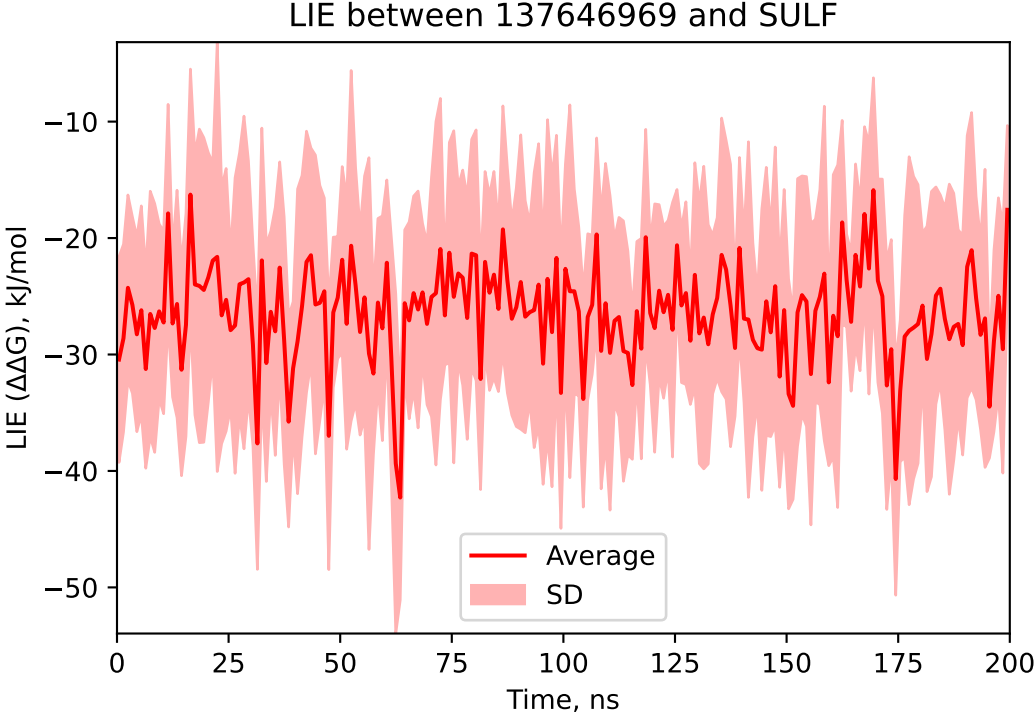

LIE between 137646969 and LYNC
LIE (ΔΔG), kJ/mol
60
50
40
30
20
10
0
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

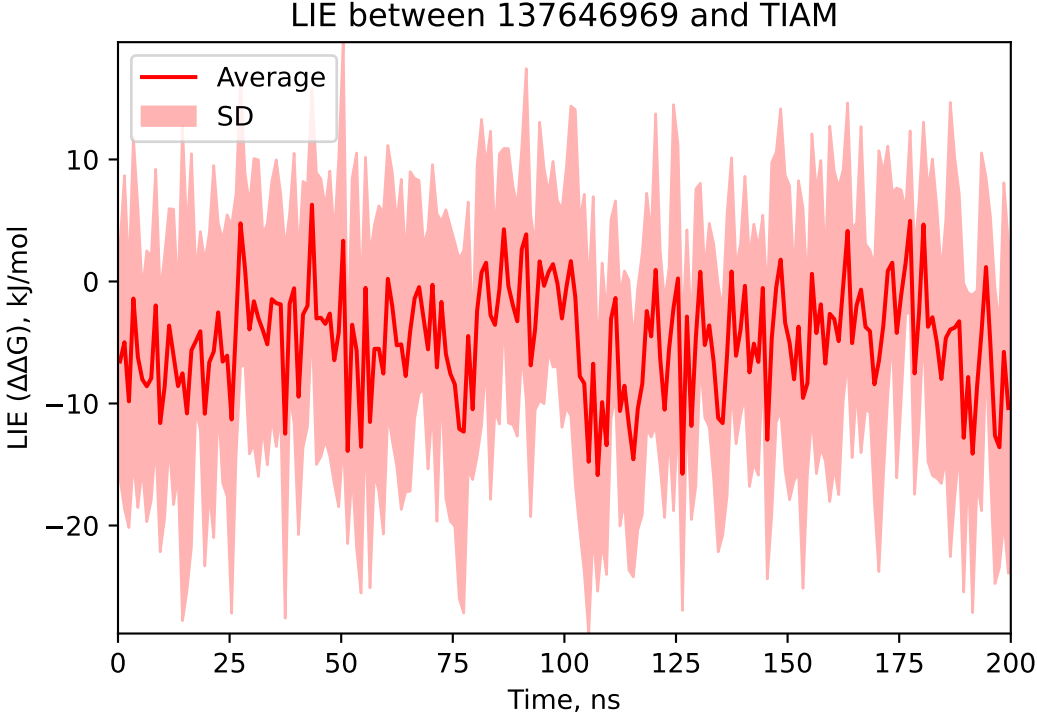

LIE between 137646969 and METR
Average
SD
−30
−40
−50
−60
−70
LIE (ΔΔG), kJ/mol
0
25
50
75
100
125
150
175
200
Time, ns

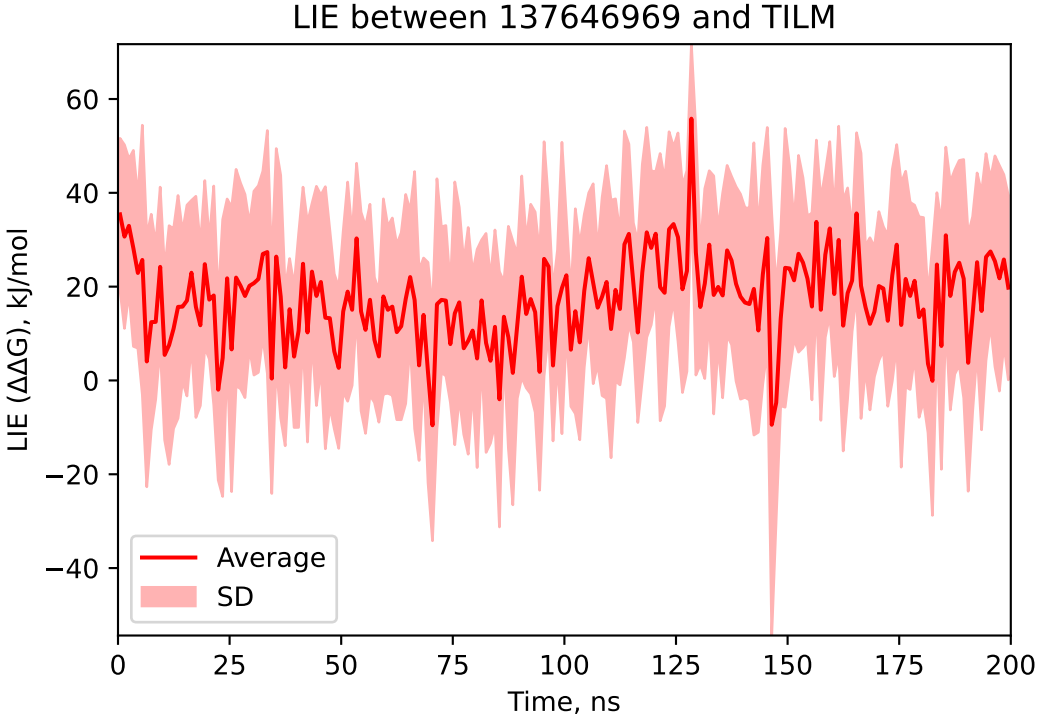

LIE between 137646969 and RONI
Average
SD
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns

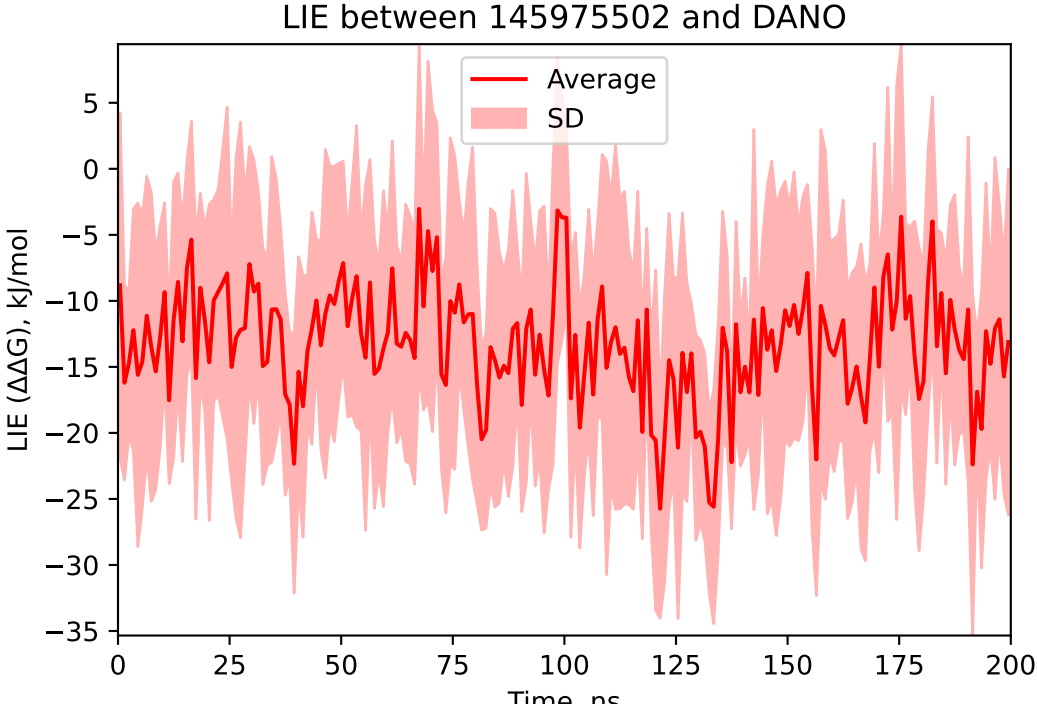

LIE between 137646969 and SPIR
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
40
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200

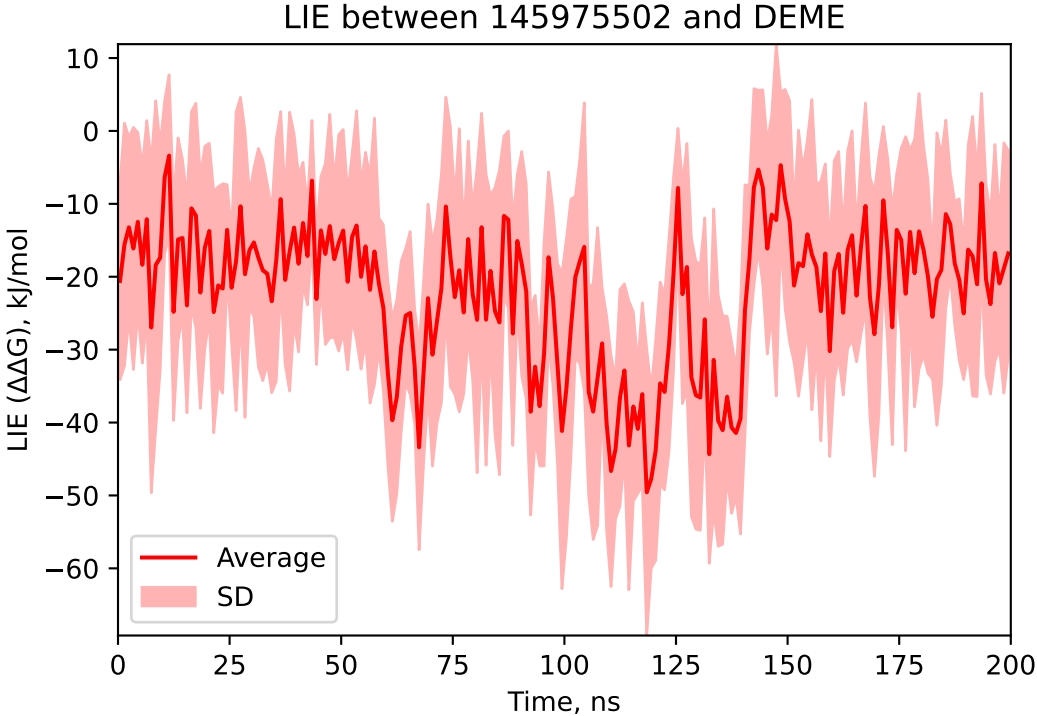

LIE between 137646969 and STRE
LIE (ΔΔG), kJ/mol
80
60
40
20
0
−20
−40
−60
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

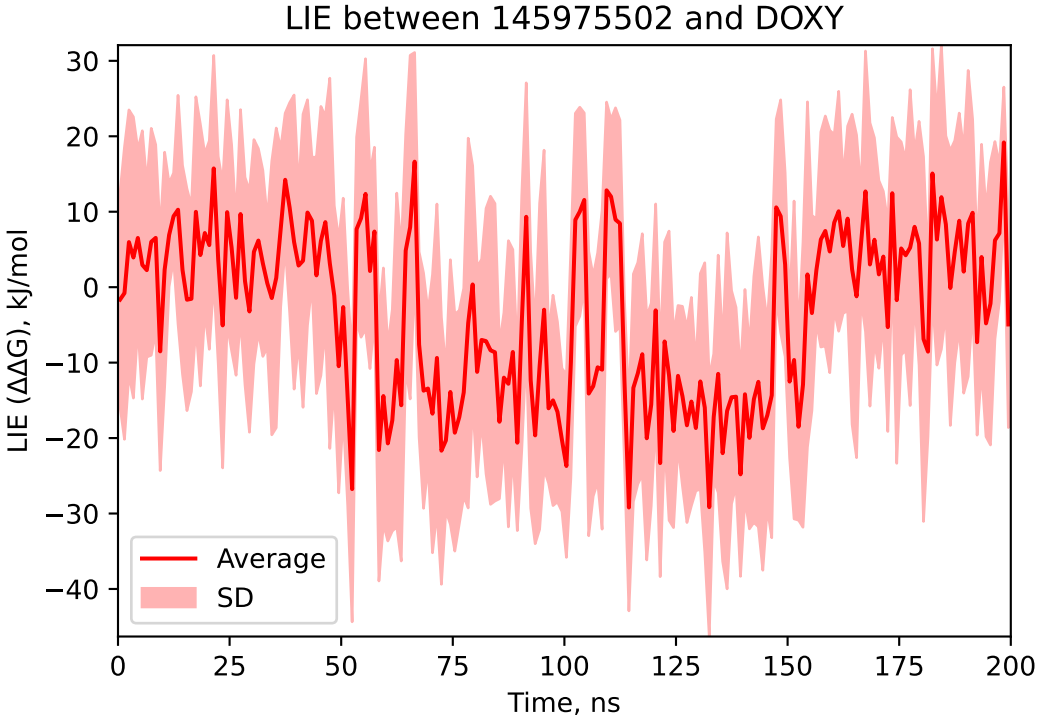

LIE between 137646969 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

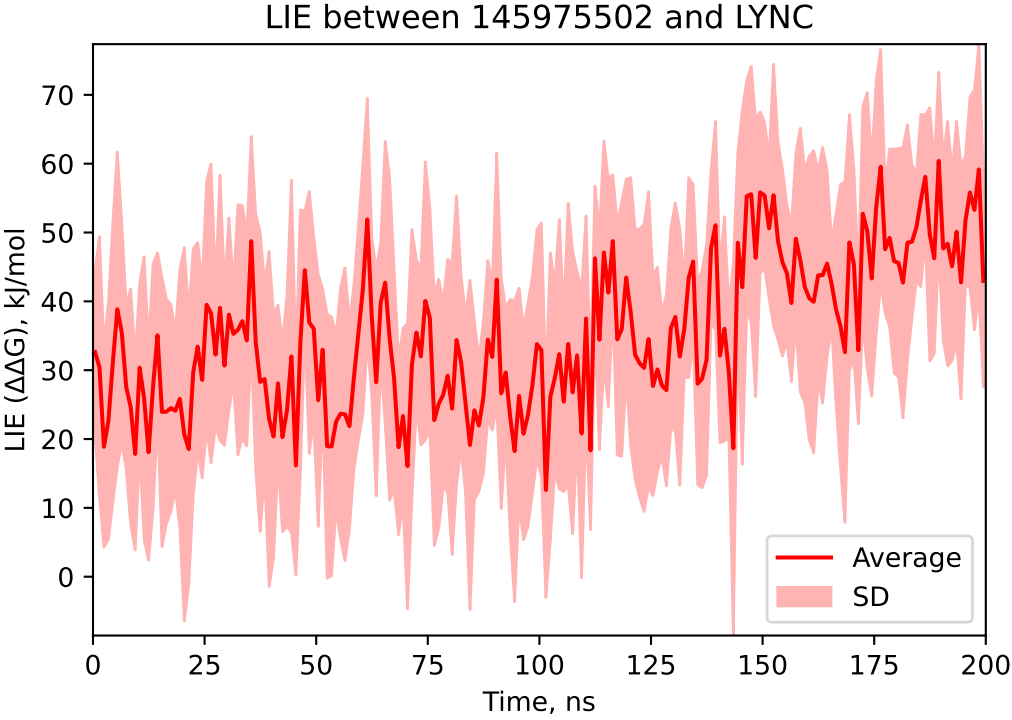

LIE between 137646969 and TIAM
Average
SD
10
0
−10
−20
LIE (ΔΔG), kJ/mol
0
25
50
75
100
125
150
175
200
Time, ns

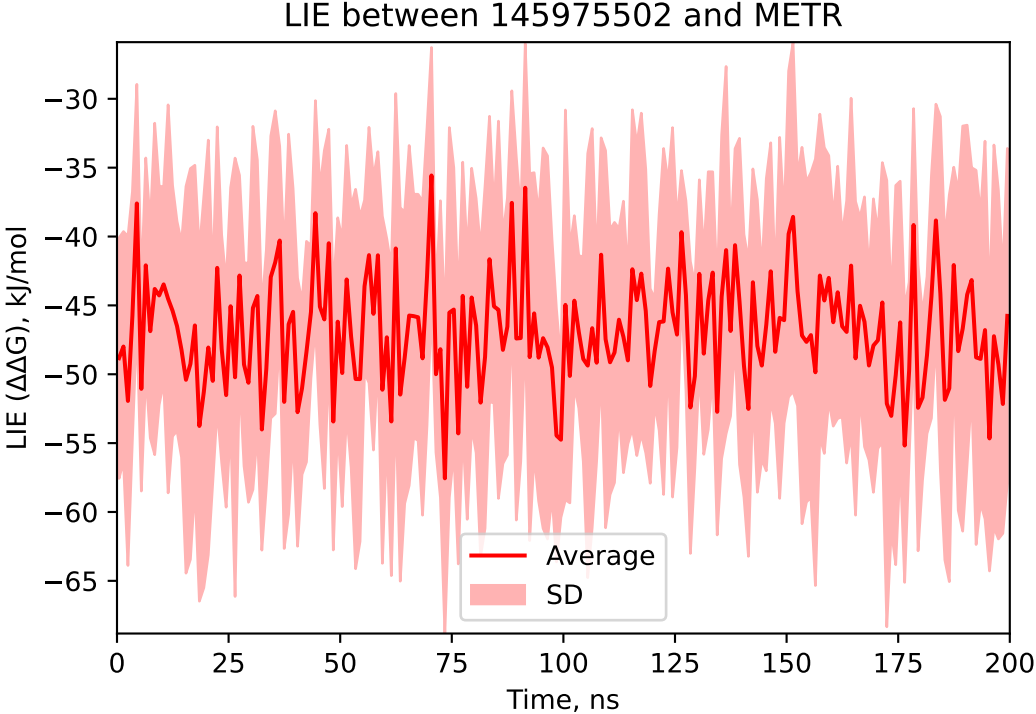

LIE between 137646969 and TILM
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

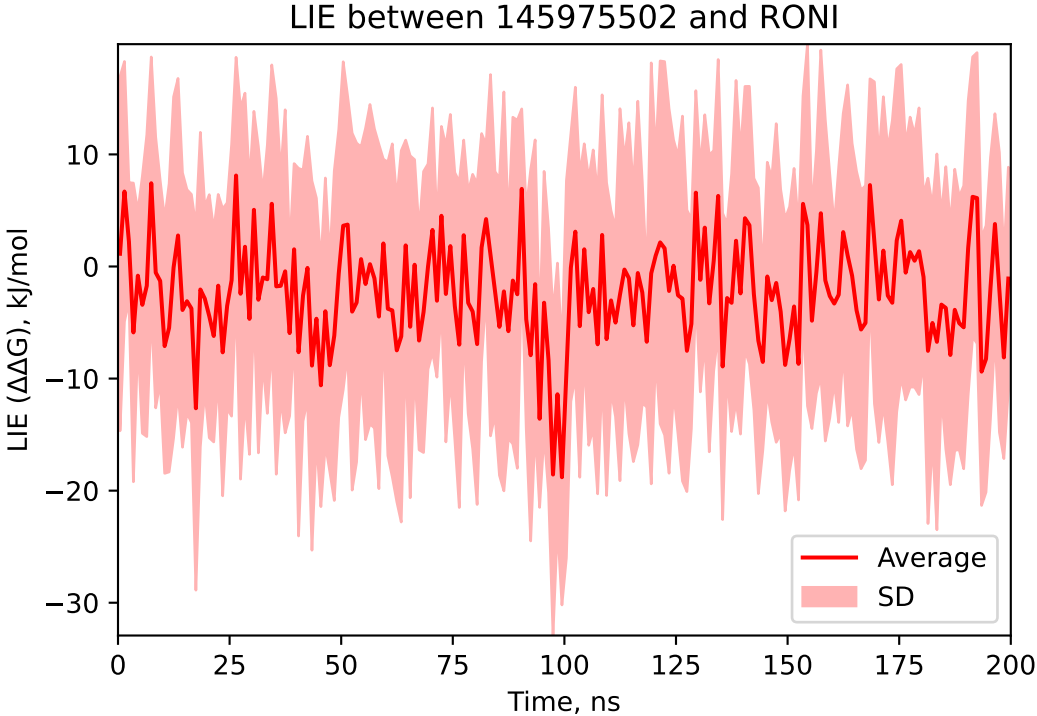

LIE between 145975502 and DANO
Average
SD
LIE (ΔΔG), kJ/mol
5
0
−5
−10
−15
−20
−25
−30
−35
0
25
50
75
100
125
150
175
200
Time, ns

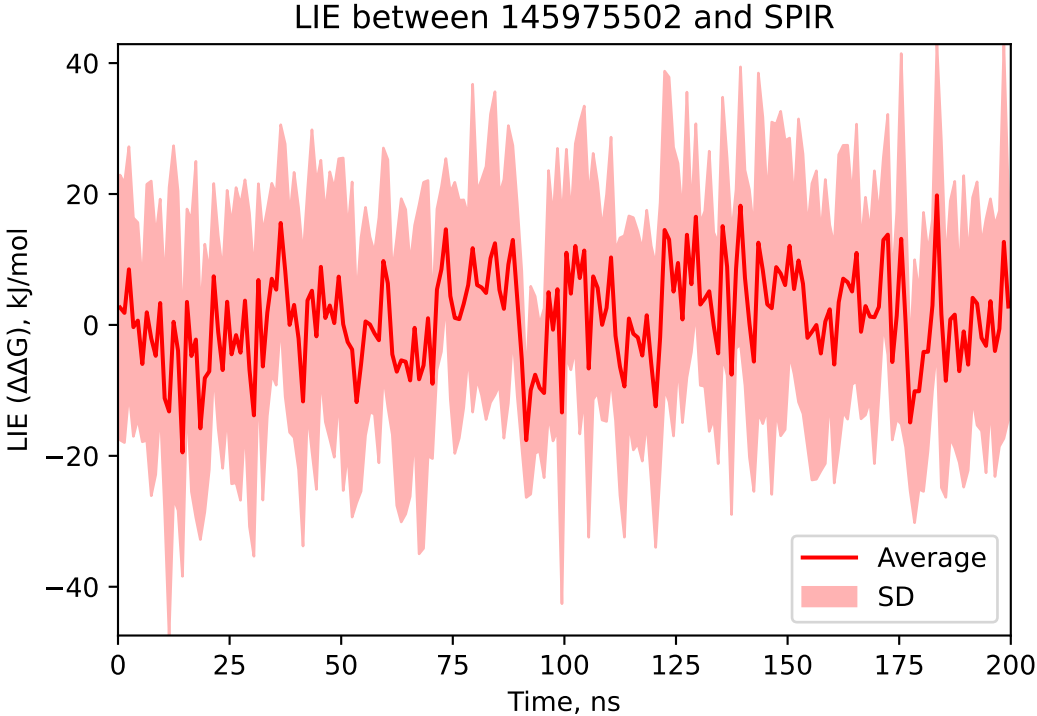

LIE between 145975502 and DEME
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
−40
−50
−60
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

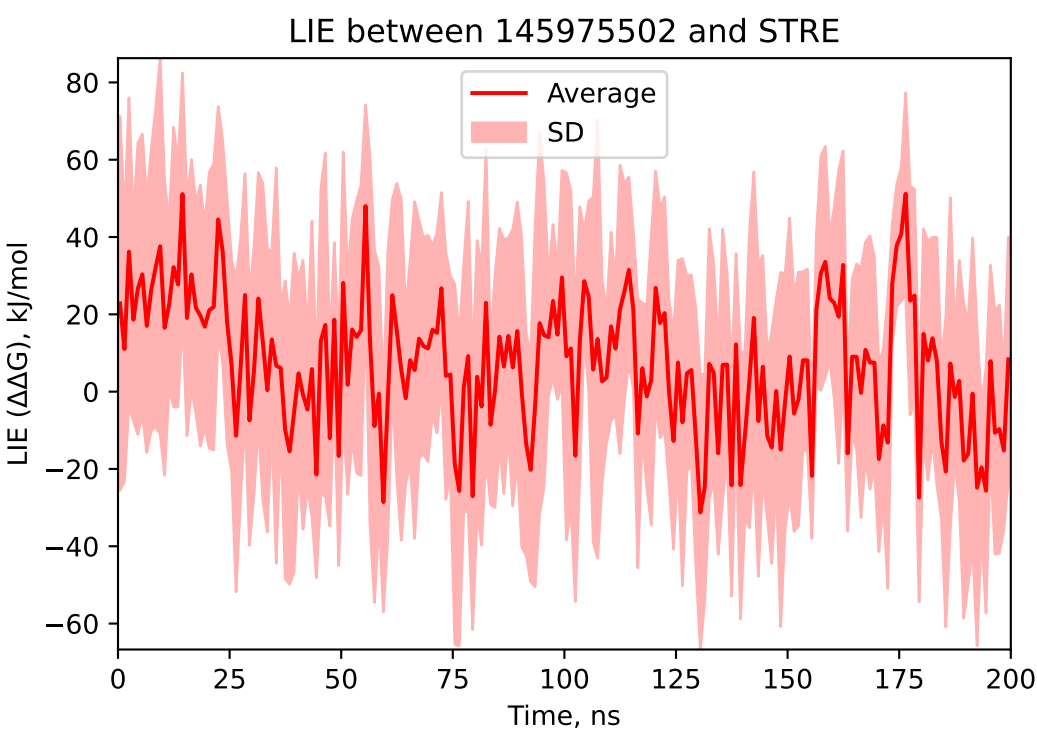

LIE between 145975502 and DOXY
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

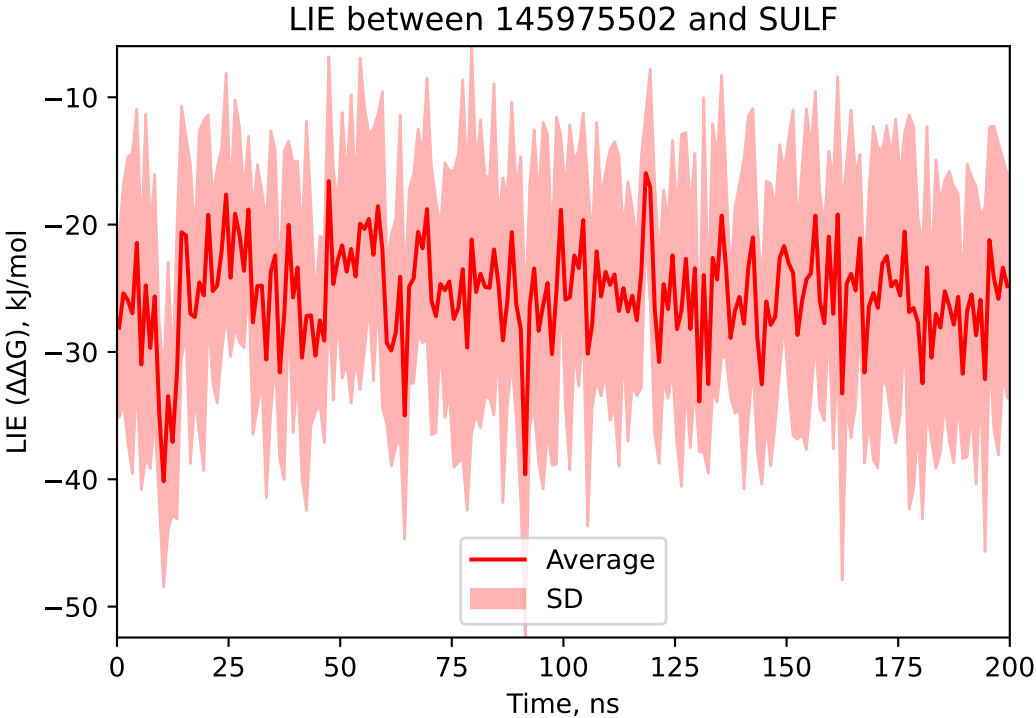

LIE between 145975502 and LYNC
LIE (ΔΔG), kJ/mol
70
60
50
40
30
20
10
0
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

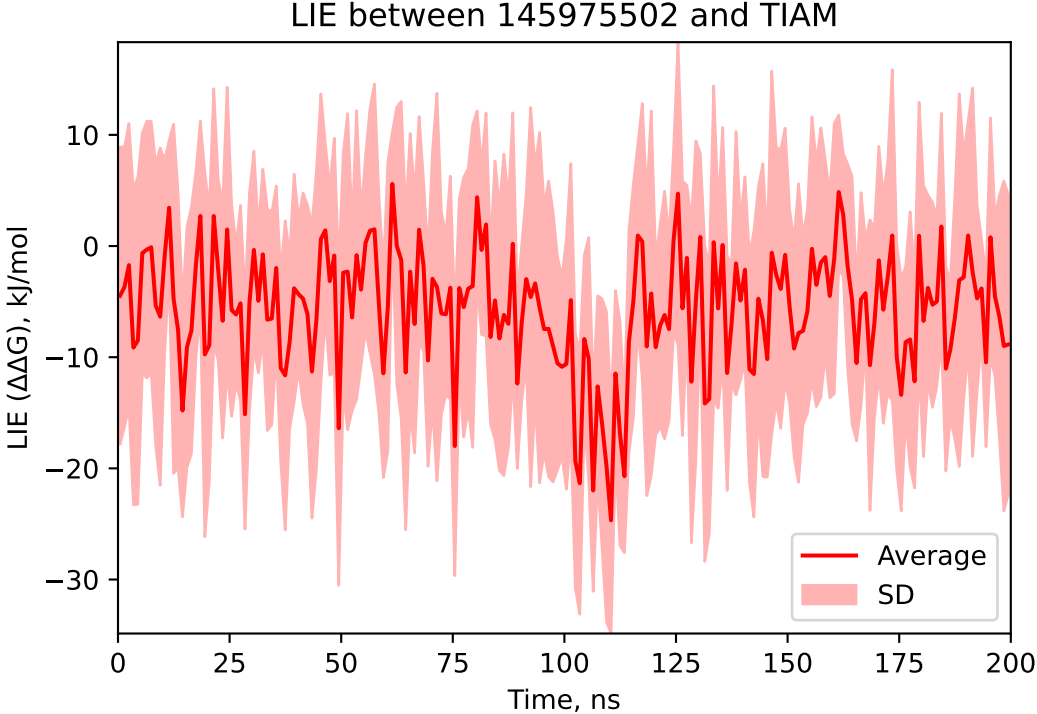

LIE between 145975502 and METR
LIE (ΔΔG), kJ/mol
−30
−35
−40
−45
−50
−55
−60
−65
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

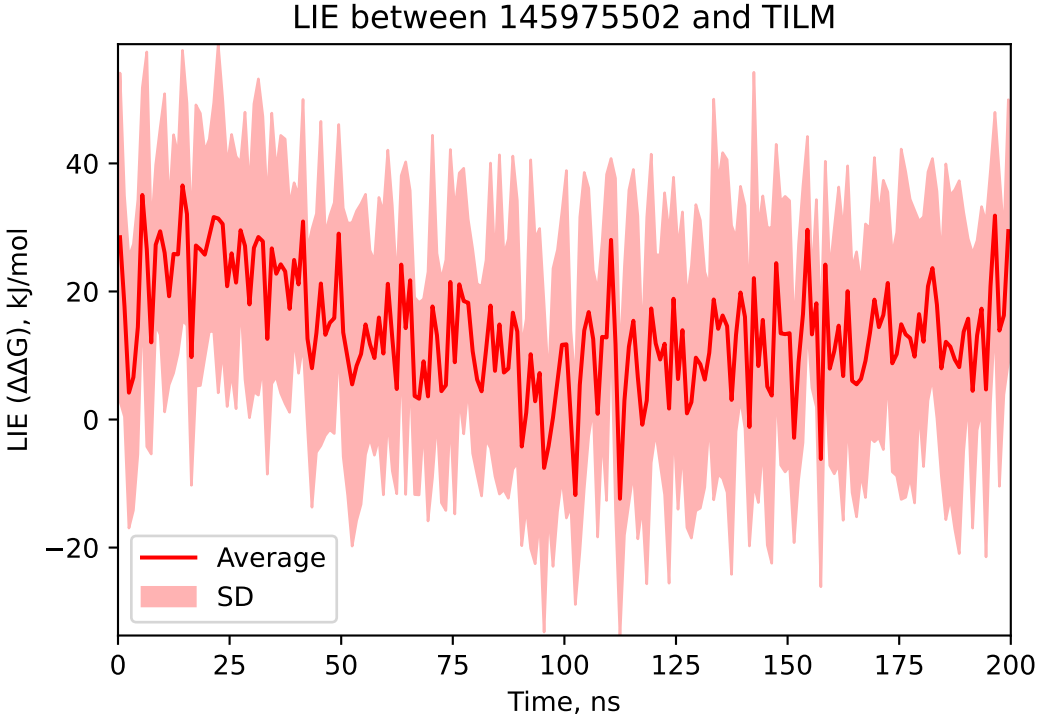

LIE between 145975502 and RONI
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

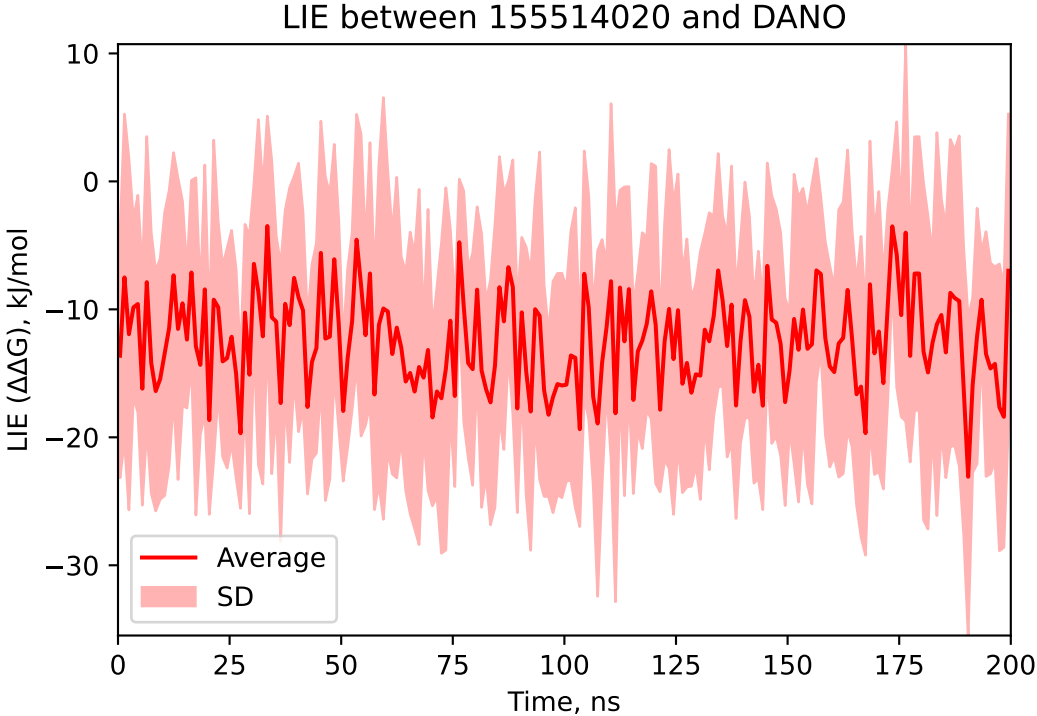

LIE between 145975502 and SPIR
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200

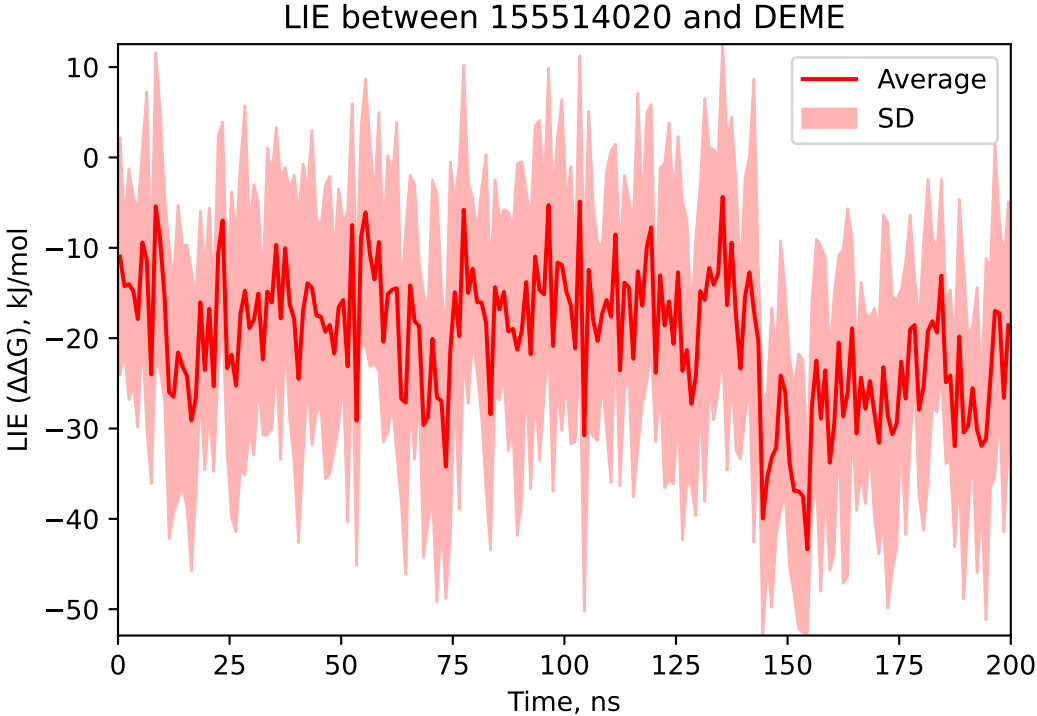

LIE between 145975502 and STRE
Average
SD
LIE (ΔΔG), kJ/mol
80
60
40
20
0
−20
−40
−60
0
25
50
75
100
125
150
175
200
Time, ns

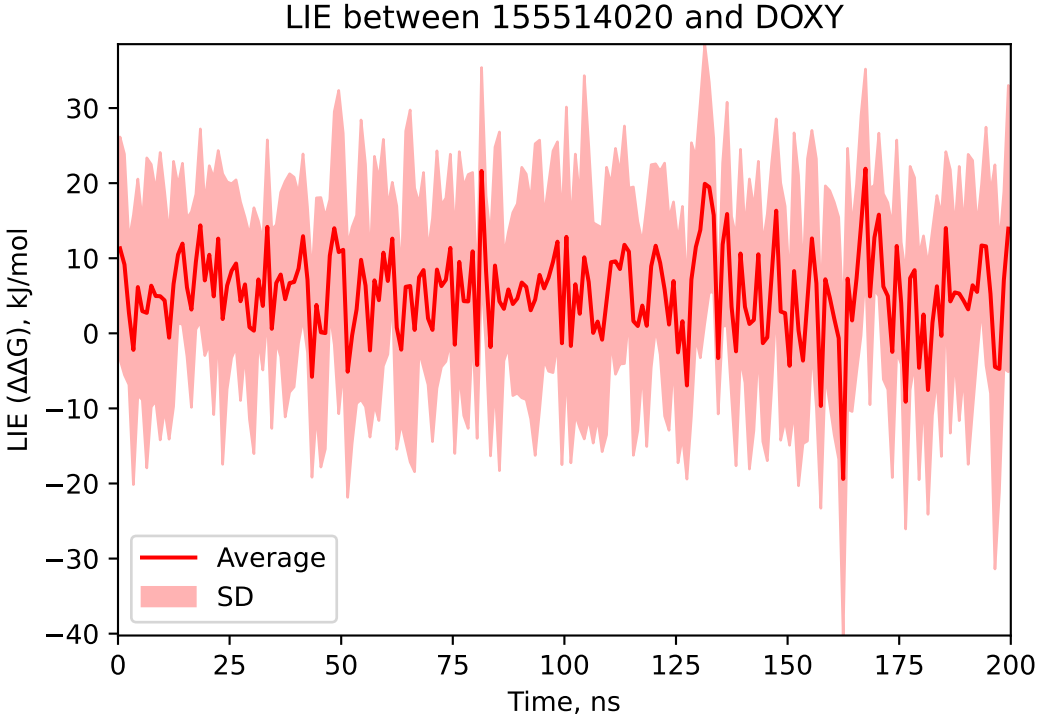

LIE between 145975502 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

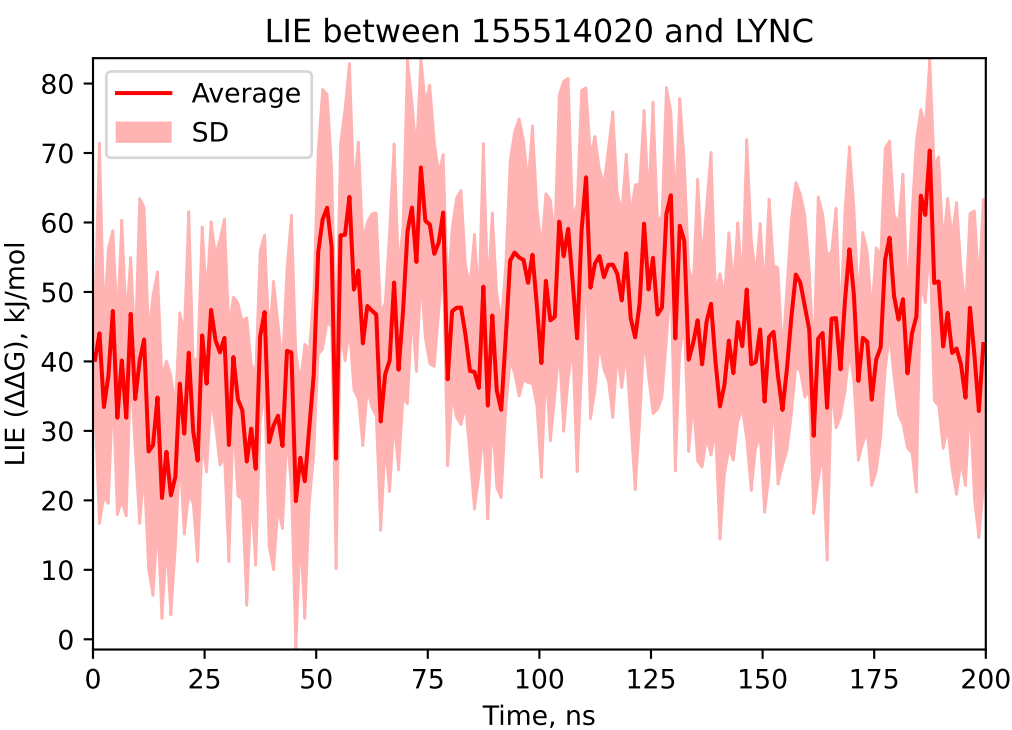

LIE between 145975502 and TIAM
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

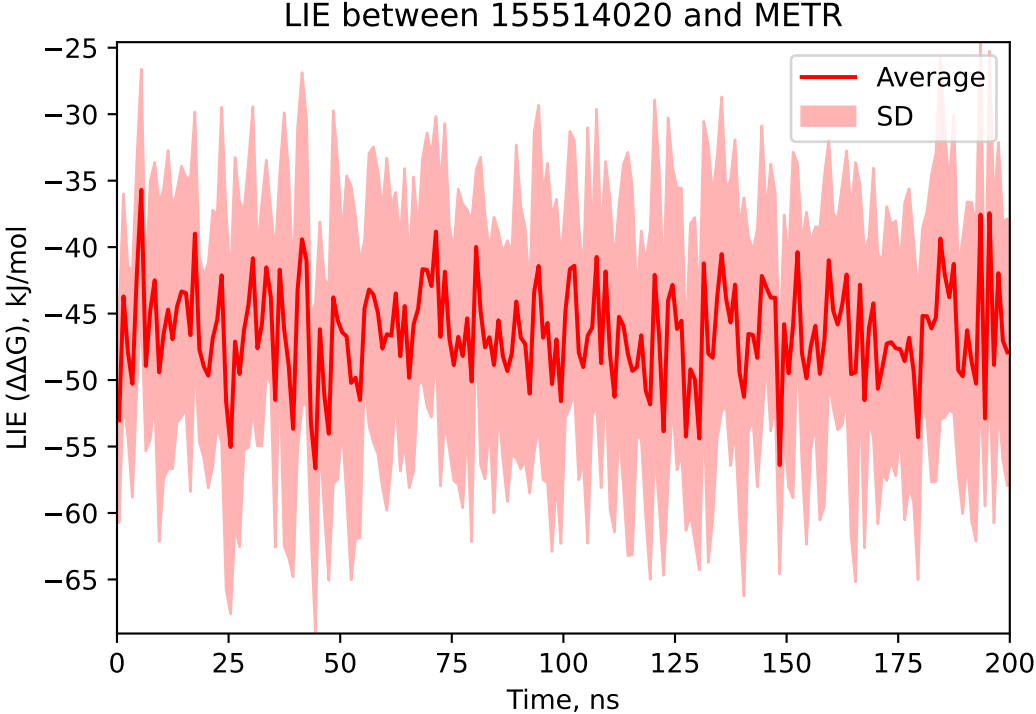

LIE between 145975502 and TILM
LIE (ΔΔG), kJ/mol
40
20
0
−20
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

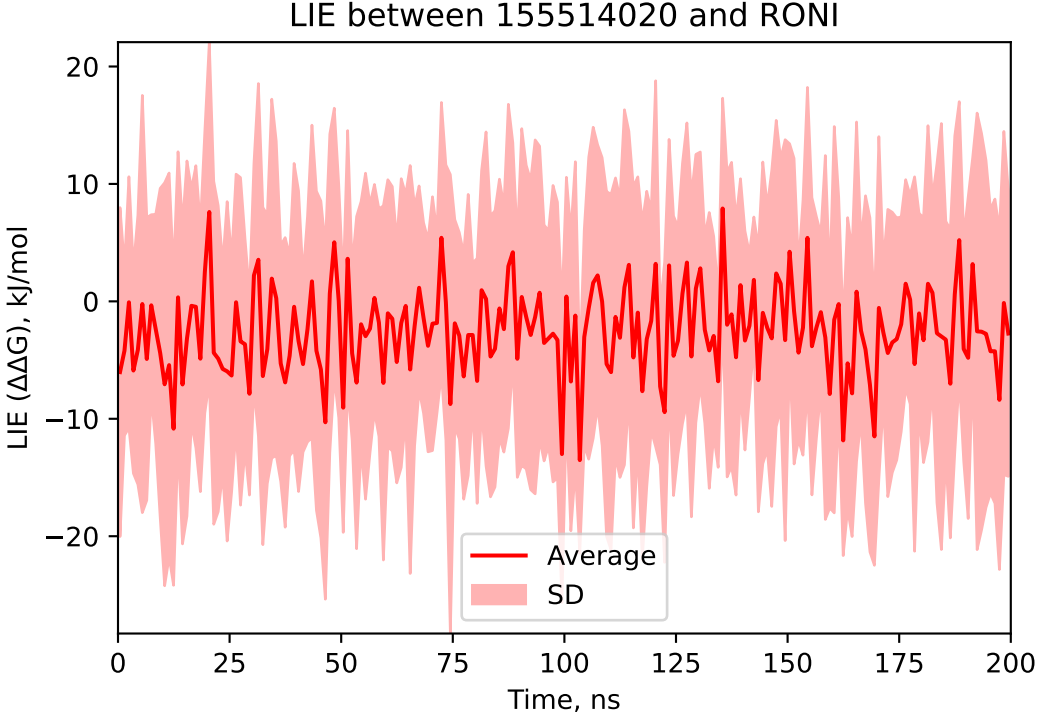

LIE between 155514020 and DANO
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

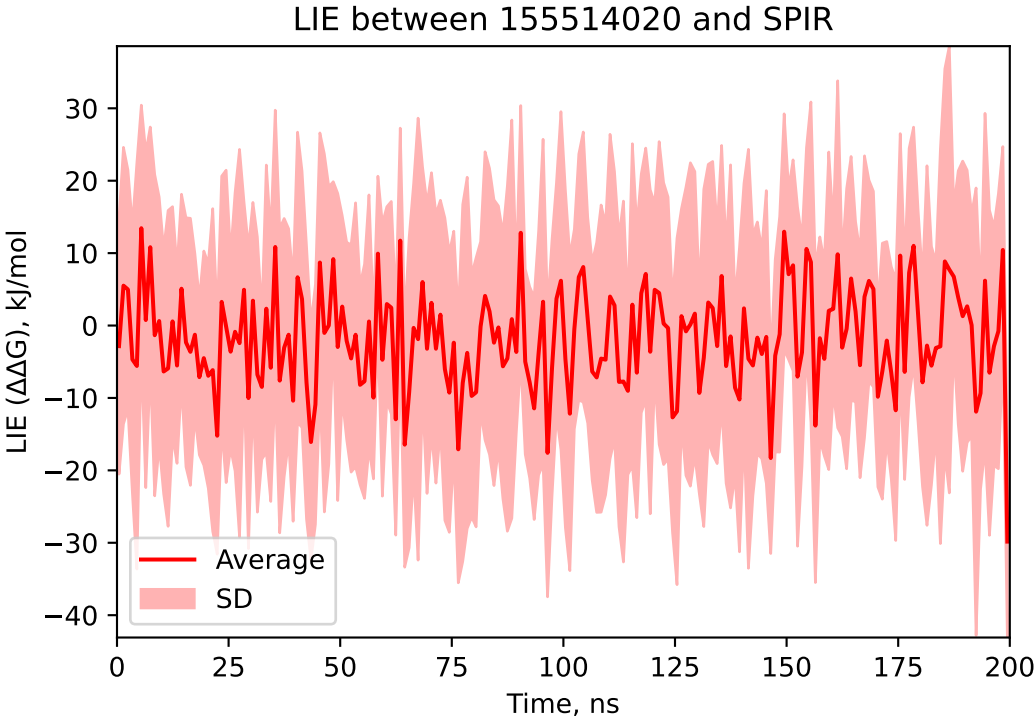

LIE between 155514020 and DEME
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
10
0
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200

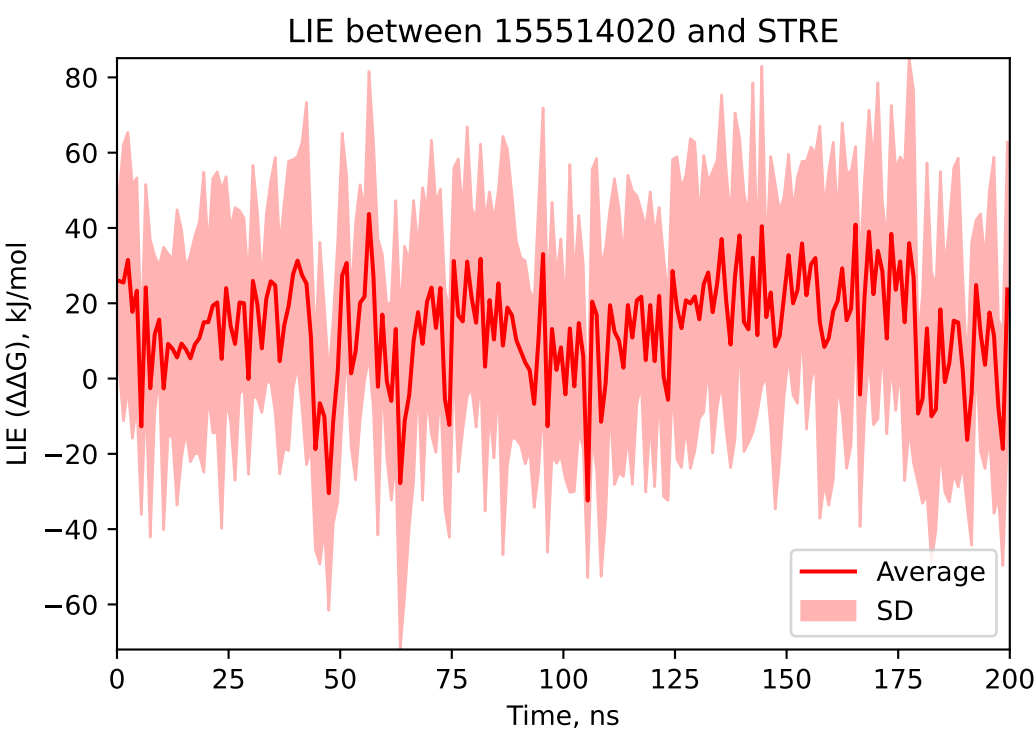

LIE between 155514020 and DOXY
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200

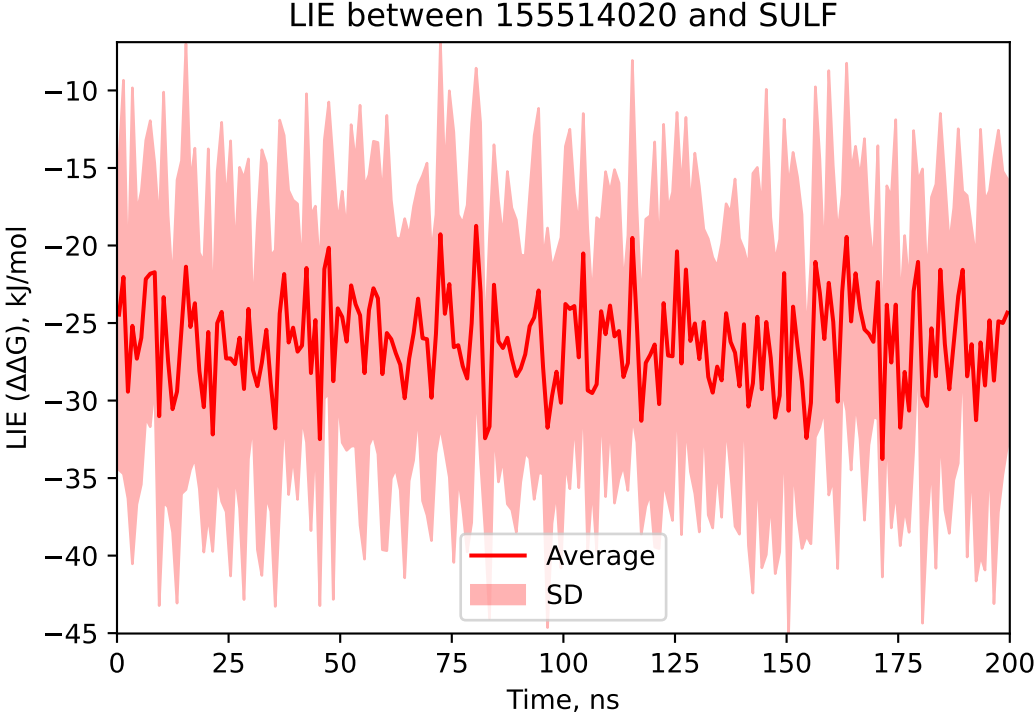

LIE between 155514020 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
0
10
20
30
40
50
60
70
80
0
25
50
75
100
125
150
175
200

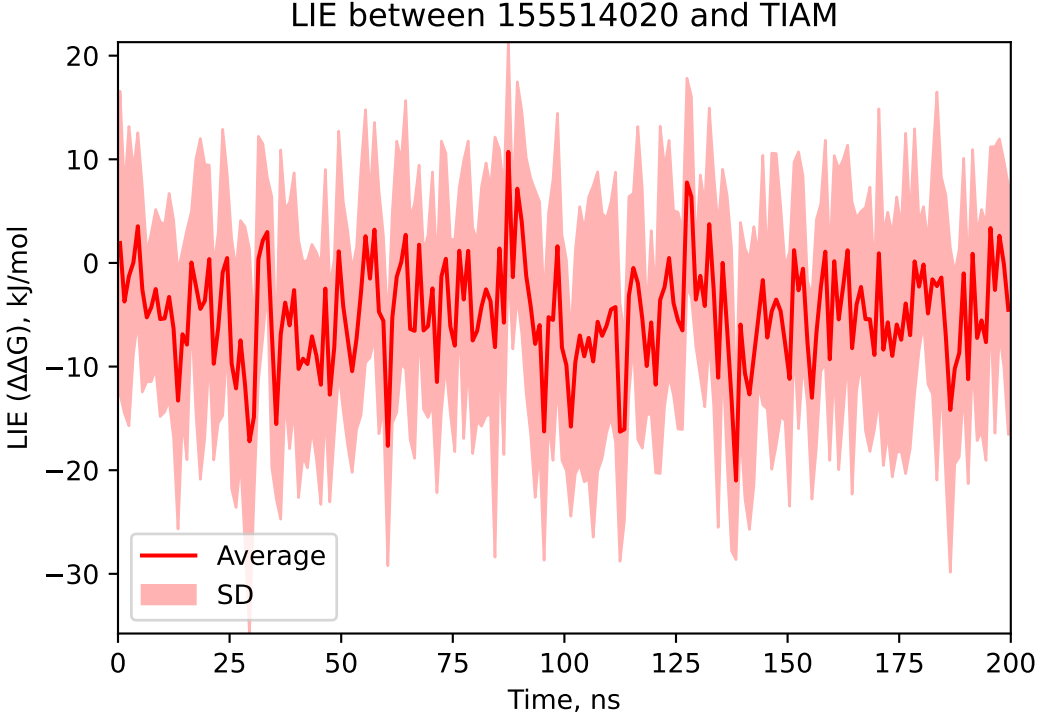

LIE between 155514020 and METR
Average
SD
LIE (ΔΔG), kJ/mol
−25
−30
−35
−40
−45
−50
−55
−60
−65
0
25
50
75
100
125
150
175
200
Time, ns

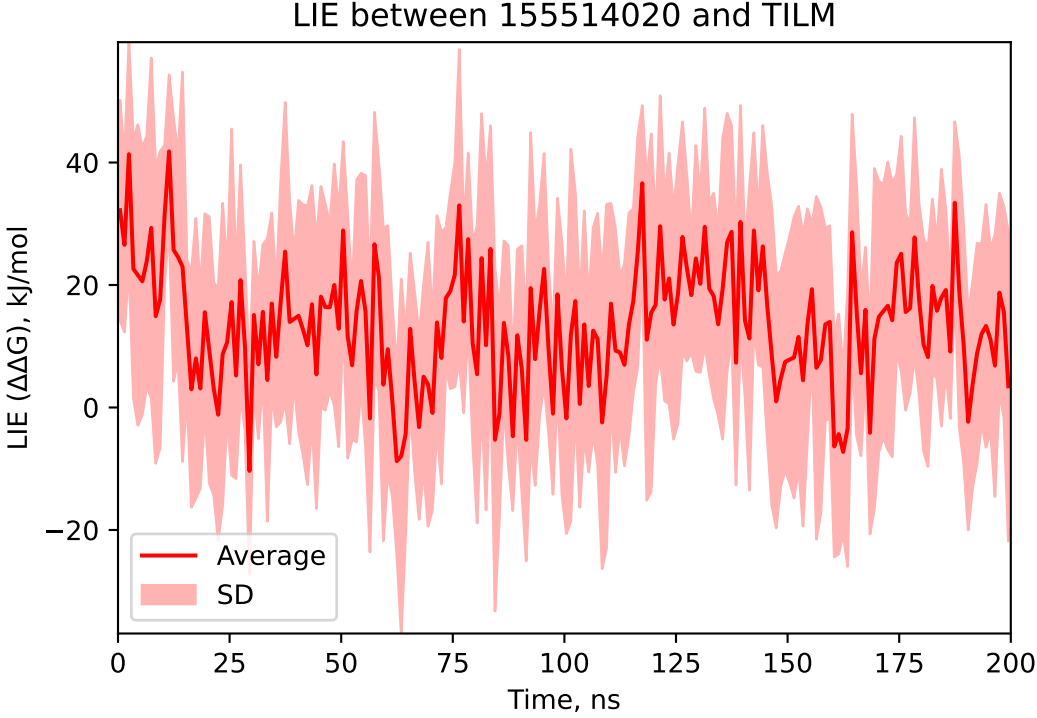

LIE between 155514020 and RONI
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

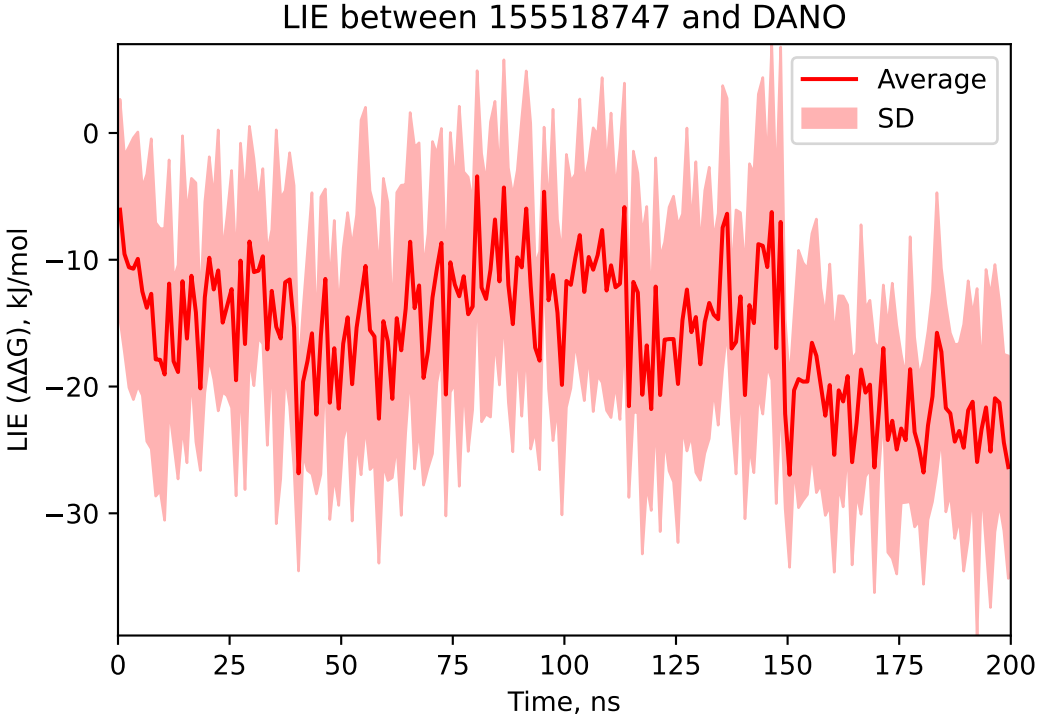

LIE between 155514020 and SPIR
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

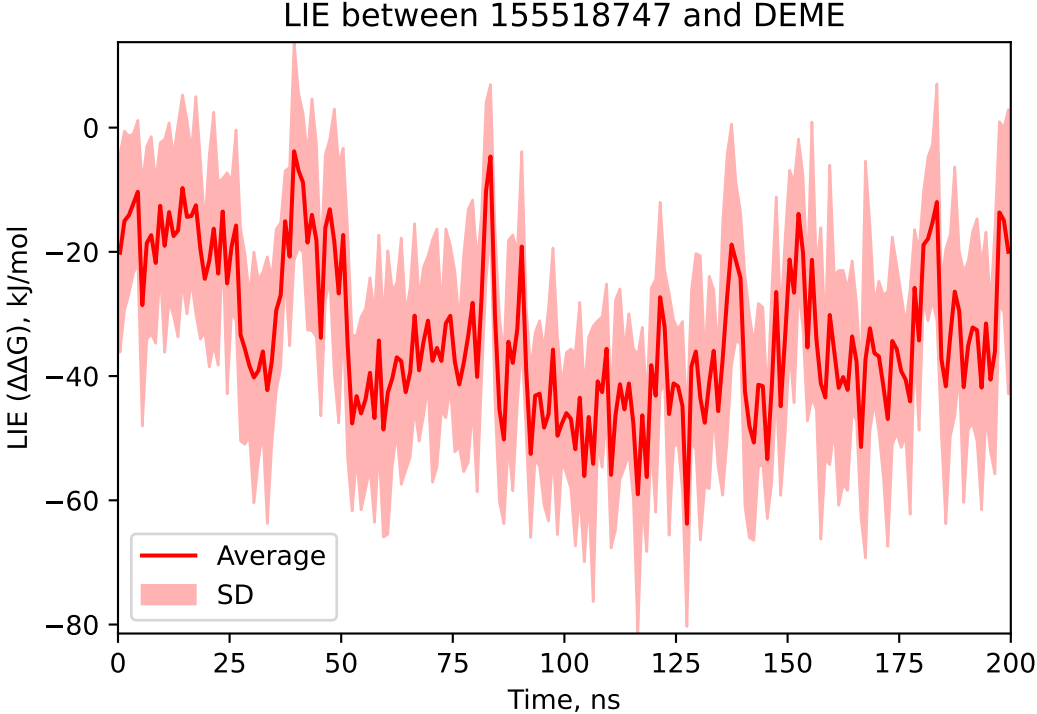

LIE between 155514020 and STRE
LIE (ΔΔG), kJ/mol
80
60
40
20
0
−20
−40
−60
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

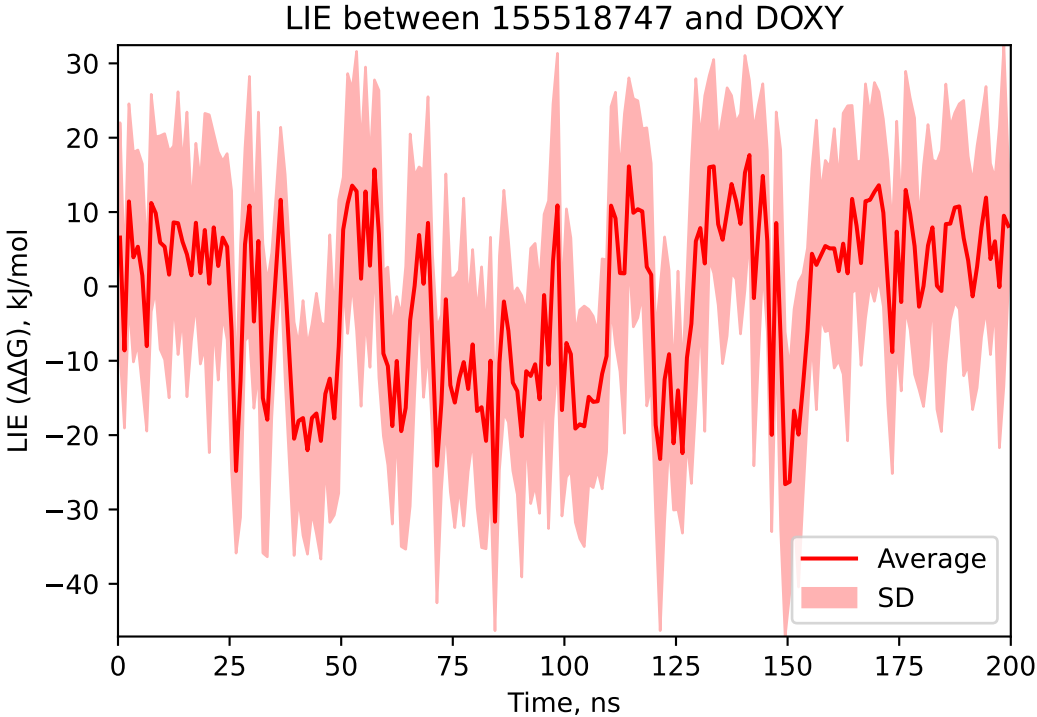

LIE between 155514020 and SULF
LIE (ΔΔG), kJ/mol
−10
−15
−20
−25
−30
−35
−40
−45
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

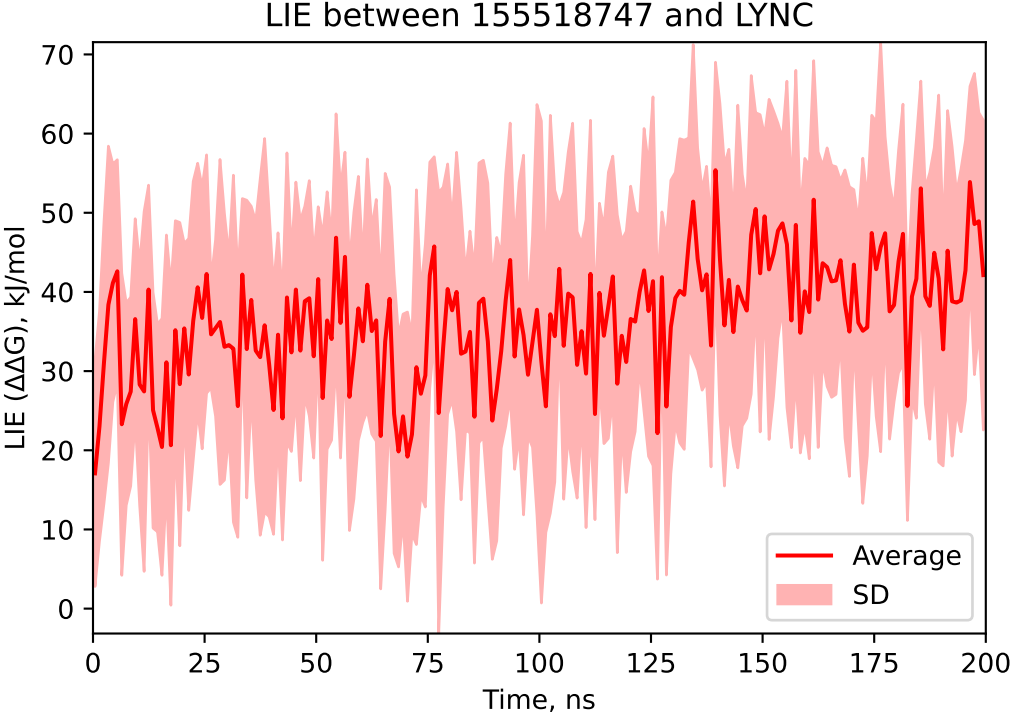

LIE between 155514020 and TIAM
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200

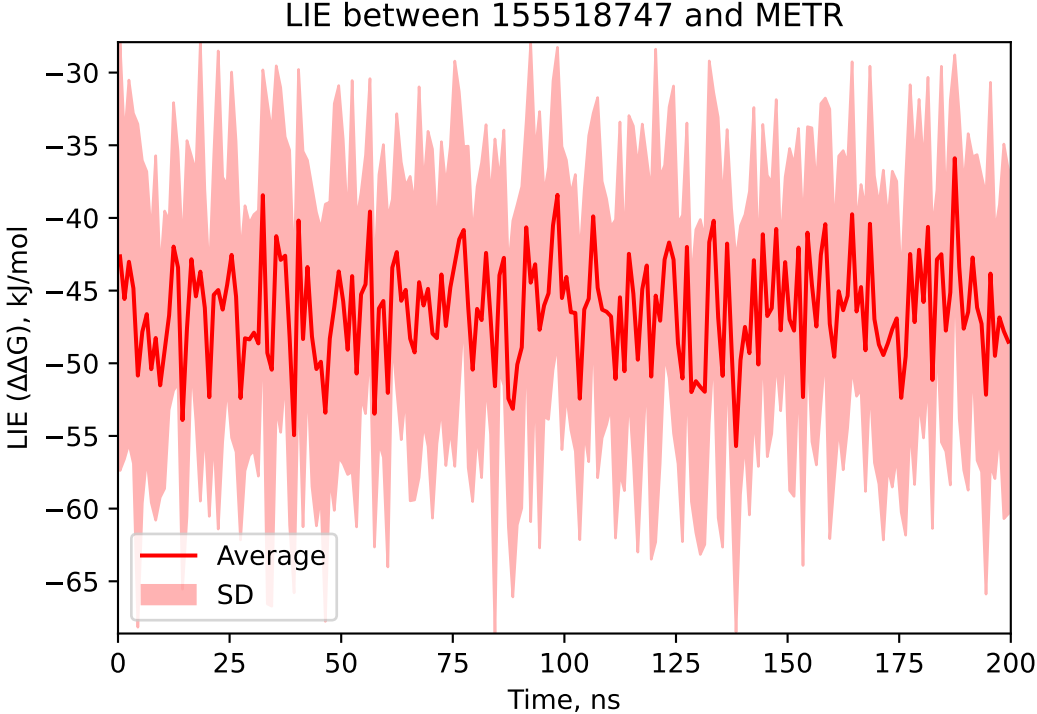

LIE between 155514020 and TILM
LIE (ΔΔG), kJ/mol
40
20
0
−20
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

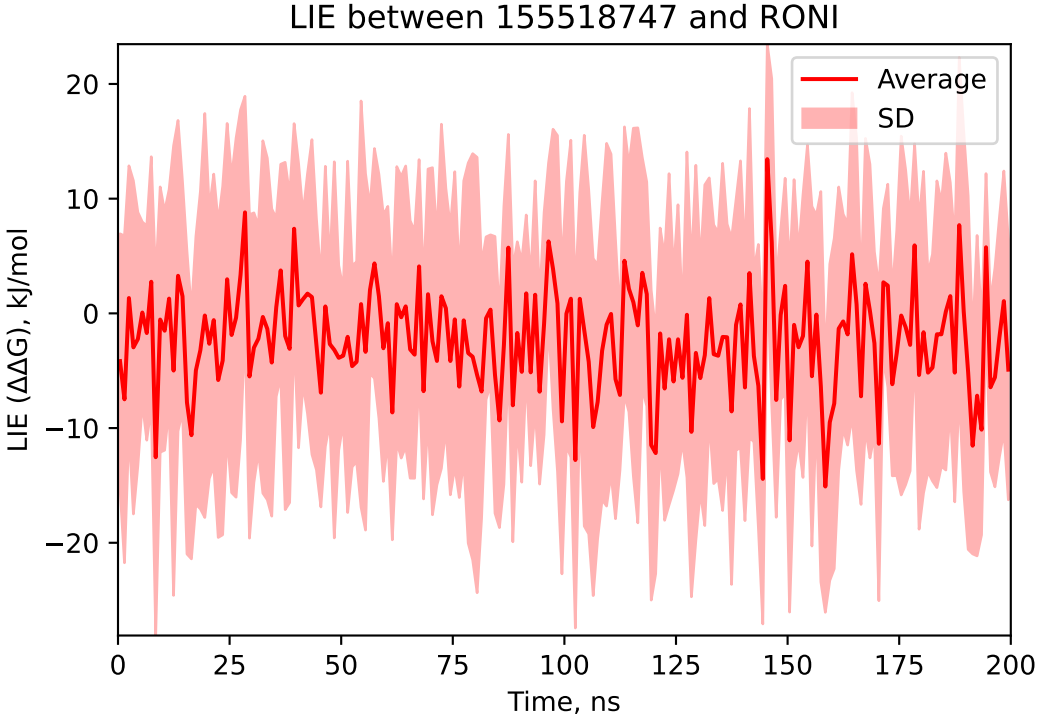

LIE between 155518747 and DANO
Average
SD
0
−10
−20
−30
LIE (ΔΔG), kJ/mol
0
25
50
75
100
125
150
175
200
Time, ns

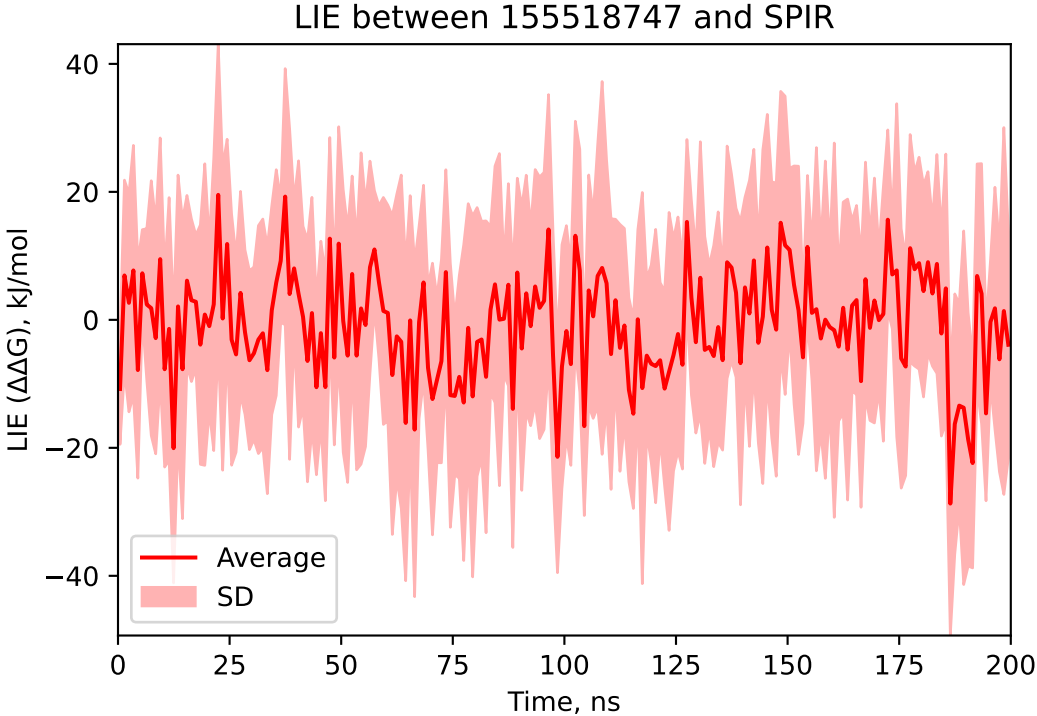

LIE between 155518747 and DEME
LIE (ΔΔG), kJ/mol
0
−20
−40
−60
−80
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

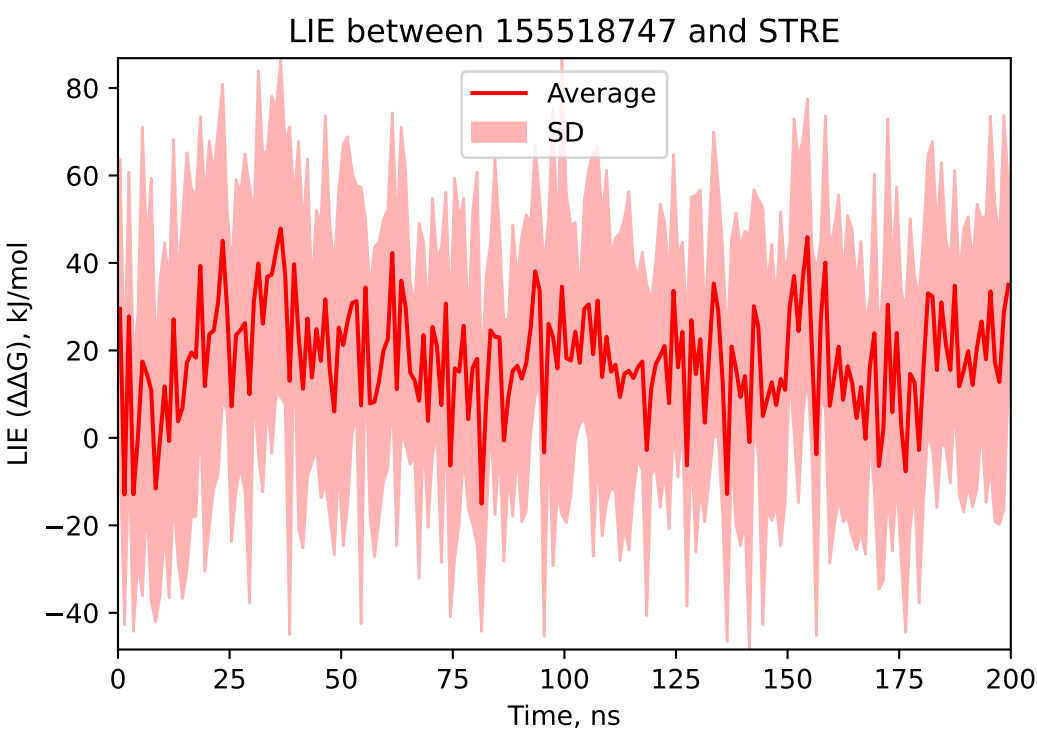

LIE between 155518747 and DOXY
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200

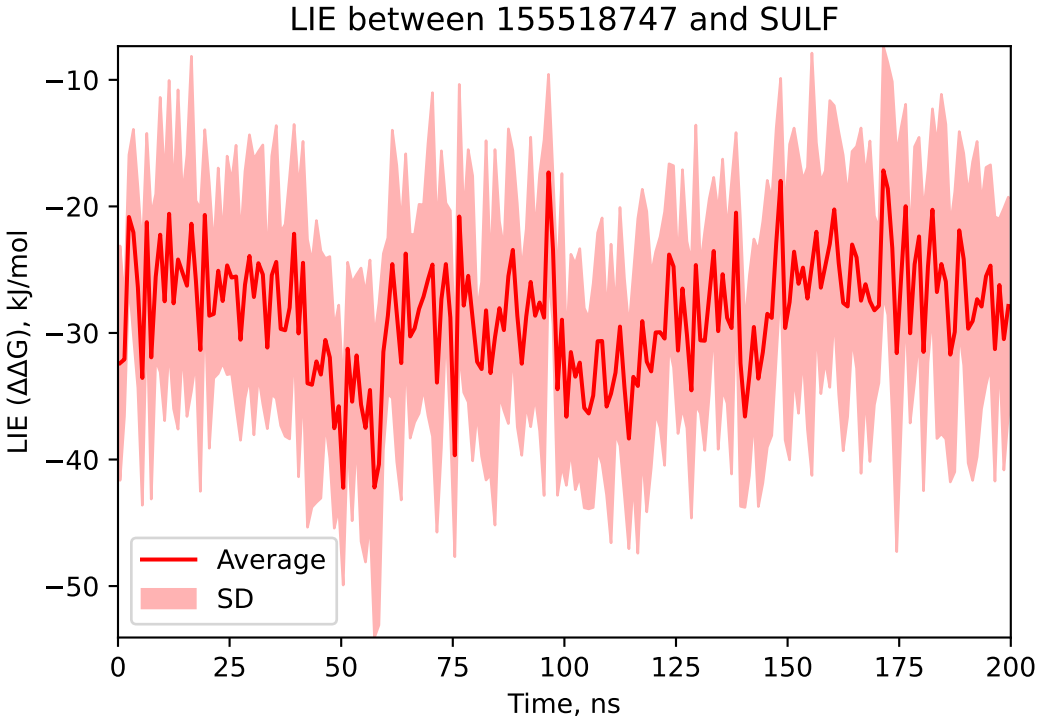

LIE between 155518747 and LYNC
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
0
10
20
30
40
50
60
70
0
25
50
75
100
125
150
175
200

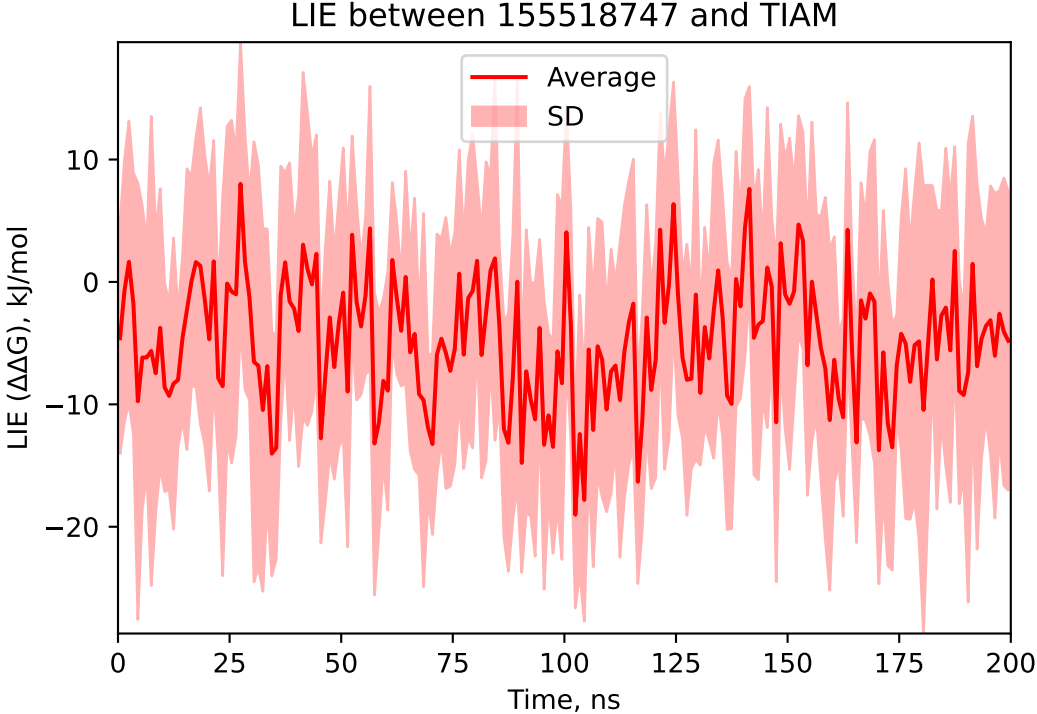

LIE between 155518747 and METR
LIE (ΔΔG), kJ/mol
−30
−35
−40
−45
−50
−55
−60
−65
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

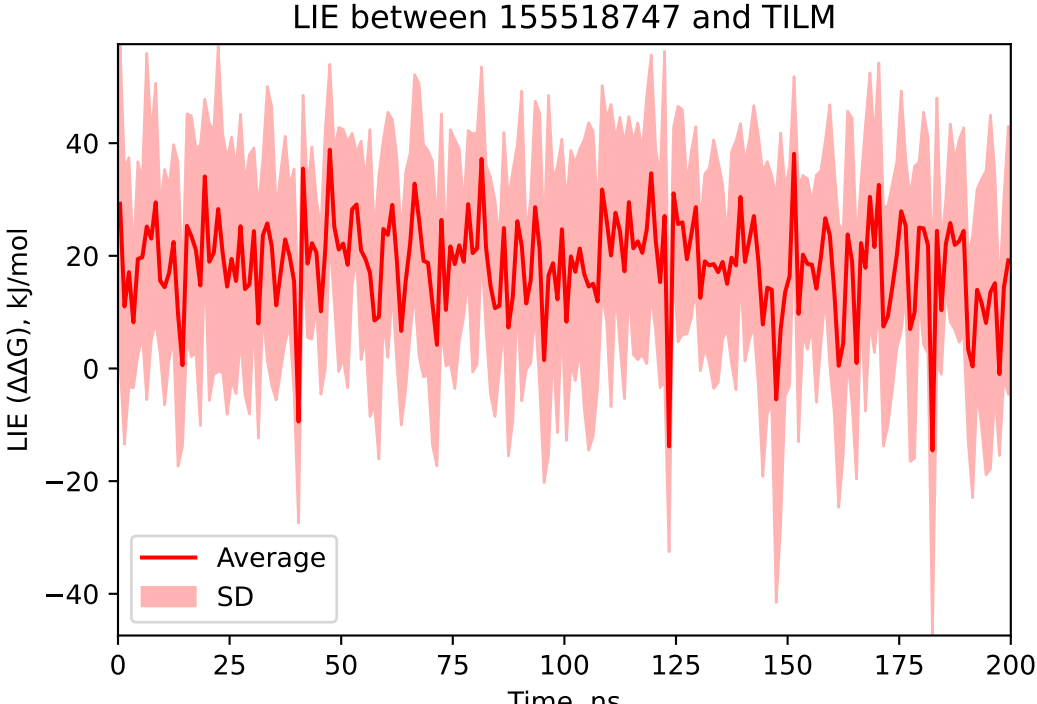

LIE between 155518747 and RONI
Average
SD
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns

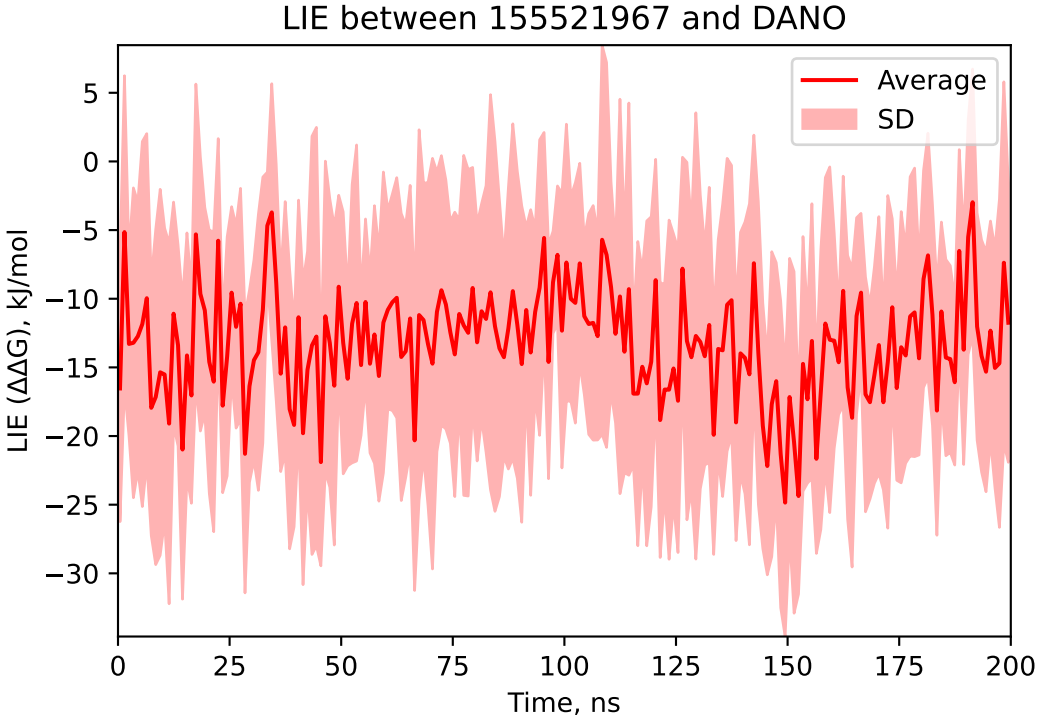

LIE between 155518747 and SPIR
LIE (ΔΔG), kJ/mol
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

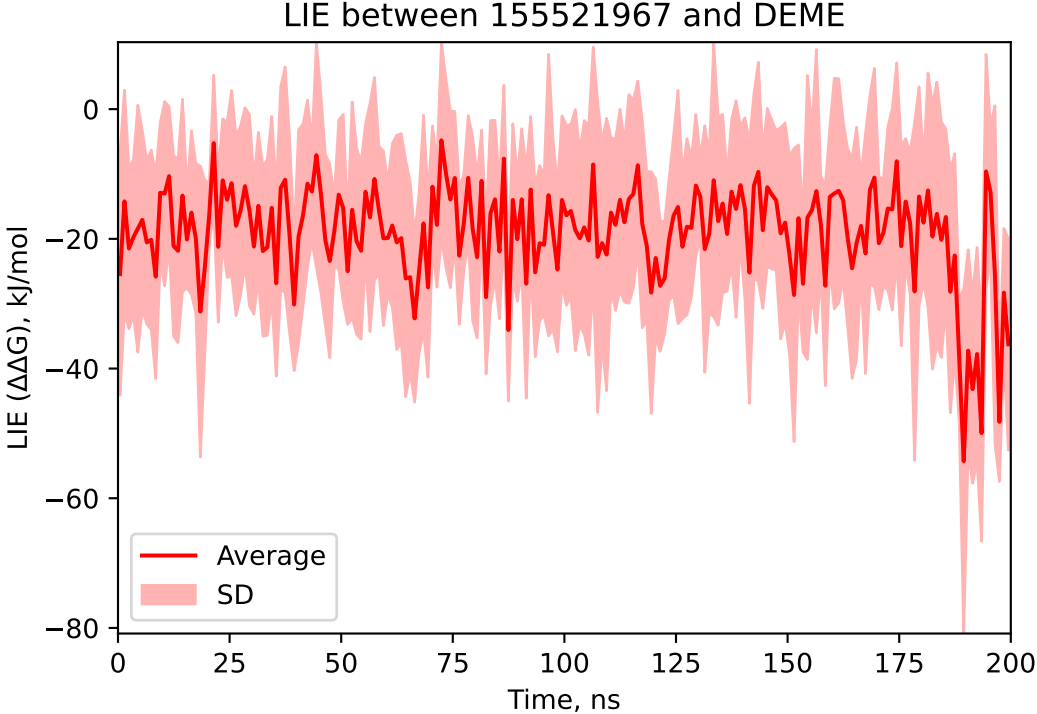

LIE between 155518747 and STRE
Average
SD
LIE (ΔΔG), kJ/mol
80
60
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns

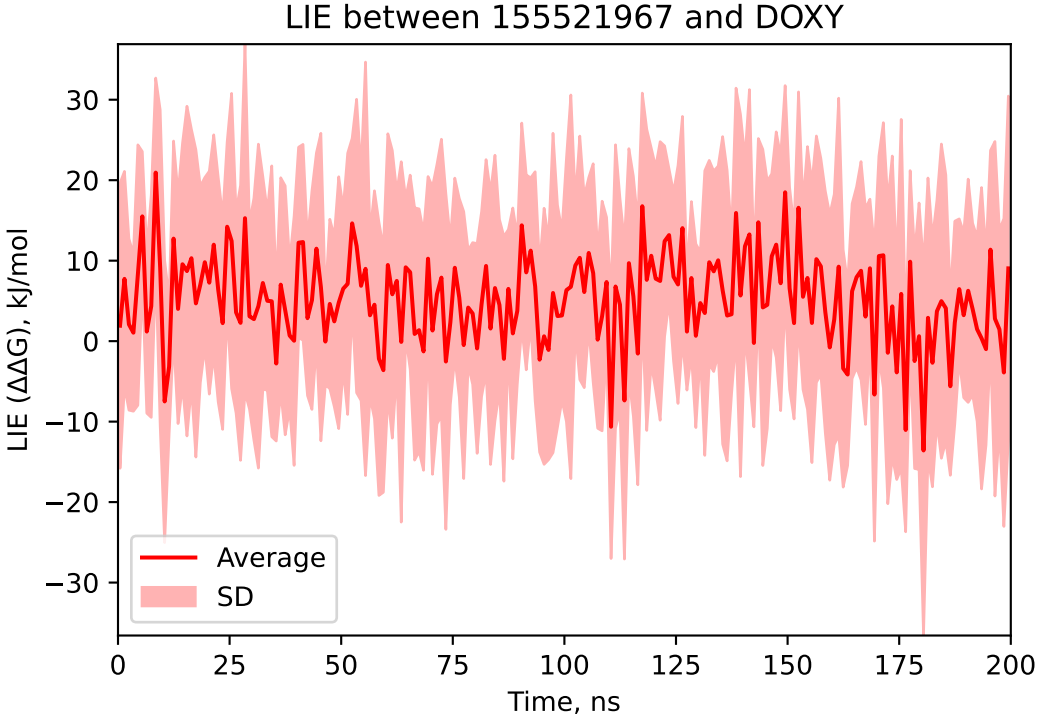

LIE between 155518747 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

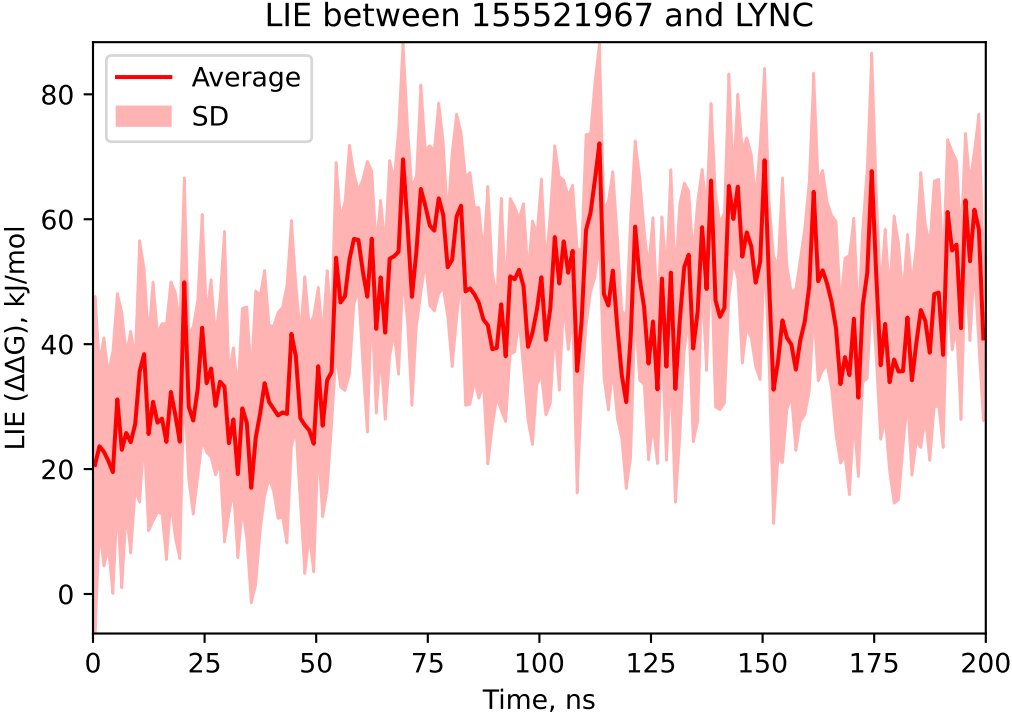

LIE between 155518747 and TIAM
Average
SD
10
0
−10
−20
LIE (ΔΔG), kJ/mol
0
25
50
75
100
125
150
175
200
Time, ns

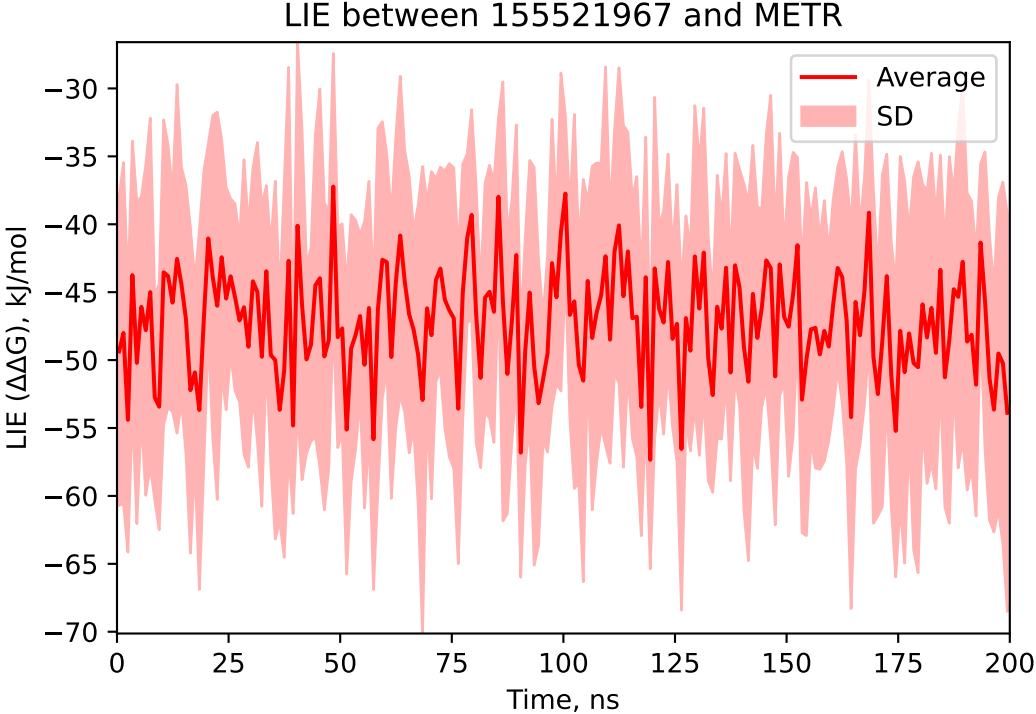

LIE between 155518747 and TILM
LIE (ΔΔG), kJ/mol
40
20
0
−20
−40
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

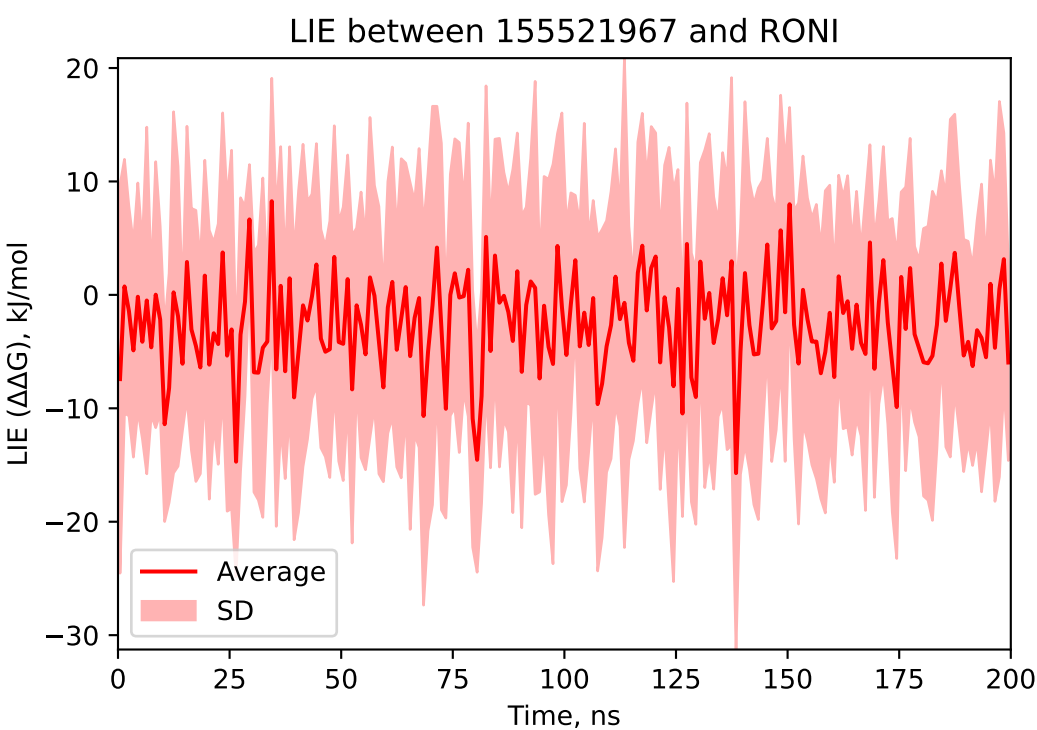

LIE between 155521967 and DANO
Average
SD
LIE (ΔΔG), kJ/mol
5
0
−5
−10
−15
−20
−25
−30
0
25
50
75
100
125
150
175
200
Time, ns

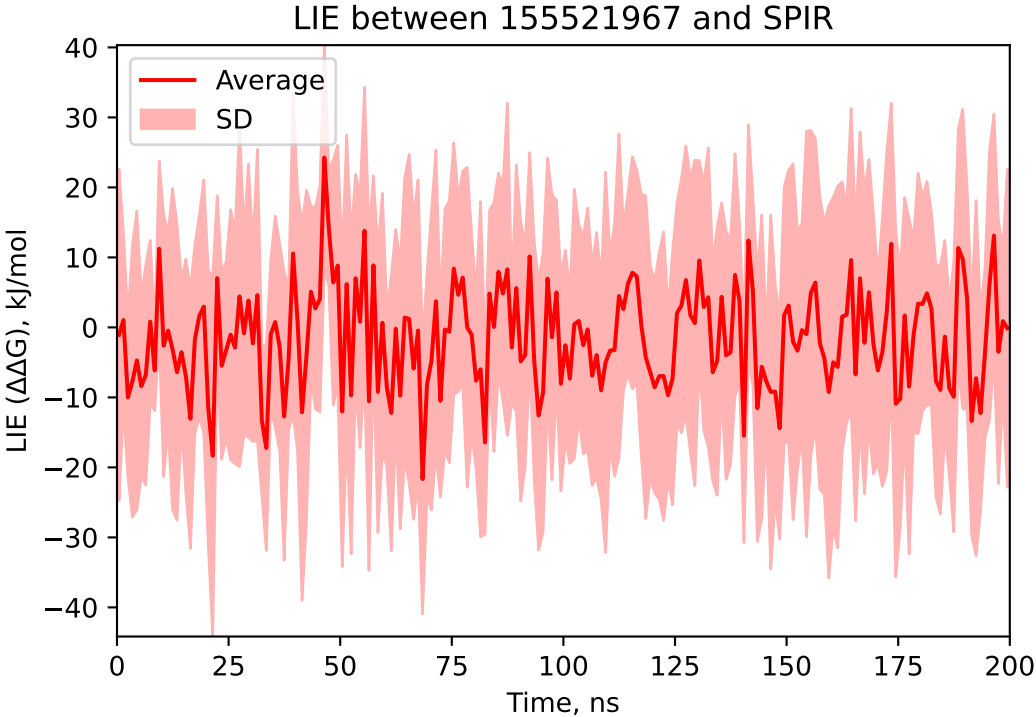

LIE between 155521967 and DEME
LIE (ΔΔG), kJ/mol
0
−20
−40
−60
−80
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

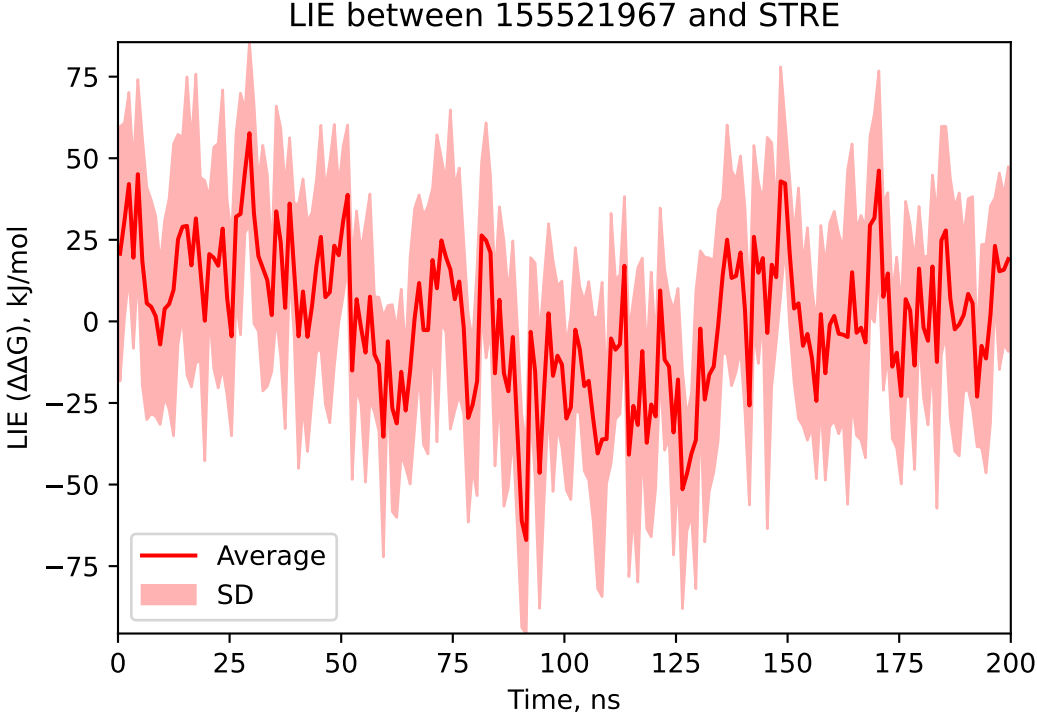

LIE between 155521967 and DOXY
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
30
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200

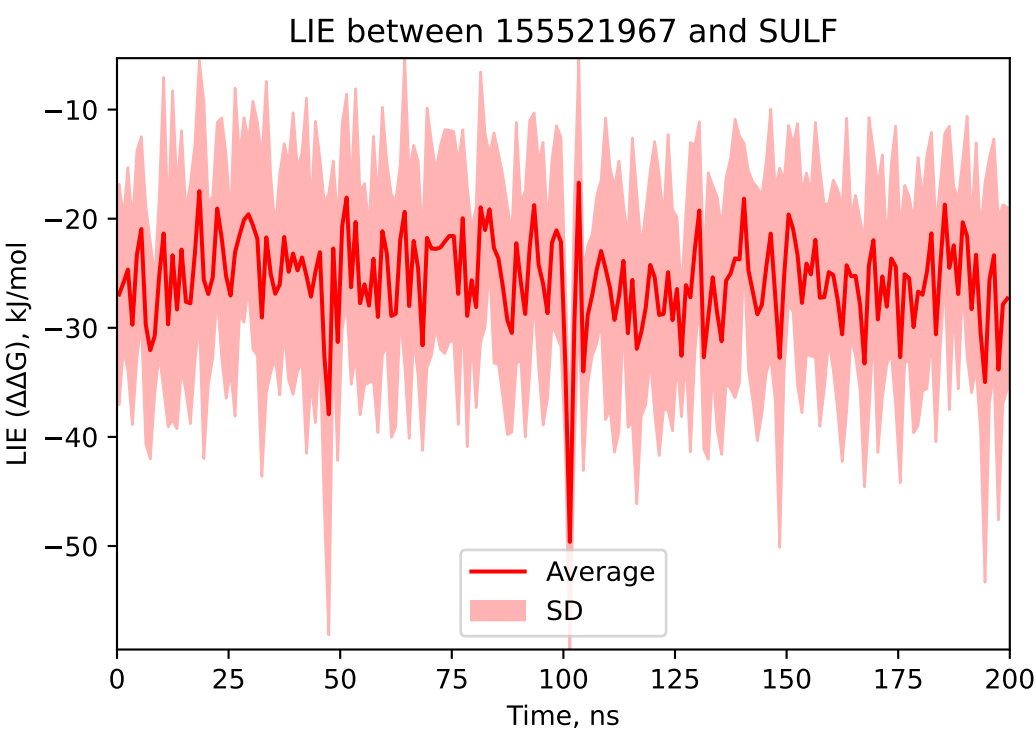

LIE between 155521967 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
0
20
40
60
80
0
25
50
75
100
125
150
175
200
Time, ns

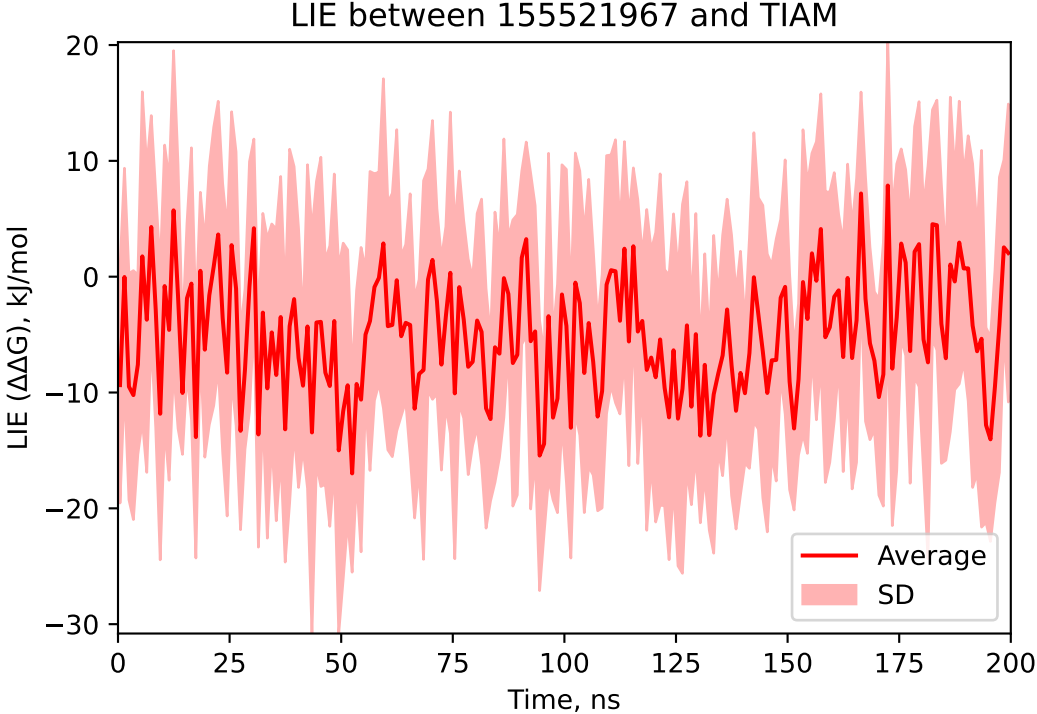

LIE between 155521967 and METR
Average
SD
LIE (ΔΔG), kJ/mol
−30
−35
−40
−45
−50
−55
−60
−65
−70
0
25
50
75
100
125
150
175
200
Time, ns

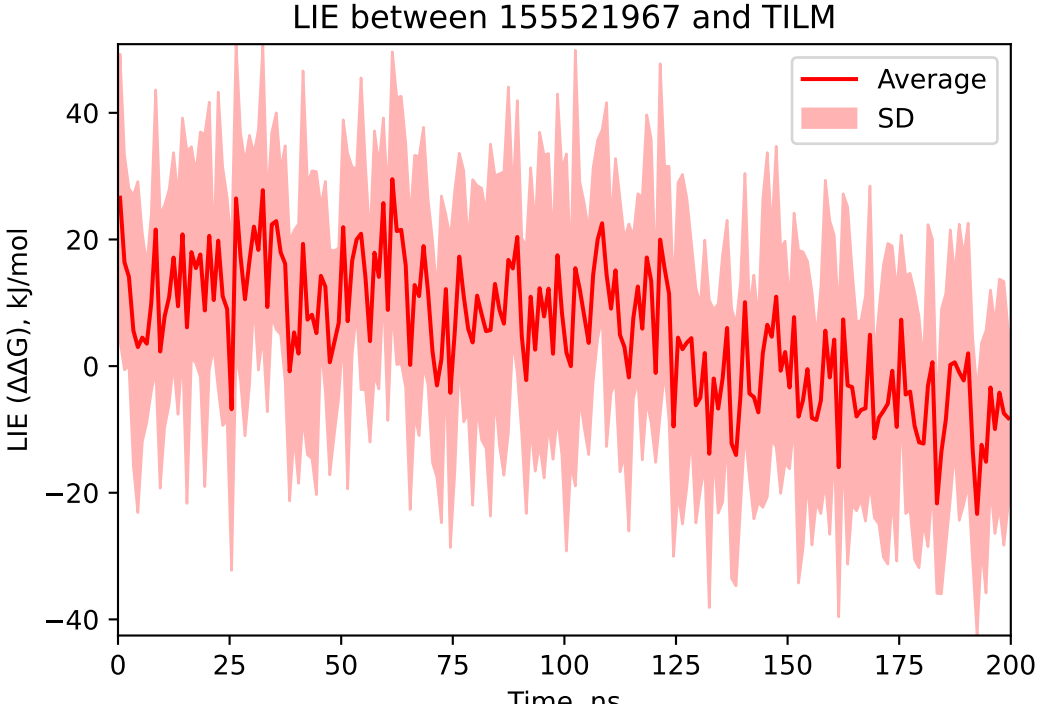

LIE between 155521967 and RONI
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200

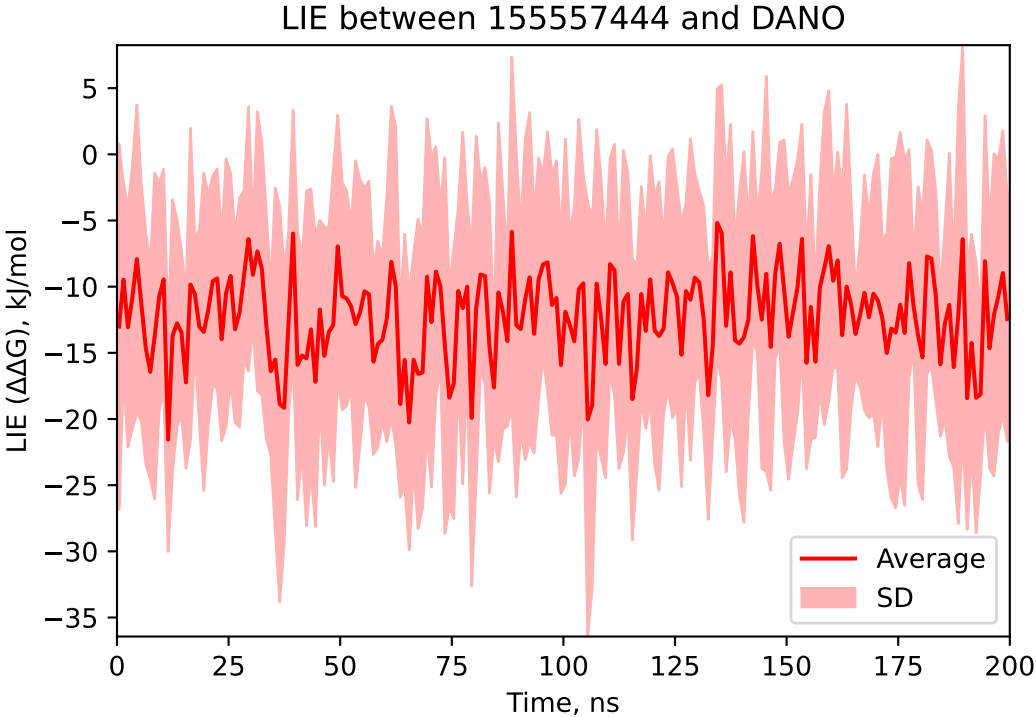

LIE between 155521967 and SPIR
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
40
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200

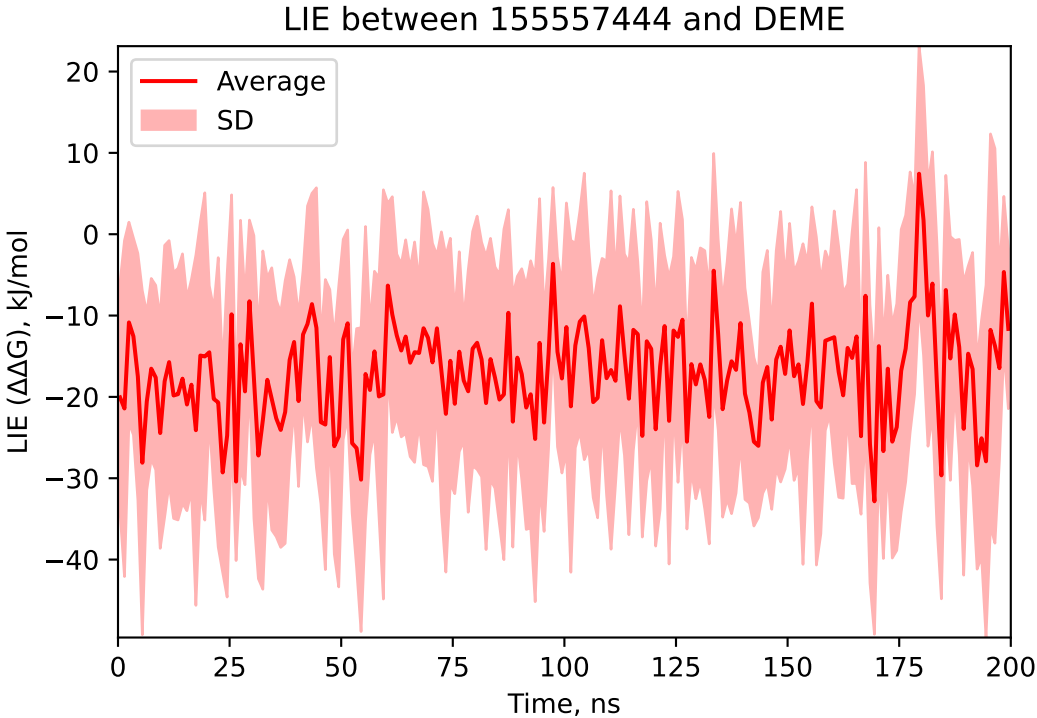

LIE between 155521967 and STRE
LIE (ΔΔG), kJ/mol
75
50
25
0
−25
−50
−75
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

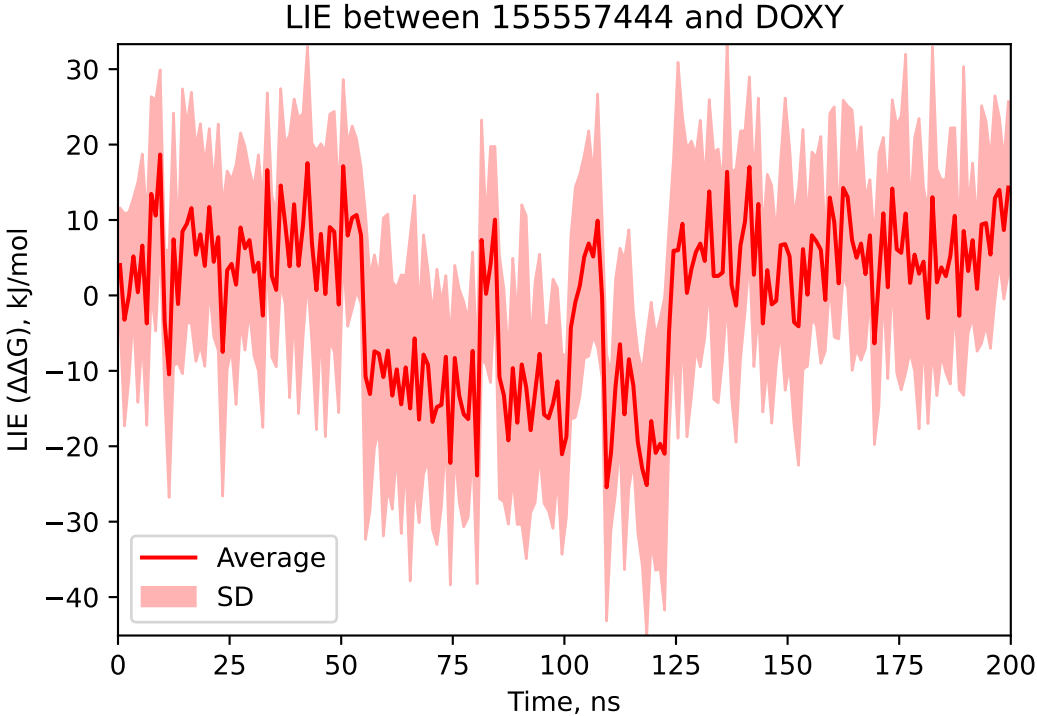

LIE between 155521967 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

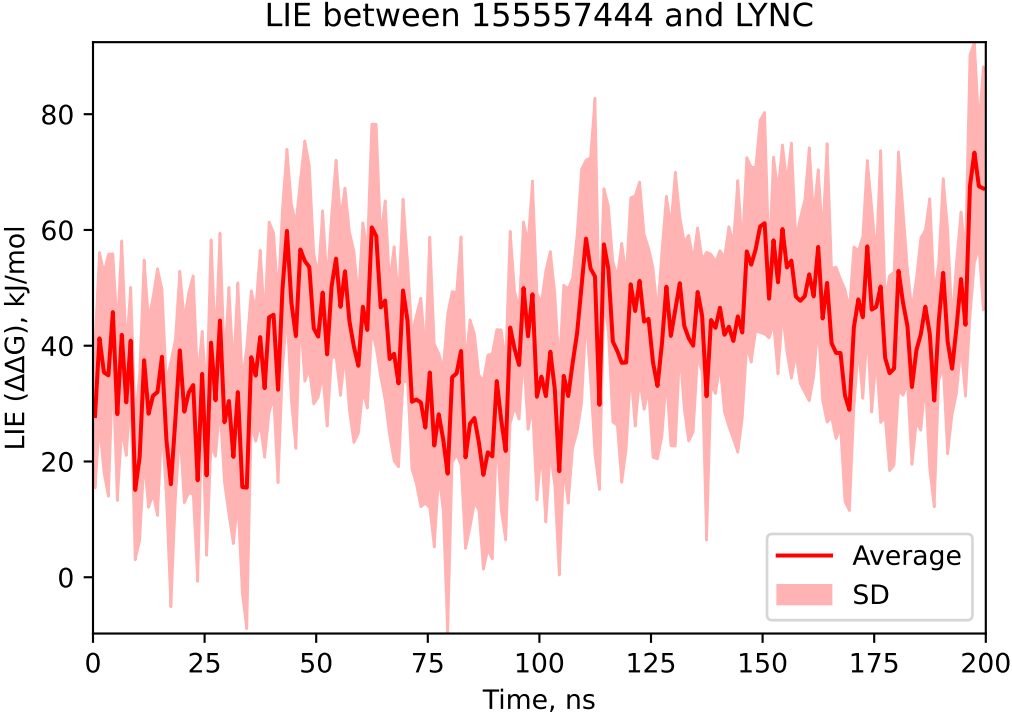

LIE between 155521967 and TIAM
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200

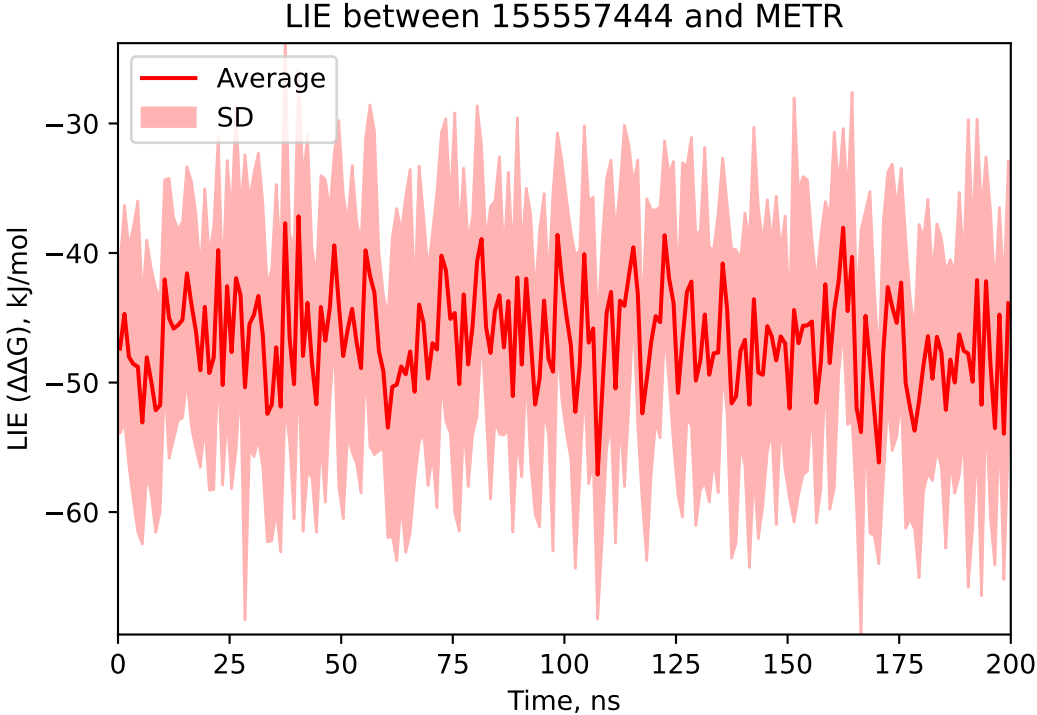

LIE between 155521967 and TILM
Average
SD
LIE (ΔΔG), kJ/mol
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns

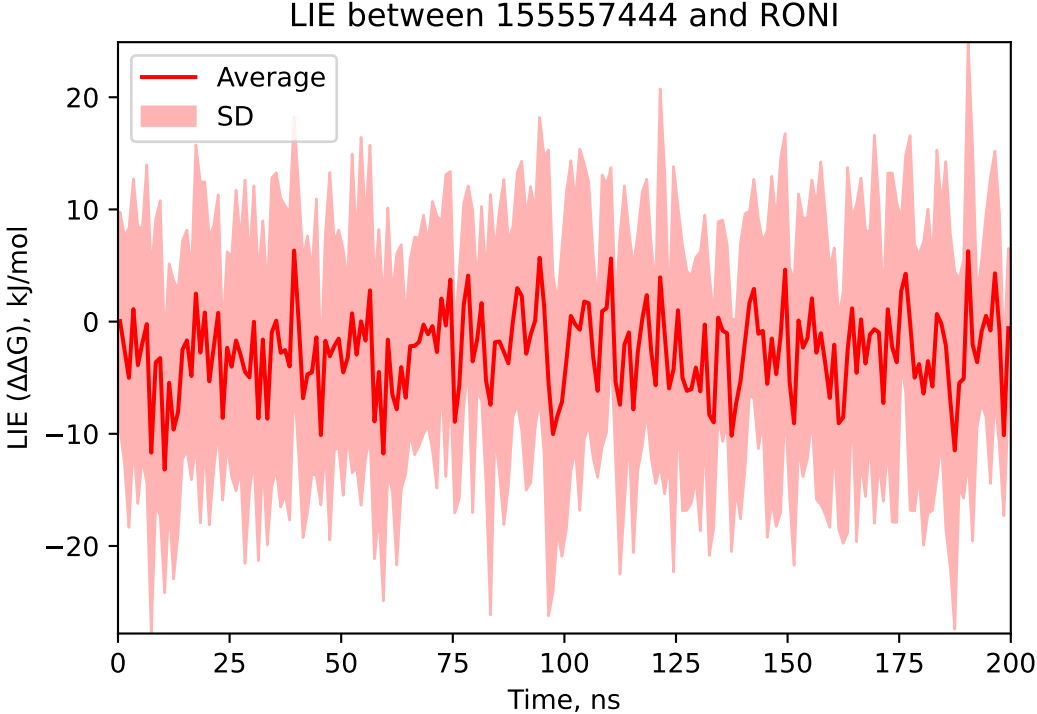

LIE between 155557444 and DANO
LIE (ΔΔG), kJ/mol
5
0
−5
−10
−15
−20
−25
−30
−35
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

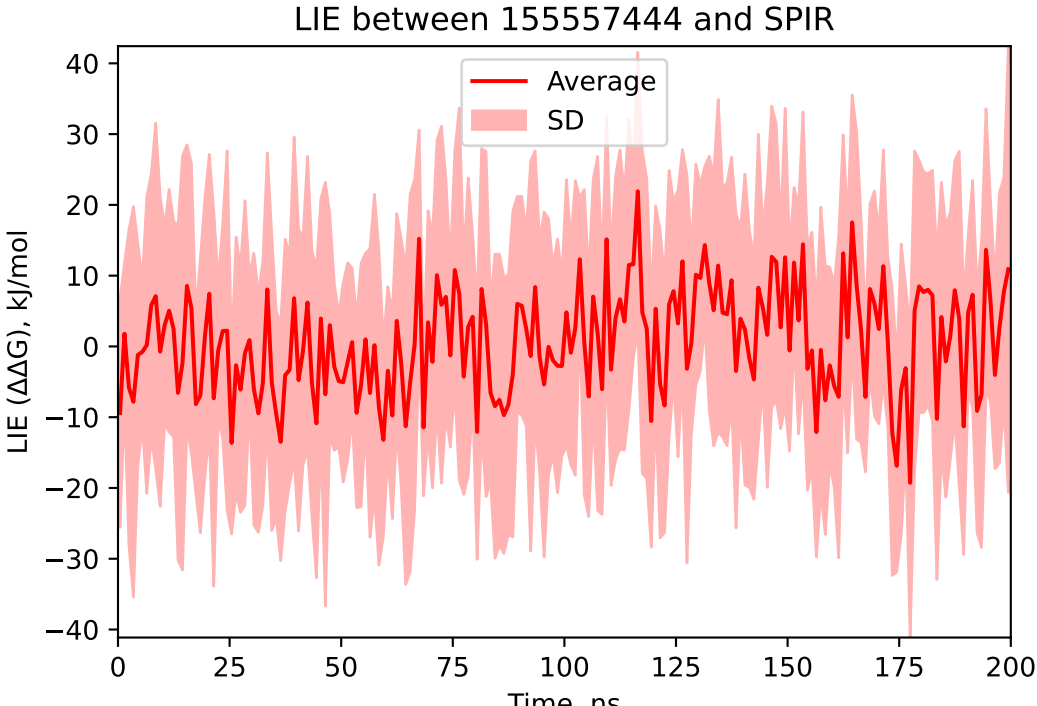

LIE between 155557444 and DEME
Average
SD
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns

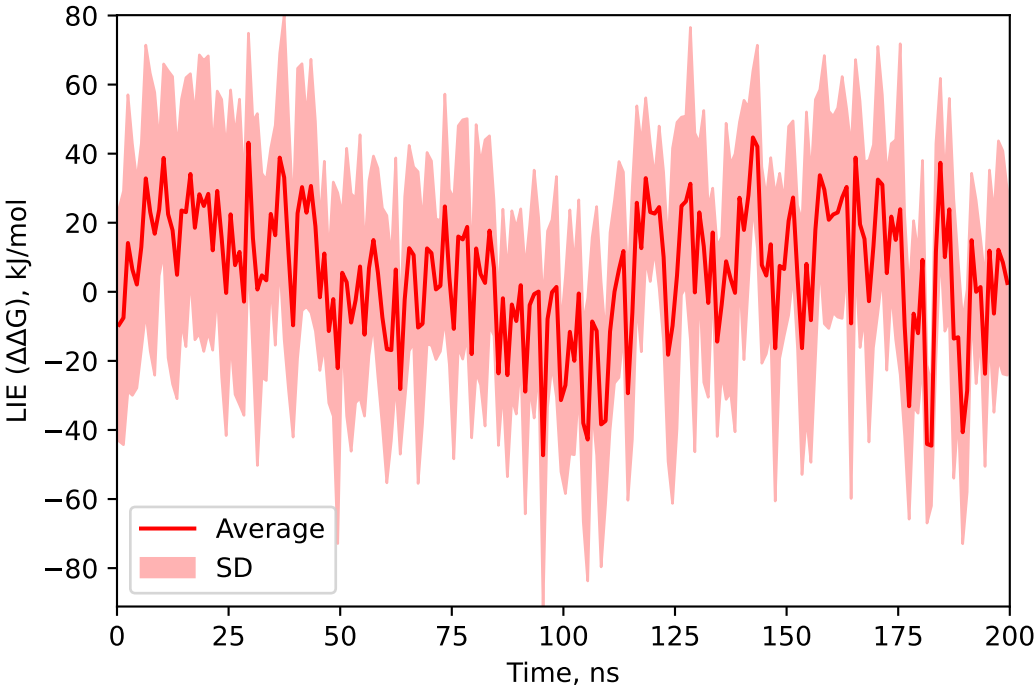

LIE between 155557444 and DOXY
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

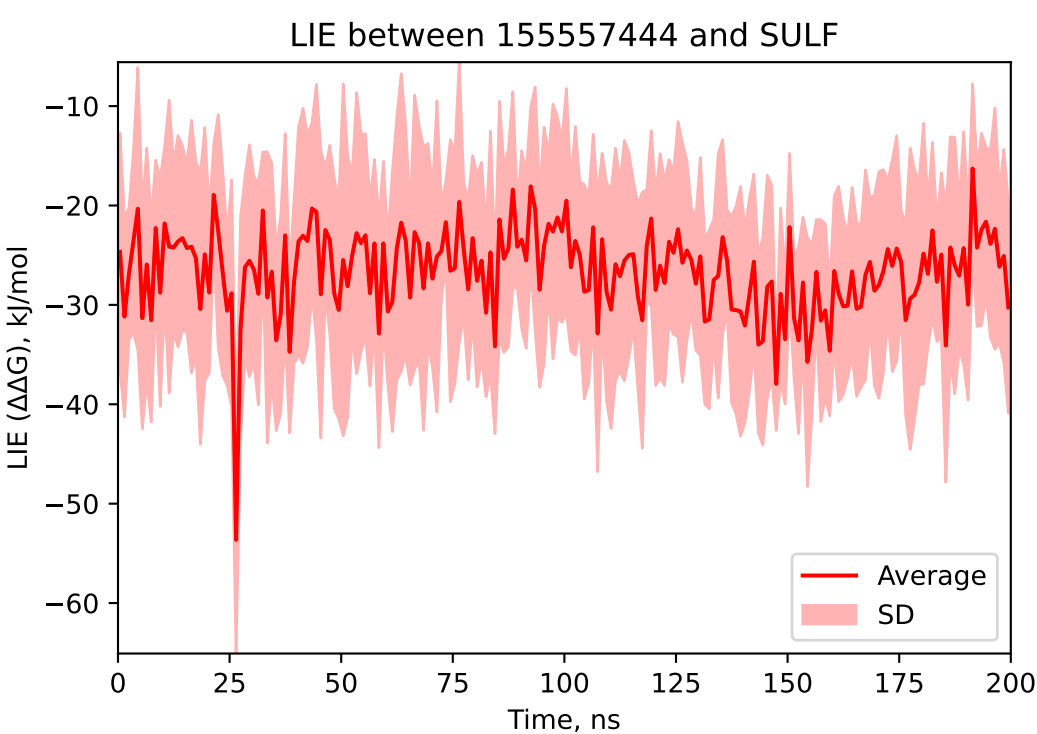

LIE between 155557444 and LYNC
LIE (ΔΔG), kJ/mol
80
60
40
20
0
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

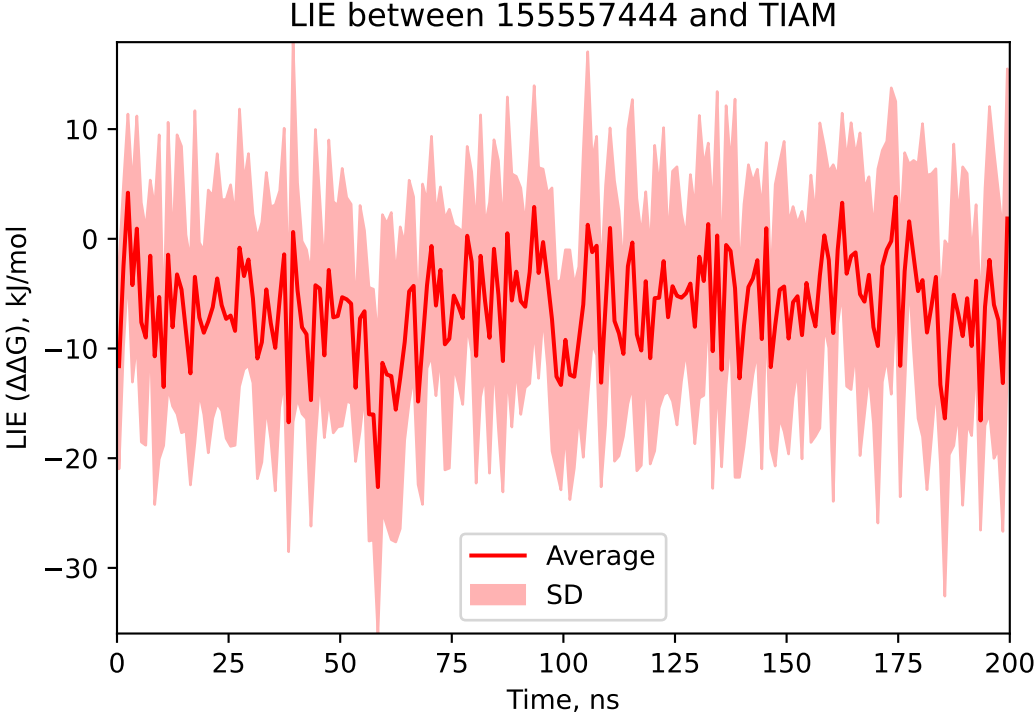

LIE between 155557444 and METR
Average
SD
−30
−40
−50
−60
LIE (ΔΔG), kJ/mol
0
25
50
75
100
125
150
175
200
Time, ns

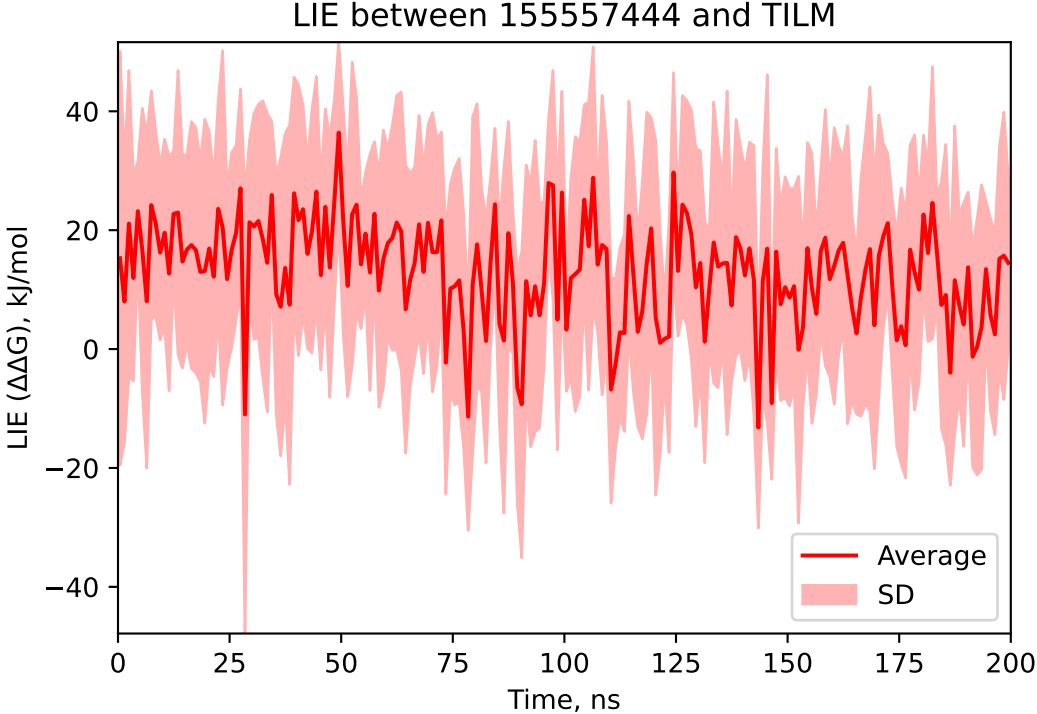

LIE between 155557444 and RONI
Average
SD
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns

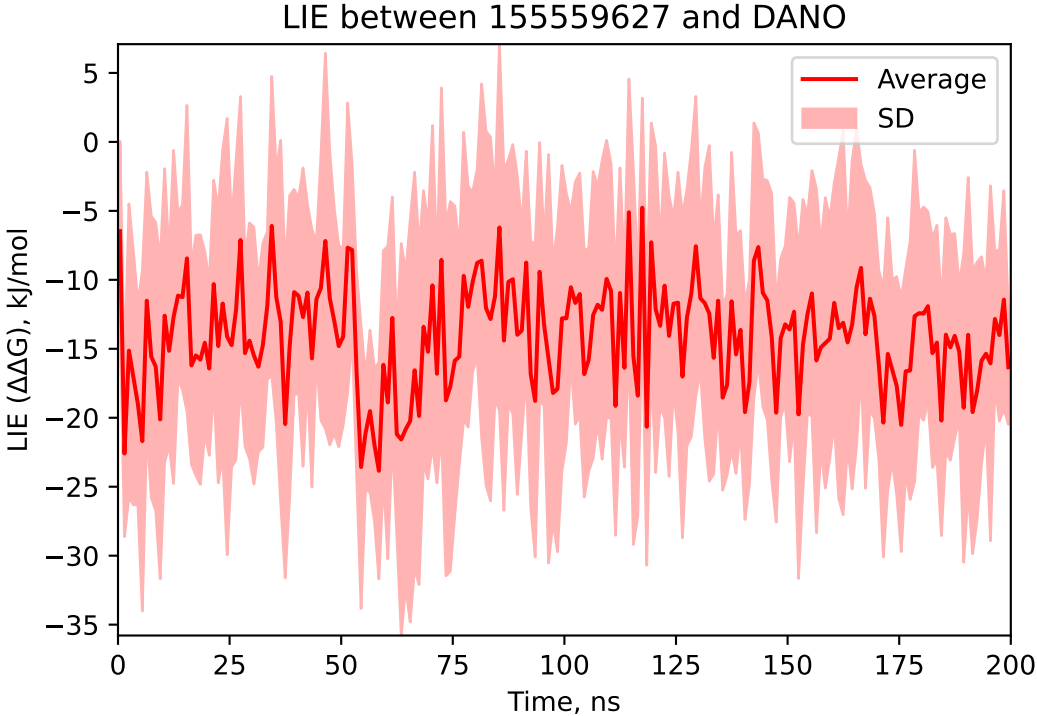

LIE between 155557444 and SPIR
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
40
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200

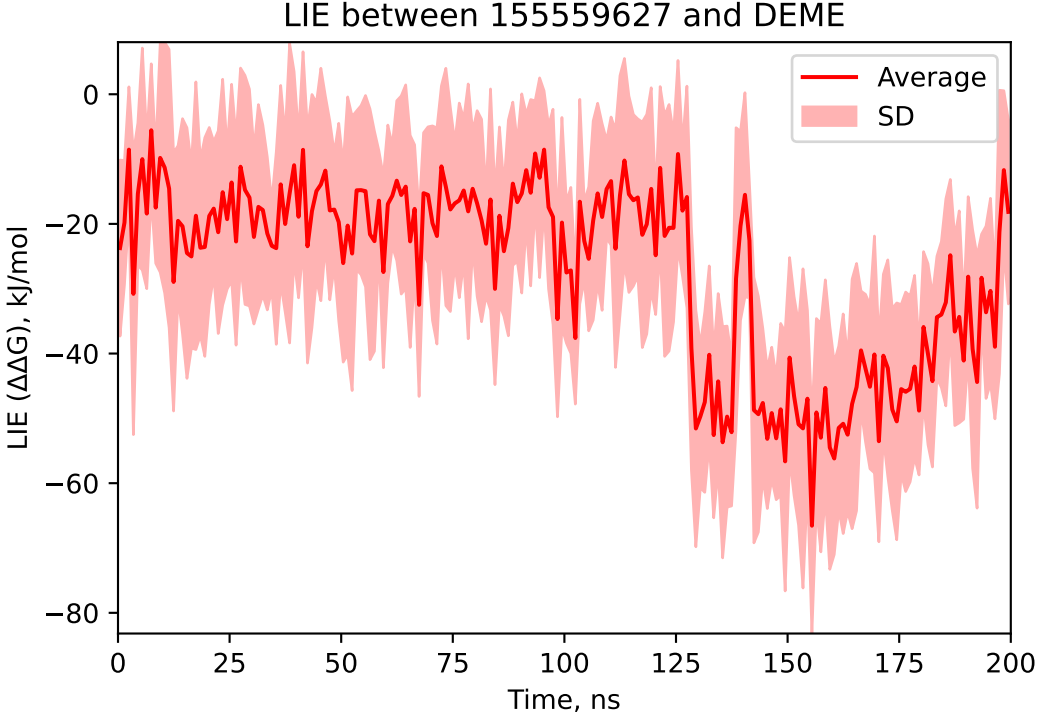

LIE between 155557444 and STRE
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
80
60
40
20
0
−20
−40
−60
−80
0
25
50
75
100
125
150
175
200

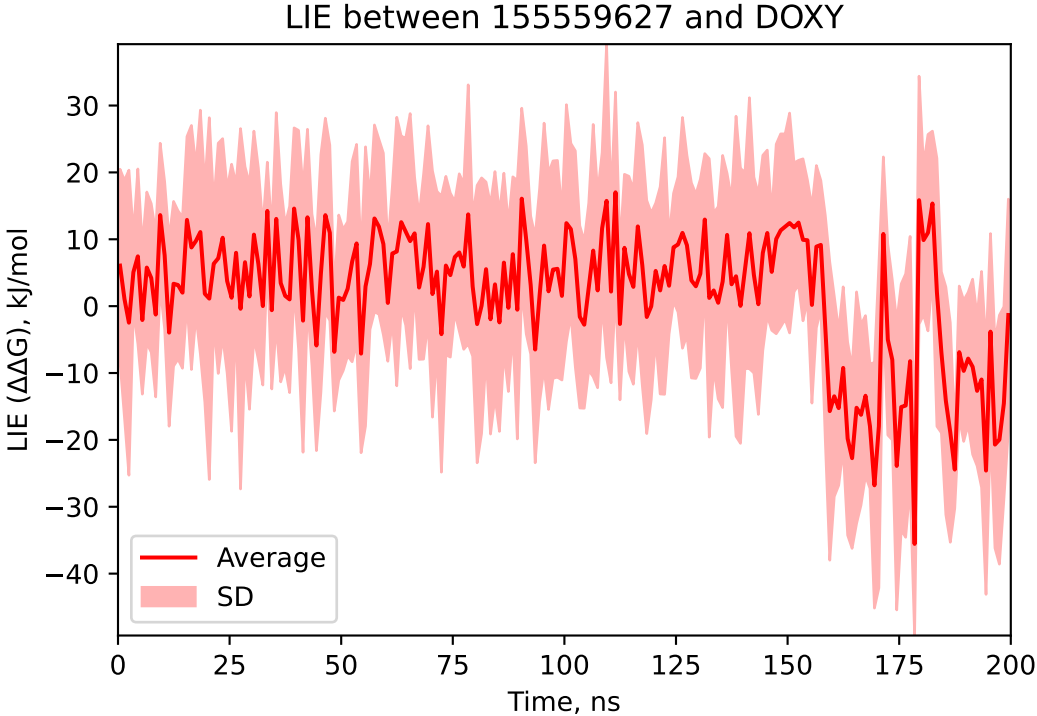

LIE between 155557444 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
−60
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

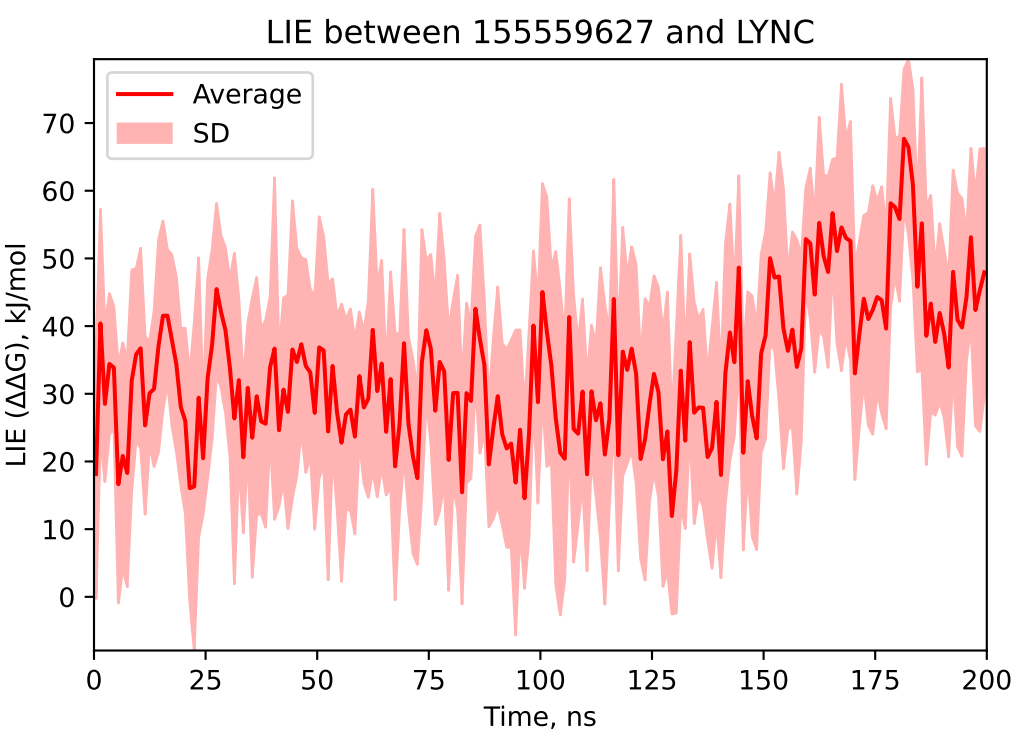

LIE between 155557444 and TIAM
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

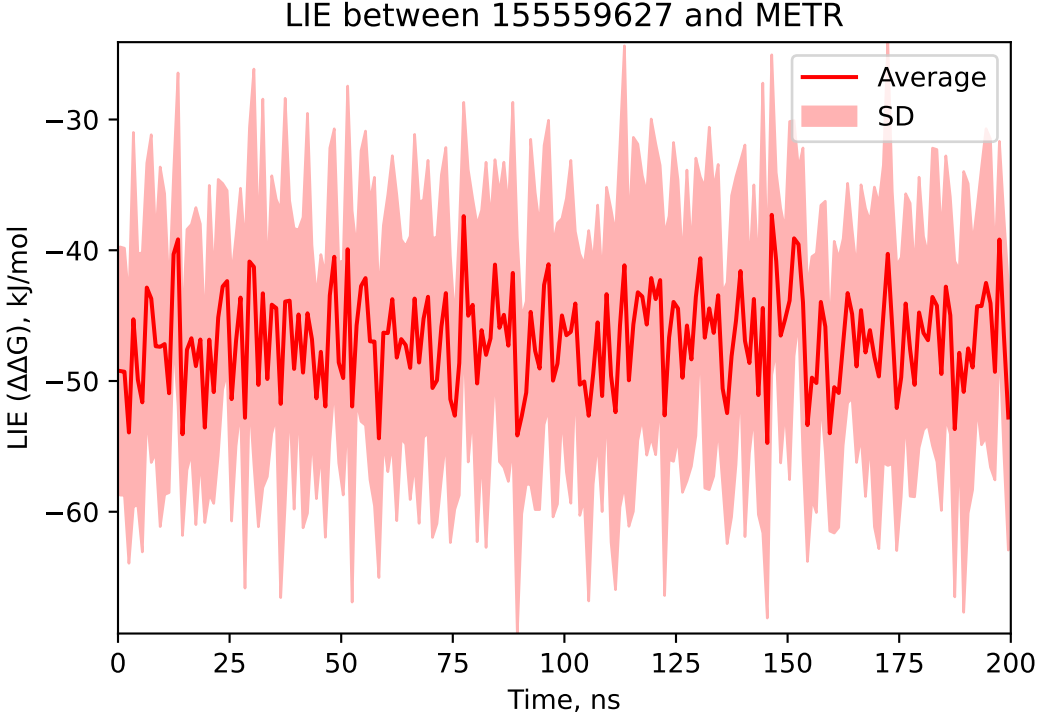

LIE between 155557444 and TILM
LIE (ΔΔG), kJ/mol
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

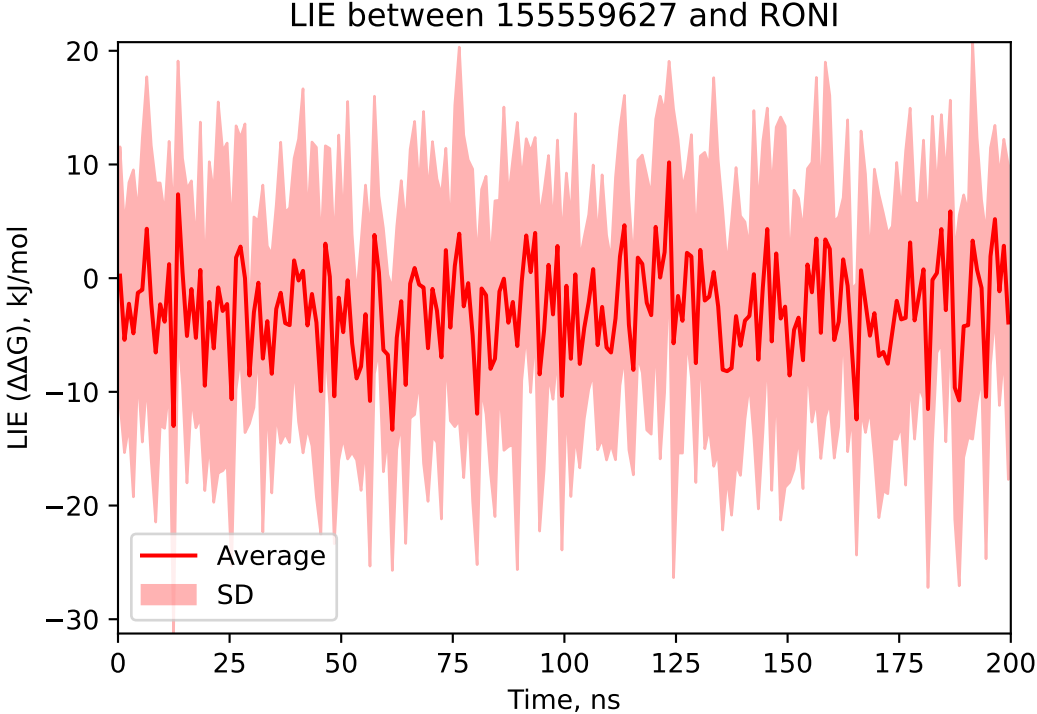

LIE between 155559627 and DANO
Average
SD
LIE (ΔΔG), kJ/mol
5
0
−5
−10
−15
−20
−25
−30
−35
0
25
50
75
100
125
150
175
200
Time, ns

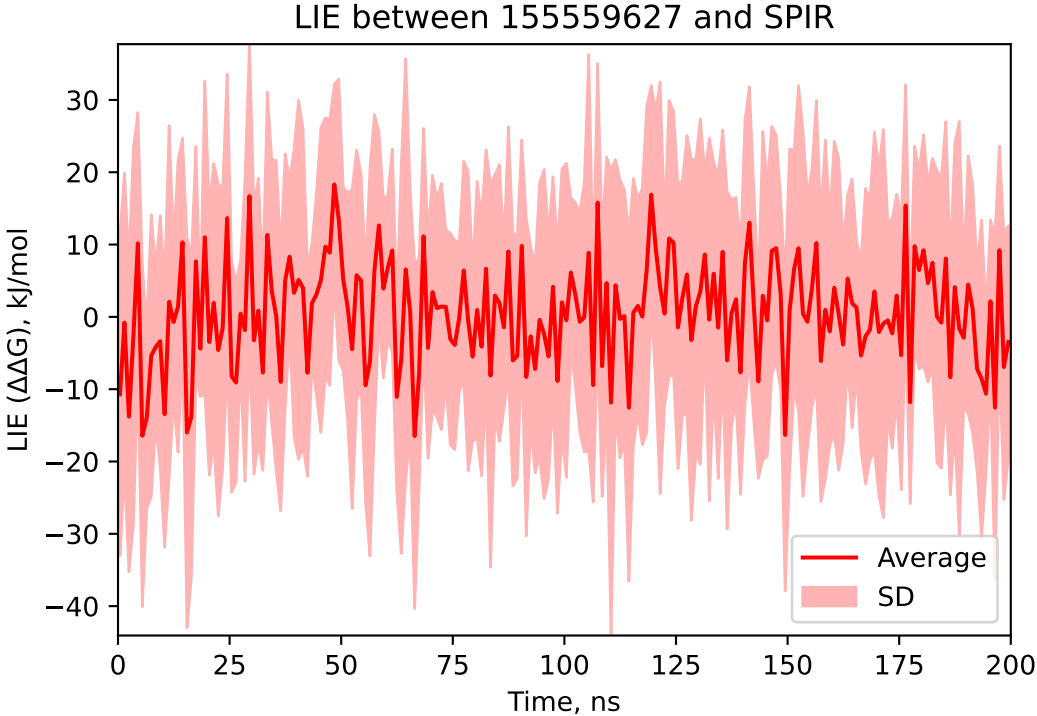

LIE between 155559627 and DEME
Average
SD
LIE (ΔΔG), kJ/mol
0
−20
−40
−60
−80
0
25
50
75
100
125
150
175
200
Time, ns

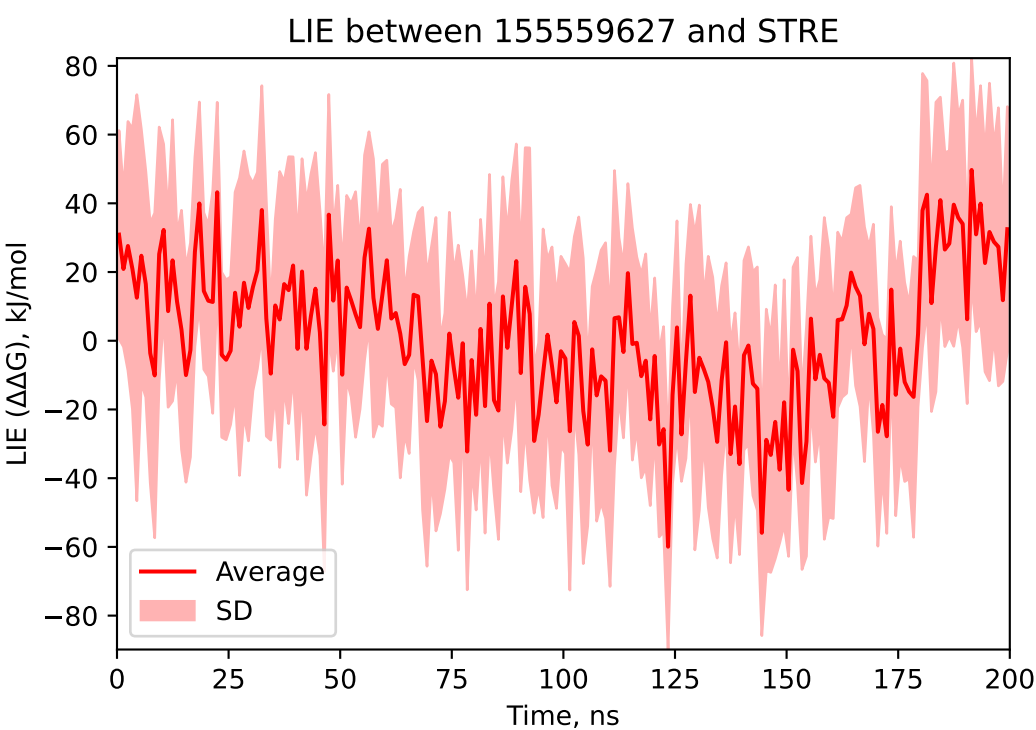

LIE between 155559627 and DOXY
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

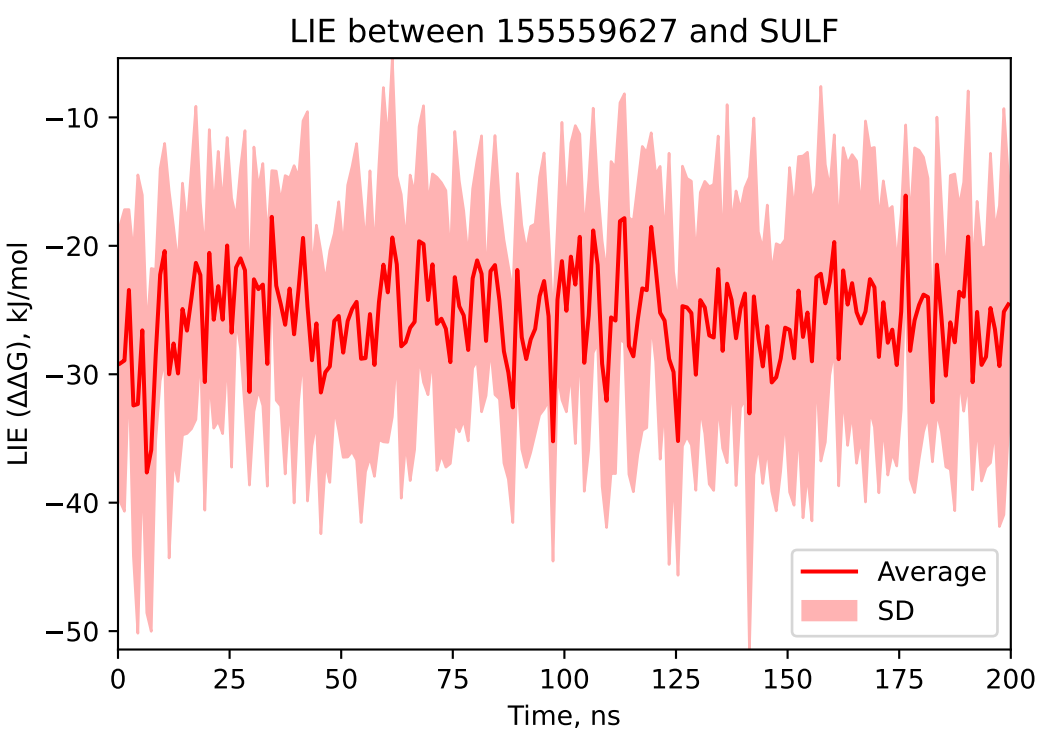

LIE between 155559627 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
70
60
50
40
30
20
10
0
0
25
50
75
100
125
150
175
200
Time, ns

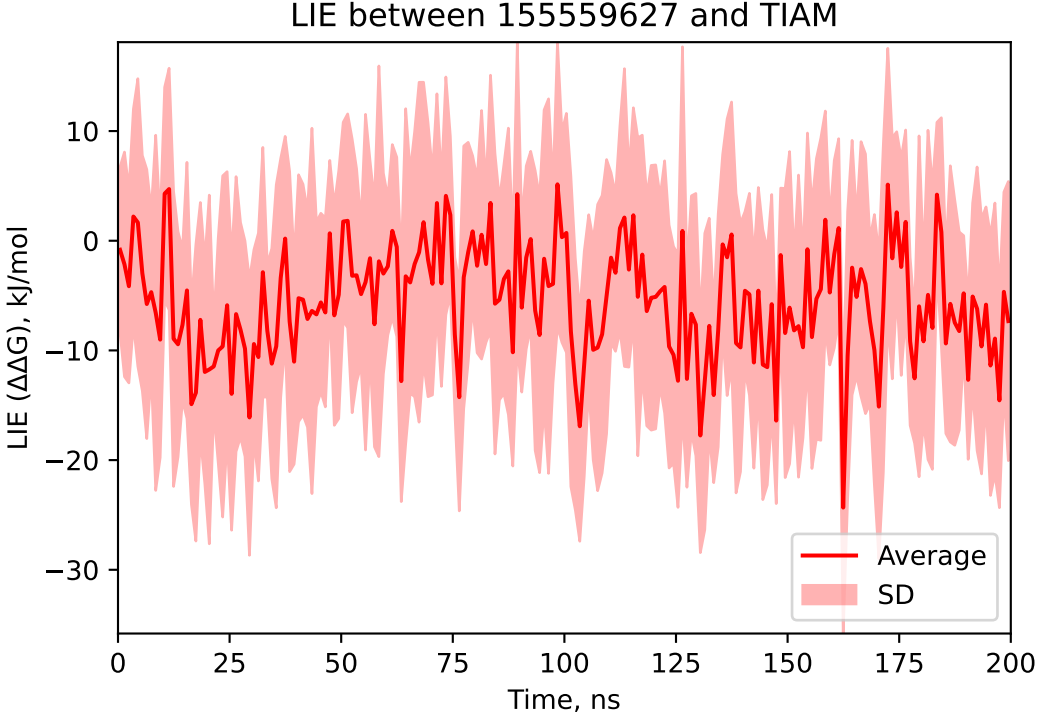

LIE between 155559627 and METR
Average
SD
−30
−40
−50
−60
LIE (ΔΔG), kJ/mol
0
25
50
75
100
125
150
175
200
Time, ns

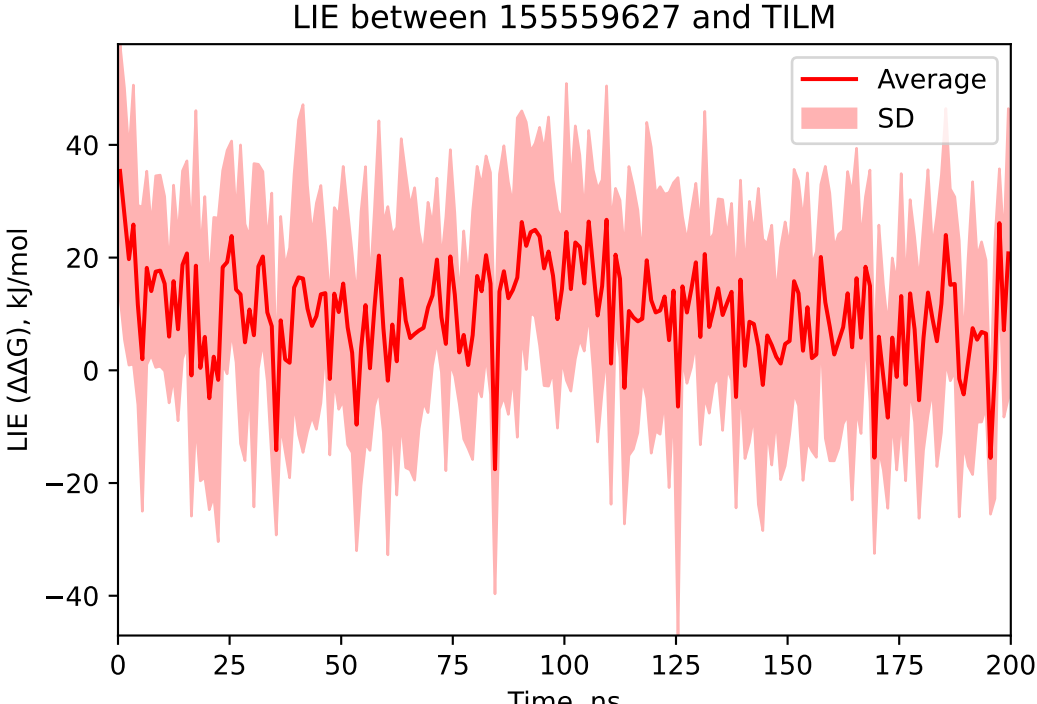

LIE between 155559627 and RONI
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200

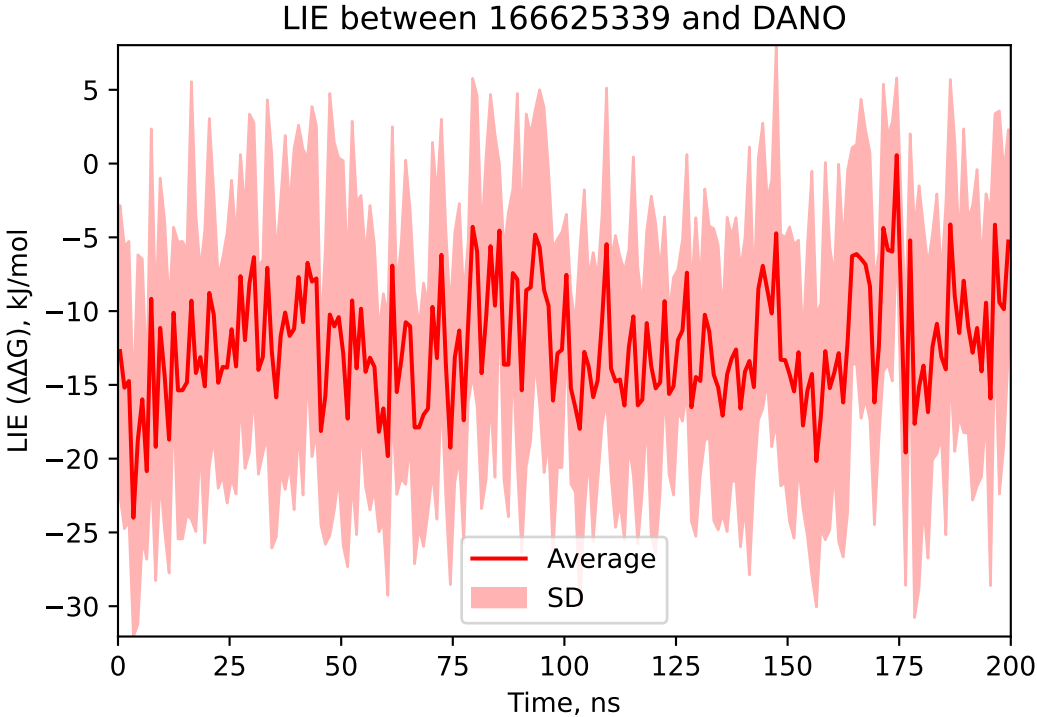

LIE between 155559627 and SPIR
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

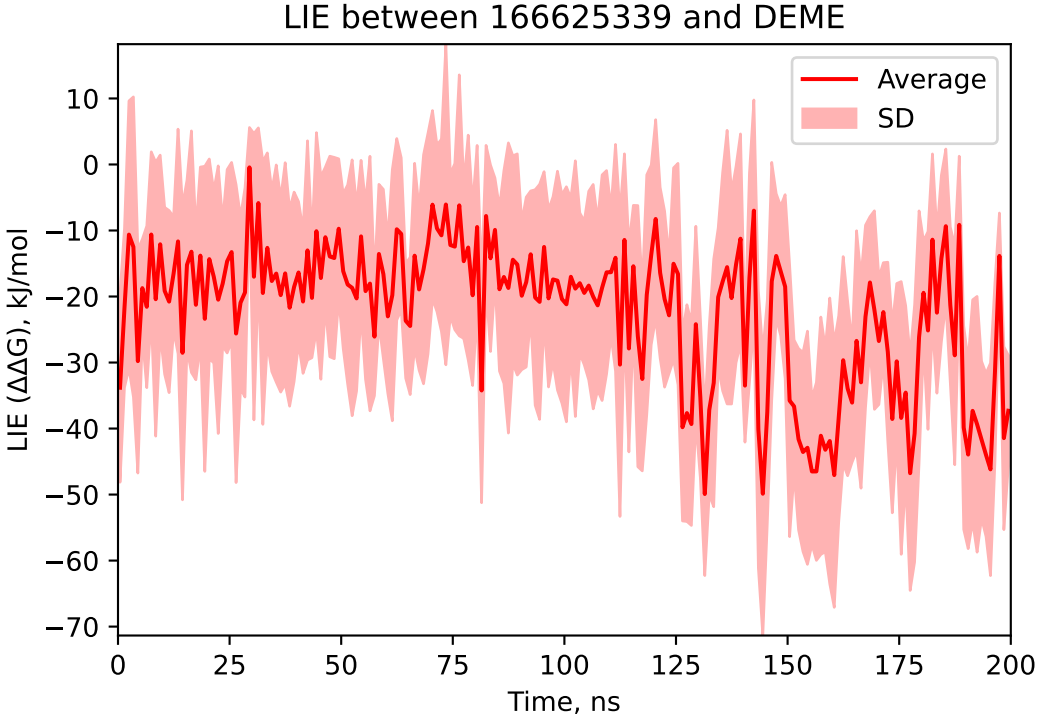

LIE between 155559627 and STRE
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
80
60
40
20
0
−20
−40
−60
−80
0
25
50
75
100
125
150
175
200

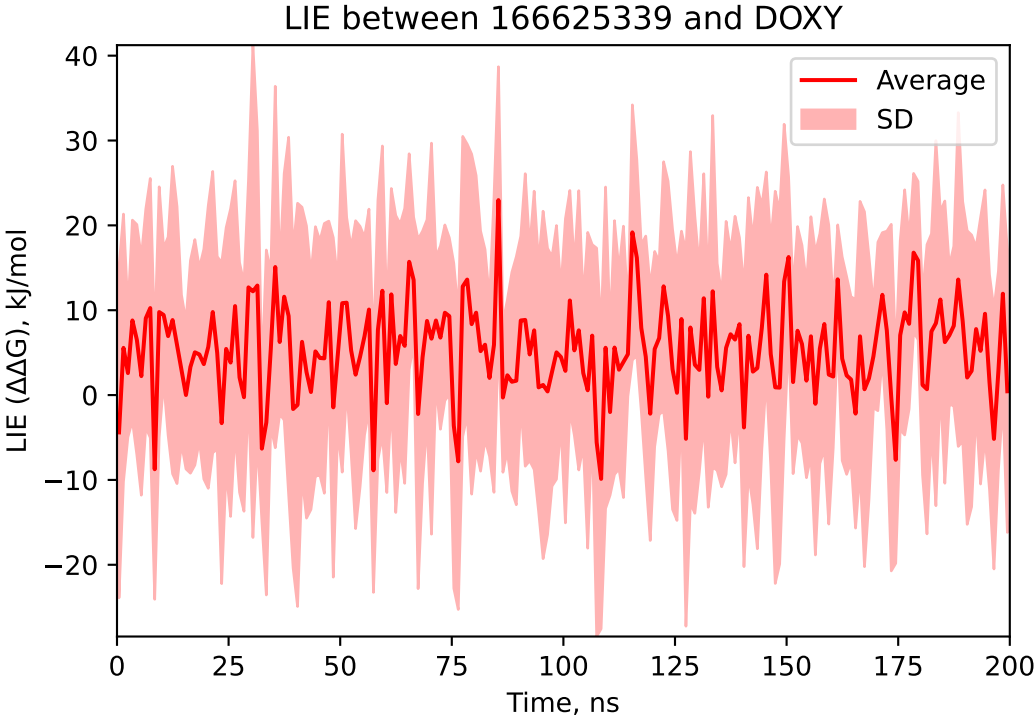

LIE between 155559627 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

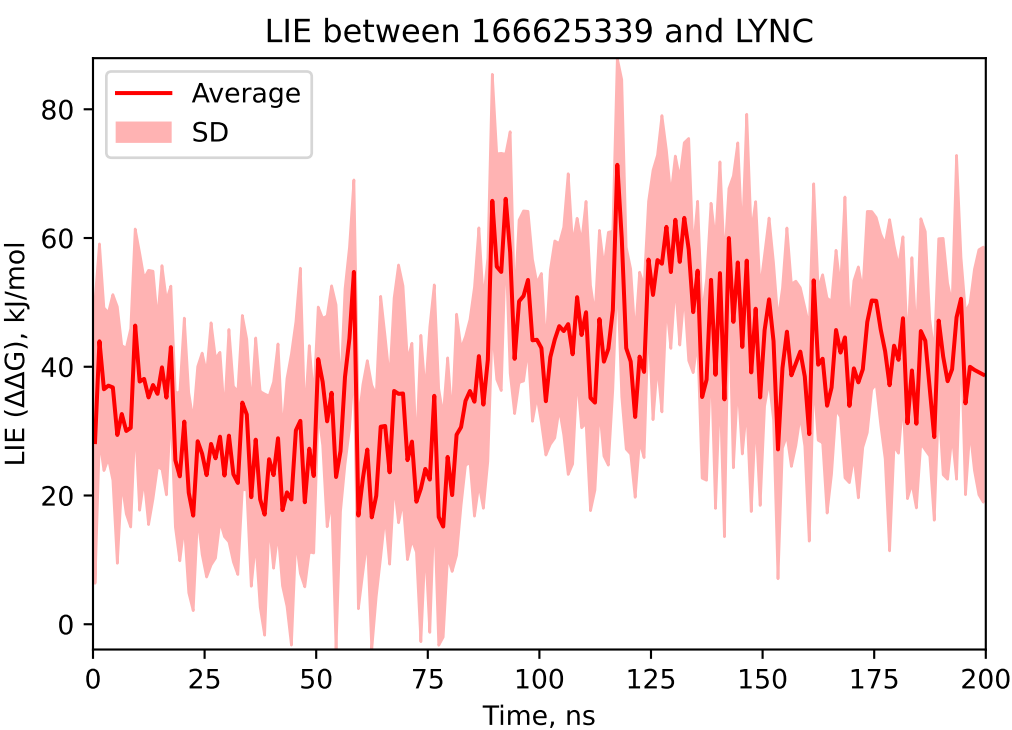

LIE between 155559627 and TIAM
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

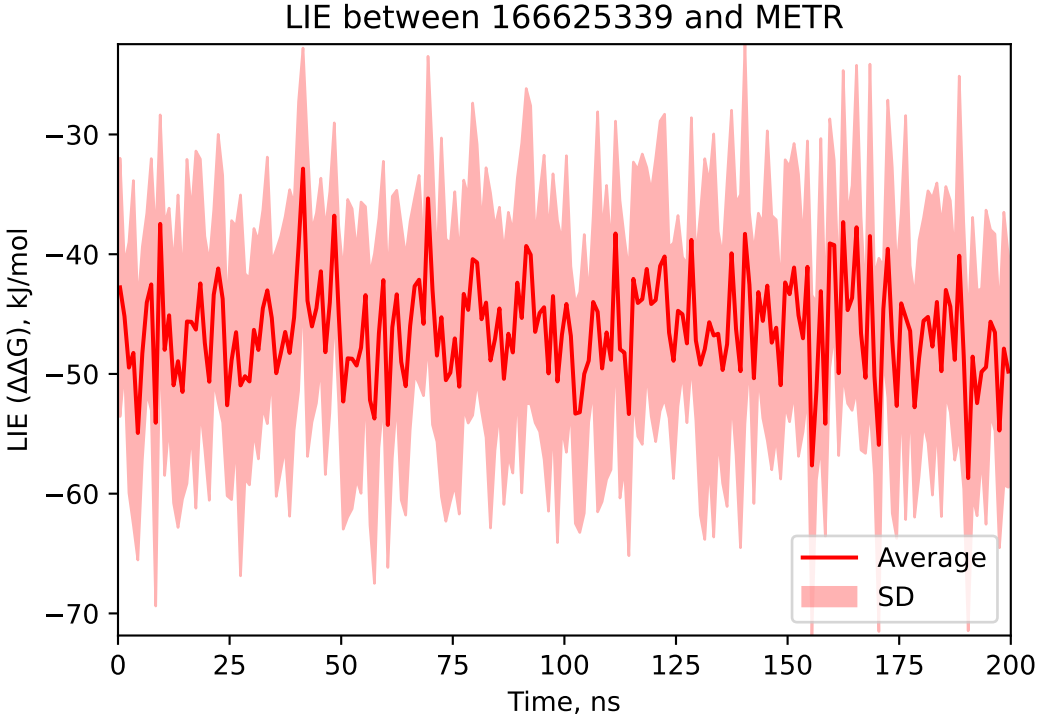

LIE between 155559627 and TILM
Average
SD
LIE (ΔΔG), kJ/mol
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns

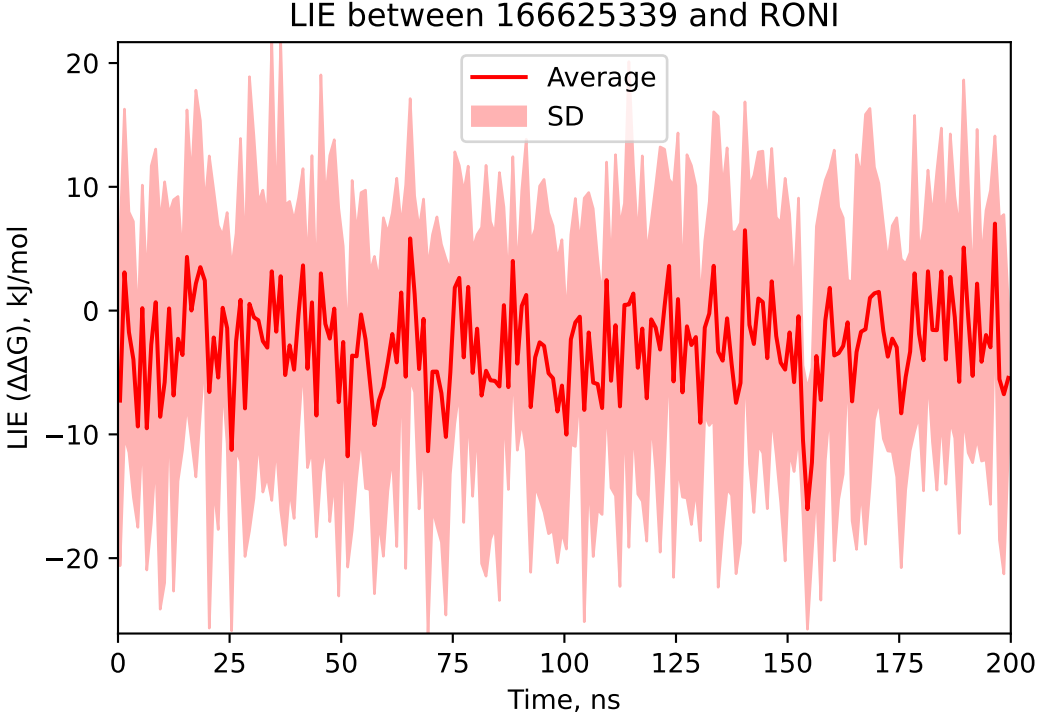

LIE between 166625339 and DANO
LIE (ΔΔG), kJ/mol
5
0
−5
−10
−15
−20
−25
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

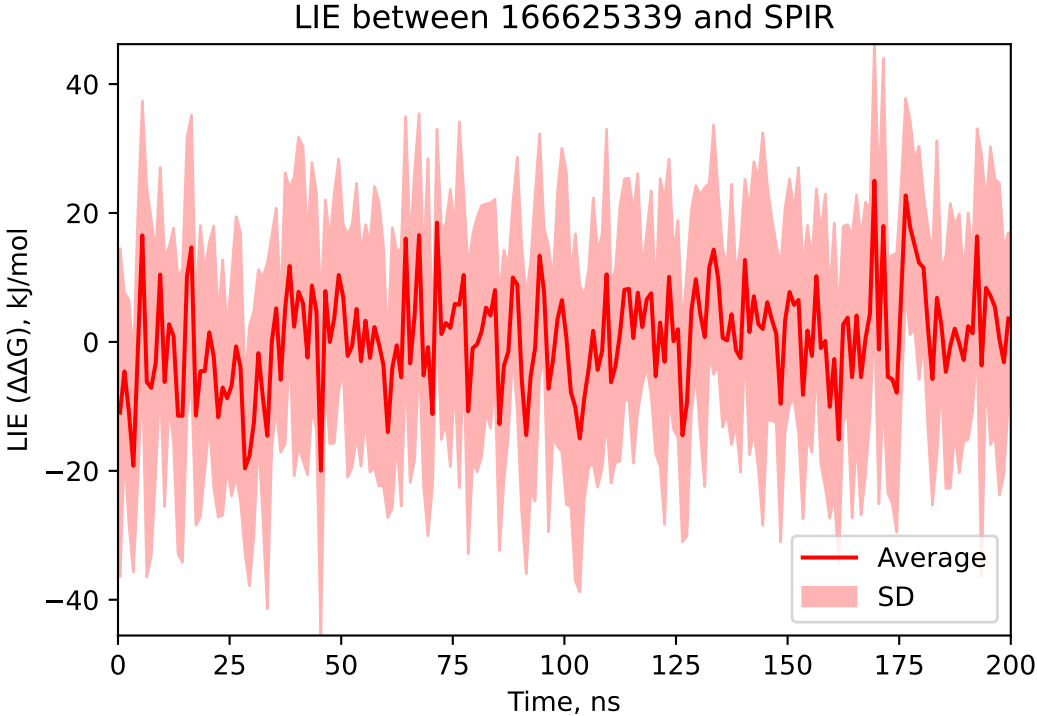

LIE between 166625339 and DEME
Average
SD
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
−40
−50
−60
−70
0
25
50
75
100
125
150
175
200
Time, ns

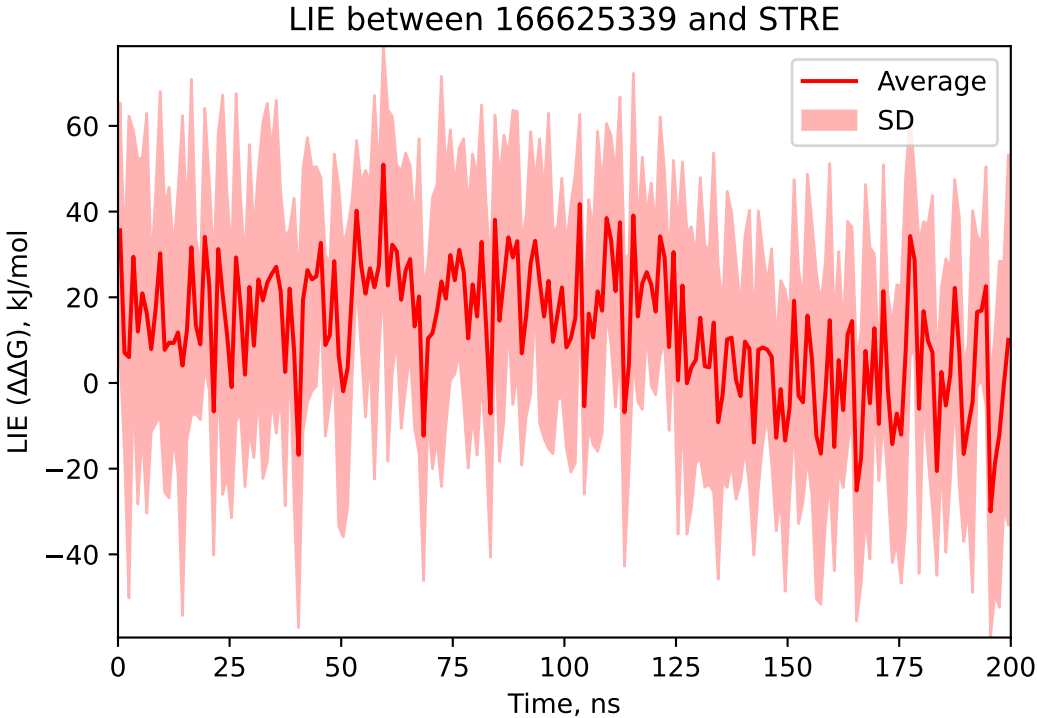

LIE between 166625339 and DOXY
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
40
30
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200

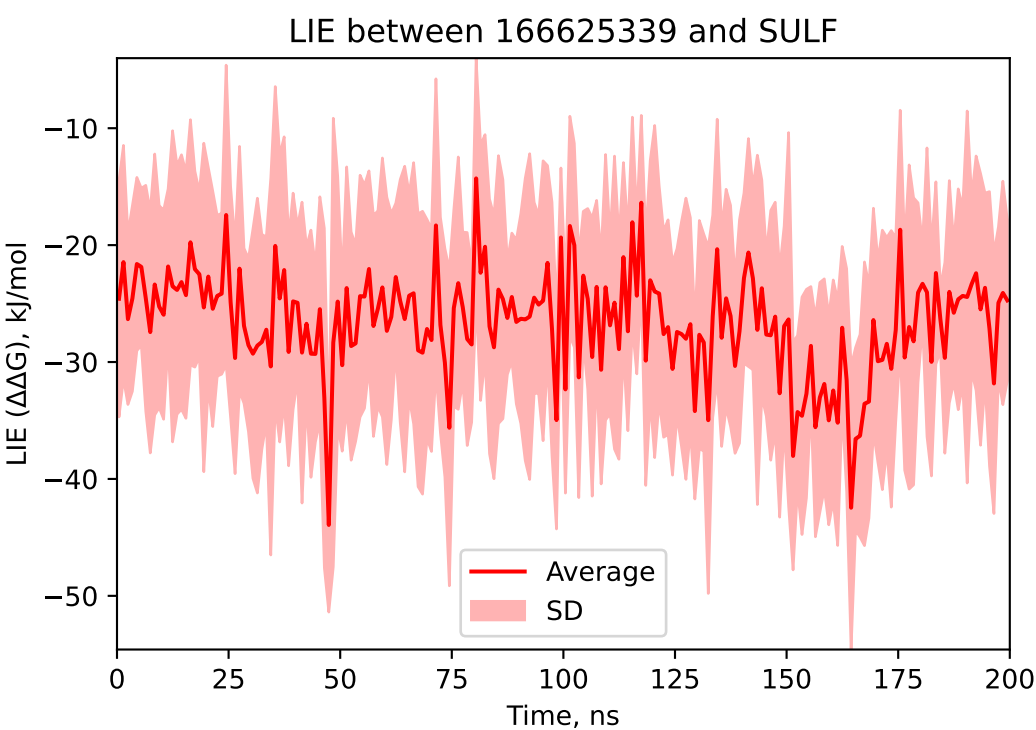

LIE between 166625339 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
0
20
40
60
80
0
25
50
75
100
125
150
175
200
Time, ns

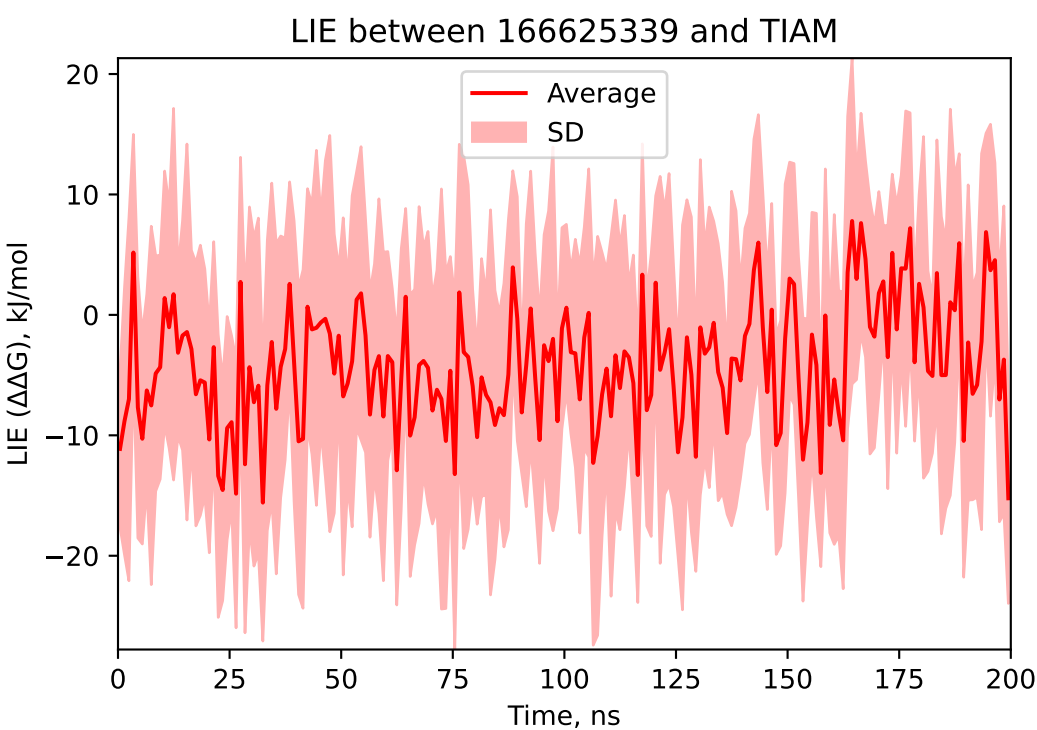

LIE between 166625339 and METR
LIE (ΔΔG), kJ/mol
−30
−40
−50
−60
−70
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

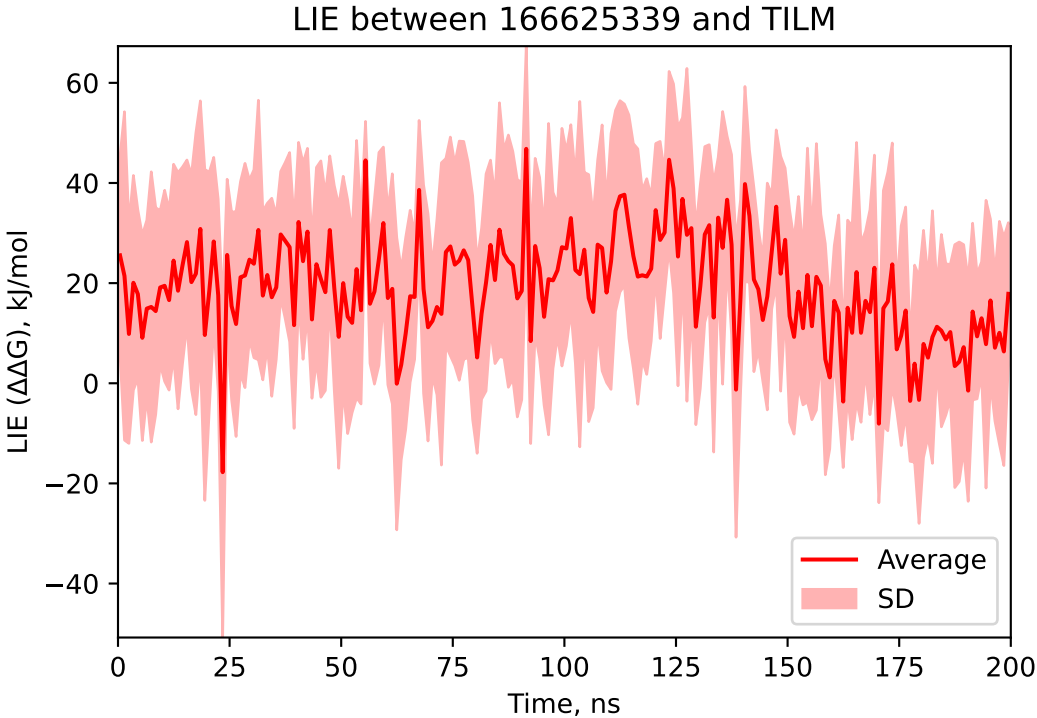

LIE between 166625339 and RONI
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200

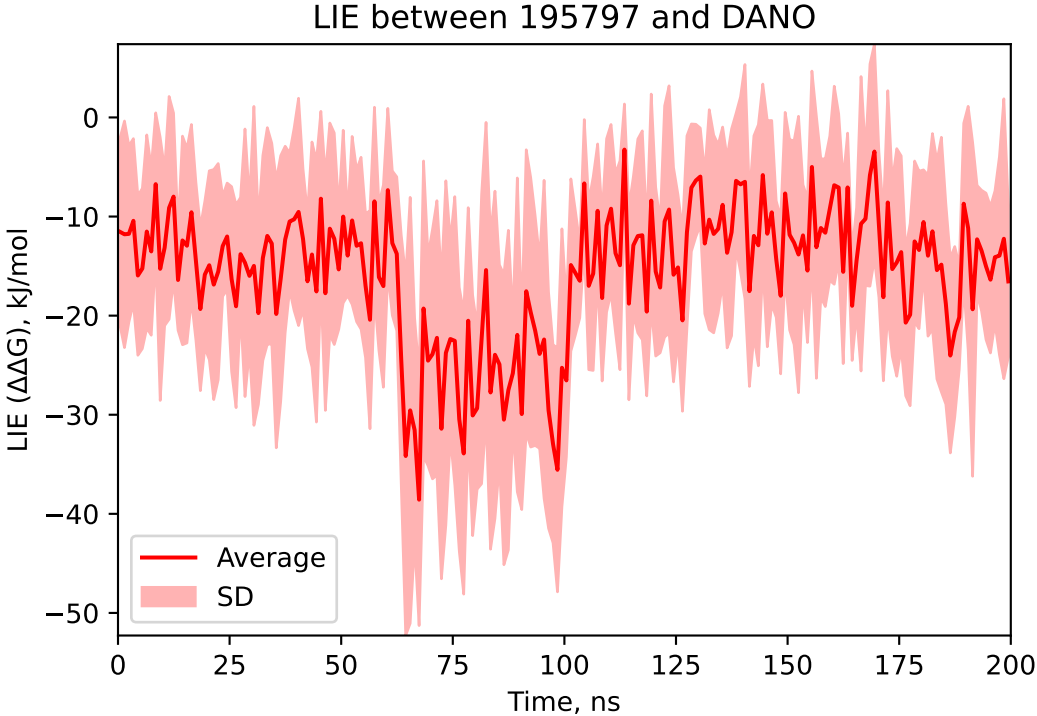

LIE between 166625339 and SPIR
LIE (ΔΔG), kJ/mol
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

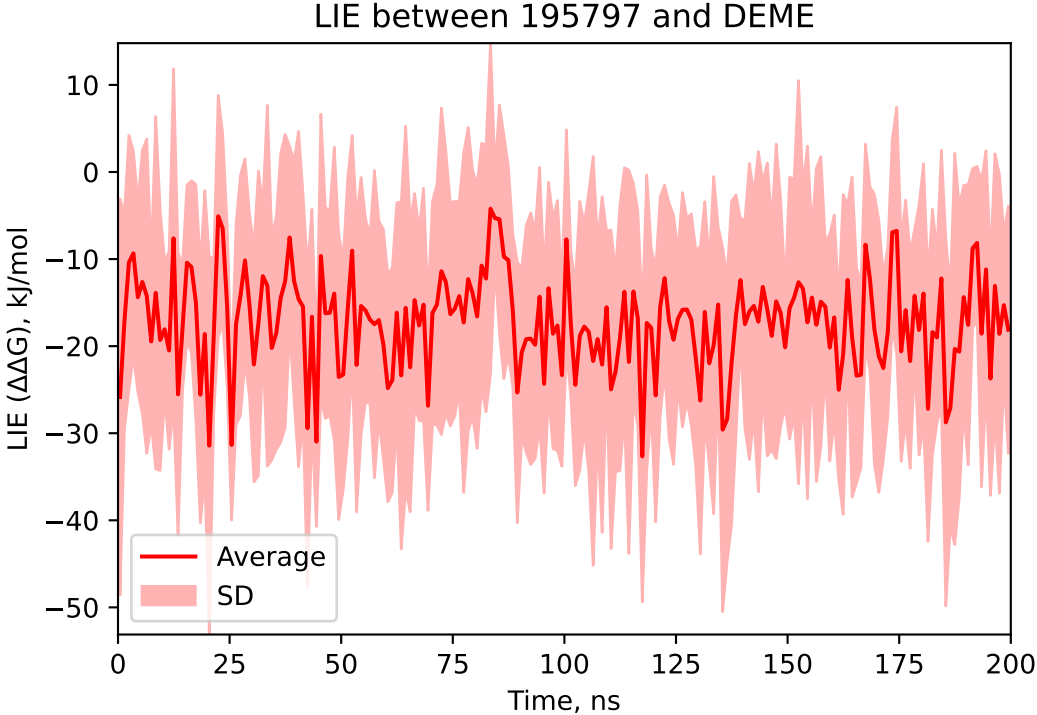

LIE between 166625339 and STRE
Average
SD
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns

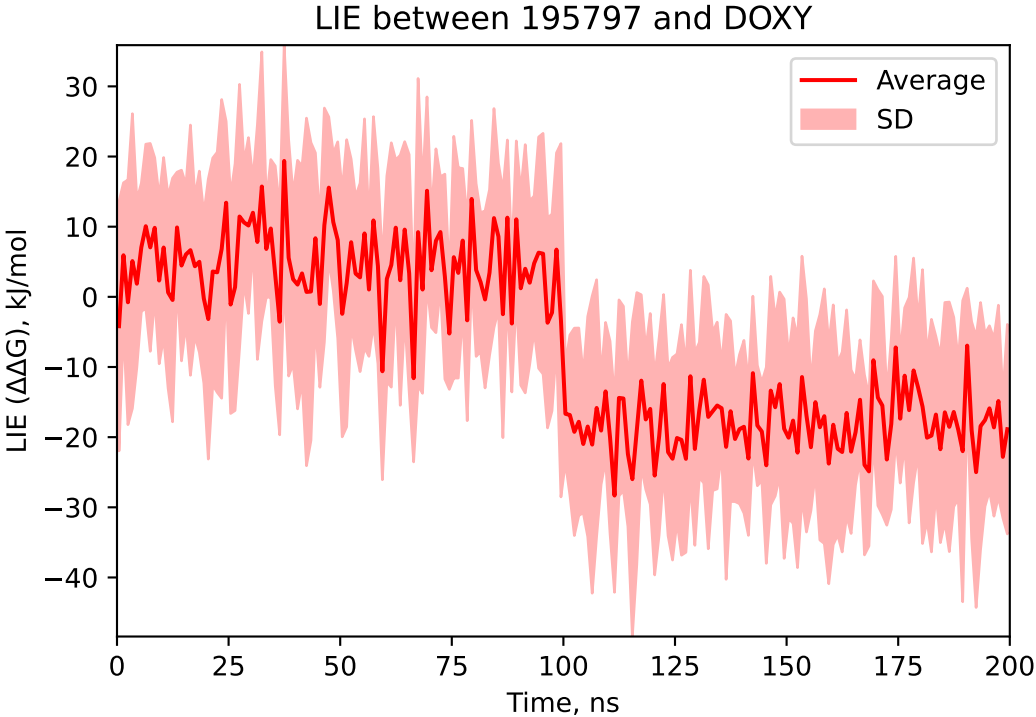

LIE between 166625339 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

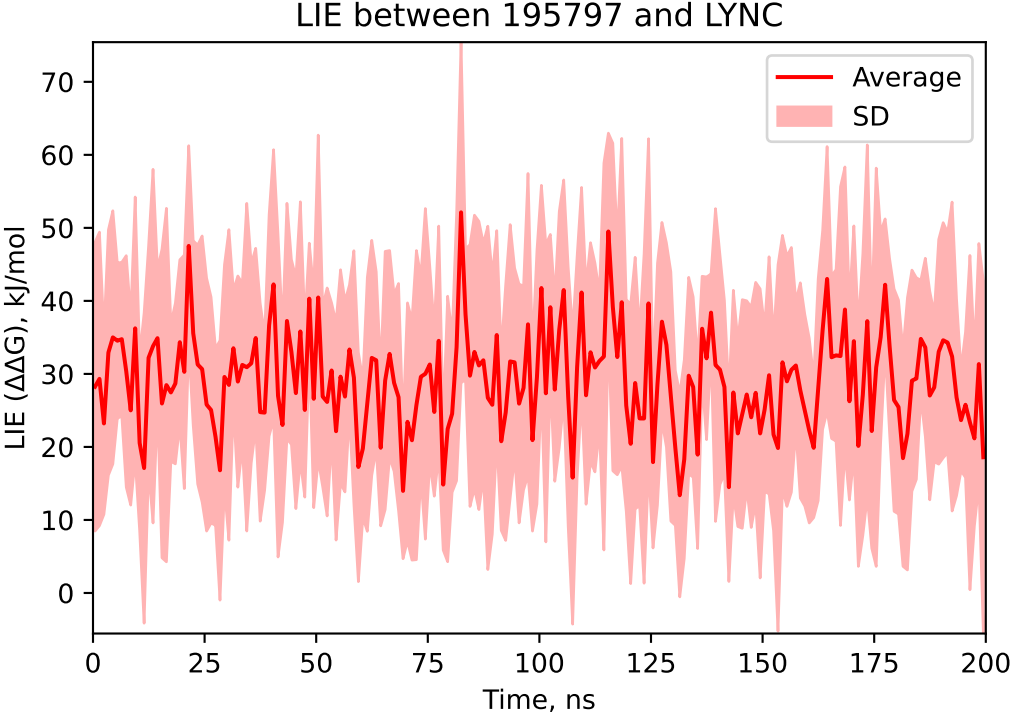

LIE between 166625339 and TIAM
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200

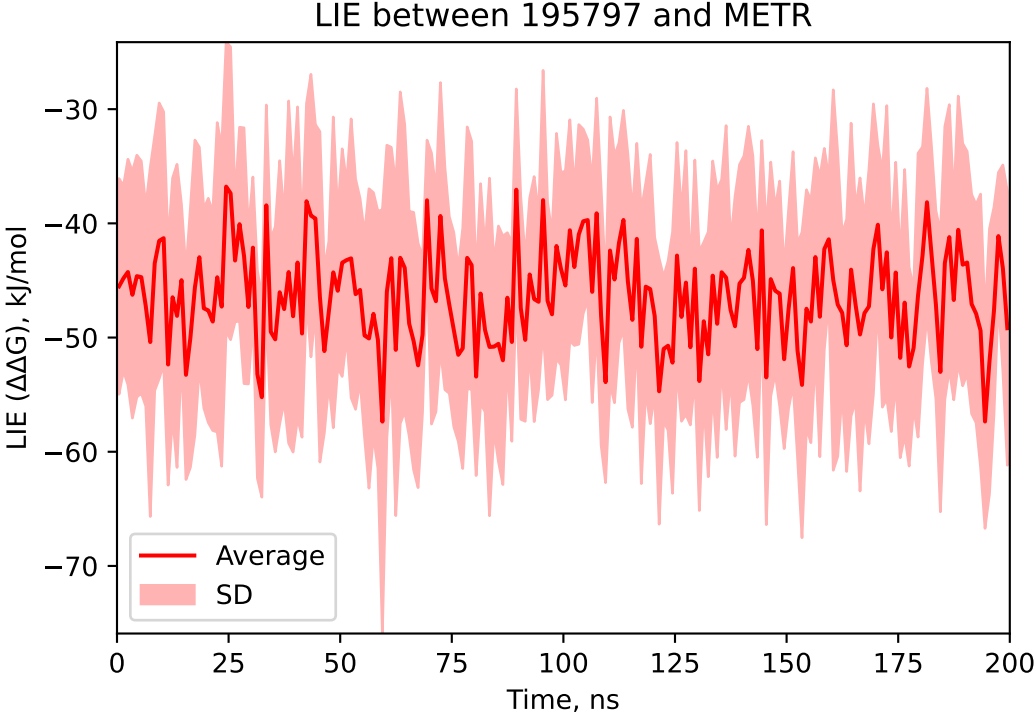

LIE between 166625339 and TILM
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

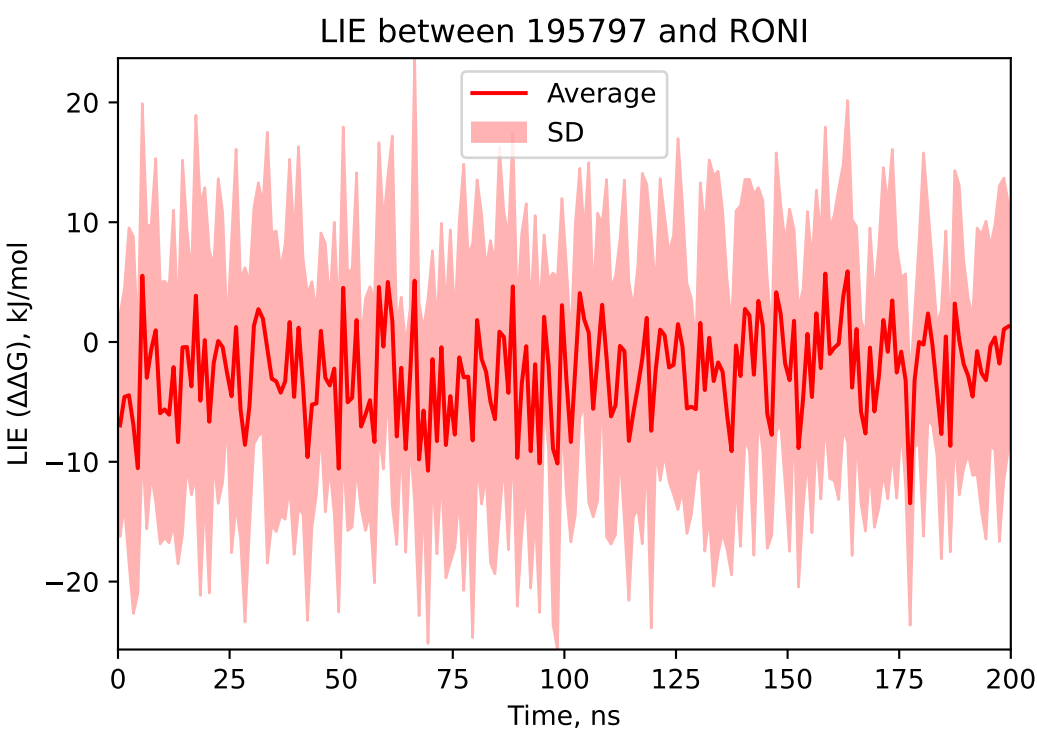

LIE between 195797 and DANO
LIE (ΔΔG), kJ/mol
0
−10
−20
−30
−40
−50
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

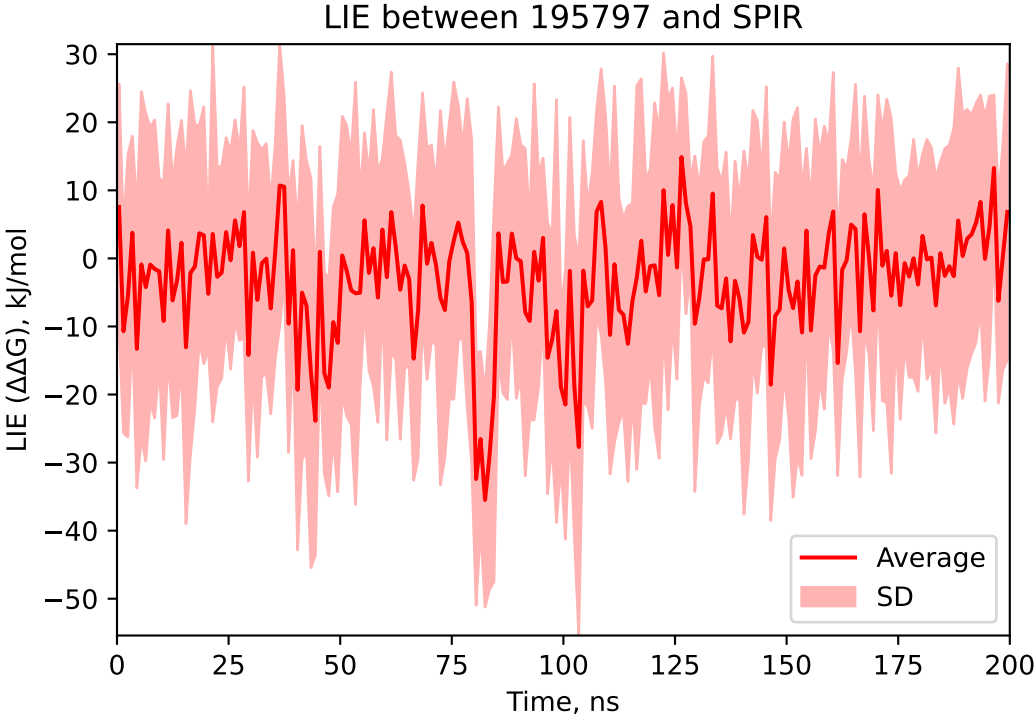

LIE between 195797 and DEME
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
−40
−50
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

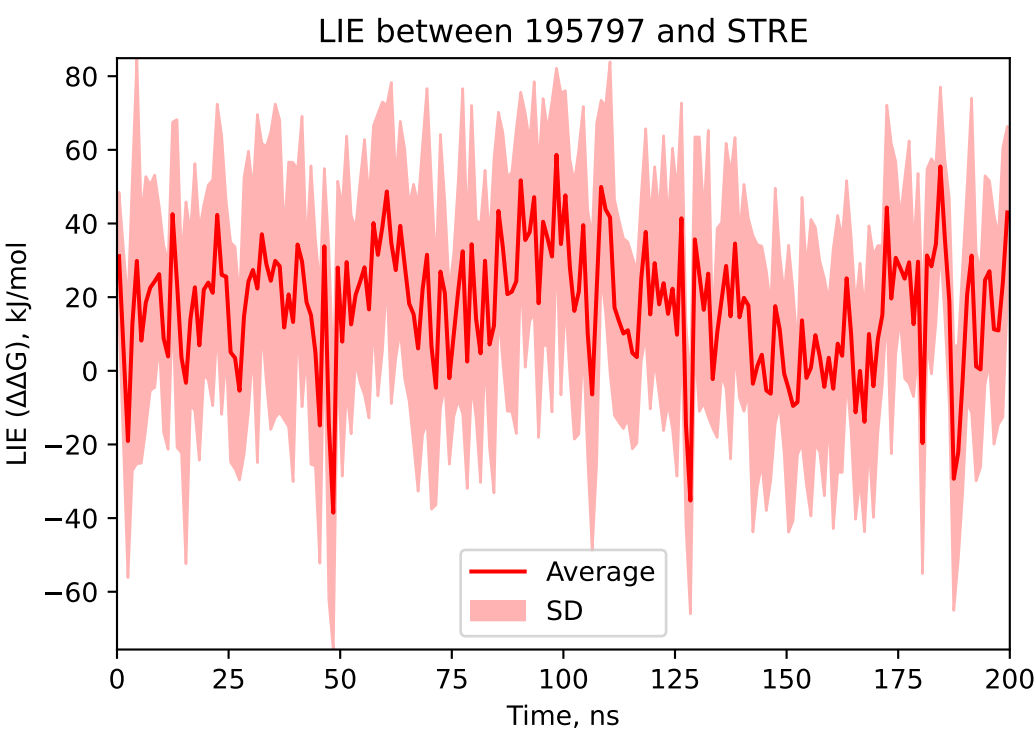

LIE between 195797 and DOXY
Average
SD
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns

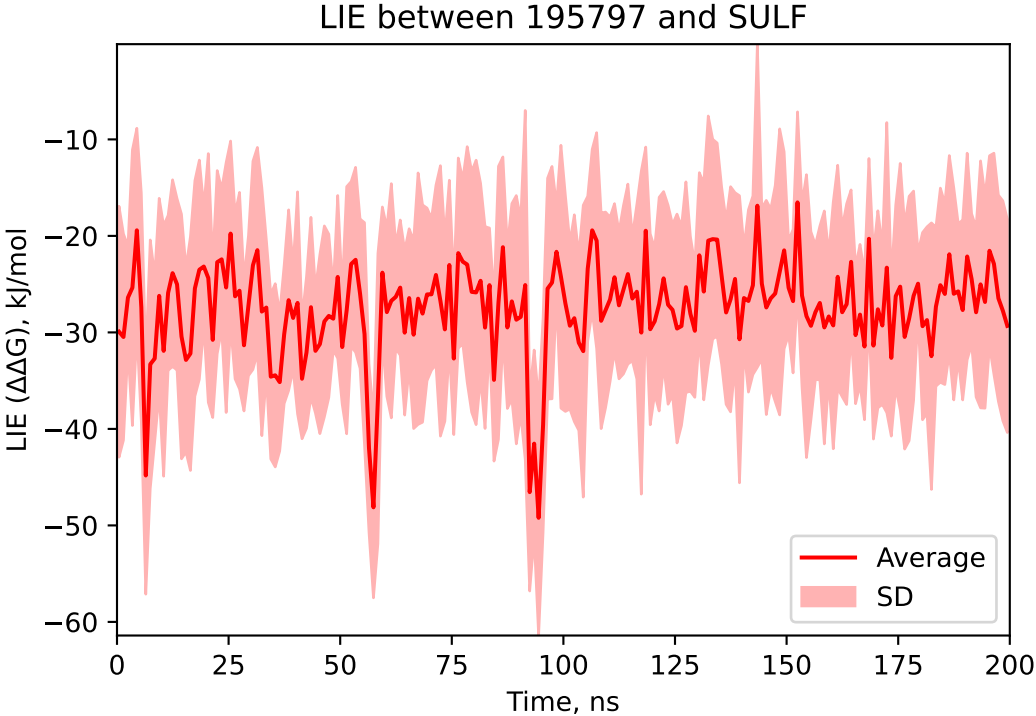

LIE between 195797 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
70
60
50
40
30
20
10
0
0
25
50
75
100
125
150
175
200
Time, ns

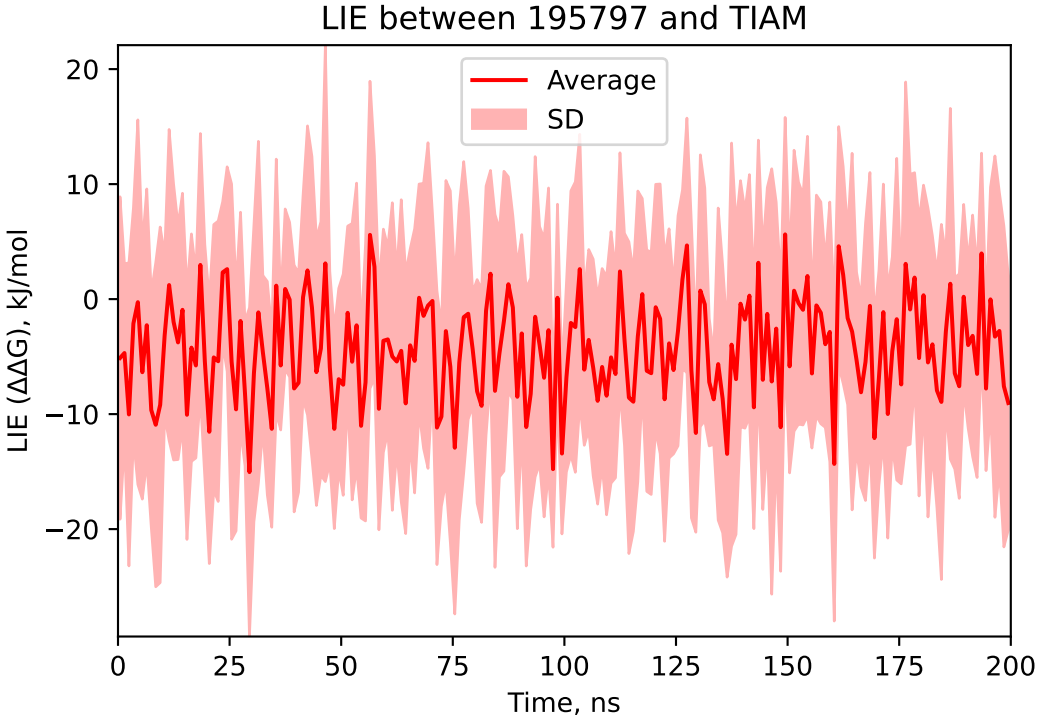

LIE between 195797 and METR
LIE (ΔΔG), kJ/mol
−30
−40
−50
−60
−70
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

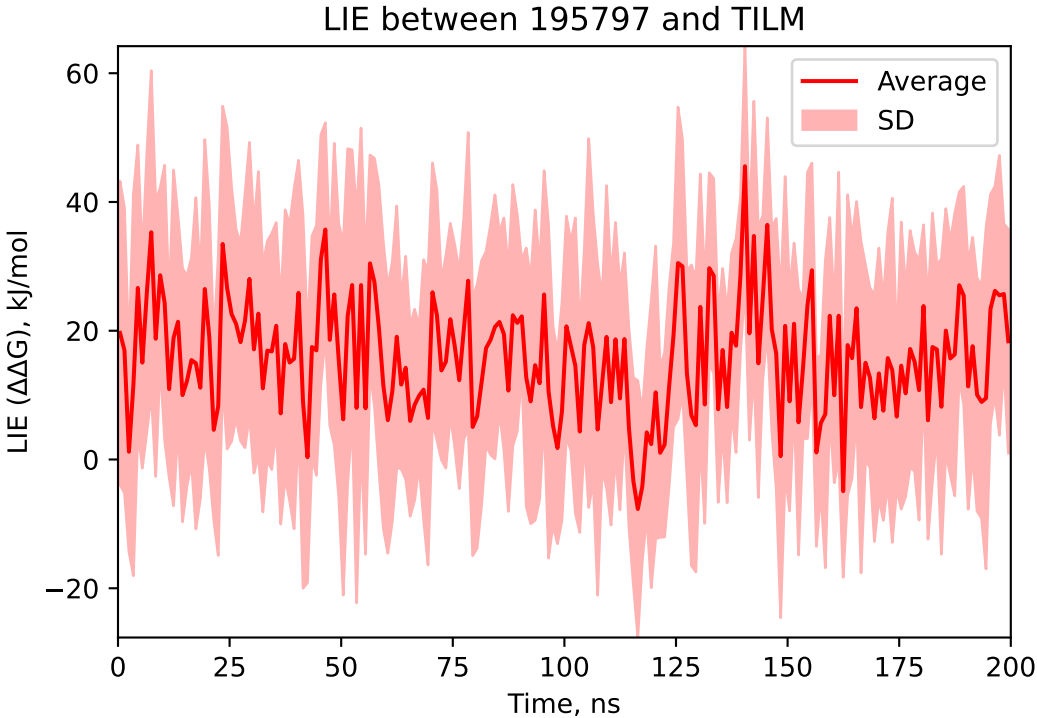

LIE between 195797 and RONI
Average
SD
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns

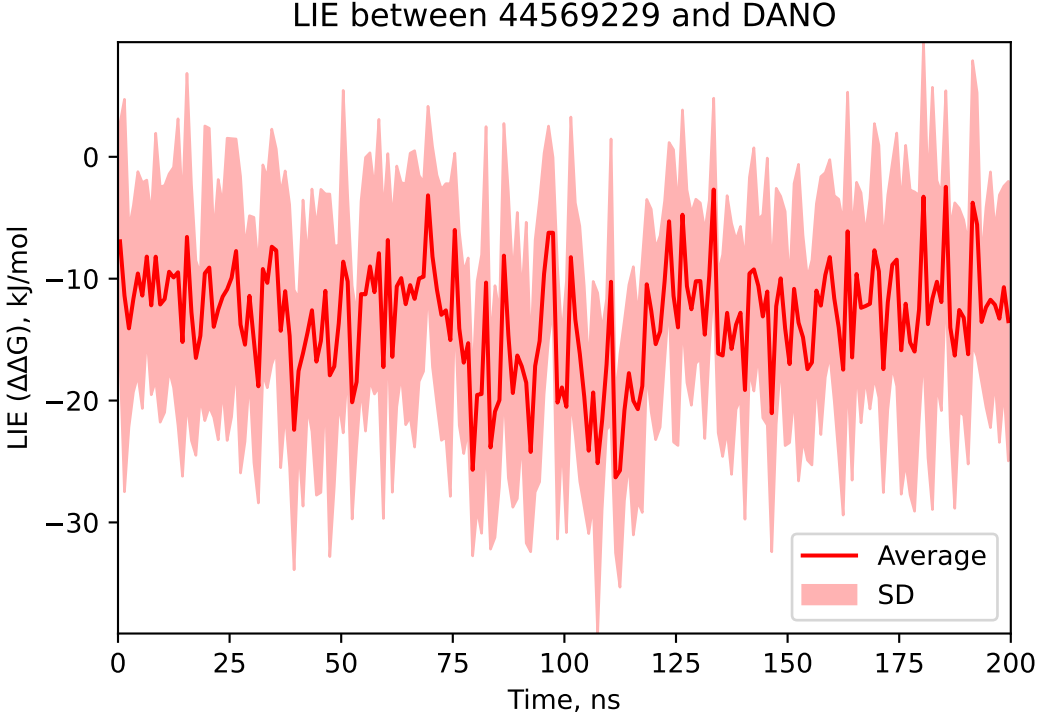

LIE between 195797 and SPIR
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

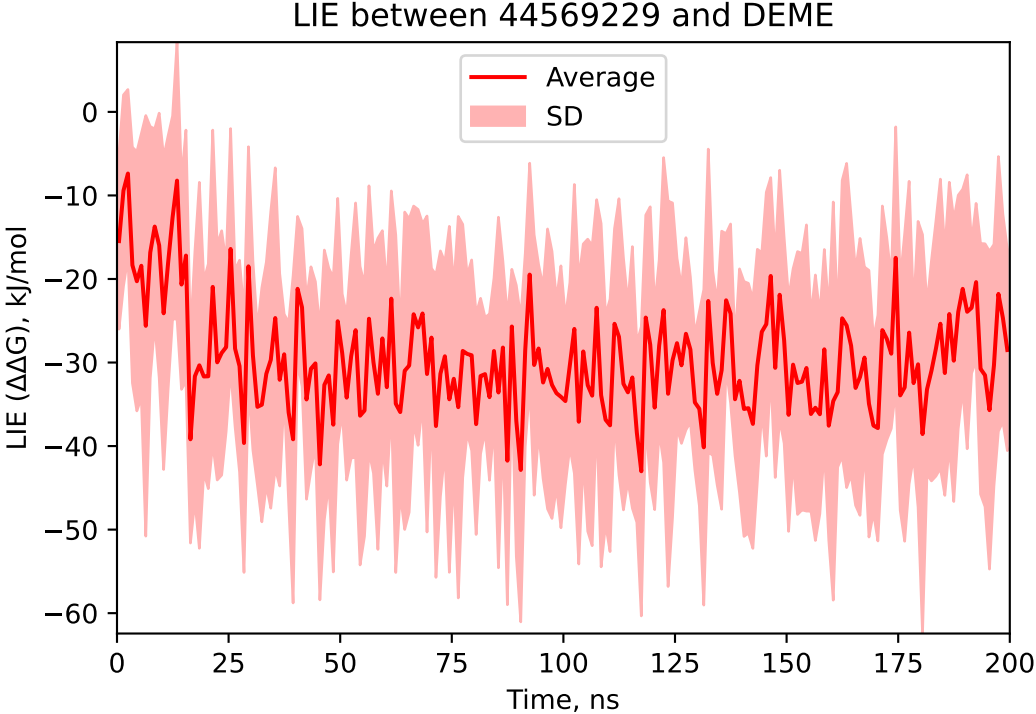

LIE between 195797 and STRE
LIE (ΔΔG), kJ/mol
80
60
40
20
0
−20
−40
−60
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

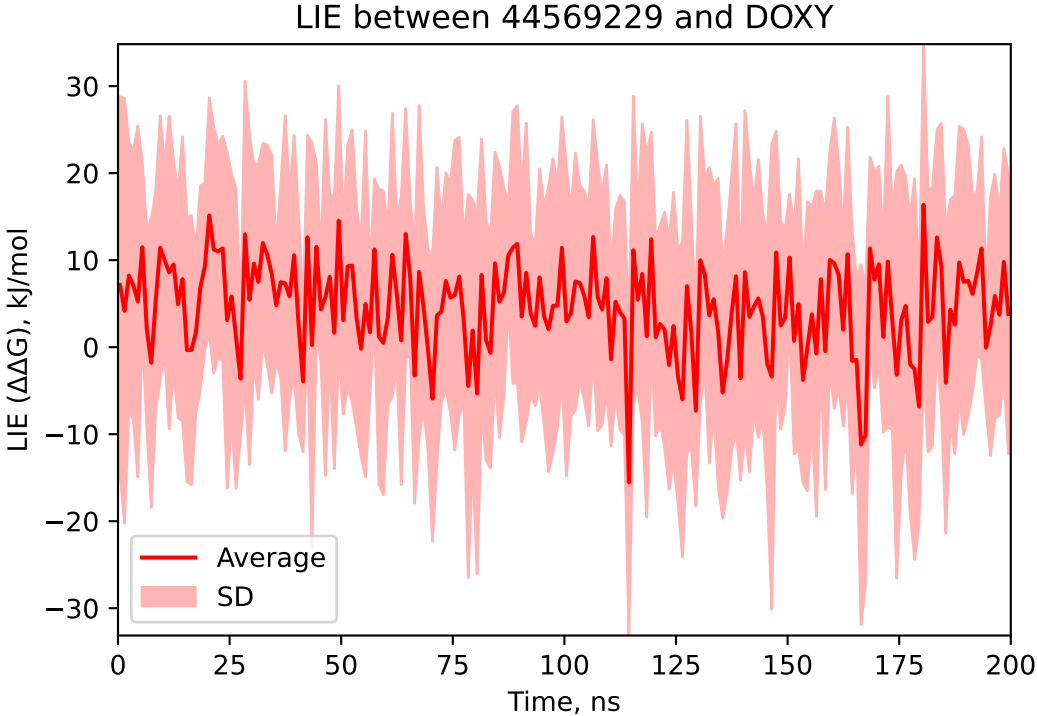

LIE between 195797 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
−60
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

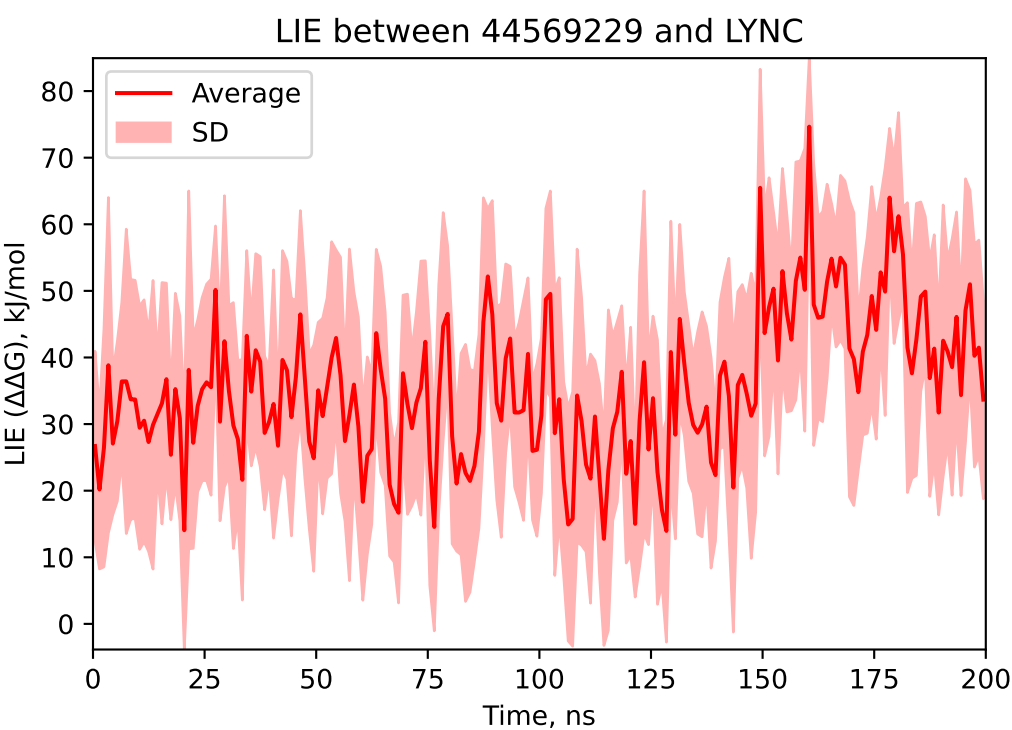

LIE between 195797 and TIAM
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200

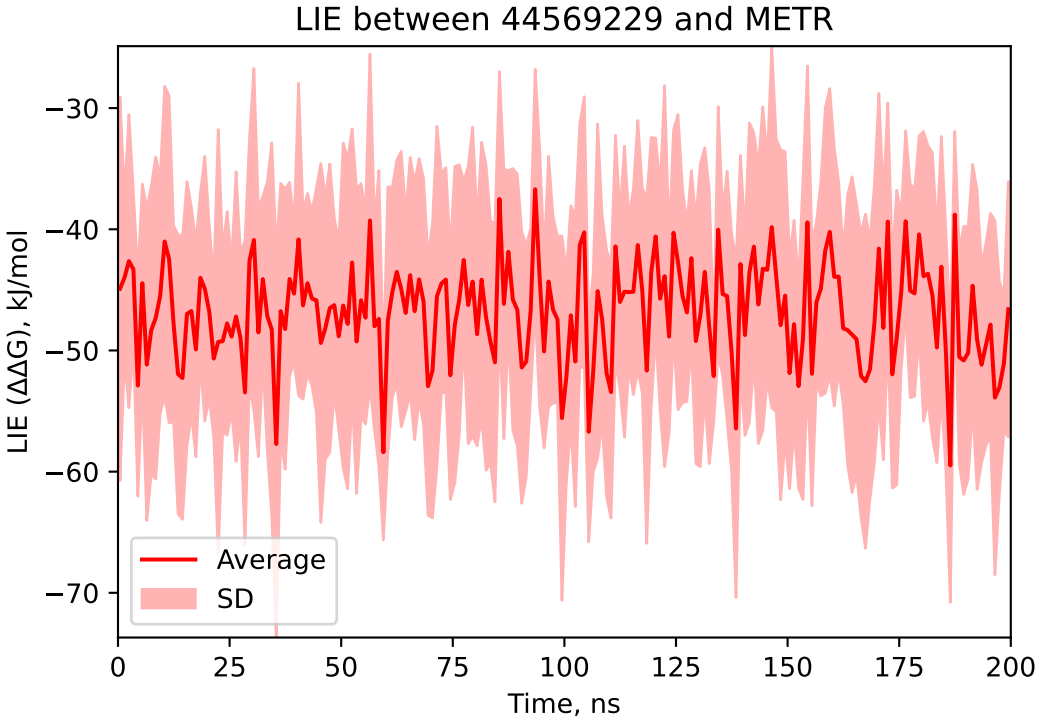

LIE between 195797 and TILM
Average
SD
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
0
25
50
75
100
125
150
175
200
Time, ns

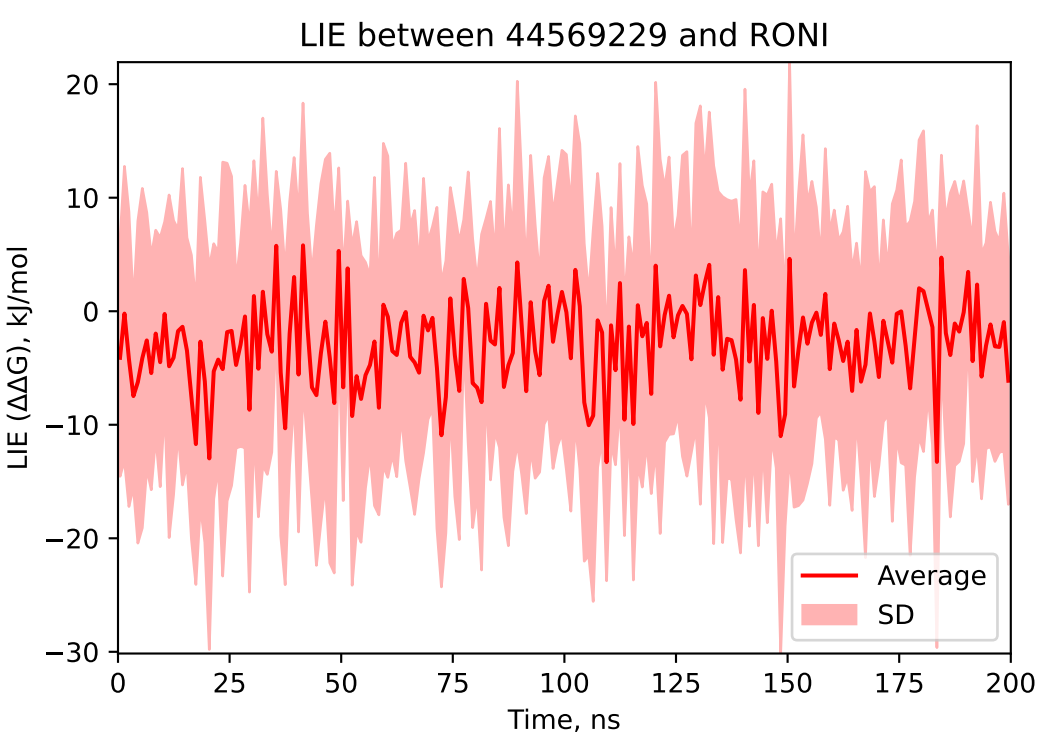

LIE between 44569229 and DANO
LIE (ΔΔG), kJ/mol
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

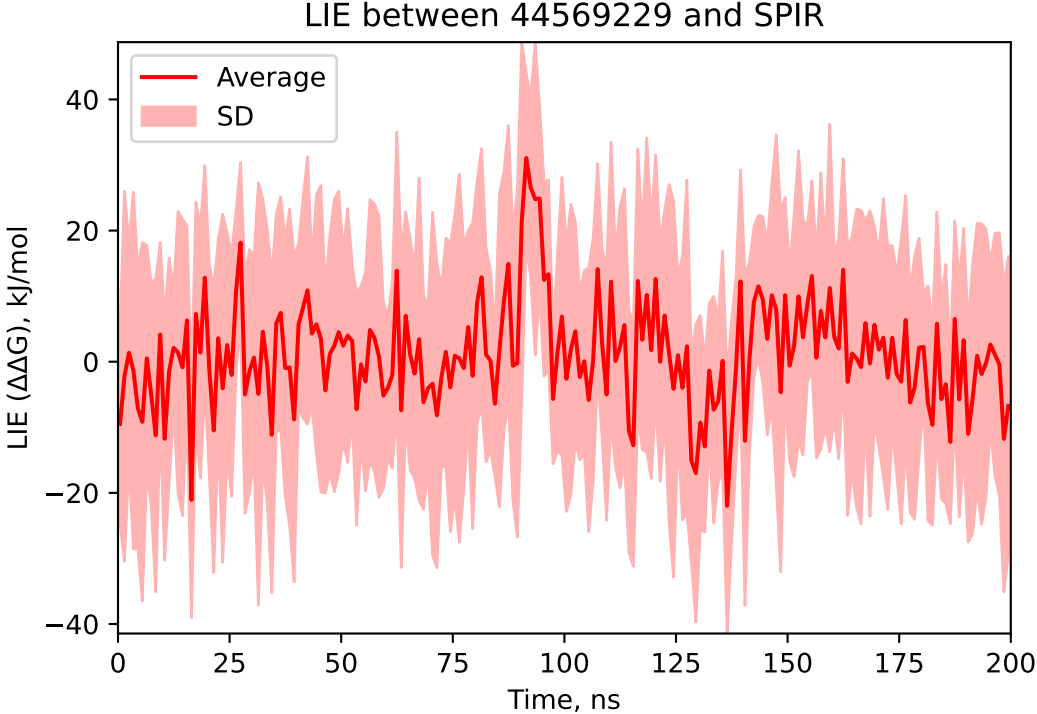

LIE between 44569229 and DEME
Average
SD
LIE (ΔΔG), kJ/mol
0
−10
−20
−30
−40
−50
−60
0
25
50
75
100
125
150
175
200
Time, ns

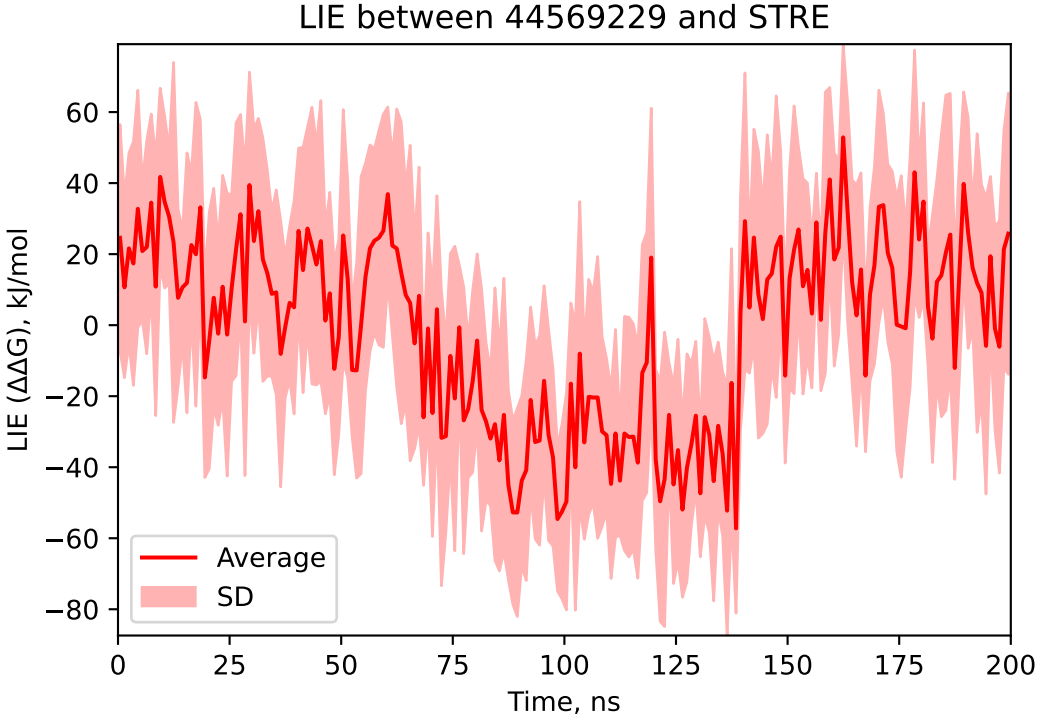

LIE between 44569229 and DOXY
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

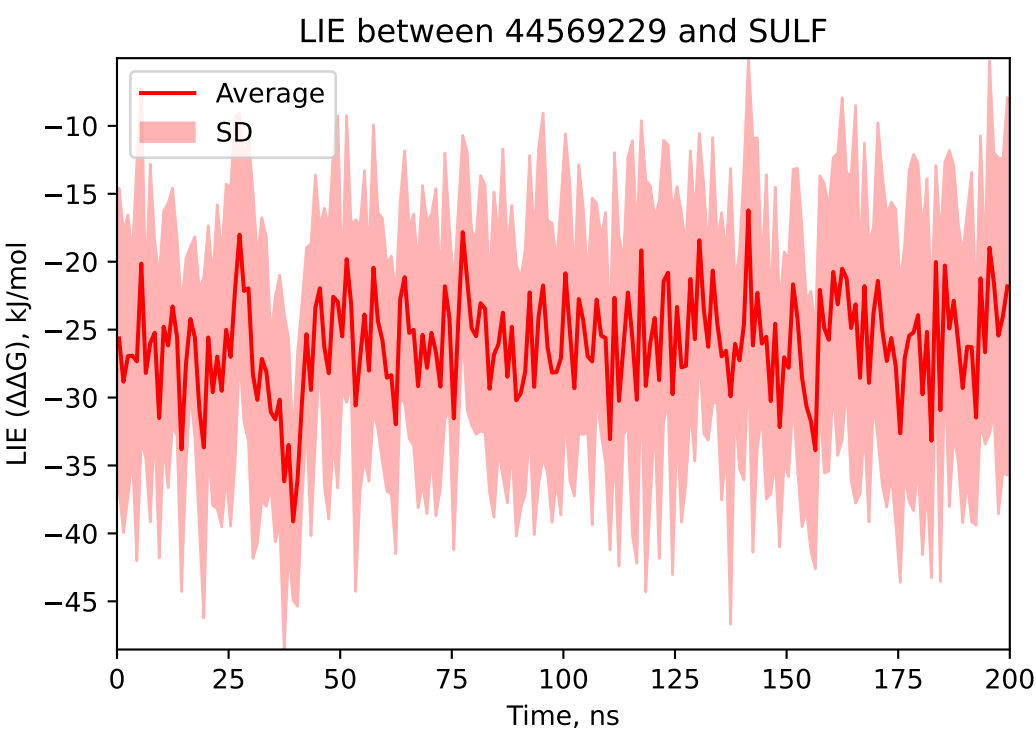

LIE between 44569229 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
0
10
20
30
40
50
60
70
80
0
25
50
75
100
125
150
175
200

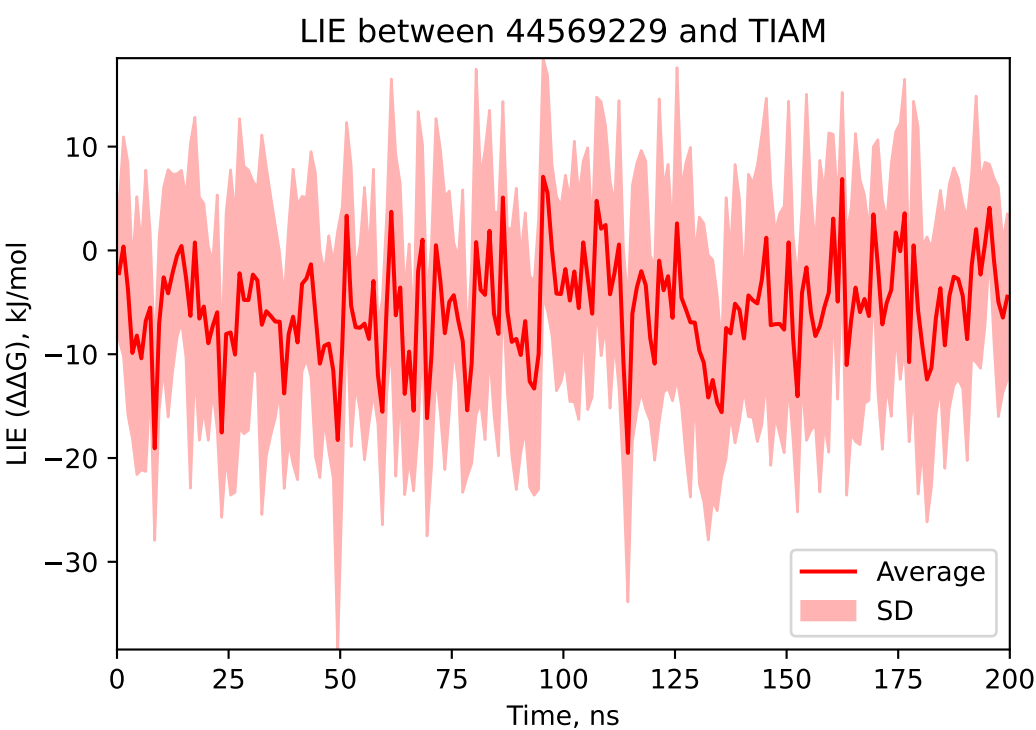

LIE between 44569229 and METR
LIE (ΔΔG), kJ/mol
−30
−40
−50
−60
−70
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

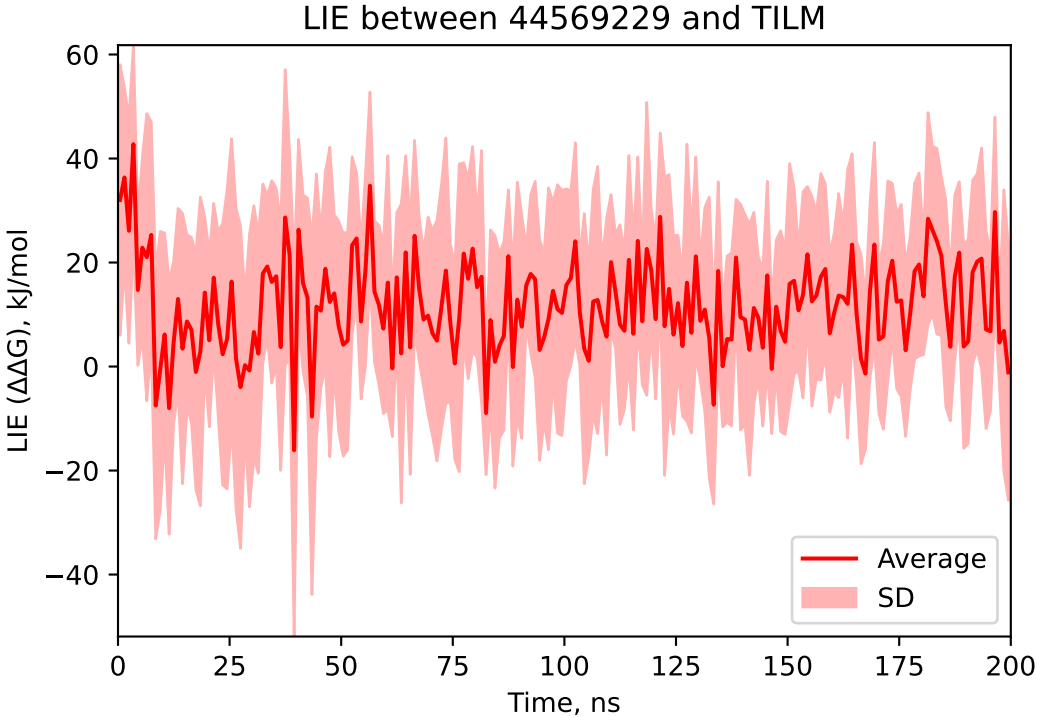

LIE between 44569229 and RONI
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200

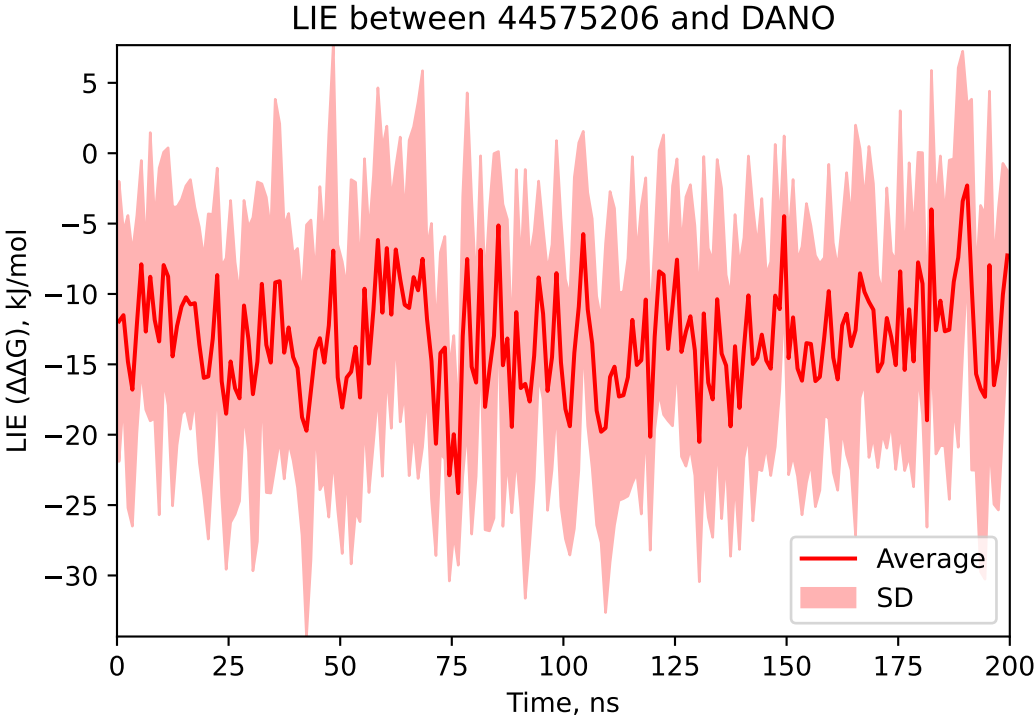

LIE between 44569229 and SPIR
Average
SD
LIE (ΔΔG), kJ/mol
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns

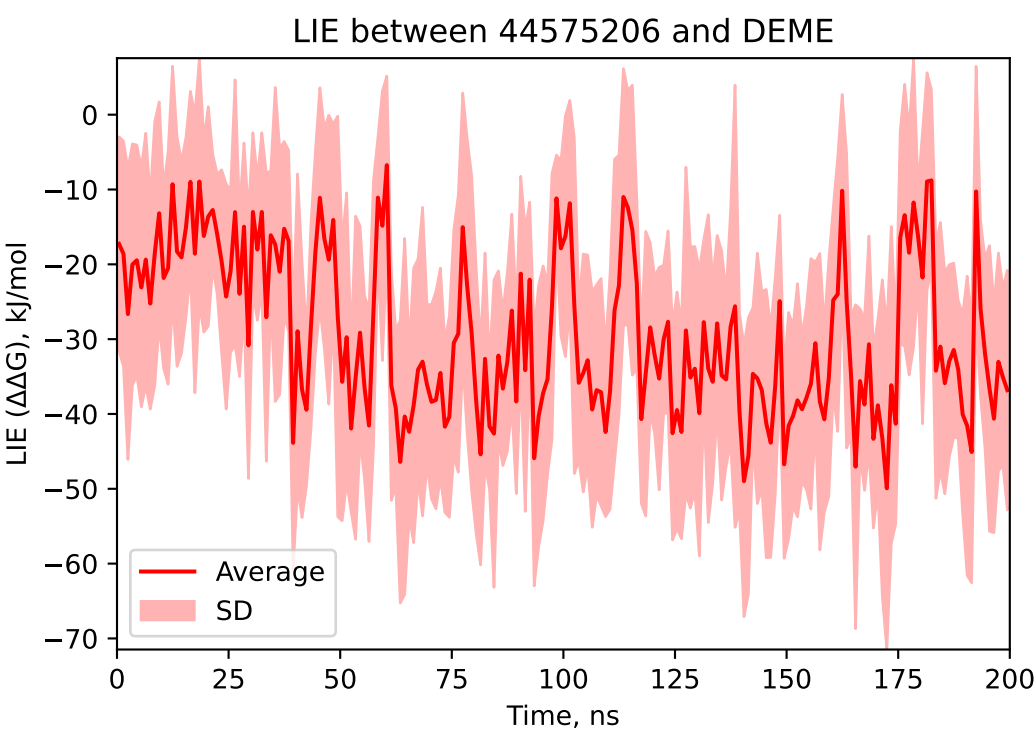

LIE between 44569229 and STRE
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
−40
−60
−80
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

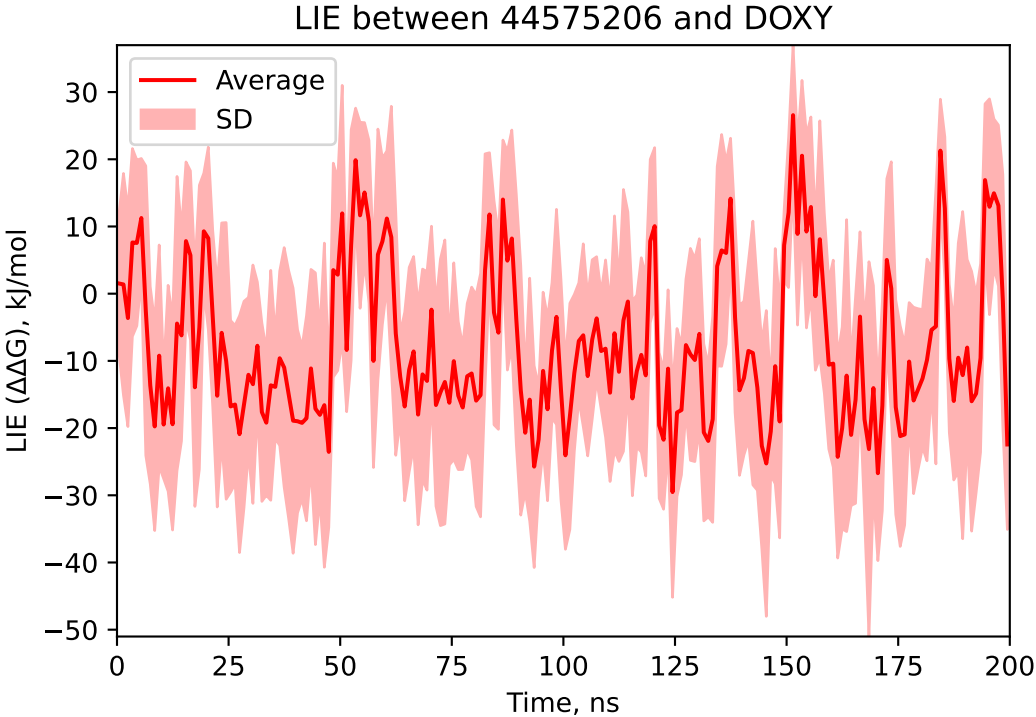

LIE between 44569229 and SULF
Average
SD
LIE (ΔΔG), kJ/mol
−10
−15
−20
−25
−30
−35
−40
−45
0
25
50
75
100
125
150
175
200
Time, ns

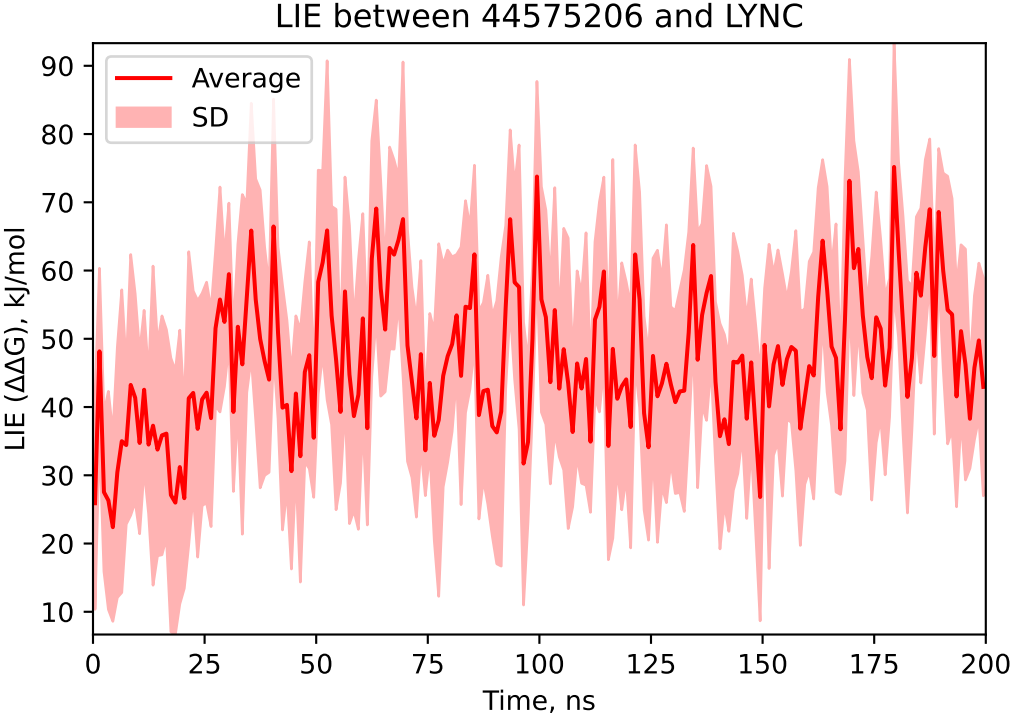

LIE between 44569229 and TIAM
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

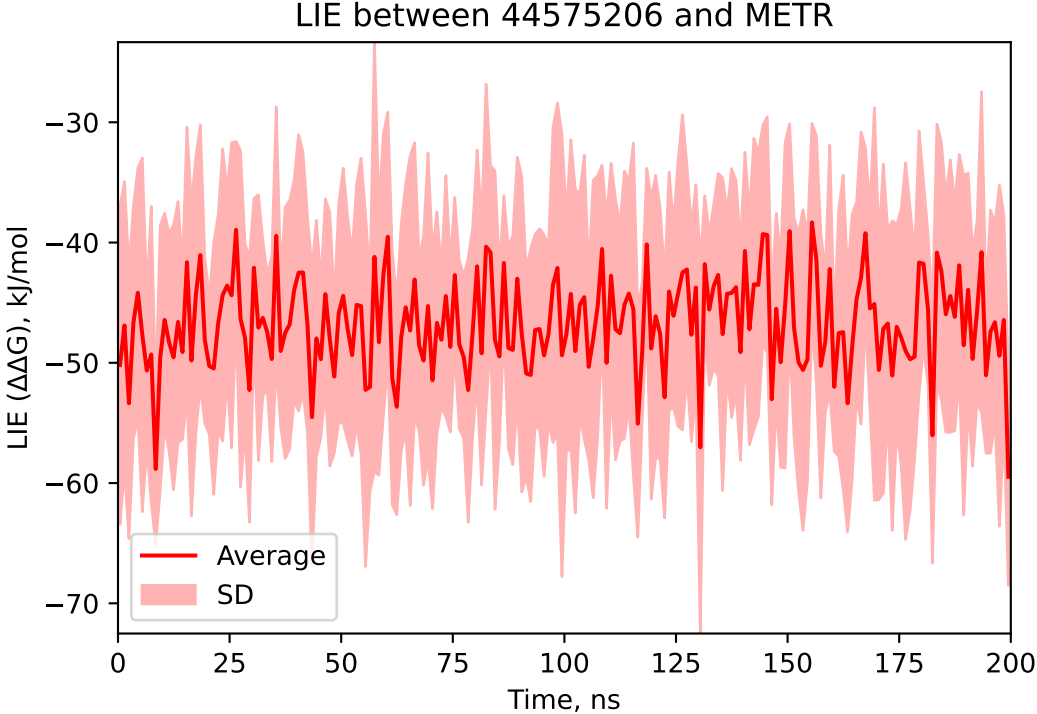

LIE between 44569229 and TILM
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

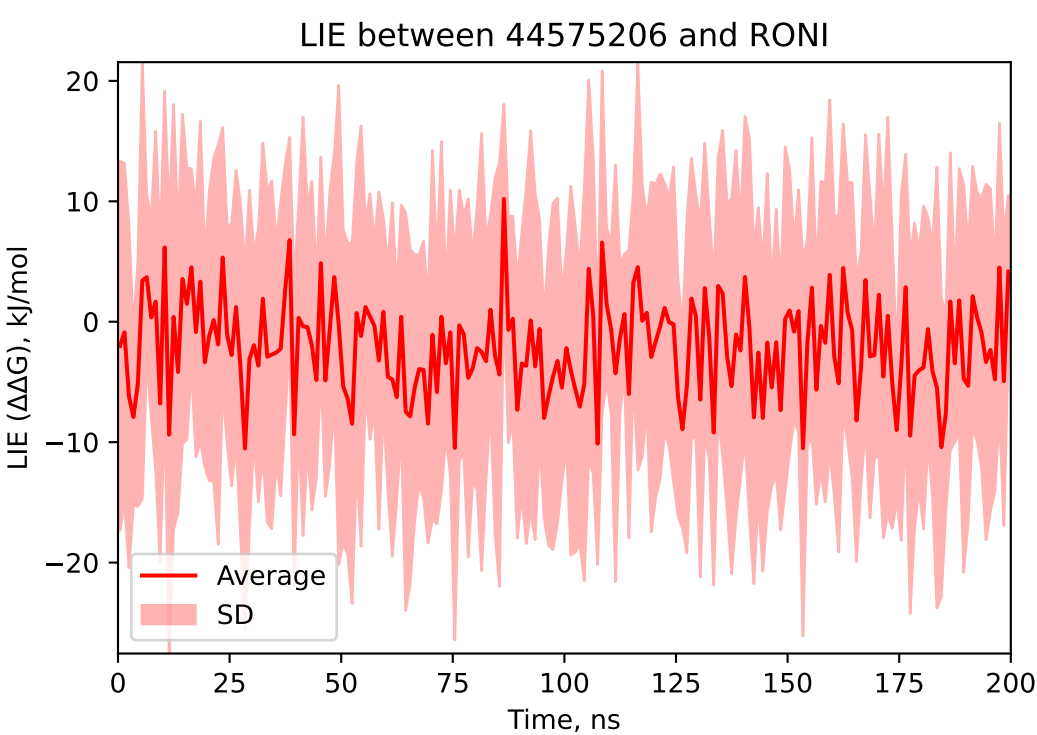

LIE between 44575206 and DANO
LIE (ΔΔG), kJ/mol
5
0
−5
−10
−15
−20
−25
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

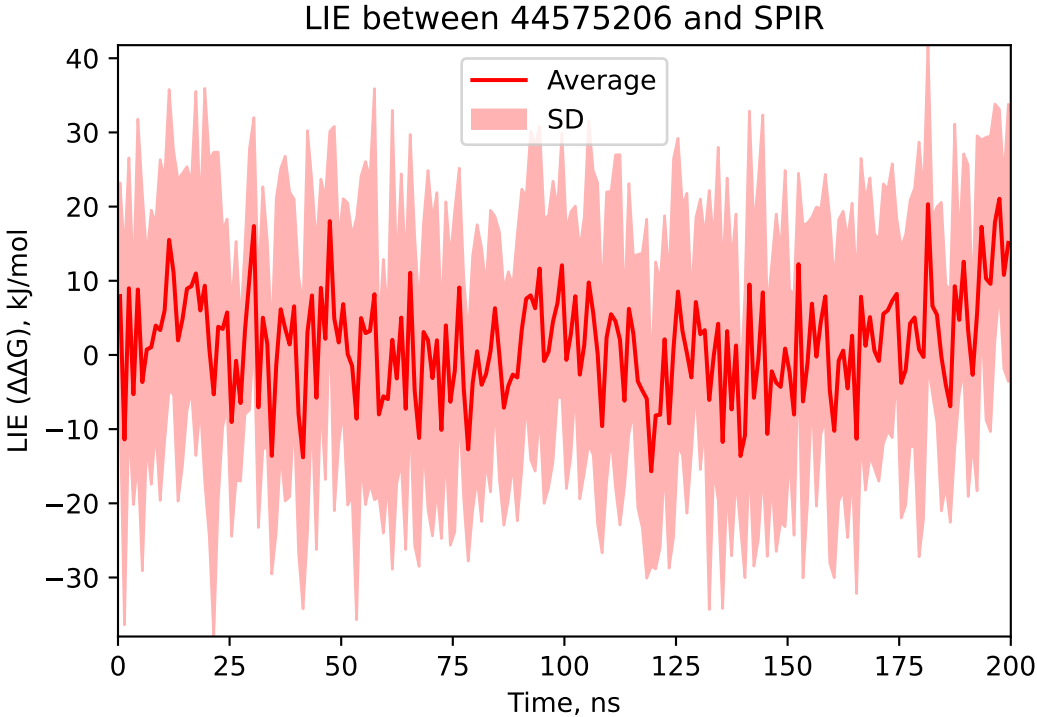

LIE between 44575206 and DEME
LIE (ΔΔG), kJ/mol
0
−10
−20
−30
−40
−50
−60
−70
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

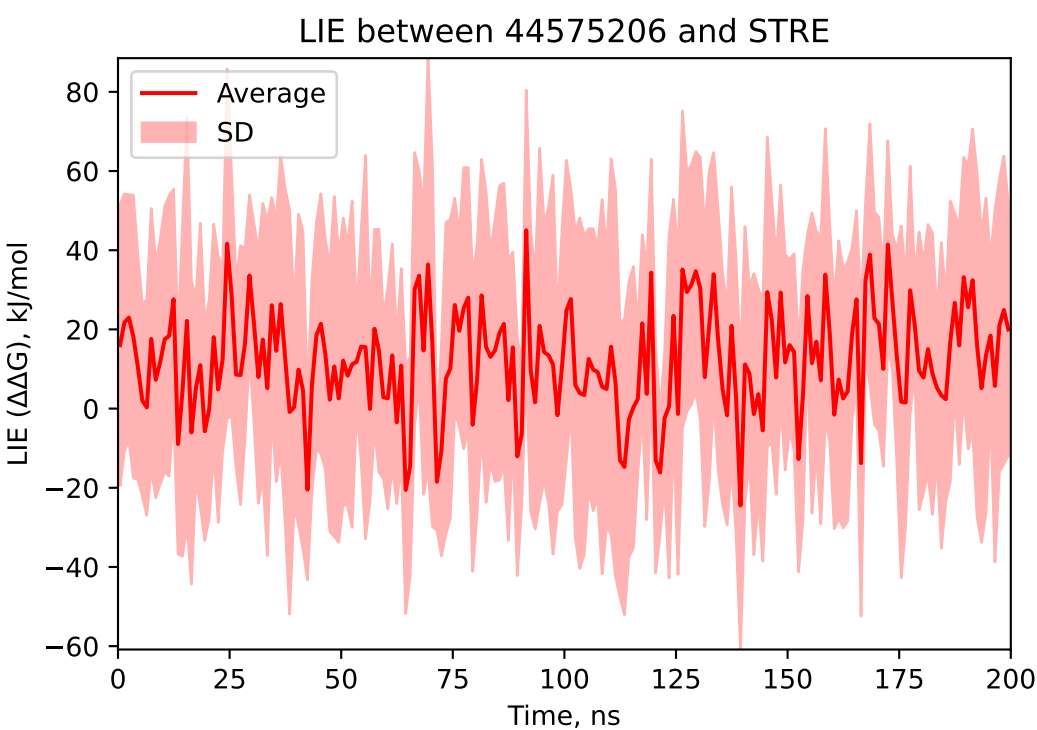

LIE between 44575206 and DOXY
Average
SD
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns

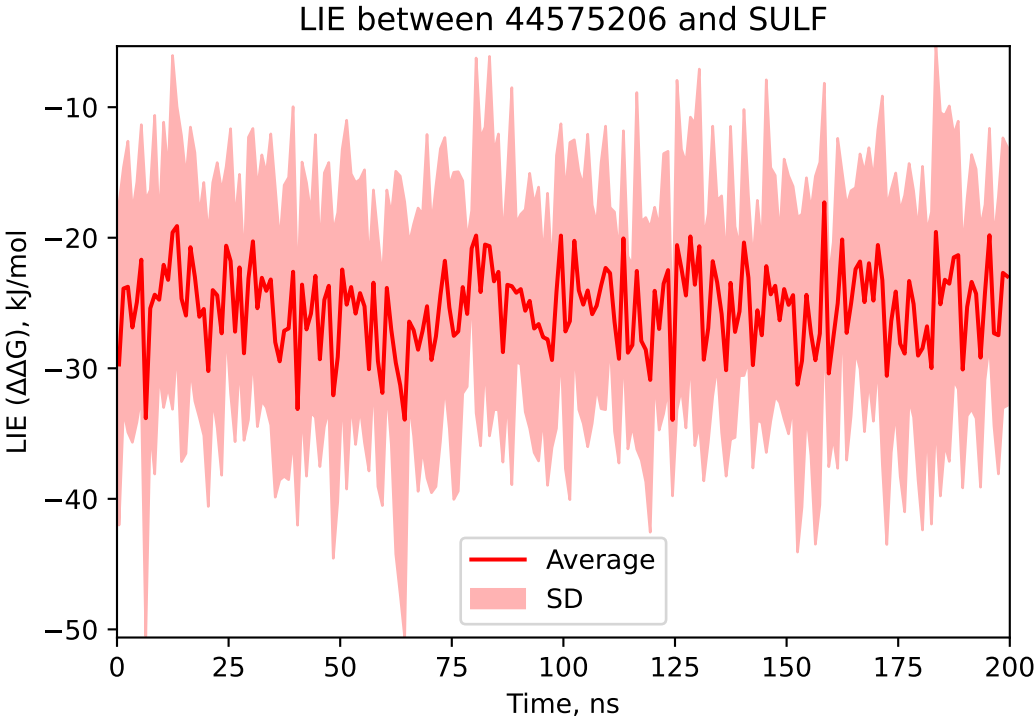

LIE between 44575206 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
10
20
30
40
50
60
70
80
90
0
25
50
75
100
125
150
175
200

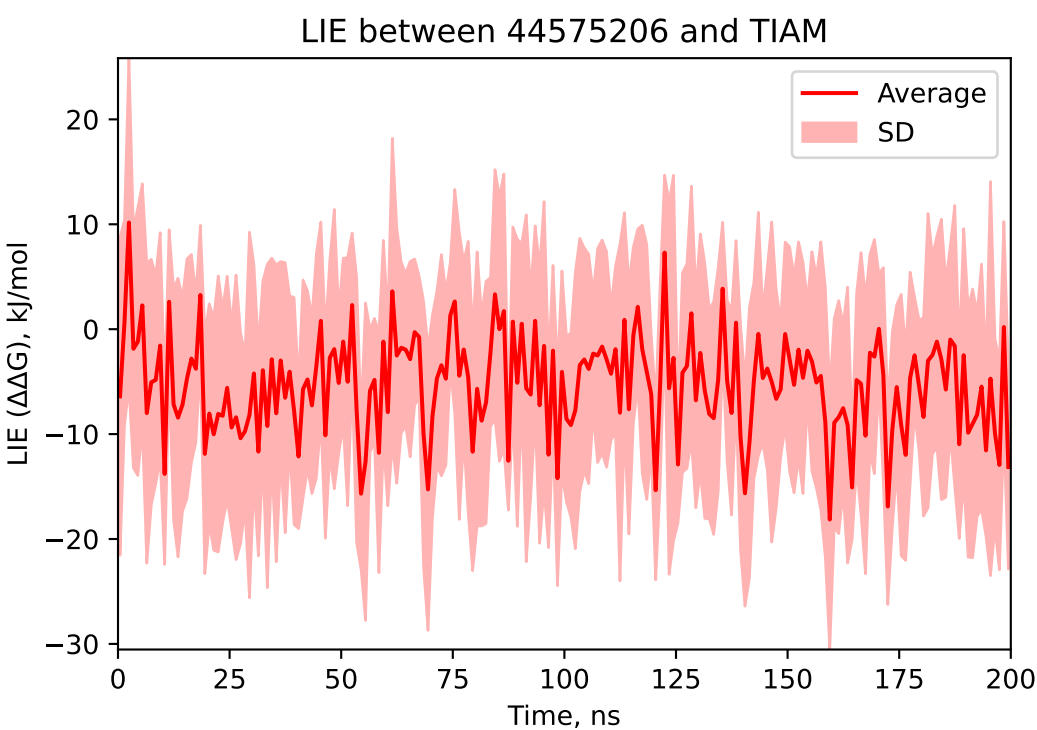

LIE between 44575206 and METR
LIE (ΔΔG), kJ/mol
−30
−40
−50
−60
−70
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

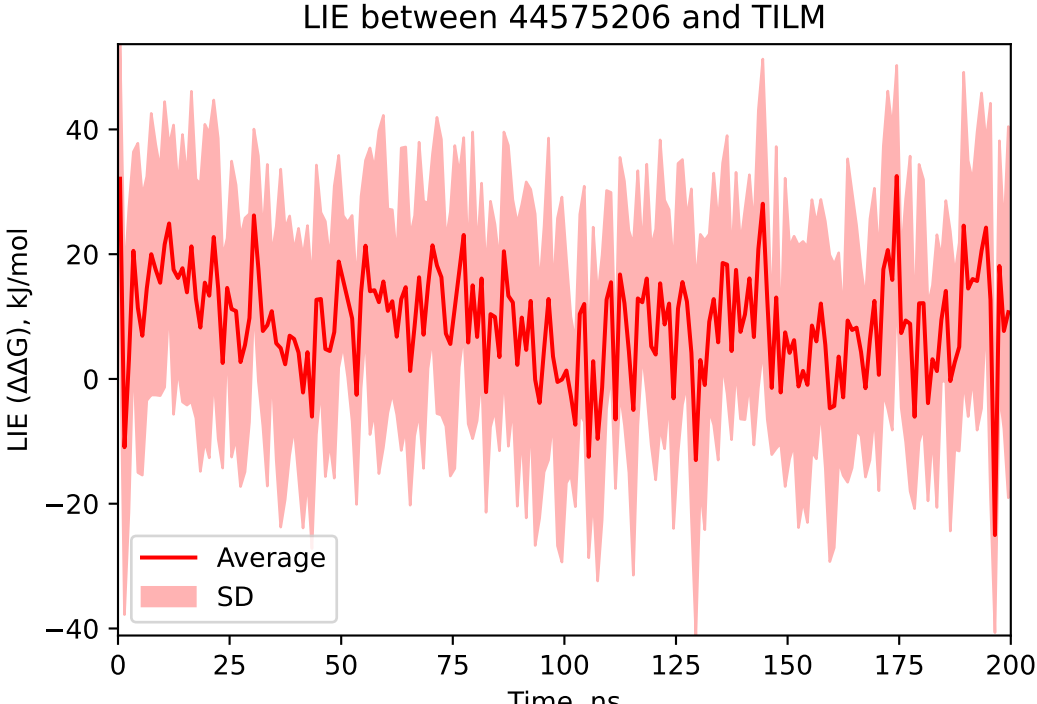

LIE between 44575206 and RONI
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

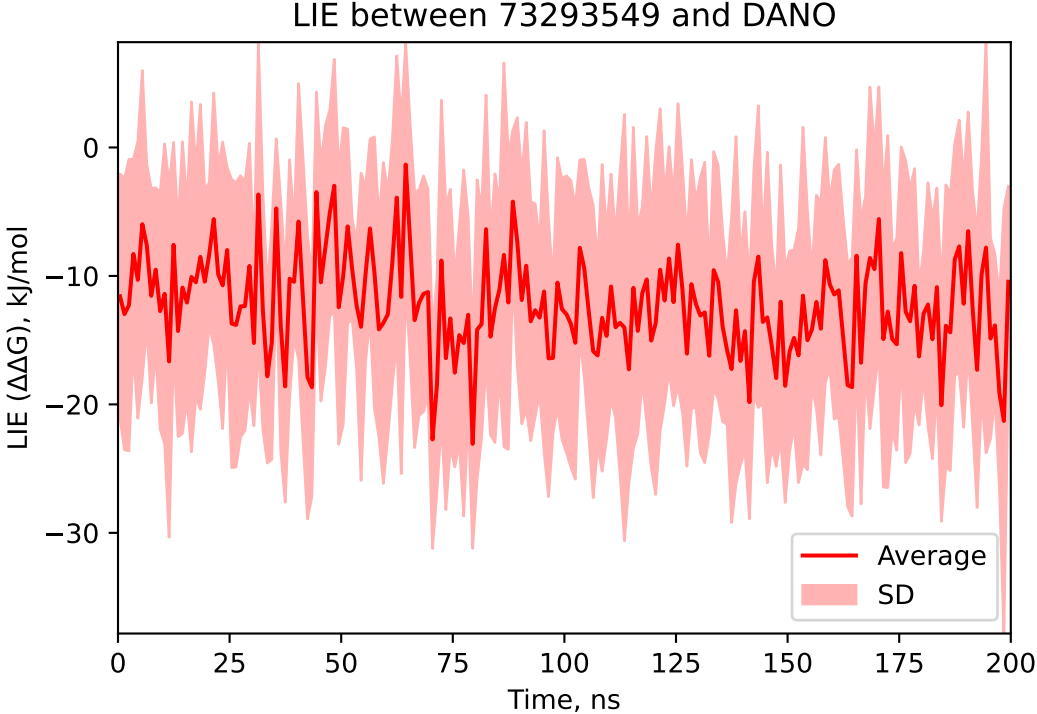

LIE between 44575206 and SPIR
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
40
30
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200

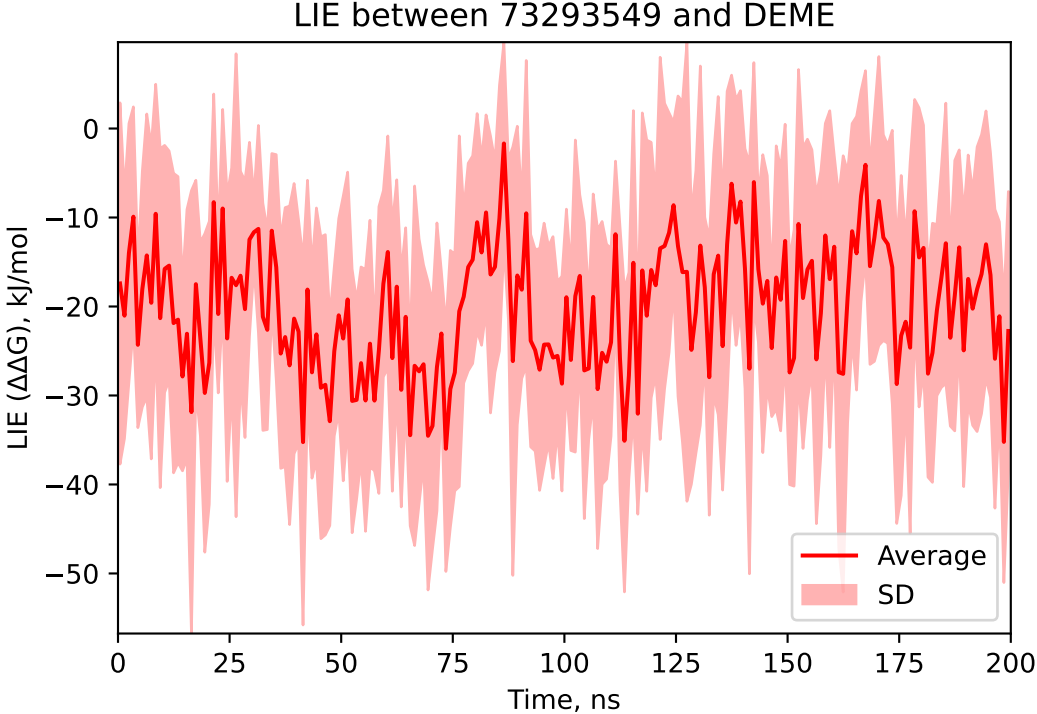

LIE between 44575206 and STRE
Average
SD
LIE (ΔΔG), kJ/mol
80
60
40
20
0
−20
−40
−60
0
25
50
75
100
125
150
175
200
Time, ns

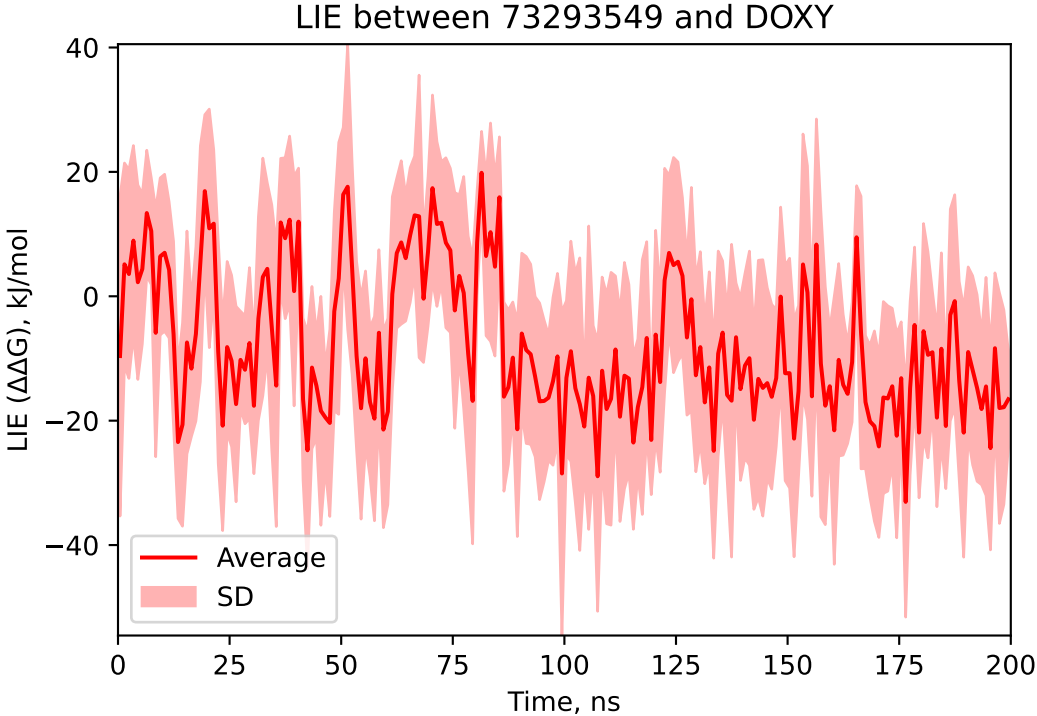

LIE between 44575206 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

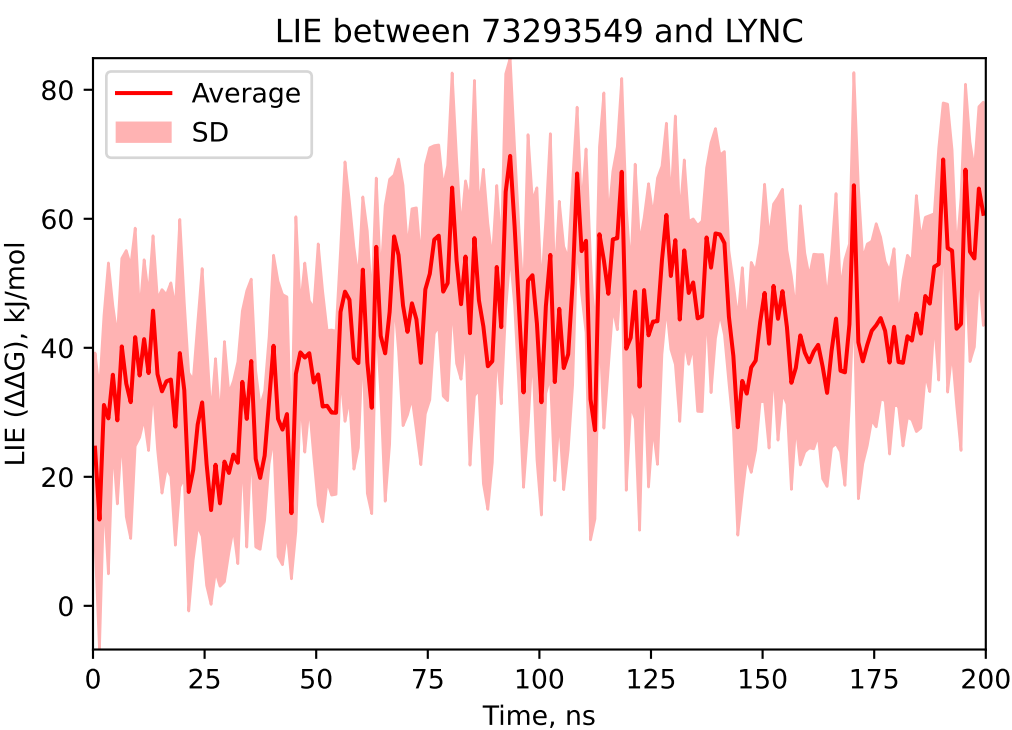

LIE between 44575206 and TIAM
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
20
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200

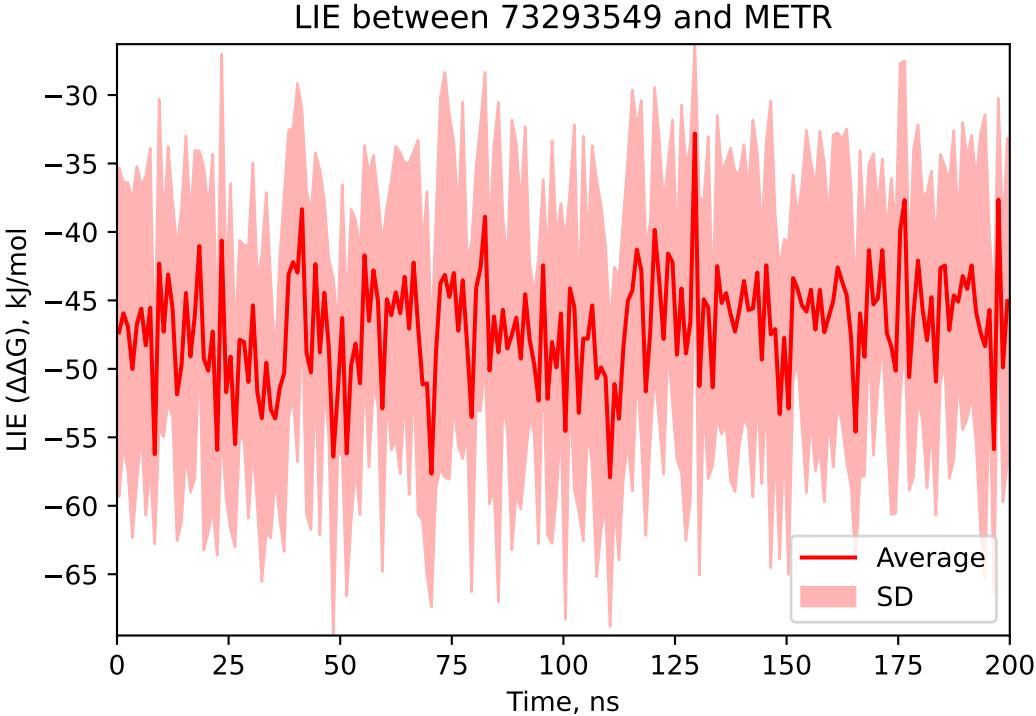

LIE between 44575206 and TILM
LIE (ΔΔG), kJ/mol
40
20
0
−20
−40
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns

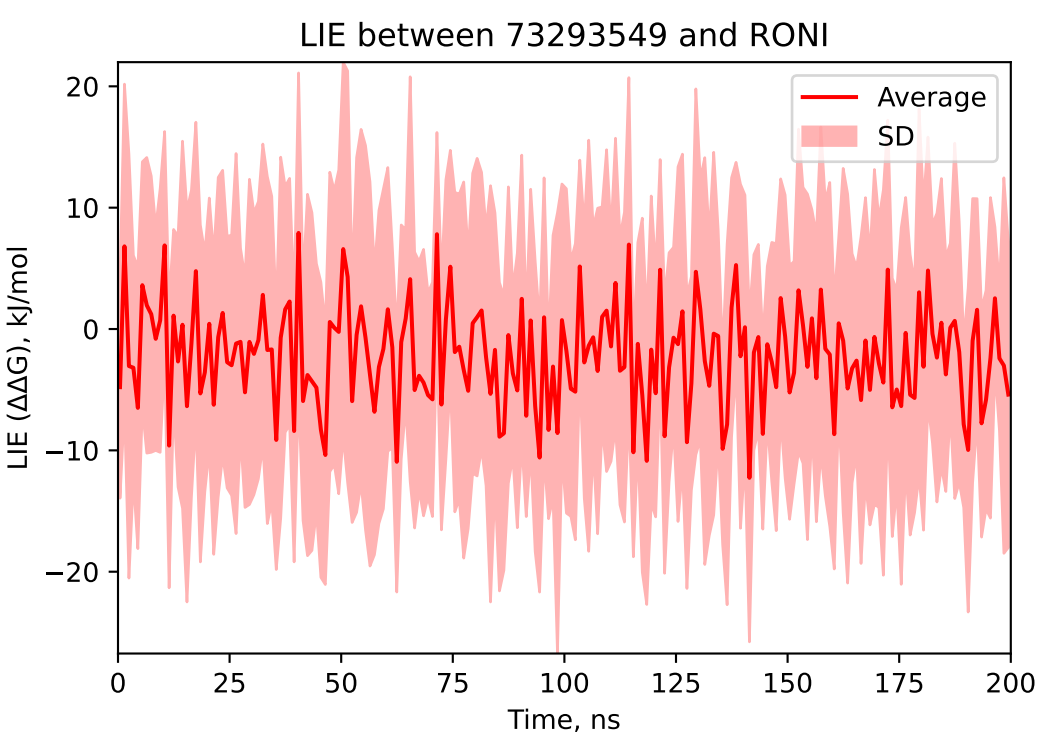

LIE between 73293549 and DANO
LIE (ΔΔG), kJ/mol
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

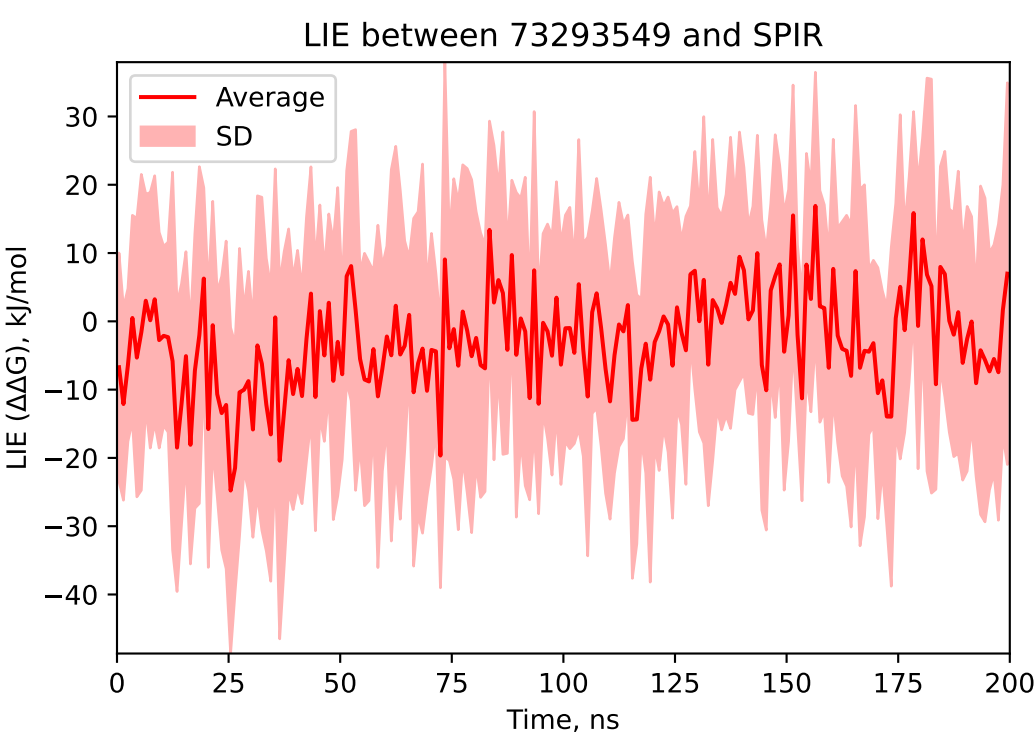

LIE between 73293549 and DEME
LIE (ΔΔG), kJ/mol
0
−10
−20
−30
−40
−50
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

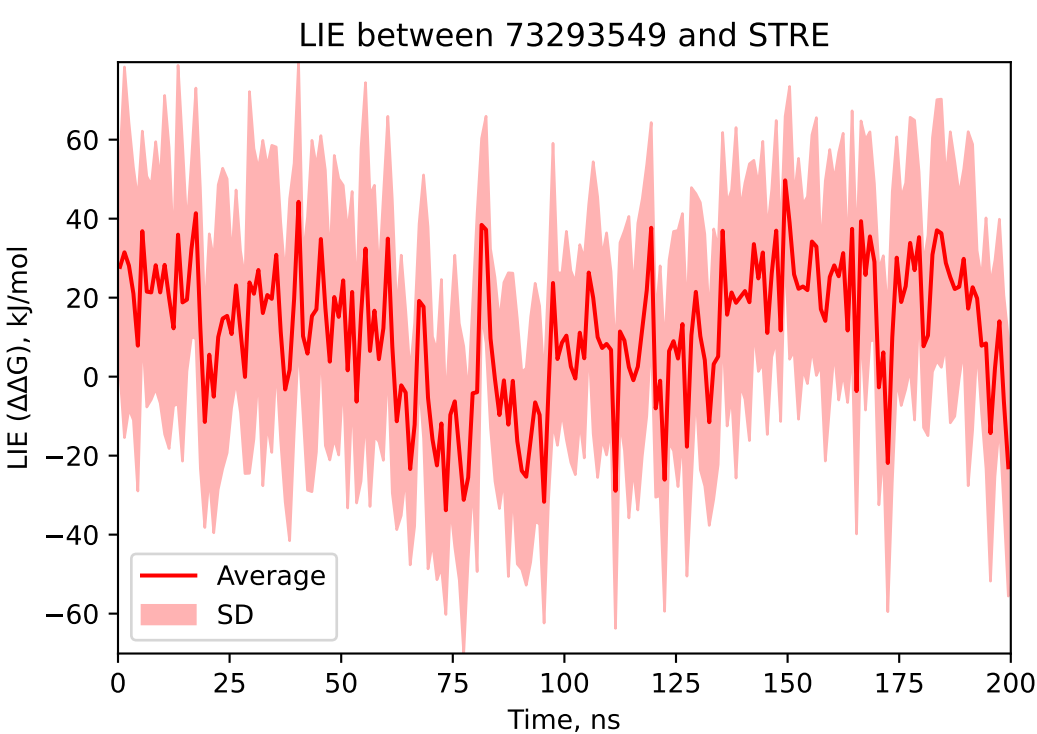

LIE between 73293549 and DOXY
LIE (ΔΔG), kJ/mol
Time, ns
Average
SD
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200

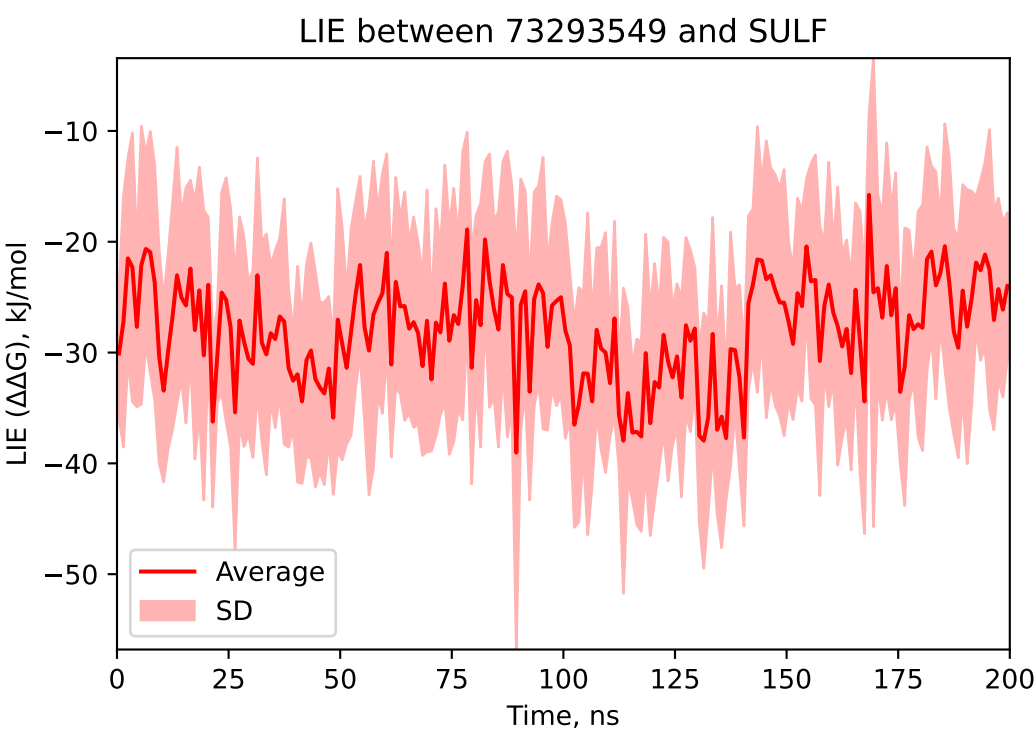

LIE between 73293549 and LYNC
Average
SD
LIE (ΔΔG), kJ/mol
Time, ns
0
20
40
60
80
0
25
50
75
100
125
150
175
200

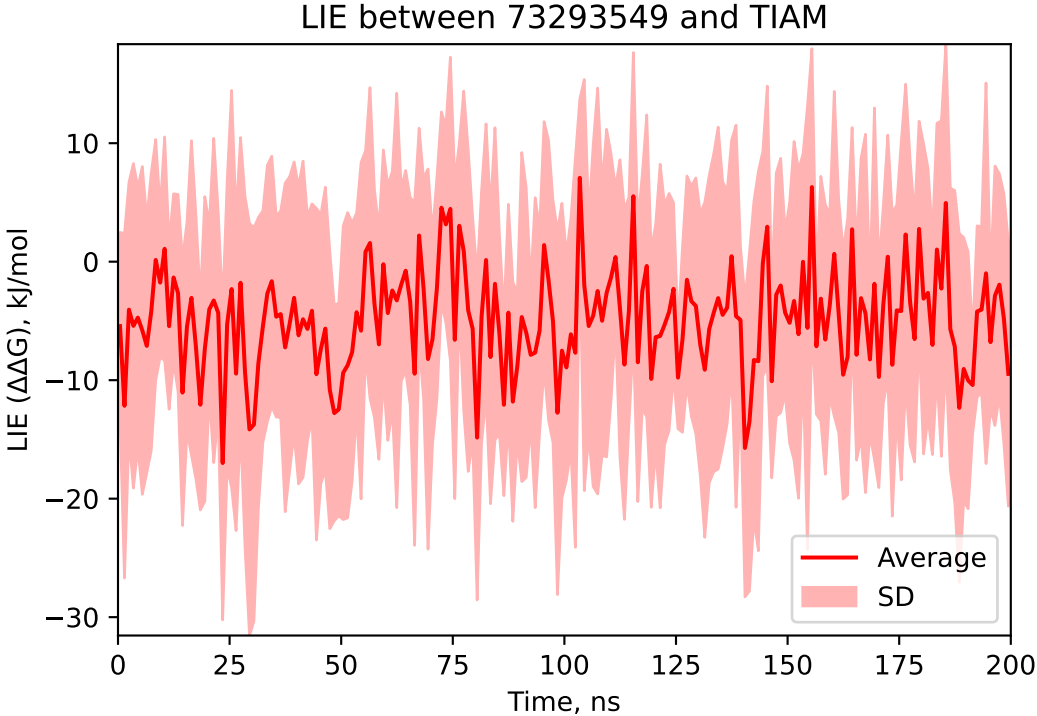

LIE between 73293549 and METR
LIE (ΔΔG), kJ/mol
−30
−35
−40
−45
−50
−55
−60
−65
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD

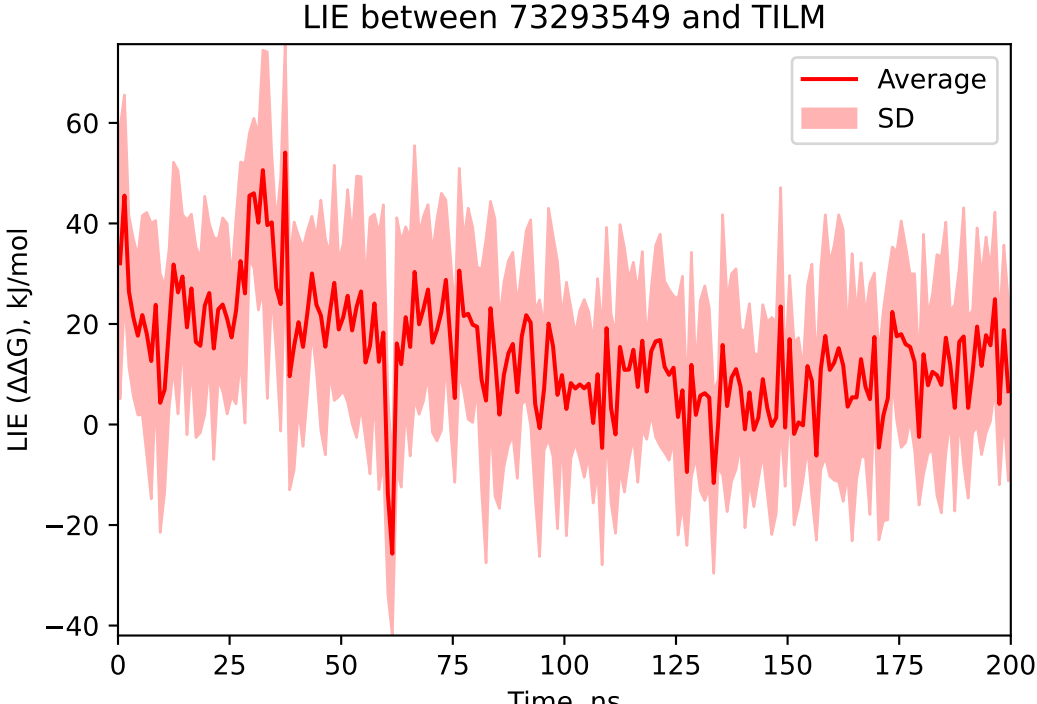

LIE between 73293549 and RONI
Average
SD
LIE (ΔΔG), kJ/mol
20
10
0
−10
−20
0
25
50
75
100
125
150
175
200
Time, ns


LIE between 73293549 and SPIR
Average
SD
LIE (ΔΔG), kJ/mol
30
20
10
0
−10
−20
−30
−40
0
25
50
75
100
125
150
175
200
Time, ns


LIE between 73293549 and STRE
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
−40
−60
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns


LIE between 73293549 and SULF
LIE (ΔΔG), kJ/mol
−10
−20
−30
−40
−50
Average
SD
0
25
50
75
100
125
150
175
200
Time, ns


LIE between 73293549 and TIAM
LIE (ΔΔG), kJ/mol
10
0
−10
−20
−30
0
25
50
75
100
125
150
175
200
Time, ns
Average
SD


LIE between 73293549 and TILM
Average
SD
LIE (ΔΔG), kJ/mol
60
40
20
0
−20
−40
0
25
50
75
100
125
150
175
200
Time, ns