25

0

25

0

4

NOE 8

25

0

50 -

0

2.5 5.0

NOE 9

NOE PMF plots

5.0

50

0

25

0

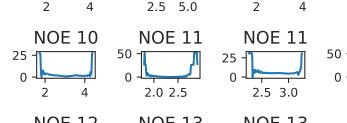
2

2

4

NOE 10

NOE 11



2.5 5.0

NOE 7

50

0

25 +

0 -

0

2

4

2

5.0

50 +

0 -

25 -

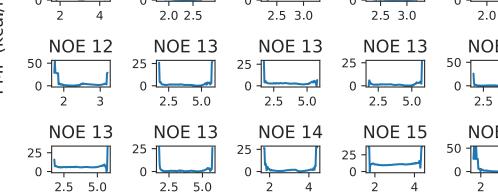
0 -

2.5

NOE 6

2.5 5.0 2 2 3 **NOE 11** 2.5 3.0 **NOE 13 NOE 13**

PMF (kcal/mol 50 T 2.0 2.5 **NOE 12 NOE 13 NOE 13** 50 -25 25 50 25 0 0 -0 0 5.0 2.5 5.0 5.0 2 3 2.5 2.5 2.5 **NOE 13 NOE 13 NOE 14 NOE 15**



5.0 **NOE 16** 3 **NOE 18 NOE 18 NOE 19 NOE 17 NOE 19** 25 + 50 25 -50 -25

0

2

3

3