

Case	Variable	No. samples	Obs. ave	Sim. ave (domain 4)	NMB (domain 4)
NUIST FR2012	C1-amine	61	4.35	8.97	106.72
	C2-amines	61	7.08	1.99	-71.50
	C3-amines	61	1.91	8.64	359.02
NUIST SDR2012	C1-amine	61	4.35	6.39	45.60
	C2-amines	61	7.08	10.56	49.12
	C3-amines	61	1.91	1.12	-41.26
Fudan FR2015	C1-amine	719	15.71	6.79 (9.26)	-56.75 (-41.03)
	C2-amines	719	40.20	1.56 (2.15)	-96.13 (-94.67)
	C3-amines	719	1.13	6.71 (9.24)	494.28 (718.61)
Fudan SDR2015	C1-amine	719	15.71	4.97 (6.61)	-68.37 (-57.95)
	C2-amines	719	40.20	16.33 (25.15)	-59.37 (-37.43)
	C3-amines	719	1.13	1.01 (1.37)	-10.84 (21.34)