Microstate ID of Deprotonated State (A)	Microstate ID of Protonated State (HA)	Molecule ID	pKa (exp)	pKa SEM (exp)	pKa ID	Microstate identification source
HN	NH					
		SM07	6.08	0.01	SM07_pKa1	NMR measurement
SM07_micro004	SM07_micro006					
SWIO7_ITTICTGGG4	514107_1111010000					
N.		SM14	5.3	0.01	SM14_pKa2	NMR measurement
H-N N-	H-N H-N					
SM14_micro001	SM14_micro002					
		SM14	2.58	0.01	SM14_pKa1	NMR measurement
		3W114	2.56	0.01	SINIT4_bra1	Nivik illeasurement
H <sub>E</sub> N T <sub>E</sub>	HAN THE					
SM14_micro002	SM14_micro003					
						Estimated based on
NH →	HN	SM02	5.03	0.01	SM02_pKa1	SM07 NMR measurement
F—F	, F					measurement
SM02_micro002	SM02_micro004					
HN	HN	SM04	6.02	0.01	SM04_pKa1	Estimated based on SM07 NMR
						measurement
SM04_micro003	SM04_micro002					
NH NH						Estimated based on
	HN ()	SM09	5.37	0.01	SM09_pKa1	SM07 NMR measurement
J	,					
SM09_micro003	SM09_micro001					
NH	NH	SM12	5.28	0.01	SM12_pKa1	Estimated based on SM07 NMR
						measurement
GI SM12_micro012	SM12_micro006					
O N	ļ. , H					
					Ch440	Estimated based on
NH		SM13	5.77	0.01	SM13_pKa1	SM07 NMR measurement
CM12	CM42					
SM13_micro005	SM13_micro001					
						Fatimated book
		SM15	8.94	0.01	SM15_pKa2	Estimated based on SM14 NMR measurement
						measarement
SM15_micro004	SM15_micro002					
OH	OH					
		SM15	4.7	0.01	SM15_pKa1	Estimated based on SM14 NMR
					p1	measurement
SM15_micro002	SM15_micro003					