Table 3.2: How to specify available Nucleic Acid force fields in LeAP

RNA			
Desired Behavior	Source this leaprc	Load these frcmods	Notes
Default AMBER ff14 (also Default AMBER ff12)	leaprc.ff14SB	n/a	Based on ff99; contains parmbsc0 α/γ dihedral modifications + χOL3 modifications.
AMBER ff99	oldff/leaprc.rna.ff99	n/a	Outdated leaprc file – you should be using corrections unless you know what you're doing.
AMBER ff99χ	oldff/leaprc.rna.ff99	frcmod.parmCHI_YIL	χ modifications based on Yildirim et al. 2010.
AMBER ff99χ+bcs0	oldff/leaprc.parmCHI_YIL.bsc	n/a	Based on ff99; contains parmbsc0 α/γ dihedral modifications + Yildirim et al. 2010 χ modifications.
AMBER ff99bsc0	oldff/leaprc.ff99bsc0	n/a	Contains only parmbsc0 α/γ dihedral modifications from Perez et al. 2006.
Modified RNA nucleotides	leaprc.ff14SB, followed by leaprc.modrna08	n/a	Contains Aduri et al. 2007 parameters for modified nucleosides, with Default AMBER ff14 modifications (see first entry in the RNA section of this table).
DNA			
Default AMBER ff14	leaprc.ff14SB	n/a	Based on ff99; contains parmbsc0 α/γ dihedral modifications.
AMBER ff99	oldff/leaprc.ff99	n/a	Outdated leaprc file – you should be using corrections unless you know what you're doing.
Recommended: AMBER ff14+ ε/ζ OL1+ χOL4	leaprc.parmbsc0_chiOL4_ezOL1	n/a	Contains ε/ζ OL1 (Zgarbova et al.) + χOL4 modifications (Krepl et al.), with Default AMBER ff14 modifications (see first entry in the DNA section of this table).