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Technical Bulletin: One-Minute NMR Reference Model Compounds
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Maleic Acid

Formula weight = 116.07 g/mol

Add 10.00 mL to 0.0232 g to yield 20.0 mM

Add 5.00 mL to 0.0116 g to yield 20.0 mM

Add 5.00 mL to 0.0232 g to yield 40.0 mM

Sigma #M0375-500G (500 grams)

- Yields a 2-proton singlet as its only NMR signal
- S/N is 4-fold greater than the equivalent concentration of the sucrose anomeric proton signal
- 20 mM maleic acid yields an 8-fold greater S/N than 10 mM sucrose
 - Makes a nice solution to shim on
- Soluble in acetone, acetonitrile, DMSO, D₂O, methanol
- Not soluble in chloroform

Astemizole

Formula weight = 458.6 g/mol

Add 1.00 mL to 0.0917 g to yield 200 mM

Sigma #A6424-1G (1 gram; discontinued, so last gram)

- Soluble in chloroform, DMSO, methanol; can degrade over weeks in DMSO (turns yellow)
- Not soluble in D₂O

Amitriptyline·HCl

Formula weight = 313.9 g/mol

Add 1.00 mL to 0.0628 g to yield a 200 mM solution

Sigma #A-8404 (10 grams)

- Soluble in chloroform, DMSO, D₂O, methanol

Naproxen (not naproxen sodium)

Formula weight = 230.27 g/mol

Add 10.00 mL to 0.0461 g to yield 20.0 mM

Add 5.00 mL to 0.0230 g to yield 20.0 mM

Add 5.00 mL to 0.0461 g to yield 40.0 mM

Sigma-Aldrich #M4015-5G (5 grams)

- Soluble in acetone, acetonitrile, chloroform, DMSO, D₂O, methanol
- Not as spectrally simple as maleic acid, but a reasonable substitute for maleic acid which is not soluble in chloroform

Sucrose

Formula weight = 342.3 g/mol

Add 10.00 mL to 0.0342 g to yield 10.0 mM

Add 5.00 mL to 0.0171 g to yield 10.0 mM

- Soluble in water and DMSO