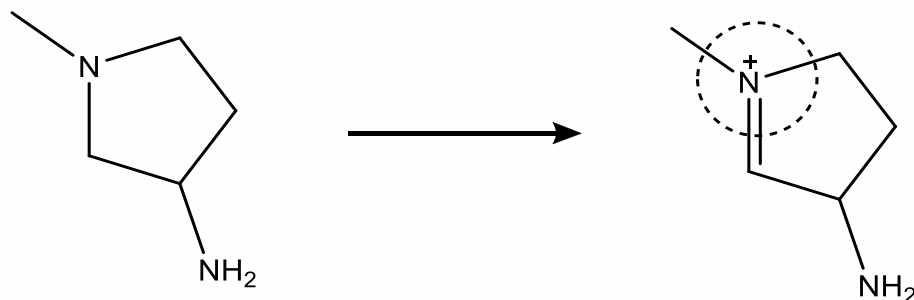


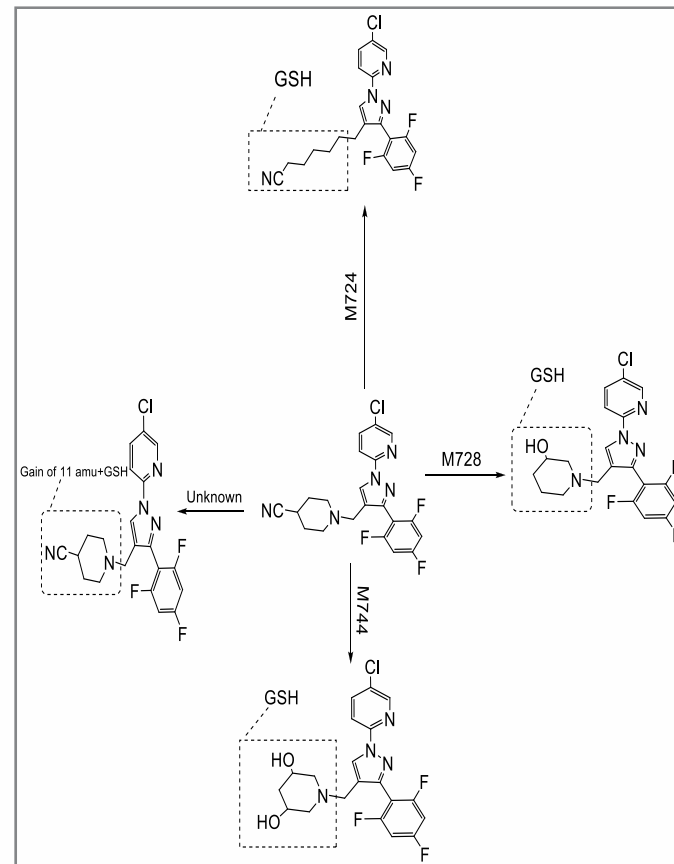
Heterocyclic compounds with pyrrolidine ring can form iminium reactive intermediates



GSH is the relevant trapping reagent to trap nitrenium intermediates

Q1Mass, m/z	Biotransformation pathway	Fragmentation Score				
		Loss of 75 amu	Loss of 129 amu	Loss of 146/147 amu	Loss of 273/ Gain of 32 amu	Parent fragment (322)
724.10	Piperidine ring opening+GSH	649.10	595.10	577.10	451.10	322.10
728.10	Loss of nitrile +Oxidation+GSH	653.10	599.10	581.20	-	322.10
744.10	Loss of nitrile +Dioxidation+GSH	669.10	615.10	-	-	322.10
748.10	Unknown	673.10	619.10	601.20	475.10	322.10
457.20	Acetaminophen (Parent+GSH)	382.10	328.10	311.00	182.10	-

## GSHTrapping



Fragmentation score and list of GSH conjugates identified for XXXX and acetaminophen

**Note: Conjugates with fragmentation score of 2 or >2 were considered as GSH conjugates**