The research and results presented in this poster are courtesy of Dr. Dave Detlefsen, Novatia LLC, Monmouth Junction, NJ

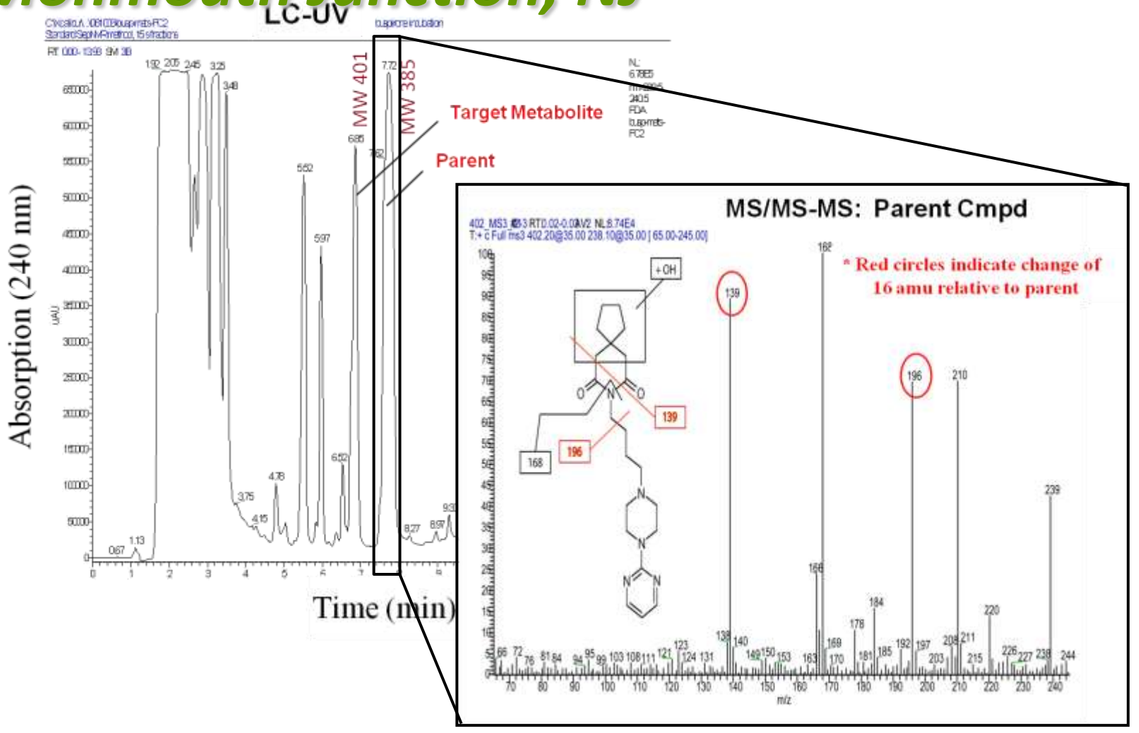
Medchem

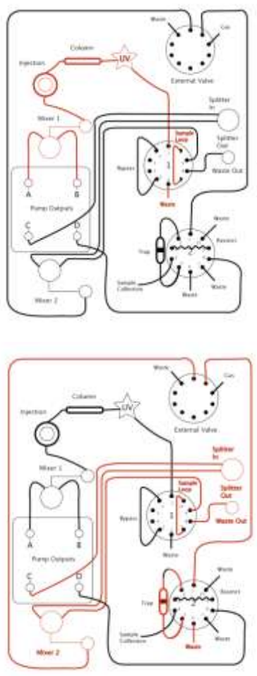
Novatia

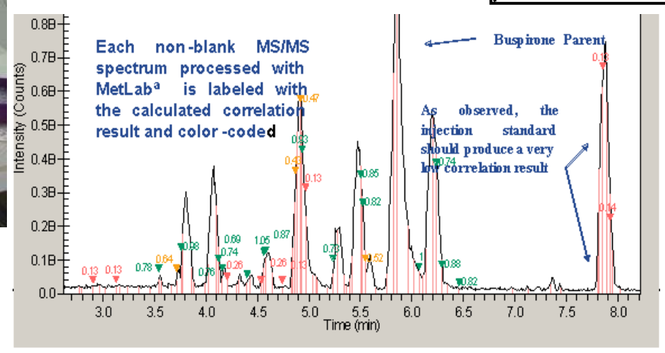
Drug of Interest

10s - 100s of ug of crude extract

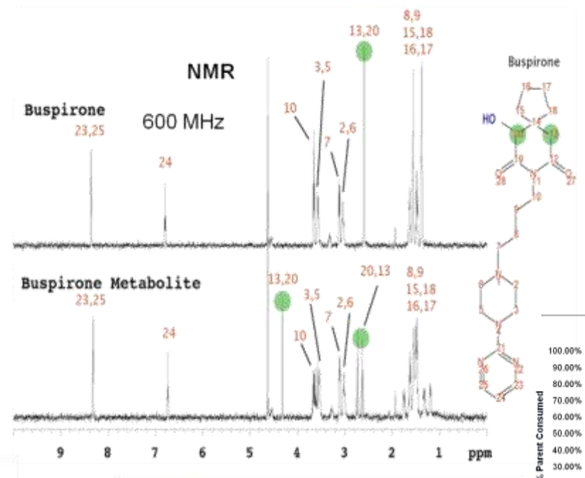
Human Liver Microsomes

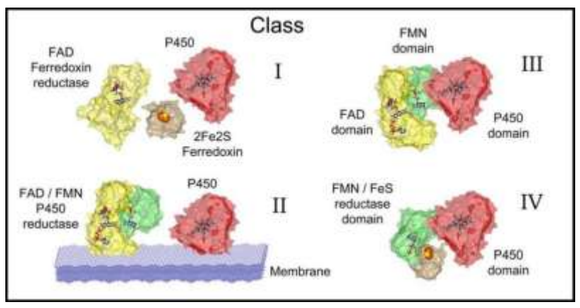


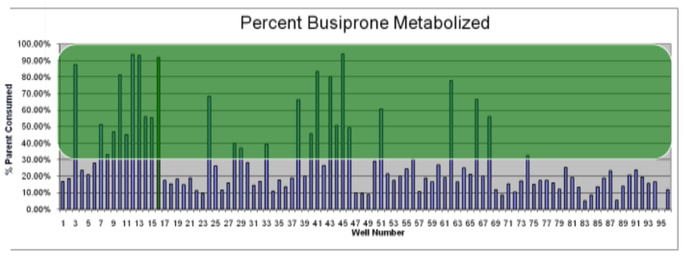




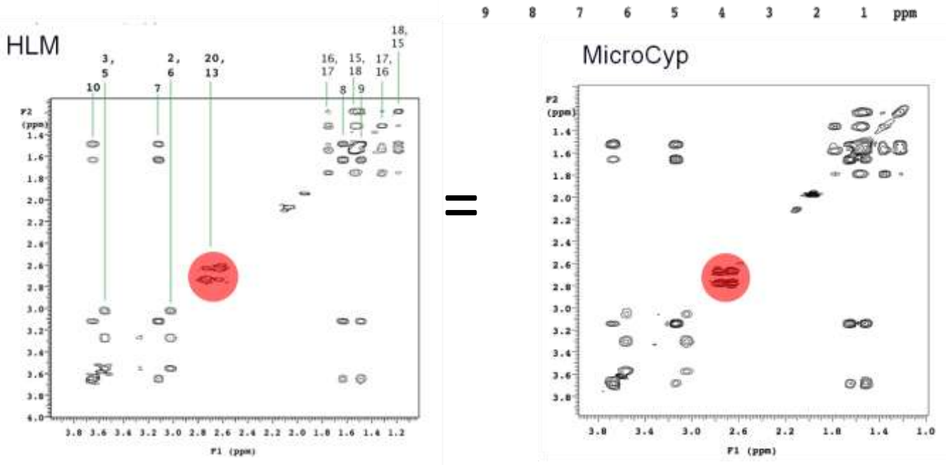
Metabolite	RT	M+H	Corr	Shifted Ions	Common Ions	Unique Ions
Dihydroxy	3.54	418	High	122(+18), 150(+18), 265(+18), 222(+18)		
Dihydroxy	3.72	418	Mid	122(+18), 150(+18), 222(+18)		235, 220
Hydroxy	3.76	402	High	265(+18), 222(+18)	122, 150	359
Hydroxy	4.12	402	High	265(+18), 222(+18), 291(+18)	122, 150	219, 220
Dihydroxy	4.16	418	High	265(+18), 222(+18)	122	297, 400, 374, 220
Dihydroxy	4.40	418	High	180(+18), 222(+18), 265(+18)		297, 164, 293, 374
Hydroxy	4.56	402	High	222(+18), 265(+18)	122, 150	358
Dihydroxy	4.58	418	High	122(+18), 150(+18), 265(+18), 222(+18)		400
Unknown	4.87	360	Mid		122, 265	343
Hydroxy	**4.93**	**402**	**High**	222(+18), 265(+18)	122, 150	359, 342
Dihydroxy	5.24	418	High	222(+18), 265(+18)		297, 293, 306, 374, 400
Hydroxy	5.50	402	High	122(+18), 150(+18)	222, 265, 180	
Unknown	5.52	372	High	150(-14)	122, 222, 265	251
Parent	5.86	386	High			
Hydroxy	6.24	402	High		222, 265, 122	358, 384







Codexis MicroCyp GM-III Series P450 Enzymes (1/well)
- 300 µl Incubation with 175 µg buspirone
- 26 wells exceed 30% (50µg) of parent consumed



Separation/ Purification	1	**Michrom Bioresources HPLC System** Paradigm MS4B quaternary pump Analytical Scale **CTC Analytics Autosampler** HTS PAL
High Sensitivity Detection	2	**Thermo Scientific DAD** SpectraSystem UV6000LP PDA **Thermo-Finnigan Mass Spec** TSQ-7000 Triple Quad MS
Fraction Collection	3	**ISCO Fraction Collector** Foxy Jr.

Sample Preparation	4	**Novatia SepNMR** Paradigm MS4B HPLC SPE **LabConco Vacuum Centrifuge** Centrivap
NMR	5	**Varian NMR** 500MHz Inova **Protasis Automation** 10 uL g-TXI probe Dual-Solvent OMNMR
Reporting	6	**Agilent** MetLab