

# SME and Me

## Dream it, Then Build it

Can SiRNA scientists eliminate the bottleneck of manual data interpretation in their new Mass Spec based workflow used for Metabolite Identification.

# SirnaMetID (2009)

## Project Scope

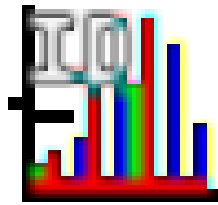
- SiRNA had developed a Mass Spec workflow to analyze drug candidate's liability to degradation in vitro and find sites of degradation for amelioration
- External vendors failed to deliver viable system to automate the analysis

## Project Findings

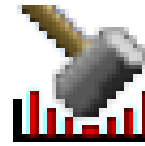
- Use open source software applications and internally developed modules which were developed in 2 months
- The SirnaMetID solution successfully achieve desired speed and quality
  - Increased data analysis throughput 25X over manual analysis
  - Able to meet Year End objectives for \$0 additional cost

# SirnaMetID (2009)

**SirnaMetID** calls executables  
and creates a transaction log

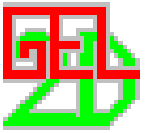


**Less than 1 minute per  
sample!**



Decon2LS.exe

- Decon2LS\* deconvolutes and de-isotopes mass spectral data



VIPER.exe

- Viper\* produces peak table with retention time and intensity



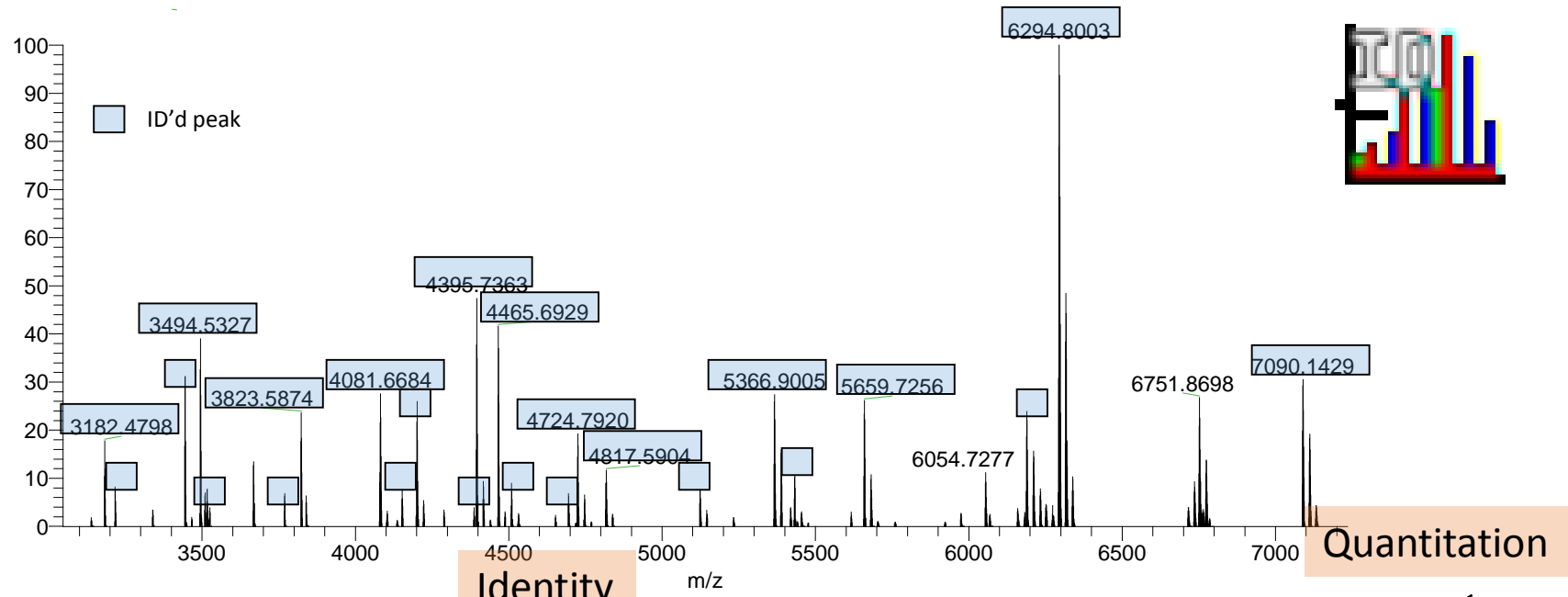
*\* Open source software from Pacific Northwest National Labs*

# SirnaMetID (2009)

luc\_80-0735-s9-02\_xt\_00001\_m\_

11/3/2009 11:13:41 AM

luc\_80-0735-s9-02\_xt\_00001\_m\_ #1 RT: 1.00  
T: FTMS - p ESI sid=20.00 Full ms [510.00-140]



	A	B	C	D	E	F	G	H	I	J	K	L
1	MW	MW_Phos	DELTA	STRAND	START	END	PROTOGE	Monoisoto	Class_Rep	Abundance	TOTAL	% parent
2				GS	1	21				0	85758132	0
3	6292.819		0.015	GS	2	21	rA;rU;fluC;	6292.804	10	2.91E+07	85758132	33.9
4	4693.611		0.0089	GS	2	16	rA;rU;fluC;	4693.62	8	756967	85758132	0.88
5	4385.59		0.0006	GS	2	15	rA;rU;fluC;	4385.589	7	502110	85758132	0.59
6	4078.553		0.003	GS	2	14	rA;rU;fluC;	4078.556	7	3.15E+06	85758132	3.67

- Output gives great results for metabolite identification