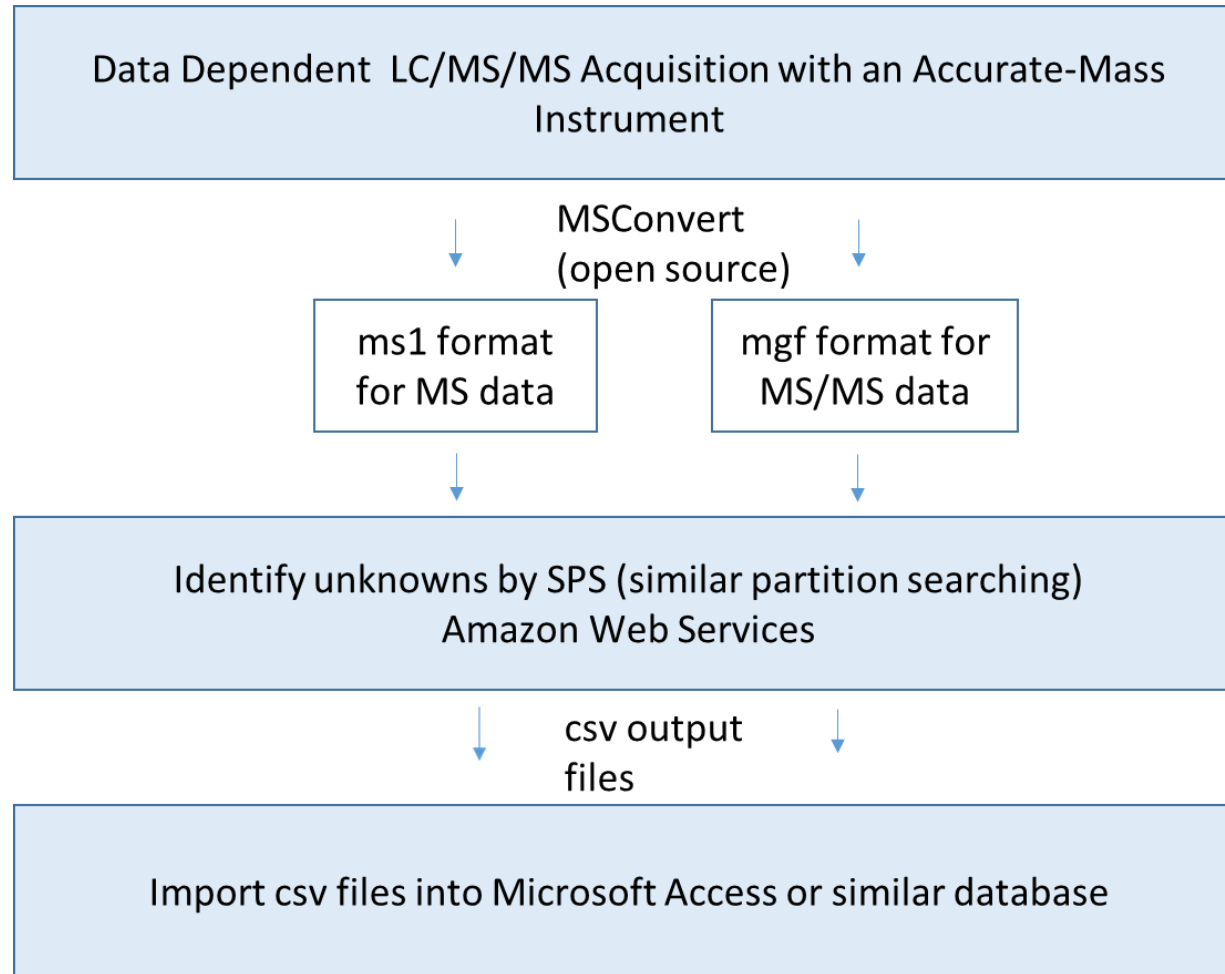


# Analyzing, Searching, and Archiving Data Generated by Data Dependent Analyses

Daniel L. Sweeney, MathSpec, Inc.



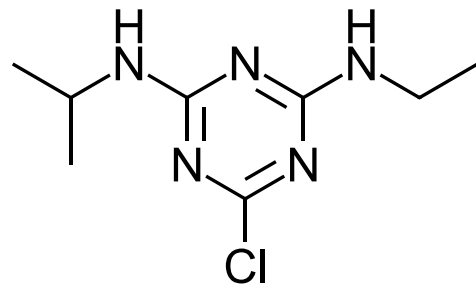
# DDA Parameter Optimization

- Exclusion list
- Dynamic exclusion list
- Precursor Isolation Window
- Collision Energy or Energies
- Mass Range
- Intensity Threshold

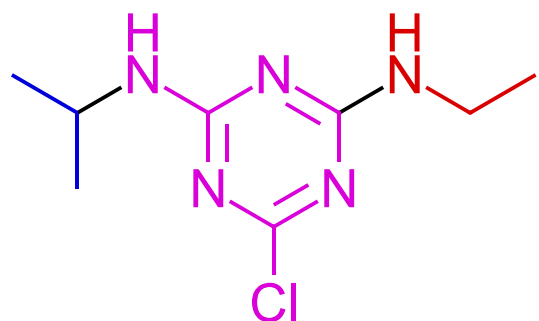
Modern instruments can generate over 10000 MS/MS spectra in a 30 minute analysis.

File Home Create External Data Database Tools Fields Table Tell me what you want to do												
Tables												
Search...												
<ul style="list-style-type: none"> <li>LCMS_Conditions</li> <li>Processed_Data</li> <li>Results</li> <li>Run_Information</li> </ul>												
Processed_Data												
RT	Intensity	MW	Adduct	Ion1	Ion2	Ion3	Ion4	Ion5	Ion6	Ion7	Ion8	Ion9
19.448	2995	920.9991	H+	87.0452	466.3612	323.2570	75.0432	166.1267	177.1031	639.6893	38	
19.458	35355	215.0929	H+	68.0240	96.0556	104.0010	79.0057	43.0291	71.0602	174.0531	10	
19.458	22979	215.0929	H+	174.0541	176.0516	96.0559	138.1007	43.0537	132.0313	104.0002	14	
Score	Num_Syr	Shift	PubChemLink	Class	Iso1	Iso2	Iso3	Iso4	PubChemID			
81	228	-----	<a href="#">2256</a>	herbicide	100	10	32	3	2256			
81	27	-----	<a href="#">24740</a>	not classified	100	10	32	3	24740			
81	22	-----	<a href="#">107944</a>	not classified	100	10	32	3	107944			
81	20	-----	<a href="#">165706</a>	not classified	100	10	32	3	165706			
81	25	-----	<a href="#">170183</a>	not classified	100	10	32	3	170183			
81	15	-----	<a href="#">202237</a>	not classified	100	10	32	3	202237			
81	15	-----	<a href="#">12306645</a>	not classified	100	10	32	3	12306645			
81	5	-----	<a href="#">16213378</a>	not classified	100	10	32	3	16213378			
70	27	-C2H4	<a href="#">15950</a>	not classified	100	13	33	4	15950			
48	26	-----	<a href="#">4611495</a>	not classified	100	15	1	0	4611495			
*	0				0	0	0	0	0			
19.460	17944	173.0461	H+	96.0557	68.0246	146.0222	132.0312	79.0063	104.0005	134.0282	13	
19.461	20591	173.0461	H+	68.0243	43.0292	104.0010	71.0599	105.9981	79.0060	61.9790	9	
19.465	1729	249.1696	H+	59.0488	64.9765	137.0971	156.0801	212.1991	175.1111	135.1156	13	
19.469	3075	249.1696	H+	97.0637	57.0706	101.1078	43.0532	221.1481	160.1125	58.0653	4	
19.496	27765	191.1303	H+	119.0493	72.0436	91.0543	100.0758	99.0777	121.0993	43.0176	9	
19.501	55470	191.1303	H+	91.0541	119.0491	72.0445	44.0126	65.0378	67.0540	118.0645	4	
19.533	15238	99.0680	H+	55.0542	44.0129	67.0545	43.0180	41.0383	72.0438	69.0327	5	
19.540	12308	99.0680	H+	51.0225	41.0380	44.0132	67.0544	58.0291	43.0181	65.0379	3	
19.552	6237	191.1299	Na+	81.0693	96.0540	57.0702	109.1013	67.0550	95.0859	93.0698	8	
19.556	13920	191.1299	Na+	96.0556	68.0244	55.0543	67.0537	93.0699	43.0543	57.0700	7	
19.559	4726	234.1586	H+	58.0648	45.0327	89.0581	95.0861	83.0834	67.0551	110.1042	12	
19.564	6072	234.1586	H+	124.0862	67.0549	57.0697	45.0330	42.0340	58.0662	55.0555	4	
19.570	33731	163.0989	H+	119.0492	44.0128	72.0439	121.1008	95.0860	93.0694	91.0542	6	
19.576	31863	163.0989	H+	91.0541	44.0128	55.0543	77.0295	79.0547	91.0793	119.0493	6	

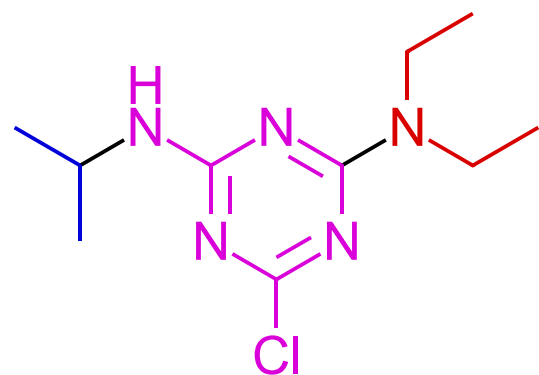
Data Courtesy of I. Ferrer and E. M. Thurman



SubGrp A	SubGrp B	SubGrp C	A+B	A+C	B+C	A+B+C
349690	1220592	580657	1570282	0	1801249	2150938
349690	1100718	700531	1450408	0	1801249	2150938
349690	1100592	700657	1450282	0	1801249	2150938
349690	820531	980718	1170221	0	1801249	2150938
349690	960687	840562	1310377	0	1801249	2150938
349690	960562	840687	1310252	0	1801249	2150938
440500	400061	1310376	840561	0	1710437	2150938
580657	400061	1170220	980718	0	1570281	2150938
410140	430548	1310250	840688	1720390	0	2150938
1279891	430548	440500	1710439	1720391	0	2150938
1250701	430548	469690	1681249	1720391	0	2150938
550170	430548	1170220	980718	1720390	0	2150938
1159891	430548	560500	1590439	1720391	0	2150938
1110671	430548	609720	1541219	1720391	0	2150938
1019860	430548	700531	1450408	1720391	0	2150938
970640	430548	749751	1401188	1720391	0	2150938
879829	430548	840562	1310377	1720391	0	2150938
440500	1240749	469690	1681249	0	1710439	2150938
580657	1129782	440500	1710439	0	1570282	2150938
440500	1100718	609720	1541218	0	1710438	2150938



SubGrp A	SubGrp B	SubGrp C	A+B	A+C	B+C	A+B+C
349690	960562	840687	1310252	0	1801249	2150938
440500	400061	1310376	840561	0	1710437	2150938
580657	400061	1170220	980718	0	1570281	2150938
410140	430548	1310250	840688	1720390	0	2150938
1279891	430548	440500	1710439	1720391	0	2150938
1250701	430548	469690	1681249	1720391	0	2150938
550170	430548	1170220	980718	1720390	0	2150938
1159891	430548	560500	1590439	1720391	0	2150938
1110671	430548	609720	1541219	1720391	0	2150938
1019860	430548	700531	1450408	1720391	0	2150938
970640	430548	749751	1401188	1720391	0	2150938
879829	430548	840562	1310377	1720391	0	2150938



550170	430548	1450533	980718	2000703	0	2431251
1390984	430548	609720	1821532	2000704	0	2431251
720813	1279891	430548	2000704	0	1710439	2431251
1250953	430548	749751	1681501	2000704	0	2431251
1159891	430548	840813	1590439	2000704	0	2431251
879829	430548	1120875	1310377	2000704	0	2431251
1019860	430548	980844	1450408	2000704	0	2431251
580657	1380905	469690	1961562	0	1850595	2431251
720813	1240749	469690	1961562	0	1710439	2431251
580657	1240875	609720	1821532	0	1850595	2431251
720813	1129782	580657	1850595	0	1710439	2431251
580657	729720	1120875	1310377	0	1850595	2431251