

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062018\
 Data File : VX002750.D
 Acq On : 20 Jun 2018 19:00
 Operator : JC/MD
 Sample : J3597-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 W-44

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	89	rBV	1678755	2023408	100.00%	18.081%
2	1.148	89	92	103	rVV	96631	165829	8.20%	1.482%
3	1.270	108	112	114	rVV	187914	211697	10.46%	1.892%
4	1.313	114	119	142	rVB	418139	1264144	62.48%	11.296%
5	2.630	330	335	341	rBV2	11399	27891	1.38%	0.249%
6	5.507	796	807	823	rBV	141728	409149	20.22%	3.656%
7	5.666	823	833	850	rVB	208309	589385	29.13%	5.267%
8	6.074	890	900	916	rBV	148392	393286	19.44%	3.514%
9	6.867	1018	1030	1046	rBV	305844	709579	35.07%	6.341%
10	8.720	1327	1334	1350	rBV	736667	1129493	55.82%	10.093%
11	10.116	1556	1563	1565	rBV	627064	873495	43.17%	7.805%
12	10.140	1565	1567	1580	rVB	559388	692367	34.22%	6.187%
13	11.140	1725	1731	1736	rBV	645491	813039	40.18%	7.265%
14	11.774	1830	1835	1839	rBV	26909	33513	1.66%	0.299%
15	11.927	1853	1860	1863	rBV	33394	52223	2.58%	0.467%
16	12.079	1880	1885	1897	rVB	751289	1034135	51.11%	9.241%
17	12.719	1986	1990	1995	rBV2	20056	32132	1.59%	0.287%
18	12.817	2003	2006	2011	rVB	35066	45653	2.26%	0.408%
19	12.878	2011	2016	2021	rVB2	22877	33218	1.64%	0.297%
20	12.957	2024	2029	2033	rBV	39643	59794	2.96%	0.534%
21	13.311	2082	2087	2092	rBV	18799	27655	1.37%	0.247%
22	13.640	2137	2141	2146	rBV	23828	35779	1.77%	0.320%
23	14.036	2202	2206	2211	rVB2	14274	22761	1.12%	0.203%
24	14.384	2256	2263	2267	rBV	103269	139627	6.90%	1.248%
25	14.432	2267	2271	2278	rVB5	25110	48421	2.39%	0.433%
26	14.737	2316	2321	2324	rBV4	23314	36273	1.79%	0.324%
27	14.853	2335	2340	2344	rVB2	54307	84019	4.15%	0.751%
28	15.243	2400	2404	2410	rVB6	15013	29073	1.44%	0.260%
29	15.676	2469	2475	2481	rVB	49179	76940	3.80%	0.688%
30	15.816	2492	2498	2504	rBV2	12829	28366	1.40%	0.253%
31	15.932	2513	2517	2523	rVB	42404	68493	3.39%	0.612%

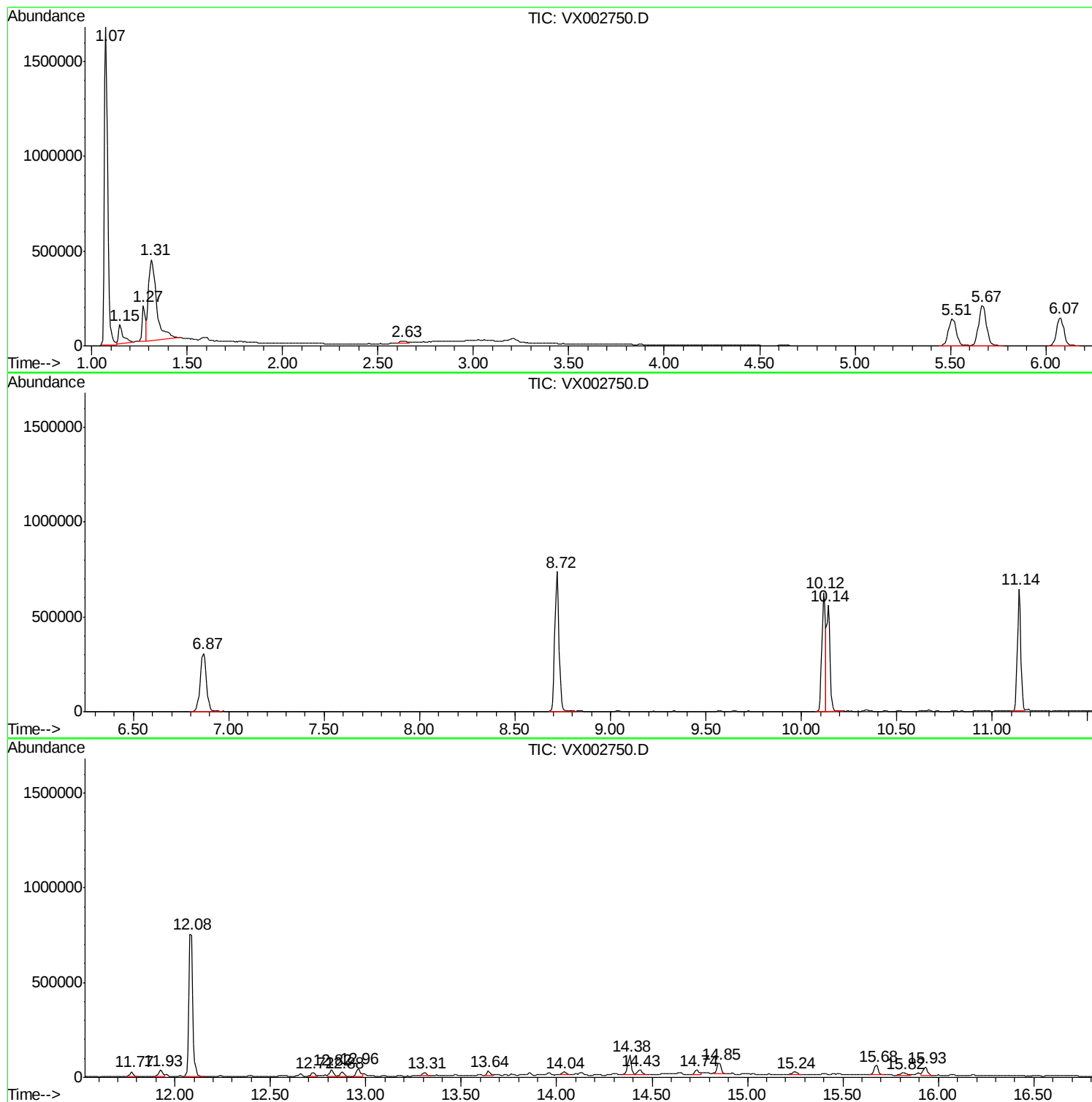
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X061518W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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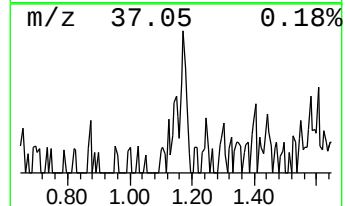
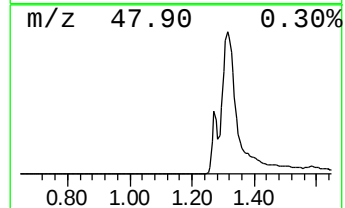
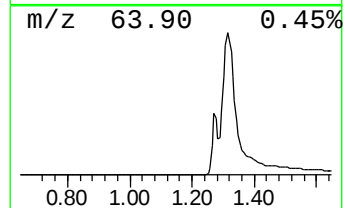
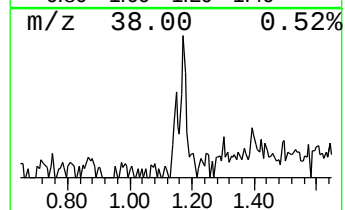
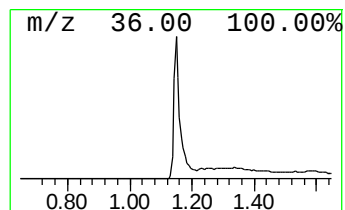
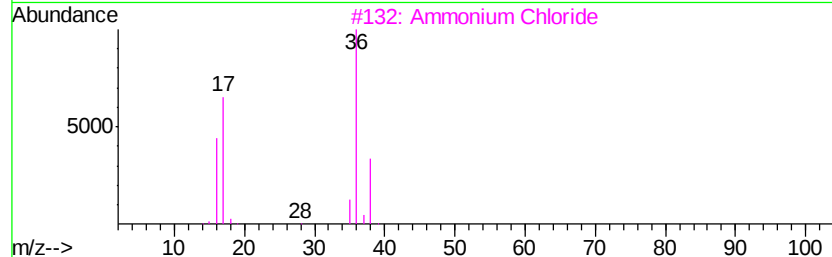
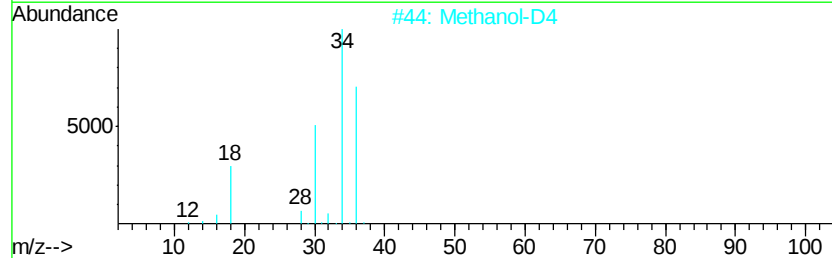
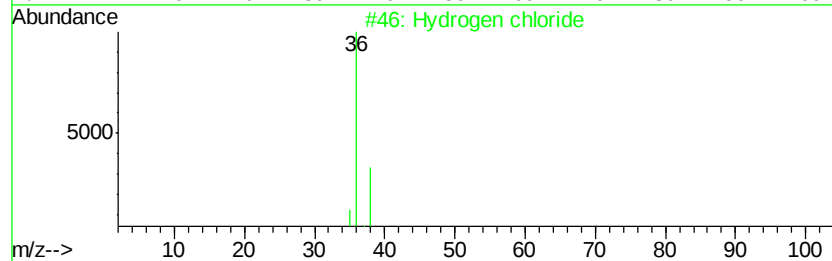
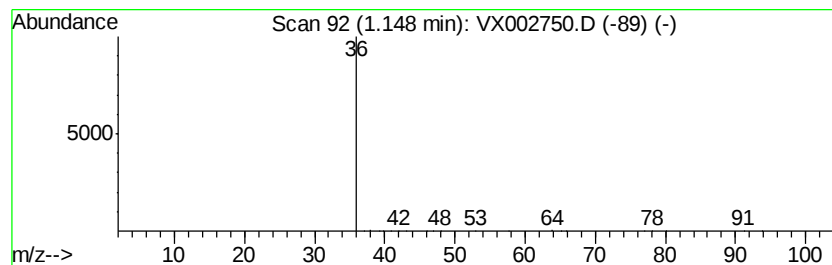
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown1.15 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.15	14.07 ug/l	165829	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydrogen chloride	36	ClH	007647-01-0	2
2		Methanol-D4	36	CD4O	000811-98-3	2
3		Ammonium Chloride	53	ClH4N	012125-02-9	1
4		2-Chloroethylamine	79	C2H6ClN	000689-98-5	1
5		Hydrogen sulfide	34	H2S	007783-06-4	1



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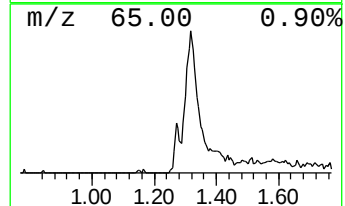
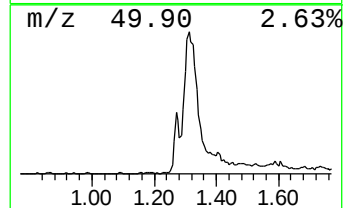
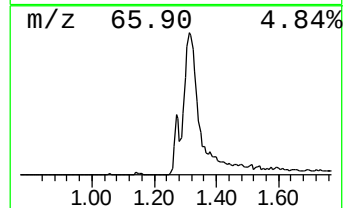
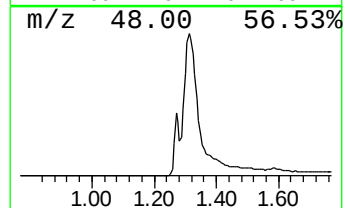
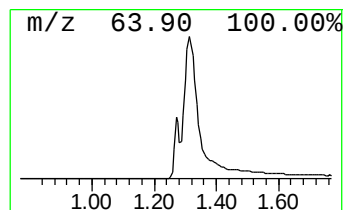
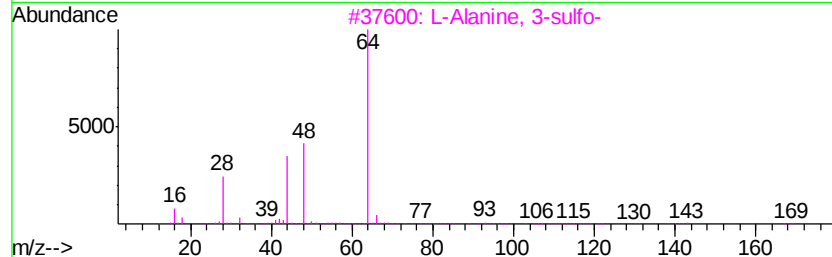
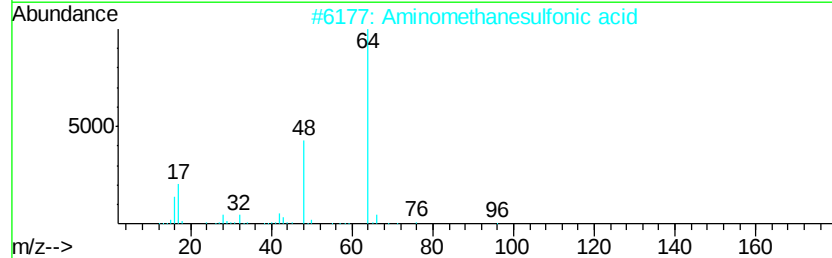
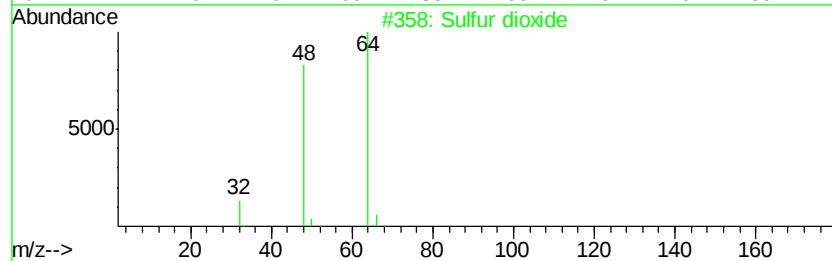
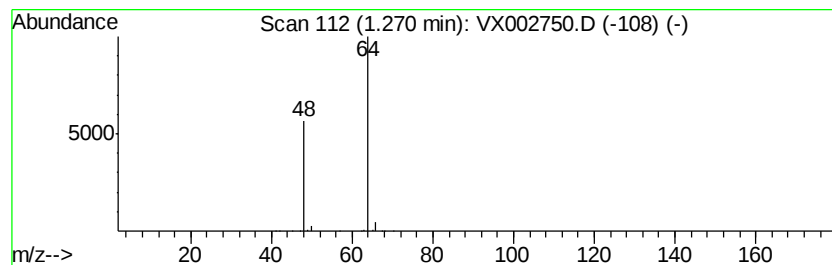
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Peak Number 3 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.27	17.96 ug/l	211697	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide		64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-		169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-		64	C2H2F2	000075-38-7	4
5	Ethyl Chloride		64	C2H5Cl	000075-00-3	3



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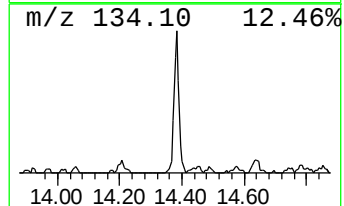
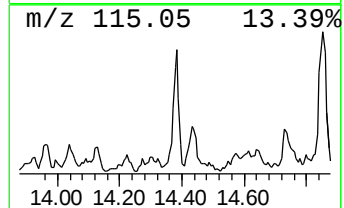
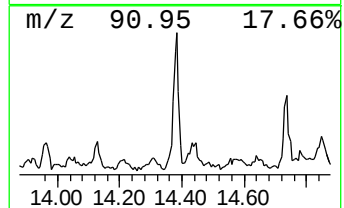
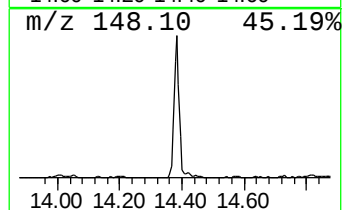
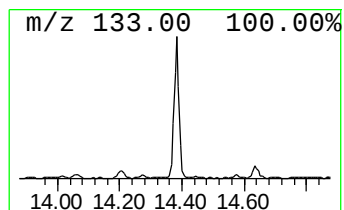
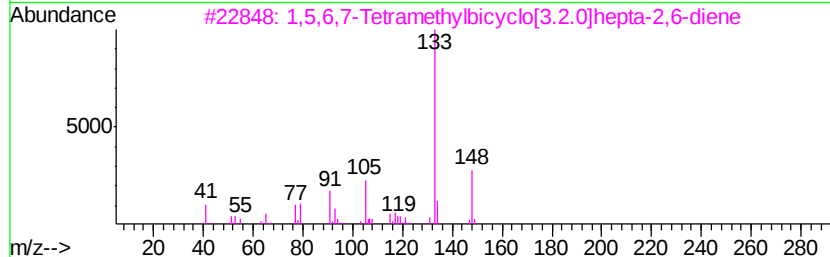
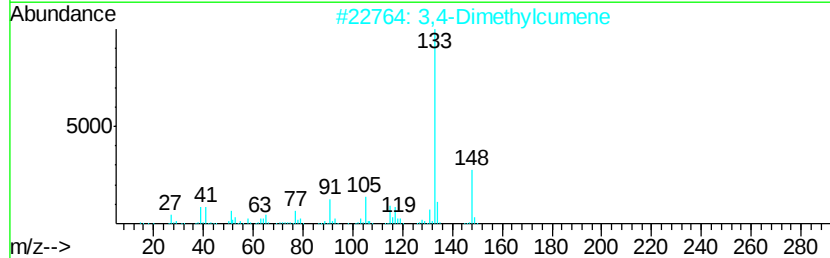
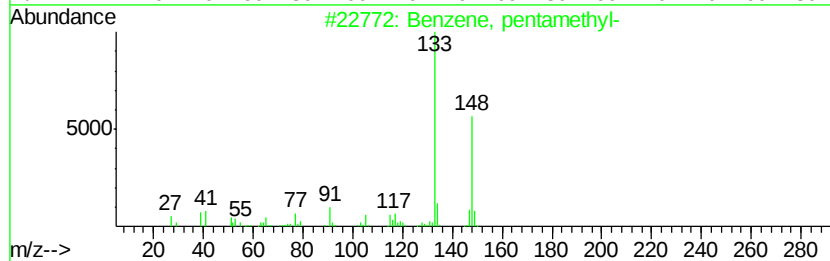
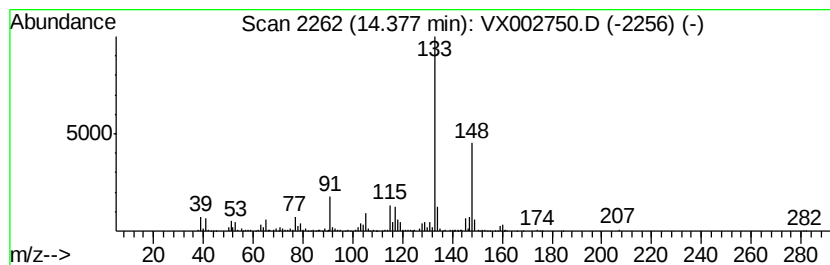
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Peak Number 5 Benzene, pentamethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	6.75 ug/l	139627	1,4-Dichlorobenzene-d4	12.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, pentamethyl-	148	C11H16	000700-12-9	95
2		3,4-Dimethylcumene	148	C11H16	1000370-34-1	87
3		1,5,6,7-Tetramethylbicyclo[3.2.0]hept-2,6-diene	148	C11H16	134329-46-7	83
4		Benzene, 1-ethyl-2,4,5-trimethyl-	148	C11H16	017851-27-3	80
5		Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.15	1.15	14.1	ug/l	165829	1	5.67	589385	50.0
Sulfur dioxide	1.27	18.0	ug/l	211697	1	5.67	589385	50.0
Benzene, pentamet...	14.38	6.8	ug/l	139627	4	12.09	1034140	50.0