

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX062518\
 Data File : VX002884.D
 Acq On : 26 Jun 2018 02:33
 Operator : JC/MD
 Sample : J3705-06
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 W-38

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\82X062518W.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	1924669	2238497	100.00%	16.507%
2	1.148	89	92	97	rBV	73202	94227	4.21%	0.695%
3	1.270	108	112	115	rBV	180846	232752	10.40%	1.716%
4	1.319	115	120	141	rVB	605377	1755171	78.41%	12.943%
5	1.581	161	163	172	rVB3	19247	33567	1.50%	0.248%
6	2.617	329	333	339	rBV3	14572	33280	1.49%	0.245%
7	5.507	795	807	821	rBV	167044	471451	21.06%	3.477%
8	5.666	821	833	846	rVV	250304	690178	30.83%	5.090%
9	6.074	888	900	915	rBV	175943	458246	20.47%	3.379%
10	6.867	1020	1030	1047	rBV	353375	822250	36.73%	6.064%
11	8.720	1327	1334	1343	rBV	855603	1304477	58.27%	9.620%
12	10.116	1557	1563	1579	rBV	729663	1016499	45.41%	7.496%
13	11.140	1725	1731	1736	rBV	773848	957327	42.77%	7.060%
14	12.079	1880	1885	1896	rVB	931149	1173863	52.44%	8.656%
15	12.238	1906	1911	1915	rBV	49942	60478	2.70%	0.446%
16	12.652	1974	1979	1985	rVB4	13956	29184	1.30%	0.215%
17	12.725	1985	1991	1996	rBV4	38054	70341	3.14%	0.519%
18	12.817	2003	2006	2011	rVB	34812	46347	2.07%	0.342%
19	12.878	2011	2016	2022	rVB2	43879	63773	2.85%	0.470%
20	12.957	2022	2029	2032	rBV	56738	95304	4.26%	0.703%
21	13.304	2082	2086	2091	rBV	32045	44985	2.01%	0.332%
22	13.469	2108	2113	2119	rBV5	26719	55147	2.46%	0.407%
23	13.640	2137	2141	2146	rBV	41503	67792	3.03%	0.500%
24	13.817	2166	2170	2173	rBV5	16188	26474	1.18%	0.195%
25	13.859	2173	2177	2181	rVB	50120	69407	3.10%	0.512%
26	13.908	2181	2185	2190	rBV6	19360	44357	1.98%	0.327%
27	13.963	2190	2194	2196	rBV2	22200	26792	1.20%	0.198%
28	14.036	2203	2206	2211	rVB3	24368	30335	1.36%	0.224%
29	14.127	2218	2221	2224	rVB4	27341	32122	1.43%	0.237%
30	14.292	2241	2248	2256	rBV4	36920	116424	5.20%	0.859%
31	14.377	2256	2262	2267	rVV	147954	218446	9.76%	1.611%
32	14.432	2267	2271	2277	rVV4	50690	88396	3.95%	0.652%
33	14.481	2277	2279	2286	rVB4	15620	24539	1.10%	0.181%
34	14.573	2287	2294	2297	rBV8	18960	43963	1.96%	0.324%

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35	14.640	2302	2305	2308	rBV2	17919	25200	1.13%	0.186%
36	14.676	2308	2311	2317	rVB5	27629	42147	1.88%	0.311%
37	14.737	2317	2321	2324	rBV3	42114	64395	2.88%	0.475%
38	14.853	2335	2340	2344	rVB	114958	172777	7.72%	1.274%
39	14.914	2346	2350	2354	rVB3	43044	61121	2.73%	0.451%
40	14.981	2354	2361	2366	rBV9	23965	59581	2.66%	0.439%
41	15.255	2400	2406	2410	rBV2	49564	83634	3.74%	0.617%
42	15.396	2425	2429	2435	rBV4	42046	76126	3.40%	0.561%
43	15.670	2471	2474	2479	rVB	18827	25920	1.16%	0.191%
44	15.737	2481	2485	2490	rVB3	21317	38775	1.73%	0.286%
45	15.810	2493	2497	2503	rBV3	27078	59265	2.65%	0.437%
46	15.895	2507	2511	2514	rVV	44698	86518	3.87%	0.638%
47	15.926	2514	2516	2523	rVB	65512	95253	4.26%	0.702%
48	16.072	2535	2540	2553	rVB2	46082	106777	4.77%	0.787%
49	16.176	2553	2557	2567	rVB2	12119	26756	1.20%	0.197%

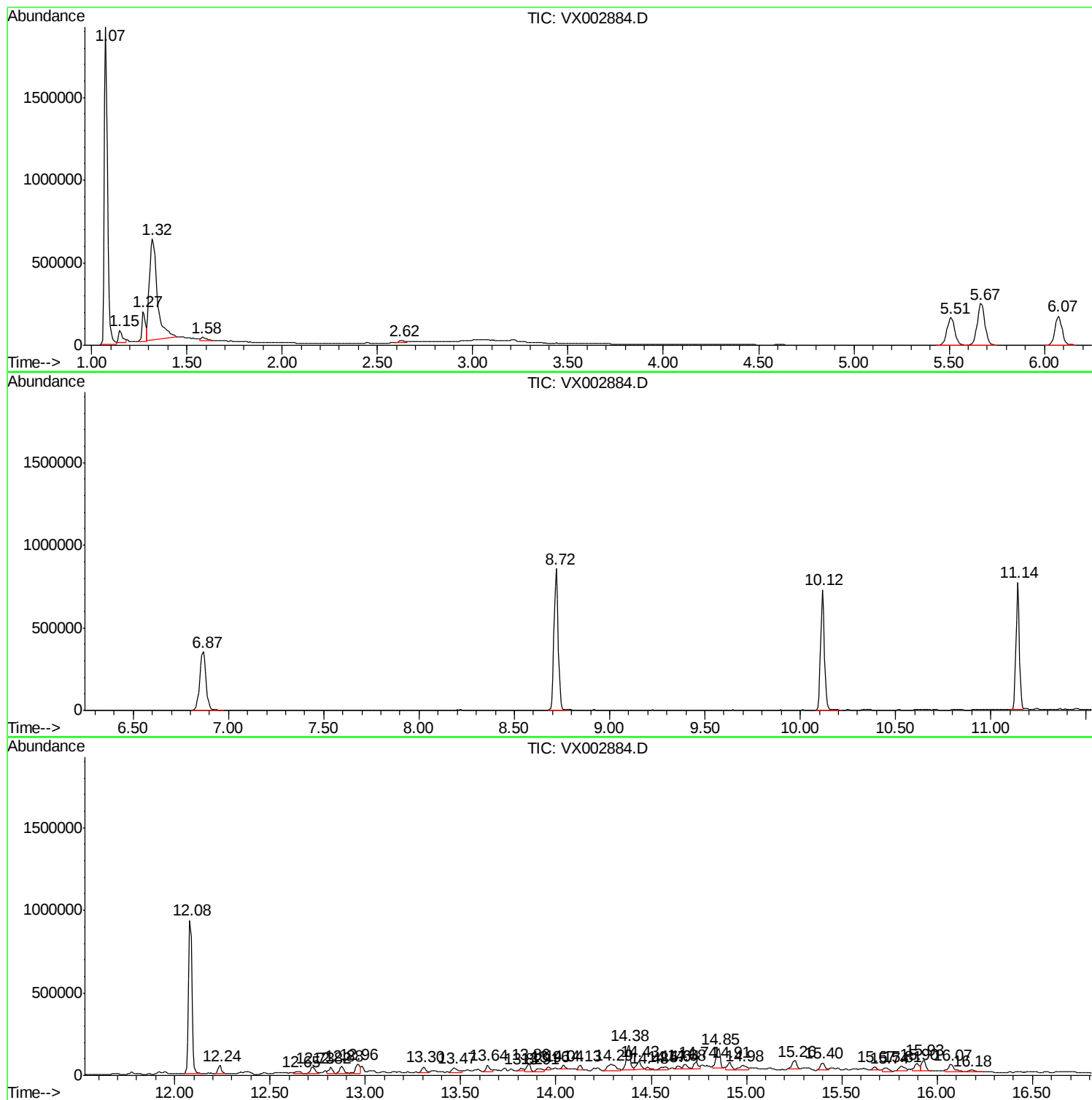
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Quant Title : SW846 8260

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



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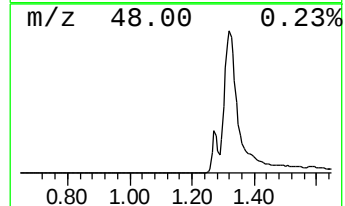
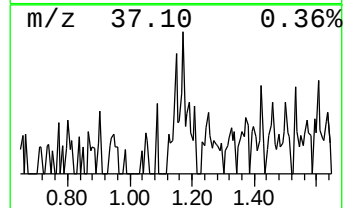
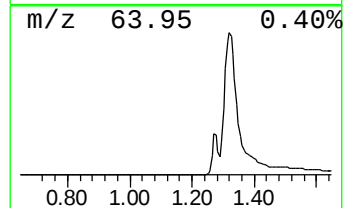
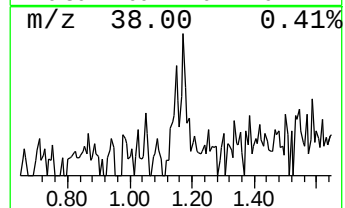
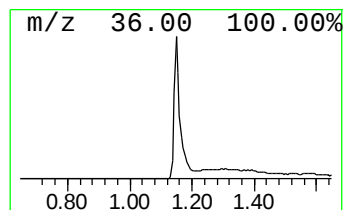
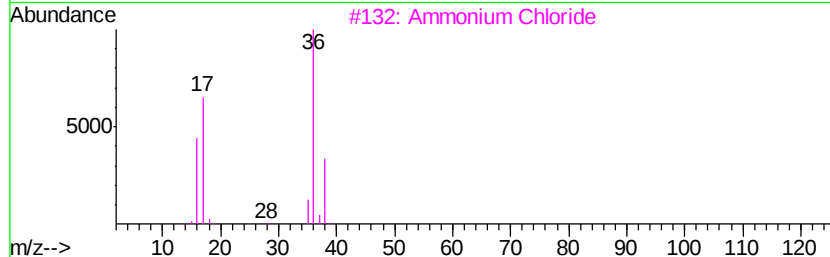
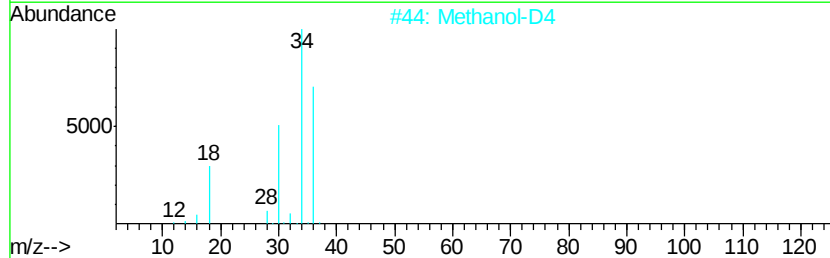
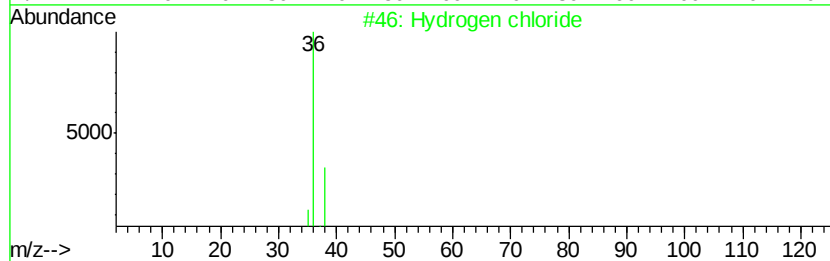
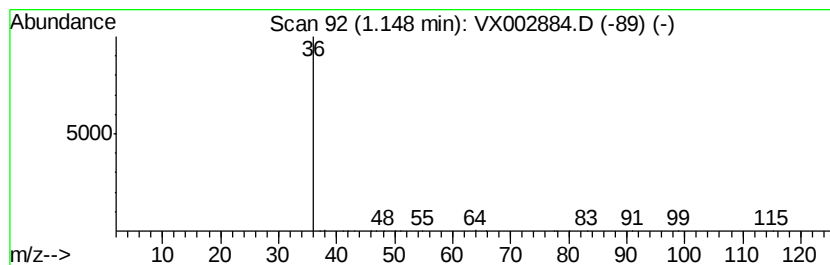
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X062518W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown1.15 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.15	6.83 ug/l	94227	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		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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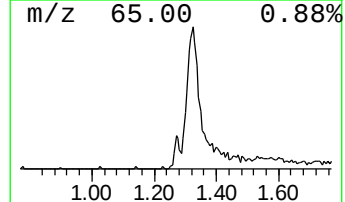
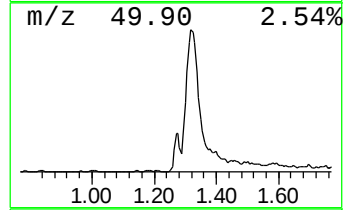
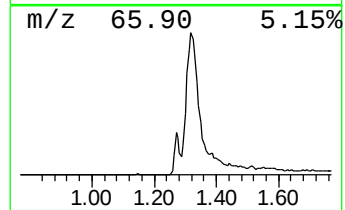
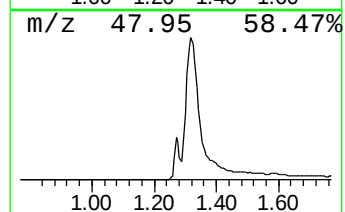
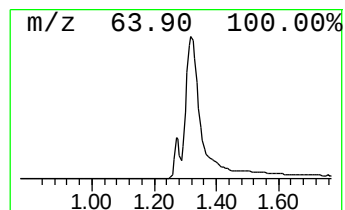
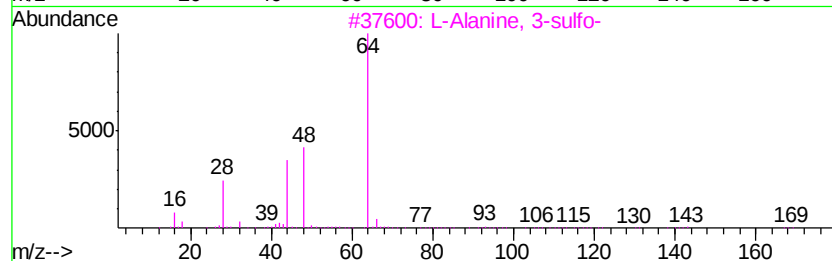
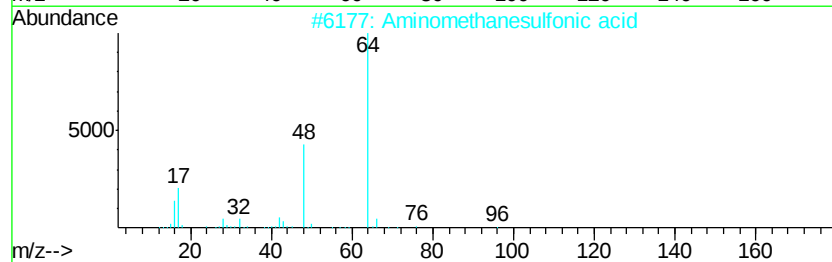
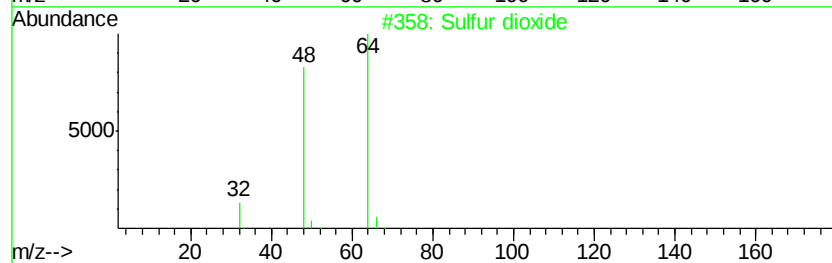
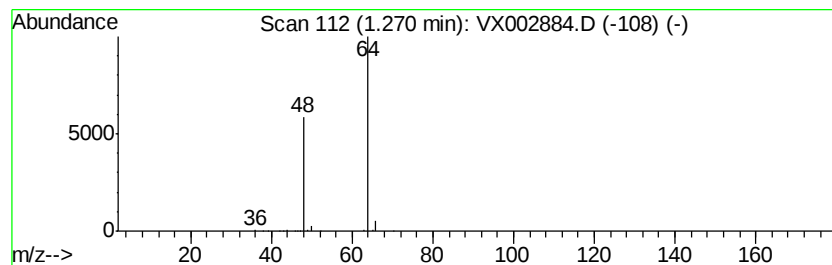
Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.27	16.86 ug/l	232752	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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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
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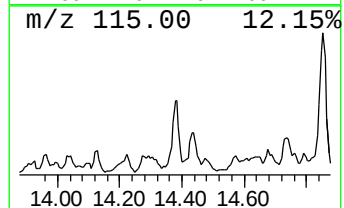
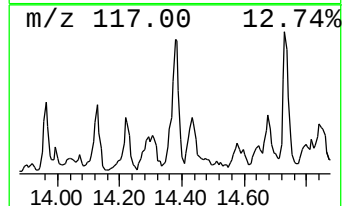
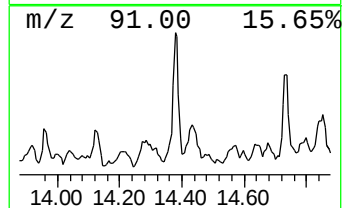
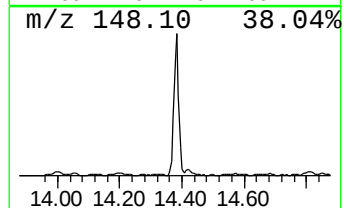
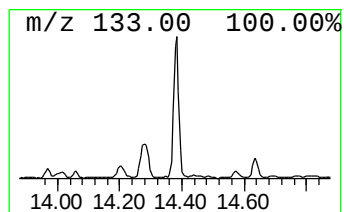
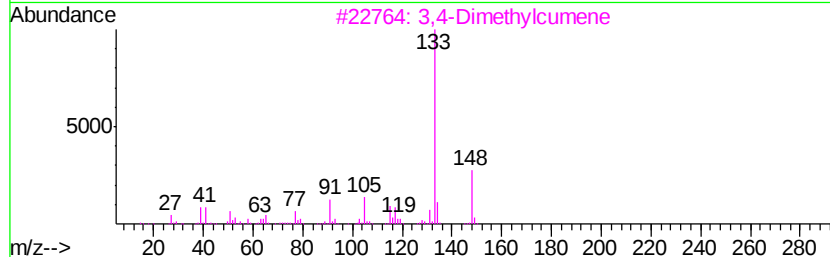
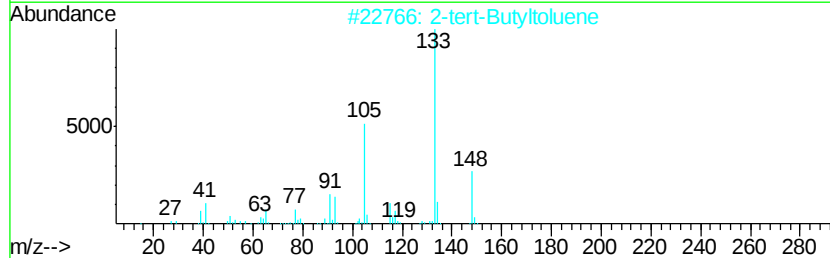
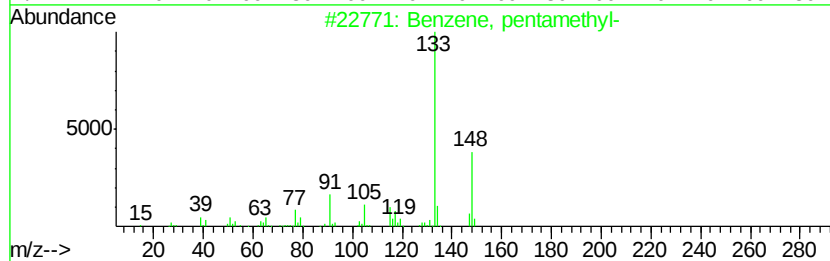
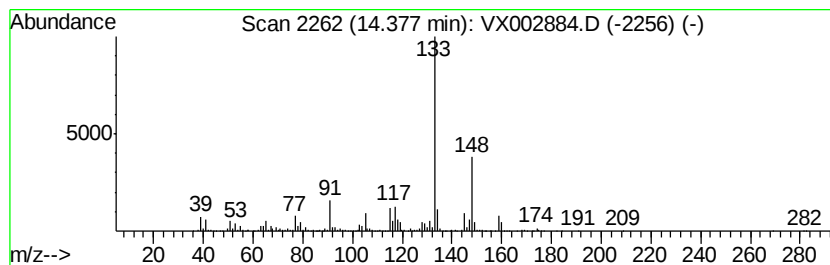
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzene, pentamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	9.30 ug/l	218446	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, pentamethyl-	148	C11H16	000700-12-9	94
2		2-tert-Butyltoluene	148	C11H16	001074-92-6	81
3		3,4-Dimethylcumene	148	C11H16	1000370-34-1	81
4		Benzene, 2,4-diethyl-1-methyl-	148	C11H16	001758-85-6	74
5		Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	74



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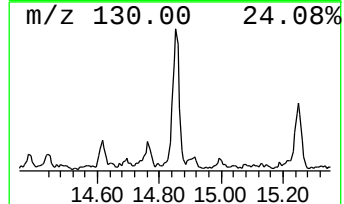
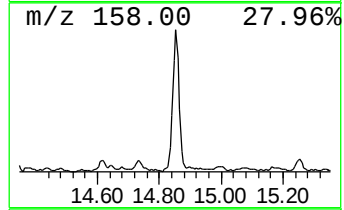
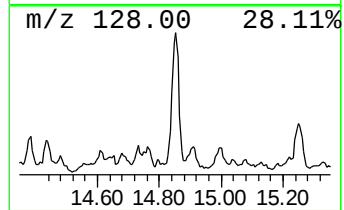
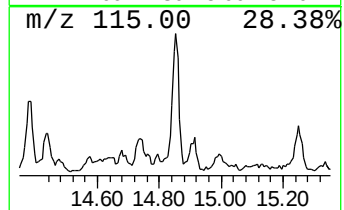
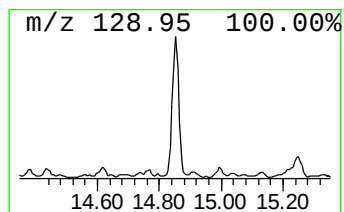
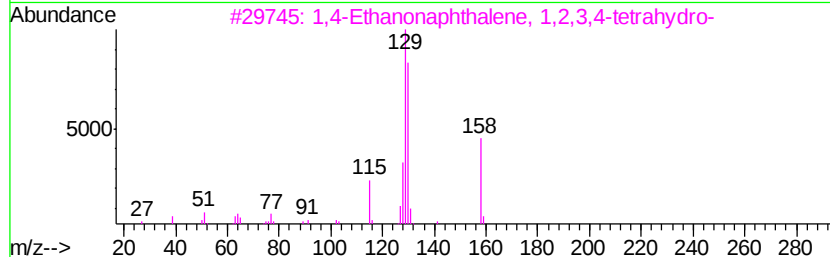
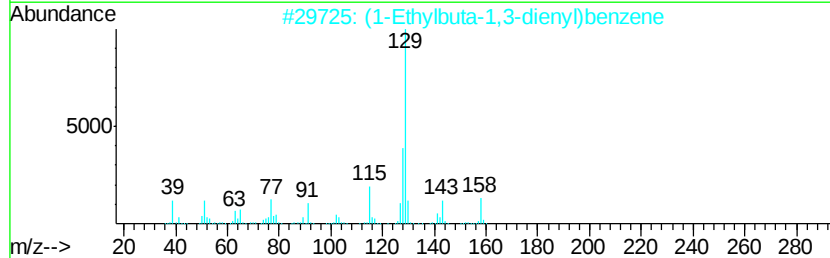
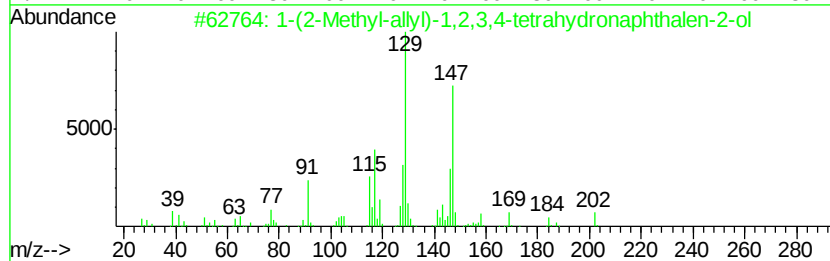
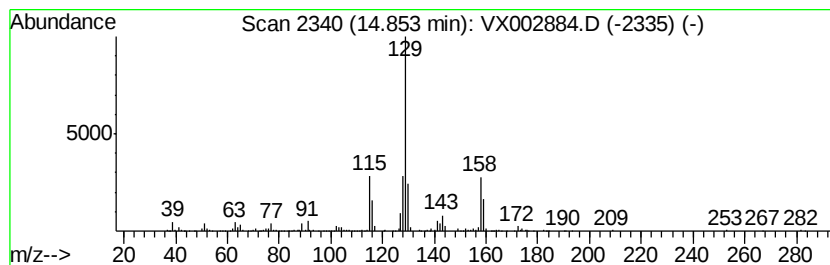
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-(2-Methyl-allyl)-1,2,3,4-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	7.36 ug/l	172777	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-(2-Methyl-allyl)-1,2,3,4-tetra...	202	C14H18O	1000192-52-9	59
2		(1-Ethylbuta-1,3-dienyl)benzene	158	C12H14	1000210-05-6	53
3		1,4-Ethanonaphthalene, 1,2,3,4-t...	158	C12H14	004175-52-4	50
4		Benzene, 1,3-hexadienyl-	158	C12H14	041635-77-2	46
5		Fluorene, 1,2,3,4,4a,9a-hexahydr...	172	C13H16	001559-97-3	42



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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
unknown1.15	1.15	6.8	ug/l	94227	1	5.67	690178	50.0
Sulfur dioxide	1.27	16.9	ug/l	232752	1	5.67	690178	50.0
Benzene, pentamet...	14.38	9.3	ug/l	218446	4	12.08	1173860	50.0
1-(2-Methyl-allyl...	14.85	7.4	ug/l	172777	4	12.08	1173860	50.0