

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061219\
 Data File : VX010256.D
 Acq On : 12 Jun 2019 17:21
 Operator : JC/SP
 Sample : K3309-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 LF001MW001-190610

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\82X060719W.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	1.367	32	35	39	rBV	20067565	41825467	63.09%	13.895%
2	2.434	204	210	214	rBV	2516237	4538880	6.85%	1.508%
3	2.477	214	217	231	rVV	3291476	5463821	8.24%	1.815%
4	4.592	553	564	570	rVV	1546553	4379813	6.61%	1.455%
5	4.665	570	576	598	rVB	1629326	4729814	7.13%	1.571%
6	5.659	731	739	755	rVB2	317082	898671	1.36%	0.299%
7	6.141	811	818	832	rVB	403758	1064041	1.60%	0.353%
8	6.860	925	936	942	rBV	459748	1117941	1.69%	0.371%
9	8.482	1193	1202	1218	rBV	730448	1404874	2.12%	0.467%
10	8.671	1218	1233	1239	rBV	22967851	58729935	88.59%	19.511%
11	8.726	1239	1242	1247	rVV	748678	1349025	2.03%	0.448%
12	8.811	1247	1256	1261	rVB2	32630665	66296748	100.00%	22.024%
13	9.091	1296	1302	1311	rBV	1511777	2152251	3.25%	0.715%
14	10.140	1465	1474	1480	rVB	9065973	13823717	20.85%	4.592%
15	10.250	1486	1492	1498	rBV	6170961	7968781	12.02%	2.647%
16	10.360	1502	1510	1516	rVB	12395243	16608808	25.05%	5.518%
17	10.701	1560	1566	1571	rBV	7775408	10180900	15.36%	3.382%
18	11.134	1632	1637	1643	rBV	944851	1208278	1.82%	0.401%
19	11.359	1669	1674	1680	rBV	564584	694317	1.05%	0.231%
20	11.432	1680	1686	1693	rVV	2113897	3630696	5.48%	1.206%
21	11.506	1693	1698	1704	rVB	2369403	2858991	4.31%	0.950%
22	11.664	1719	1724	1729	rBV	1297701	1595648	2.41%	0.530%
23	11.804	1742	1747	1753	rVB	6659042	7947917	11.99%	2.640%
24	12.024	1776	1783	1787	rBV	1491235	1835284	2.77%	0.610%
25	12.097	1787	1795	1798	rVV2	2921778	5261000	7.94%	1.748%
26	12.140	1798	1802	1808	rVB	3455023	4183401	6.31%	1.390%
27	12.298	1821	1828	1830	rBV	635499	822696	1.24%	0.273%
28	12.396	1836	1844	1849	rVB	16516062	23514248	35.47%	7.812%
29	13.828	2073	2079	2085	rVB	3760189	4931036	7.44%	1.638%

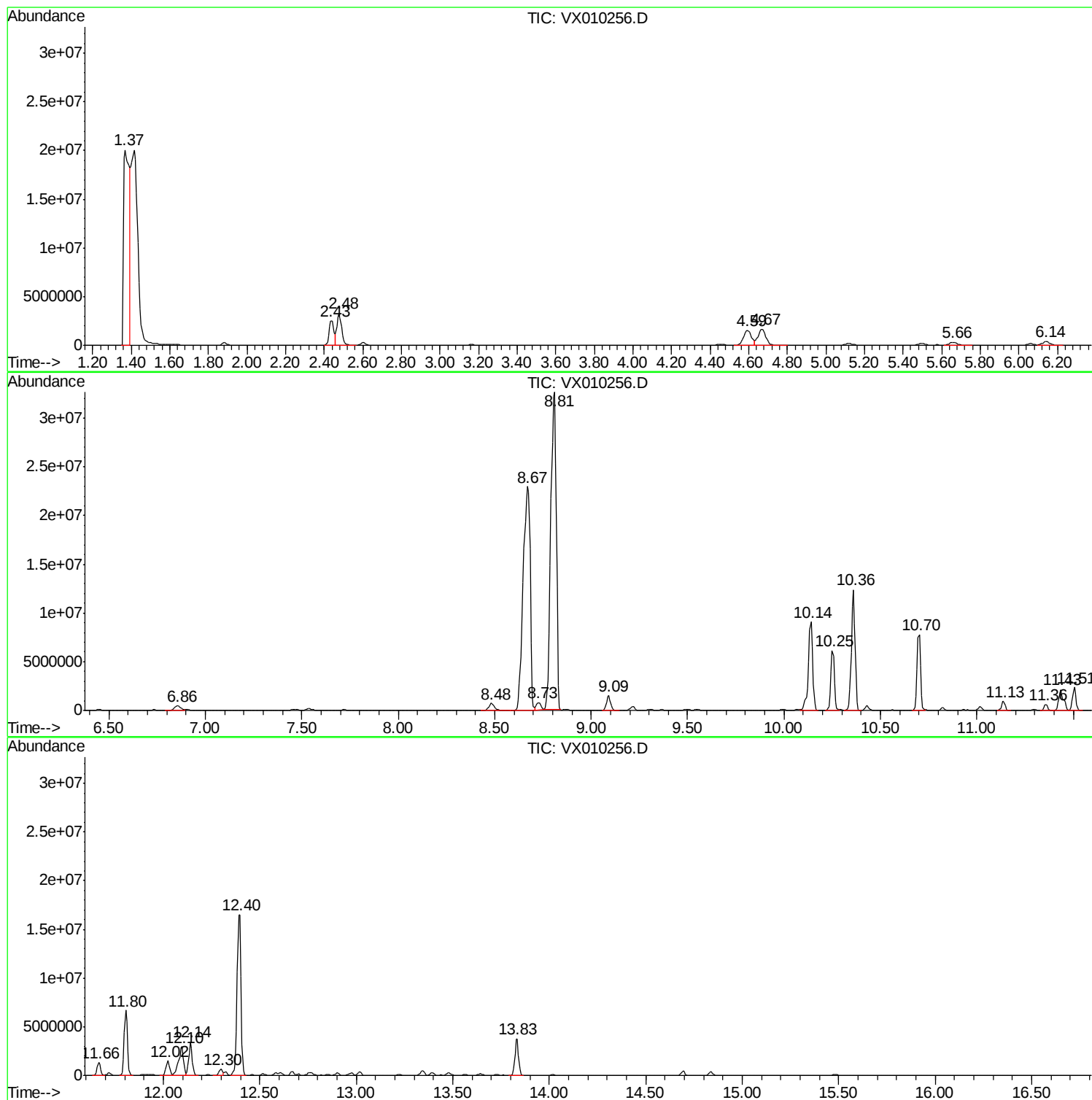
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Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX061219\
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Sample : K3309-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LF001MW001-190610

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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



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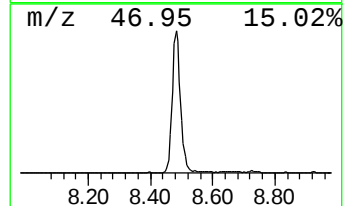
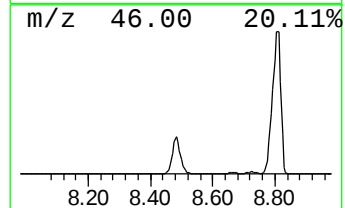
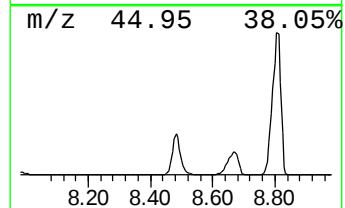
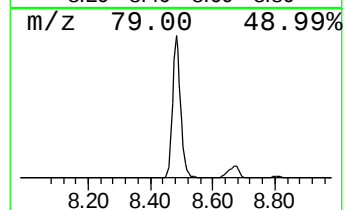
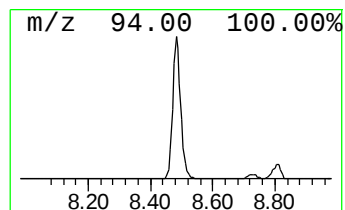
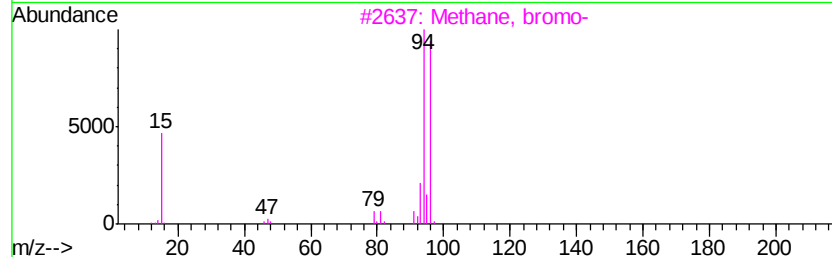
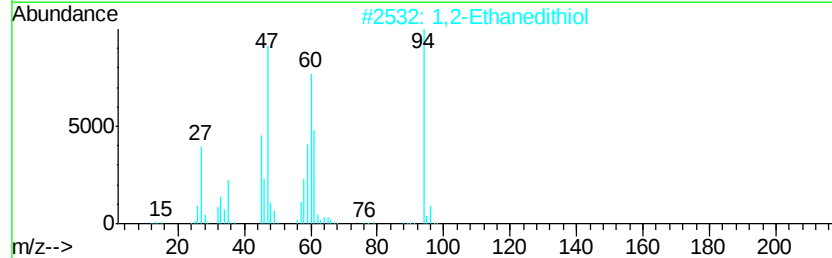
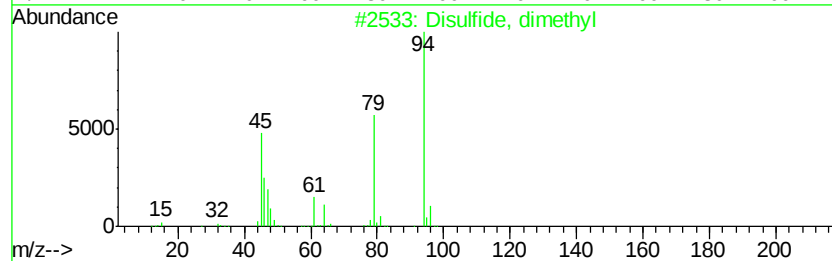
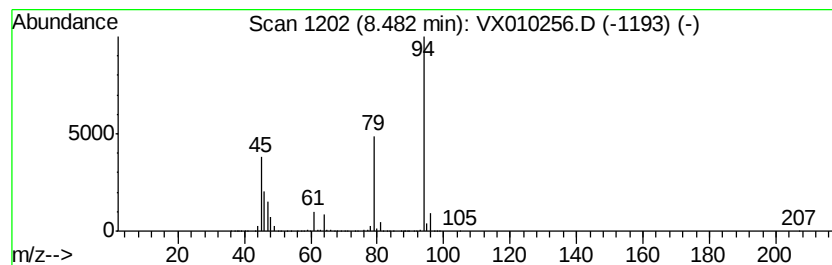
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X060719W.M
Quant Title : SW846 8260

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

Peak Number 1 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.48	62.83 ug/l	1404870	1,4-Difluorobenzene	6.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
2	1,2-Ethanedithiol	94	C2H6S2	000540-63-6	58
3	Methane, bromo-	94	CH3Br	000074-83-9	5
4	Ethanol	46	C2H6O	000064-17-5	4
5	Fampridine	94	C5H6N2	000504-24-5	4



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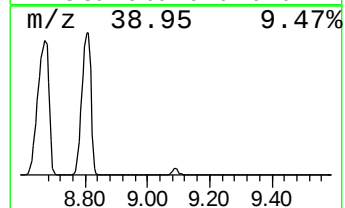
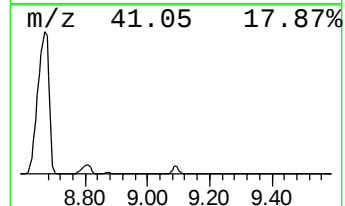
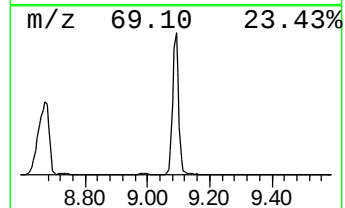
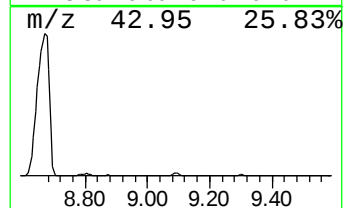
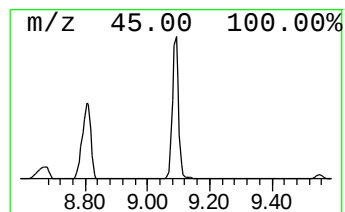
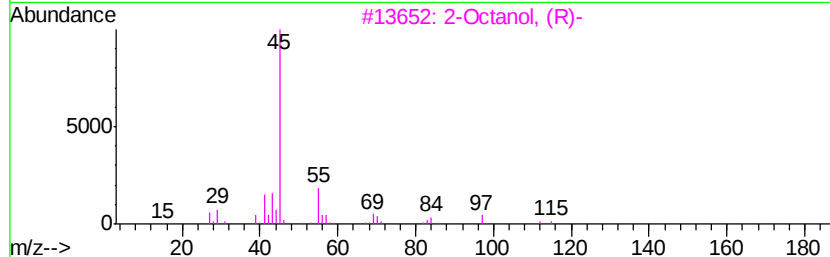
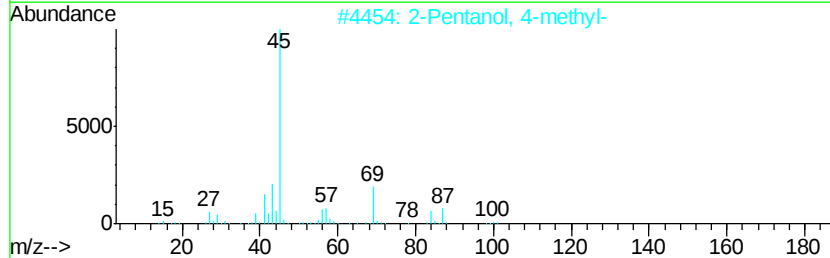
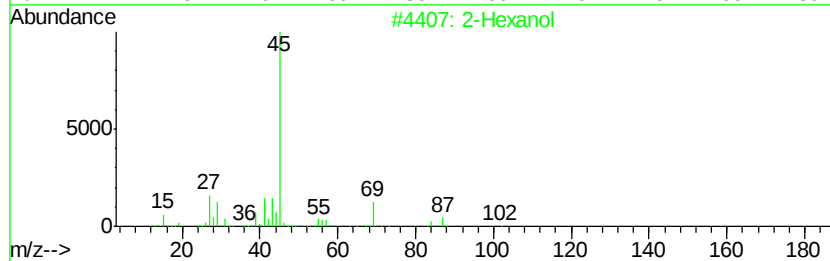
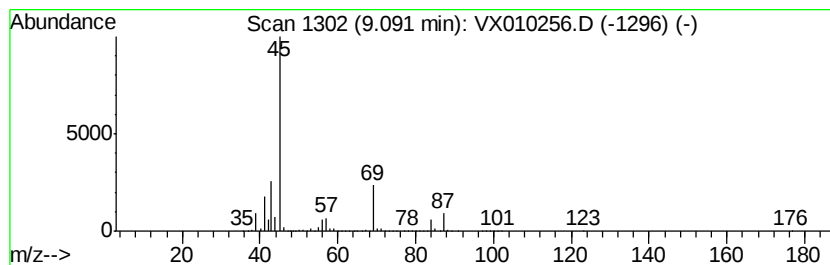
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Quant Title : SW846 8260

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

Peak Number 2 2-Hexanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	7.78 ug/l	2152250	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanol	102	C6H14O	000626-93-7	83
2		2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	83
3		2-Octanol, (R)-	130	C8H18O	005978-70-1	78
4		2-Octanol, (S)-	130	C8H18O	006169-06-8	78
5		2-Octanol	130	C8H18O	000123-96-6	64



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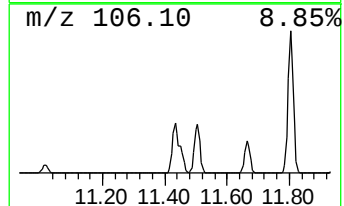
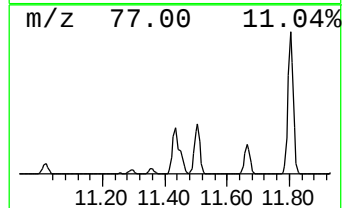
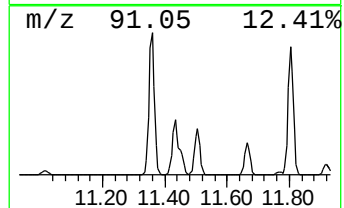
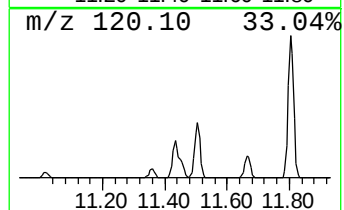
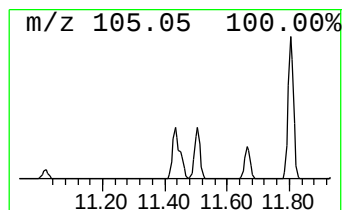
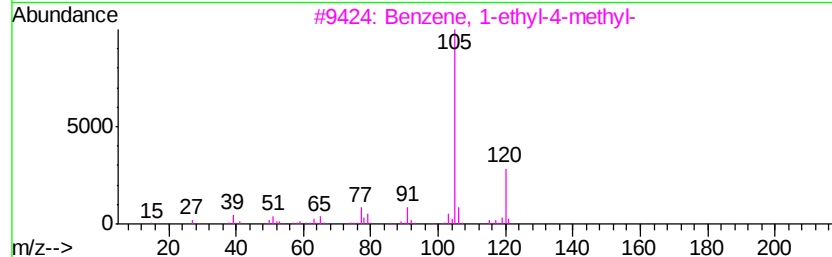
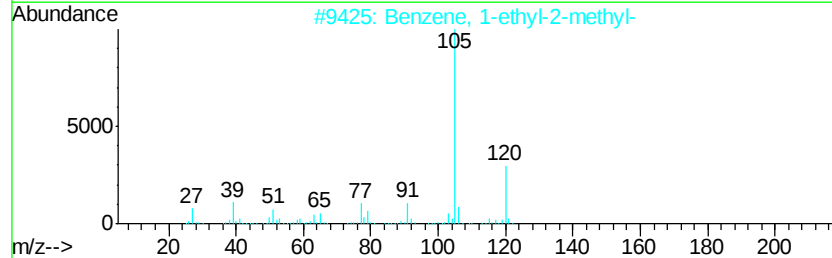
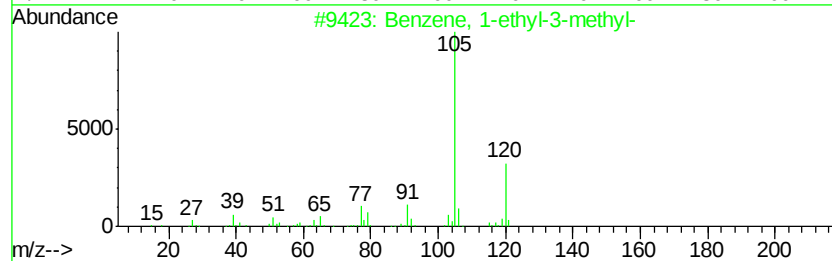
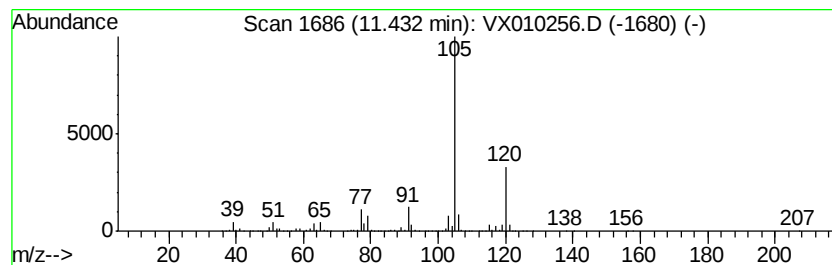
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Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	34.51 ug/l	3630700	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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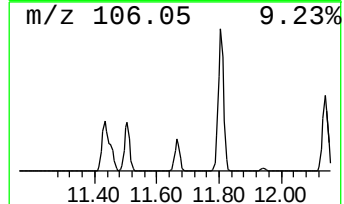
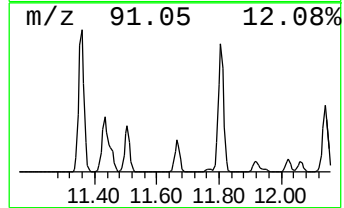
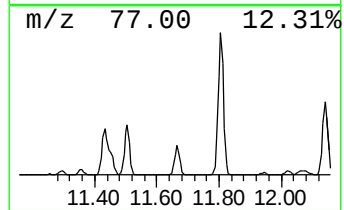
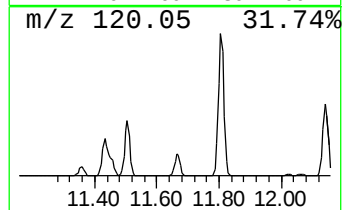
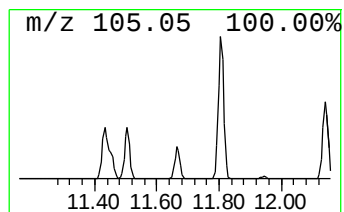
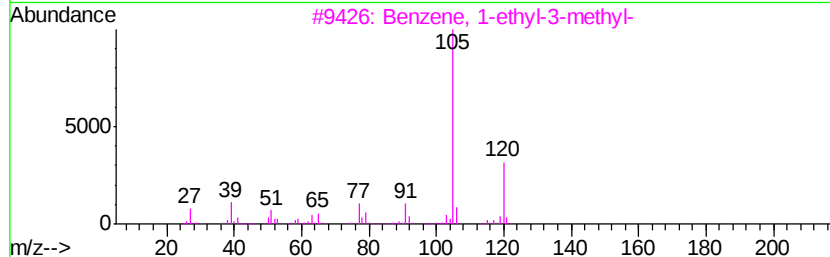
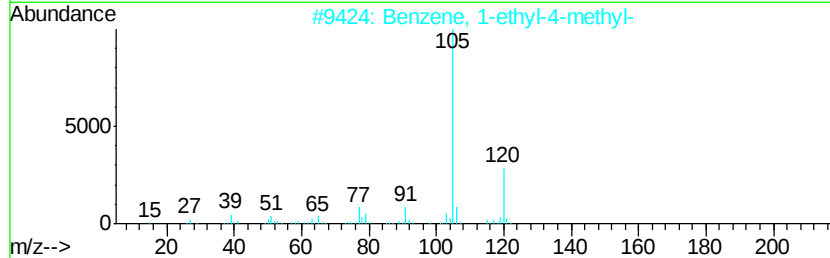
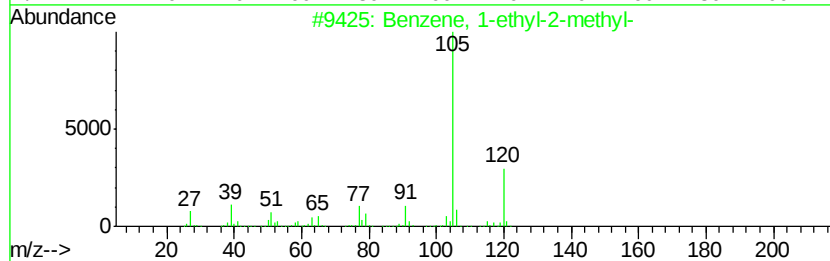
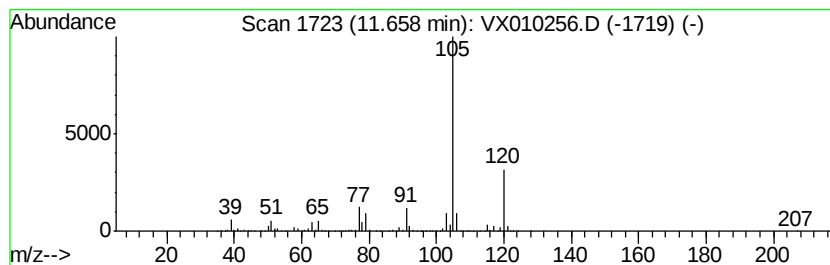
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Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	15.16 ug/l	1595650	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5		Mesitylene	120	C9H12	000108-67-8	91



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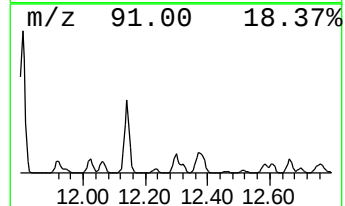
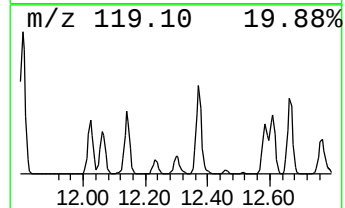
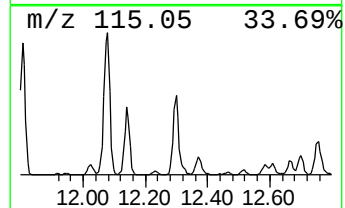
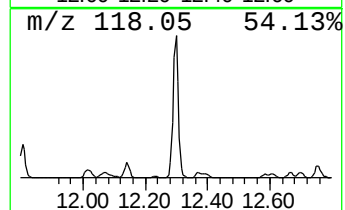
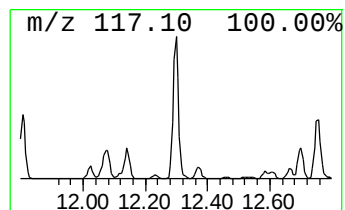
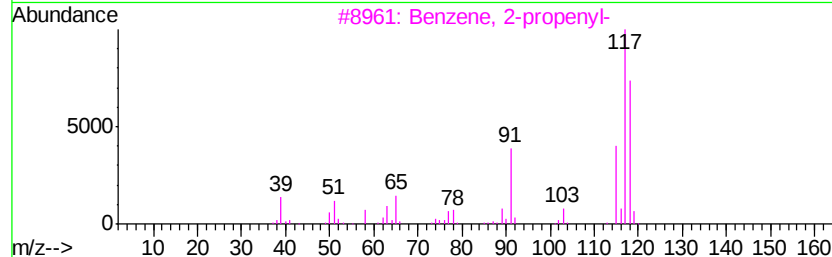
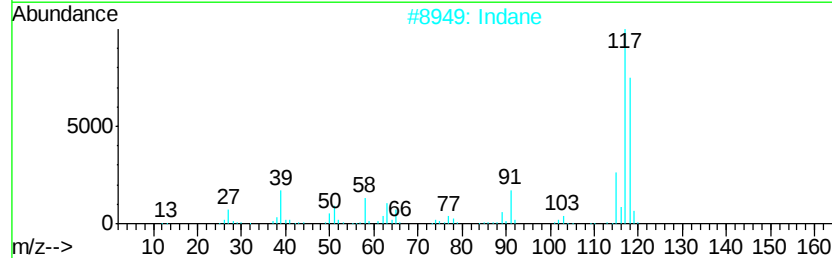
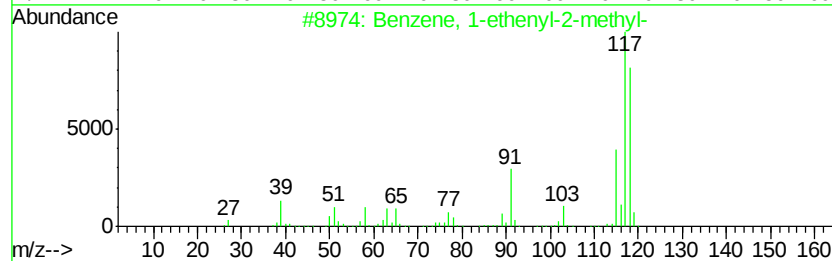
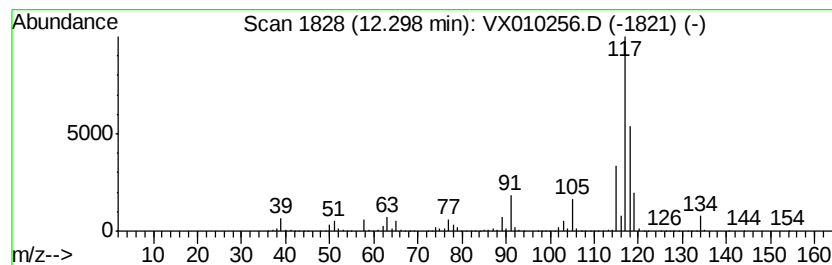
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Peak Number 5 Benzene, 1-ethenyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	7.82 ug/l	822696	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1-ethenyl-2-methyl-	118 C9H10	000611-15-4 87
2		Indane	118 C9H10	000496-11-7 76
3		Benzene, 2-propenyl-	118 C9H10	000300-57-2 76
4		Benzene, cyclopropyl-	118 C9H10	000873-49-4 70
5		Deltacyclene	118 C9H10	007785-10-6 58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, dimethyl	8.48	62.8	ug/l	1404870	2	6.86	1117940	50.0
2-Hexanol	9.09	7.8	ug/l	2152250	3	10.12	13823700	50.0
Benzene, 1-ethyl-...	11.43	34.5	ug/l	3630700	4	12.08	5261000	50.0
Benzene, 1-ethyl-...	11.66	15.2	ug/l	1595650	4	12.08	5261000	50.0
Benzene, 1-etheny...	12.30	7.8	ug/l	822696	4	12.08	5261000	50.0