

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120121\
 Data File : VX025412.D
 Acq On : 01 Dec 2021 14:48
 Operator : JC/MD
 Sample : M4866-19
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 16953

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
 Title : SW846 8260

Signal : TIC: VX025412.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.124	3	6	7	rBV	14782	11342	1.30%	0.200%
2	1.246	22	26	42	rBV	388188	870590	100.00%	15.377%
3	2.380	205	212	217	rBV	5898	9518	1.09%	0.168%
4	2.532	229	237	243	rBV	9774	21862	2.51%	0.386%
5	2.959	300	307	313	rBV2	3967	8742	1.00%	0.154%
6	3.696	420	428	441	rBV4	3783	10277	1.18%	0.182%
7	5.391	695	706	719	rBV	71118	202204	23.23%	3.571%
8	5.556	722	733	749	rVB	115134	320061	36.76%	5.653%
9	5.958	789	799	816	rBV	70270	188791	21.69%	3.335%
10	6.763	921	931	949	rVV	179273	423467	48.64%	7.480%
11	8.653	1234	1241	1248	rBV	367242	579518	66.57%	10.236%
12	8.720	1248	1252	1260	rVB	8475	13846	1.59%	0.245%
13	10.055	1465	1471	1486	rVB	378912	506727	58.21%	8.950%
14	11.085	1634	1640	1646	rBV	296235	389481	44.74%	6.879%
15	11.366	1680	1686	1691	rBV	115946	143878	16.53%	2.541%
16	11.421	1691	1695	1697	rVV	11028	15001	1.72%	0.265%
17	11.457	1697	1701	1706	rVV	70901	89451	10.27%	1.580%
18	11.506	1706	1709	1717	rVB2	7673	10559	1.21%	0.187%
19	11.750	1744	1749	1756	rVB	23721	30632	3.52%	0.541%
20	11.975	1780	1786	1787	rBV	13733	16851	1.94%	0.298%
21	12.018	1787	1793	1801	rVV3	463728	769348	88.37%	13.589%
22	12.091	1801	1805	1808	rVV	9963	12490	1.43%	0.221%
23	12.323	1839	1843	1847	rBV4	6984	14054	1.61%	0.248%
24	12.536	1871	1878	1879	rBV3	6316	10701	1.23%	0.189%
25	12.555	1879	1881	1886	rVV2	9396	10452	1.20%	0.185%
26	12.616	1886	1891	1894	rVV	7337	9065	1.04%	0.160%
27	12.664	1895	1899	1903	rVV	17329	21957	2.52%	0.388%
28	12.701	1903	1905	1914	rVB3	5525	9666	1.11%	0.171%
29	12.853	1927	1930	1935	rVB3	11104	15124	1.74%	0.267%
30	12.920	1935	1941	1944	rBV3	10048	16719	1.92%	0.295%
31	12.963	1944	1948	1952	rVB	14775	19086	2.19%	0.337%
32	13.054	1960	1963	1971	rVB5	10736	20182	2.32%	0.356%
33	13.170	1974	1982	1985	rBV4	12128	25452	2.92%	0.450%
34	13.292	1997	2002	2013	rVB3	40145	84782	9.74%	1.497%
35	13.426	2018	2024	2029	rVB	24817	39467	4.53%	0.697%
36	13.591	2046	2051	2054	rBV3	18178	29579	3.40%	0.522%

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37	13.664	2061	2063	2069	rVB2	8790	11961	1.37%	0.211%
38	13.749	2069	2077	2079	rBV5	12413	23750	2.73%	0.419%
39	13.786	2079	2083	2092	rVV2	48846	107638	12.36%	1.901%
40	13.884	2095	2099	2103	rVV	157504	196149	22.53%	3.465%
41	13.926	2103	2106	2108	rVV3	14715	22081	2.54%	0.390%
42	13.963	2108	2112	2122	rVB	65320	94728	10.88%	1.673%
43	14.079	2127	2131	2139	rBV2	18018	30692	3.53%	0.542%
44	14.231	2149	2156	2167	rVB2	26489	57968	6.66%	1.024%
45	14.323	2167	2171	2176	rVV2	6504	8745	1.00%	0.154%
46	14.371	2176	2179	2184	rVB2	9373	11798	1.36%	0.208%
47	14.481	2192	2197	2203	rBV2	21919	28858	3.31%	0.510%
48	14.640	2215	2223	2226	rBV2	23470	39658	4.56%	0.700%
49	14.780	2241	2246	2250	rBV	19973	25274	2.90%	0.446%
50	15.182	2308	2312	2320	rVB2	6785	13439	1.54%	0.237%
51	15.597	2376	2380	2387	rVB3	9284	17946	2.06%	0.317%

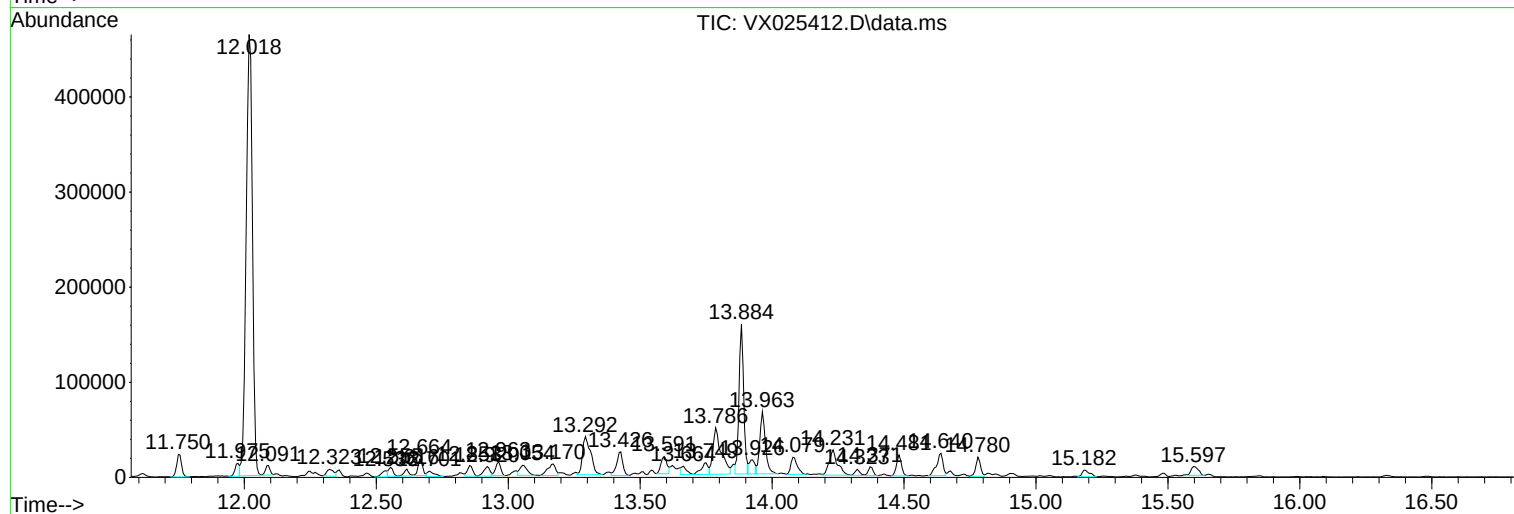
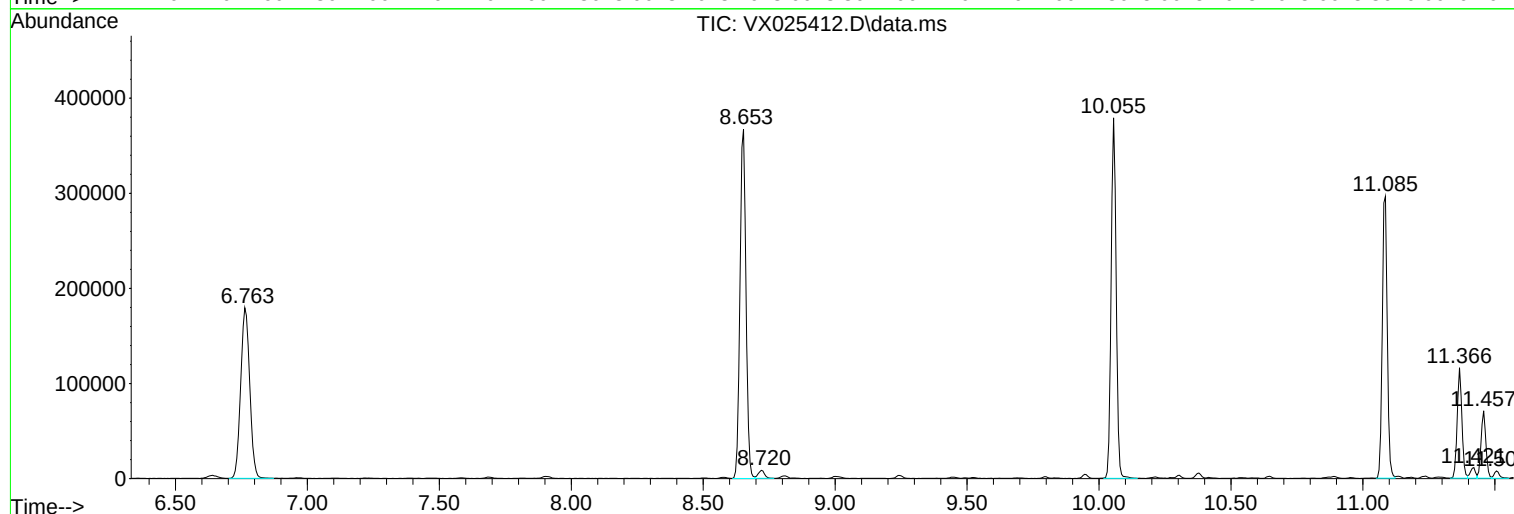
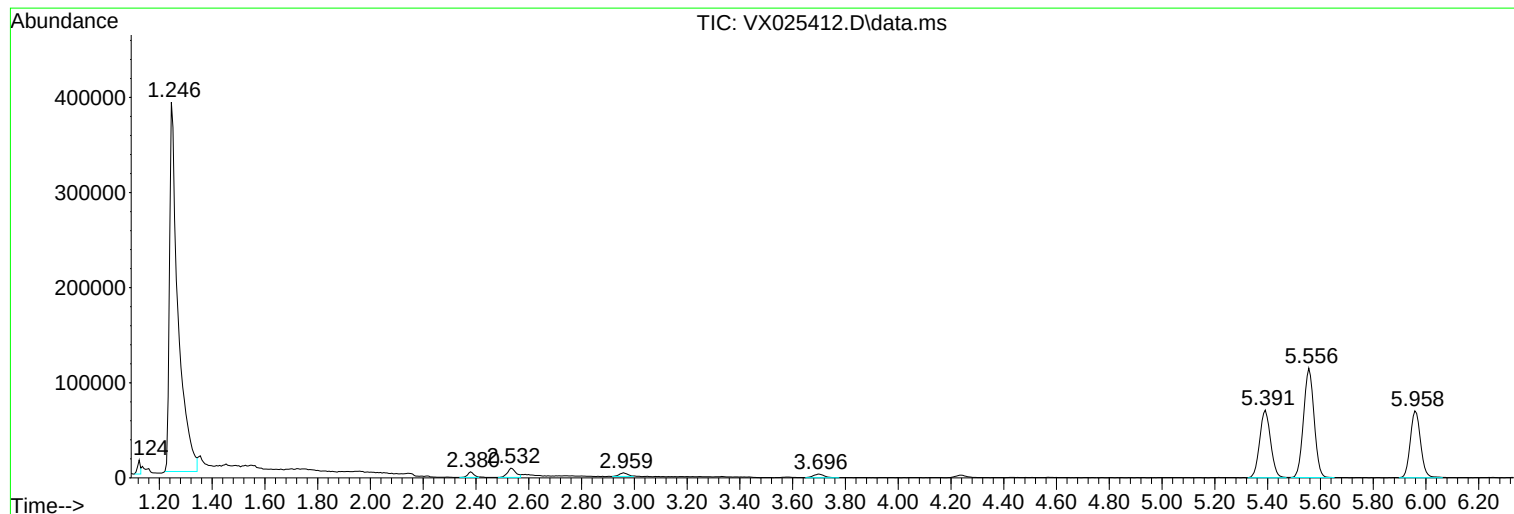
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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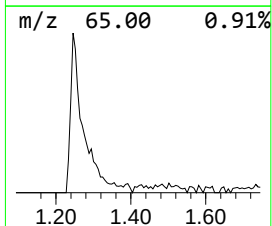
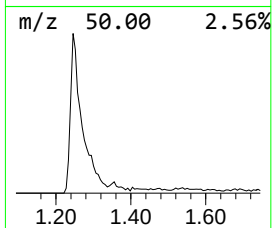
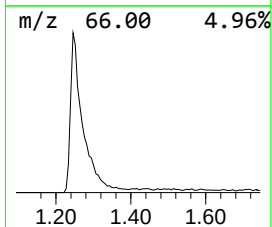
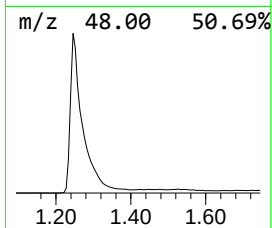
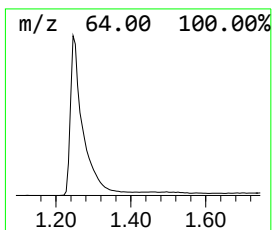
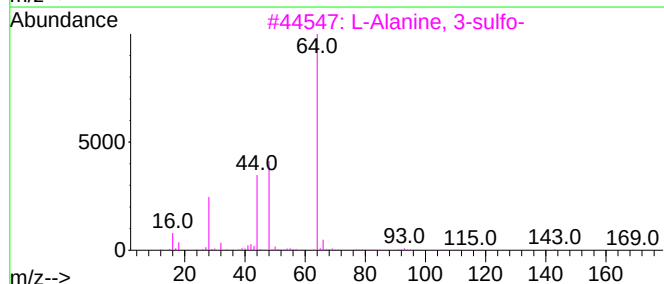
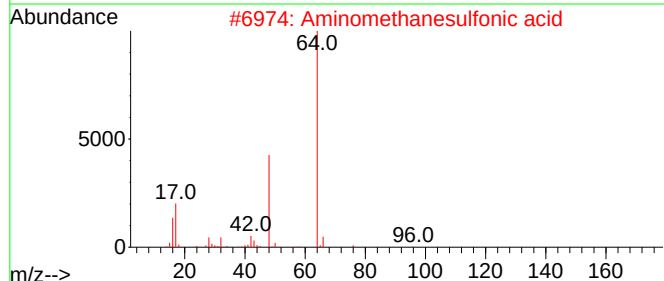
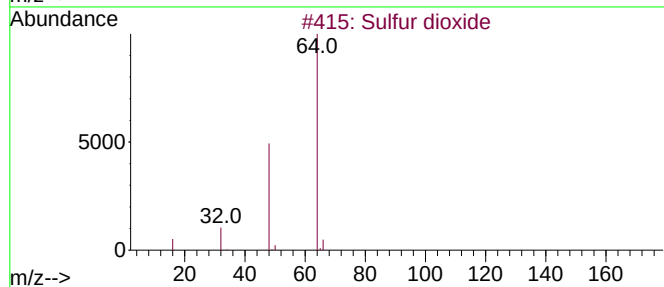
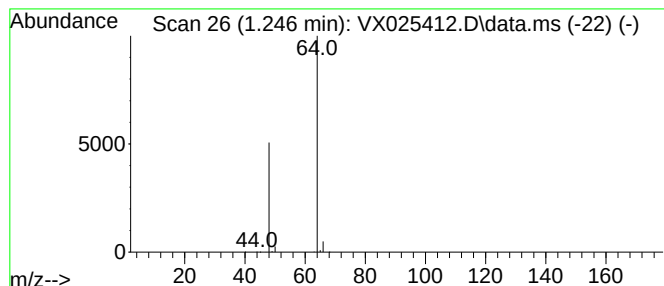
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	136.00 ug/l	870590	Pentafluorobenzene	5.556

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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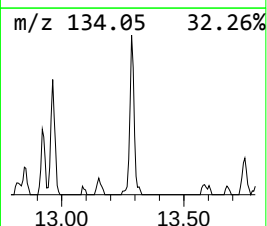
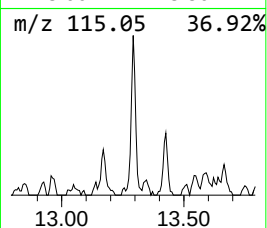
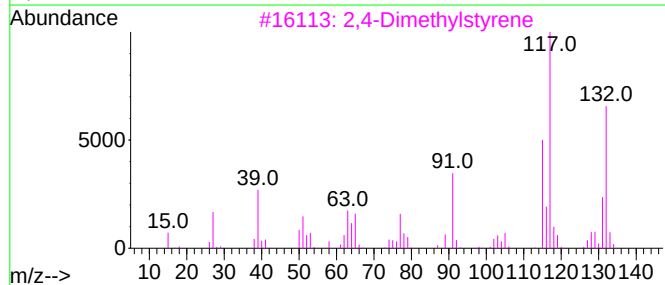
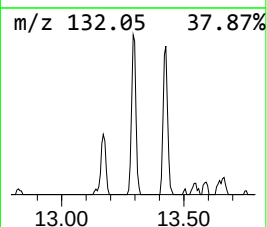
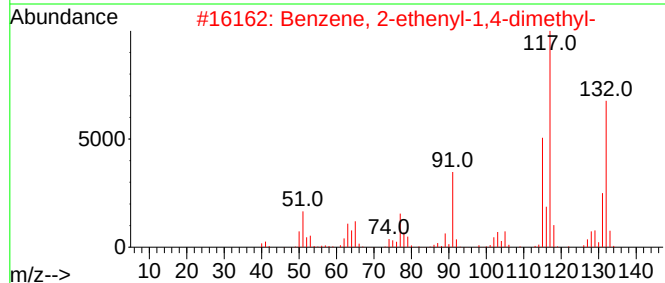
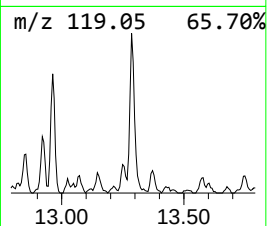
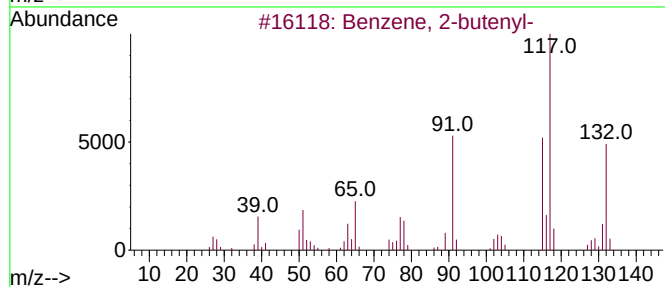
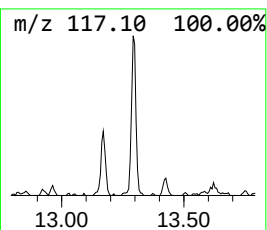
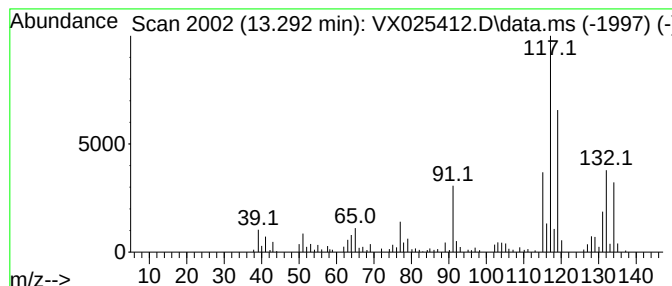
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 2-butenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	5.51 ug/l	84782	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	86
3			2,4-Dimethylstyrene	132	C10H12	002234-20-0	86
4			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	86
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	70



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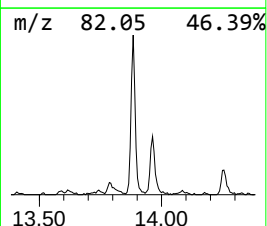
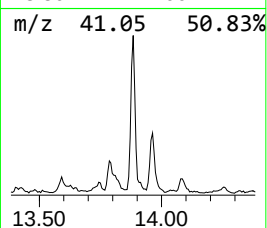
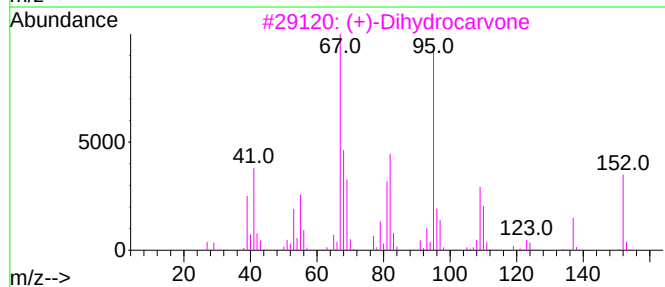
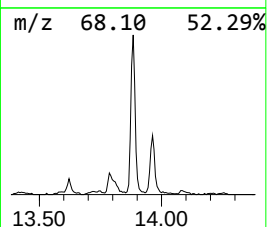
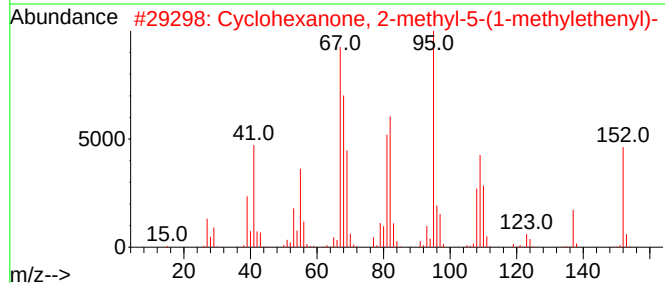
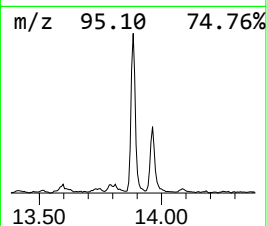
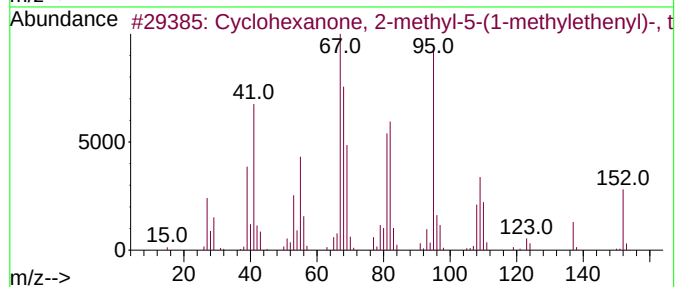
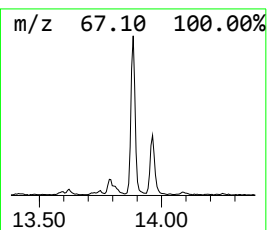
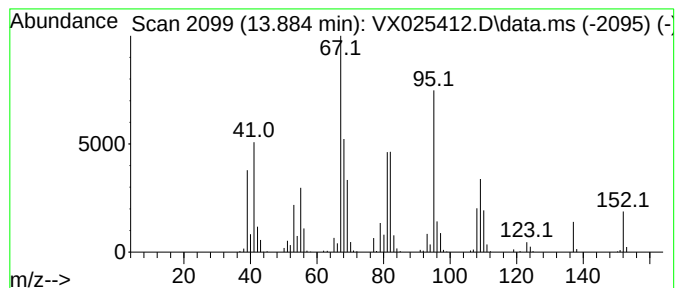
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cyclohexanone, 2-methyl-5-(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.884	12.75 ug/l	196149	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	005948-04-9	98
2			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	97
3			(+)-Dihydrocarvone	152	C10H16O	005524-05-0	93
4			cis-Dihydrocarvone	152	C10H16O	003792-53-8	93
5			3-Nonyne	124	C9H16	020184-89-8	70



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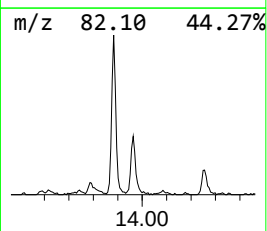
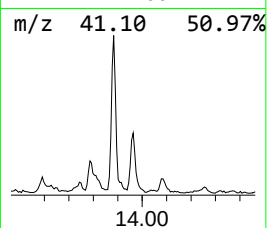
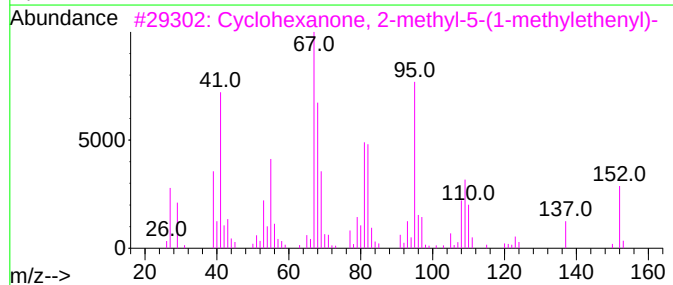
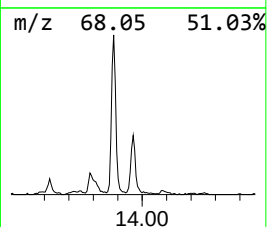
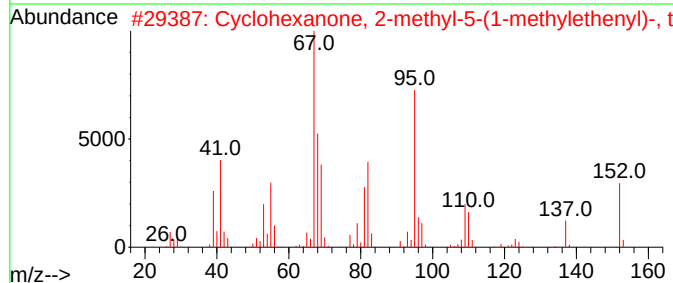
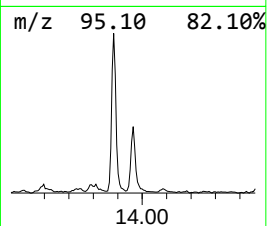
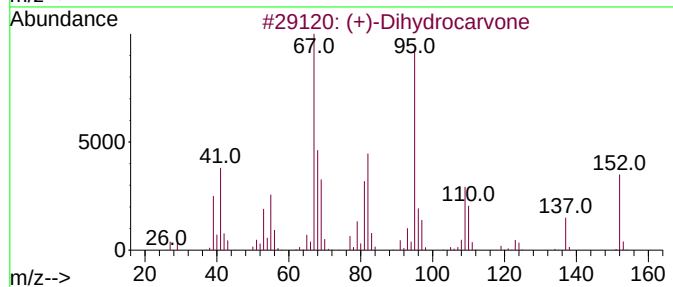
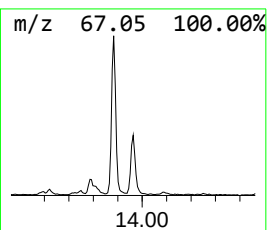
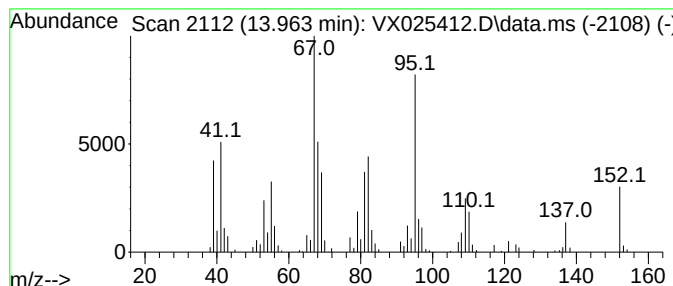
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (+)-Dihydrocarvone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	6.16 ug/l	94728	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(+)-Dihydrocarvone	152	C10H16O	005524-05-0	97
2			Cyclohexanone, 2-methyl-5-(1-methylethenyl)-	152	C10H16O	005948-04-9	97
3			Cyclohexanone, 2-methyl-5-(1-methylethenyl)-	152	C10H16O	007764-50-3	94
4			trans-4a-Methyl-decahydronaphthalene	152	C11H20	002547-27-5	74
5			3-Nonyne	124	C9H16	020184-89-8	70



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	136.0	ug/l	870590	1	5.556	320061	50.0
Benzene, 2-bute...	13.292	5.5	ug/l	84782	4	12.024	769348	50.0
Cyclohexanone, ...	13.884	12.8	ug/l	196149	4	12.024	769348	50.0
(+)-Dihydrocarvone	13.963	6.2	ug/l	94728	4	12.024	769348	50.0