

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120121\
 Data File : VX025413.D
 Acq On : 01 Dec 2021 15:12
 Operator : JC/MD
 Sample : M4866-20
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 16954

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: VX025413.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	7956	8719	1.02%	0.153%
2	1.246	21	26	42	rBV	386703	832233	97.80%	14.591%
3	2.380	206	212	223	rVB	5602	9469	1.11%	0.166%
4	5.391	693	706	722	rBV	70518	204230	24.00%	3.581%
5	5.556	722	733	753	rVB	114400	324777	38.17%	5.694%
6	5.958	789	799	810	rBV	70844	189992	22.33%	3.331%
7	6.763	921	931	946	rBV	181639	429188	50.44%	7.525%
8	8.653	1234	1241	1248	rBV	369745	589475	69.28%	10.335%
9	8.720	1248	1252	1259	rVB	4911	8796	1.03%	0.154%
10	10.055	1465	1471	1488	rVB	386813	516388	60.69%	9.054%
11	10.378	1518	1524	1528	rBV	6055	8678	1.02%	0.152%
12	11.085	1634	1640	1646	rBV	293871	397386	46.70%	6.967%
13	11.366	1681	1686	1691	rBV	85765	107626	12.65%	1.887%
14	11.414	1691	1694	1697	rVV	8266	11417	1.34%	0.200%
15	11.457	1697	1701	1706	rVV	49238	62262	7.32%	1.092%
16	11.506	1706	1709	1717	rVV2	7718	10115	1.19%	0.177%
17	11.750	1740	1749	1755	rBV	24163	31052	3.65%	0.544%
18	11.975	1779	1786	1787	rBV	14437	18851	2.22%	0.331%
19	12.018	1787	1793	1801	rVV3	502903	850914	100.00%	14.919%
20	12.085	1801	1804	1808	rVV	8488	10257	1.21%	0.180%
21	12.323	1839	1843	1846	rBV3	6717	12271	1.44%	0.215%
22	12.359	1846	1849	1854	rVB2	7227	9485	1.11%	0.166%
23	12.555	1878	1881	1885	rVB3	8915	11102	1.30%	0.195%
24	12.664	1895	1899	1903	rVV	28982	34172	4.02%	0.599%
25	12.701	1903	1905	1914	rVB4	5774	9561	1.12%	0.168%
26	12.817	1918	1924	1927	rBV5	5709	9634	1.13%	0.169%
27	12.853	1927	1930	1935	rVB2	12902	17070	2.01%	0.299%
28	12.920	1935	1941	1944	rBV3	9643	16679	1.96%	0.292%
29	12.963	1944	1948	1952	rVB2	13540	18366	2.16%	0.322%
30	13.054	1952	1963	1972	rBV7	10378	29752	3.50%	0.522%
31	13.170	1974	1982	1985	rBV4	10349	22616	2.66%	0.397%
32	13.292	1997	2002	2013	rVB3	36598	83837	9.85%	1.470%
33	13.426	2018	2024	2028	rVB2	22230	35953	4.23%	0.630%
34	13.591	2046	2051	2054	rBV4	19252	32242	3.79%	0.565%
35	13.749	2069	2077	2079	rBV5	15048	28652	3.37%	0.502%
36	13.786	2079	2083	2092	rVV2	52780	120852	14.20%	2.119%

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37	13.884	2092	2099	2104	rVV	185000	250023	29.38%	4.384%
38	13.926	2104	2106	2108	rVV3	16523	20318	2.39%	0.356%
39	13.963	2108	2112	2123	rVV2	74868	114342	13.44%	2.005%
40	14.079	2127	2131	2144	rVB4	19980	36310	4.27%	0.637%
41	14.231	2149	2156	2158	rBV	23366	37469	4.40%	0.657%
42	14.323	2167	2171	2176	rBV3	7118	9558	1.12%	0.168%
43	14.371	2176	2179	2184	rVB	9182	11862	1.39%	0.208%
44	14.481	2192	2197	2203	rBV3	20259	28158	3.31%	0.494%
45	14.615	2215	2219	2220	rBV2	8468	8986	1.06%	0.158%
46	14.640	2220	2223	2226	rVV	18045	22565	2.65%	0.396%
47	14.780	2241	2246	2250	rBV	14820	20058	2.36%	0.352%
48	15.182	2308	2312	2320	rVB3	6970	13576	1.60%	0.238%
49	15.597	2376	2380	2386	rVV2	8399	16398	1.93%	0.287%

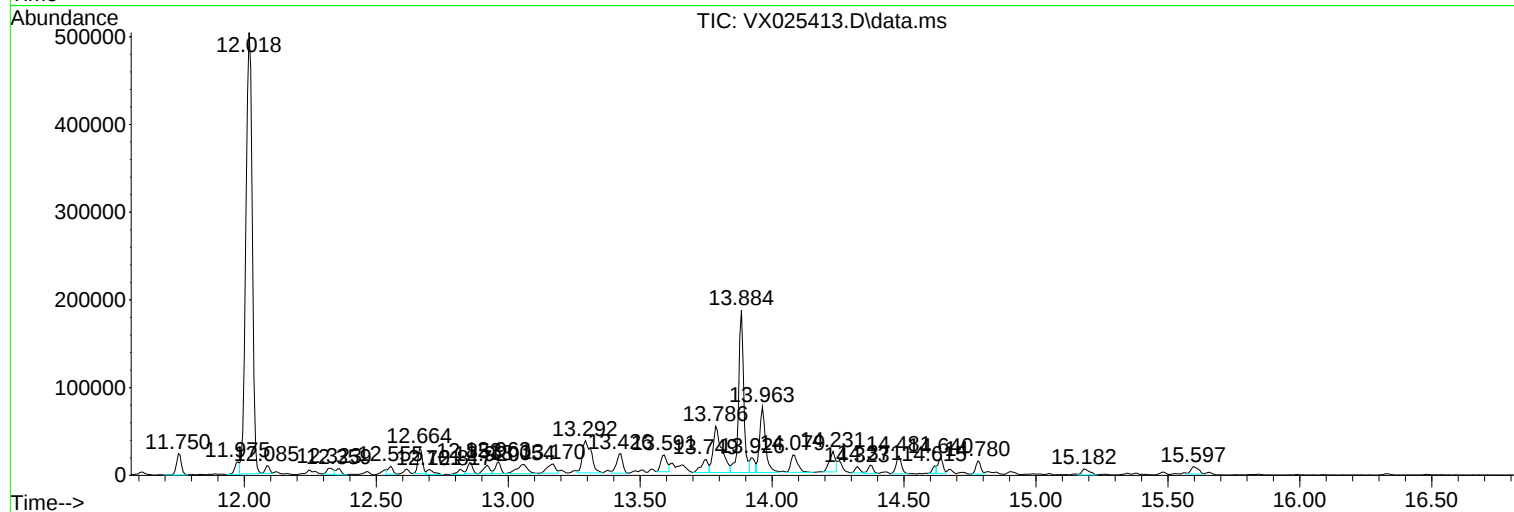
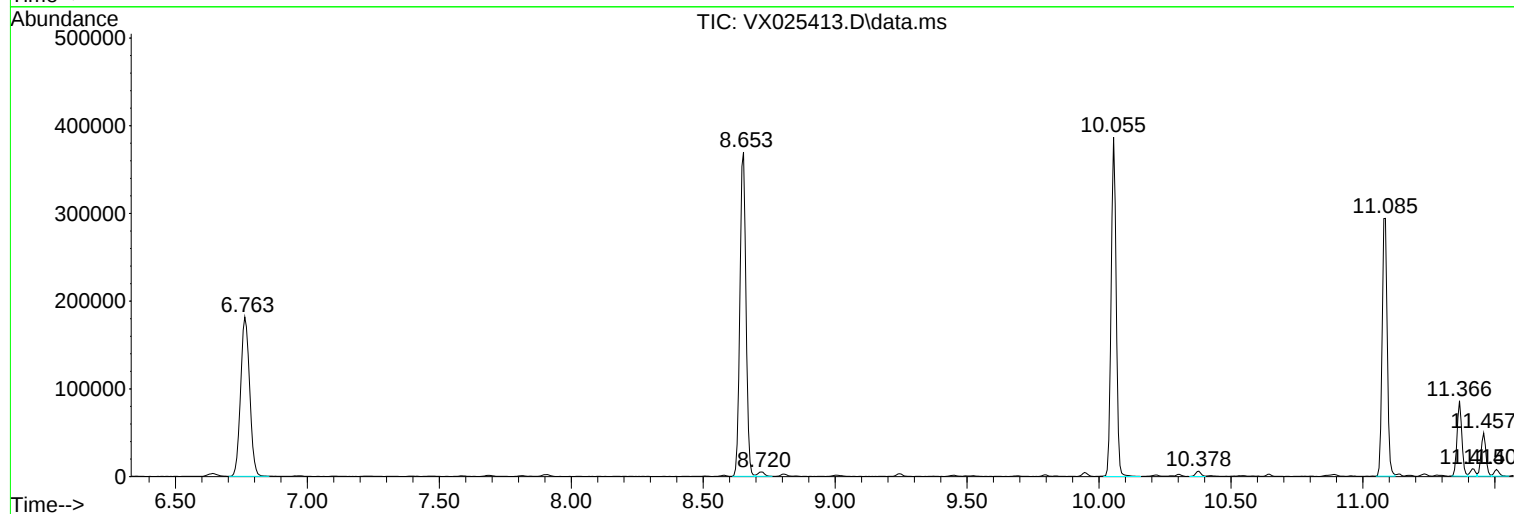
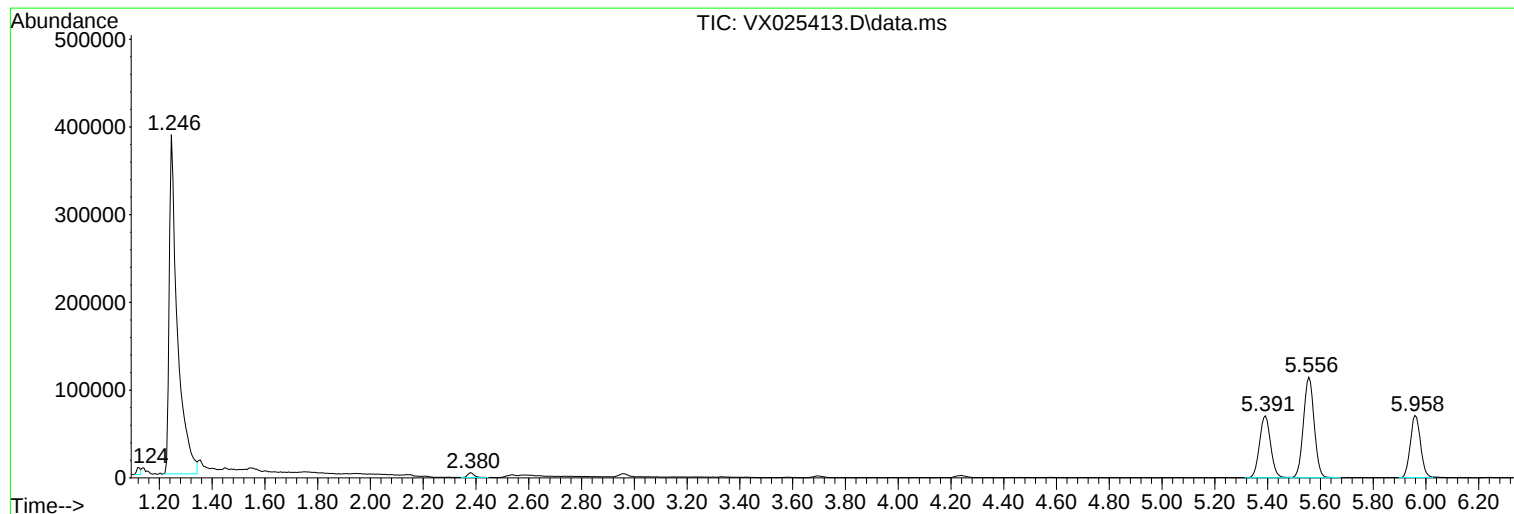
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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



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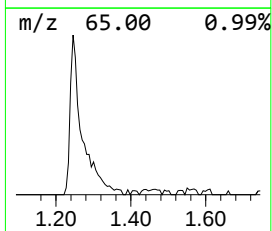
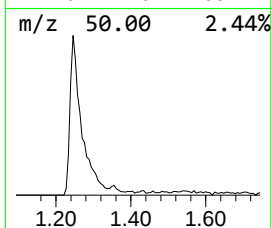
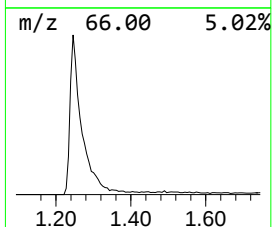
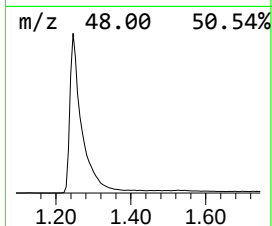
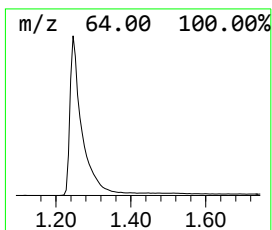
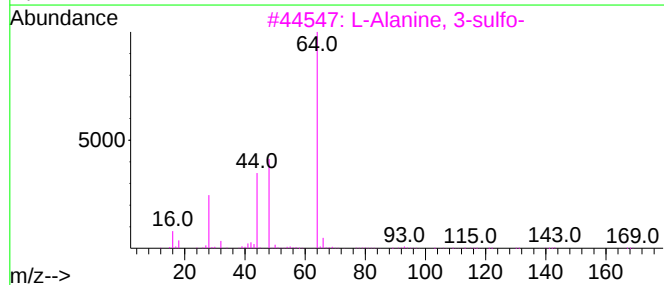
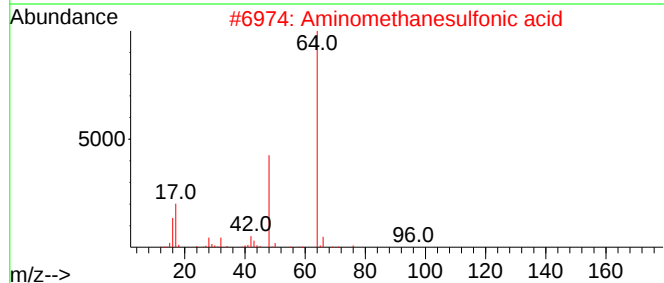
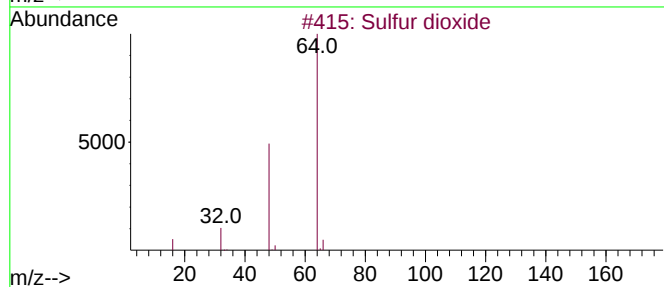
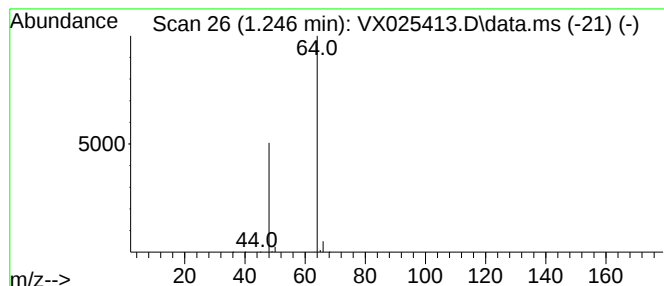
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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	128.12 ug/l	832233	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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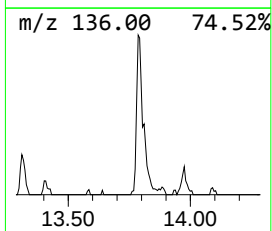
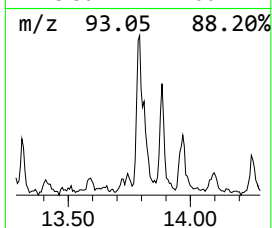
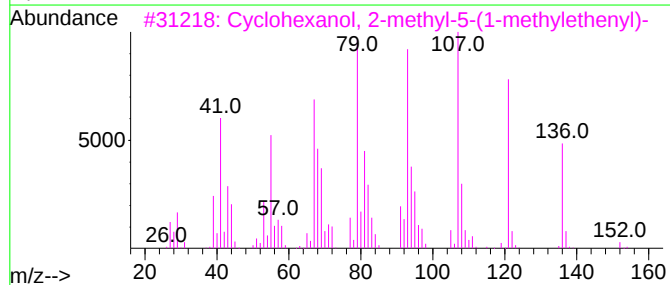
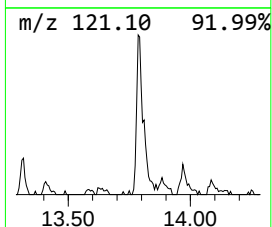
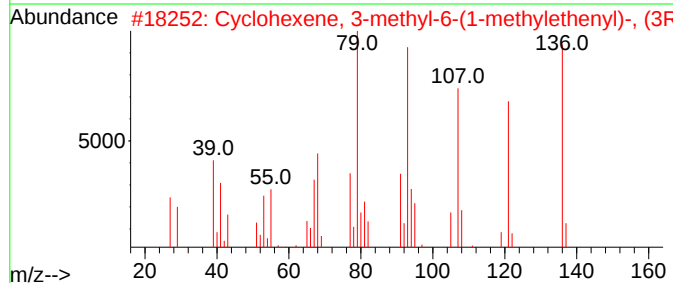
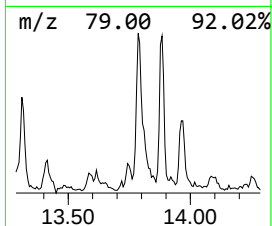
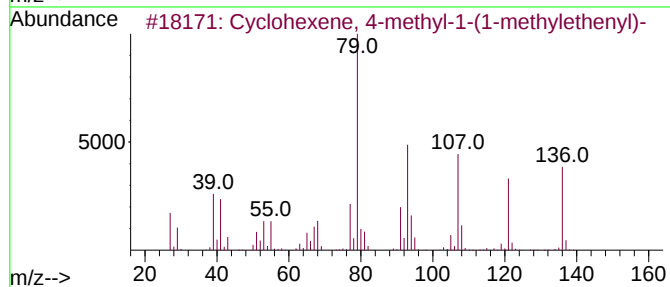
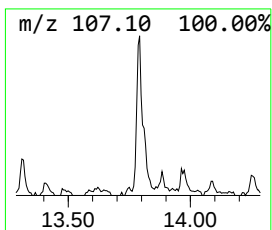
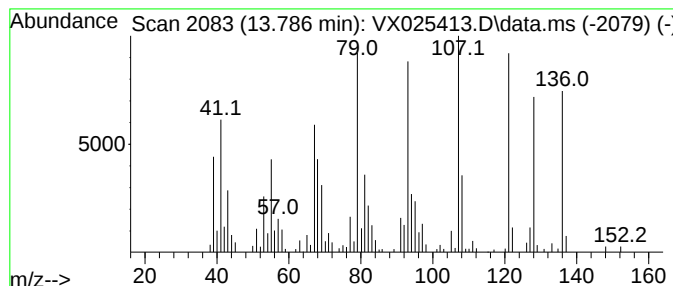
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexene, 4-methyl-1-(1-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.786	7.10 ug/l	120852	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 4-methyl-1-(1-methy...	136	C10H16	000586-67-4	93
2			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	005113-87-1	90
3			Cyclohexanol, 2-methyl-5-(1-meth...	154	C10H18O	000619-01-2	87
4			1,5-Cyclooctadiene, 1,5-dimethyl-	136	C10H16	003760-14-3	70
5			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	006876-12-6	70



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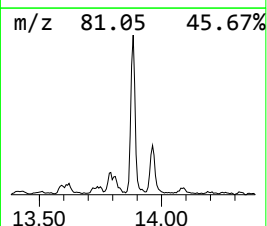
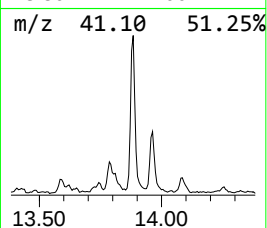
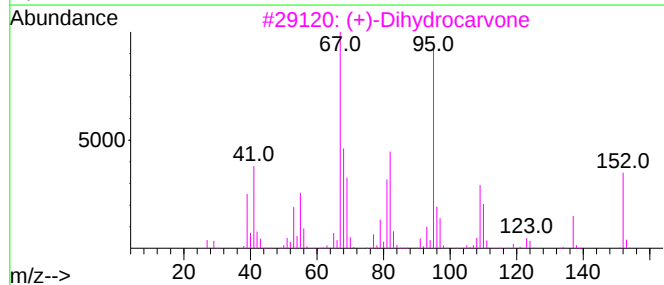
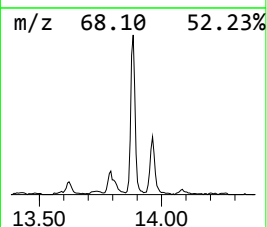
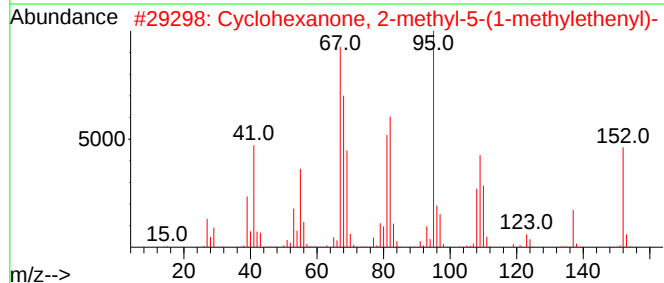
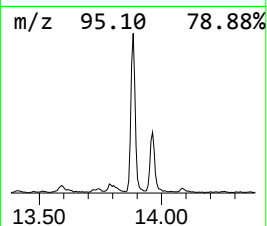
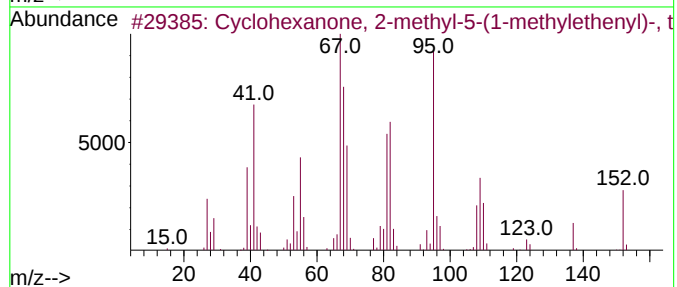
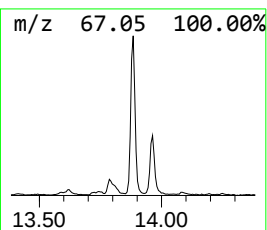
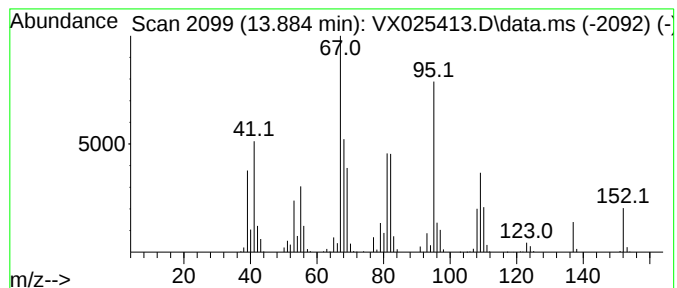
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Cyclohexanone, 2-methyl-5-(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.884	14.69 ug/l	250023	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	95
4			cis-Dihydrocarvone	152	C10H16O	003792-53-8	94
5			3-Nonyne	124	C9H16	020184-89-8	64



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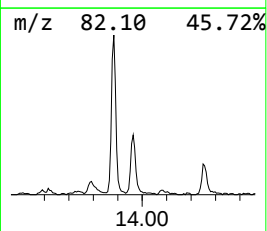
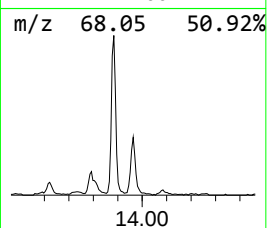
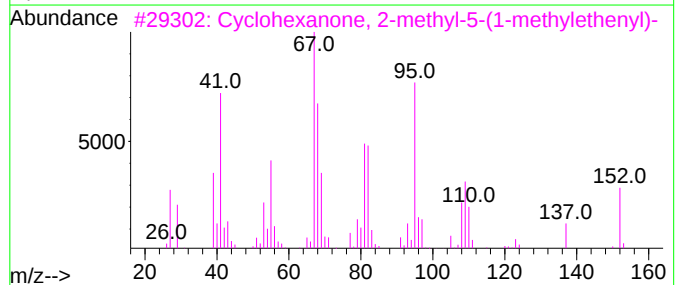
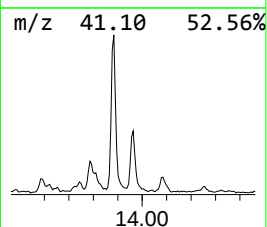
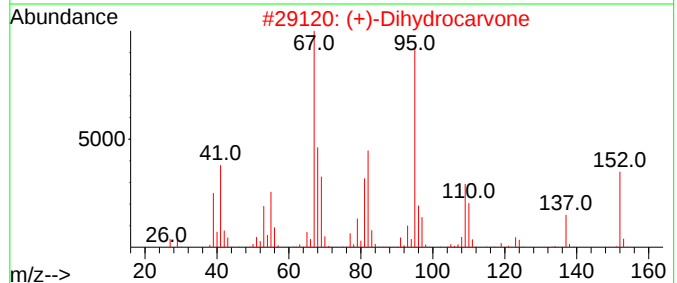
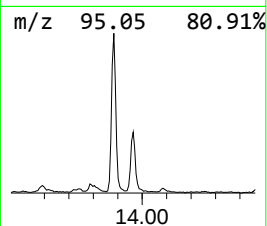
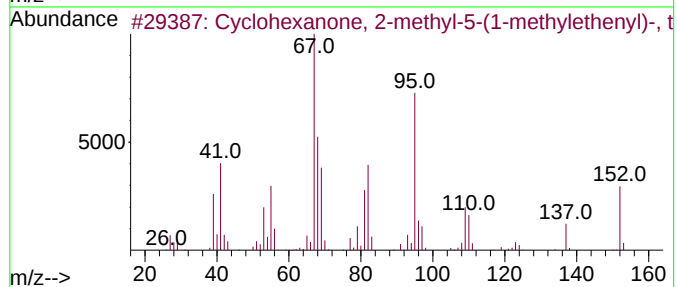
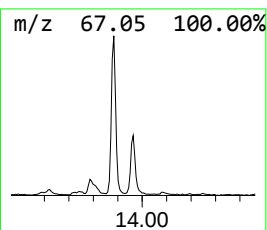
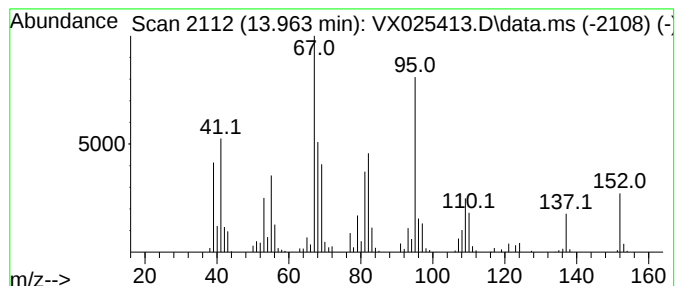
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Peak Number 4 (+)-Dihydrocarvone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	6.72 ug/l	114342	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	96
2			(+)-Dihydrocarvone	152	C10H16O	005524-05-0	96
3			Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	94
4			trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	81
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	128.1	ug/l	832233	1	5.556	324777	50.0
Cyclohexene, 4-...	13.786	7.1	ug/l	120852	4	12.024	850914	50.0
Cyclohexanone, ...	13.884	14.7	ug/l	250023	4	12.024	850914	50.0
(+)-Dihydrocarvone	13.963	6.7	ug/l	114342	4	12.024	850914	50.0